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THE EFFECT OF pH AND PULSED ULTRAVIOLET LIGHT EMITTING DIODE DUTY CYCLES ON THE FIRST ORDER RATE CONSTANT AND BYPRODUCT PROFILE OF THE ADVANCED OXIDATION OF TARTRAZINE

THESIS

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AFIT ENV-MS-16-M-186

DEPARTMENT OF THE AIR FORCE
AIR UNIVERSITY

AIR FORCE INSTITUTE OF TECHNOLOGY

Wright-Patterson Air Force Base, Ohio

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THESIS

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Abstract

Water treatment capability is required for military operations, production of drinking water, and industrial wastewater treatment. The Advanced Oxidation Process (AOP) is one of many viable steps for treating water; however, it is important to understand the byproducts of the treatment process to avoid creating other constituents more severe than the first. Tartrazine (TAR) was oxidized with pulsed Ultra-Violet (UV) Light Emitting Diodes (LEDs) in combination with hydrogen peroxide (H_2O_2) in an AOP at the laboratory scale.

The relative concentration of TAR was reduced from 1 to between 1 – 0.75 over pH values between 6 and 9, and at Duty Cycles (DCs) ranging from 0% to100%. The first order rate constant for TAR removal was statistically and positively correlated with DC, was statistically and negatively correlated with pH, and was typically greatest at pH6. DC and pH were variables in a regression model of the first order rate constant with adjusted R^2 of 0.85.

Chromatographic contrast angle determinations revealed that the byproduct profile was most significantly influenced by pH 7 under both positive and negative ionization, by the 70% DC for the positive ionization, and 50% DC for the negative ionization. DC and pH were variables in regression models to predict positive and negative Chromatographic Contrast Angle (CCA) with adjusted R^2 of 0.76, and 0.68, respectively.

Chemical byproduct analysis indicated that OH addition, H abstraction, and electron transfer without molecule transfer were among the plausible reaction mechanisms for TAR degradation. Of six metabolites identified, two potentially novel metabolites demonstrated that TAR was likely cleaved. These metabolites were (1-(2-hydroxy-4-sulfonatophenyl)-5-oxo-4,5-dihydro-1H-pyrazol-4-yl)diazen-1-ide and (E)-4-(hydroxydiazenyl)-5-oxo-1-(4-sulfonatophenyl)-4,5-dihydro-1H-pyrazole-3-carboxylate. Two other potentially novel metabolites were identified: (E)-4-((2-hydroxy-4-sulfonatophenyl)diazenyl)-5-oxo-1-(4-sulfonatophenyl)-4,5-dihydro-1H-pyrazole-3-carboxylate, and (E)-4-((1-(4-sulfonatophenyl)-4,5-dihydro-1H-pyrazol-4-yl)diazenyl)benzenesulfonate. There were several potential isomers for each metabolite identified.

This research is the first to determine the optimal pH for UV LED-driven oxidation of TAR, the first to use CCA to evaluate byproduct profiles, and the first to identify novel TAR-related byproducts from UV LED-based AOP. This study is the first to develop regression models for the prediction of TAR removal and the byproduct profile given pH and DC; given the assumption that all other operating conditions are analogous to those of this study.

To my Wife, Son, and Daughter. To paraphrase Voyager: My attachment to my family is not something that can be described as a mere emotion. My family is part of my identity. Without them, I would be incomplete.

Acknowledgments

First, I would like to thank Dr. Willie Harper, Jr., my thesis advisor, for his guidance and support in the completion of my thesis research. Second, I would like to thank committee members Dr. Michael Miller and Lt Col David Kempisty for their technical expertise. I would also like to thank Dr. Daniel Felker and Dr. Edward White, for their instruction and assistance with challenging research questions and analysis. Lastly, I would like to thank Dr. Catherine Almquist of Miami (OH) University, Mr. Nathaniel Godby, Ms. Sarah Fyda, Ms. Lana Amer, Ms. Kandace Bailey, Capt Kelsey Duckworth, Maj. Michael Spencer, Maj. Robert Scott, Capt. Patrick Mudimbi, and Capt. Drew Gallucci, whose previous work, concurrent work, and invaluable training have directly contributed to the successful completion of my study.

Brandon M. Stewart

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Glossary of Acronyms and Abbreviations

AFIT – Air Force Institute of Technology

ANOVA – Analysis of the Variance

AOP – Advanced Oxidation Process

BEAR – Base Expeditionary Airfield Resources

BOD – Biological Oxygen Demand

CBRN – Chemical, Biological, Radiological, Nuclear

CCA – Chromatographic Contrast Angle

CSTR – Continuous Stirred-Tank Reactor

DC – Duty Cycle

DOC – Dissolved Organic Carbon

DOD – Department of Defense

DV – Dummy Variable

EPA – Environmental Protection Agency

HPLC – High Performance Liquid Chromatography

IUPAC – International Union of Pure and Applied Chemistry

LED – Light Emitting Diode

LS Means – Least Squares Means

MS – Mass Spectroscopy

NOM – Natural Organic Matter

PFR – Plug Flow Reactor

ROWPU – Reverse Osmosis Water Purification Unit

SSE – Sum Squares Error

SSR – Sum Squares Regression

TS – Test Statistic

US – United States

USAF – United States Air Force

UV – Ultraviolet

VIF – Variance Inflation Factor

VUV – Vacuum Ultraviolet

WPAFB – Wright Patterson Air Force Base

COO^- – Carboxylic Acid Group (Deprotonated)

CN – Cyanide

HO· – Hydroxyl Radical

NaOH – Sodium Hydroxide

Sulf – Sulfonic Acid Group

$2\dot{O}_2^-$ – Super Anoxide Radical

Tar – Tartrazine

TCS – Triclosan

UV-Vis – Ultraviolet, Visible Spectrum

PULSED ULTRAVIOLET LIGHT EMITTING DIODES FOR ADVANCED OXIDATION OF TARTRAZINE

I: Introduction

1.1 Chapter Overview

This chapter discusses the problem, background, research, and investigative questions for the application of Ultraviolet (UV) Light Emitting Diodes (LEDs) in water treatment processes. Additionally, it articulates the scope, assumptions, and limitations of the research. This section also provides a description of the methodology used to conduct the experiments, and highlights the remaining sections of this thesis.

1.2 General Issue

The purpose of this thesis is to increase knowledge of the utilization of UV LEDs for use in water treatment through an Advanced Oxidation Process (AOP). Specifically, this research effort attempts to identify optimal operating parameters such as pH and DC for the AOP of Tartrazine (TAR), to categorize reaction mechanisms, and to suggest possible byproduct structures.

Understanding options to treat water is of particular importance in the military environment (*Quadrennial Defense Review*, 2014). The Air Force needs water treatment capabilities to answer the threat of chemical weapons attack, accidental industrial chemical release, or other military operations resulting in environmental contamination (Duckworth et al., 2014; Mudimbi, 2015; Scott, 2015; Spencer, 2014). There are several types of AOP reactions; this thesis will focus on UV-hydrogen peroxide (UV/H_2O_2) process. When UV light comes in contact with H_2O_2, it produces two hydroxyl radicals

(HO·) (Andreozzi, et al., 1999; Legrini, et al., 1993; Tayade, et al., 2009; S. H. Vilhunen & Sillanpää, 2009). These hydroxyl radicals are more powerful oxidants than chlorine or ozone and react quickly and efficiently with contaminants (Munter, 2001). There is discussion of how pH affects the AOP (Andreozzi et al., 1999; Vescovi, Coleman, & Amal, 2010) and the extent of these effects is not fully understood. Additionally, operating conditions for AOP vary substantially based on the constituent in question. Andreozzi (1999) demonstrated that the H_2O_2 photolysis of benzene, toluene, and other organic compounds was pH dependent and that degradation increased with higher pH. Imoberdorf (2011) did not observe significant effects in degradation of natural organic matter when adjusting pH between 5 and 9. Conversely, another study found UV radiation alone degrades TAR relatively quickly at a pH of 6 (dos Santos, et al., 2014). The AOP reaction often does not completely mineralize compounds (i.e. the end products are not solely CO_2 and H_2O). It is important to fully identify the byproducts of the reaction in the context of water treatment because the byproducts (also called intermediate oxidation products) may be more harmful or toxic than the original compound (Munter, 2001).

Using LEDs for conducting AOP reactions comes with multiple benefits. LEDs are superior to traditional mercury lamps in several respects. LEDs require very little energy, are cost-comparative, produce significantly less heat, efficiently produce light, are more compact, more robust, require no warm up time (instant on/off), run on direct current, which allows for operation with batteries or solar panels, are not manufactured with mercury, which carries many negative health implications, and have longer lifetimes (Autin et al., 2013; *Crystal IS*, 2013). While LEDs are a rapidly improving technology, their potential is not fully realized. Downsides to LEDs include: extreme sensitivity to negative current or electrical shorts, potential corrosion of the metal casings, and emitting a single wavelength; as opposed to mercury lamps, which are polychromatic.

1.3 Problem Statement

The EPA and the Air Force Institute of Technology (AFIT) are investigating the use of LEDs due to the interest in treatment methods and improving the health of deployed service members. UV LEDs are still in the developmental stage; however, the method has proven to be a viable and efficient means for driving the AOP (Duckworth et al., 2014; Mudimbi, 2015; Scott, 2015; Spencer, 2014). Notwithstanding, thorough research and investigative questions are required to advance the understanding of treatment methods, system components, and operating conditions.

1.4 Research Objectives/Questions/Hypotheses

This research effort addresses two main questions: 1.) What operating conditions promote the most effective use of UV LEDs for degradation of TAR? 2.) What reactions occur and how are they characterized? In order to conduct this study, the following investigative questions and respective hypotheses were formulated:

1. How does pH affect the reaction? Considering the conclusions of (Farhataziz, AB, Ross, & Ross, 1977; Imoberdorf & Mohseni, 2011; Legrini et al., 1993), there is no consensus on the effect pH has on the AOP reactions, particularly of the UV/H_2O_2 AOP. To adequately answer this question, the removal of TAR must be

quantified at a variety of pH levels and DCs. The hypothesis for this research question is that pH plays a significant role in the degradation of TAR.

2. What byproducts are generated in the AOP of TAR? Is the byproduct profile influenced by pH? The hypothesis for this research question is that pH does affect the byproduct profile.
3. Which reaction mechanisms play a role in the AOP of TAR? According to Benjamin (2013), Hydroxyl radicals can decompose a compound in three different ways: Hydrogen Abstraction, Electron Abstraction, or OH addition. Based on the composition of TAR, the most likely method is electron transfer or OH addition. Given this hypothesis, the byproducts of the reaction must be identified.

1.5 Methodology

To answer the investigative questions, experiments were conducted – hereafter referred to as the AOP Experiments. The AOP Experiment involved manipulating both pH and DCs. DC indicates the amount of time the LEDs are on. For example, the 100% DC refers to the LEDs remaining on continuously. The 30% DC means the lights are on for 30% of the time and off for 70% of the time. This experiment was conducted at AFIT.

Two kinds of control experiments exist for the AOP Experiment. The first control did not incorporate H_2O_2 in the solution mixture; thus preventing the AOP, resulting in negligible TAR reduction unless there is some effect due to pH adjustor, UV radiation, or some interaction of the two. The second control experiment operated at the 0% DC to see if pH adjustor and H_2O_2 interact without UV radiation. The baseline for this experiment is 100% DC at pH 7. The solution flows from the source solution beaker into the reactor, and then into the Ultraviolet-Visible Spectrum (UV-Vis) spectrophotometer. The spectrophotometer measures absorbance, which is used to calculate concentration and the first order rate constant of the AOP.

The effluent from each experiment was collected, filtered, and processed by High Performance Liquid Chromatography (HPLC). Both positive and negative ionization readings were collected, resulting in chromatograms and mass spectroscopy (MS) plots for each experiment. Chromatographic Contrast Angles (CCAs) were calculated from the chromatograms and were used to analyze the effect of pH on the byproduct profile. The chromatograms and the MS plots were used in chemical analysis to identify potential byproduct structures and reaction mechanisms associated with those structures.

The statistical methods used in this study included one-way Analysis of Variance (ANOVA), Tukey Analysis, and Linear Regression Analysis. The software used to conduct this analysis was JMP Pro® versions 11 and 12.

1.6 Assumptions/Limitations

The limitations of this research are as follows:

1. The LEDs used are small and operate at low power. The assumption is that as technology improves, and as the number of manufacturing vendors increases, LEDs will become more versatile, more powerful, and less expensive.

2. The LEDs for this research were supplied by a single manufacturer (Sensor Electronic Technology, Inc.), due to the limited number of UV LED vendors. In addition to LED limitations, only non-toxic chemicals are allowed in the laboratory due to safety

and disposal requirements. Because of this limitation, TAR was selected as a “witness dye.”

3. This research is a laboratory study; the kinetic and hydraulic characteristics observed during this research may or may not be observed at a larger scale.

II. Literature Review

2.1 Chapter Overview

This section elucidates the relevant literature and background to UV LED applications in AOP processes. Specifically, it develops the key issues of operating conditions and byproducts generated when UV LEDs are used in the UV/H_2O_2 AOP. These areas include UV light and usage, Advanced Oxidation Processes, and AOP byproduct analysis; to include Chromatographic Contrast Angle (CCA) analysis and Mass Spectroscopy analysis.

2.2 Background

Whether accidental or malicious, water contamination is a threat to public safety and health. The United States Military must safeguard clean water against Chemical, Biological, Radiological, or Nuclear (CBRN) contamination, because water is a fundamental, precious resource (*Quadrennial Defense Review*, 2014). Industrial accidents, in which chemicals are released, create adverse human and environmental health effects, requiring expensive medical treatment and remediation (Barrett, 2014; Fitzsimmons, 2014) . The EPA sponsors this research in an effort to find safe and viable methods to decontaminate water.

2.3 UV Light and LED Usage

The UV spectrum spans between 100 and 400 nm. This is further categorized into Vacuum (100-200 nm), C (200-280 nm), B (280-315 nm), and A (315-400 nm) (*Crystal IS*, 2013). It is well established that UV light can degrade molecular structures, as well as inactivate microorganisms by damaging RNA and or DNA (Andreozzi et al., 1999; Cassan, Mercier, Castex, & Rambaud, 2006; dos Santos et al., 2014; Munter, 2001). UV light is traditionally produced with low-pressure mercury lamps (Bettles, Schujman, Smart, Liu, & Schowalter, 2007; Würtele, Kolbe, Lipsz, & Külberg, 2011), but these lamps have several drawbacks, particularly with respect to AOP, to include: high energy consumption, high heat emission, short lifespan, instability, and disposal issues with respect to mercury as an environmental contaminant (Autin et al., 2013).

LEDs have many properties and characteristics that make them superior to mercury lamps (Autin et al., 2013; *Crystal IS*, 2013, US EPA, 2000; Vilhunen & Sillanpää, 2009). These properties include: LEDs do not contain mercury, and therefore do not pose the associated health risks (OSHA, 2012; US EPA, 2000, US EPA, 2013); LEDs are expected to become more effective and less expensive with time according to Haitz's Law (Autin et al., 2013; Lenk & Lenk, 2011); LEDs require no warm up time, which saves energy and increases the blub lifecycle by incorporating pulsing DCs (Autin et al., 2013; Tran, et al., 2014); LEDs generate significantly less heat and are more robust than traditional lamps (Bettles et al., 2007).

2.4 Advanced Oxidation of Tartrazine

2.4.1 Advanced Oxidation Processes (AOP)

The AOP creates hydroxyl radicals (HO·), which hold a single, unpaired electron in an orbital (Benjamin & Lawler, 2013), and which quickly oxidize compounds (Andreozzi et al., 1999), to include disinfection byproducts (DBP) (Chin & Bérubé, 2005; Toor & Mohseni, 2007). HO· radicals are short lived but are very powerful oxidizing agents – twice as potent as chlorine and 1.3 times more so than ozone (Legrini et al., 1993; Munter, 2001).

There are two general categories of AOP: photochemical and non-photochemical, which refers to whether or not a UV light source is required for the reaction. Within the non-photochemical category, there are four AOP varieties: combining Ozone with 1.) high pH; 2.) H_2O_2; 3.) some other catalyst (Cortes, et al., 1998; Munter, 2001; Paillard, et al., 1988); and 4.) Fenton's reaction using H_2O_2 and Fe^{+2} (Fenton, 1884).

The photochemical category includes combining UV radiation with: 1) H_2O_2, see Equation 1; 2) Ozone and H_2O_2; 3) TiO_2; and other titanium or molybdenum composite materials (Andreozzi et al., 1999; Liu et al., 2015; Munter, 2001; Schröder & Meesters, 2005; Varshney & Kanel, 2016). This research focuses on the UV/H_2O_2 AOP as a continuation of that conducted by Duckworth (2014), Spencer (2014), Scott (2015), and Mudimbi (2015) using H_2O_2 to degrade a "witness dye". There are a few noteworthy formulas due to their potential role in the AOP reaction:

Equation 1: Photochemical AOP UV/H_2O_2

$$H_2O_2 \overset{hv}{\rightarrow} 2\dot{O}H$$

Equation 2: Atmospheric Acidification/Hydroxyl Radical Sink

$$HCO_3^- + \dot{O}H \leftrightarrow HC\dot{O}_3 + OH^- \leftrightarrow C\dot{O}_3 + H_2O$$

Equation 3: Peroxide/Hydroxyl Radical Sink

$$H_2O_2 + 2\dot{O}H \leftrightarrow O_2 + 2H_2O$$

These formulas are significant because they indicate potential sinks for radicals, just through interaction of hydroxyl radicals and peroxide, as well as the acidification of water due to exposure to atmospheric CO_2. Equation 2 plays a large role in this study because H_2CO_3 pKa_1 and pKa_2 are 6.35 and 10.33 (Benjamin, 2014), respectively – the pH of the solutions in this experiment was between 6 and 10, making HCO_3^- the most prevalent form of carbonic acid in the solution (at pH less than 6.35 it is not the most prevalent form, but is close to the same concentration as H_2CO_3); log concentration of HCO_3^- was calculated with VMINTEQ and increases linearly from approximately -5 to -1 between pH = 6.35 and 10.33 (Gustafsson, 2012). HO_2^- forms in acid/base equilibrium with H_2O_2, see Equation 3. However, this attribute has much less influence because the pKa for that reaction is 11.6 (Buxton, Greenstock, Helman, & Ross, 1988; Legrini et al., 1993) and the pH was less for all experiments of this study.

The "witness dye," as coined by Scott (2015), is used in place of toxic contaminants due to the limitations of lab safety requirements and the ease of disposal of the witness dye. Degradation of the witness dye is characterized by absorbance, which is measured by a UV-Vis Spectrophotometer. The decrease in absorbance over time demonstrates that the AOP reaction occurs and degrades the dyes. Duckworth (2014) leveraged DCs of 10%, 50%, 70%, and 100% for the H_2O_2/UV AOP to degrade methylene blue and observed the log of the degradation rate constant increased linearly with increase in DC. Spencer (2014) developed a stainless steel reactor for use in both AOP and disinfection processes and measured the output angle for UV radiation in water to be between 43 and 46 degrees. Scott (2015) incorporated brilliant blue and methylene blue in the AOP experiment and observed degradation rate constant results consistent with Duckworth (2014). Scott (2015) also demonstrated that fouling of the UV LED lens is greater with methylene blue than that of brilliant blue due to the cationic nature of methylene blue interacting with the LED surface. Mudimbi (2015) observed slight fouling of the LED lens with use of TAR compared to methylene blue, and increased correlation of results with the computer model of the Continuous Stirred-Tank Reactor (CSTR) reactor by incorporating a magnetic stir bar. This greatly reduced the amount of variation between the measured concentration and the models predicted concentration. Mudimbi (2015) also established the AOP conditions in the CSTR reactor could provide up to 23% removal of TAR during 100% DC.

Whether acidic or basic conditions are favorable to the AOP is inconsistent in the literature. Duckworth (2014), Mudimbi (2015), and Scott (2015) did not discuss is what effect, if any, pH of their solutions had on the AOP reaction. This is of interest due to the fact that pH is commonly addressed in AOP literature and does not have the same effect on one contaminant as it does another. In addition, the pH condition may also affect the reaction mechanism of degradation. Measurements taken in the lab demonstrate the pH of the supplied distilled, de-ionized (DI) water was not consistent from one day to the next and could have significantly affected their data. Each contaminant is unique and, thus, the AOP operating procedures could be different from one contaminant to the next. Andreozzi (1999) confirmed that acidity decreased HO· production for organic compounds such as toluene, benzene, chlorobenzyne, tri/tetra-chloroethelyne, and butanol. However, Alpert (2010), showed that higher alkalinity scavenges HO· in the UV/H_2O_2 AOP of methylene blue, and that this scavenging effect was strongest in the presence of dissolved organic carbon (DOC) between concentrations of 0 to 2 mg/L. Jin-hui (2012) demonstrated that pH was not as important for degradation of organic matter as exposure time or light intensity; conversely, Jyothi (2014) established that pH had great effect on phenol and ZnO. Legrini (1993) found that the production of HO· from

H_2O_2 was pH dependent and increased with more alkaline solutions. As previously discussed, the operating conditions of this research are such that this phenomenon does not have an effect. Tayade (2009) showed optimum operation for degradation of Methylene Blue dye at pH 9. Vescovi (2010) examined dioxane, and determined that AOP was optimal at neutral pH.

TAR has three Na^+ ions that may separate from the structure due to interaction with water, which means that in evaluation of the Mass Spectroscopy, masses of 534, 511, 488, and 465 can indicate TAR because the mass weight of Na^+ is 23. TAR can be considered acidic: both the sulfonic acid groups' pKa are 2, and the azo group pKa is 10.86 (Gómez, Arancibia, Rojas, & Nagles, 2012). Therefore, in this study's experimental conditions, it is expected that the H in the azo group does not dissociate. In addition, sulfonic acid grouped with a benzene ring (hereafter referred to the Sulfonic Acid Group) is a common product in both the manufacture and degradation of TAR.

This thesis effort is similar to the work conducted by dos Santos (2014), which examined the effect of pH and UV radiation on TAR, found optimal removal of TAR at pH 6, and identified byproducts of this reaction. However, the work done by dos Santos (2014) is distinct from this research effort: dos Santos (2014) used UV light alone, and not AOP, to degrade TAR. In addition, operating conditions were substantially different from those of this study: light intensity was 10 times greater and initial concentration of TAR was 5 times less.

2.4.2 AOP Reaction Mechanisms

There are three main mechanisms by which HO· radicals degrade a compound. They are: Hydrogen Abstraction, OH Addition, or Electron Transfer (Benjamin &

Lawler, 2013; Legrini et al., 1993; Vilhunen & Sillanpää, 2009). Hydrogen Abstraction occurs at saturated organic compounds (i.e. no double bonds). The chemical makeup of TAR is depicted in Figure 1with a potential Hydrogen Abstraction opportunity highlighted. Legrini (1993) investigated hydroxyl radical production in the H_2O_2/UV, Ozone/UV, Ozone/H_2O_2/UV, TiO_2/UV, and vacuum ultraviolet (VUV) AOPs of organic substrates and observed the primary reaction mechanism of hydroxyl radicals to be hydrogen abstraction, which generates radical chain reactions in the presence of dissolved oxygen. Wang (2014) investigated UV radiation on humic acid and observed formation of hydroxyl radicals and suggested that hydrogen abstraction contributed to the formation of acidic functional groups and that OH addition contributed to the split of the carbon chain. Durme, Dewulf, & Sysmans, (2007) studied the mineralization of toluene using non-thermal plasma (DC positive corona discharge) and found formation of hydroxyl radicals, and products to suggest hydrogen abstraction occurred at carbon rings.

OH Addition, also known as electrophilic addition (Aleboyeh, Aleboyeh, & Moussa, 2003; Legrini et al., 1993), occurs at unsaturated bonds (Benjamin & Lawler, 2013), or in the presence of natural organic matter (NOM), can occur at double bonds (Matilainen & Sillanpää, 2010). There are 9 hydrogen atoms in TAR; each represents an opportunity for OH addition, both at the benzene rings and at the N-H bond in the azo group (Figure 2). Legrini (1993) also suggested OH addition as a viable mechanism for the AOPs of organic substrates, particularly for chlorinated phenols. Gonzalez, Oliveros, Wörner, & Braun (2004) explored VUV photolysis in the reduction of aromatic hydrocarbons and found evidence to suggest electrophilic addition of OH was a main facilitator of the degradation of the substrate. Gao, Ji, Li, & An (2014) explored the hydroxyl radical reduction of triclosan (TCS) and proposed 12 OH addition opportunity locations, as triclosan is a chlorinated phenoxyphenol containing a benzene ring, a phenolic ring, and three chlorine substituents.

The third mechanism for mineralization is electron transfer. This could occur at any location, but perhaps the most apparent indicator would be the loss of either sulfonic acid or the deprotonated carboxylic acid (COO^-) groups. There may be interaction with any of these structures and other constituents in the water after any of the reaction mechanisms have occurred. Gao (2014) observed one electron transfer route in the investigation of TCS in secondary reaction progressions. Gonzalez (2004) evaluated organic compounds, corresponding radicals, and $NO^{\cdot}$ radicals and observed electron transfer from $NO^{\cdot}$ to NO^- yielding N_2O. Jyothi (2014) evaluated AOPs utilizing oscillation in photo and sono signals to produce radicals for the degradation of phenol and ZnO and observed electron transfer and that the transfer was pH dependent.

Under similar AOP conditions, the mineralization progresses more quickly for brilliant blue than for TAR (Mudimbi, 2015; Scott, 2015), likely due to the fact that there are many more available double bonds than TAR. Due to the structure of TAR, it is expected that OH addition or electron transfer is the most likely mode for the mineralization of TAR.

Analysis of the byproduct profile for the AOP of TAR has not been conducted previously; however, other studies of the degradation of TAR have observed the following byproduct structures. Maslowska (1996) studied the voltammetric reduction of TAR and observed addition of 2 hydrogens at both nitrogen locations in the azo group. Weisz (2014) showed that TAR is not a pure substance: Pk 5 and Pk7 (manufactured isomers) form as well as the main structure of TAR, see Figure 3 and following discussion. The structures are distinguished by the number of sulfonic acid groups that form. dos Santos (2014) showed an addition of 2 hydrogen atoms as well, but indicated their locations were in place of two removed Na^+ due to ionization. dos Santos (2014) also showed fissure of the double nitrogen bond in the azo group, followed by loss of the COO^- group in subsequent byproduct formations.

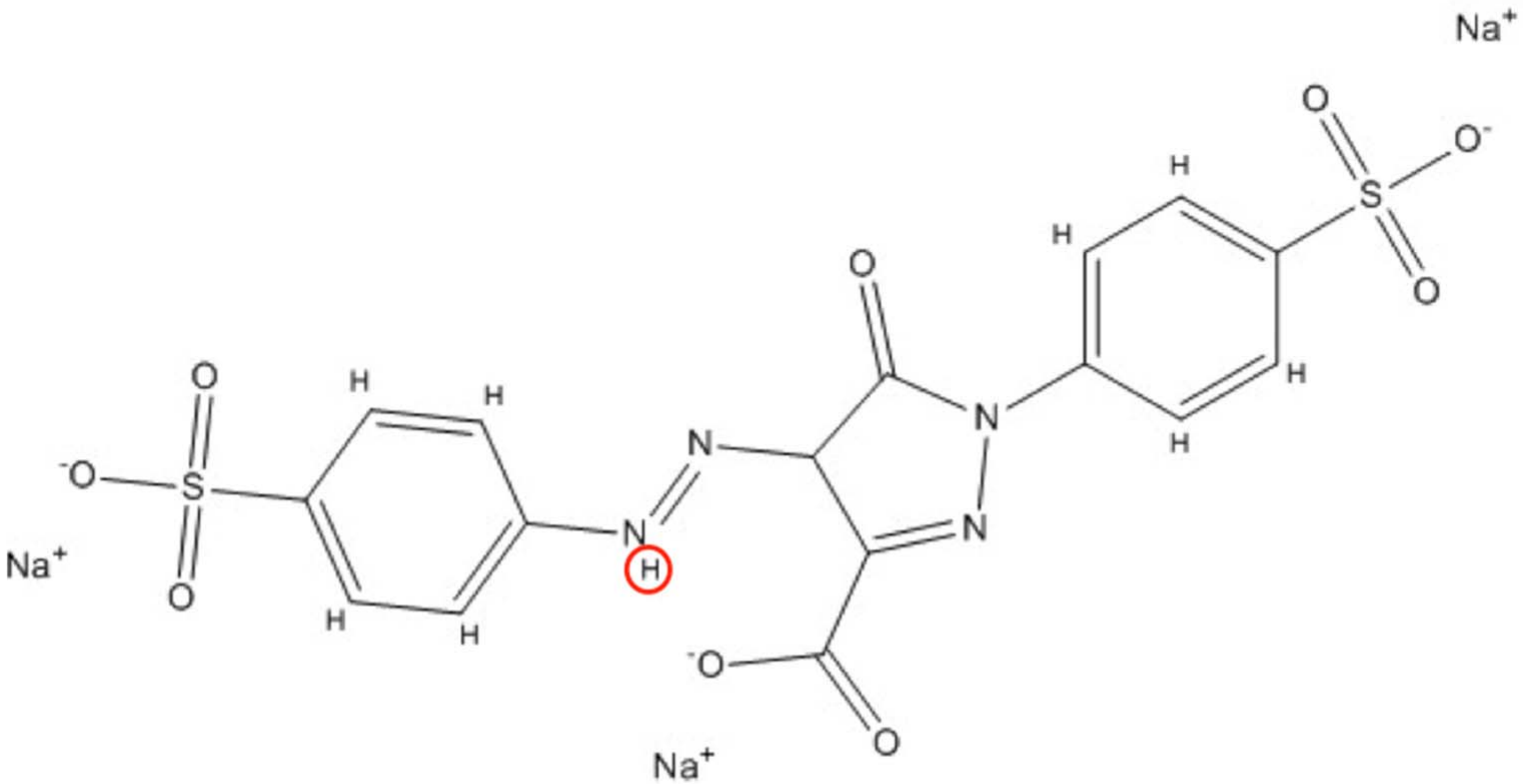


Figure 1: Tartrazine (H Abstraction Location)

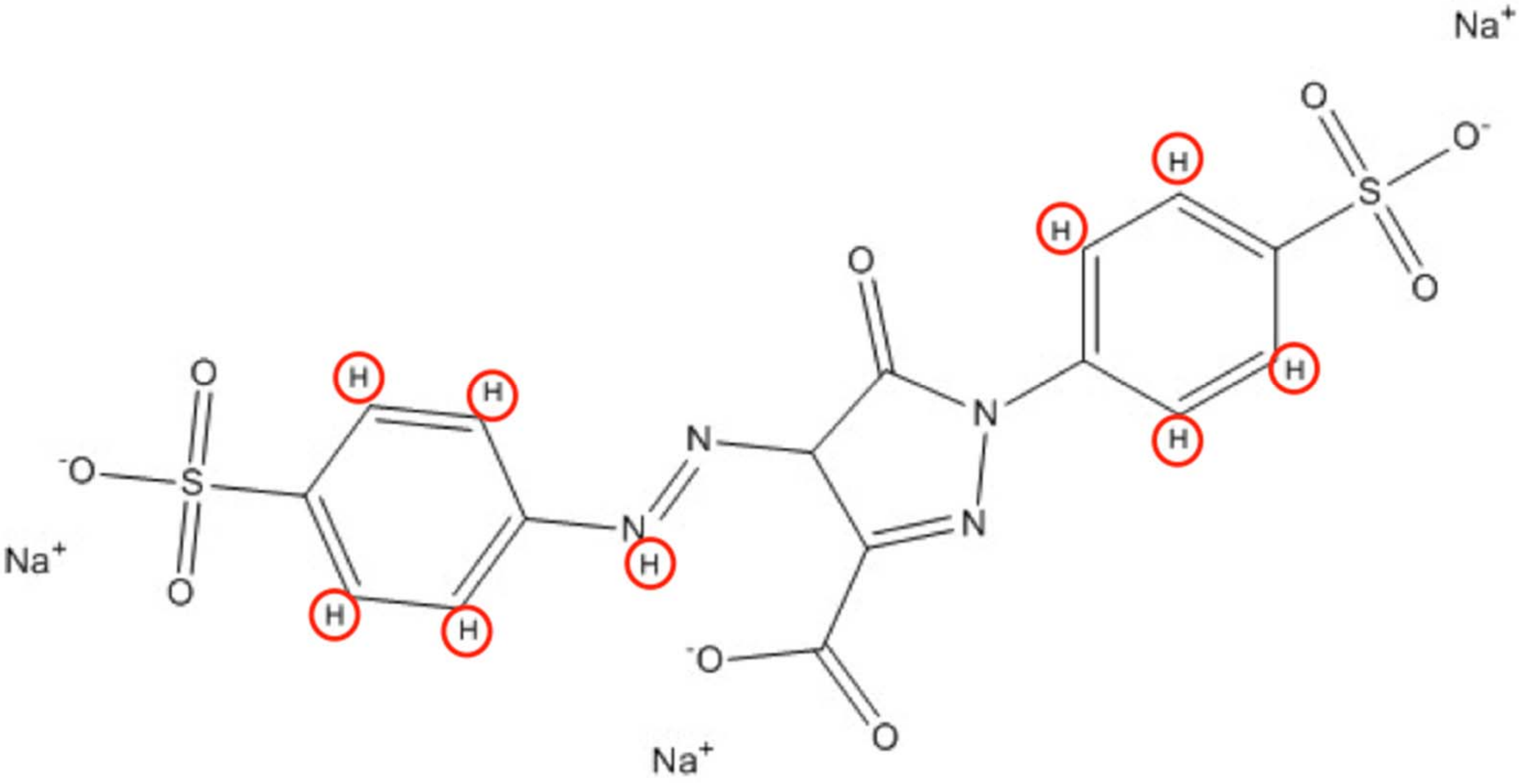


Figure 2: Tartrazine (OH Addition Locations)

2.5 Spectral Chromatographic Contrast Angle

One method of comparing byproduct profiles without identifying the structures is in the calculation of CCAs (Wan, Vidavsky, & Gross, 2002). The CCA is denoted by θ, and is a vector in multi-dimensional space. High angles (up to 90 degrees) indicate differing byproduct profiles, while low angles indicate strong similarity. This is the most reliable comparison method for library searches for compound identification (Wan et al., 2002). Theta is calculated by Equation 4, where a and b are the two spectra under comparison and i is the number of points in each data set; i also indicates the number of dimensions of space in which the vector exists.

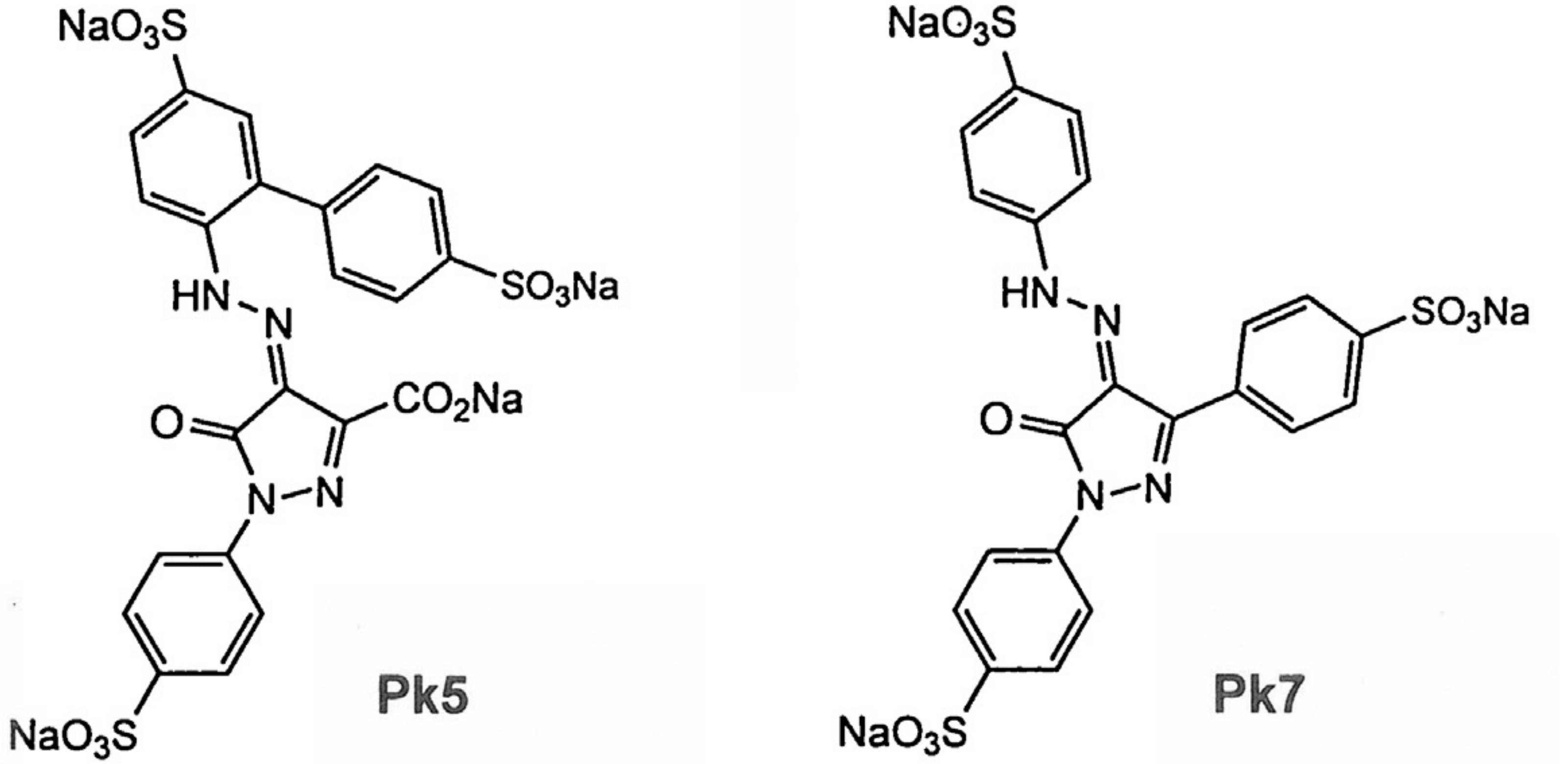
Equation 4: Chromatographic Contrast Angle Calculation

$$cos\theta = \frac{\sum_i a_i b_i}{\sqrt{\sum_i a_i^2 \sum_i b_i^2}}$$

This method has been widely used in a variety of applications. Li (2001) used this method in HPLC analysis of fatty acids, specifically for photodiode array detector produced spectra. The produced spectra were compared with the spectra library for spectrum matching. The method of using contrast angles was also used to analyze sample purity, and used to indicate photometric error, or solution imprecision. Kushnir (2005) showed that contrast angle calculation is useful for LC-MS for identification of compounds, particularly if two or more mass transitions are used. In this case, calculation complexity can be greatly reduced. In addition, Zhang (2011) used spectral contrast angles to analyze peptide modification trends, and recommended the method as statistically acceptable to compare protein/ligand structures. However, the “self-angles” for the protein/ligands used were much greater (up to 35 degrees in some cases) than those used by Wan (2002).

2.6 Tartrazine and Chromatography

TAR is defined as $C_{16}H_9N_4Na_3O_9S_2$, has a molecular weight of 534.4, and is commonly recognized as is represented in Figure 1 (Weisz et al., 2014). However, TAR is a manufactured product and it is not a pure substance. Other isomers of the molecule are depicted in Figure 3, (Weisz et al., 2014).



Pk5

Pk7

Figure 3: Tartrazine Manufacturing Isomers

These manufactured isomers, Pk5 and Pk7, are different from the main structure of TAR due to an extra sulfonic acid group, either forming off a benzene ring or forming in place of the COO^- location. Their molecular weights are 713.5 and 646.5, respectively. According to Weisz (2014), Pk5 is detected by UV-Vis, with peaks at 258 and 428.1 nm, whereas Pk7 is characterized by peaks at 276.9 and 404.1 nm.

Other studies have been conducted on decomposition products of TAR. In the UV decomposition of TAR study, several noteworthy products emerged: fully ionized TAR with the addition of 2 Hydrogen atoms, the fissure of the double nitrogen bond of the azo group, and secondary products losing the COO^- group (dos Santos et al., 2014). Maslowska (1996) observed both TAR plus 2 hydrogen atoms (although, proposed a different structure than dos Santos (2014)), as well as a “reduction of [the] azo group… result[ing] in the formation of a hydrazine compound” in evaluating the voltammetric reduction of TAR.

2.7 Objectives

The purpose of this study is to evaluate degradation of TAR using operating conditions such as DC and pH to characterize ideal operation procedures and to identify reaction mechanisms that occur in the H_2O_2/UV LED AOP of TAR. The objectives of this work are:

- Determine the effects of pH and DC on the removal of TAR
- Determine the effect of pH and DC on the byproduct profile
- Propose chemical structures of measured byproducts

III. Methodology

3.1 Materials and Equipment

Materials and equipment between the AOP Experiment are varied and will be discussed individually in the following subsections. However, operating parameters are as follows. Water was conveyed through PharMed® BPT tubing (inner diameter of 0.8 millimeters, Valley Forge, PA) via a digital pump – Easy-Load II Masterflex, model 77200-50 (Cole Parmer, Vernon Hills, IL) at rate of 0.7 mL/minute.

DC programs for both reactors' LEDs were controlled by Data Acquisition System Laboratory (DASYLab, version 12, Stamford, CT). Power was delivered to the circuit board by the driver box measurement computing device (USB-2408-2AO, Norton, MA), and the circuit board delivered 20 mA to each LED (Duckworth et al., 2014; Spencer, 2014). The luminous flux and optical power output of bulbs were measured through Labsphere® integrating sphere (Labsphere ® North Sutton, NH), which was calibrated with a Deuterium Lamp (S/N 667329).

To ensure LEDs are functioning properly (correct voltage and DC waveform) at each experiment without deconstructing the reactor, each LED signal was measured by oscilloscope (OWON PDS5022T, Zhangzhou, China). Kimtech Kimwipes ® (Kimberly-Clark, Roswell, GA) were used to clean the cuvette and the pH meter diode.

Finally, in order to ensure complete mixing of the solutions within the reactors, both reactors contained a magnetic stir bar and were placed on a Corning Stirrer Table; model PC-210, S/N 220197028704 (Corning, Inc. Corning, NY).

3.1.1 AOP Experiment

In order to answer the first research question, two Independent Variables (IVs) of pH and DC were adjusted with the anticipation of observing significant differences between the respective first order rate constants (k_S). The pH was adjusted to levels of 6, 7, 8, or 9; the DCs were adjusted from 0%, 5%, 10%, 20%, 30%, 50%, 70%, and 100%: the total number of planned experiments was 36. The order in which the experiments were executed was randomized to prevent introducing a learning curve into the data. Intentional repeat experiments were scheduled to be conducted when degradation behavior was not anticipated or when errors were made in the preparation stages. A total of 6 additional experiments were conducted: an accidental repeat pH 8 at 70% DC, an error in pH adjustment led to an experiment operated at pH 5 at 70% DC, a repeat of pH 9 at 50% DC was conducted because the first iteration did not use a mix table, an experiment operated at pH 7 and 50% DC was operated at 1.5 mL/min instead of 0.7 mL/min, and unexpected results led to the repeat of experiment conditions pH 6 at 70% DC and pH 8 at 100% DC.

The solution for each AOP experiment consisted of Hydrogen Peroxide (30% in water, Fisher Scientific, Pittsburgh, PA), TAR (Acid Yellow 23, CAS: 1934-21-0, Sigma-Aldrich Co, St. Louis, MO), reverse osmosis, purified, deionized water (DI Water, AFIT ENV Lab), and stock solutions of NaOH (1.0, 0.1, or 0.01 M, AFIT ENV Lab) or as required for pH adjustment. It is important to note that the pH level of the DI water was not consistent throughout the experiment and ranged from 4.1 to 7.4. This variation is not caused due to the pH meter, which was calibrated before each use; it is likely due to a malfunction in the storage or production of the DI water.

The exact amounts for the solution, measuring and mixing procedures are detailed as follows. Mass was measured using a Mettler Type AT 261 Delta Range SNR L43911 mass scale (Hightstown, NJ). It is important to note that the mass scale was not perfectly balanced and the fisheye was not centered. The amount desired for TAR was 0.02672 g, which equates to 0.05 mmol/L. The mean measurement for TAR was .026728 g with a standard deviation of 1.97e-5 g. The preferred amount of H_2O_2 was 2.87953 g (30% in water) (Mudimbi, 2015), which is approximately 25 mmol/L. The mean measurement for H_2O_2 was 2.878817 g with a standard deviation of 2.599e-3 g. H_2O_2 is volatile and the precision of the conveying implement was low. This explains why the standard deviation for H_2O_2 mass measurement was much higher than that of TAR. 1000 mL of DI water was measured with volumetric flasks ± 0.6 mL.

Upon completion of mass measurement, TAR was added to the DI water, followed by the H_2O_2. The solution was mixed for 10 – 15 minutes and a pH reading was made. A determination was then made for how much NaOH was required and at what concentration. This was measured and added to the solution, mixed, and a new pH reading was made using SevenMulti pH Meter, S/N 1229425365 (Mettler-Toledo Group, Schwerzenbach, Switzerland), see Appendix A for calibration procedures. This process was repeated until arriving on the desired pH level as described in the experiment schedule, see Appendix B. In the event of overshooting the desired pH, a future scheduled experiment was conducted instead. Upon complete mixing of the solution at the desired pH, the solution was poured into the reactor. The reactor was designed and constructed by Duckworth (2014) and Spencer (2014), and houses seven 245 nm UV LEDs from Sensor Electronic Technology, Inc. (Columbia, SC). The reactor was constructed of 316 stainless steel; inflow and outflow ports were 1 inch in diameter, see Figure 4.

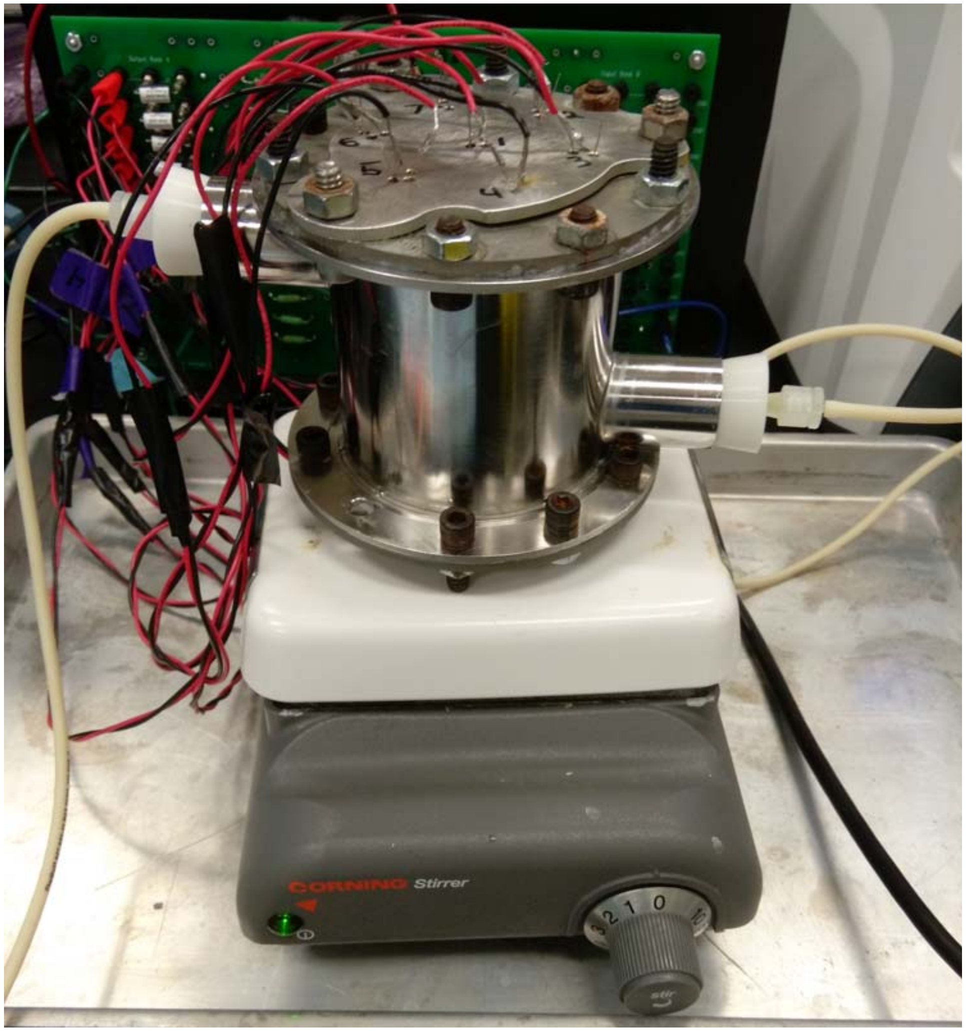


Figure 4: AOP Reactor

This reactor contained a half-inch stir bar to meet the assumptions of a CSTR. After the reactor is full and placed on the mix table, calibration curve mixtures were prepared.

The calibration curve mixtures were comprised of 0% solution, 25%, 50%, 75%, and 100%. For 0% solution, 10 mL of DI water was all that is required. For 25% solution calibration, 7.5 mL of DI water was combined with 2.5 mL of the solution. For 50% solution calibration, 5 mL of DI water was combined with 5 mL of solution. For 75%, 2.5 mL of DI water was combined with 7.5 mL of the solution. For 100%, 10 mL of solution was required.

The outflow of the CSTR was connected to a continual flow, quartz cuvette for use in Agilent Technologies Cary 60 UV-Vis Spectrophotometer (Santa Clara, CA). See entire setup in Figure 5.

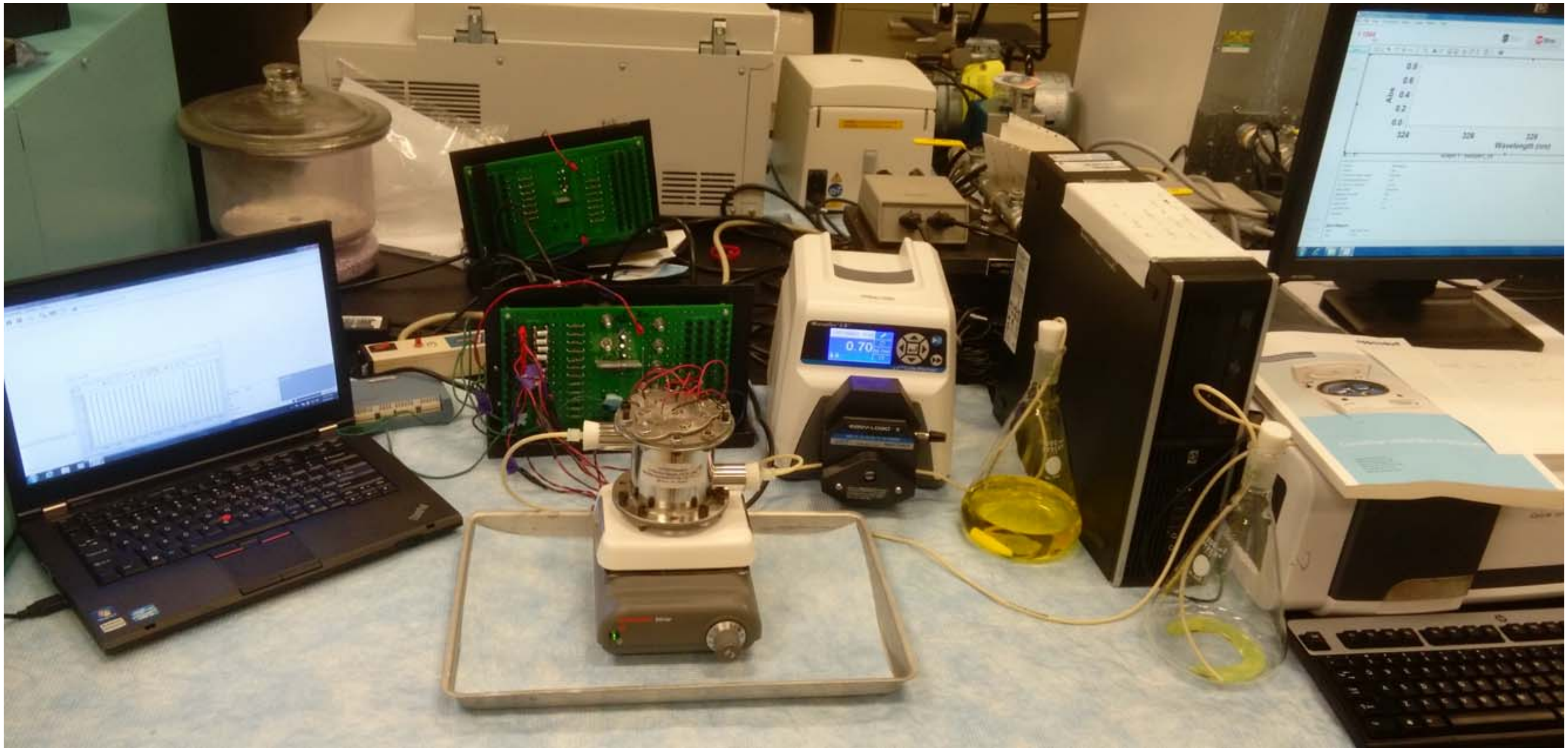


Figure 5: AOP Experimental Setup

The Cary 60 Scan program was set up to measure absorbance every five minutes for five hours between 425 and 435 nm; the absorbance peak for TAR is 430 nm. Five hours was selected as the experiment operating time due to previous research operating conditions (Mudimbi, 2015; Scott, 2015). It should be noted, that the full residence time for this reactor at flow rate of 0.7 mL/min is 500 minutes; however, steady state removal was achieved prior to the 300 minutes of operation. After the experiment concluded, calibration curve mixtures were individually loaded into the cuvette through a syringe and the absorbance was measured through Cary 60 Rapid Result function at 430 nm. These values were entered into the excel program which calculated the calibration curve equation and R^2. The data collected by Cary 60 was added to this spreadsheet and the model was created using solver to find k_s (min^{-1}) see Equation 5, where C_F is the final concentration, C_I is the initial concentration, τ is residence time in the reactor, and t is the retention time (see data and charts in Appendix C and D, respectively). To calculate the adjusted first order rate constant ($k_{s,adj}$), k_s is divided by the duty cycle (DC), see Equation 6.

Equation 5: CSTR Equation

$$\frac{C_F}{C_I} = (\frac{1}{1 + \tau k_s})(1 + \tau k_s e^{-\left(\frac{1}{\tau}+K\right)t})$$

Equation 6: Adjusted First Order Rate Constant

$$k_{s,adj} = \frac{k_s}{DC}$$

In the effort to answer the second research question, the byproducts of this AOP were examined. Using the chromatography of untreated TAR as a baseline and foundation for the analysis method, effluent streams from the AOP Experiment were compared to that of the baseline. Using the information from Benjamin & Lawler (2013) and dos Santos et al. (2014), potential degradation mechanisms were selected that might explain the observed changes in the chromatography. Special attention was paid to the byproducts in experiments in which the pH of the solution increases.

Thirty minutes prior to the completion of each experiment, the outflow from the cuvette was transferred to a different storage beaker. The pH of this effluent was measured, and approximately 10 mL was taken for use in byproduct analysis. The 10 mL of effluent was filtered through a 0.2 µm hydrophilic syringe filter (Minisart from Sartorius Stedim Biotech, Goettingen Germany). This was stored in the dark at 2 degrees Celsius until analysis by High Performance Liquid Chromatography (HPLC).

3.1.2 Byproduct Analysis

3.1.2.1 Chromatographic Contrast Angle Analysis

The first step to determine how byproducts were formed was to calculate CCAs for each experiment effluent chromatography. The byproducts were analyzed using HPLC, both a positive ionization and a negative ionization analysis was conducted (see method files in Appendix H and I, respectively). The HPLC was an Agilent Technology 1260 Infinity combined with 6130 Quadrupole LC/MS (Agilent Technologies, Santa Clara, CA). The method included use of a SUPELCO Analytical column (Ascentis ® Express C18, Cat#53829-U, 15 cm x 4.6mm, 2.7 µm) and a particle fragmentor, with acetonitrile as the mobile phase. Using Equation 4, the CCA was calculated between the 0% DC experiments and the H_2O_2 Control experiments within each pH level. In addition, the CCAs were calculated between each experiment and the 0% DC of the respective pH level. Wan (2002) individually measured the same analyte 28 times to calculate a “self-spectral angle”. In theory, if two vectors are identical, their CCA should equal zero. However, in application, the readings are not so precise. Wan's (2002) calculations for the self-spectral angle contrast yielded 2.7° ± 1.6°, and 2.2° ± 1.0° for analytes a and b. This study did not include the calculation of a self-spectral angle because of the large number of experiments to analyze. Therefore, for the purpose of this study any CCAs calculated less than 5° will be considered for similarity. Each data set for the analytes of this study included over 120 points; therefore, this study’s CCAs are calculated in 120-dimensional space and cannot be graphically represented on traditional Cartesian axes.

3.1.2.2 Mass Spectroscopy Analysis

Analysis of the MS spectra suggested byproduct structures. See Positive and Negative Chromatograms, and MS plots in Appendix J and K, respectively. Factors that were considered were mass to charge ratios (kinetic energy) reported by the MS, but also the fact that in this method, a doubly charged particle with a mass of 26 will be indistinguishable from a single-charge particle with a mass of 13. This study’s AOP experiments were conducted over several months, and the byproducts of each experiment were stored at 2 degrees C until completion of all AOP experiments, so that each experiment’s effluent could be processed by the HPLC on the same day. However, due to the randomization of the experiment order, any effect time could have on byproduct profiles (whether long term reactions continued or if steady state was reached upon completion of the experiment) should not be statistically significant with respect to any DC or pH regression analysis.

3.2 H_2O_2 Control AOP Experiment (0% DC)

There may be interaction with the dye and the pH adjustors. In order to form a baseline, a complete solution was mixed at each pH level and transferred through the CSTR reactor but the UV LEDs were not powered. The k_s was expected to be close to or equal to zero. Effluent samples from each of these experiments were stored in the refrigerator to be evaluated via HPLC along with the other experiment effluents.

3.3 UV Control AOP Experiment (100% no H_2O_2)

In order to ensure that there is no interaction between the pH adjustor and the UV radiation, a solution was mixed without H_2O_2 and transferred through the CSTR reactor while running the 100% DC. The k_s was expected to be close to or equal to zero. Effluent samples from each of these experiments were also collected and stored for evaluation with the byproducts in the HPLC.

3.4 Statistical Methods

The purpose of this section is to outline the statistical methods used for data analysis for this research effort. This section provides computer program information and execution procedures for Analysis of Variance (ANOVA), Tukey, and Linear Regression analyses. These analyses were conducted to predict the first order rate constant, as well as chromatographic contrast angles. These were the "response" variables, and are denoted by Y_1 or Y_2. Predictor variables, such as pH, DC, operator of the experiment, spin table speeds, date of the experiment, etc. were used in analysis and are denoted by $X_1, \ldots X_i$. P-values were considered statistically significant if they were less than 0.05 (95% confidence).

In order to gain a better understanding of statistical significance of the levels within pH and DC, dummy variables (DVs) can be incorporated into models. DVs are binary; pH levels are represented by three dummy variables, for example, pH 6, pH 7, and pH 8 (this assumes that pH 9 is the baseline). DC levels are represented by seven DVs, for example, DC 5, 10, 20, 30, 50, 70, and 100 (which assumes DC 0 is the baseline). All regression models in this study include DVs.

3.4.1 Analysis of Variance

One-way Analysis of Variance (ANOVA) analyses were conducted for each response variable. This uses the F-Test and is statistically significant when the p-value is less than 0.05. Each ANOVA test incorporated pH and DCs as predictors. The ANOVA report is generated in JMP® by the "Fit Y by X" analytical tool. Then, "Means and ANOVA" option is chosen for the plot which reports the means, standard deviation error, and upper/lower 95% for each category within each X variable. The "Prob > F" displays the p-value of the test. The F-test only shows that one of the categories within pH or DC is significant; it does not specify which pH level or DC is significant. To better clarify statistical distinctions, Tukey analyses was performed.

3.4.2 Tukey Analysis

Tukey Analysis was conducted for each response variable. This uses the Q-Test and is statistically significant at $\alpha = 0.05$. Each Tukey analysis incorporated pH and DCs as predictors. The report is generated in JMP® by the "Fit Model" tool. Then under each variable, "LS Means Plots" and "LS Means Tukey HSD" options are selected. These display the LS Means plot, which shows means and error bars; and the Tukey table, which shows statistically significant comparisons in red. This also displays a table where each level (i.e. pH levels 6 through 9 or DC levels between 5% and 100%) is categorized by letter groups (see Appendix). These letters connect levels which are not statistically different; therefore, levels not connected by the same letter are significantly different. While the Tukey analysis provides insight to what levels are distinct, it doesn't provide the whole picture. To better understand what levels are significant predictors, regression analysis must be conducted.

3.4.3 Linear Regression Analysis

3.4.3.1 Effect Tests

Linear regression is an iterative process. Evaluating ANOVA and Tukey analyses gives an idea of what might be significant, but another tool in selecting viable predictor variables is to use a Stepwise fit. The stopping rule is p-value threshold (set to 0.25 to enter and to leave), and the direction is mixed. Every conceivable predictor variable is loaded and compared against one another. After the rules are established, the model computes and shows all variables ranked by the p-value for that particular arrangement of variables. However, these are suggested variables and their respective p-values will change with any change in the model, in addition, may not uphold required assumptions, or meet reasonable p-values. Ideally, all significant predictor variables have p-value of less than 0.05. Having too many predictor variables can also have a negative effect on the validity of the model. For this reason, the adjusted R^2 will be the preferred value used in this research effort for amount of understood variance. The adjusted R^2 carries a penalty for increasing the number of variables, as well as for variables of low added benefit. After each model is generated, four columns must be added to the data table: the residuals of the model, the studentized residuals of the model, Cook's D Influence, and the residuals of the model squared, each to be discussed in coming sections.

3.4.3.2 Required Assumptions in Regression Modelling

There are three assumptions that must be upheld in order to produce a valid regression model. They are normally distributed residuals, constant variance, and independence. Each of these assumptions requires a test.

Whether the residuals are normally distributed is evaluated with the Shapiro-Wilks Test (W-Test). A distribution is created for the residuals of the model. Then, a "continuous, normal fit" tool is selected and under the "fitted normal" dropdown menu, the "goodness of fit test" is selected, which reports the Shapiro-Wilks test. The assumption of normality is upheld with p-values of greater than 0.05.

The assumption of constant variance is tested by the Breusch-Pagan test. This requires an additional model to be generated with all the same X variables as the original model, only the Y variable is the residuals of the model squared. This creates a Sum of Squares Regression (SSR) model. The only value of interest reported by this SSR model is located under the Analysis of Variance heading; the value for the model-sum of squares is required for the calculation of the Breusch-Pagan test statistic (TS). In addition, three values required for the Breusch-Pagan test are found in the original model. The values are: N (located after "observations or sum wgts"), degrees of freedom (located under the ANOVA heading; the value for model-DF), and the Sum of Squares Error (SSE) (located under the ANOVA heading; the value for error-sum of squares). These values are incorporated into the following excel equations for the TS (Equation 7) and p-value (Equation 8). The final step in testing for constant variance is the χ-distribution in excel, coded “Chidist(TS, degrees of freedom)”. The resulting p-value is compared with α, and if the p-value is greater than 0.05, then the assumption of constant variance is upheld.

Equation 7: Breusch-Pagan Test Statistic

$$TS = \frac{\frac{SSR}{2}}{(\frac{SSE}{N})^2}$$

Equation 8: Breusch-Pagan P-Value

$$p - value = \chi(TS, DF)$$

Finally, the assumption of independence is tested with the Durbin-Watson test. This is found in the original model report, under “Row Diagnostics” then “Durbin-Watson Test”. This displays the TS, but not the p-value. This is corrected by selecting the drop down for Durbin-Watson, and selecting “significance p-value”. If the p-value is greater than 0.05, then the assumption of independence is upheld.

If any of these tests are not upheld, the model may still be valid. However, outlier detection must be conducted (to make the case that a robust deviation has occurred). If any cohorts exist, they should be identified and incorporated to the model. The residual by predicted plot must also appear to have no trend. If none of these steps resolve the issue, other variable combinations must be considered, and the assumptions tests must be conducted again.

3.4.3.3 Outlier and Influence Detection and Processing

Outliers and overly influential points are mainly detected by two respective tools. The first is a histogram of the studentized residuals. The desired outcome is that no points fall outside ± 3 standard deviations. The second tool is an overlay plot of Cook’s D

Influence. In this plot, it is important that no points rank higher than 0.5. Any points that are identified by these tools can be evaluated – if any explanation can be offered as to why these points in particular can be grouped together (for example, all conducted on the same day, or during some condition that did not apply to the rest), a cohort variable may be created. Overly influential points may cause issues with the assumptions tests, but if all the assumption tests pass, then the points may still be included. If not, there may be a reasonable case to have the points excluded from the model due to the fact they were overly influential.

3.4.3.4 Model Formation

Once a model is formulated in which all the tests pass and a reasonable adjusted R^2 is achieved, the model may be evaluated for functionality. Variance Inflation Factor (VIF) scores must be less than 2 for all parameters. All models in this study are linear, and the equation for the model is generated in the original model report under “Parameter Estimates”. The base formula for linear regression is shown in Equation 9, where Y is the model’s predicted value, e is the intercept, X_i are the predictor variables, and β_i are the respective predictor variable coefficients.

Equation 9: Linear Regression Model

$$Y = e + \sum_{i=1}^{n} \beta_i X_i$$

3.4.3.5 Error Analysis

Once the formula is entered into a column in the data sheet, a new column is generated to calculate the model’s Average Predictive Error (APE), which is defined by the absolute value of the true response value minus the model's predicted value divided by the true response value, see Equation 10.

Equation 10: Regression Model APE Score

$$APE\ (\%) = \frac{\left|Y_{true} - Y_{predicted}\right|}{Y_{true}} * 100\%$$

Finally, these values are used to create a histogram of all the APEs. This research report will state each regression model's respective mean APE, the median APE, the maximum APE, and the amount of the deviation from the true value generated by that specific maximum error.

IV. Results and Discussion

4.1 The Effect of pH and Duty Cycle on the Relative Concentration of Tartrazine

Figure 6 shows the effect of DC on the relative concentration of TAR at pH 6. The x-axis shows the time of the experiment; the y-axis shows the relative concentration (C/C_0). Over the course of 300 minutes, the relative concentration of TAR decreased to 0.98, 0.97, 0.91, 0.90, 0.87, 0.75 - 0.83, and 0.76 for DCs of 5%, 10%, 20%, 30%, 50%, 70%, 70% repeat experiment, and 100% respectively. Noteworthy results include the first iteration of the 70% DC, for which the C/C_0 was approximately 0.75 -- the greatest level of removal observed in this study, and an improvement of 2% removal compared to the optimal removal observed by Mudimbi (2015) at 100% DC. However, Mudimbi (2015) did not record the pH of this solution. The pH 6 at 70% DC condition was repeated approximately two months later, and only achieved relative C/C_0 reduction of approximately 0.83. This may be attributed to the decrease in output capability of the LEDs due to operating time. The second highest concentration reduction was for the 100% DC, approximately 0.76. A possible explanation for the decreased performance at the 100% DC may have been due to different operators between the three experiments. However, this explanation was not found to be a significant predictive factor for the first order rate constant. The rest of the data set results were as expected, with the first order rate constant gradually increasing with increasing DC level. These results mean that operating the experiment at pH 6 can increase the proficiency of the AOP of TAR. Additionally, optimal TAR removal may be accomplished with greater efficiency than the 100% DC.

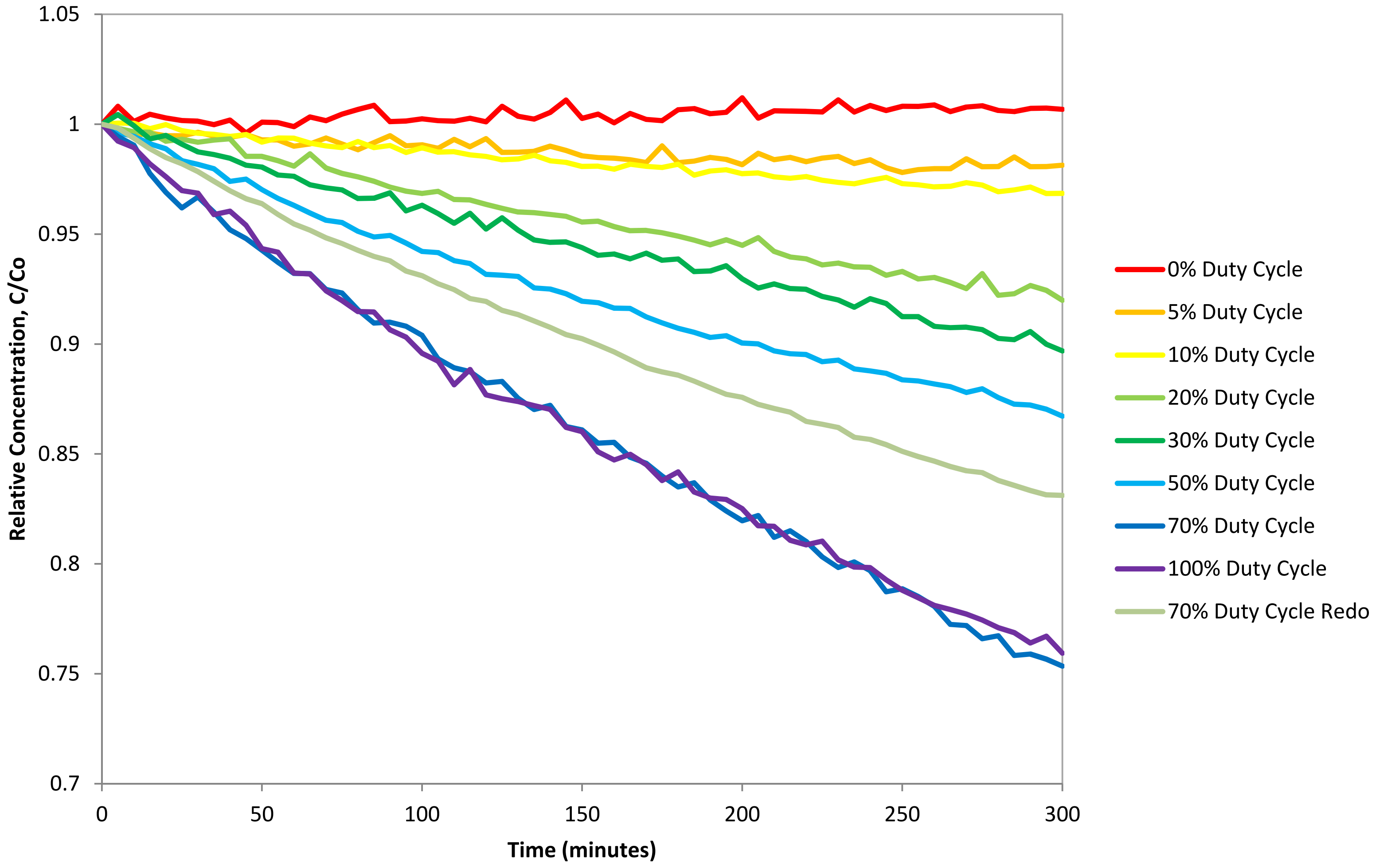


Figure 6: The Effect of Duty Cycle on the Removal of Tartrazine at pH 6

Figure 7 shows the effect of DC on the relative concentration of TAR at pH 7. The x-axis shows the time of the experiment; the y-axis shows the relative concentration (C/C_0). The magnitudes of the relative concentration of TAR were recorded as follows: 0.98, 0.96, 0.95, 0.91, 0.88, 0.89, 0.80 for DCs of 5%, 10%, 20%, 30%, 50%, 70%, and 100%, respectively. These first order rate constants appeared as expected, gradually increasing between 0% and 100% DCs, with one exception. The reduction in relative concentration for the 50% DC (0.88) narrowly exceeded the reduction for that of the 70% DC (0.89). This was not due to the degradation of the LEDs over time, because the 50% was conducted a month after the 70%. This will be discussed further for the pH 8 and 9 sections. Also, the 100% DC (20% removal) substantially outperformed the 50% DC (12% removal). This data set demonstrated that at pH 7, the removal of TAR generally follows AOP/dye reduction trends previously observed by Duckworth (2014), Mudimbi (2015) and Scott (2015).

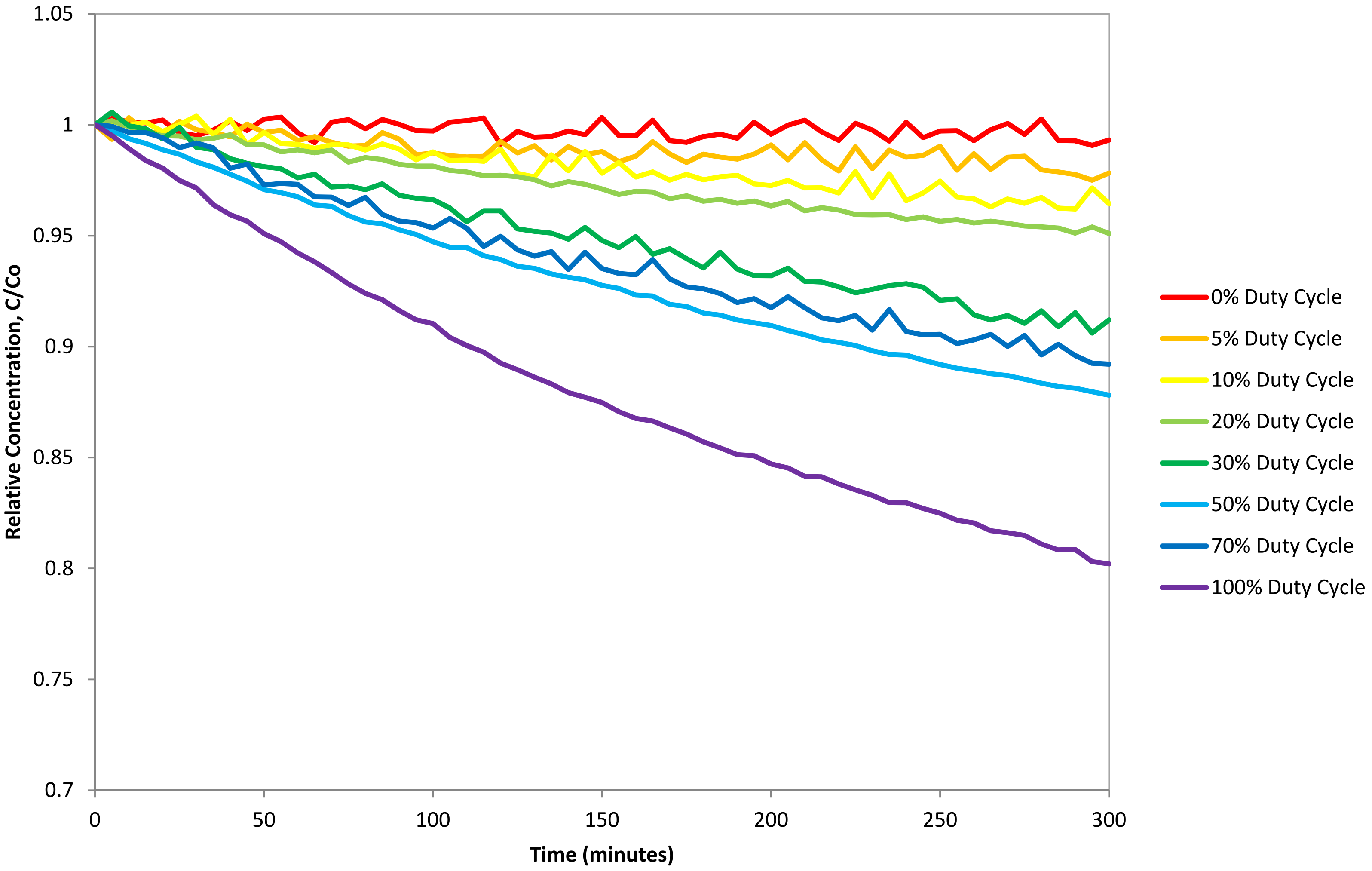


Figure 7: The Effect of Duty Cycle on the Removal of Tartrazine at pH 7

Figure 8 shows the effect of DC on the relative concentration of TAR at pH 8. The x-axis shows the time of the experiment; the y-axis shows the relative concentration (C/C_0). The observed concentration of TAR after 300 minutes was 1.00, 0.99, 0.97, 0.96, 0.84, 0.87 - 0.91, 0.90-0.90 for DC levels of 5%, 10%, 20%, 30%, 50%, 70%, 70% duplicate, 100%, and 100% duplicate, respectively. In this operating condition, the greatest removal was observed during the 50% DC (16% removal), the second greatest removal was observed during one of the 70% DC iterations (13% removal), and the third greatest removal was observed for both the 100% DC iterations (10% removal). This inversion of the relationship between removal and the DC was not expected. It is likely the abundance of OH^- and the bicarbonate (see Equation 2) in the solution may have a scavenging effect on the hydroxyl radicals (Alpert et al., 2010). This may also indicate an interaction between this scavenging effect and the higher DCs. This data showed that at higher pH levels the first order rate constant is negatively correlated with higher DC, resulting in diminished TAR removal.

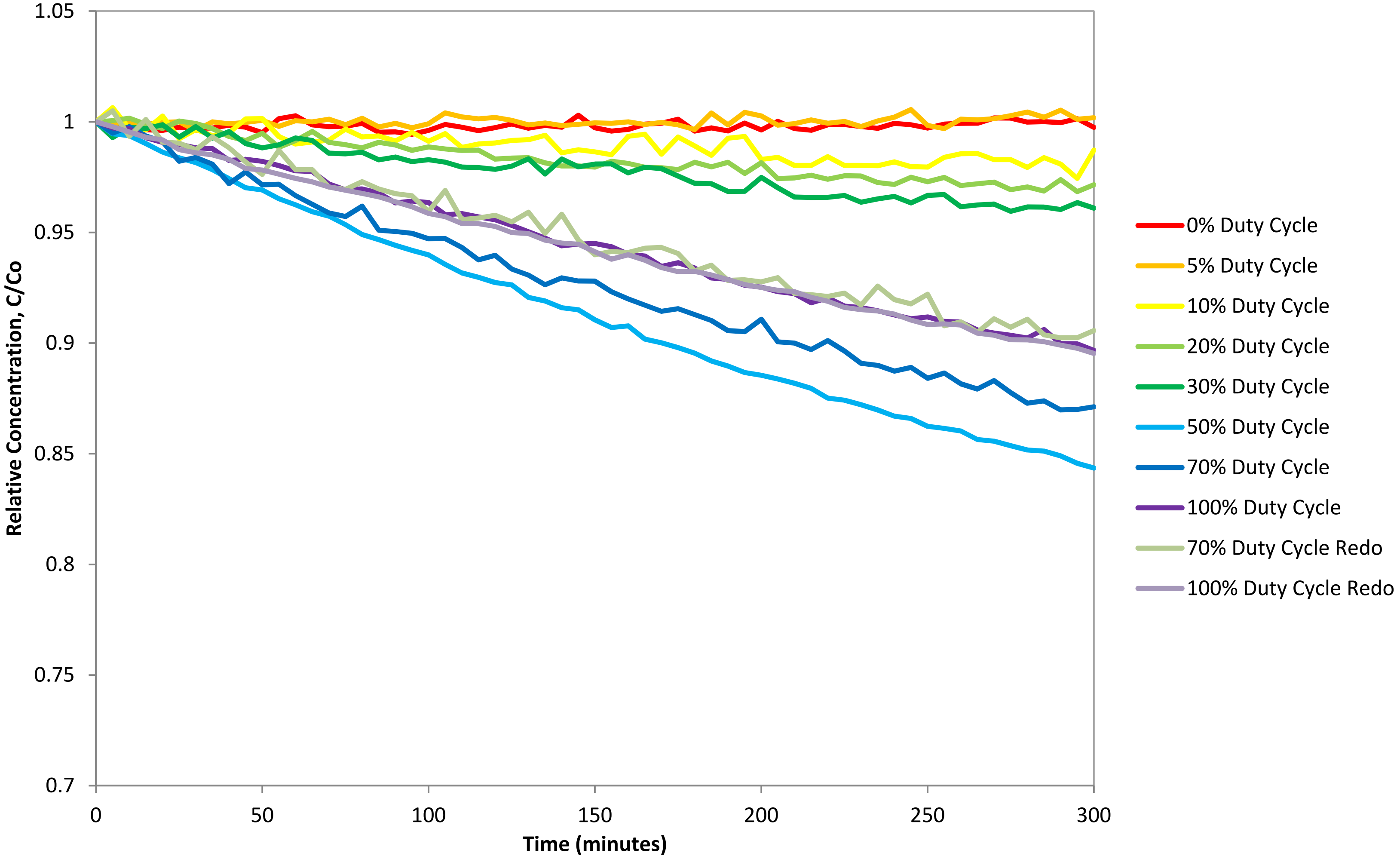


Figure 8: The Effect of Duty Cycle on the Removal of Tartrazine at pH 8

Figure 9 shows the effect of DC on the relative concentration of TAR at pH 9. The x-axis shows the time of the experiment; the y-axis shows the relative concentration (C/C_0). The relative concentrations of TAR at the end of 300 minutes were recorded as follows: 0.99, 0.98, 0.98, 0.98, 0.94 - 0.97, 0.94, and 0.94 for DC levels of 5%, 10%, 20%, 30%, 50%, 50% experiment repeat, 70%, and 100%, respectively. Under this operating condition, the removal of TAR was similar for all DC levels. The top three TAR removal conditions were 50%, 70%, and 100% (the magnitude of each of these three concentrations was within C/C_0 of .005); however, the same inversion observed during pH 8 experiments occurred, with the greatest removal of TAR occurring at the 50% DC (only 6% removal). Because this inversion behavior was observed for all experiment conditions except pH 6, the most likely explanation is that bicarbonate (the dominant carbonate species at pH values >6.35) interacts with hydroxyl radicals resulting in less TAR removal. This is supported by the negative correlative relationship between bicarbonate concentration and TAR removal between pH 8 and pH 9 conditions observed in this study. For the pH 9 experiments, however, the differences in the first order rate constants between these levels were much less than for the pH 8 experiments. This data set showed further diminishment of performance of the AOP. Within the pH 9 condition, improvement between DCs was negative or marginal with DC increases. As with the pH 8 experiments, the positive correlative relationship between DC and first order rate constant does not apply. This additional decrease in performance relative to the pH 8 experiments supports the indication of a scavenging effect due to the increase in the concentration of OH^-.

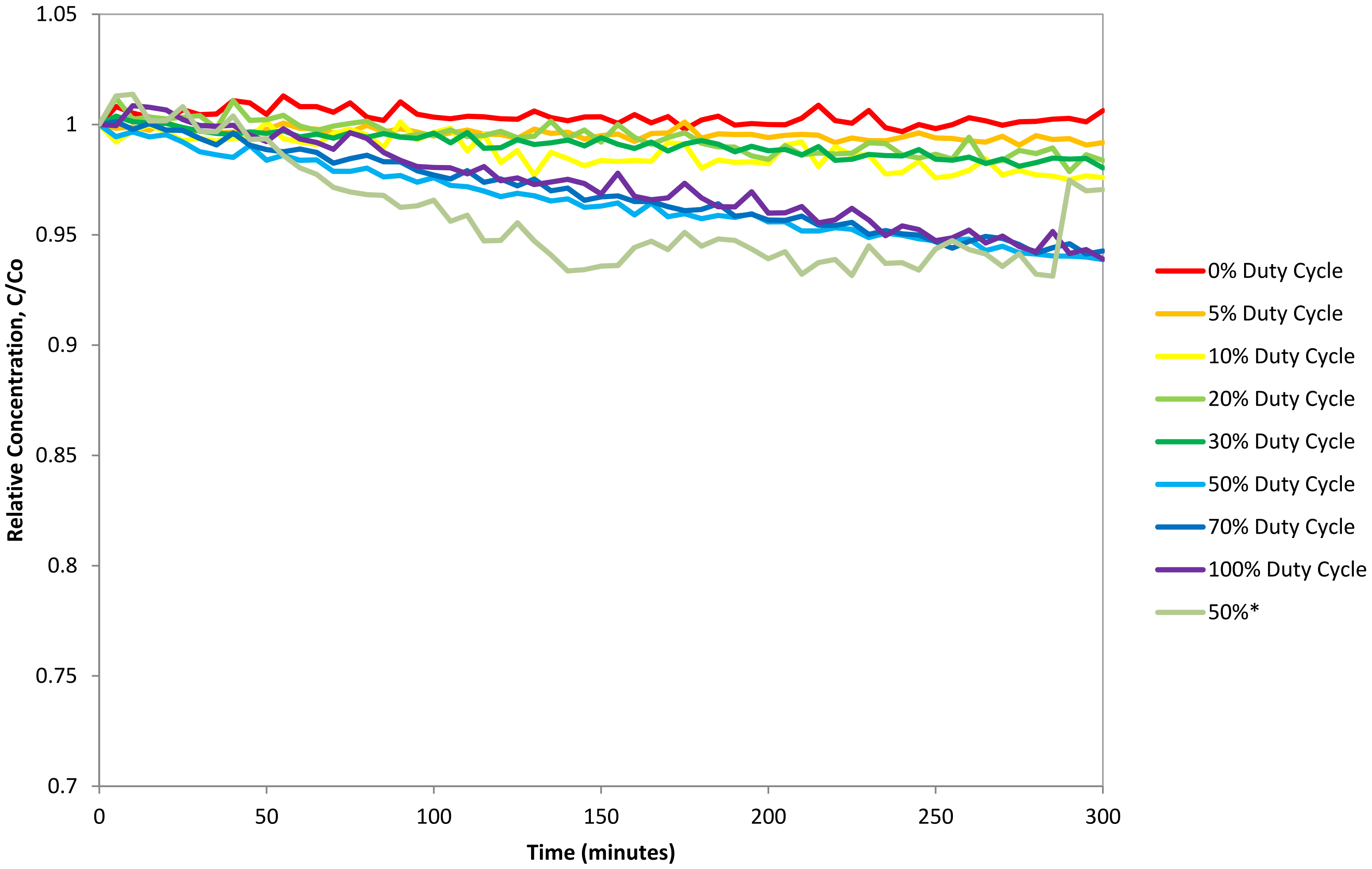


Figure 9: The Effect of Duty Cycle on the Removal of Tartrazine at pH 9

4.2 Statistical Analysis of First Order Rate Constants

Figure 10 shows the one-way ANOVA of k_s by nominal pH .The x-axis shows the pH of the experiment and the y-axis shows the first order rate constant. The ANOVA triangles indicate the specific pH level mean response, and the upper and lower 95% values, while the line through the entire plot shows the mean response for all data points. Mean response for the all points was 3.91E-4 min^{-1}, and the mean response within the pH levels were: 6.22E-4 min^{-1}, 4.18E-4 min^{-1}, 3.54E-4 min^{-1}, 1.74E-4 min^{-1} for pH 6, 7, 8, and 9, respectively. The mean values of pH 6 and 7 outperformed the overall mean, while pH 8 and 9 did not exceed the overall mean. The data points at pH 9 were clustered, and became more widespread at lower pH levels. This is due to the fact that at pH 9, significantly less removal was observed. The reported p-value was 0.0471, which denotes the high confidence that pH is a statistically significant predictor of the first order rate constant.

Figure 11 shows one-way ANOVA of k_s by DC. The x-axis shows the DC of the experiment and the y-axis shows the first order rate constant. The ANOVA triangles indicate the specific DC level mean response, and the upper and lower 95% values, while the line through the entire plot shows the mean response for all data points. Mean response for the all points was 3.91E-4 min^{-1}, and the mean response within the DC levels were: 5.4E-5 min^{-1}, 1.22E-4 min^{-1}, 1.95E-4 min^{-1}, 2.85E-4 min^{-1}, 4.88E-4 min^{-1}, 6.51E-4 min^{-1}, and 6.89E-4 min^{-1} for DCs 5%, 10%, 20%, 30%, 50%, 70%, and 100%, respectively. The mean values for DC levels 50%, 70%, and 100% exceeded the overall mean, while the DC levels 5%, 10%, 20%, and 30% did not exceed the overall mean. The points were closely positioned in the lower DCs, and more spread out at higher DCs. The pH had much greater influence on the first order rate constant at higher DCs. The p-value was 0.0017, which indicates high level of confidence of statistical significance of DC as a predictor variable for the first order rate constant. This finding was consistent with other research findings with respect to degradation of dye using AOP (Duckworth, 2014; Mudimbi, 2015; Scott, 2015).

Tukey analysis (Appendix E) showed a statistically significant (with 95% confidence) distinction between pH groups as described as follows. Levels 6 and 7 were connected by group A, and Levels 7, 8, and 9 were connected by group B. Levels not connected by the same letter are significantly different. This means that responses between pH 6 and 7 were not significantly different, but pH 6 responses were significantly different from those of pH 8 and 9. Tukey analysis of the first order rate constant by DC (Appendix E) showed distinction between DC groups as follows. DC Levels 100%, 70%, and 50% were connected by group A; DC Levels 70%, 50%, and 30% are connected by group B; DC Levels 50%, 30%, 20%, and 10% were connected by group C; lastly, DC Levels 30%, 20%, 10%, and 5% were connected by group D. This means the 100% DC was significantly different than DCs of 30% and below, the 70% DC was significantly different than DCs of 20% and below, and that the 50% DC was significantly different than the 5% DC. This result is consistent with other AOP research conducted by Duckworth (2014), Mudimbi (2015), and Scott (2015).

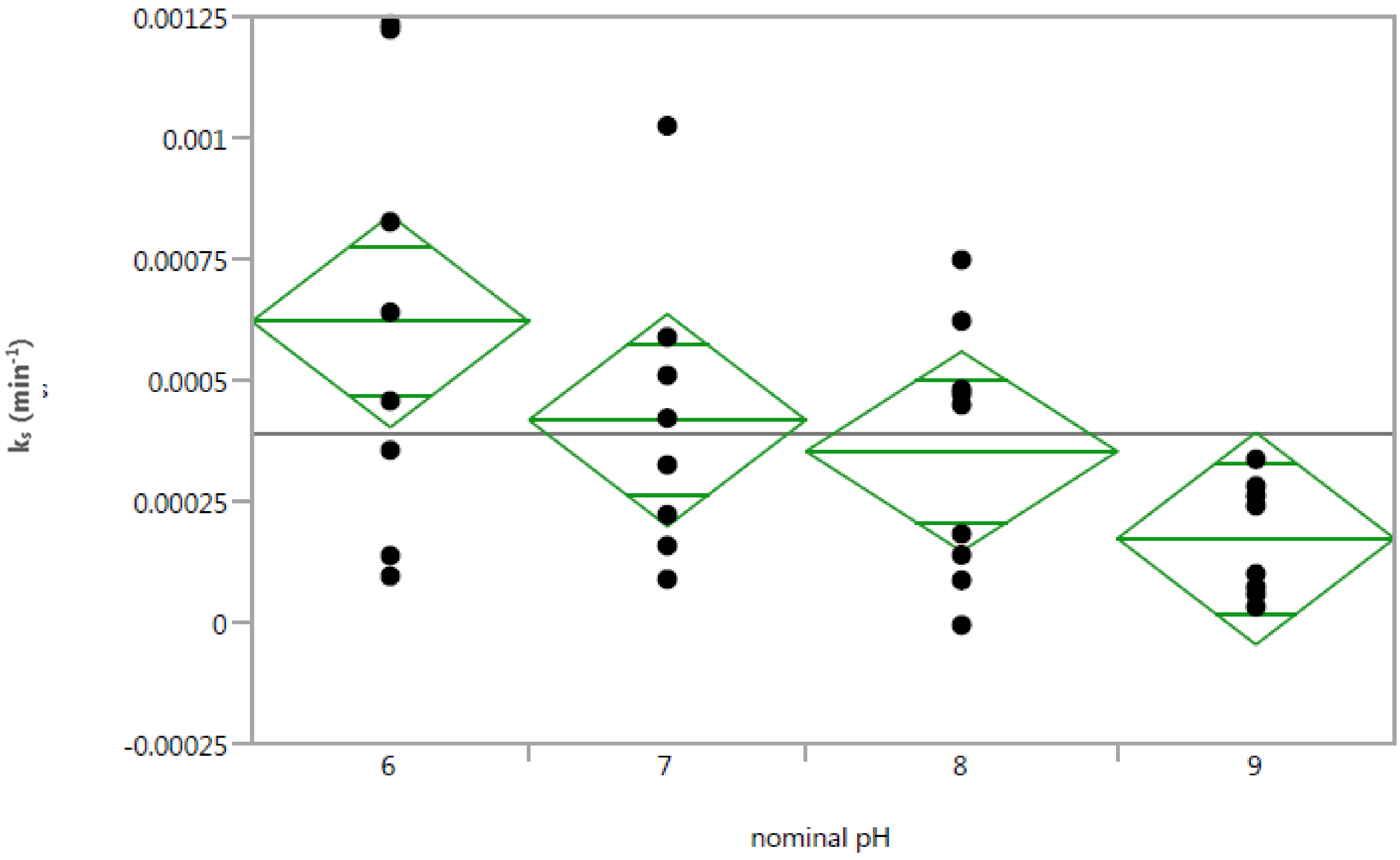


Figure 10: AOP ANOVA of ks by nominal pH; p-value = 0.0471 means there is a statistically significant distinction between at least two pH groups. Each point represents one experiment. Within each pH category, experiments operated at DCs between 5% and 100% are represented.

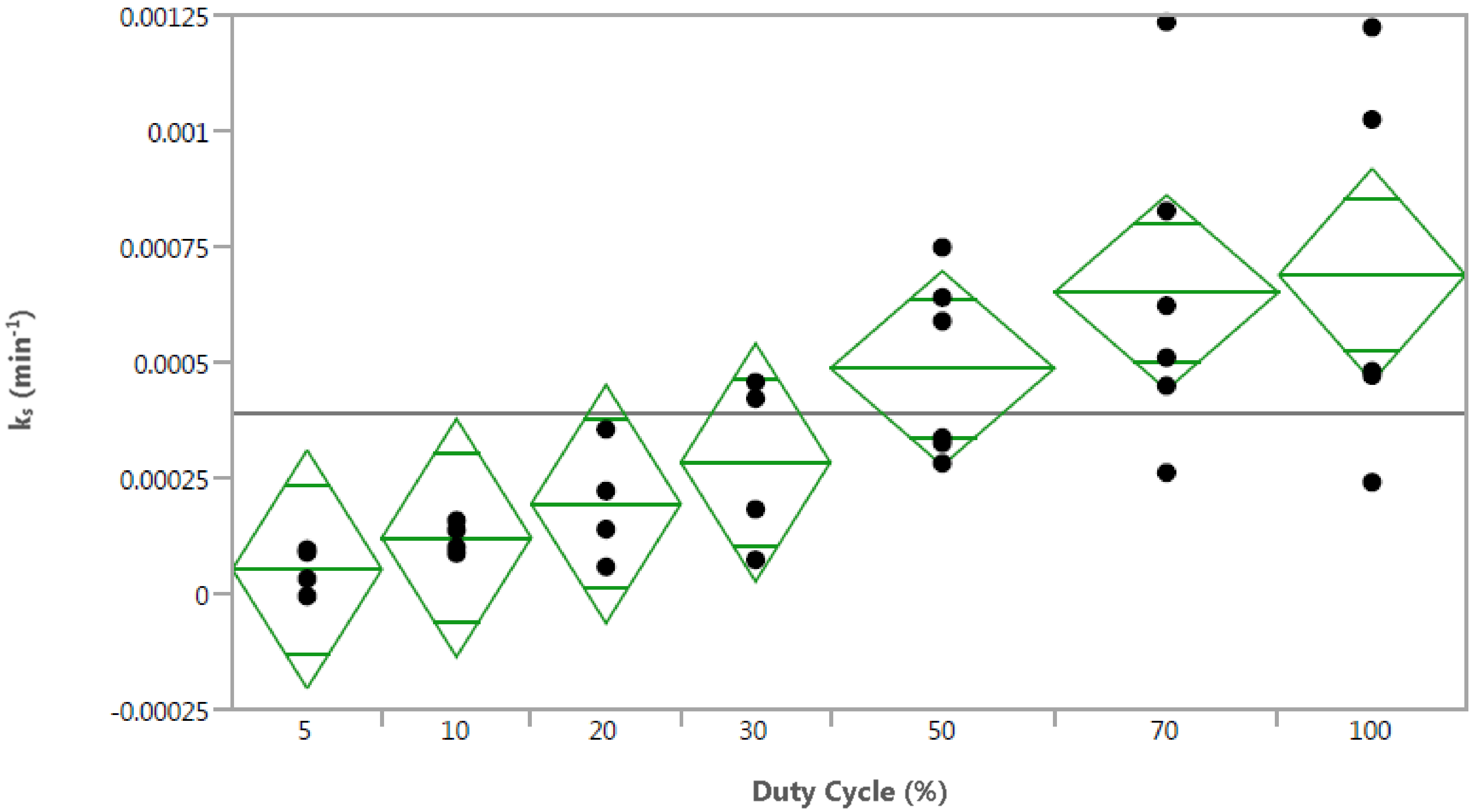


Figure 11: AOP ANOVA of ks by Duty Cycle; p-value = 0.0017 means there is a statistically significant distinction between at least two DC groups. Each point represents one experiment. Within each DC category, experiments operated at nominal pH levels between 6 and 9 are represented.

Figure 12 shows the one-way ANOVA of $k_{s,adj}$ (k_s/DC) by nominal pH. The adjusted first order rate constant is the first order rate constant divided by the DC; thus, the $k_{s,adj}$(DC=100%) = k_s(DC=100%). The x-axis shows the pH of the experiment and the y-axis shows the adjusted first order rate constant. The ANOVA triangles indicate the specific pH level mean response, and the upper and lower 95% values, while the line through the entire plot shows the mean response for all data points. Mean response for the all points was 9.64E-4 min^{-1}, and the mean responses within the pH levels were: 1.511E-3 min^{-1}, 1.19E-3 min^{-1}, 6.79E-4 min^{-1}, 5.13E-4 min^{-1} for pH 6, 7, 8, and 9, respectively. The mean values of pH 6 and 7 surpassed the overall mean, while pH 8 and 9 were below the overall mean. The reported p-value was <0.0001, which denotes the high confidence that pH is a statistically significant predictor of the adjusted first order rate constant.

Figure 13 shows the one-way ANOVA of $k_{s,adj}$ by DC. The x-axis shows the DC of the experiment and the y-axis shows the adjusted first order rate constant. The ANOVA triangles indicate the specific DC level mean response, and the upper and lower 95% values, while the line through the entire plot shows the mean response for all data points. The mean response for the all points was 9.64E-4 min^{-1}, and the mean responses within the DC levels were: 1.088E-3 min^{-1}, 1.223E-3 min^{-1}, 9.75E-4 min^{-1}, 9.49E-4 min^{-1}, 9.75E-4 min^{-1}, 9.30E-4 min^{-1}, and 6.89E-4 min^{-1} for DC levels of 5%, 10%, 20%, 30%, 50%, 70%, and 100%, respectively. The mean values of DCs 5%, 10%, 20%, and 50% exceeded the overall mean, while DCs 30%, 70%, and 100% did not exceed the overall mean. The mean value for the 10% DC was the greatest out of each of the DCs, similar to the first order rate constant. This is a unique deviation, as Mudimbi (2015) and Scott

(2015) observed greatest values for the adjusted first order rate constant in the 5% DC. However, the trend of the entire study agrees with that observed by Mudimbi (2015) and Scott (2015). While the greatest values for this study were also from the 5% DC, the mean of the 10% group was greatest. The result was influenced by the pH 8 experiment at 5% DC, which did not produce a positive k_s (slightly negative). Theoretically, the k_s for this point should be 0, because there was no TAR removal observed. The Tukey analysis' of the adjusted first order rate constant by DC reported a p-value of 0.8827, which exhibits insufficient evidence to suggest that DC is a statistically significant predictor of the adjusted first order rate constant.

Tukey analysis of $k_{s,adj}$ by pH and DC (Appendix E) shows a statistically significant (with 95% confidence) distinction between pH groups as described as follows. Levels 6 and 7 were connected by group A, Levels 7, and 8 were connected by group B, and Levels 8 and 9 were connected by group C. Tukey analysis shows that levels not connected by the same letter are significantly different. This means that responses for pH 6 and 7 were not significantly different, but pH 6 responses were significantly different from those of pH 8 and 9. Tukey analysis of the adjusted first order rate constant by DC (Appendix E) showed no distinction between DC groups, as all DC levels are connected by the same letter.

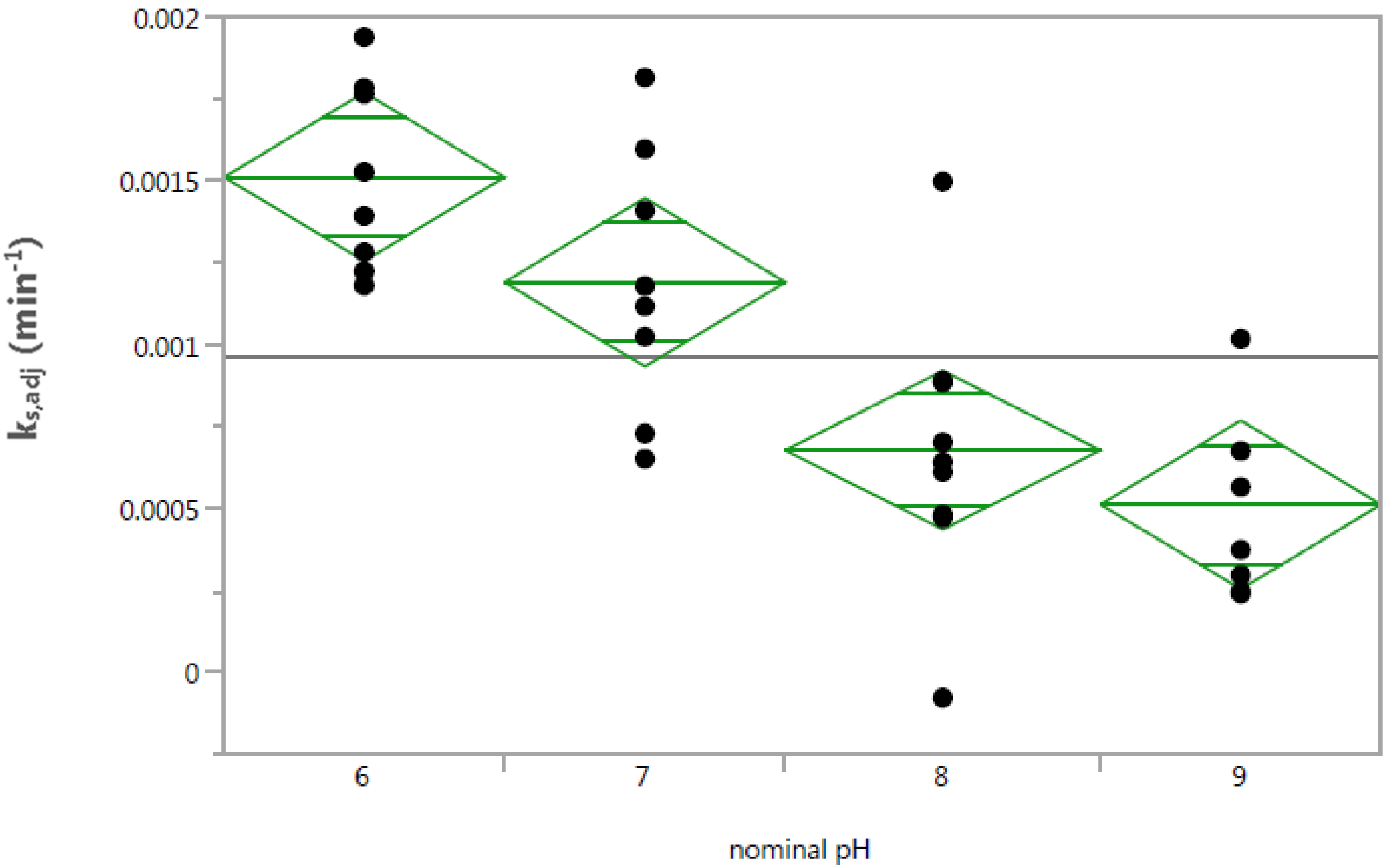


Figure 12: ANOVA of AOP ks,adj by Nominal pH; p-value < 0.0001 means there is a statistically significant distinction between at least two pH groups. Each point represents one experiment. Within each pH category, experiments operated at DCs between 5% and 100% are represented.

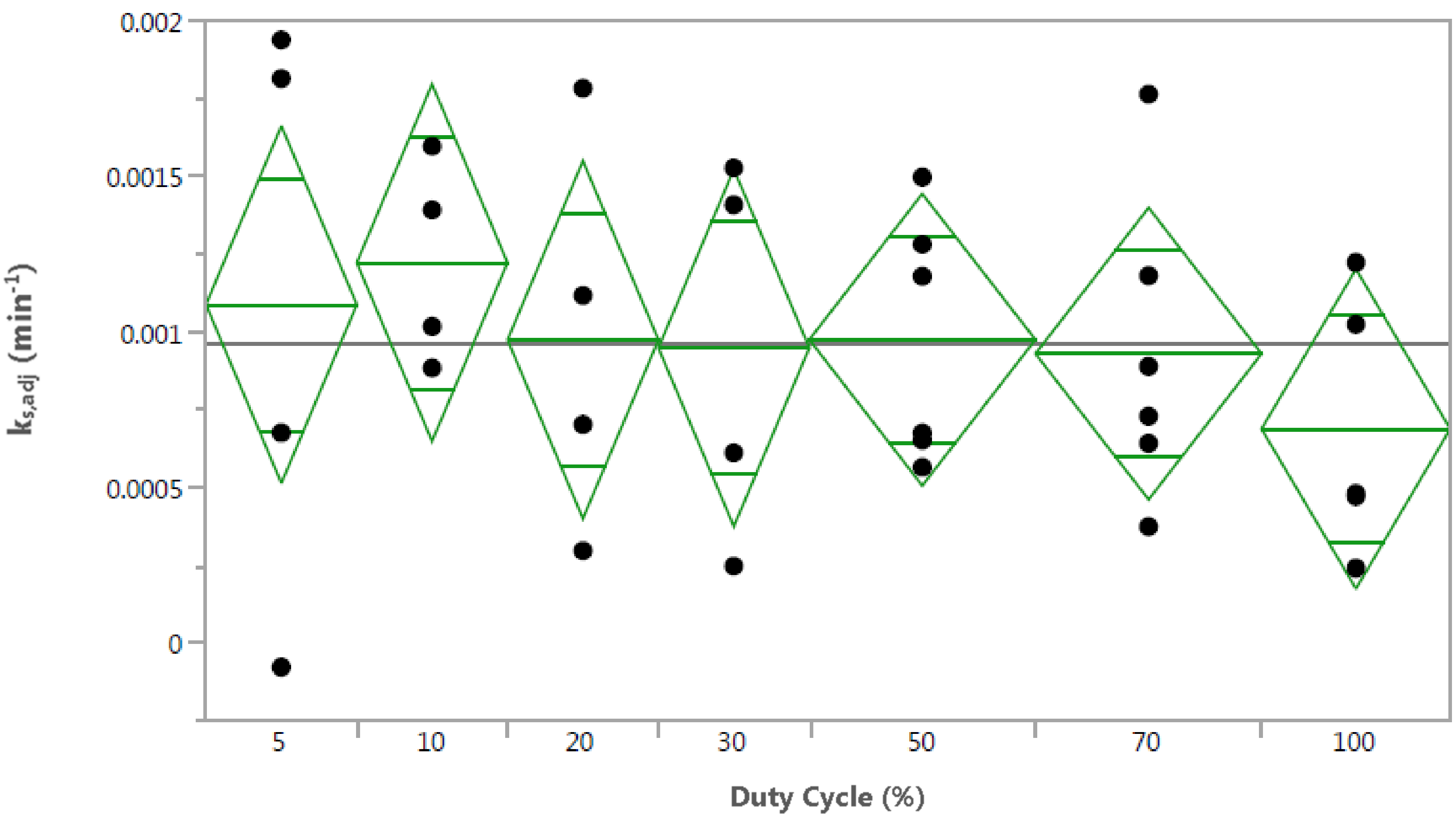


Figure 13: ANOVA of AOP ks,adj by Nominal Duty Cycle; p-value = 0.8827 means there is insufficient evidence to suggest a statistically significant distinction between at least two DC groups. Each point represents one experiment. Within each DC category, experiments operated at nominal pH levels between 6 and 9 are represented. This result is anticipated due to the definition of the adjusted first order rate constant.

Using the above information, a linear regression analysis was conducted using primary dependent variables pH and DC to predict k_s only, as $k_{s,adj}$ can be calculated given k_s and DC. Points that were excluded from the model were H_2O_2 control and the 0% DC experiments, but their purpose was not to predict removal, but rather to establish that the UV radiation alone could not account for significant removal of TAR, or that adding hydrogen peroxide to the solution at a given pH level could not account for significant removal of TAR. The other exclusion was the experiment dated 29 May 15. This point was excluded because the pH of the solution for the experiment fell outside the operating procedures set for this study, which caused unacceptable amount of influence as detected by the statistical parameter Cook's D. The resulting model upheld the three assumptions for linear regression models: independence (Durbin Watson Test), normally distributed residuals (Shapiro-Wilks Test), and constant variance (Breusch-Pagan Test). The adjusted R^2 for this model was .85, all Variance Inflation Factor (VIF) scores fell below 2.0, no significant outliers or overly influential points were detected (by studentized residuals, and Cooks D influence overlay plots), with one exception. This was the point for the experiment dated 30 July 15, with operating conditions of pH 7 and 100% DC. This point was overly influential, but did not cause failure of any of the three assumptions tests, and the model incorporated a term specifically to deal this this singular point. The model's mean predictive error was 7.93E-5 min^{-1} with standard deviation of 6.34E-5 min^{-1}. The Median error was 6.43E-5 min^{-1}. The maximum error was 2.20E-4 min^{-1}.

The high APE scores for this model resulted from the fact that the model does not incorporate terms to specifically deal with pH 9 at duty cycles less than 30%, and at pH 8 at low duty cycles. These terms, however, do not represent operating conditions of interest due to the low first order rate constants. See the regression model (Equation 11) and assumption tests in Appendix F. Figure 14 shows the comparison between the true apparent first order rate constant and the AOP Regression models predicted value. The x-axis shows the experiment number and the y-axis shows the first order rate constant. Figure 15 shows the relationship between the true (observed) first order rate constant (x-axis) and that predicted by the regression model (y-axis). The plot shows a linear trend about tightly clustered points, which is indicative of the strong adjusted R^2 for the model.

Equation 11: AOP Regression Model

$$\begin{aligned} Y_{AOP} = {} & (7.8989E-5) - 0.00017(pH9) + 8.9044E-5(pH7) + 0.0002688(pH6) \\ & + 0.0001608(DC\ 30) + 0.0003848(DC\ 50) + 0.0004662(DC\ 70) \\ & + 0.0006139(DC\ 100) \\ & + 0.0004428(pH6 - 0.24242)(DC\ 70 - 0.18182) \\ & + 0.0006832(pH6 - 0.24242)(DC\ 100 - 0.15152) \\ & + 0.0005658(pH7 - 0.24242)(DC\ 100 - 0.15152) \end{aligned}$$

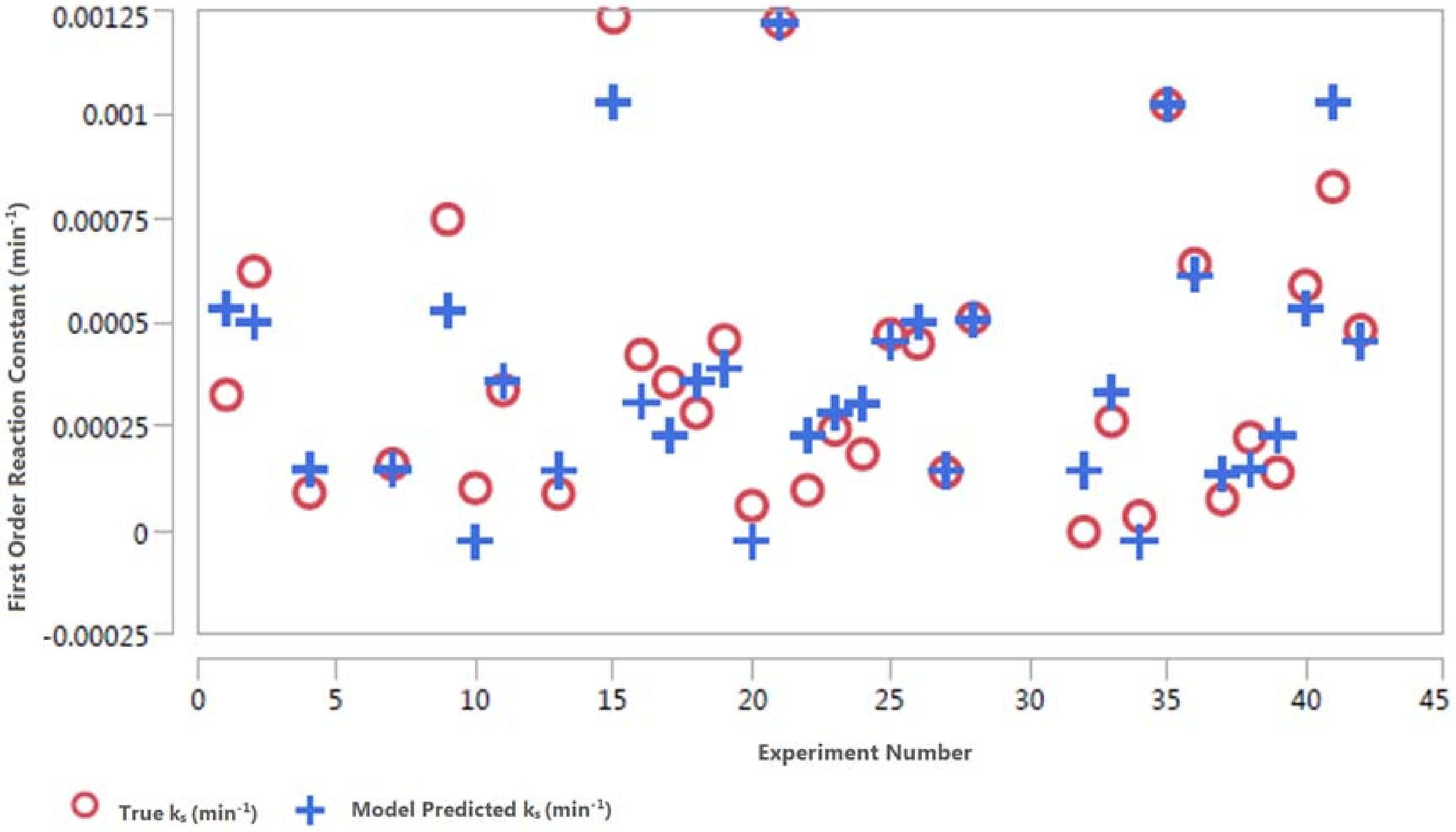


Figure 14: AOP Regression Model Predicted vs. Actual Response

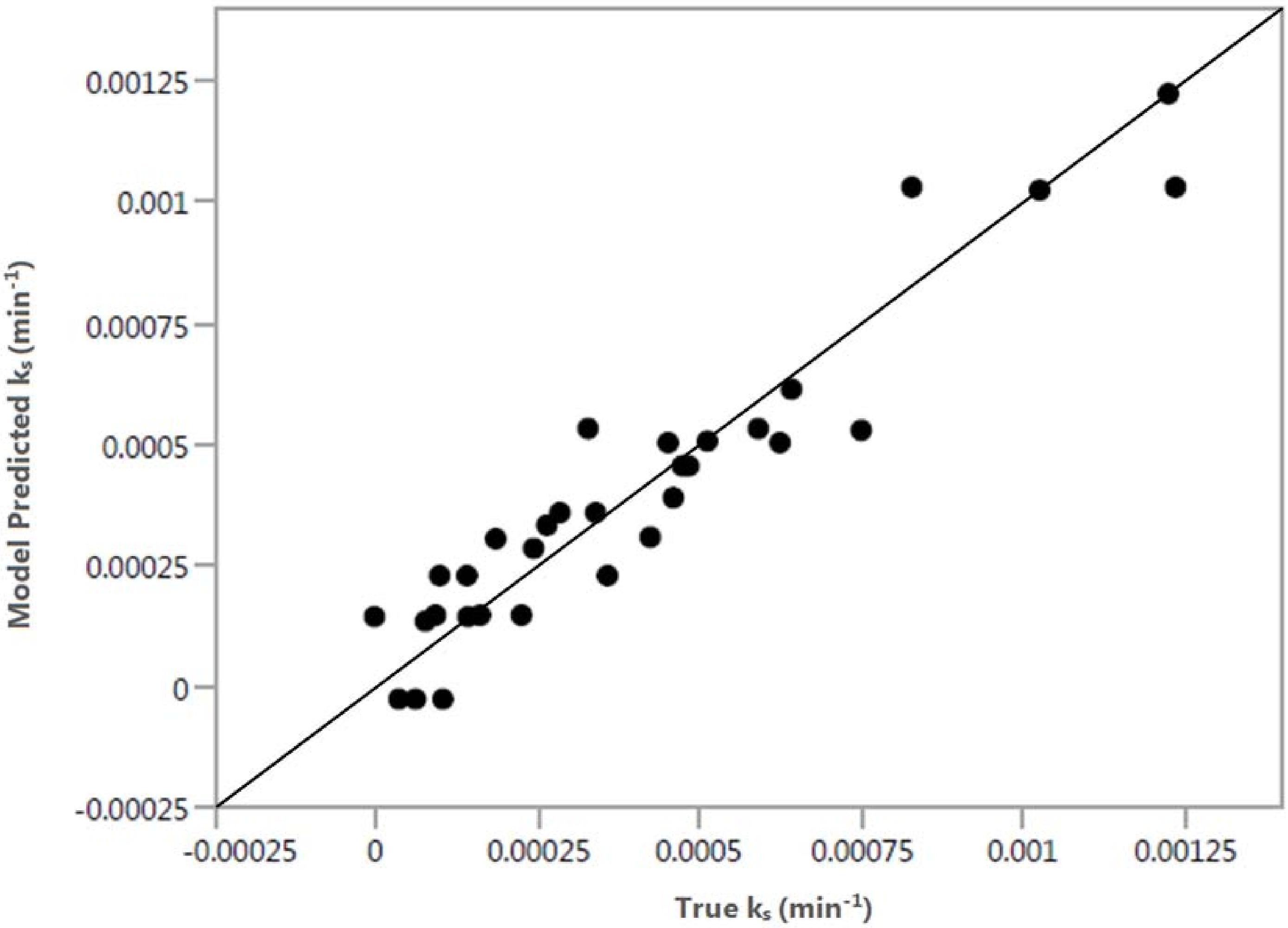


Figure 15: True vs Predicted First Order Rate Constant

4.3 The Effect of pH and Duty Cycle on the AOP Byproduct Profile

4.3.1 Chromatographic Contrast Angle Analysis

The purpose of this section is to determine the impact of pH and/or DC on the AOP byproduct profile. To establish the relationships between the pH levels, CCAs were calculated between the 0% DC experiments among the different pH levels (all 6 unique pairings). Since each experiment had two chromatographs (from positive and negative ionization), a total of 12 calculations were made (Figure 16, Figure 17). In similar fashion, CCAs were calculated between H_2O_2 control experiments for both the positive and the negative runs (Figure 18, Figure 19). Comparisons made with pH 7 tended to produce larger CCAs, see summaries in Appendix L.

4.3.1.1 The Effect of pH on Chromatographic Contrast Angles

Figure 16 shows the effect of pH on the 0% DC CCAs under positive ionization. The x-axis shows the pH labels for the 2 chromatograms being compared, and the y-axis shows the values of the CCAs. The CCA value for the pH 7/9 comparison was 24.9°, the highest value observed in this study. The second and third highest values were 24.7°, and 24.0° from the pH 7/8 and pH 6/7 comparisons respectively. These data mean that the byproduct profile observed at pH 7 was most different from those observed at pH 6, 8, and 9 at 0% DC under positive ionization. Smaller values were observed at comparisons pH 6/8 (6.7°), pH 6/9 (7.9°), and pH 8/9 (11.2°).

The chromatographs of the positive run appear to have three main peaks; hereafter referred to as peaks 1-3 from left to right. In comparison pH 6/8, there are no shifts, the magnitudes of the first two peaks are nearly identical, and the third peak is slightly smaller in the pH 8 chromatogram. This explains why the CCA was low for this comparison. Similar, slight deviations and no shifts were observed for the other low CCA comparisons. However, the larger CCA comparisons contained greater deviations. The pH 6/7 comparison peak 2 greatly increased from pH 6 to pH 7. Also, slight increases in peaks 1 and 3 were observed. The comparison of pH 7/8 also produced large distinction, due to the magnitude of the pH 7 chromatograms peak 2, but no shifts were observed. Similarly, the peak 2 of the chromatogram of pH 9 was dwarfed by comparison to pH 7. This suggests that without UV radiation, pH 7 influences the byproduct profile more so than the other pH conditions.

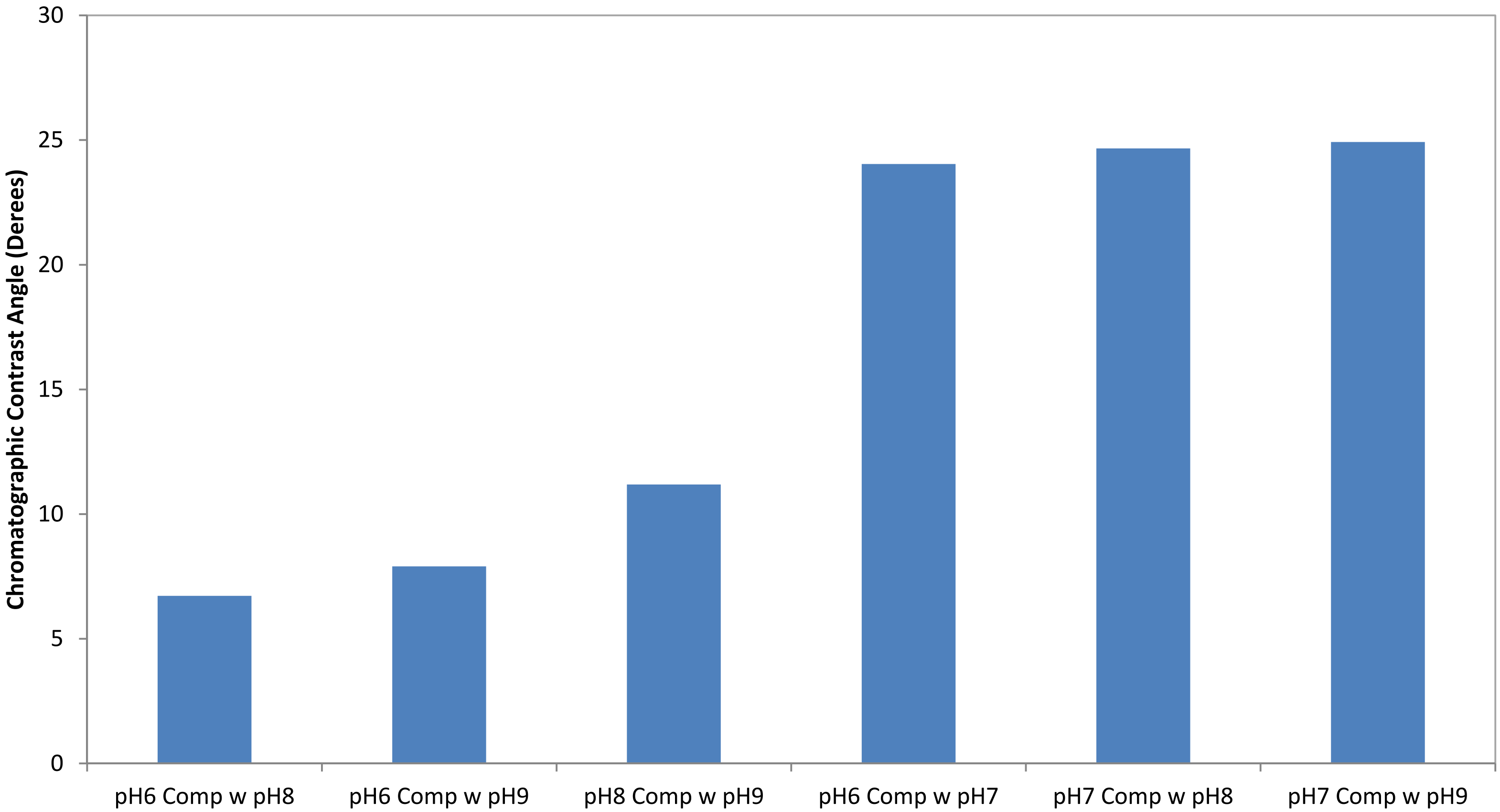


Figure 16: The Effect of pH on Chromatographic Contrast Angles for 0% DC under Positive Ionization

Figure 17 shows the effect of pH on the 0% DC CCAs under negative ionization. The x-axis shows the pH labels for the 2 chromatograms being compared, and the y-axis shows the values of the CCAs. The CCA value for the pH 7/8 comparison was 37.8°, the highest value observed in this study. The second and third highest values were 30.2°, and 23.1° from the pH 8/9 and pH 6/7 comparisons respectively. The smaller angles produced were 20.6° (pH 6/8), 16.7° (pH 6/9), and 16.6° (pH 7/9). The similarities between chromatograms were less than that of the positive ionization condition.

The associated chromatographs did not follow the pattern observed for the positive ionization byproduct profile. The largest peak 1 was evenly matched for pH 7 and pH 9; pH 7 had the largest peak 2; and pH 8 had the largest peak 3. Noticeable shifts occurred in peak 1 between pH 6/9, 7/8, and 8/9. This suggests that pH impacts the byproduct profile under negative ionization in the presence of H_2O_2 without UV radiation.

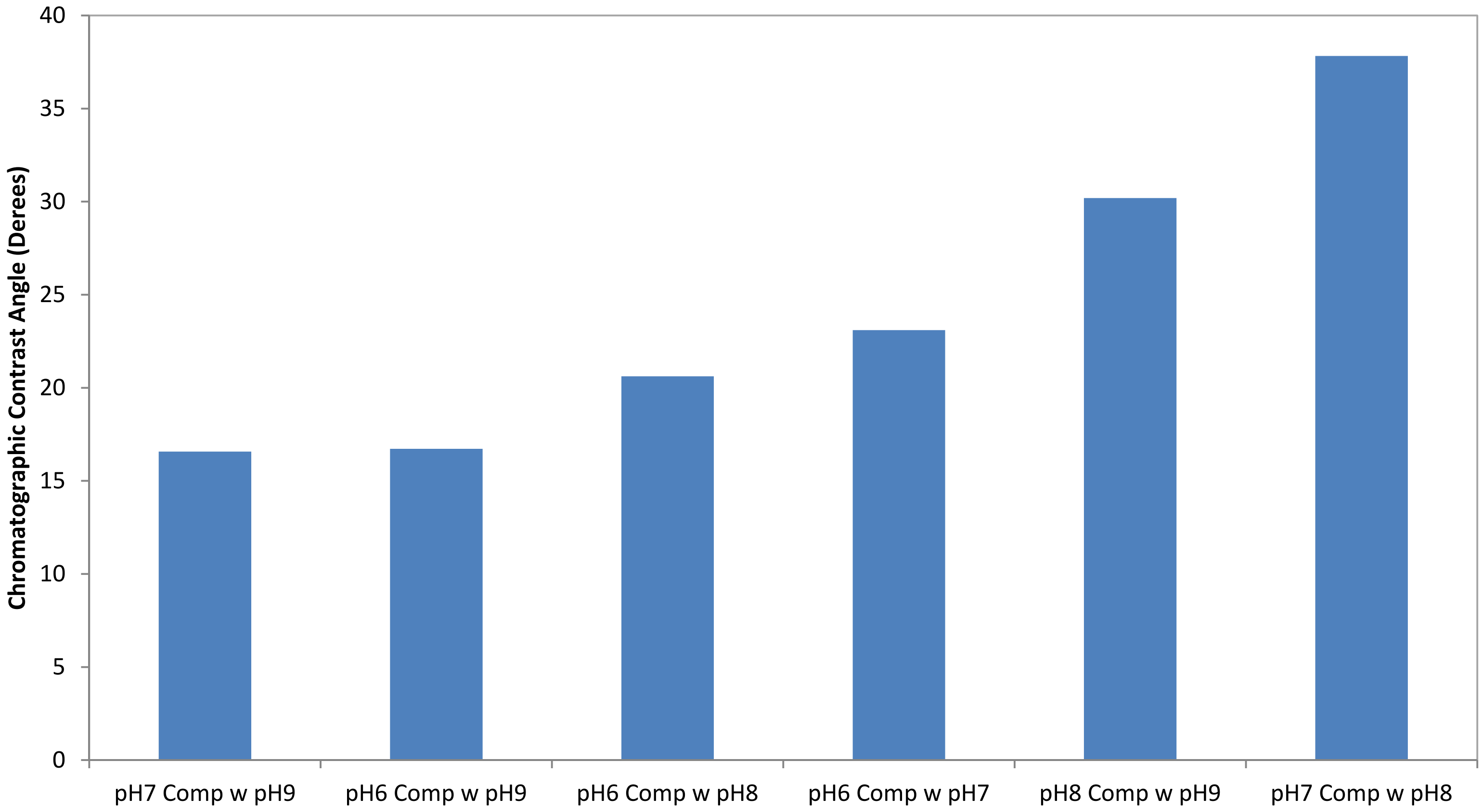


Figure 17: The Effect of pH on Chromatographic Contrast Angles for 0% DC under Negative Ionization

Figure 18 shows the effect of pH on the H_2O_2 control CCAs under positive ionization. The x-axis shows the pH labels for the 2 chromatograms being compared, and the y-axis shows the values of the CCAs. This chart is similar to Figure 16 in that the largest CCA values were created in comparisons made with pH 7, and the order of comparisons from largest to smallest was similar. The values in this chart were different from Figure 16 with respect to the magnitude of the (positive) CCAs of the H_2O_2 control experiments, which were much less than that of the 0% DC (positive) CCAs. The CCA value for the pH 7/9 comparison was 9.4°, the highest value observed in this study. The second and third highest values were 9.2°, and 7.1° from the pH 7/8 and pH 6/7 comparisons respectively. These data mean that the byproduct profile observed at pH 7 was most different from those observed at pH 6, 8, and 9. Smaller values were observed at comparisons pH 8/9 (2.9°), pH 6/8 (5.2°), and pH 6/9 (6.9°).

In contrast from the 0% DC chromatograms, in which only pH 7 had a substantial peak 2, the H_2O_2 control chromatograms of pH 7 are the only ones which do not have a peak 2. The only other main difference between the pH conditions is slight changes in magnitudes of the three peaks. No considerable shifts were observed. This is why the CCAs are considerably lower for this figure.

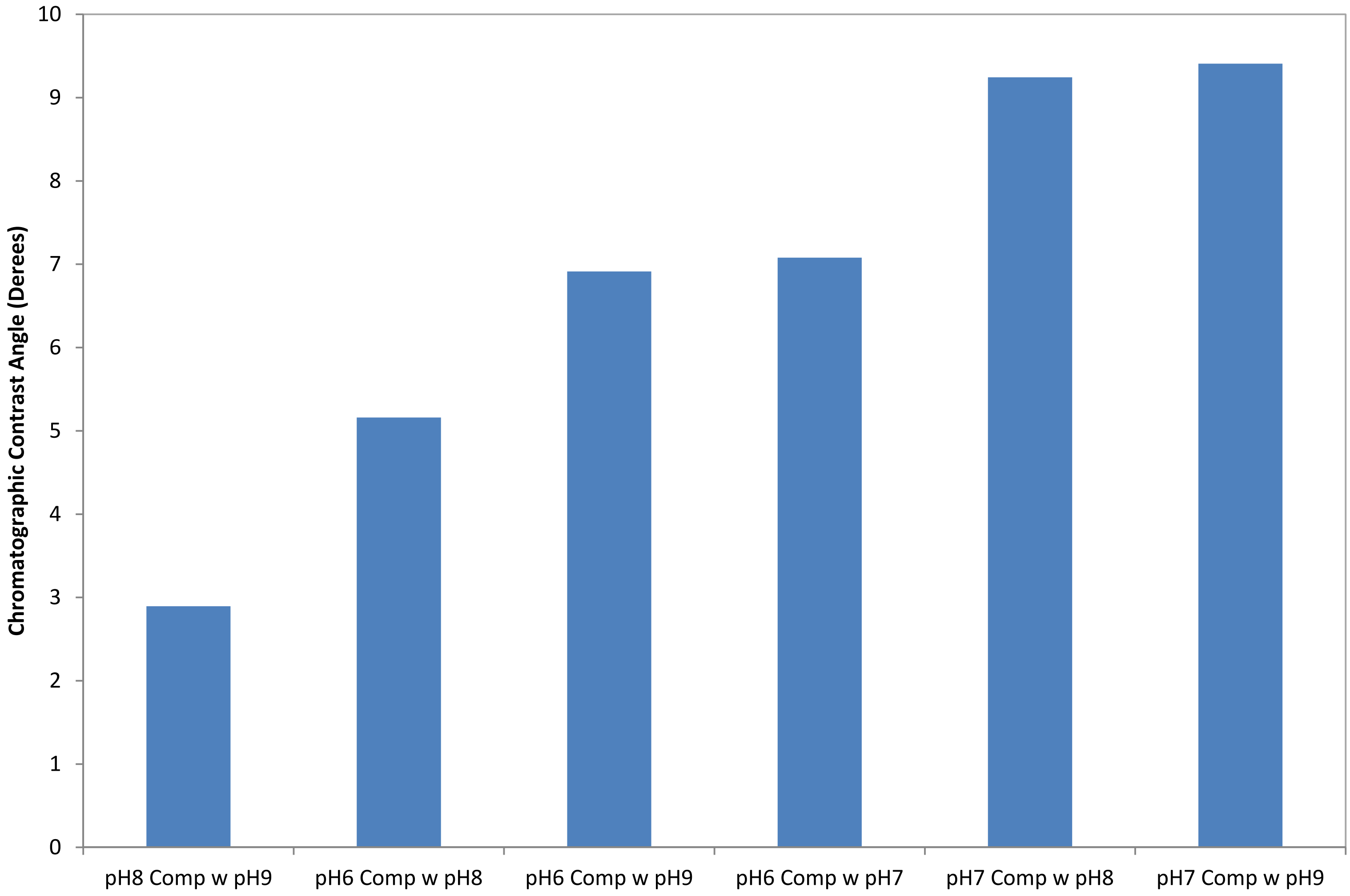


Figure 18: The Effect of pH on Chromatographic Contrast Angles for H_2O_2 Controls under Positive Ionization

Figure 19 shows the effect of pH on the H_2O_2 control CCAs under negative ionization. The x-axis shows the pH labels for the 2 chromatograms being compared, and the y-axis shows the values of the CCAs. The CCA value for the pH 7/9 comparison was 17.9°, the highest value observed in this study. The second and third highest values were 17.5°, and 12.5° from the pH 6/9 and pH 7/8 comparisons respectively. Smaller values were observed at comparisons pH 6/7 (3.6°), pH 8/9 (6.3°), and pH 6/8 (12.1°).

The associated chromatograms were very similar. The trend was a large peak 1, and miniscule peaks 2 and 3. Slight peak 1 shifts were observed for pH comparisons 6/8, 6/9, 7/8, and 7/9. Other than these reasons, the CCA's were driven by distinctions in the magnitudes of the respective pH comparisons peaks 1. This means that without peroxide and under UV radiation, peak 1 is most affected by pH.

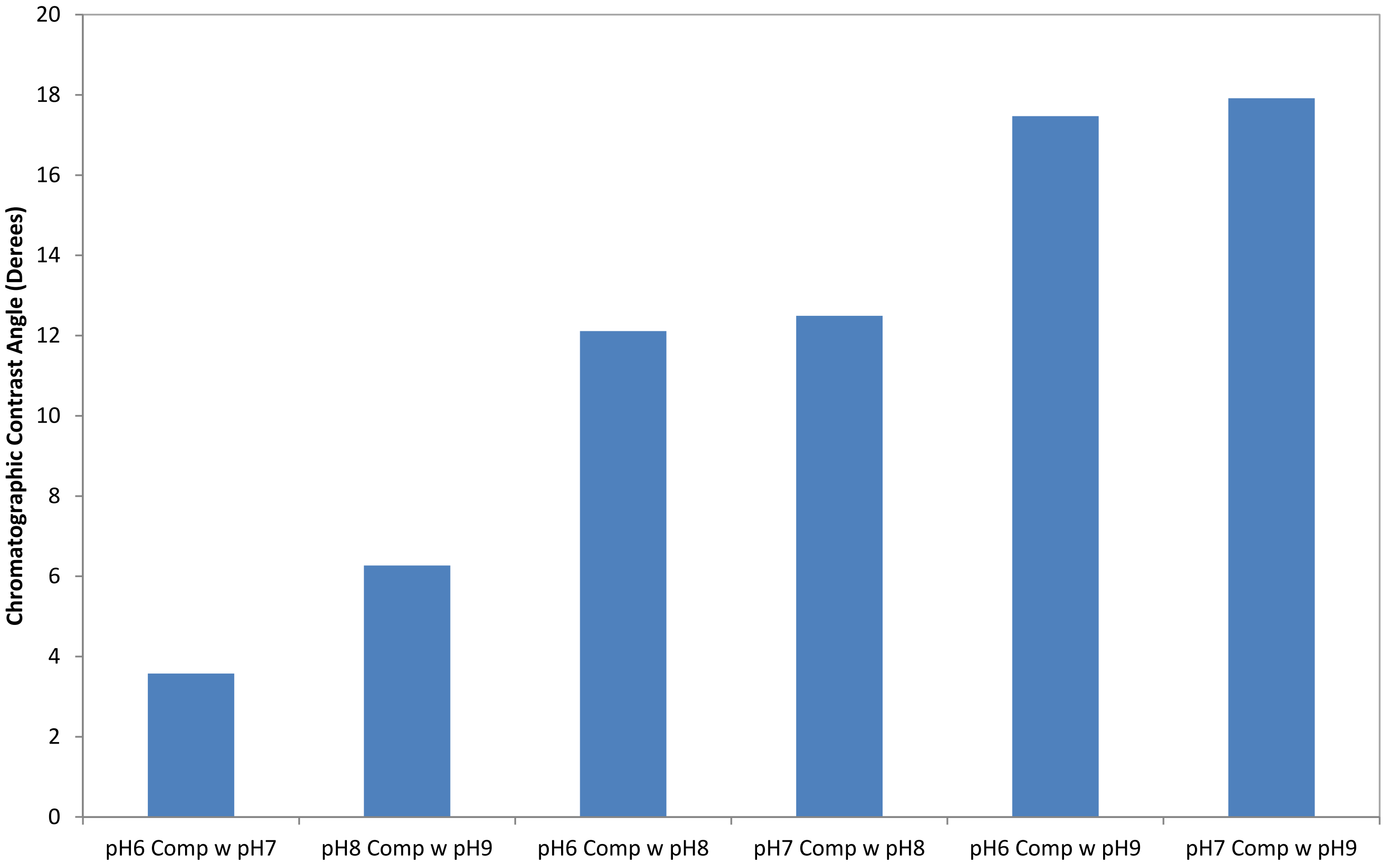


Figure 19: The Effect of pH on Chromatographic Contrast Angles for H_2O_2 Controls under Negative Ionization

4.3.1.2 The Effect of Duty Cycle on Chromatographic Contrast Angles

Finally, the CCAs were calculated for every experiment relative to the 0% DC of the corresponding pH level for both the positive and negative run (Figure 20, Figure 21).

Figure 20 shows the effect of DCs on CCA for the positive ionization. The x-axis shows the DC and the y-axis shows the contrast angle in degrees. There were few CCAs under 5°, all of which were at pH 6, for DCs 5%, 20%, and 100%. The CCAs did not correlate directly to TAR removal, otherwise a larger CCA would have been observed between pH 6 DCs 0% and 100%. Also, pH 7 was associated with high CCA values within each DC category, ranging from 10° to 30°.

Figure 21 shows the effect of DC on the CCA in the negative ionization condition. The x-axis shows the DC and the y-axis shows the contrast angle in degrees. There were only three comparisons in which the CCA was less than 5°: (all at pH 6) H_2O_2 Ctrl, 10%, and 20% DC. This reiterates the point that the CCA did not directly relate to the removal of TAR. The condition pH 7 consistently created relatively large CCAs (ranging from 11° to 44°), but wasn't always the greatest angle within a DC category. These exceptions were pH 8 during the H_2O_2 control comparison, as well as pH 9 during the 5% DC.

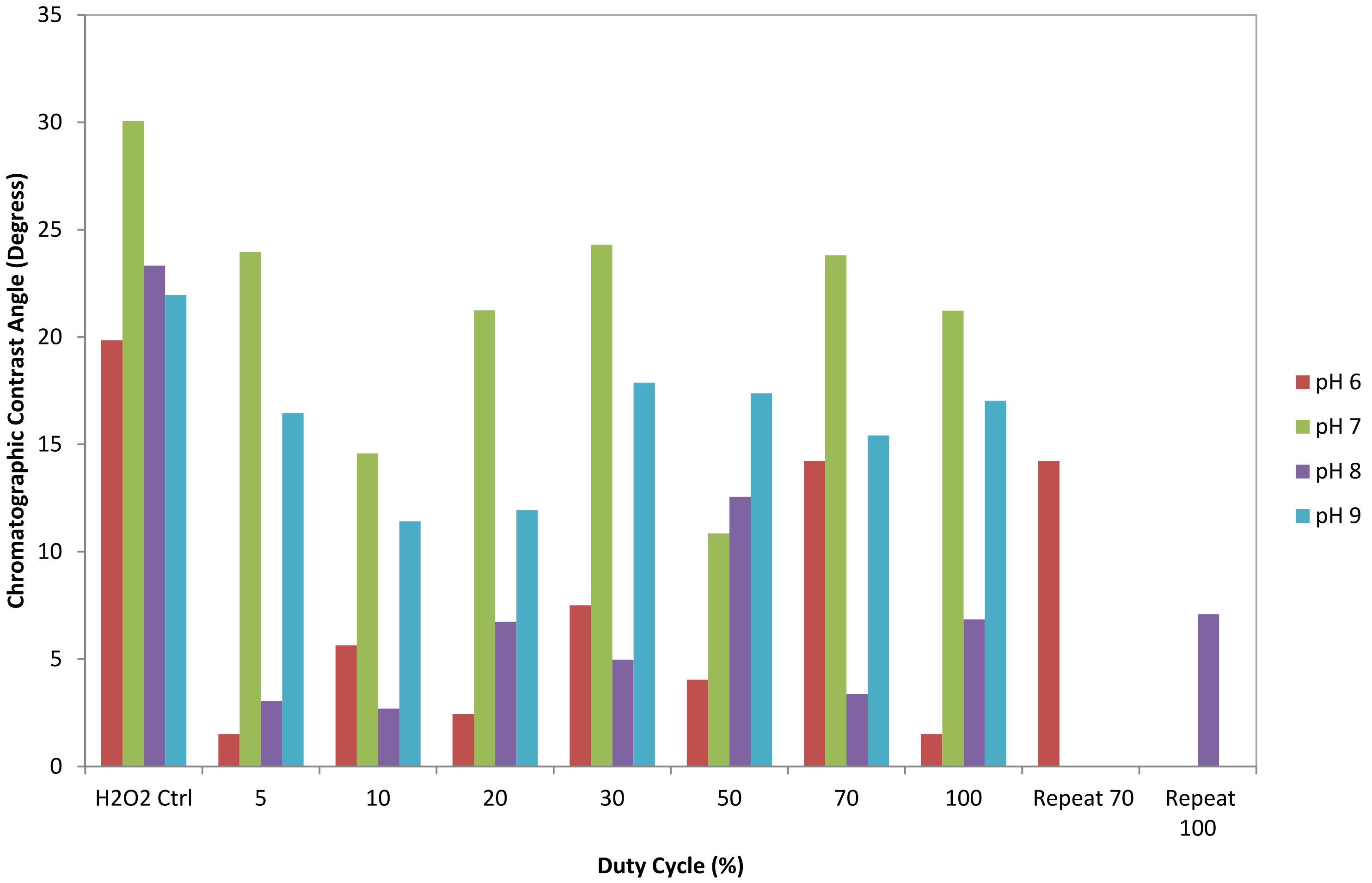


Figure 20: The Effect of Duty Cycle on Chromatographic Contrast Angles under Positive Ionization. Each chromatogram was compared to the 0% DC chromatogram of the respective pH level.

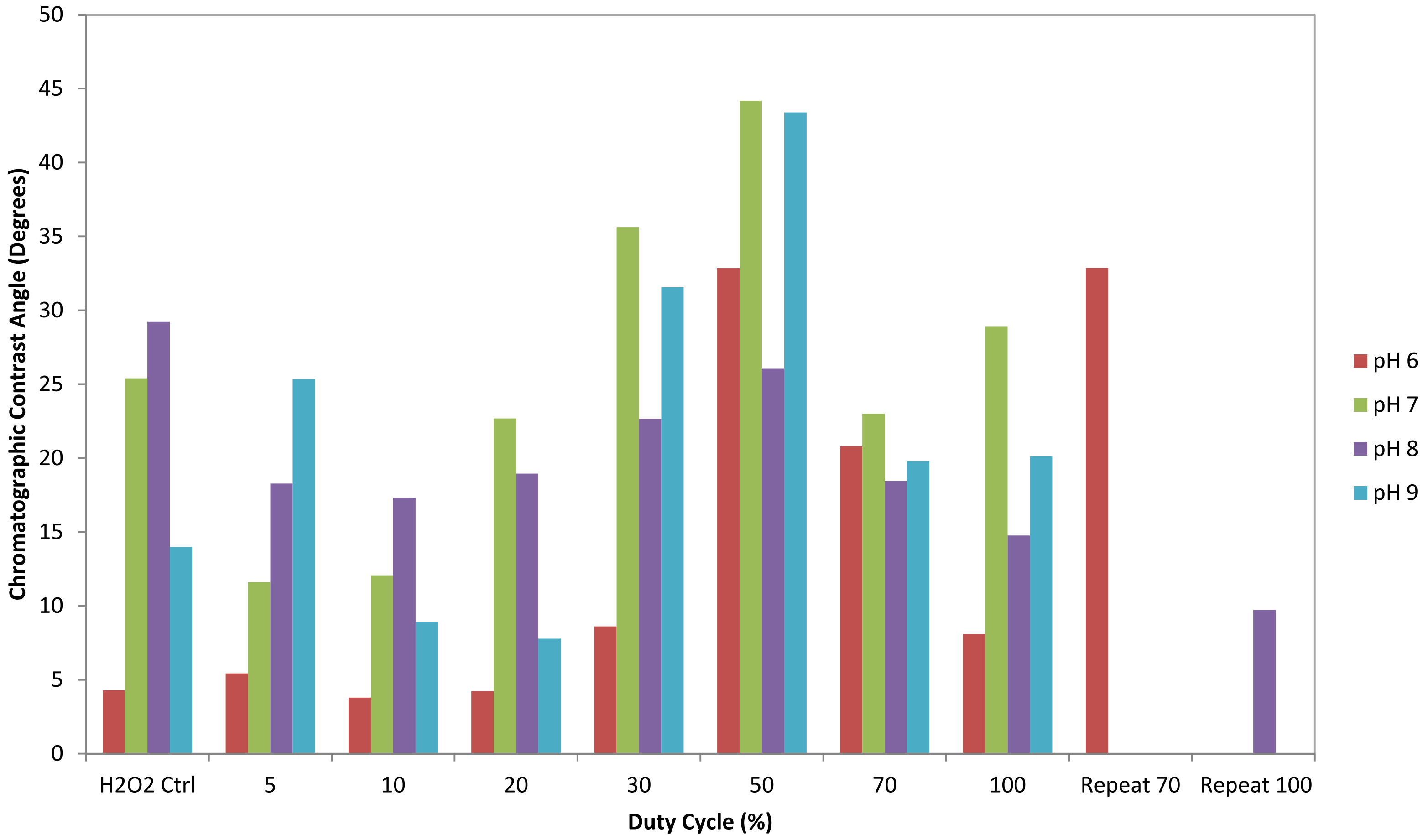


Figure 21: The Effect of Duty Cycle on Contrast Angles under Negative Ionization. Each chromatogram was compared to the 0% DC chromatogram of the respective pH level.

4.3.1.3 Statistical Evaluation of the effect of pH and Duty Cycle on CCA

In consideration of both positive and negative CCAs, pH level 7 was associated with larger CCAs. In addition, DCs 30%, 50%, and 70% appeared to create larger CCAs for the negative run. One-Way ANOVA and Tukey analyses were conducted for both positive and negative CCAs. See summary statistics, ANOVA, LS Means diagrams (positive and negative), and Tukey (positive and negative) reports in Appendix M.

Figure 22 shows the one-way ANOVA of the positive CCA by DC. The x-axis shows the DC, and the y axis shows the positive CCA in degrees. The triangles depict the mean, upper 95%, and lower 95% for each DC category. The line through the middle of the figure shows the mean of all responses in the data set, which is 11.5°. The means for each DC are 11.2°, 8.6°, 10.6°, 13.7°, 11.2°, 14.2°, and 10.7° for DCs 5%, 10%, 20%, 30%, 50%, 70%, and 100%, respectively. The p-value was 0.9519, which demonstrates insufficient evidence to suggest that DC alone cannot be used as a statistically significant predictor variable for the positive CCA.

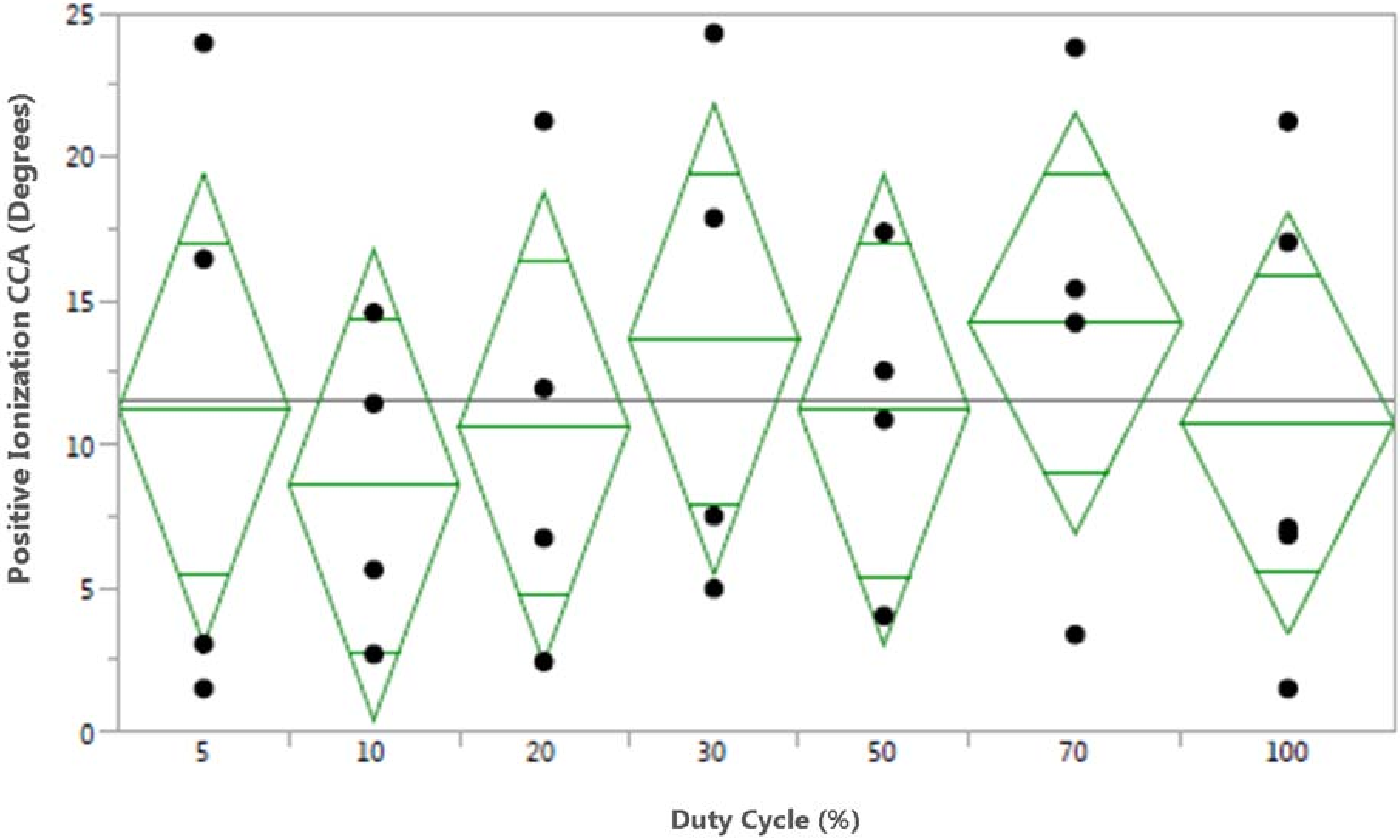


Figure 22: ANOVA of Positive Ionization CCA by Duty Cycle; p-value = 0.9519 indicates insufficient evidence to suggest that DC is a statistically significant predictor of the Positive Ionization CCA. Each point represents one experiment. Within each DC category, experiments operated at nominal pH levels between 6 and 9 are represented.

Figure 23 shows the one-way ANOVA of the positive CCA by pH level. The x-axis shows the nominal pH, and the y axis shows the positive CCA in degrees. The triangles depict the mean, upper 95%, and lower 95% for each pH category. The line through the middle of the figure shows the mean of all responses in the data set (which is 11.5°). The means for the pH levels are 6.4°, 20.0°, 5.9°, and 15.4° for pH levels 6, 7, 8, and 9, respectively. The pH 9 was tightly clustered, which may be attributable to the fact that pH 9 produced the least amount of variance with respect to the first order rate constant, and thus, would have less effect on changing the byproduct profile. The p-value was less than 0.0001, which demonstrated that pH is a statistically significant predictor variable for the positive CCA.

Tukey analysis (Appendix M) of the positive CCA by pH (p-value = 0.00004), DC (p-value = .00075), and the interaction of pH and DC (p-value = .00097) produced strong indication that pH and DCs together were strong predictors of CCA. DCs were grouped into the following letter categories: 70% and 30% were group A, 100%, 5%, and 50% were group B, 5%, 50%, and 20% were group C, and 10% was group D. Levels not connected by the same letter are significantly different. Each of the pH levels were grouped into separate letter groups. This means that several DCs were unique, and that each pH level was statistically distinct.

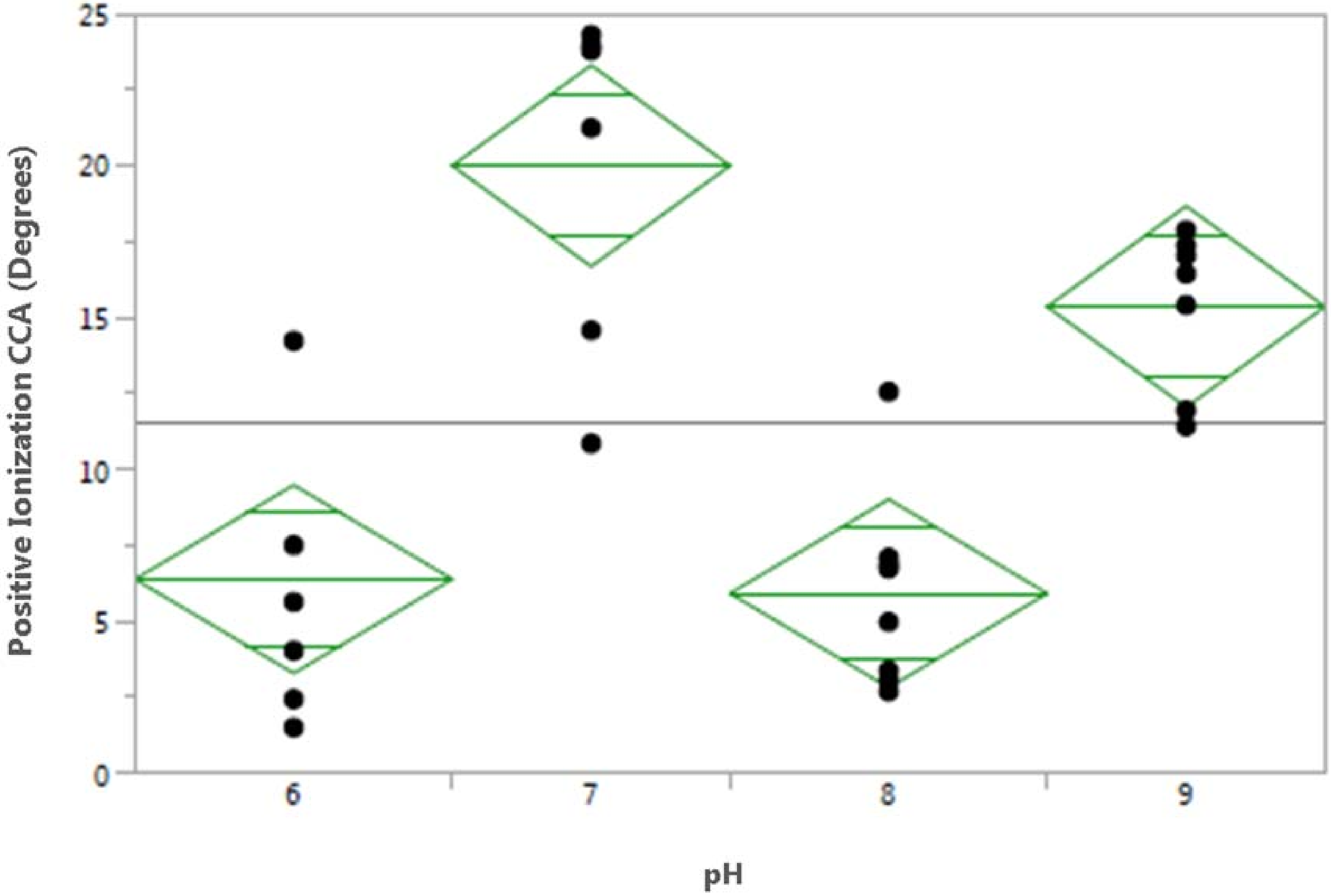


Figure 23: ANOVA of Positive Ionization CCA by pH; p-value = 0.0001 indicates there is a statistically significant distinction between at least two pH groups. Each point represents one experiment. Within each pH category, experiments operated at DCs between 5% and 100% are represented.

Figure 24 shows the one-way ANOVA of the negative CCA by DC. The x-axis shows the DC, and the y axis shows the negative CCA in degrees. The triangles depict the mean, upper 95%, and lower 95% for each DC category. The line through the middle of the figure shows the mean of all responses in the data set (which is 19.9°). The means for the DCs were 15.2°, 10.5°, 13.4°, 24.6°, 36.6°, 23.0°, and 16.3° for DC levels 5%, 10%, 20%, 30%, 50%, 70%, and 100%, respectively. The p-value was 0.0035, which demonstrated that DC is a statistically significant predictor variable for the negative CCA.

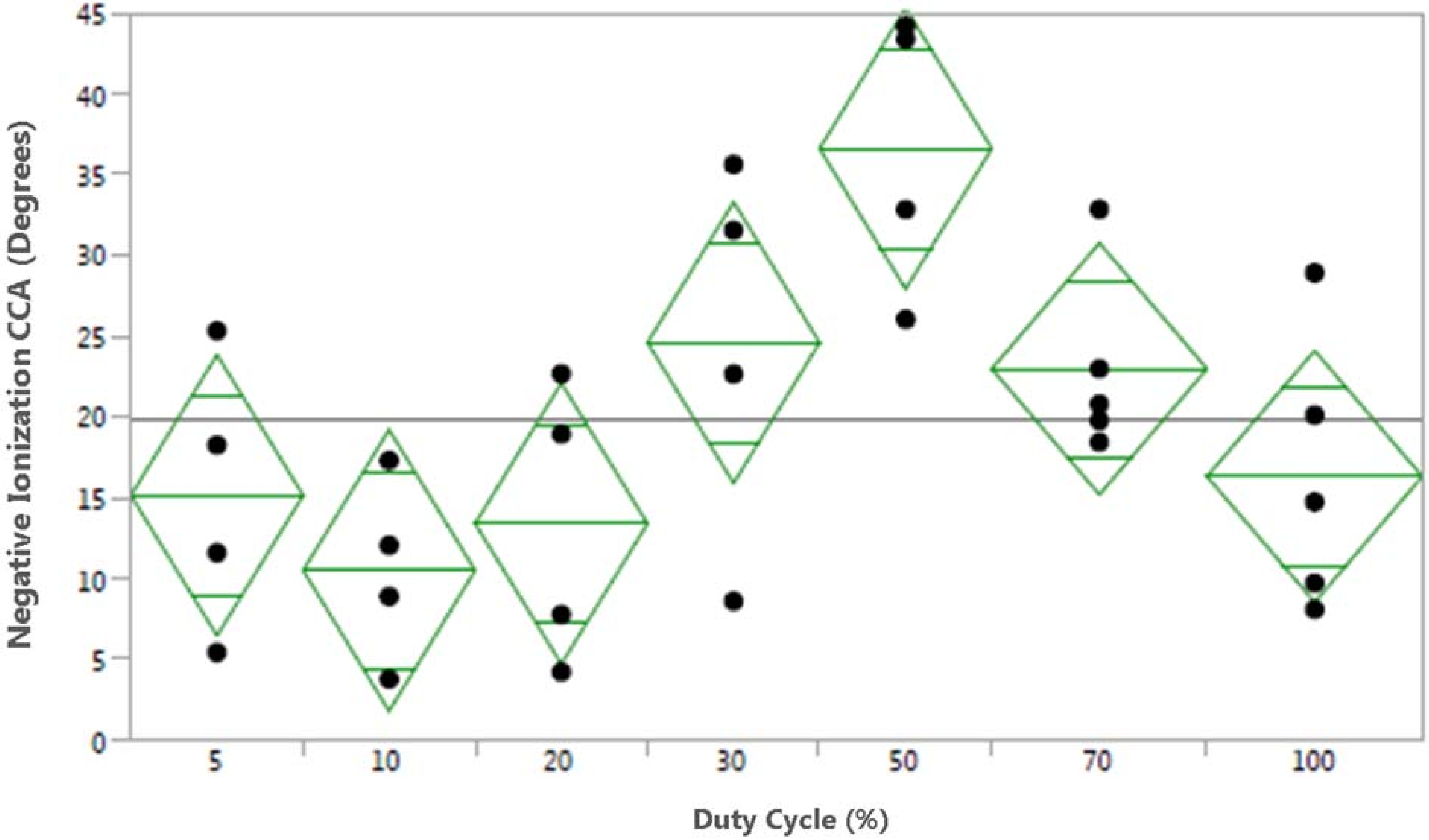


Figure 24: ANOVA of Negative Ionization CCA by Duty Cycle; p-value =0.0035 indicates statistically significant distinction between at least two DC groups. Each point represents one experiment. Within each DC category, experiments operated at pH levels between 6 and 9 are represented.

Figure 25 shows the one-way ANOVA of the negative CCA by pH level. The x-axis shows the nominal pH, and the y axis shows the negative CCA in degrees. The triangles depict the mean, upper 95%, and lower 95% for each pH category. The line through the middle of the figure shows the mean of all responses in the data set (which is 19.9°). The means for the pH levels were 14.6°, 25.4°, 18.3°, and 22.4° for pH levels 6, 7, 8, and 9, respectively. The p-value was 0.2544, which demonstrates the insufficient evidence to suggest that pH alone is a statistically significant predictor variable for the negative CCA.

The Tukey analysis of the negative CCA (Appendix M) by pH (p-value = .04282) and DC (p-value = .00105) produced significant evidence that pH and DC together were strong predictors. The DC groups were A: 50%, 30%, and 70%, and B: 30%, 70%, 100%, 5%, 20%, and 10%. This means that 50% is significantly different than 100%, 5%, 20%, and 10%, but the 30% and 70% could belong to either group. The pH groups were A: 7, 9, and 8, and B: 9, 8, and 6. This means that pH 7 and 6 were statistically different, but pH 8 and 9 could belong to either group.

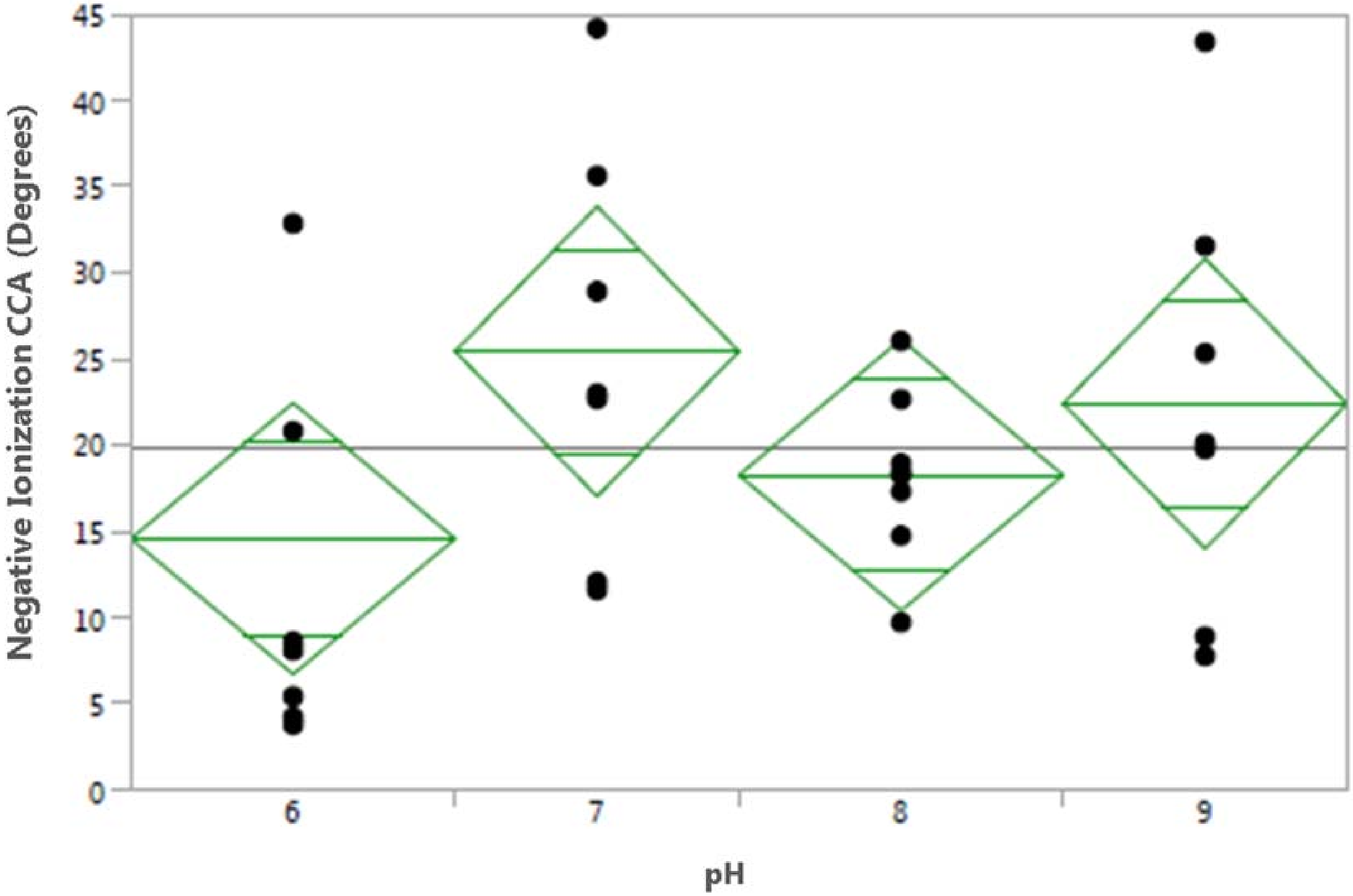


Figure 25: ANOVA of Negative Ionization CCA by pH; p-value = 0.2544 indicates insufficient evidence to suggest that pH is a statistically significant predictor of the Negative Ionization CCA. Each point represents one experiment. Within each pH category, experiments conducted at DCs between 5% and 100% are represented.

4.3.1.4 Regression Analysis of Positive and Negative Ionization CCAs

A linear regression model was constructed with pH (nominal), DC (nominal), and interaction terms. The model upheld the three assumptions for linear regression models: independence (Durbin Watson Test), normally distributed residuals (Shapiro-Wilks Test), and constant variance (Breusch-Pagan Test). The significant predictor variables were pH 6, pH 7, pH 8, DC 70, and DC 70 * pH 6. The adjusted R^2 for this model was .76, all VIF scores fell below 2.0, no significant outliers or overly influential points were detected (by studentized residuals, and Cooks D influence overlay plots), and the model's mean predictive error was 2.51° with standard deviation of 2.02°. The maximum error was 9.07°. See model (Equation 12) and assumption tests in Appendix N. Figure 26 shows the relationship between the true (observed) positive ionization chromatographic contrast angle (x-axis) and that predicted by the regression model (y-axis). The plot shows a linear trend, but it is apparent the model predicted the same value for several different conditions. This is due to the fact that the model incorporated dummy variables which did not cover many operating conditions such as pH 9 and most duty cycles.

Equation 12: Positive Ionization CCA Regression Model

$$Y_{(+)CCA} = (14.84291) - 9.853601(pH6) - 9.429323(pH8) + 3.1633158(DC\ 70) \\ + 4.637696(pH7) + 9.9500619(pH6 - 0.26667)(DC\ 70 - 0.16667)$$

The resulting negative run model upheld the three assumptions for linear regression models: independence (Durbin-Watson Test), normally distributed residuals (Shapiro-Wilks Test), and constant variance (Breusch-Pagan Test). The significant predictor variables were pH 6, pH 8, DC 30, DC 50, DC 70, and DC 70 * pH 6. The adjusted R^2 for the model was .68, all VIF scores fell below 2.0, no significant outliers or overly influential points were detected (by studentized residuals, and Cooks D influence overlay plots), and the model's mean predictive error was 4.50° with standard deviation of 3.11°. The maximum error was 10.90°. See model (Equation 13) and assumption tests in Appendix O. Figure 26 shows the relationship between the true (observed) negative ionization chromatographic contrast angle (x-axis) and that predicted by the regression model (y-axis). This model incorporated more duty cycle conditions, resulting in a stronger linear trend than that of the positive CCA.

Equation 13: Negative Ionization CCA Regression Model

$$\begin{aligned} Y_{(-)CCA} = {} & (17.87982) - 10.64895(pH6) - 5.000822(pH8) + 10.593667(DC\ 30) \\ & + 22.596346(DC\ 50) + 8.3034399(DC\ 70) \\ & + 18.489657(pH6 - 0.26667)(DC\ 70 - 0.16667) \end{aligned}$$

As expected, the randomization of the experiment order prevented bias of time: no significant effects were observed in the regression analysis that could be attributable to the date on which the experiment was run. This is true for both the positive and negative ionization conditions.

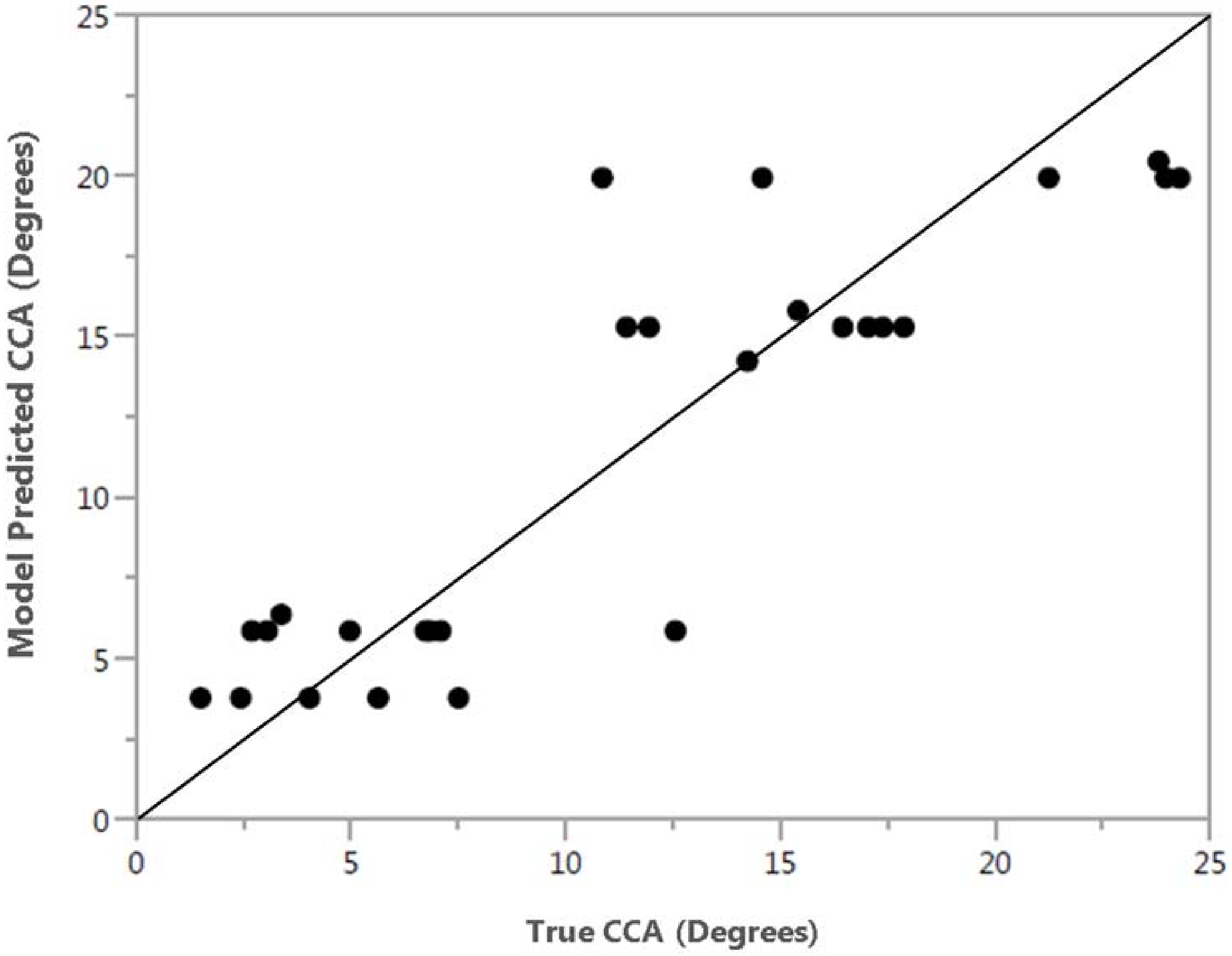


Figure 26: True vs Predicted Positive CCA

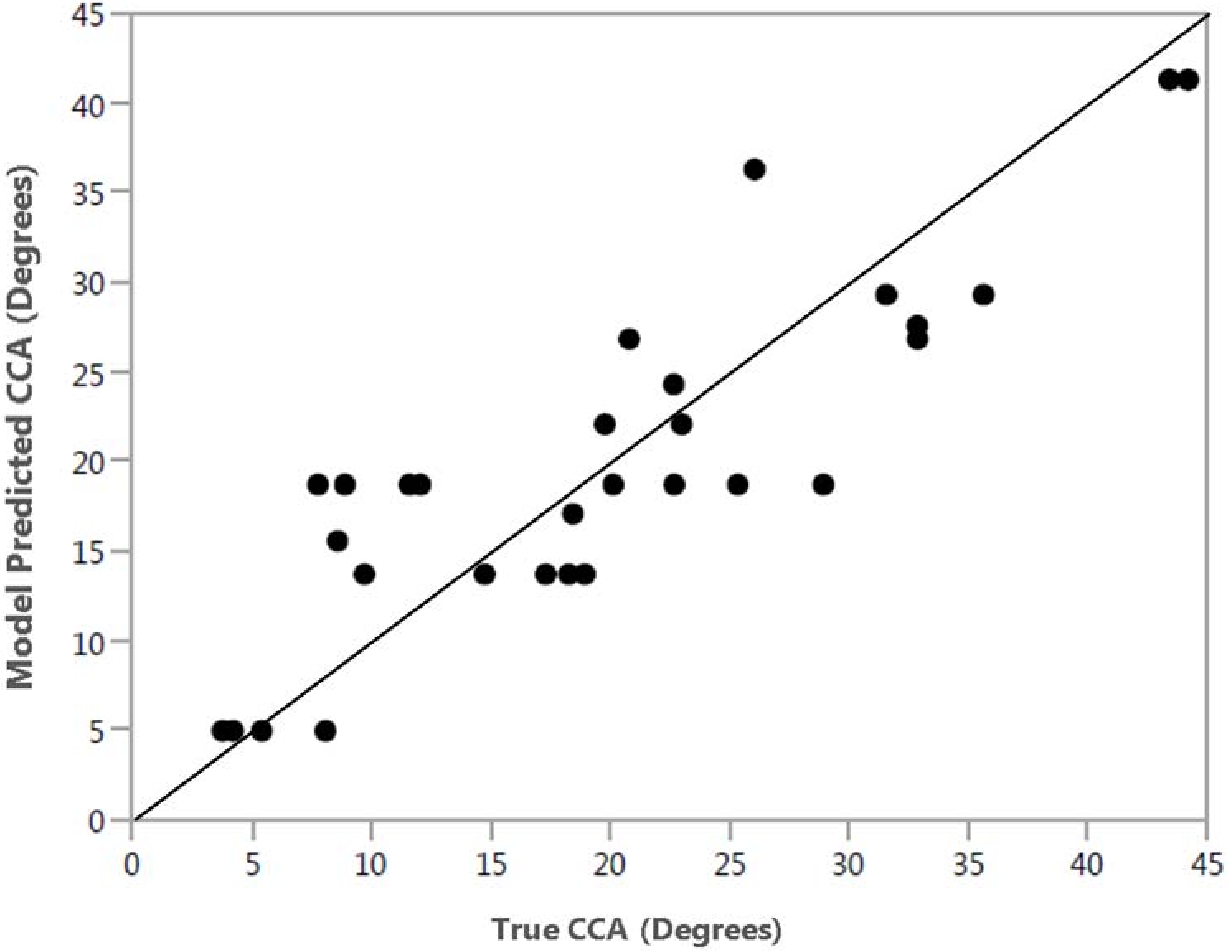


Figure 27: True vs Predicted Negative CCA

4.3.2 Mass Spectroscopy Analysis

Mass Spectroscopy analysis of the AOP byproducts suggests several isomers within each proposed structure. In chromatographs of all experimental conditions, three main peaks emerged for both ionization HPLC settings. These peaks are characterized in Table 1.

Table 1: Proposed Byproduct Structures Naming Convention

Retention Time	**Proposed Structure**	**Ionization**	**Product Name**
2.846	Tartrazine (abbrev TAR)	Negative	A
3.303	TAR + OH	Negative	B
3.909	TAR – O – COO + (CN)**	Negative	C
3.126	TAR + 2H	Positive	D
3.612	TAR – sulfonic acid (sulf) – COO + OH + (CN)**	Positive	E
3.938	TAR – sulf + O + (CN)**	Positive	F

**CN from mobile phase and not from AOP reactions

There are several isomers for each proposed structure. TAR (Product A) may retain between zero and three Na^+ ions, thereby changing the charge of the main structure between neutral and -3, and reducing the mass of the main structure by 22.99 for every Na^+ lost. This phenomenon will be present in each remaining proposed structure, where the number of Na^+ is not constant; however, the main structures are not be affected. See each structure's mass with the variation in ionization in Table 2. It is likely that this ionization is due to the interaction of TAR with water and not due to the AOP.

Table 2: Each Product's Potential Mass Due to Ionization

Mass	**A**	**B**	**C**	**D**	**E**	**F**
- 0Na	534.36	551.37	474.35	536.38	328.22	371.22
- 1Na	511.32	528.38	451.36	513.39	305.23	348.23
- 2Na	488.38	505.39	428.37	490.40	282.24	325.24
- 3Na	465.39	482.40	405.38	467.41	-	-

Product B (Tar + OH) has 9 isomers, at each H location within the TAR structure as previously discussed. Product C is only a reduction of TAR and does not have any proposed isomers. The CN may take multiple locations (most likely at the local positive end of the main TAR structure left by the removal of O), but as the CN is due to the mobile phase, its location is trivial (this is also applicable for Products E and F). Product D likely has few simple isomers. The H's potentially bond at the local negative regions left by ionization, or at the azo group. The formation order for Product E is unclear. The OH addition may occur before or after the loss of the sulfonic acid group or COO^- group. However, the OH locations will follow the same trends as discussed for Product B. Finally, Product F formation order is also unclear. Possible locations for the addition of oxygen are at such a location that hydrogen abstraction can occur, followed by OH addition.

4.3.3 Byproduct and Mechanisms Associated with UV LED AOP of Tartrazine

4.3.3.1 Product A: Ionized Tartrazine

Product A is the base case of TAR, which may be partially ionized in solution. It is not clear whether the 9th hydrogen atom is bonded to the nitrogen in the azo group, or bonded to the stand-alone oxygen opposite the COO^- group. For the purposes of this study, it will be assumed that TAR's 9th Hydrogen atom is bonded to the N in the azo group, denoted by IUPAC name (E)-5-oxo-1-(4-sulfonatophenyl)-4-((4-sulfonatophenyl)diazenyl)-4,5-dihydro-1H-pyrazole-3-carboxylate.

4.3.3.2 Product B: Tartrazine + OH

The most likely mechanism to account for the structure of Product B is OH addition. See Figure 28 with the caveat that the OH can join the main TAR structure at any of the locations detailed in Figure 2. These locations were determined using information from Benjamin (2013); however, the specific structures have not been previously proposed in the literature review of this study. The IUPAC names for the shown possible isomers in Figure 28 are:

- (E)-4-((2-hydroxy-4-sulfonatophenyl)diazenyl)-5-oxo-1-(4-sulfonatophenyl)-4,5-dihydro-1H-pyrazole-3-carboxylate
- (E)-4-(2-hydroxy-2-(4-sulfonatophenyl)-2λ^4-diazenyl)-5-oxo-1-(4-sulfonatophenyl)-4,5-dihydro-1H-pyrazole-3-carboxylate

4.3.3.3 Product C: Tartrazine – O – COO Group

Product C is most likely caused by electron transfer, suggested by the fact that the main structure only loses atoms other than hydrogen. The presence of CN is attributable to the mobile phase. The loss of the COO^- group may not be attributable to the AOP reaction, but to UV radiation alone. This structure is similar to that of dos Santos (2014), who observed the loss of the COO^- group in subsequent reactions bud did not also observe a loss of O. The IUPAC name for the proposed structure is (E)-4-((1-(4-sulfonatophenyl)-4,5-dihydro-1H-pyrazol-4-yl)diazenyl)benzenesulfonate.

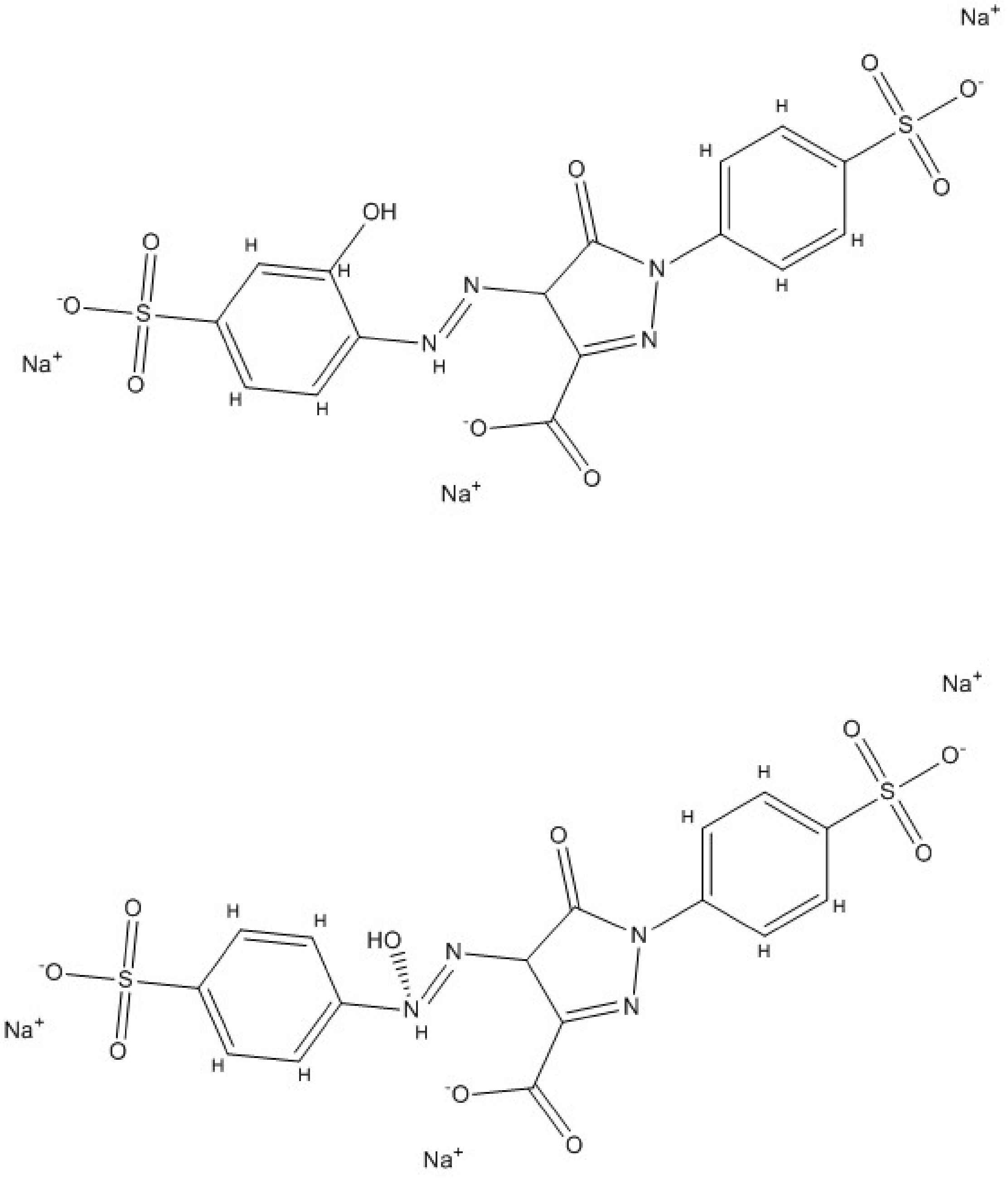


Figure 28: Tartrazine + OH Potential Isomers

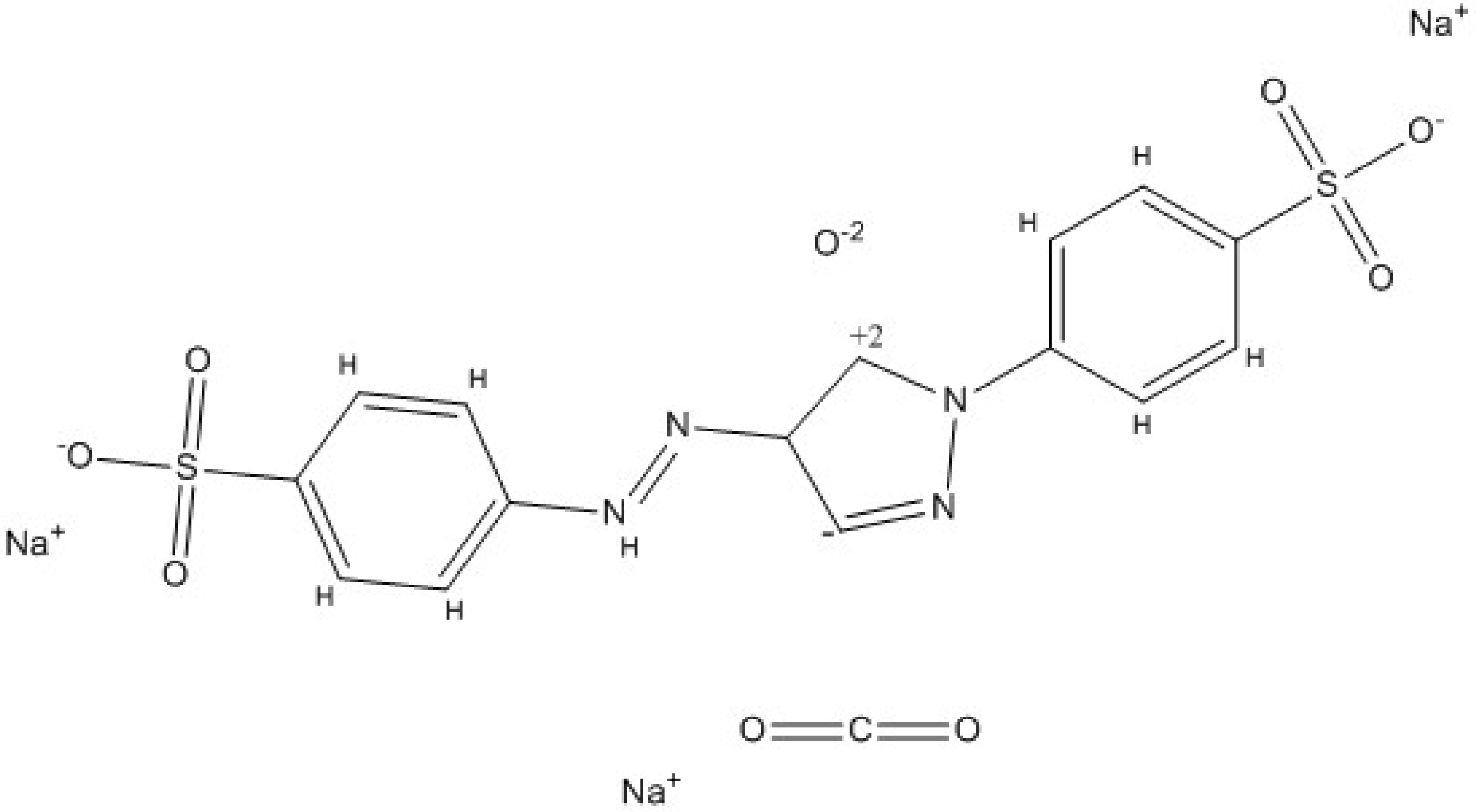


Figure 29: Tartrazine – O – COO + (CN) Potential Isomers

4.3.3.4 Product D: Tartrazine + 2H

The net result of Product D is an increase from 9 to 11 hydrogen atoms. This could be interaction with the free H's in the water as depicted in Figure 30, or two OH additions and a loss of two oxygen atoms. Due to the fact that the sulfonic acid groups have pKa of 2, the third isomer within Figure 30 seems unlikely. In addition, dos Santos (2014) proposed the same structure as the first isomer within Figure 31.

It should also be noted, that a fourth isomer is possible as presented by Maslowska (1996). That isomer instead presents hydrogen bonds with both Nitrogen atoms within the azo group, and with the single oxygen opposite the COO^- group depicted in Figure 31.

The IUPAC names for each of the four possible isomers for Product D are listed below:

- (E)-4-(3-carboxy-5-oxo-4-((4-sulfophenyl)diazenyl)-4,5-dihydro-1H-pyrazol-1-yl)benzenesulfonate
- (E)-4-((3-carboxy-5-oxo-1-(4-sulfophenyl)-4,5-dihydro-1H-pyrazol-4-yl)diazenyl)benzenesulfonate
- (E)-5-oxo-1-(4-sulfophenyl)-4-((4-sulfophenyl)diazenyl)-4,5-dihydro-1H-pyrazole-3-carboxylate
- (E)-5-hydroxy-1-(4-sulfonatophenyl)-4-((4-sulfonatophenyl)diazenyl)-4,5-dihydro-1H-pyrazole-3-carboxylate

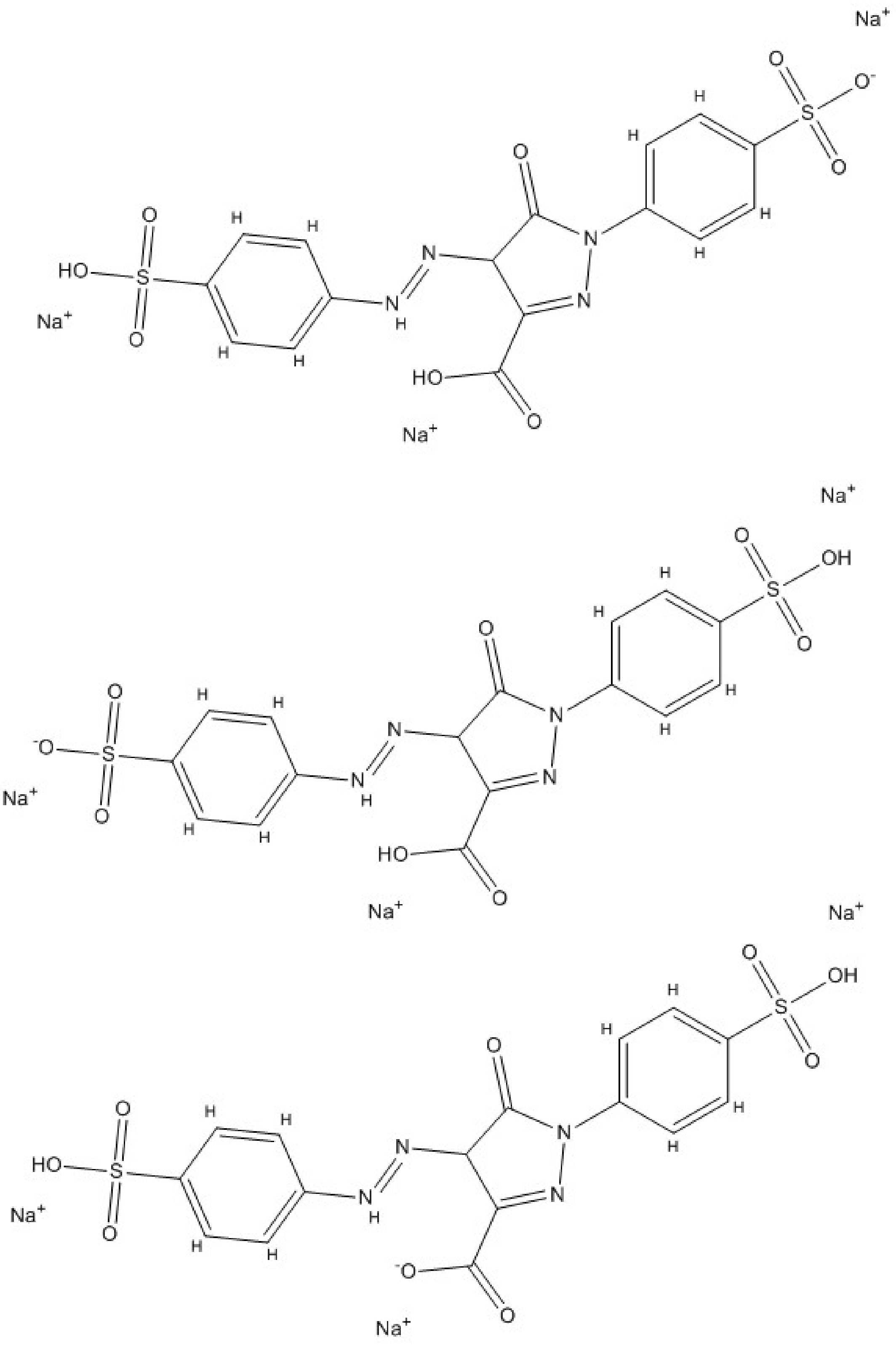


Figure 30: Tartrazine + 2H Potential Isomers

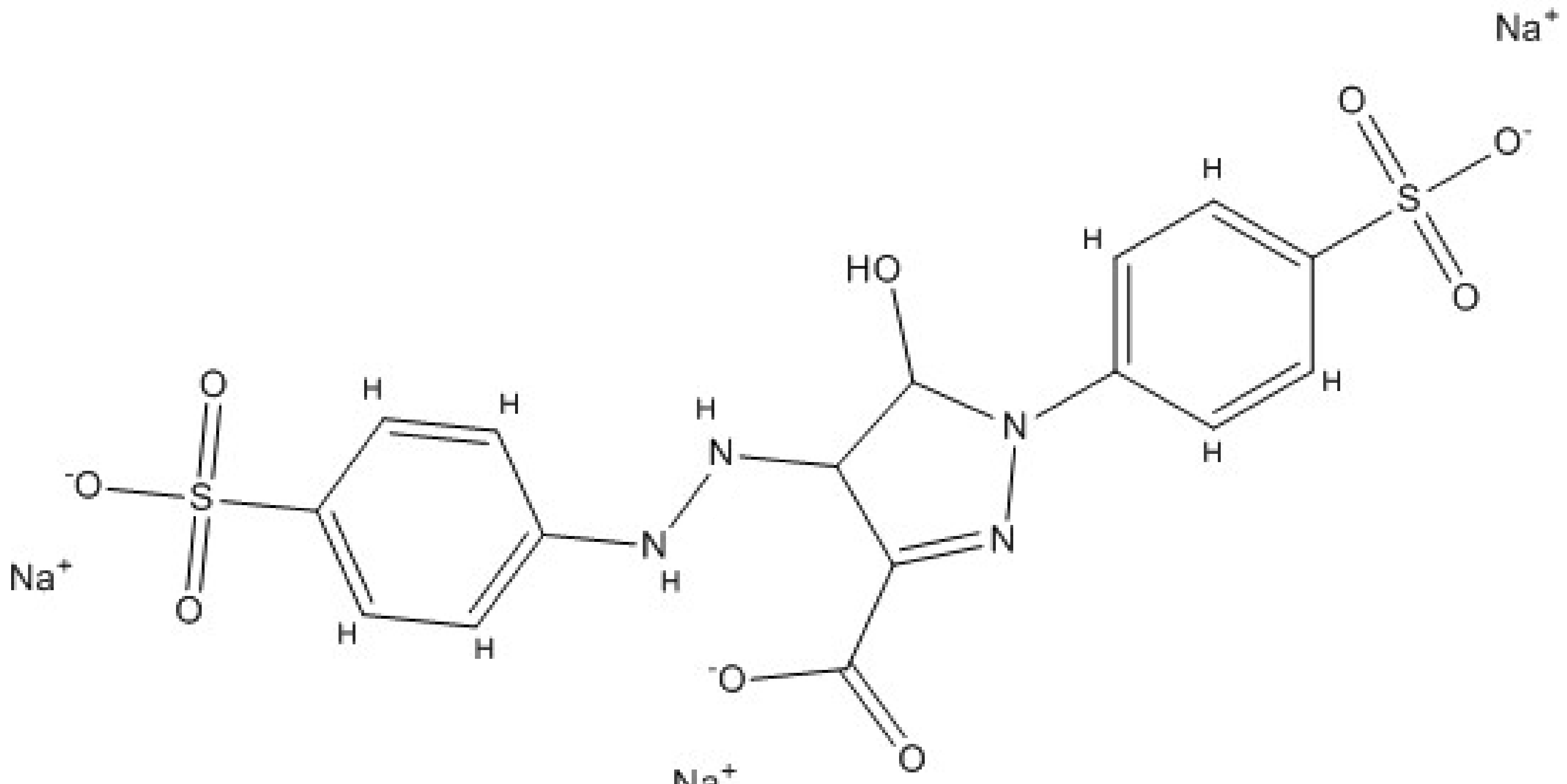


Figure 31: Tartrazine + 2H Most Likely Isomer

4.3.3.5 Product E: Tartrazine – Sulfonic Acid Group – COO Group + OH

The reaction mechanisms for Product E are likely twofold: OH addition and Electron transfer, see Figure 32. The OH Addition is indicated by the increase of OH. The Electron Transfer is indicated by the loss of the sulfonic acid group and the COO^- group. There are intermediate groups within this proposed structure. TAR – sulfonic acid group could be one of two structures, denoted by IUPAC names:

- (3-carboxylato-5-oxo-1-(4-sulfonatophenyl)-4,5-dihydro-1H-pyrazol-4-yl)diazen-1-ide
- (E)-3-carboxylato-5-oxo-4-((4-sulfonatophenyl)diazenyl)-4,5-dihydropyrazol-1-ide

The sulfonic acid group is expressed as 4-methylbenzenesulfonate. The order of the reaction mechanisms is undetermined. The IUPAC names for Product E's proposed isomers are:

- (1-(2-hydroxy-4-sulfonatophenyl)-5-oxo-4,5-dihydro-1H-pyrazol-4-yl)diazen-1-ide
- (Z)-4-(4-(hydroxydiazenyl)-5-oxo-4,5-dihydro-1H-pyrazol-1-yl)benzenesulfonate
- monosodium mono((E)-4-((3-hydroxy-4-sulfonatophenyl)diazenyl)-5-oxo-4,5-dihydropyrazol-1-ide)
- (Z)-4-(2-hydroxy-2-(4-sulfonatophenyl)-2l4-diazenyl)-5-oxo-4,5-dihydropyrazol-1-ide

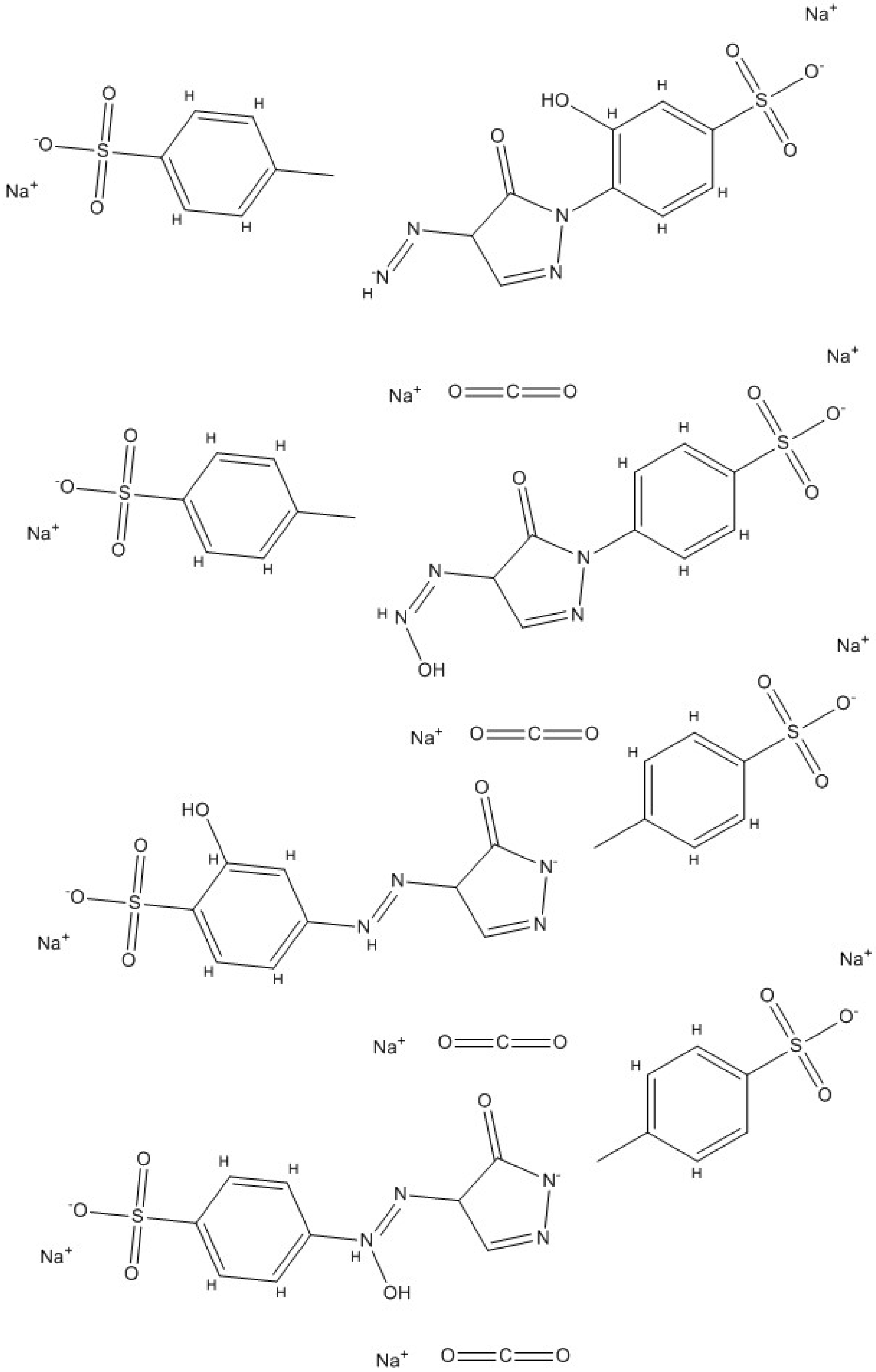


Figure 32: Tartrazine – Sulfonic Acid – COO + OH + (CN) Potential Isomers

4.3.3.6 Product F: Tartrazine – Sulfonic Acid Group + O

The reaction mechanism for Product F is one of two possibilities. First, the main structure of TAR (before or after loss of the sulfonic acid group) could pick up an oxygen atom from the water or from other possible reactions. If there had been a gain of two oxygen atoms, this could suggest a super anoxide radical ($2\dot{O}_2^-$) was created in the reactor, and propagation of the radical would be possible (Benjamin & Lawler, 2013). The results of the AOP experiment are consistent with the explanation that super anoxide radicals are not created in these conditions; otherwise a greater decrease in concentration of TAR would be expected. Second, and more likely, there could be a hydrogen abstraction followed by an OH addition, the net result of which would only be an increase by one oxygen atom, see Figure 33. The location of CN from the mobile phase was not determined. Product F's proposed IUPAC name is (E)-4-(hydroxydiazenyl)-5-oxo-1-(4-sulfonatophenyl)-4,5-dihydro-1H-pyrazole-3-carboxylate.

4.3.4 Byproduct Structure Summary

In summary, six products were consistently observed regardless of pH or DC of the experiments. Of these products, there were several proposed structures and respective isomers. To summarize and to simplify, the first isomer of each structure is included in Table 3; the structures mass calculations are shown in Appendix P.

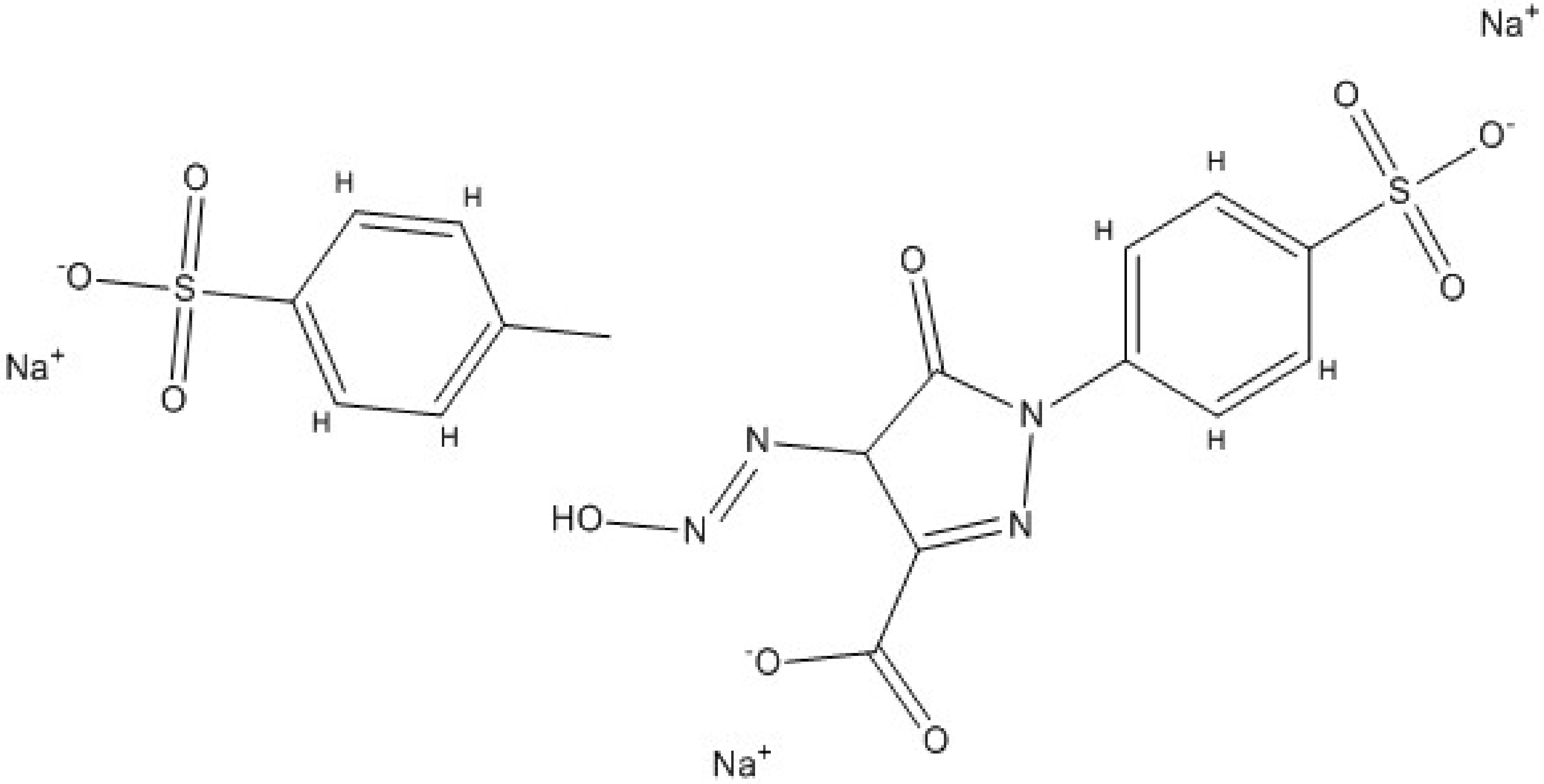
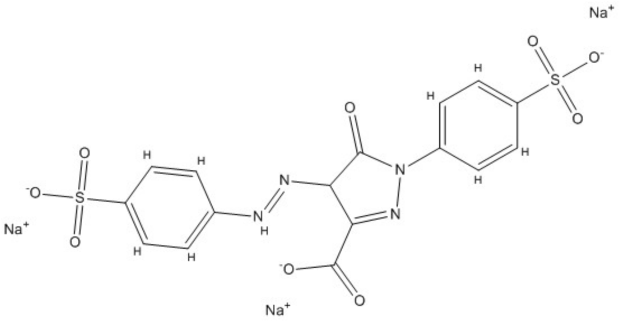
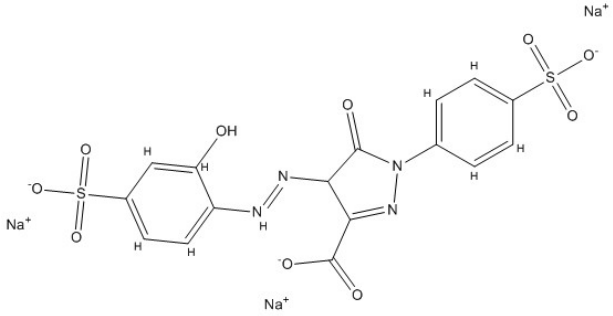
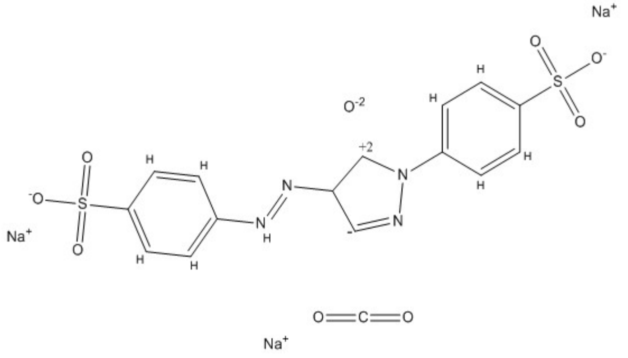
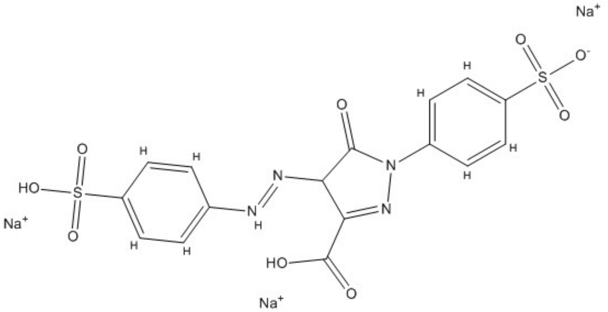
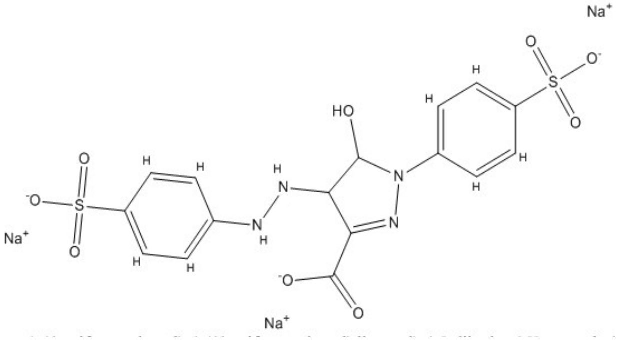
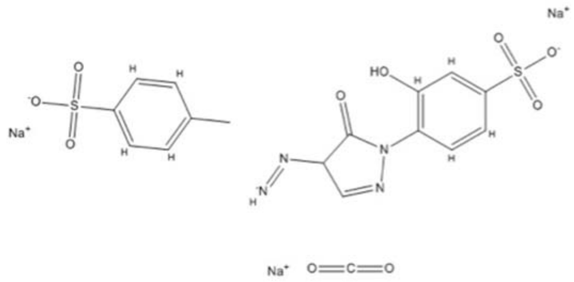
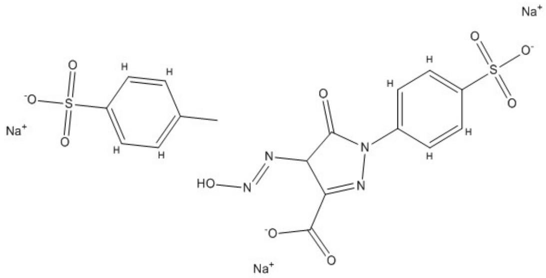
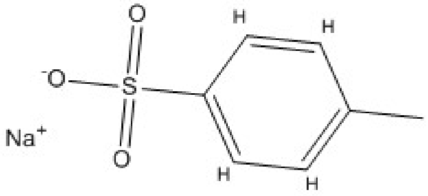


Figure 33: Tartrazine – Sulfonic Acid + O + (CN) Potential Isomer Structure

Table 3: Proposed Structures by Mass, IUPAC Name. Reaction Mechanisms denoted by H, E, or O for Hydrogen Abstraction, Electron Transfer, or OH addition, respectively.

Product (Mass) **Reaction Mechanism**	Structure	IUPAC Name	Reported by Others
A (534.36, 511.37, 488.38, 465.39) **None**		(E)-5-oxo-1-(4-sulfonatophenyl)-4-((4-sulfonatophenyl)diazenyl)-4,5-dihydro-1H-pyrazole-3-carboxylate	(Al-Dawery 2013; dos Santos et al., 2014; Maslowska & Janiak, 1996; Weisz et al., 2014)
B (551.37 528.38 505.39 482.40) **O**		(E)-4-((2-hydroxy-4-sulfonatophenyl)diazenyl)-5-oxo-1-(4-sulfonatophenyl)-4,5-dihydro-1H-pyrazole-3-carboxylate	No

C (474.35 451.36 428.37 405.38) **E**		(E)-4-((1-(4-sulfonatophenyl)-4,5-dihydro-1H-pyrazol-4-yl)diazenyl)benzenesulfonate	No
D (536.38 513.39 490.40 467.41) **E**	 	(E)-4-(3-carboxy-5-oxo-4-((4-sulfophenyl)diazenyl)-4,5-dihydro-1H-pyrazol-1-yl)benzenesulfonate or (E)-5-hydroxy-1-(4-sulfonatophenyl)-4-((4-sulfonatophenyl)diazenyl)-4,5-dihydro-1H-pyrazole-3-carboxylate	(dos Santos et al., 2014) (Maslowska & Janiak, 1996)

E (328.22 305.23 282.24) OH Add **E**		(1-(2-hydroxy-4-sulfonatophenyl)-5-oxo-4,5-dihydro-1H-pyrazol-4-yl)diazen-1-ide	No
F (371.22 348.23 325.24) **H, E, O**		(E)-4-(hydroxydiazenyl)-5-oxo-1-(4-sulfonatophenyl)-4,5-dihydro-1H-pyrazole-3-carboxylate	No
Sulfonic Acid Group (179.14 156.15) **E**		4-methylbenzenesulfonate	(Weisz et al., 2014)

4.4 Investigative Questions Answered

The first investigative question asked how pH affects the AOP of TAR and the associated hypothesis was that pH was significant. This hypothesis was supported by the data and analysis. The pH of the solution significantly affected the first order rate constant; this study observed a negative correlative relationship. Optimal TAR removal reported by Mudimbi (2015) was about 22%. This study observed optimal removal of 25%, with corresponding k_s of 1.2346E-03 min^{-1}.

The second investigative question of this research was what byproducts are generated and does pH influence the byproduct profile? The AOP of TAR produces several byproducts, each with a variety of possible structures, masses, and charge. Possible products are described in Table 3. The pH of the solution significantly influenced the CCAs in this study.

The third investigative question of the research was what reaction mechanisms occur in the AOP of TAR? The observations made in this study suggest that primary mechanisms of the AOP of TAR are OH Addition and Electron Transfer; but observations were also made that also indicate Hydrogen Abstraction.

4.5 Summary

In summary, this section developed the results and analysis conducted on the AOP Experiment, and the associated byproduct analysis. The pH of the solution significantly affected the first order rate constant. The byproduct profile of TAR remained consistent throughout the experiment, but the magnitudes of the peaks (amounts of each byproduct) varied greatly as detected by the CCA analysis, particularly at pH 7 and DC levels between 30% and 70%. The main reaction mechanisms of the AOP of TAR are likely OH Addition and Electron Transfer.

V. Conclusions and Recommendations

5.1 Chapter Overview

This chapter presents the outcomes of this study, discusses the significance of the findings and provides recommendations for further research in this field. The operating conditions for the UV/H_2O_2 AOP of TAR are discussed. The suggested byproducts from this reaction are characterized and potential reaction mechanisms identified.

5.2 Conclusions of Research

The conclusions of this study are as follows:

- The relative concentration of TAR was reduced from 1 to between 1 – 0.75 over the pH and DC values investigated in this effort. The first order rate constant for TAR removal was statistically and positively correlated with DC, statistically and negatively correlated with pH, and typically greatest at pH6. DC and pH were used as predictor variables in a regression model of the first order rate constant with adjusted R^2 of 0.85.
- Chromatographic contrast angle determinations revealed that the byproduct profile was most significantly influenced by pH and duty cycle. CCA under positive ionization is predicted by significant factors of pH 6, pH 7, pH 8, and 70% DC. The CCA under negative ionization is predicted by pH 6, pH 8, 30% DC, 50% DC, 70% DC. These factors were used as variables in regression models to predict positive and negative CCA with adjusted R^2 of 0.76, and 0.68, respectively.

- Chemical byproduct analysis indicated that OH addition (Products B, E, and F), electron transfer without molecule transfer (Products C, D, E, and F), and possibly H abstraction (Product F) were among the plausible reaction mechanisms for TAR degradation.
- Four potentially novel metabolites were identified, two of which demonstrate that TAR was likely cleaved. These metabolites were (1-(2-hydroxy-4-sulfonatophenyl)-5-oxo-4,5-dihydro-1H-pyrazol-4-yl)diazen-1-ide and (E)-4-(hydroxydiazenyl)-5-oxo-1-(4-sulfonatophenyl)-4,5-dihydro-1H-pyrazole-3-carboxylate (Products E and F, respectively). The other novel metabolites proposed by this study are: (E)-4-((2-hydroxy-4-sulfonatophenyl)diazenyl)-5-oxo-1-(4-sulfonatophenyl)-4,5-dihydro-1H-pyrazole-3-carboxylate, and (E)-4-((1-(4-sulfonatophenyl)-4,5-dihydro-1H-pyrazol-4-yl)diazenyl)benzenesulfonate (Products B and C, respectively).

5.3 Significance of Research

This research explained what effect pH has on the apparent first order rate constant for the LED driven UV/H_2O_2 AOP of TAR. This research also demonstrated pH can be used in conjunction with DC as a predictor for the first order rate constant as well as the positive and negative CCAs of the chromatograms of the byproducts. This capability was not previously available and no regression models existed. Additionally, this research offered suggestion of byproduct structures and identified possible AOP reaction mechanisms.

These are significant findings, because understanding AOP ideal operating conditions, mechanisms, and products can help the USAF in treatment of military wastewater, preserving the local environment, and safeguarding military members in chemical attack situations.

Byproducts are just as important to understand as the original substance because they may be toxic as well. It is not acceptable to conduct an AOP on CBRN contaminants and expect complete mineralization. Understanding the AOP reaction mechanisms leads to better understanding of the how byproducts are formed which may help in predicting AOP outcomes for contaminants for which laboratory testing has not been conducted or data may not be available.

The creation of linear regression models for reactor performance and byproduct profile has not been accomplished in other studies on TAR. These models are practically applicable to future research as follows. The AOP regression model provides a baseline against which future researchers can compare additional independent variable (other than pH or DC) testing in the AOP of TAR without having to conduct the conditions represented in this study again. The byproduct profile models are also useful as future research on byproduct formation can save time and effort by using the model as a baseline.

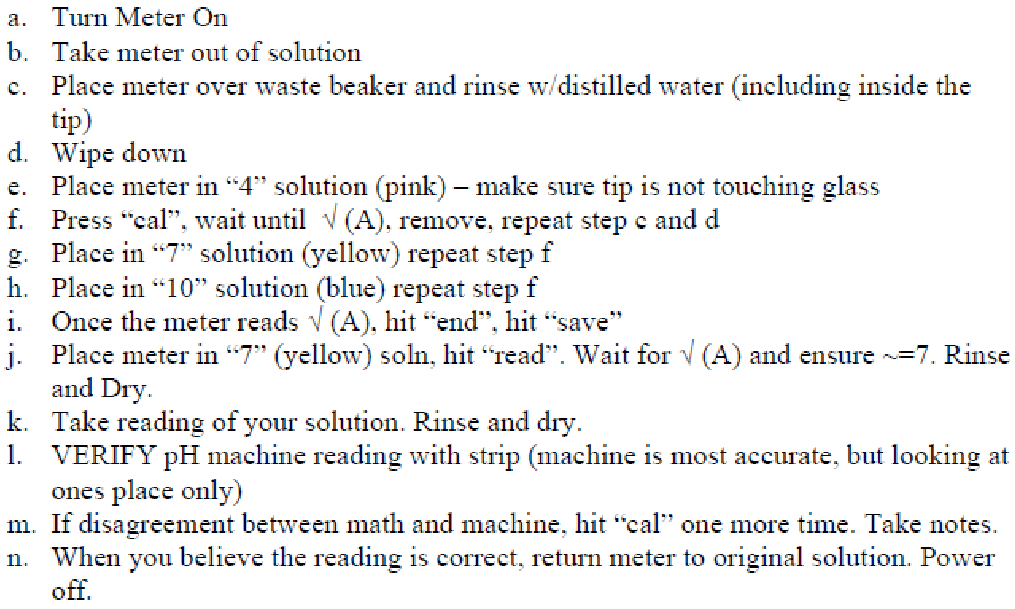
5.4 Recommendations for Future Research

Future research in this field should consider a variety of topics, to include: evaluation of more acidic pH levels, implementation of more powerful LEDs which will provide greater understanding of the UV dose effects, executing AOPs on other contaminants (perhaps mild chemical or nerve agents), construction of large scale reactor capable of handling greater flow rates, and creating exact mass characterization using time of flight MS. Future TAR byproduct research should include measurement by UV-Vis at peaks 258, 277, and 404 to detect and substantiate manufacturing isomers Pk5 and Pk7. Future research could also incorporate hydroxyl radical sensors to quantify concentrations of the radicals during the reaction. Future research should also attempt to construct predictive models for byproducts depending on the constituent.

5.5 Summary

To conclude, wastewater treatment is vital to the success of USAF operations. Incorporating UV LEDs into these treatment methods can be beneficial with further study and design. This study observed that the LED UV/H_2O_2 AOP of TAR is significantly affected by the pH of the solution. The first order rate constant can be reasonably predicted by DC and pH levels. Operating conditions can be manipulated to maximize k_s (DCs 70-100%) or to maximize $k_{s,adj}$ (DCs of 5-10%), at pH 6. Evaluation of the AOP reaction byproducts suggested reaction mechanisms of OH Addition and Electron Transfer.

Appendix A: pH Meter Calibration Procedures



a. Turn Meter On
b. Take meter out of solution
c. Place meter over waste beaker and rinse w/distilled water (including inside the tip)
d. Wipe down
e. Place meter in “4” solution (pink) – make sure tip is not touching glass
f. Press “cal”, wait until √ (A), remove, repeat step c and d
g. Place in “7” solution (yellow) repeat step f
h. Place in “10” solution (blue) repeat step f
i. Once the meter reads √ (A), hit “end”, hit “save”
j. Place meter in “7” (yellow) soln, hit “read”. Wait for √ (A) and ensure ~=7. Rinse and Dry.
k. Take reading of your solution. Rinse and dry.
l. VERIFY pH machine reading with strip (machine is most accurate, but looking at ones place only)
m. If disagreement between math and machine, hit “cal” one more time. Take notes.
n. When you believe the reading is correct, return meter to original solution. Power off.

Appendix B: AOP Experiment Schedule

Data Point	Duty Cycle (%)	pH	H_2O_2 Ctrl	Date Completed
1	70	8	N	9-Jul-15
2	0	7	N	7-Mar-15
3	5	7	N	13-Mar-15
4	0	9	N	16-Mar-15
5	100	9	Y	8-Apr-15
6	10	7	N	9-Apr-15
7	100	8	Y	16-Apr-15
8	50	8	N	23-Apr-15
9	10	9	N	30-Apr-15
10	50	9	N	7-May-15
11	0	6	N	14-May-15
12	10	8	N	27-May-15
13	70	6	N	1-Jun-15
14	20	6	N	9-Jun-15
15	30	6	N	17-Jun-15
16	100	6	N	26-Jun-15
17	30	7	N	3-Jun-15
18	20	9	N	22-Jun-15
19	5	6	N	29-Jun-15
20	30	8	N	2-Jul-15
21	70	7	N	13-Jul-15
22	100	9	N	1-Jul-15
23	100	8	N	6-Jul-15
24	20	8	N	10-Jul-15
25	100	7	Y	14-Jul-15
26	0	8	N	15-Jul-15
27	100	6	Y	17-Jul-15
28	70	9	N	23-Jul-15
29	5	8	N	21-Jul-15
30	100	7	N	30-Jul-15
31	20	7	N	6-Aug-15
32	50	7	N	11-Aug-15
33	10	6	N	7-Aug-15
34	5	9	N	28-Jul-15
35	30	9	N	5-Aug-15
36	50	6	N	4-Aug-15
37	100	8	N	13-Aug-15
38	70	6	N	12-Aug-15

Appendix C: AOP Experiment Data

		13-Feb-15		7-Mar-15		13-Mar-15		16-Mar-15		8-Apr-15		9-Apr-15		16-Apr-15	
	pH	pH8		pH7		pH7		pH9		pH9**		pH7		pH8**	
	DC	70		0		5		0		100		10		100	
Ks	Ks, adj	6.2298E-04	8.8997E-04	1.9741E-05	0.0000E+00	9.0691E-05	1.8138E-03	-1.5526E-05	0.0000E+00	4.3388E-05	0.0000E+00	1.5964E-04	1.5964E-03	9.4125E-07	0.0000E+00
R	R^2	0.9978	0.9956	0.3996	0.1597	0.8335	0.6948	0.5228	0.2733	0.6083	0.3700	0.9601	0.9218	0.4793	0.2297
	Time	C/C0	Model	C/C0	Model	C/C0	Model	C/C0	Model	C/C0	Model	C/C0	Model	C/C0	Model
0	0	1	1	1	1	1	1	1	1	1	1	1	1	1	1
5	5	0.994883616	0.996906027	1.002841314	0.999901808	0.993421847	0.999548993	1.00815327	1.000077233	1.01111733	0.999784204	1.00153689	0.999206227	0.99915669	0.999995318
10	10	0.997830417	0.993853506	1.001375868	0.999804639	1.003211288	0.999102843	1.005193723	1.000153675	1.002195819	0.999570682	0.99981983	0.998421273	1.000096142	0.999990684
20	15	0.993565127	0.990841882	1.000850807	0.999708482	0.997051685	0.998661497	1.003418424	1.000229334	1.003827837	0.999359409	1.001117373	0.997645038	1.00141169	0.999986099
30	20	0.991033129	0.987870608	1.002115296	0.999613327	0.995962653	0.998224903	1.001855958	1.000304217	1.004641429	0.999150361	0.996977577	0.996877428	0.995958994	0.99998156
50	25	0.982201934	0.984939141	0.996355313	0.999519163	1.001571016	0.997793011	1.006745796	1.000378334	0.998126533	0.998943516	1.00016749	0.996118345	1.005674378	0.999977069
70	30	0.983873936	0.98204695	0.995113173	0.99942598	0.997784799	0.99736577	1.004454909	1.000451692	1.001092779	0.99873885	1.003887451	0.995367695	0.994432121	0.999972624
100	35	0.980823281	0.979193508	0.997616426	0.999333768	0.996638757	0.99694313	1.004740494	1.000524298	1.009848248	0.998536339	0.995545091	0.994625385	0.996820088	0.999968224
100**	40	0.972074146	0.976378295	1.001692766	0.999242517	0.994549523	0.996525041	1.010861687	1.000596161	0.994483474	0.998335963	1.002465322	0.993891321	0.997530537	0.99996387
	45	0.977349636	0.9736008	0.997506781	0.999152216	1.000280639	0.996111454	1.009838871	1.000667287	1.000009004	0.998137697	0.991082152	0.993165413	0.995073732	0.999959562
	50	0.971521415	0.970860518	1.002577507	0.999062856	0.99657221	0.995702321	1.00459725	1.000737685	0.997592392	0.997941519	0.996559434	0.992447568	0.994768777	0.999955297
	55	0.971727282	0.968156949	1.003421016	0.998974426	0.997526343	0.995297593	1.012936466	1.000807362	0.996888236	0.997747409	0.991511496	0.991737699	0.997428327	0.999951077
	60	0.966684261	0.965489602	0.99639846	0.998886918	0.992964053	0.994897224	1.008106274	1.000876325	0.999481946	0.997555343	0.991155065	0.991035716	0.991469289	0.9999469
	65	0.962761128	0.962857991	0.991971745	0.998800322	0.994639857	0.994501166	1.008105371	1.000944581	0.998526675	0.9973653	0.989326733	0.990341532	0.993962709	0.999942766
	70	0.958838301	0.960261638	1.001175823	0.998714628	0.992071047	0.994109373	1.005601199	1.001012139	1.00820193	0.99717726	0.990964962	0.989655059	0.995432775	0.999938675
	75	0.9572061	0.95770007	1.00232501	0.998629826	0.990318861	0.993721799	1.009842147	1.001079005	0.995983744	0.9969912	0.990934951	0.988976213	0.994351463	0.999934626
	80	0.961845369	0.955172822	0.998248397	0.998545908	0.990573303	0.993338399	1.003334715	1.001145185	1.001018629	0.9968071	0.988597598	0.988304909	0.994907078	0.99993062
	85	0.950988349	0.952679433	1.002348272	0.998462864	0.996460898	0.992959128	1.001845678	1.001210688	0.996682471	0.99662494	0.991374333	0.987641063	0.999171336	0.999926654
	90	0.950463246	0.95021945	1.000212177	0.998380685	0.993526435	0.99258394	1.010283177	1.00127552	1.000419474	0.996444699	0.989069739	0.986984591	0.994127689	0.999922729
	95	0.94959619	0.947792425	0.997374055	0.998299362	0.986432474	0.992212793	1.004712929	1.001339688	0.992262763	0.996266357	0.984193729	0.986335413	0.993535248	0.999918845
	100	0.947106348	0.945397917	0.99719417	0.998218887	0.987311628	0.991845642	1.003318334	1.001403198	0.994742269	0.996089893	0.987759833	0.985693446	0.99416671	0.999915001
	105	0.947218388	0.94303549	1.001180567	0.998139249	0.986045943	0.991482446	1.002630695	1.001466058	0.99236538	0.995915288	0.983850507	0.985058612	0.998003297	0.999911197
	110	0.943234374	0.940704715	1.00188077	0.998060442	0.985508653	0.99112316	1.003741062	1.001528274	0.99468434	0.995742523	0.984075165	0.98443083	0.997322978	0.999907432
	115	0.937620205	0.938405166	1.003042181	0.997982455	0.985782567	0.990767743	1.003449377	1.001589853	1.000883637	0.995571577	0.983517746	0.983810023	1.002226544	0.999903705
	120	0.939688901	0.936136426	0.991297813	0.997905281	0.992506058	0.990416154	1.002624482	1.001650801	0.994696456	0.995402433	0.989026731	0.983196112	0.995392288	0.999900018
	125	0.933443216	0.933898083	0.997033076	0.997828911	0.987337323	0.99006835	1.002360361	1.001711125	0.9925154	0.99523507	0.978069312	0.982589022	0.997113328	0.999896368
	130	0.930711184	0.931689728	0.994379765	0.997753336	0.990533556	0.989724292	1.006065953	1.001770831	0.989905602	0.995069471	0.976476522	0.981988676	0.996512099	0.999892756
	135	0.92635002	0.92951096	0.994693562	0.997678549	0.984126336	0.989383939	1.003165036	1.001829925	0.991191964	0.994905615	0.986461338	0.981394999	1.002181141	0.999889181
	140	0.929493991	0.927361383	0.997151936	0.99760454	0.990129661	0.989047251	1.001731693	1.001888414	0.992539565	0.994743486	0.979239204	0.980807919	0.992581149	0.999885644
	145	0.928041157	0.925240606	0.995571461	0.997531303	0.986528529	0.988714189	1.003429721	1.001946304	0.997082945	0.994583065	0.987908723	0.98022736	0.99675031	0.999882142
	150	0.927970352	0.923148242	1.003290845	0.997458829	0.987944672	0.988384713	1.003486544	1.002003601	0.997249847	0.994424334	0.9781902	0.979653251	0.996766944	0.999878677
	155	0.923185278	0.921083911	0.995182682	0.99738711	0.983347051	0.988058785	1.000508244	1.002060311	0.989190589	0.994267275	0.982994777	0.97908552	0.995576412	0.999875248
	160	0.919977562	0.919047237	0.995004712	0.997316137	0.985815991	0.987736367	1.004470951	1.00211644	0.995522759	0.994111871	0.976438903	0.978524096	1.004089862	0.999871854
	165	0.91719969	0.917037851	1.002066311	0.997245905	0.992375374	0.987417421	1.000795185	1.002171994	0.989880047	0.993958104	0.978748887	0.977968909	0.995256601	0.999868495
	170	0.914369021	0.915055385	0.992799747	0.997176403	0.986833157	0.987101909	1.003584714	1.002226979	0.995464896	0.993805956	0.975000182	0.97741989	0.998667609	0.999865171
	175	0.915552755	0.913099481	0.992072817	0.997107626	0.983000569	0.986789795	0.997798471	1.002281401	0.994965645	0.993655412	0.977626653	0.976876971	1.001115103	0.999861881
	180	0.912892961	0.911169781	0.994682068	0.997039566	0.986757476	0.986481042	1.002028461	1.002335266	0.993488613	0.993506453	0.975195886	0.976340083	0.997238867	0.999858625
	185	0.910236951	0.909265935	0.995757549	0.996972214	0.985415107	0.986175614	1.003779923	1.002388579	0.994855348	0.993359064	0.976590331	0.97580916	0.995076348	0.999855403
	190	0.905589907	0.907387596	0.99391646	0.996905564	0.984496407	0.985873475	0.999721871	1.002441345	0.988310858	0.993213227	0.977213582	0.975284135	0.997492561	0.999852214
	195	0.90519393	0.905534422	1.001189506	0.996839608	0.986766912	0.985574589	1.000450179	1.002493572	0.988535624	0.993068926	0.973328772	0.974764942	0.998489657	0.999849058
	200	0.910742307	0.903706077	0.995755269	0.99677434	0.990915269	0.985278922	1.000004406	1.002545263	0.983112712	0.992926146	0.972627429	0.974251518	1.001174211	0.999845934
	205	0.900592213	0.901902228	0.999840457	0.996709751	0.984201213	0.984986439	0.999848847	1.002596425	0.986135629	0.99278487	0.974934982	0.973743797	1.003456516	0.999842843
	210	0.89998904	0.900122546	1.002086927	0.996645835	0.991922497	0.984697106	1.002880808	1.002647062	0.988573294	0.992645082	0.971487442	0.973241717	1.000380174	0.999839783
	215	0.897092784	0.898366709	0.996815882	0.996582585	0.984207537	0.984410888	1.008746918	1.002697181	0.98885632	0.992506766	0.97158688	0.972745215	1.002092845	0.999836756
	220	0.901116601	0.896634395	0.992968596	0.996519994	0.979158947	0.984127752	1.001796085	1.002746787	0.985460736	0.992369908	0.969249104	0.972254229	1.000378082	0.999833759
	225	0.896437838	0.89492529	1.000686064	0.996458055	0.99004053	0.983847665	1.000561791	1.002795885	0.990410746	0.992234491	0.978892389	0.971768697	0.995408086	0.999830794
	230	0.890848431	0.893239084	0.997620076	0.996396762	0.980246072	0.983570595	1.006355265	1.002844479	0.986630312	0.992100501	0.967014887	0.97128856	0.996767153	0.999827859
	235	0.889920188	0.891575469	0.992626612	0.996336106	0.988536864	0.983296507	0.998602581	1.002892576	0.997581203	0.991967923	0.977909959	0.970813756	1.000697371	0.999824954
	240	0.887337951	0.889934143	1.001109415	0.996276083	0.985379877	0.983025372	0.996772944	1.002940181	0.98424283	0.991836741	0.965767431	0.970344227	0.99836234	0.999822079
	245	0.889022641	0.888314807	0.994178626	0.996216685	0.986164883	0.982757156	1.000009941	1.002987297	0.987097123	0.991706941	0.969287779	0.969879915	1.001736418	0.999819234
	250	0.884067513	0.886717167	0.997191798	0.996157906	0.990341946	0.982491829	0.998117607	1.003033931	0.991295906	0.991578509	0.974566189	0.969420761	1.002062298	0.999816419
	255	0.886478161	0.885140931	0.997303907	0.996099739	0.979542969	0.982229358	0.999936624	1.003080088	0.99375138	0.991451429	0.967327674	0.968966707	1.008062554	0.999813632
	260	0.881614915	0.883585813	0.992831583	0.996042178	0.986921383	0.981969714	1.00310471	1.003125771	0.998422866	0.991325688	0.966624958	0.968517698	1.00950249	0.999810874
	265	0.879242228	0.882051531	0.997806528	0.995985216	0.979901697	0.981712866	1.001679614	1.003170987	0.991942397	0.991201272	0.962991647	0.968073678	0.999277207	0.999808145
	270	0.883053731	0.880537804	1.0005766	0.995928848	0.985382486	0.981458784	0.999680411	1.003215739	0.993517081	0.991078167	0.966522245	0.96763459	1.001303517	0.999805444
	275	0.877630287	0.879044358	0.995630663	0.995873068	0.98588324	0.981207438	1.001225368	1.003260034	0.995096995	0.990956358	0.964615399	0.96720038	1.001931004	0.999802771
	280	0.872821782	0.877570921	1.00263014	0.995817868	0.979705471	0.980958799	1.001440912	1.003303874	1.004428911	0.990835832	0.967205201	0.966770994	1.002212736	0.999800125
	285	0.87390596	0.876117224	0.992878105	0.995763244	0.978741904	0.980712837	1.002422381	1.003347265	0.989884748	0.990716577	0.962355609	0.966346378	1.000777821	0.999797507
	290	0.869814305	0.874683004	0.992749394	0.995709188	0.977547281	0.980469524	1.002727961	1.003390212	0.994296909	0.990598577	0.962032359	0.96592648	1.007290592	0.999794916
	295	0.870005234	0.873268	0.990713642	0.995655696	0.975005872	0.980228831	1.001204017	1.003432719	0.99359613	0.990481821	0.971491247	0.965511246	1.001875034	0.999792351
	300	0.87121731	0.871871953	0.993133612	0.99560276	0.978226997	0.979990729	1.006271103	1.003474791	0.997311749	0.990366294	0.964441674	0.965100626	1.007439042	0.999789813

23-Apr-15		30-Apr-15		7-May-15		14-May-15		27-May-15		1-Jun-15		9-Jun-15		17-Ju
pH8		pH9		pH9		pH6		pH8		pH6		pH6		pH
50		10		50		0		10		70		20		3
7.4882E-04	**1.4976E-03**	**1.0181E-04**	**1.0181E-03**	**3.3801E-04**	**6.7602E-04**	**-3.5141E-05**	**0.0000E+00**	**8.8471E-05**	**8.8471E-04**	**1.2346E-03**	**1.7637E-03**	**3.5649E-04**	**1.7825E-03**	**4.5805E-04**
0.9991	**0.9981**	**0.8198**	**0.6720**	**0.8141**	**0.6627**	**0.6116**	**0.3740**	**0.8486**	**0.7200**	**0.9968**	**0.9937**	**0.9961**	**0.9922**	**0.9963**
C/C0	**Model**	**C/C0**	**Model**	**C/C0**	**Model**	**C/C0**	**Model**	**C/C0**	**Model**	**C/C0**	**Model**	**C/C0**	**Model**	**C/C0**
1	1	1	1	1	1	1	1	1	1	1	1	1	1	1
0.994597073	0.996282187	0.992018544	0.999493686	1.012971099	0.998320097	1.008136475	1.000174812	1.006367094	0.999560027	0.994361427	0.993877778	0.998099167	0.998228338	1.004368995
0.993773284	0.992616491	0.997197563	0.998992851	1.013750328	0.996660339	1.001201371	1.000347851	0.996882422	0.999124788	0.990420004	0.987856024	0.996515787	0.996478081	0.999260907
0.990129273	0.989002183	0.999869108	0.998497438	1.001583726	0.995020482	1.00453596	1.000519134	0.99638312	0.99869423	0.977588755	0.981933088	0.996335631	0.994748972	0.993291516
0.986310516	0.985438541	0.996481392	0.998007386	1.001679449	0.993400289	1.002853808	1.00068868	1.002614452	0.998268305	0.969034947	0.97610735	0.992274916	0.993040754	0.994902731
0.983676384	0.981924855	0.992690501	0.997522639	1.008097443	0.991799524	1.001665785	1.000856505	0.99233323	0.997846961	0.961898533	0.970377214	0.993141558	0.991353176	0.990869282
0.98159279	0.978460426	0.993741339	0.997043138	0.996818204	0.990217954	1.00137142	1.001022627	0.996497885	0.997430149	0.966911779	0.964741111	0.991819745	0.989685987	0.987399462
0.978347578	0.975044563	0.99249312	0.996568827	0.996704273	0.988655348	0.999830995	1.001187064	0.993795301	0.997017822	0.959998857	0.959197498	0.992794586	0.988038942	0.986169726
0.97427794	0.971676584	0.993786428	0.99609965	1.003869762	0.987111479	1.001886094	1.001349832	0.995054152	0.99660993	0.95197979	0.953744858	0.993361212	0.986411797	0.98453602
0.970195578	0.968355819	0.993591671	0.995635551	0.993161364	0.985586124	0.995985214	1.001510949	1.001298316	0.996206426	0.94799634	0.948381698	0.985343361	0.984804311	0.981358357
0.969233943	0.965081606	1.001228097	0.995176475	0.993490074	0.984079058	1.000898184	1.001670432	1.001405758	0.995807263	0.94266658	0.943106548	0.985375611	0.983216248	0.980534927
0.965222201	0.961853292	0.993617177	0.994722368	0.985996023	0.982590064	1.000724305	1.001828296	0.993314856	0.995412394	0.937227998	0.937917966	0.983407652	0.981647372	0.976909586
0.9624902	0.958670234	0.992124065	0.994273176	0.980360157	0.981118925	0.998915283	1.001984559	0.98996723	0.995021773	0.932124947	0.93281453	0.980908573	0.980097452	0.976324104
0.95938188	0.955531796	0.990914676	0.993828846	0.977402579	0.979665426	1.003252408	1.002139236	0.990822427	0.994635353	0.932001695	0.927794842	0.986481025	0.978566259	0.972418699
0.957375372	0.952437355	0.995981848	0.993389325	0.971491883	0.978229356	1.001607516	1.002292344	0.991689418	0.994253091	0.92482579	0.92285753	0.980076492	0.977053566	0.971022305
0.953561068	0.949386293	0.997805926	0.992954562	0.969443369	0.976810505	1.004548496	1.002443898	0.996684321	0.993874941	0.923213475	0.91800124	0.977629938	0.975559149	0.970142756
0.949094752	0.946378002	0.995243065	0.992524504	0.968211392	0.975408669	1.006712125	1.002593915	0.993159266	0.993500859	0.915615842	0.913224644	0.97603164	0.974082789	0.966198205
0.946753597	0.943411882	0.989626348	0.9920991	0.967867074	0.974023642	1.008574076	1.00274241	0.99357938	0.993130801	0.909527654	0.908526432	0.974055067	0.972624267	0.966282542
0.944182876	0.940487342	1.001235635	0.991678301	0.962442941	0.972655222	1.001157147	1.002889398	0.991338643	0.992764724	0.909923639	0.903905321	0.971387703	0.971183367	0.968776702
0.941945848	0.937603799	0.993088359	0.991262057	0.963141386	0.971303212	1.001442457	1.003034895	0.995260678	0.992402585	0.908097778	0.899360043	0.969517964	0.969759876	0.960573908
0.939882188	0.93476068	0.996420354	0.990850318	0.96564027	0.969967413	1.002476334	1.003178915	0.991217203	0.992044341	0.903973134	0.894889354	0.96847957	0.968353584	0.963130869
0.935565064	0.931957416	0.998333936	0.990443035	0.956125054	0.968647632	1.001612158	1.003321475	0.994627688	0.991689952	0.893245259	0.890492031	0.969472058	0.966964284	0.959344916
0.931749274	0.929193449	0.988142186	0.990040161	0.95888383	0.967343677	1.001353776	1.003462588	0.988393698	0.991339375	0.889182046	0.886166869	0.965730478	0.965591769	0.954935926
0.929729301	0.926468228	0.995652768	0.989641647	0.947220439	0.966055357	1.002724732	1.003602269	0.989956926	0.990992569	0.88743819	0.881912685	0.965565239	0.964235838	0.95949545
0.927350928	0.923781211	0.98275347	0.989247446	0.947420504	0.964782486	1.001091332	1.003740533	0.990387732	0.990649494	0.882298377	0.877728313	0.963556836	0.962896289	0.952288899
0.926309236	0.921131862	0.988181353	0.988857512	0.955417022	0.963524878	1.00814135	1.003877394	0.991609905	0.99031011	0.883031062	0.873612608	0.961735734	0.961572926	0.957432101
0.920642282	0.918519652	0.977035606	0.988471798	0.94720565	0.962282349	1.003591461	1.004012867	0.9918708	0.989974376	0.875310471	0.869564443	0.960023566	0.960265551	0.951765052
0.919037648	0.91594406	0.98734149	0.98809026	0.940853502	0.96105472	1.002321142	1.004146965	0.993917972	0.989642255	0.870259391	0.865582709	0.959708423	0.958973973	0.947337391
0.91601914	0.913404575	0.984600563	0.98771285	0.93363651	0.959841812	1.005366009	1.004279703	0.986020829	0.989313706	0.872085351	0.861666318	0.958948405	0.957698	0.946219258
0.91503651	0.910900689	0.981302755	0.987339526	0.934168853	0.958643447	1.010974149	1.004411093	0.987372866	0.988988691	0.862482049	0.857814195	0.958094055	0.956437444	0.946439383
0.910517283	0.908431903	0.983701546	0.986970243	0.935809285	0.957459452	1.002632569	1.004541151	0.986418133	0.988667173	0.860944816	0.854025287	0.955443812	0.955192118	0.943881786
0.907051517	0.905997726	0.983229392	0.986604956	0.936079655	0.956289654	1.004580649	1.004669889	0.985140878	0.988349113	0.85488393	0.850298556	0.955883751	0.953961838	0.940342373
0.907795991	0.903597672	0.983763661	0.986243623	0.94424666	0.955133884	1.000621114	1.004797322	0.993482694	0.988034475	0.855242569	0.846632982	0.953416501	0.952746423	0.940974638
0.901783891	0.901231263	0.983295007	0.985886201	0.947106583	0.953991972	1.004871299	1.004923461	0.994377939	0.987723222	0.848481957	0.843027561	0.951535732	0.951545694	0.938772742
0.900144797	0.898898027	0.991789869	0.985532647	0.943326077	0.952863753	1.002204023	1.00504832	0.985363409	0.987415317	0.845798111	0.839481306	0.951685425	0.950359471	0.941315913
0.897941276	0.896597499	0.991204927	0.985182921	0.951071176	0.951749063	1.001598927	1.005171913	0.993166718	0.987110724	0.839989093	0.835993247	0.950639048	0.949187581	0.938100908
0.895415195	0.894329221	0.980226075	0.984836979	0.944883272	0.950647739	1.006604408	1.005294251	0.989105876	0.986809408	0.835022943	0.832562427	0.949095165	0.948029851	0.938696892
0.891913907	0.892092741	0.983954784	0.984494782	0.948138941	0.94955962	1.007083564	1.005415348	0.984901044	0.986511334	0.836894635	0.829187909	0.947298538	0.946886108	0.932948051
0.889653658	0.889887612	0.982856299	0.984156288	0.94747223	0.94848455	1.004789119	1.005535217	0.99256749	0.986216466	0.829092136	0.825868767	0.945114707	0.945756184	0.93319682
0.886735458	0.887713396	0.983018013	0.983821459	0.943584036	0.94742237	1.005410465	1.00565387	0.993369355	0.98592477	0.824070602	0.822604093	0.947414511	0.944639913	0.935572483
0.88546876	0.885569658	0.982215164	0.983490253	0.939173087	0.946372928	1.01202265	1.005771318	0.983033374	0.985636212	0.819611208	0.819392994	0.944916482	0.943537128	0.929648496
0.883759999	0.883455972	0.990628732	0.983162632	0.942370639	0.945336069	1.002773136	1.005887575	0.9839629	0.985350758	0.821950262	0.81623459	0.948346807	0.942447668	0.925492519
0.881861861	0.881371917	0.992073121	0.982838557	0.932176747	0.944311643	1.006048875	1.006002653	0.980267608	0.985068375	0.812058723	0.813128016	0.94208703	0.941371371	0.927312404
0.879559515	0.879317077	0.980953687	0.98251799	0.93742363	0.943299501	1.005901576	1.006116563	0.980300722	0.98478903	0.815080342	0.810072423	0.939611167	0.940308078	0.925220624
0.87513116	0.877291042	0.989928443	0.982200892	0.938790941	0.942299496	1.005776796	1.006229317	0.984223794	0.984512689	0.810226231	0.807066972	0.938787805	0.939257632	0.924856541
0.874182779	0.87529341	0.986135601	0.981887227	0.931593644	0.941311482	1.005523986	1.006340927	0.98026709	0.984239322	0.803182939	0.804110842	0.936012557	0.938219878	0.921642172
0.872185603	0.87332378	0.98621676	0.981576956	0.944962495	0.940335315	1.011022436	1.006451405	0.980270395	0.983968895	0.798337507	0.801203223	0.93679348	0.937194663	0.920074769
0.869776374	0.871381762	0.977611935	0.981270044	0.936996151	0.939370853	1.005534665	1.006560762	0.98014889	0.983701377	0.800832088	0.798343319	0.935105682	0.936181834	0.916732886
0.866986477	0.869466967	0.978274605	0.980966453	0.93734411	0.938417956	1.008499788	1.00666901	0.981888251	0.983436737	0.796926353	0.795530346	0.93489023	0.935181243	0.92061909
0.865920822	0.867579015	0.983371792	0.980666149	0.934005501	0.937476486	1.006253863	1.006776159	0.979724694	0.983174944	0.787321979	0.792763536	0.931264728	0.934192741	0.918410405
0.862428865	0.865717529	0.975771033	0.980369094	0.943588719	0.936546305	1.008142976	1.006882221	0.979553162	0.982915968	0.788665072	0.79004213	0.933030785	0.933216182	0.91242298
0.861480909	0.863882138	0.97675942	0.980075255	0.947373461	0.935627277	1.008063232	1.006987207	0.983922917	0.982659777	0.785113686	0.787365382	0.929616638	0.932251423	0.912451729
0.860254398	0.862072476	0.979284729	0.979784597	0.943285053	0.93471927	1.00875225	1.007091127	0.985556974	0.982406342	0.780715188	0.784732562	0.930324238	0.93129832	0.908044861
0.85641104	0.860288183	0.984522364	0.979497084	0.941318587	0.93382215	1.005722357	1.007193994	0.985654112	0.982155633	0.772469363	0.782142946	0.928018656	0.930356733	0.907469351
0.855657658	0.858528903	0.977221143	0.979212683	0.935655371	0.932935788	1.007827601	1.007295816	0.982881089	0.981907622	0.771947932	0.779595827	0.925223764	0.929426522	0.907685764
0.853640654	0.856794284	0.979198791	0.978931361	0.941372022	0.932060054	1.00836224	1.007396606	0.982905908	0.981662278	0.765957546	0.777090507	0.932031364	0.928507551	0.906573252
0.851707629	0.855083983	0.97722296	0.978653083	0.932127028	0.931194822	1.006273247	1.007496373	0.979432954	0.981419574	0.767336473	0.7746263	0.922197453	0.927599683	0.902549351
0.851223789	0.853397657	0.976613521	0.978377817	0.931239591	0.930339964	1.005750796	1.007595128	0.983842432	0.981179481	0.758367568	0.772202532	0.922881941	0.926702783	0.901994952
0.849060244	0.85173497	0.975034673	0.978105531	0.974636149	0.929495357	1.007174798	1.007692881	0.980877788	0.98094197	0.759006936	0.769818538	0.926614487	0.925816721	0.905678003
0.845666158	0.850095592	0.976747576	0.977836192	0.969931493	0.928660877	1.007297837	1.007789642	0.974441355	0.980707015	0.75668641	0.767473667	0.924415529	0.924941364	0.899881743
0.843545556	0.848479195	0.975949639	0.977569768	0.970535553	0.927836404	1.006762733	1.007885421	0.987259138	0.980474587	0.753475526	0.765167275	0.919925066	0.924076584	0.896856205

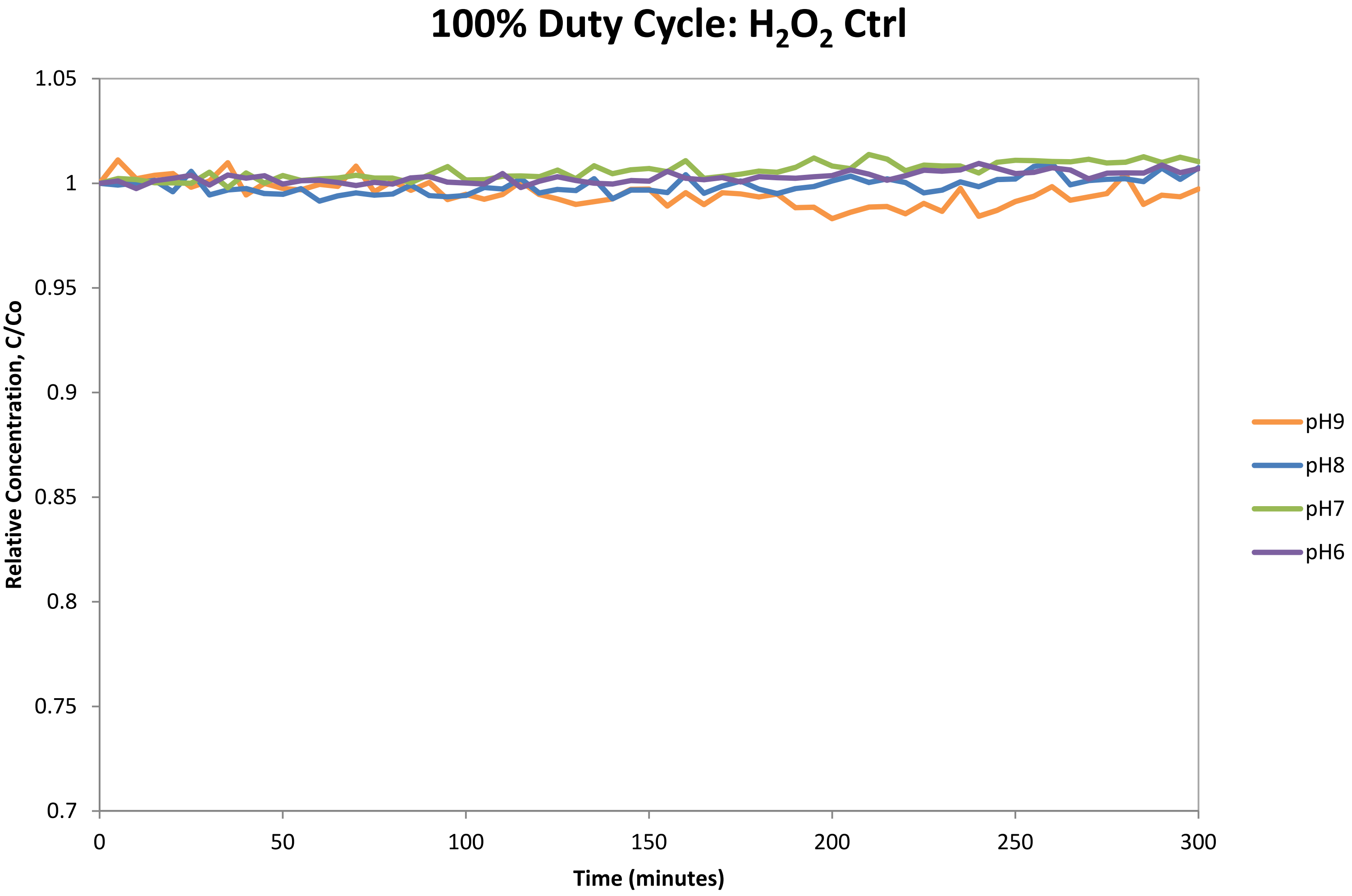
n-15	26-Jun-15		3-Jun-15		22-Jun-15		29-Jun-15		2-Jul-15		13-Jul-15		1-Jul-15	
6	pH6		pH7		pH9		pH6		pH8		pH7		pH9	
0	100		30		20		5		30		70		100	
1.5268E-03	1.2235E-03	1.2235E-03	4.2257E-04	1.4086E-03	5.9627E-05	2.9814E-04	9.6902E-05	1.9380E-03	1.8371E-04	6.1237E-04	5.1079E-04	7.2970E-04	2.4222E-04	2.4222E-04
0.9926	0.9988	0.9975	0.9948	0.9896	0.8901	0.7922	0.9293	0.8636	0.9761	0.9528	0.9957	0.9914	0.9832	0.9667
Model	C/C0	Model	C/C0	Model	C/C0	Model	C/C0	Model	C/C0	Model	C/C0	Model	C/C0	Model
1	1	1	1	1	1	1	1	1	1	1	1	1	1	1
0.997724185	0.99228707	0.993932541	1.005650807	0.997900289	1.011995806	0.999703449	0.997820953	0.99951811	0.992882062	0.999086617	0.999361021	0.997462491	0.999495752	0.998795868
0.995477008	0.989339249	0.987964321	0.999545502	0.995826633	1.002378692	0.999410045	0.994800583	0.999041424	0.997619785	0.998183489	0.996532431	0.994957574	1.008559141	0.997605605
0.99325811	0.981991732	0.982093716	0.998239116	0.993778708	1.003381845	0.999119756	0.995992794	0.998569885	0.996954798	0.997290502	0.996392757	0.99248483	1.007825919	0.996429051
0.991067134	0.976111047	0.976319129	0.993694924	0.991756196	1.002571405	0.998832549	0.994727876	0.998103439	0.998682918	0.996407542	0.994194503	0.990043847	1.00660386	0.995266048
0.988903729	0.969764647	0.970638991	0.998833932	0.989758779	1.003255996	0.99854839	0.994709776	0.997642031	0.993066093	0.995534497	0.989676042	0.987634217	1.002252542	0.99411644
0.986767547	0.968657644	0.965051756	0.989826513	0.987786149	1.00405697	0.998267247	0.996286954	0.997185605	0.99782787	0.994671254	0.991781653	0.985255536	0.99951808	0.992980074
0.984658247	0.958861818	0.959555905	0.988822669	0.985837995	0.998271607	0.997989089	0.994612397	0.996734108	0.992616696	0.993817705	0.989623104	0.982907407	0.999173764	0.991856795
0.982575491	0.960411902	0.954149943	0.984681051	0.983914016	1.010776239	0.997713883	0.99407939	0.996287487	0.995569466	0.992973739	0.980416211	0.980589439	0.999668355	0.990746454
0.980518943	0.954076869	0.9488324	0.982603936	0.982013911	1.001874036	0.997441599	0.995276051	0.995845689	0.990183498	0.99213925	0.982270146	0.978301242	0.995250668	0.989648902
0.978488275	0.943420506	0.94360183	0.981104035	0.980137384	1.002169163	0.997172205	0.992811844	0.995408662	0.988202583	0.991314131	0.972866594	0.976042436	0.992284629	0.988563991
0.97648316	0.941821469	0.93845681	0.980197289	0.978284141	1.004165143	0.99690567	0.992831765	0.994976355	0.989620885	0.990498276	0.973518807	0.973812642	0.998084171	0.987491576
0.974503277	0.93221129	0.933395942	0.976080803	0.976453895	0.999310973	0.996641965	0.989982592	0.994548716	0.992689244	0.989691583	0.973092019	0.971611488	0.993465456	0.986431512
0.972548309	0.931860434	0.928417848	0.97766509	0.97464636	0.997304865	0.996381058	0.991005325	0.994125695	0.991597694	0.988893947	0.967471042	0.969438606	0.991861135	0.985383658
0.970617942	0.924254088	0.923521175	0.971903006	0.972861254	0.999302632	0.996122922	0.993731334	0.993707243	0.985832311	0.988105268	0.967346352	0.967293633	0.98876674	0.984347873
0.968711866	0.9197844	0.918704592	0.97244189	0.971098299	1.000541265	0.995867525	0.991038999	0.99329331	0.985500875	0.987325444	0.963607747	0.965176211	0.996351562	0.983324018
0.966829777	0.914772825	0.913966787	0.970780256	0.96935722	1.001567324	0.995614839	0.988348281	0.992883847	0.986239757	0.986554377	0.967297023	0.963085985	0.993621758	0.982311955
0.964971371	0.914572622	0.909306474	0.97333563	0.967637745	0.997573776	0.995364836	0.991626206	0.992478806	0.982797307	0.985791967	0.959615606	0.961022606	0.987376118	0.981311549
0.963136351	0.906508837	0.904722383	0.968188995	0.965939607	0.99436432	0.995117486	0.99475528	0.992078138	0.984074876	0.985038119	0.956581278	0.95898573	0.98374405	0.980322666
0.961324422	0.903139372	0.90021327	0.96681328	0.96426254	0.995446187	0.994872762	0.990164609	0.991681798	0.981990432	0.984292734	0.955883017	0.956975016	0.981027191	0.979345172
0.959535295	0.895802424	0.895777906	0.966246723	0.962606283	0.995298425	0.994630636	0.990630673	0.991289738	0.982908149	0.98355572	0.953436151	0.954990128	0.980554313	0.978378936
0.957768682	0.892222086	0.891415087	0.962517165	0.960970578	0.997495393	0.994391079	0.989044698	0.990901912	0.981757972	0.98282698	0.957819641	0.953030734	0.980340956	0.97742383
0.956024299	0.881471305	0.887123625	0.956224409	0.95935517	0.994511817	0.994154066	0.993086387	0.990518274	0.979518618	0.982106424	0.953347228	0.951096507	0.977670878	0.976479724
0.954301868	0.88839299	0.882902354	0.961175087	0.957759808	0.994963775	0.993919568	0.989705926	0.990138779	0.979302194	0.981393958	0.945057896	0.949187123	0.980947807	0.975546492
0.952601111	0.876863228	0.878750125	0.961208529	0.956184241	0.996934731	0.99368756	0.99338631	0.989763383	0.978542145	0.980689492	0.949759016	0.947302264	0.97453162	0.974624008
0.950921757	0.875104267	0.874665809	0.953076272	0.954628225	0.994011332	0.993458014	0.987134834	0.98939204	0.979949414	0.979992937	0.943599576	0.945441615	0.975766282	0.97371215
0.949263535	0.873873133	0.870648296	0.951989409	0.953091518	0.994696056	0.993230905	0.987224629	0.989024707	0.983256519	0.979304202	0.940778861	0.943604864	0.972780997	0.972810794
0.94762618	0.871994928	0.866696493	0.95117145	0.951573878	1.001520188	0.993006207	0.98768048	0.988661342	0.976411773	0.978623201	0.942774111	0.941791704	0.97395785	0.97191982
0.94600943	0.870302667	0.862809324	0.94840457	0.950075071	0.993854236	0.992783893	0.989993816	0.9883019	0.983225665	0.977949846	0.934795846	0.940001833	0.975156211	0.971039108
0.944413024	0.862069388	0.858985734	0.953695338	0.948594862	0.997462093	0.99256394	0.98805038	0.987946341	0.979676222	0.977284053	0.942540263	0.938234952	0.973222231	0.970168539
0.942836707	0.860171839	0.855224681	0.947867348	0.94713302	0.992012837	0.992346321	0.985625812	0.987594621	0.980888427	0.976625735	0.935201087	0.936490765	0.968466803	0.969307998
0.941280226	0.850961071	0.851525144	0.944602066	0.945689318	1.000002714	0.992131013	0.984812701	0.987246699	0.980963155	0.975974809	0.932963349	0.93476898	0.977934988	0.968457367
0.939743332	0.847224997	0.847886115	0.949591955	0.94426353	0.994131621	0.99191799	0.984476273	0.986902534	0.976947188	0.975331192	0.932334761	0.933069311	0.967426662	0.967616535
0.938225778	0.849813987	0.844306606	0.941685479	0.942855434	0.99101008	0.991707228	0.983859639	0.986562087	0.979468329	0.974694802	0.939266181	0.931391472	0.965883985	0.966785386
0.936727321	0.845176399	0.840785643	0.944092125	0.941464811	0.994101433	0.991498703	0.982539814	0.986225315	0.978859981	0.974065557	0.930575655	0.929735184	0.966772276	0.965963811
0.93524772	0.83790326	0.837322268	0.939695782	0.940091443	0.996246565	0.991292392	0.990097364	0.985892181	0.975497584	0.973443378	0.926929255	0.928100169	0.973374492	0.965151698
0.933786738	0.841862668	0.83391554	0.93546215	0.938735118	0.991517516	0.99108827	0.982504119	0.985562644	0.972201319	0.972828185	0.926025913	0.926486155	0.96675755	0.964348939
0.932344141	0.832653993	0.830564531	0.942526808	0.937395622	0.989867572	0.990886316	0.98319912	0.985236666	0.971997788	0.9722199	0.923948412	0.924892871	0.962698974	0.963555426
0.930919697	0.829966099	0.827268331	0.934951623	0.936072748	0.989757346	0.990686505	0.984873778	0.984914209	0.968543086	0.971618445	0.919901911	0.923320052	0.962637604	0.962771053
0.929513178	0.829325806	0.824026043	0.931998466	0.934766289	0.985778296	0.990488815	0.983986041	0.984595233	0.968588693	0.971023743	0.921585985	0.921767435	0.969491122	0.961995713
0.928124359	0.825120031	0.820836786	0.931946543	0.933476041	0.984174694	0.990293223	0.981615977	0.984279703	0.97484921	0.970435719	0.91754539	0.92023476	0.959837799	0.961229304
0.926753016	0.817308595	0.817699691	0.935337868	0.932201804	0.990413935	0.990099708	0.986774339	0.983967579	0.970215401	0.969854297	0.922427529	0.91872177	0.959916703	0.960471722
0.92539893	0.817054253	0.814613906	0.929462745	0.930943378	0.986312941	0.989908247	0.98384336	0.983658827	0.96598038	0.969279404	0.917501312	0.917228214	0.962808015	0.959722866
0.924061884	0.810758702	0.811578592	0.929098209	0.929700567	0.987081674	0.989718818	0.984902496	0.983353409	0.965757734	0.968710967	0.912942163	0.915753841	0.955465728	0.958982635
0.922741663	0.808694849	0.808592923	0.926961348	0.928473178	0.986655005	0.9895314	0.982957948	0.983051289	0.965835221	0.968148911	0.9117143	0.914298406	0.956809295	0.958250929
0.921438055	0.810327785	0.805656087	0.924262427	0.92726102	0.986958539	0.989345971	0.984587202	0.982752431	0.966744471	0.967593167	0.914090837	0.912861664	0.961996848	0.957527652
0.920150852	0.801799485	0.802767286	0.925776701	0.926063902	0.991743926	0.989162511	0.985372606	0.982456802	0.96364853	0.967043663	0.907437452	0.911443376	0.956732445	0.956812704
0.918879847	0.798563622	0.799925733	0.927507175	0.924881639	0.991362207	0.988980998	0.982115613	0.982164364	0.965170746	0.966500329	0.916674424	0.910043305	0.949632282	0.956105991
0.917624836	0.798285301	0.797130656	0.92834557	0.923714047	0.986278781	0.988801411	0.983798563	0.981875085	0.966259858	0.965963096	0.906830193	0.908661217	0.954009696	0.955407418
0.916385618	0.79274201	0.794381295	0.926759523	0.922560943	0.984874908	0.988623731	0.980215052	0.98158893	0.963334991	0.965431896	0.905240512	0.90729688	0.952356676	0.954716891
0.915161994	0.788021967	0.791676902	0.920840593	0.921422147	0.986484866	0.988447937	0.978058049	0.981305865	0.966729718	0.964906659	0.905525	0.905950067	0.947357685	0.954034318
0.913953767	0.78457932	0.789016742	0.921531629	0.920297482	0.98434364	0.988274009	0.979363617	0.981025857	0.967100345	0.964387321	0.901348779	0.904620553	0.948644539	0.953359605
0.912760745	0.781086772	0.786400091	0.91432235	0.919186773	0.99419385	0.988101928	0.979740999	0.980748873	0.961598468	0.963873814	0.903015134	0.903308116	0.95210188	0.952692665
0.911582736	0.779256772	0.783826237	0.912041356	0.918089846	0.98237189	0.987931673	0.979723404	0.98047488	0.962425677	0.963366072	0.905543813	0.902012535	0.946361997	0.952033405
0.910419551	0.777194713	0.781294481	0.913985779	0.917006531	0.983825811	0.987763225	0.984277673	0.980203846	0.962784181	0.962864032	0.900106588	0.900733596	0.949427145	0.951381739
0.909271003	0.774451334	0.778804134	0.91051349	0.915936658	0.988260726	0.987596565	0.980637736	0.979935738	0.959555589	0.962367629	0.904947491	0.899471083	0.944739593	0.950737579
0.908136908	0.770965116	0.776354518	0.916148065	0.914880061	0.986828519	0.987431674	0.980717824	0.979670527	0.961517774	0.9618768	0.896264294	0.898224786	0.942303968	0.950100838
0.907017085	0.768712276	0.773944969	0.908911796	0.913836574	0.989328823	0.987268534	0.985075716	0.979408179	0.961464854	0.961391482	0.901040993	0.896994497	0.951476467	0.94947143
0.905911353	0.764013968	0.771574829	0.915293926	0.912806036	0.978677308	0.987107125	0.980604771	0.979148664	0.960357526	0.960911614	0.895985384	0.89578001	0.941490061	0.948849272
0.904819535	0.767097086	0.769243455	0.906145894	0.911788286	0.986291094	0.98694743	0.980685667	0.978891952	0.963495994	0.960437133	0.892459625	0.894581122	0.943296985	0.94823428
0.903741457	0.759384805	0.766950212	0.912106675	0.910783165	0.983669045	0.986789429	0.981317671	0.978638013	0.9610025	0.959967981	0.892068604	0.893397633	0.939009025	0.947626371

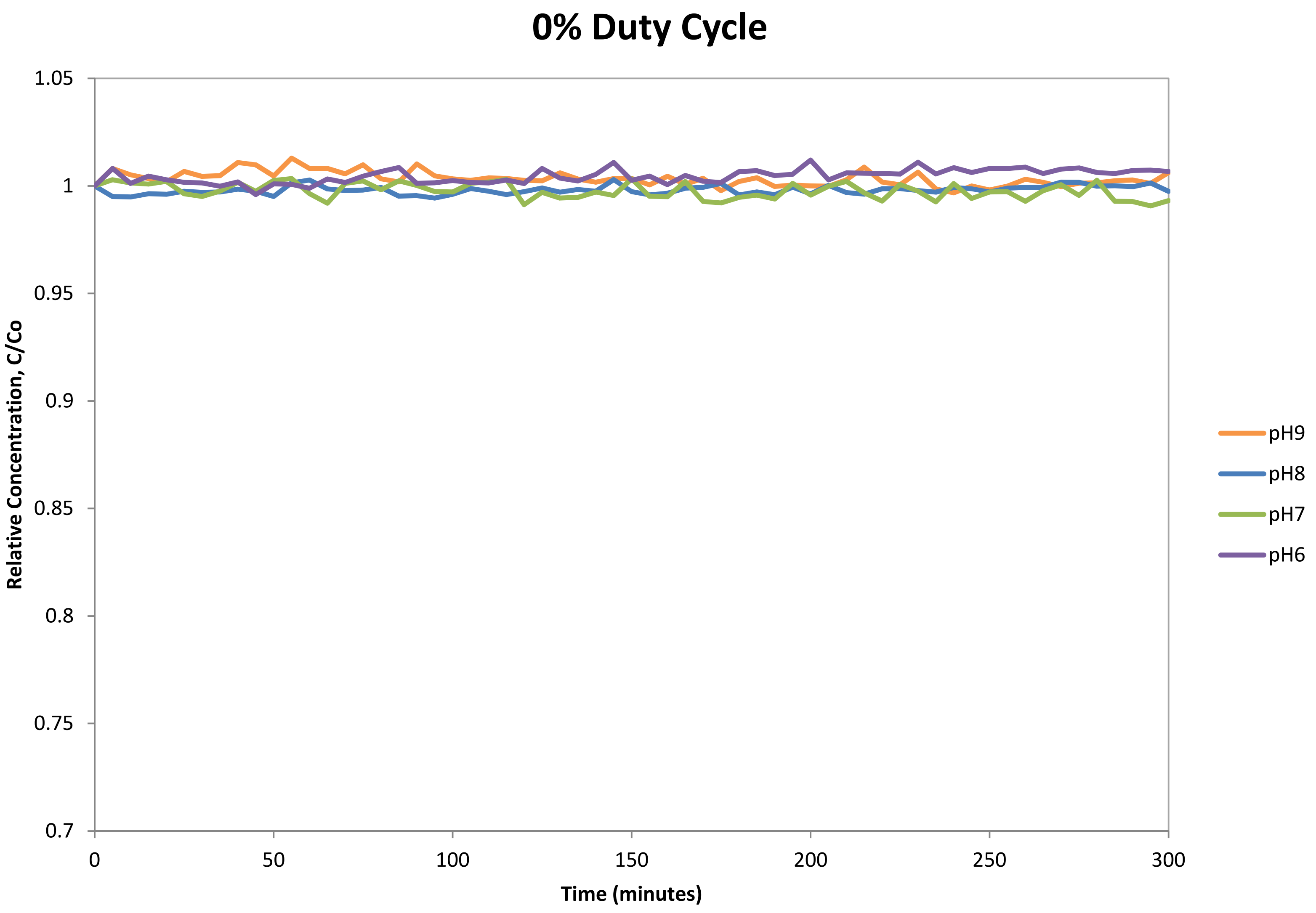
6-Jul-15		10-Jul-15		14-Jul-15		15-Jul-15		17-Jul-15		23-Jul-15		21-Jul-15		30-Ju
pH8		pH8		pH7**		pH8		pH6**		pH9		pH8		pH
100		20		100		0		100		70		5		10
4.7230E-04	**4.7230E-04**	**1.4060E-04**	**7.0298E-04**	**-4.7812E-05**	**0.0000E+00**	**9.8817E-06**	**0.0000E+00**	**-2.4032E-05**	**0.0000E+00**	0.000262708	**3.7530E-04**	-3.79936E-06	**-7.5987E-05**	0.001024644
0.9977	**0.9953**	**0.9787**	**0.9579**	**0.8340**	**0.6956**	**0.3427**	**0.1175**	**0.6713**	**0.4507**	**0.9944**	**0.9889**	**0.3542**	**0.1255**	**0.9993**
C/C0	**Model**	**C/C0**	**Model**	**C/C0**	**Model**	**C/C0**	**Model**	**C/C0**	**Model**	**C/C0**	**Model**	**C/C0**	**Model**	**C/C0**
1	1	1	1	1	1	1	1	1	1	1	1	1	1	1
0.997170663	0.99765345	1.000551918	0.999300895	1.002222037	1.000237852	0.995018068	0.999950848	1.001128948	1.000119547	1.001339935	0.998694104	0.999104594	1.000018899	0.995171525
0.996834668	0.995336594	1.001638722	0.998609491	1.001774452	1.000473306	0.994845137	0.999902205	0.997509661	1.000237874	0.997734395	0.997403382	0.999103452	1.000037603	0.989223724
0.992852232	0.993049055	0.998907635	0.997925703	1.000272237	1.000706386	0.996354253	0.999854067	1.001205212	1.000354994	1.000374472	0.996127656	0.998835992	1.000056114	0.983907632
0.990703158	0.990790464	0.997010796	0.997249447	1.000189694	1.000937115	0.996104346	0.999806428	1.002422797	1.000470919	0.997491141	0.994866753	0.999762094	1.000074435	0.980472444
0.989869775	0.988560454	1.000369683	0.99658064	0.999960053	1.001165518	0.997531113	0.999759283	1.003816134	1.000585662	0.997316592	0.9936205	0.999977432	1.000092567	0.974903496
0.988245176	0.986358662	0.999264922	0.995919201	1.005260456	1.001391618	0.997050272	0.999712627	0.999173775	1.000699234	0.993707719	0.992388728	0.996095436	1.000110512	0.971468523
0.987879358	0.984184733	0.996952407	0.995265047	0.997933778	1.001615439	0.997165679	0.999666455	1.004002838	1.000811648	0.990756977	0.991171267	0.999955401	1.000128273	0.963968594
0.982579763	0.982038313	0.993390431	0.994618099	1.004949816	1.001837002	0.998475012	0.999620761	1.002475432	1.000922915	0.996156308	0.989967952	0.999091093	1.00014585	0.959483218
0.983073748	0.979919054	0.991554646	0.993978278	1.00011609	1.002056331	0.997538035	0.999575541	1.003601337	1.001033047	0.99063154	0.988778619	0.999703725	1.000163247	0.956576894
0.98211807	0.977826612	0.994834754	0.993345504	1.003709134	1.002273449	0.995084065	0.99953079	0.999613205	1.001142056	0.988637691	0.987603104	1.000657433	1.000180464	0.950910378
0.980227264	0.975760649	0.988451327	0.9927197	1.001385022	1.002488377	1.001432258	0.999486503	1.001200142	1.001249953	0.987700729	0.986441247	0.99793434	1.000197503	0.947330025
0.977867826	0.973720829	0.991525683	0.99210079	1.002113783	1.002701139	1.002737652	0.999442675	1.001432077	1.001356749	0.988893257	0.98529289	1.000455931	1.000214368	0.942213911
0.977532965	0.971706822	0.995641661	0.991488698	1.002466687	1.002911755	0.998605694	0.999399302	1.000377973	1.001462455	0.987339386	0.984157876	1.000005306	1.000231058	0.938269998
0.971922328	0.9697183	0.990693289	0.990883347	1.003837804	1.003120247	0.997832578	0.999356378	0.998918311	1.001567084	0.982485675	0.983036049	1.00119336	1.000247577	0.933414062
0.969263389	0.967754941	0.989666264	0.990284665	1.00255883	1.003326637	0.998020307	0.999313899	1.000478373	1.001670645	0.984527685	0.981927257	0.998648193	1.000263925	0.928180352
0.969644353	0.965816427	0.988206069	0.989692578	1.002484454	1.003530946	0.999323912	0.999271861	0.999620405	1.001773149	0.986072373	0.980831348	1.001623902	1.000280106	0.923978845
0.967848421	0.963902444	0.990695374	0.989107012	1.000299935	1.003733195	0.995247091	0.999230259	1.002622787	1.001874608	0.983087075	0.979748172	0.997682463	1.000296119	0.921158888
0.963362459	0.96201268	0.989531992	0.988527897	1.00410331	1.003933405	0.995465731	0.999189088	1.003213933	1.001975032	0.983041771	0.978677581	0.99929011	1.000311967	0.916231769
0.964179963	0.96014683	0.987132357	0.987955161	1.008007435	1.004131596	0.994357852	0.999148344	1.000552507	1.002074432	0.9790555	0.97761943	0.997339305	1.000327653	0.912102199
0.963520649	0.958304591	0.988684769	0.987388734	1.001557832	1.004327788	0.996126185	0.999108023	1.000150399	1.002172817	0.977097772	0.976573573	0.999081891	1.000343176	0.910350736
0.957991209	0.956485664	0.987715438	0.986828546	1.001706696	1.004522002	0.998802494	0.999068119	0.999609757	1.002270199	0.975345611	0.975539868	1.004031174	1.00035854	0.904151912
0.958485193	0.954689754	0.987041297	0.986274528	1.003329746	1.004714258	0.997549134	0.999028629	1.004694993	1.002366588	0.979074819	0.974518174	1.002246004	1.000373745	0.900510499
0.957009444	0.952916569	0.987147996	0.985726614	1.003489093	1.004904576	0.995973186	0.998989549	0.997991989	1.002461993	0.973789768	0.97350835	1.00134368	1.000388794	0.897515761
0.955731048	0.951165824	0.983133273	0.985184735	1.003181544	1.005092974	0.997347083	0.998950874	1.00095989	1.002556425	0.975341258	0.97251026	1.001941871	1.000403688	0.892534475
0.953139829	0.949437232	0.983578607	0.984648825	1.00633881	1.005279473	0.999024952	0.9989126	1.003165457	1.002649894	0.972214538	0.971523767	1.000667239	1.000418428	0.889591212
0.950305355	0.947730514	0.983760147	0.984118818	1.002183304	1.005464091	0.997111257	0.998874723	1.001346788	1.002742409	0.975260921	0.970548735	0.998593653	1.000433017	0.886207608
0.947419573	0.946045394	0.981473813	0.983594649	1.008418384	1.005646847	0.99838598	0.998837238	1.000037726	1.002833981	0.969935396	0.969585033	0.999515321	1.000447455	0.883202639
0.94397936	0.944381597	0.980006553	0.983076254	1.004565021	1.005827761	0.99756083	0.998800143	0.99963227	1.002924618	0.971204518	0.968632527	0.998296169	1.000461745	0.879258942
0.944733881	0.942738855	0.980025321	0.982563569	1.006480502	1.006006851	1.002946505	0.998763432	1.001261903	1.003014331	0.965636964	0.967691089	0.998878845	1.000475887	0.877190011
0.945012765	0.9411169	0.979531329	0.982056532	1.007047378	1.006184135	0.997330017	0.998727101	1.001030677	1.003103129	0.967164033	0.966760589	0.999545144	1.000489884	0.874791657
0.943507859	0.93951547	0.982213874	0.98155508	1.005586875	1.006359631	0.995834387	0.998691147	1.005692711	1.003191021	0.967672376	0.965840901	0.999269086	1.000503736	0.870658534
0.940169992	0.937934304	0.981196349	0.981059152	1.010767216	1.006533358	0.996591749	0.998655566	1.002404542	1.003278016	0.965105833	0.964931898	0.99996467	1.000517446	0.867608659
0.939380644	0.936373147	0.979484293	0.980568686	1.002378847	1.006705333	0.998929596	0.998620354	1.001668272	1.003364124	0.965085834	0.964033457	0.998820141	1.000531014	0.866451643
0.934629343	0.934831746	0.979201268	0.980083623	1.00335325	1.006875574	0.999338949	0.998585507	1.002759189	1.003449354	0.962757103	0.963145455	0.99974416	1.000544443	0.863354546
0.936299311	0.933309849	0.97839158	0.979603903	1.004389782	1.007044098	1.001156094	0.998551022	1.000642462	1.003533714	0.960999365	0.962267771	0.998626162	1.000557734	0.860635709
0.933900909	0.931807211	0.981726833	0.979129468	1.005808681	1.007210923	0.995786649	0.998516894	1.003179959	1.003617213	0.961477573	0.961400285	0.996483259	1.000570887	0.857079316
0.929401804	0.930323588	0.979666296	0.978660258	1.00527734	1.007376066	0.997216997	0.998483119	1.002687996	1.003699861	0.964051054	0.960542878	1.00394473	1.000583905	0.854364356
0.928813012	0.928858738	0.981719883	0.978196217	1.007642061	1.007539544	0.995887854	0.998449695	1.002375842	1.003781666	0.958494043	0.959695433	0.998625826	1.000596789	0.851301235
0.926111908	0.927412425	0.976669097	0.977737288	1.012137119	1.007701373	0.999418791	0.998416618	1.003136148	1.003862636	0.959300263	0.958857834	1.004272842	1.00060954	0.850826863
0.925286598	0.925984415	0.981548306	0.977283414	1.008230566	1.007861571	0.99629482	0.998383883	1.003728917	1.00394278	0.956666648	0.958029967	1.002632887	1.00062216	0.84710802
0.923272429	0.924574474	0.97429634	0.976834539	1.007008202	1.008020153	1.000227233	0.998351488	1.006410626	1.004022107	0.956551552	0.95721172	0.998474767	1.00063465	0.845327536
0.922314083	0.923182375	0.974607286	0.976390609	1.01373214	1.008177136	0.996922573	0.998319429	1.004358195	1.004100625	0.958492615	0.956402979	0.999145096	1.000647011	0.84144409
0.91824171	0.921807893	0.97585385	0.975951569	1.011527648	1.008332537	0.996187409	0.998287702	1.001513513	1.004178341	0.954323904	0.955603636	1.000865718	1.000659245	0.841266456
0.920474783	0.920450803	0.974028723	0.975517365	1.005996721	1.00848637	0.998674437	0.998256305	1.003664721	1.004255265	0.954212617	0.95481358	0.99936218	1.000671353	0.838106254
0.916709717	0.919110886	0.975635585	0.975087944	1.00866502	1.008638653	0.998754279	0.998225232	1.006268746	1.004331404	0.955633773	0.954032703	1.000191494	1.000683336	0.835408416
0.916033724	0.917787924	0.975475826	0.974663253	1.008265437	1.0087894	0.997857402	0.998194482	1.00580163	1.004406767	0.950190362	0.9532609	0.997788184	1.000695196	0.83296241
0.914647911	0.916481704	0.972593437	0.97424324	1.008280776	1.008938626	0.99707629	0.998164051	1.006375131	1.00448136	0.951903477	0.952498064	1.000361427	1.000706934	0.829660218
0.912766779	0.915192013	0.971674038	0.973827854	1.004940105	1.009086349	0.999282857	0.998133935	1.009500528	1.004555193	0.950421508	0.951744091	1.002119327	1.00071855	0.829640242
0.910995332	0.913918642	0.974905604	0.973417043	1.010050704	1.009232581	0.998671214	0.998104132	1.007115863	1.004628273	0.949928266	0.950998879	1.005520742	1.000730047	0.82699038
0.911851132	0.912661385	0.972946784	0.973010758	1.010976663	1.009377339	0.997161382	0.998074638	1.004673088	1.004700607	0.946856441	0.950262325	0.998357426	1.000741426	0.824872989
0.909748294	0.911420037	0.974839685	0.972608948	1.010819412	1.009520638	0.998951794	0.998045449	1.005202473	1.004772203	0.94394835	0.949534329	0.996930727	1.000752687	0.821742239
0.909439787	0.910194397	0.97117576	0.972211564	1.010400518	1.009662492	0.99930589	0.998016563	1.007437044	1.004843069	0.94704548	0.948814792	1.001184695	1.000763832	0.820487387
0.90592138	0.908984267	0.972031324	0.971818557	1.010216231	1.009802915	0.999339068	0.997987977	1.006387807	1.004913212	0.949304283	0.948103615	1.00083865	1.000774863	0.817009231
0.904519955	0.90778945	0.972737092	0.97142988	1.011488362	1.009941922	1.001735274	0.997959687	1.002138937	1.004982639	0.948352968	0.947400702	1.001390496	1.00078578	0.816062586
0.903545796	0.906609753	0.969329316	0.971045483	1.009671205	1.010079528	1.001660804	0.99793169	1.004826832	1.005051359	0.945616637	0.946705955	1.002791671	1.000796584	0.814899916
0.902338789	0.905444983	0.97059766	0.970665321	1.010016385	1.010215746	0.999829934	0.997903984	1.004963539	1.005119377	0.941723424	0.946019281	1.004381854	1.000807277	0.810993802
0.906141351	0.904294954	0.96871507	0.970289347	1.012635577	1.010350591	1.00005108	0.997876564	1.004854417	1.005186701	0.944165891	0.945340585	1.002007158	1.00081786	0.808357832
0.899784732	0.903159476	0.973866646	0.969917514	1.009923579	1.010484076	0.99961022	0.99784943	1.008709189	1.005253339	0.945930432	0.944669774	1.005286395	1.000828334	0.808499928
0.899610197	0.902038368	0.968440502	0.969549777	1.012422047	1.010616215	1.001382611	0.997822576	1.005046801	1.005319297	0.941314396	0.944006758	1.00113976	1.000838701	0.803065861
0.896744564	0.900931446	0.971543125	0.969186091	1.010377123	1.010747022	0.997503425	0.997796001	1.007017795	1.005384582	0.94269705	0.943351446	1.001831113	1.00084896	0.802056326

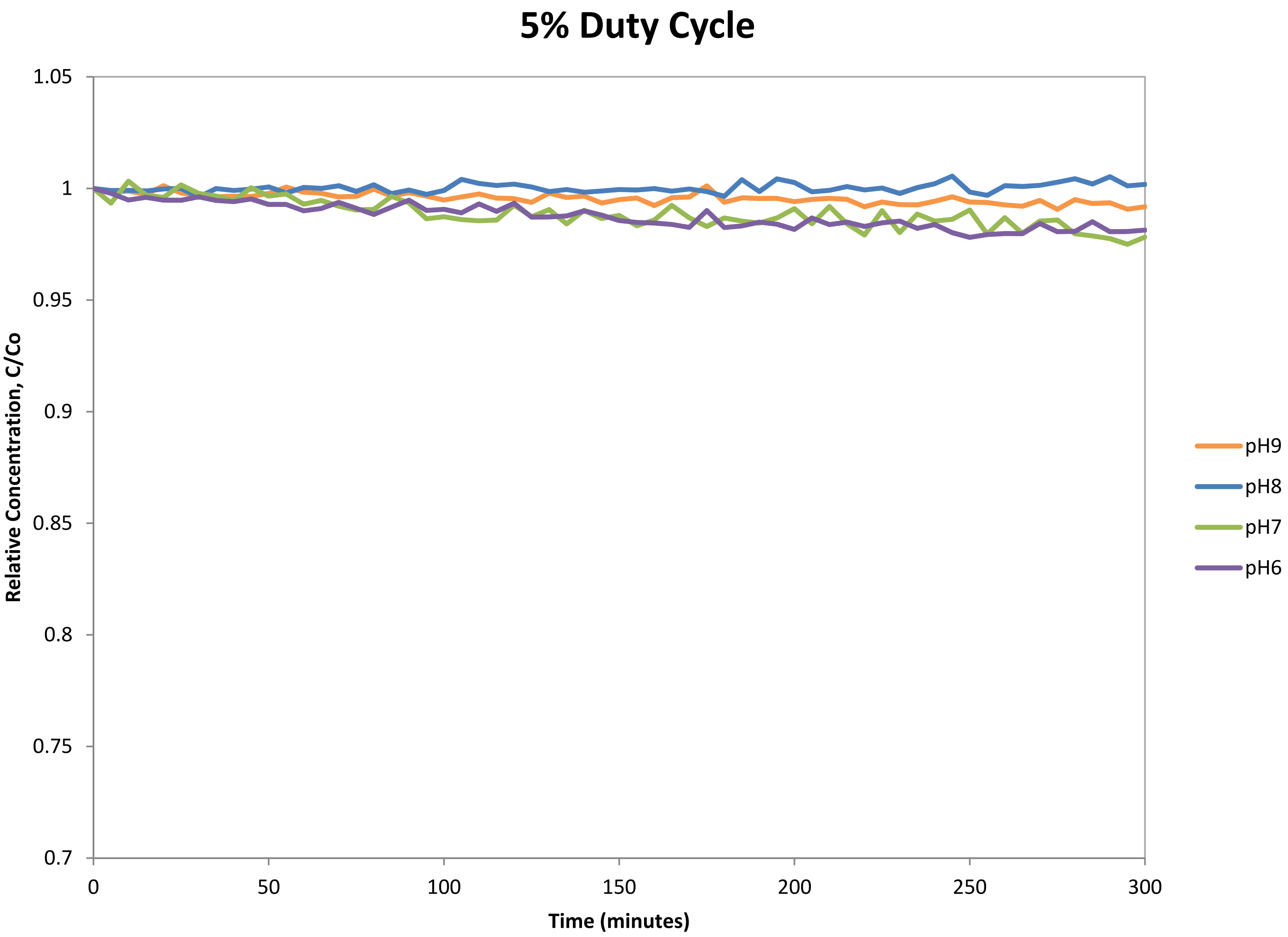
ul-15	6-Aug-15		11-Aug-15		7-Aug-15		28-Jul-15		5-Aug-15		4-Aug-15		Repeats	29-May-15	
H7	pH7		pH7		pH6		pH9		pH9		pH6			pH5	
0	20		50		10		5		30		50			70	
1.0246E-03	0.00022352	1.1176E-03	5.8957E-04	1.1791E-03	0.000139229	1.3923E-03	3.38367E-05	6.7673E-04	7.4676E-05	2.4892E-04	0.000640741	1.2815E-03		1.2624E-03	1.8034E-03
0.9987	0.9970	0.9941	0.9999	0.9997	0.9927	0.9855	0.7590	0.5760	0.9442	0.8915	0.9994	0.9988		0.9981	0.9961
Model	C/C0	Model	C/C0	Model	C/C0	Model	C/C0	Model	C/C0	Model	C/C0	Model		C/Co	Model
1	1	1	1	1	1	1	1	1	1	1	1	1		1	1
0.994916273	1.001846165	0.998888795	0.997407965	0.997071692	1.000511574	0.999307695	0.998287411	0.999831705	1.003779525	0.999628619	0.996130568	0.996817945		0.99398293	0.993740482
0.989910719	0.999030093	0.997790287	0.993678017	0.994182134	1.000371757	0.998623011	0.99881067	0.999665176	1.001268164	0.999261208	0.994472113	0.993678801		0.986527369	0.98758454
0.984982137	0.996789706	0.996704329	0.991569131	0.991330814	0.997908948	0.997945864	0.997413015	0.999500393	1.000677147	0.998897725	0.991065463	0.99058199		0.982251475	0.981530459
0.980129343	0.995047619	0.995630778	0.988730219	0.988517225	0.999804757	0.997276172	1.001231464	0.999337338	1.000534404	0.998538127	0.988826995	0.987526941		0.973998457	0.975576555
0.975351171	0.99489666	0.994569493	0.98671632	0.985740868	0.997114037	0.996613852	0.997960409	0.999175993	0.998644458	0.998182373	0.983396448	0.98451309		0.971163595	0.969721169
0.970646474	0.993238353	0.993520333	0.98326016	0.983001251	0.995879747	0.995958824	0.996952716	0.99901634	0.997088459	0.997830421	0.981734639	0.981539883		0.963744546	0.963962672
0.966014122	0.993902753	0.992483161	0.980834724	0.980297886	0.995431548	0.995311006	0.996301747	0.998858361	0.995983965	0.997482232	0.97974561	0.97860677		0.95910776	0.95829946
0.961453002	0.995487262	0.991457838	0.977677439	0.977630296	0.994456529	0.99467032	0.996521449	0.998702039	0.995552947	0.997137764	0.973975995	0.975713211		0.956458847	0.952729957
0.956962021	0.990955572	0.99044423	0.974601914	0.974998005	0.995314707	0.994036686	0.996388979	0.998547356	0.996632769	0.996796979	0.9750151	0.972858673		0.948232605	0.947252611
0.952540097	0.99093516	0.989442202	0.970765916	0.972400548	0.991864357	0.993410029	0.997793943	0.998394296	0.99593822	0.996459836	0.97022782	0.97004263		0.94490223	0.941865899
0.948186171	0.987822216	0.988451624	0.969359118	0.969837462	0.993689059	0.992790269	1.000637385	0.998242841	0.997146393	0.996126297	0.966224281	0.967264562		0.944917787	0.93656832
0.943899196	0.988647557	0.987472362	0.967518433	0.967308294	0.993621002	0.992177333	0.998292445	0.998092974	0.994390812	0.995796324	0.963051871	0.964523957		0.938179672	0.9313584
0.939678142	0.987341076	0.986504289	0.963880279	0.964812594	0.991404942	0.991571144	0.997858764	0.997944679	0.995648769	0.995469877	0.959621305	0.961820311		0.931547603	0.926234687
0.935521997	0.988584077	0.985547277	0.963241592	0.96234992	0.990090835	0.990971628	0.99617769	0.997797939	0.993821236	0.99514692	0.956327415	0.959153124		0.92494559	0.921195757
0.931429761	0.983174221	0.984601199	0.959111054	0.959919834	0.989342094	0.990378712	0.996454973	0.997652738	0.996231195	0.994827416	0.955285516	0.956521906		0.921483451	0.916240204
0.927400453	0.985191197	0.98366593	0.956197566	0.957521905	0.992093357	0.989792323	0.999681411	0.99750906	0.994244325	0.994511326	0.951297847	0.95392617		0.921551821	0.911366651
0.923433104	0.984322902	0.982741346	0.955375632	0.955155709	0.989361585	0.98921239	0.996579788	0.997366888	0.995904737	0.994198616	0.948717295	0.951365439		0.91135707	0.906573741
0.919526762	0.98218065	0.981827327	0.952671277	0.952820823	0.990287058	0.98863884	0.998125014	0.997226208	0.994307472	0.993889248	0.94941141	0.94883924		0.910991627	0.901860137
0.915680489	0.98138974	0.98092375	0.950535936	0.950516836	0.987162731	0.988071605	0.996564479	0.997087003	0.993704267	0.993583186	0.945908873	0.946347109		0.90438845	0.89722453
0.91189336	0.98138189	0.980030496	0.947267128	0.948243337	0.989264454	0.987510614	0.994805619	0.996949258	0.996084854	0.993280397	0.942098561	0.943888584		0.8958319	0.892665627
0.908164467	0.979443758	0.979147449	0.94479665	0.945999923	0.987274345	0.986955799	0.99618962	0.996812957	0.99168619	0.992980844	0.941578785	0.941463214		0.896243488	0.88818216
0.904492914	0.978744253	0.97827449	0.944555588	0.943786196	0.987480587	0.986407091	0.997523074	0.996678086	0.996358151	0.992684493	0.937923031	0.939070551		0.88794369	0.883772881
0.900877819	0.977040524	0.977411506	0.940961338	0.941601763	0.986068258	0.985864424	0.995631882	0.996544629	0.989217636	0.99239131	0.936595149	0.936710154		0.8862966	0.879436561
0.897318314	0.977223447	0.976558381	0.939227157	0.939446237	0.985351967	0.985327731	0.995409766	0.996412572	0.989446362	0.992101261	0.931652303	0.934381587		0.882268252	0.875171994
0.893813545	0.976569926	0.975715003	0.936234759	0.937319235	0.983797971	0.984796946	0.993785445	0.996281899	0.993146219	0.991814312	0.931284292	0.932084423		0.878881044	0.870977993
0.890362669	0.975231818	0.974881261	0.935286251	0.935220379	0.984171687	0.984272005	0.997919517	0.996152597	0.990943839	0.99153043	0.930748088	0.929818236		0.875514685	0.866853389
0.886964858	0.972439186	0.974057045	0.932712461	0.933149297	0.985870184	0.983752842	0.995945023	0.996024651	0.991742582	0.991249583	0.925509984	0.92758261		0.869682719	0.862797035
0.883619295	0.974319221	0.973242246	0.931228008	0.931105622	0.983361205	0.983239394	0.996583305	0.995898047	0.99296757	0.990971738	0.925039045	0.925377132		0.864138196	0.8588078
0.880325178	0.973189383	0.972436756	0.930152355	0.929088991	0.982621067	0.982731599	0.993477544	0.995772771	0.990284829	0.990696863	0.922908421	0.923201396		0.857506761	0.854884575
0.877081716	0.971042981	0.971640469	0.927610494	0.927099046	0.98076348	0.982229394	0.994977326	0.995648808	0.994027934	0.990424927	0.919462992	0.921055001		0.855882002	0.851026268
0.873888129	0.968585241	0.97085328	0.926216581	0.925135434	0.980921699	0.981732717	0.995714219	0.995526146	0.99105655	0.990155897	0.918791451	0.918937551		0.852055796	0.847231803
0.87074365	0.970031129	0.970075085	0.923183247	0.923197806	0.979535614	0.981241508	0.992334347	0.99540477	0.989116894	0.989889742	0.91627907	0.916848655		0.848704254	0.843500125
0.867647525	0.969627711	0.96930578	0.922729177	0.921285818	0.981809604	0.980755706	0.995861583	0.995284666	0.992012134	0.989626433	0.916189553	0.914787929		0.84328578	0.839830195
0.864599009	0.966658885	0.968545266	0.919053621	0.919399132	0.980825548	0.980275253	0.99613528	0.995165823	0.988022386	0.989365938	0.912346944	0.912754993		0.839272089	0.83622099
0.861597371	0.967944393	0.96779344	0.918131567	0.917537413	0.980287513	0.979800088	1.001129336	0.995048225	0.991217797	0.989108228	0.909667041	0.910749471		0.836324885	0.832671507
0.85864189	0.965523663	0.967050204	0.915119044	0.915700329	0.981819948	0.979330155	0.993826337	0.994931861	0.992746407	0.988853273	0.907137896	0.908770995		0.832471374	0.829180757
0.855731856	0.966369865	0.96631546	0.914174583	0.913887556	0.976799922	0.978865395	0.995778626	0.994816718	0.991085334	0.988601043	0.905321865	0.906819199		0.831363718	0.825747768
0.85286657	0.964600748	0.965589111	0.91204808	0.912098771	0.978681574	0.978405751	0.995456037	0.994702781	0.987645336	0.988351509	0.903005336	0.904893724		0.822985445	0.822371584
0.850045344	0.965622471	0.96487106	0.910733817	0.910333656	0.979303456	0.977951167	0.995514445	0.99459004	0.990124243	0.988104642	0.903811151	0.902994215		0.822195979	0.819051265
0.847267501	0.96341988	0.964161213	0.909524292	0.9085919	0.977479081	0.977501587	0.994081622	0.994478481	0.98812232	0.987860414	0.900401763	0.901120322		0.816456352	0.815785888
0.844532373	0.965440221	0.963459476	0.90723176	0.906873192	0.977778643	0.977056957	0.995091867	0.994368092	0.988720533	0.987618797	0.90002509	0.899271698		0.818427187	0.812574542
0.841839304	0.961190372	0.962765757	0.905344435	0.905177228	0.976056299	0.976617221	0.99550686	0.994258861	0.986121205	0.987379763	0.89687056	0.897448005		0.808916494	0.809416334
0.839187646	0.962605755	0.962079964	0.903019176	0.903503706	0.975395216	0.976182326	0.995109244	0.994150775	0.989965053	0.987143283	0.895579613	0.895648904		0.804670022	0.806310385
0.836576764	0.961548143	0.961402006	0.901946716	0.90185233	0.976188059	0.975752219	0.991811848	0.994043823	0.983760296	0.986909332	0.895192827	0.893874065		0.802782319	0.80325583
0.83400603	0.959502232	0.960731795	0.900474008	0.900222806	0.974497185	0.975326846	0.993902812	0.993937992	0.984299767	0.986677881	0.891981972	0.89212316		0.797925134	0.800251817
0.831474827	0.959408134	0.96006924	0.898137573	0.898614846	0.973514979	0.974906157	0.992740445	0.993833271	0.98645082	0.986448904	0.892701567	0.890395867		0.795456615	0.797297513
0.828982546	0.95951726	0.959414255	0.896457101	0.897028165	0.97289484	0.974490098	0.99262618	0.993729649	0.985940133	0.986222375	0.888712222	0.888691867		0.795397719	0.794392092
0.82652859	0.95731467	0.958766754	0.896130916	0.895462479	0.974419435	0.97407862	0.994254915	0.993627113	0.985745331	0.985998267	0.887791411	0.887010847		0.788306649	0.791534748
0.824112369	0.95848421	0.958126651	0.893922538	0.893917512	0.975810747	0.973671671	0.996236581	0.993525652	0.988665316	0.985776555	0.886705648	0.885352495		0.784047583	0.788724683
0.821733302	0.956463534	0.95749386	0.891913599	0.89239299	0.972958215	0.973269203	0.993903709	0.993425256	0.984262833	0.985557213	0.883701597	0.883716507		0.780619047	0.785961116
0.819390819	0.957323082	0.9568683	0.890285524	0.890888642	0.972461558	0.972871165	0.993639183	0.993325912	0.98379958	0.985340215	0.883217974	0.882102581		0.777241311	0.783243278
0.817084357	0.955713	0.956249887	0.889133642	0.8894042	0.971490025	0.972477509	0.992627353	0.99322761	0.985246465	0.985125537	0.88182628	0.88051042		0.77633384	0.780570412
0.814813361	0.956539462	0.95563854	0.887779697	0.887939403	0.971760404	0.972088186	0.992018034	0.99313034	0.982349463	0.984913154	0.880636584	0.878939729		0.769063963	0.777941773
0.812577288	0.955626192	0.955034177	0.886977604	0.886493989	0.973419046	0.971703149	0.994645083	0.993034089	0.98441982	0.984703041	0.87795059	0.87739022		0.766975441	0.77535663
0.810375599	0.954395976	0.954436719	0.885284645	0.885067701	0.972283193	0.971322351	0.990620449	0.992938848	0.981058464	0.984495174	0.879635643	0.875861606		0.763763229	0.772814264
0.808207765	0.953974614	0.953846088	0.883495787	0.883660288	0.969264927	0.970945745	0.994973396	0.992844605	0.982712414	0.984289528	0.875678093	0.874353607		0.763045994	0.770313965
0.806073267	0.953467006	0.953262204	0.882014868	0.8822715	0.970145318	0.970573285	0.993214329	0.992751351	0.984788793	0.984086081	0.872585196	0.872865943		0.758171505	0.767855039
0.803971592	0.951147999	0.952684992	0.881249151	0.880901089	0.971427412	0.970204925	0.99356588	0.992659075	0.984360051	0.983884809	0.872256187	0.871398341		0.756287241	0.7654368
0.801902234	0.9539468	0.952114374	0.87963744	0.879548812	0.968430053	0.96984062	0.990678167	0.992567766	0.984584812	0.983685688	0.870374444	0.869950531		0.754566703	0.763058576
0.799864697	0.950973039	0.951550276	0.878121001	0.87821443	0.968474045	0.969480326	0.991779713	0.992477415	0.980345117	0.983488696	0.867198346	0.868522244		0.751660721	0.760719703

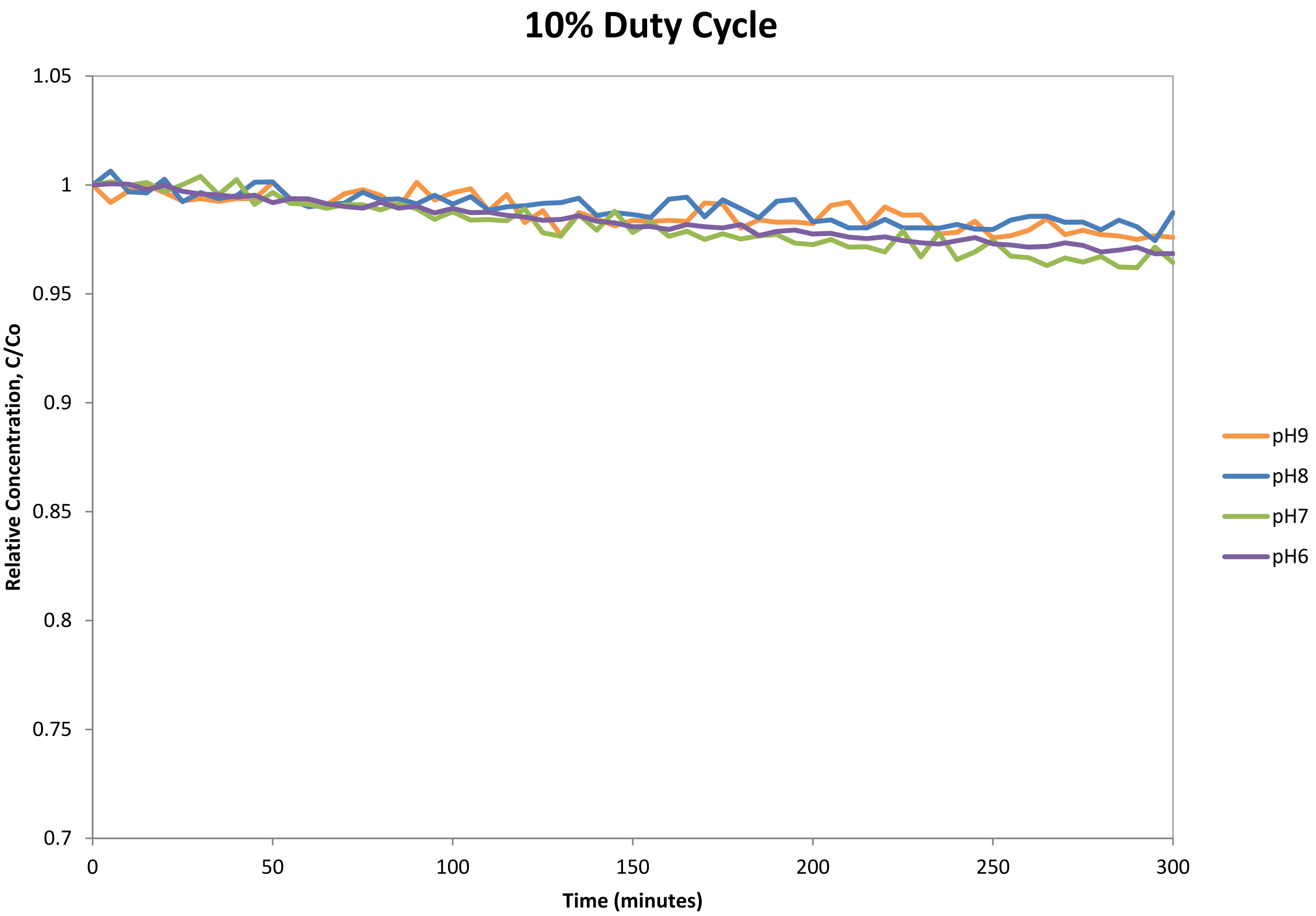
15-Jun-15		9-Jul-15		12-Aug-15		13-Aug-15	
pH9		pH8		pH6		pH8	
50		70		70		100	
2.8300E-04	**5.6600E-04**	**4.5001E-04**	**6.4288E-04**	**8.2701E-04**	**1.1814E-03**	0.000481987	**4.8199E-04**
0.9950	**0.9899**	**0.9915**	**0.9831**	**0.9995**	**0.9990**	**0.9988**	**0.9977**
C/Co	**Model**	**C/Co**	**Model**	**C/Co**	**Model**	**C/Co**	**Model**
1	1	1	1	1	1	1	1
0.994477902	0.998593308	1.004943956	0.997764068	0.998282809	0.995894796	0.997813881	0.997605403
0.996676647	0.997203101	0.993460191	0.995556183	0.993596411	0.991848723	0.995402067	0.995241222
0.994427577	0.995829187	1.001026193	0.993375995	0.988843975	0.987860928	0.993018866	0.992907072
0.995406017	0.994471373	0.990786588	0.991223155	0.98484553	0.983930573	0.991842235	0.990602569
0.992027601	0.993129472	0.990366077	0.989097321	0.982016246	0.980056829	0.987444385	0.988327339
0.987673831	0.991803298	0.987422259	0.986998153	0.978447546	0.976238882	0.986019029	0.986081008
0.986264787	0.990492665	0.993180886	0.984925318	0.974036397	0.972475928	0.985068163	0.983863211
0.985105792	0.989197391	0.988282502	0.982878485	0.969708438	0.968767174	0.98299217	0.981673584
0.990509363	0.987917297	0.981823828	0.980857328	0.966128415	0.965111841	0.978922535	0.979511769
0.983842915	0.986652205	0.976228504	0.978861525	0.963837407	0.961509158	0.97822842	0.977377414
0.98606528	0.985401939	0.987093813	0.976890757	0.958973303	0.957958367	0.976337925	0.97527017
0.983771914	0.984166325	0.978360987	0.974944711	0.954602291	0.954458721	0.97443389	0.973189692
0.983929065	0.982945192	0.978355924	0.973023076	0.951779397	0.951009483	0.972872795	0.97113564
0.978758384	0.981738369	0.970507164	0.971125547	0.948329879	0.947609927	0.970562802	0.969107679
0.978758599	0.980545689	0.96945174	0.969251821	0.945722363	0.944259337	0.969090269	0.967105477
0.980225147	0.979366986	0.972925283	0.967401599	0.94260617	0.940957008	0.967639719	0.965128707
0.976254526	0.978202097	0.969646575	0.965574587	0.939832384	0.937702246	0.966101934	0.963177046
0.976872073	0.97705086	0.967500167	0.963770493	0.937874701	0.934494364	0.963880572	0.961250175
0.973860653	0.975913114	0.966616676	0.96198903	0.933226311	0.931332687	0.961604356	0.959347779
0.975945179	0.974788702	0.959438504	0.960229914	0.931048541	0.928216551	0.958583988	0.957469547
0.972364814	0.973677467	0.968962638	0.958492864	0.927374563	0.925145299	0.957136858	0.955615173
0.97178905	0.972579255	0.955836643	0.956777604	0.924749781	0.922118284	0.954013272	0.953784353
0.969837984	0.971493913	0.956532549	0.955083861	0.920716131	0.91913487	0.954004828	0.951976788
0.967354228	0.97042129	0.957792935	0.953411365	0.919395387	0.916194428	0.952742497	0.950192183
0.968805987	0.969361238	0.954811716	0.951759848	0.915331353	0.91329634	0.949908394	0.948430246
0.967727326	0.968313608	0.959128125	0.950129049	0.913370082	0.910439995	0.949481778	0.946690689
0.965350969	0.967278257	0.949609399	0.948518706	0.91050649	0.907624792	0.946524219	0.944973228
0.966268459	0.966255038	0.958185828	0.946928564	0.907598499	0.904850138	0.945235648	0.943277582
0.962459296	0.965243811	0.946582493	0.945358369	0.904315027	0.90211545	0.944711886	0.941603474
0.963001032	0.964244435	0.939914713	0.943807871	0.90243235	0.899420152	0.941312916	0.939950631
0.9644347	0.963256771	0.941386506	0.942276823	0.899552501	0.896763676	0.937960844	0.938318783
0.95907327	0.962280681	0.940893836	0.94076498	0.896432216	0.894145464	0.939913591	0.936707662
0.964366355	0.96131603	0.942850704	0.939272102	0.892825565	0.891564963	0.937517689	0.935117005
0.958202086	0.960362685	0.943190314	0.937797951	0.88917345	0.889021632	0.934137213	0.933546553
0.959568485	0.959420511	0.940456522	0.936342292	0.887321326	0.886514934	0.932272399	0.93199605
0.957285888	0.95848938	0.932615358	0.934904893	0.88584827	0.884044341	0.932419304	0.93046524
0.958776414	0.95756916	0.935182164	0.933485525	0.883140185	0.881609335	0.930781581	0.928953875
0.957907886	0.956659725	0.928329446	0.932083962	0.880076127	0.879209402	0.928666228	0.927461707
0.959585428	0.955760948	0.928606392	0.93069998	0.877125587	0.876844037	0.926446262	0.925988493
0.955853225	0.954872703	0.927682853	0.92933336	0.875762407	0.874512742	0.925153643	0.924533992
0.955901612	0.953994869	0.929537872	0.927983882	0.872542954	0.872215026	0.923907084	0.923097966
0.951710306	0.953127321	0.922418047	0.926651332	0.870689876	0.869950407	0.92322581	0.92168018
0.951707506	0.952269941	0.921867491	0.925335498	0.869003742	0.867718406	0.920628289	0.920280403
0.953174054	0.951422609	0.921074858	0.924036171	0.864820078	0.865518554	0.918911846	0.918898406
0.95252097	0.950585206	0.922569323	0.922753142	0.863533026	0.863350389	0.916142297	0.917533963
0.948779722	0.949757618	0.917174243	0.921486208	0.862016749	0.861213453	0.915104196	0.916186851
0.950764458	0.948939728	0.925744917	0.920235166	0.857611093	0.859107298	0.914515671	0.91485685
0.949783577	0.948131423	0.919669928	0.918999818	0.856583032	0.857031478	0.913104063	0.913543743
0.948173087	0.947332591	0.917728136	0.917779966	0.854248466	0.854985559	0.910394601	0.912247316
0.947218409	0.94654312	0.922089946	0.916575416	0.85117925	0.852969108	0.908385326	0.910967355
0.94761125	0.945762902	0.90782912	0.915385976	0.848794848	0.850981702	0.908653593	0.909703652
0.947988297	0.944991827	0.909591957	0.914211457	0.846726112	0.849022922	0.908172332	0.908456001
0.942846692	0.944229788	0.904832825	0.913051671	0.844283633	0.847092356	0.90451389	0.907224198
0.944808957	0.94347668	0.910984689	0.911906434	0.842329257	0.845189597	0.903535527	0.906008041
0.941809598	0.942732398	0.907139947	0.910775563	0.841507156	0.843314245	0.901473701	0.904807332
0.941291912	0.941996838	0.910741116	0.909658877	0.837992217	0.841465905	0.90146742	0.903621874
0.940402636	0.941269899	0.903715429	0.9085562	0.835732209	0.839644188	0.900637428	0.902451474
0.940325246	0.940551478	0.902390653	0.907467354	0.833351115	0.837848711	0.899086243	0.90129594
0.939913308	0.939841477	0.90243732	0.906392168	0.831403915	0.836079095	0.89762704	0.900155084
0.938775492	0.939139797	0.905675864	0.905330469	0.831095479	0.834334969	0.895323118	0.899028719

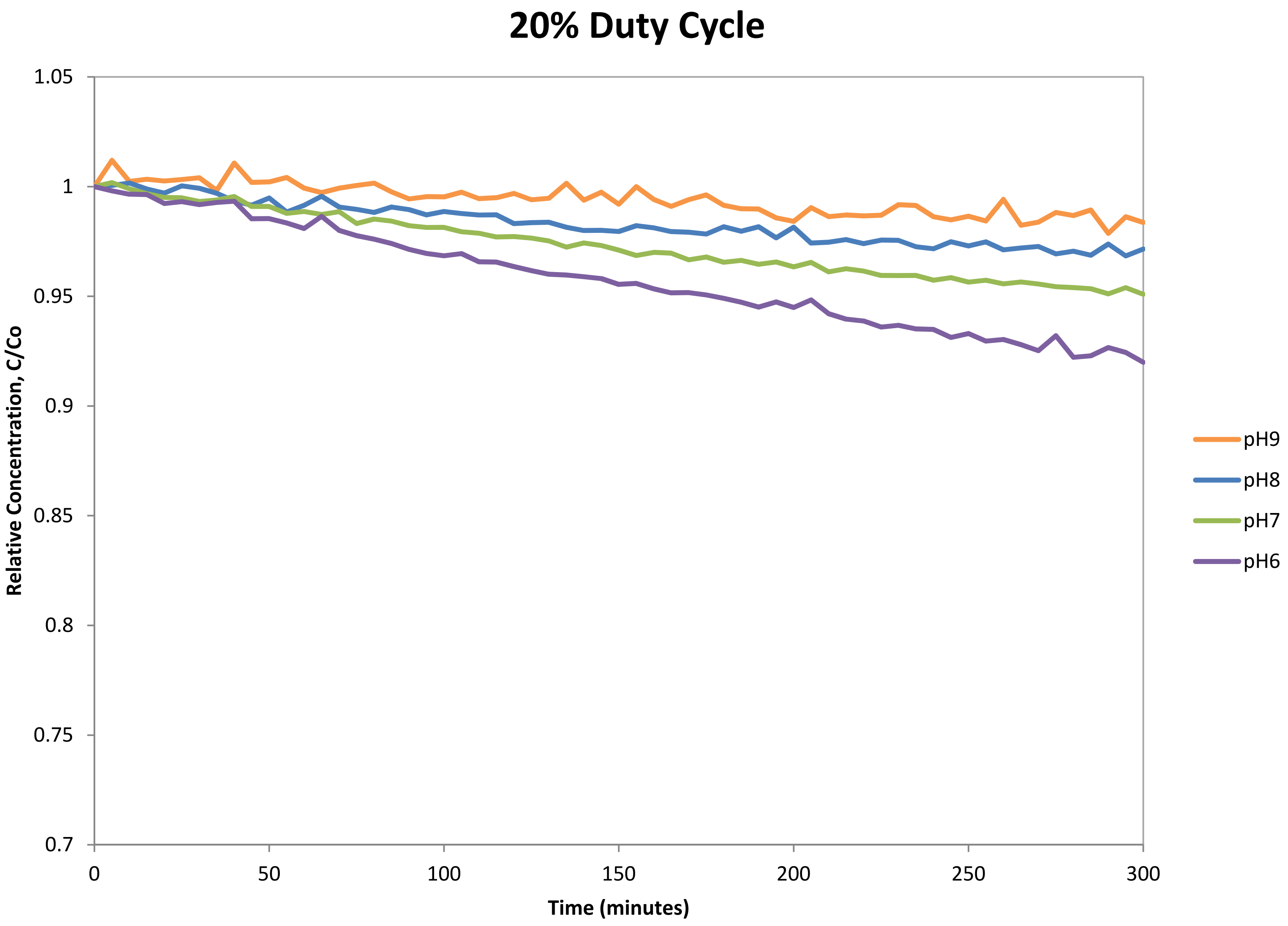
Appendix D: AOP Experiment Charts by Duty Cycle

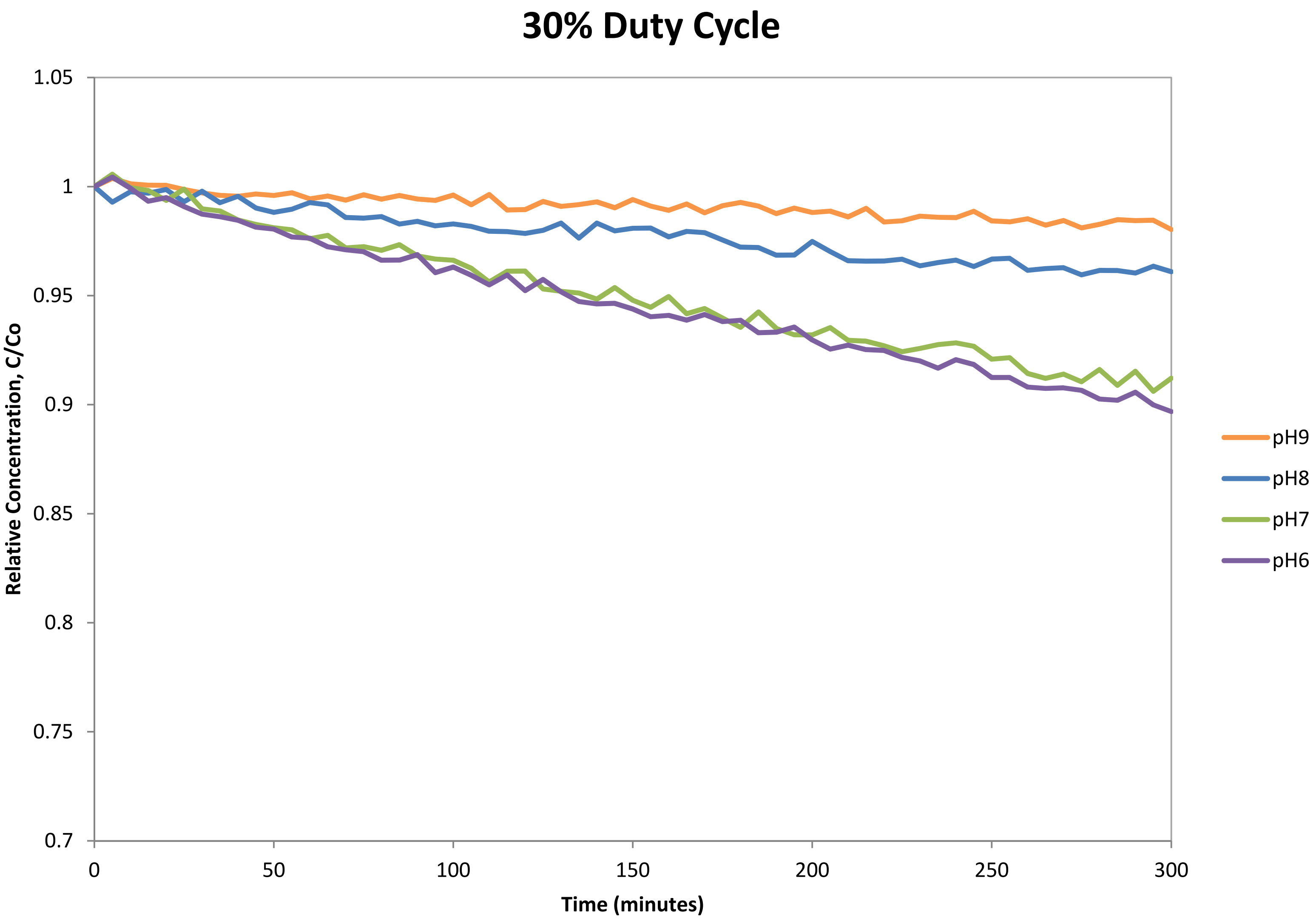


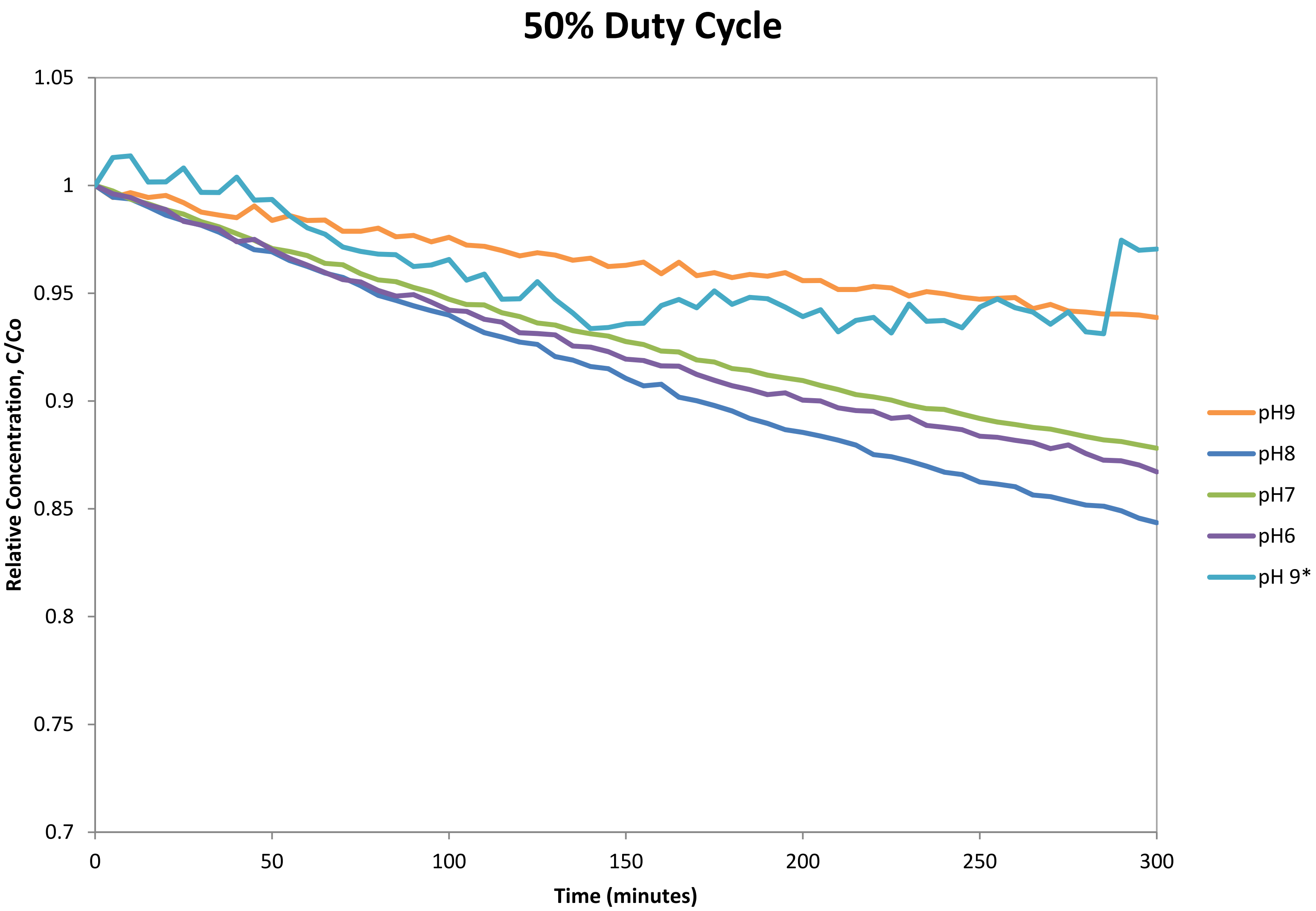

0% Duty Cycle
1.05
1
0.95
0.9
0.85
0.8
0.75
0.7
Relative Concentration, C/Co
0
50
100
150
200
250
300
Time (minutes)
pH9
pH8
pH7
pH6

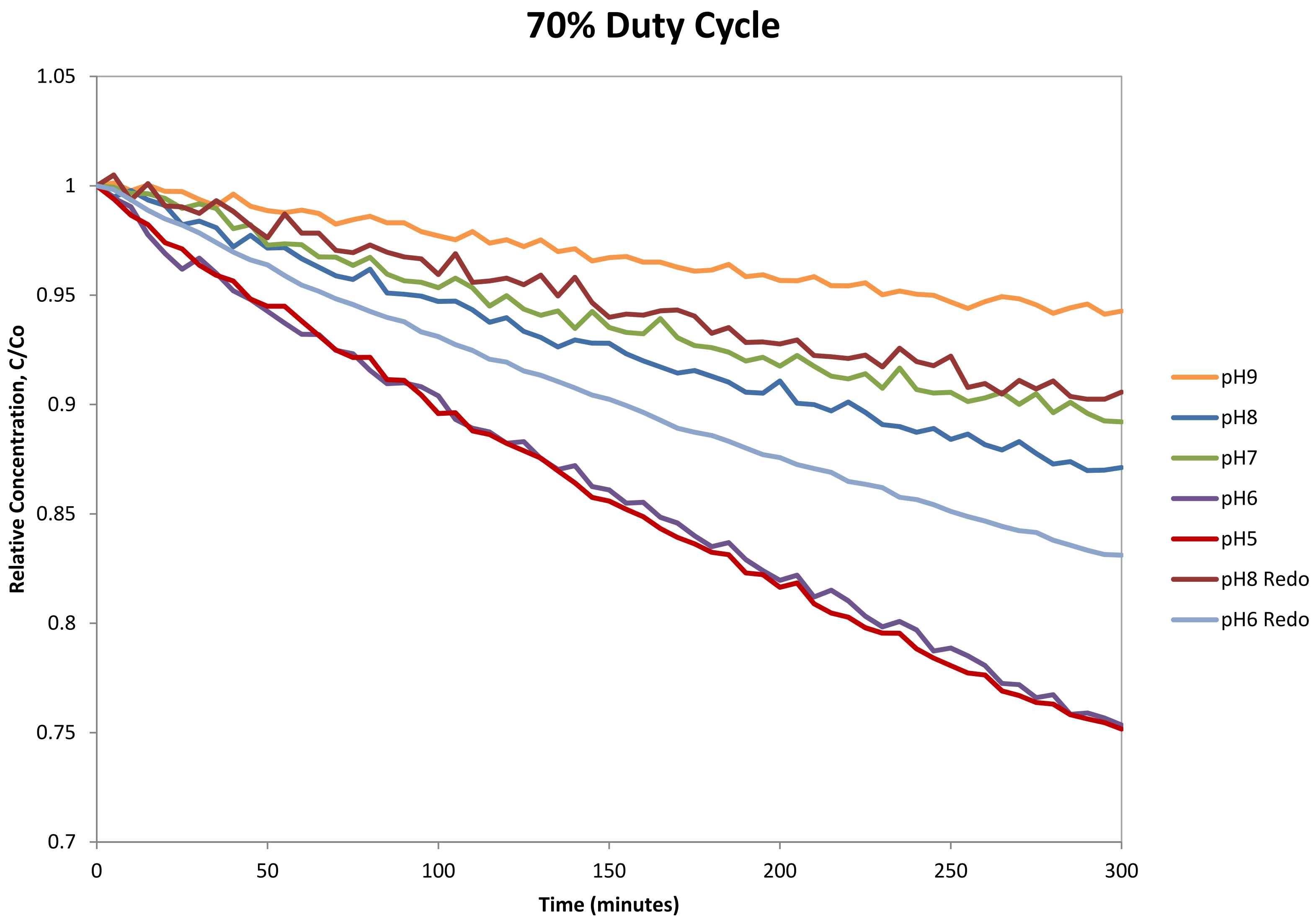

5% Duty Cycle
1.05
1
0.95
0.9
0.85
0.8
0.75
0.7
Relative Concentration, C/Co
0
50
100
150
200
250
300
Time (minutes)
pH9
pH8
pH7
pH6

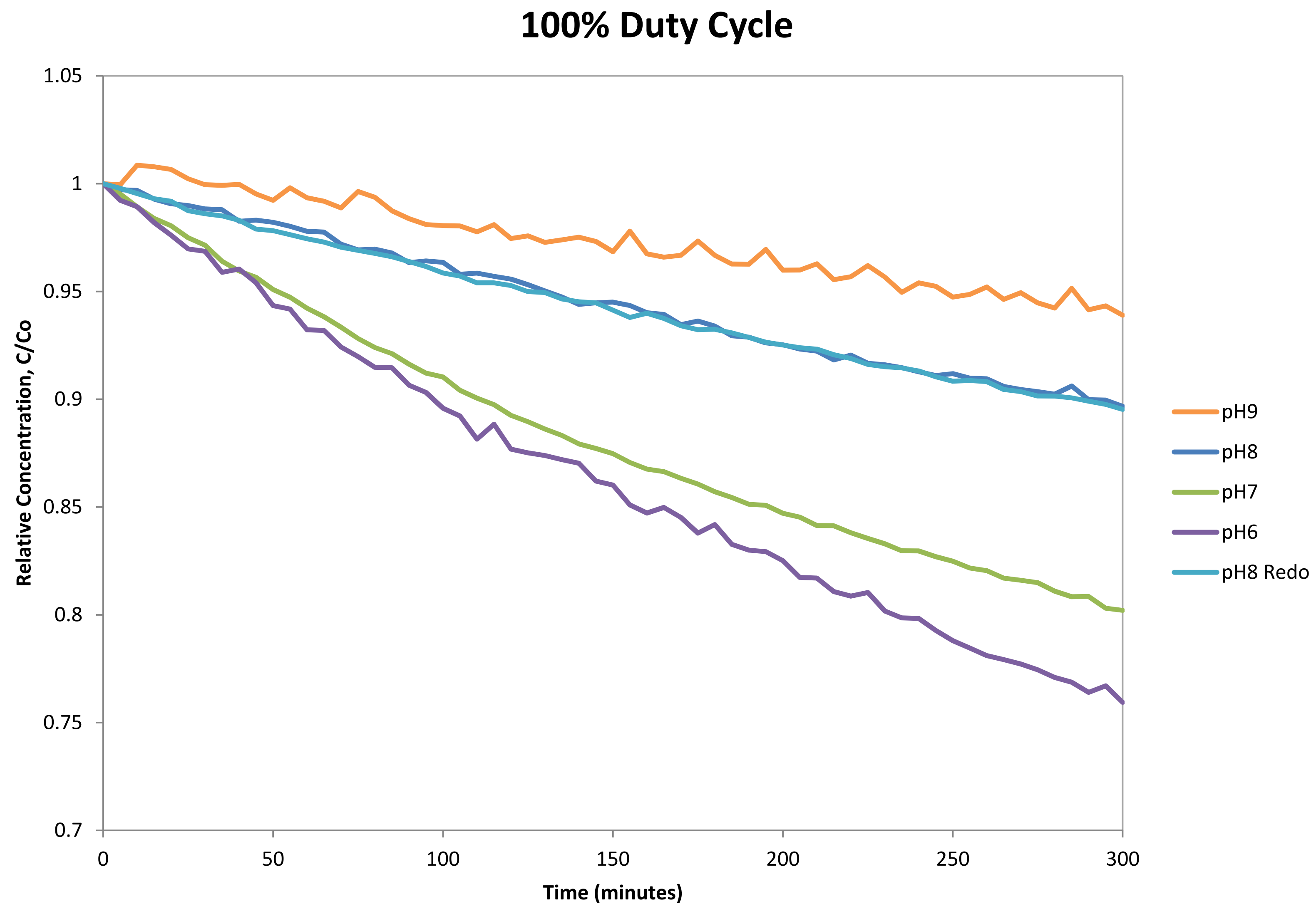

10% Duty Cycle
1.05
1
0.95
0.9
0.85
0.8
0.75
0.7
Relative Concentration, C/Co
0
50
100
150
200
250
300
Time (minutes)
pH9
pH8
pH7
pH6


20% Duty Cycle
1.05
1
0.95
0.9
0.85
0.8
0.75
0.7
Relative Concentration, C/Co
0
50
100
150
200
250
300
Time (minutes)
pH9
pH8
pH7
pH6

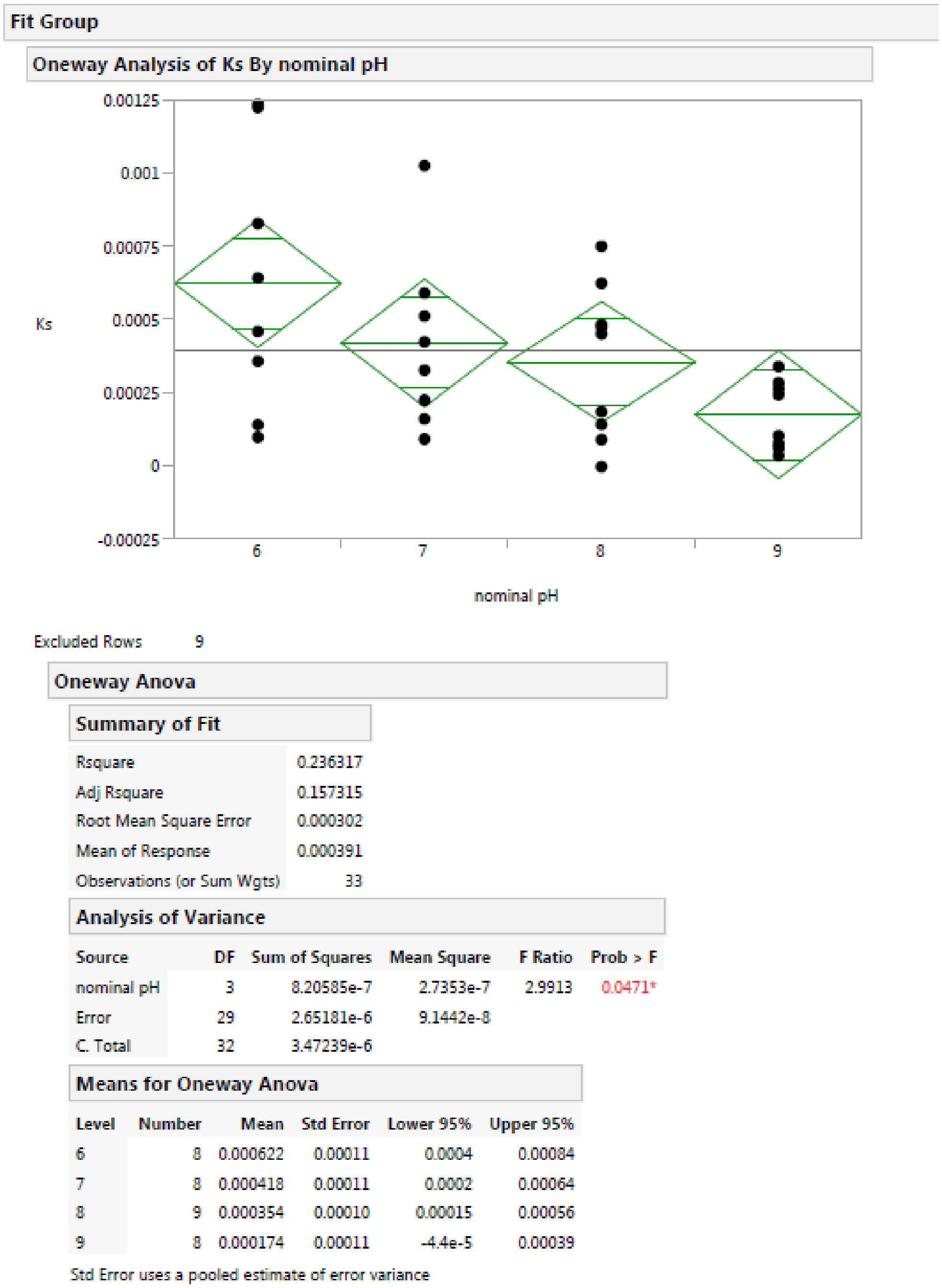

30% Duty Cycle
Relative Concentration, C/Co
1.05
1
0.95
0.9
0.85
0.8
0.75
0.7
0
50
100
150
200
250
300
Time (minutes)
pH9
pH8
pH7
pH6


50% Duty Cycle
Relative Concentration, C/Co
1.05
1
0.95
0.9
0.85
0.8
0.75
0.7
0
50
100
150
200
250
300
Time (minutes)
pH9
pH8
pH7
pH6
pH 9*


70% Duty Cycle
Relative Concentration, C/Co
1.05
1
0.95
0.9
0.85
0.8
0.75
0.7
0
50
100
150
200
250
300
Time (minutes)
pH9
pH8
pH7
pH6
pH5
pH8 Redo
pH6 Redo


100% Duty Cycle
Relative Concentration, C/Co
1.05
1
0.95
0.9
0.85
0.8
0.75
0.7
0
50
100
150
200
250
300
Time (minutes)
pH9
pH8
pH7
pH6
pH8 Redo

Appendix E: AOP ANOVA and Tukey Analyses



Fit Group

Oneway Analysis of Ks By nominal pH

Excluded Rows 9

Oneway Anova

Summary of Fit

Rsquare	0.236317
Adj Rsquare	0.157315
Root Mean Square Error	0.000302
Mean of Response	0.000391
Observations (or Sum Wgts)	33

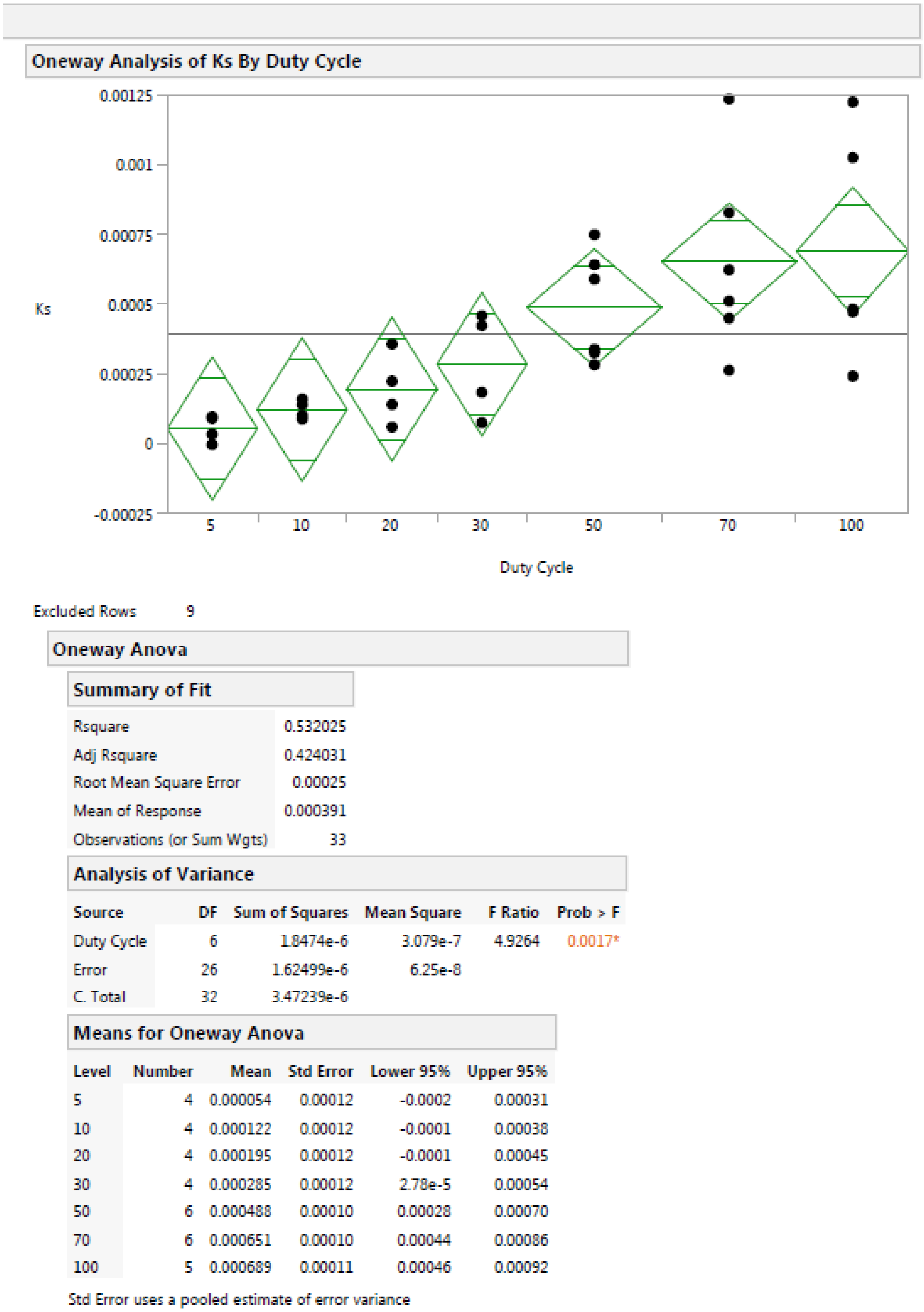
Analysis of Variance

Source	DF	Sum of Squares	Mean Square	F Ratio	Prob > F
nominal pH	3	8.20585e-7	2.7353e-7	2.9913	0.0471*
Error	29	2.65181e-6	9.1442e-8		
C. Total	32	3.47239e-6			

Means for Oneway Anova

Level	Number	Mean	Std Error	Lower 95%	Upper 95%
6	8	0.000622	0.00011	0.0004	0.00084
7	8	0.000418	0.00011	0.0002	0.00064
8	9	0.000354	0.00010	0.00015	0.00056
9	8	0.000174	0.00011	-4.4e-5	0.00039

Std Error uses a pooled estimate of error variance



Oneway Analysis of Ks By Duty Cycle

Excluded Rows 9

Oneway Anova

Summary of Fit

Rsquare	0.532025
Adj Rsquare	0.424031
Root Mean Square Error	0.00025
Mean of Response	0.000391
Observations (or Sum Wgts)	33

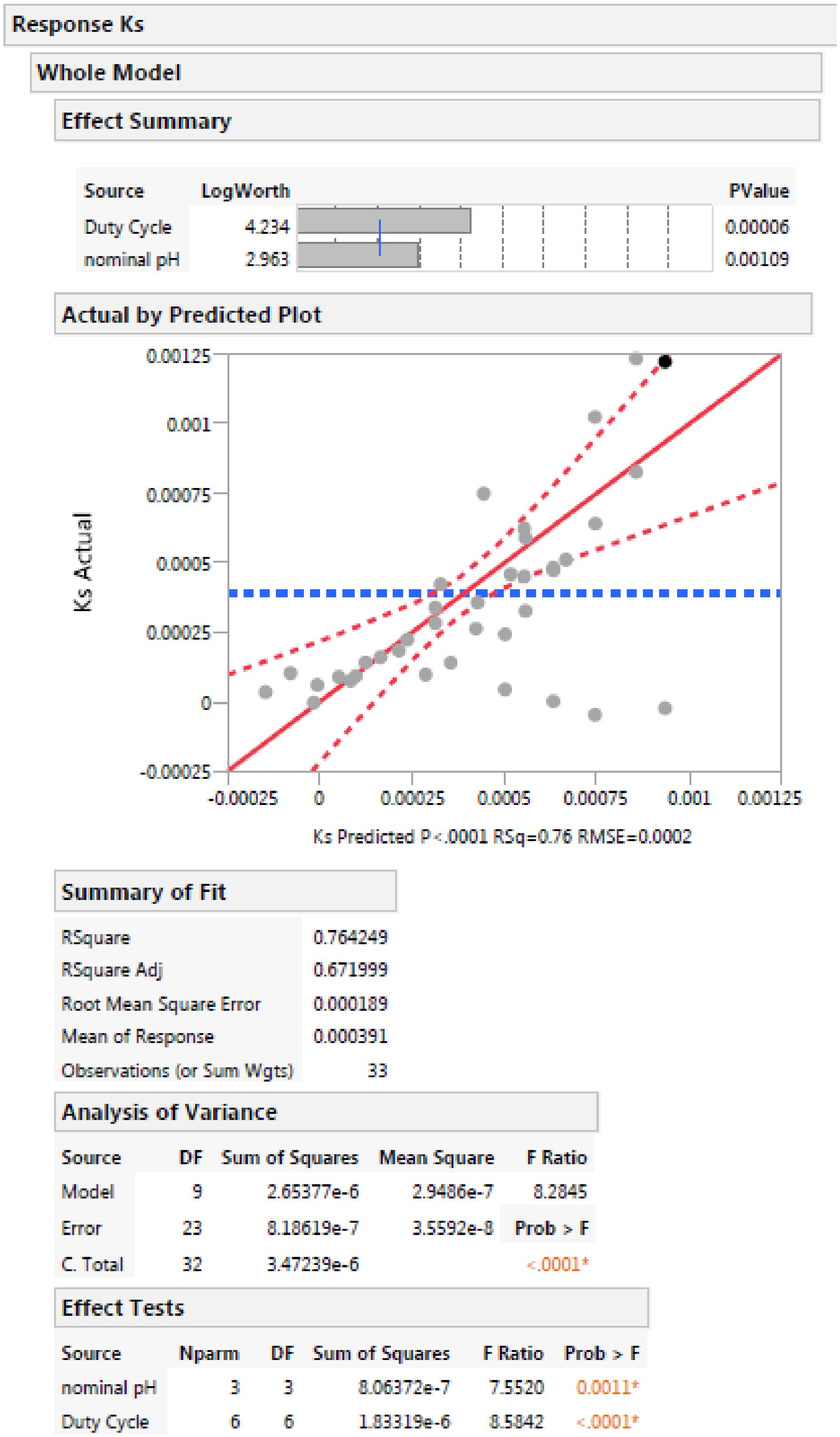
Analysis of Variance

Source	DF	Sum of Squares	Mean Square	F Ratio	Prob > F
Duty Cycle	6	1.8474e-6	3.079e-7	4.9264	0.0017*
Error	26	1.62499e-6	6.25e-8		
C. Total	32	3.47239e-6			

Means for Oneway Anova

Level	Number	Mean	Std Error	Lower 95%	Upper 95%
5	4	0.000054	0.00012	-0.0002	0.00031
10	4	0.000122	0.00012	-0.0001	0.00038
20	4	0.000195	0.00012	-0.0001	0.00045
30	4	0.000285	0.00012	2.78e-5	0.00054
50	6	0.000488	0.00010	0.00028	0.00070
70	6	0.000651	0.00010	0.00044	0.00086
100	5	0.000689	0.00011	0.00046	0.00092

Std Error uses a pooled estimate of error variance



Response Ks

Whole Model

Effect Summary

Source	LogWorth	PValue
Duty Cycle	4.234	0.00006
nominal pH	2.963	0.00109

Actual by Predicted Plot

Summary of Fit

RSquare	0.764249
RSquare Adj	0.671999
Root Mean Square Error	0.000189
Mean of Response	0.000391
Observations (or Sum Wgts)	33

Analysis of Variance

Source	DF	Sum of Squares	Mean Square	F Ratio
Model	9	2.65377e-6	2.9486e-7	8.2845
Error	23	8.18619e-7	3.5592e-8	Prob > F
C. Total	32	3.47239e-6		<.0001*

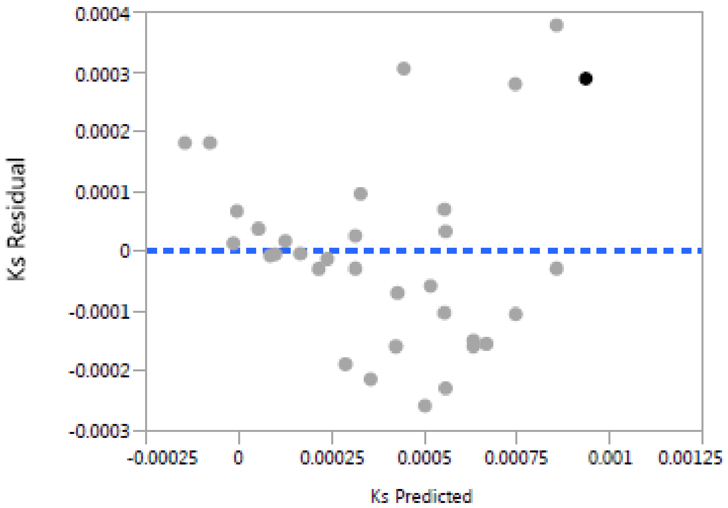
Effect Tests

Source	Nparm	DF	Sum of Squares	F Ratio	Prob > F
nominal pH	3	3	8.06372e-7	7.5520	0.0011*
Duty Cycle	6	6	1.83319e-6	8.5842	<.0001*

Response Ks

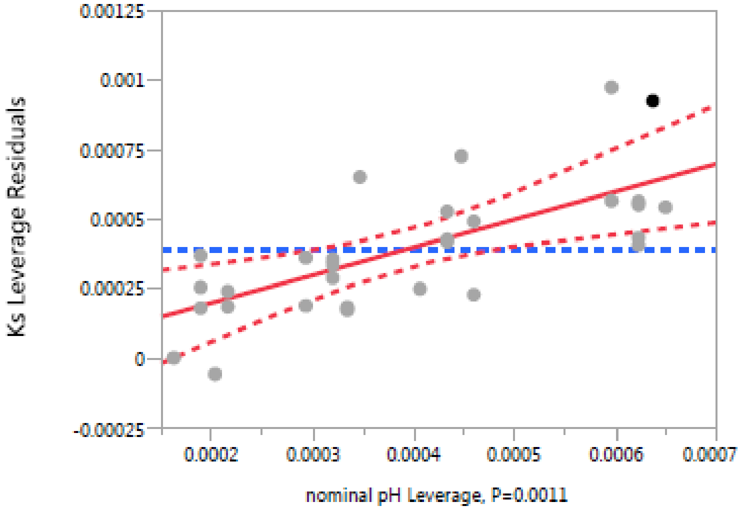
Whole Model

Residual by Predicted Plot



nominal pH

Leverage Plot



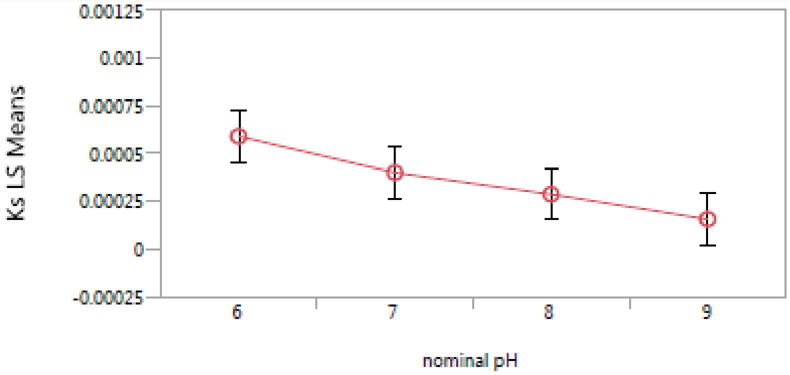
Least Squares Means Table

Level	Least Sq Mean	Std Error	Mean
6	0.00058861	0.00006734	0.000622
7	0.00039879	0.00006734	0.000418
8	0.00028569	0.00006389	0.000354
9	0.00015480	0.00006734	0.000174

Response Ks

nominal pH

LS Means Plot



LSMeans Differences Tukey HSD

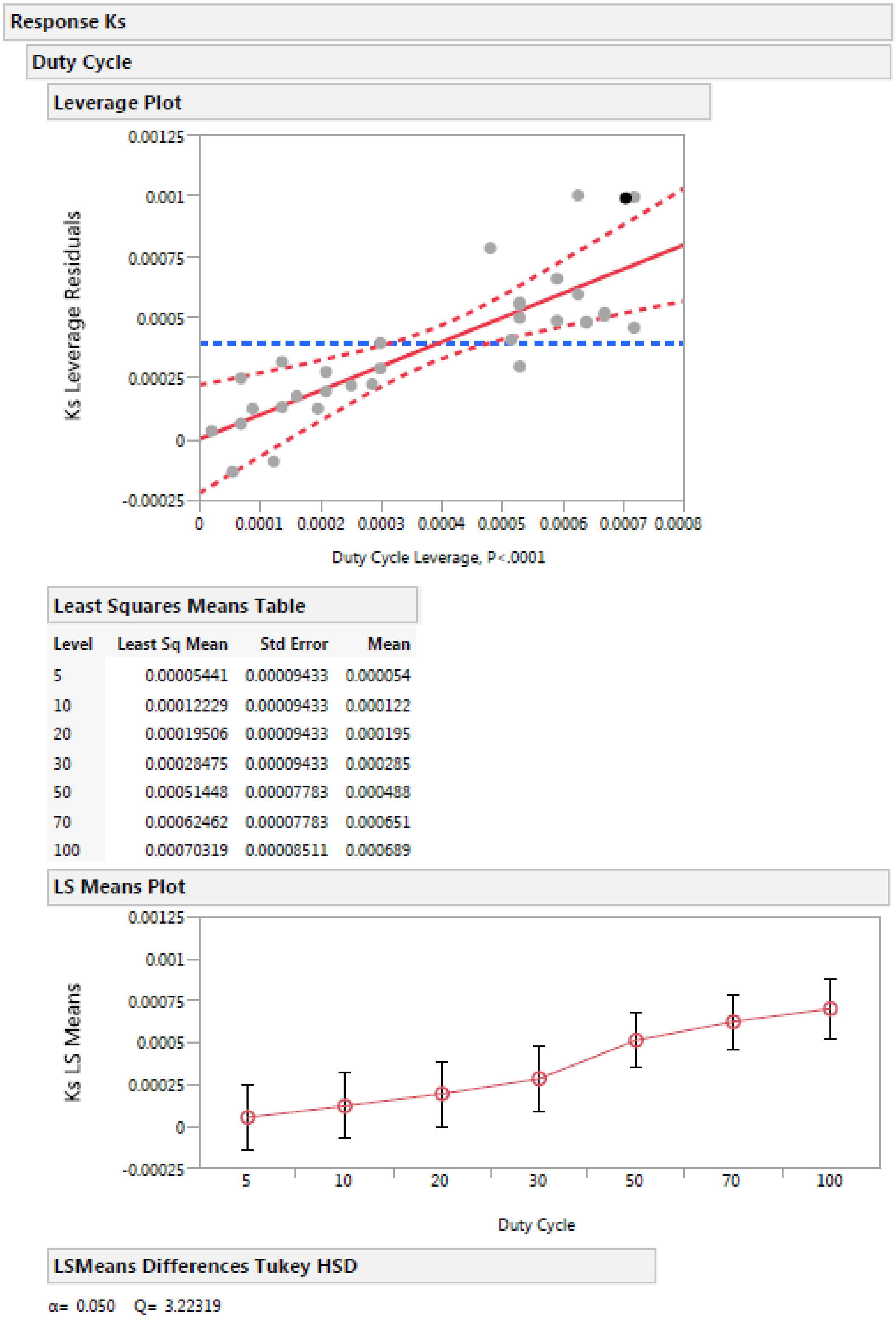
α= 0.050 Q= 2.76731

LSMean[j]

LSMean[i]	Mean[i]-Mean[j] Std Err Dif Lower CL Dif Upper CL Dif	6	7	8	9
6		0	0.00019	0.0003	0.00043
		0	0.0001	9.21e-5	0.0001
		0	-0.0001	4.8e-5	0.00017
		0	0.00045	0.00056	0.0007
7		-0.0002	0	0.00011	0.00024
		0.0001	0	9.31e-5	9.43e-5
		-0.0005	0	-0.0001	-1.7e-5
		7.4e-5	0	0.00037	0.00051
8		-0.0003	-0.0001	0	0.00013
		9.21e-5	9.31e-5	0	9.31e-5
		-0.0006	-0.0004	0	-0.0001
		-4.8e-5	0.00014	0	0.00039
9		-0.0004	-0.0002	-0.0001	0
		0.0001	9.43e-5	9.31e-5	0
		-0.0007	-0.0005	-0.0004	0
		-0.0002	1.7e-5	0.00013	0

Level			Least Sq Mean
6	A		0.00058861
7	A	B	0.00039879
8		B	0.00028569
9		B	0.00015480

Levels not connected by same letter are significantly different.



Response Ks

Duty Cycle

Leverage Plot

Least Squares Means Table

Level	Least Sq Mean	Std Error	Mean
5	0.00005441	0.00009433	0.000054
10	0.00012229	0.00009433	0.000122
20	0.00019506	0.00009433	0.000195
30	0.00028475	0.00009433	0.000285
50	0.00051448	0.00007783	0.000488
70	0.00062462	0.00007783	0.000651
100	0.00070319	0.00008511	0.000689

LS Means Plot

LSMeans Differences Tukey HSD

α= 0.050 Q= 3.22319

Response Ks

Duty Cycle

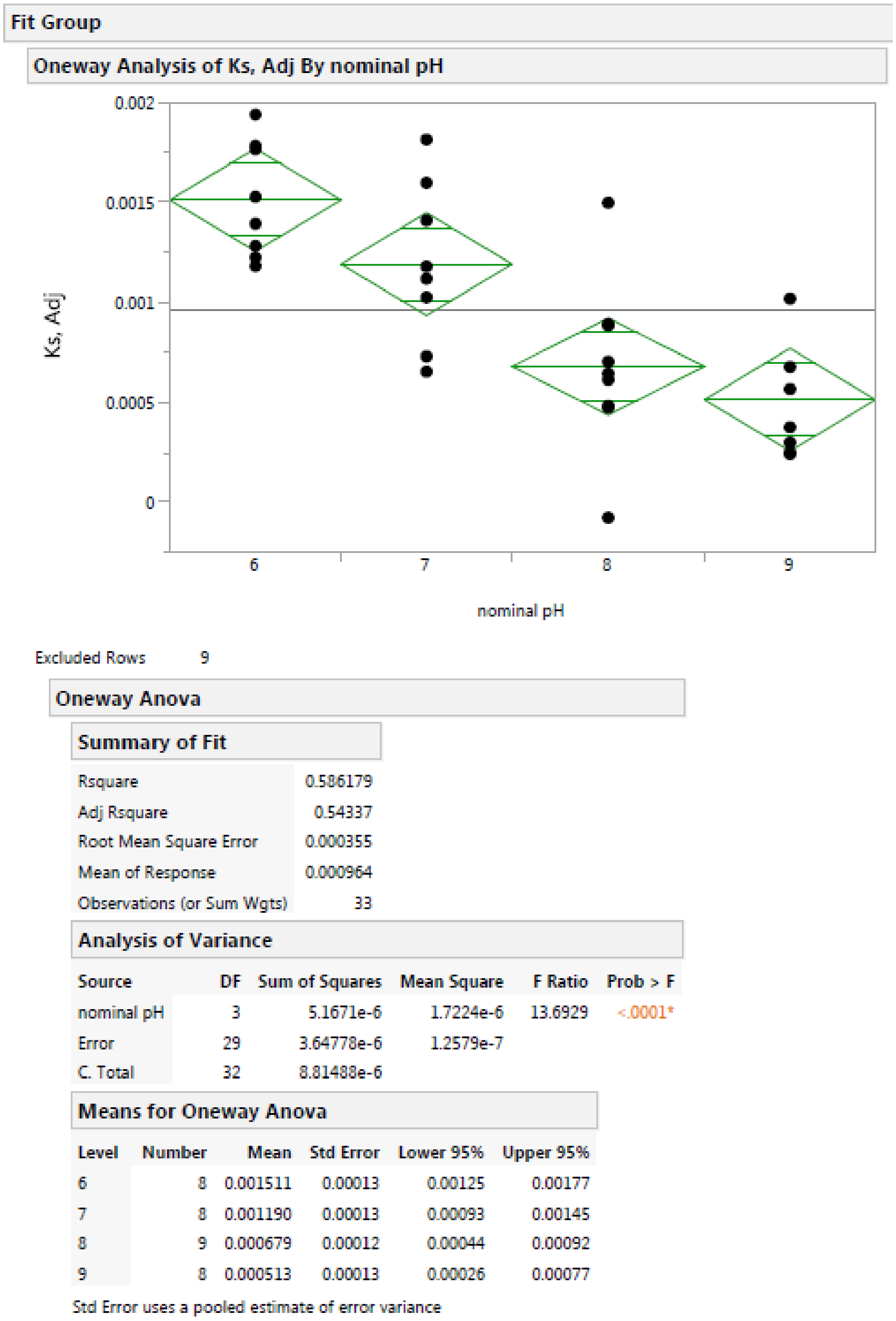
LSMeans Differences Tukey HSD

LSMean[j]

LSMean[i]	Mean[i]-Mean[j] Std Err Dif Lower CL Dif Upper CL Dif	5	10	20	30	50	70	100
5		0	-0.0001	-0.0001	-0.0002	-0.0005	-0.0006	-0.0006
		0	0.00013	0.00013	0.00013	0.00012	0.00012	0.00013
		0	-0.0005	-0.0006	-0.0007	-0.0009	-0.001	-0.0011
		0	0.00036	0.00029	0.0002	-0.0001	-0.0002	-0.0002
10		6.79e-5	0	-0.0001	-0.0002	-0.0004	-0.0005	-0.0006
		0.00013	0	0.00013	0.00013	0.00012	0.00012	0.00013
		-0.0004	0	-0.0005	-0.0006	-0.0008	-0.0009	-0.001
		0.0005	0	0.00036	0.00027	1.98e-6	-0.0001	-0.0002
20		0.00014	7.28e-5	0	-0.0001	-0.0003	-0.0004	-0.0005
		0.00013	0.00013	0	0.00013	0.00012	0.00012	0.00013
		-0.0003	-0.0004	0	-0.0005	-0.0007	-0.0008	-0.0009
		0.00057	0.0005	0	0.00034	7.48e-5	-3.5e-5	-0.0001
30		0.00023	0.00016	0.00009	0	-0.0002	-0.0003	-0.0004
		0.00013	0.00013	0.00013	0	0.00012	0.00012	0.00013
		-0.0002	-0.0003	-0.0003	0	-0.0006	-0.0007	-0.0008
		0.00066	0.00059	0.00052	0	0.00016	5.43e-5	-8.9e-6
50		0.00046	0.00039	0.00032	0.00023	0	-0.0001	-0.0002
		0.00012	0.00012	0.00012	0.00012	0	0.00011	0.00012
		6.59e-5	-2e-6	-0.0001	-0.0002	0	-0.0005	-0.0006
		0.00085	0.00079	0.00071	0.00062	0	0.00025	0.00019
70		0.00057	0.0005	0.00043	0.00034	0.00011	0	-0.0001
		0.00012	0.00012	0.00012	0.00012	0.00011	0	0.00011
		0.00018	0.00011	3.54e-5	-0.0001	-0.0002	0	-0.0004
		0.00096	0.0009	0.00082	0.00073	0.00047	0	0.00029
100		0.00065	0.00058	0.00051	0.00042	0.00019	7.86e-5	0
		0.00013	0.00013	0.00013	0.00013	0.00012	0.00011	0
		0.00024	0.00017	0.0001	8.92e-6	-0.0002	-0.0003	0
		0.00106	0.00099	0.00092	0.00083	0.00056	0.00045	0

Level					Least Sq Mean
100	A				0.00070319
70	A	B			0.00062462
50	A	B	C		0.00051448
30		B	C	D	0.00028475
20			C	D	0.00019506
10			C	D	0.00012229
5				D	0.00005441

Levels not connected by same letter are significantly different.



Excluded Rows 9

Oneway Anova

Summary of Fit

Rsquare	0.586179
Adj Rsquare	0.54337
Root Mean Square Error	0.000355
Mean of Response	0.000964
Observations (or Sum Wgts)	33

Analysis of Variance

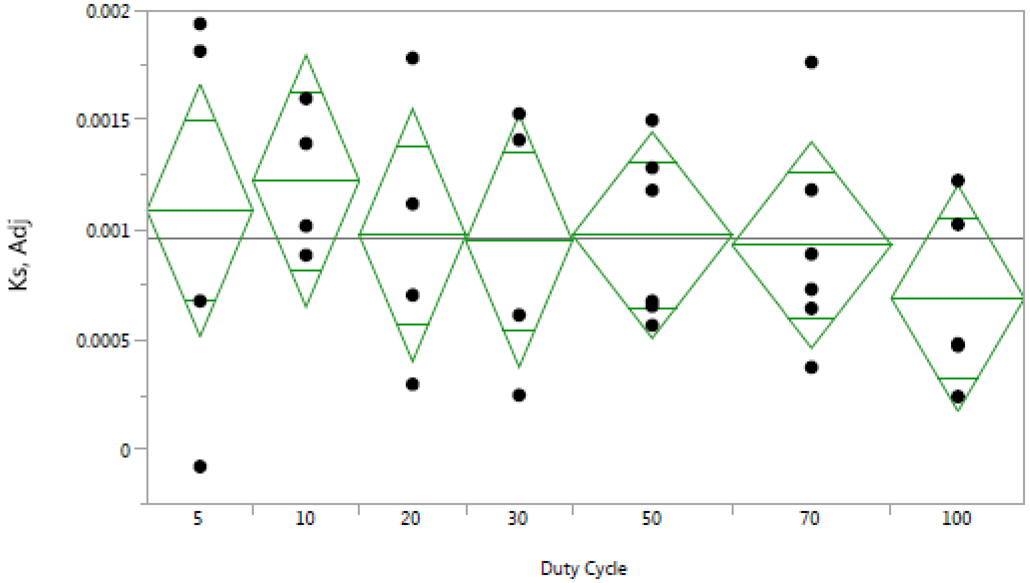
Source	DF	Sum of Squares	Mean Square	F Ratio	Prob > F
nominal pH	3	5.1671e-6	1.7224e-6	13.6929	<.0001*
Error	29	3.64778e-6	1.2579e-7		
C. Total	32	8.81488e-6			

Means for Oneway Anova

Level	Number	Mean	Std Error	Lower 95%	Upper 95%
6	8	0.001511	0.00013	0.00125	0.00177
7	8	0.001190	0.00013	0.00093	0.00145
8	9	0.000679	0.00012	0.00044	0.00092
9	8	0.000513	0.00013	0.00026	0.00077

Std Error uses a pooled estimate of error variance

Oneway Analysis of Ks, Adj By Duty Cycle



Excluded Rows 9

Oneway Anova

Summary of Fit

Rsquare	0.081336
Adj Rsquare	-0.13066
Root Mean Square Error	0.000558
Mean of Response	0.000964
Observations (or Sum Wgts)	33

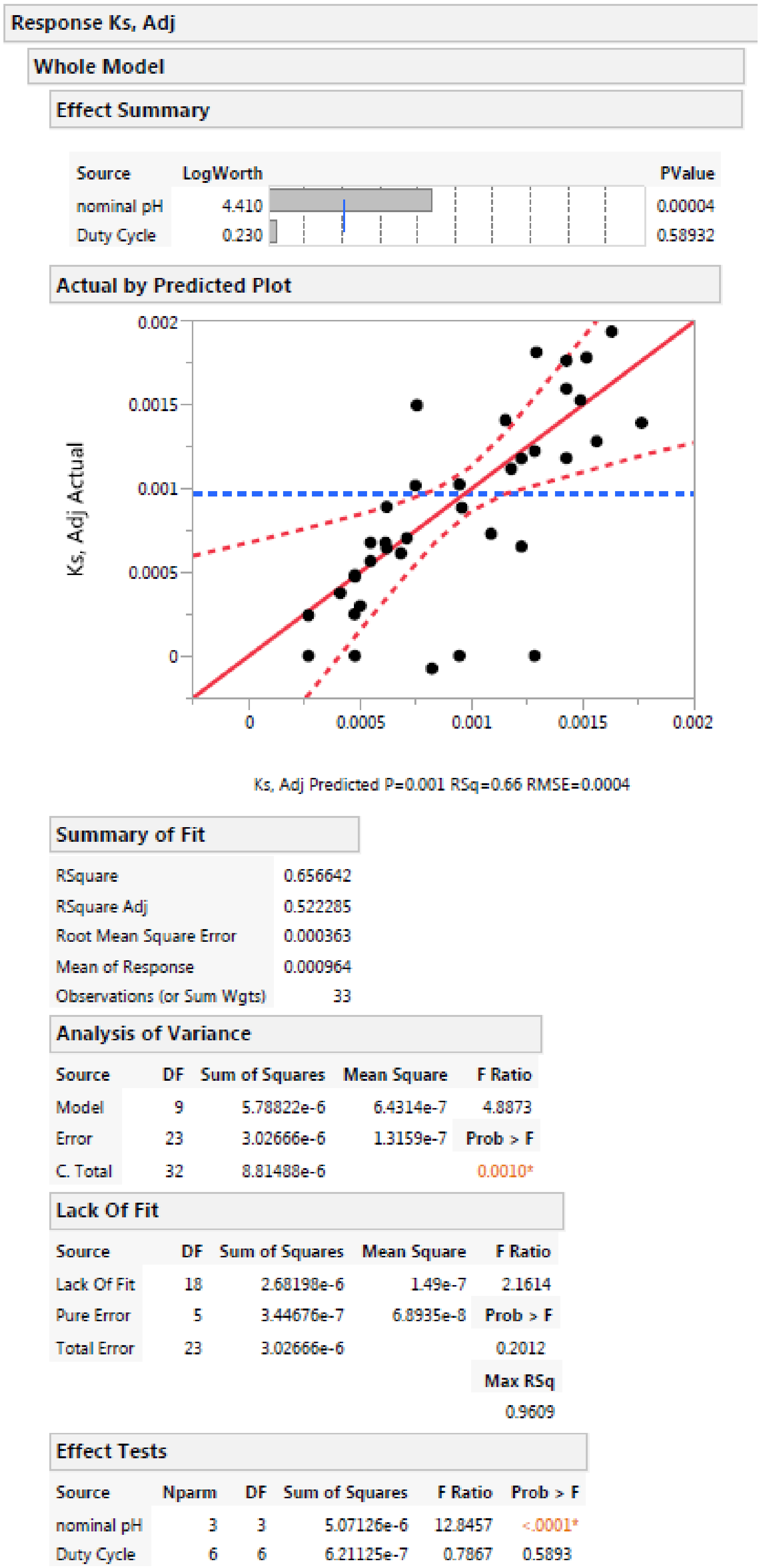
Analysis of Variance

Source	DF	Sum of Squares	Mean Square	F Ratio	Prob > F
Duty Cycle	6	7.16966e-7	1.1949e-7	0.3837	0.8827
Error	26	8.09791e-6	3.1146e-7		
C. Total	32	8.81488e-6			

Means for Oneway Anova

Level	Number	Mean	Std Error	Lower 95%	Upper 95%
5	4	0.001088	0.00028	0.00051	0.00166
10	4	0.001223	0.00028	0.00065	0.00180
20	4	0.000975	0.00028	0.00040	0.00155
30	4	0.000949	0.00028	0.00038	0.00152
50	6	0.000975	0.00023	0.00051	0.00144
70	6	0.000930	0.00023	0.00046	0.00140
100	5	0.000689	0.00025	0.00018	0.00120

Std Error uses a pooled estimate of error variance



Response Ks, Adj

Whole Model

Effect Summary

Source	LogWorth	PValue
nominal pH	4.410	0.00004
Duty Cycle	0.230	0.58932

Actual by Predicted Plot

Summary of Fit

RSquare	0.656642
RSquare Adj	0.522285
Root Mean Square Error	0.000363
Mean of Response	0.000964
Observations (or Sum Wgts)	33

Analysis of Variance

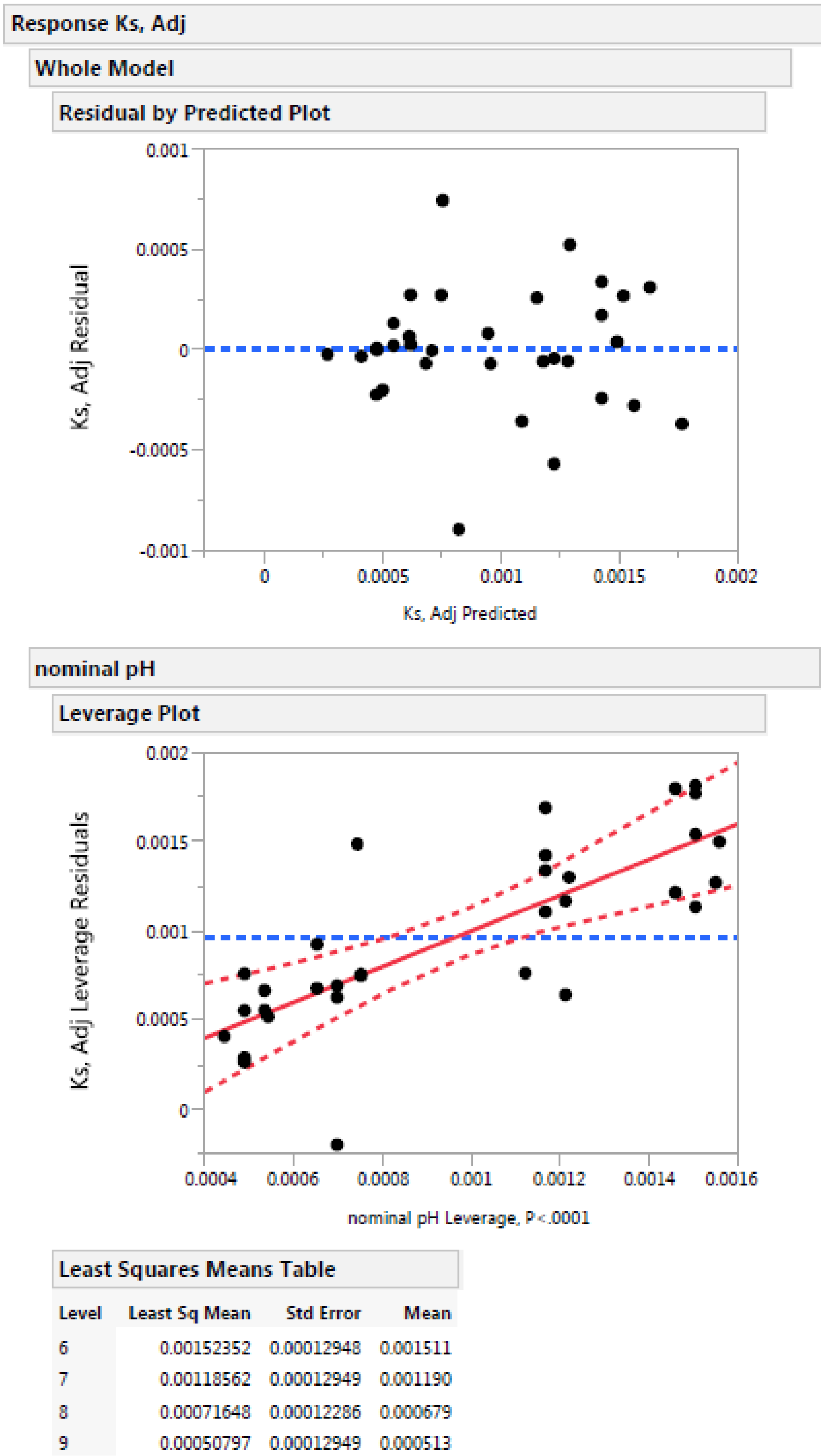
Source	DF	Sum of Squares	Mean Square	F Ratio
Model	9	5.78822e-6	6.4314e-7	4.8873
Error	23	3.02666e-6	1.3159e-7	Prob > F
C. Total	32	8.81488e-6		0.0010*

Lack Of Fit

Source	DF	Sum of Squares	Mean Square	F Ratio
Lack Of Fit	18	2.68198e-6	1.49e-7	2.1614
Pure Error	5	3.44676e-7	6.8935e-8	Prob > F
Total Error	23	3.02666e-6		0.2012
				Max RSq
				0.9609

Effect Tests

Source	Nparm	DF	Sum of Squares	F Ratio	Prob > F
nominal pH	3	3	5.07126e-6	12.8457	<.0001*
Duty Cycle	6	6	6.21125e-7	0.7867	0.5893



Response Ks, Adj

Whole Model

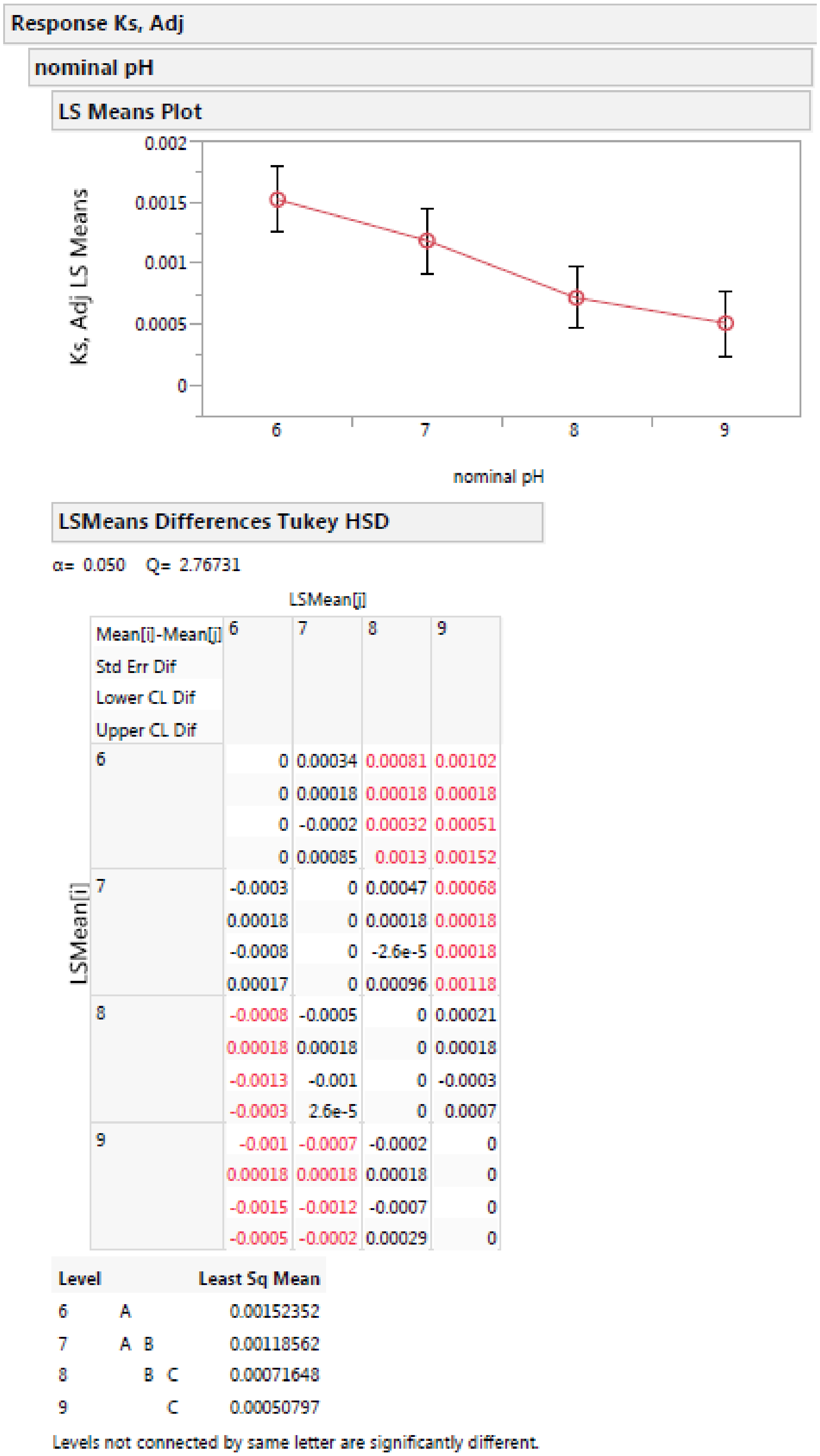
Residual by Predicted Plot

nominal pH

Leverage Plot

Least Squares Means Table

Level	Least Sq Mean	Std Error	Mean
6	0.00152352	0.00012948	0.001511
7	0.00118562	0.00012949	0.001190
8	0.00071648	0.00012286	0.000679
9	0.00050797	0.00012949	0.000513



Response Ks, Adj

nominal pH

LS Means Plot

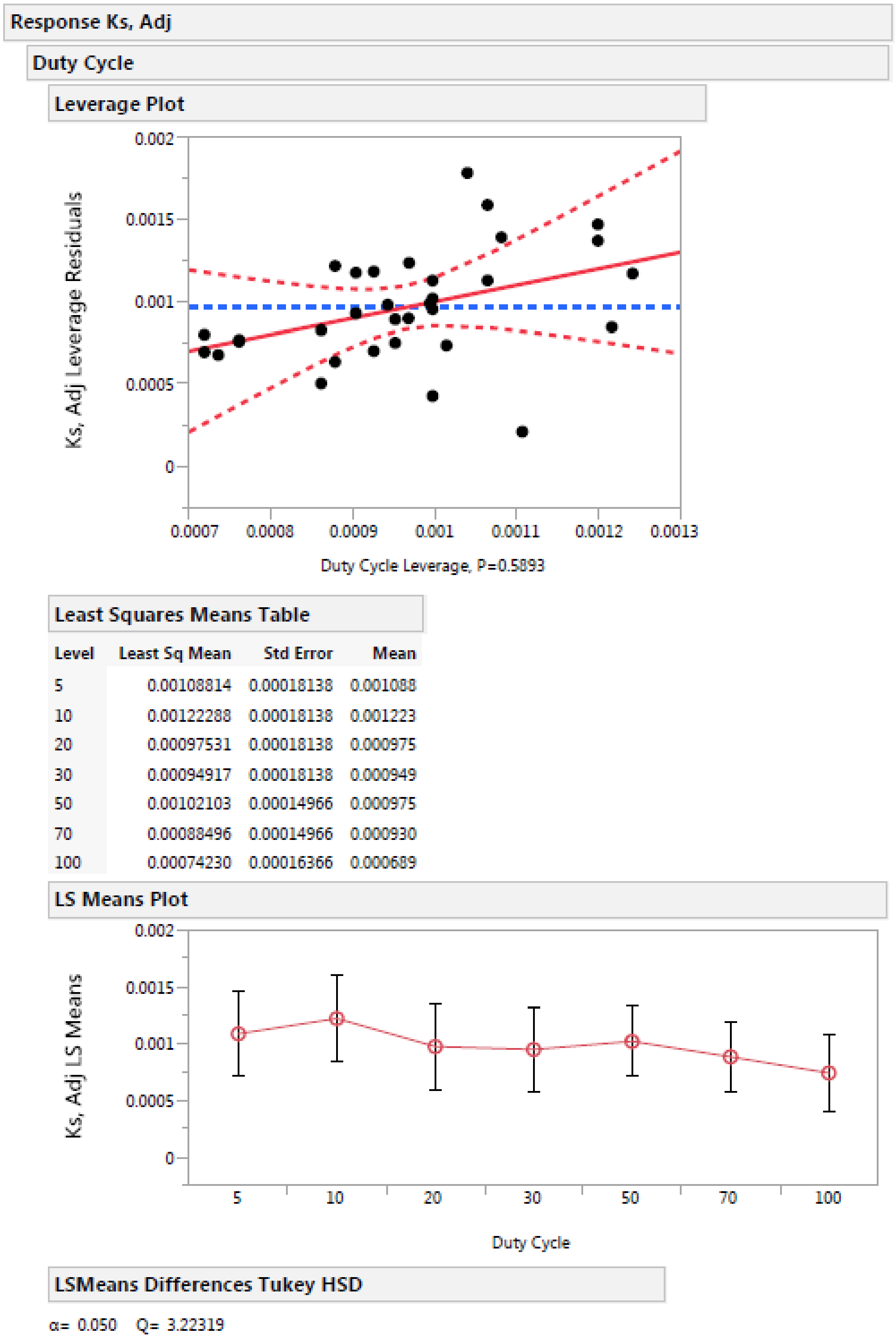
LSMeans Differences Tukey HSD

α= 0.050 Q= 2.76731

LSMean[i]		LSMean[j] 6	7	8	9
	Mean[i]-Mean[j] Std Err Dif Lower CL Dif Upper CL Dif				
6		0	0.00034	0.00081	0.00102
		0	0.00018	0.00018	0.00018
		0	-0.0002	0.00032	0.00051
		0	0.00085	0.0013	0.00152
7		-0.0003	0	0.00047	0.00068
		0.00018	0	0.00018	0.00018
		-0.0008	0	-2.6e-5	0.00018
		0.00017	0	0.00096	0.00118
8		-0.0008	-0.0005	0	0.00021
		0.00018	0.00018	0	0.00018
		-0.0013	-0.001	0	-0.0003
		-0.0003	2.6e-5	0	0.0007
9		-0.001	-0.0007	-0.0002	0
		0.00018	0.00018	0.00018	0
		-0.0015	-0.0012	-0.0007	0
		-0.0005	-0.0002	0.00029	0

Level				Least Sq Mean
6	A			0.00152352
7	A	B		0.00118562
8		B	C	0.00071648
9			C	0.00050797

Levels not connected by same letter are significantly different.



Response Ks, Adj

Duty Cycle

Leverage Plot

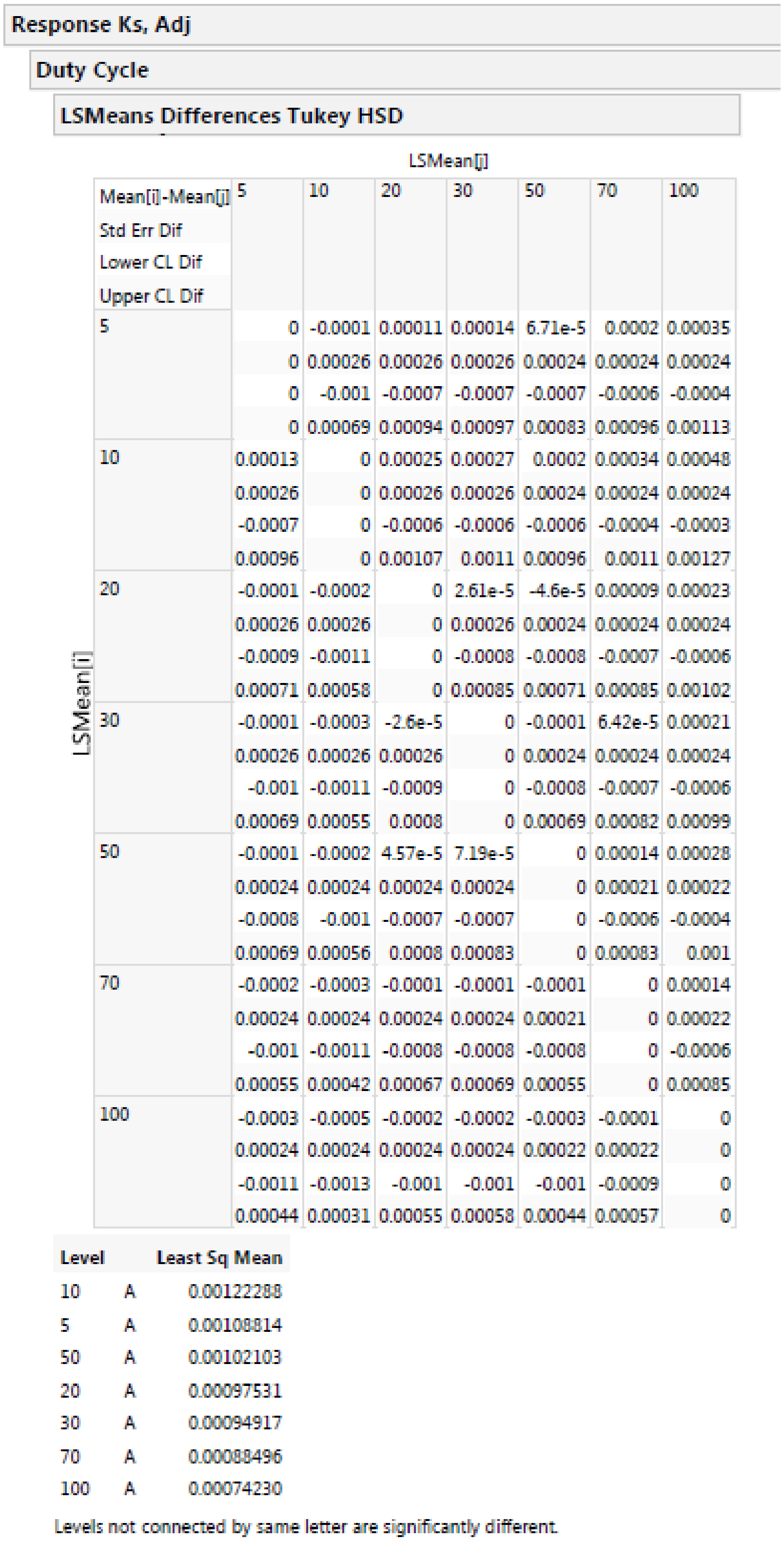
Least Squares Means Table

Level	Least Sq Mean	Std Error	Mean
5	0.00108814	0.00018138	0.001088
10	0.00122288	0.00018138	0.001223
20	0.00097531	0.00018138	0.000975
30	0.00094917	0.00018138	0.000949
50	0.00102103	0.00014966	0.000975
70	0.00088496	0.00014966	0.000930
100	0.00074230	0.00016366	0.000689

LS Means Plot

LSMeans Differences Tukey HSD

α= 0.050 Q= 3.22319



Response Ks, Adj

Duty Cycle

LSMeans Differences Tukey HSD

LSMean[j]

LSMean[i]	Mean[i]-Mean[j] Std Err Dif Lower CL Dif Upper CL Dif	5	10	20	30	50	70	100
	5	0	-0.0001	0.00011	0.00014	6.71e-5	0.0002	0.00035
		0	0.00026	0.00026	0.00026	0.00024	0.00024	0.00024
		0	-0.001	-0.0007	-0.0007	-0.0007	-0.0006	-0.0004
		0	0.00069	0.00094	0.00097	0.00083	0.00096	0.00113
	10	0.00013	0	0.00025	0.00027	0.0002	0.00034	0.00048
		0.00026	0	0.00026	0.00026	0.00024	0.00024	0.00024
		-0.0007	0	-0.0006	-0.0006	-0.0006	-0.0004	-0.0003
		0.00096	0	0.00107	0.0011	0.00096	0.0011	0.00127
	20	-0.0001	-0.0002	0	2.61e-5	-4.6e-5	0.00009	0.00023
		0.00026	0.00026	0	0.00026	0.00024	0.00024	0.00024
		-0.0009	-0.0011	0	-0.0008	-0.0008	-0.0007	-0.0006
		0.00071	0.00058	0	0.00085	0.00071	0.00085	0.00102
	30	-0.0001	-0.0003	-2.6e-5	0	-0.0001	6.42e-5	0.00021
		0.00026	0.00026	0.00026	0	0.00024	0.00024	0.00024
		-0.001	-0.0011	-0.0009	0	-0.0008	-0.0007	-0.0006
		0.00069	0.00055	0.0008	0	0.00069	0.00082	0.00099
	50	-0.0001	-0.0002	4.57e-5	7.19e-5	0	0.00014	0.00028
		0.00024	0.00024	0.00024	0.00024	0	0.00021	0.00022
		-0.0008	-0.001	-0.0007	-0.0007	0	-0.0006	-0.0004
		0.00069	0.00056	0.0008	0.00083	0	0.00083	0.001
	70	-0.0002	-0.0003	-0.0001	-0.0001	-0.0001	0	0.00014
		0.00024	0.00024	0.00024	0.00024	0.00021	0	0.00022
		-0.001	-0.0011	-0.0008	-0.0008	-0.0008	0	-0.0006
		0.00055	0.00042	0.00067	0.00069	0.00055	0	0.00085
	100	-0.0003	-0.0005	-0.0002	-0.0002	-0.0003	-0.0001	0
		0.00024	0.00024	0.00024	0.00024	0.00022	0.00022	0
		-0.0011	-0.0013	-0.001	-0.001	-0.001	-0.0009	0
		0.00044	0.00031	0.00055	0.00058	0.00044	0.00057	0

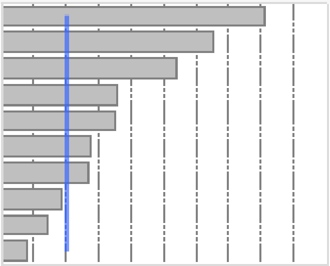
Level		Least Sq Mean
10	A	0.00122288
5	A	0.00108814
50	A	0.00102103
20	A	0.00097531
30	A	0.00094917
70	A	0.00088496
100	A	0.00074230

Levels not connected by same letter are significantly different.

Appendix F: AOP Regression Report

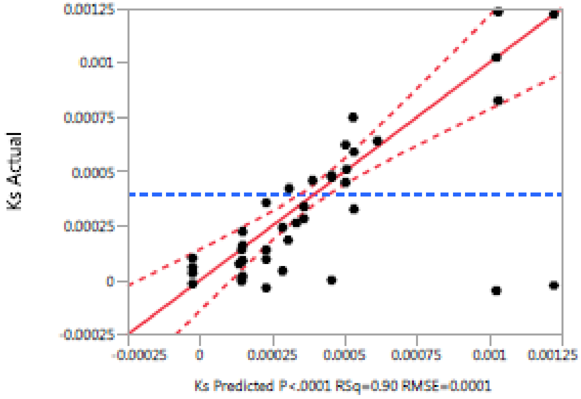
Response Ks

Effect Summary



Source	LogWorth	PValue
DV DC 100	8.138	0.00000
DV DC 70	6.563	0.00000
DV DC 50	5.380	0.00000
DV pH6	3.578	0.00026
DV pH6*DV DC 100	3.489	0.00032
DV pH7*DV DC 100	2.802	0.00158
DV pH6*DV DC 70	2.681	0.00209
DV pH9	1.905	0.01245
DV DC 30	1.426	0.03747
DV pH7	0.778	0.16680 ^

Actual by Predicted Plot



Summary of Fit

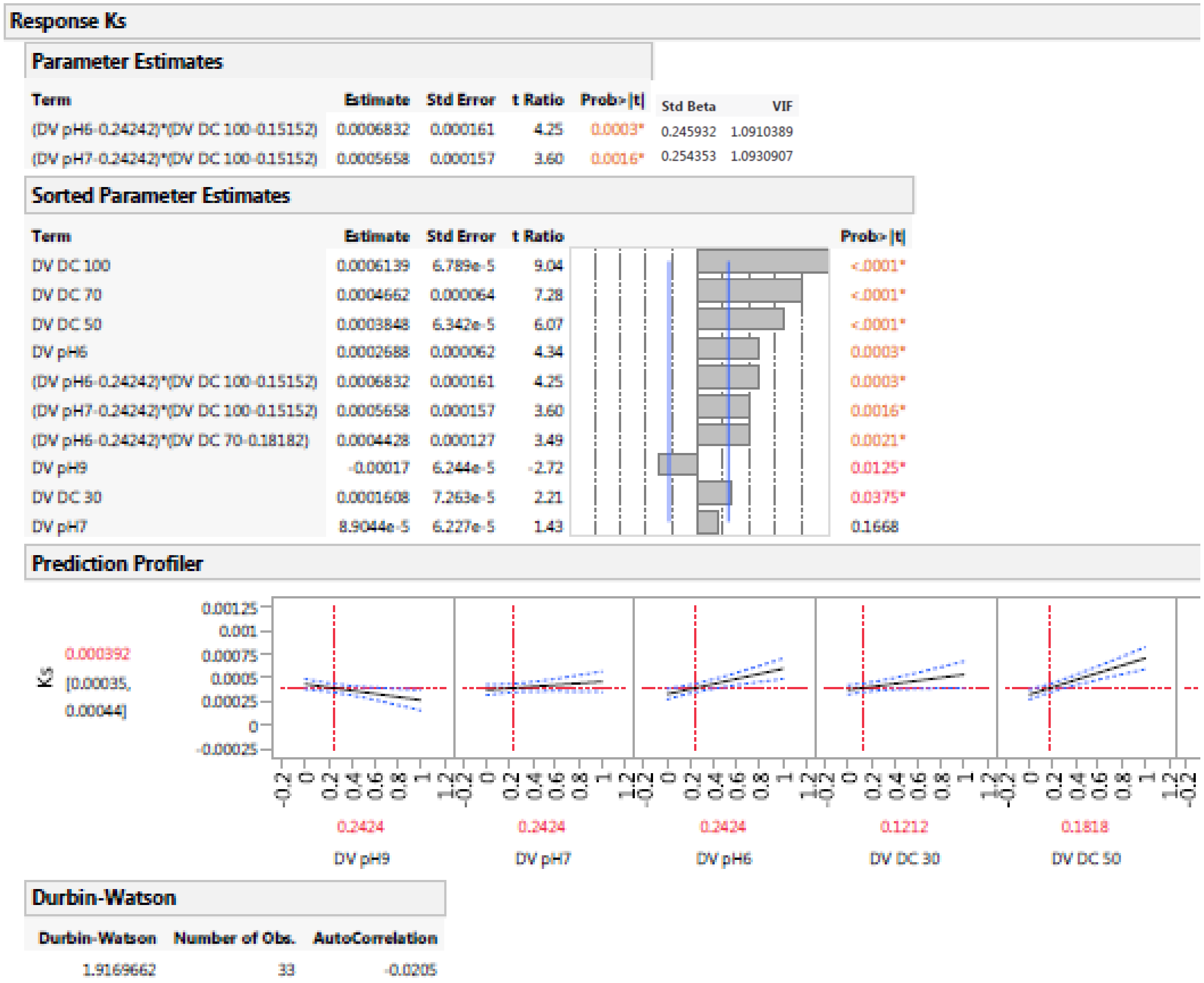
RSquare	0.899731
RSquare Adj	0.854155
Root Mean Square Error	0.000126
Mean of Response	0.000391
Observations (or Sum Wgts)	33

Analysis of Variance

Source	DF	Sum of Squares	Mean Square	F Ratio
Model	10	3.12422e-6	3.1242e-7	19.7410
Error	22	3.48172e-7	1.5826e-8	**Prob > F**
C. Total	32	3.47239e-6		<.0001*

Parameter Estimates

Term	Estimate	Std Error	t Ratio	Prob>|t|	Std Beta	VIF
Intercept	7.8989e-5	5.237e-5	1.51	0.1457	0	.
DV pH9	-0.00017	6.244e-5	-2.72	0.0125*	0.355112	1.4702044
DV pH7	8.9044e-5	6.227e-5	1.43	0.1668	0.117639	1.485137
DV pH6	0.0002688	0.000062	4.34	0.0003*	0.161821	1.1717172
DV DC 30	0.0001608	7.263e-5	2.21	0.0375*	0.457516	1.247506
DV DC 50	0.0003848	6.342e-5	6.07	<.0001*	0.554353	1.2731293
DV DC 70	0.0004662	0.000064	7.28	<.0001*	0.678575	1.2353928
DV DC 100	0.0006139	6.789e-5	9.04	<.0001*	-0.22452	1.4929043
(DV pH6-0.24242)*(DV DC 70-0.18182)	0.0004428	0.000127	3.49	0.0021*	0.307121	1.1433804



Response Ks

Parameter Estimates

Term	Estimate	Std Error	t Ratio	Prob>|t|	Std Beta	VIF
(DV pH6-0.24242)*(DV DC 100-0.15152)	0.0006832	0.000161	4.25	0.0003*	0.245932	1.0910389
(DV pH7-0.24242)*(DV DC 100-0.15152)	0.0005658	0.000157	3.60	0.0016*	0.254353	1.0930907

Sorted Parameter Estimates

Term	Estimate	Std Error	t Ratio	Prob>|t|
DV DC 100	0.0006139	6.789e-5	9.04	<.0001*
DV DC 70	0.0004662	0.000064	7.28	<.0001*
DV DC 50	0.0003848	6.342e-5	6.07	<.0001*
DV pH6	0.0002688	0.000062	4.34	0.0003*
(DV pH6-0.24242)*(DV DC 100-0.15152)	0.0006832	0.000161	4.25	0.0003*
(DV pH7-0.24242)*(DV DC 100-0.15152)	0.0005658	0.000157	3.60	0.0016*
(DV pH6-0.24242)*(DV DC 70-0.18182)	0.0004428	0.000127	3.49	0.0021*
DV pH9	-0.00017	6.244e-5	-2.72	0.0125*
DV DC 30	0.0001608	7.263e-5	2.21	0.0375*
DV pH7	8.9044e-5	6.227e-5	1.43	0.1668

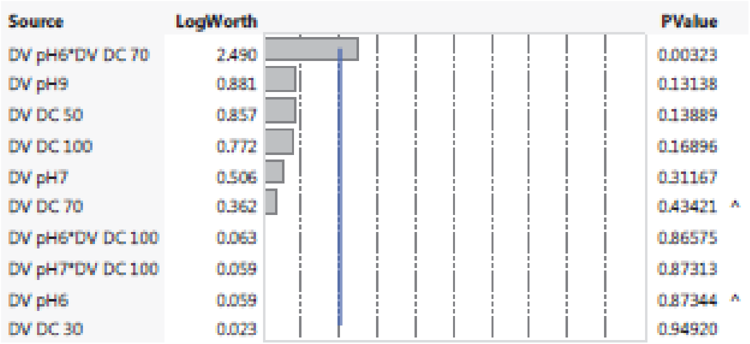
Prediction Profiler

Durbin-Watson

Durbin-Watson	Number of Obs.	AutoCorrelation
1.9169662	33	-0.0205

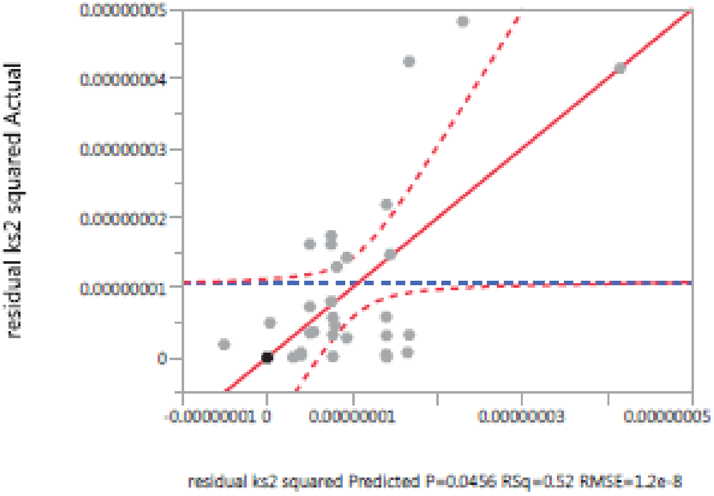
Response residual ks2 squared

Effect Summary



Source	LogWorth	PValue
DV pH6*DV DC 70	2.490	0.00323
DV pH9	0.881	0.13138
DV DC 50	0.857	0.13889
DV DC 100	0.772	0.16896
DV pH7	0.506	0.31167
DV DC 70	0.362	0.43421 ^
DV pH6*DV DC 100	0.063	0.86575
DV pH7*DV DC 100	0.059	0.87313
DV pH6	0.059	0.87344 ^
DV DC 30	0.023	0.94920

Actual by Predicted Plot



Summary of Fit

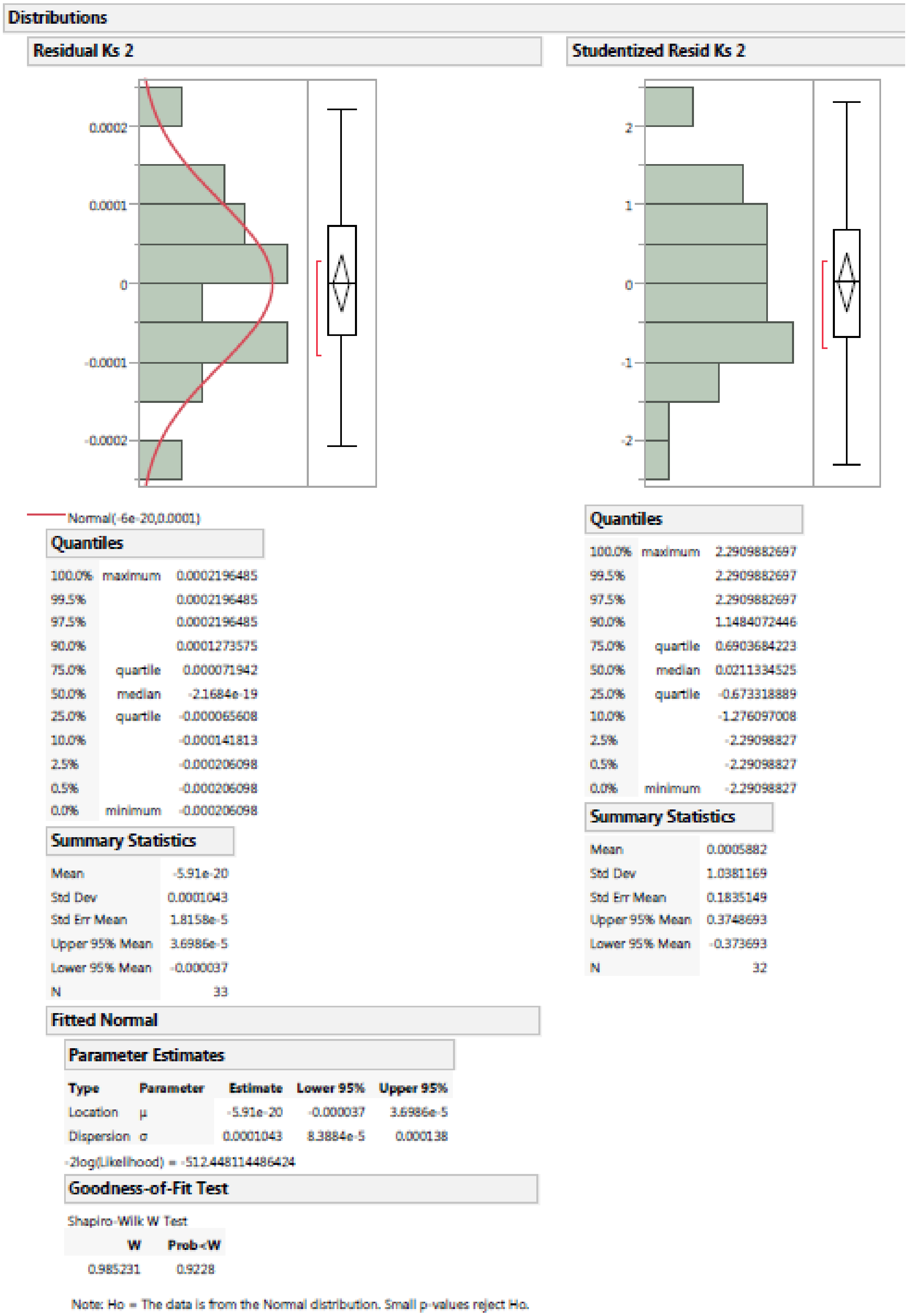
RSquare	0.516492
RSquare Adj	0.296716
Root Mean Square Error	1.159e-8
Mean of Response	1.055e-8
Observations (or Sum Wgts)	33

Analysis of Variance

Source	DF	Sum of Squares	Mean Square	F Ratio
Model	10	3.1588e-15	3.159e-16	2.3501
Error	22	2.9571e-15	1.344e-16	**Prob > F**
C. Total	32	6.1159e-15		0.0456*

Lack Of Fit

Source	DF	Sum of Squares	Mean Square	F Ratio
Lack Of Fit	9	1.6727e-15	1.859e-16	1.8811
Pure Error	13	1.2844e-15	9.88e-17	**Prob > F**
Total Error	22	2.9571e-15		0.1456
				Max RSq
				0.7900



Distributions

Residual Ks 2

Normal(-6e-20,0.0001)

Quantiles

100.0%	maximum	0.0002196485
99.5%		0.0002196485
97.5%		0.0002196485
90.0%		0.0001273575
75.0%	quartile	0.000071942
50.0%	median	-2.1684e-19
25.0%	quartile	-0.000065608
10.0%		-0.000141813
2.5%		-0.000206098
0.5%		-0.000206098
0.0%	minimum	-0.000206098

Summary Statistics

Mean	-5.91e-20
Std Dev	0.0001043
Std Err Mean	1.8158e-5
Upper 95% Mean	3.6986e-5
Lower 95% Mean	-0.000037
N	33

Fitted Normal

Parameter Estimates

Type	Parameter	Estimate	Lower 95%	Upper 95%
Location	μ	-5.91e-20	-0.000037	3.6986e-5
Dispersion	σ	0.0001043	8.3884e-5	0.000138

-2log(Likelihood) = -512.448114486424

Goodness-of-Fit Test

Shapiro-Wilk W Test

W	Prob<W
0.985231	0.9228

Note: Ho = The data is from the Normal distribution. Small p-values reject Ho.

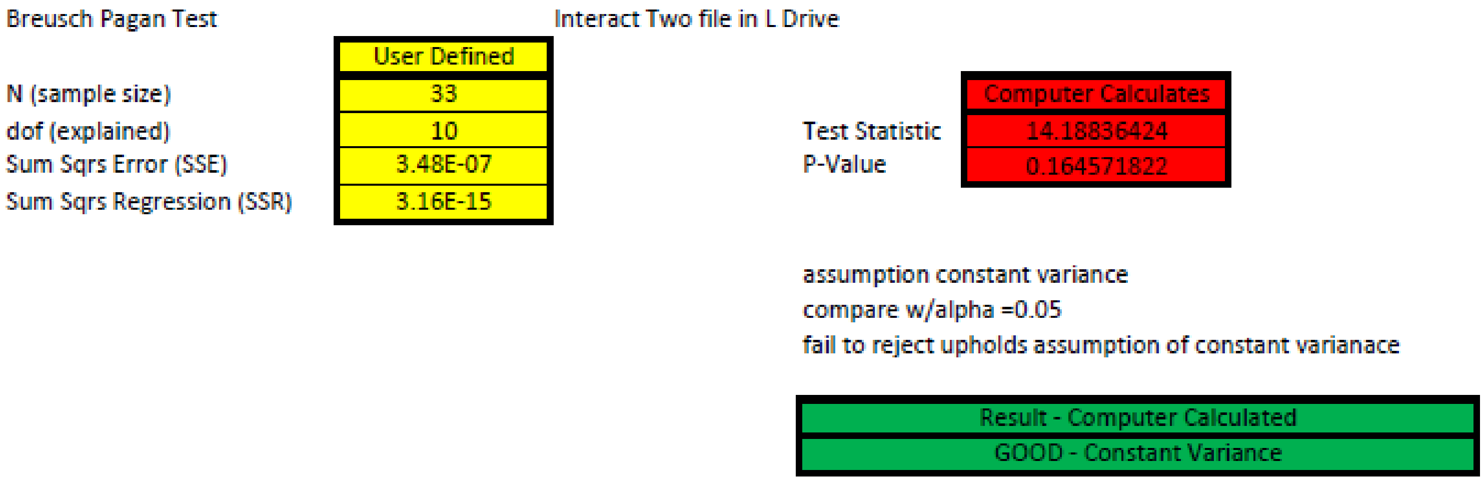
Studentized Resid Ks 2

Quantiles

100.0%	maximum	2.2909882697
99.5%		2.2909882697
97.5%		2.2909882697
90.0%		1.1484072446
75.0%	quartile	0.6903684223
50.0%	median	0.0211334525
25.0%	quartile	-0.673318889
10.0%		-1.276097008
2.5%		-2.29098827
0.5%		-2.29098827
0.0%	minimum	-2.29098827

Summary Statistics

Mean	0.0005882
Std Dev	1.0381169
Std Err Mean	0.1835149
Upper 95% Mean	0.3748693
Lower 95% Mean	-0.373693
N	32



Breusch Pagan Test

Interact Two file in L Drive

	User Defined
N (sample size)	33
dof (explained)	10
Sum Sqrs Error (SSE)	3.48E-07
Sum Sqrs Regression (SSR)	3.16E-15

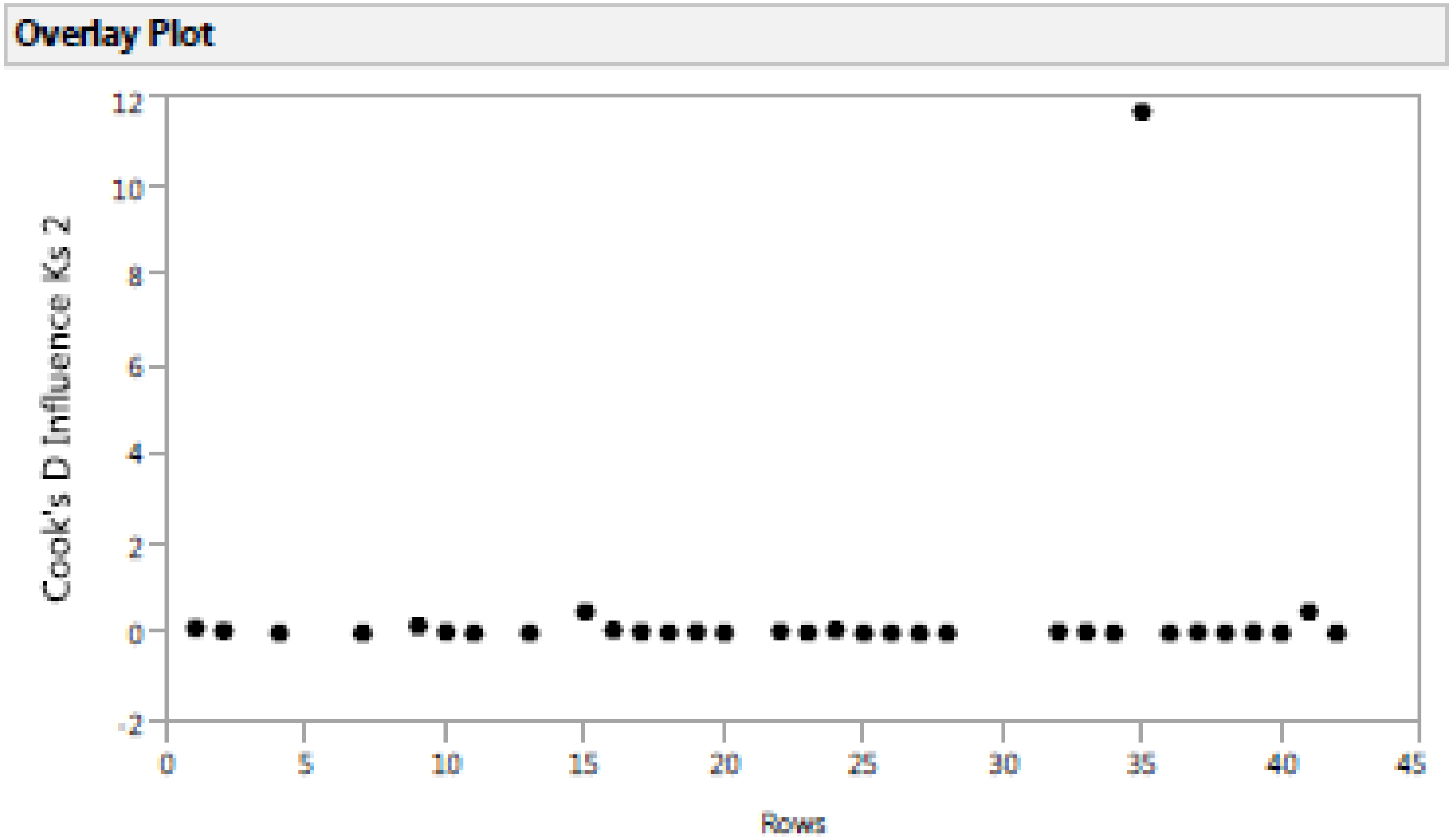
	Computer Calculates
Test Statistic	14.18836424
P-Value	0.164571822

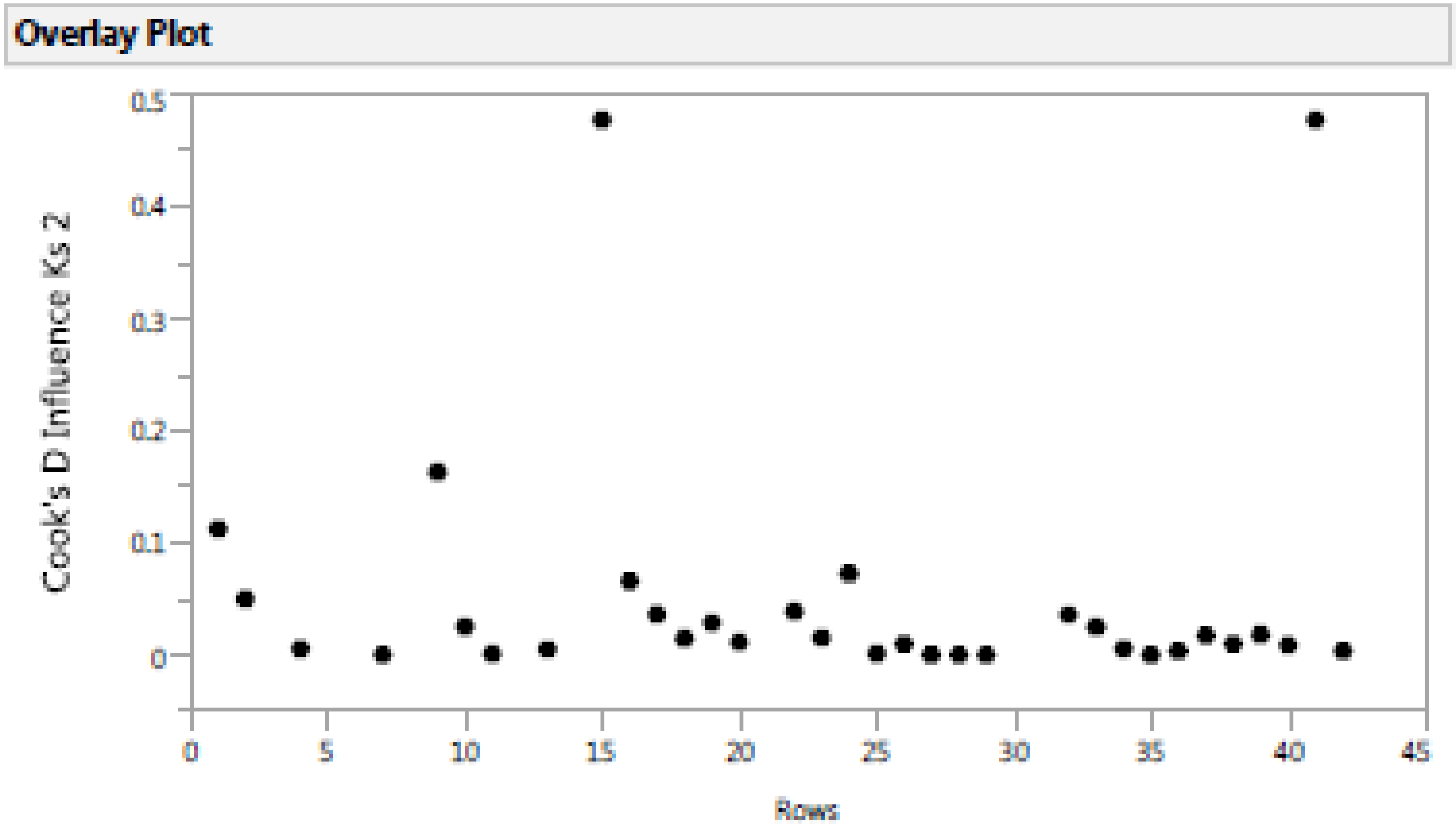
assumption constant variance

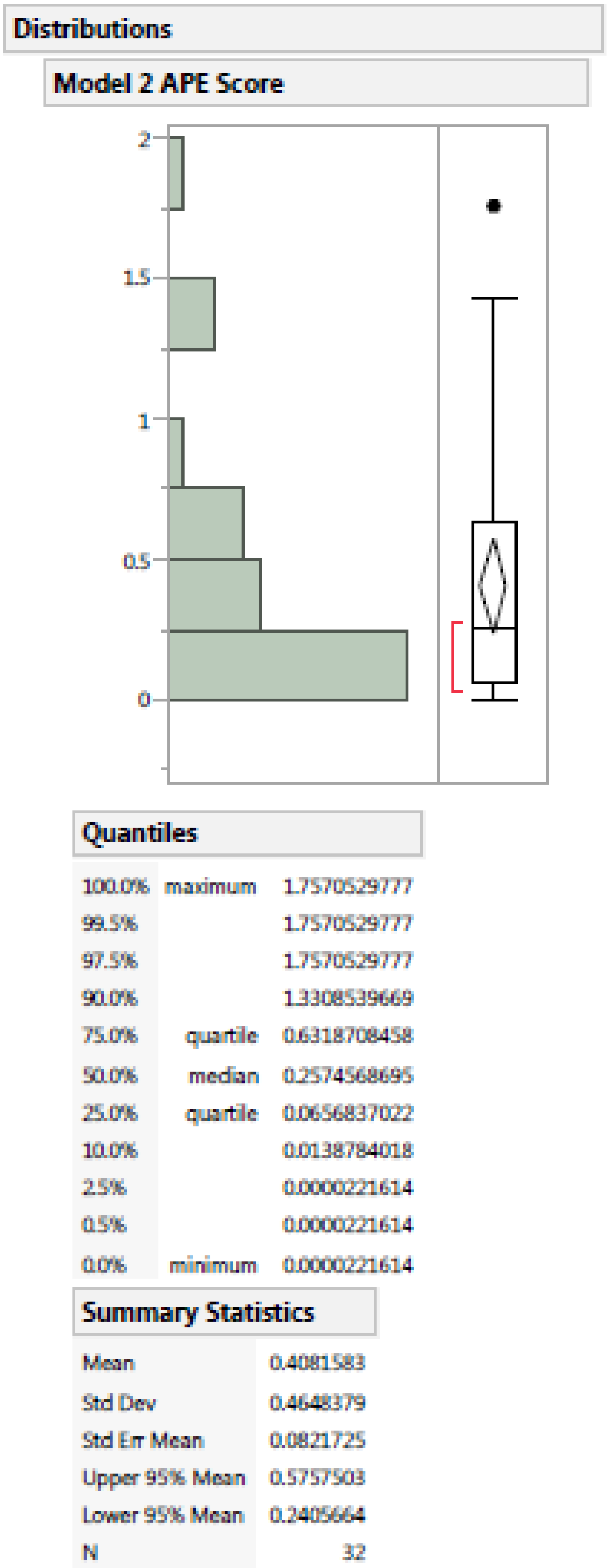
compare w/alpha =0.05

fail to reject upholds assumption of constant varianace

Result - Computer Calculated
GOOD - Constant Variance


Overlay Plot
Cook's D Influence Ks 2
12
10
8
6
4
2
0
-2
0
5
10
15
20
25
30
35
40
45
Rows


Overlay Plot
Cook's D Influence Ks 2
0.5
0.4
0.3
0.2
0.1
0
0
5
10
15
20
25
30
35
40
45
Rows



Distributions

Model 2 APE Score

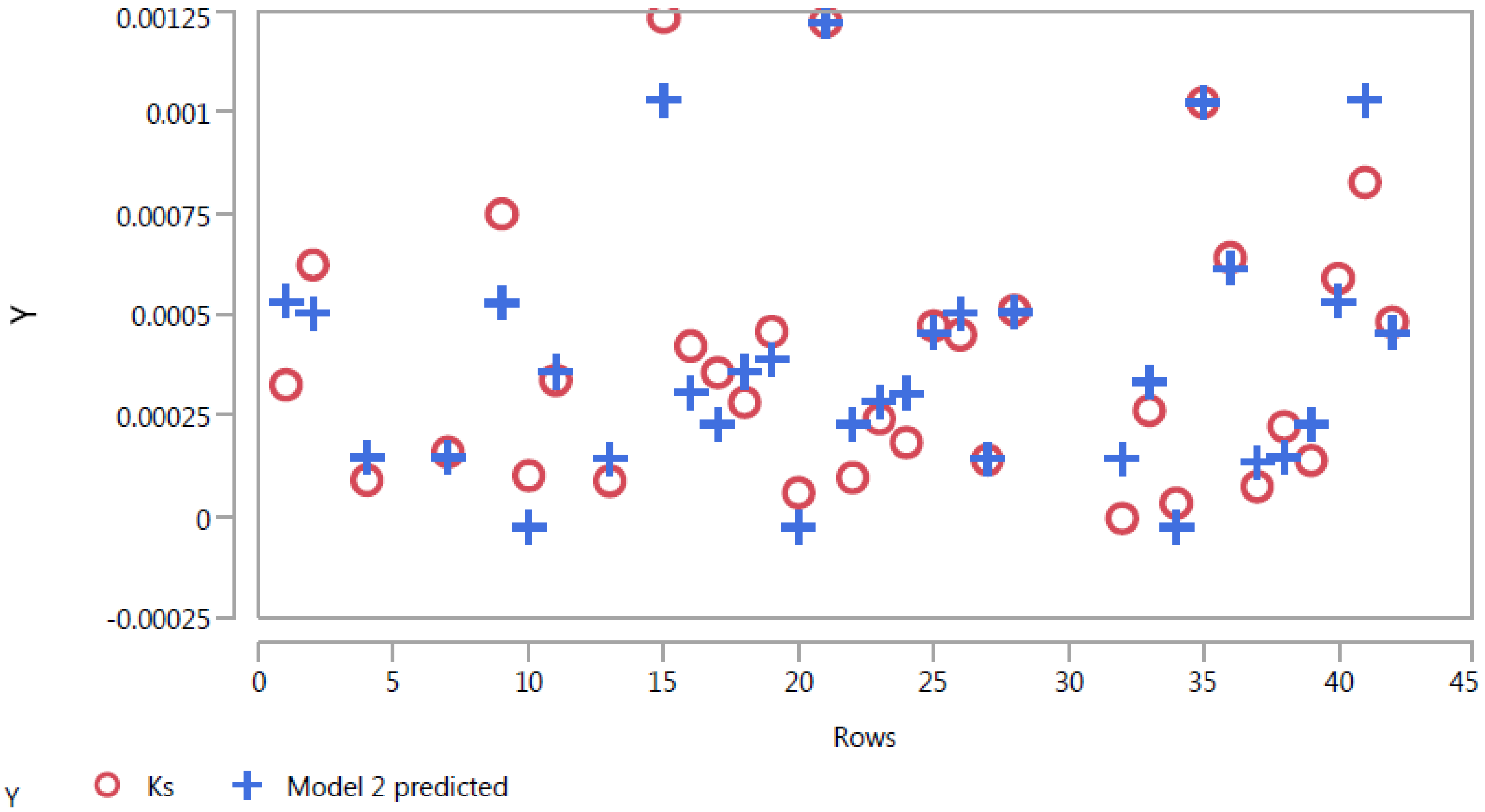
Quantiles

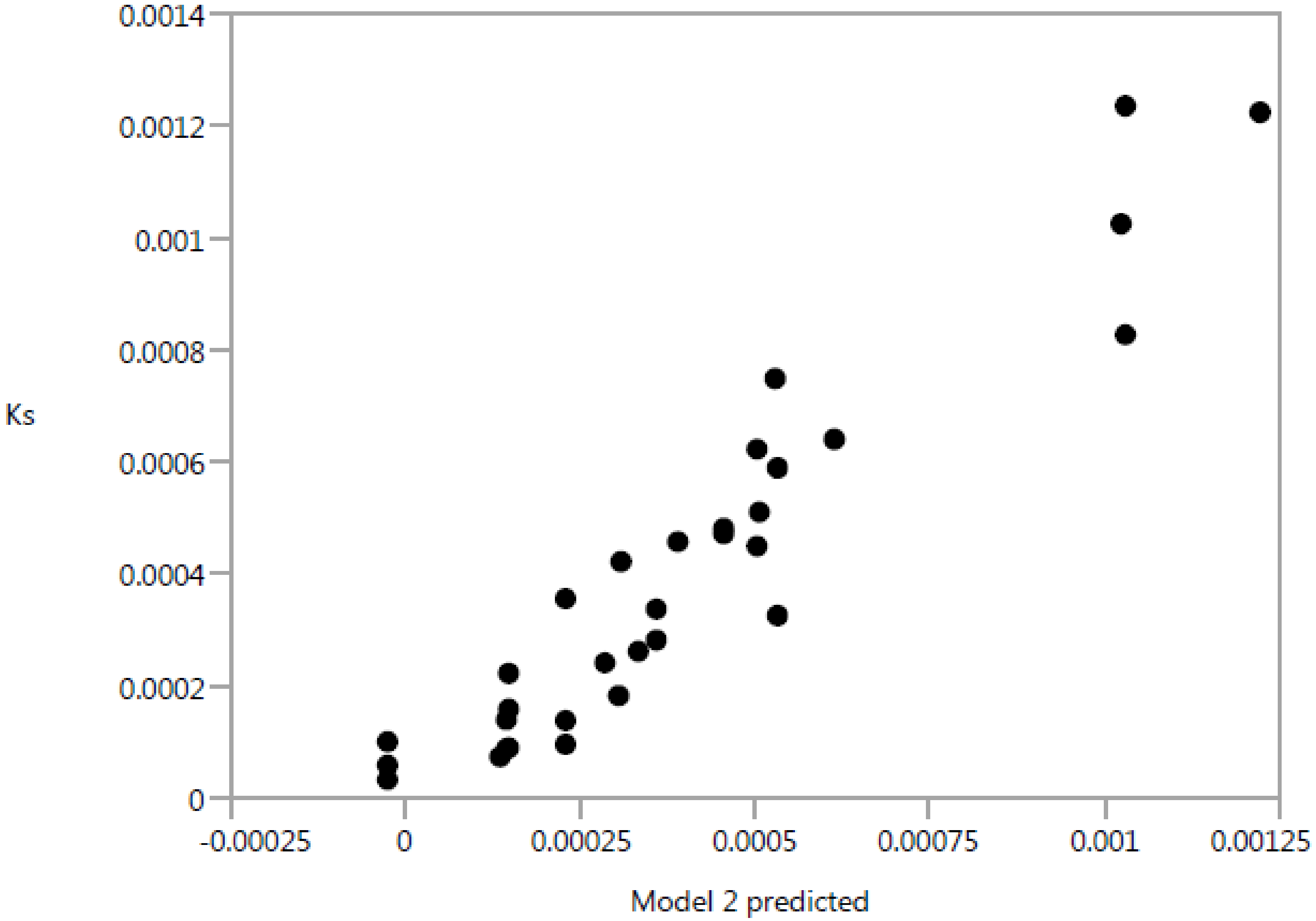
100.0%	maximum	1.7570529777
99.5%		1.7570529777
97.5%		1.7570529777
90.0%		1.3308539669
75.0%	quartile	0.6318708458
50.0%	median	0.2574568695
25.0%	quartile	0.0656837022
10.0%		0.0138784018
2.5%		0.0000221614
0.5%		0.0000221614
0.0%	minimum	0.0000221614

Summary Statistics

Mean	0.4081583
Std Dev	0.4648379
Std Err Mean	0.0821725
Upper 95% Mean	0.5757503
Lower 95% Mean	0.2405664
N	32

Overlay Plot



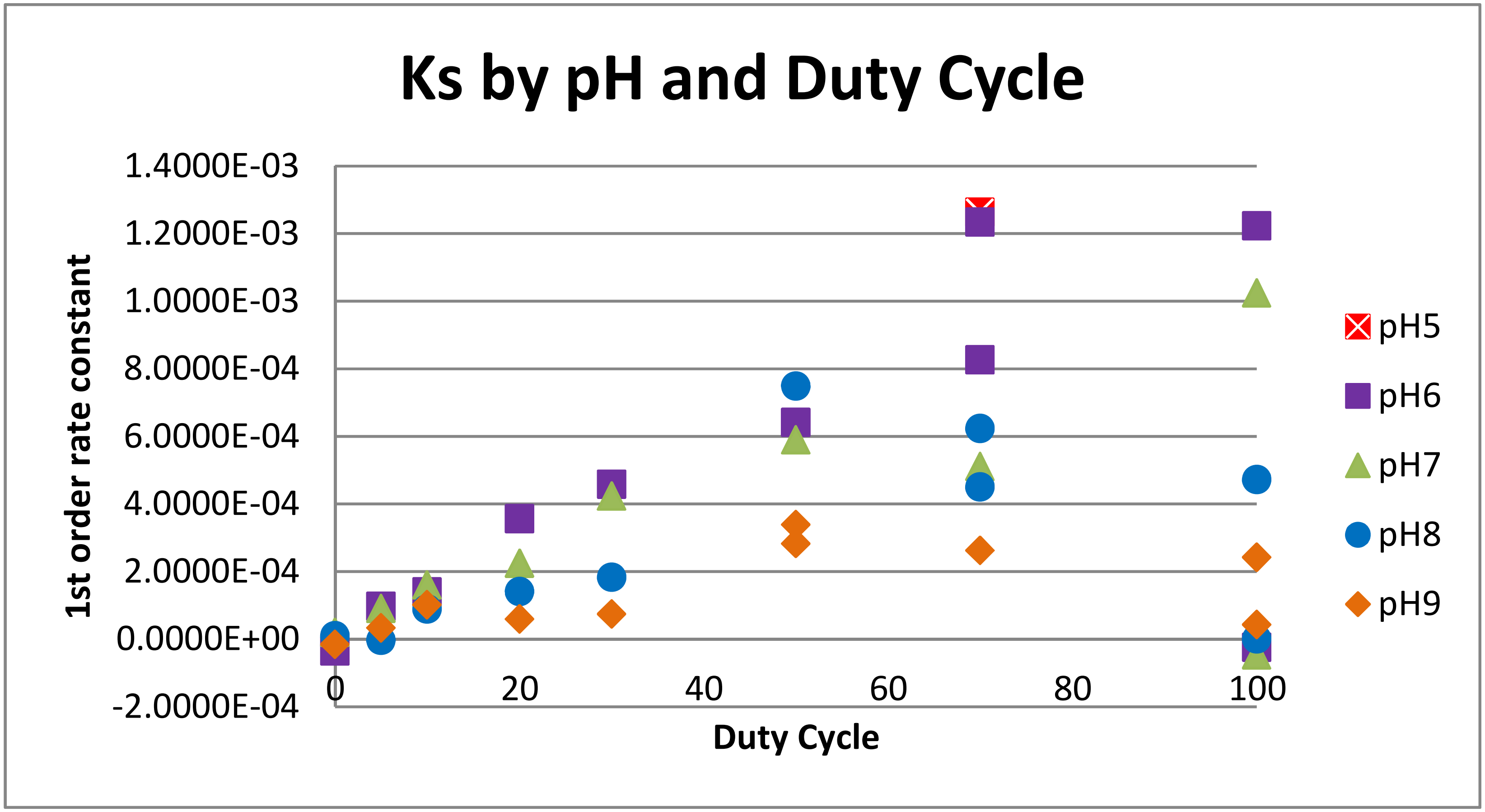


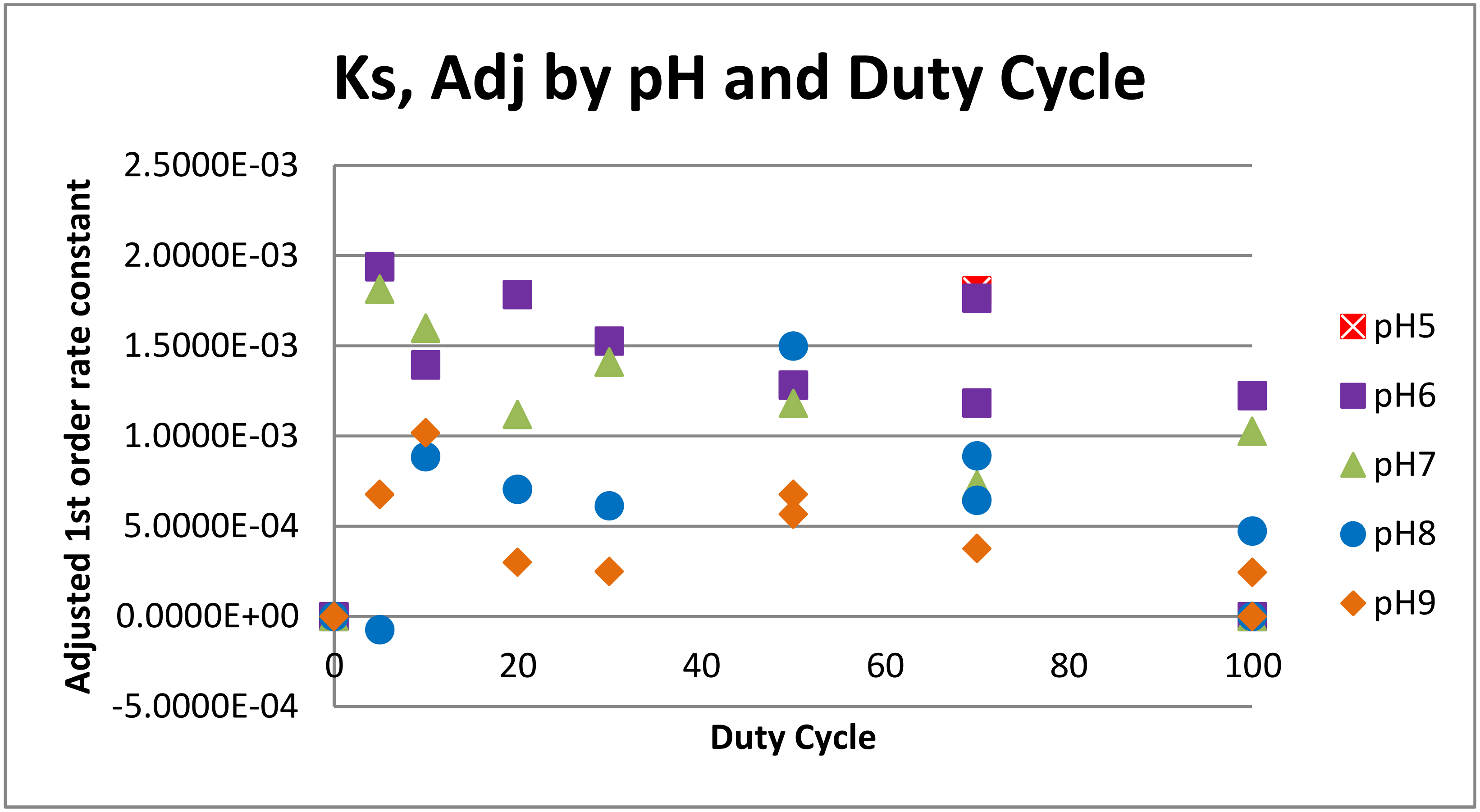
Ks
0.0014
0.0012
0.001
0.0008
0.0006
0.0004
0.0002
0
-0.00025
0
0.00025
0.0005
0.00075
0.001
0.00125
Model 2 predicted

Appendix G: First Order Reaction Constant (Apparent and Adjusted) Charts

Ks	pH5	pH6	pH7	pH8	pH9
100		-2.4032E-05	-4.7812E-05	9.4125E-07	4.3388E-05
0		-3.5141E-05	1.9741E-05	9.8817E-06	-1.5526E-05
5		9.6902E-05	9.0691E-05	-3.7994E-06	3.3837E-05
10		1.3923E-04	1.5964E-04	8.8471E-05	1.0181E-04
20		3.5649E-04	2.2352E-04	1.4060E-04	5.9627E-05
30		4.5805E-04	4.2257E-04	1.8371E-04	7.4676E-05
50		6.4074E-04	5.8957E-04	7.4882E-04	3.3801E-04
70	1.2624E-03	1.2346E-03	5.1079E-04	6.2298E-04	2.6271E-04
100		1.2235E-03	1.0246E-03	4.7230E-04	2.4222E-04
50					2.8300E-04
70		8.2701E-04		4.5001E-04	
100				4.8199E-04	

Ks, adj	pH5	pH6	pH7	pH8	pH9
100		0.0000E+00	0.0000E+00	0.0000E+00	0.0000E+00
0		0.0000E+00	0.0000E+00	0.0000E+00	0.0000E+00
5		1.9380E-03	1.8138E-03	-7.5987E-05	6.7673E-04
10		1.3923E-03	1.5964E-03	8.8471E-04	1.0181E-03
20		1.7825E-03	1.1176E-03	7.0298E-04	2.9814E-04
30		1.5268E-03	1.4086E-03	6.1237E-04	2.4892E-04
50		1.2815E-03	1.1791E-03	1.4976E-03	6.7602E-04
70	1.8034E-03	1.7637E-03	7.2970E-04	8.8997E-04	3.7530E-04
100		1.2235E-03	1.0246E-03	4.7230E-04	2.4222E-04
50					5.6600E-04
70		1.1814E-03		6.4288E-04	
100				4.8199E-04	


Ks by pH and Duty Cycle
1st order rate constant
1.4000E-03
1.2000E-03
1.0000E-03
8.0000E-04
6.0000E-04
4.0000E-04
2.0000E-04
0.0000E+00
-2.0000E-04
0
20
40
60
80
100
Duty Cycle
pH5
pH6
pH7
pH8
pH9


Ks, Adj by pH and Duty Cycle
Adjusted 1st order rate constant
2.5000E-03
2.0000E-03
1.5000E-03
1.0000E-03
5.0000E-04
0.0000E+00
-5.0000E-04
0
20
40
60
80
100
Duty Cycle
pH5
pH6
pH7
pH8
pH9

Appendix H: Positive Ionization HPLC Method File

```
Data File  : D:\data\tarr\20150824_TAR_STEWART 2015-08-24 09-11-48\tar1000017.D
Acq. Method: 1500819A_TAR_MS.M


The Acq. Method's Instrument Parameters for the Run were :


=====================================================================
                    Fraction Collector
=====================================================================

Fraction Collector (G1364C)
===========================

Peak Detector Mode:            at least one peak detector
Rinse Needle At Start Of Collection:                No
Rinse Needle Between Collection:                    No

Fraction Trigger Mode
Fraction Trigger Mode:                        Off

Fill Volume
Fill Volume Mode:                       As Configured

Peak Detectors
Peak Detector
  Detector type with serial number   Unit   Up Slope

-----------------------------------------------------
             G1315C:DEAA200974    mAU      5.00
             G1321B:DEABW04663     LU      5.00


  Down Slope   Threshold   Upper Threshold   Mode

--------------------------------------------------
       5.00      5.000        3000.000    Off
       5.00      5.000        3000.000    Off




Stop Time
Stoptime Mode:                       As pump/injector

Post Time
Posttime Mode:                                Off
```

```
Timetable



Instrument Curves
Store Temperature:                     No





=====================================================
                 FLD
=====================================================

FLD (G1321B)
============

Detection Mode:               Fluorescence Mode
Fit spectra range on:                Yes
PMT gain:                         10
Baseline Behaviour Mode:              Append
Peakwidth:       > 0.2 min (4 s resp. time) (2.31 Hz)
Analog Output Source Channel 1:             1
Analog Output Source Channel 2:             2
Signal polarity:              Positive (+)

Signal A

Excitation
Use Signal:                      Yes
Signal:                      Signal A
Wavelength Mode:                   Wavel. Set
Excitation Wavelength:               200 nm

Emission
Use Signal:                      Yes
Signal:                      Signal A
Wavelength Mode:                   Wavel. Set
Emission Wavelength:                 410 nm

Multiple Wavelengths
Multi Wavelength Mode:             Multi Emission
```

```
Emission Signals
Emission Signal
  Use   Signal      Mode   Em. Wavel.
                      nm
---------------------------------------
  Yes Signal B Wavel. Set        500
  Yes Signal C Wavel. Set        650
  Yes Signal D Wavel. Set        700




Acquire Spectra
Acquire Spectra Mode:                          None

Fluorescence Scan Range

Excitation Scan
Scan Excitation WL From:                      220 nm
Scan Excitation WL To:                      380 nm
Scan Excitation WL Step:                      5 nm

Emission Scan
Scan Emission WL From:                        300 nm
Scan Emission WL To:                        500 nm
Scan Emission WL Step:                        5 nm

Lamp Settings
Lamp on only during run:                        Yes
Lamp on required for analysis:                     No
Lamp economy mode on:                              No
Lamp energy reference mode on:                      Yes

Analog Output 1
Analog 1 Zero Offset:                         5 %
Analog 1 Attenuation:                       100 LU

Analog Output 2
Analog 2 Zero Offset:                         5 %
Analog 2 Attenuation:                       100 LU

Stoptime
Stoptime Mode:                       As pump/injector

Posttime
Posttime Mode:                              Off
```

```
Timetable






=============================================================
                    DAD
=============================================================

DAD (G1315C)
============

Peakwidth:        >0.10 min  (2.0 s response time) (2.5 Hz)
Slit:                                 4 nm
UV Lamp Required:                            No
Vis Lamp Required:                           No

Analog Output 1
Analog 1 Zero Offset:                        5 %
Analog 1 Attenuation:                     1000 mAU

Analog Output 2
Analog 2 Zero Offset:                        5 %
Analog 2 Attenuation:                     1000 mAU

Signals
Signal table
  Use Sig.   Signal   Wavelength   Bandwidth   Use Ref.
                        nm         nm
---------------------------------------------------------
     Yes Signal A        414        200       Yes
      No Signal B
     Yes Signal C        430          5       Yes
      No Signal D
      No Signal E
      No Signal F
      No Signal G
      No Signal H


  Ref Wavel.   Ref Bandw.
        nm          nm
--------------------------
```

```
        360         100

        360         100







Prepare Mode
Margin for negative Absorbance:                 100 mAU

Autobalance
Autobalance Prerun:                             Yes
Autobalance Postrun:                             No

Spectrum
Spectrum Store:                              None

Stoptime
Stoptime Mode:                         As pump/injector

Posttime
Posttime Mode:                                Off

Timetable



Instrument Curves
Store Board Temperature:                          No
Store Optical Unit Temperature:                     No
Store UV Lamp Anode Voltage:                        No



=====================================================================
                    Column Comp.
=====================================================================
```

```
Column Comp. (G1316A)
====================

Valve Position:                    Port 1 -> 2

Left Temperature Control
Temperature Control Mode:                 Not Controlled

Enable Analysis Left Temperature
Enable Analysis Left Temperature On:                  Yes
Enable Analysis Left Temperature Value:           0.80 °C

Right Temperature Control
Right temperature Control Mode:           Temperature Set
Right temperature:                        35.00 °C

Enable Analysis Right Temperature
Enable Analysis Right Temperature On:                 Yes
Enable Analysis Right Temperature Value:          0.80 °C

Stop Time
Stoptime Mode:                     As pump/injector

Post Time
Posttime Mode:                            Off

Timetable




Instrument Curves
Store Left Temperature:                        Yes
Store Right Temperature:                         No






==========================================================
                 HiP Sampler
==========================================================

HiP Sampler (G1367E)
===================
```

Auxiliary
Draw Speed: 100.0 µl/min
Eject Speed: 100.0 µl/min
Draw Position Offset: 0.0 mm
Wait Time After Drawing: 2.0 s
Sample Flush Out Factor: 5.0
Vial/Well bottom sensing: No

Injection
Injection Mode: Standard injection
Injection Volume: 5.00 µL

High throughput
Automaitc Delay Volume Reduction: No

Overlapped Injection
Enable Overlapped Injection: No

Valve Switching
Valve Movements: 0

Valve Switch Time 1
Switch Time 1 Enabled: No

Valve Switch Time 2
Switch Time 2 Enabled: No

Valve Switch Time 3
Switch Time 3 Enabled: No

Valve Switch Time 4
Switch Time 4 Enabled: No

Stop Time
Stoptime Mode: As pump/No limit

Post Time
Posttime Mode: Off

Timetable

Instrument Curves
Store Temperature: No

```
====================================================
                Valve
====================================================

Valve (G1170A)
==============

Position Switching Mode:              Use valve position
Valve position:                              1
After Run Position Switching Mode:          Do not switch

Stop Time
Stoptime Mode:                    As pump/injector

Post Time
Posttime Mode:                               Off

Timetable

Position Description
  Position   Position Description

---------------------------------
     1            MS
     2            FLD
     3            DAD
     4         Channel 4
     5         Channel 5
     6         Channel 6
     7         Channel 7
     8         Channel 8
     9          by pass
    10         Channel 10
    11         Channel 11
    12         Channel 12
```

```
====================================================
              Quat. Pump
====================================================

Quat. Pump (G1311B)
===================

Low Pressure Limit:                0.00 bar
High Pressure Limit:             550.00 bar
Flow:                        0.350 ml/min
Maximum Flow Gradient:            100.000 ml/min²
Primary Channel:                 Automatic

Stop Time
Stoptime Mode:                    Time set
Stoptime:                      25.00 min

Post Time
Posttime Mode:                       Off

Compress
Compressibility Mode:      Compressibility Value Set
Compressibility:              100 10e-6/bar

Stroke
Automatic Stroke Calculation:            Yes

Timetable

Solvent Composition
  Channel  Name 1  Used  Percent
                  %
-----------------------------------
     A        Yes    40.0
     B        Yes    50.0
     C        Yes    10.0
     D         No
```

```
Instrument Curves
Store Pressure:                    Yes
Store Flow:                        Yes
Store Solvent Ratio A:                 Yes
Store Solvent Ratio B:                 Yes
Store Solvent Ratio C:                 Yes
Store Solvent Ratio D:                 Yes
Store Direction of Piston A:               No




=============================================
              Mass Spectrometer Detector
=============================================


General Information
------- -----------

Use MSD              : Enabled
Tune File            : atunes.tun
StopTime             : No Limit
Time Filter          : Enabled
Data Storage         : Condensed
Peakwidth            : 0.10 min
Fast Scan            : Disabled
Fast Scan Data Reconstruction: Disabled
Polarity Switch Delay    : 50 ms
Ionization Switch Delay  : 50 ms


Signals
-------

[Signal 1]

Not Active


[Signal 2]

Ionization Mode        : API-ES
Polarity               : Positive
Fragmentor Ramp        : Disabled
Percent Cycle Time     : 100.00 %
```

```
Scan Parameters

  Time |      Mass Range    |Frag- | Gain|Thres-| Step-
 (min) |    Low   |  High   |mentor| EMV | hold | size
-------|----------|---------|------|-----|------|-------
   0.00    100.00    700.00    70    1.0     150  0.10


[Signal 3]

Not Active


[Signal 4]

Not Active



Spray Chamber
----- -------

[MSZones]

Gas Temp              : 300 C              maximum 350 C
DryingGas             : 10.0 l/min          maximum 13.0 l/min
Neb Pres              : 45 psig             maximum 60 psig
Quad Temp               : 0 C               maximum 0 C

VCap (Positive)         : 3000 V
VCap (Negative)          : 3500 V

[Time Table]

Time Table is empty.



                 END OF MS ACQUISITION PARAMETERS

========================================================
                        FIA Series
========================================================

FIA Series in this Method   :     Disabled
```

```
Time Setting
   Time between Injections   :     0.15 min
   Injection Loop Flush Time :     0.17 min

=========================================================
                       Column(s)
=========================================================

Column Description :  Ascentis Exp C18
Serial#           :  USMD005296
Product#          :  53822-U          Batch# :
Diameter          :  2.1 mm          Length :   50.0 mm
Particle size      :  2.7 µm      Void volume :   60.0 %
Maximum Pressure   :  400.0 bar      Maximum pH :      9.0
    Minimum pH :      2.0
Maximum Temperature:   60.0 °C
Comment           :
```

Appendix I: Negative Ionization HPLC Method File

```
                 Method Information

        Method: D:\METHOD\1500819A_TAR_MS.M
      Modified: 8/25/2015 at 1:15:13 PM


                 Method Audit Trail

Operator   : user
Date       : 8/19/2015 11:13:50 AM
Change Info: This method was created at 8/19/2015 11:13:50 AM and based on
             method D:\METHOD\1500819_TAR_MS.M

Operator   : user
Date       : 8/19/2015 11:13:52 AM
Change Info: Method saved. User comment: ""

Operator   : user
Date       : 8/24/2015 9:01:21 AM
Change Info: Method saved. User comment: ""



                 Run Time Checklist

        Pre-Run Cmd/Macro:  off

         Data Acquisition:  on

   Standard Data Analysis:  on

 Customized Data Analysis:  off

            Save GLP Data:  off

       Post-Run Cmd/Macro:  off


    Save Method with Data:  off



              Injection Source and Location

  Injection Source:   HipAls
```

```
  Injection Location: HipAls

==================================================================================


The Acq. Method's Instrument Parameters for the Run were :

Data File  : D:\data\tarr\20150820_TAR_STEWART 2015-08-20 13-47-13\tar1000035.D
Acq. Method: 1500819A_TAR_MS_NEG.M


The Acq. Method's Instrument Parameters for the Run were :



==============================================================================
                   Fraction Collector
==============================================================================

Fraction Collector (G1364C)
==========================

Peak Detector Mode:            at least one peak detector
Rinse Needle At Start Of Collection:                  No
Rinse Needle Between Collection:                      No

Fraction Trigger Mode
Fraction Trigger Mode:                           Off

Fill Volume
Fill Volume Mode:                         As Configured

Peak Detectors
Peak Detector
  Detector type with serial number   Unit   Up Slope

----------------------------------------------------
             G1315C:DEAA200974    mAU       5.00
             G1321B:DEABW04663     LU       5.00


  Down Slope   Threshold   Upper Threshold   Mode

-------------------------------------------------
      5.00      5.000        3000.000    Off
      5.00      5.000        3000.000    Off
```

```
Stop Time
Stoptime Mode:                  As pump/injector

Post Time
Posttime Mode:                          Off

Timetable




Instrument Curves
Store Temperature:                         No





=======================================================
                    FLD
=======================================================

FLD (G1321B)
============

Detection Mode:                 Fluorescence Mode
Peakwidth:          > 0.2 min (4 s resp. time) (2.31 Hz)
PMT gain:                           10
Baseline Behaviour Mode:                Append
Fit spectra range on:                  Yes
Analog Output Source Channel 1:                1
Analog Output Source Channel 2:                2
Signal polarity:                Positive (+)

Stoptime
Stoptime Mode:                  As pump/injector

Posttime
Posttime Mode:                          Off

Multiple Wavelengths
Multi Wavelength Mode:                Multi Emission

Emission Signals
```

```
Emission Signal
  Use   Signal      Mode   Em. Wavel.
                      nm
--------------------------------------
  Yes Signal B Wavel. Set       500
  Yes Signal C Wavel. Set       650
  Yes Signal D Wavel. Set       700




Acquire Spectra
Acquire Spectra Mode:                          None

Analog Output 1
Analog 1 Attenuation:                        100 LU
Analog 1 Zero Offset:                          5 %

Analog Output 2
Analog 2 Attenuation:                        100 LU
Analog 2 Zero Offset:                          5 %

Lamp Settings
Lamp on only during run:                        Yes
Lamp on required for analysis:                    No
Lamp economy mode on:                             No
Lamp energy reference mode on:                      Yes

Fluorescence Scan Range

Excitation Scan
Scan Excitation WL From:                       220 nm
Scan Excitation WL To:                       380 nm
Scan Excitation WL Step:                       5 nm

Emission Scan
Scan Emission WL From:                         300 nm
Scan Emission WL To:                         500 nm
Scan Emission WL Step:                         5 nm

Signal A

Excitation
Use Signal:                              Yes
Signal:                              Signal A
Wavelength Mode:                           Wavel. Set
Excitation Wavelength:                        200 nm
```

```
Emission
Use Signal:                         Yes
Signal:                          Signal A
Wavelength Mode:                      Wavel. Set
Emission Wavelength:                    410 nm

Timetable








=============================================================
                  DAD
=============================================================

DAD (G1315C)
============

Peakwidth:       >0.10 min  (2.0 s response time) (2.5 Hz)
Slit:                             4 nm
UV Lamp Required:                           No
Vis Lamp Required:                          No

Analog Output 1
Analog 1 Attenuation:                  1000 mAU
Analog 1 Zero Offset:                     5 %

Analog Output 2
Analog 2 Attenuation:                  1000 mAU
Analog 2 Zero Offset:                     5 %

Signals
Signal table
  Use Sig.   Signal   Wavelength   Bandwidth   Use Ref.
                     nm         nm
-----------------------------------------------------
     Yes Signal A        414        200       Yes
      No Signal B
     Yes Signal C        430          5       Yes
      No Signal D
      No Signal E
      No Signal F
```

```
    No Signal G
    No Signal H


  Ref Wavel.  Ref Bandw.
      nm         nm
--------------------------
     360        100

     360        100








Prepare Mode
Margin for negative Absorbance:            100 mAU

Autobalance
Autobalance Prerun:                      Yes
Autobalance Postrun:                      No

Spectrum
Spectrum Store:                        None

Stoptime
Stoptime Mode:                   As pump/injector

Posttime
Posttime Mode:                          Off

Timetable




Instrument Curves
Store Board Temperature:                    No
Store Optical Unit Temperature:               No
Store UV Lamp Anode Voltage:                  No
```

```
==================================================
             Column Comp.
==================================================

Column Comp. (G1316A)
====================

Valve Position:                         Port 1 -> 2

Left Temperature Control
Temperature Control Mode:                  Not Controlled

Enable Analysis Left Temperature
Enable Analysis Left Temperature On:                  Yes
Enable Analysis Left Temperature Value:            0.80 °C

Right Temperature Control
Right temperature Control Mode:            Temperature Set
Right temperature:                          35.00 °C

Enable Analysis Right Temperature
Enable Analysis Right Temperature On:                 Yes
Enable Analysis Right Temperature Value:           0.80 °C

Stop Time
Stoptime Mode:                          As pump/injector

Post Time
Posttime Mode:                                Off

Timetable




Instrument Curves
Store Left Temperature:                        Yes
Store Right Temperature:                        No
```

```
=====================================================
                HiP Sampler
=====================================================

HiP Sampler (G1367E)
====================



Auxiliary
Draw Speed:                       100.0 µl/min
Eject Speed:                     100.0 µl/min
Draw Position Offset:                   0.0 mm
Wait Time After Drawing:                  2.0 s
Sample Flush Out Factor:                  5.0
Vial/Well bottom sensing:                  No

Injection
Injection Mode:                 Standard injection
Injection Volume:                      5.00 µL

High throughput
Automaitc Delay Volume Reduction:               No

Overlapped Injection
Enable Overlapped Injection:                 No

Valve Switching
Valve Movements:                        0

Valve Switch Time 1
Switch Time 1 Enabled:                   No

Valve Switch Time 2
Switch Time 2 Enabled:                   No

Valve Switch Time 3
Switch Time 3 Enabled:                   No

Valve Switch Time 4
Switch Time 4 Enabled:                   No

Stop Time
Stoptime Mode:                   As pump/No limit

Post Time
Posttime Mode:                         Off
```

```
Timetable



Instrument Curves
Store Temperature:                    No




=====================================================
                Valve
=====================================================

Valve (G1170A)
==============

Position Switching Mode:          Use valve position
Valve position:                       1
After Run Position Switching Mode:      Do not switch

Stop Time
Stoptime Mode:                  As pump/injector

Post Time
Posttime Mode:                       Off

Timetable

Position Description
  Position   Position Description

----------------------------------
     1            MS
     2            FLD
     3            DAD
     4         Channel 4
     5         Channel 5
     6         Channel 6
     7         Channel 7
     8         Channel 8
     9          by pass
    10         Channel 10
    11         Channel 11
```

```
                    Method Information

          Method: D:\METHOD\1500819A_TAR_MS.M
         Modified: 8/25/2015 at 1:15:13 PM


                    Method Audit Trail

Operator   : user
Date       : 8/19/2015 11:13:50 AM
Change Info: This method was created at 8/19/2015 11:13:50 AM and based on
       method D:\METHOD\1500819_TAR_MS.M

Operator   : user
Date       : 8/19/2015 11:13:52 AM
Change Info: Method saved. User comment: ""

Operator   : user
Date       : 8/24/2015 9:01:21 AM
Change Info: Method saved. User comment: ""



                    Run Time Checklist

          Pre-Run Cmd/Macro:  off

           Data Acquisition:  on

     Standard Data Analysis:  on

   Customized Data Analysis:  off

              Save GLP Data:  off

         Post-Run Cmd/Macro:  off


      Save Method with Data:  off



               Injection Source and Location

   Injection Source:   HipAls
```

```
    D        No




Instrument Curves
Store Pressure:                     Yes
Store Flow:                       Yes
Store Solvent Ratio A:                 Yes
Store Solvent Ratio B:                 Yes
Store Solvent Ratio C:                 Yes
Store Solvent Ratio D:                 Yes
Store Direction of Piston A:              No




===============================================
               Mass Spectrometer Detector
===============================================


General Information
------- -----------

Use MSD              : Enabled
Tune File            : atunes.tun
StopTime             : No Limit
Time Filter          : Enabled
Data Storage         : Condensed
Peakwidth            : 0.10 min
Fast Scan            : Disabled
Fast Scan Data Reconstruction: Disabled
Polarity Switch Delay    : 50 ms
Ionization Switch Delay  : 50 ms


Signals
-------

[Signal 1]

Ionization Mode         : API-ES
Polarity             : Negative
```

```
Fragmentor Ramp         : Disabled
Percent Cycle Time      : 100.00 %

Scan Parameters

  Time |      Mass Range     |Frag- | Gain|Thres-| Step-
 (min) |    Low    |  High   |mentor| EMV | hold | size
-------|----------|---------|------|-----|------|-------
   0.00    100.00    550.00    70    1.0     150  0.10


[Signal 2]

Not Active


[Signal 3]

Not Active


[Signal 4]

Not Active



Spray Chamber
----- -------

[MSZones]

Gas Temp              : 300 C              maximum 350 C
DryingGas             : 10.0 l/min          maximum 13.0 l/min
Neb Pres              : 45 psig            maximum 60 psig
Quad Temp             : 0 C                maximum 0 C

VCap (Positive)        : 3000 V
VCap (Negative)        : 3500 V

[Time Table]

Time Table is empty.


               END OF MS ACQUISITION PARAMETERS
```

```
=====================================================
                    FIA Series
=====================================================

FIA Series in this Method  :     Disabled

Time Setting
   Time between Injections  :     0.15 min
   Injection Loop Flush Time :     0.17 min

=====================================================
                    Column(s)
=====================================================

Column Description :  Ascentis Exp C18
Serial#           :  USMD005296
Product#          :  53822-U          Batch# :
Diameter          :  2.1 mm          Length :   50.0 mm
Particle size      :  2.7 µm      Void volume :   60.0 %
Maximum Pressure   :  400.0 bar      Maximum pH :      9.0
    Minimum pH :      2.0
Maximum Temperature:   60.0 °C
Comment           :




The Data Analysis Parameters of the used Method are :

=====================================================
                  Integration Events
=====================================================



-----------------------------------------------------------------------
           Non signal specific Integration Events
-----------------------------------------------------------------------

           Event                              Value
|-------------------------------------------------------|-------------|
 Tangent Skim Mode                               Standard
 Baseline Correction                            Advanced
 Tail Peak Skim Height Ratio                       0.000
 Front Peak Skim Height Ratio                        0.000
```

```
Skim Valley Ratio                          20.000
Peak to Valley Ratio                       500.000

-----------------------------------------------------------------------
             Default Integration Event Table "Event"
-----------------------------------------------------------------------

             Event                        Value     Time
|-----------------------------------------------|-------------|-------|
Initial Slope Sensitivity                    1.000   Initial
Initial Peak Width                           0.020   Initial
Initial Area Reject                          1.000   Initial
Initial Height Reject                        1.700   Initial
Initial Shoulders                            OFF     Initial

-----------------------------------------------------------------------
        Detector Default Integration Event Table "Event_DAD"
-----------------------------------------------------------------------

             Event                        Value     Time
|-----------------------------------------------|-------------|-------|
Initial Slope Sensitivity                    5.000   Initial
Initial Peak Width                           0.020   Initial
Initial Area Reject                          5.000   Initial
Initial Height Reject                        1.000   Initial
Initial Shoulders                            OFF     Initial

-----------------------------------------------------------------------
        Detector Default Integration Event Table "Event_ADC"
-----------------------------------------------------------------------

             Event                        Value     Time
|-----------------------------------------------|-------------|-------|
Initial Slope Sensitivity                    1.000   Initial
Initial Peak Width                           0.020   Initial
Initial Area Reject                          1.000   Initial
Initial Height Reject                        1.700   Initial
Initial Shoulders                            OFF     Initial

-----------------------------------------------------------------------
        Detector Default Integration Event Table "Event_FLD"
-----------------------------------------------------------------------

             Event                        Value     Time
|-----------------------------------------------|-------------|-------|
Initial Slope Sensitivity                    1.000   Initial
Initial Peak Width                           0.020   Initial
```

```
Initial Area Reject                    1.000   Initial
Initial Height Reject                   1.700   Initial
Initial Shoulders                     OFF     Initial

-----------------------------------------------------------------------
       Detector Default Integration Event Table "Event_MSD"
-----------------------------------------------------------------------

           Event                        Value     Time
|-----------------------------------------------|-------------|-------|
Initial Slope Sensitivity                10000.000   Initial
Initial Peak Width                        0.020   Initial
Initial Area Reject                    1000.000   Initial
Initial Height Reject                   100.000   Initial
Initial Shoulders                     OFF     Initial

-----------------------------------------------------------------------
      Signal Specific Integration Event Table "Event_MSD1SPC"
-----------------------------------------------------------------------

           Event                        Value     Time
|-----------------------------------------------|-------------|-------|
Initial Slope Sensitivity(Full Scan)               1.000   Initial
Initial Peak Width(Full Scan)                    0.250   Initial
Initial Slope Sensitivity(Cond. Scan/SIM)           0.100   Initial
Initial Peak Width(Cond. Scan/SIM)               0.050   Initial
Initial Area Reject                    0.000   Initial
Initial Height Reject                   5.000   Initial
Initial Shoulders                     OFF     Initial

-----------------------------------------------------------------------
       Detector Default Integration Event Table "Event_VWD"
-----------------------------------------------------------------------

           Event                        Value     Time
|-----------------------------------------------|-------------|-------|
Initial Slope Sensitivity                   1.000   Initial
Initial Peak Width                        0.020   Initial
Initial Area Reject                    1.000   Initial
Initial Height Reject                   1.700   Initial
Initial Shoulders                     OFF     Initial

-----------------------------------------------------------------------
       Detector Default Integration Event Table "Event_ECD"
-----------------------------------------------------------------------

           Event                        Value     Time
```

```
|-----------------------------------------------|-------------|-------|
 Initial Slope Sensitivity                     1.000   Initial
 Initial Peak Width                           0.020   Initial
 Initial Area Reject                          1.000   Initial
 Initial Height Reject                         1.700   Initial
 Initial Shoulders                           OFF     Initial

---------------------------------------------------------------------
       Detector Default Integration Event Table "Event_MWD"
---------------------------------------------------------------------

           Event                          Value     Time
|-----------------------------------------------|-------------|-------|
 Initial Slope Sensitivity                     1.000   Initial
 Initial Peak Width                           0.020   Initial
 Initial Area Reject                          1.000   Initial
 Initial Height Reject                         1.700   Initial
 Initial Shoulders                           OFF     Initial

---------------------------------------------------------------------
      Signal Specific Integration Event Table "Event_MSD1TIC"
---------------------------------------------------------------------

           Event                          Value     Time
|-----------------------------------------------|-------------|-------|
 Initial Slope Sensitivity                  4255.241   Initial
 Initial Peak Width                           0.157   Initial
 Initial Area Reject                     13989.271   Initial
 Initial Height Reject                     743.464   Initial
 Initial Shoulders                           OFF     Initial

Apply Method's Manual Integration Events: No




=====================================================================
                   Specify Report
=====================================================================

Calculate:                 Area Percent
Use Multiplier & Dilution Factor with ISTDs

Use Sample Data from Data File
Destination:                 Screen
Quantitative Results sorted by: Signal
```

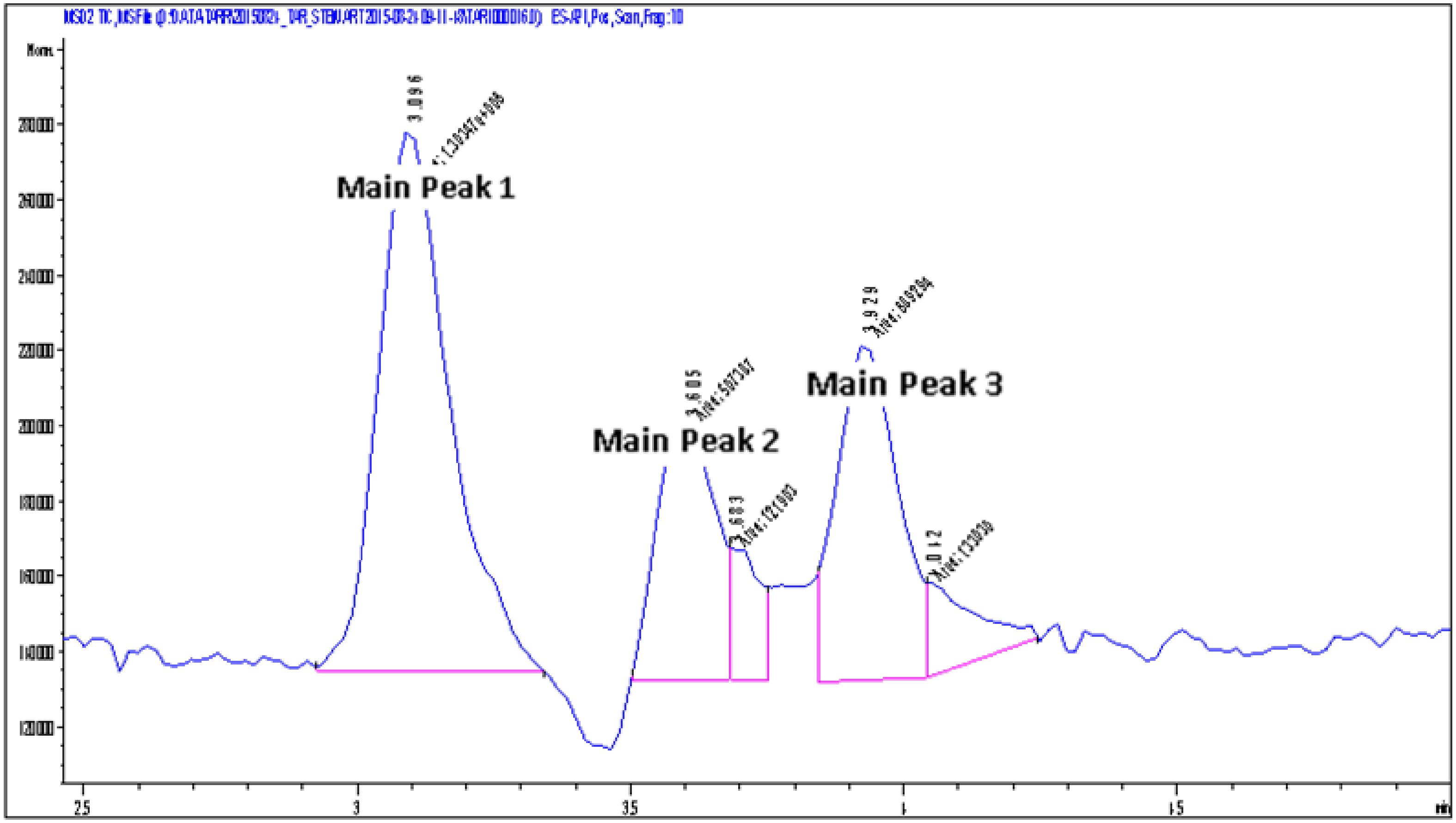
```
Report Style:                  Short
Sample info on each page:       No
Add Chromatogram Output:        Yes
Chromatogram Output:           Portrait
Size in Time direction:        100 % of Page
Size in Response direction:      40 % of Page
Uncalibrated Peaks:            Report with Calibrated Peaks


===========================================================
                    Signal Options
===========================================================

Include: Axes, Retention Times, Baselines, Tick Marks
Font:    Times New Roman, Size: 8

Ranges:  Full
Multi Chromatograms: Overlaid, Each in full Scale

===========================================================
                    Calibration Table
===========================================================



Calib. Data Modified  :


Rel. Reference Window :      5.000 %
Abs. Reference Window :      0.000 min
Rel. Non-ref. Window  :      5.000 %
Abs. Non-ref. Window  :      0.000 min
Uncalibrated Peaks    :      not reported
Partial Calibration   :      Yes, identified peaks are recalibrated
Correct All Ret. Times:      No, only for identified peaks

Curve Type            :      Linear
Origin                :      Included
Weight                :      Equal

Recalibration Settings:
Average Response      :      Average all calibrations
Average Retention Time:      Floating Average New 75%

Calibration Report Options :
  Printout of recalibrations within a sequence:
    Calibration Table after Recalibration
```

Normal Report after Recalibration
If the sequence is done with bracketing:
Results of first cycle (ending previous bracket)

```
=========================================================
                   Peak Sum Table
=========================================================

***No Entries in table***
=========================================================



=========================================================
              Sample related custom fields
=========================================================

Custom Field              Type    Mand.  Default Value
------------------------------------------------------------------------
None defined

=========================================================
             Compound related custom fields
=========================================================

Custom Field              Type    Mand.  Default Value
------------------------------------------------------------------------
None defined
```

Appendix J: Positive Ionization HPLC Chromatograms and Mass Spectroscopy

Example Positive Chromatogram

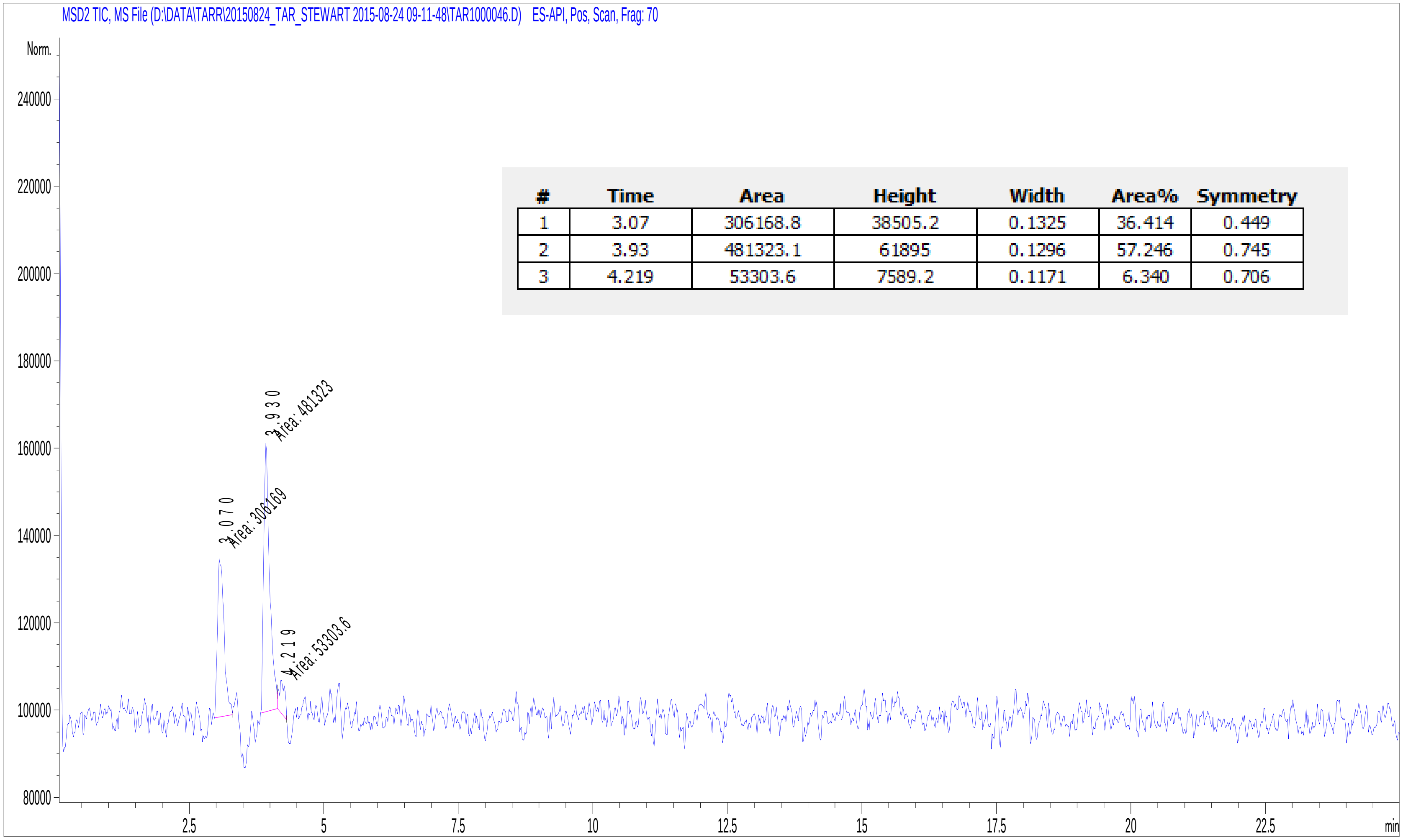


Baselines, Standards, Misc.

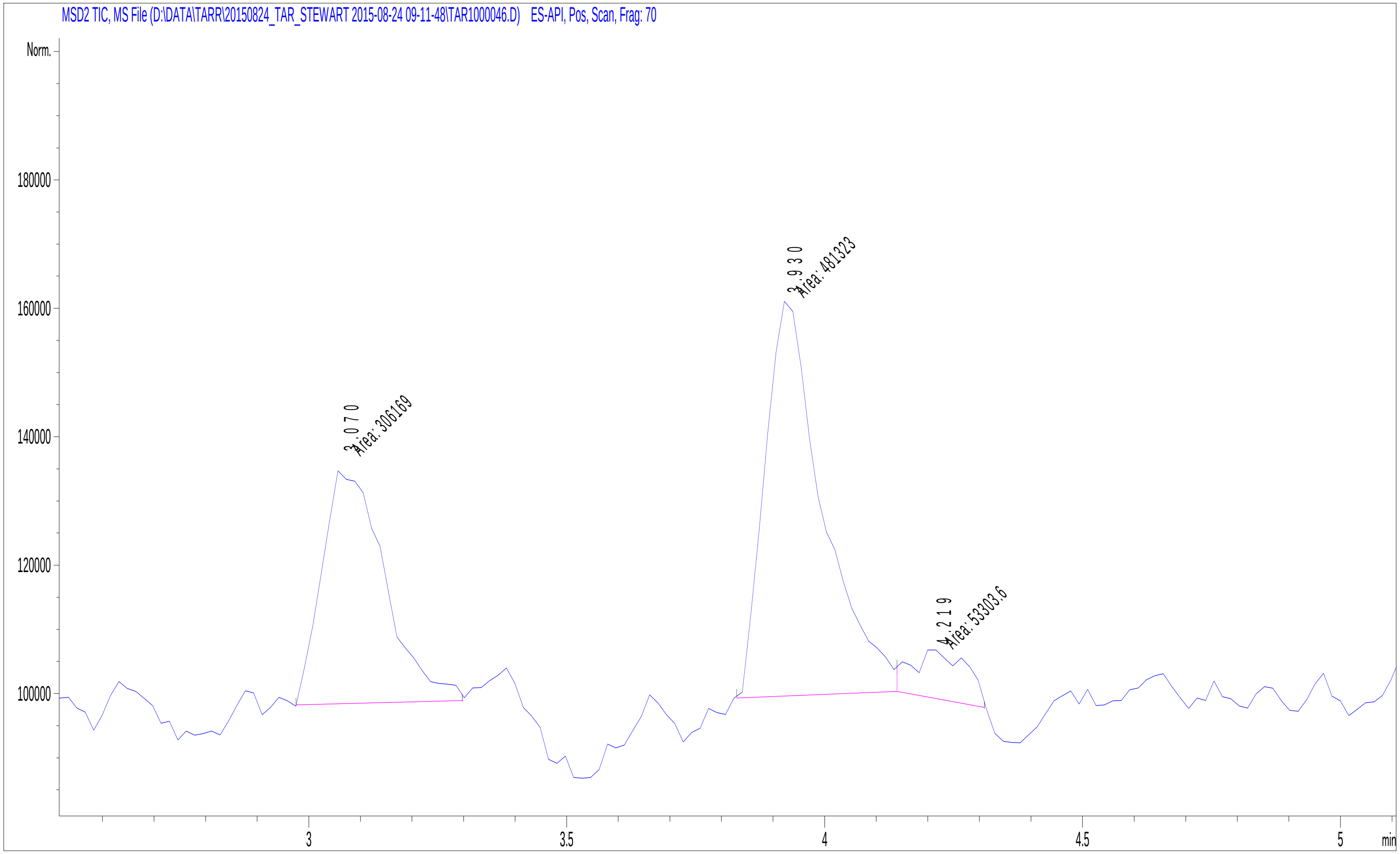
20-Aug-15

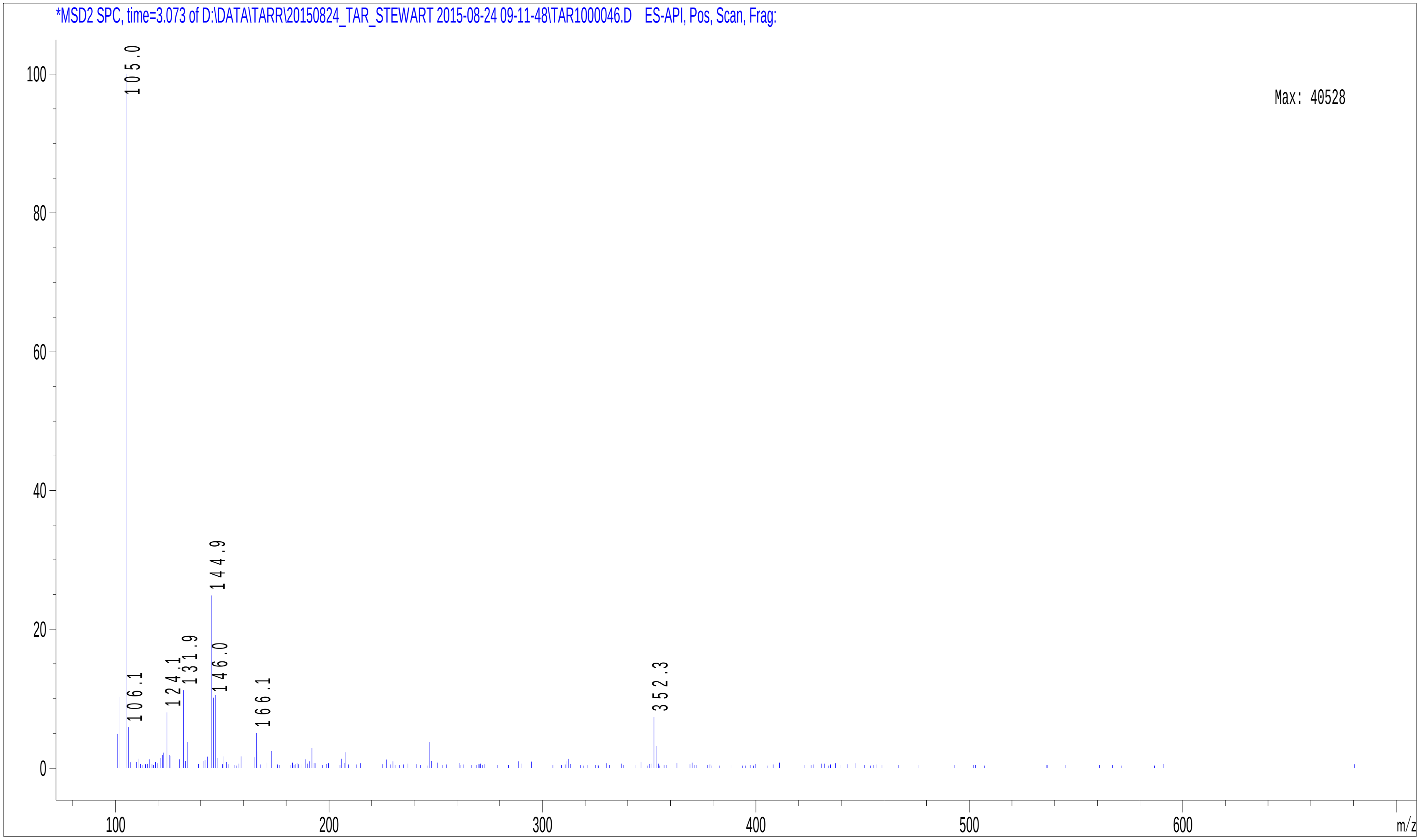
Baseline - DI Water

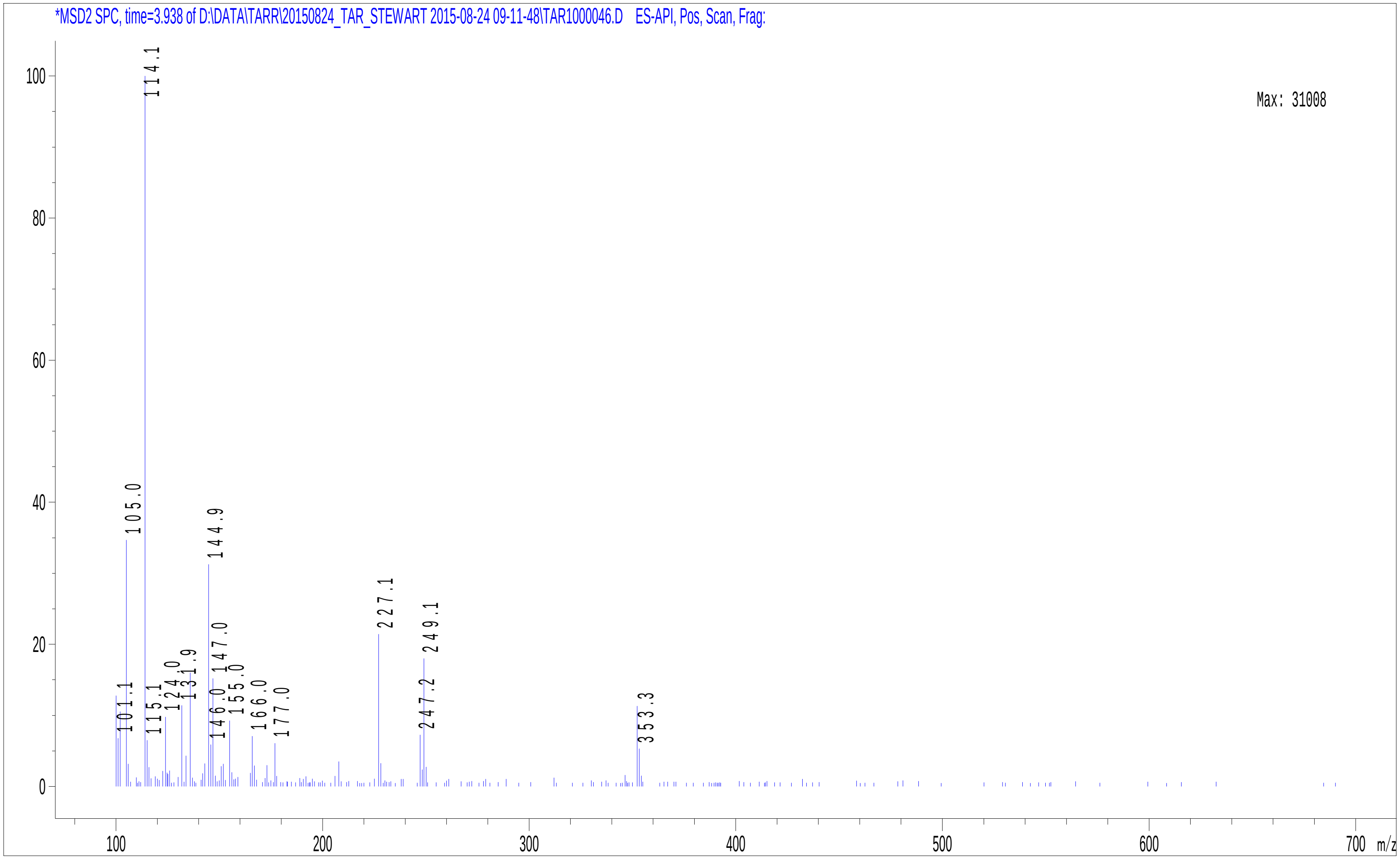
P2-A-01

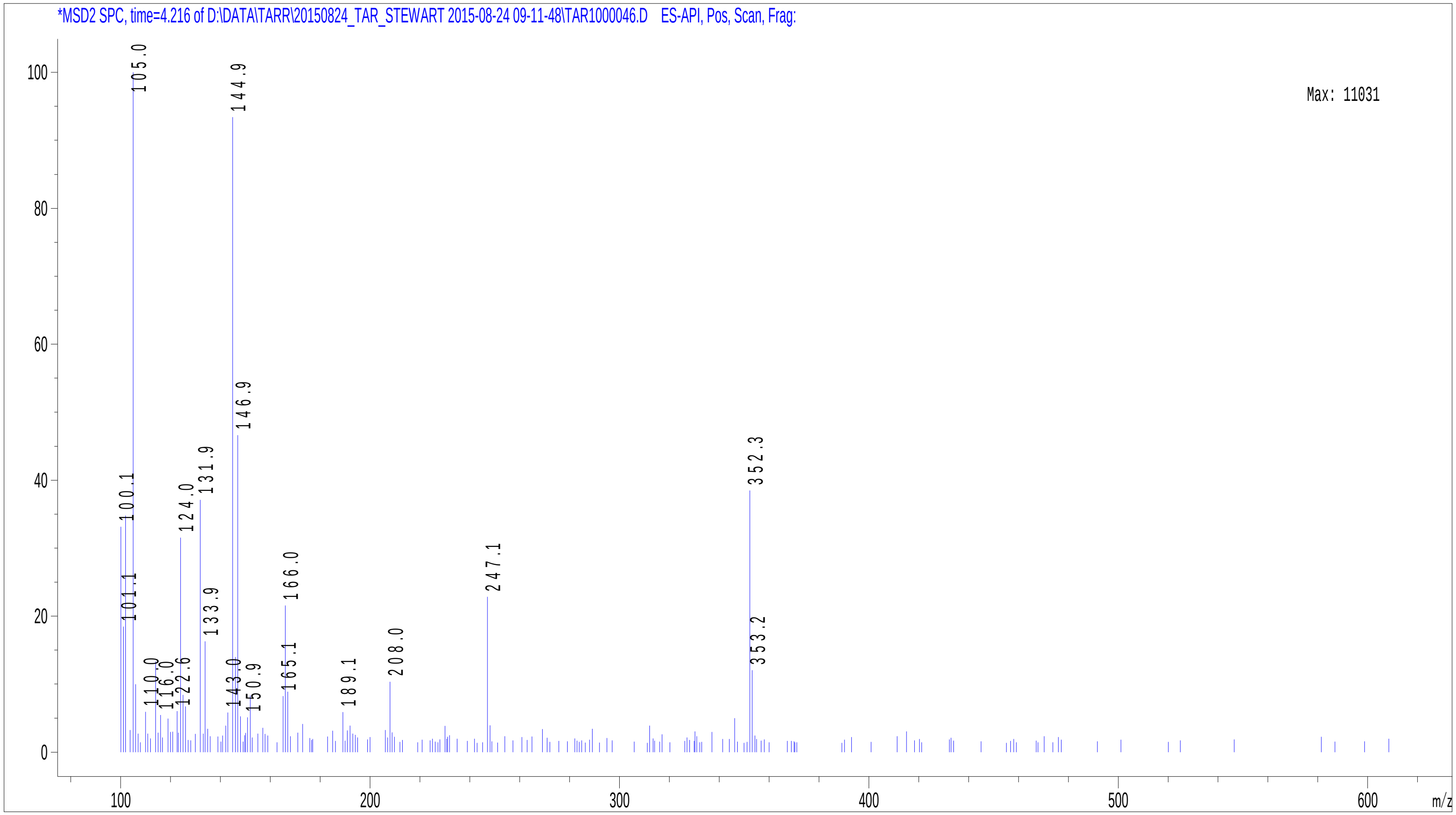


#	Time	Area	Height	Width	Area%	Symmetry
1	3.07	306168.8	38505.2	0.1325	36.414	0.449
2	3.93	481323.1	61895	0.1296	57.246	0.745
3	4.219	53303.6	7589.2	0.1171	6.340	0.706


MSD2 TIC, MS File (D:\DATA\TARR\20150824_TAR_STEWART 2015-08-24 09-11-48\TAR1000046.D) ES-API, Pos, Scan, Frag: 70
Norm.
180000
160000
140000
120000
100000
3.070
Area: 306169
3.930
Area: 481323
4.219
Area: 53303.6
3
3.5
4
4.5
5
min


*MSD2 SPC, time=3.073 of D:\DATA\TARR\20150824_TAR_STEWART 2015-08-24 09-11-48\TAR1000046.D ES-API, Pos, Scan, Frag:
Max: 40528
105.0
106.1
124.1
131.9
144.9
146.0
166.1
352.3
100
80
60
40
20
0
100
200
300
400
500
600
m/z

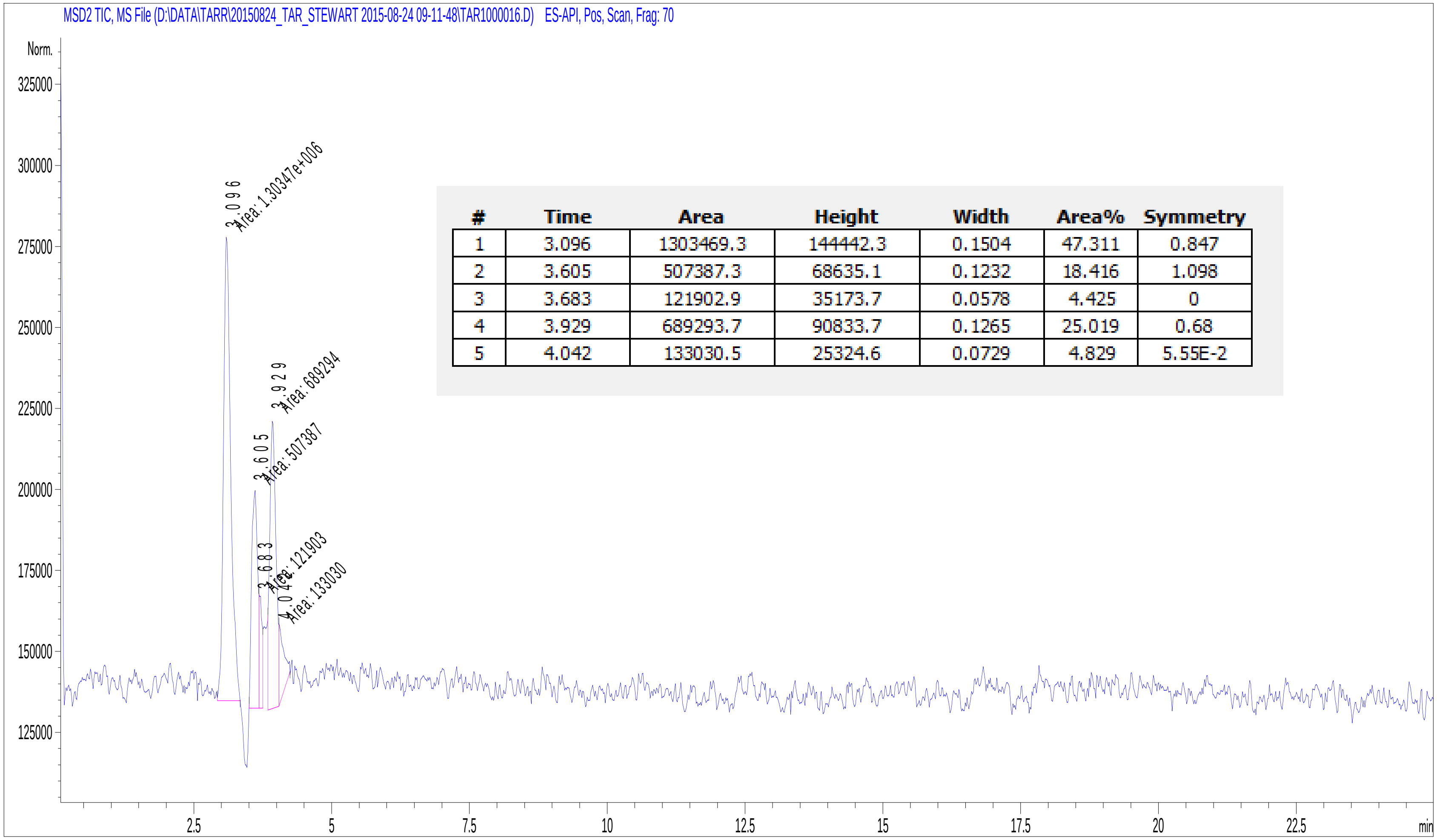

*MSD2 SPC, time=3.938 of D:\DATA\TARR\20150824_TAR_STEWART 2015-08-24 09-11-48\TAR1000046.D ES-API, Pos, Scan, Frag:
Max: 31008
114.1
105.0
144.9
227.1
249.1
147.0
131.9
124.0
155.0
115.1
101.1
166.0
177.0
146.0
247.2
353.3
0
20
40
60
80
100
100
200
300
400
500
600
700
m/z

*MSD2 SPC, time=4.216 of D:\DATA\TARR\20150824_TAR_STEWART 2015-08-24 09-11-48\TAR1000046.D ES-API, Pos, Scan, Frag:
Max: 11031
100
80
60
40
20
0
105.0
144.9
146.9
100.1
101.1
124.0
131.9
133.9
110.0
116.0
122.6
143.0
150.9
165.1
166.0
189.1
208.0
247.1
352.3
353.2
100
200
300
400
500
600
m/z

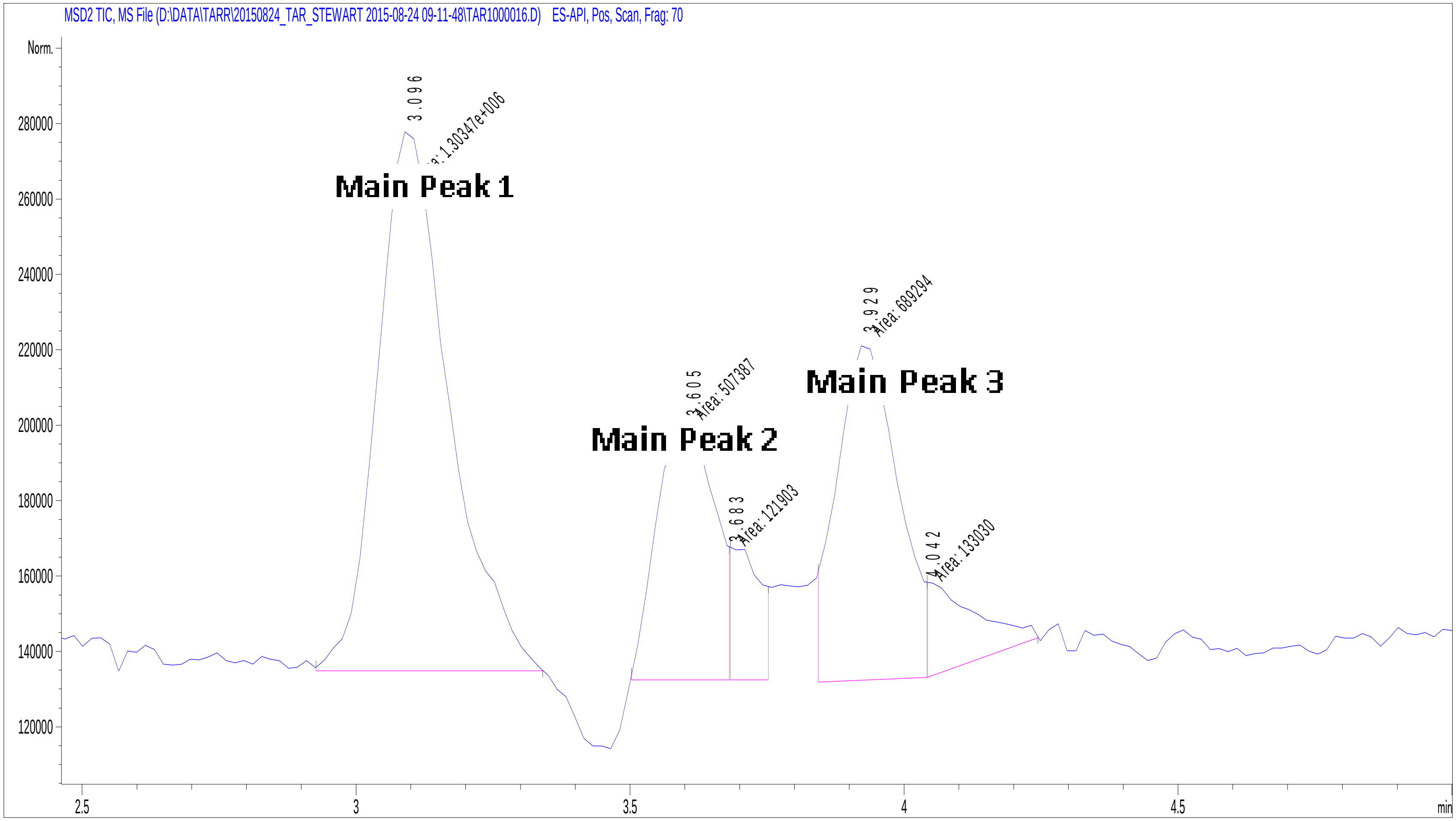
29-May-15

pH5 - repeat

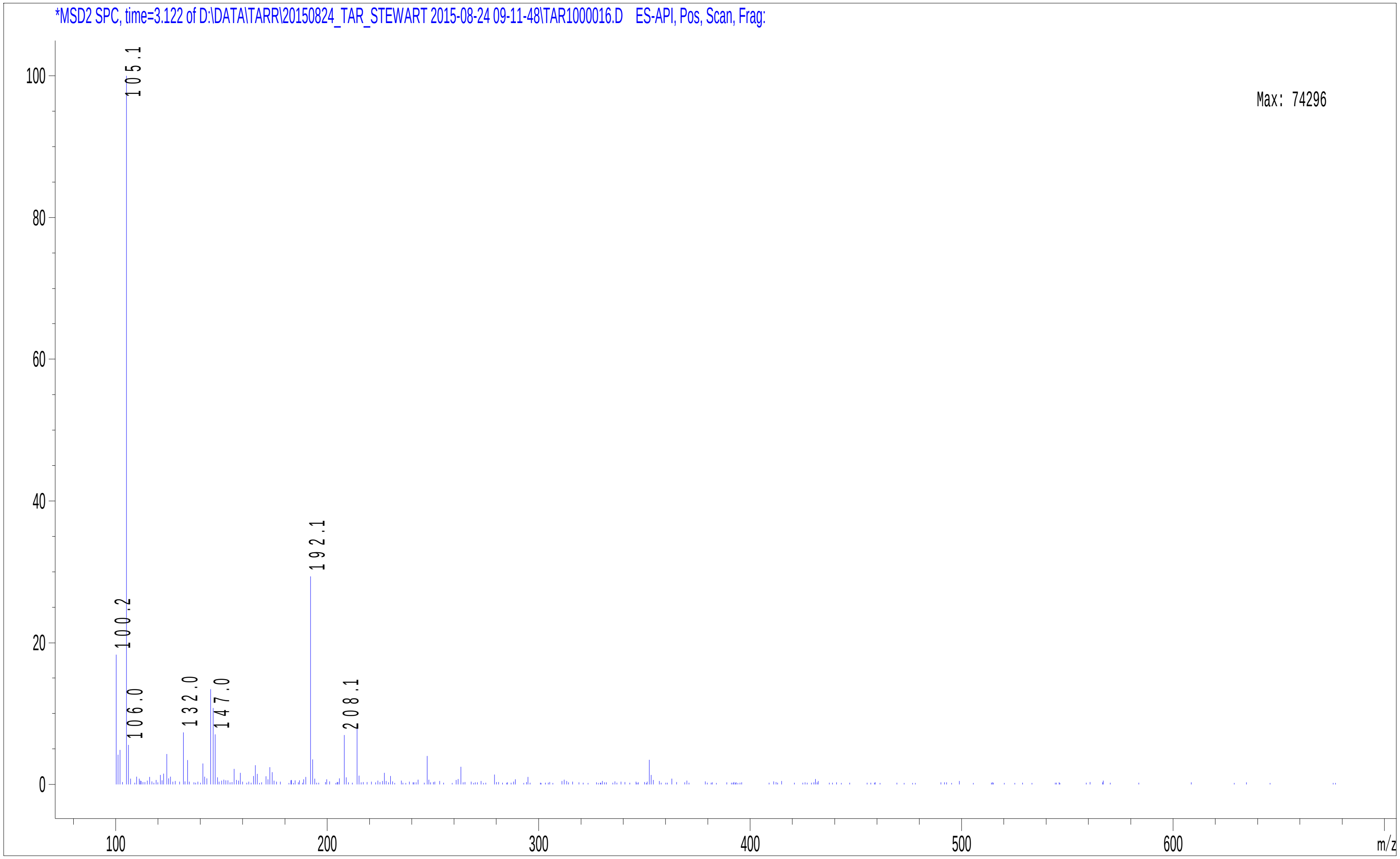
P2-B-03

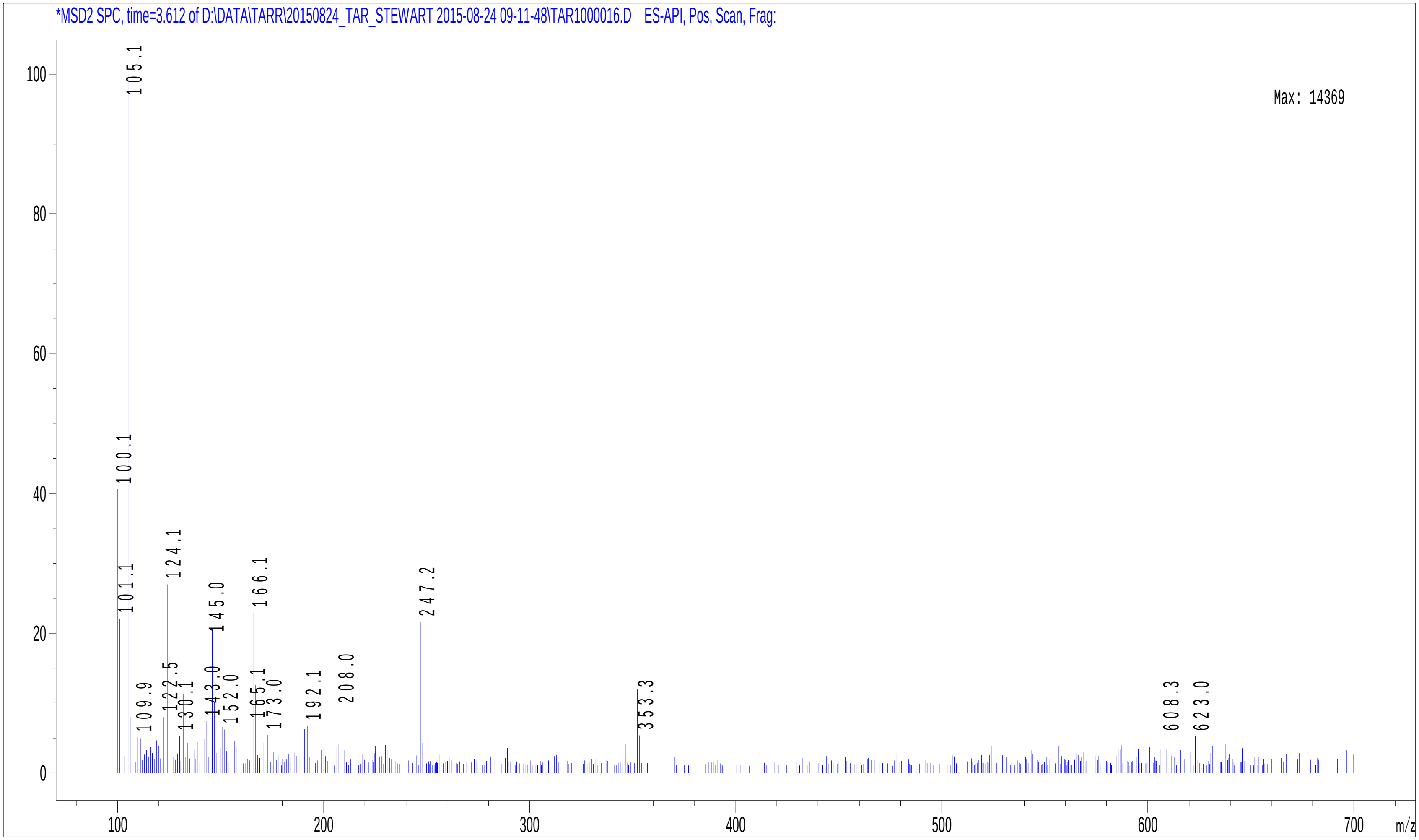


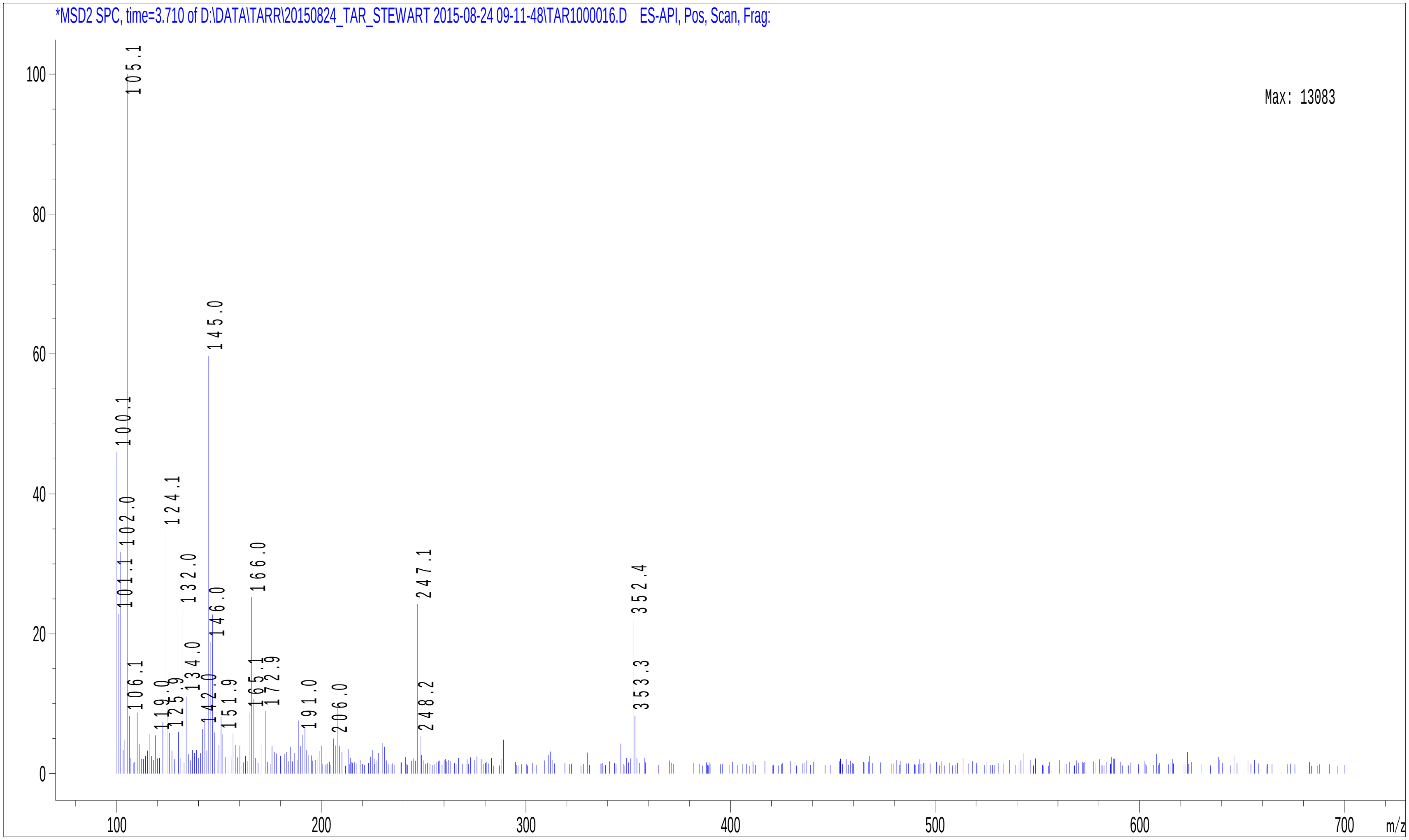
#	Time	Area	Height	Width	Area%	Symmetry
1	3.096	1303469.3	144442.3	0.1504	47.311	0.847
2	3.605	507387.3	68635.1	0.1232	18.416	1.098
3	3.683	121902.9	35173.7	0.0578	4.425	0
4	3.929	689293.7	90833.7	0.1265	25.019	0.68
5	4.042	133030.5	25324.6	0.0729	4.829	5.55E-2

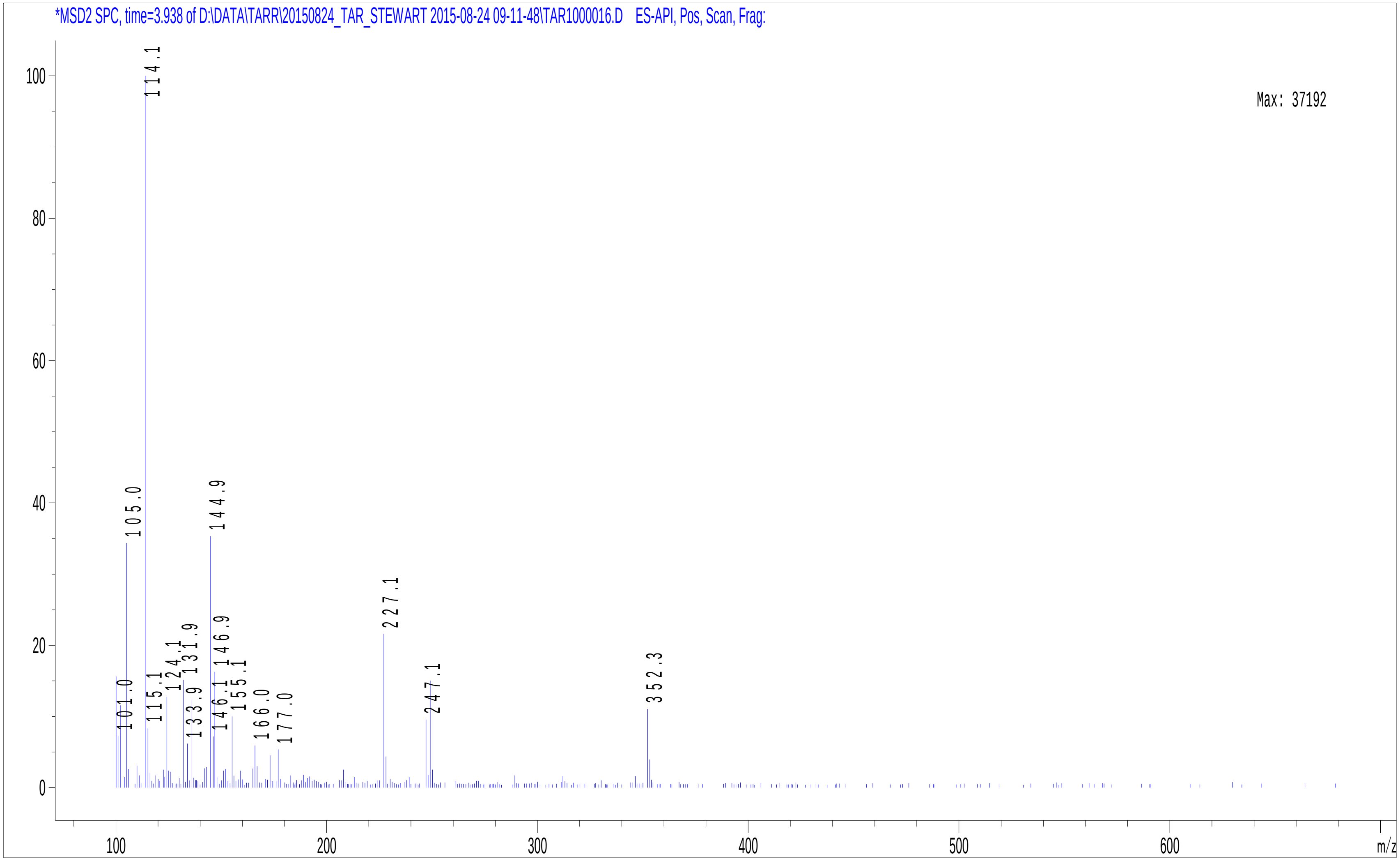

MSD2 TIC, MS File (D:\DATA\TARR\20150824_TAR_STEWART 2015-08-24 09-11-48\TAR1000016.D) ES-API, Pos, Scan, Frag: 70
Norm.
280000
260000
240000
220000
200000
180000
160000
140000
120000
3.096
Area: 1.30347e+006
Main Peak 1
3.605
Area: 507387
Main Peak 2
3.683
Area: 121903
3.929
Area: 689294
Main Peak 3
4.042
Area: 133030
2.5
3
3.5
4
4.5
min

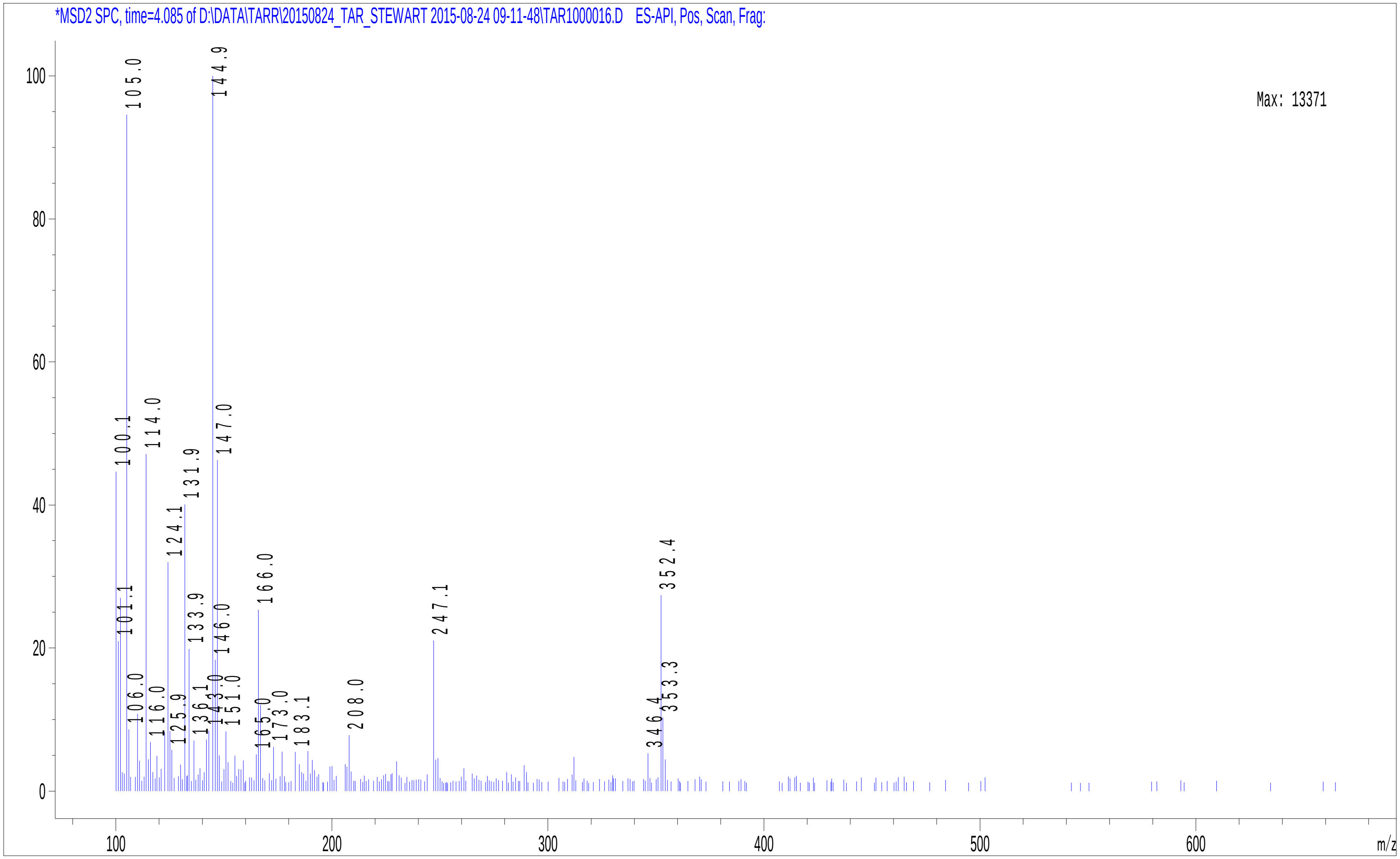
Main Peak 3


*MSD2 SPC, time=3.122 of D:\DATA\TARR\20150824_TAR_STEWART 2015-08-24 09-11-48\TAR1000016.D ES-API, Pos, Scan, Frag:
Max: 74296
105.1
100.2
106.0
132.0
147.0
192.1
208.1
0
20
40
60
80
100
100
200
300
400
500
600
m/z

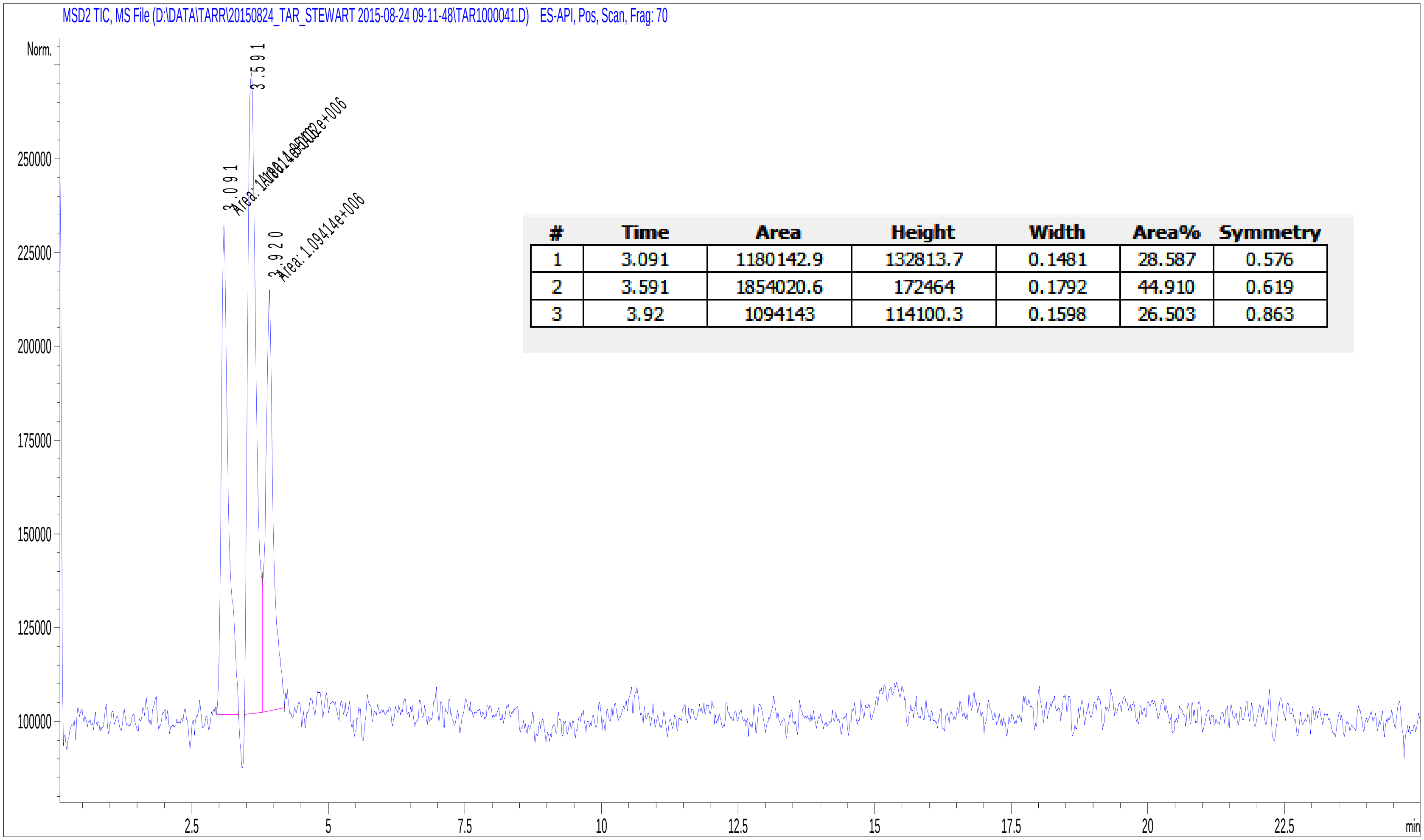

*MSD2 SPC, time=3.612 of D:\DATA\TARR\20150824_TAR_STEWART 2015-08-24 09-11-48\TAR1000016.D ES-API, Pos, Scan, Frag:
Max: 14369
105.1
100.1
101.1
124.1
109.9
122.5
130.1
143.0
145.0
152.0
165.1
166.1
173.0
192.1
208.0
247.2
353.3
608.3
623.0
0
20
40
60
80
100
100
200
300
400
500
600
700
m/z


*MSD2 SPC, time=3.710 of D:\DATA\TARR\20150824_TAR_STEWART 2015-08-24 09-11-48\TAR1000016.D ES-API, Pos, Scan, Frag:
Max: 13083
105.1
145.0
100.1
124.1
102.0
101.1
132.0
166.0
146.0
247.1
352.4
106.1
119.0
125.9
134.0
142.0
151.9
165.1
172.9
191.0
206.0
248.2
353.3
0
20
40
60
80
100
100
200
300
400
500
600
700
m/z

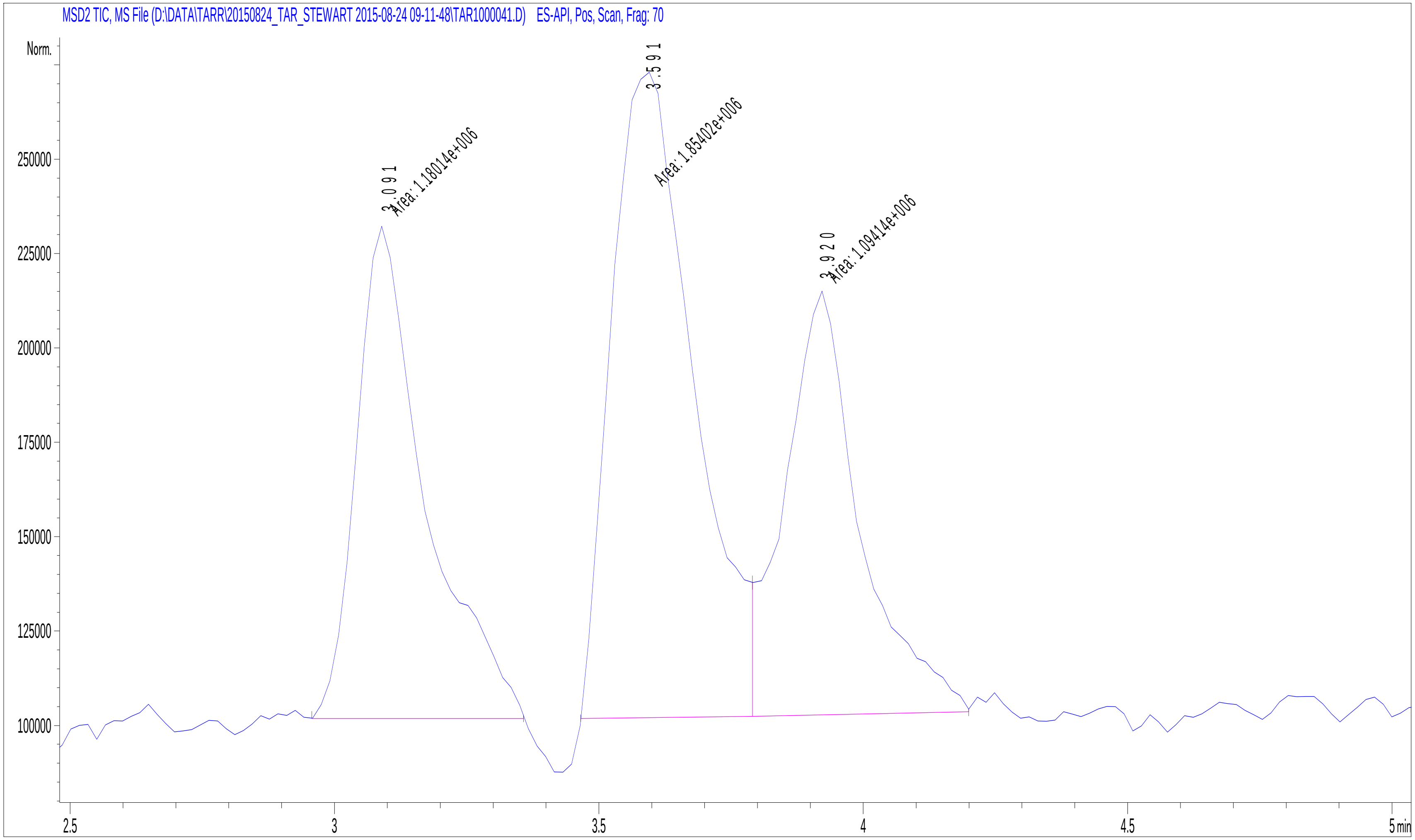

*MSD2 SPC, time=3.938 of D:\DATA\TARR\20150824_TAR_STEWART 2015-08-24 09-11-48\TAR1000016.D ES-API, Pos, Scan, Frag:
Max: 37192
114.1
105.0
144.9
227.1
101.0
115.1
124.1
131.9
133.9
146.9
146.1
155.1
166.0
177.0
247.1
352.3
0
20
40
60
80
100
100
200
300
400
500
600
m/z

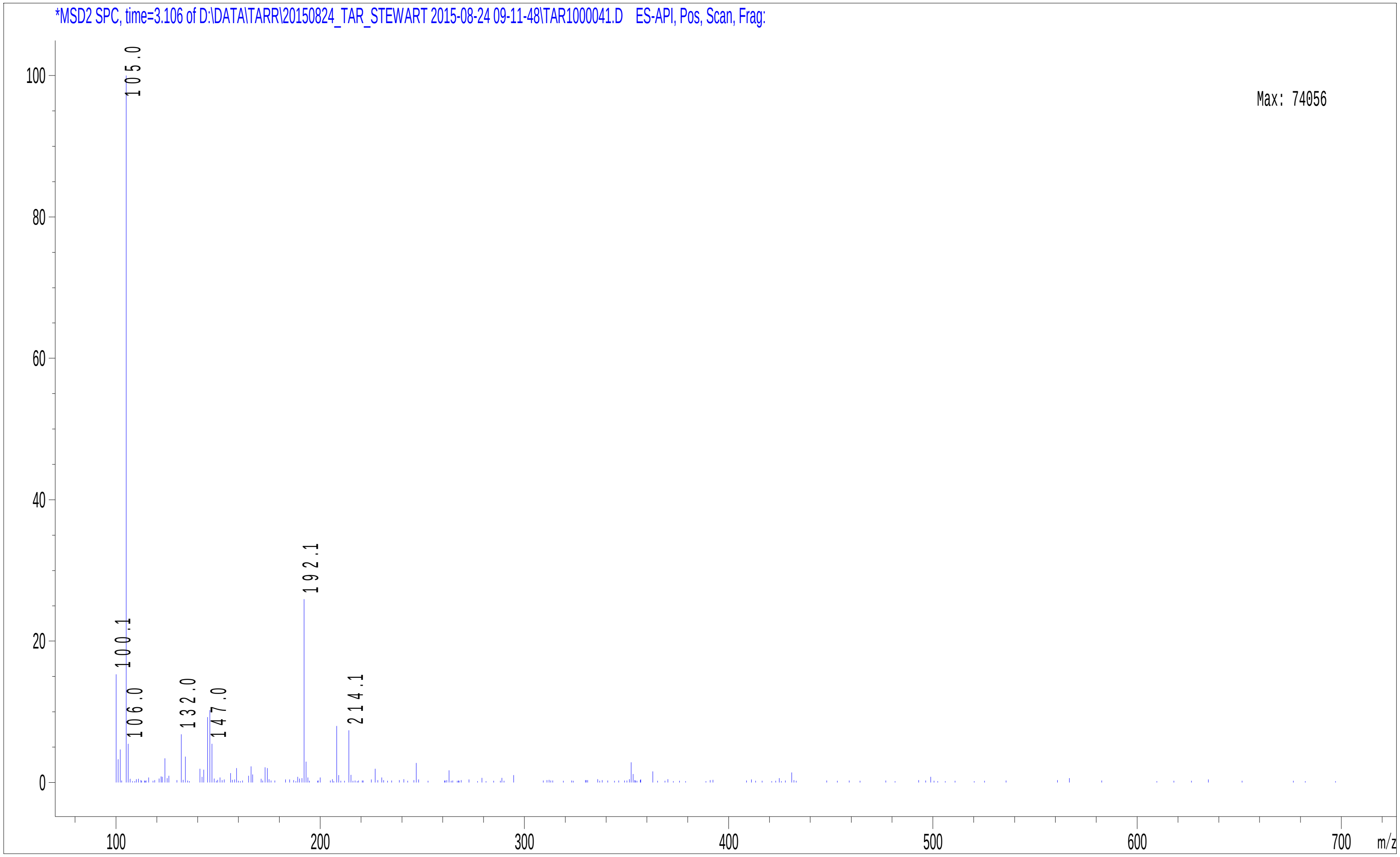

*MSD2 SPC, time=4.085 of D:\DATA\TARR\20150824_TAR_STEWART 2015-08-24 09-11-48\TAR1000016.D ES-API, Pos, Scan, Frag:
Max: 13371
105.0
144.9
100.1
114.0
147.0
131.9
124.1
166.0
101.1
133.9
146.0
247.1
352.4
106.0
116.0
125.9
136.1
143.0
151.0
165.0
173.0
183.1
208.0
353.3
346.4
0
20
40
60
80
100
100
200
300
400
500
600
m/z

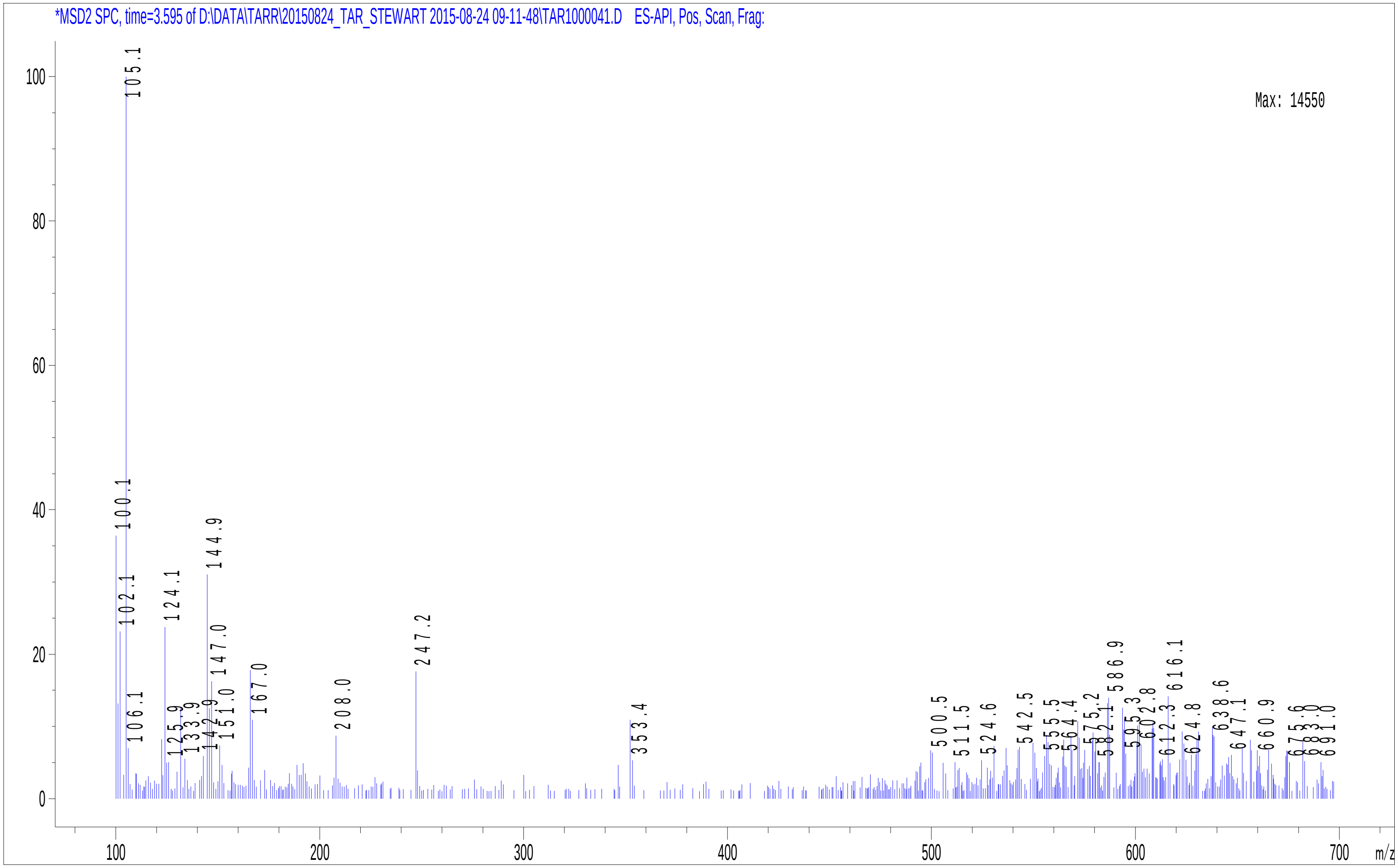
11-Aug-15
UNTREATED SOLUTION
P2-E-05

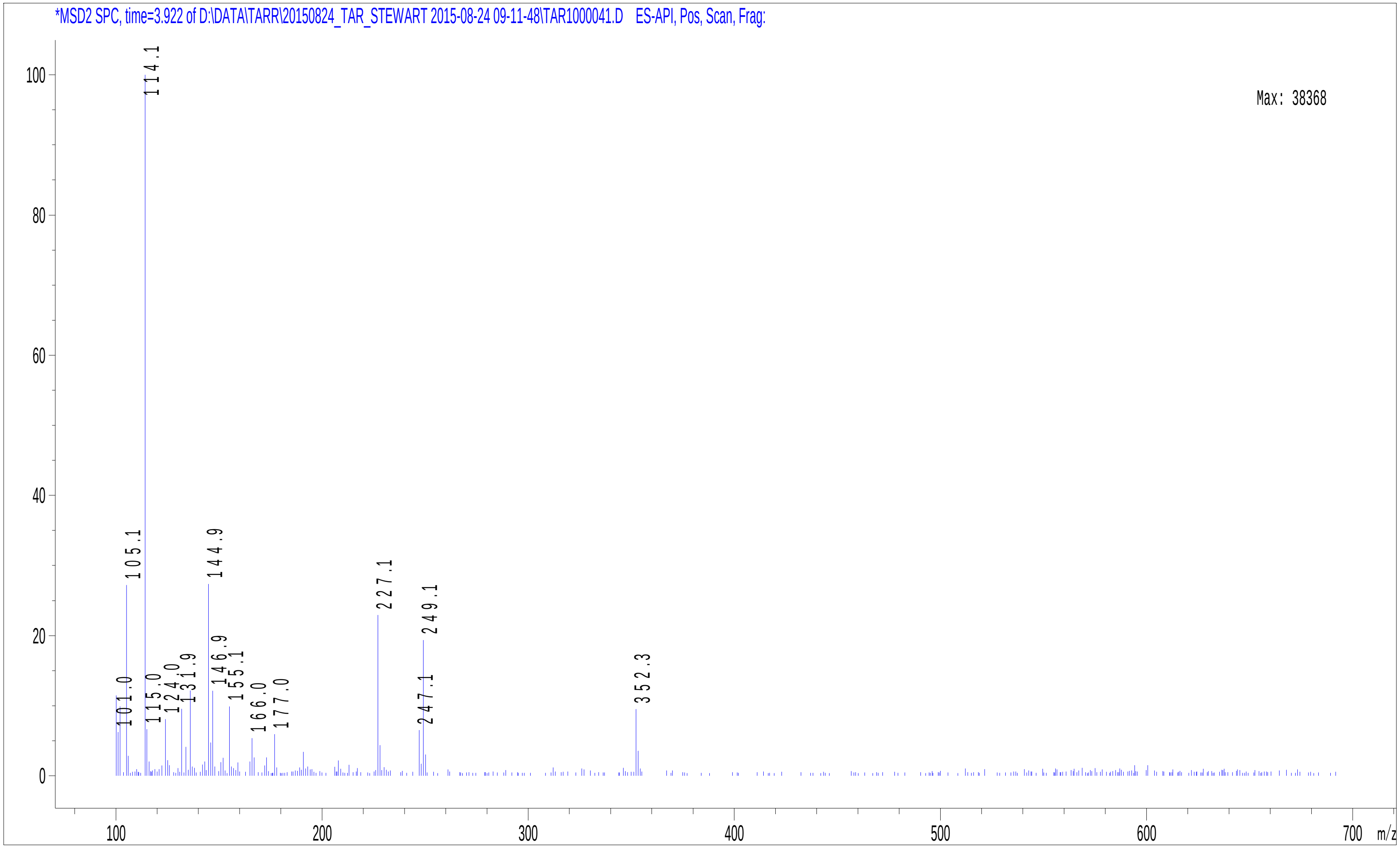


#	Time	Area	Height	Width	Area%	Symmetry
1	3.091	1180142.9	132813.7	0.1481	28.587	0.576
2	3.591	1854020.6	172464	0.1792	44.910	0.619
3	3.92	1094143	114100.3	0.1598	26.503	0.863


MSD2 TIC, MS File (D:\DATA\TARR\20150824_TAR_STEWART 2015-08-24 09-11-48\TAR1000041.D) ES-API, Pos, Scan, Frag: 70
Norm.
250000
225000
200000
175000
150000
125000
100000
3.091
Area: 1.18014e+006
3.591
Area: 1.85402e+006
3.920
Area: 1.09414e+006
2.5
3
3.5
4
4.5
5
min


*MSD2 SPC, time=3.106 of D:\DATA\TARR\20150824_TAR_STEWART 2015-08-24 09-11-48\TAR1000041.D ES-API, Pos, Scan, Frag:
Max: 74056
105.0
100.1
106.0
132.0
147.0
192.1
214.1
0
20
40
60
80
100
100
200
300
400
500
600
700
m/z

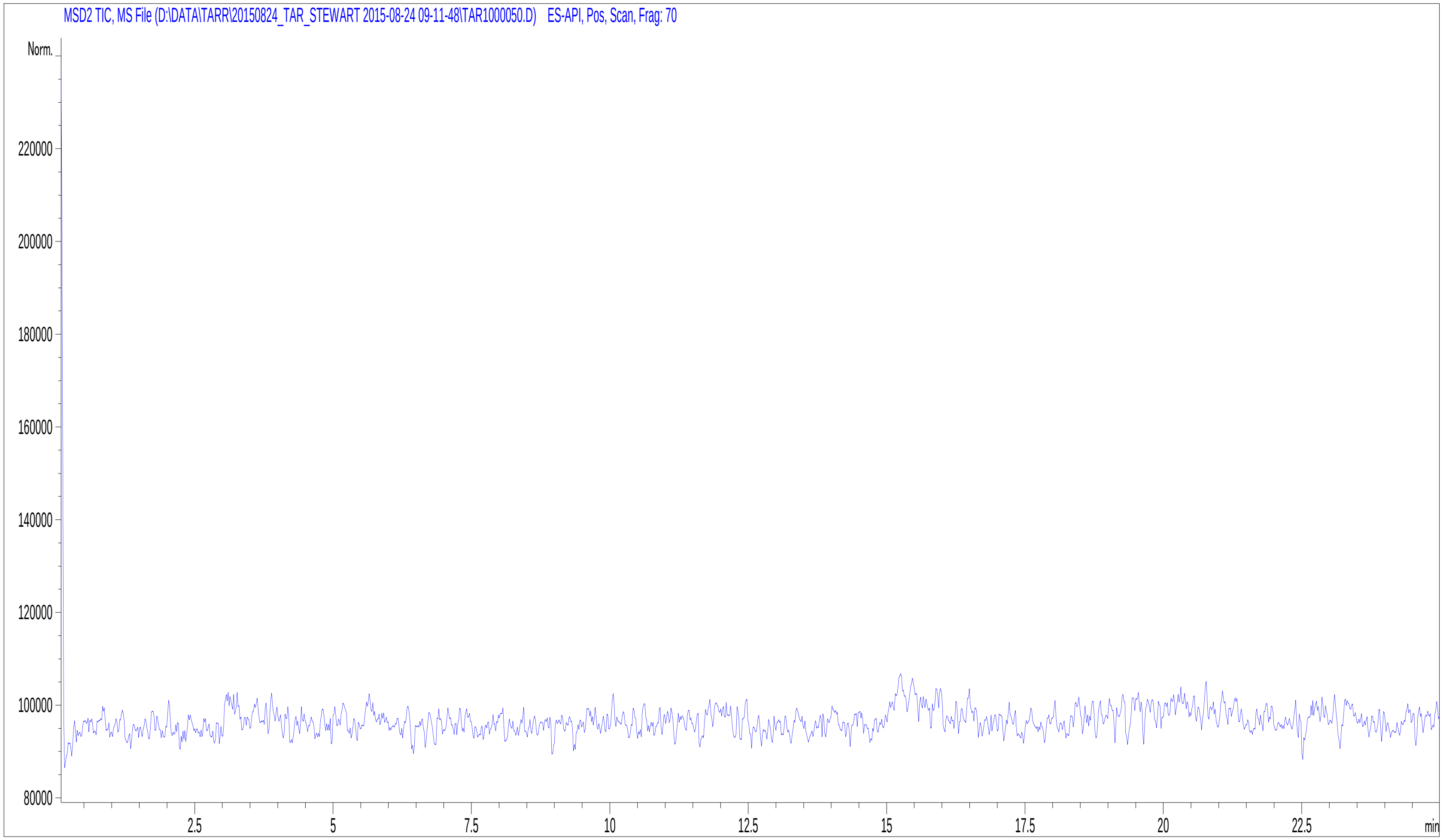

*MSD2 SPC, time=3.595 of D:\DATA\TARR\20150824_TAR_STEWART 2015-08-24 09-11-48\TAR1000041.D   ES-API, Pos, Scan, Frag:
Max: 14550
0
20
40
60
80
100
100
200
300
400
500
600
700
m/z
100.1
102.1
105.1
106.1
124.1
125.9
133.9
142.9
144.9
147.0
151.0
167.0
208.0
247.2
353.4
500.5
511.5
524.6
542.5
555.5
564.4
575.2
582.1
586.9
595.3
602.8
612.3
616.1
624.8
638.6
647.1
660.9
675.6
683.0
691.0


*MSD2 SPC, time=3.922 of D:\DATA\TARR\20150824_TAR_STEWART 2015-08-24 09-11-48\TAR1000041.D ES-API, Pos, Scan, Frag:
Max: 38368
114.1
105.1
144.9
227.1
249.1
101.0
115.0
124.0
131.9
146.9
155.1
166.0
177.0
247.1
352.3
0
20
40
60
80
100
200
300
400
500
600
700
m/z

--

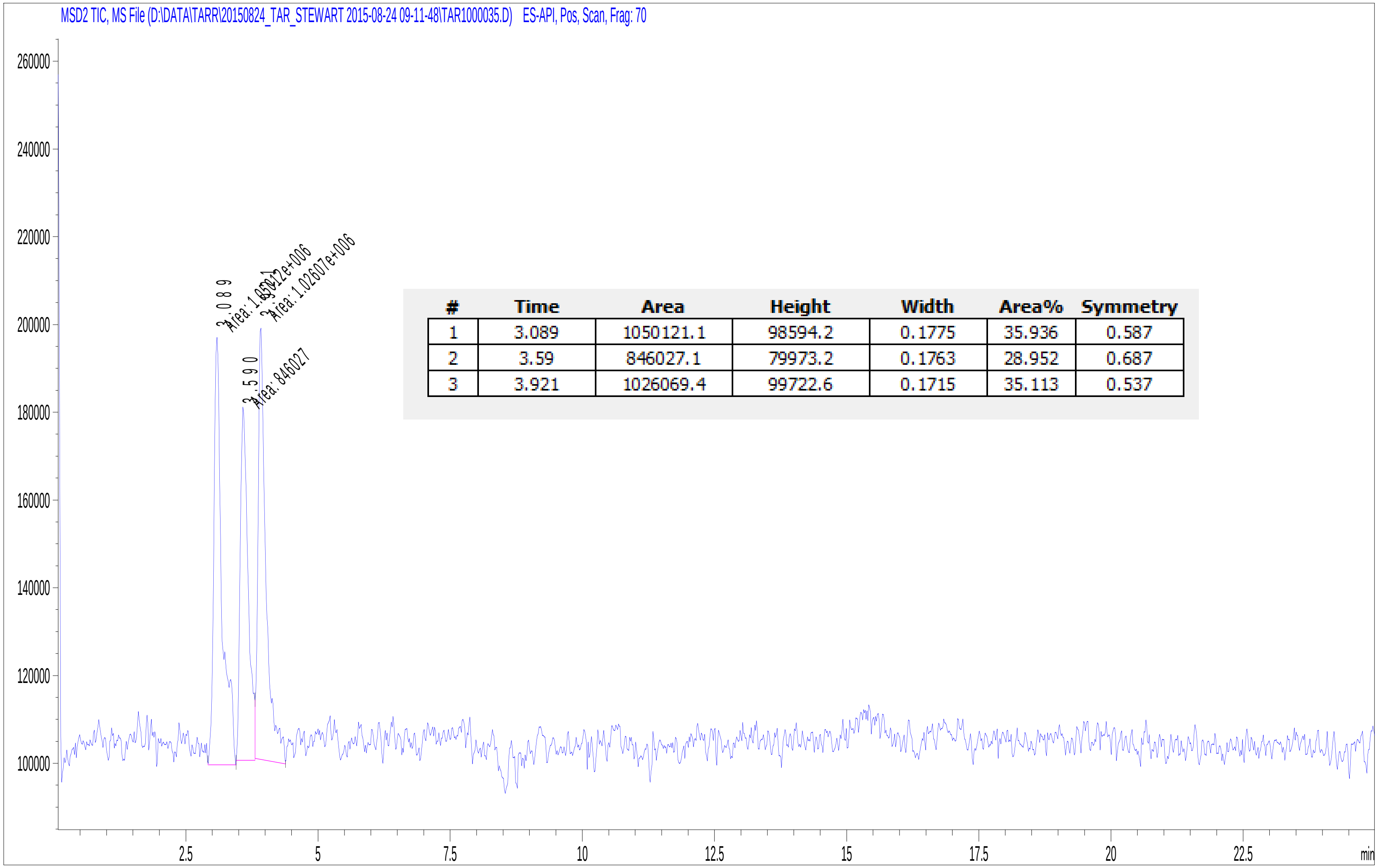
Standard

P1-A-09

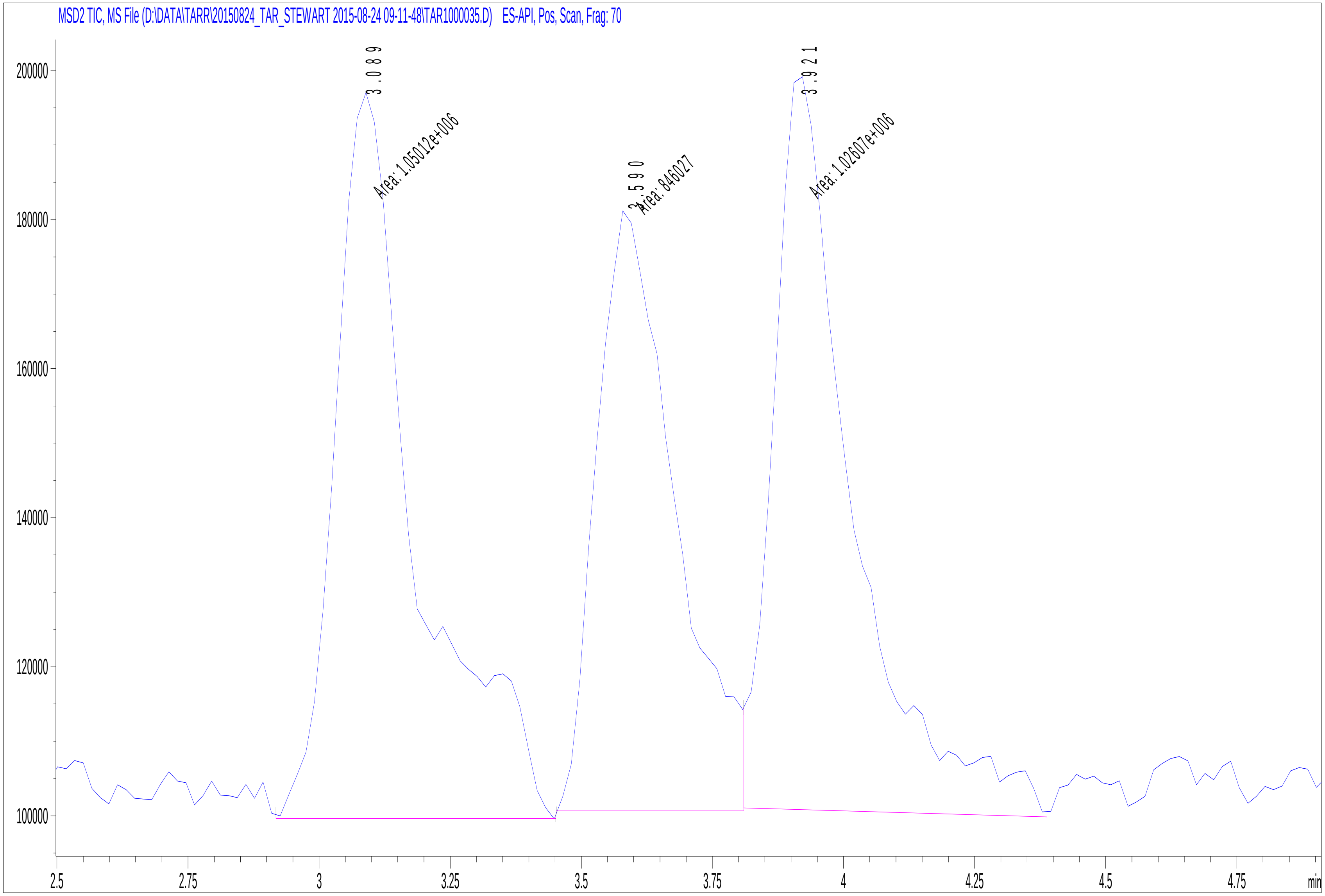


pH 6

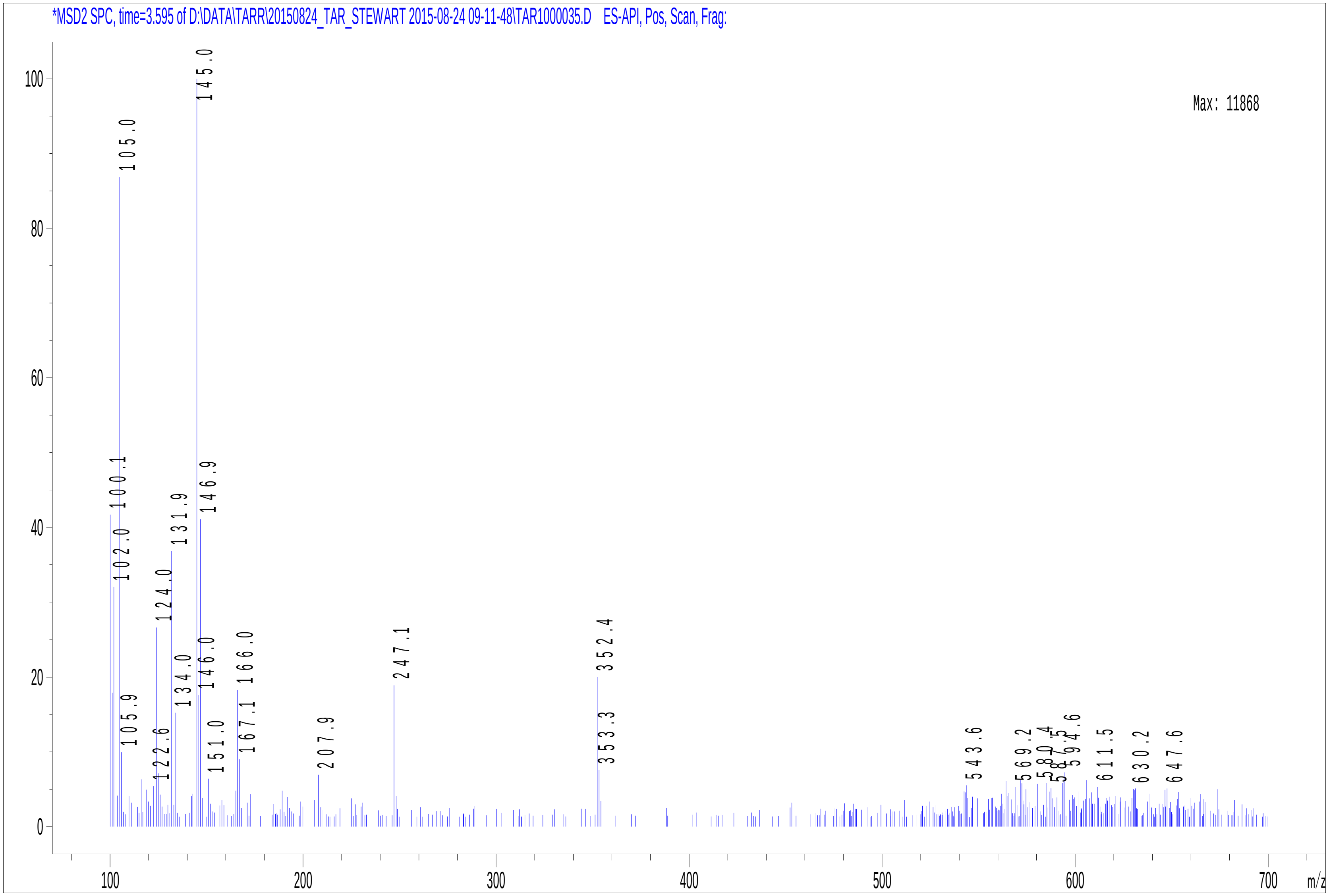
17-Jul-15
H2O2 Ctrl
P2-D-02

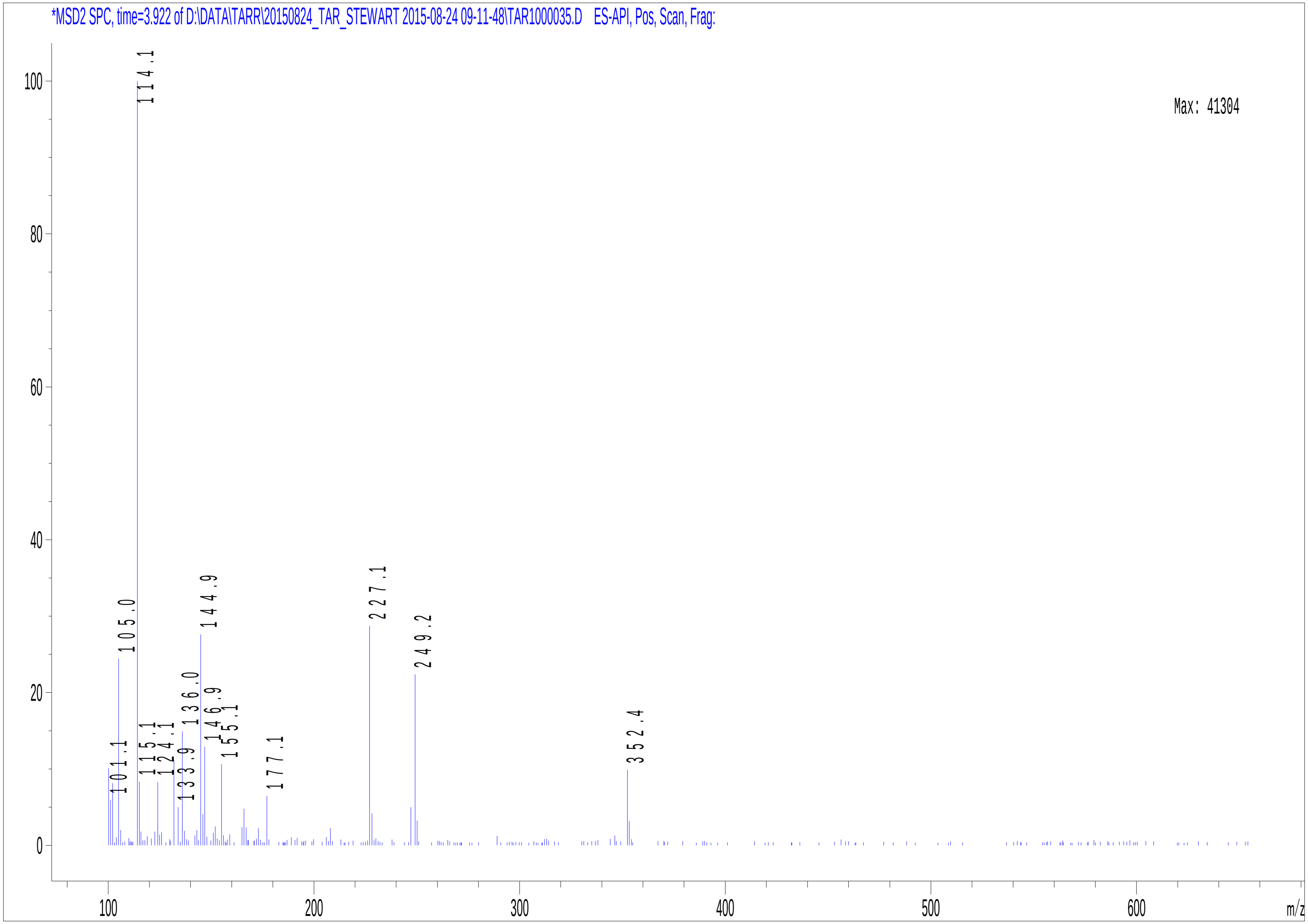


#	Time	Area	Height	Width	Area%	Symmetry
1	3.089	1050121.1	98594.2	0.1775	35.936	0.587
2	3.59	846027.1	79973.2	0.1763	28.952	0.687
3	3.921	1026069.4	99722.6	0.1715	35.113	0.537

MSD2 TIC, MS File (D:\DATA\TARR\20150824_TAR_STEWART 2015-08-24 09-11-48\TAR1000035.D) ES-API, Pos, Scan, Frag: 70
200000
180000
160000
140000
120000
100000
3.089
Area: 1.05012e+006
3.590
Area: 846027
3.921
Area: 1.02607e+006
2.5
2.75
3
3.25
3.5
3.75
4
4.25
4.5
4.75
min


*MSD2 SPC, time=3.089 of D:\DATA\TARR\20150824_TAR_STEWART 2015-08-24 09-11-48\TAR1000035.D ES-API, Pos, Scan, Frag:
Max: 82368
105.1
100.1
131.9
146.9
100
80
60
40
20
0
100
200
300
400
500
600
m/z

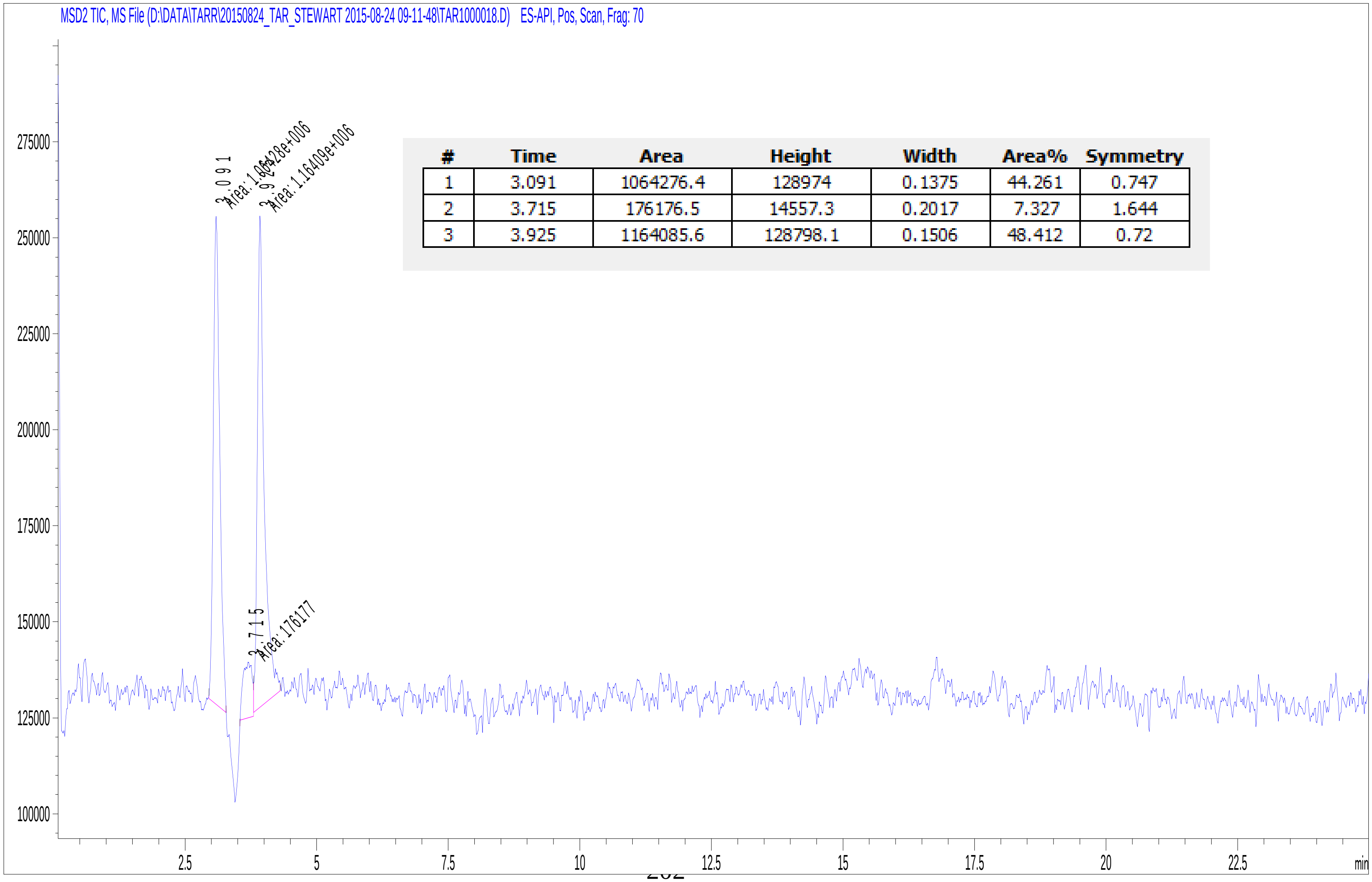

*MSD2 SPC, time=3.595 of D:\DATA\TARR\20150824_TAR_STEWART 2015-08-24 09-11-48\TAR1000035.D ES-API, Pos, Scan, Frag:
Max: 11868
100
80
60
40
20
0
100
200
300
400
500
600
700
m/z
145.0
105.0
100.1
146.9
102.0
131.9
124.0
352.4
247.1
146.0
134.0
166.0
105.9
167.1
122.6
151.0
207.9
353.3
543.6
569.2
580.4
587.5
594.6
611.5
630.2
647.6


*MSD2 SPC, time=3.922 of D:\DATA\TARR\20150824_TAR_STEWART 2015-08-24 09-11-48\TAR1000035.D ES-API, Pos, Scan, Frag:
Max: 41304
114.1
105.0
101.1
115.1
124.1
133.9
136.0
144.9
146.9
155.1
177.1
227.1
249.2
352.4
0
20
40
60
80
100
100
200
300
400
500
600
m/z

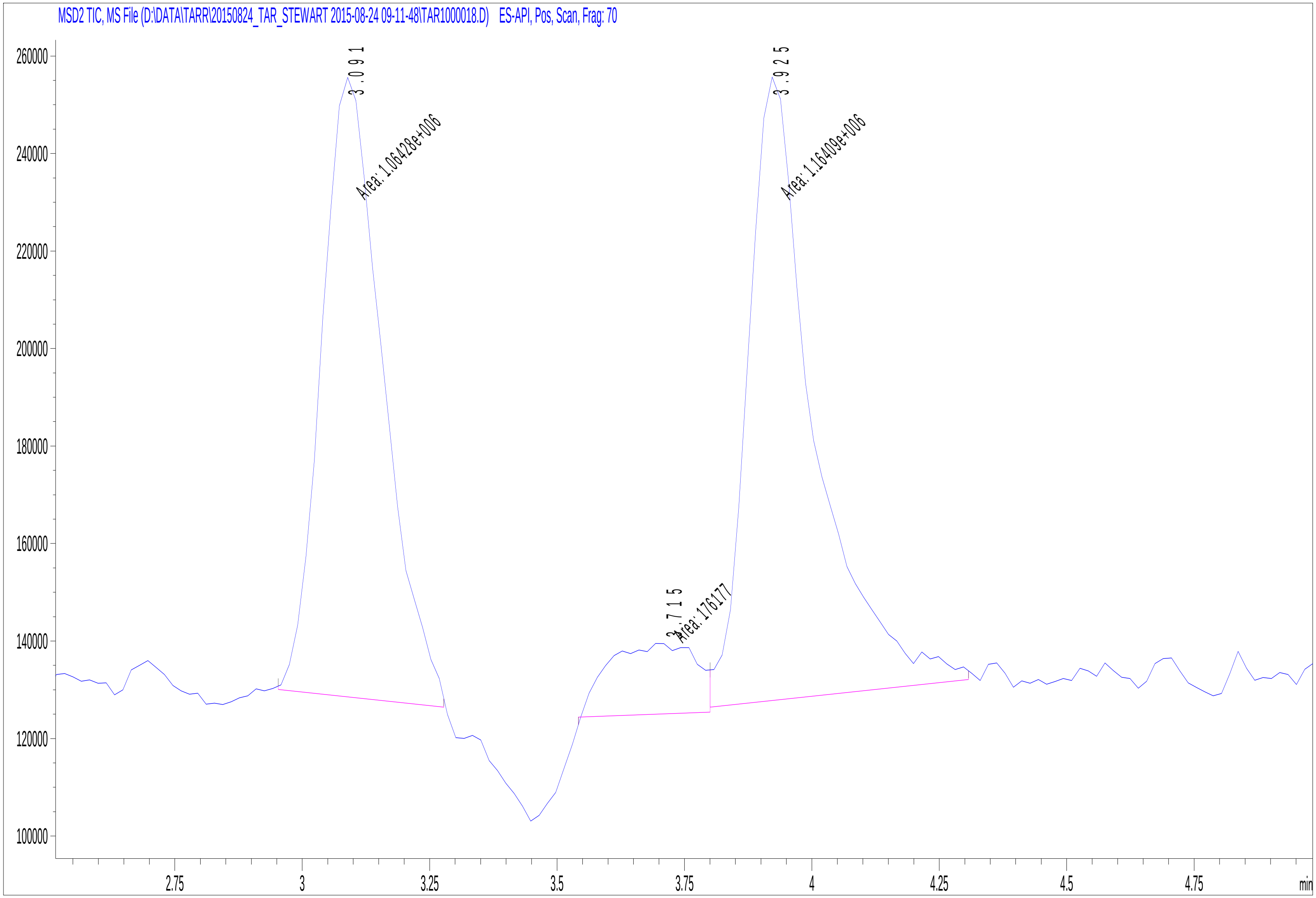
14-May-15

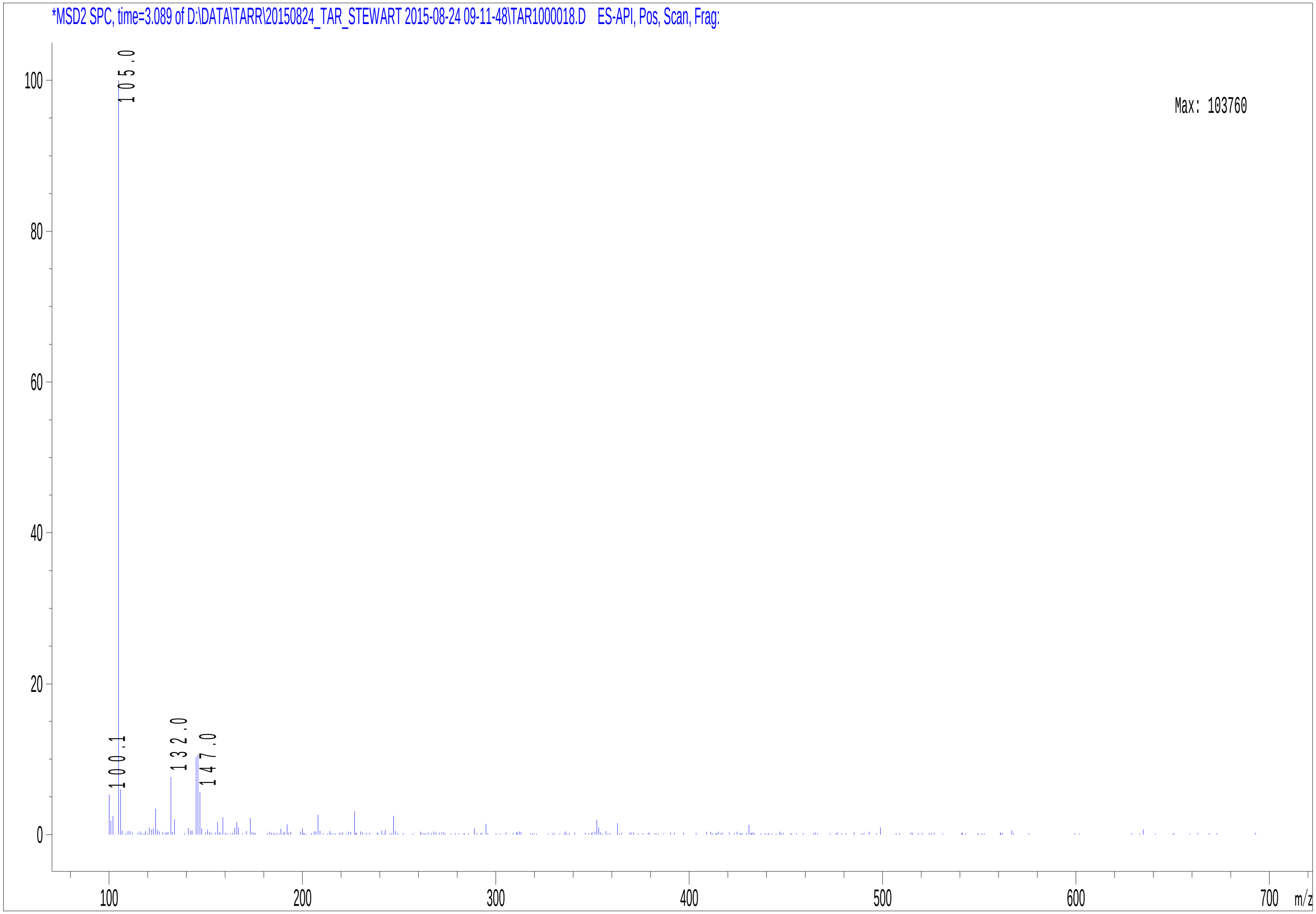
0 DC

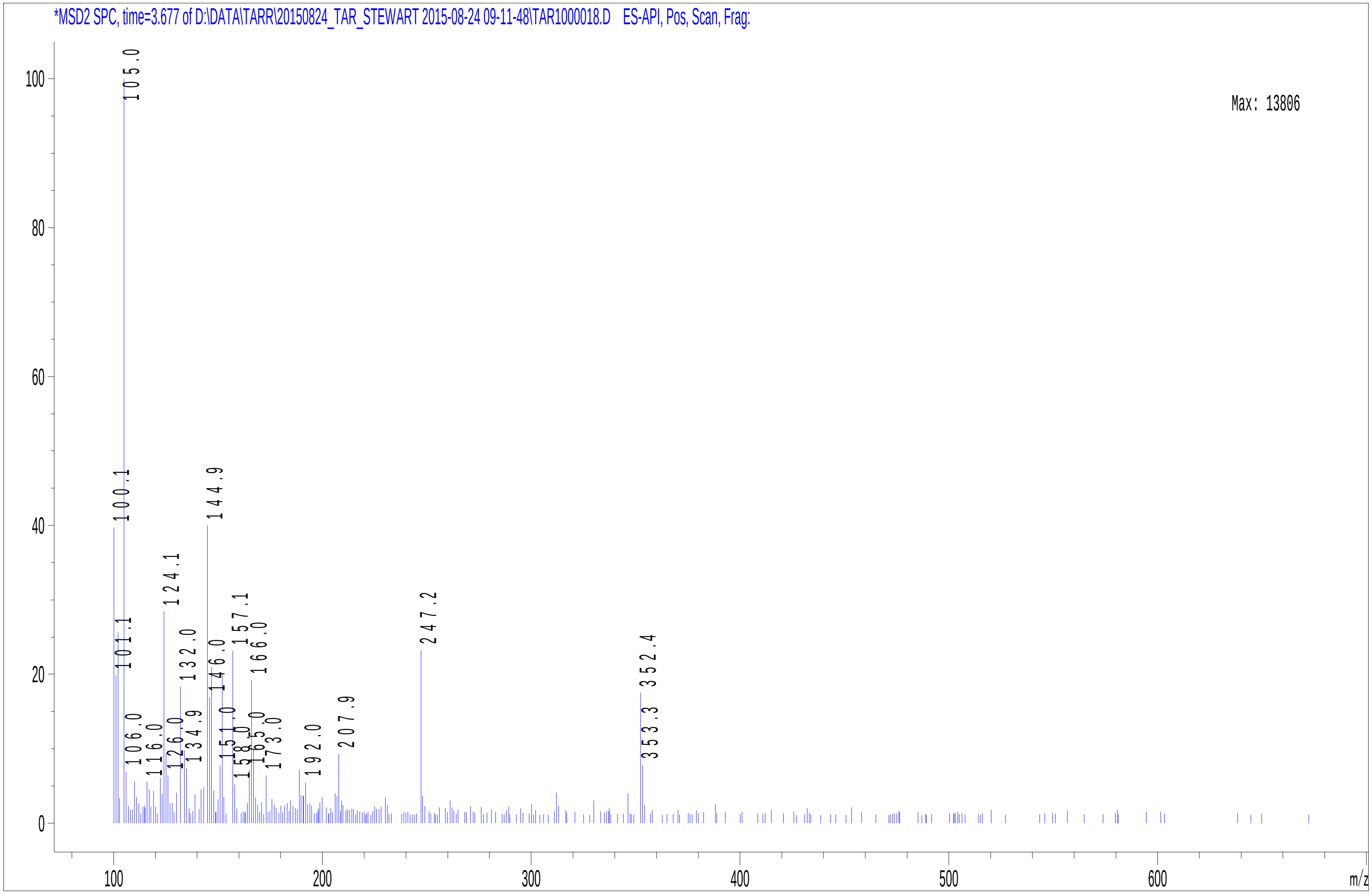
P2-B-01

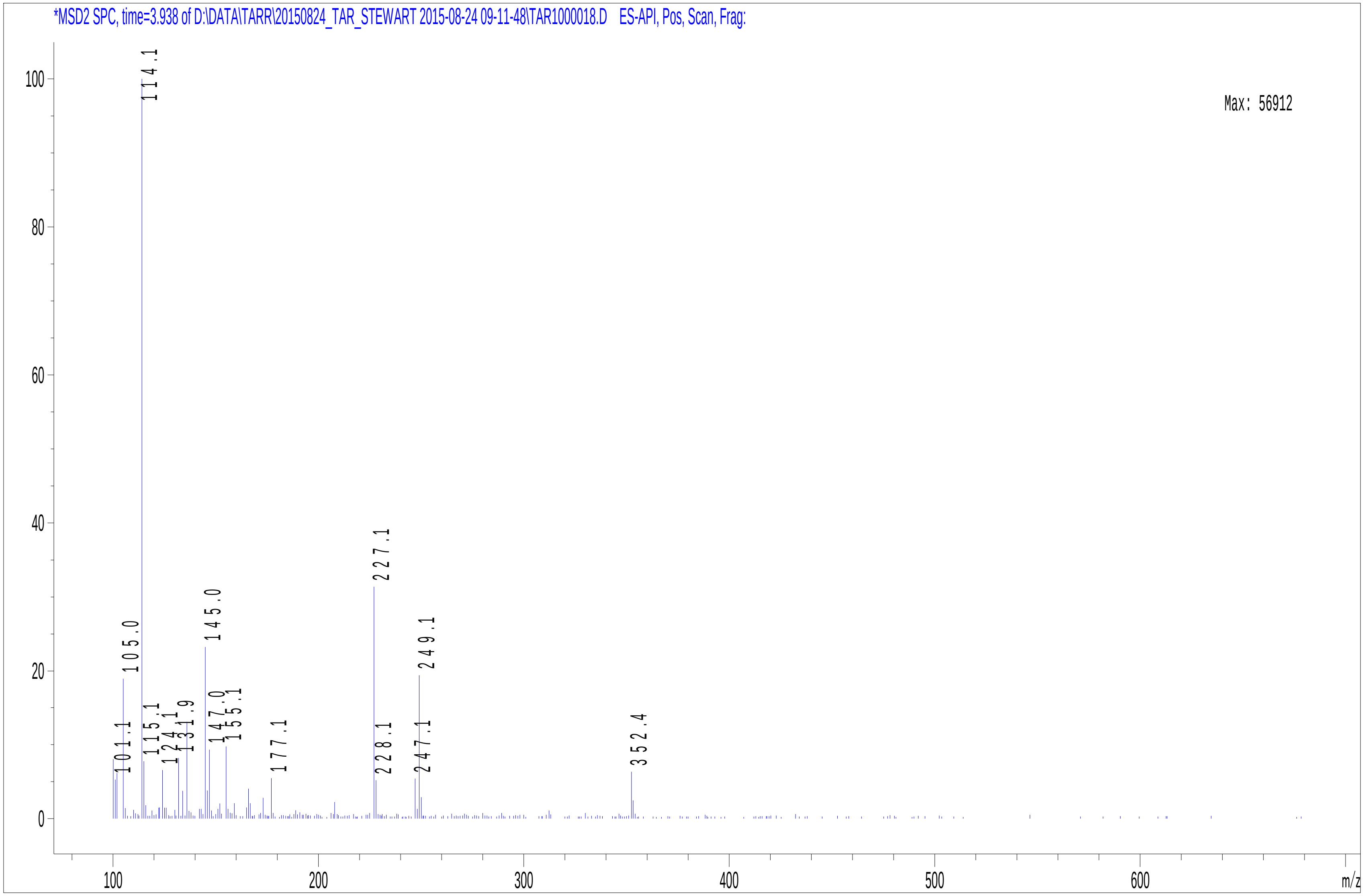


#	Time	Area	Height	Width	Area%	Symmetry
1	3.091	1064276.4	128974	0.1375	44.261	0.747
2	3.715	176176.5	14557.3	0.2017	7.327	1.644
3	3.925	1164085.6	128798.1	0.1506	48.412	0.72


MSD2 TIC, MS File (D:\DATA\TARR\20150824_TAR_STEWART 2015-08-24 09-11-48\TAR1000018.D)   ES-API, Pos, Scan, Frag: 70
260000
240000
220000
200000
180000
160000
140000
120000
100000
3.091
Area: 1.06428e+006
3.715
Area: 176177
3.925
Area: 1.16409e+006
2.75
3
3.25
3.5
3.75
4
4.25
4.5
4.75
min


*MSD2 SPC, time=3.089 of D:\DATA\TARR\20150824_TAR_STEWART 2015-08-24 09-11-48\TAR1000018.D ES-API, Pos, Scan, Frag:
Max: 103760
105.0
100.1
132.0
147.0
0
20
40
60
80
100
100
200
300
400
500
600
700
m/z

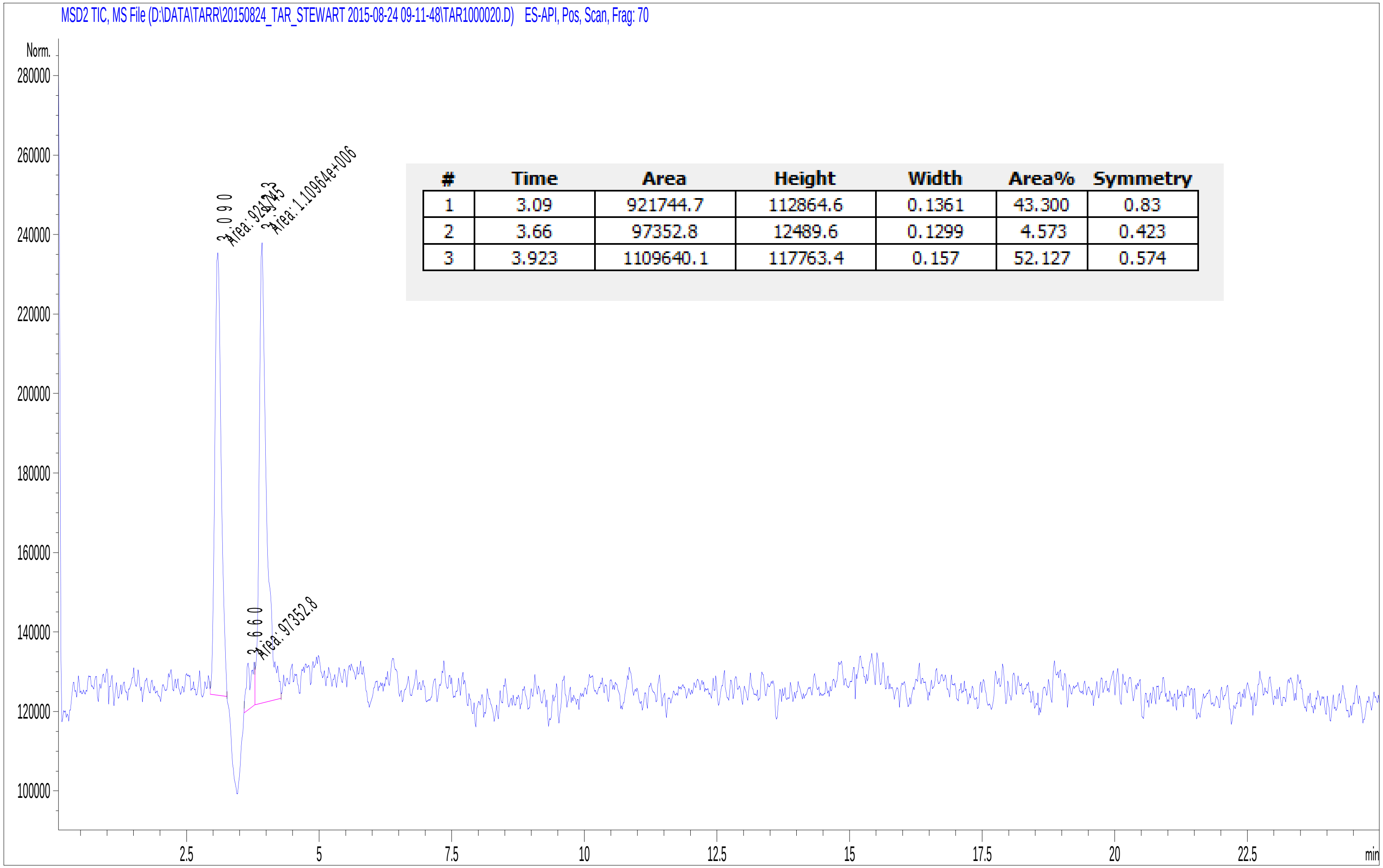

*MSD2 SPC, time=3.677 of D:\DATA\TARR\20150824_TAR_STEWART 2015-08-24 09-11-48\TAR1000018.D ES-API, Pos, Scan, Frag:
Max: 13806
105.0
100.1
144.9
124.1
101.1
247.2
157.1
166.0
132.0
146.0
352.4
353.3
106.0
116.0
126.0
134.9
151.0
158.0
165.0
173.0
192.0
207.9
0
20
40
60
80
100
100
200
300
400
500
600
m/z


*MSD2 SPC, time=3.938 of D:\DATA\TARR\20150824_TAR_STEWART 2015-08-24 09-11-48\TAR1000018.D ES-API, Pos, Scan, Frag:
Max: 56912
114.1
105.0
101.1
115.1
124.1
131.9
145.0
147.0
155.1
177.1
227.1
228.1
249.1
247.1
352.4
0
20
40
60
80
100
100
200
300
400
500
600
m/z

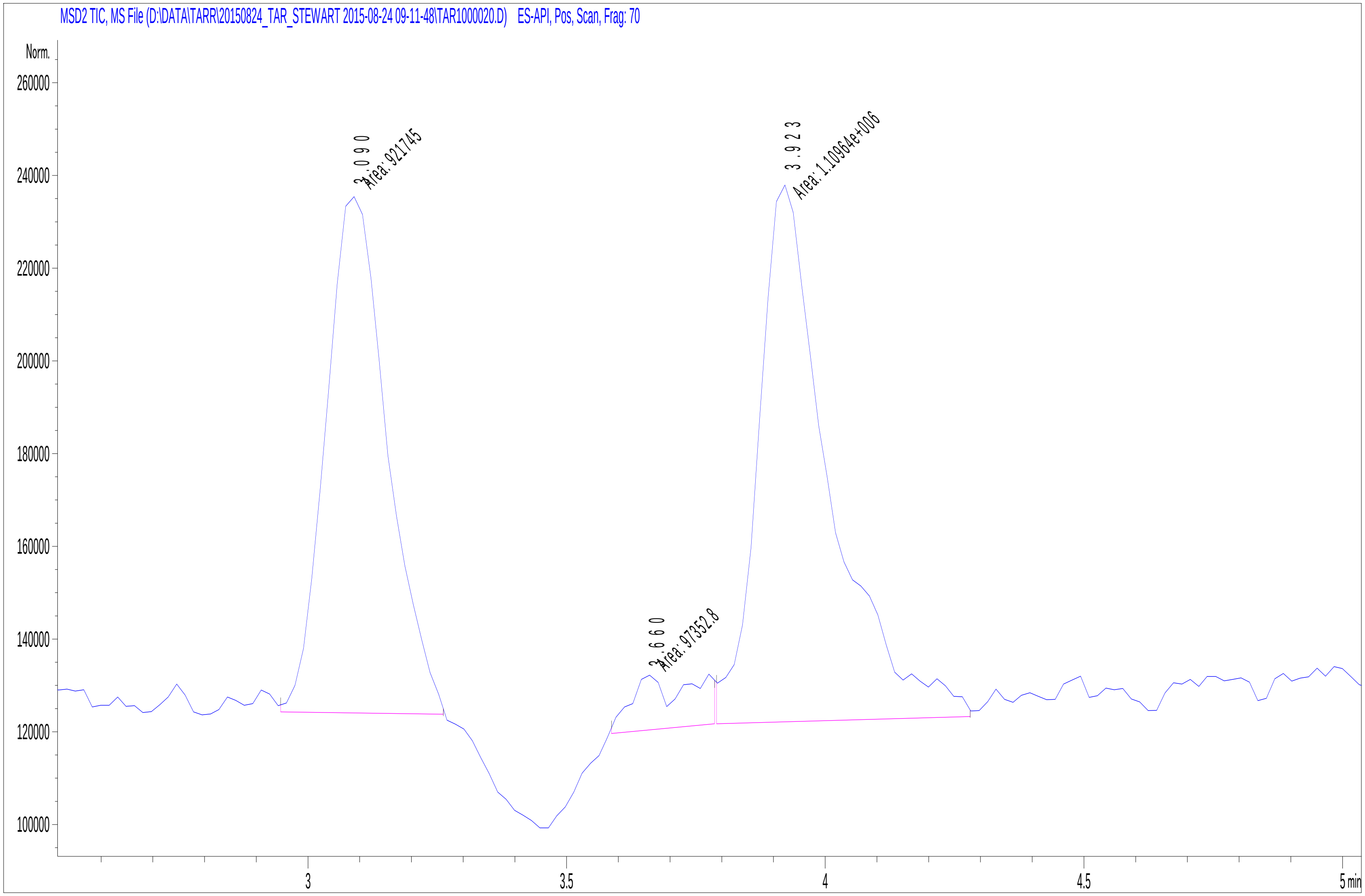
29-Jun-15

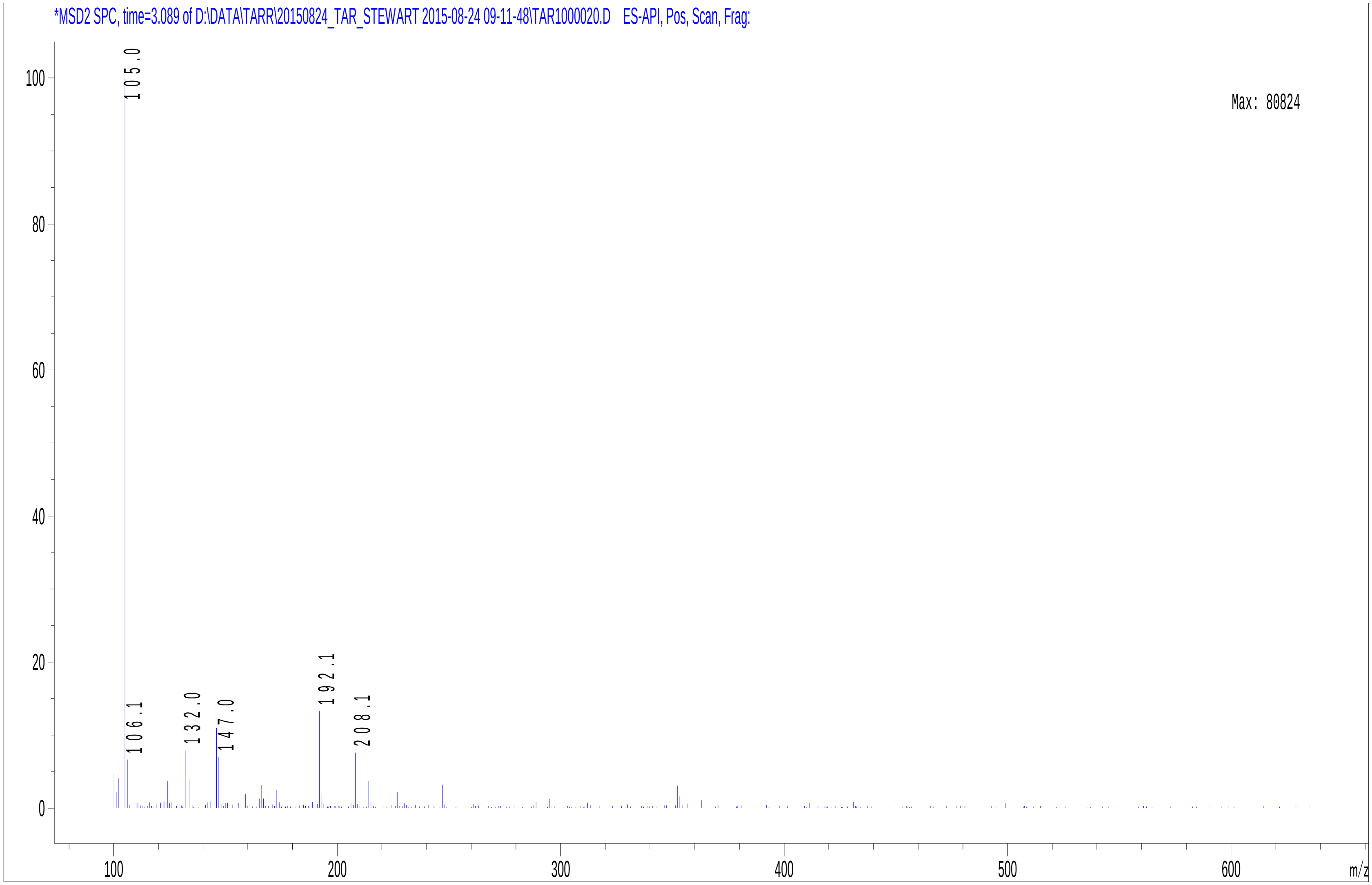
5 DC

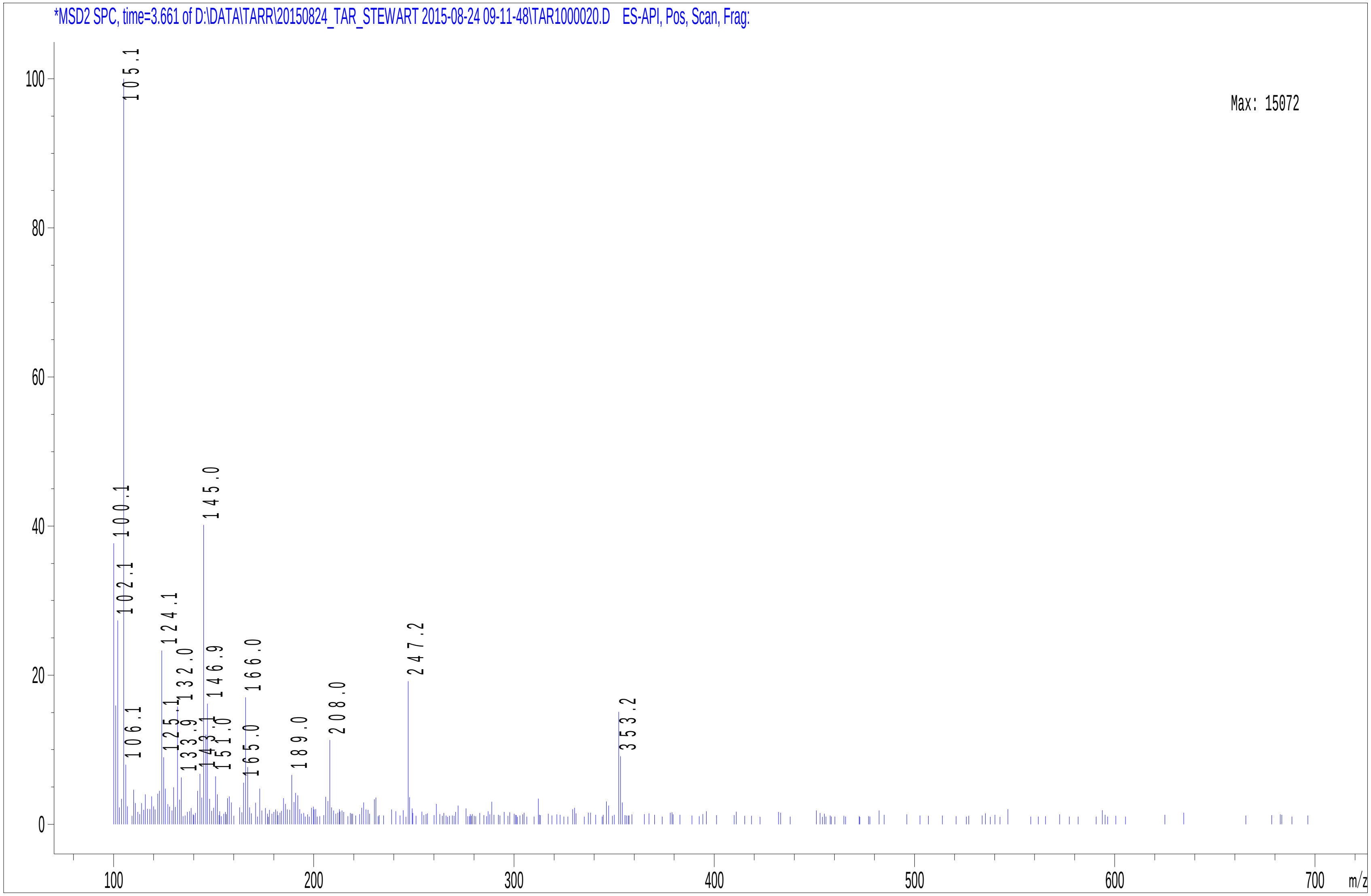
P2-C-02

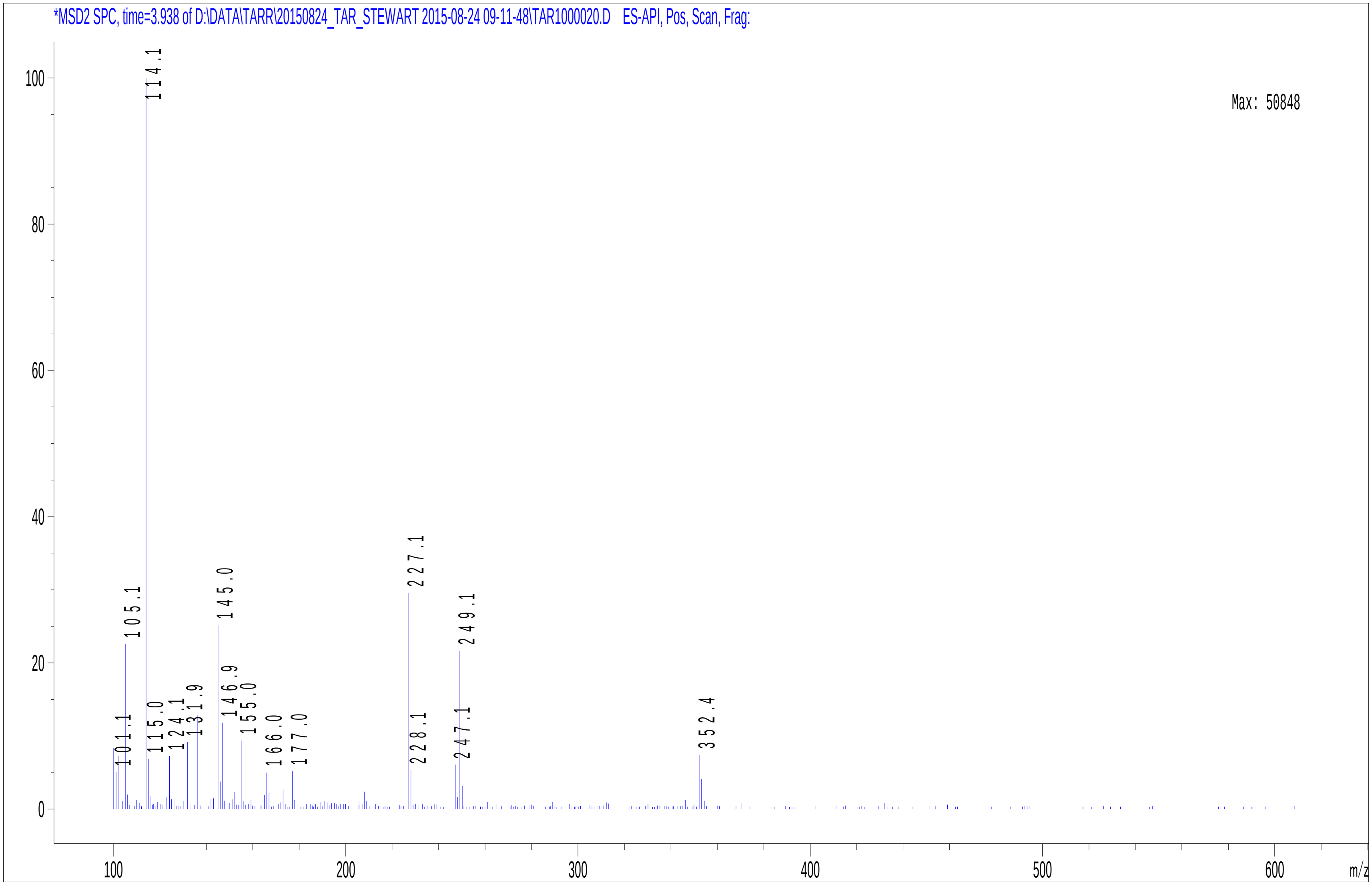


#	Time	Area	Height	Width	Area%	Symmetry
1	3.09	921744.7	112864.6	0.1361	43.300	0.83
2	3.66	97352.8	12489.6	0.1299	4.573	0.423
3	3.923	1109640.1	117763.4	0.157	52.127	0.574


MSD2 TIC, MS File (D:\DATA\TARR\20150824_TAR_STEWART 2015-08-24 09-11-48\TAR1000020.D) ES-API, Pos, Scan, Frag: 70
Norm.
260000
240000
220000
200000
180000
160000
140000
120000
100000
3.090
Area: 921745
3.660
Area: 97352.8
3.923
Area: 1.10964e+006
3
3.5
4
4.5
5 min


*MSD2 SPC, time=3.089 of D:\DATA\TARR\20150824_TAR_STEWART 2015-08-24 09-11-48\TAR1000020.D ES-API, Pos, Scan, Frag:
Max: 80824
105.0
106.1
132.0
147.0
192.1
208.1
100
80
60
40
20
0
100
200
300
400
500
600
m/z

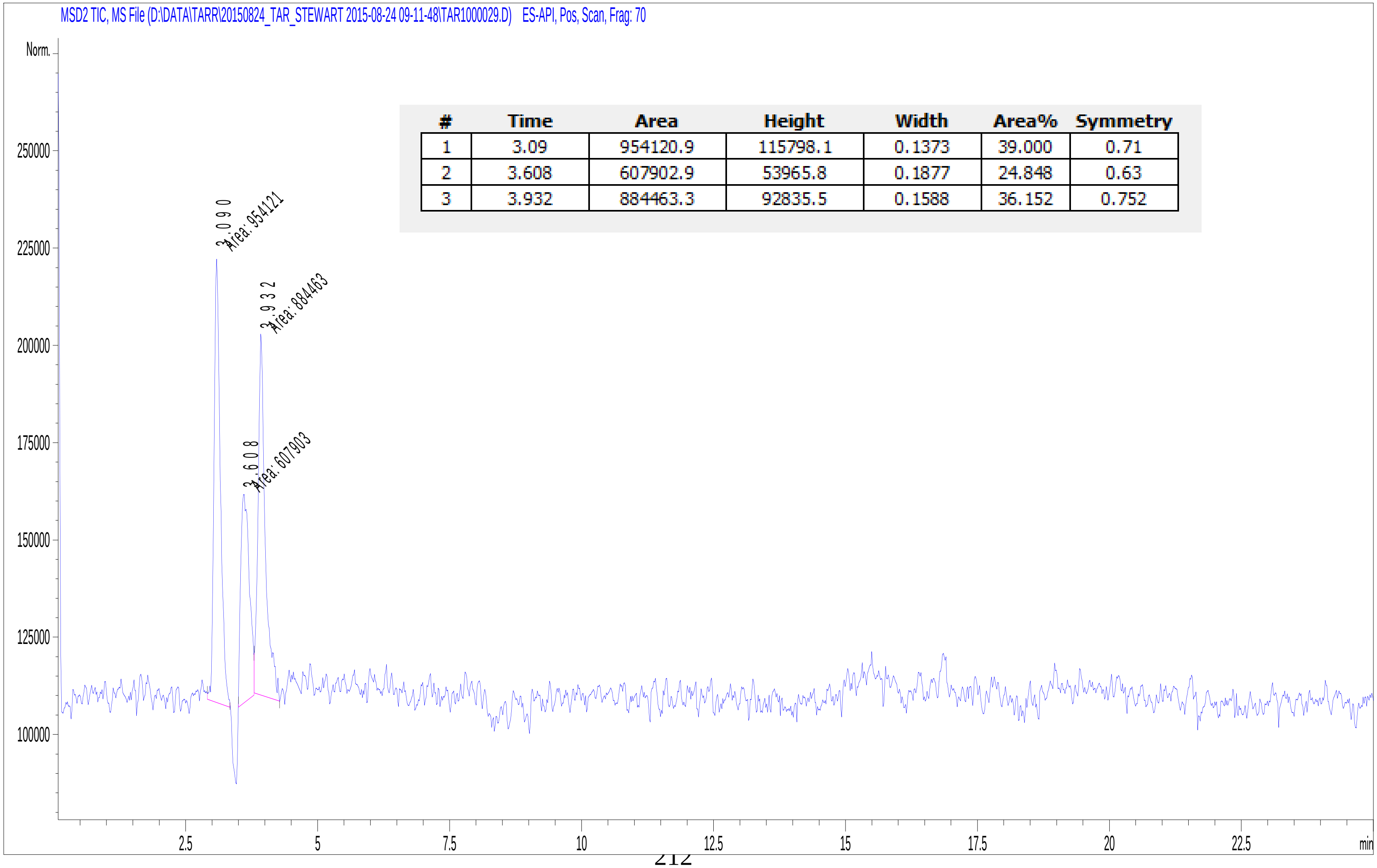

*MSD2 SPC, time=3.661 of D:\DATA\TARR\20150824_TAR_STEWART 2015-08-24 09-11-48\TAR1000020.D ES-API, Pos, Scan, Frag:
Max: 15072
105.1
100.1
102.1
106.1
124.1
125.1
132.0
133.9
143.1
145.0
146.9
151.0
165.0
166.0
189.0
208.0
247.2
353.2
0
20
40
60
80
100
100
200
300
400
500
600
700
m/z


*MSD2 SPC, time=3.938 of D:\DATA\TARR\20150824_TAR_STEWART 2015-08-24 09-11-48\TAR1000020.D ES-API, Pos, Scan, Frag:
Max: 50848
114.1
105.1
101.1
115.0
124.1
131.9
145.0
146.9
155.0
166.0
177.0
227.1
228.1
249.1
247.1
352.4
0
20
40
60
80
100
100
200
300
400
500
600
m/z

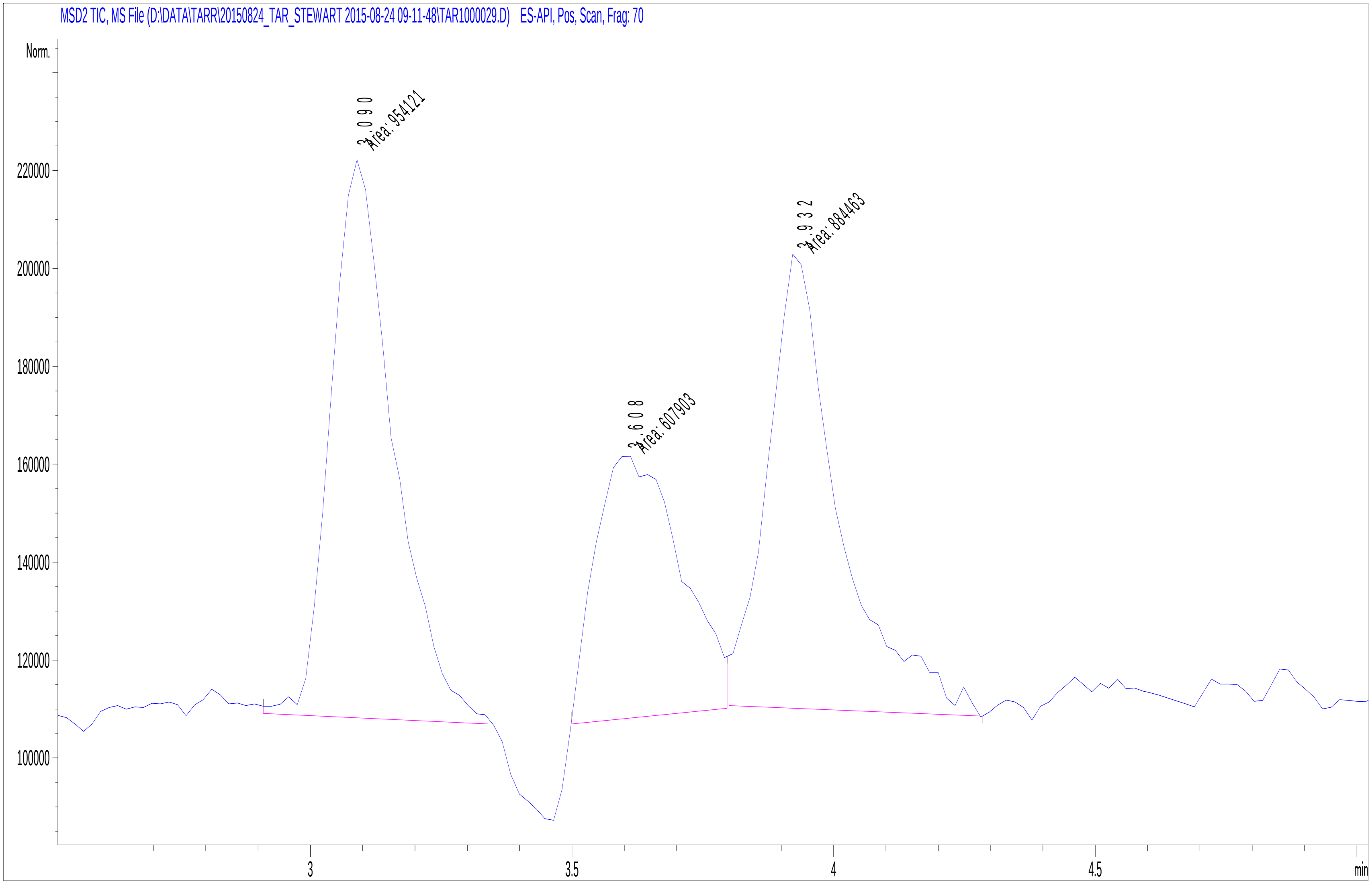
7-Aug-15

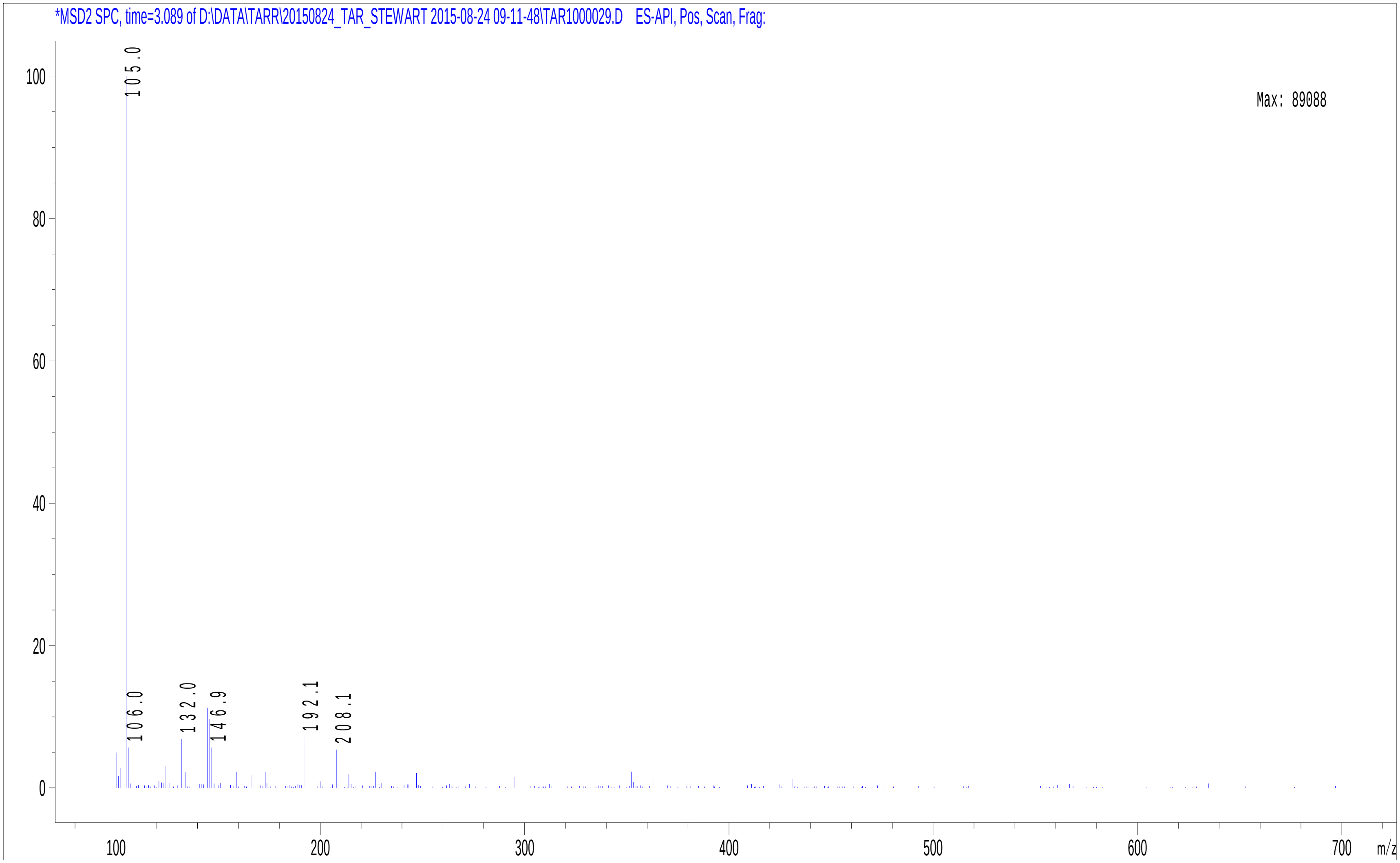
10 DC

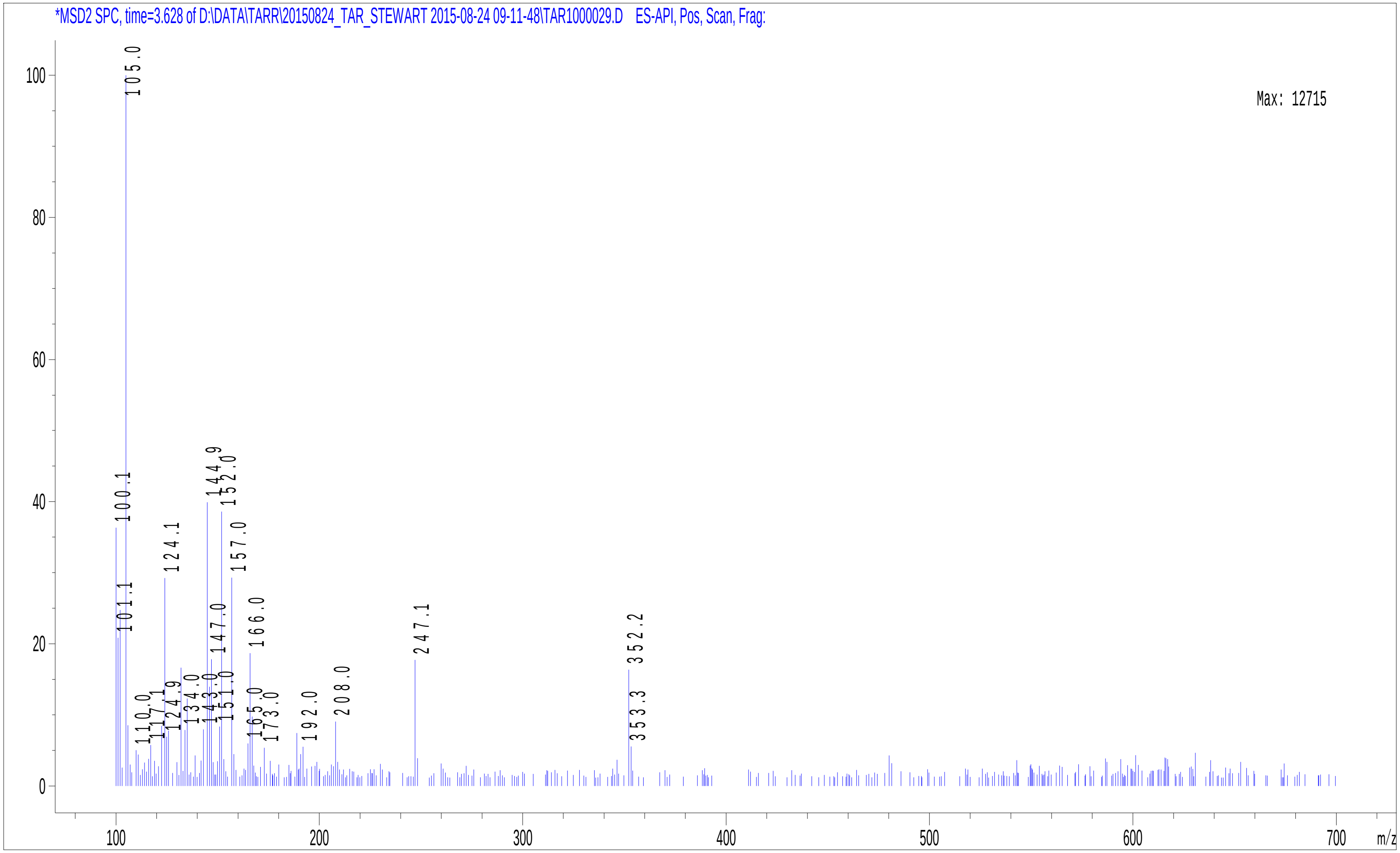
P2-D-08

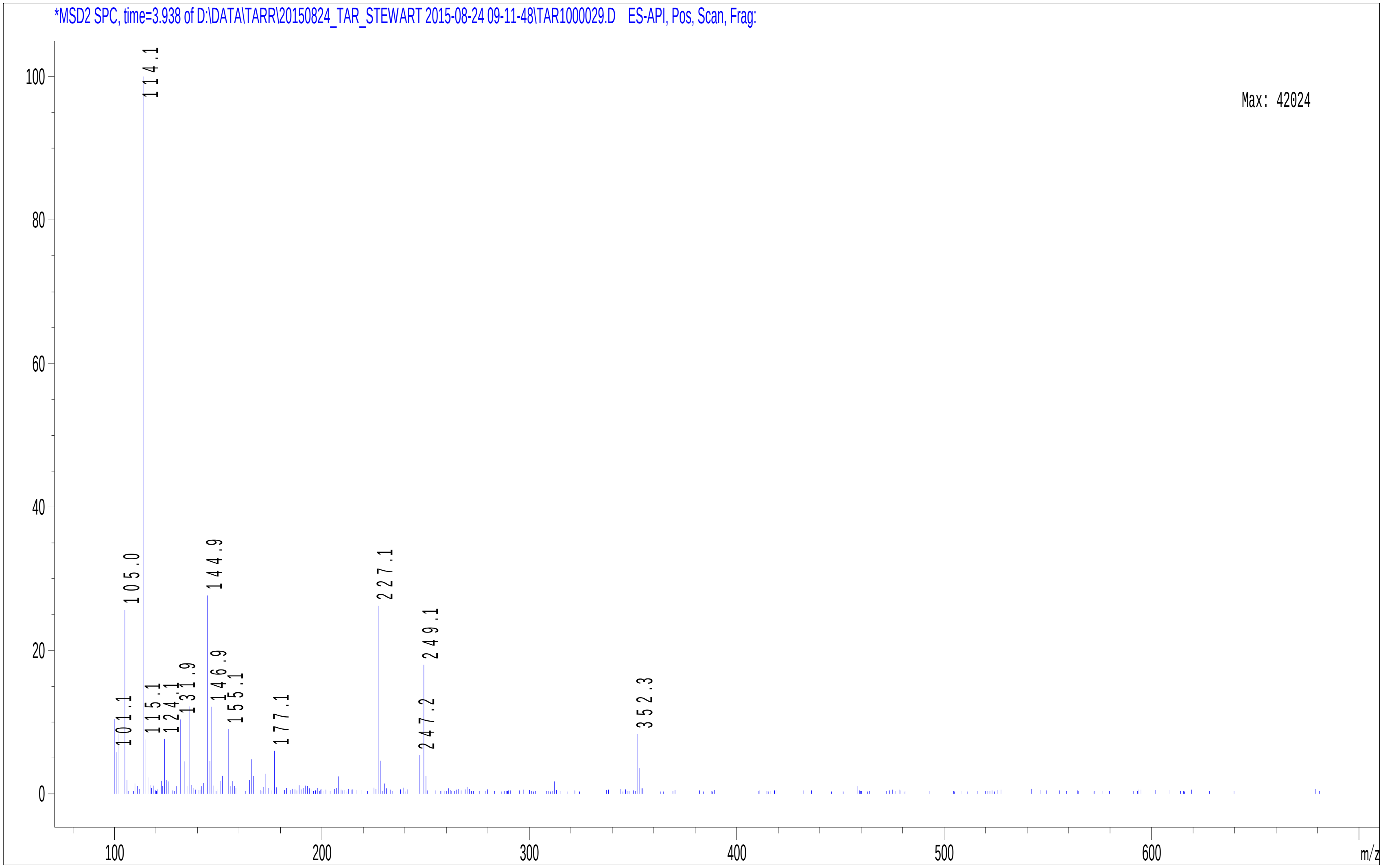


#	Time	Area	Height	Width	Area%	Symmetry
1	3.09	954120.9	115798.1	0.1373	39.000	0.71
2	3.608	607902.9	53965.8	0.1877	24.848	0.63
3	3.932	884463.3	92835.5	0.1588	36.152	0.752


MSD2 TIC, MS File (D:\DATA\TARR\20150824_TAR_STEWART 2015-08-24 09-11-48\TAR1000029.D)   ES-API, Pos, Scan, Frag: 70
Norm.
220000
200000
180000
160000
140000
120000
100000
3.090
Area: 954121
3.608
Area: 607903
3.932
Area: 884463
3
3.5
4
4.5
min


*MSD2 SPC, time=3.089 of D:\DATA\TARR\20150824_TAR_STEWART 2015-08-24 09-11-48\TAR1000029.D ES-API, Pos, Scan, Frag:
Max: 89088
105.0
106.0
132.0
146.9
192.1
208.1
0
20
40
60
80
100
100
200
300
400
500
600
700
m/z

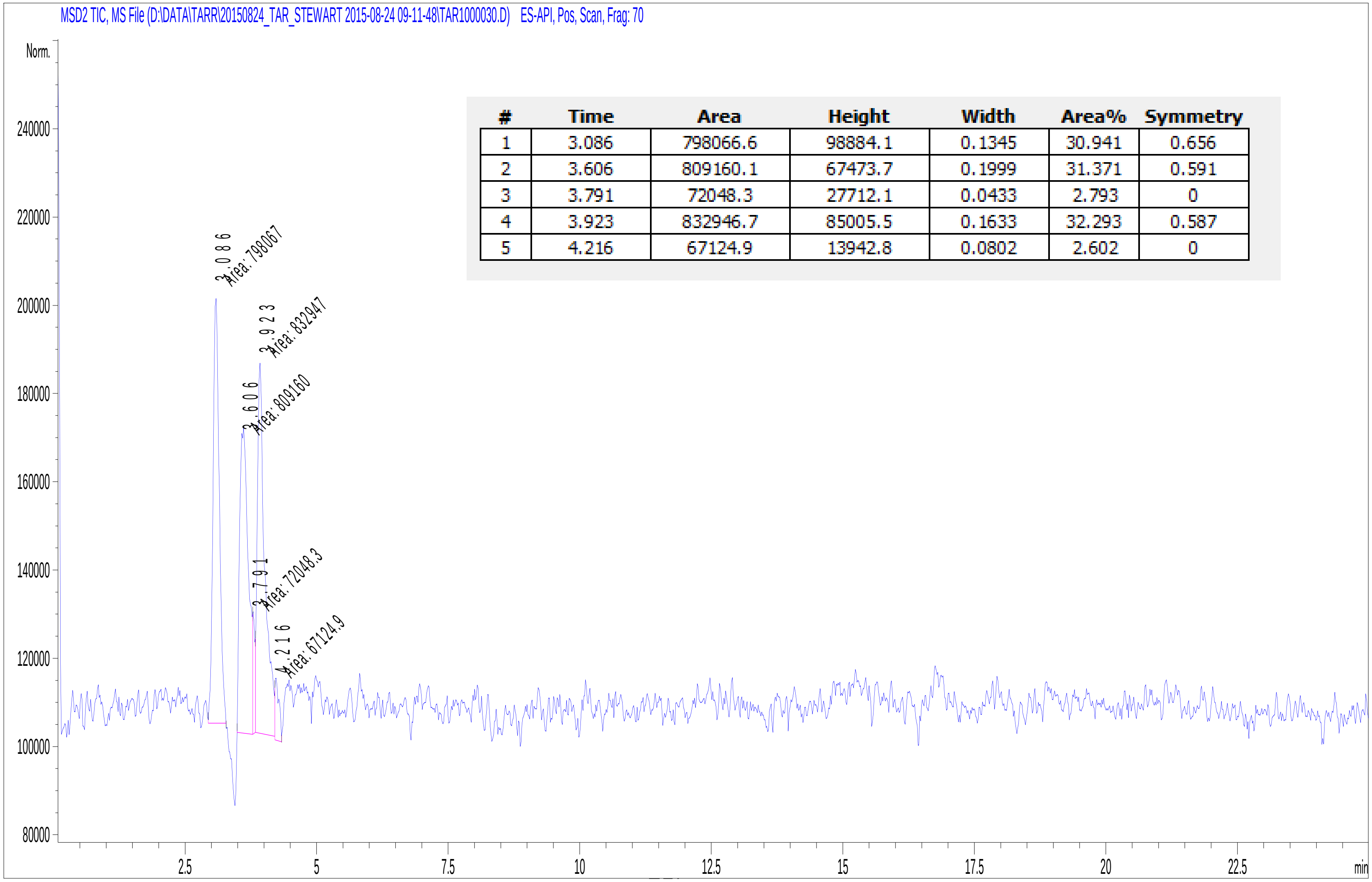

*MSD2 SPC, time=3.628 of D:\DATA\TARR\20150824_TAR_STEWART 2015-08-24 09-11-48\TAR1000029.D   ES-API, Pos, Scan, Frag:
Max: 12715
105.0
100.1
101.1
110.0
117.1
124.1
124.9
134.0
143.0
144.9
147.0
151.0
152.0
157.0
165.0
166.0
173.0
192.0
208.0
247.1
352.2
353.3
0
20
40
60
80
100
100
200
300
400
500
600
700
m/z


*MSD2 SPC, time=3.938 of D:\DATA\TARR\20150824_TAR_STEWART 2015-08-24 09-11-48\TAR1000029.D ES-API, Pos, Scan, Frag:
Max: 42024
114.1
105.0
101.1
115.1
124.1
131.9
144.9
146.9
155.1
177.1
227.1
247.2
249.1
352.3
0
20
40
60
80
100
200
300
400
500
600
m/z

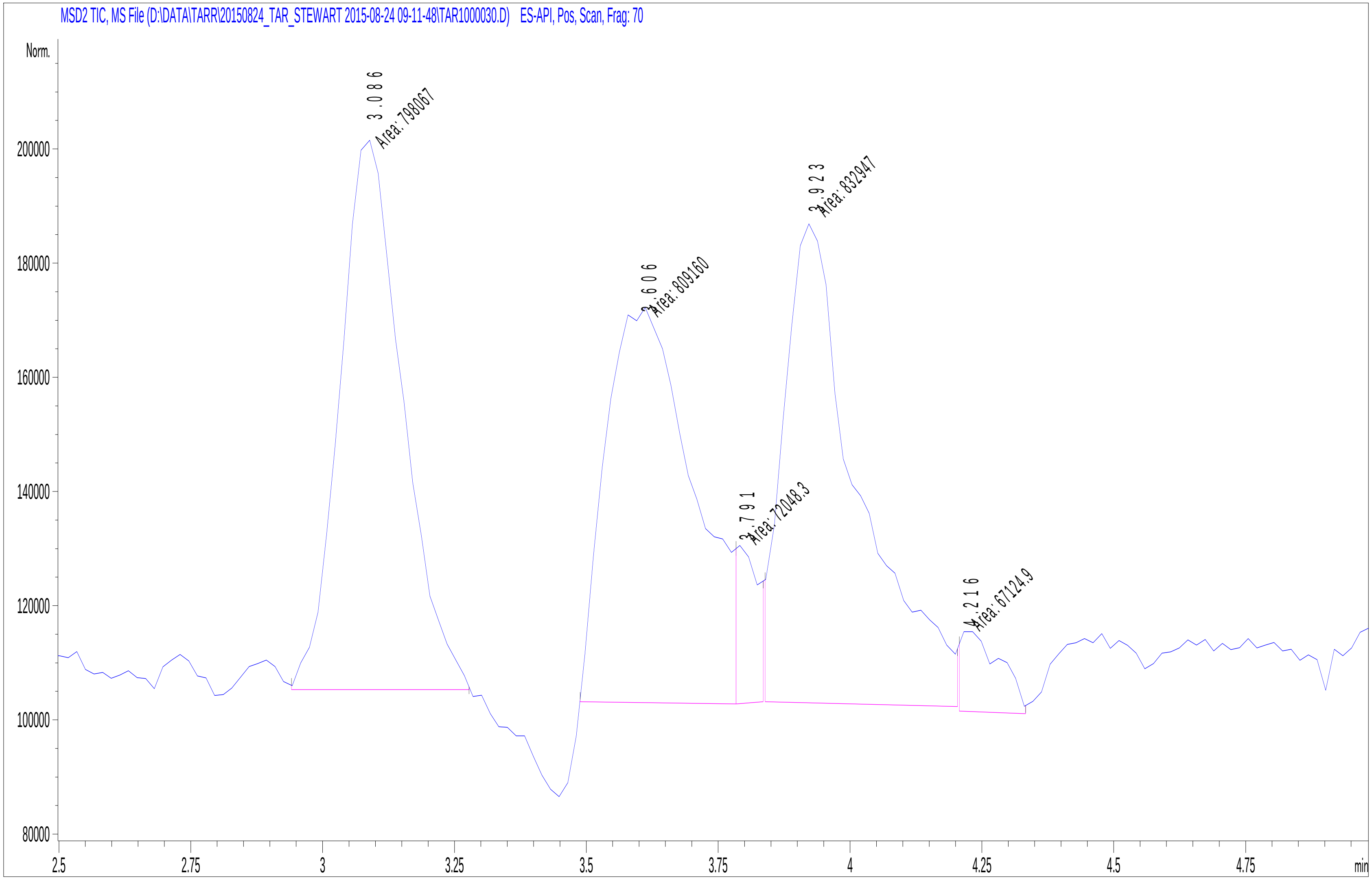
31-Jul-15

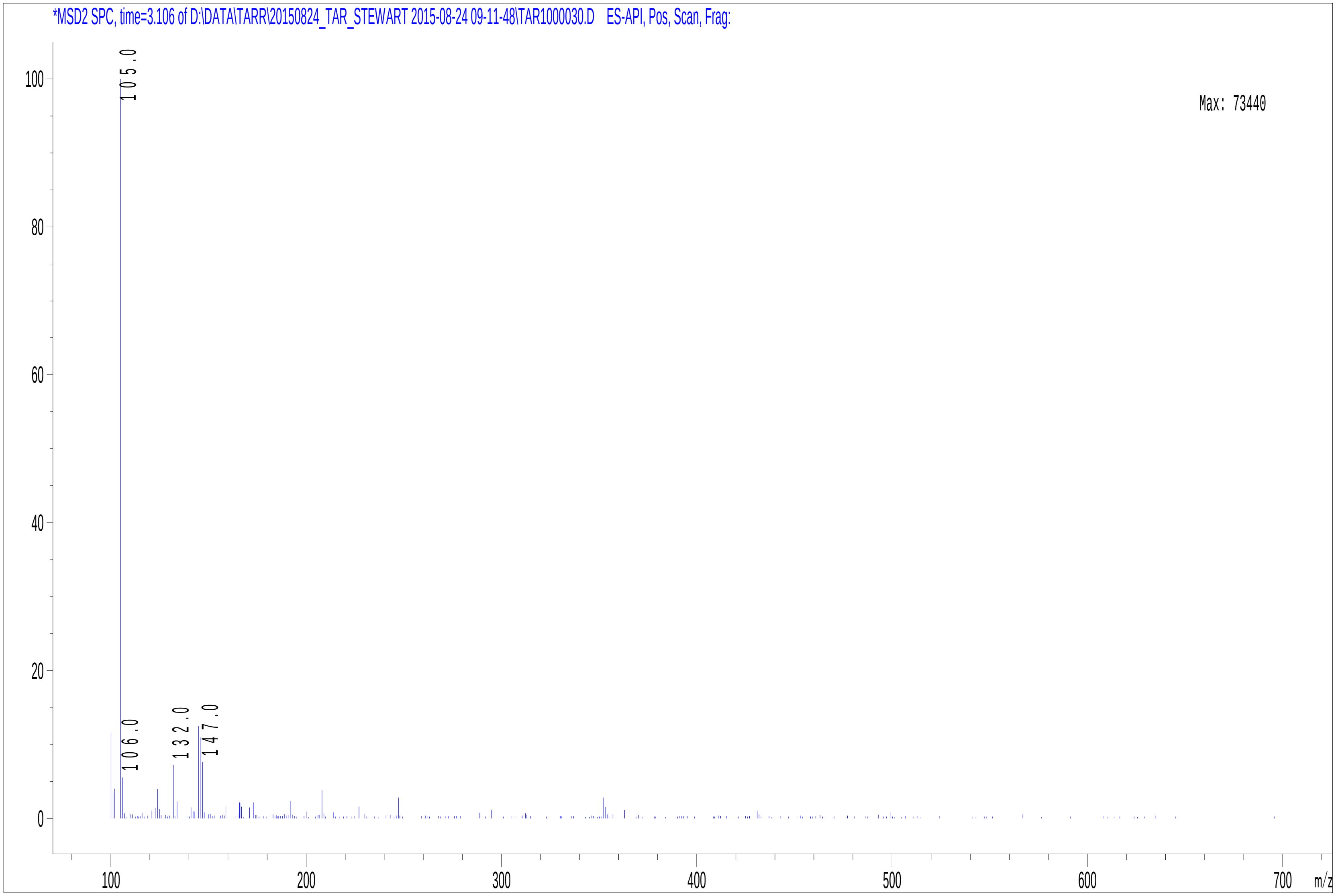
10 DC Problem (removal went up)

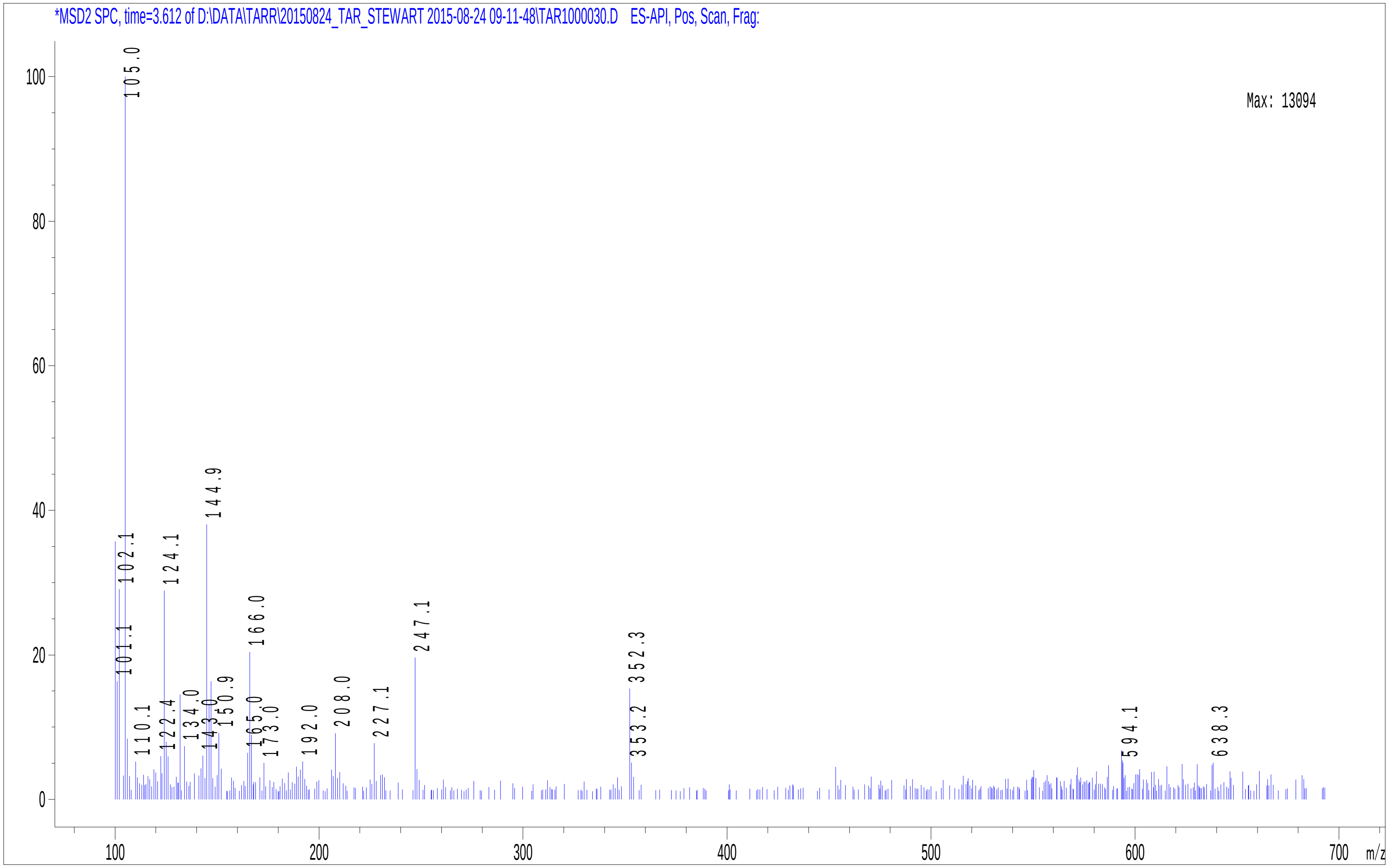
P2-D-07

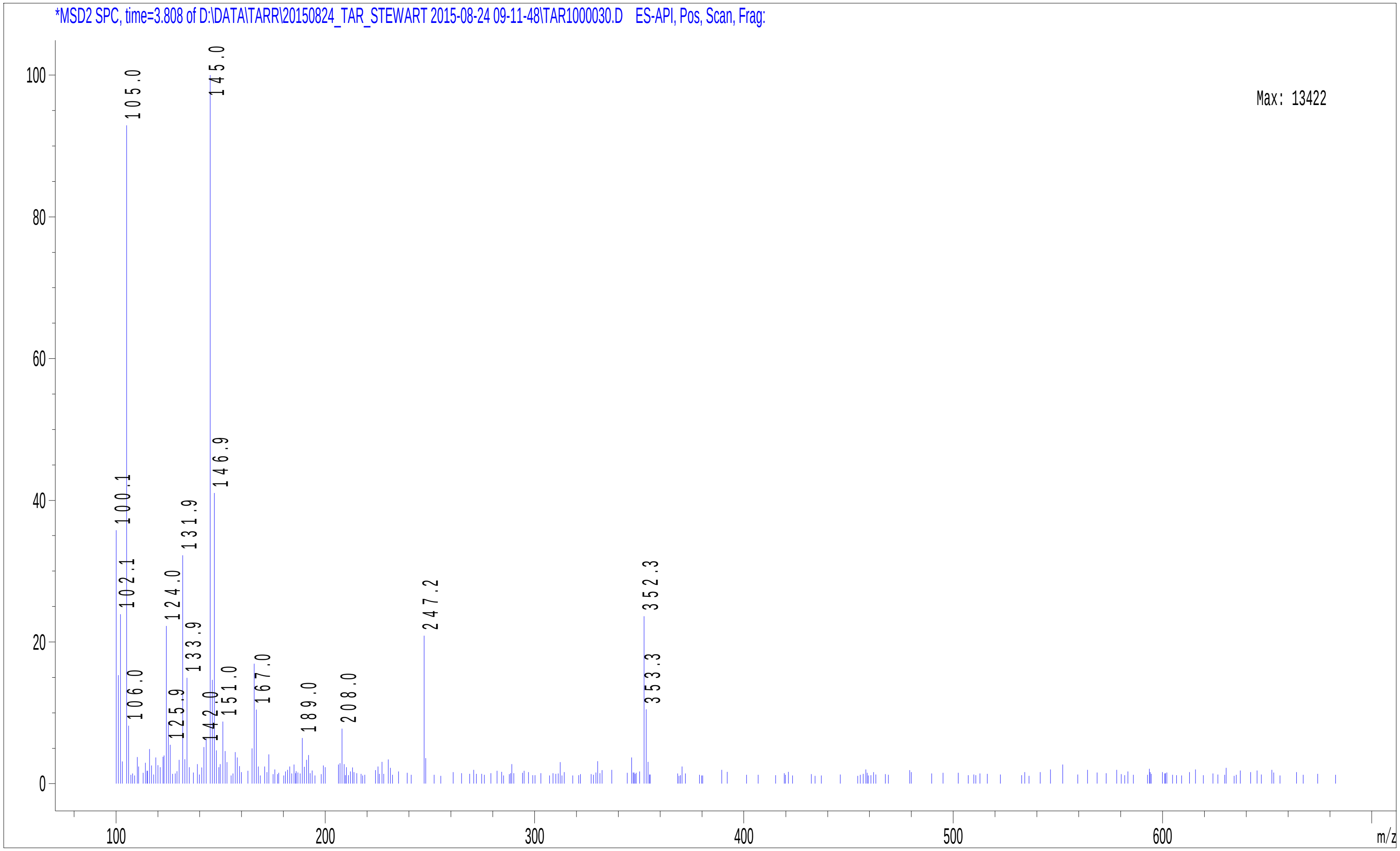


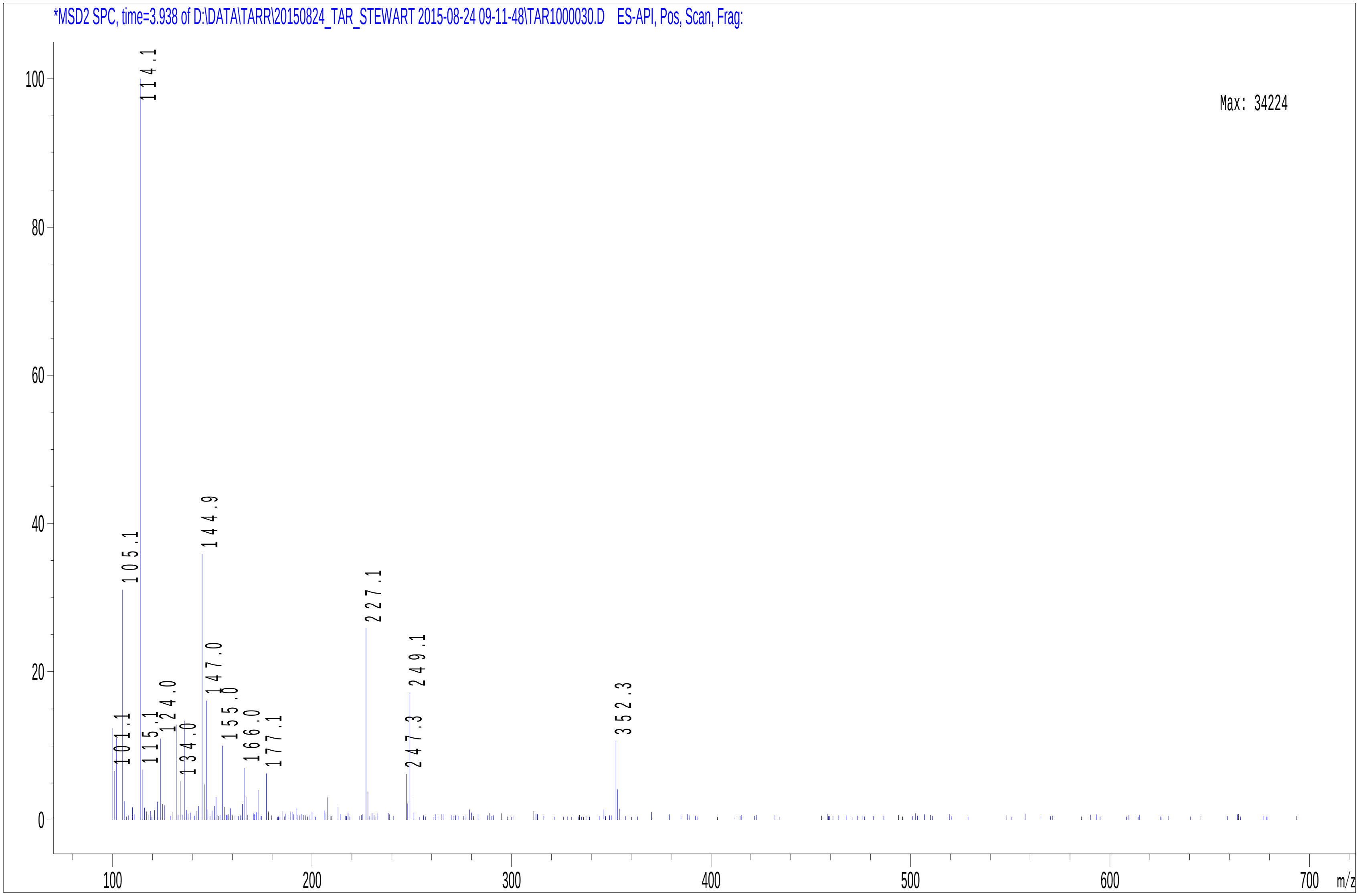
#	Time	Area	Height	Width	Area%	Symmetry
1	3.086	798066.6	98884.1	0.1345	30.941	0.656
2	3.606	809160.1	67473.7	0.1999	31.371	0.591
3	3.791	72048.3	27712.1	0.0433	2.793	0
4	3.923	832946.7	85005.5	0.1633	32.293	0.587
5	4.216	67124.9	13942.8	0.0802	2.602	0


MSD2 TIC, MS File (D:\DATA\TARR\20150824_TAR_STEWART 2015-08-24 09-11-48\TAR1000030.D) ES-API, Pos, Scan, Frag: 70
Norm.
200000
180000
160000
140000
120000
100000
80000
2.5
2.75
3
3.25
3.5
3.75
4
4.25
4.5
4.75
min
3.086
Area: 798067
3.606
Area: 809160
3.791
Area: 72048.3
3.923
Area: 832947
4.216
Area: 67124.9


*MSD2 SPC, time=3.106 of D:\DATA\TARR\20150824_TAR_STEWART 2015-08-24 09-11-48\TAR1000030.D ES-API, Pos, Scan, Frag:
Max: 73440
105.0
106.0
132.0
147.0
100
80
60
40
20
0
100
200
300
400
500
600
700
m/z


*MSD2 SPC, time=3.612 of D:\DATA\TARR\20150824_TAR_STEWART 2015-08-24 09-11-48\TAR1000030.D   ES-API, Pos, Scan, Frag:
Max: 13094
105.0
102.1
101.1
110.1
122.4
124.1
134.0
143.0
144.9
150.9
165.0
166.0
173.0
192.0
208.0
227.1
247.1
352.3
353.2
594.1
638.3
0
20
40
60
80
100
100
200
300
400
500
600
700
m/z

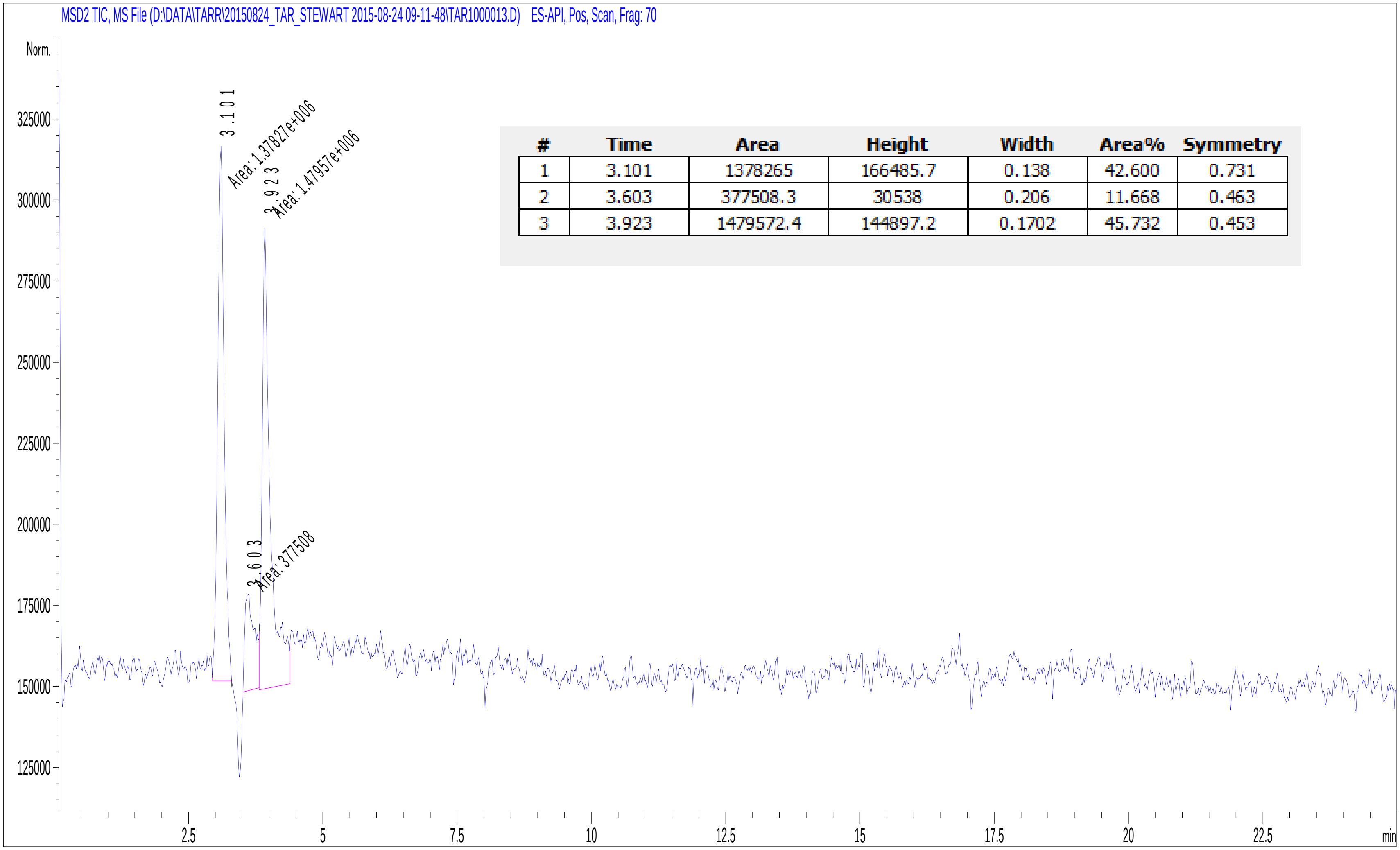

*MSD2 SPC, time=3.808 of D:\DATA\TARR\20150824_TAR_STEWART 2015-08-24 09-11-48\TAR1000030.D ES-API, Pos, Scan, Frag:
Max: 13422
100
80
60
40
20
0
100.1
102.1
105.0
106.0
124.0
125.9
131.9
133.9
142.0
145.0
146.9
151.0
167.0
189.0
208.0
247.2
352.3
353.3
100
200
300
400
500
600
m/z


*MSD2 SPC, time=3.938 of D:\DATA\TARR\20150824_TAR_STEWART 2015-08-24 09-11-48\TAR1000030.D ES-API, Pos, Scan, Frag:
Max: 34224
114.1
105.1
101.1
115.1
124.0
134.0
144.9
147.0
155.0
166.0
177.1
227.1
249.1
247.3
352.3
0
20
40
60
80
100
100
200
300
400
500
600
700
m/z

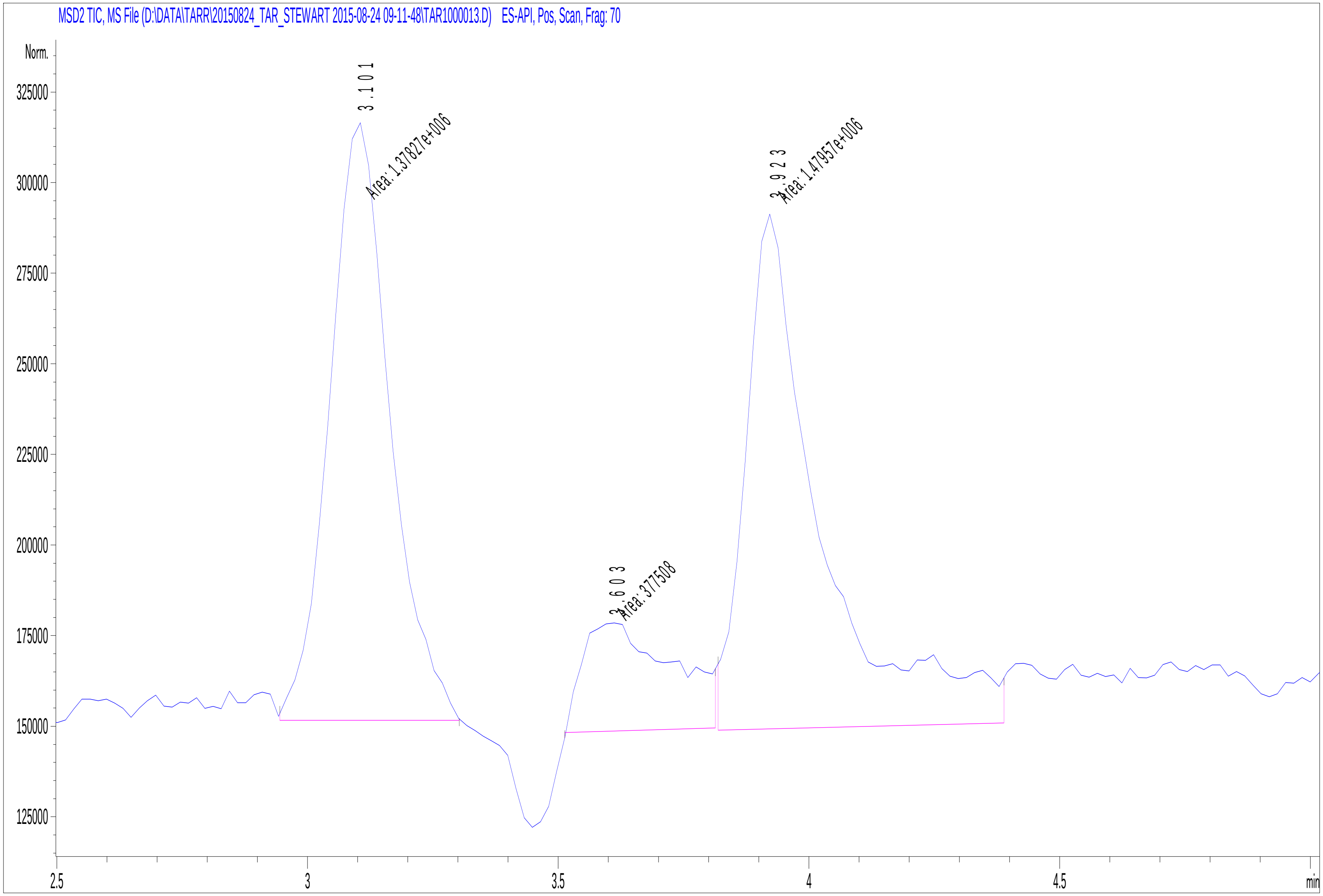
9-Jun-15

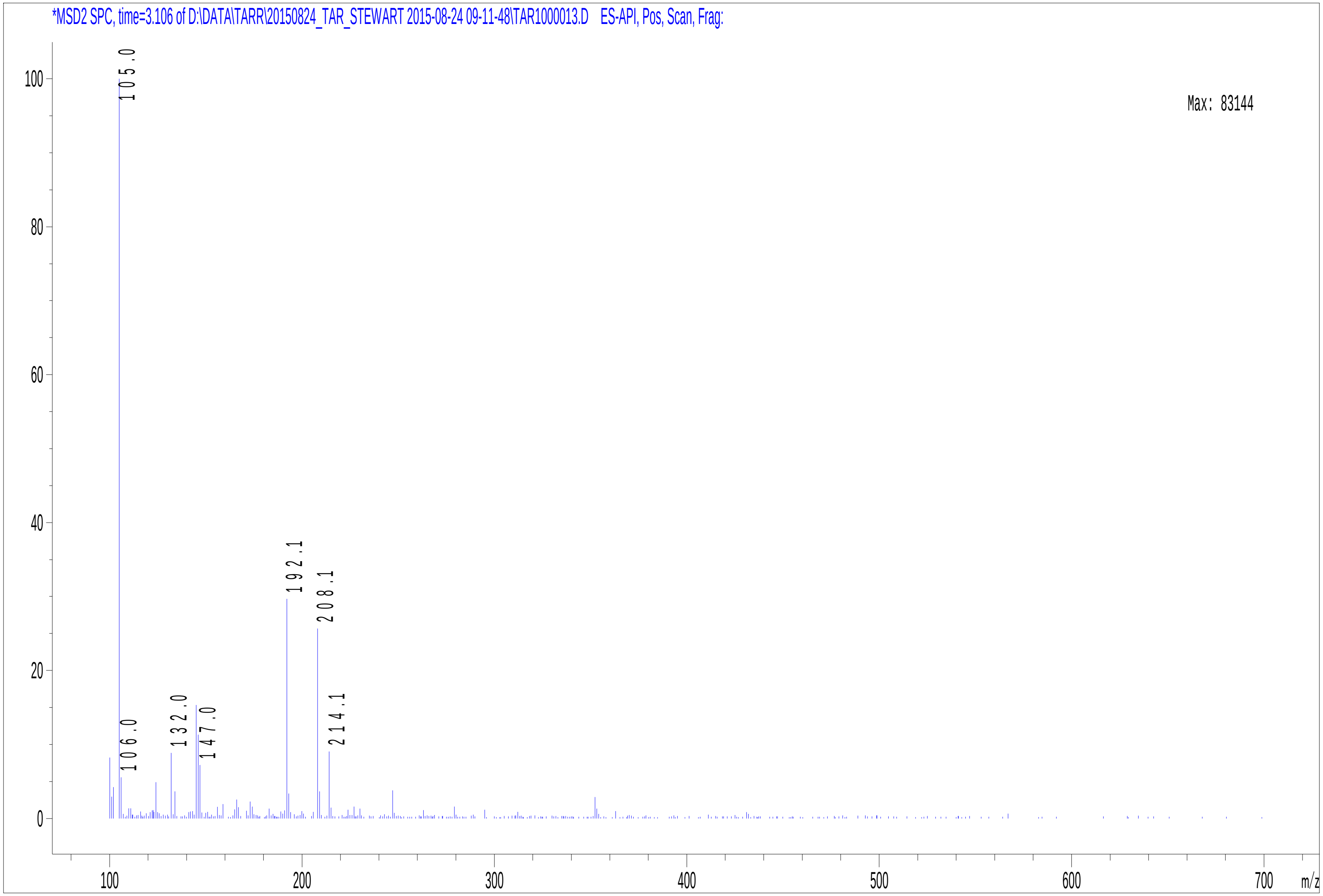
20 DC

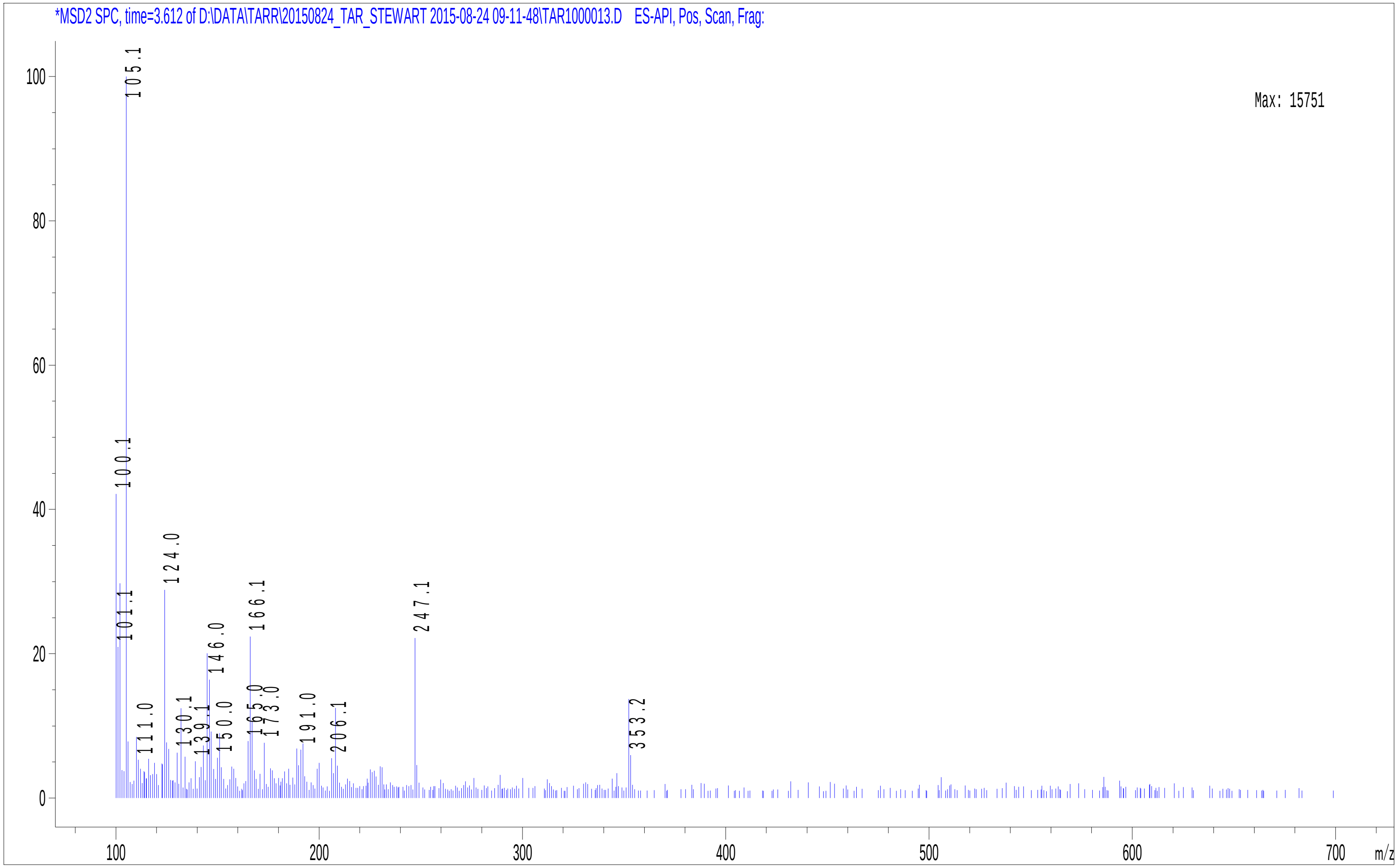
P2-B-06

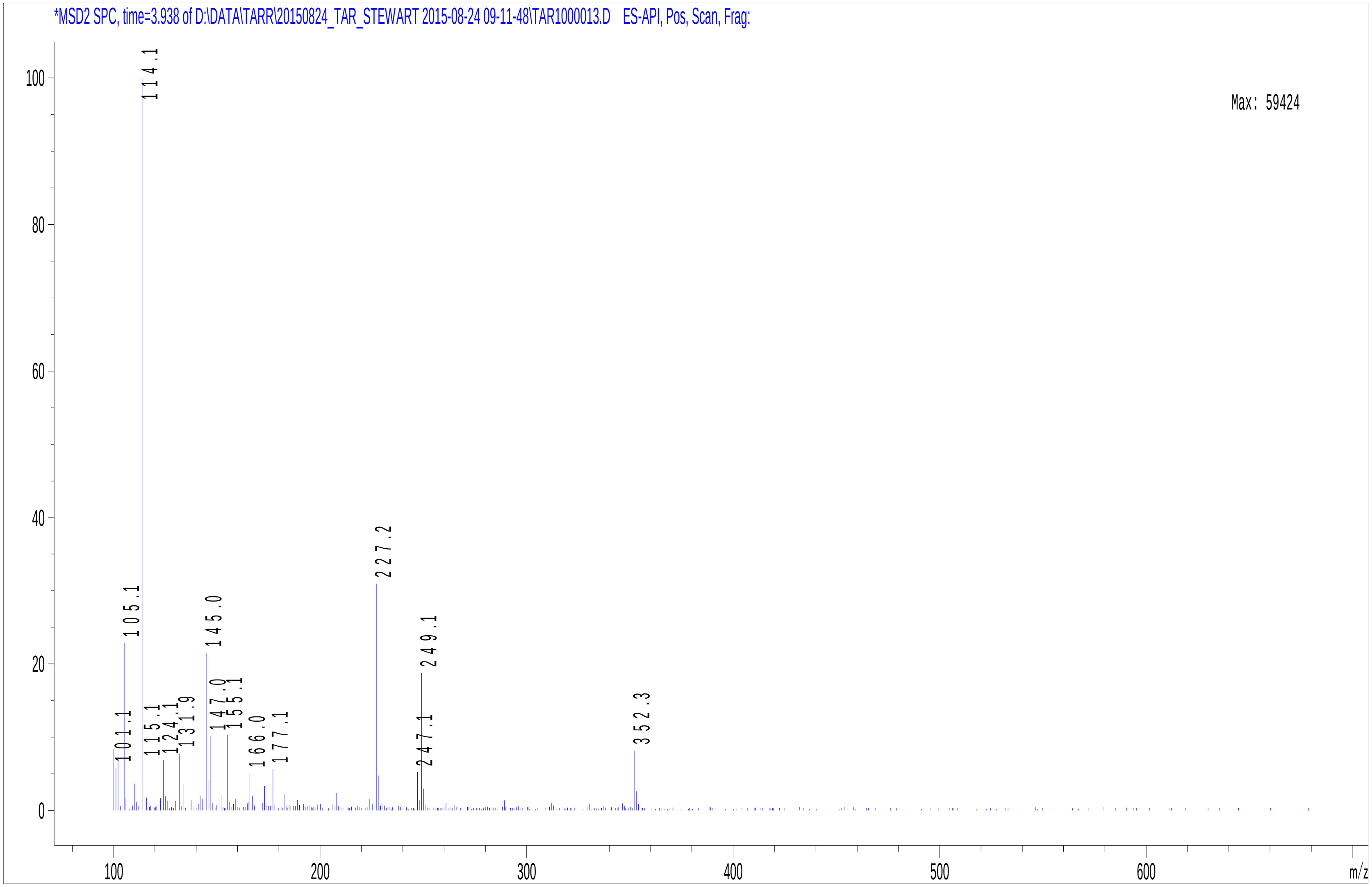


#	Time	Area	Height	Width	Area%	Symmetry
1	3.101	1378265	166485.7	0.138	42.600	0.731
2	3.603	377508.3	30538	0.206	11.668	0.463
3	3.923	1479572.4	144897.2	0.1702	45.732	0.453


MSD2 TIC, MS File (D:\DATA\TARR\20150824_TAR_STEWART 2015-08-24 09-11-48\TAR1000013.D) ES-API, Pos, Scan, Frag: 70
Norm.
325000
300000
275000
250000
225000
200000
175000
150000
125000
3.101
Area: 1.37827e+006
3.603
Area: 377508
3.923
Area: 1.47957e+006
2.5
3
3.5
4
4.5
min


*MSD2 SPC, time=3.106 of D:\DATA\TARR\20150824_TAR_STEWART 2015-08-24 09-11-48\TAR1000013.D ES-API, Pos, Scan, Frag:
Max: 83144
105.0
106.0
132.0
147.0
192.1
208.1
214.1
100
80
60
40
20
0
100
200
300
400
500
600
700
m/z

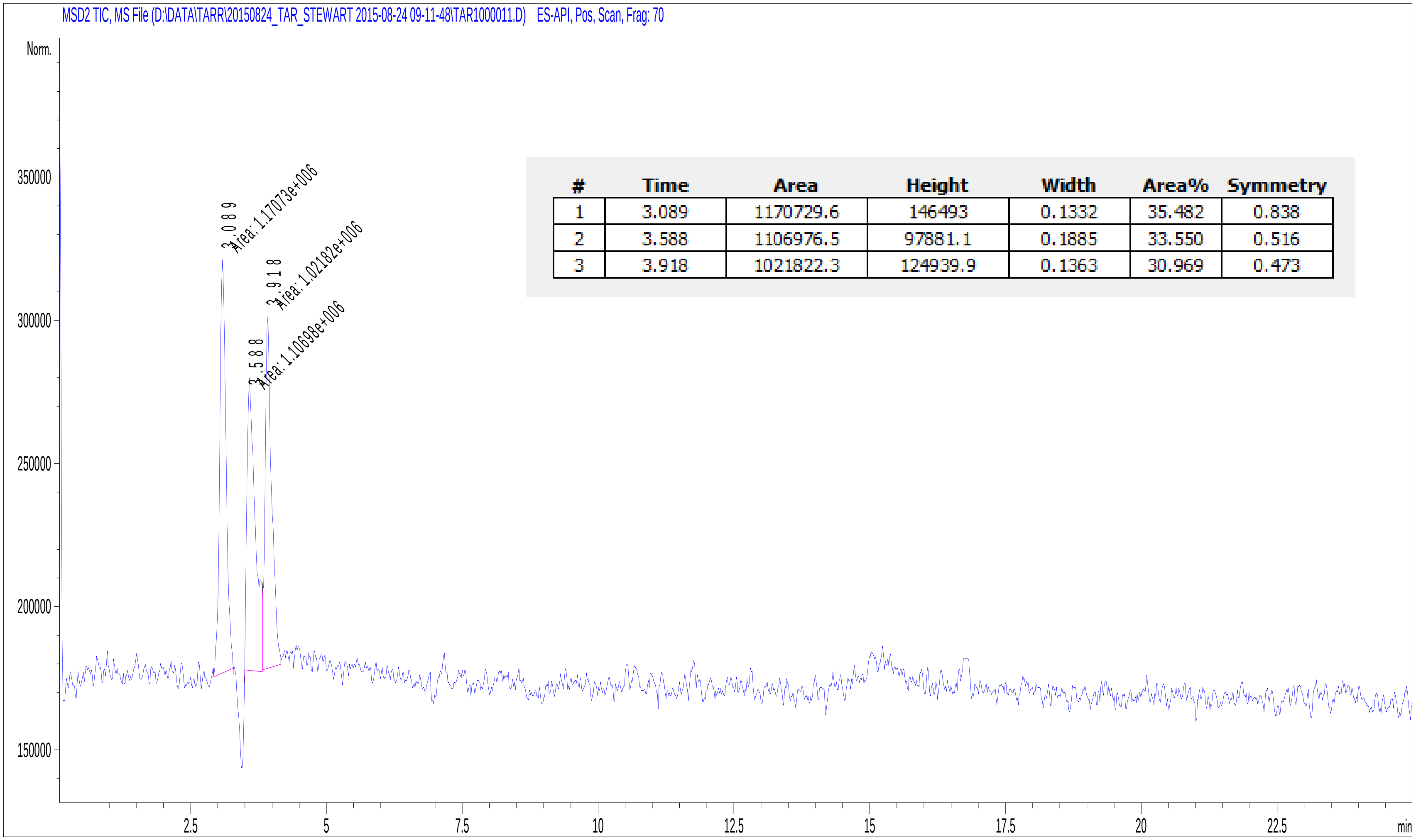
*MSD2 SPC, time=3.612 of D:\DATA\TARR\20150824_TAR_STEWART 2015-08-24 09-11-48\TAR1000013.D ES-API, Pos, Scan, Frag:
Max: 15751
105.1
100.1
101.1
111.0
124.0
130.1
139.1
146.0
150.0
165.0
166.1
173.0
191.0
206.1
247.1
353.2
0
20
40
60
80
100
100
200
300
400
500
600
700
m/z


*MSD2 SPC, time=3.938 of D:\DATA\TARR\20150824_TAR_STEWART 2015-08-24 09-11-48\TAR1000013.D ES-API, Pos, Scan, Frag:
Max: 59424
114.1
105.1
101.1
115.1
124.1
131.9
145.0
147.0
155.1
166.0
177.1
227.2
247.1
249.1
352.3
0
20
40
60
80
100
100
200
300
400
500
600
m/z

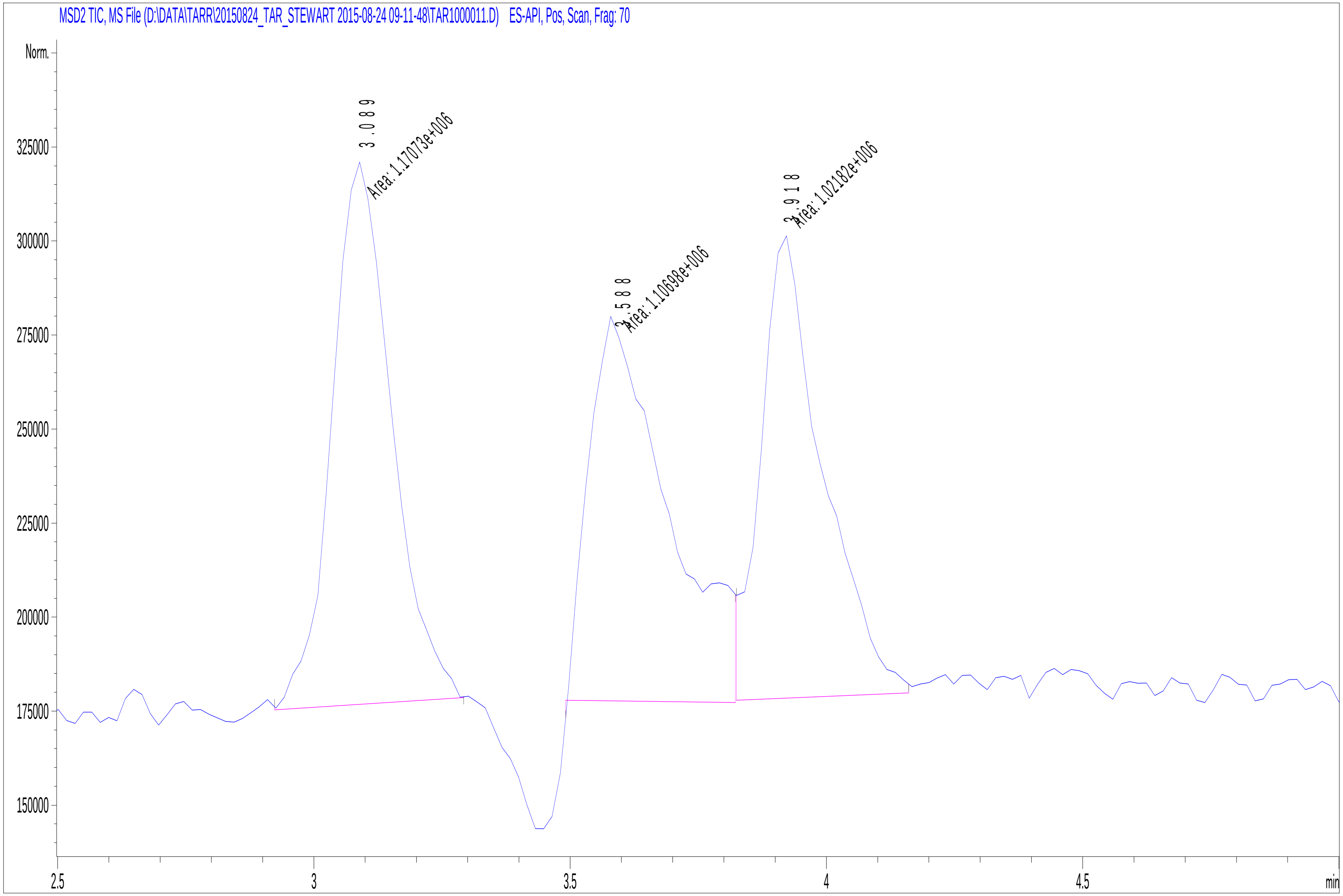
17-Jun-15

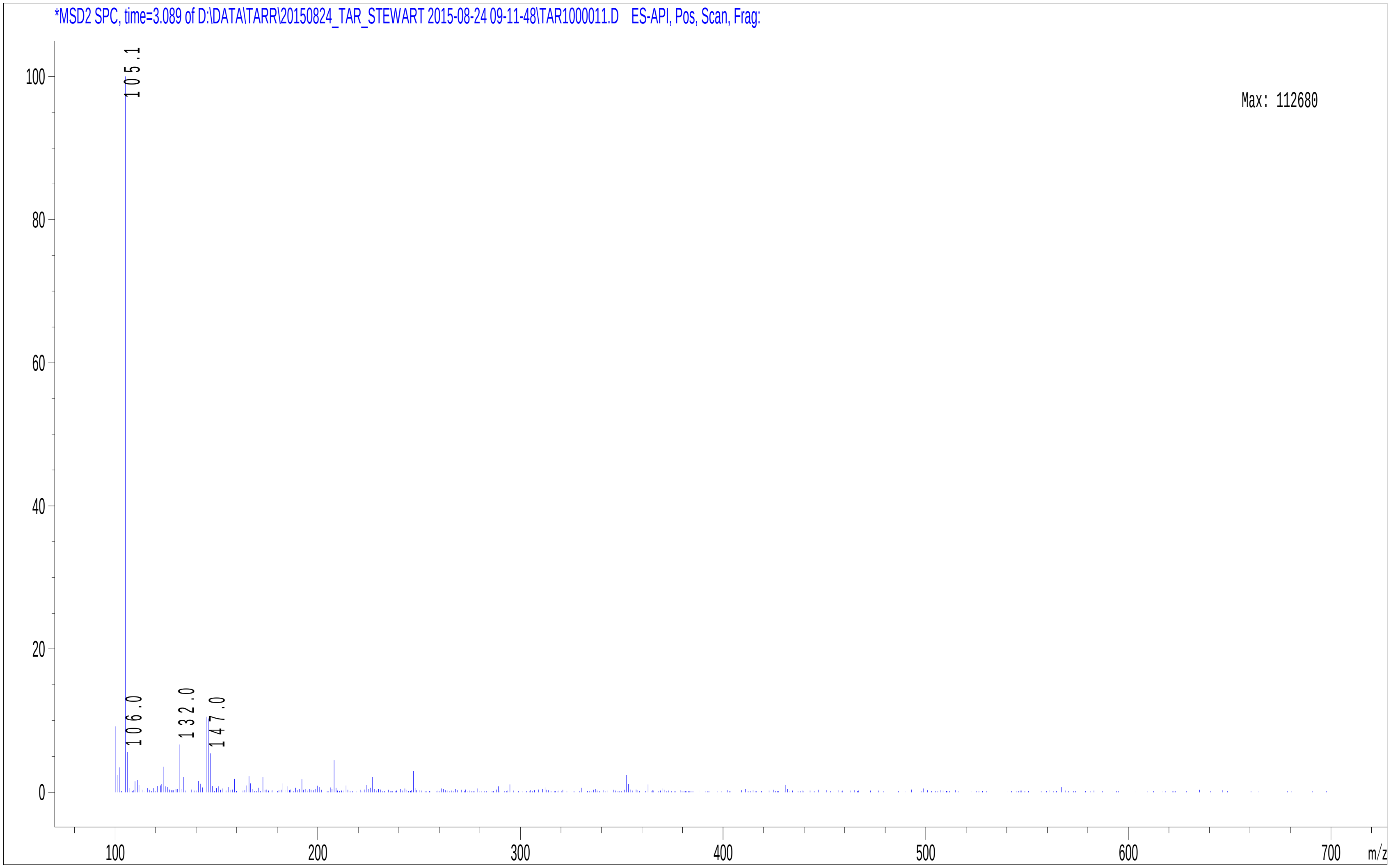
30 DC

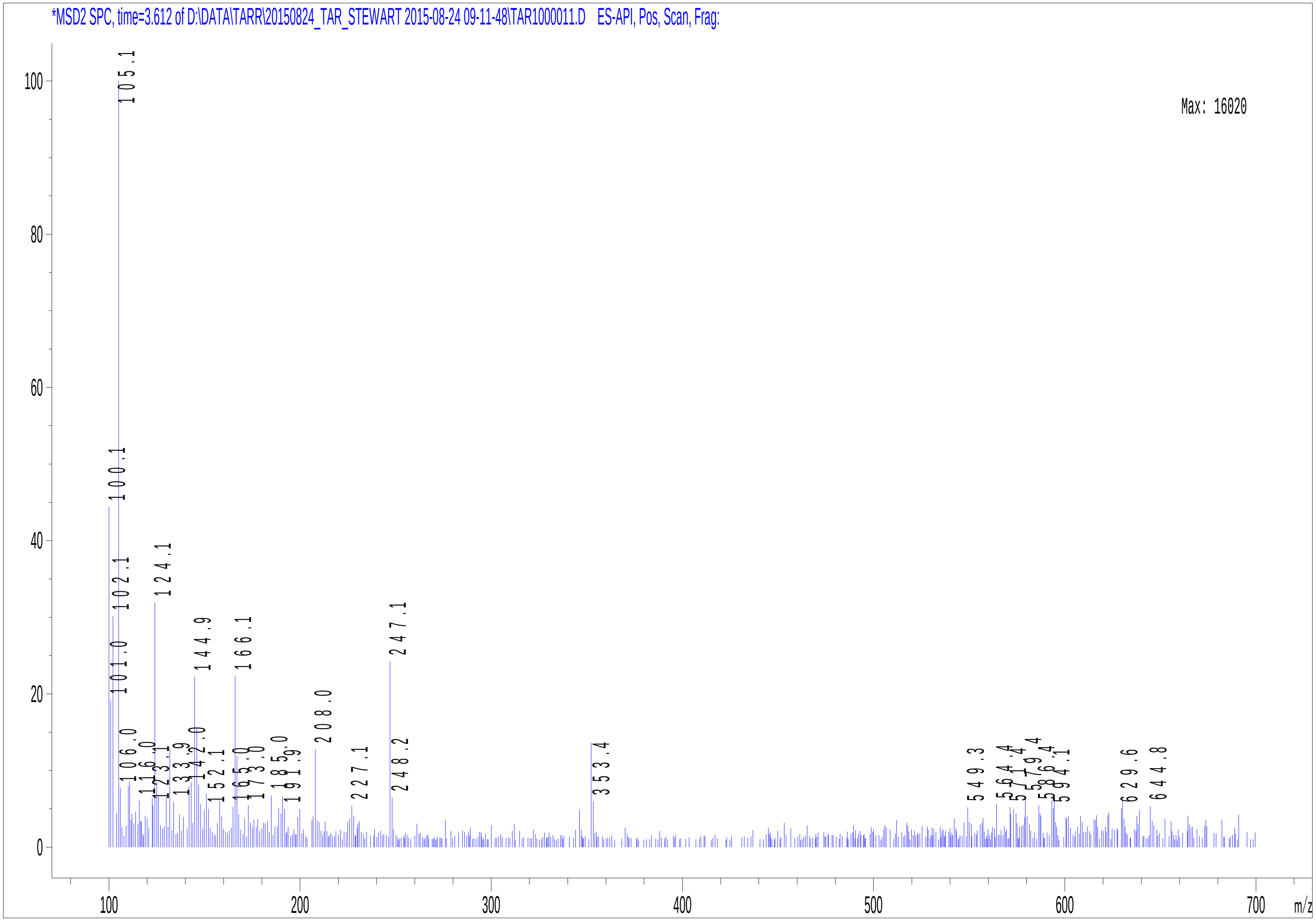
P2-B-08

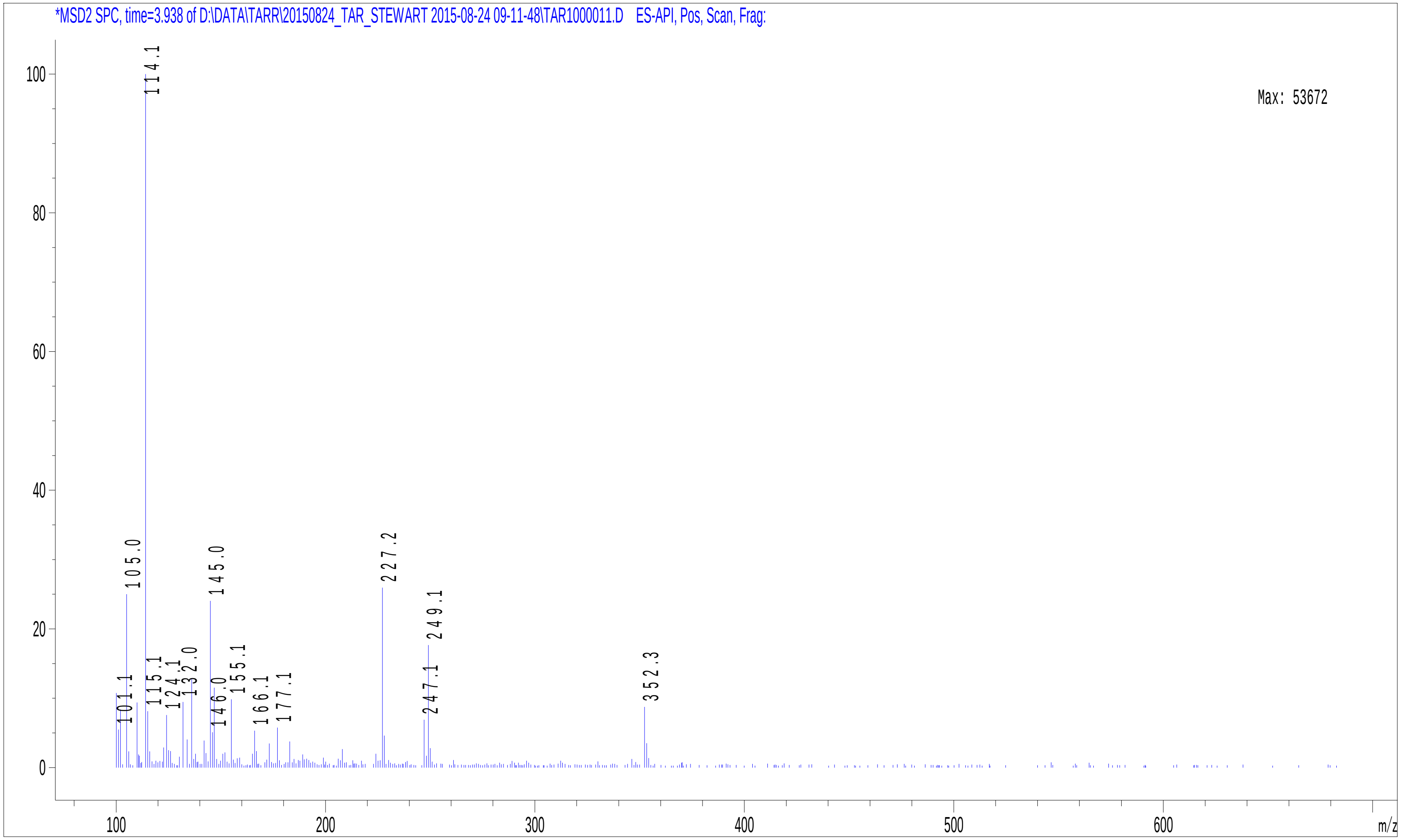


#	Time	Area	Height	Width	Area%	Symmetry
1	3.089	1170729.6	146493	0.1332	35.482	0.838
2	3.588	1106976.5	97881.1	0.1885	33.550	0.516
3	3.918	1021822.3	124939.9	0.1363	30.969	0.473


MSD2 TIC, MS File (D:\DATA\TARR\20150824_TAR_STEWART 2015-08-24 09-11-48\TAR1000011.D) ES-API, Pos, Scan, Frag: 70
Norm.
325000
300000
275000
250000
225000
200000
175000
150000
3.089
Area: 1.17073e+006
3.588
Area: 1.10698e+006
3.918
Area: 1.02182e+006
2.5
3
3.5
4
4.5
min


*MSD2 SPC, time=3.089 of D:\DATA\TARR\20150824_TAR_STEWART 2015-08-24 09-11-48\TAR1000011.D ES-API, Pos, Scan, Frag:
Max: 112680
105.1
106.0
132.0
147.0
100
80
60
40
20
0
100
200
300
400
500
600
700
m/z

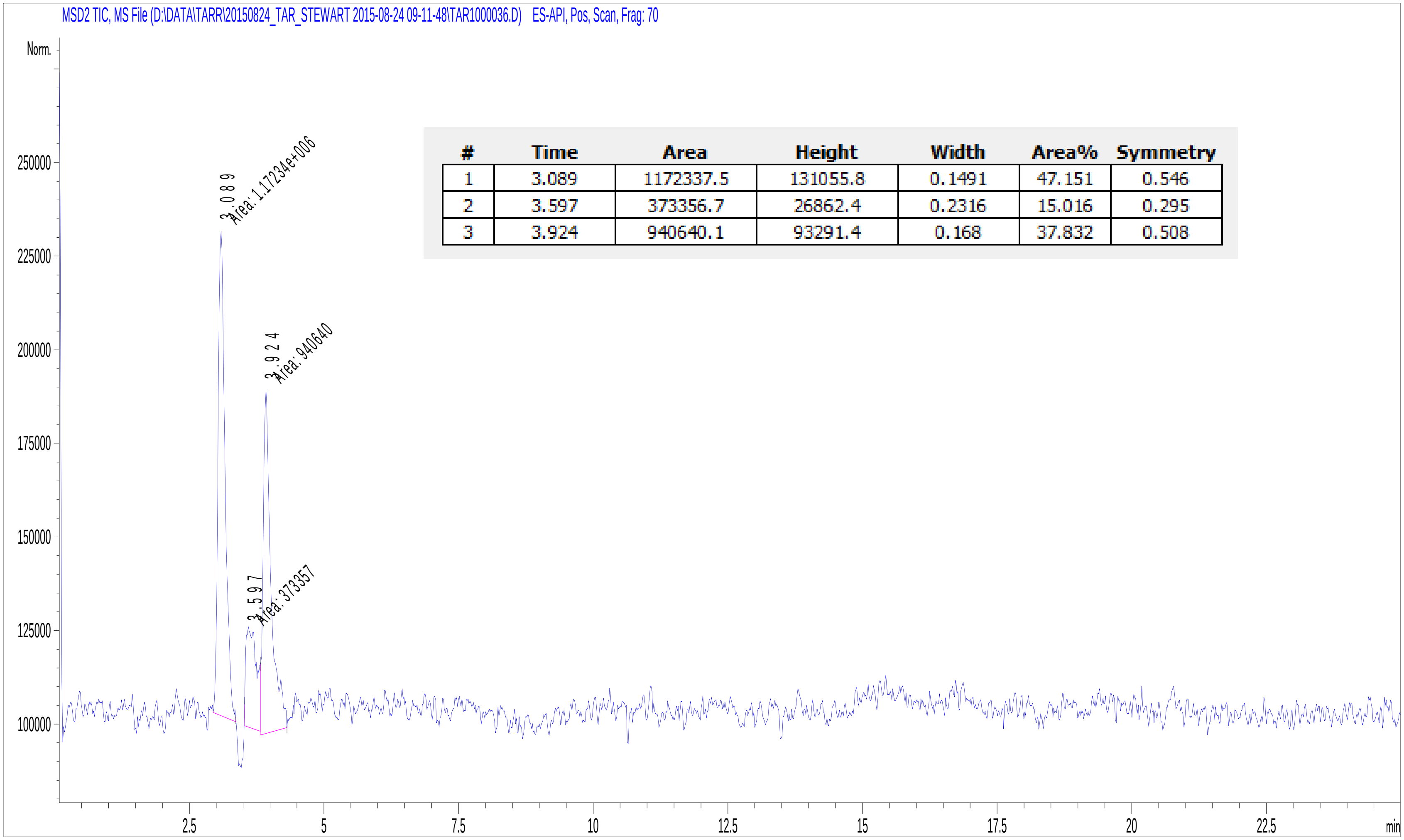

*MSD2 SPC, time=3.612 of D:\DATA\TARR\20150824_TAR_STEWART 2015-08-24 09-11-48\TAR1000011.D ES-API, Pos, Scan, Frag:
Max: 16020
100
80
60
40
20
0
100
200
300
400
500
600
700
m/z
105.1
100.1
102.1
101.0
124.1
144.9
166.1
247.1
208.0
106.0
116.0
123.1
133.9
142.0
152.1
165.0
173.0
185.0
191.9
227.1
248.2
353.4
549.3
564.4
571.4
579.4
586.4
594.1
629.6
644.8


*MSD2 SPC, time=3.938 of D:\DATA\TARR\20150824_TAR_STEWART 2015-08-24 09-11-48\TAR1000011.D ES-API, Pos, Scan, Frag:
Max: 53672
100
80
60
40
20
0
114.1
105.0
101.1
115.1
124.1
132.0
145.0
146.0
155.1
166.1
177.1
227.2
249.1
247.1
352.3
100
200
300
400
500
600
m/z

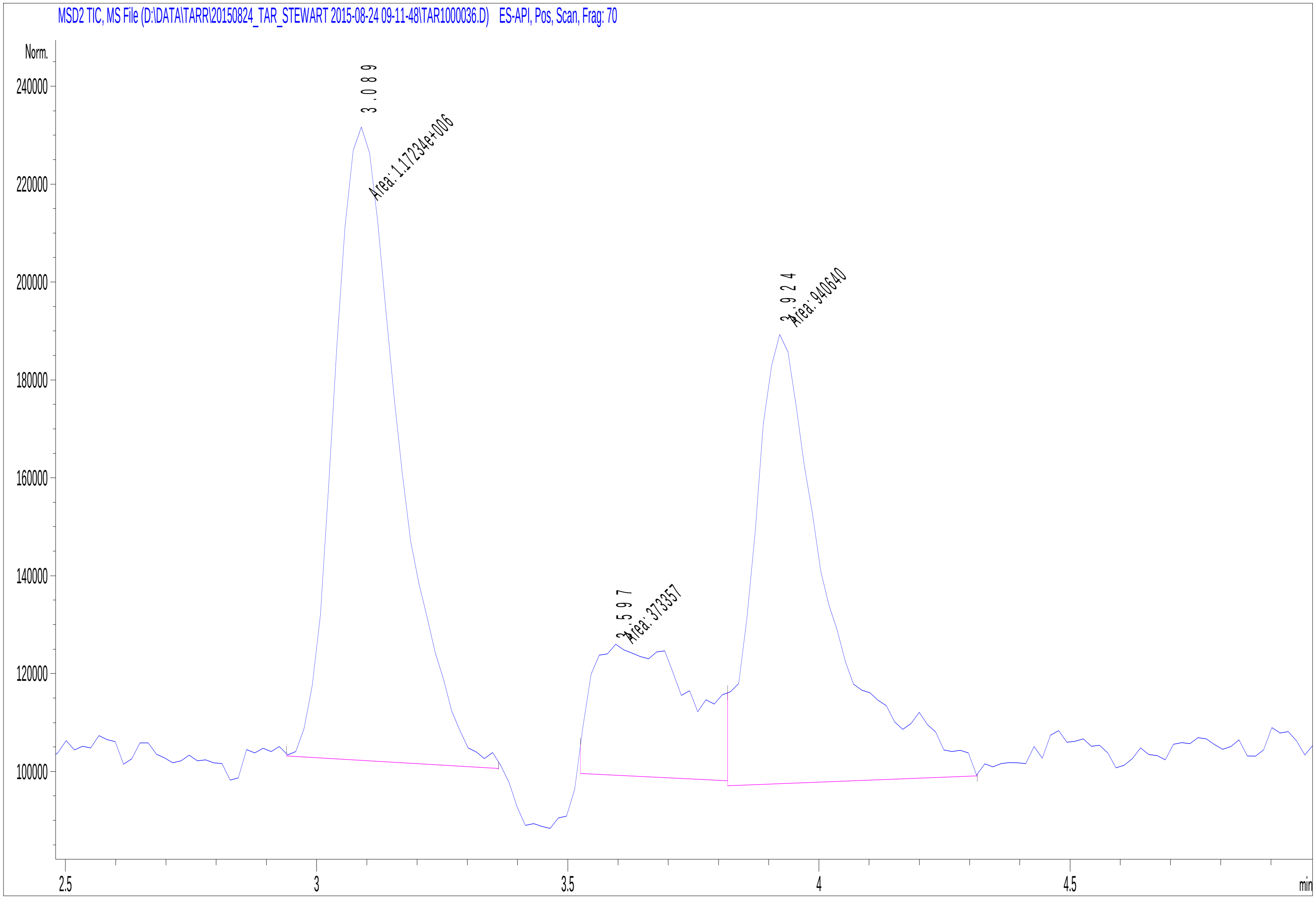
4-Aug-15

50 DC

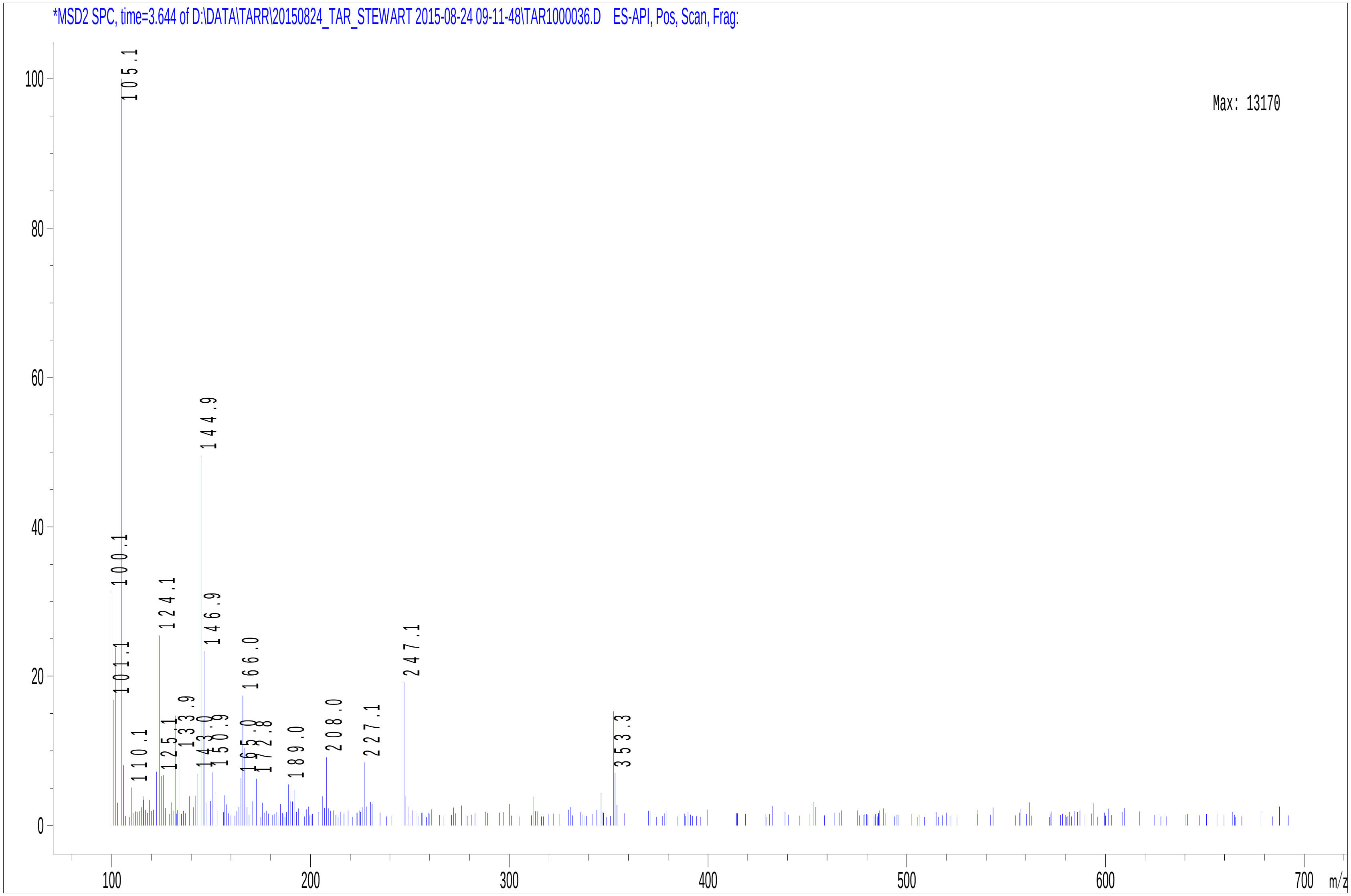
P2-E-01

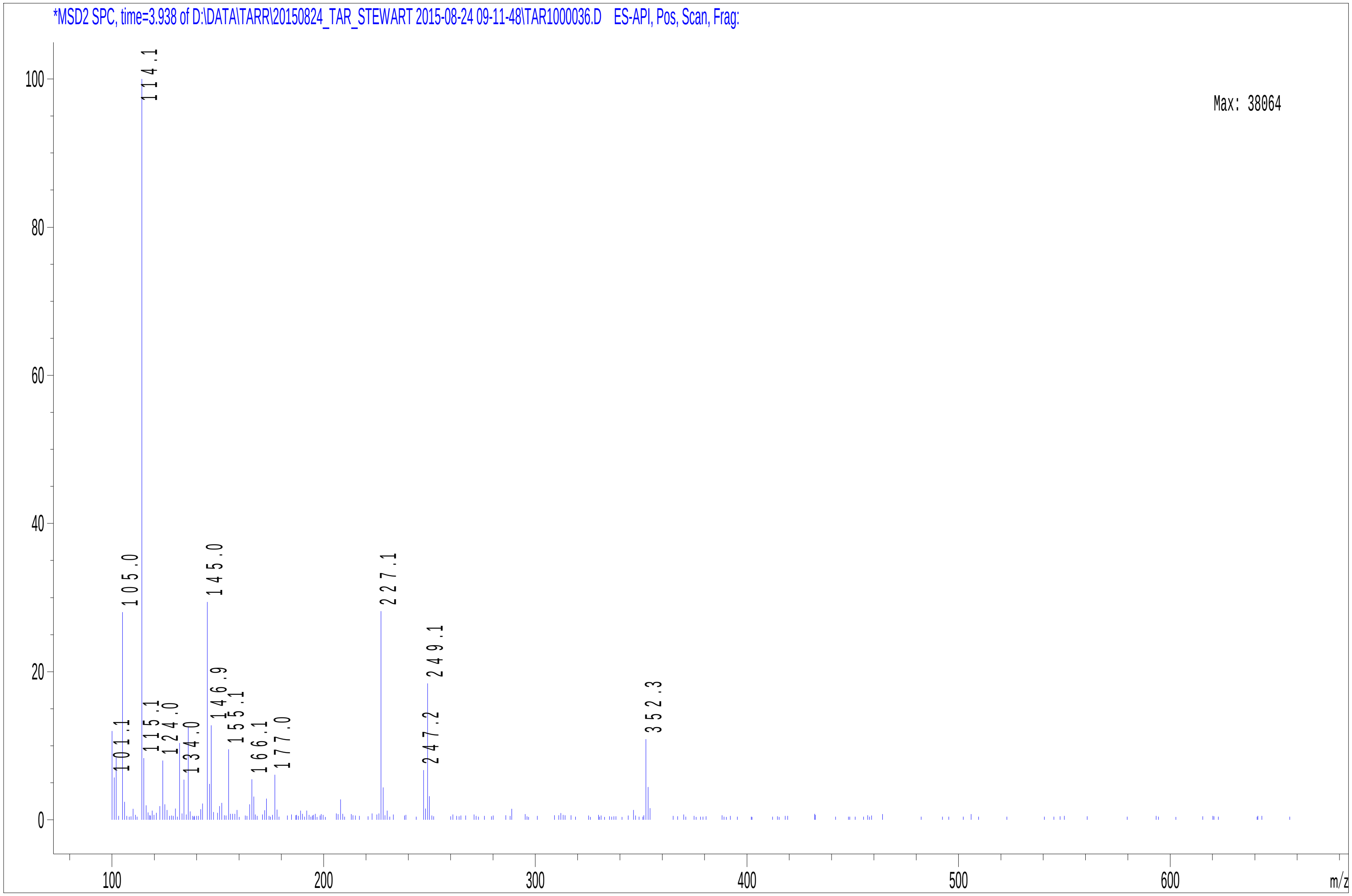


#	Time	Area	Height	Width	Area%	Symmetry
1	3.089	1172337.5	131055.8	0.1491	47.151	0.546
2	3.597	373356.7	26862.4	0.2316	15.016	0.295
3	3.924	940640.1	93291.4	0.168	37.832	0.508


MSD2 TIC, MS File (D:\DATA\TARR\20150824_TAR_STEWART 2015-08-24 09-11-48\TAR1000036.D) ES-API, Pos, Scan, Frag: 70
Norm.
240000
220000
200000
180000
160000
140000
120000
100000
3.089
Area: 1.17234e+006
3.597
Area: 373357
3.924
Area: 940640
2.5
3
3.5
4
4.5
min


*MSD2 SPC, time=3.106 of D:\DATA\TARR\20150824_TAR_STEWART 2015-08-24 09-11-48\TAR1000036.D ES-API, Pos, Scan, Frag:
Max: 99208
105.0
106.0
132.0
144.9
100
80
60
40
20
0
100
200
300
400
500
600
700
m/z

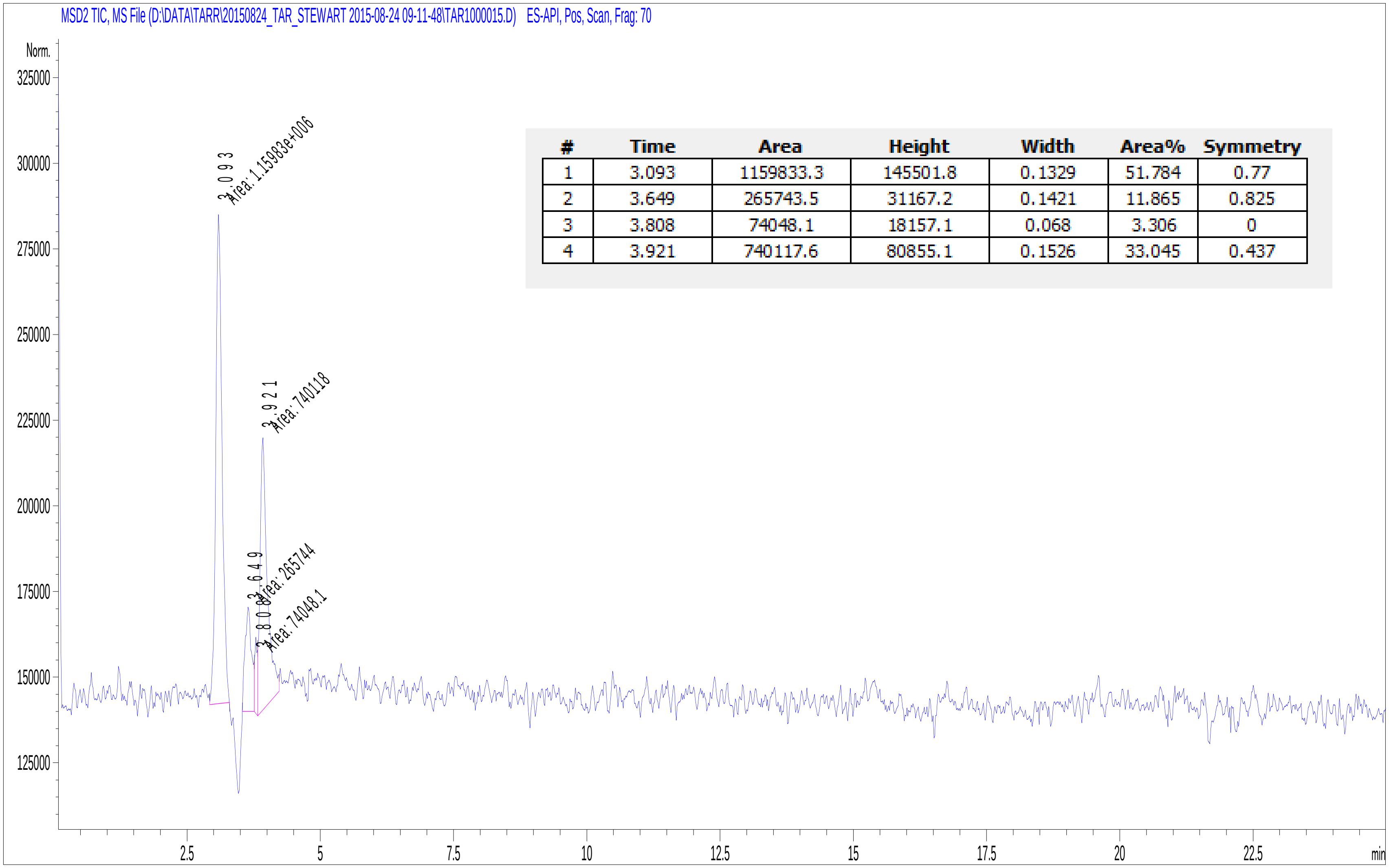

*MSD2 SPC, time=3.644 of D:\DATA\TARR\20150824_TAR_STEWART 2015-08-24 09-11-48\TAR1000036.D ES-API, Pos, Scan, Frag:
Max: 13170
105.1
144.9
100.1
124.1
146.9
101.1
166.0
247.1
133.9
125.1
110.1
143.0
150.9
165.0
172.8
189.0
208.0
227.1
353.3
0
20
40
60
80
100
100
200
300
400
500
600
700
m/z


*MSD2 SPC, time=3.938 of D:\DATA\TARR\20150824_TAR_STEWART 2015-08-24 09-11-48\TAR1000036.D ES-API, Pos, Scan, Frag:
Max: 38064
114.1
105.0
145.0
227.1
249.1
101.1
115.1
124.0
134.0
146.9
155.1
166.1
177.0
247.2
352.3
0
20
40
60
80
100
100
200
300
400
500
600
m/z

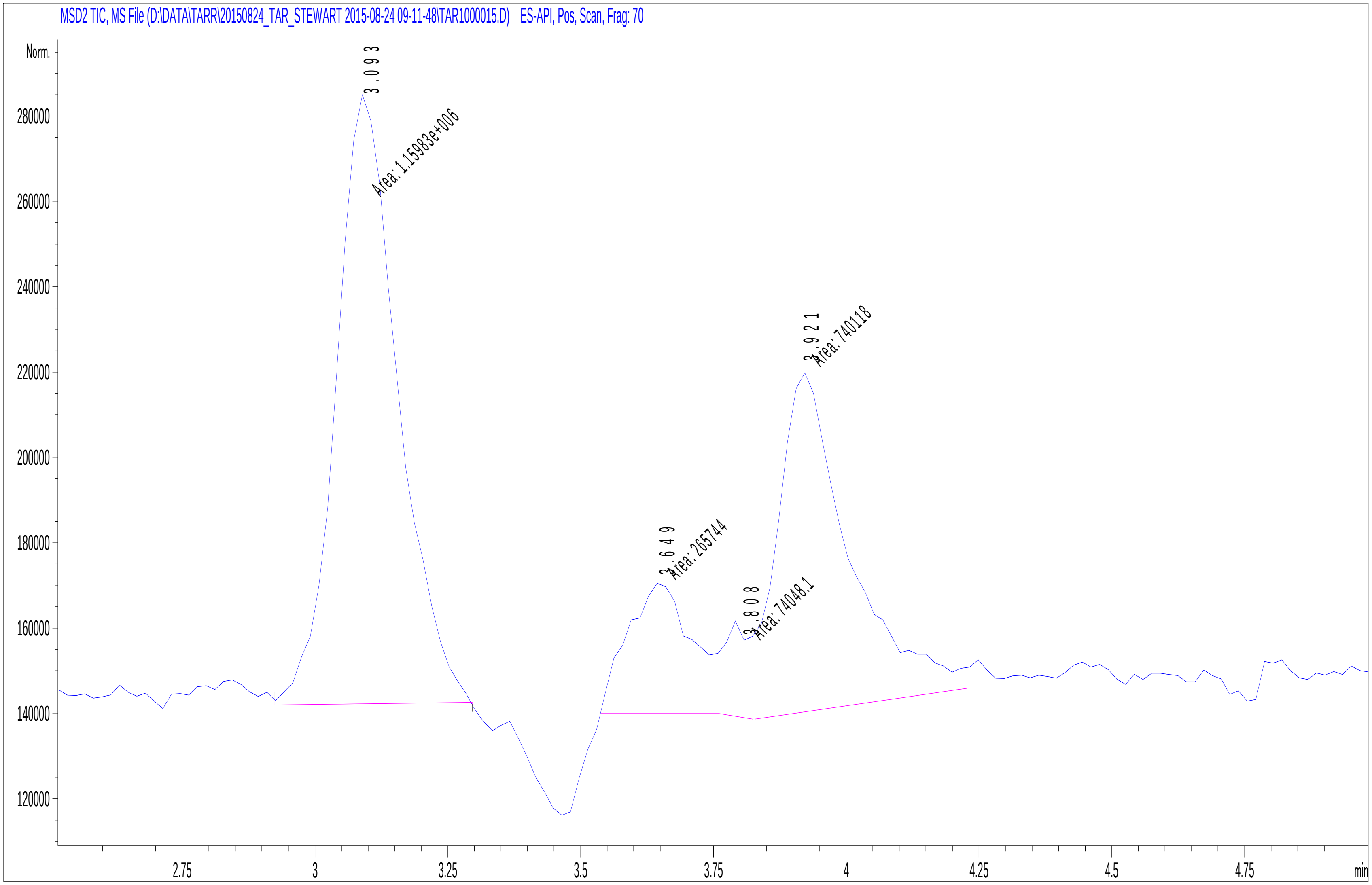
1-Jun-15

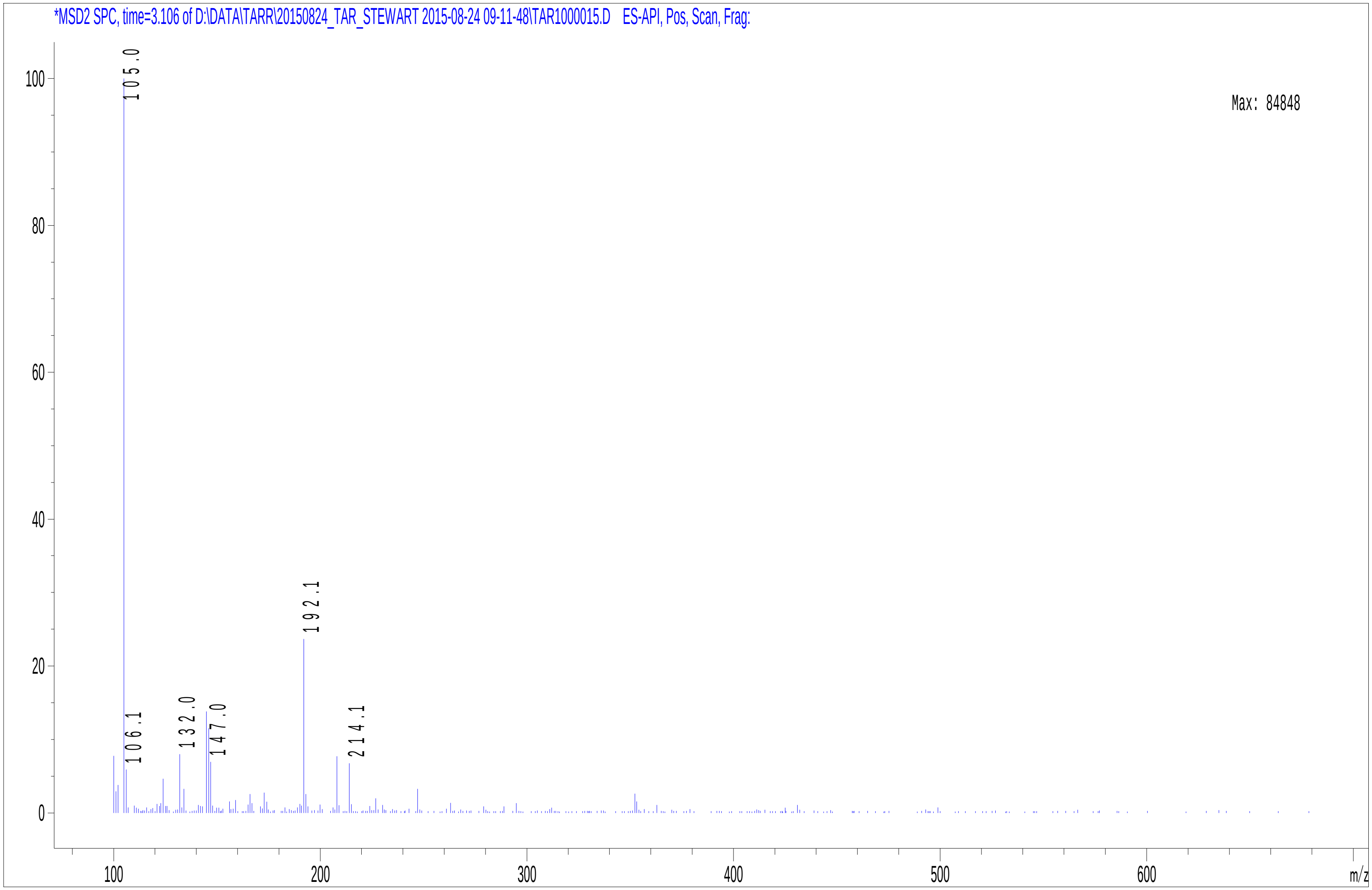
70 DC

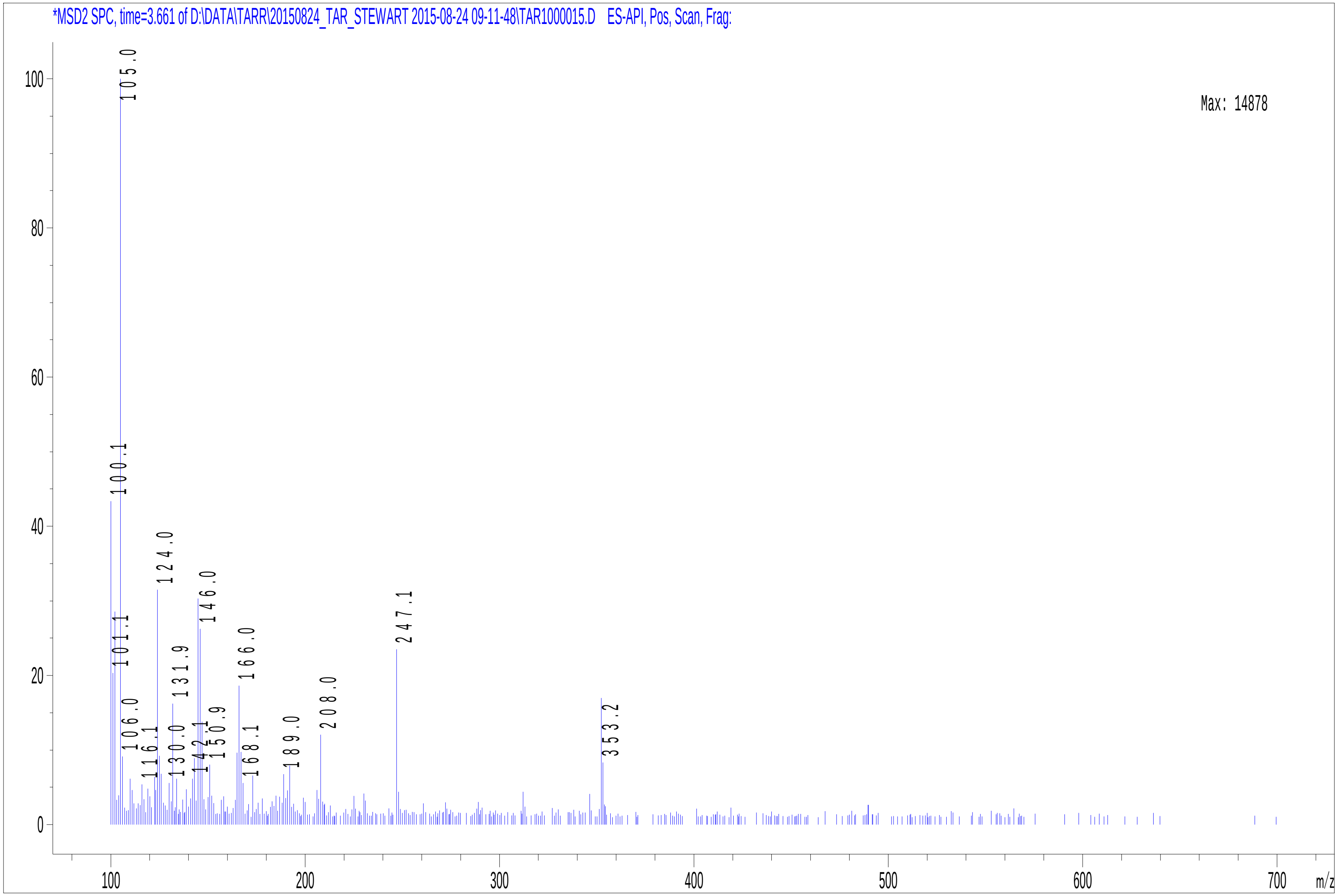
P2-B-04

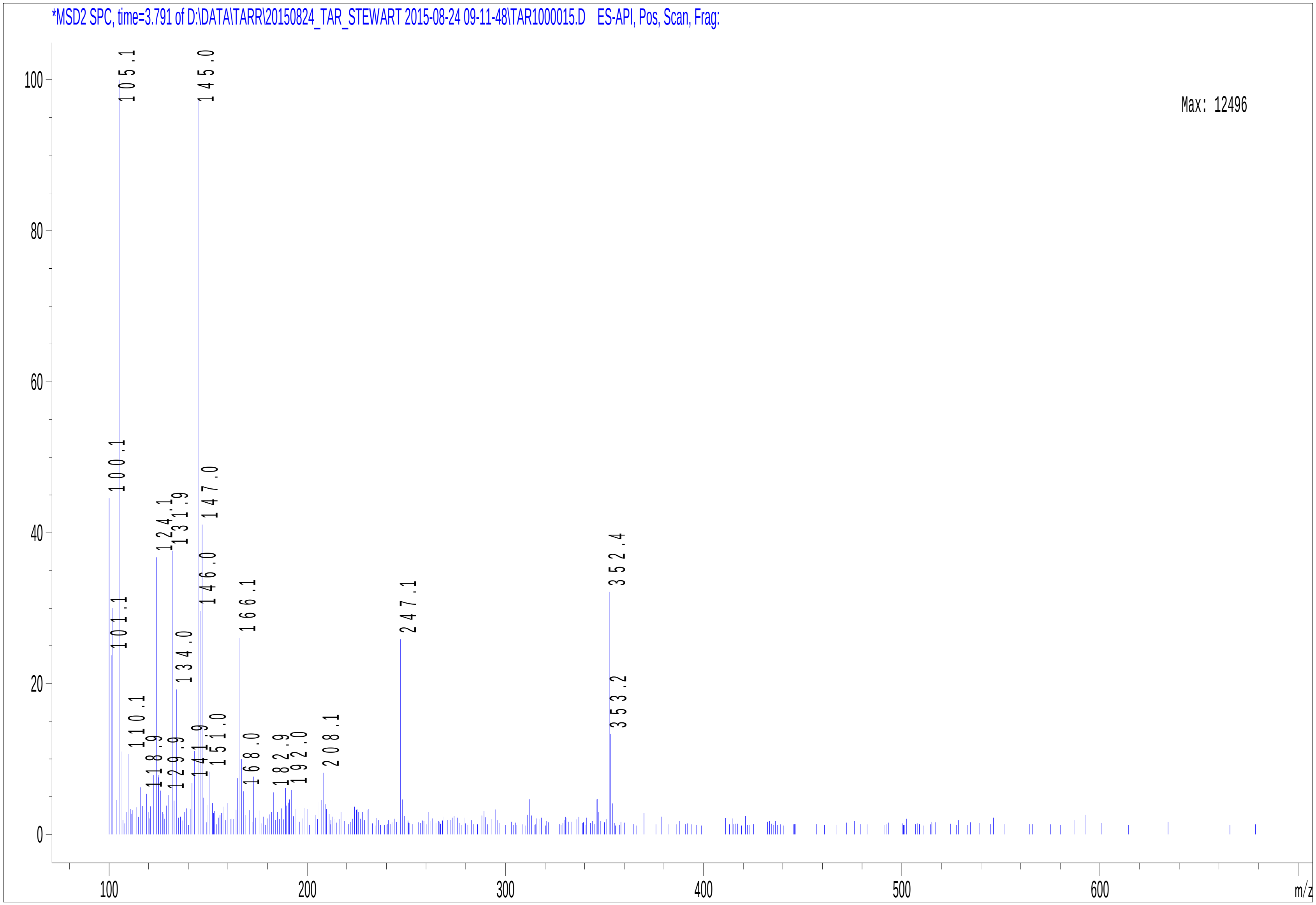


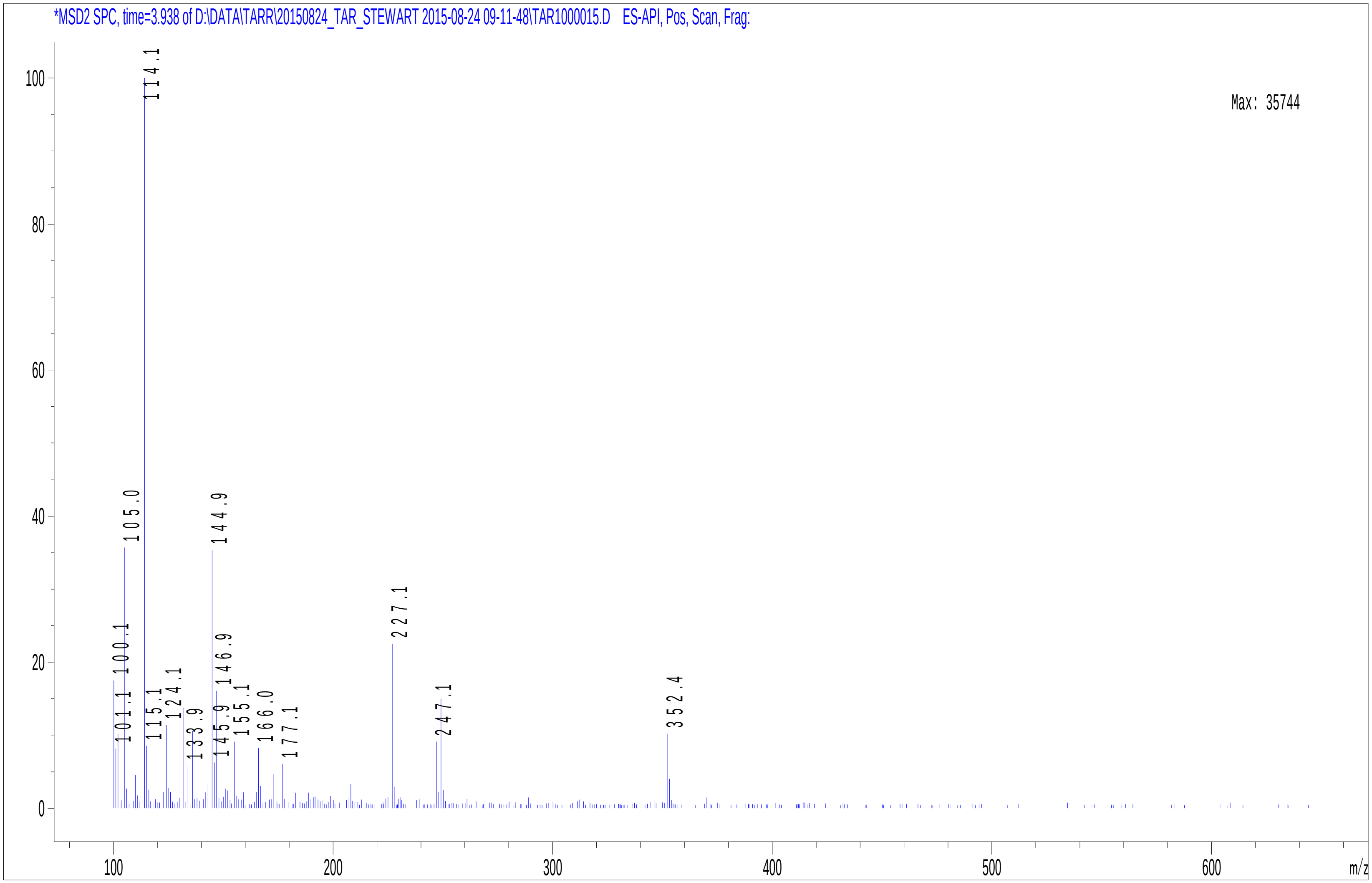
#	Time	Area	Height	Width	Area%	Symmetry
1	3.093	1159833.3	145501.8	0.1329	51.784	0.77
2	3.649	265743.5	31167.2	0.1421	11.865	0.825
3	3.808	74048.1	18157.1	0.068	3.306	0
4	3.921	740117.6	80855.1	0.1526	33.045	0.437


MSD2 TIC, MS File (D:\DATA\TARR\20150824_TAR_STEWART 2015-08-24 09-11-48\TAR1000015.D)   ES-API, Pos, Scan, Frag: 70
Norm.
280000
260000
240000
220000
200000
180000
160000
140000
120000
3.093
Area: 1.15983e+006
3.649
Area: 265744
3.808
Area: 74048.1
3.921
Area: 740118
2.75
3
3.25
3.5
3.75
4
4.25
4.5
4.75
min


*MSD2 SPC, time=3.106 of D:\DATA\TARR\20150824_TAR_STEWART 2015-08-24 09-11-48\TAR1000015.D ES-API, Pos, Scan, Frag:
Max: 84848
105.0
106.1
132.0
147.0
192.1
214.1
100
80
60
40
20
0
100
200
300
400
500
600
m/z


*MSD2 SPC, time=3.661 of D:\DATA\TARR\20150824_TAR_STEWART 2015-08-24 09-11-48\TAR1000015.D ES-API, Pos, Scan, Frag:
Max: 14878
105.0
100.1
124.0
146.0
101.1
131.9
166.0
247.1
208.0
106.0
116.1
130.0
142.1
150.9
168.1
189.0
353.2
0
20
40
60
80
100
100
200
300
400
500
600
700
m/z

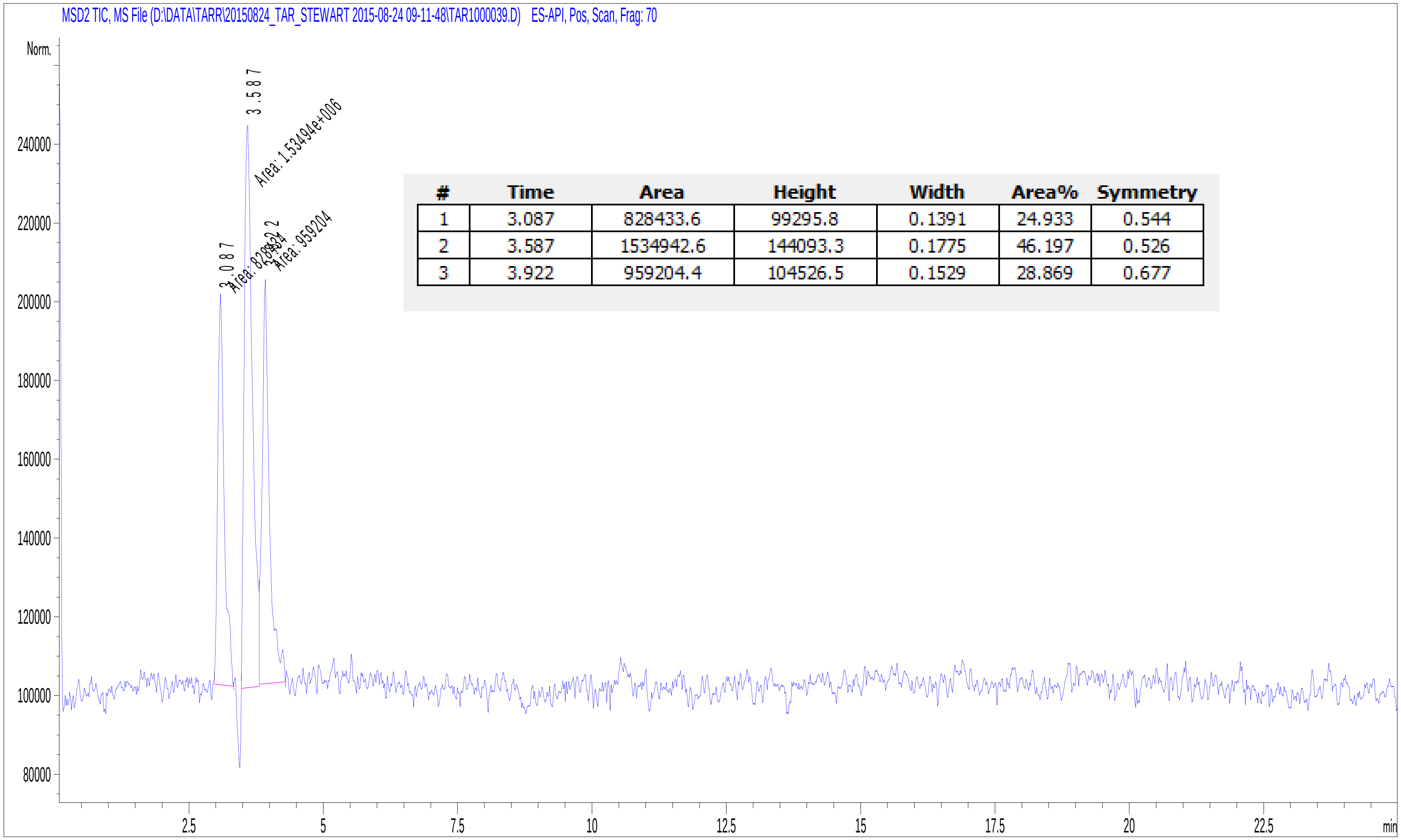

*MSD2 SPC, time=3.791 of D:\DATA\TARR\20150824_TAR_STEWART 2015-08-24 09-11-48\TAR1000015.D ES-API, Pos, Scan, Frag:
Max: 12496
100
80
60
40
20
0
100.1
101.1
105.1
110.1
118.9
124.1
129.9
131.9
134.0
141.9
145.0
146.0
147.0
151.0
166.1
168.0
182.9
192.0
208.1
247.1
352.4
353.2
100
200
300
400
500
600
m/z


*MSD2 SPC, time=3.938 of D:\DATA\TARR\20150824_TAR_STEWART 2015-08-24 09-11-48\TAR1000015.D ES-API, Pos, Scan, Frag:
Max: 35744
114.1
105.0
144.9
227.1
100.1
146.9
124.1
115.1
101.1
133.9
145.9
155.1
166.0
177.1
247.1
352.4
0
20
40
60
80
100
100
200
300
400
500
600
m/z

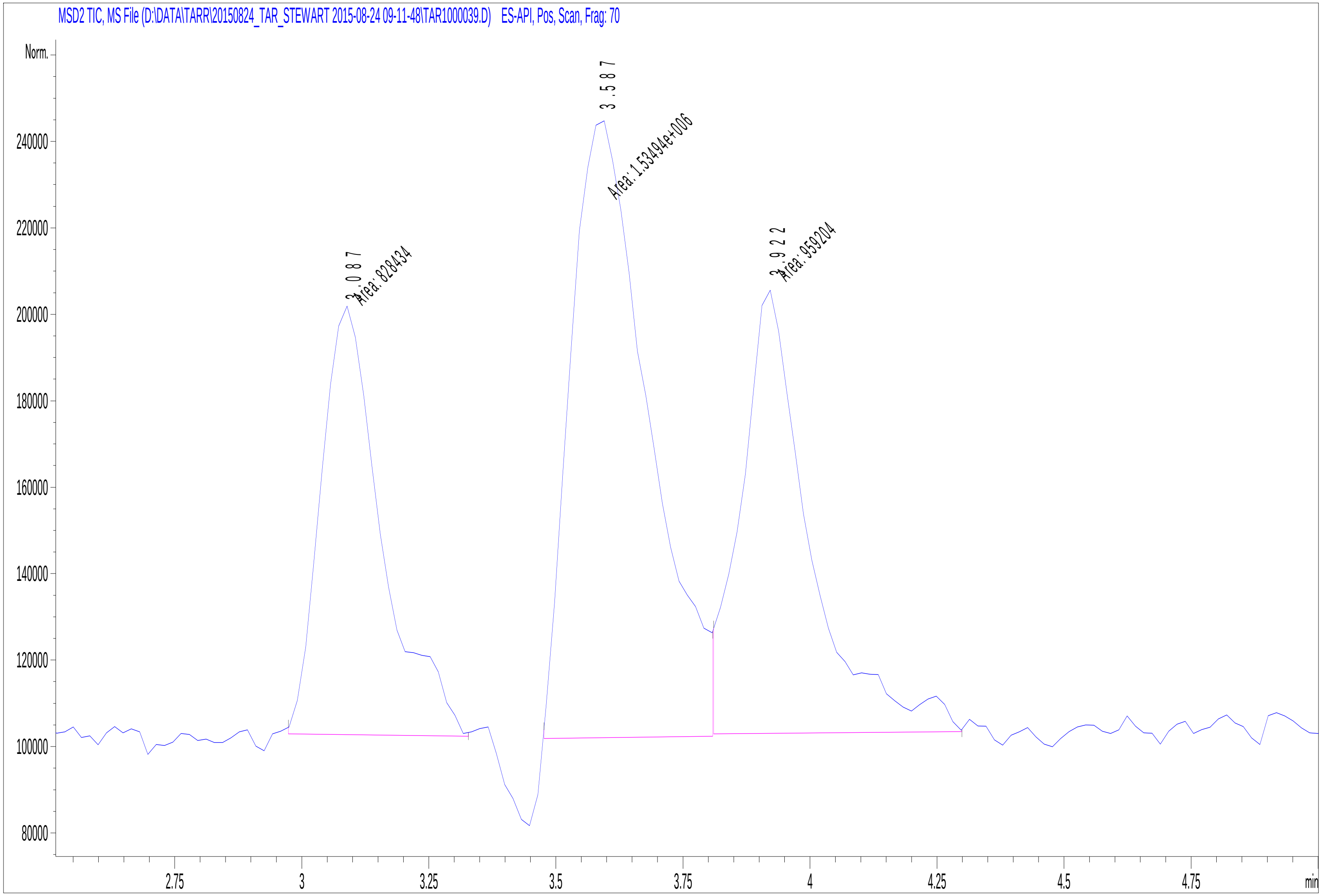
12-Aug-15

70 DC repeat

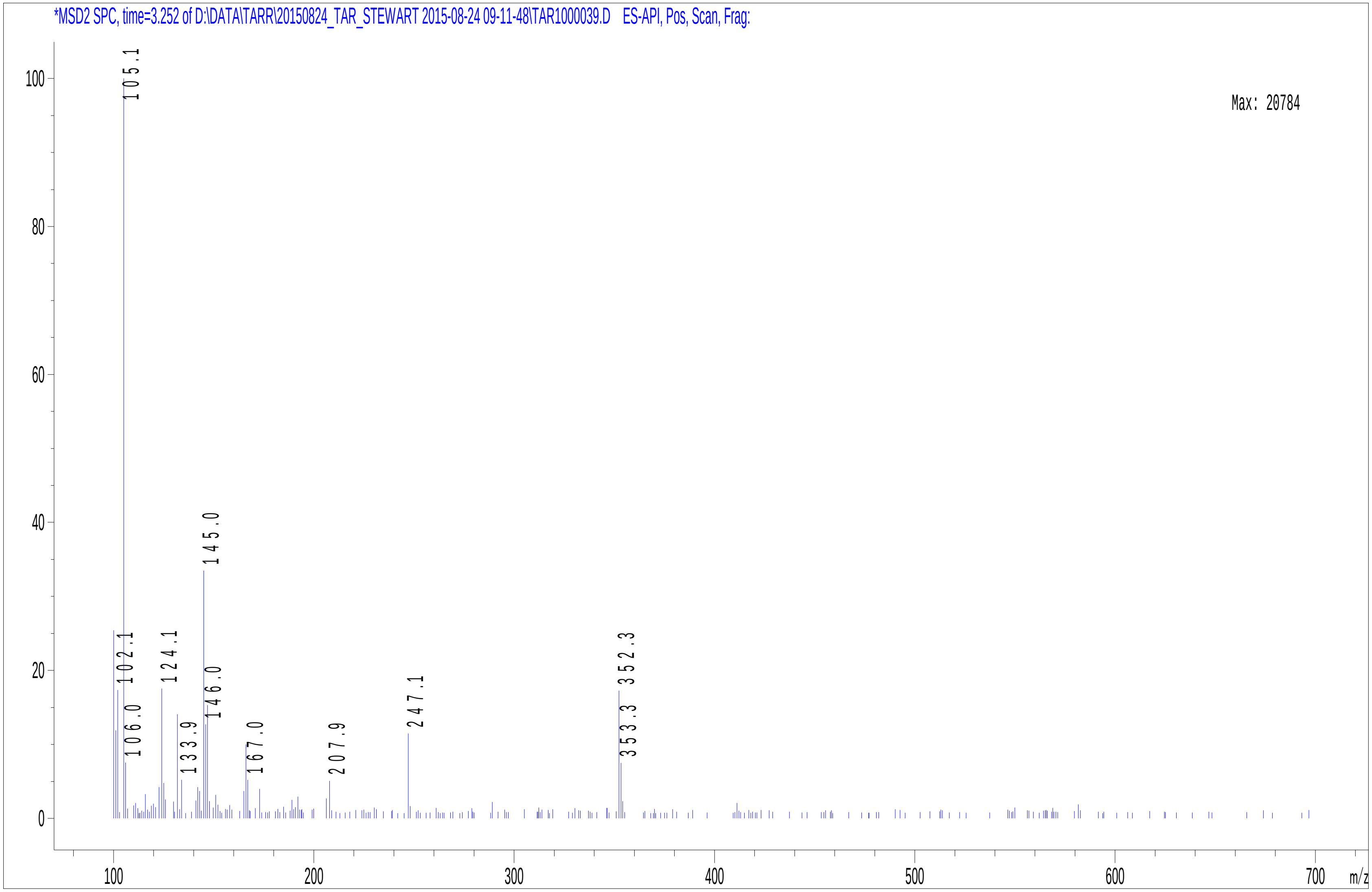
P2-E-03

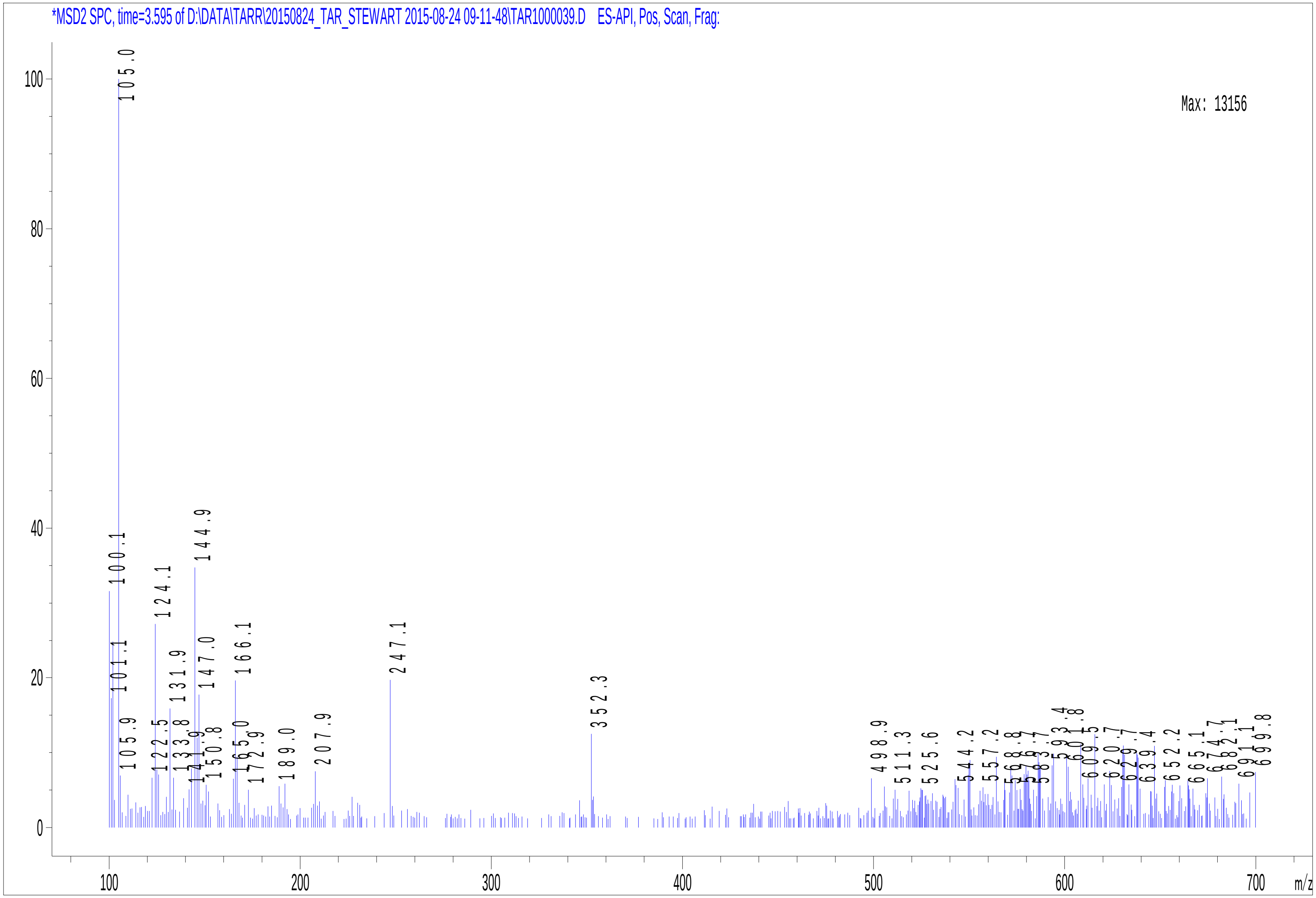


#	Time	Area	Height	Width	Area%	Symmetry
1	3.087	828433.6	99295.8	0.1391	24.933	0.544
2	3.587	1534942.6	144093.3	0.1775	46.197	0.526
3	3.922	959204.4	104526.5	0.1529	28.869	0.677

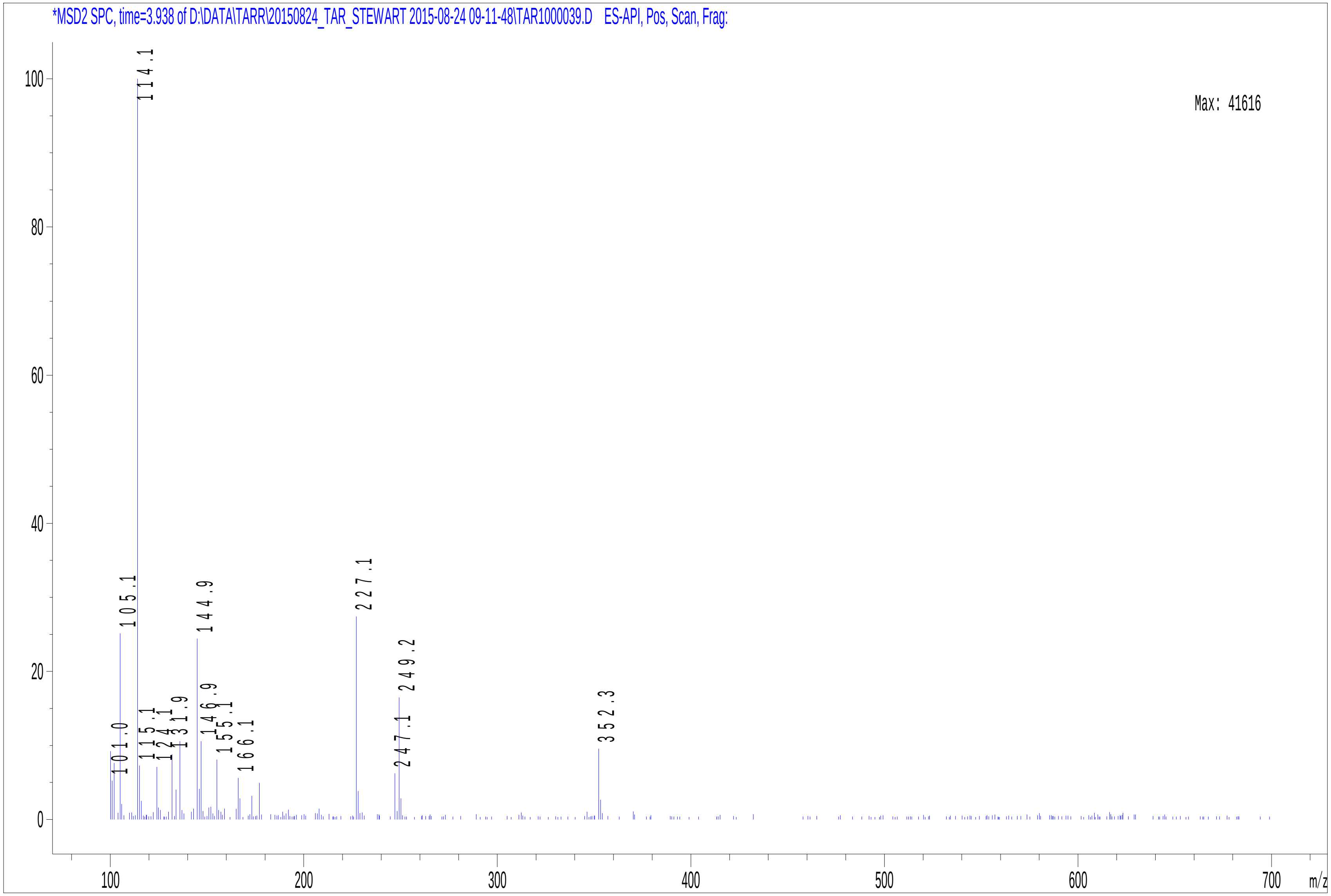

MSD2 TIC, MS File (D:\DATA\TARR\20150824_TAR_STEWART 2015-08-24 09-11-48\TAR1000039.D) ES-API, Pos, Scan, Frag: 70
Norm.
240000
220000
200000
180000
160000
140000
120000
100000
80000
3.087
Area: 828434
3.587
Area: 1.53494e+006
3.922
Area: 959204
2.75
3
3.25
3.5
3.75
4
4.25
4.5
4.75
min


*MSD2 SPC, time=3.089 of D:\DATA\TARR\20150824_TAR_STEWART 2015-08-24 09-11-48\TAR1000039.D ES-API, Pos, Scan, Frag:
Max: 83392
105.0
106.0
131.9
146.9
0
20
40
60
80
100
100
200
300
400
500
600
700
m/z


*MSD2 SPC, time=3.252 of D:\DATA\TARR\20150824_TAR_STEWART 2015-08-24 09-11-48\TAR1000039.D ES-API, Pos, Scan, Frag:
Max: 20784
105.1
102.1
106.0
124.1
133.9
145.0
146.0
167.0
207.9
247.1
352.3
353.3
0
20
40
60
80
100
100
200
300
400
500
600
700
m/z



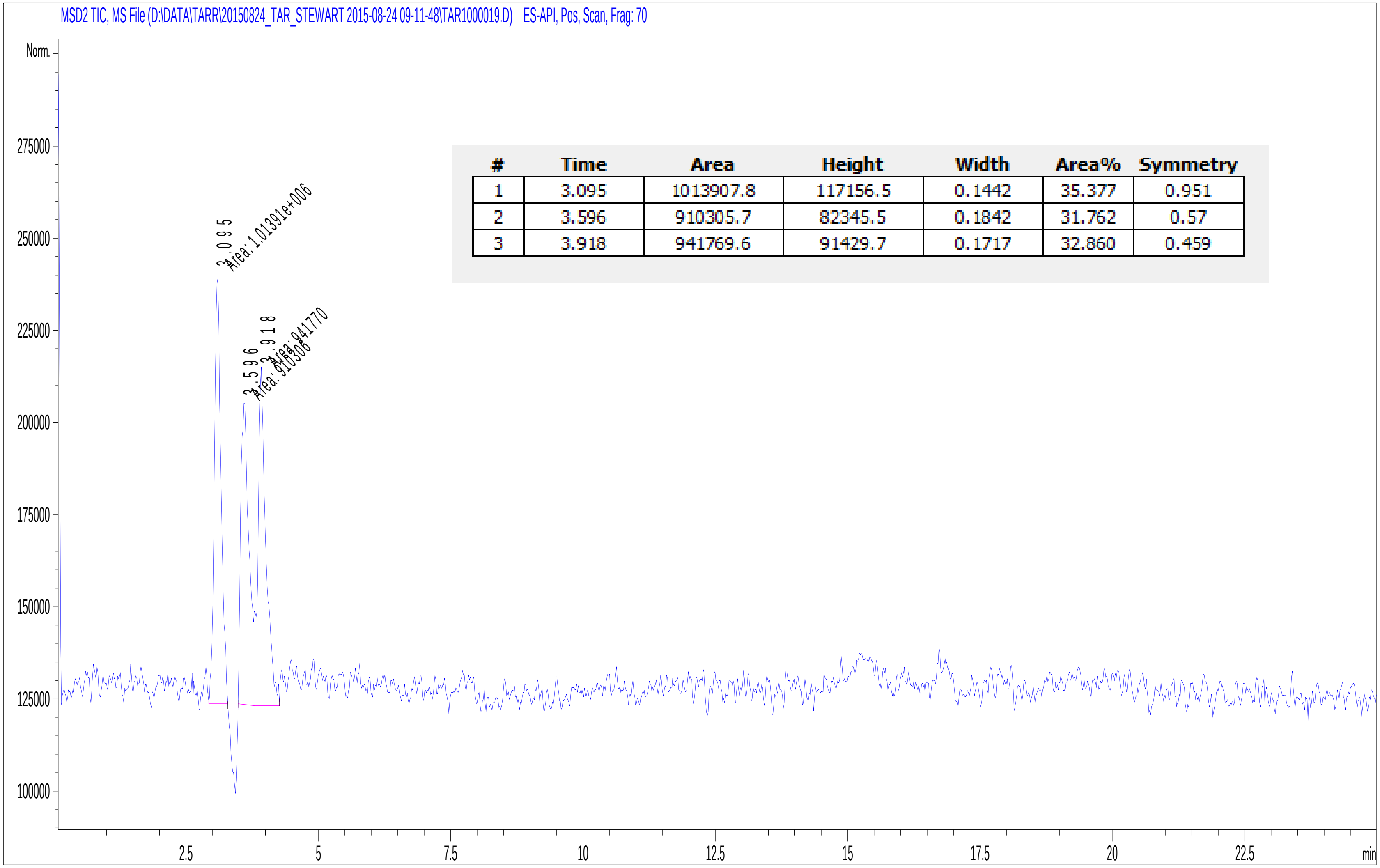
*MSD2 SPC, time=3.595 of D:\DATA\TARR\20150824_TAR_STEWART 2015-08-24 09-11-48\TAR1000039.D ES-API, Pos, Scan, Frag:
Max: 13156
0
20
40
60
80
100
100
200
300
400
500
600
700
m/z
105.0
100.1
101.1
105.9
122.5
124.1
131.9
133.8
141.9
144.9
147.0
150.8
165.0
166.1
172.9
189.0
207.9
247.1
352.3
498.9
511.3
525.6
544.2
557.2
568.8
583.7
593.4
601.8
609.5
620.7
629.7
639.4
652.2
665.1
674.7
682.1
691.1
699.8


*MSD2 SPC, time=3.938 of D:\DATA\TARR\20150824_TAR_STEWART 2015-08-24 09-11-48\TAR1000039.D ES-API, Pos, Scan, Frag:
Max: 41616
114.1
105.1
144.9
227.1
249.2
101.0
115.1
124.1
131.9
146.9
155.1
166.1
247.1
352.3
100
80
60
40
20
0
100
200
300
400
500
600
700
m/z

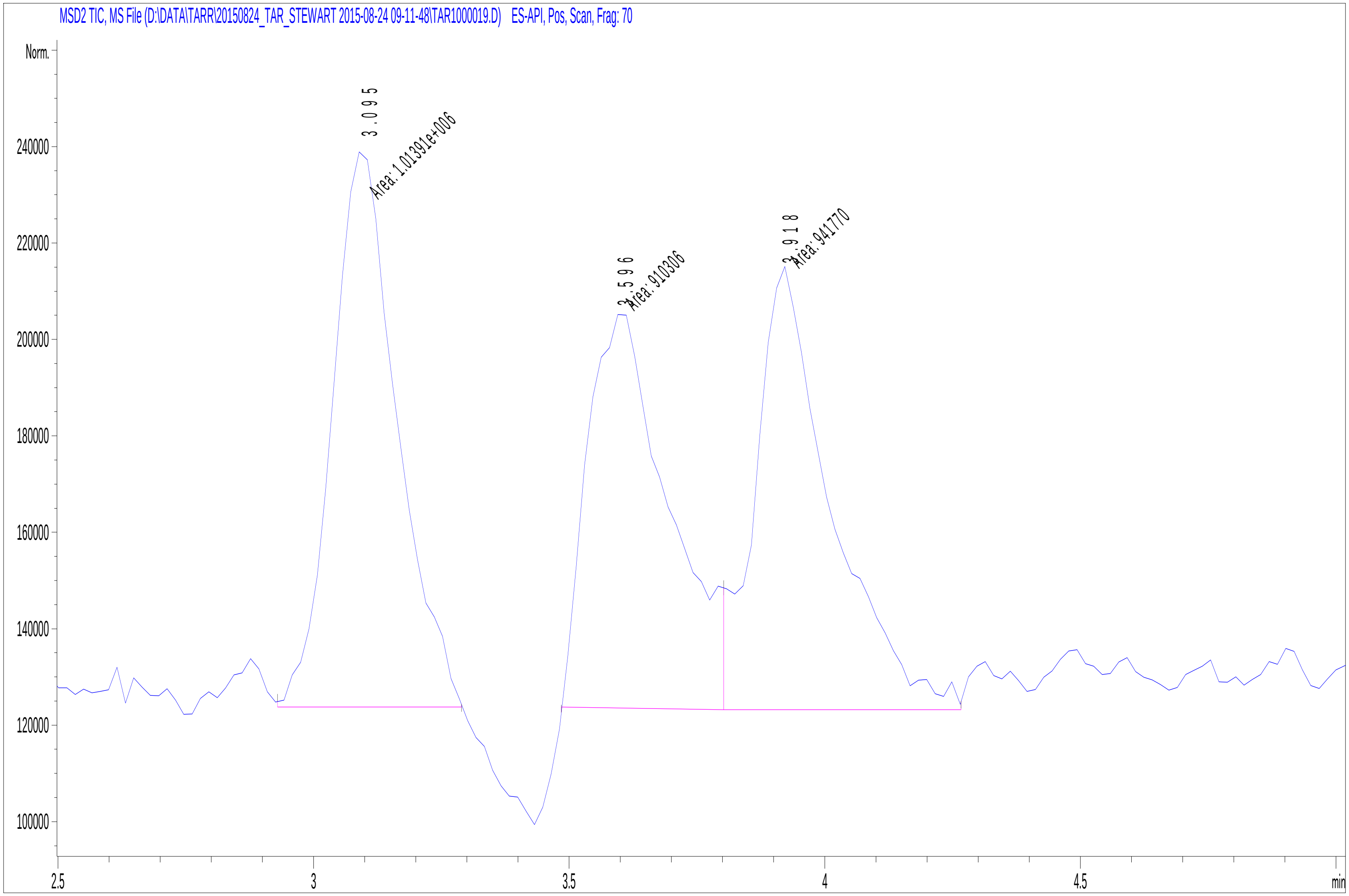
26-Jun-15

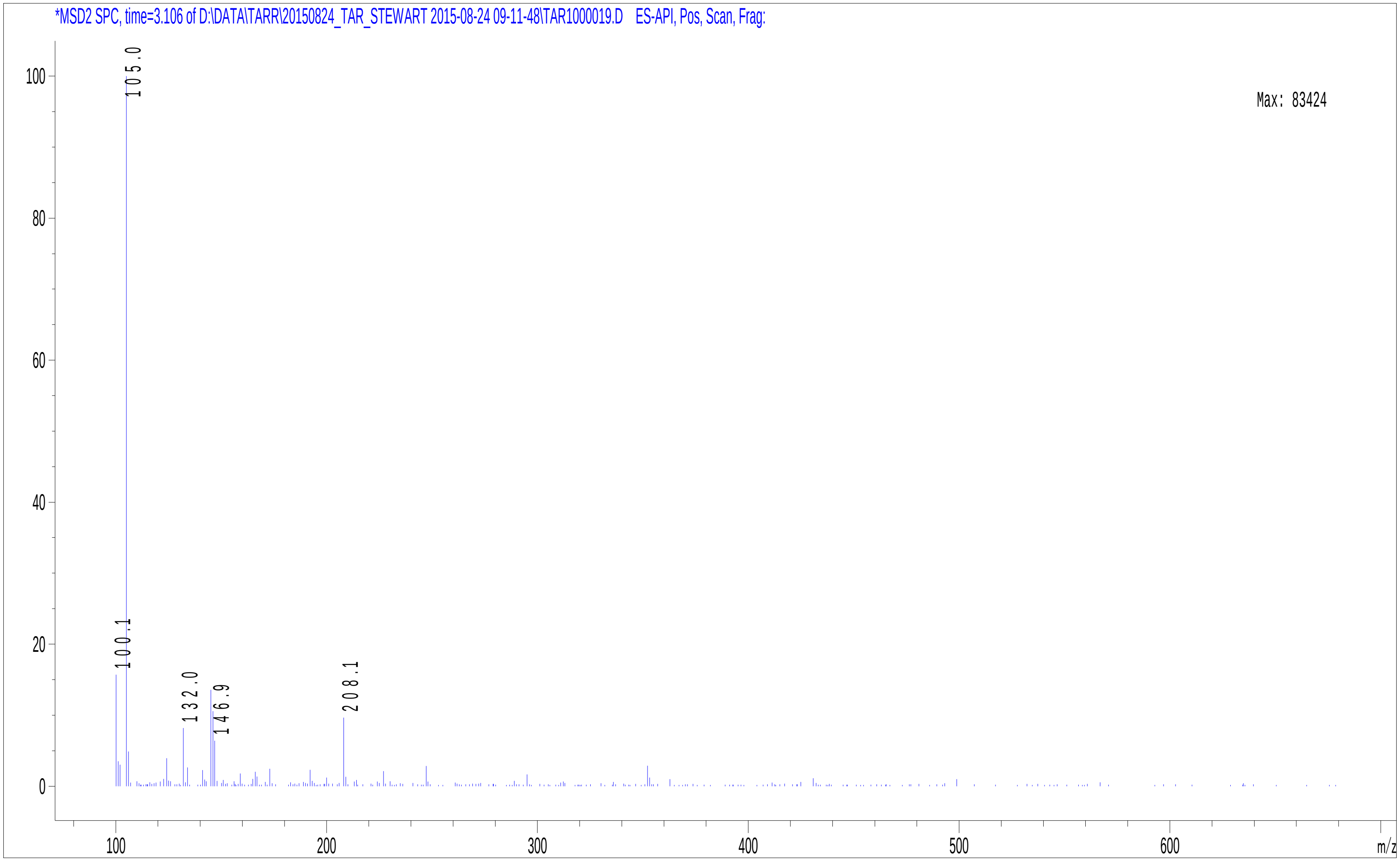
100 DC

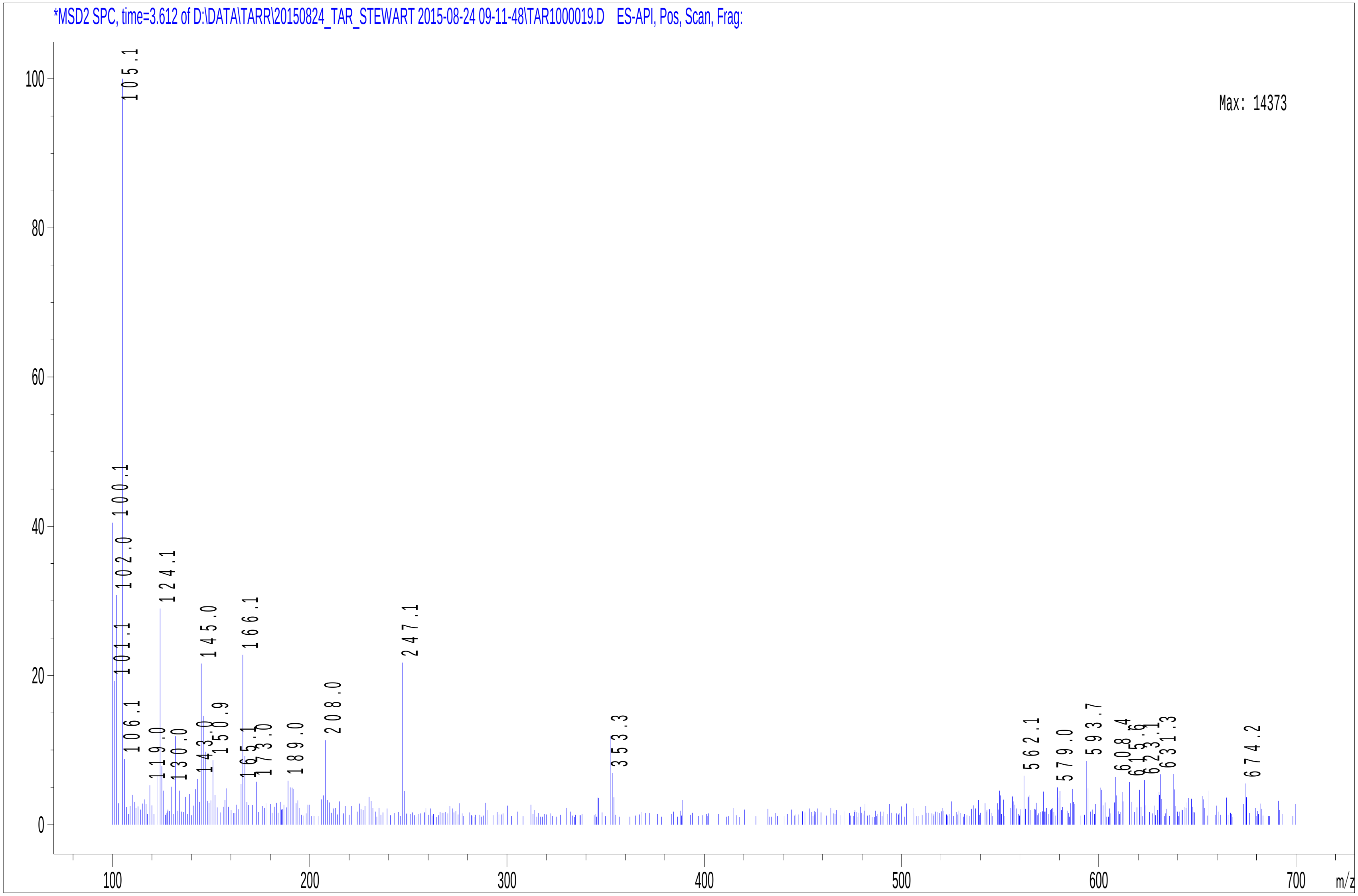
P2-C-01

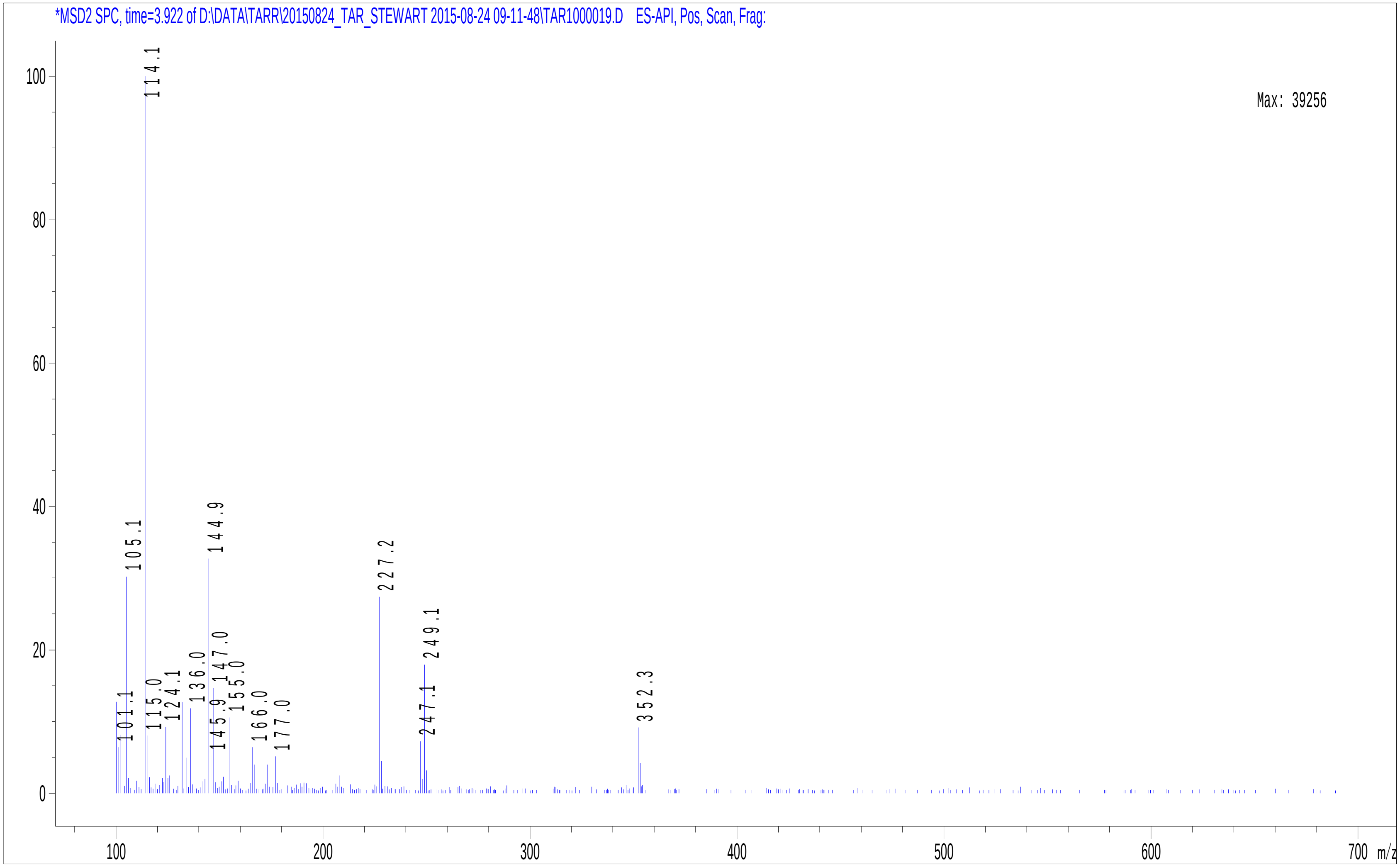


#	Time	Area	Height	Width	Area%	Symmetry
1	3.095	1013907.8	117156.5	0.1442	35.377	0.951
2	3.596	910305.7	82345.5	0.1842	31.762	0.57
3	3.918	941769.6	91429.7	0.1717	32.860	0.459


MSD2 TIC, MS File (D:\DATA\TARR\20150824_TAR_STEWART 2015-08-24 09-11-48\TAR1000019.D) ES-API, Pos, Scan, Frag: 70
Norm.
240000
220000
200000
180000
160000
140000
120000
100000
3.095
Area: 1.01391e+006
3.596
Area: 910306
3.918
Area: 941770
2.5
3
3.5
4
4.5
min


*MSD2 SPC, time=3.106 of D:\DATA\TARR\20150824_TAR_STEWART 2015-08-24 09-11-48\TAR1000019.D ES-API, Pos, Scan, Frag:
Max: 83424
105.0
100.1
132.0
146.9
208.1
100
80
60
40
20
0
100
200
300
400
500
600
m/z

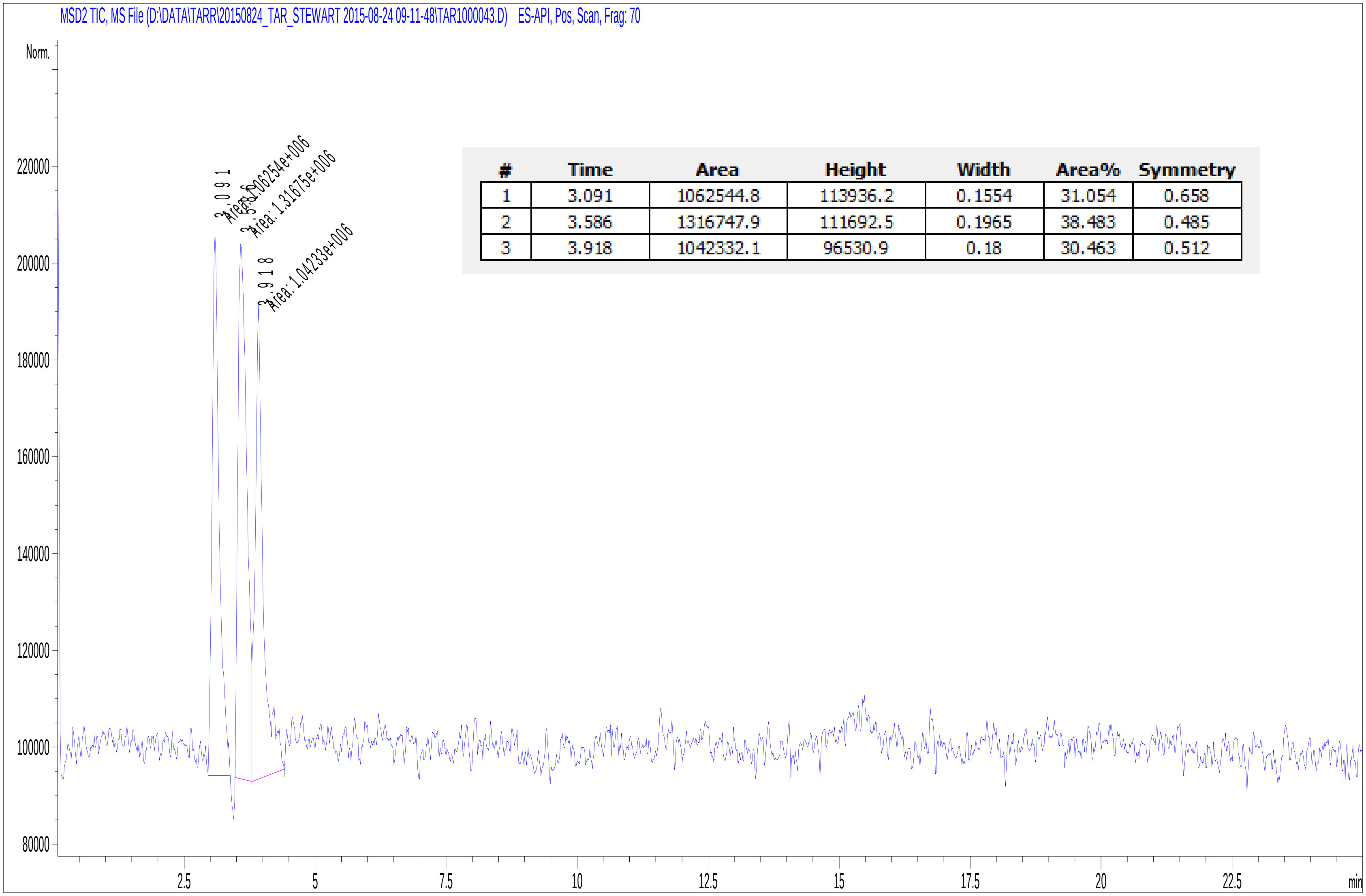

*MSD2 SPC, time=3.612 of D:\DATA\TARR\20150824_TAR_STEWART 2015-08-24 09-11-48\TAR1000019.D ES-API, Pos, Scan, Frag:
Max: 14373
105.1
100.1
102.0
124.1
101.1
145.0
166.1
247.1
106.1
119.0
130.0
143.0
150.9
165.1
173.0
189.0
208.0
353.3
562.1
579.0
593.7
608.4
615.6
623.1
631.3
674.2
0
20
40
60
80
100
100
200
300
400
500
600
700
m/z


*MSD2 SPC, time=3.922 of D:\DATA\TARR\20150824_TAR_STEWART 2015-08-24 09-11-48\TAR1000019.D ES-API, Pos, Scan, Frag:
Max: 39256
114.1
105.1
144.9
227.2
249.1
247.1
352.3
101.1
115.0
124.1
136.0
145.9
147.0
155.0
166.0
177.0
0
20
40
60
80
100
100
200
300
400
500
600
700
m/z

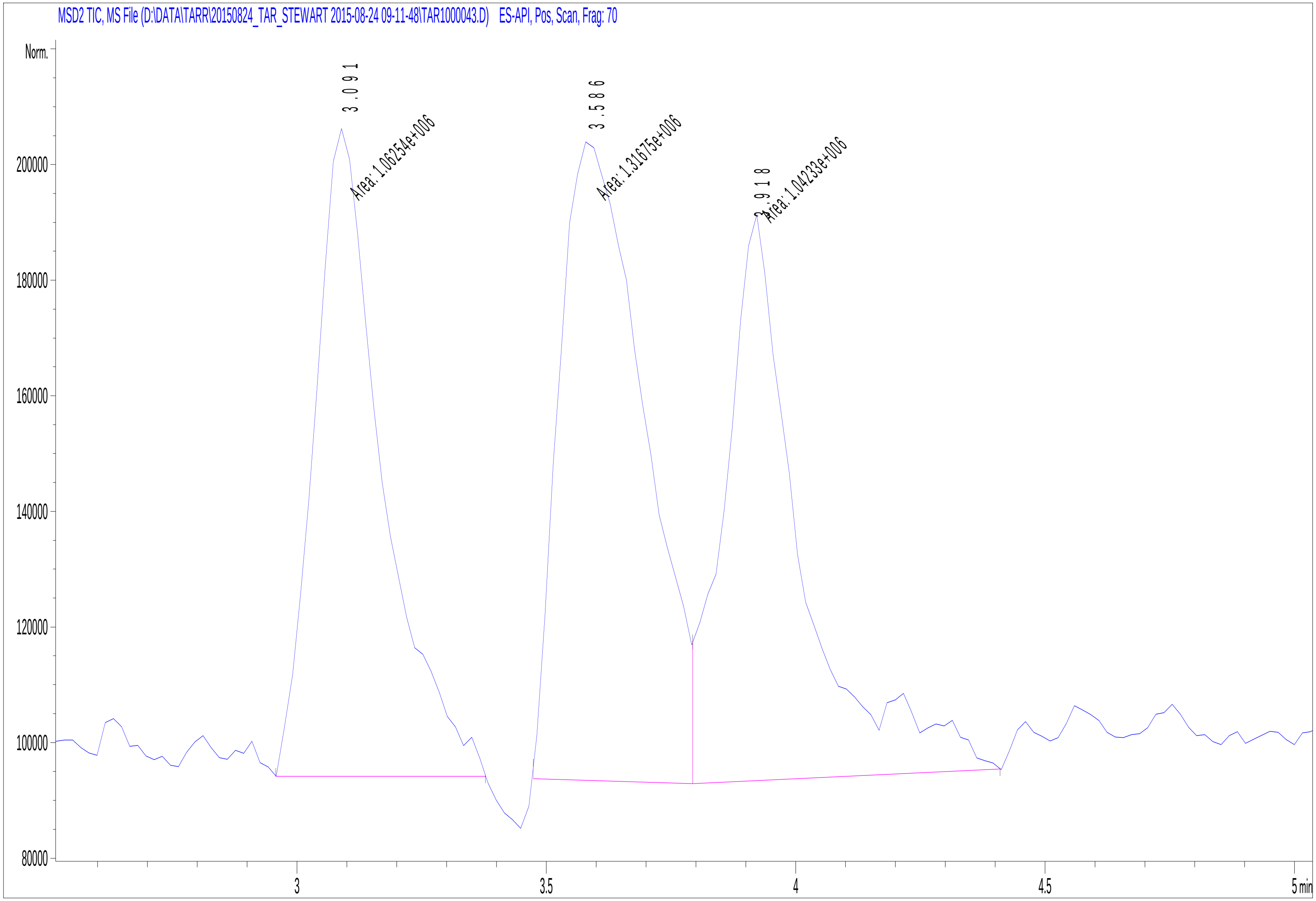
24-Jun-15

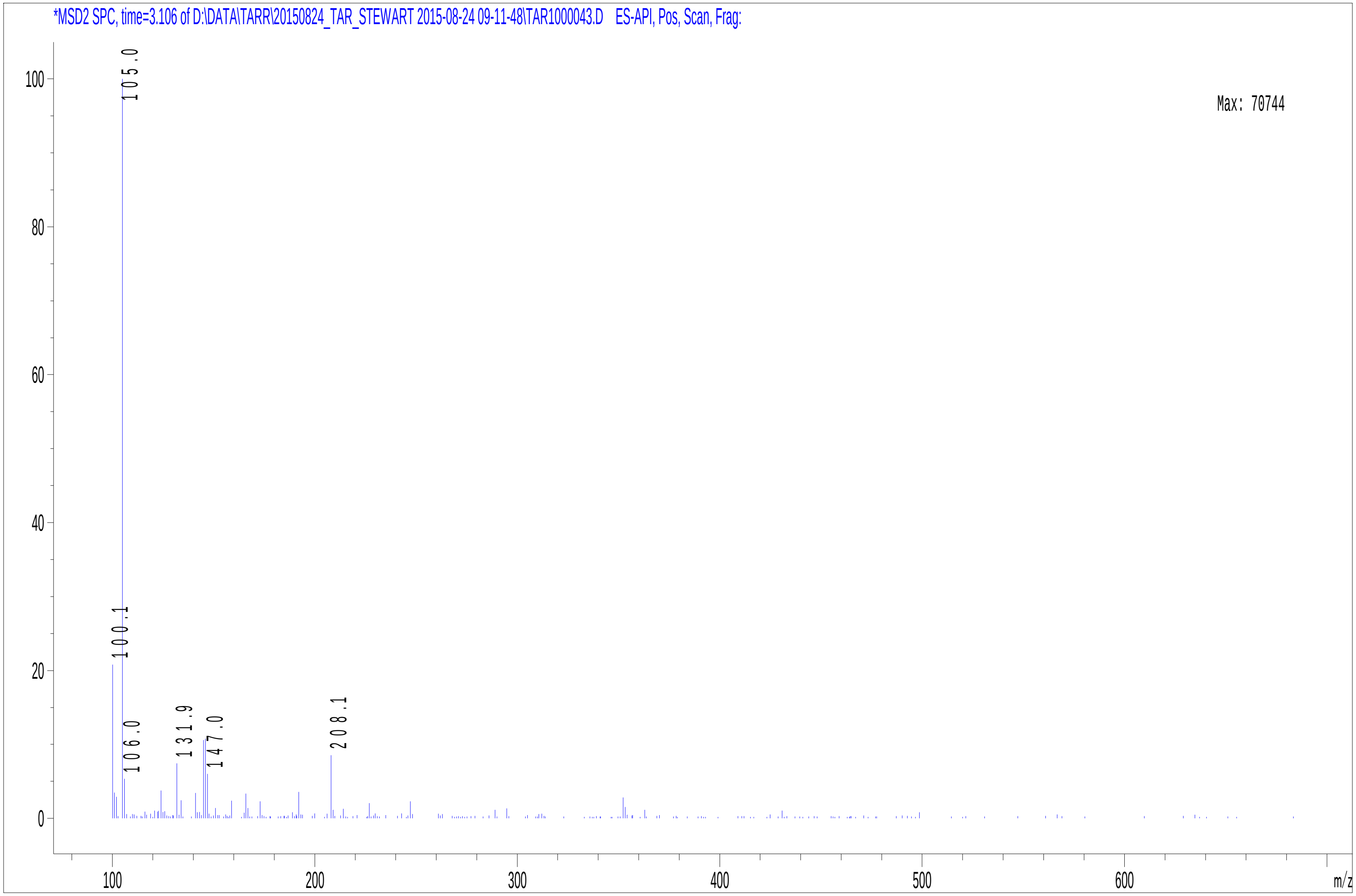
100 DC problem (no romoval)

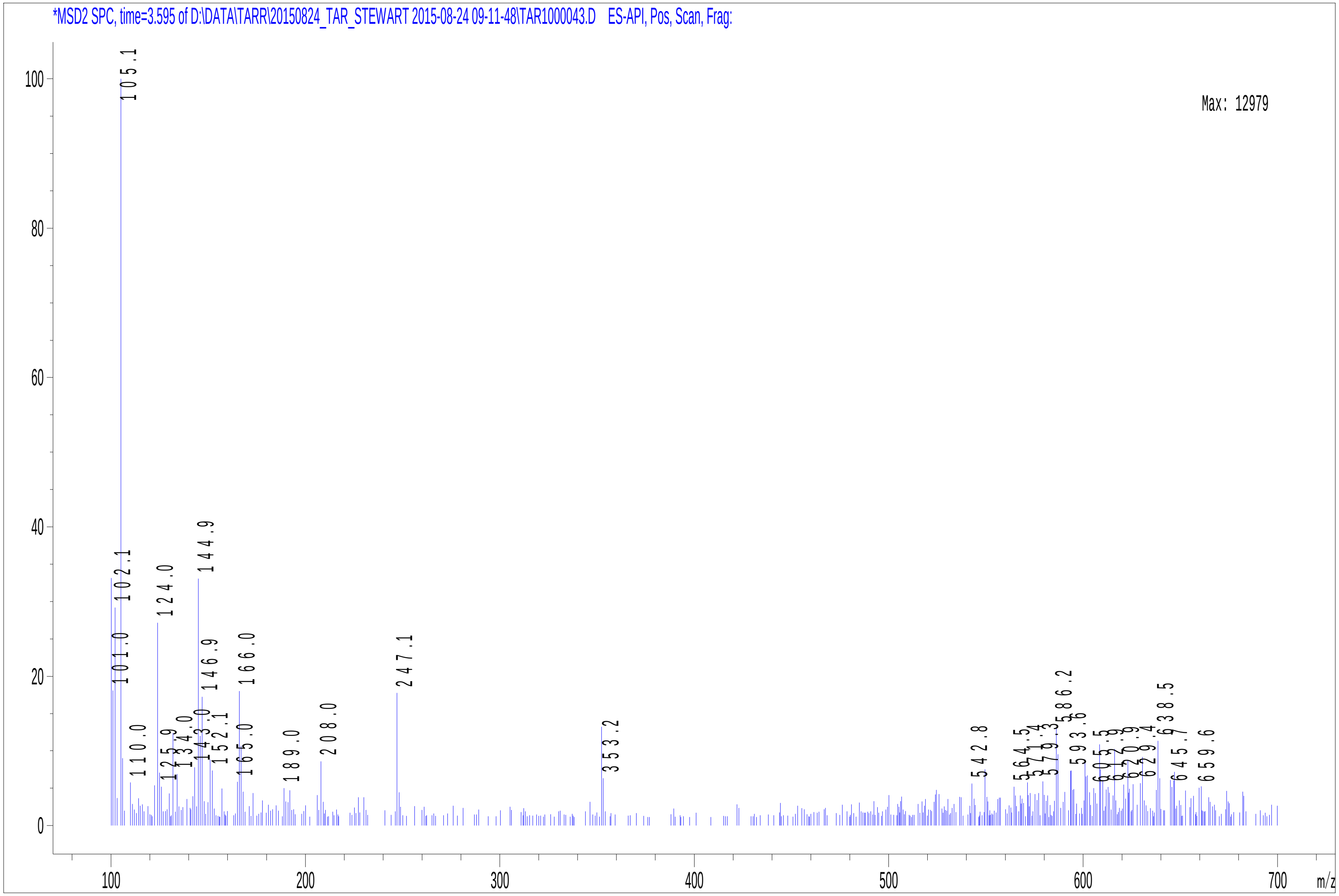
P2-E-07

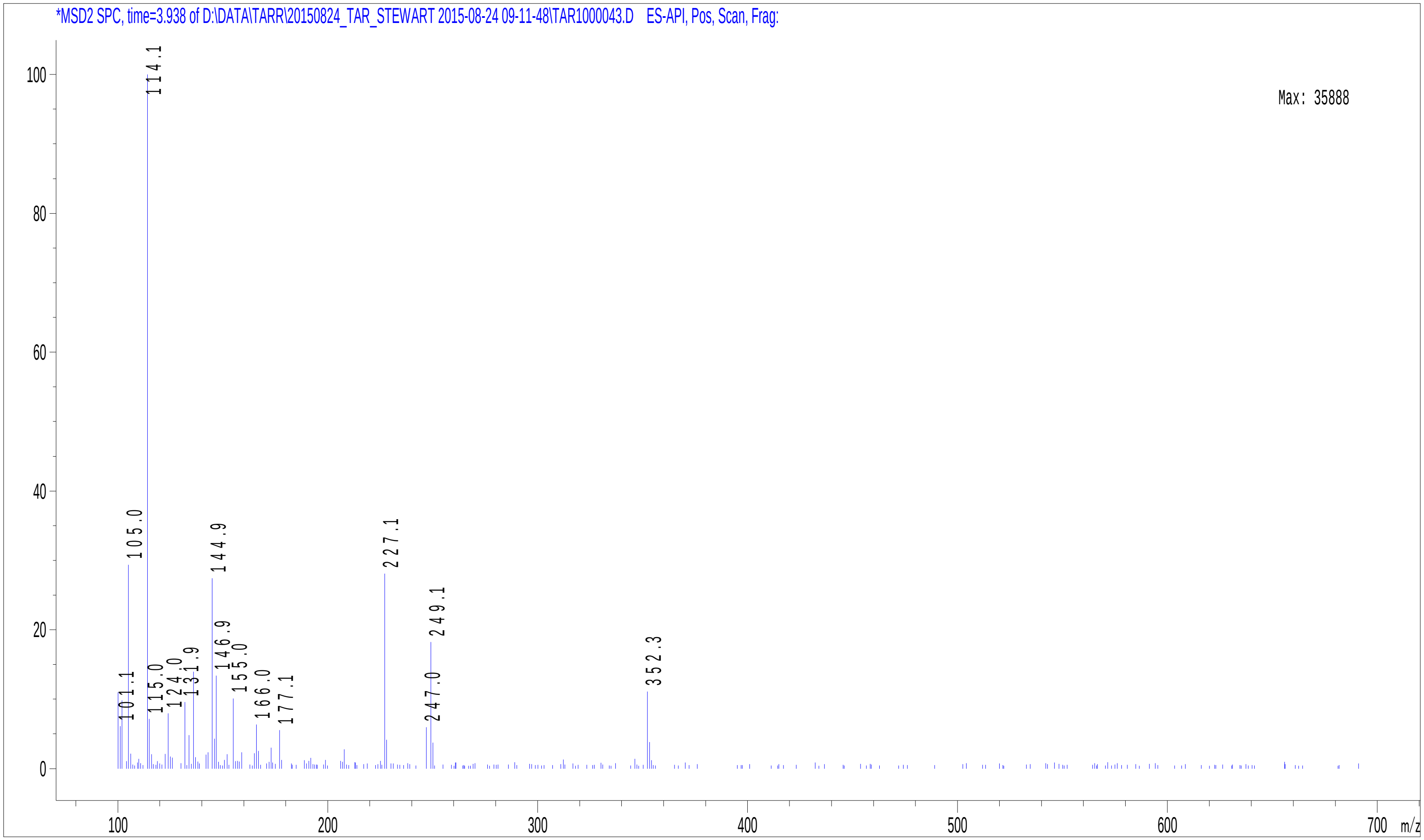


#	Time	Area	Height	Width	Area%	Symmetry
1	3.091	1062544.8	113936.2	0.1554	31.054	0.658
2	3.586	1316747.9	111692.5	0.1965	38.483	0.485
3	3.918	1042332.1	96530.9	0.18	30.463	0.512


MSD2 TIC, MS File (D:\DATA\TARR\20150824_TAR_STEWART 2015-08-24 09-11-48\TAR1000043.D) ES-API, Pos, Scan, Frag: 70
Norm.
3.091
Area: 1.06254e+006
3.586
Area: 1.31675e+006
3.918
Area: 1.04233e+006
200000
180000
160000
140000
120000
100000
80000
3
3.5
4
4.5
5 min

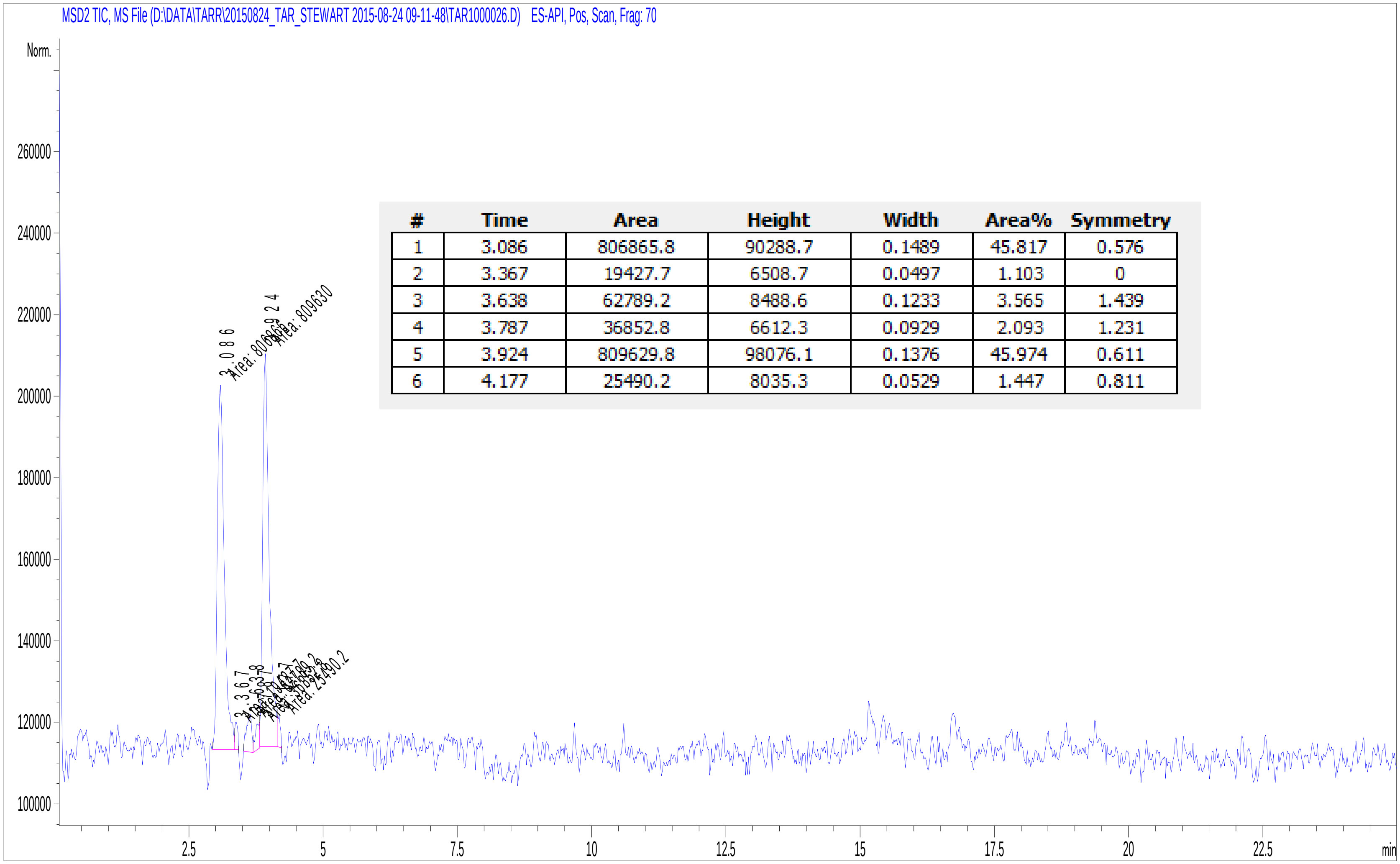

*MSD2 SPC, time=3.106 of D:\DATA\TARR\20150824_TAR_STEWART 2015-08-24 09-11-48\TAR1000043.D ES-API, Pos, Scan, Frag:
Max: 70744
105.0
100.1
106.0
131.9
147.0
208.1
0
20
40
60
80
100
100
200
300
400
500
600
m/z


*MSD2 SPC, time=3.595 of D:\DATA\TARR\20150824_TAR_STEWART 2015-08-24 09-11-48\TAR1000043.D ES-API, Pos, Scan, Frag:
Max: 12979
100
80
60
40
20
0
105.1
102.1
101.0
110.0
124.0
125.9
134.0
143.0
144.9
146.9
152.1
165.0
166.0
189.0
208.0
247.1
353.2
542.8
564.5
571.4
579.3
586.2
593.6
605.5
613.9
620.9
629.4
638.5
645.7
659.6
100
200
300
400
500
600
700
m/z

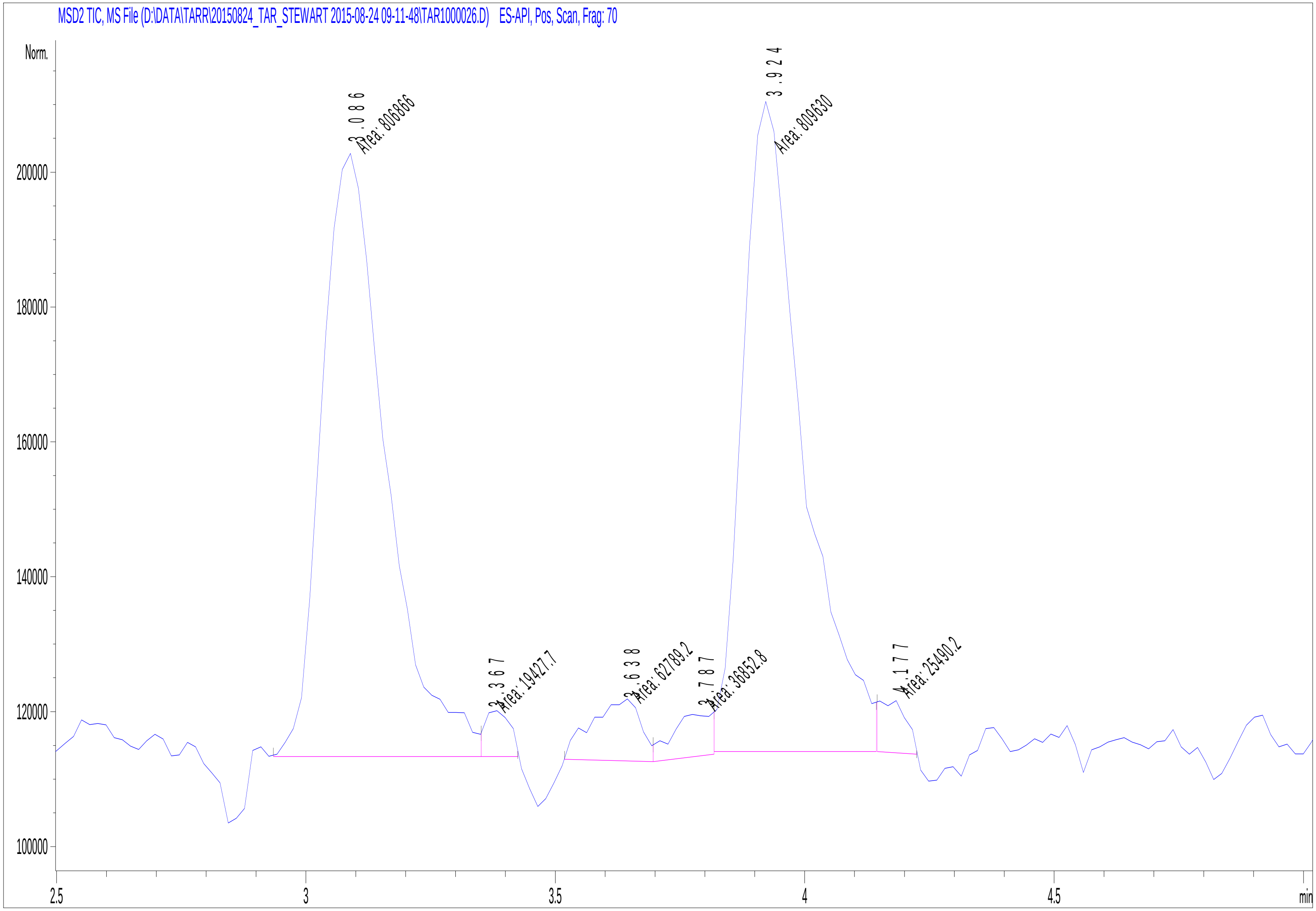

*MSD2 SPC, time=3.938 of D:\DATA\TARR\20150824_TAR_STEWART 2015-08-24 09-11-48\TAR1000043.D ES-API, Pos, Scan, Frag:
Max: 35888
114.1
105.0
144.9
227.1
249.1
146.9
155.0
131.9
124.0
115.0
101.1
166.0
177.1
247.0
352.3
0
20
40
60
80
100
100
200
300
400
500
600
700
m/z

pH 7

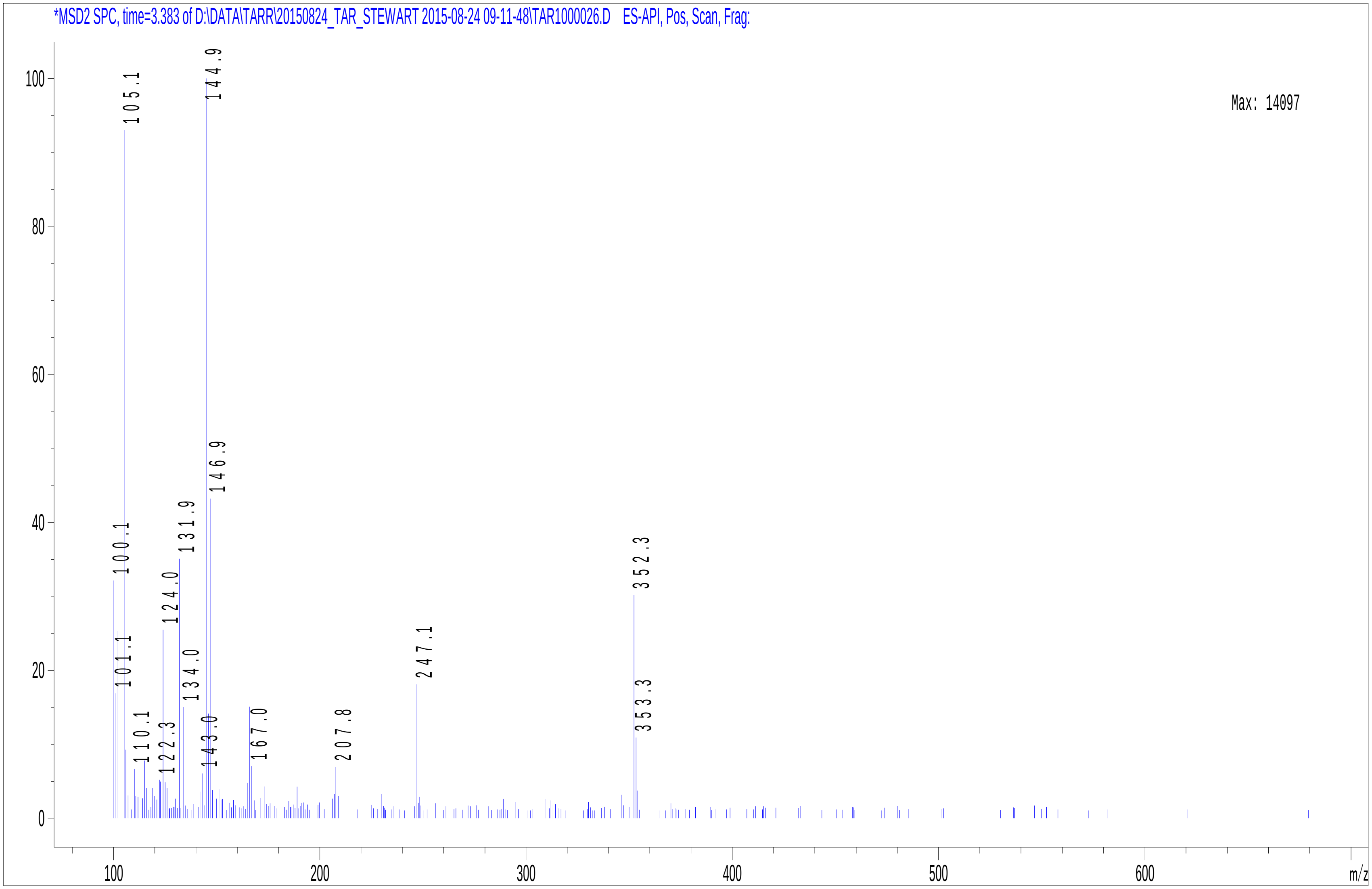
14-Jul-15
H2O2 Ctrl
P2-C-08

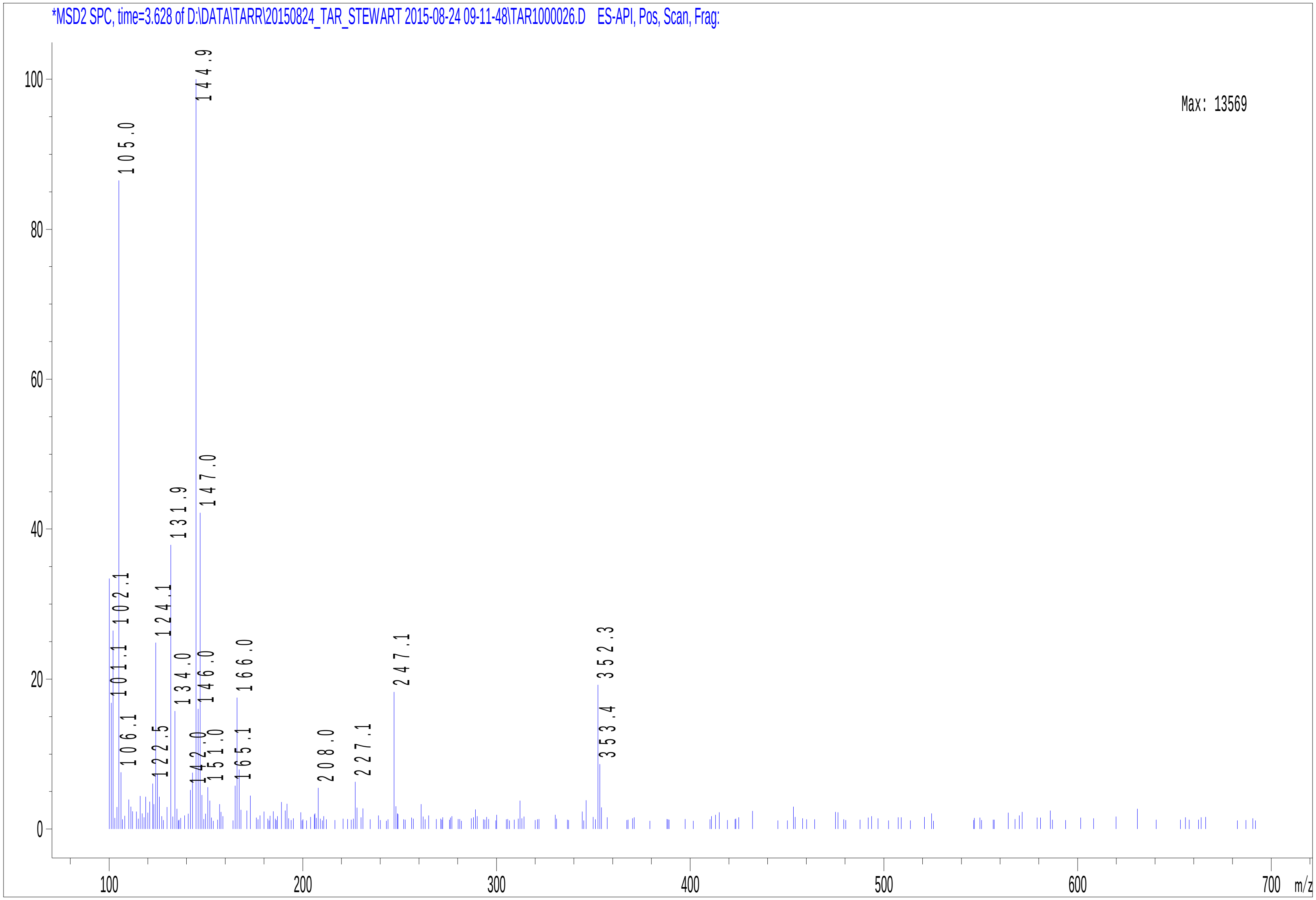


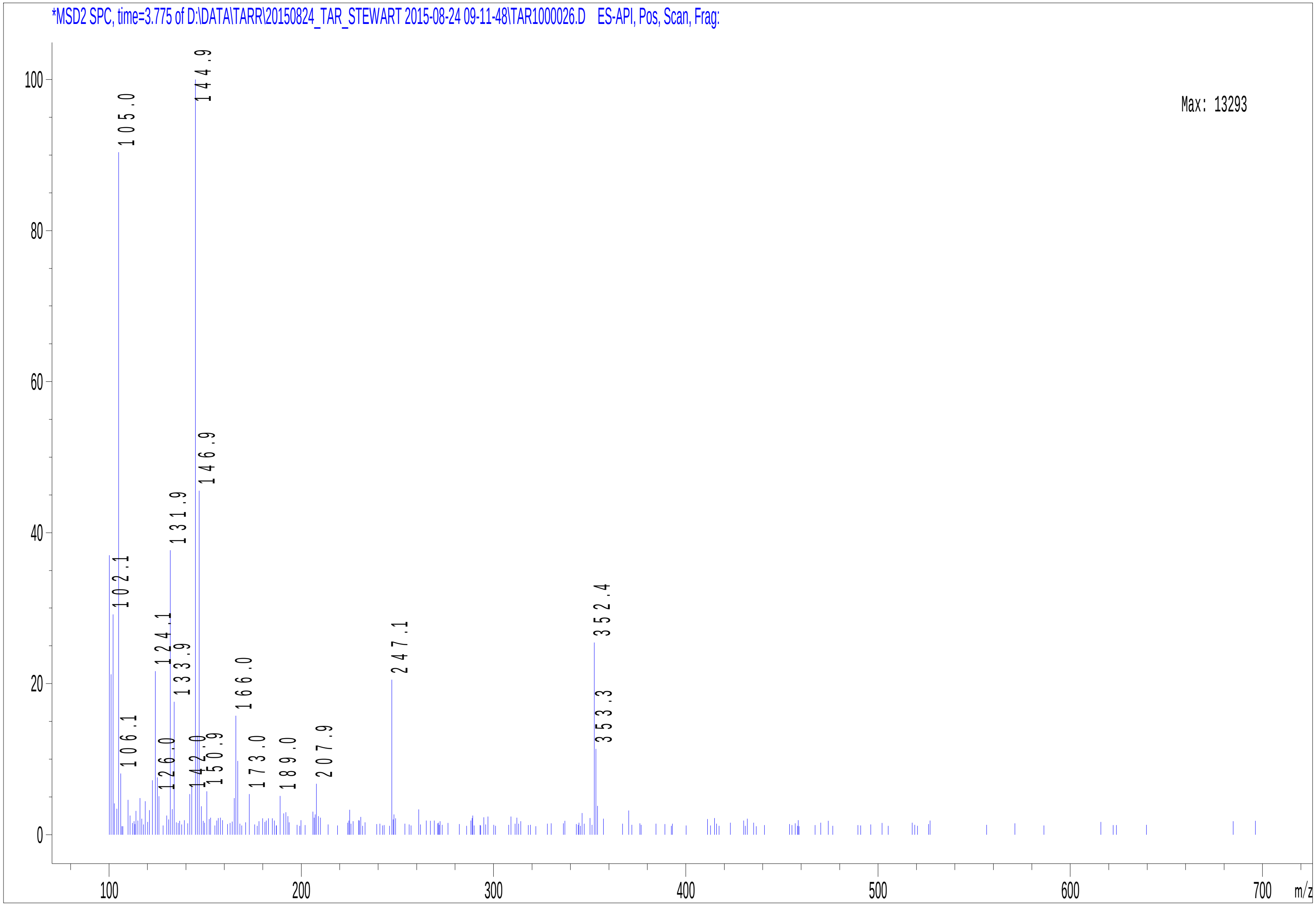
#	Time	Area	Height	Width	Area%	Symmetry
1	3.086	806865.8	90288.7	0.1489	45.817	0.576
2	3.367	19427.7	6508.7	0.0497	1.103	0
3	3.638	62789.2	8488.6	0.1233	3.565	1.439
4	3.787	36852.8	6612.3	0.0929	2.093	1.231
5	3.924	809629.8	98076.1	0.1376	45.974	0.611
6	4.177	25490.2	8035.3	0.0529	1.447	0.811

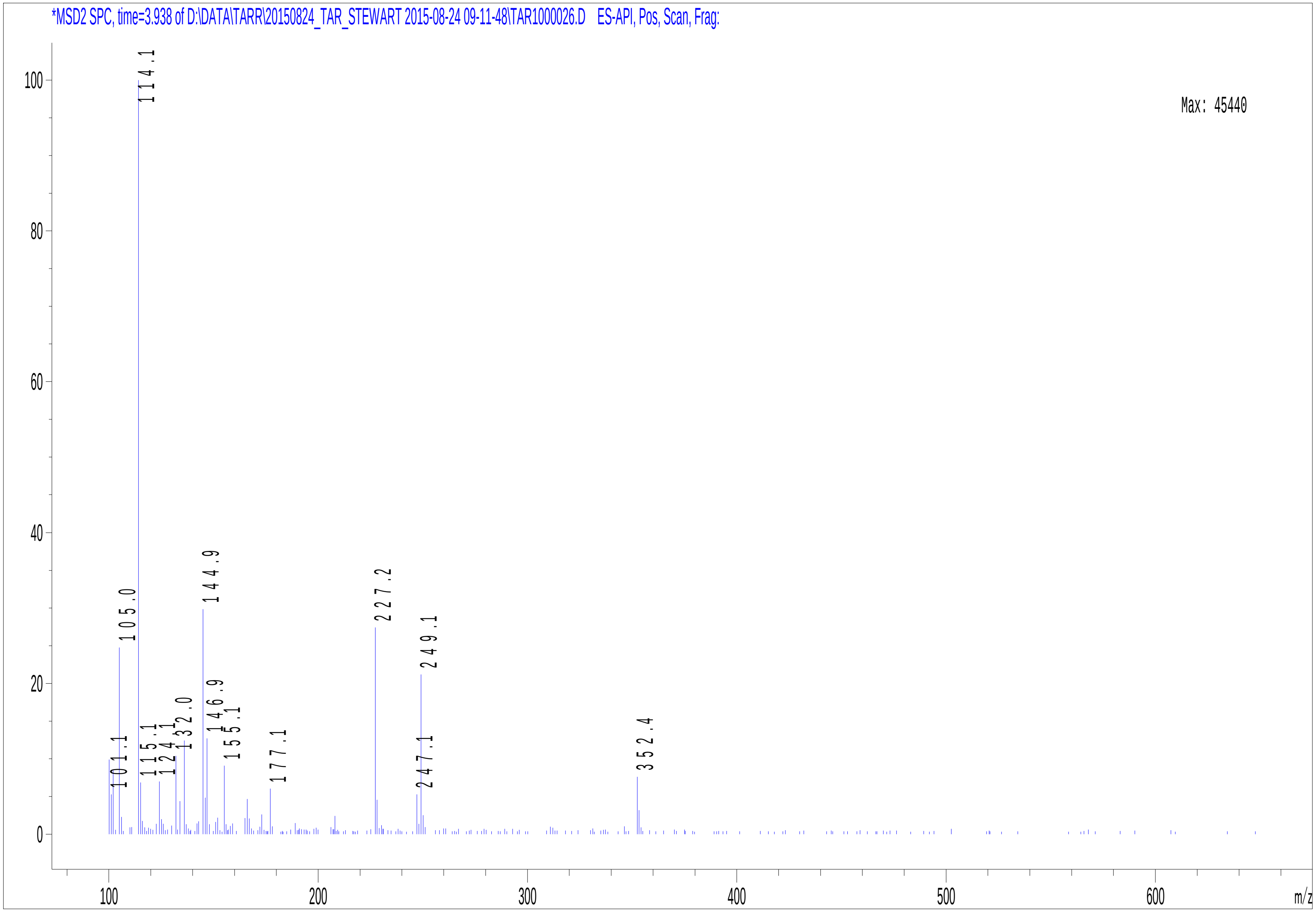

MSD2 TIC, MS File (D:\DATA\TARR\20150824_TAR_STEWART 2015-08-24 09-11-48\TAR1000026.D) ES-API, Pos, Scan, Frag: 70
Norm.
200000
180000
160000
140000
120000
100000
3.086
Area: 806866
3.924
Area: 809630
3.367
Area: 19427.7
3.638
Area: 62789.2
3.787
Area: 36852.8
4.177
Area: 25490.2
2.5
3
3.5
4
4.5
min

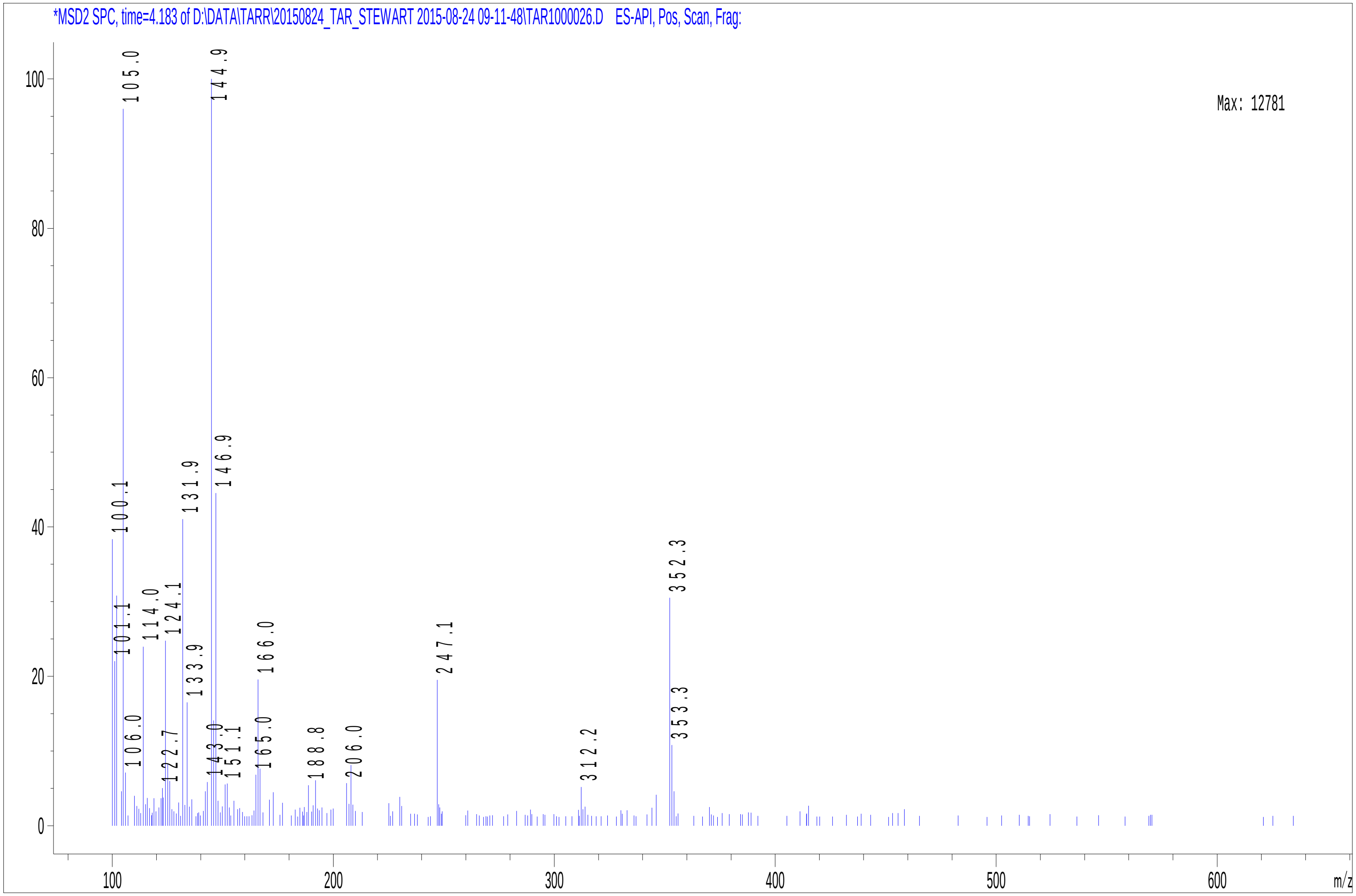

*MSD2 SPC, time=3.106 of D:\DATA\TARR\20150824_TAR_STEWART 2015-08-24 09-11-48\TAR1000026.D ES-API, Pos, Scan, Frag:
Max: 75704
105.0
106.0
131.9
147.0
100
80
60
40
20
0
100
200
300
400
500
600
700
m/z


*MSD2 SPC, time=3.383 of D:\DATA\TARR\20150824_TAR_STEWART 2015-08-24 09-11-48\TAR1000026.D ES-API, Pos, Scan, Frag:
Max: 14097
100
80
60
40
20
0
100.1
101.1
105.1
110.1
122.3
124.0
131.9
134.0
143.0
144.9
146.9
167.0
207.8
247.1
352.3
353.3
100
200
300
400
500
600
m/z


*MSD2 SPC, time=3.628 of D:\DATA\TARR\20150824_TAR_STEWART 2015-08-24 09-11-48\TAR1000026.D ES-API, Pos, Scan, Frag:
Max: 13569
144.9
105.0
147.0
131.9
102.1
124.1
101.1
134.0
146.0
166.0
106.1
122.5
142.0
151.0
165.1
208.0
227.1
247.1
352.3
353.4
0
20
40
60
80
100
100
200
300
400
500
600
700
m/z


*MSD2 SPC, time=3.775 of D:\DATA\TARR\20150824_TAR_STEWART 2015-08-24 09-11-48\TAR1000026.D ES-API, Pos, Scan, Frag:
Max: 13293
144.9
105.0
146.9
131.9
102.1
352.4
124.1
133.9
247.1
166.0
353.3
106.1
126.0
142.0
150.9
173.0
189.0
207.9
100
80
60
40
20
0
100
200
300
400
500
600
700
m/z

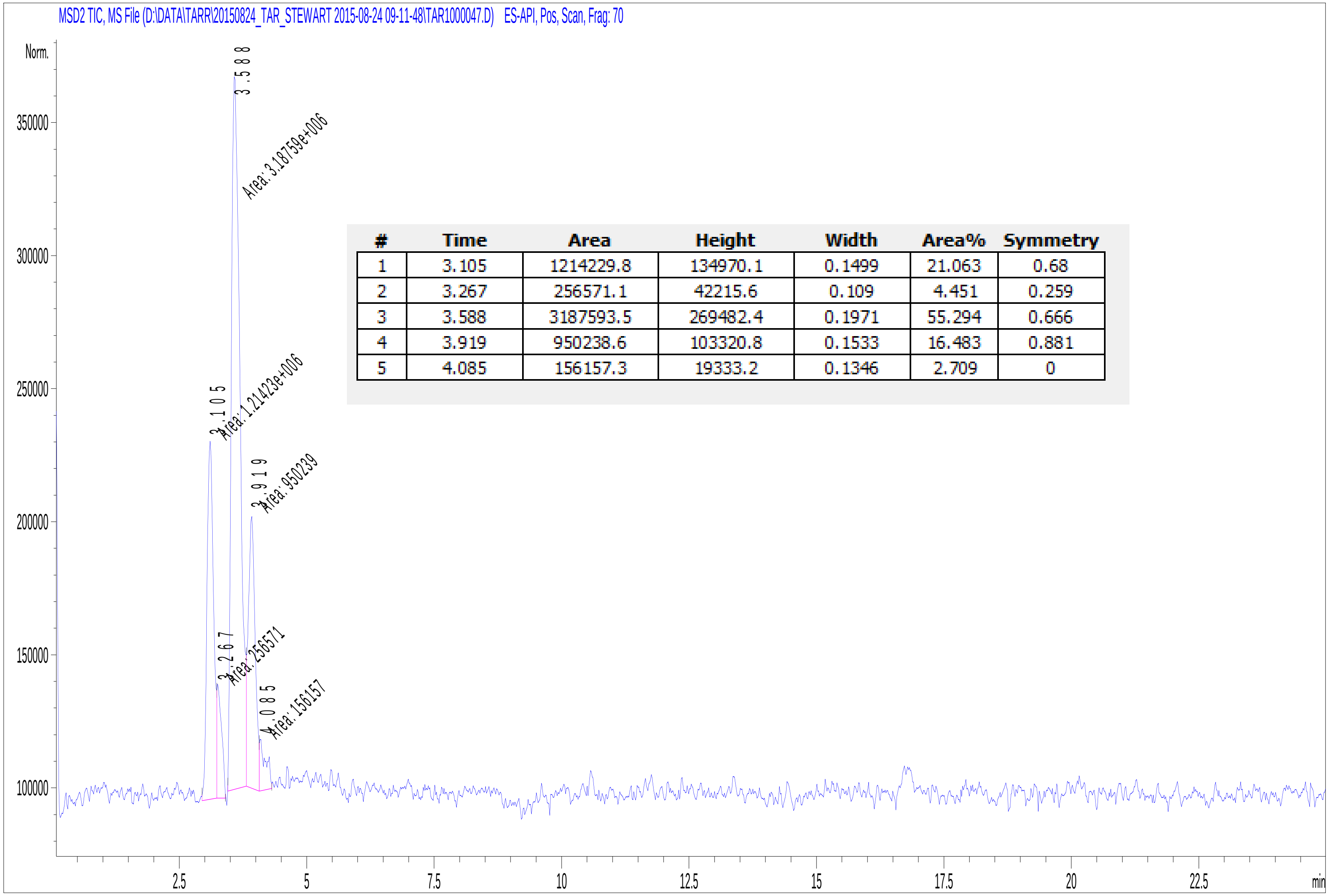

*MSD2 SPC, time=3.938 of D:\DATA\TARR\20150824_TAR_STEWART 2015-08-24 09-11-48\TAR1000026.D ES-API, Pos, Scan, Frag:
Max: 45440
114.1
105.0
144.9
227.2
249.1
101.1
115.1
124.1
132.0
146.9
155.1
177.1
247.1
352.4
0
20
40
60
80
100
200
300
400
500
600
m/z


*MSD2 SPC, time=4.183 of D:\DATA\TARR\20150824_TAR_STEWART 2015-08-24 09-11-48\TAR1000026.D ES-API, Pos, Scan, Frag:
Max: 12781
105.0
144.9
146.9
131.9
100.1
101.1
114.0
124.1
133.9
166.0
247.1
352.3
353.3
106.0
122.7
143.0
151.1
165.0
188.8
206.0
312.2
0
20
40
60
80
100
100
200
300
400
500
600
m/z

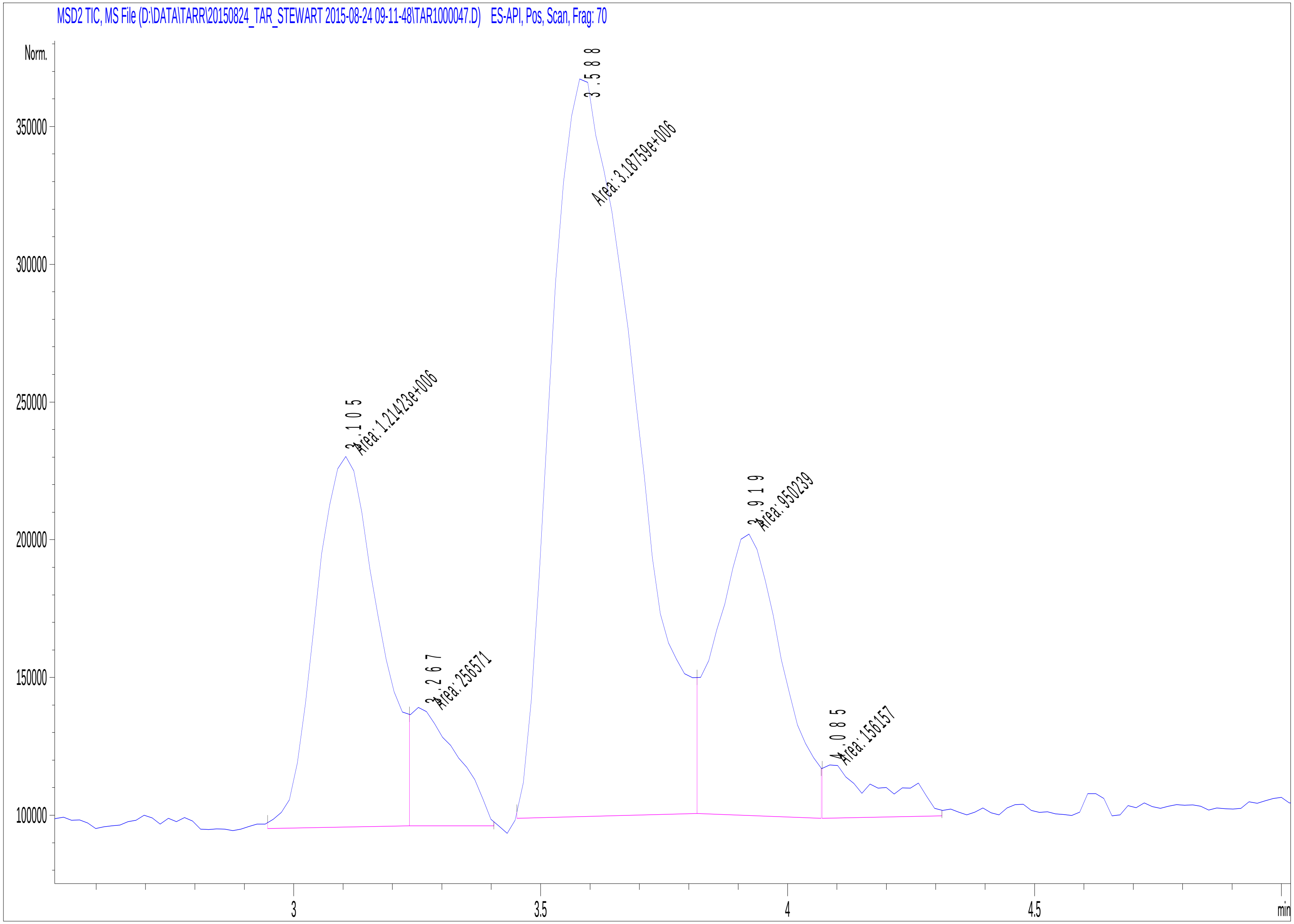
7-Mar-15

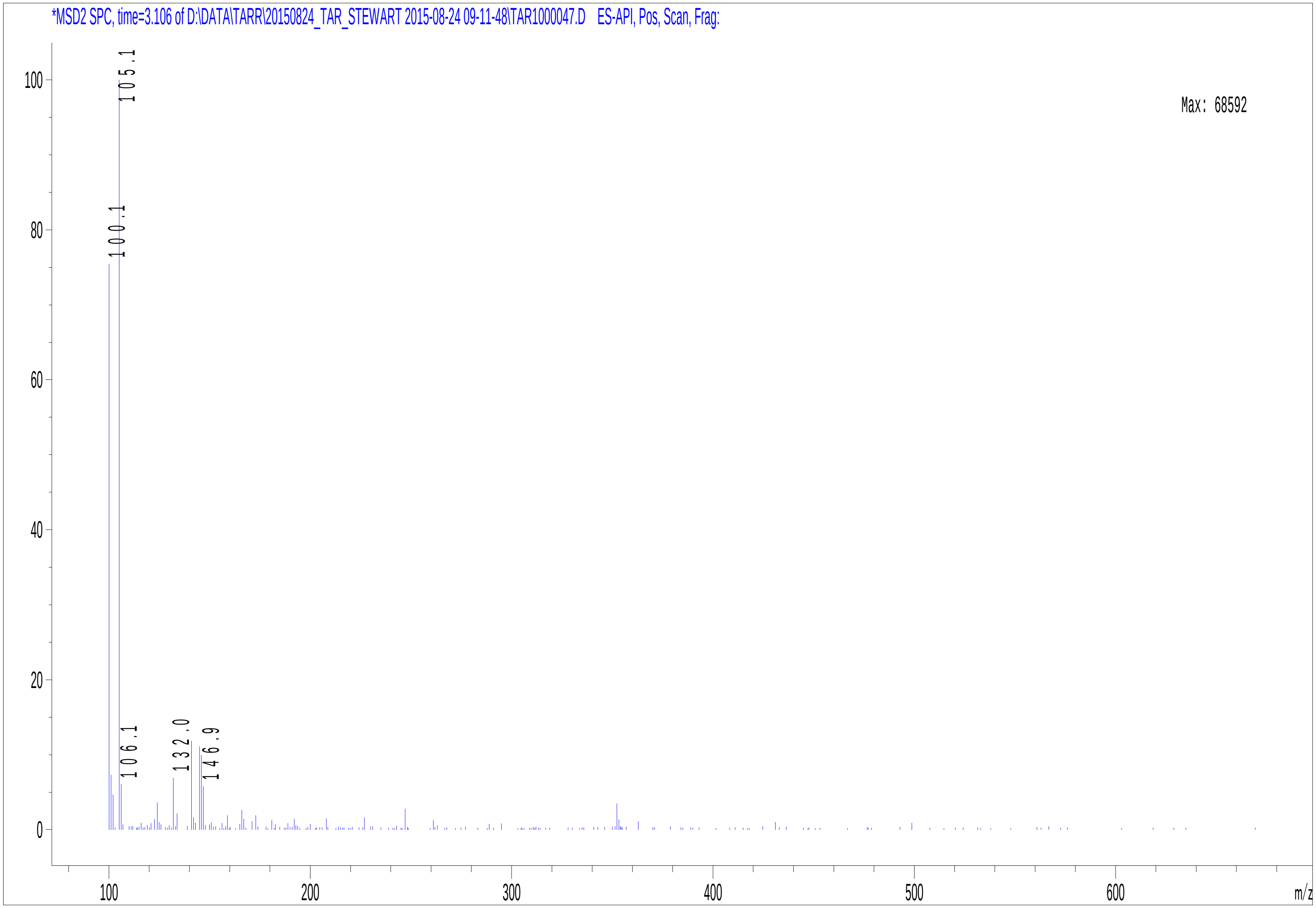
0 DC

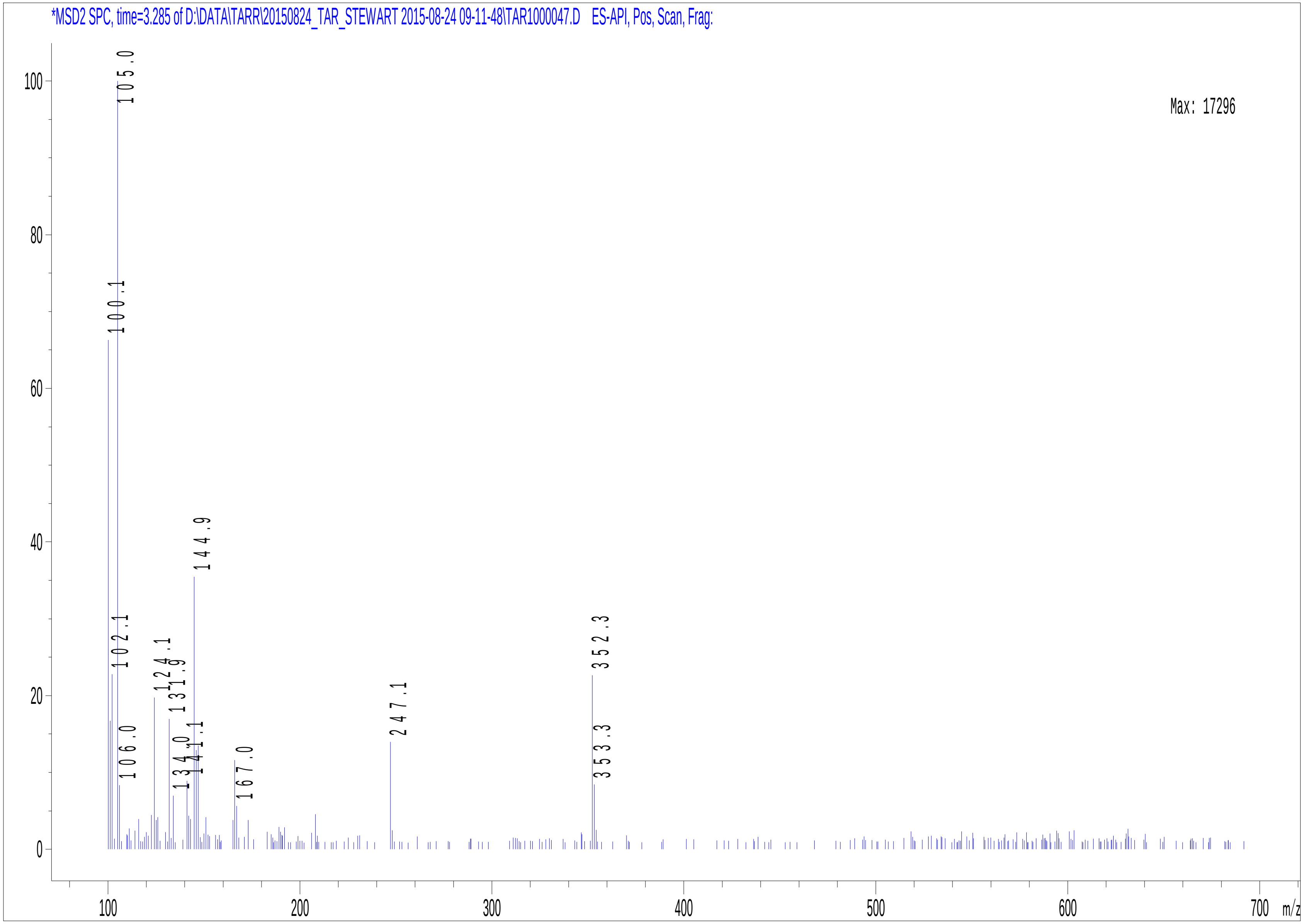
P2-A-02

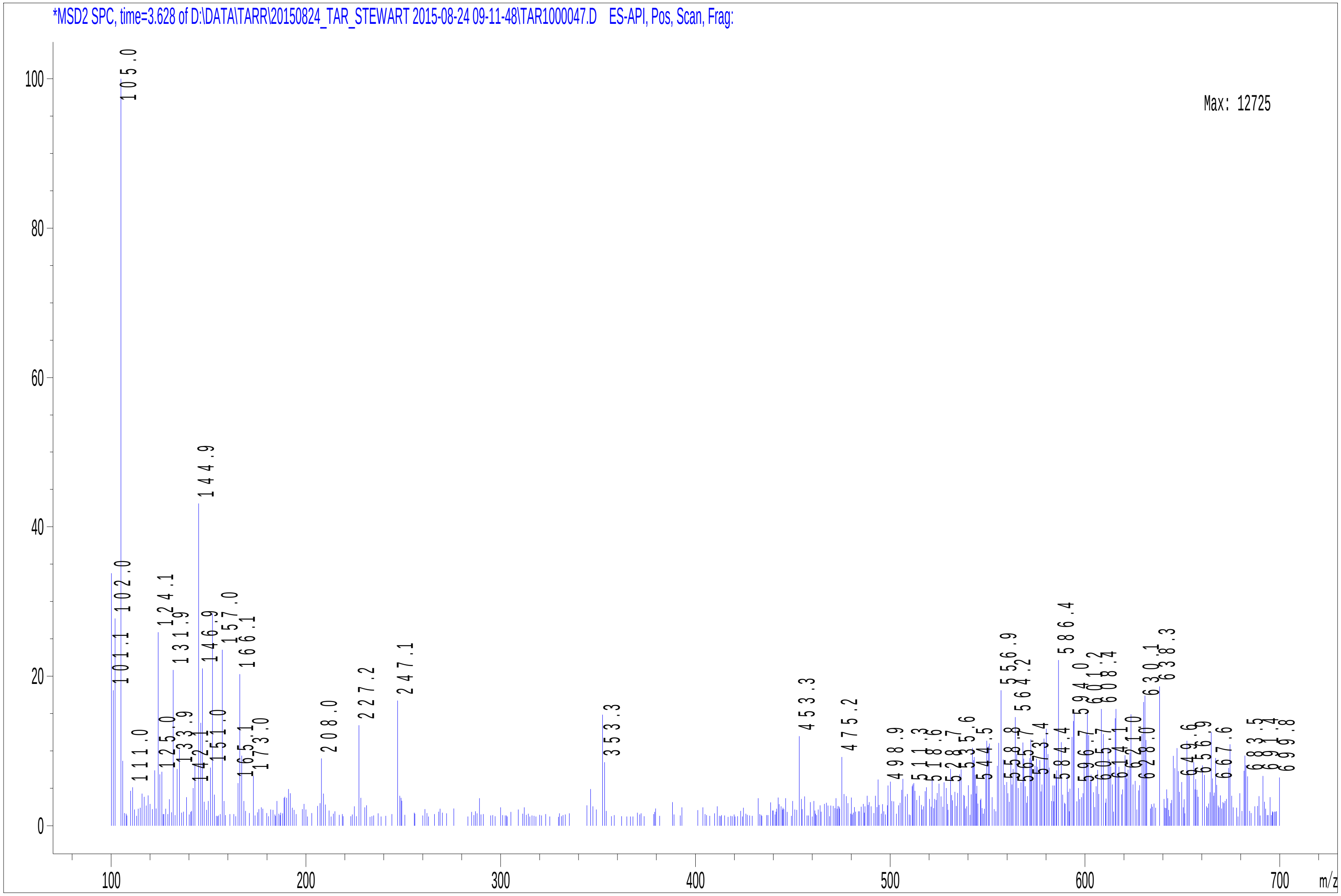


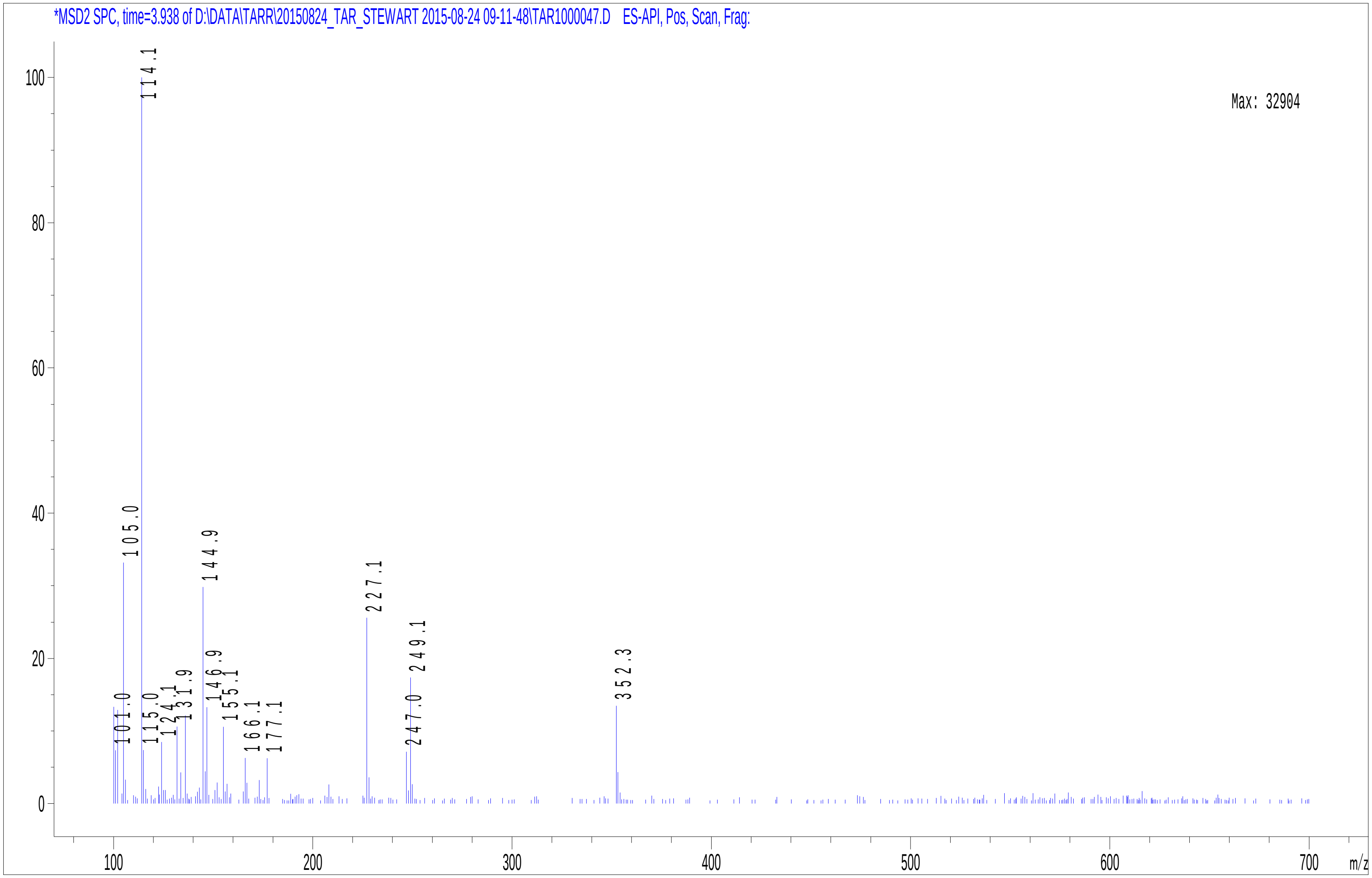
#	Time	Area	Height	Width	Area%	Symmetry
1	3.105	1214229.8	134970.1	0.1499	21.063	0.68
2	3.267	256571.1	42215.6	0.109	4.451	0.259
3	3.588	3187593.5	269482.4	0.1971	55.294	0.666
4	3.919	950238.6	103320.8	0.1533	16.483	0.881
5	4.085	156157.3	19333.2	0.1346	2.709	0

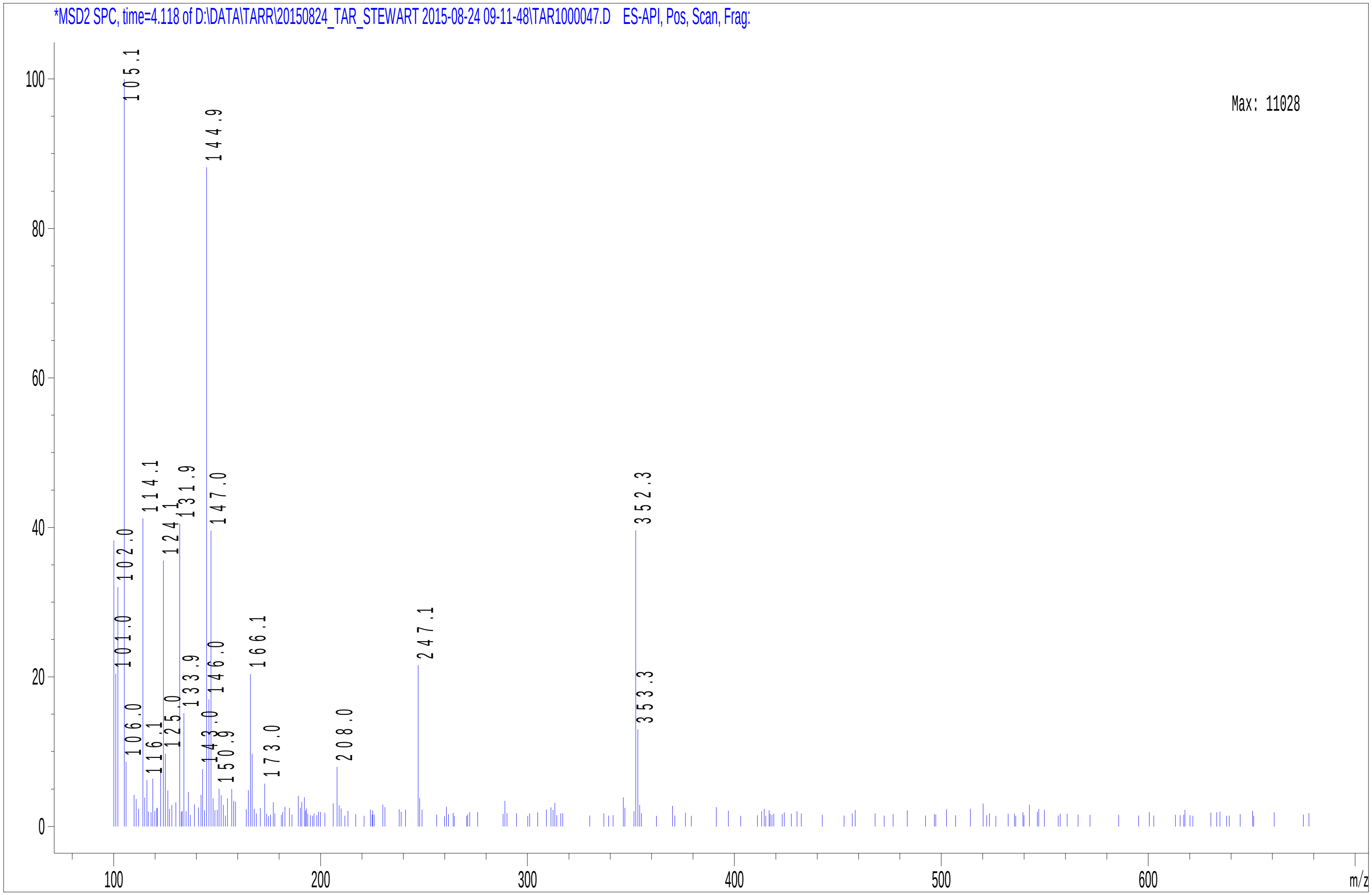

MSD2 TIC, MS File (D:\DATA\TARR\20150824_TAR_STEWART 2015-08-24 09-11-48\TAR1000047.D) ES-API, Pos, Scan, Frag: 70
Norm.
350000
300000
250000
200000
150000
100000
3.105
Area: 1.21423e+006
3.267
Area: 256571
3.588
Area: 3.18759e+006
3.919
Area: 950239
4.085
Area: 156157
3
3.5
4
4.5
min


*MSD2 SPC, time=3.106 of D:\DATA\TARR\20150824_TAR_STEWART 2015-08-24 09-11-48\TAR1000047.D ES-API, Pos, Scan, Frag:
Max: 68592
105.1
100.1
106.1
132.0
146.9
100
80
60
40
20
0
100
200
300
400
500
600
m/z


*MSD2 SPC, time=3.285 of D:\DATA\TARR\20150824_TAR_STEWART 2015-08-24 09-11-48\TAR1000047.D ES-API, Pos, Scan, Frag:
Max: 17296
105.0
100.1
102.1
106.0
124.1
131.9
134.0
141.1
144.9
167.0
247.1
352.3
353.3
0
20
40
60
80
100
100
200
300
400
500
600
700
m/z


*MSD2 SPC, time=3.628 of D:\DATA\TARR\20150824_TAR_STEWART 2015-08-24 09-11-48\TAR1000047.D   ES-API, Pos, Scan, Frag:
Max: 12725
100
80
60
40
20
0
100
200
300
400
500
600
700
m/z
105.0
101.1
102.0
111.0
124.1
125.0
131.9
133.9
142.1
144.9
146.9
151.0
157.0
165.1
166.1
173.0
208.0
227.2
247.1
353.3
453.3
475.2
498.9
511.3
518.6
528.7
535.6
544.5
556.9
558.8
564.2
565.7
573.4
584.4
586.4
594.0
596.7
601.2
605.7
608.4
614.1
621.0
628.0
630.1
638.3
649.6
656.9
667.6
683.5
691.4
699.8

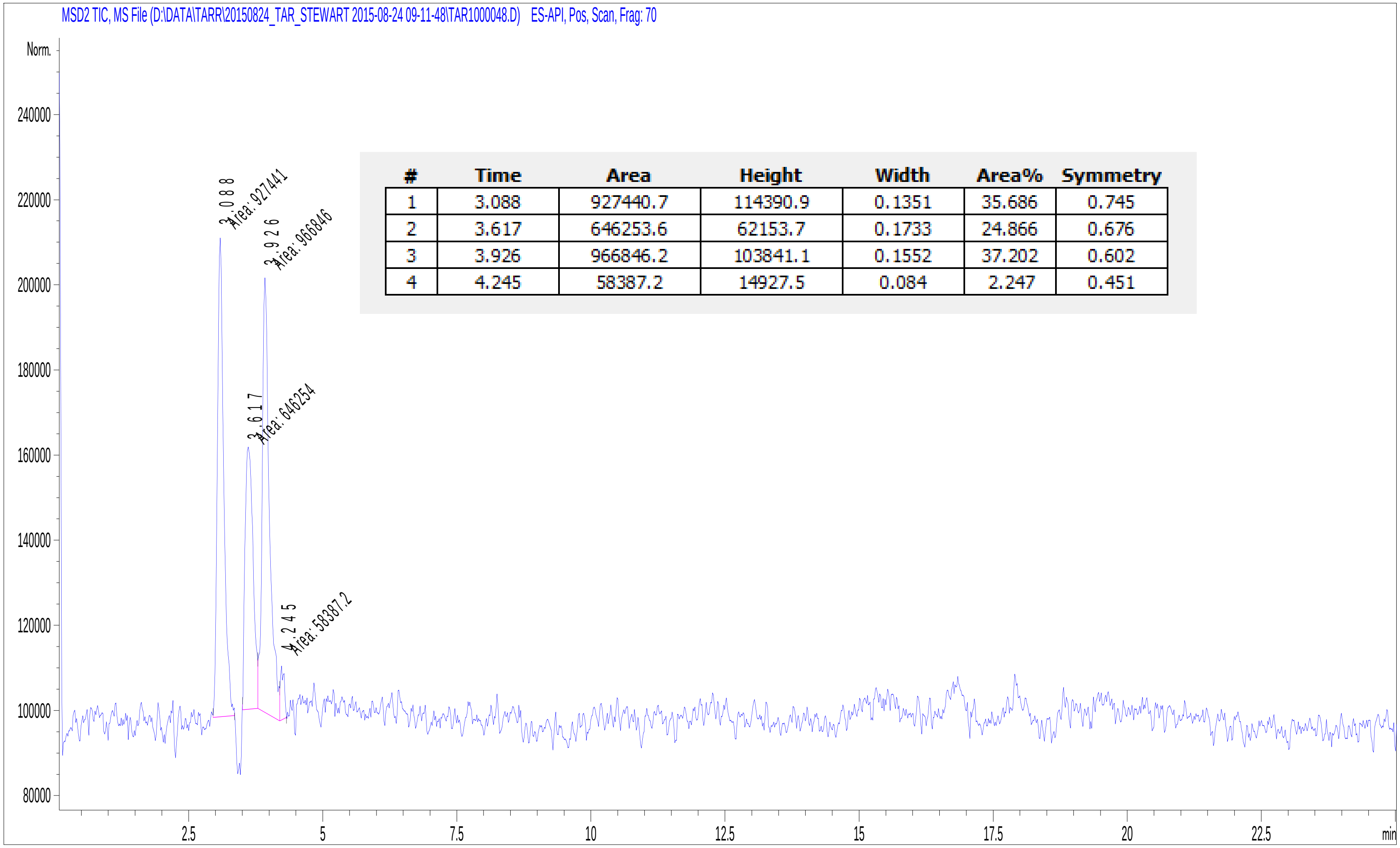

*MSD2 SPC, time=3.938 of D:\DATA\TARR\20150824_TAR_STEWART 2015-08-24 09-11-48\TAR1000047.D ES-API, Pos, Scan, Frag:
Max: 32904
114.1
105.0
144.9
227.1
249.1
352.3
101.0
115.0
124.1
131.9
146.9
155.1
166.1
177.1
247.0
0
20
40
60
80
100
100
200
300
400
500
600
700
m/z


*MSD2 SPC, time=4.118 of D:\DATA\TARR\20150824_TAR_STEWART 2015-08-24 09-11-48\TAR1000047.D ES-API, Pos, Scan, Frag:
Max: 11028
105.1
144.9
114.1
124.1
131.9
147.0
352.3
102.0
101.0
106.0
116.1
125.0
133.9
146.0
143.0
150.9
166.1
173.0
208.0
247.1
353.3
0
20
40
60
80
100
100
200
300
400
500
600
m/z

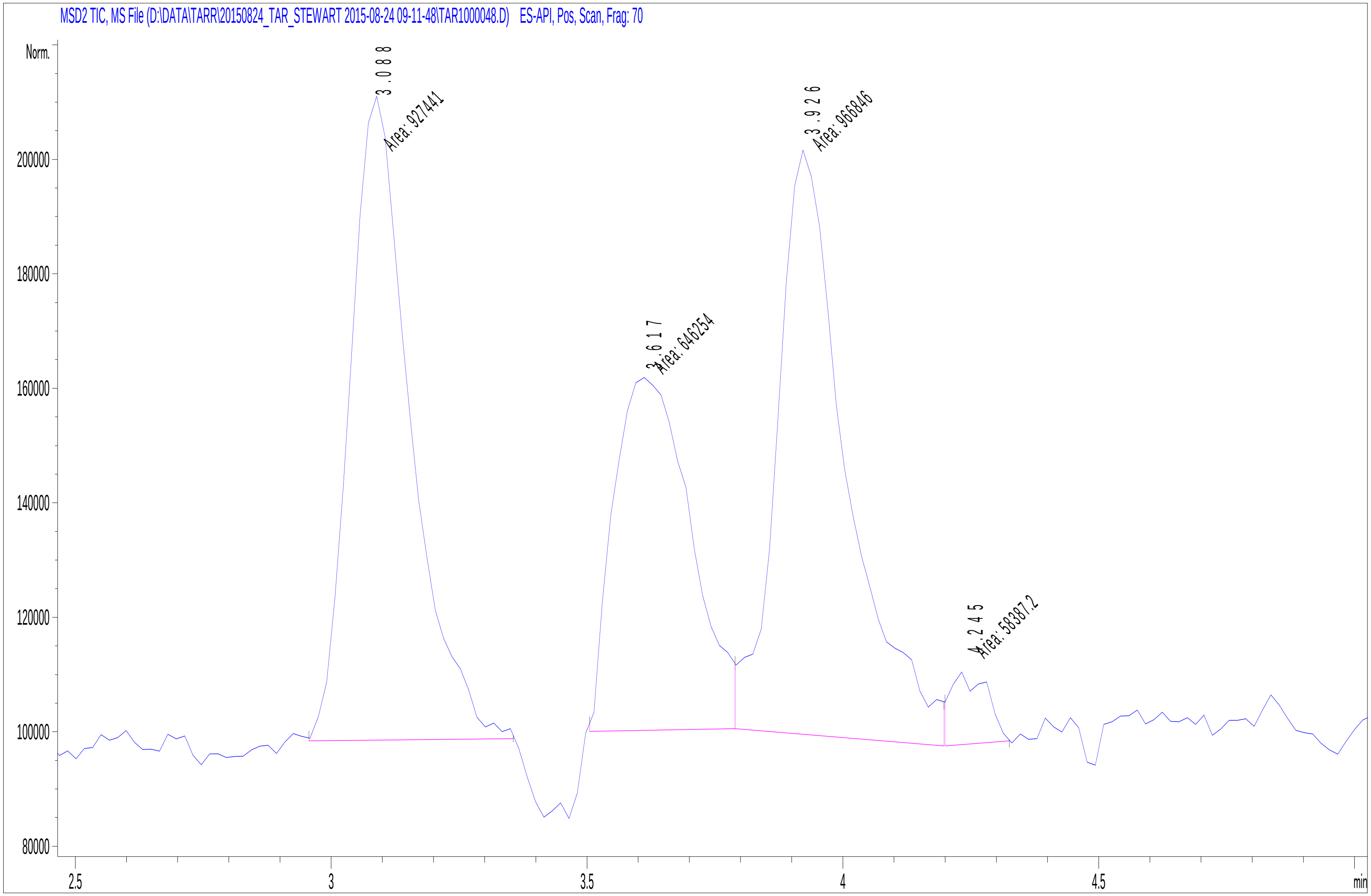
13-Mar-15

5 DC

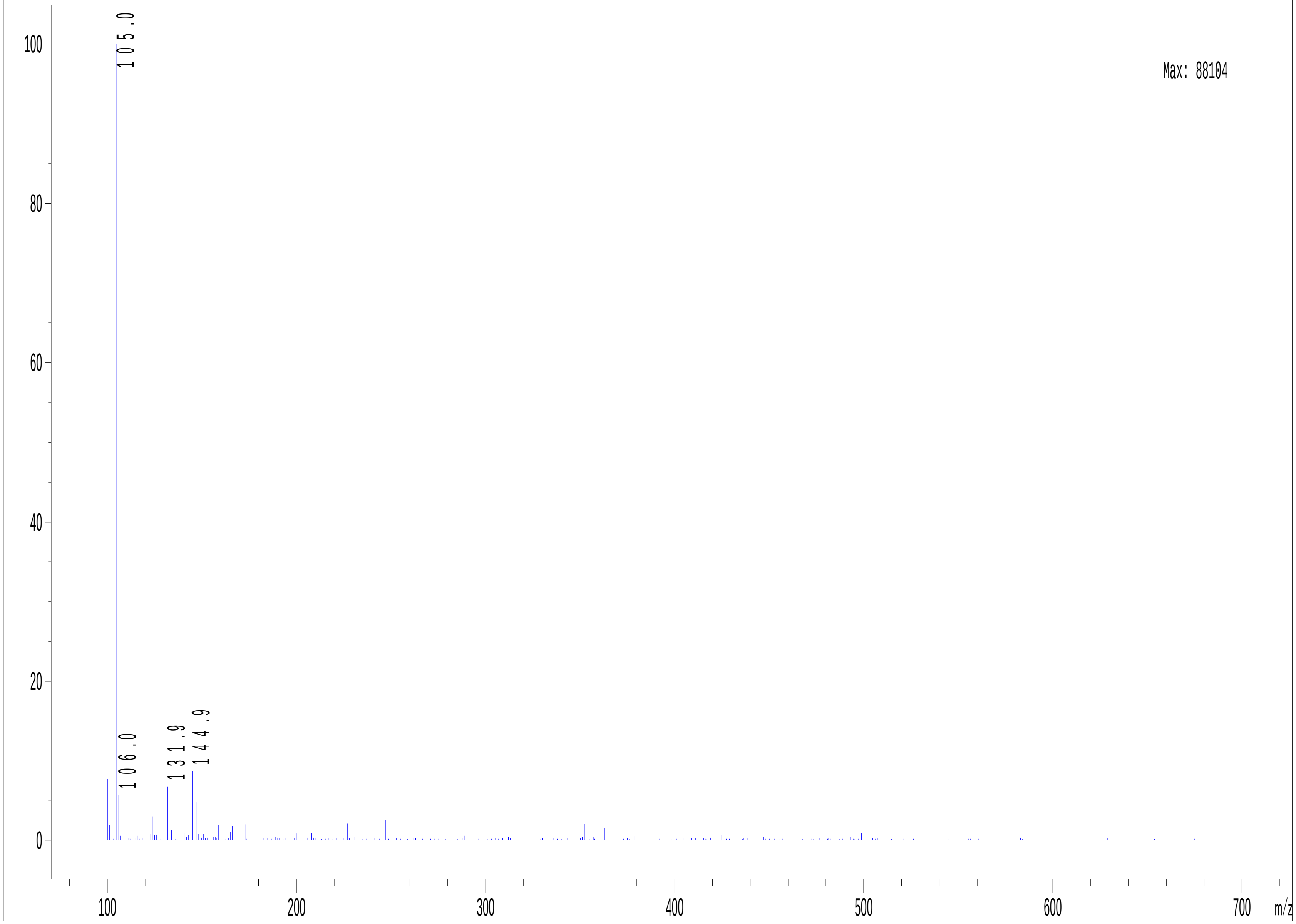
P2-A-03

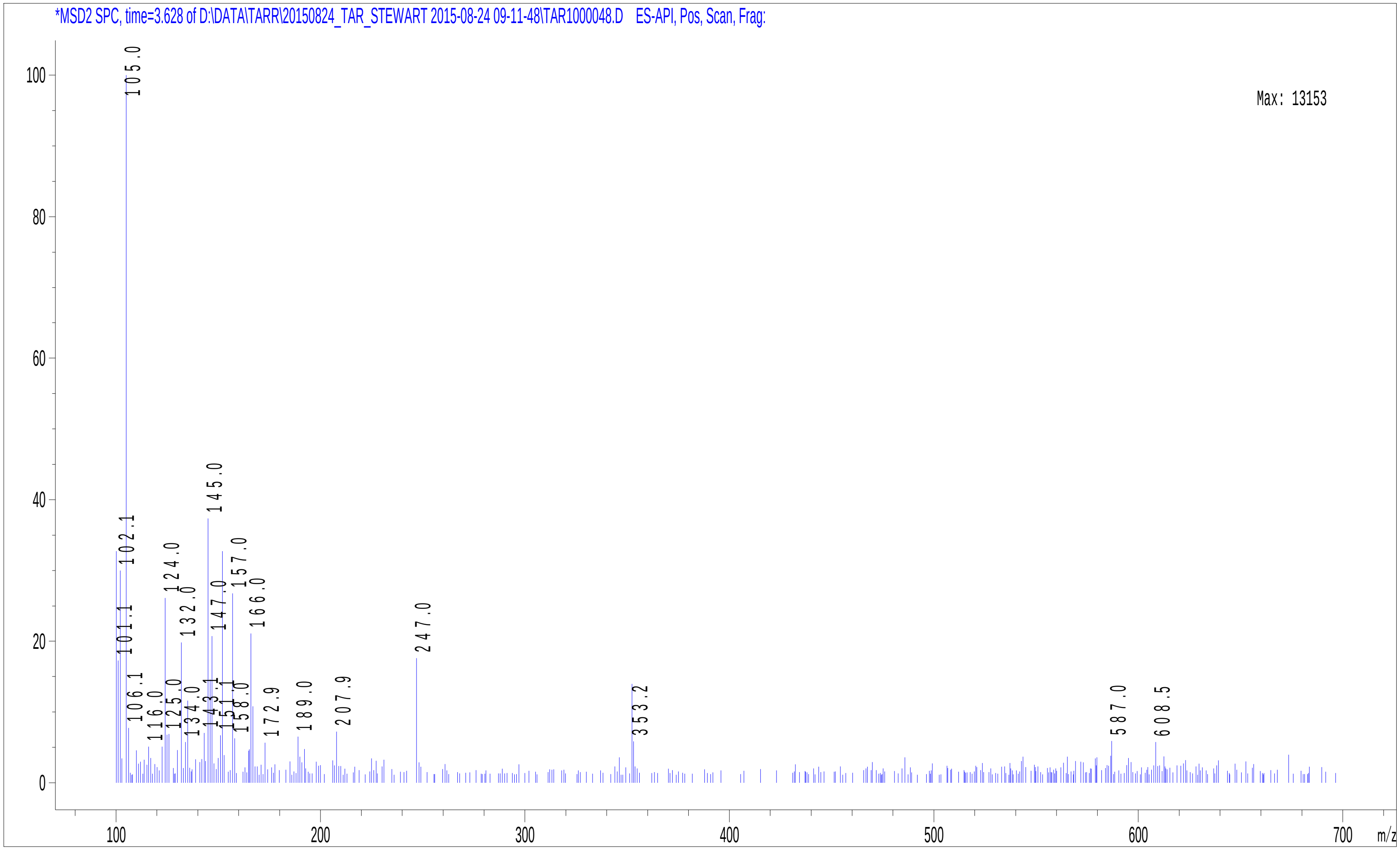


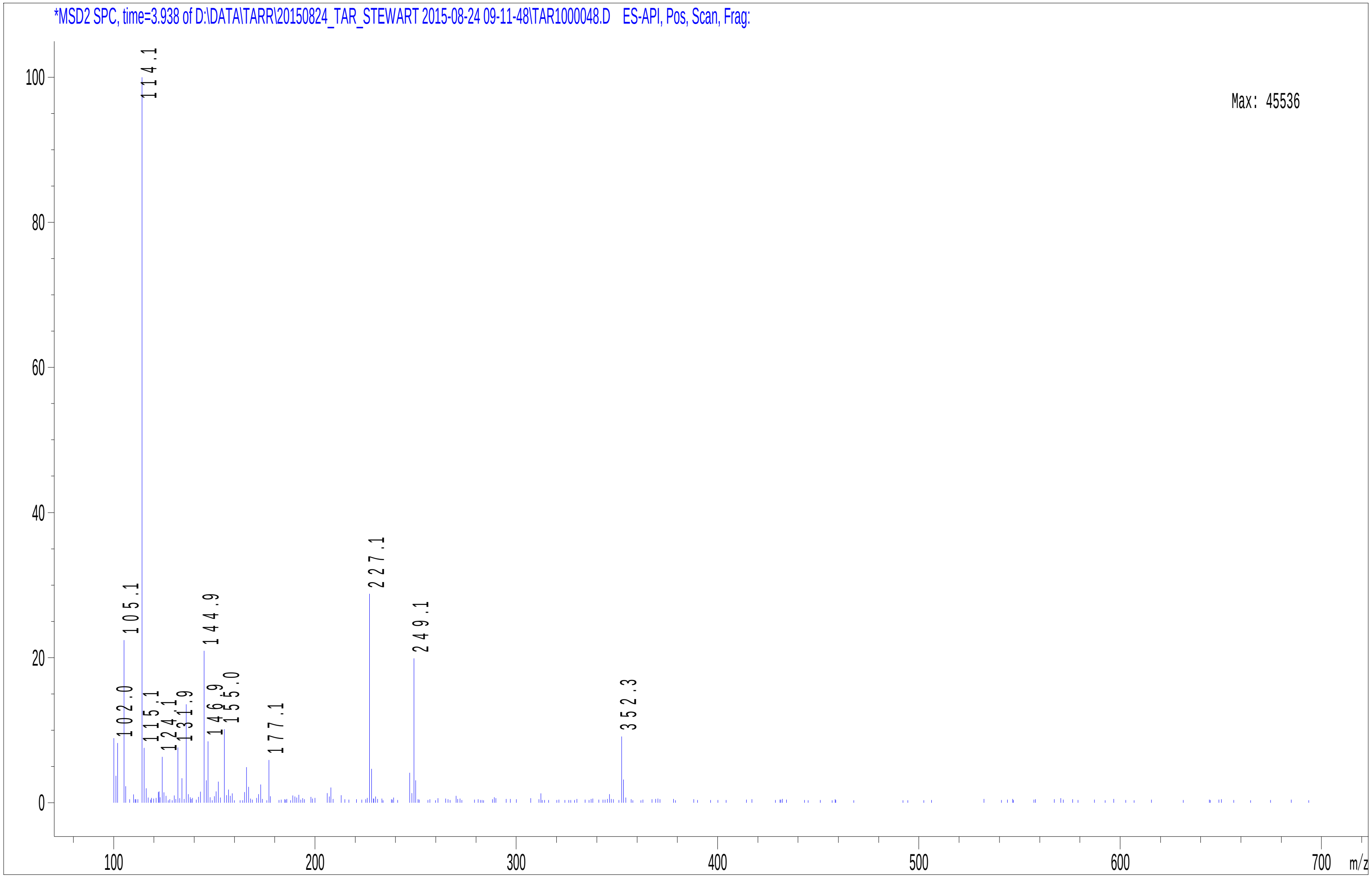
#	Time	Area	Height	Width	Area%	Symmetry
1	3.088	927440.7	114390.9	0.1351	35.686	0.745
2	3.617	646253.6	62153.7	0.1733	24.866	0.676
3	3.926	966846.2	103841.1	0.1552	37.202	0.602
4	4.245	58387.2	14927.5	0.084	2.247	0.451

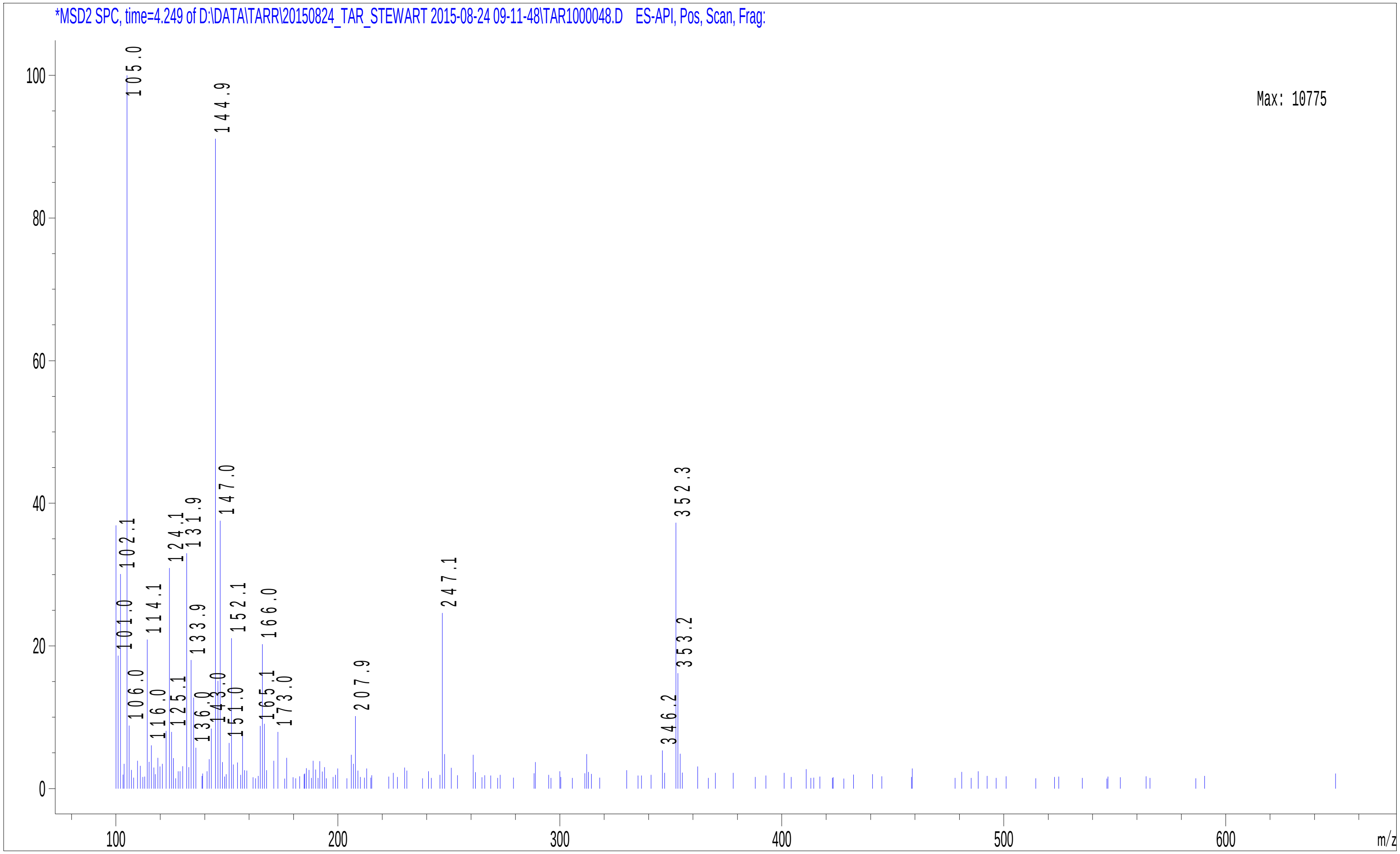

MSD2 TIC, MS File (D:\DATA\TARR\20150824_TAR_STEWART 2015-08-24 09-11-48\TAR1000048.D) ES-API, Pos, Scan, Frag: 70
Norm.
200000
180000
160000
140000
120000
100000
80000
3.088
Area: 927441
3.617
Area: 646254
3.926
Area: 966846
4.245
Area: 58387.2
2.5
3
3.5
4
4.5
min

*MSD2 SPC, time=3.106 of D:\DATA\TARR\20150824_TAR_STEWART 2015-08-24 09-11-48\TAR1000048.D   ES-API, Pos, Scan, Frag:




*MSD2 SPC, time=3.628 of D:\DATA\TARR\20150824_TAR_STEWART 2015-08-24 09-11-48\TAR1000048.D ES-API, Pos, Scan, Frag:
Max: 13153
105.0
102.1
101.1
106.1
116.0
124.0
125.0
132.0
134.0
143.1
145.0
147.0
151.1
157.0
158.0
166.0
172.9
189.0
207.9
247.0
353.2
587.0
608.5
100
80
60
40
20
0
100
200
300
400
500
600
700
m/z

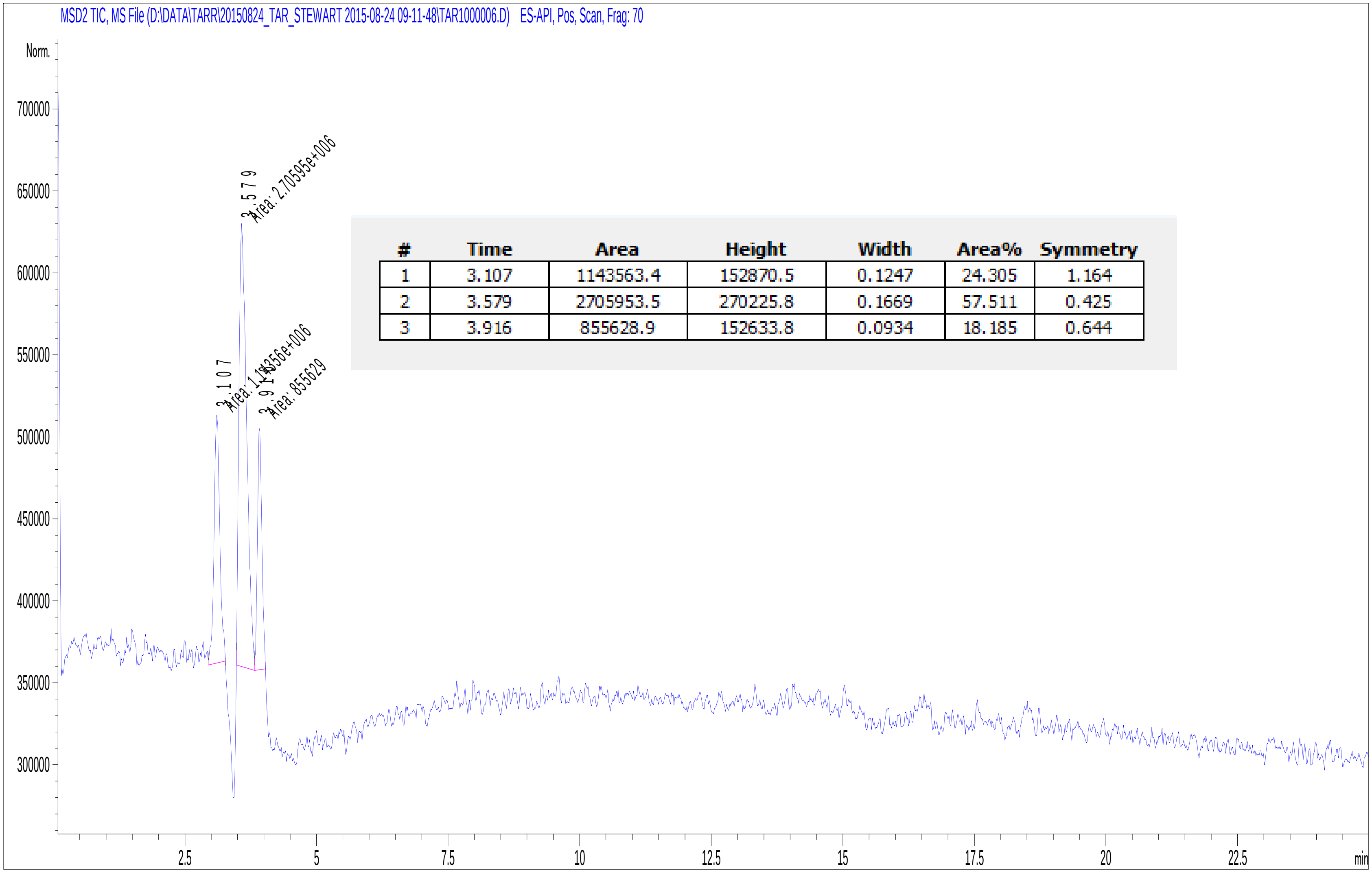

*MSD2 SPC, time=3.938 of D:\DATA\TARR\20150824_TAR_STEWART 2015-08-24 09-11-48\TAR1000048.D ES-API, Pos, Scan, Frag:
Max: 45536
114.1
105.1
102.0
115.1
124.1
131.9
144.9
146.9
155.0
177.1
227.1
249.1
352.3
0
20
40
60
80
100
100
200
300
400
500
600
700
m/z


*MSD2 SPC, time=4.249 of D:\DATA\TARR\20150824_TAR_STEWART 2015-08-24 09-11-48\TAR1000048.D ES-API, Pos, Scan, Frag:
Max: 10775
105.0
144.9
147.0
352.3
102.1
124.1
131.9
101.0
114.1
133.9
152.1
166.0
247.1
353.2
207.9
106.0
116.0
125.1
136.0
143.0
151.0
165.1
173.0
346.2
0
20
40
60
80
100
100
200
300
400
500
600
m/z

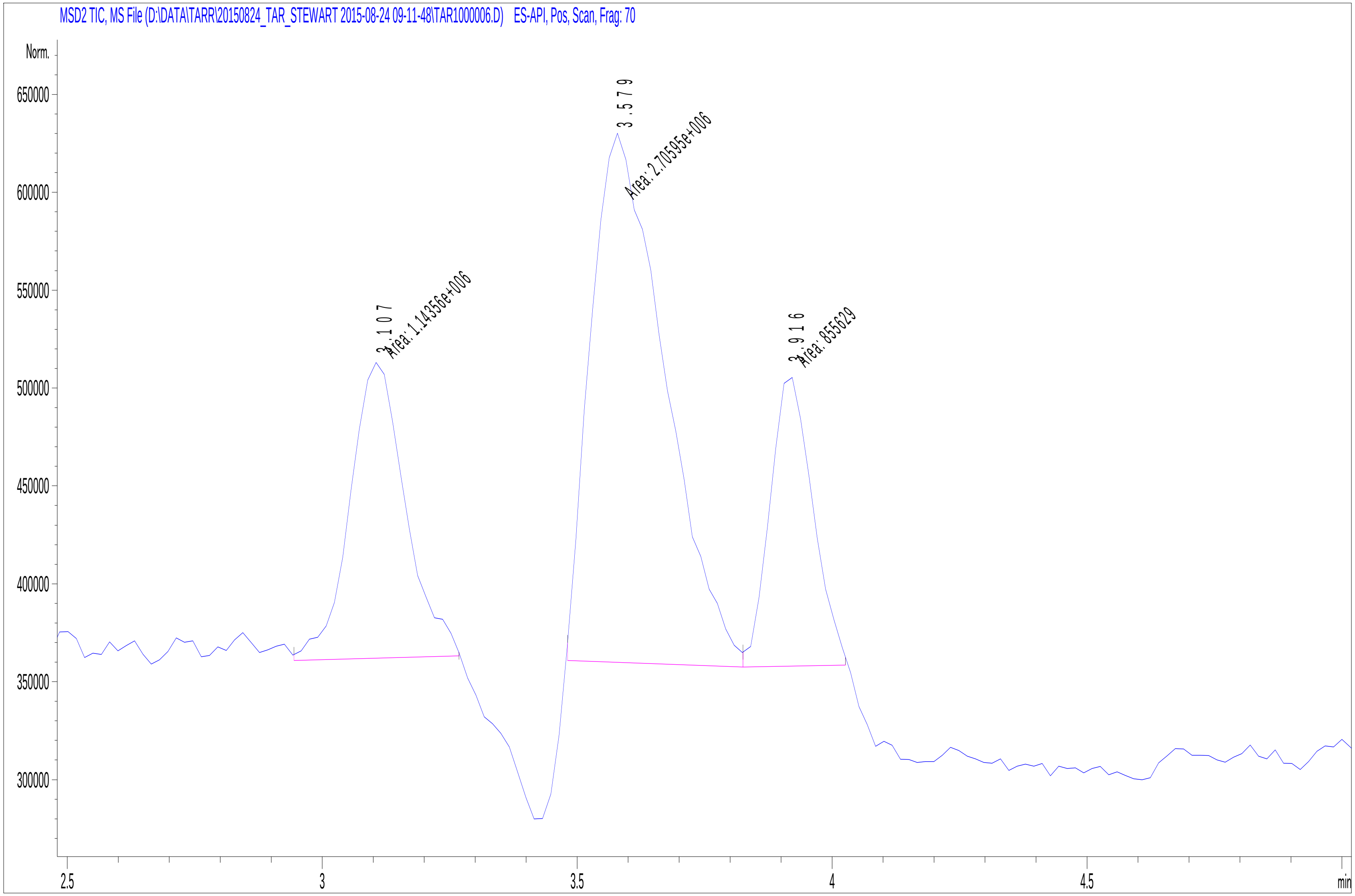
9-Apr-15

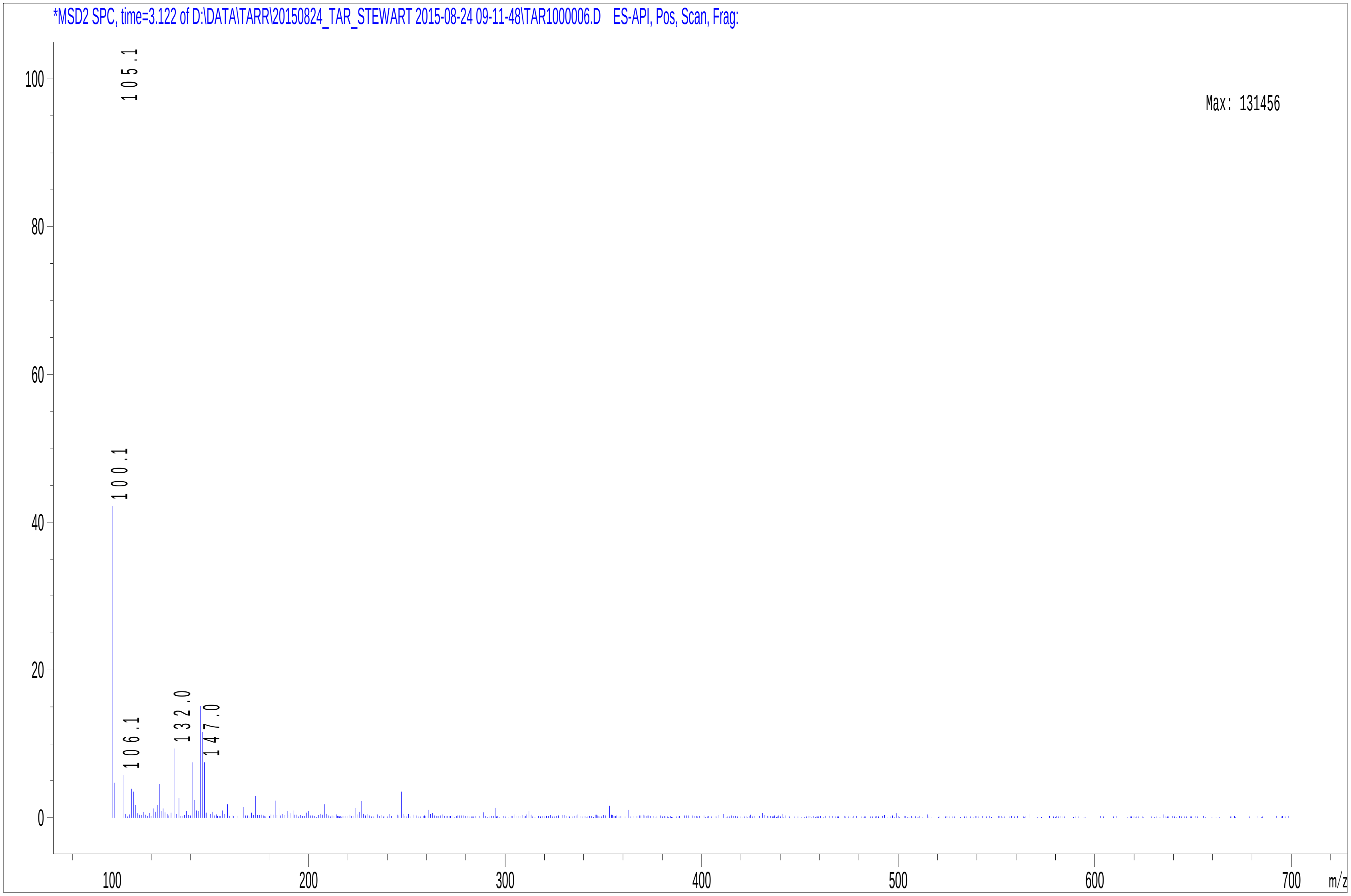
10 DC

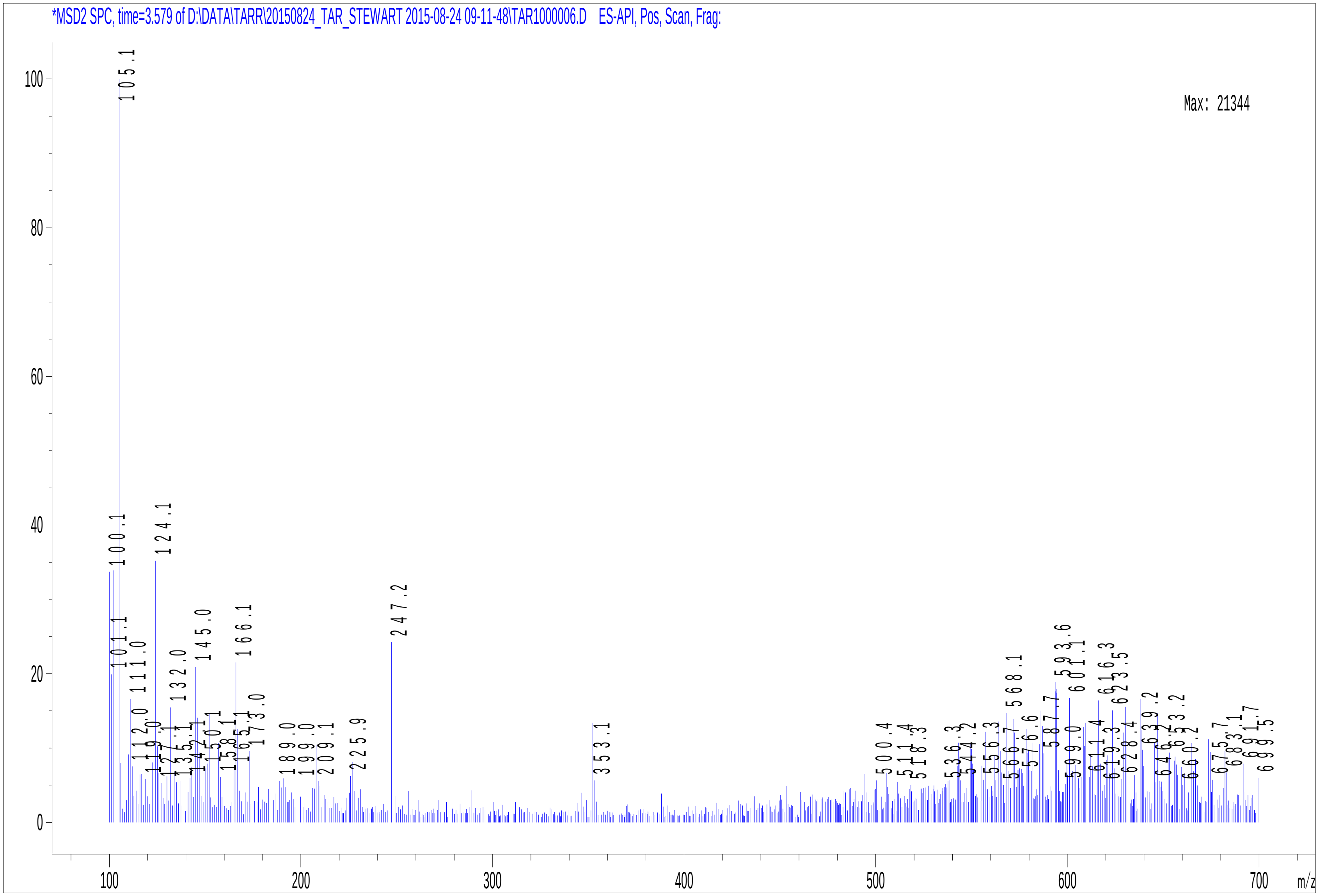
P2-A-06

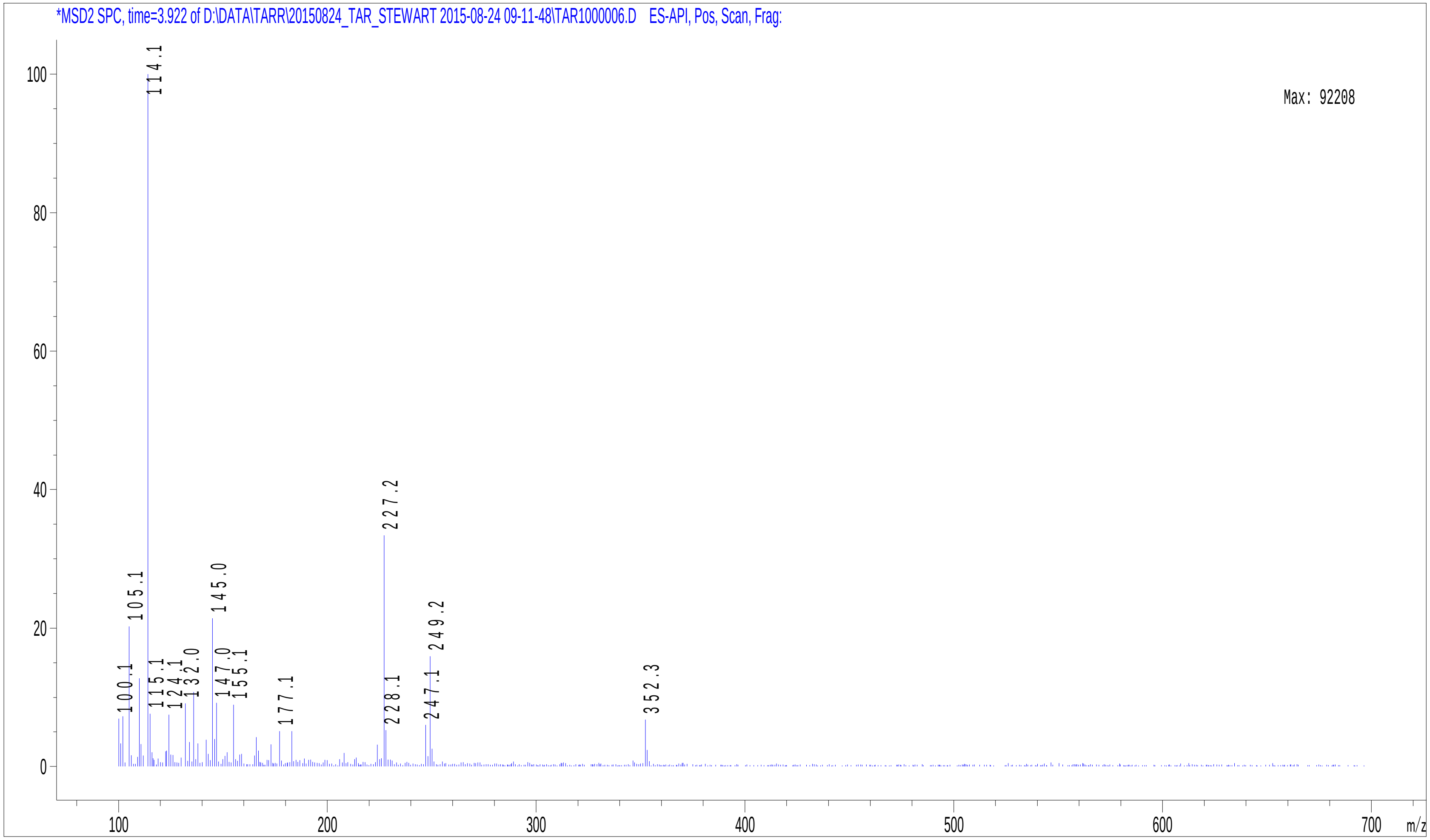


#	Time	Area	Height	Width	Area%	Symmetry
1	3.107	1143563.4	152870.5	0.1247	24.305	1.164
2	3.579	2705953.5	270225.8	0.1669	57.511	0.425
3	3.916	855628.9	152633.8	0.0934	18.185	0.644


MSD2 TIC, MS File (D:\DATA\TARR\20150824_TAR_STEWART 2015-08-24 09-11-48\TAR1000006.D) ES-API, Pos, Scan, Frag: 70
Norm.
650000
600000
550000
500000
450000
400000
350000
300000
3.107
Area: 1.14356e+006
3.579
Area: 2.70595e+006
3.916
Area: 855629
2.5
3
3.5
4
4.5
min


*MSD2 SPC, time=3.122 of D:\DATA\TARR\20150824_TAR_STEWART 2015-08-24 09-11-48\TAR1000006.D ES-API, Pos, Scan, Frag:
Max: 131456
105.1
100.1
106.1
132.0
147.0
0
20
40
60
80
100
100
200
300
400
500
600
700
m/z

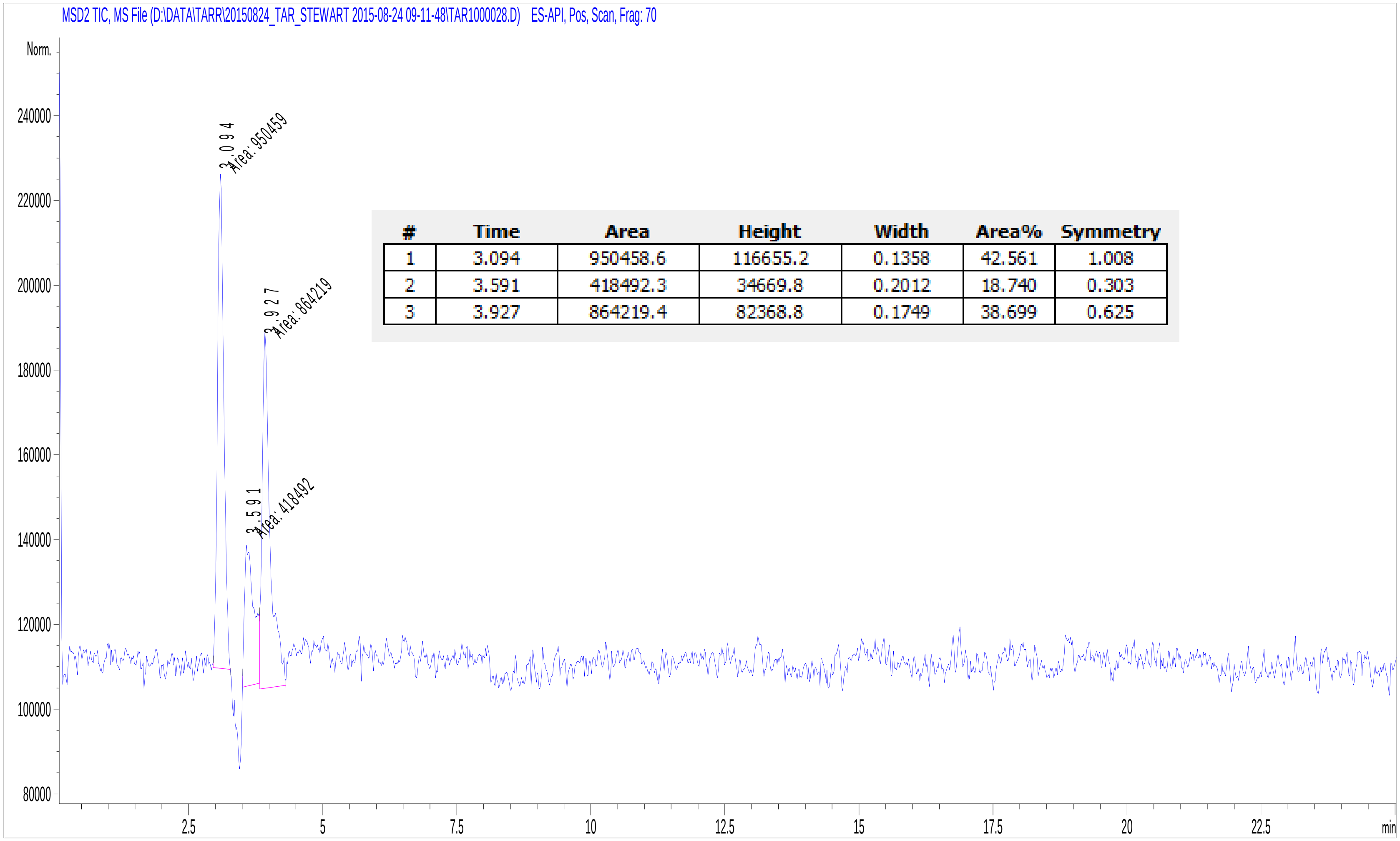

*MSD2 SPC, time=3.579 of D:\DATA\TARR\20150824_TAR_STEWART 2015-08-24 09-11-48\TAR1000006.D ES-API, Pos, Scan, Frag:
Max: 21344
100
80
60
40
20
0
100
200
300
400
500
600
700
m/z
105.1
100.1
124.1
101.1
111.0
132.0
145.0
166.1
112.0
119.0
127.1
135.1
139.1
142.1
150.1
158.1
165.1
173.0
189.0
199.0
209.1
225.9
247.2
353.1
500.4
511.4
518.3
536.3
544.2
556.3
566.7
568.1
576.6
587.7
593.6
599.0
601.1
611.4
616.3
619.3
623.5
628.4
639.2
646.2
653.2
660.2
675.7
683.1
691.7
699.5


*MSD2 SPC, time=3.922 of D:\DATA\TARR\20150824_TAR_STEWART 2015-08-24 09-11-48\TAR1000006.D   ES-API, Pos, Scan, Frag:
Max: 92208
114.1
227.2
105.1
145.0
249.2
100.1
115.1
124.1
132.0
147.0
155.1
177.1
228.1
247.1
352.3
0
20
40
60
80
100
100
200
300
400
500
600
700
m/z

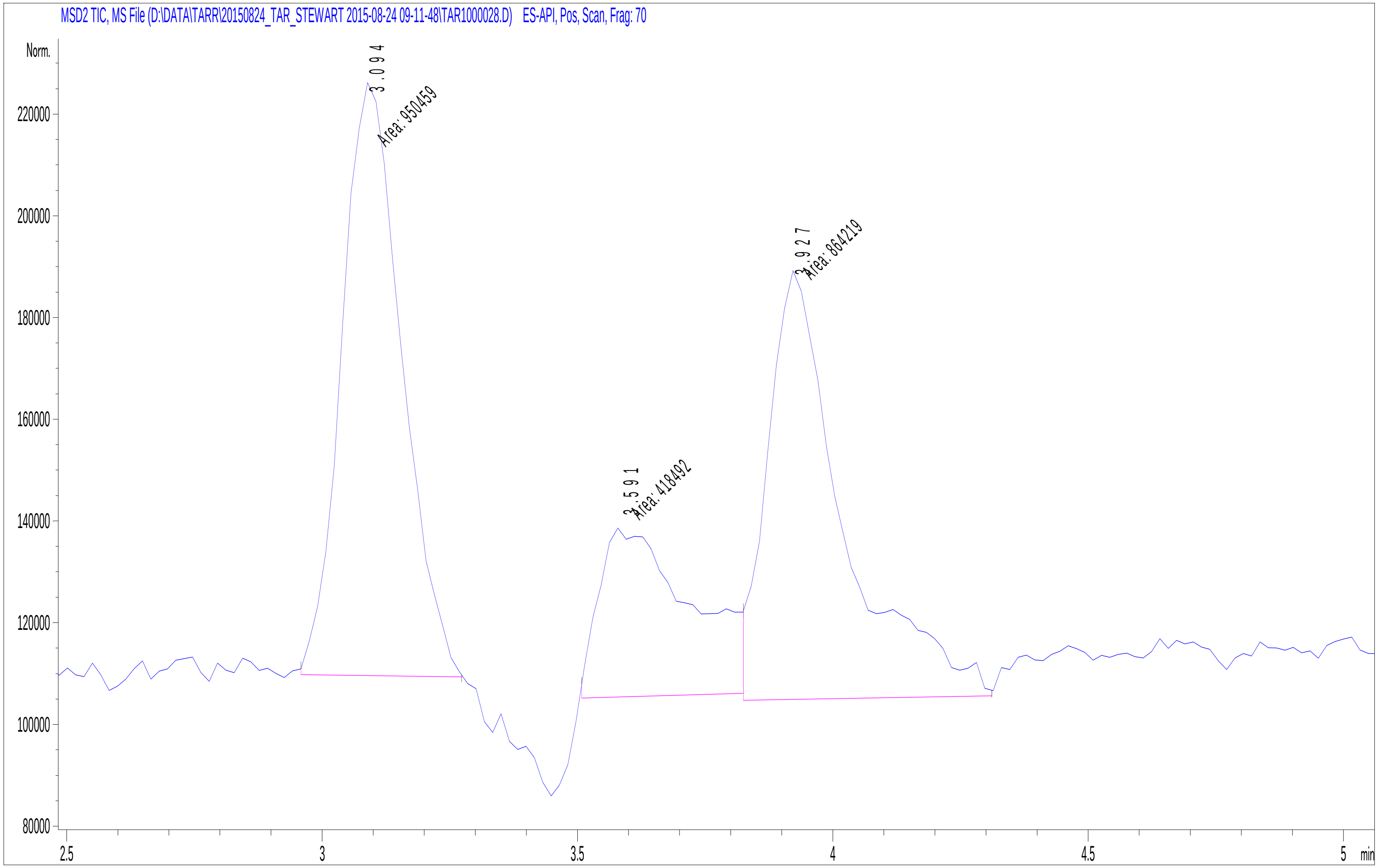
6-Aug-15

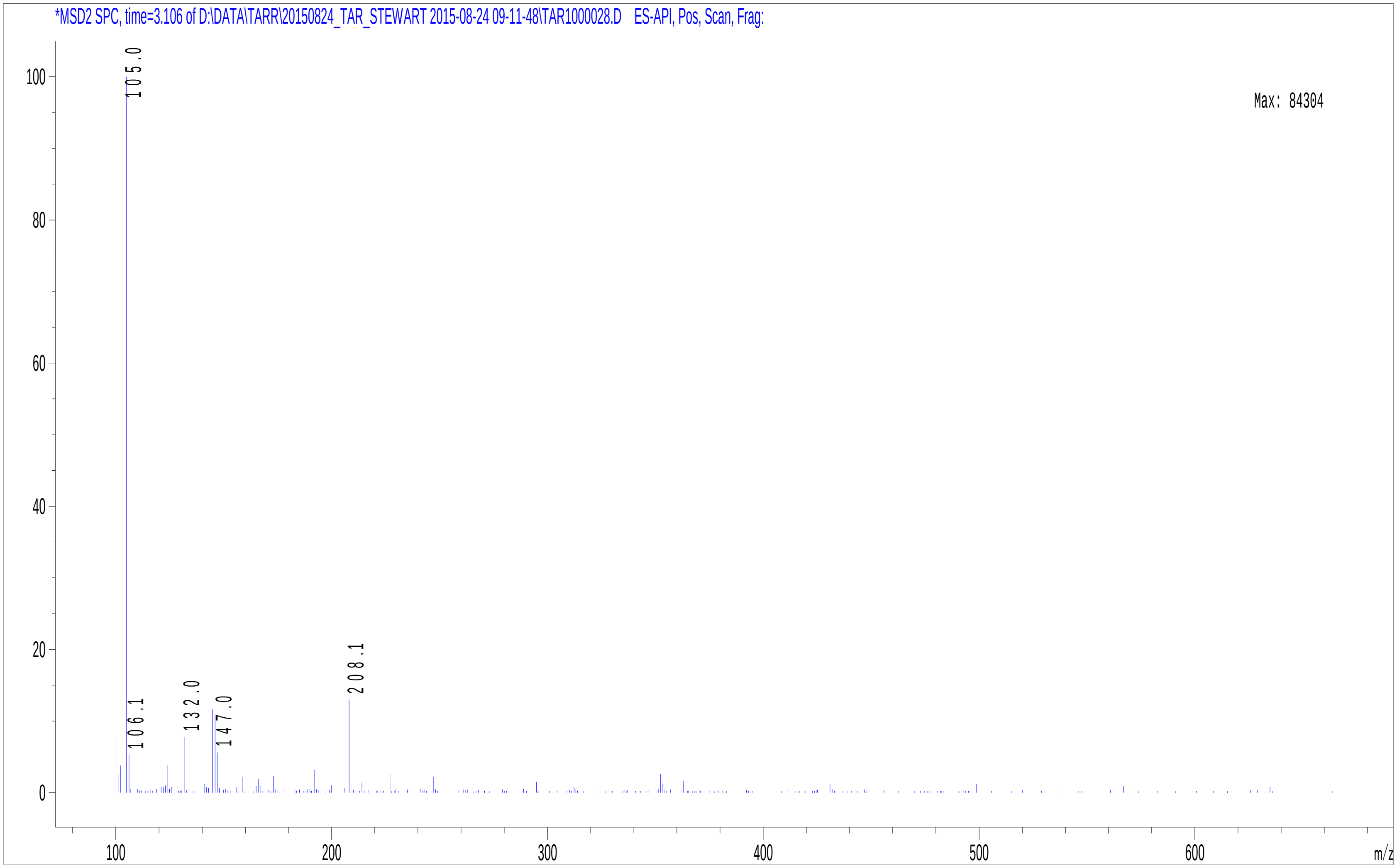
20 DC

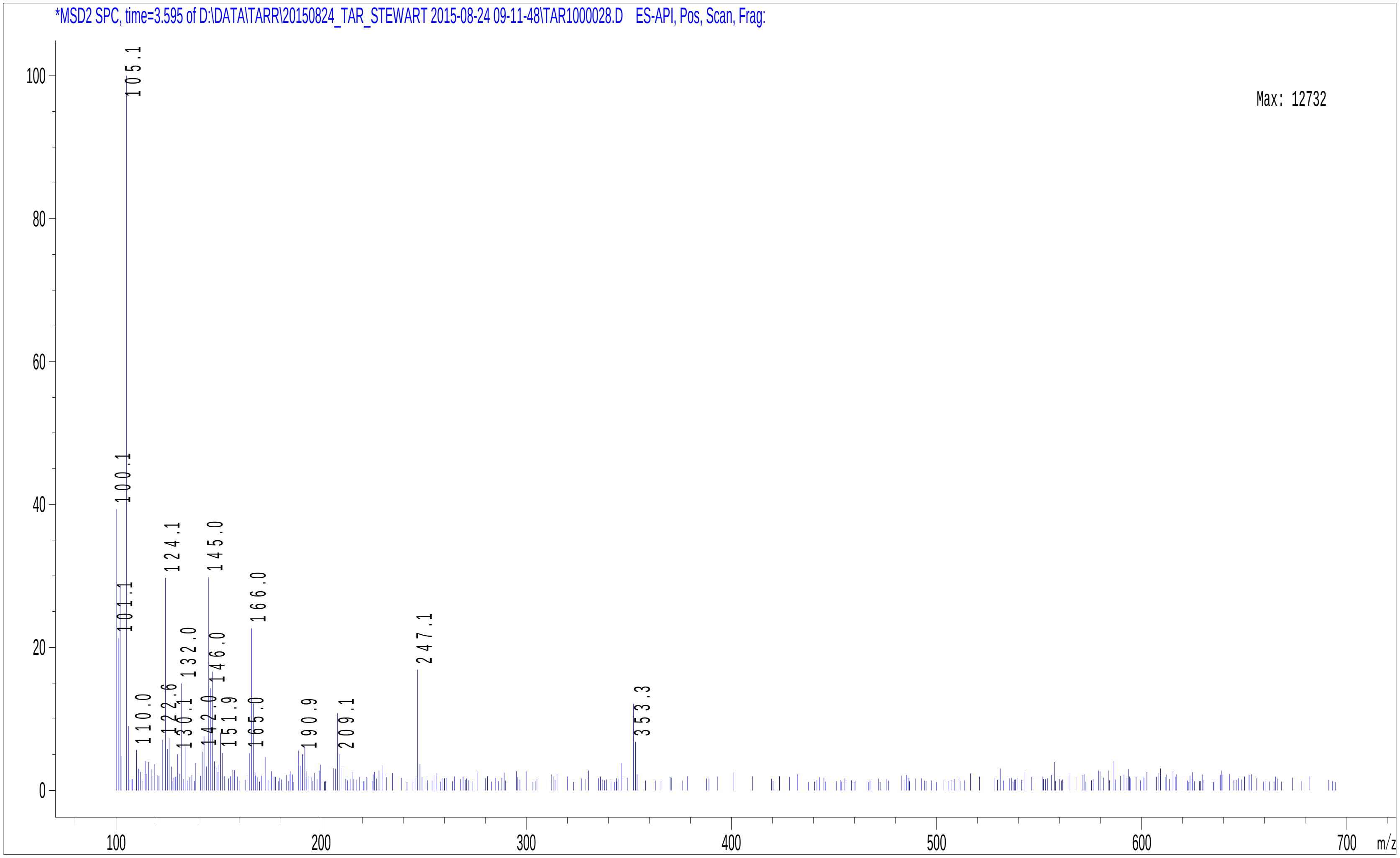
P2-D-09

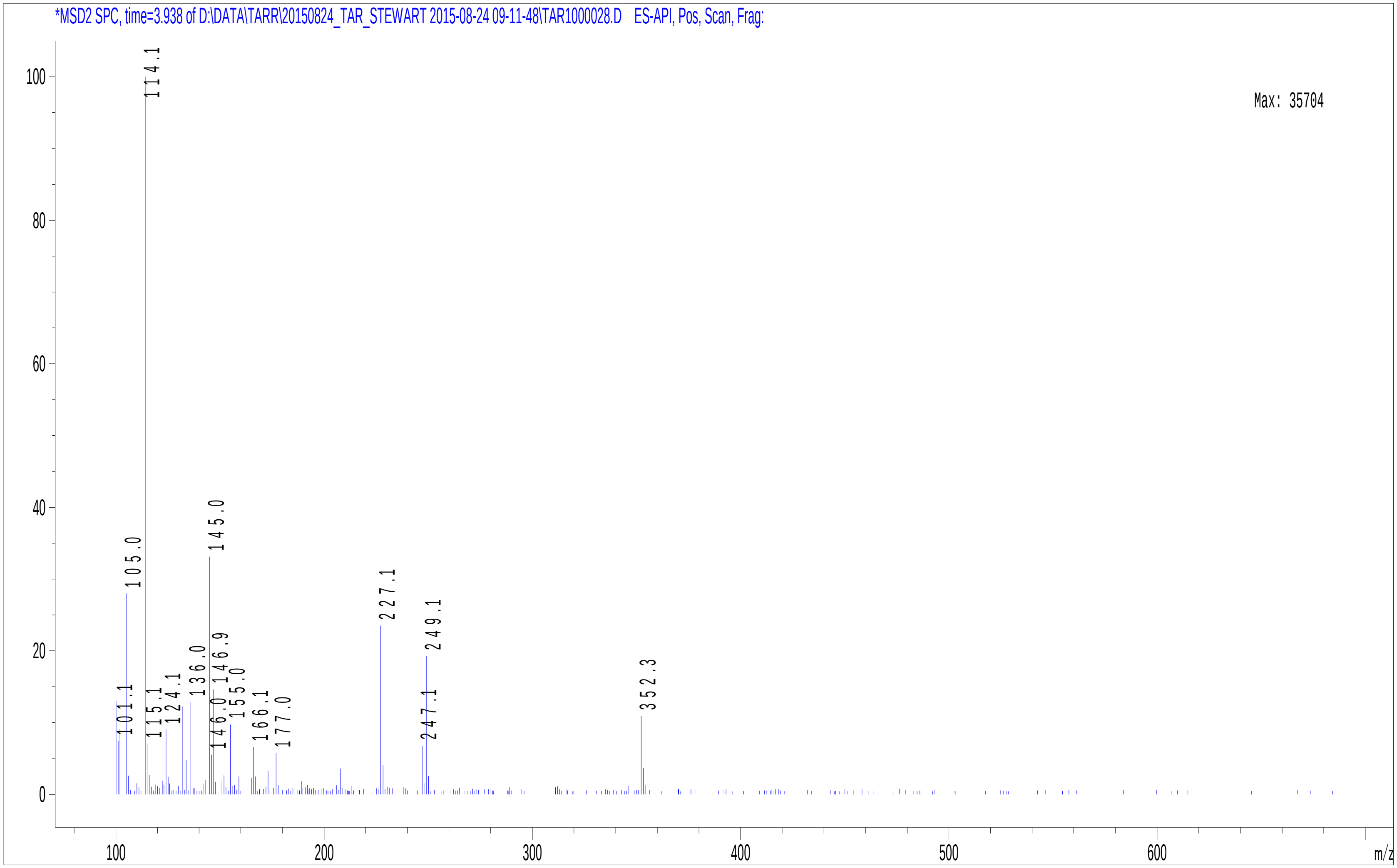


#	Time	Area	Height	Width	Area%	Symmetry
1	3.094	950458.6	116655.2	0.1358	42.561	1.008
2	3.591	418492.3	34669.8	0.2012	18.740	0.303
3	3.927	864219.4	82368.8	0.1749	38.699	0.625


MSD2 TIC, MS File (D:\DATA\TARR\20150824_TAR_STEWART 2015-08-24 09-11-48\TAR1000028.D) ES-API, Pos, Scan, Frag: 70
Norm.
220000
200000
180000
160000
140000
120000
100000
80000
3.094
Area: 950459
3.591
Area: 418492
3.927
Area: 864219
2.5
3
3.5
4
4.5
5
min


*MSD2 SPC, time=3.106 of D:\DATA\TARR\20150824_TAR_STEWART 2015-08-24 09-11-48\TAR1000028.D ES-API, Pos, Scan, Frag:
Max: 84304
105.0
106.1
132.0
147.0
208.1
100
80
60
40
20
0
100
200
300
400
500
600
m/z

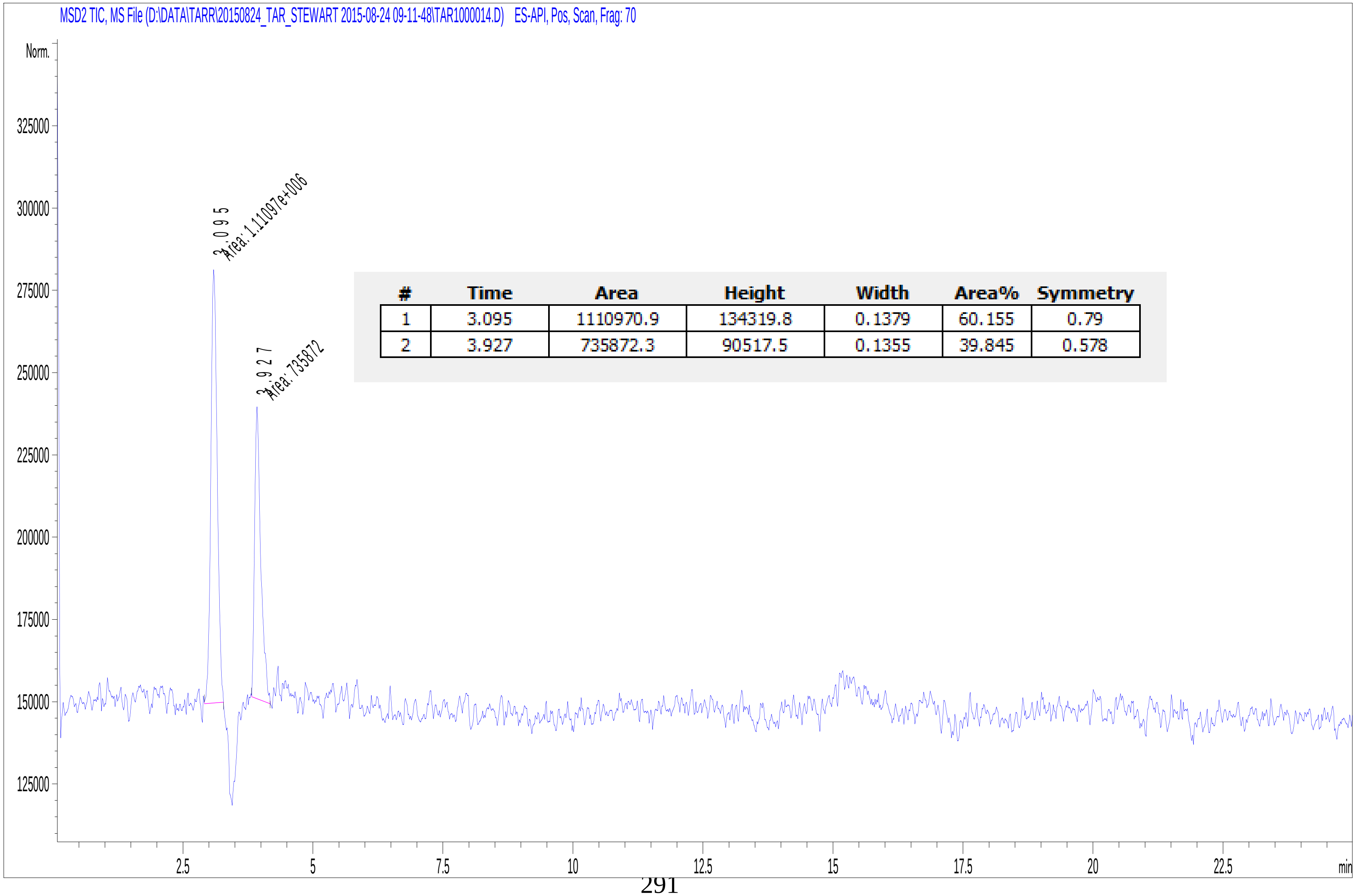

*MSD2 SPC, time=3.595 of D:\DATA\TARR\20150824_TAR_STEWART 2015-08-24 09-11-48\TAR1000028.D ES-API, Pos, Scan, Frag:
Max: 12732
105.1
100.1
101.1
110.0
122.6
124.1
130.1
132.0
142.0
145.0
146.0
151.9
165.0
166.0
190.9
209.1
247.1
353.3
100
80
60
40
20
0
100
200
300
400
500
600
700
m/z


*MSD2 SPC, time=3.938 of D:\DATA\TARR\20150824_TAR_STEWART 2015-08-24 09-11-48\TAR1000028.D   ES-API, Pos, Scan, Frag:
Max: 35704
114.1
105.0
145.0
227.1
249.1
352.3
101.1
115.1
124.1
136.0
146.9
146.0
155.0
166.1
177.0
247.1
0
20
40
60
80
100
100
200
300
400
500
600
m/z

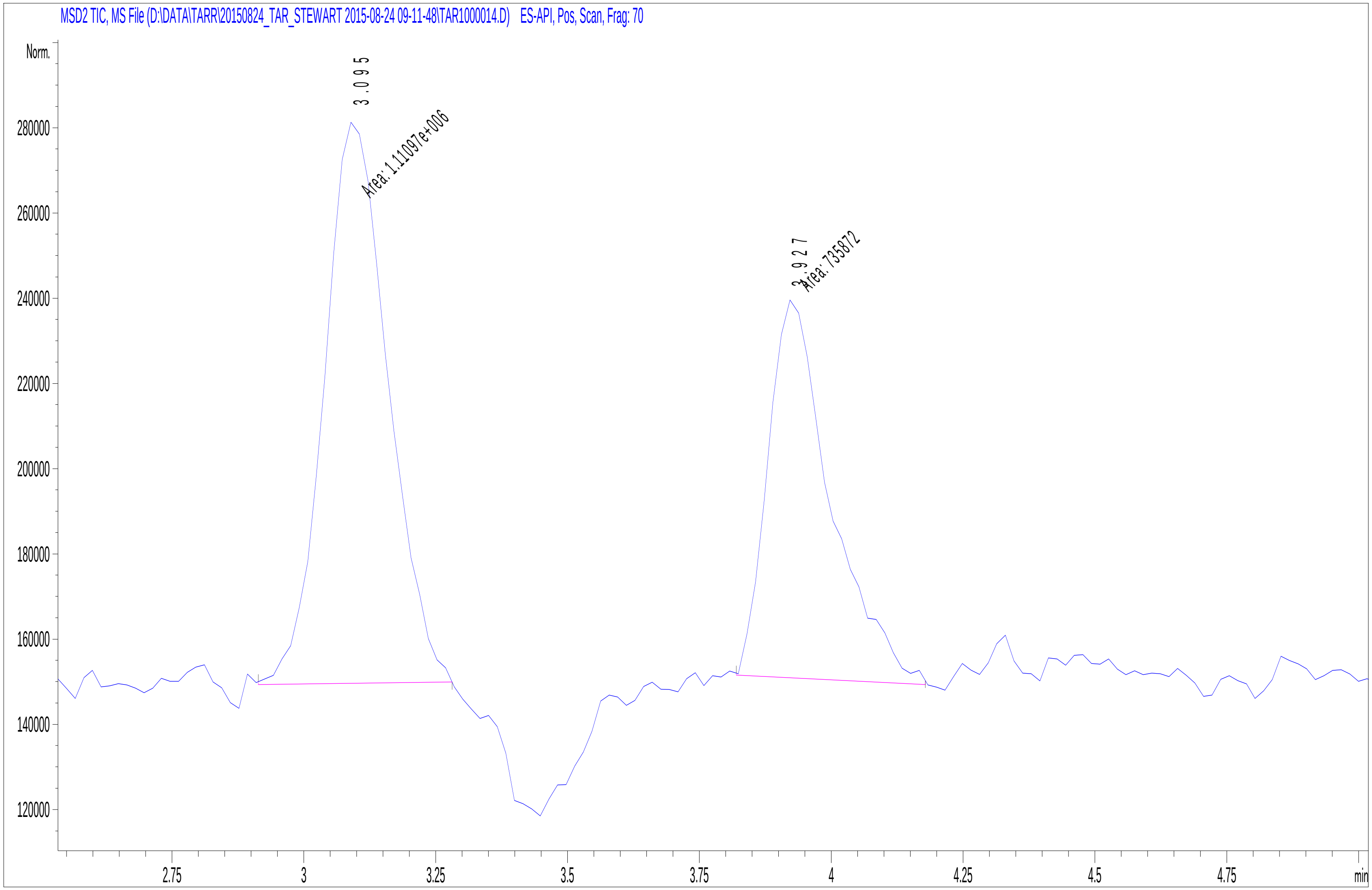
3-Jun-15

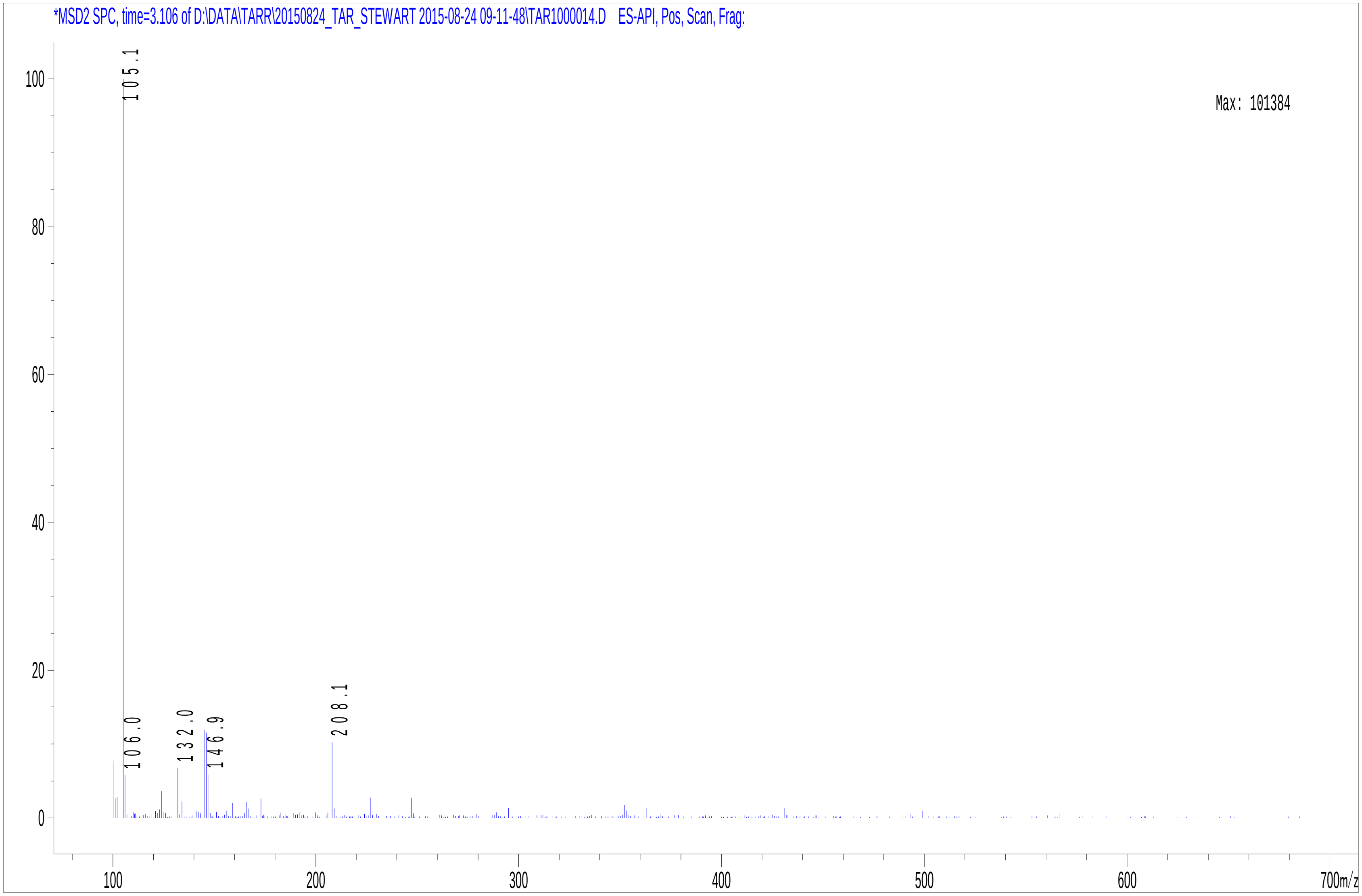
30 DC

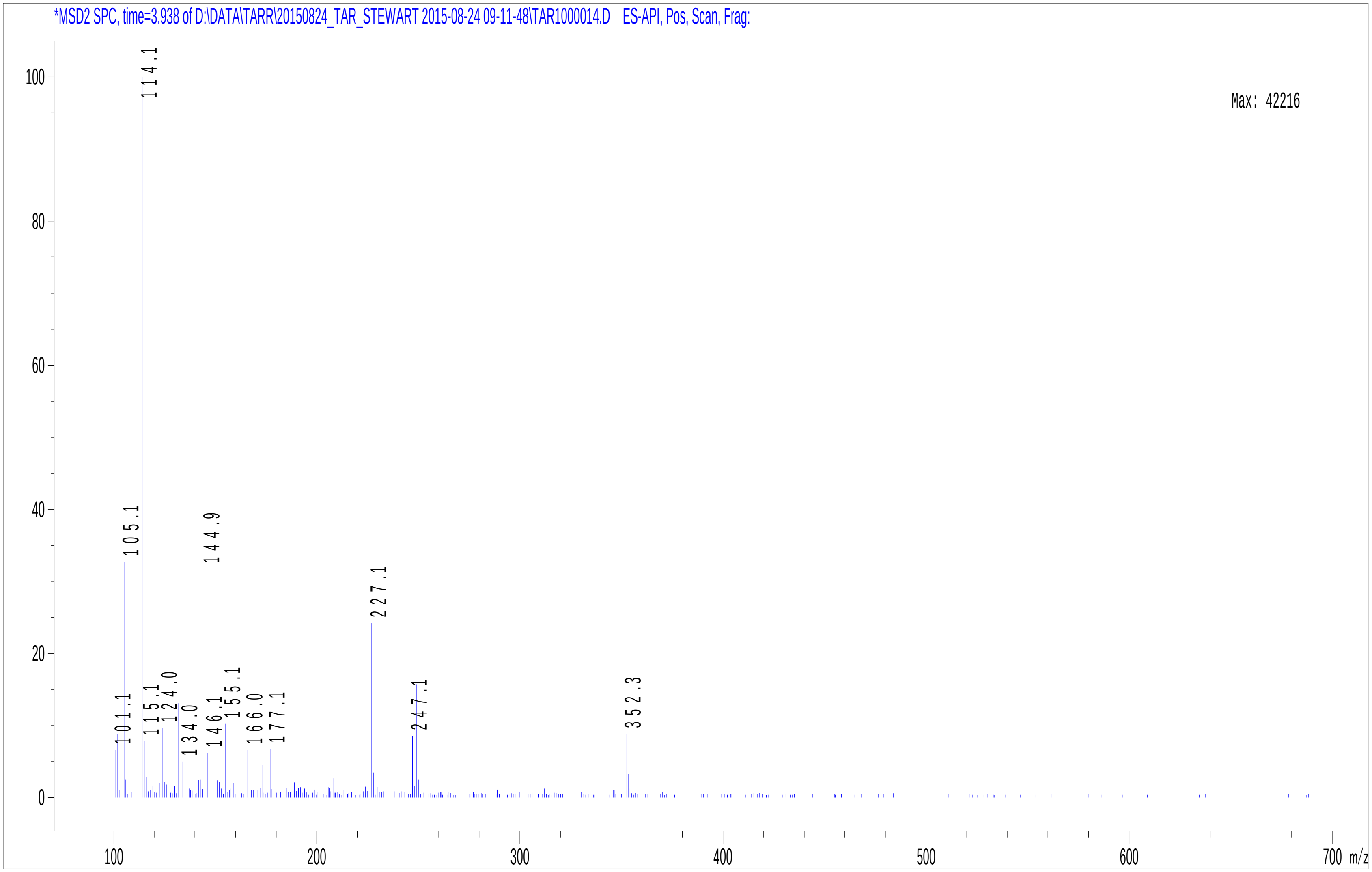
P2-B-05



#	Time	Area	Height	Width	Area%	Symmetry
1	3.095	1110970.9	134319.8	0.1379	60.155	0.79
2	3.927	735872.3	90517.5	0.1355	39.845	0.578


MSD2 TIC, MS File (D:\DATA\TARR\20150824_TAR_STEWART 2015-08-24 09-11-48\TAR1000014.D) ES-API, Pos, Scan, Frag: 70
Norm.
280000
260000
240000
220000
200000
180000
160000
140000
120000
3.095
Area: 1.11097e+006
3.927
Area: 735872
2.75
3
3.25
3.5
3.75
4
4.25
4.5
4.75
min

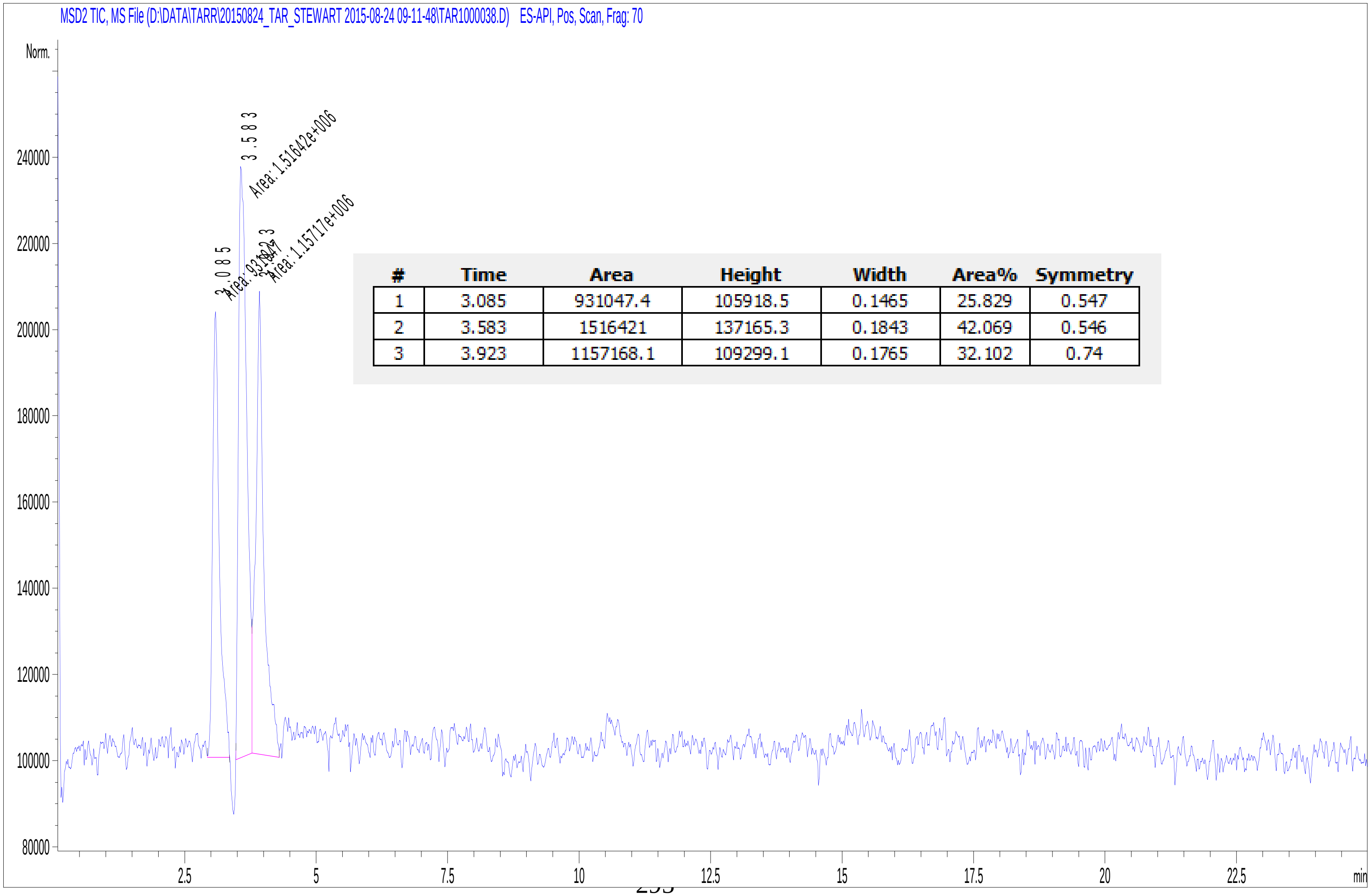

*MSD2 SPC, time=3.106 of D:\DATA\TARR\20150824_TAR_STEWART 2015-08-24 09-11-48\TAR1000014.D ES-API, Pos, Scan, Frag:
Max: 101384
105.1
106.0
132.0
146.9
208.1
100
80
60
40
20
0
100
200
300
400
500
600
700m/z


*MSD2 SPC, time=3.938 of D:\DATA\TARR\20150824_TAR_STEWART 2015-08-24 09-11-48\TAR1000014.D ES-API, Pos, Scan, Frag:
Max: 42216
114.1
105.1
144.9
227.1
101.1
115.1
124.0
134.0
146.1
155.1
166.0
177.1
247.1
352.3
0
20
40
60
80
100
100
200
300
400
500
600
700
m/z

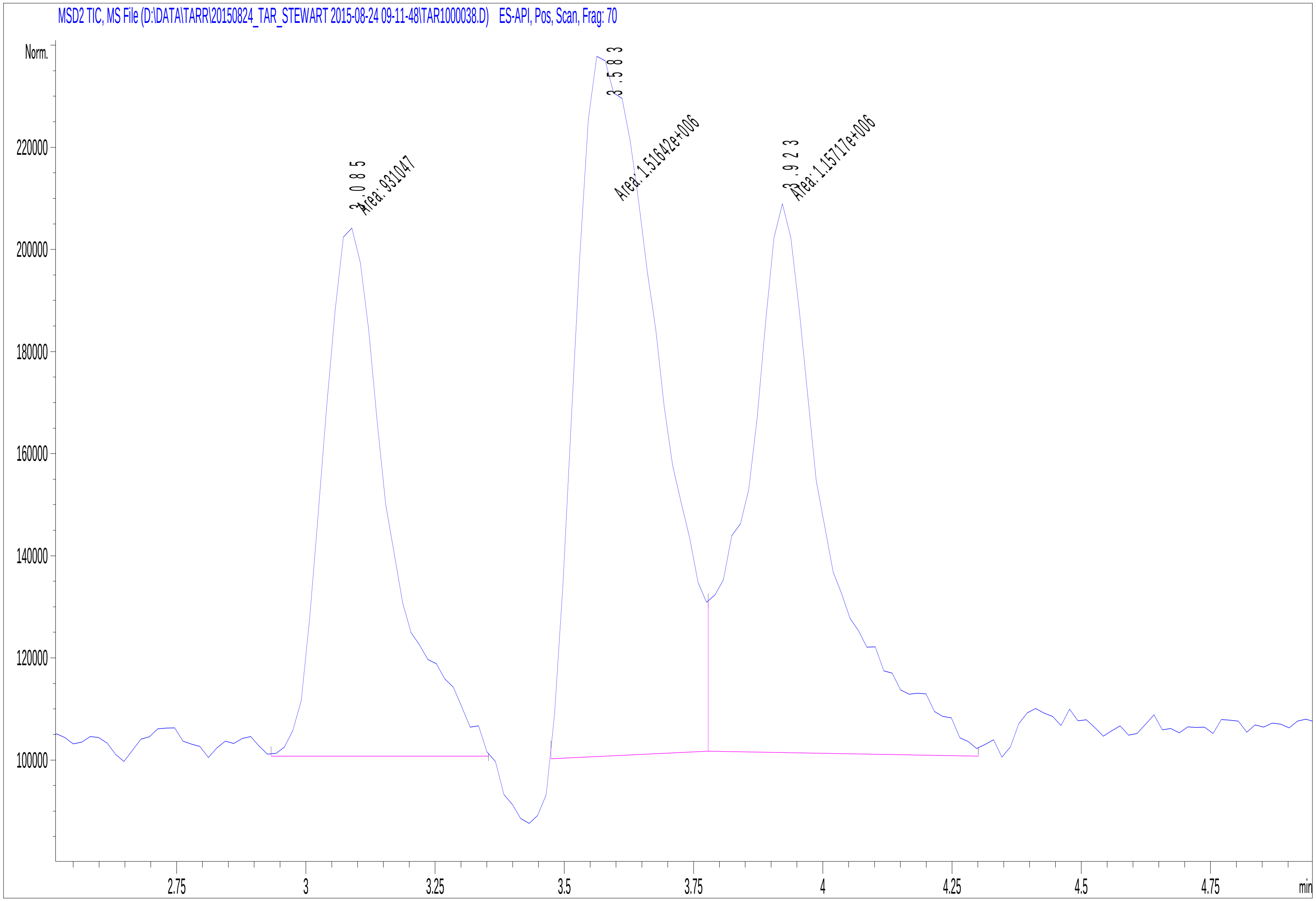
11-Aug-15

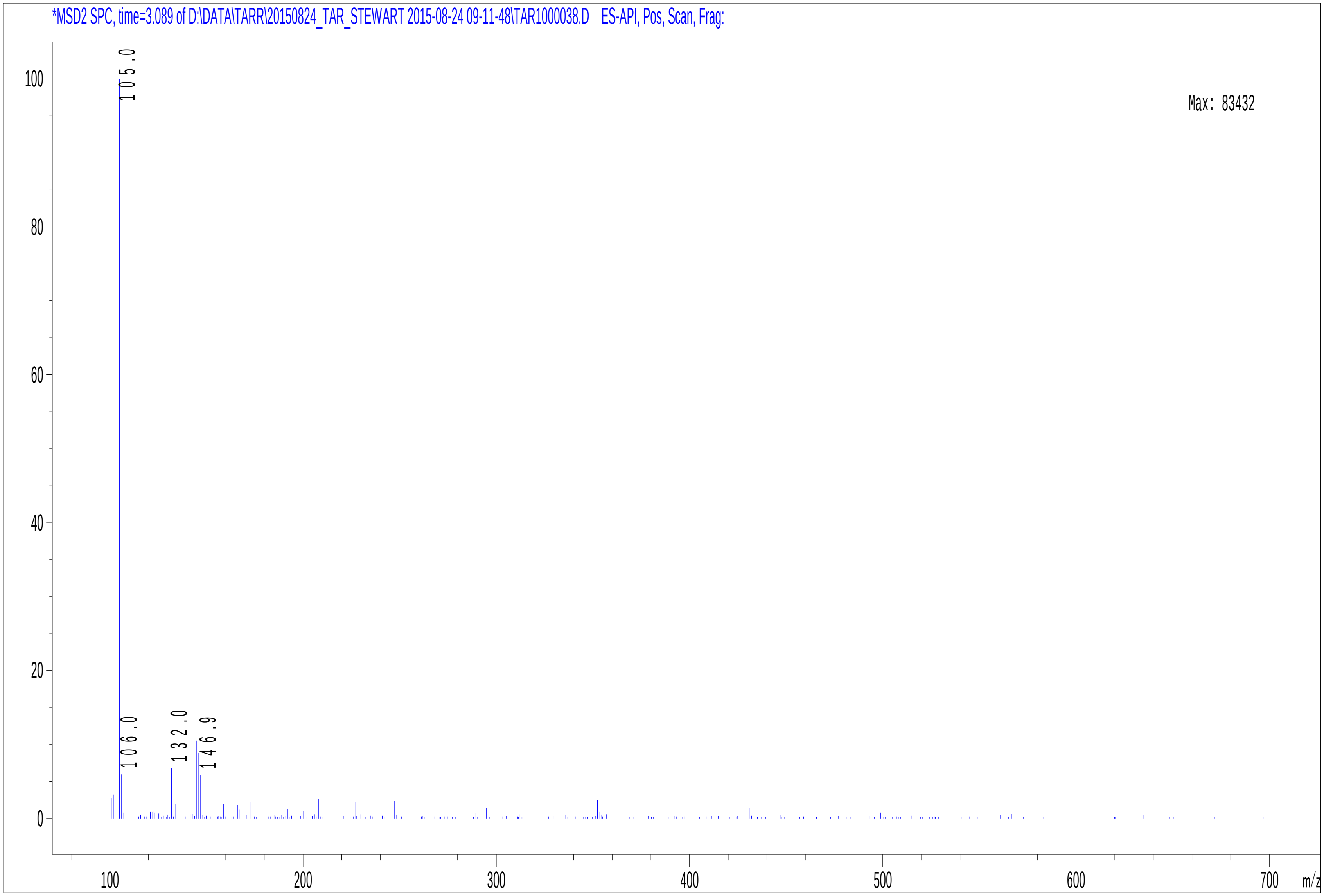
50 DC

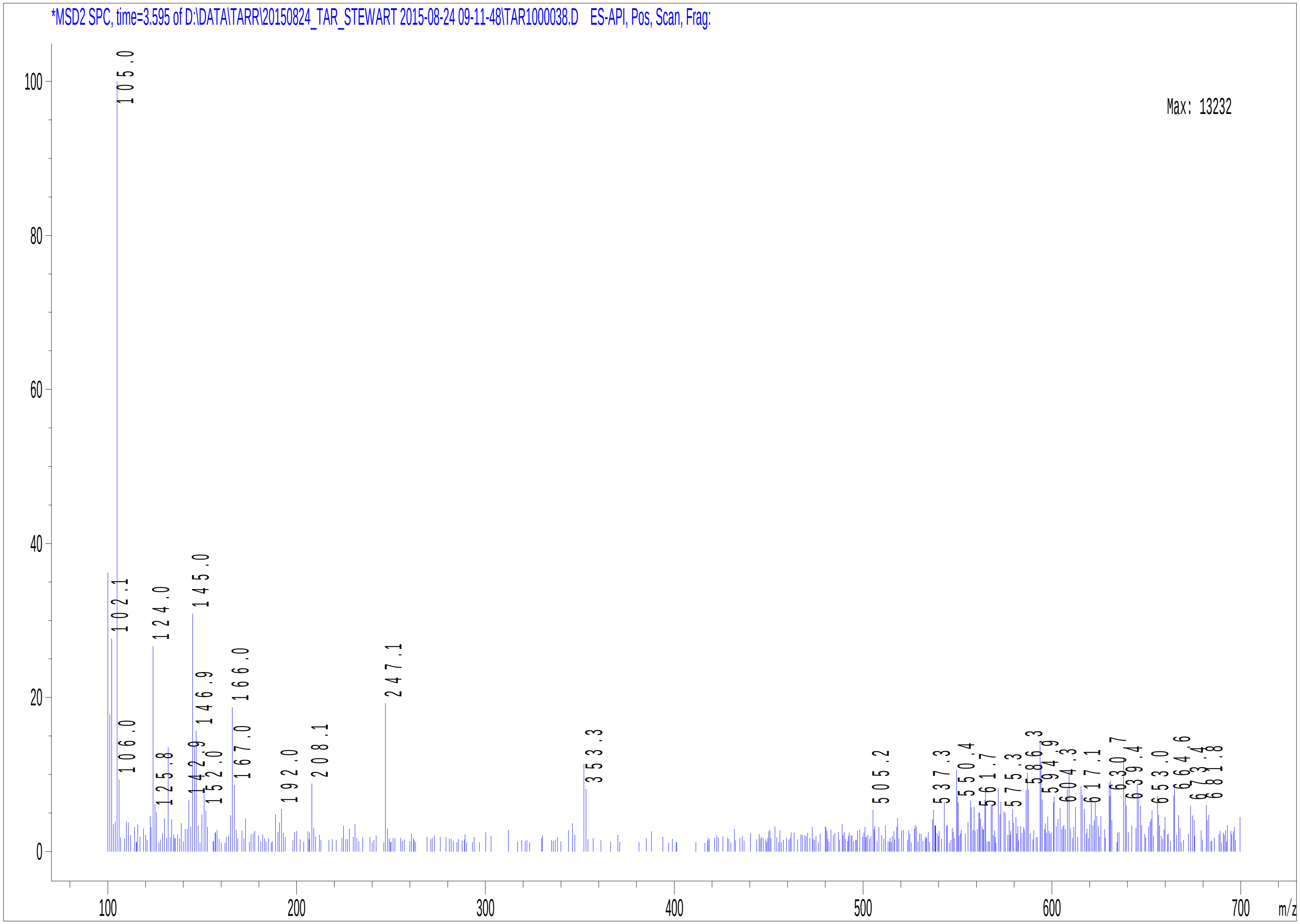
P2-E-02

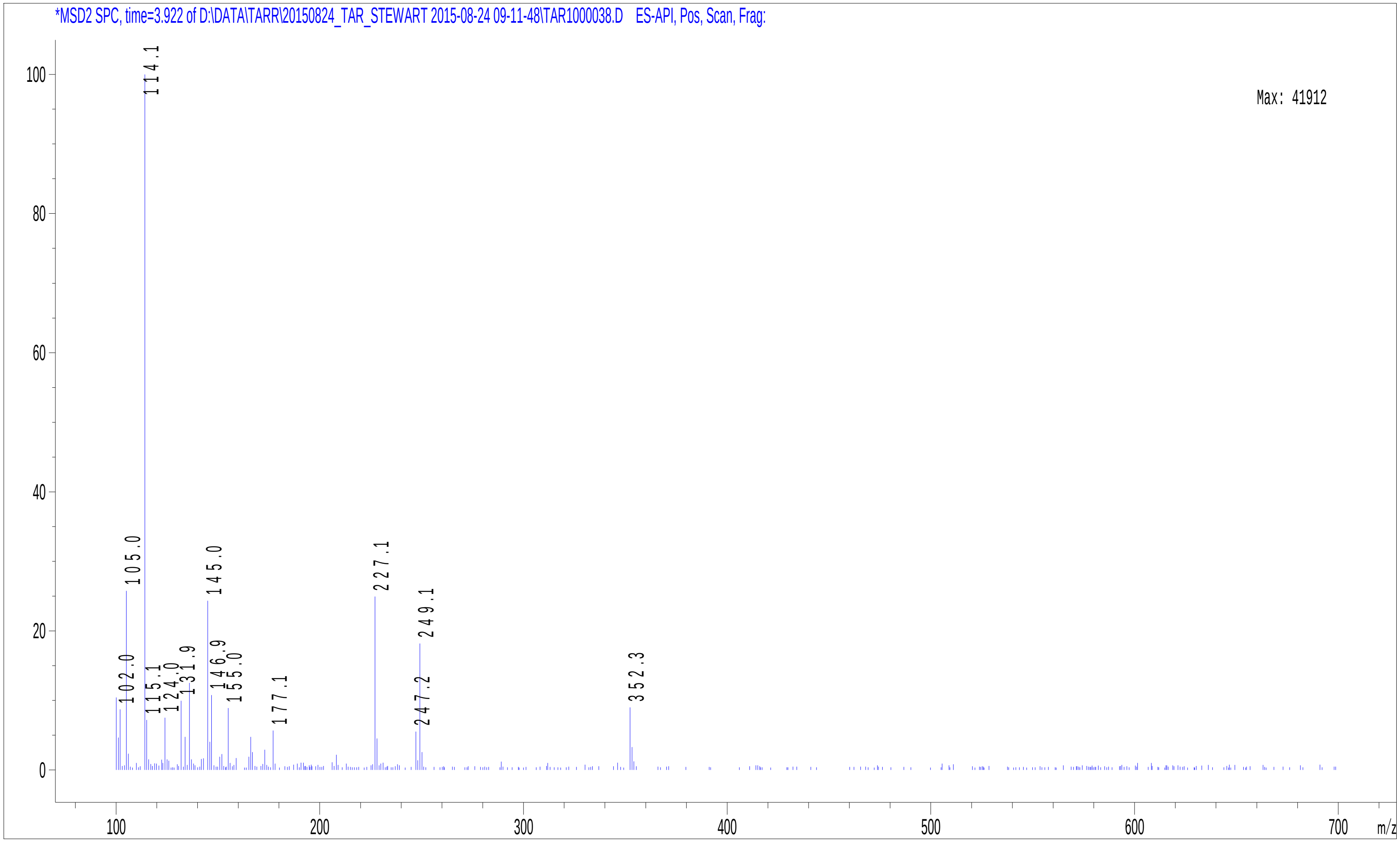


#	Time	Area	Height	Width	Area%	Symmetry
1	3.085	931047.4	105918.5	0.1465	25.829	0.547
2	3.583	1516421	137165.3	0.1843	42.069	0.546
3	3.923	1157168.1	109299.1	0.1765	32.102	0.74


MSD2 TIC, MS File (D:\DATA\TARR\20150824_TAR_STEWART 2015-08-24 09-11-48\TAR1000038.D)   ES-API, Pos, Scan, Frag: 70
Norm.
220000
200000
180000
160000
140000
120000
100000
3.085
Area: 931047
3.583
Area: 1.51642e+006
3.923
Area: 1.15717e+006
2.75
3
3.25
3.5
3.75
4
4.25
4.5
4.75
min


*MSD2 SPC, time=3.089 of D:\DATA\TARR\20150824_TAR_STEWART 2015-08-24 09-11-48\TAR1000038.D ES-API, Pos, Scan, Frag:
Max: 83432
105.0
106.0
132.0
146.9
100
80
60
40
20
0
100
200
300
400
500
600
700
m/z

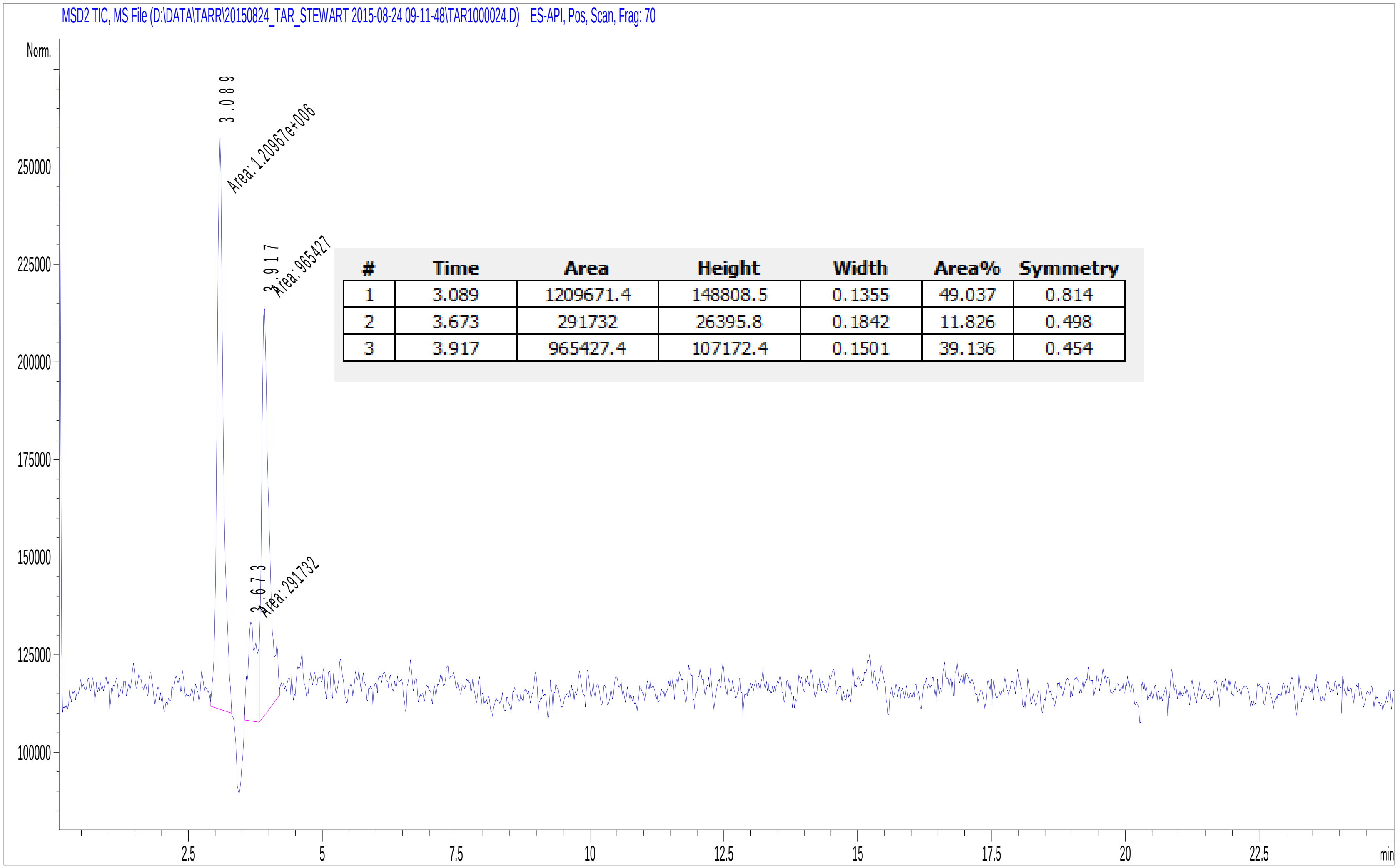

*MSD2 SPC, time=3.595 of D:\DATA\TARR\20150824_TAR_STEWART 2015-08-24 09-11-48\TAR1000038.D ES-API, Pos, Scan, Frag:
Max: 13232
105.0
102.1
106.0
124.0
125.8
142.9
145.0
146.9
152.0
166.0
167.0
192.0
208.1
247.1
353.3
505.2
537.3
550.4
561.7
575.3
586.3
594.9
604.3
617.1
630.7
639.4
653.0
664.6
673.4
681.8
0
20
40
60
80
100
100
200
300
400
500
600
700
m/z


*MSD2 SPC, time=3.922 of D:\DATA\TARR\20150824_TAR_STEWART 2015-08-24 09-11-48\TAR1000038.D ES-API, Pos, Scan, Frag:
Max: 41912
114.1
105.0
102.0
115.1
124.0
131.9
145.0
146.9
155.0
177.1
227.1
249.1
247.2
352.3
0
20
40
60
80
100
100
200
300
400
500
600
700
m/z

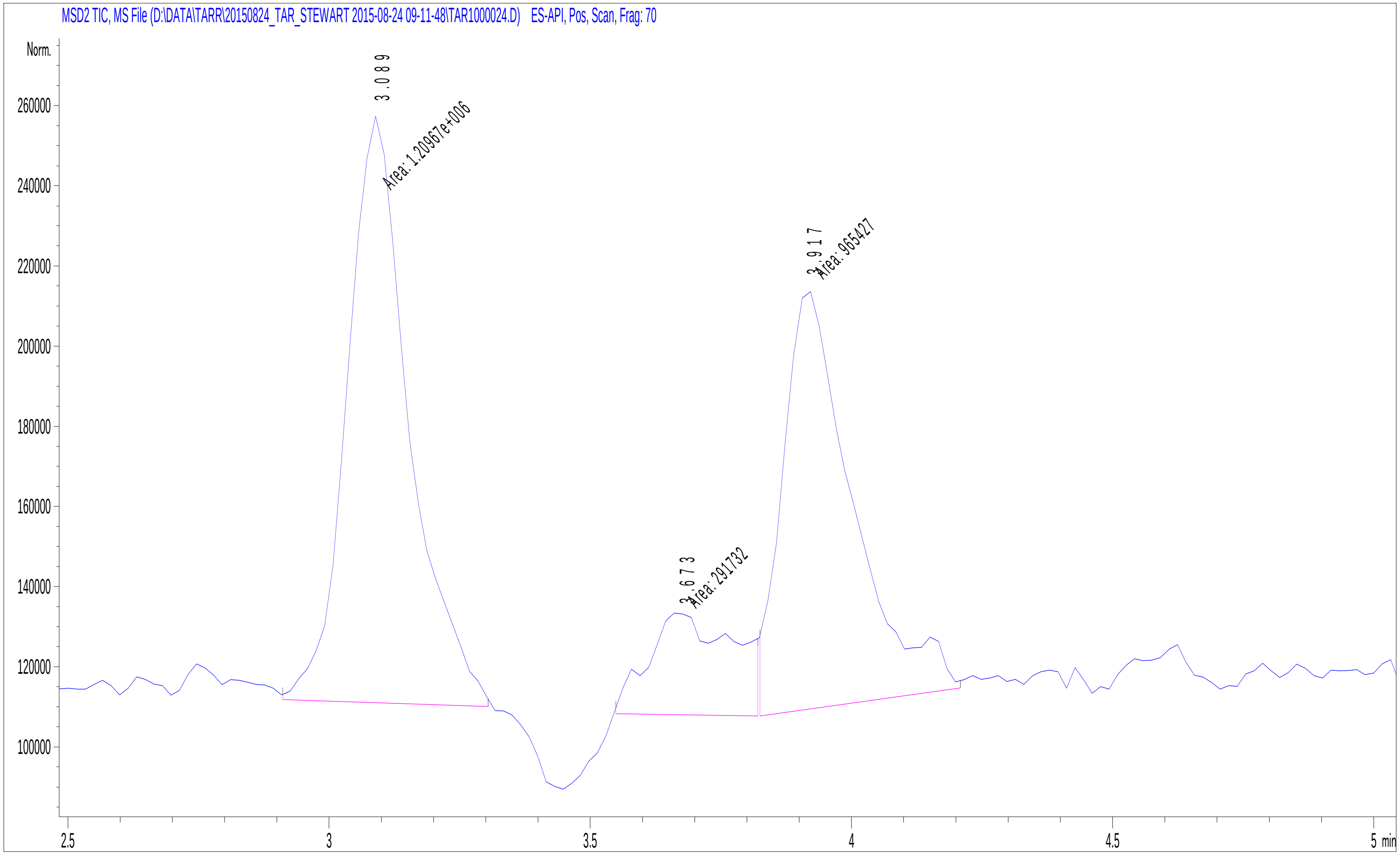
13-Jul-15

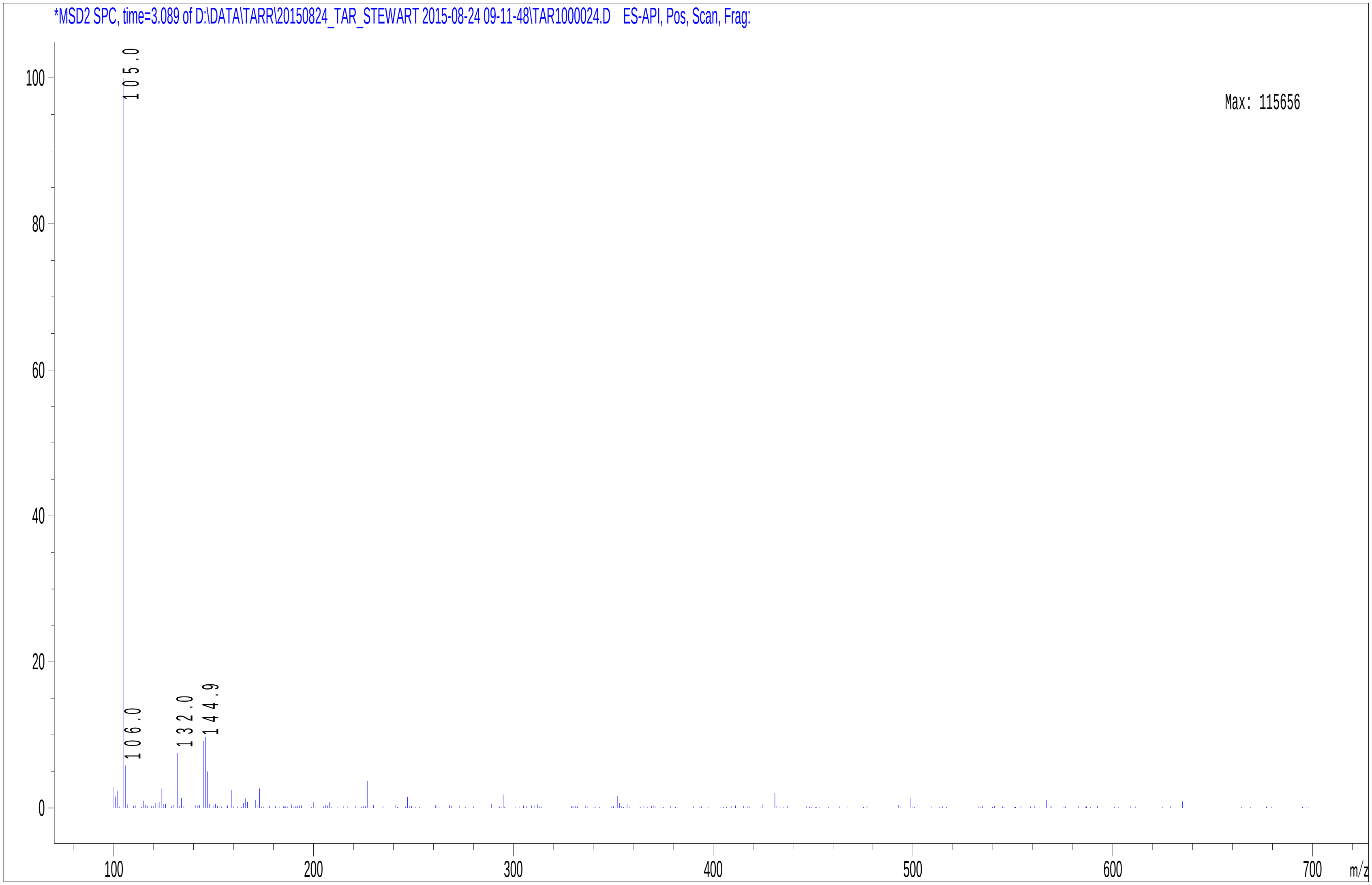
70 DC

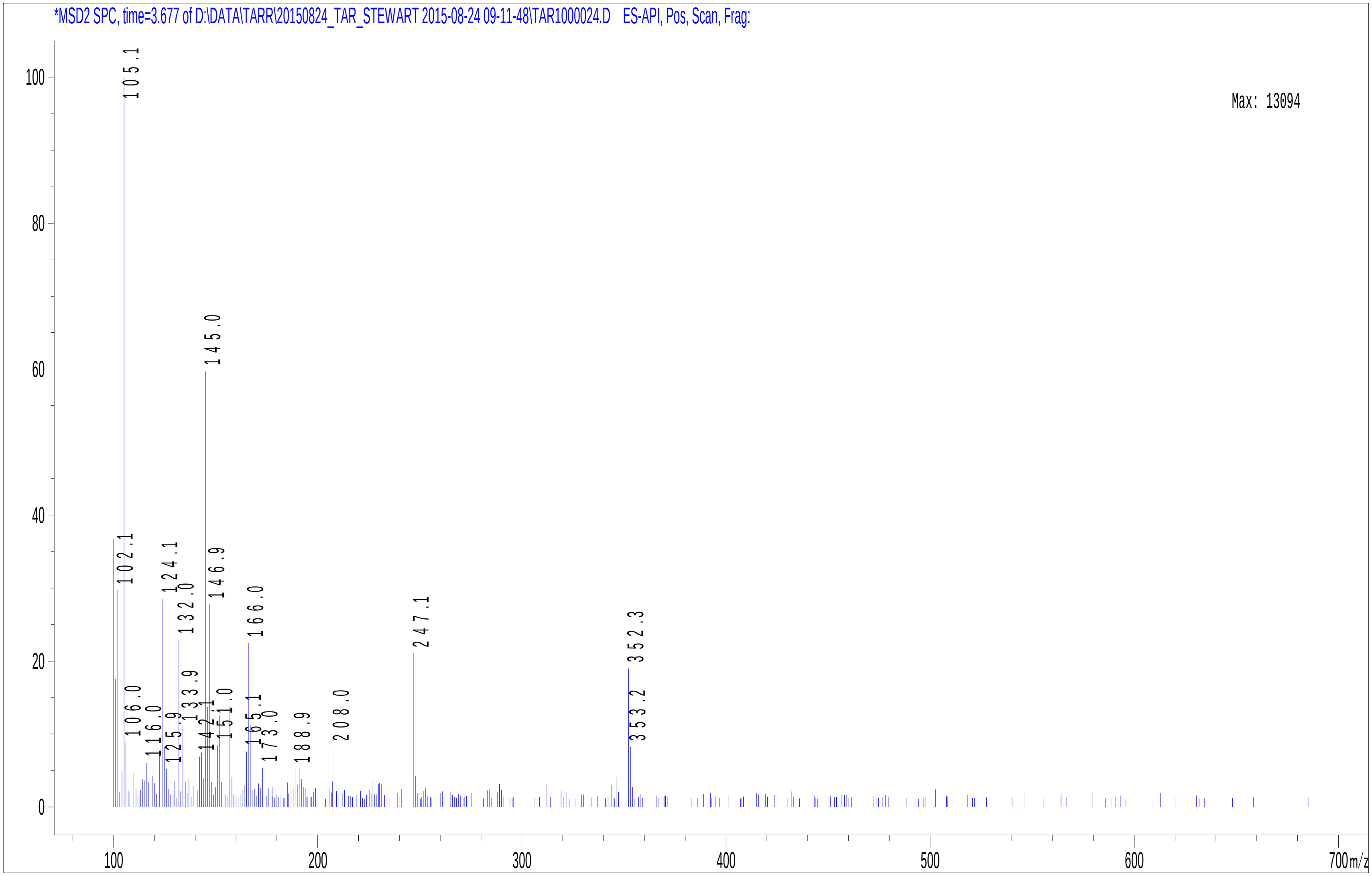
P2-C-06

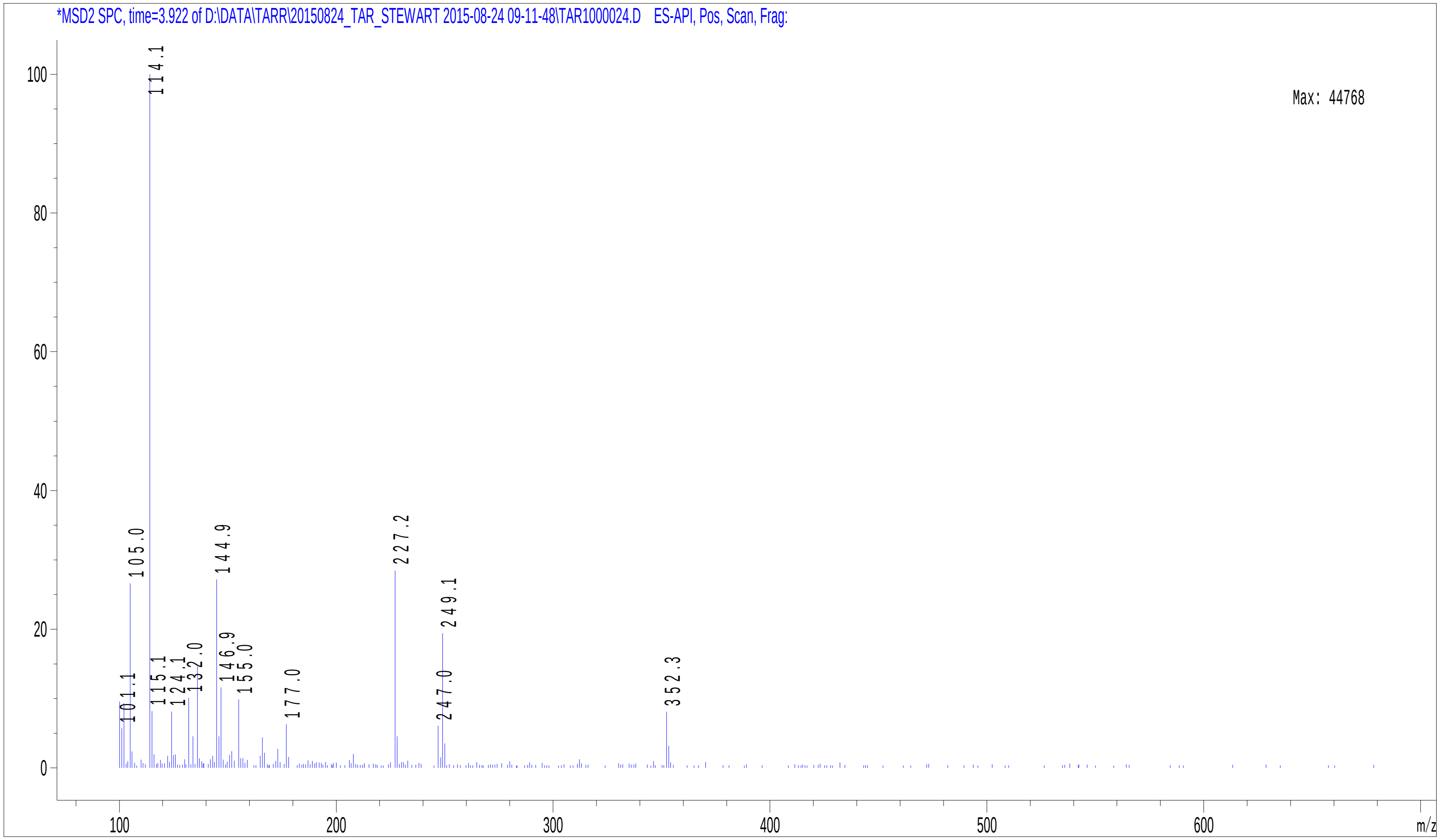


#	Time	Area	Height	Width	Area%	Symmetry
1	3.089	1209671.4	148808.5	0.1355	49.037	0.814
2	3.673	291732	26395.8	0.1842	11.826	0.498
3	3.917	965427.4	107172.4	0.1501	39.136	0.454


MSD2 TIC, MS File (D:\DATA\TARR\20150824_TAR_STEWART 2015-08-24 09-11-48\TAR1000024.D) ES-API, Pos, Scan, Frag: 70
Norm.
260000
240000
220000
200000
180000
160000
140000
120000
100000
3.089
Area: 1.20967e+006
3.673
Area: 291732
3.917
Area: 965427
2.5
3
3.5
4
4.5
5
min


*MSD2 SPC, time=3.089 of D:\DATA\TARR\20150824_TAR_STEWART 2015-08-24 09-11-48\TAR1000024.D ES-API, Pos, Scan, Frag:
Max: 115656
105.0
106.0
132.0
144.9
100
80
60
40
20
0
100
200
300
400
500
600
700
m/z

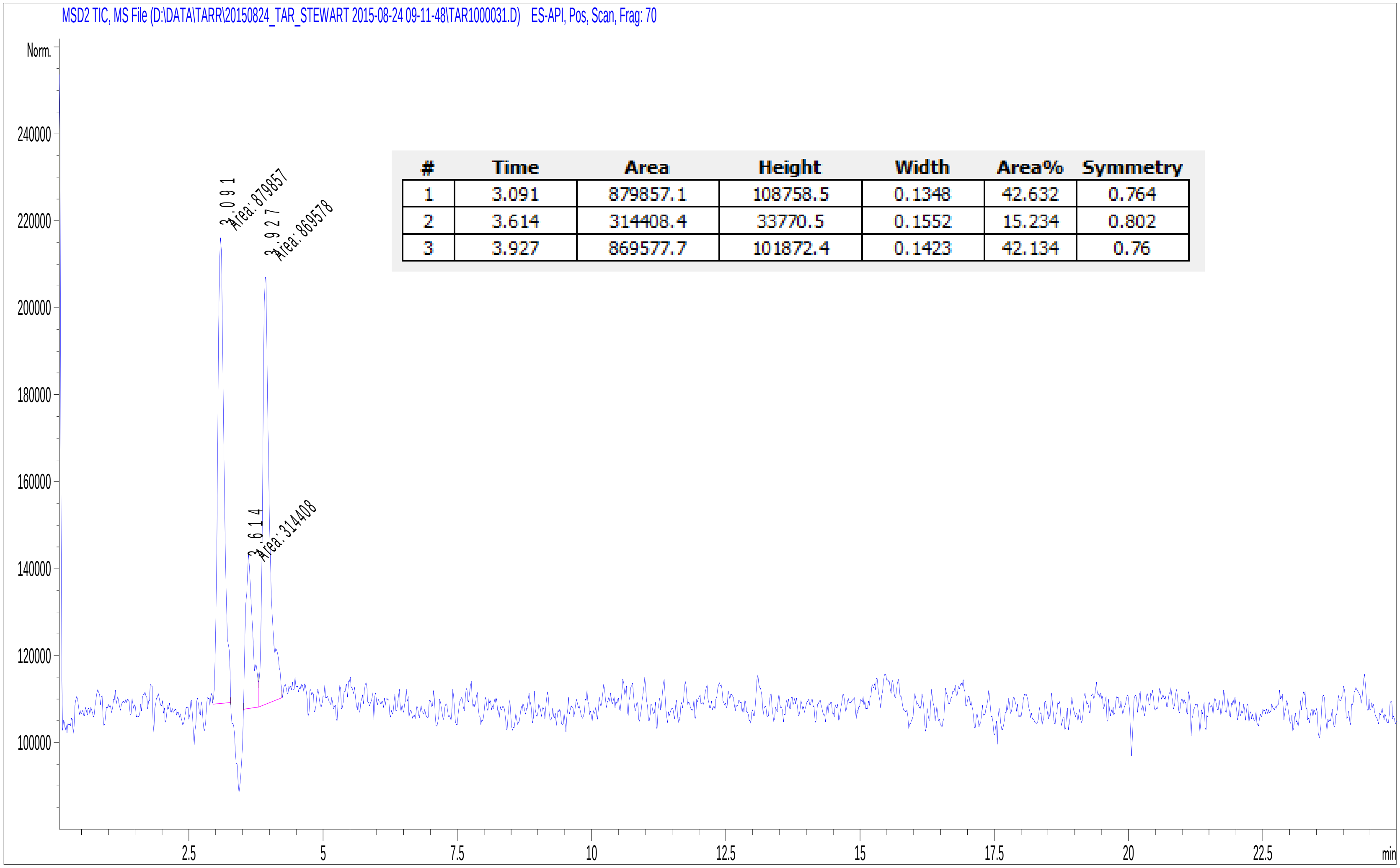

*MSD2 SPC, time=3.677 of D:\DATA\TARR\20150824_TAR_STEWART 2015-08-24 09-11-48\TAR1000024.D ES-API, Pos, Scan, Frag:
Max: 13094
105.1
102.1
106.0
116.0
125.9
124.1
132.0
133.9
142.1
145.0
146.9
151.0
165.1
166.0
173.0
188.9
208.0
247.1
352.3
353.2
0
20
40
60
80
100
100
200
300
400
500
600
700
m/z


*MSD2 SPC, time=3.922 of D:\DATA\TARR\20150824_TAR_STEWART 2015-08-24 09-11-48\TAR1000024.D ES-API, Pos, Scan, Frag:
Max: 44768
114.1
105.0
144.9
227.2
249.1
101.1
115.1
124.1
132.0
146.9
155.0
177.0
247.0
352.3
0
20
40
60
80
100
100
200
300
400
500
600
m/z

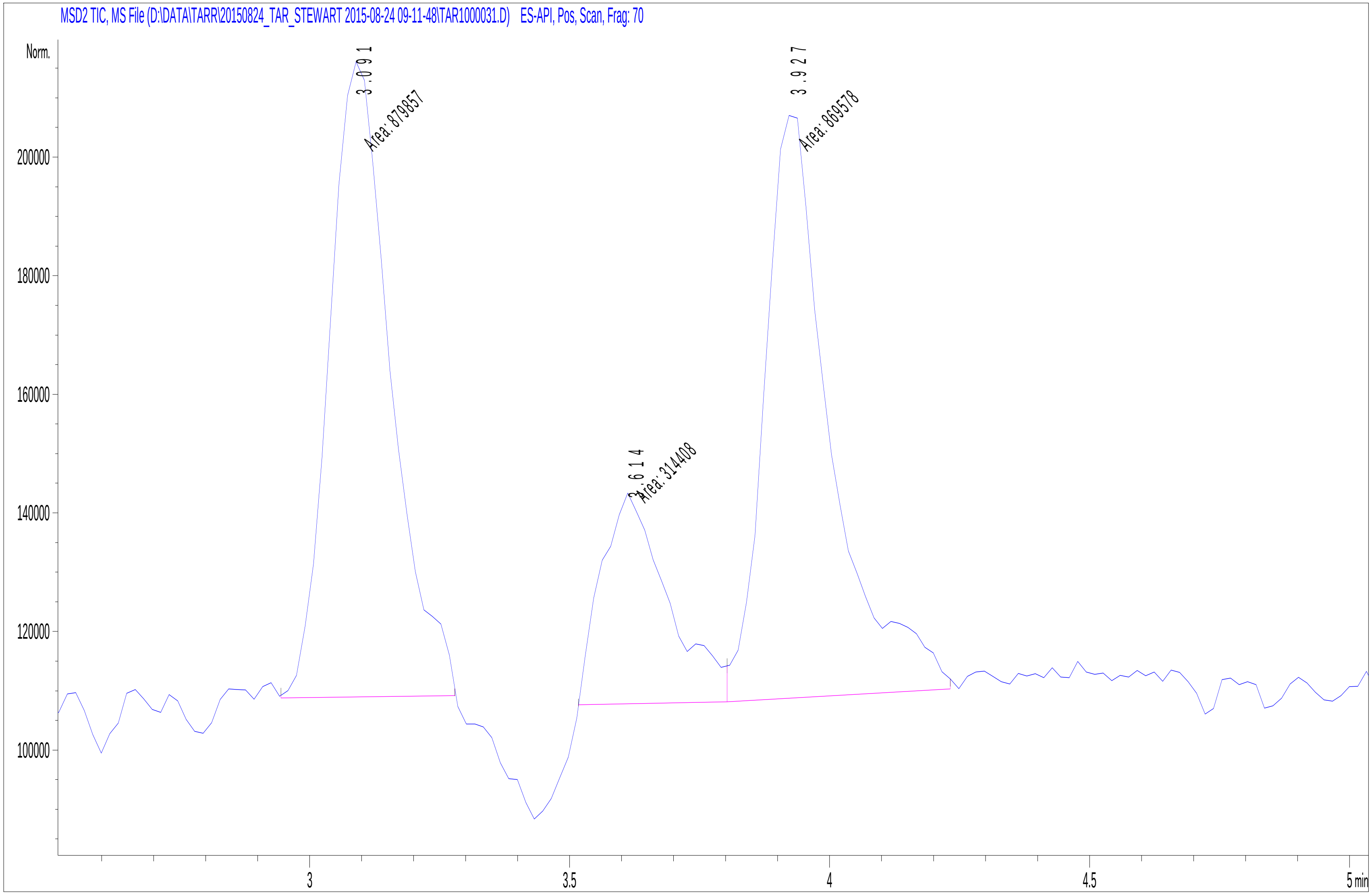
30-Jul-15

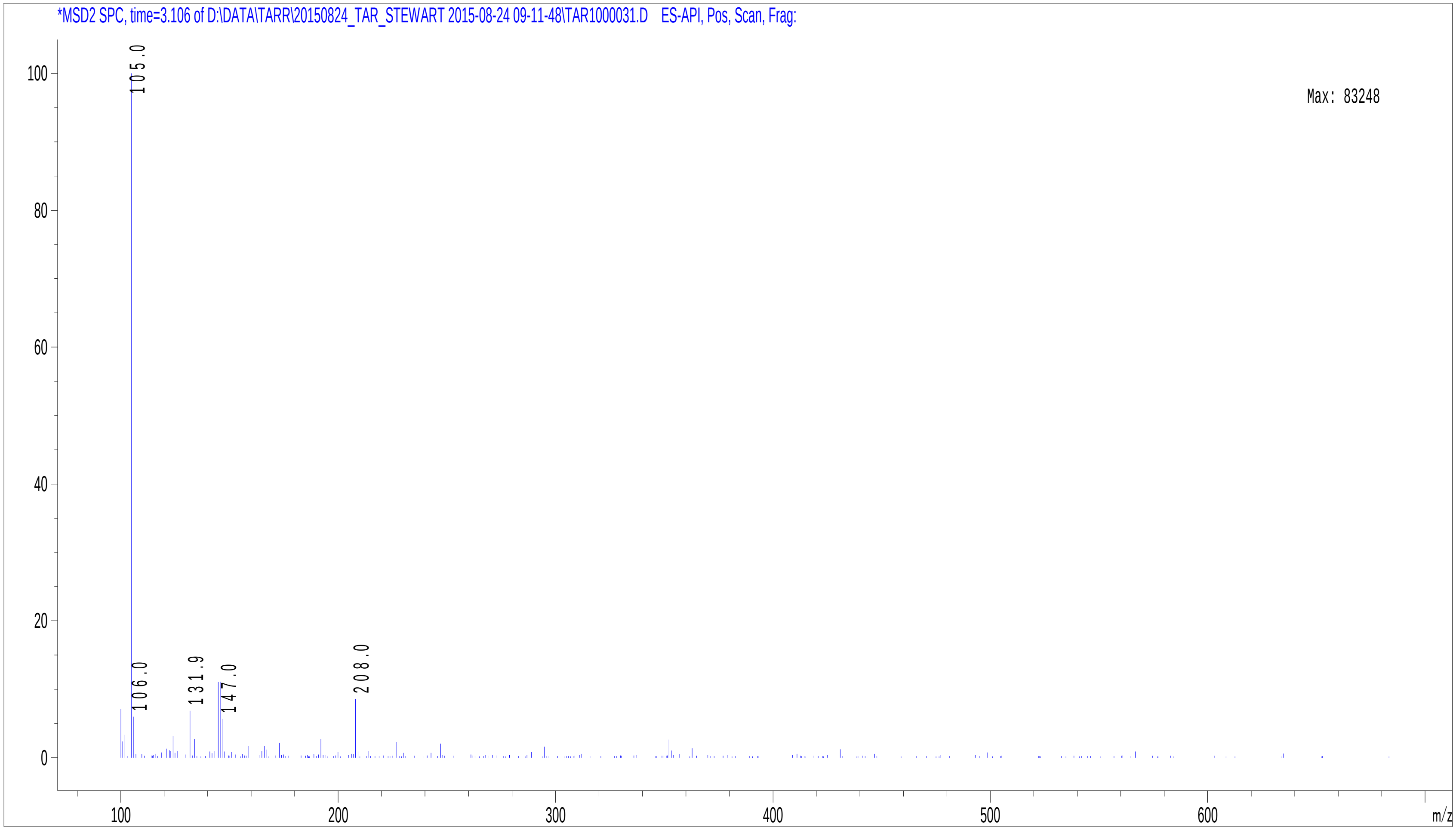
100 DC

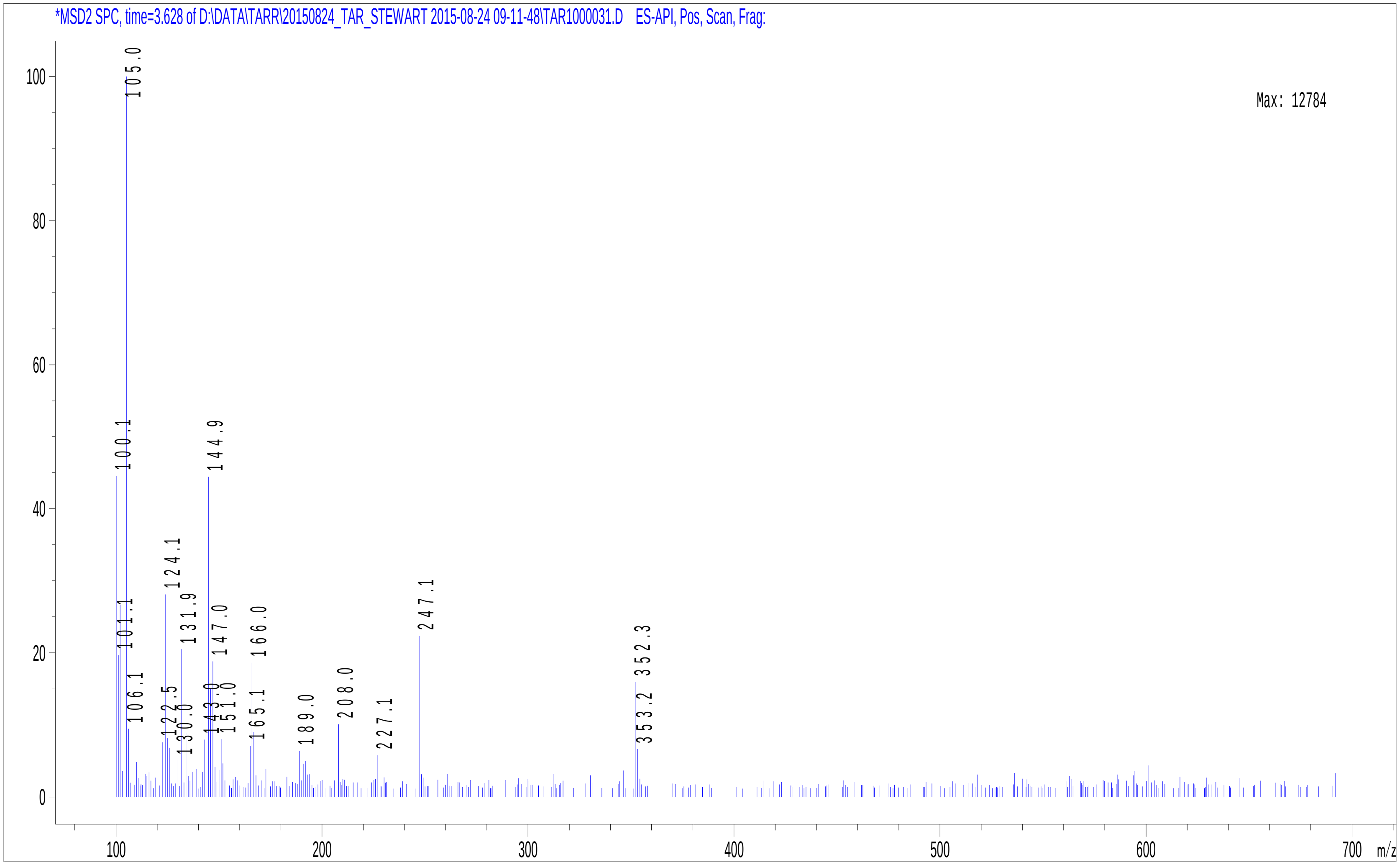
P2-D-06

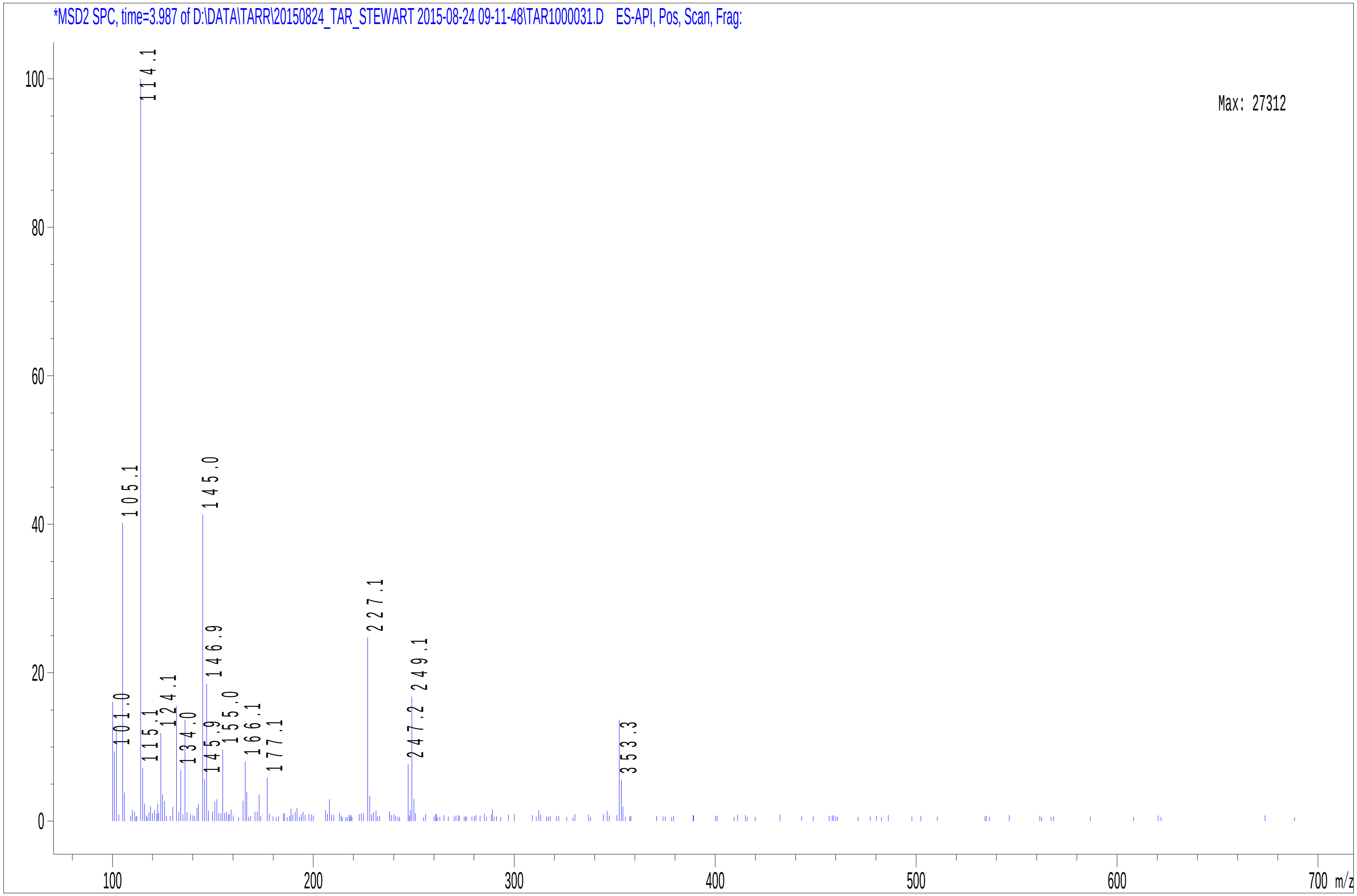


#	Time	Area	Height	Width	Area%	Symmetry
1	3.091	879857.1	108758.5	0.1348	42.632	0.764
2	3.614	314408.4	33770.5	0.1552	15.234	0.802
3	3.927	869577.7	101872.4	0.1423	42.134	0.76


MSD2 TIC, MS File (D:\DATA\TARR\20150824_TAR_STEWART 2015-08-24 09-11-48\TAR1000031.D) ES-API, Pos, Scan, Frag: 70
Norm.
200000
180000
160000
140000
120000
100000
3.091
Area: 879857
3.614
Area: 314408
3.927
Area: 869578
3
3.5
4
4.5
5 min


*MSD2 SPC, time=3.106 of D:\DATA\TARR\20150824_TAR_STEWART 2015-08-24 09-11-48\TAR1000031.D ES-API, Pos, Scan, Frag:
Max: 83248
105.0
106.0
131.9
147.0
208.0
100
80
60
40
20
0
100
200
300
400
500
600
m/z

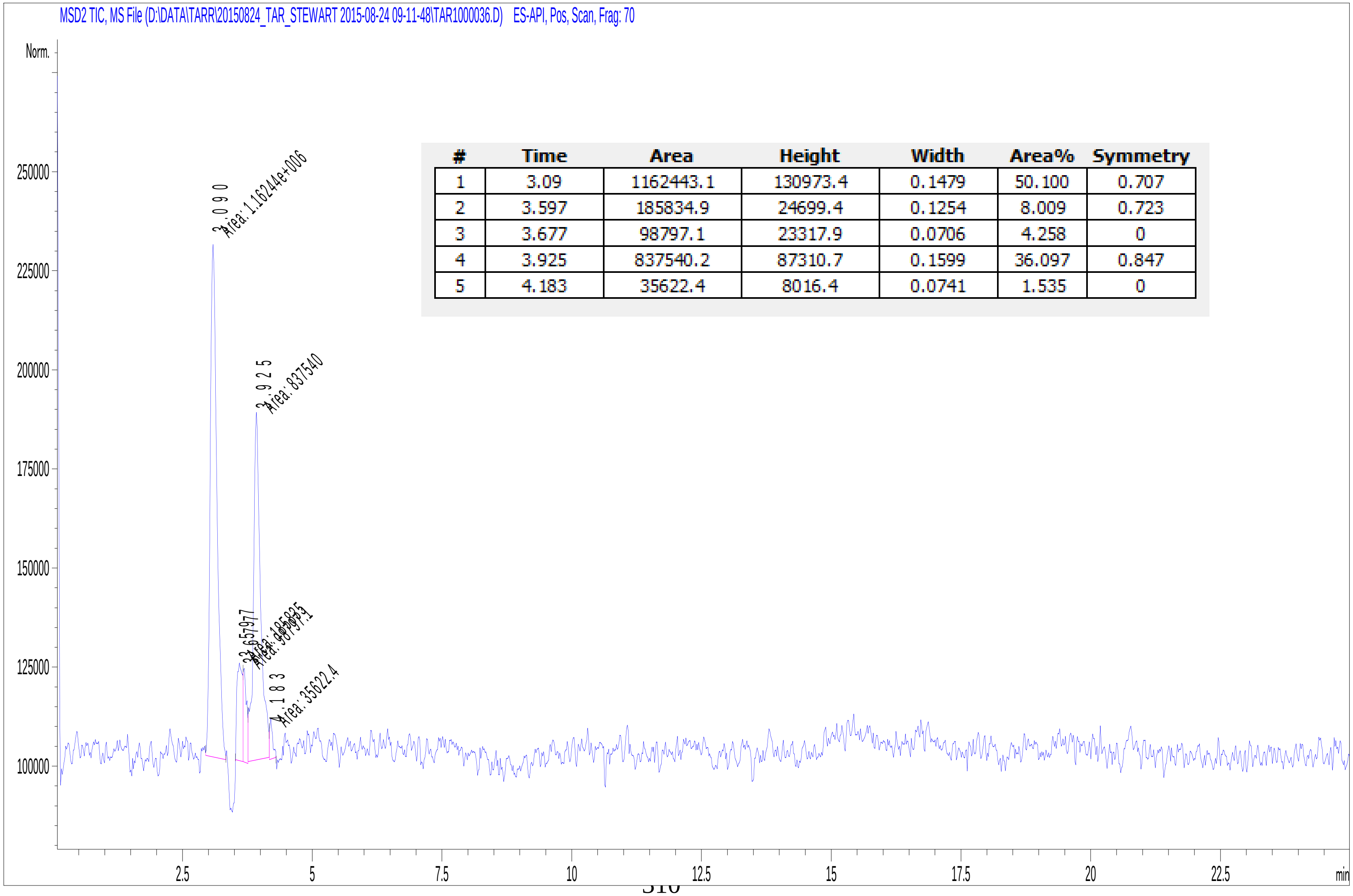

*MSD2 SPC, time=3.628 of D:\DATA\TARR\20150824_TAR_STEWART 2015-08-24 09-11-48\TAR1000031.D ES-API, Pos, Scan, Frag:
Max: 12784
100
80
60
40
20
0
105.0
100.1
144.9
124.1
101.1
131.9
147.0
166.0
247.1
352.3
106.1
122.5
130.0
143.0
151.0
165.1
189.0
208.0
227.1
353.2
100
200
300
400
500
600
700
m/z


*MSD2 SPC, time=3.987 of D:\DATA\TARR\20150824_TAR_STEWART 2015-08-24 09-11-48\TAR1000031.D ES-API, Pos, Scan, Frag:
Max: 27312
114.1
105.1
145.0
227.1
146.9
249.1
101.0
115.1
124.1
134.0
145.9
155.0
166.1
177.1
247.2
353.3
0
20
40
60
80
100
100
200
300
400
500
600
700 m/z

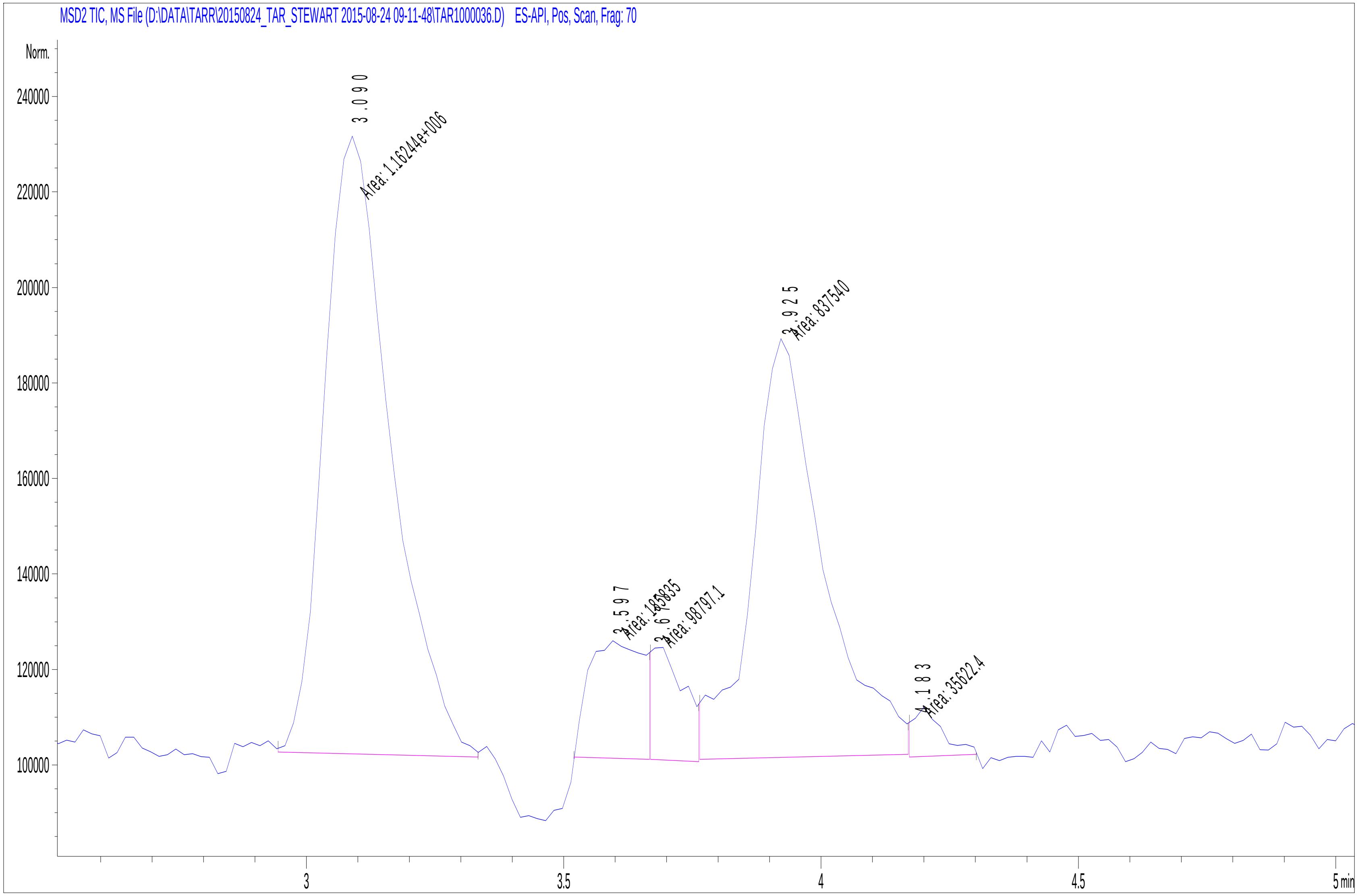
16-Jul-15

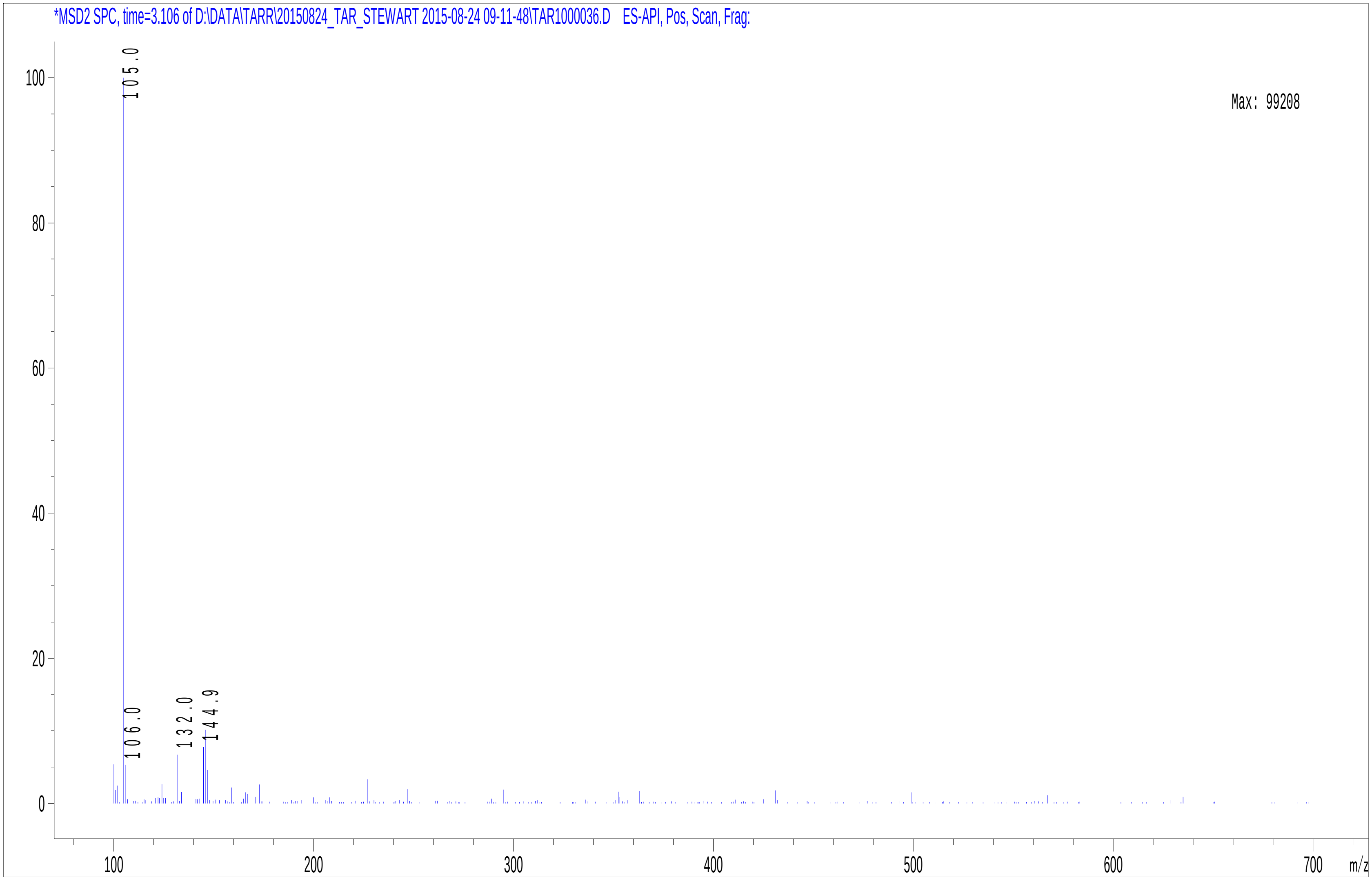
100 DC Problem no removal

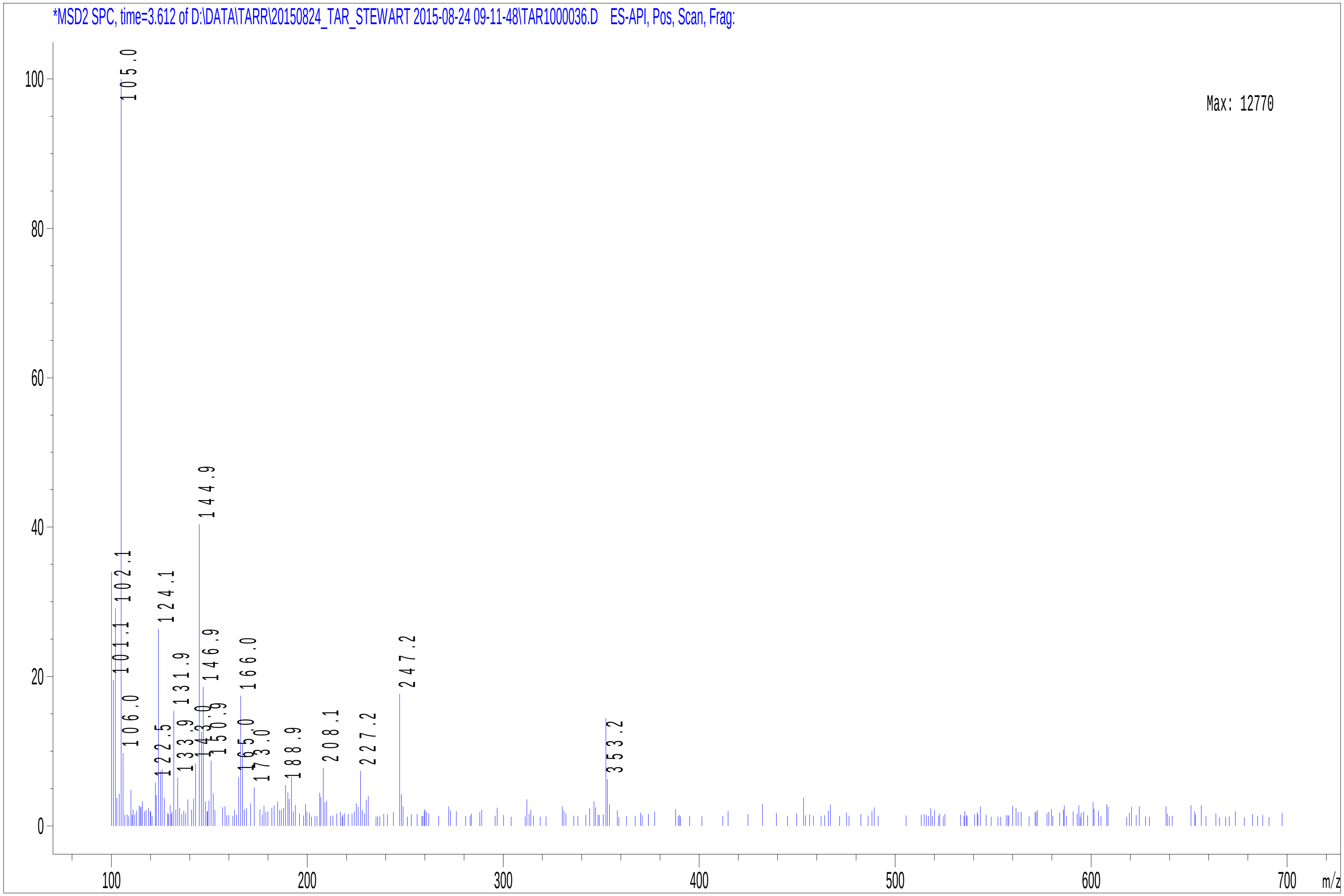
P2-D-01

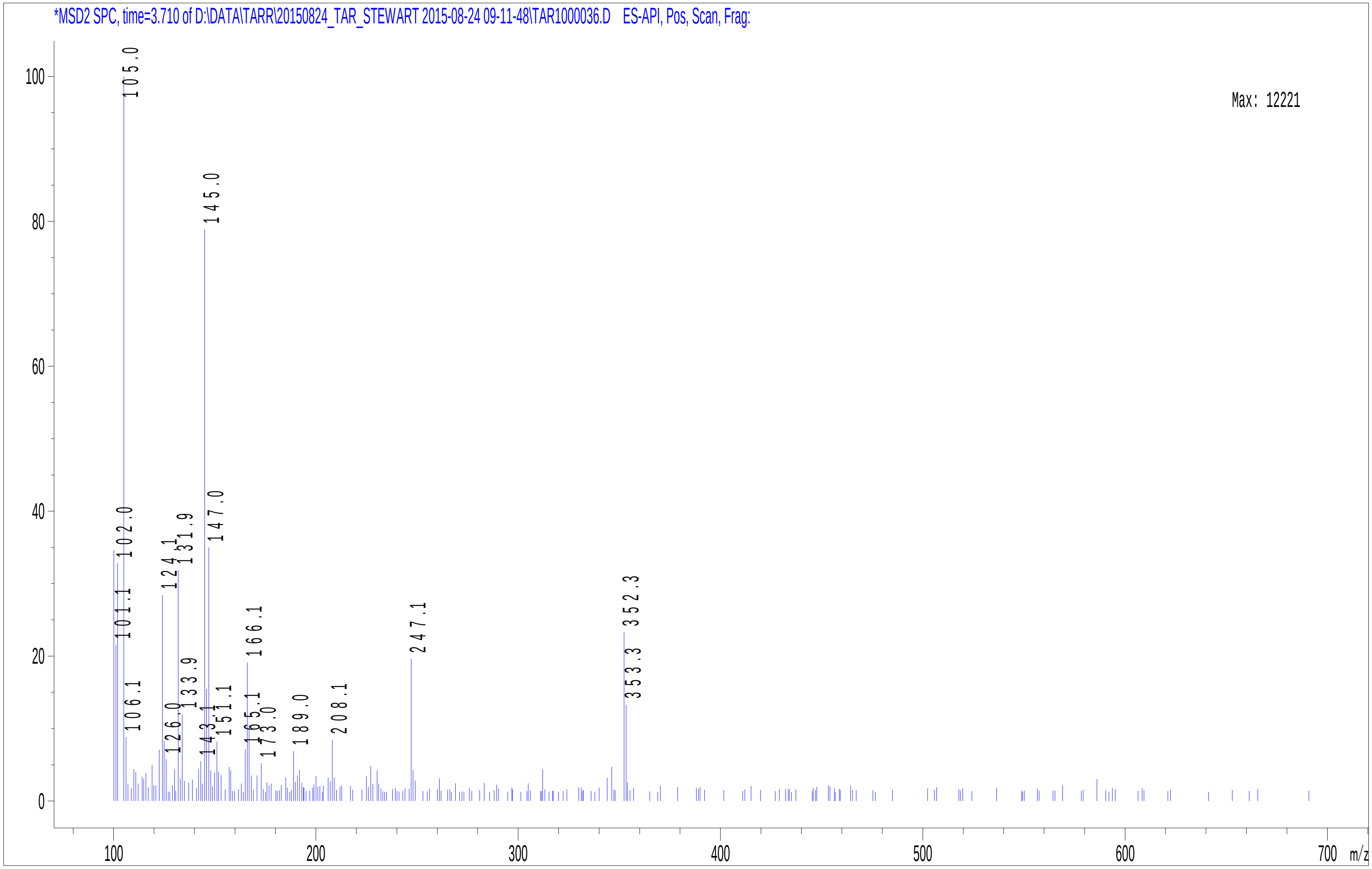


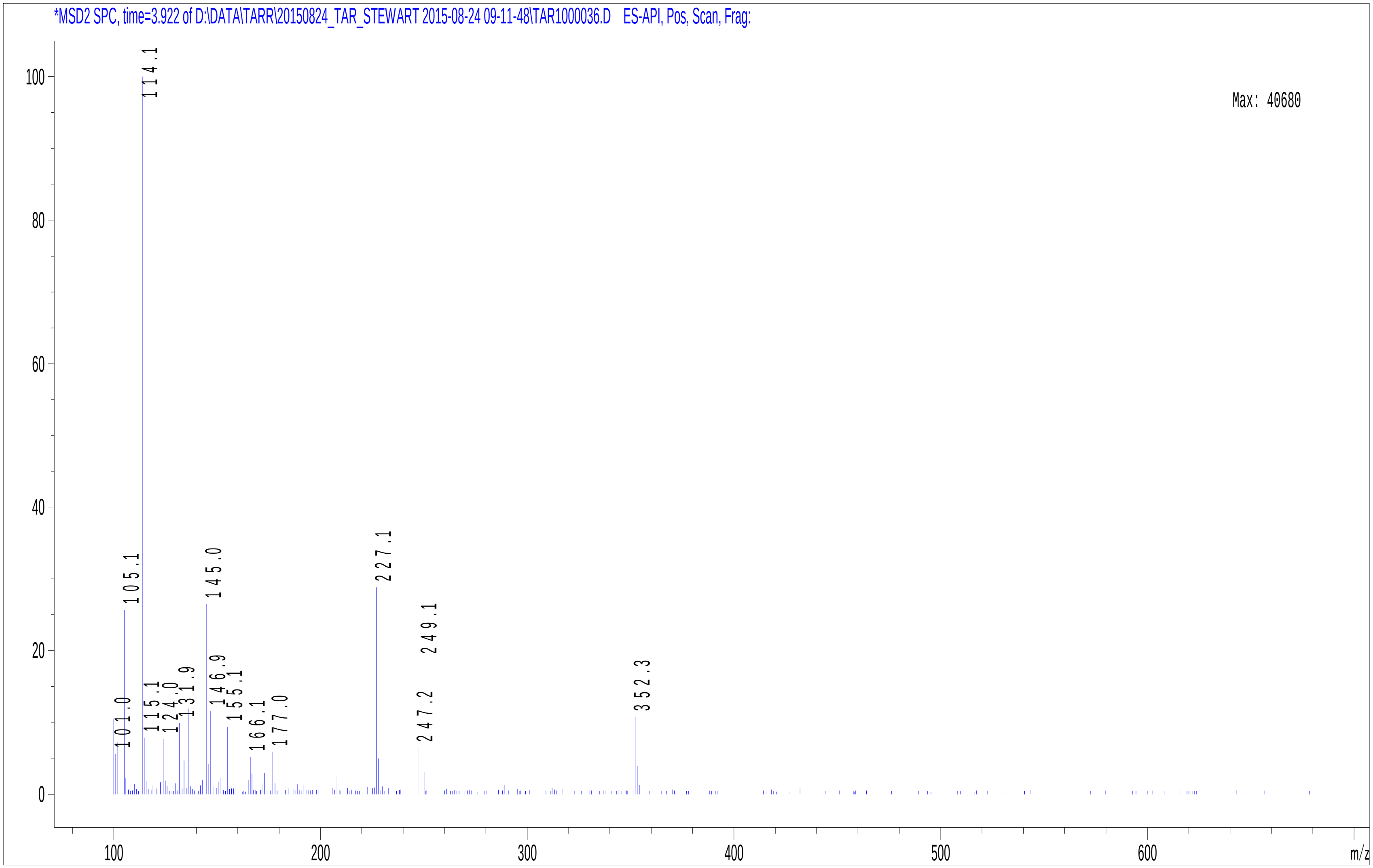
#	Time	Area	Height	Width	Area%	Symmetry
1	3.09	1162443.1	130973.4	0.1479	50.100	0.707
2	3.597	185834.9	24699.4	0.1254	8.009	0.723
3	3.677	98797.1	23317.9	0.0706	4.258	0
4	3.925	837540.2	87310.7	0.1599	36.097	0.847
5	4.183	35622.4	8016.4	0.0741	1.535	0

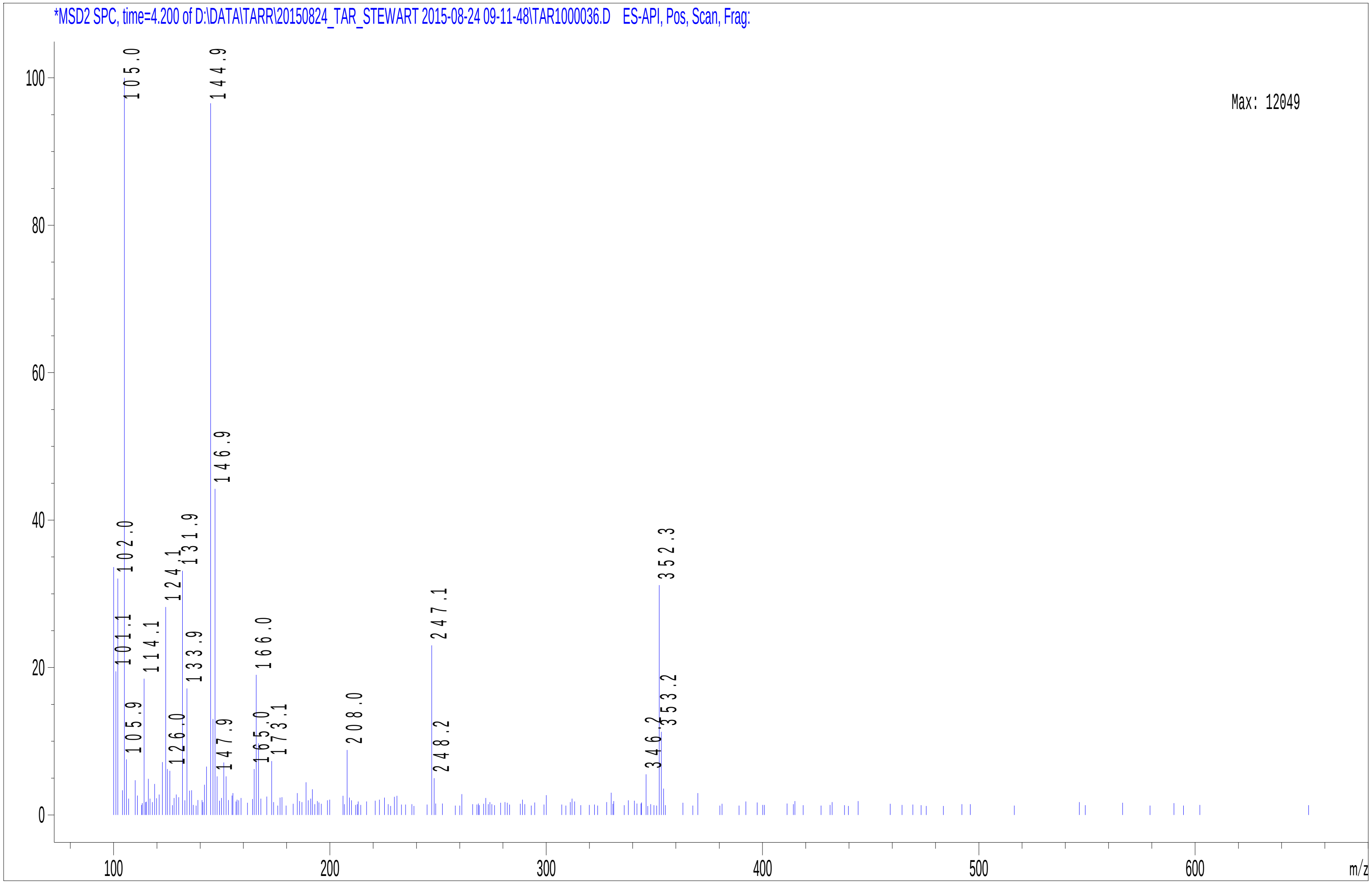

MSD2 TIC, MS File (D:\DATA\TARR\20150824_TAR_STEWART 2015-08-24 09-11-48\TAR1000036.D)   ES-API, Pos, Scan, Frag: 70
Norm.
240000
220000
200000
180000
160000
140000
120000
100000
3.090
Area: 1.16244e+006
3.597
Area: 185835
3.67
Area: 98797.1
3.925
Area: 837540
4.183
Area: 35622.4
3
3.5
4
4.5
5 min


*MSD2 SPC, time=3.106 of D:\DATA\TARR\20150824_TAR_STEWART 2015-08-24 09-11-48\TAR1000036.D ES-API, Pos, Scan, Frag:
Max: 99208
105.0
106.0
132.0
144.9
0
20
40
60
80
100
100
200
300
400
500
600
700
m/z


*MSD2 SPC, time=3.612 of D:\DATA\TARR\20150824_TAR_STEWART 2015-08-24 09-11-48\TAR1000036.D ES-API, Pos, Scan, Frag:
Max: 12770
105.0
144.9
102.1
124.1
101.1
131.9
146.9
166.0
106.0
122.5
133.9
143.0
150.9
165.0
173.0
188.9
208.1
227.2
247.2
353.2
0
20
40
60
80
100
100
200
300
400
500
600
700
m/z

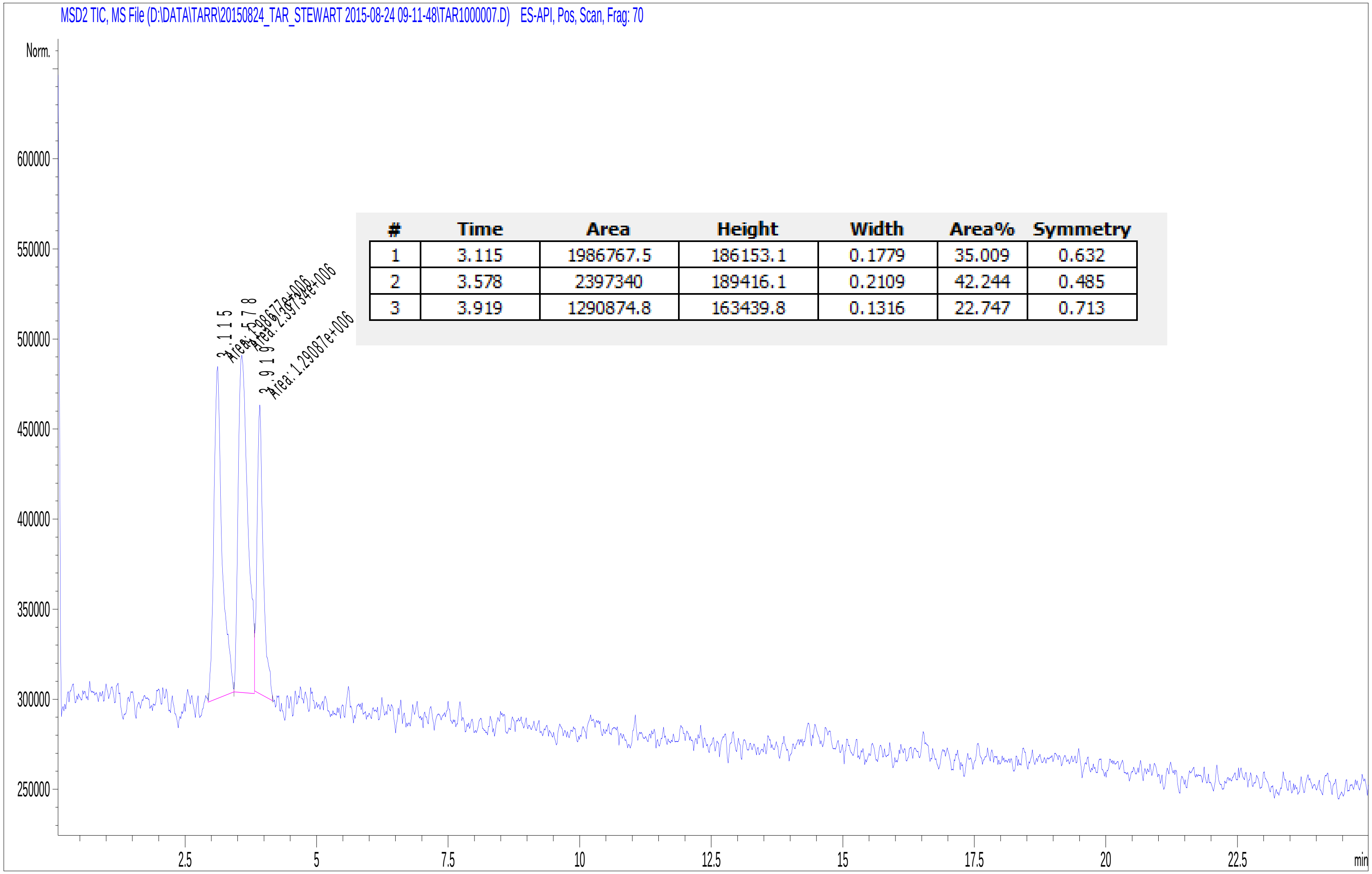

*MSD2 SPC, time=3.710 of D:\DATA\TARR\20150824_TAR_STEWART 2015-08-24 09-11-48\TAR1000036.D ES-API, Pos, Scan, Frag:
Max: 12221
105.0
145.0
102.0
147.0
131.9
124.1
101.1
352.3
166.1
247.1
353.3
133.9
106.1
126.0
143.1
151.1
165.1
173.0
189.0
208.1
0
20
40
60
80
100
100
200
300
400
500
600
700
m/z


*MSD2 SPC, time=3.922 of D:\DATA\TARR\20150824_TAR_STEWART 2015-08-24 09-11-48\TAR1000036.D ES-API, Pos, Scan, Frag:
Max: 40680
100
80
60
40
20
0
114.1
105.1
101.0
115.1
124.0
131.9
145.0
146.9
155.1
166.1
177.0
227.1
247.2
249.1
352.3
100
200
300
400
500
600
m/z

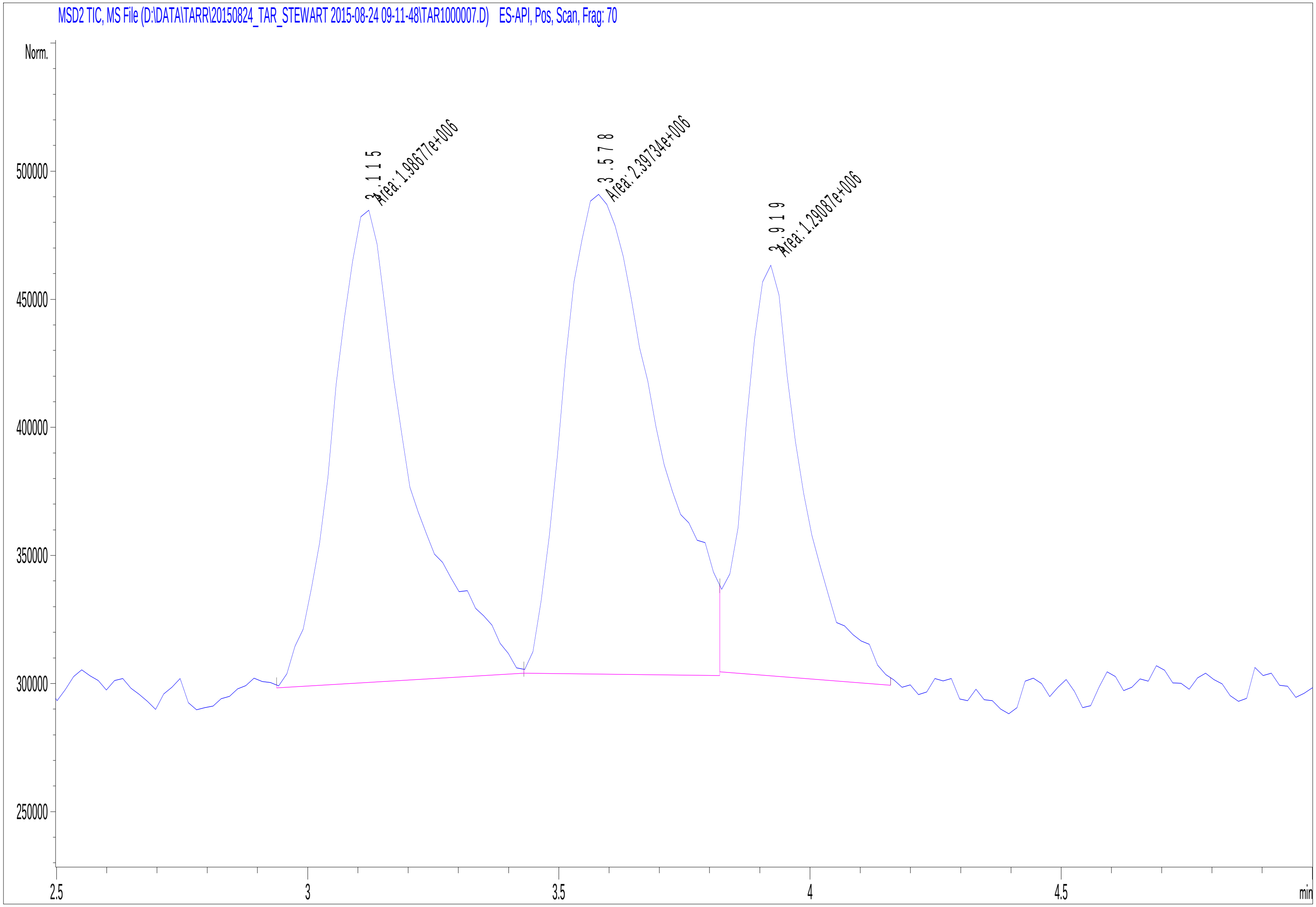

*MSD2 SPC, time=4.200 of D:\DATA\TARR\20150824_TAR_STEWART 2015-08-24 09-11-48\TAR1000036.D ES-API, Pos, Scan, Frag:
Max: 12049
105.0
144.9
146.9
102.0
131.9
124.1
101.1
114.1
133.9
166.0
247.1
352.3
105.9
126.0
147.9
165.0
173.1
208.0
248.2
346.2
353.2
100
80
60
40
20
0
100
200
300
400
500
600
m/z

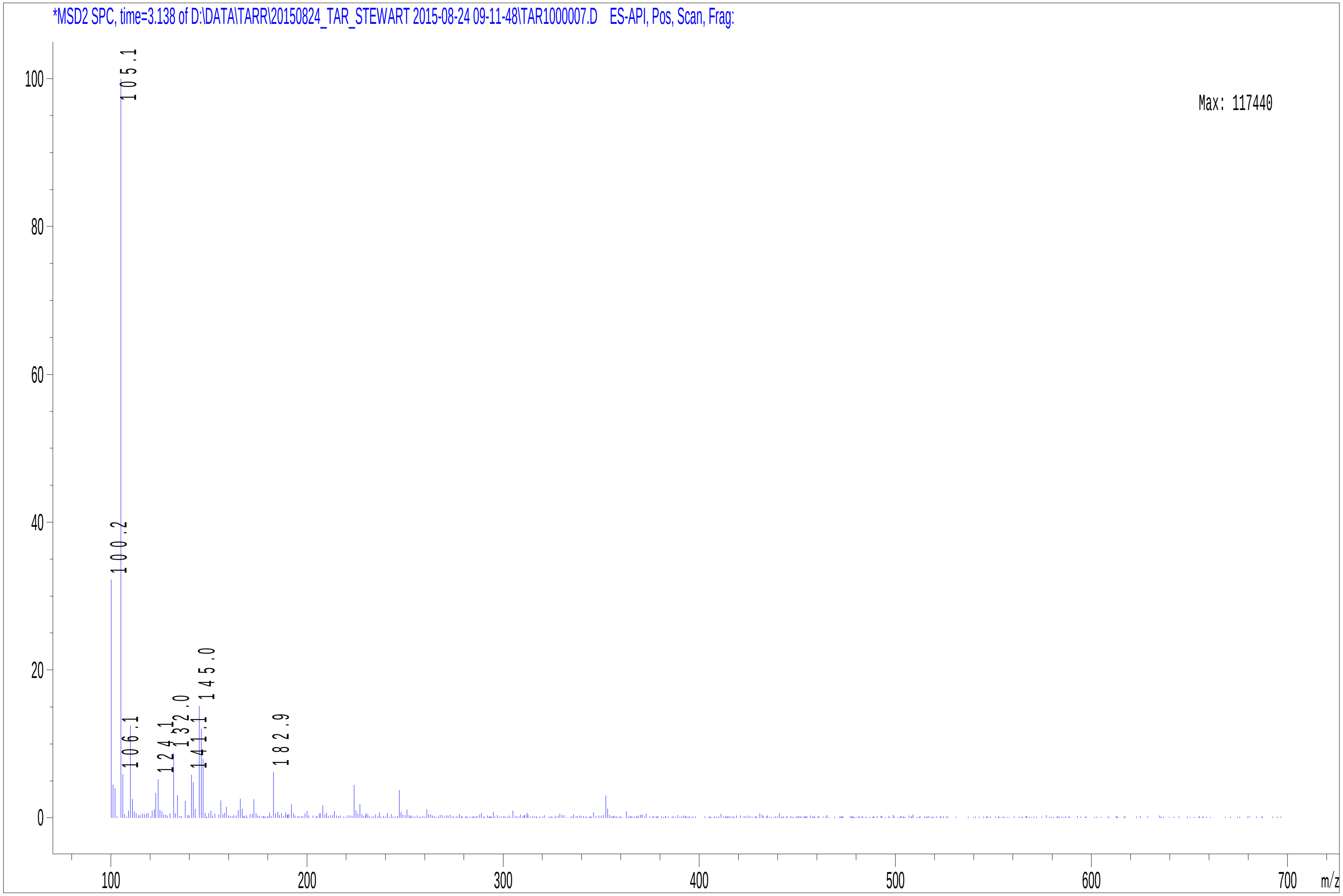
pH 8

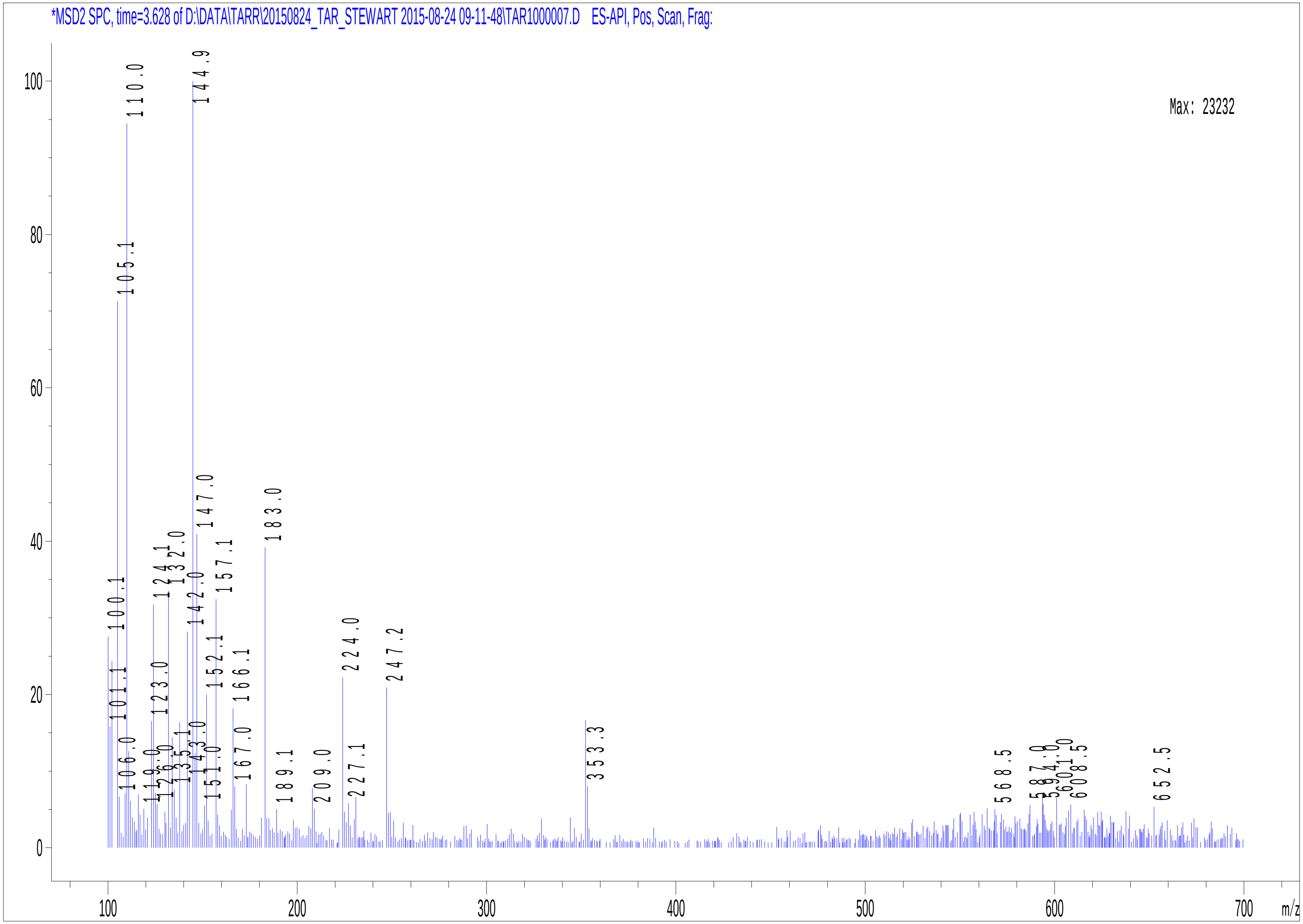
16-Apr-15
H2O2 Ctrl
P2-A-07

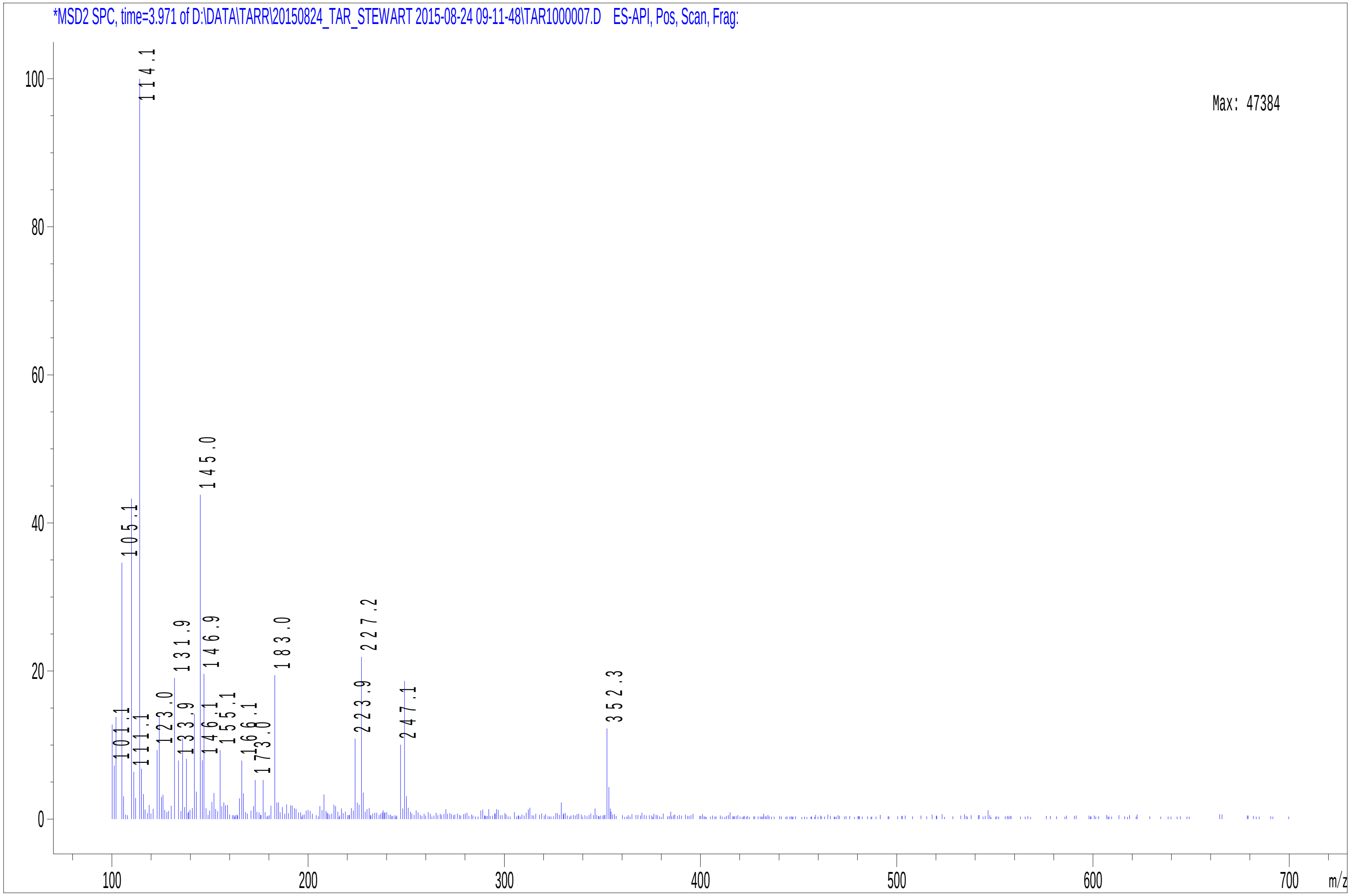


#	Time	Area	Height	Width	Area%	Symmetry
1	3.115	1986767.5	186153.1	0.1779	35.009	0.632
2	3.578	2397340	189416.1	0.2109	42.244	0.485
3	3.919	1290874.8	163439.8	0.1316	22.747	0.713


MSD2 TIC, MS File (D:\DATA\TARR\20150824_TAR_STEWART 2015-08-24 09-11-48\TAR1000007.D)   ES-API, Pos, Scan, Frag: 70
Norm.
500000
450000
400000
350000
300000
250000
3.115
Area: 1.98677e+006
3.578
Area: 2.39734e+006
3.919
Area: 1.29087e+006
2.5
3
3.5
4
4.5
min


*MSD2 SPC, time=3.138 of D:\DATA\TARR\20150824_TAR_STEWART 2015-08-24 09-11-48\TAR1000007.D ES-API, Pos, Scan, Frag:
Max: 117440
105.1
100.2
106.1
124.1
132.0
141.1
145.0
182.9
0
20
40
60
80
100
100
200
300
400
500
600
700
m/z


*MSD2 SPC, time=3.628 of D:\DATA\TARR\20150824_TAR_STEWART 2015-08-24 09-11-48\TAR1000007.D ES-API, Pos, Scan, Frag:
Max: 23232
100
80
60
40
20
0
100.1
101.1
105.1
106.0
110.0
119.0
123.0
124.1
126.0
132.0
135.1
142.0
143.0
144.9
147.0
151.0
152.1
157.1
166.1
167.0
183.0
189.1
209.0
224.0
227.1
247.2
353.3
568.5
587.0
594.0
601.0
608.5
652.5
100
200
300
400
500
600
700
m/z


*MSD2 SPC, time=3.971 of D:\DATA\TARR\20150824_TAR_STEWART 2015-08-24 09-11-48\TAR1000007.D ES-API, Pos, Scan, Frag:
Max: 47384
114.1
145.0
105.1
131.9
146.9
183.0
227.2
123.0
133.9
101.1
111.1
146.1
155.1
166.1
173.0
223.9
247.1
352.3
0
20
40
60
80
100
200
300
400
500
600
700
m/z

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0 DC

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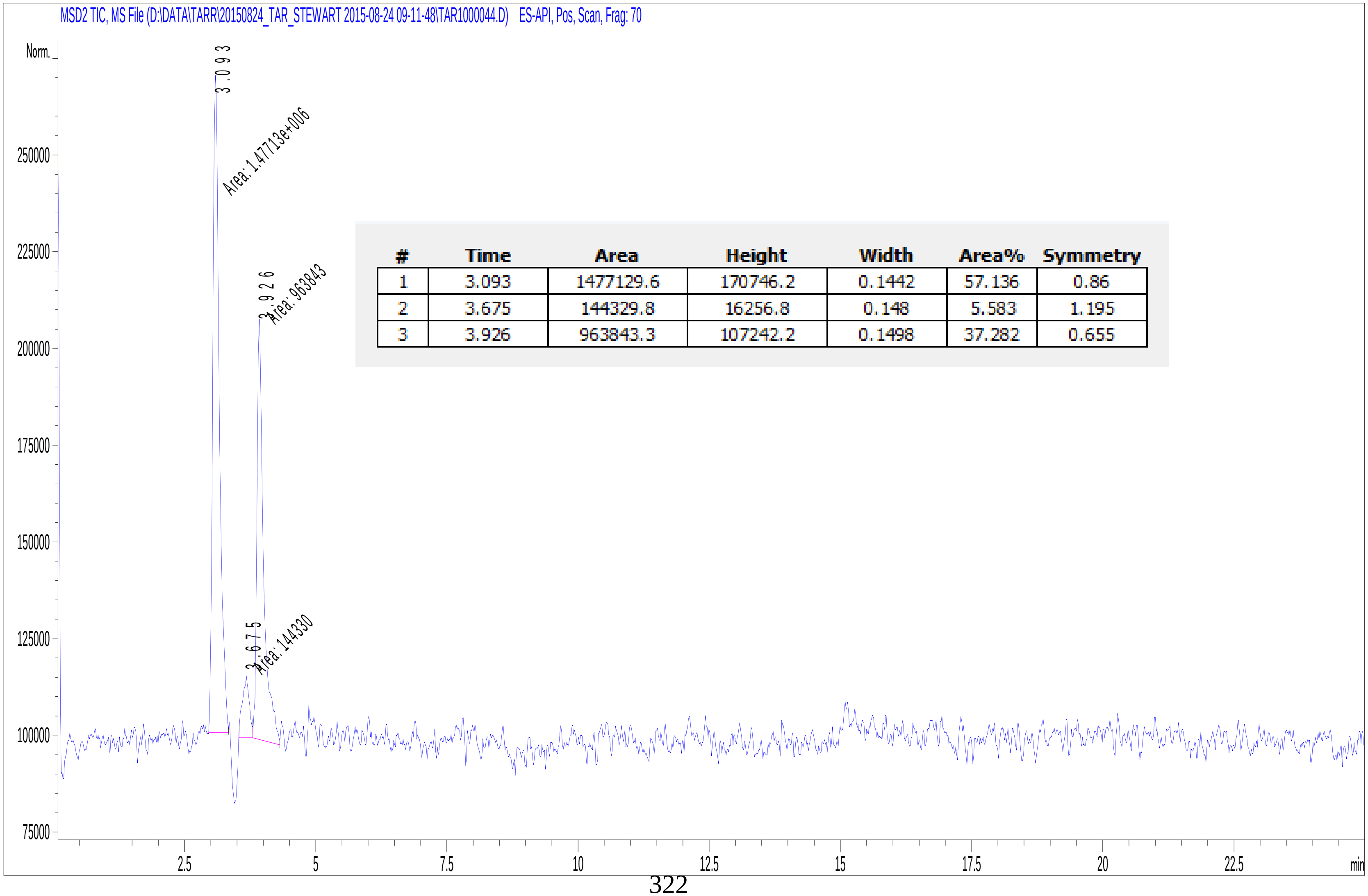
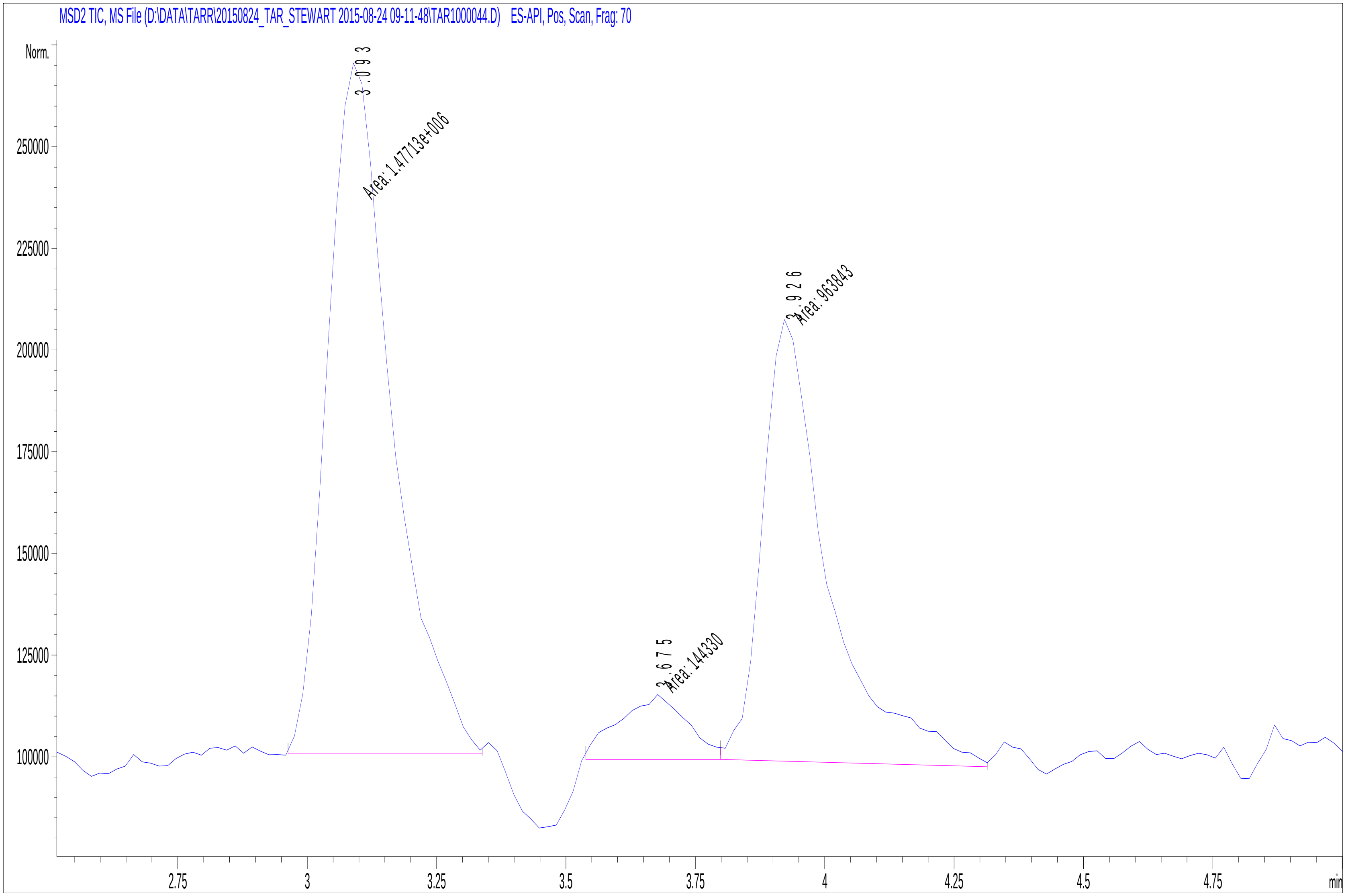
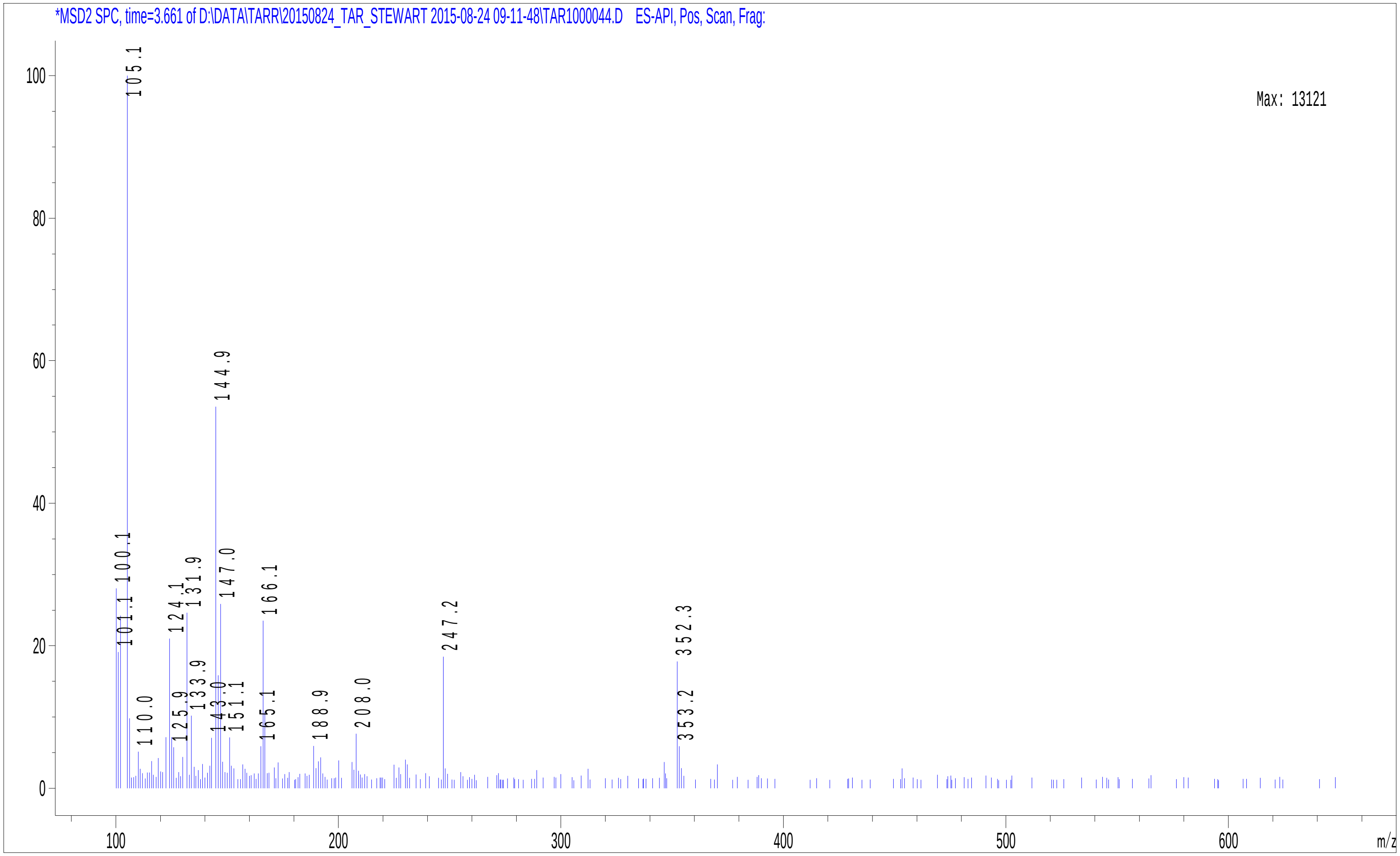
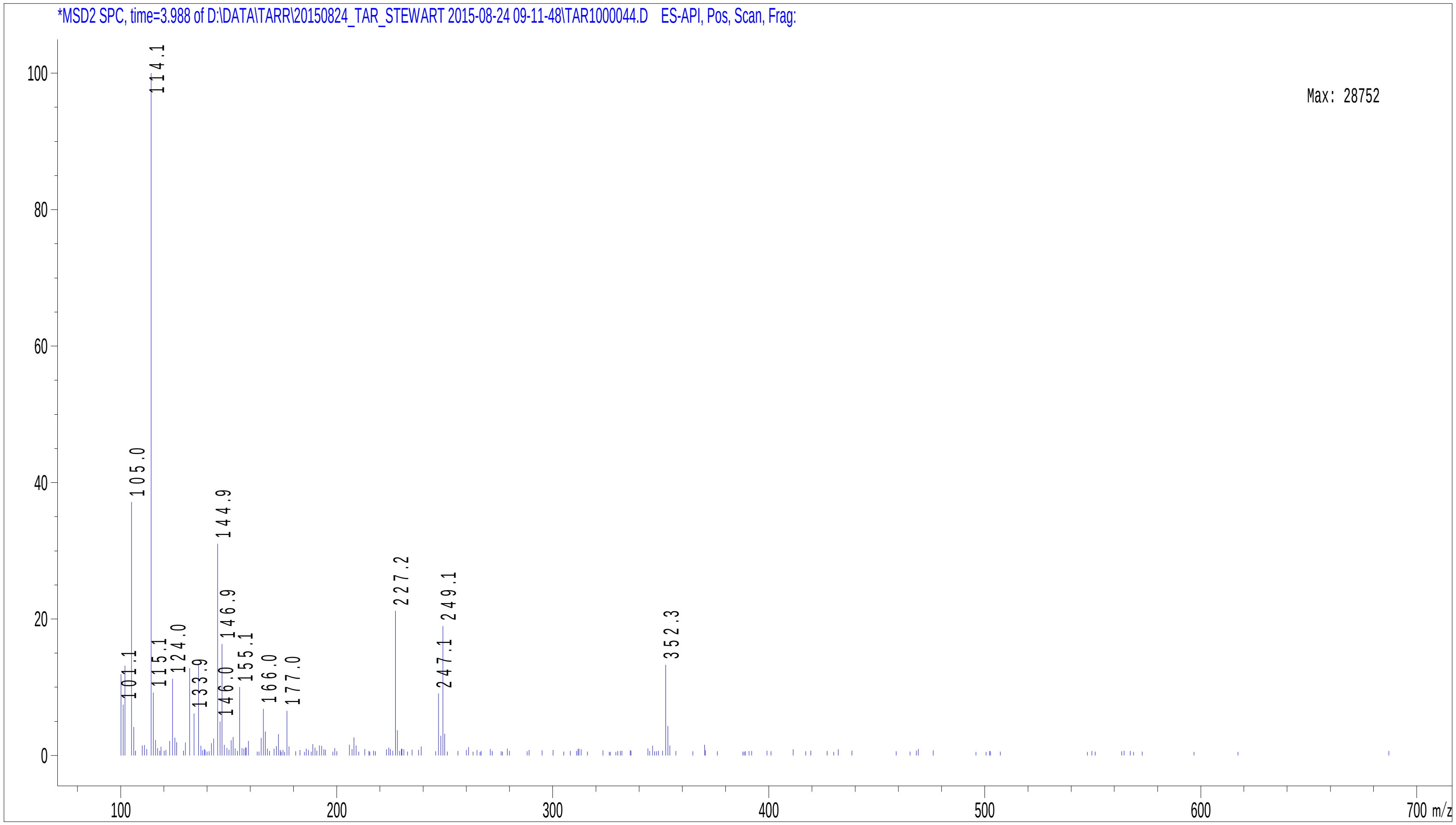


#	Time	Area	Height	Width	Area%	Symmetry
1	3.093	1477129.6	170746.2	0.1442	57.136	0.86
2	3.675	144329.8	16256.8	0.148	5.583	1.195
3	3.926	963843.3	107242.2	0.1498	37.282	0.655


MSD2 TIC, MS File (D:\DATA\TARR\20150824_TAR_STEWART 2015-08-24 09-11-48\TAR1000044.D) ES-API, Pos, Scan, Frag: 70
Norm.
3.093
Area: 1.47713e+006
3.675
Area: 144330
3.926
Area: 963843
250000
225000
200000
175000
150000
125000
100000
2.75
3
3.25
3.5
3.75
4
4.25
4.5
4.75
min


*MSD2 SPC, time=3.138 of D:\DATA\TARR\20150824_TAR_STEWART 2015-08-24 09-11-48\TAR1000044.D ES-API, Pos, Scan, Frag:
Max: 101936
105.0
106.0
131.9
144.9
100
80
60
40
20
0
100
200
300
400
500
600
700
m/z

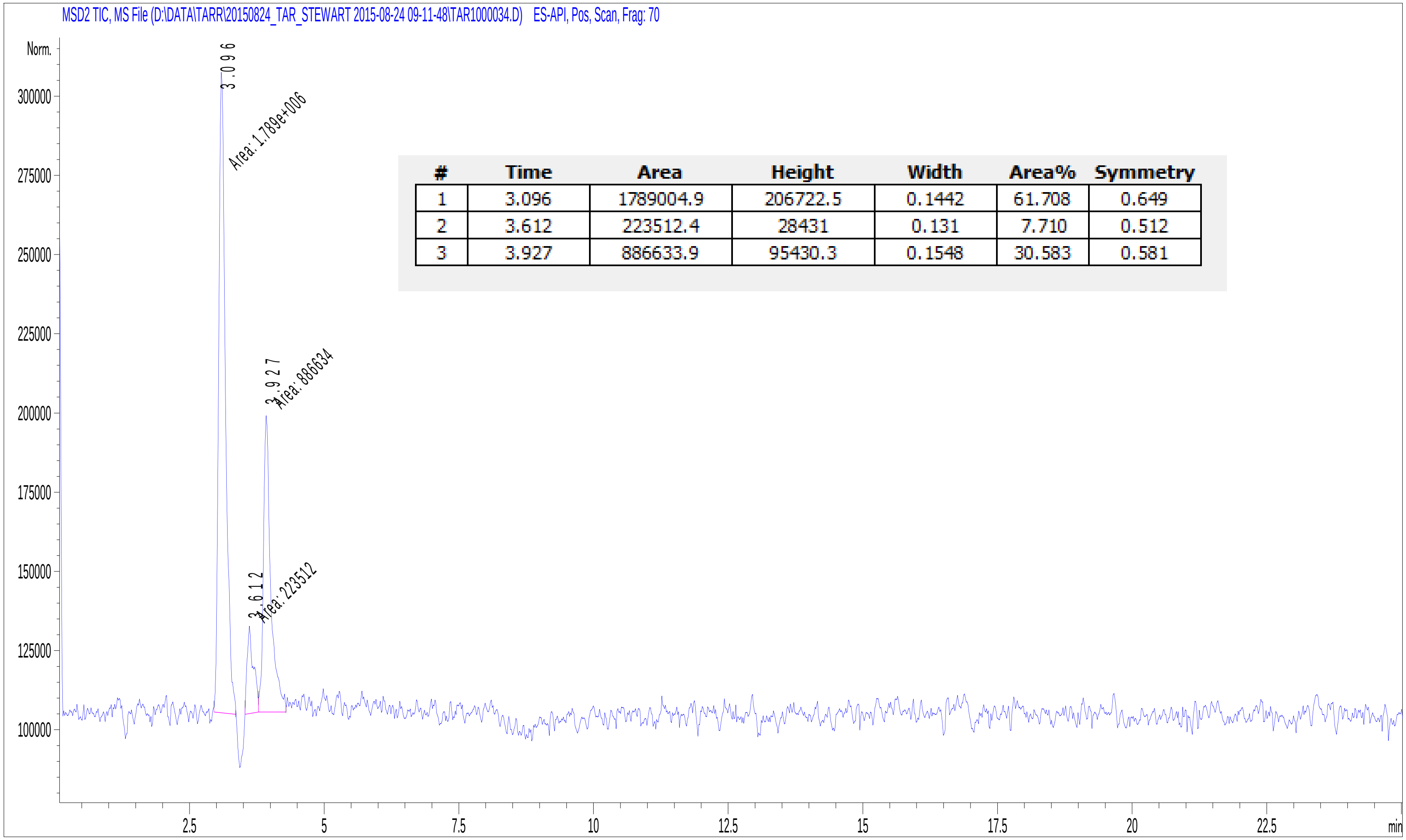

*MSD2 SPC, time=3.661 of D:\DATA\TARR\20150824_TAR_STEWART 2015-08-24 09-11-48\TAR1000044.D ES-API, Pos, Scan, Frag:
Max: 13121
105.1
144.9
100.1
101.1
124.1
131.9
147.0
166.1
110.0
125.9
133.9
143.0
151.1
165.1
188.9
208.0
247.2
352.3
353.2
100
80
60
40
20
0
100
200
300
400
500
600
m/z


*MSD2 SPC, time=3.988 of D:\DATA\TARR\20150824_TAR_STEWART 2015-08-24 09-11-48\TAR1000044.D ES-API, Pos, Scan, Frag:
Max: 28752
114.1
105.0
144.9
227.2
249.1
146.9
124.0
115.1
155.1
352.3
101.1
133.9
166.0
177.0
146.0
247.1
0
20
40
60
80
100
100
200
300
400
500
600
700 m/z

21-Jul-15

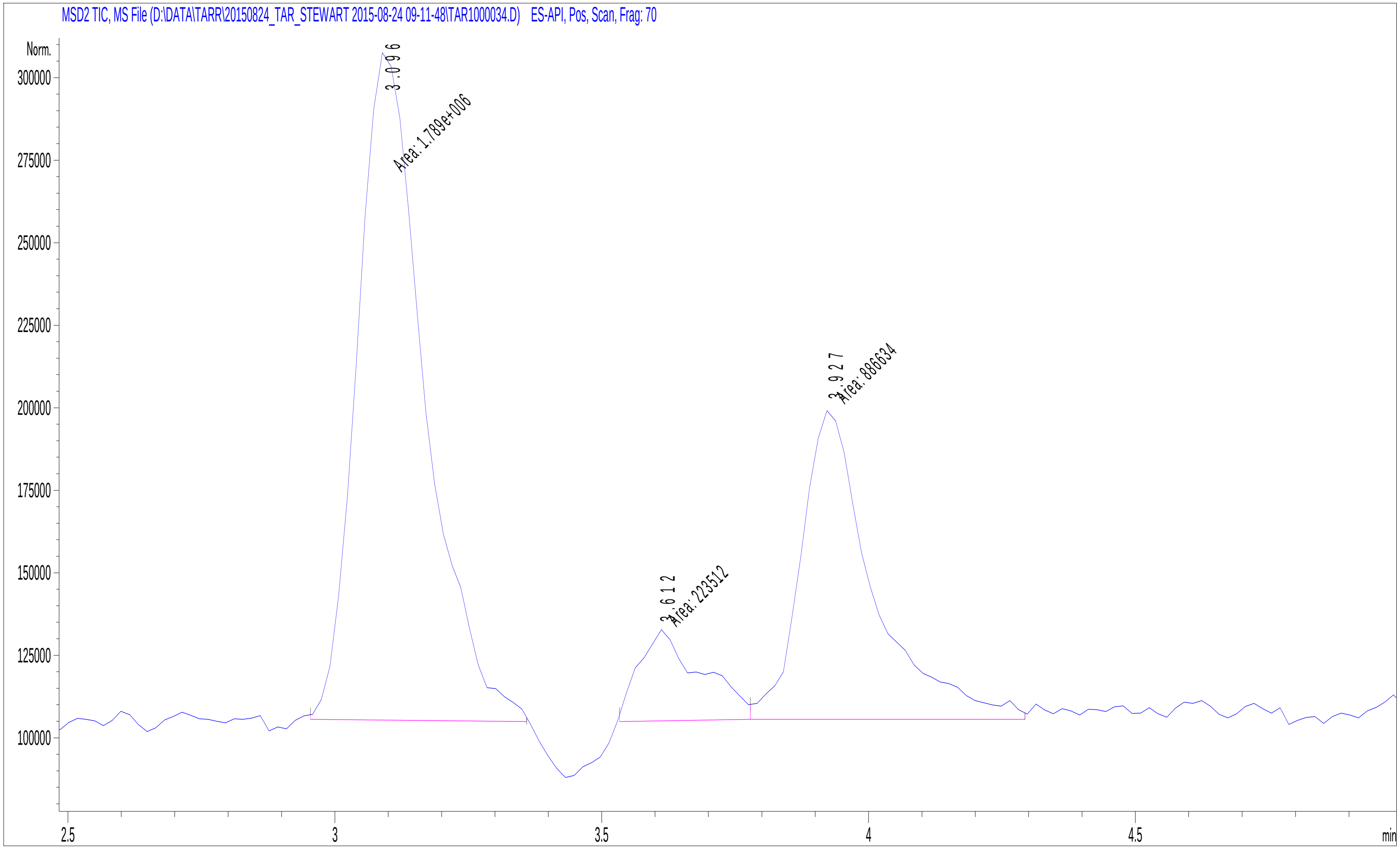
5 DC

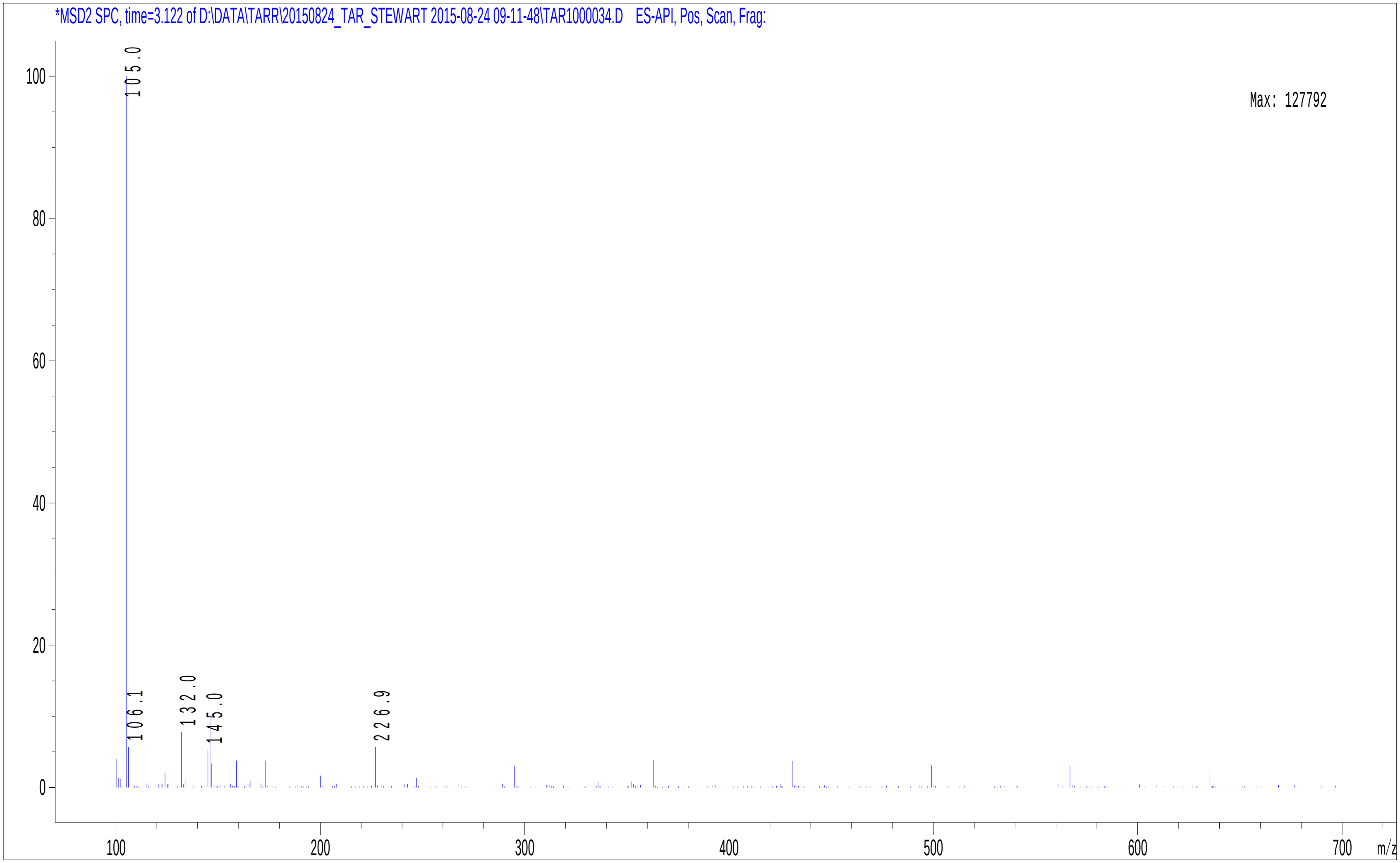
P2-D-03

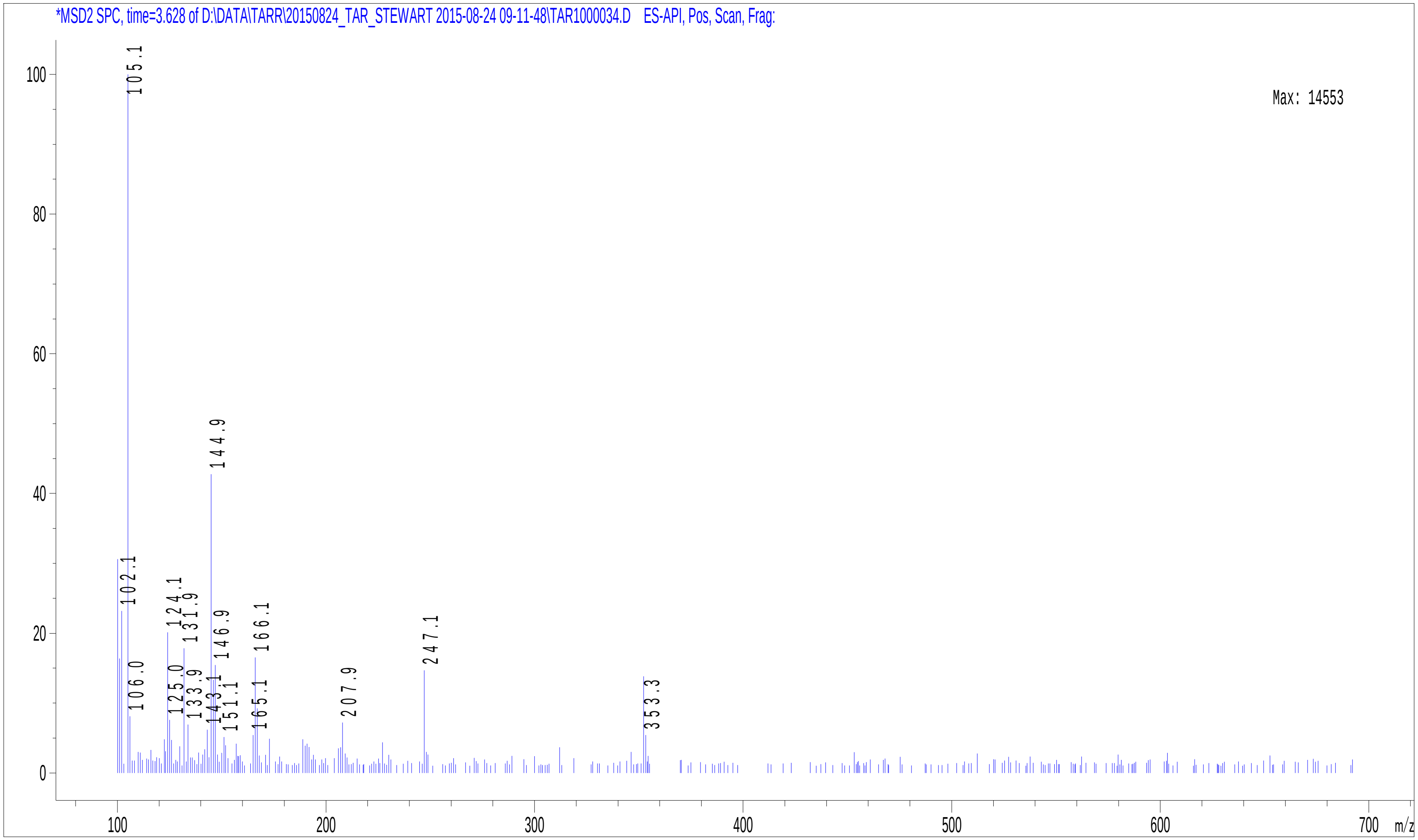


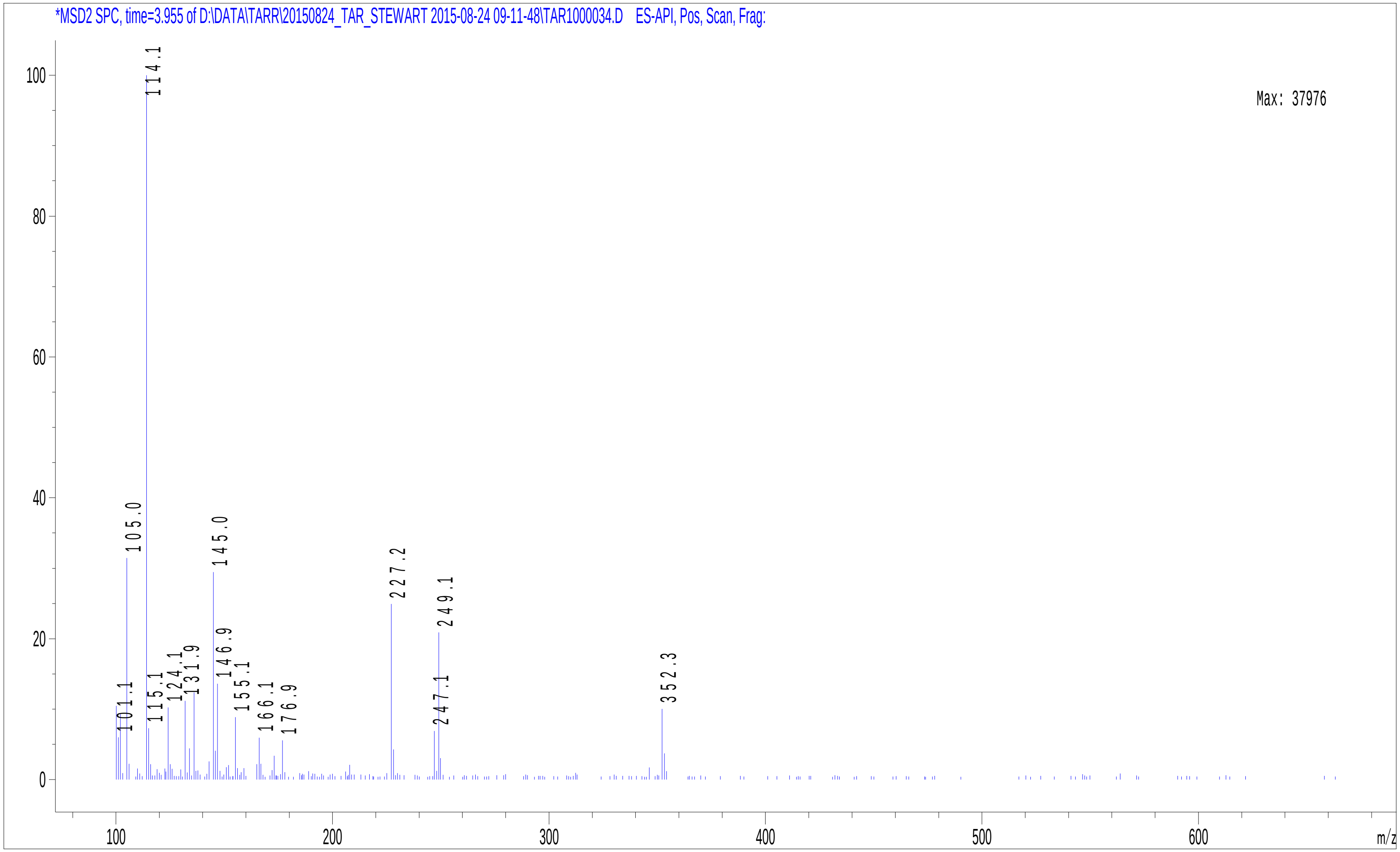
MSD2 TIC, MS File (D:\DATA\TARR\20150824_TAR_STEWART 2015-08-24 09-11-48\TAR1000034.D) ES-API, Pos, Scan, Frag: 70

#	Time	Area	Height	Width	Area%	Symmetry
1	3.096	1789004.9	206722.5	0.1442	61.708	0.649
2	3.612	223512.4	28431	0.131	7.710	0.512
3	3.927	886633.9	95430.3	0.1548	30.583	0.581


MSD2 TIC, MS File (D:\DATA\TARR\20150824_TAR_STEWART 2015-08-24 09-11-48\TAR1000034.D) ES-API, Pos, Scan, Frag: 70
Norm.
300000
275000
250000
225000
200000
175000
150000
125000
100000
3.096
Area: 1.789e+006
3.612
Area: 223512
3.927
Area: 886634
2.5
3
3.5
4
4.5
min


*MSD2 SPC, time=3.122 of D:\DATA\TARR\20150824_TAR_STEWART 2015-08-24 09-11-48\TAR1000034.D ES-API, Pos, Scan, Frag:
Max: 127792
105.0
106.1
132.0
145.0
226.9
0
20
40
60
80
100
100
200
300
400
500
600
700
m/z

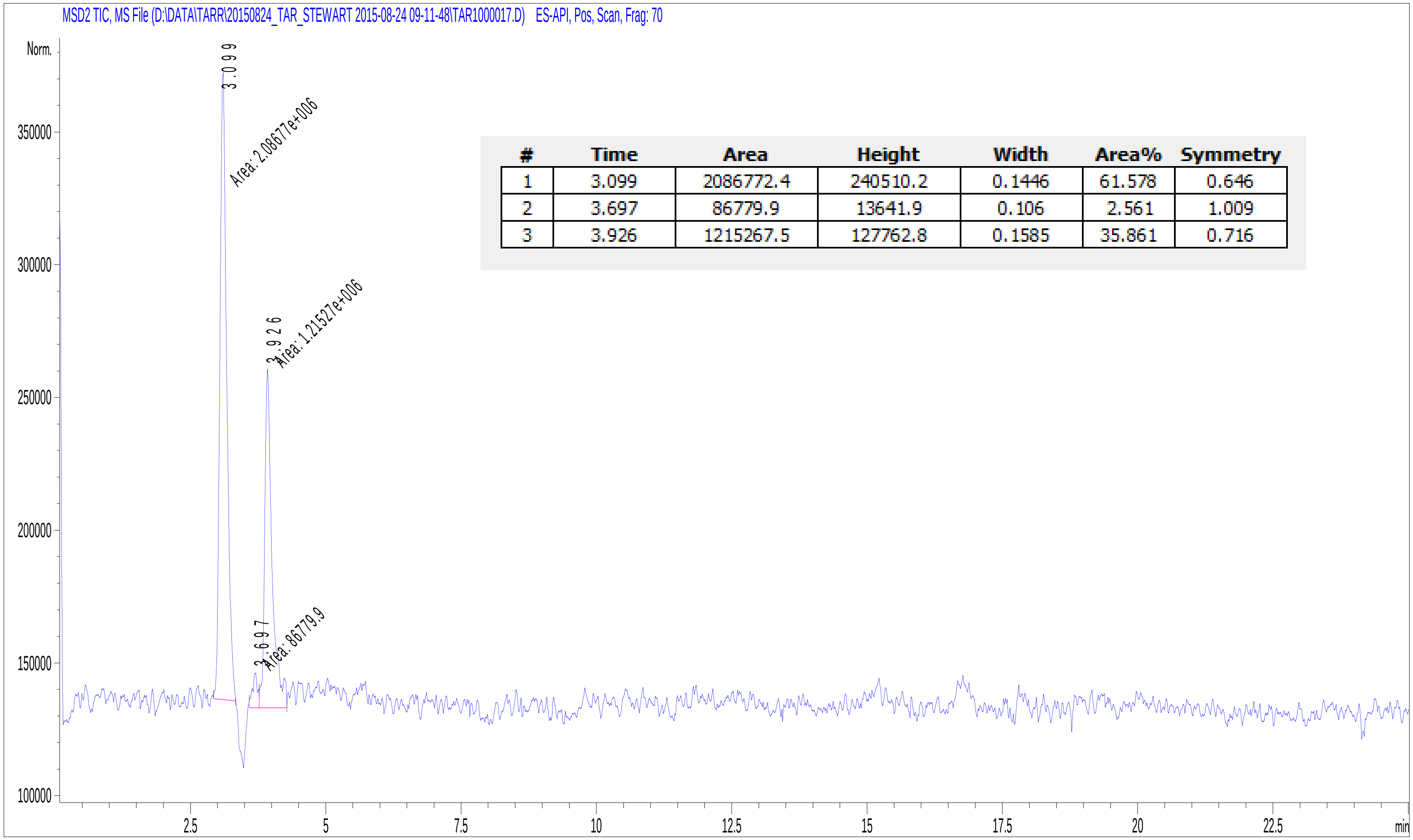

*MSD2 SPC, time=3.628 of D:\DATA\TARR\20150824_TAR_STEWART 2015-08-24 09-11-48\TAR1000034.D ES-API, Pos, Scan, Frag:
Max: 14553
105.1
144.9
102.1
124.1
131.9
146.9
166.1
106.0
125.0
133.9
143.1
151.1
165.1
207.9
247.1
353.3
0
20
40
60
80
100
100
200
300
400
500
600
700
m/z


*MSD2 SPC, time=3.955 of D:\DATA\TARR\20150824_TAR_STEWART 2015-08-24 09-11-48\TAR1000034.D ES-API, Pos, Scan, Frag:
Max: 37976
114.1
105.0
145.0
227.2
249.1
352.3
101.1
115.1
124.1
131.9
146.9
155.1
166.1
176.9
247.1
0
20
40
60
80
100
100
200
300
400
500
600
m/z

27-May-15

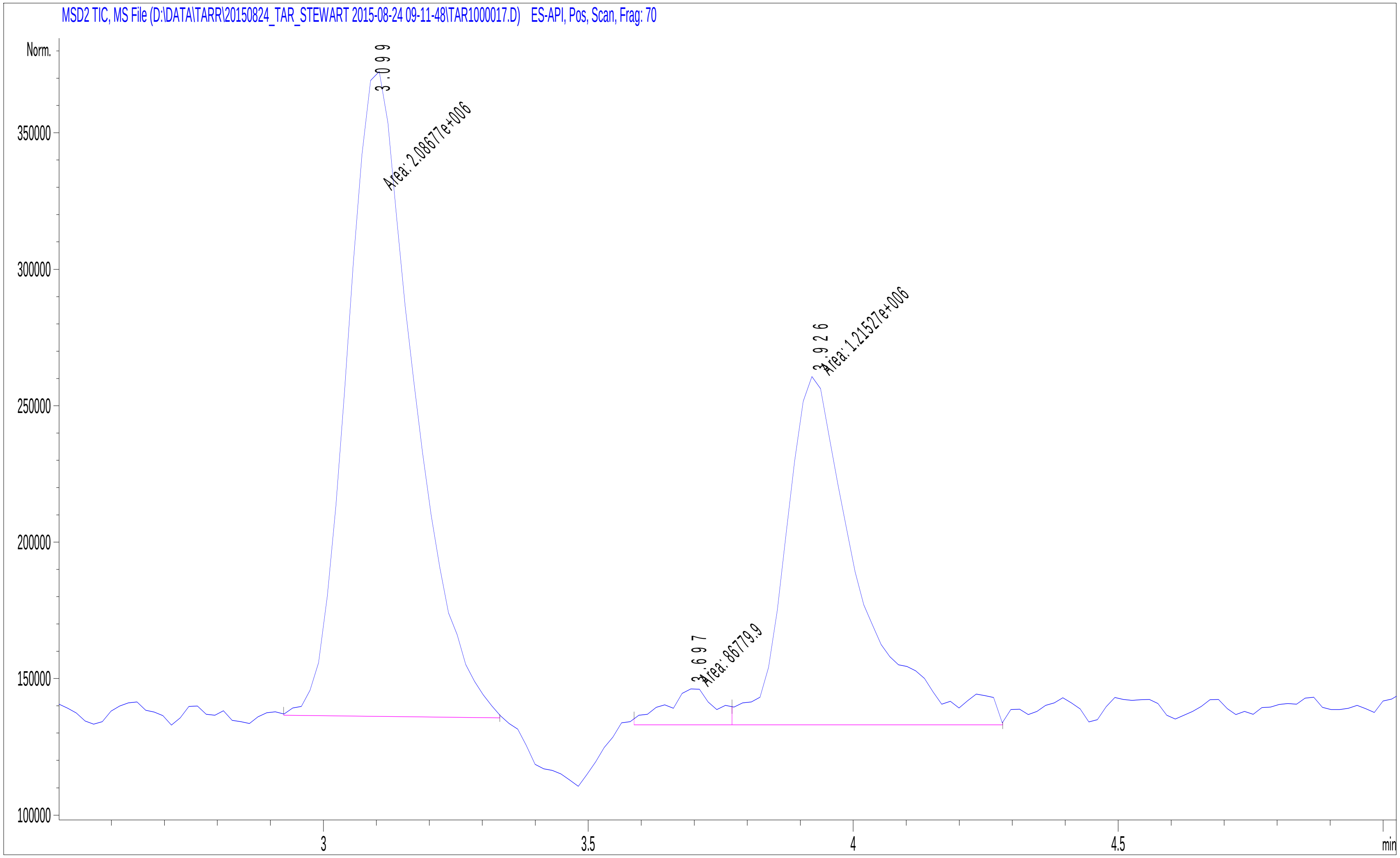
10 DC

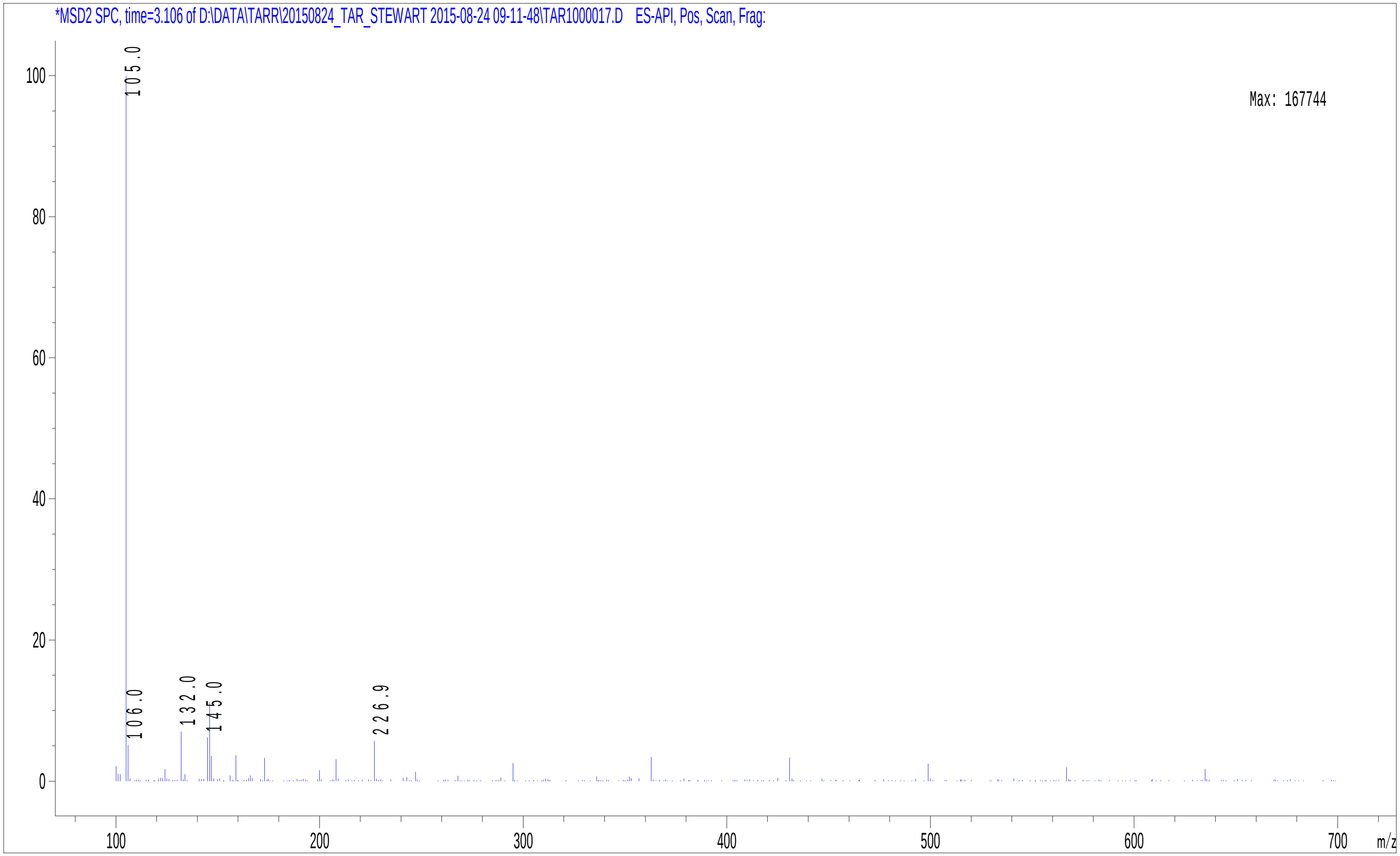
P2-B-02

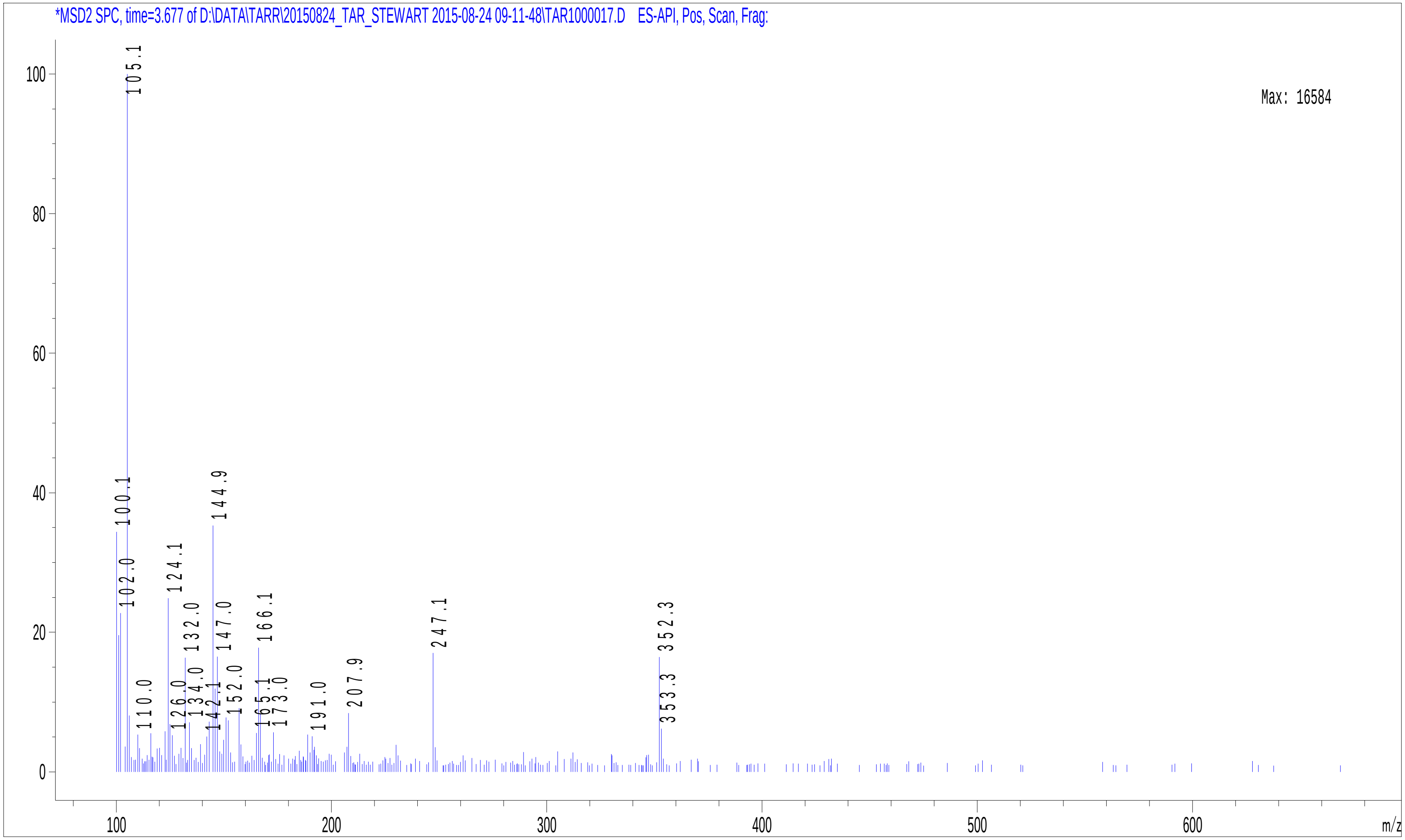


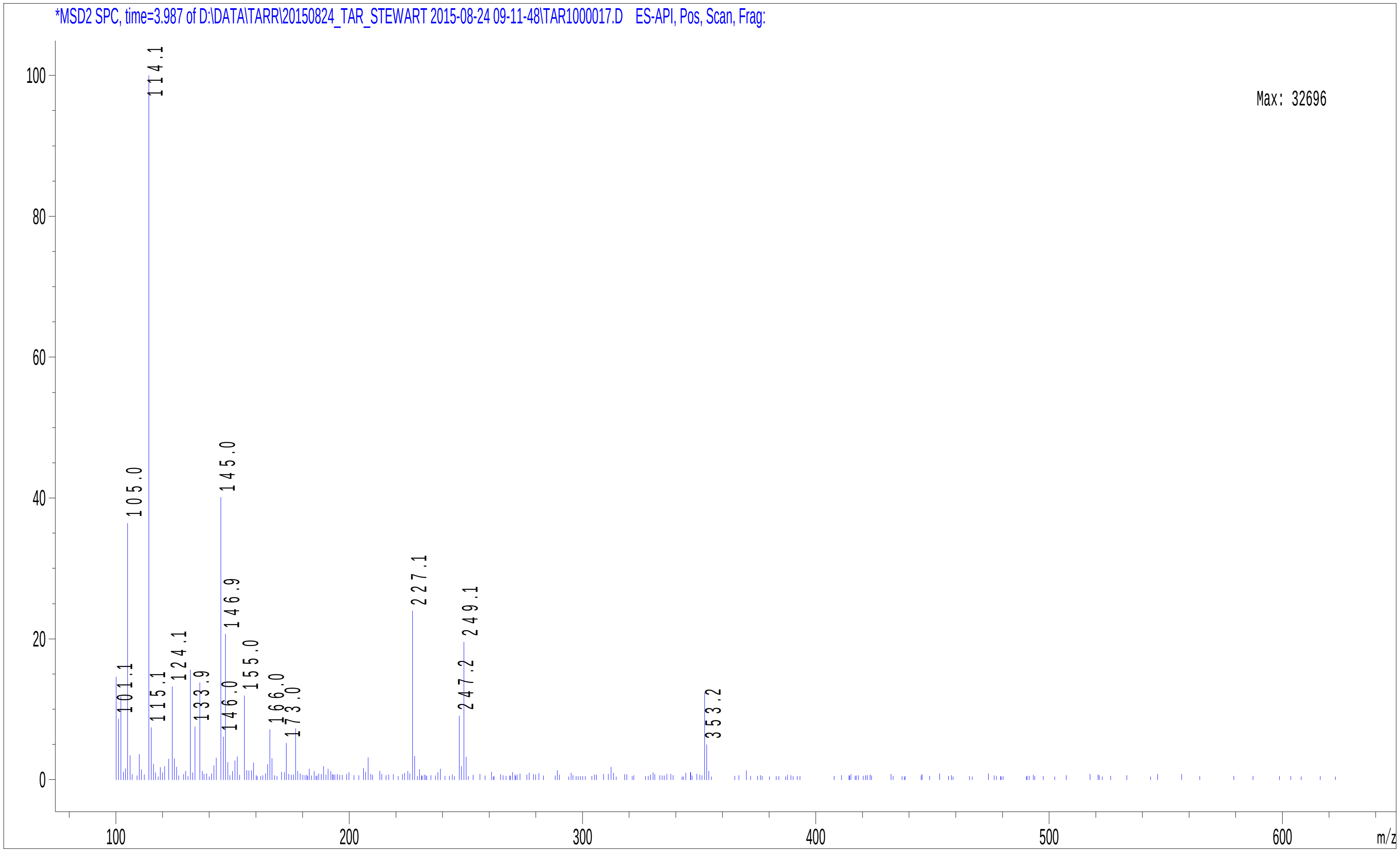
MSD2 TIC, MS File (D:\DATA\TARR\20150824_TAR_STEWART 2015-08-24 09-11-48\TAR1000017.D) ES-API, Pos, Scan, Frag: 70

#	Time	Area	Height	Width	Area%	Symmetry
1	3.099	2086772.4	240510.2	0.1446	61.578	0.646
2	3.697	86779.9	13641.9	0.106	2.561	1.009
3	3.926	1215267.5	127762.8	0.1585	35.861	0.716


MSD2 TIC, MS File (D:\DATA\TARR\20150824_TAR_STEWART 2015-08-24 09-11-48\TAR1000017.D) ES-API, Pos, Scan, Frag: 70
Norm.
350000
300000
250000
200000
150000
100000
3.099
Area: 2.08677e+006
3.697
Area: 86779.9
3.926
Area: 1.21527e+006
3
3.5
4
4.5
min


*MSD2 SPC, time=3.106 of D:\DATA\TARR\20150824_TAR_STEWART 2015-08-24 09-11-48\TAR1000017.D ES-API, Pos, Scan, Frag:
Max: 167744
105.0
106.0
132.0
145.0
226.9
100
80
60
40
20
0
100
200
300
400
500
600
700
m/z

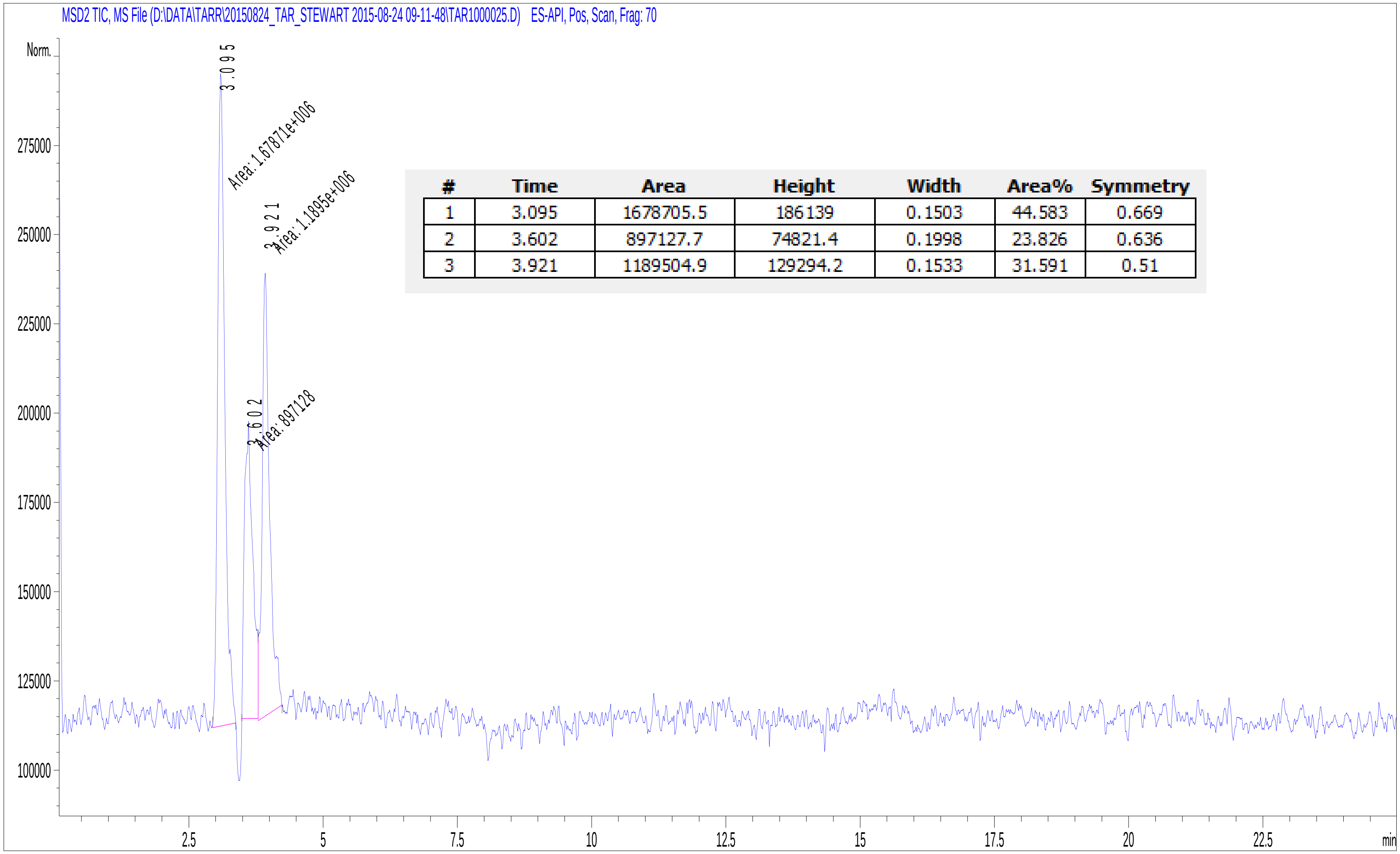

*MSD2 SPC, time=3.677 of D:\DATA\TARR\20150824_TAR_STEWART 2015-08-24 09-11-48\TAR1000017.D ES-API, Pos, Scan, Frag:
Max: 16584
105.1
100.1
144.9
102.0
124.1
132.0
147.0
166.1
247.1
352.3
207.9
110.0
126.0
134.0
142.1
152.0
165.1
173.0
191.0
353.3
0
20
40
60
80
100
100
200
300
400
500
600
m/z


*MSD2 SPC, time=3.987 of D:\DATA\TARR\20150824_TAR_STEWART 2015-08-24 09-11-48\TAR1000017.D ES-API, Pos, Scan, Frag:
Max: 32696
114.1
105.0
101.1
115.1
124.1
133.9
145.0
146.9
146.0
155.0
166.0
173.0
227.1
249.1
247.2
353.2
0
20
40
60
80
100
100
200
300
400
500
600
m/z

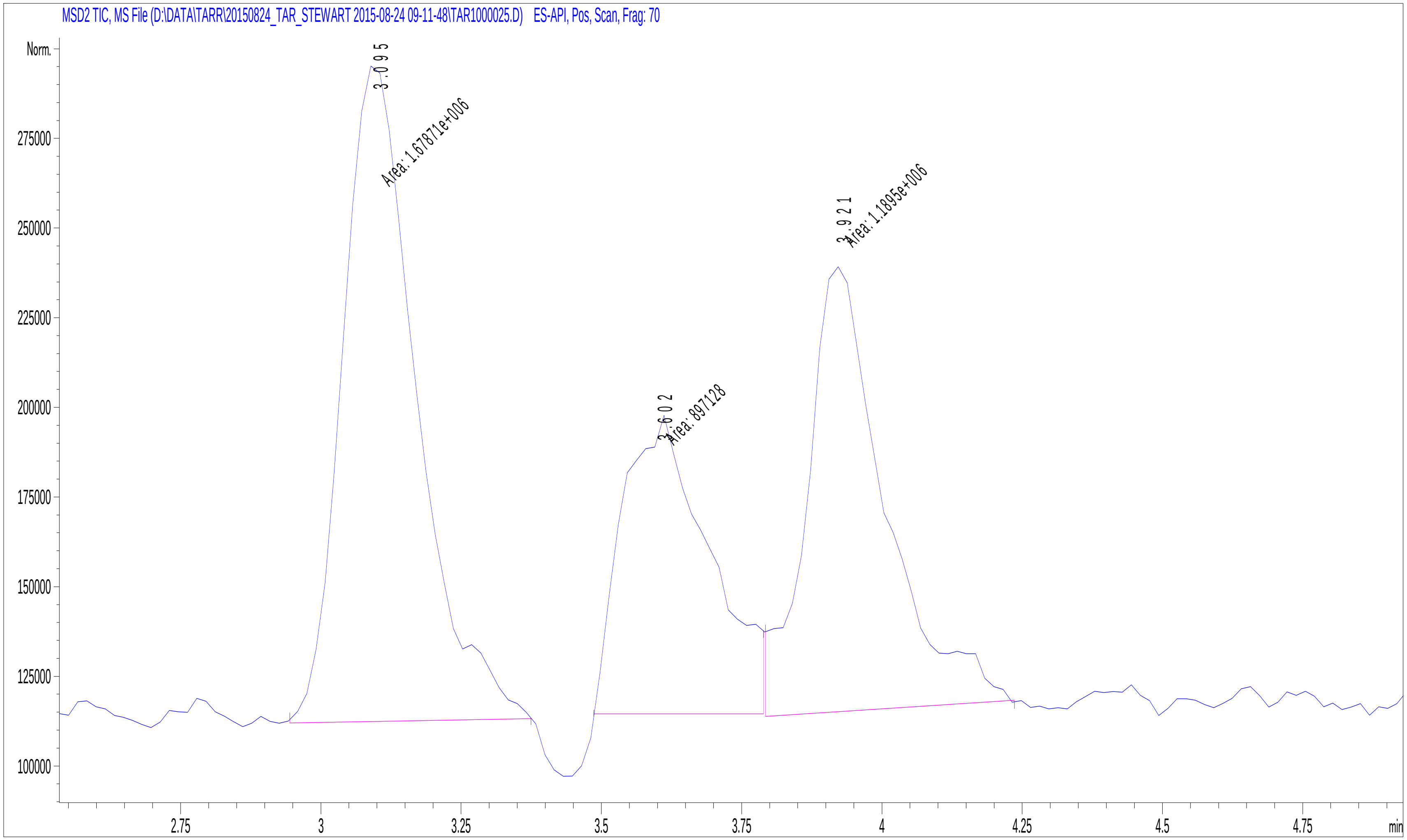
10-Jul-15

20 DC

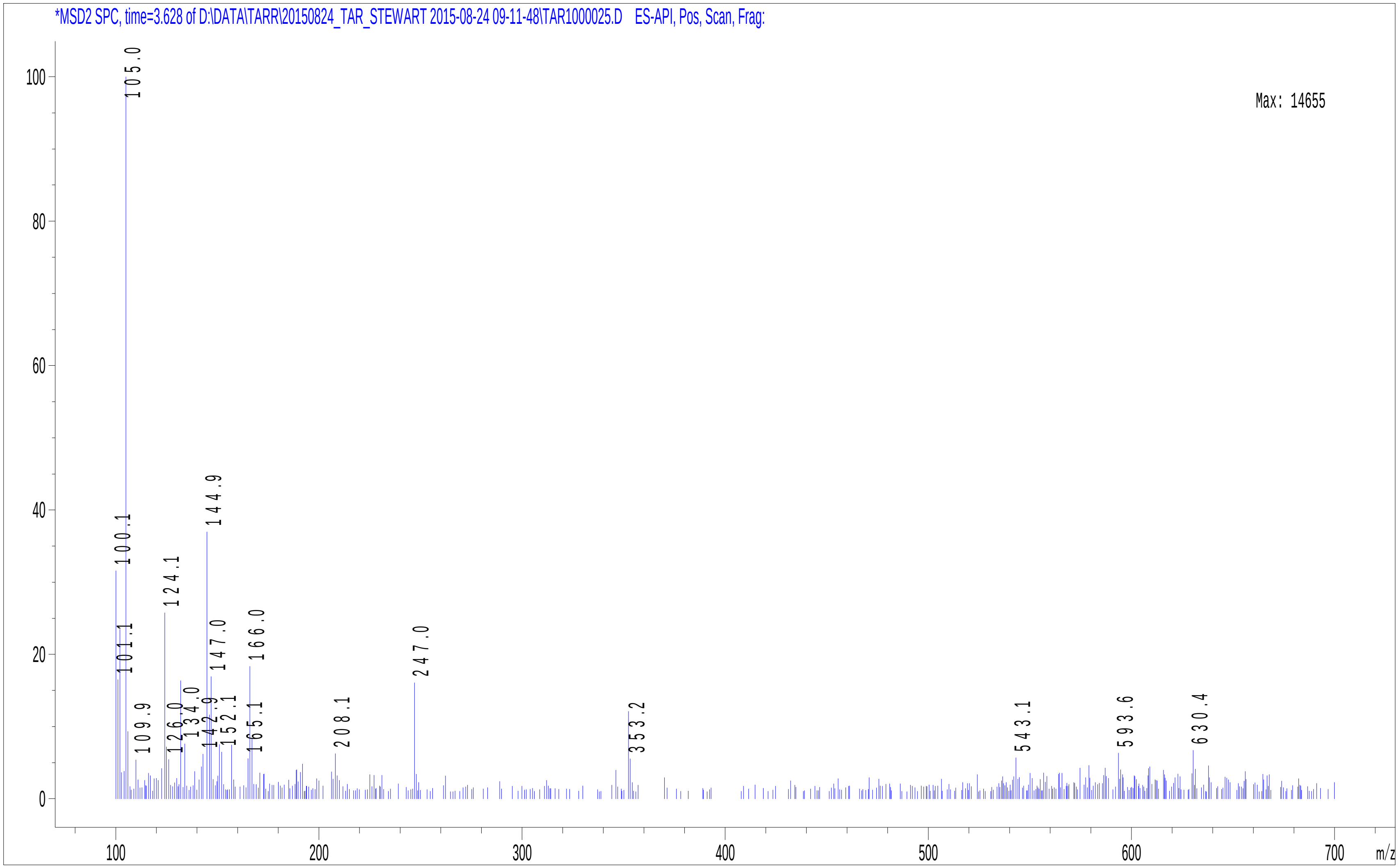
P2-C-07



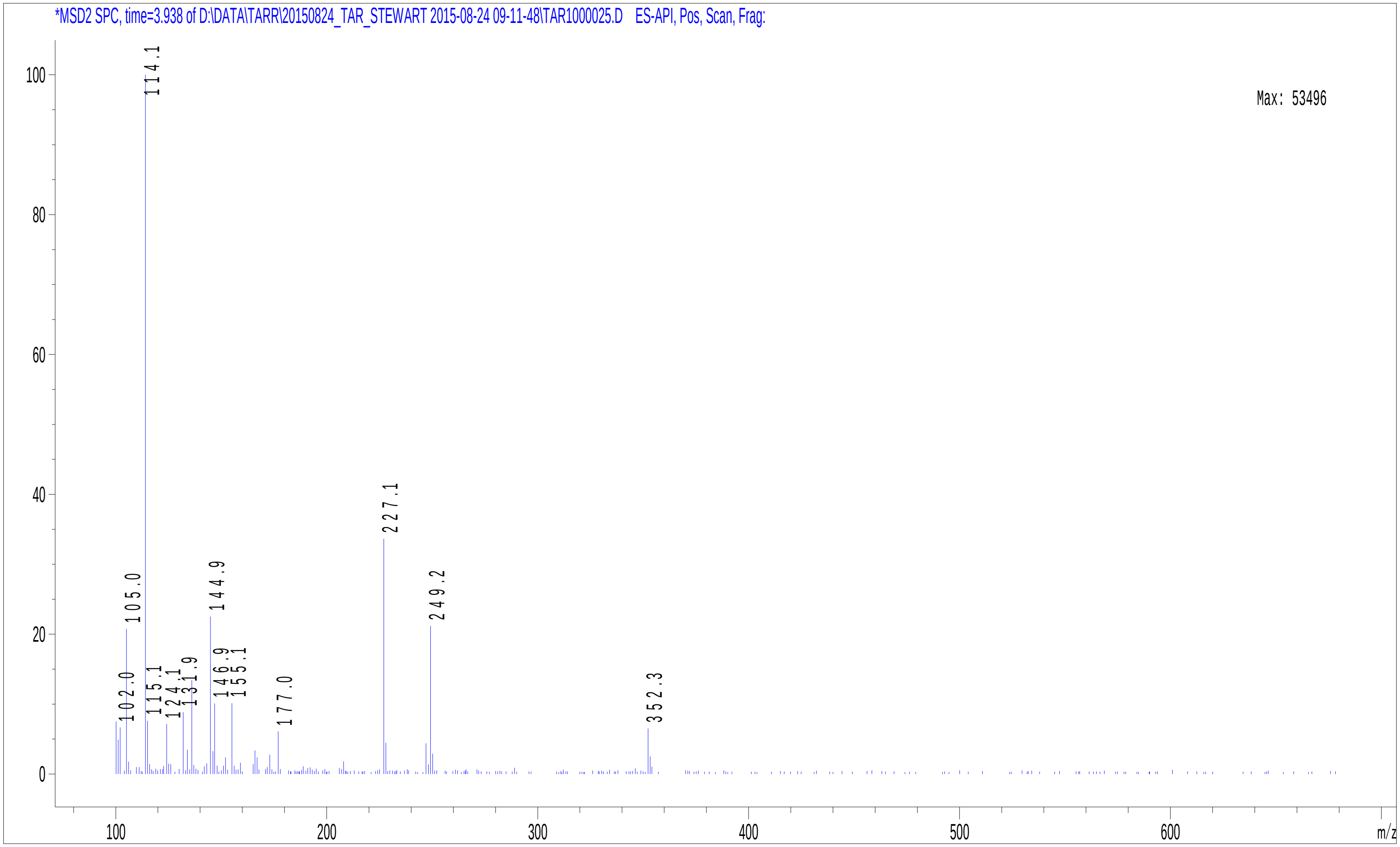
#	Time	Area	Height	Width	Area%	Symmetry
1	3.095	1678705.5	186139	0.1503	44.583	0.669
2	3.602	897127.7	74821.4	0.1998	23.826	0.636
3	3.921	1189504.9	129294.2	0.1533	31.591	0.51


MSD2 TIC, MS File (D:\DATA\TARR\20150824_TAR_STEWART 2015-08-24 09-11-48\TAR1000025.D)   ES-API, Pos, Scan, Frag: 70
Norm.
275000
250000
225000
200000
175000
150000
125000
100000
2.75
3
3.25
3.5
3.75
4
4.25
4.5
4.75
min
3.095
Area: 1.67871e+006
3.602
Area: 897128
3.921
Area: 1.1895e+006


*MSD2 SPC, time=3.122 of D:\DATA\TARR\20150824_TAR_STEWART 2015-08-24 09-11-48\TAR1000025.D ES-API, Pos, Scan, Frag:
Max: 116248
105.0
106.0
132.0
145.0
100
80
60
40
20
0
100
200
300
400
500
600
700
m/z



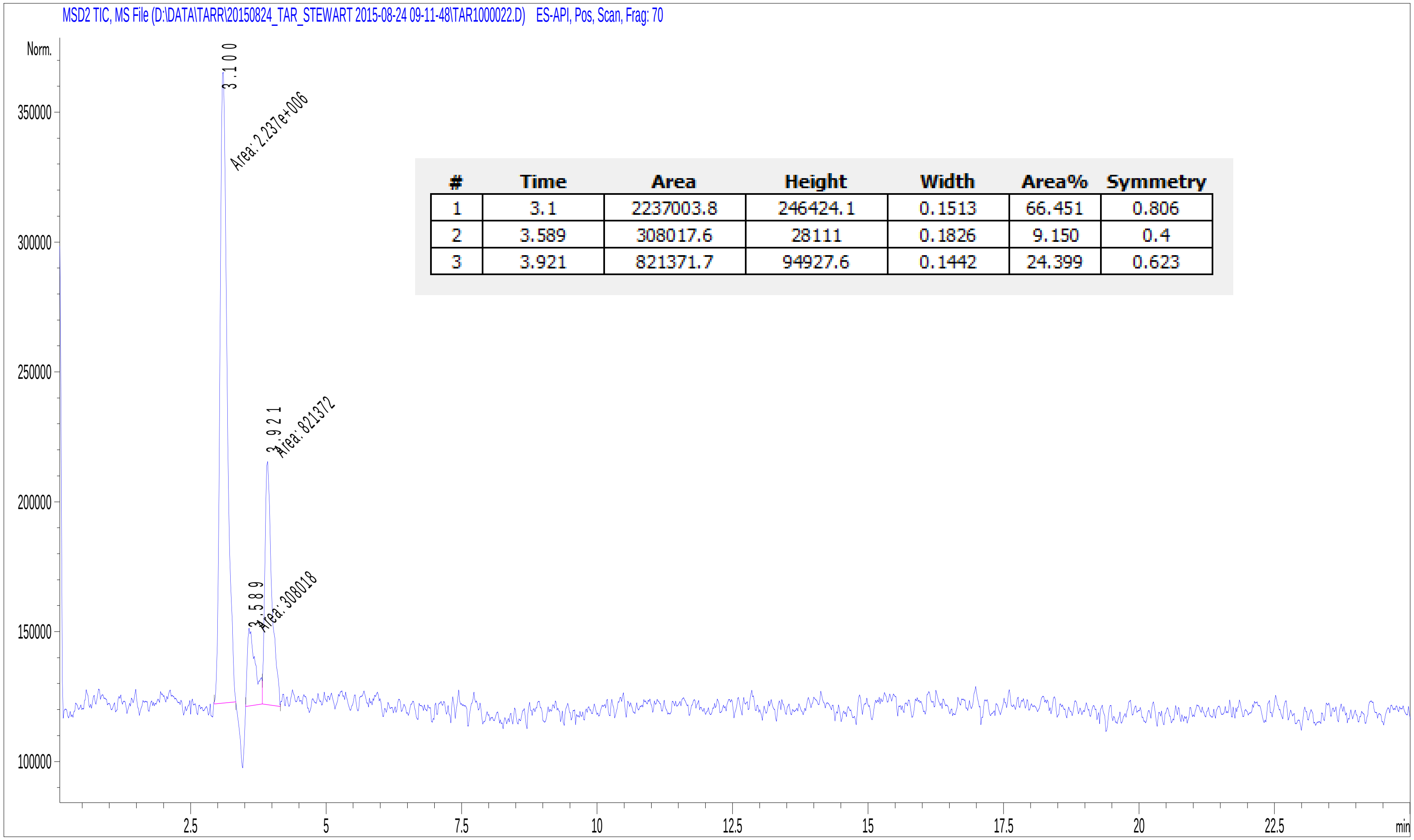
*MSD2 SPC, time=3.628 of D:\DATA\TARR\20150824_TAR_STEWART 2015-08-24 09-11-48\TAR1000025.D ES-API, Pos, Scan, Frag:
Max: 14655
105.0
100.1
101.1
109.9
124.1
126.0
134.0
142.9
144.9
147.0
152.1
165.1
166.0
208.1
247.0
353.2
543.1
593.6
630.4
0
20
40
60
80
100
100
200
300
400
500
600
700
m/z


*MSD2 SPC, time=3.938 of D:\DATA\TARR\20150824_TAR_STEWART 2015-08-24 09-11-48\TAR1000025.D ES-API, Pos, Scan, Frag:
Max: 53496
100
80
60
40
20
0
114.1
105.0
102.0
115.1
124.1
131.9
144.9
146.9
155.1
177.0
227.1
249.2
352.3
100
200
300
400
500
600
m/z

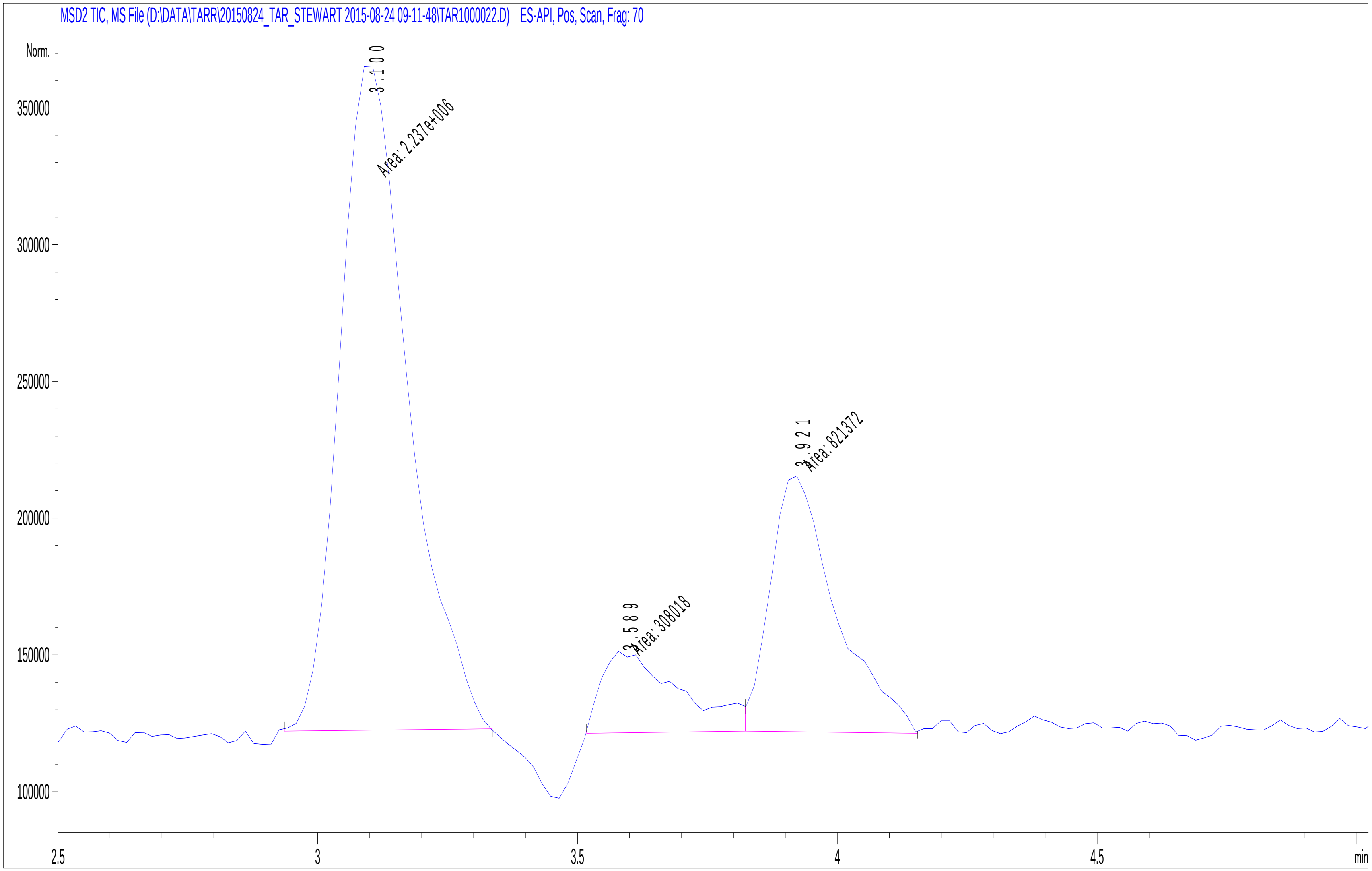
2-Jul-15

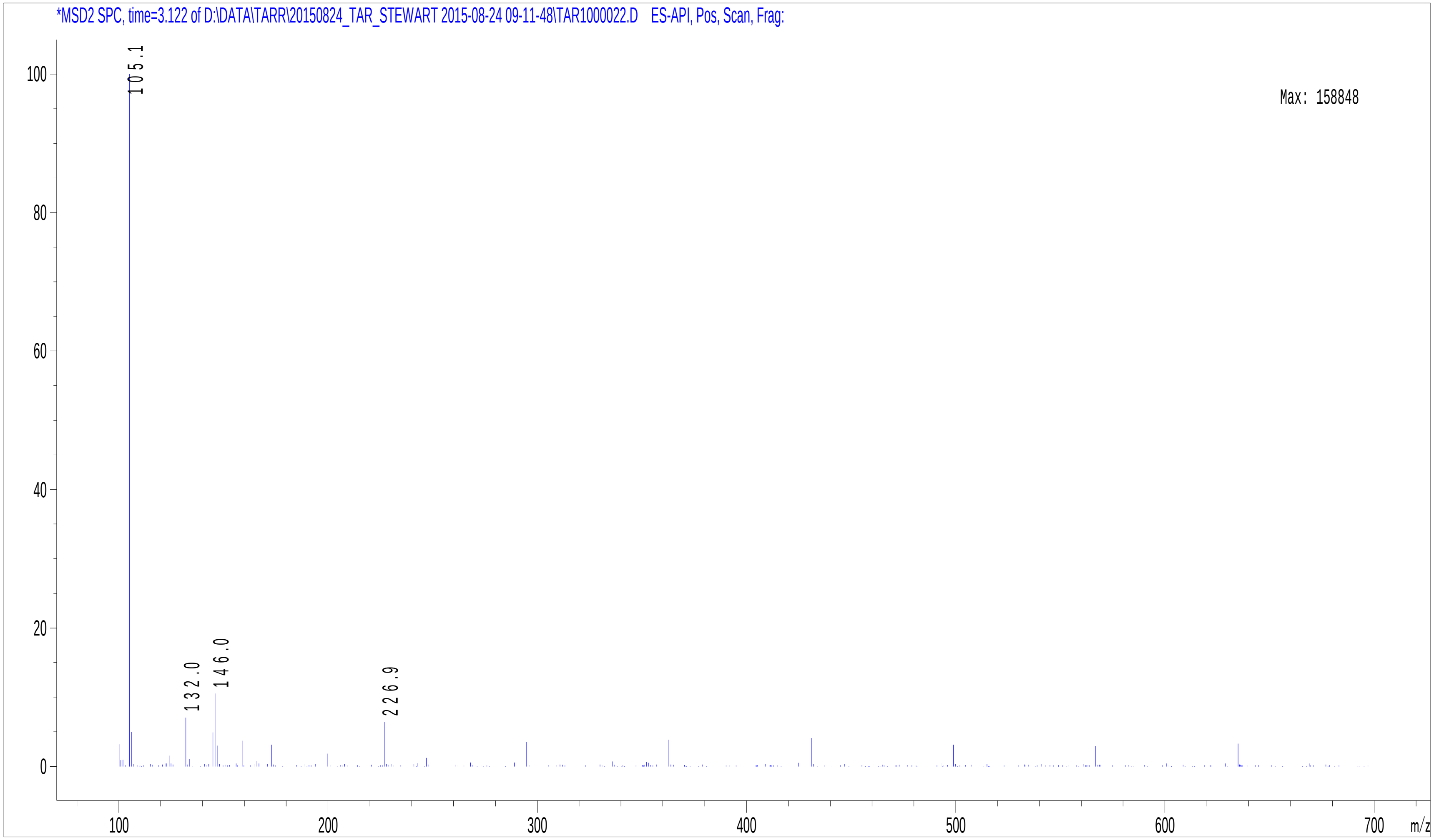
30 DC

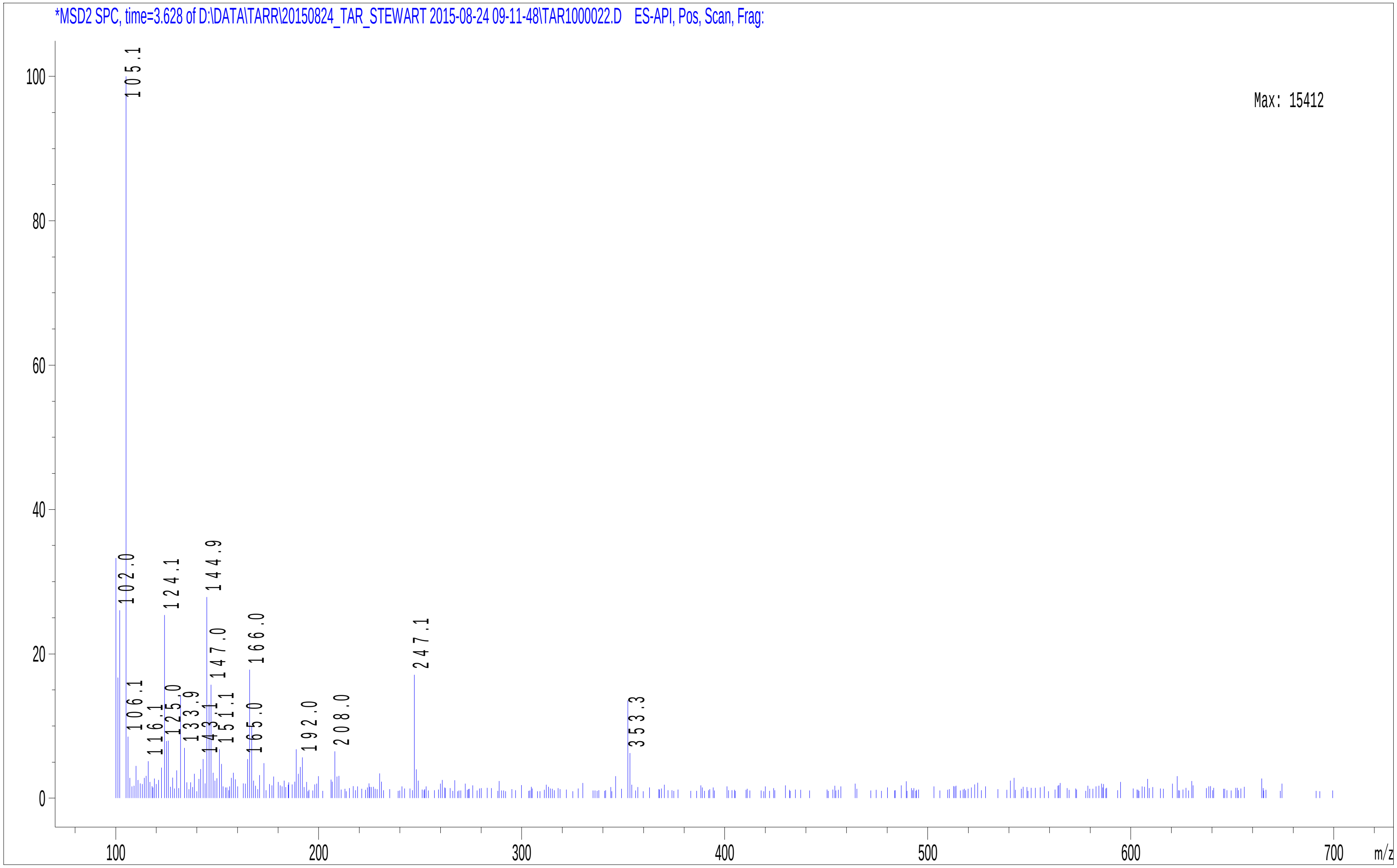
P2-C-04

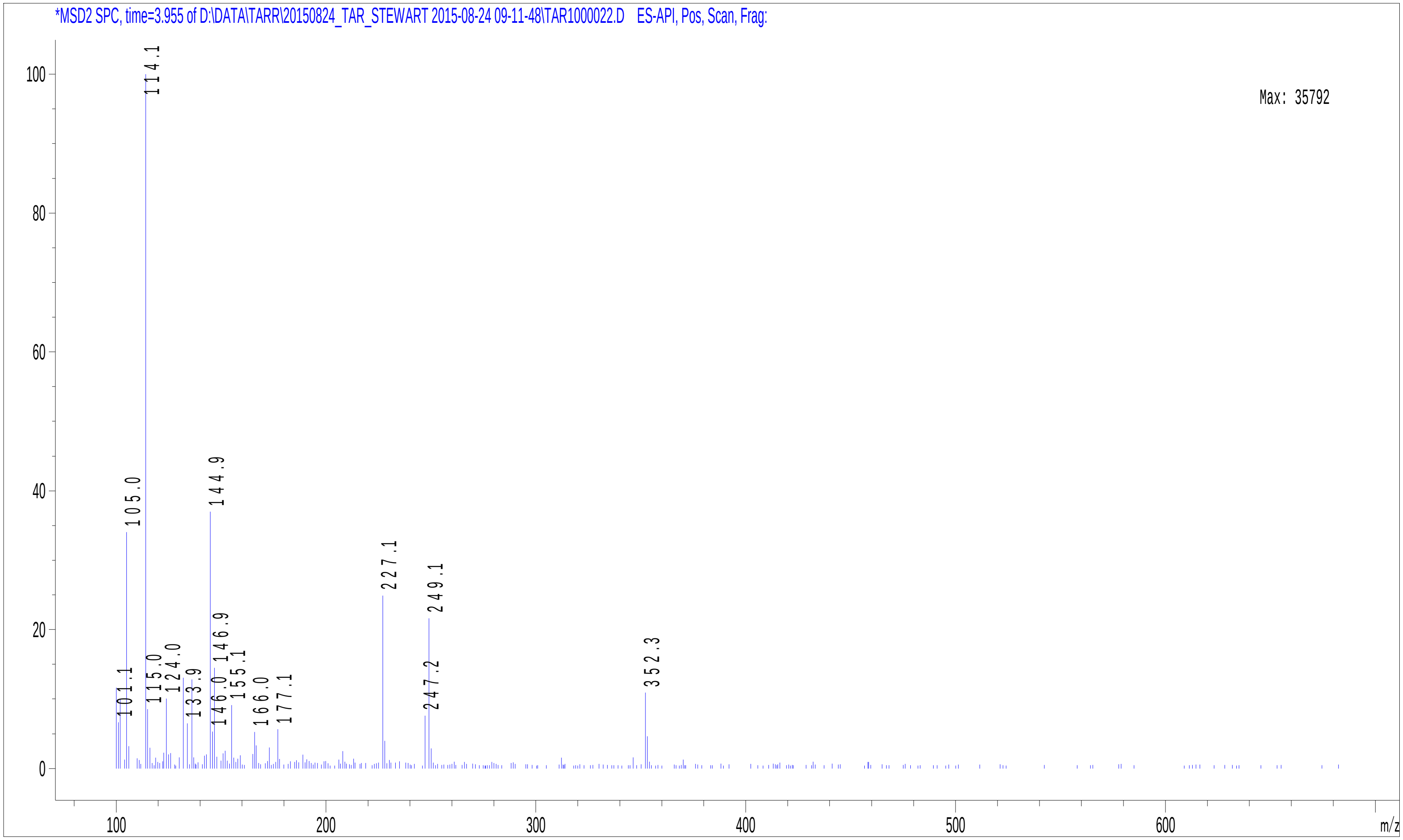


#	Time	Area	Height	Width	Area%	Symmetry
1	3.1	2237003.8	246424.1	0.1513	66.451	0.806
2	3.589	308017.6	28111	0.1826	9.150	0.4
3	3.921	821371.7	94927.6	0.1442	24.399	0.623


MSD2 TIC, MS File (D:\DATA\TARR\20150824_TAR_STEWART 2015-08-24 09-11-48\TAR1000022.D) ES-API, Pos, Scan, Frag: 70
Norm.
350000
300000
250000
200000
150000
100000
3.100
Area: 2.237e+006
3.589
Area: 308018
3.921
Area: 821372
2.5
3
3.5
4
4.5
min


*MSD2 SPC, time=3.122 of D:\DATA\TARR\20150824_TAR_STEWART 2015-08-24 09-11-48\TAR1000022.D ES-API, Pos, Scan, Frag:
Max: 158848
105.1
132.0
146.0
226.9
0
20
40
60
80
100
100
200
300
400
500
600
700
m/z

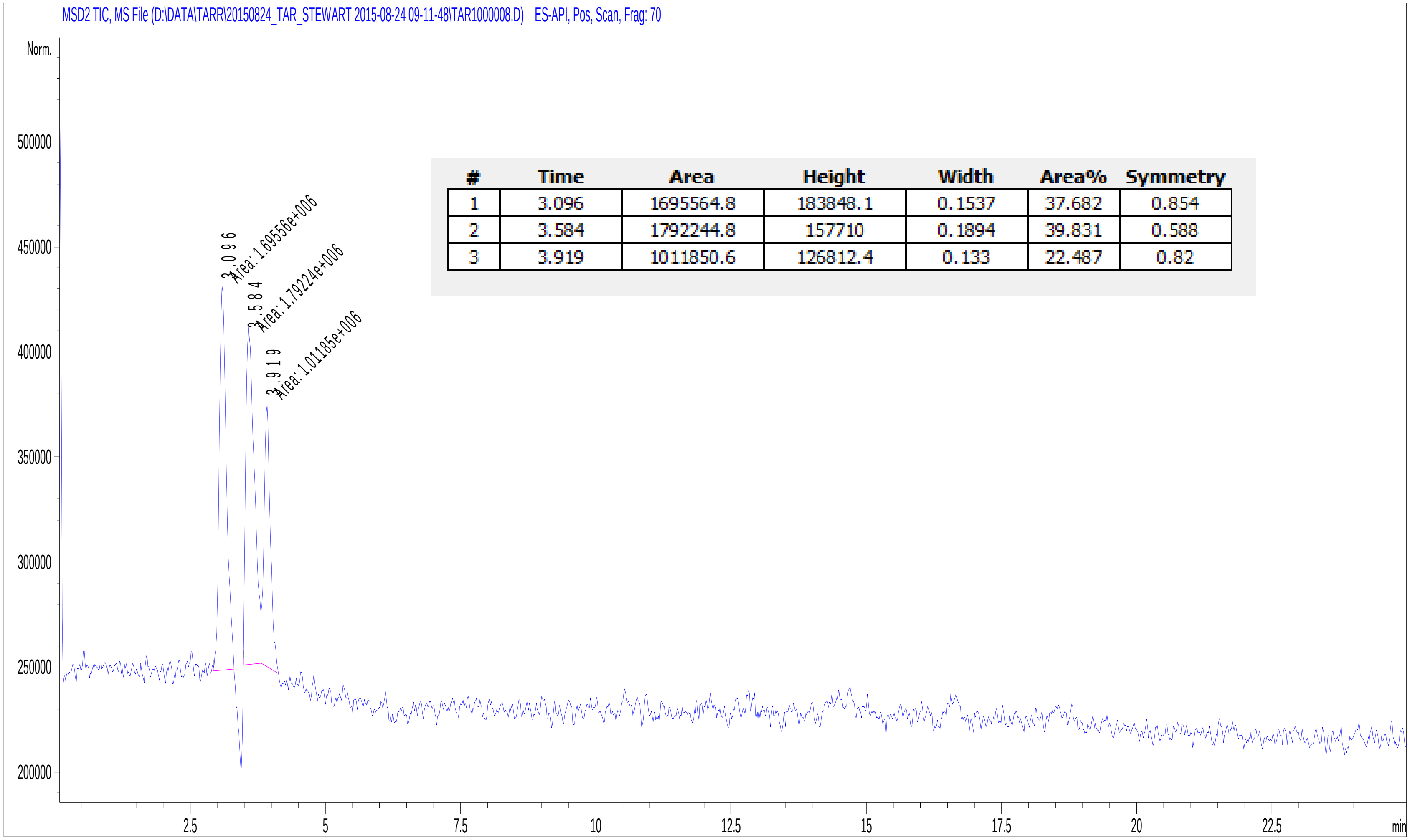

*MSD2 SPC, time=3.628 of D:\DATA\TARR\20150824_TAR_STEWART 2015-08-24 09-11-48\TAR1000022.D ES-API, Pos, Scan, Frag:
Max: 15412
105.1
102.0
106.1
116.1
124.1
125.0
133.9
143.1
144.9
147.0
151.1
165.0
166.0
192.0
208.0
247.1
353.3
0
20
40
60
80
100
100
200
300
400
500
600
700
m/z


*MSD2 SPC, time=3.955 of D:\DATA\TARR\20150824_TAR_STEWART 2015-08-24 09-11-48\TAR1000022.D   ES-API, Pos, Scan, Frag:
Max: 35792
114.1
105.0
144.9
227.1
249.1
146.9
352.3
124.0
115.0
155.1
133.9
101.1
146.0
247.2
177.1
166.0
0
20
40
60
80
100
100
200
300
400
500
600
m/z

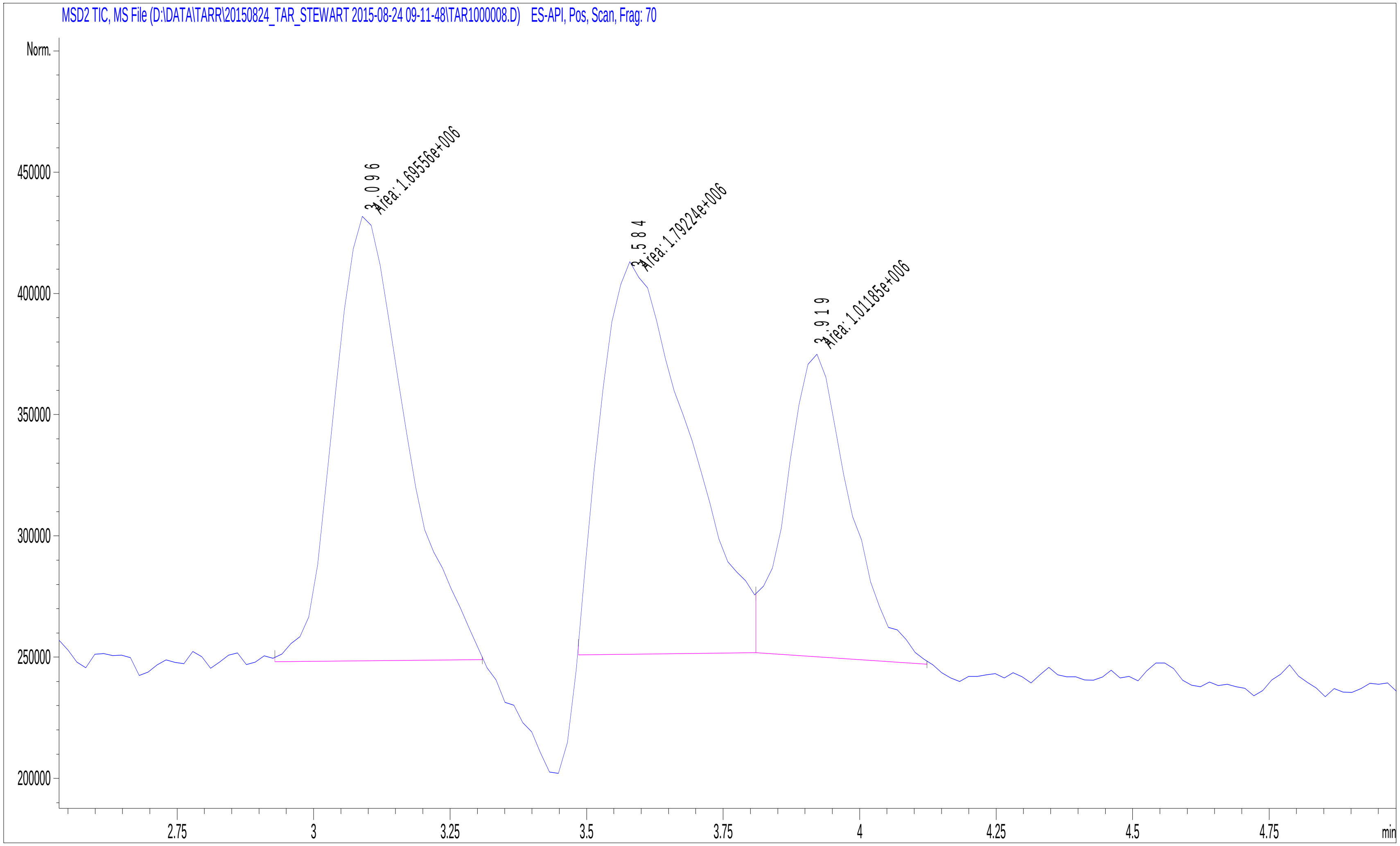
23-Apr-15

50 DC

P2-A-08

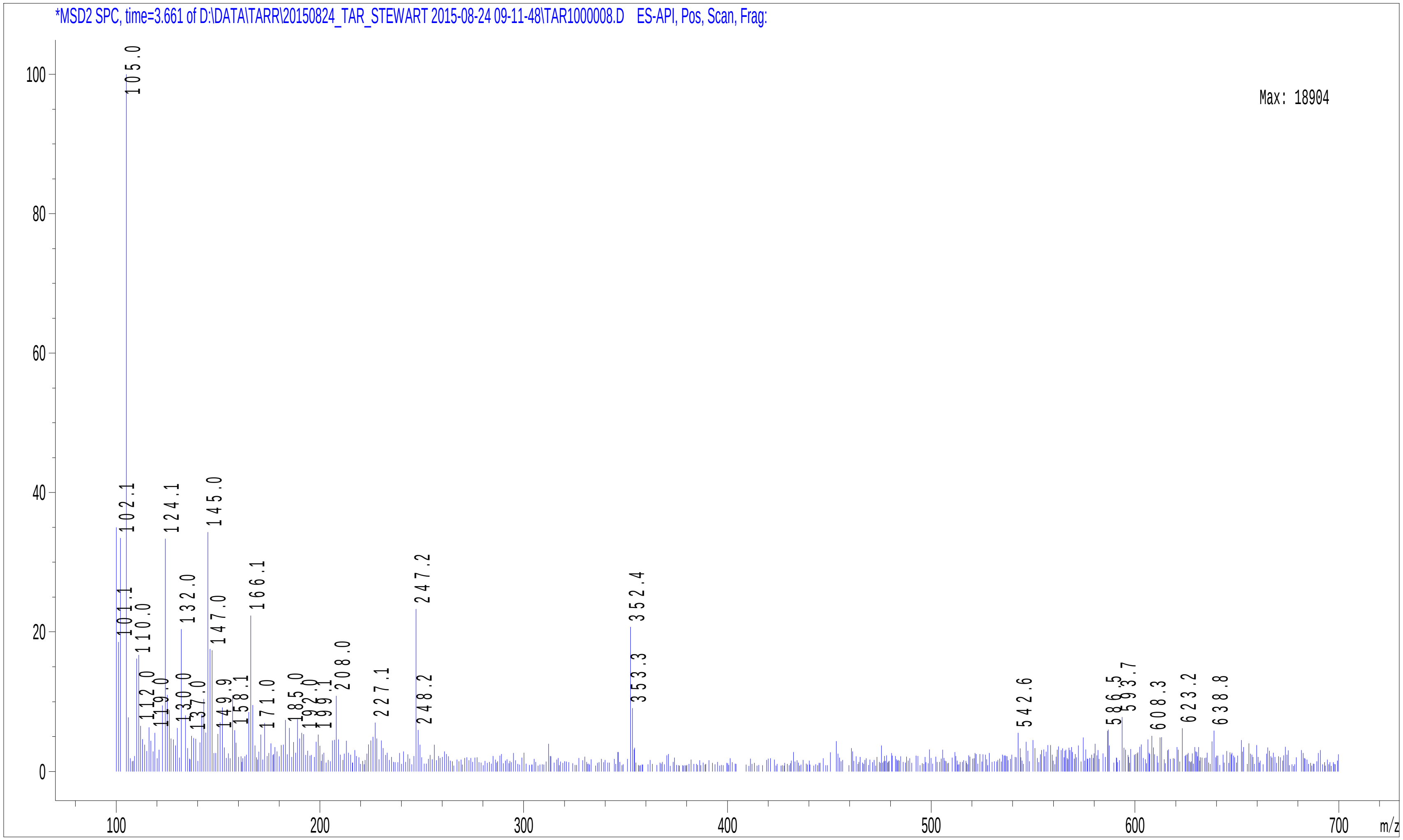


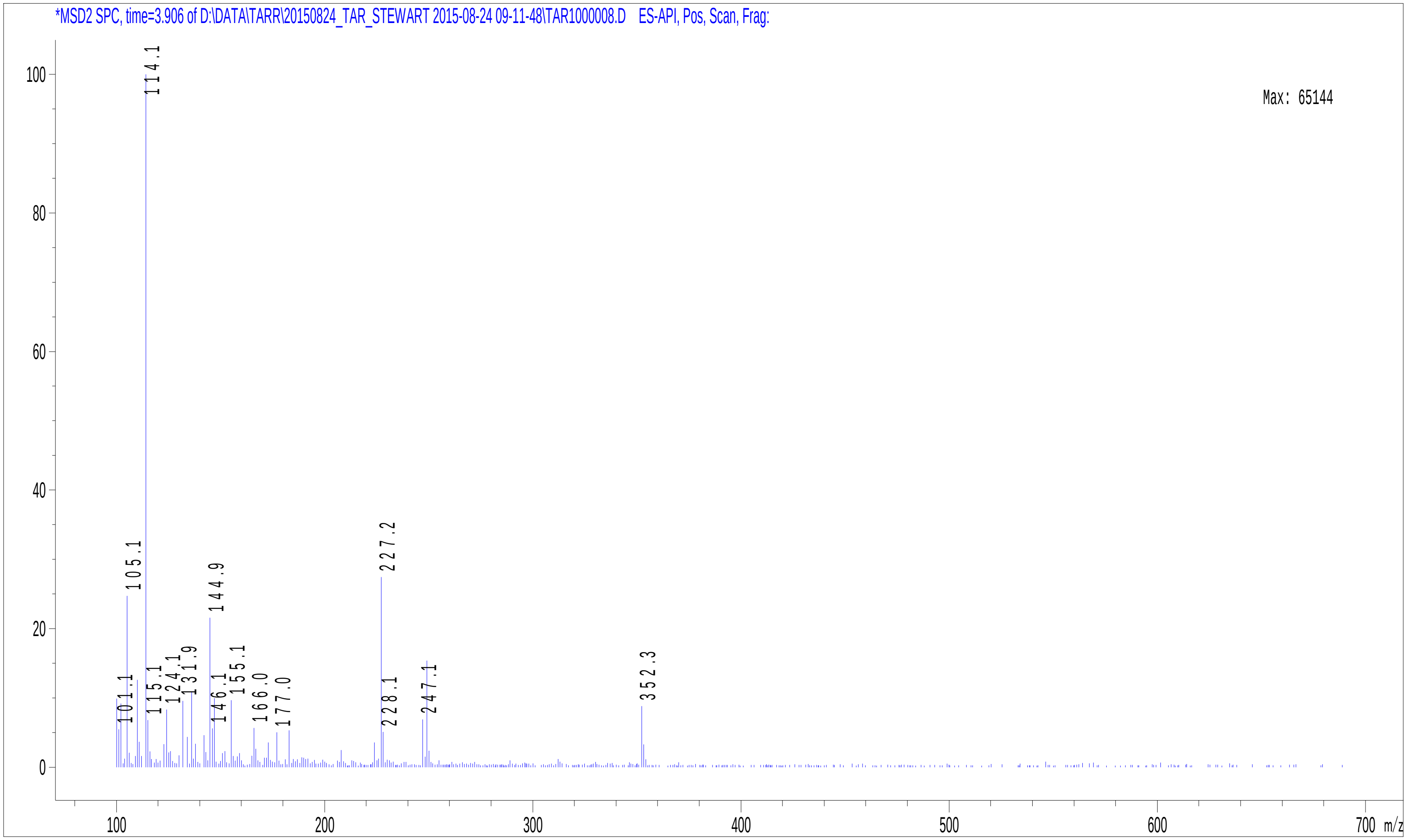
#	Time	Area	Height	Width	Area%	Symmetry
1	3.096	1695564.8	183848.1	0.1537	37.682	0.854
2	3.584	1792244.8	157710	0.1894	39.831	0.588
3	3.919	1011850.6	126812.4	0.133	22.487	0.82



MSD2 TIC, MS File (D:\DATA\TARR\20150824_TAR_STEWART 2015-08-24 09-11-48\TAR1000008.D) ES-API, Pos, Scan, Frag: 70
Norm.
450000
400000
350000
300000
250000
200000
3.096
Area: 1.69556e+006
3.584
Area: 1.79224e+006
3.919
Area: 1.01185e+006
2.75
3
3.25
3.5
3.75
4
4.25
4.5
4.75
min


*MSD2 SPC, time=3.105 of D:\DATA\TARR\20150824_TAR_STEWART 2015-08-24 09-11-48\TAR1000008.D ES-API, Pos, Scan, Frag:
Max: 141696
105.1
100.1
106.1
132.0
145.0
100
80
60
40
20
0
100
200
300
400
500
600
700
m/z

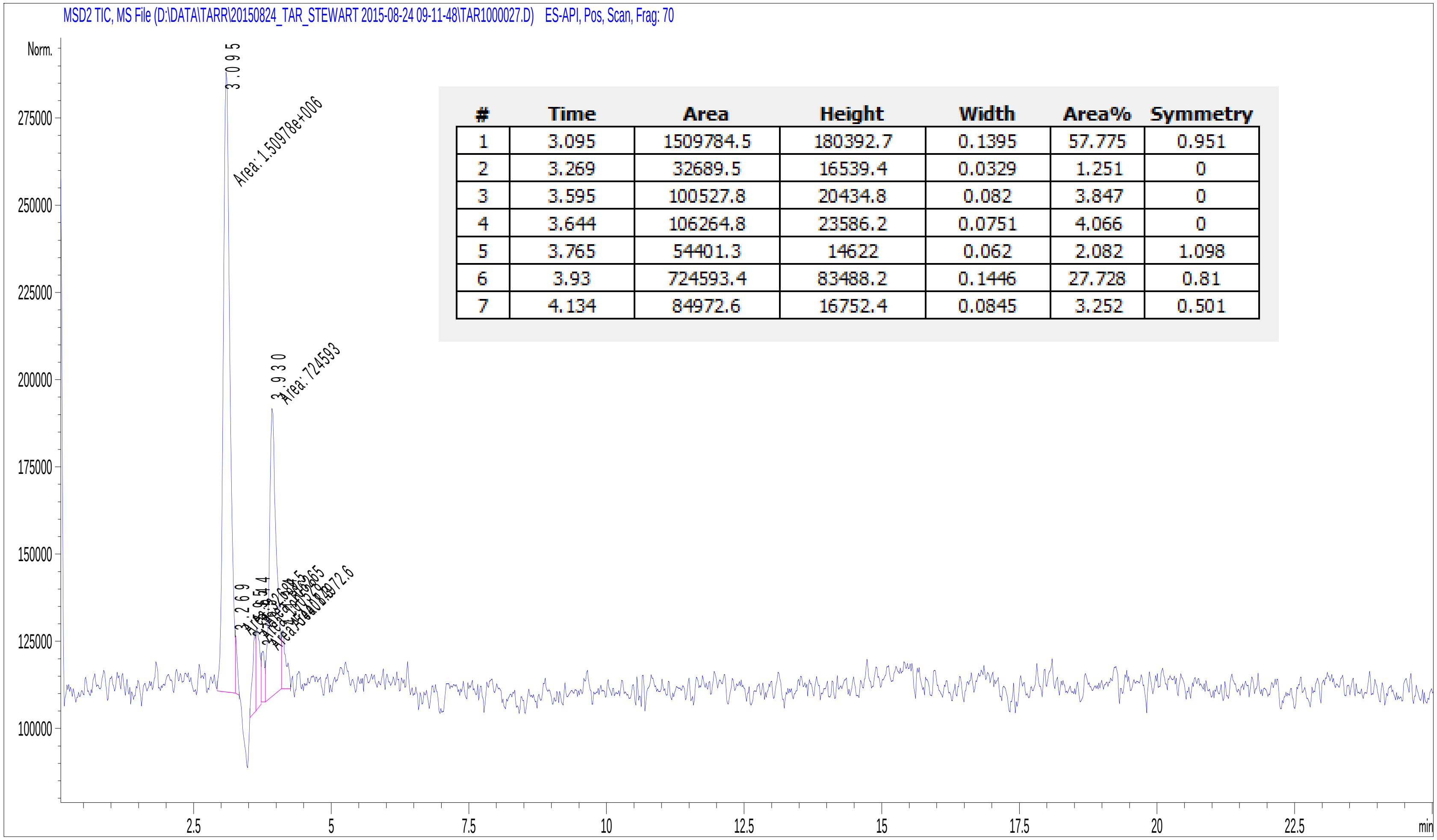

*MSD2 SPC, time=3.661 of D:\DATA\TARR\20150824_TAR_STEWART 2015-08-24 09-11-48\TAR1000008.D ES-API, Pos, Scan, Frag:
Max: 18904
105.0
102.1
101.1
110.0
112.0
119.0
124.1
130.0
132.0
137.0
145.0
147.0
149.9
158.1
166.1
171.0
185.0
192.0
199.1
208.0
227.1
247.2
248.2
352.4
353.3
542.6
586.5
593.7
608.3
623.2
638.8
100
80
60
40
20
0
100
200
300
400
500
600
700
m/z


*MSD2 SPC, time=3.906 of D:\DATA\TARR\20150824_TAR_STEWART 2015-08-24 09-11-48\TAR1000008.D ES-API, Pos, Scan, Frag:
Max: 65144
114.1
105.1
144.9
227.2
101.1
115.1
124.1
131.9
146.1
155.1
166.0
177.0
228.1
247.1
352.3
0
20
40
60
80
100
100
200
300
400
500
600
700
m/z

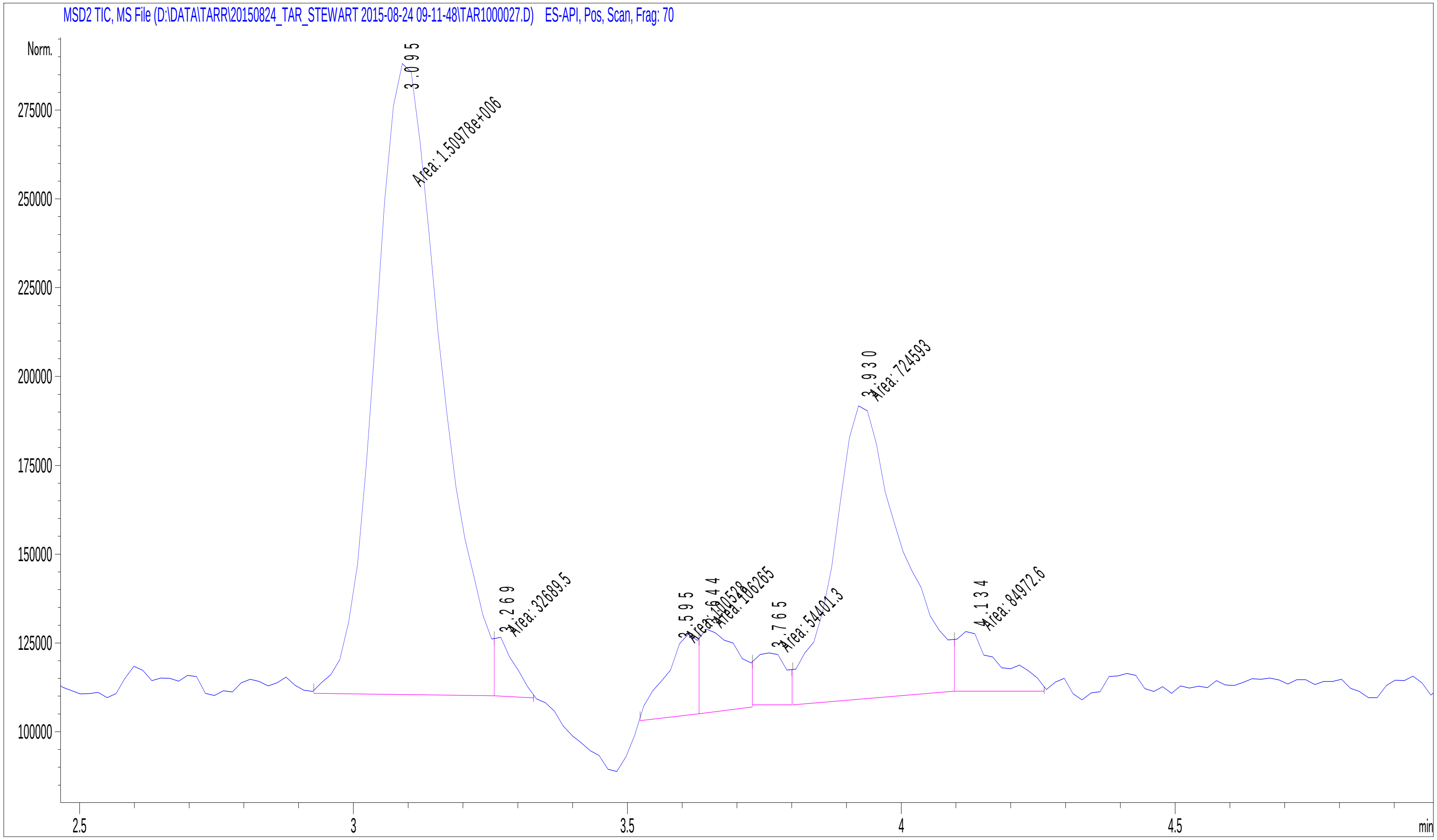
9-Jul-15

70 DC

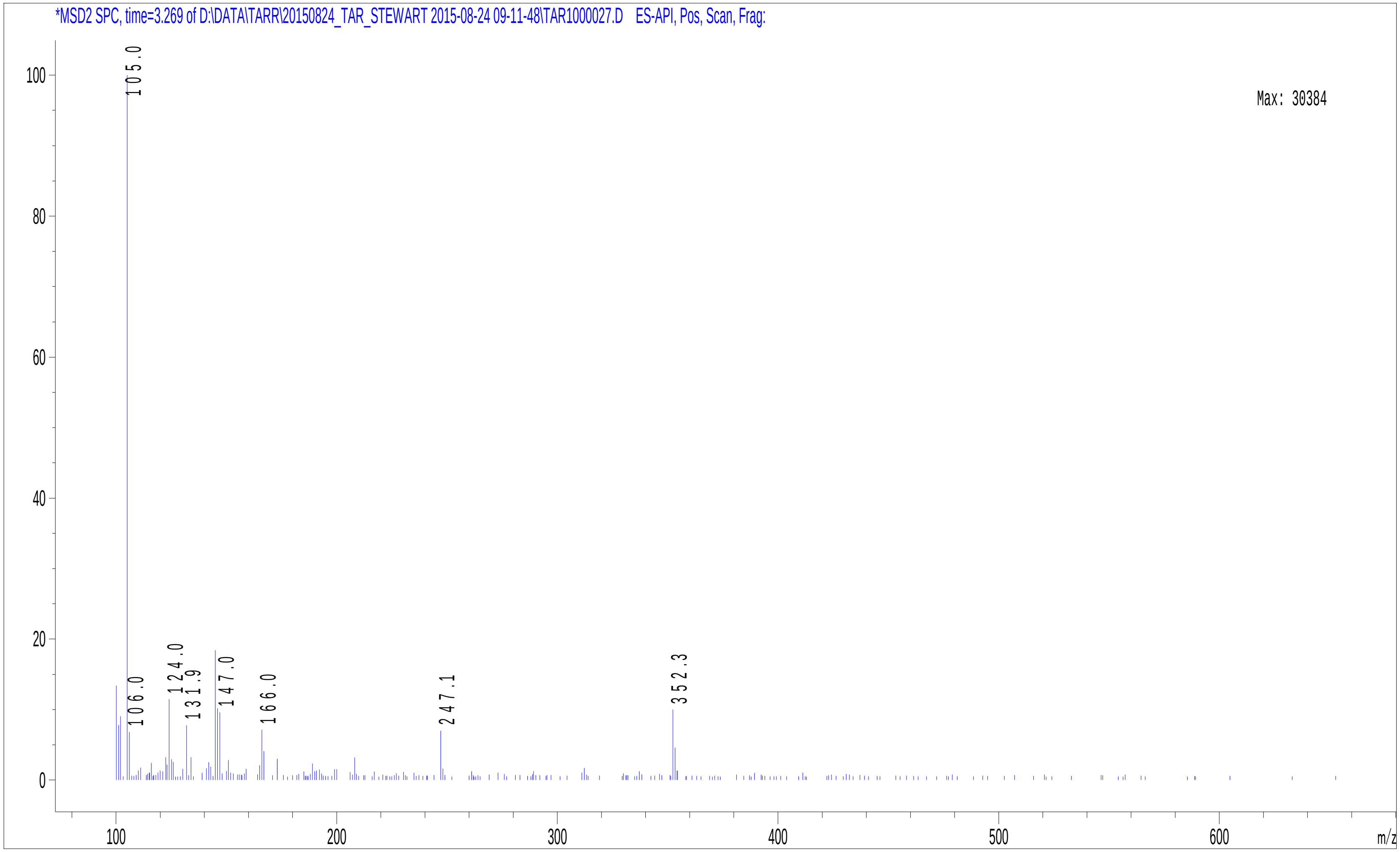
P2-C-09

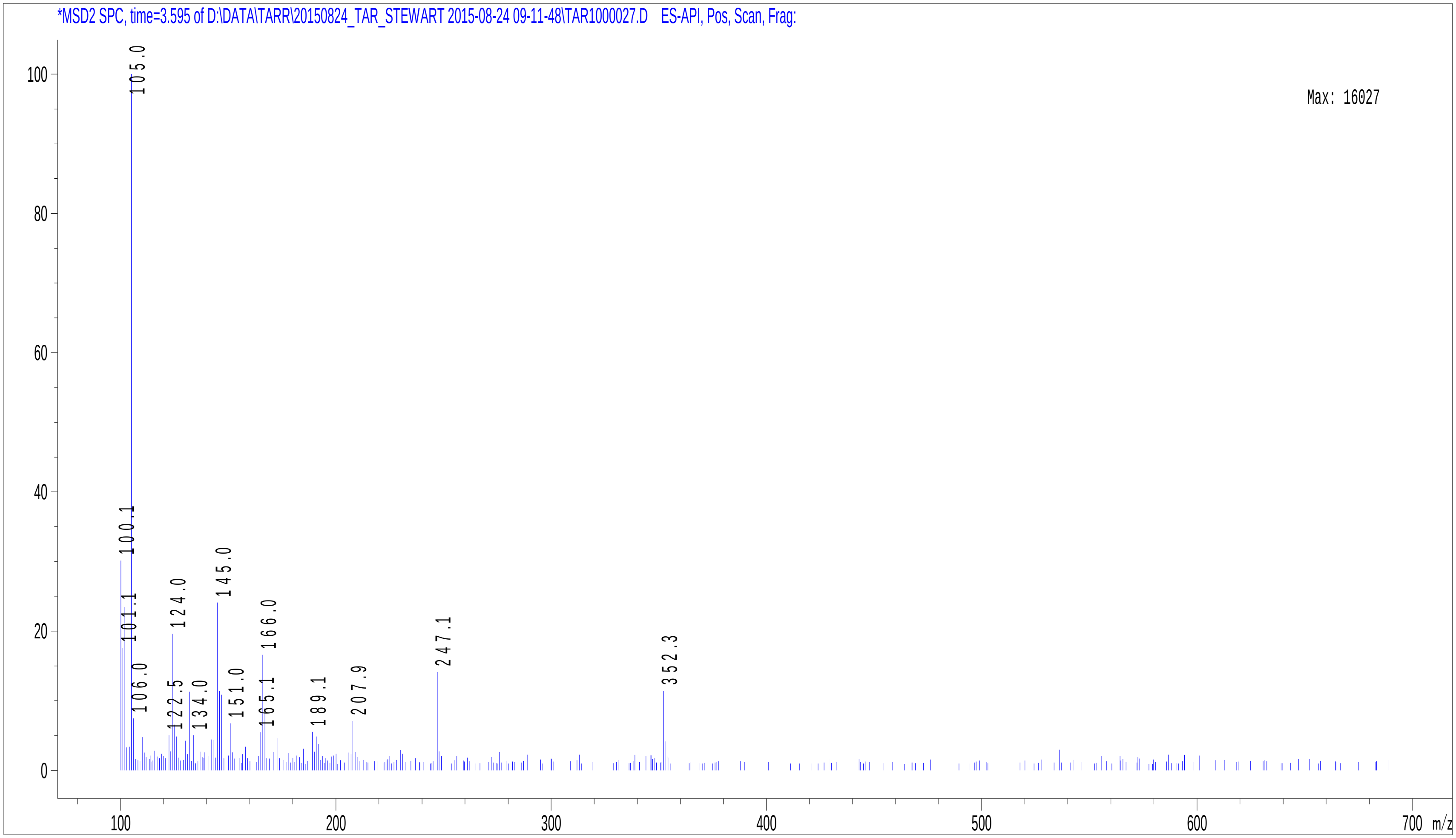


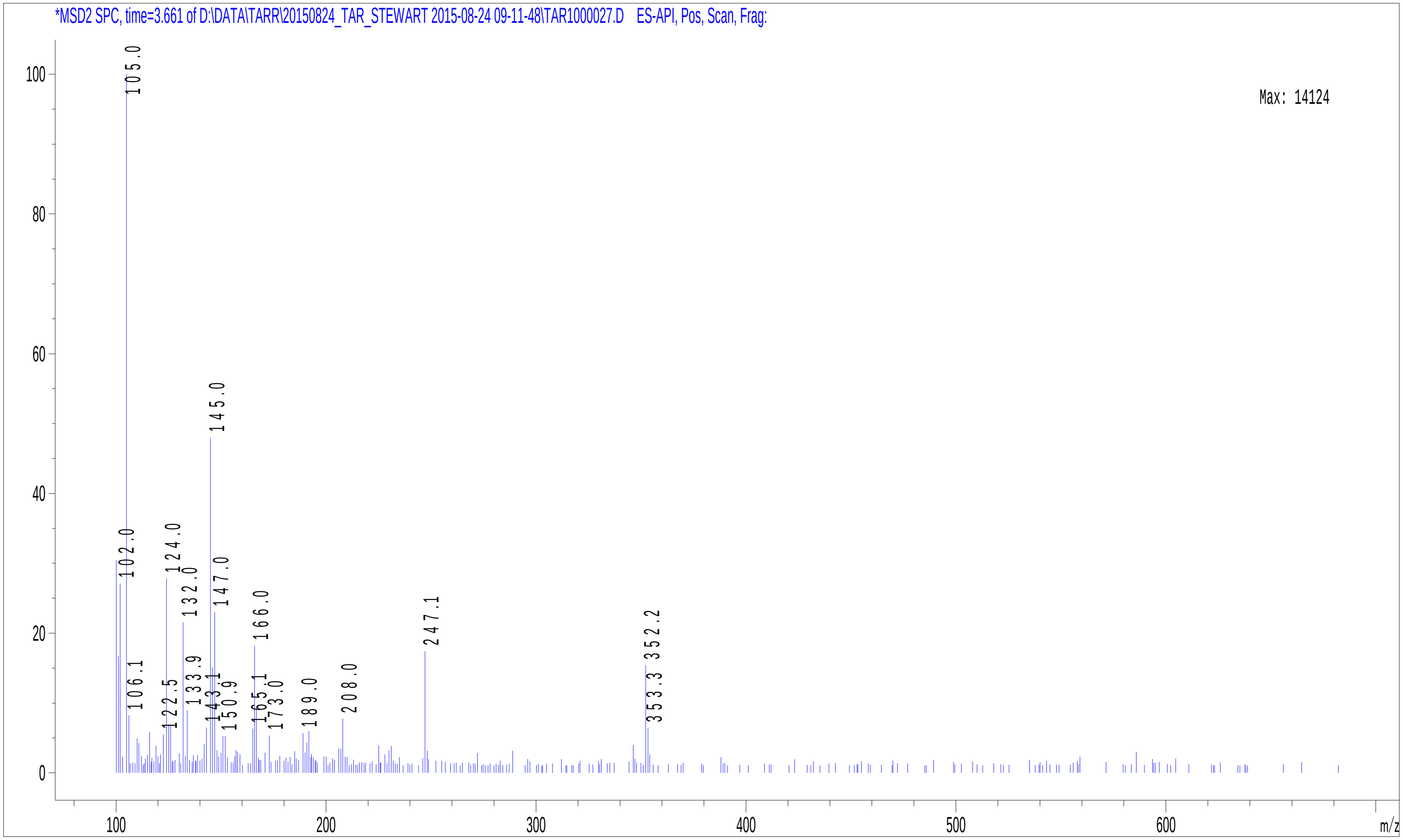
#	Time	Area	Height	Width	Area%	Symmetry
1	3.095	1509784.5	180392.7	0.1395	57.775	0.951
2	3.269	32689.5	16539.4	0.0329	1.251	0
3	3.595	100527.8	20434.8	0.082	3.847	0
4	3.644	106264.8	23586.2	0.0751	4.066	0
5	3.765	54401.3	14622	0.062	2.082	1.098
6	3.93	724593.4	83488.2	0.1446	27.728	0.81
7	4.134	84972.6	16752.4	0.0845	3.252	0.501

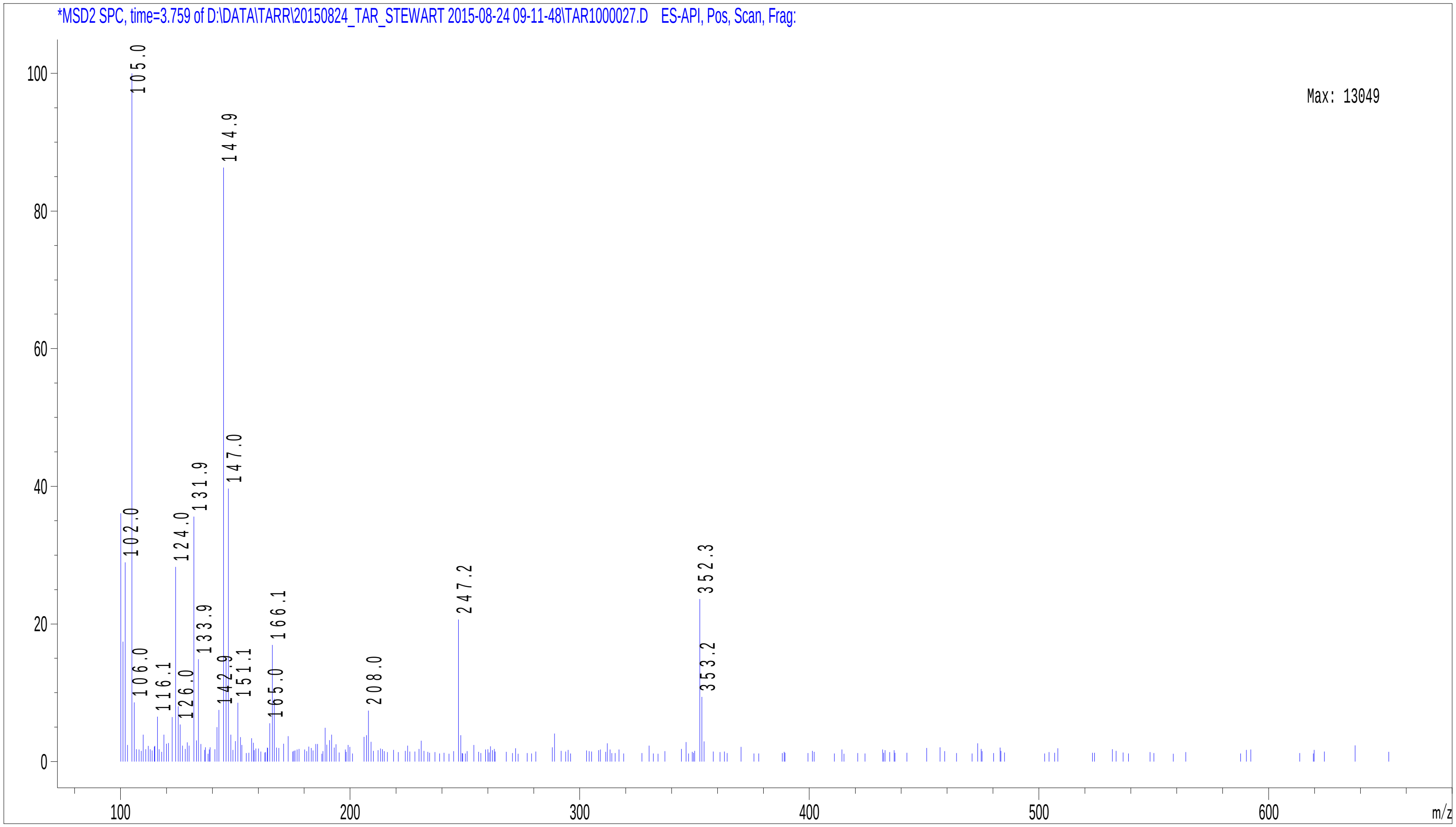

MSD2 TIC, MS File (D:\DATA\TARR\20150824_TAR_STEWART 2015-08-24 09-11-48\TAR1000027.D) ES-API, Pos, Scan, Frag: 70
Norm.
275000
250000
225000
200000
175000
150000
125000
100000
2.5
3
3.5
4
4.5
min
3.095
Area: 1.50978e+006
3.269
Area: 32689.5
3.595
Area: 100528
3.644
Area: 106265
3.765
Area: 54401.3
3.930
Area: 724593
4.134
Area: 84972.6

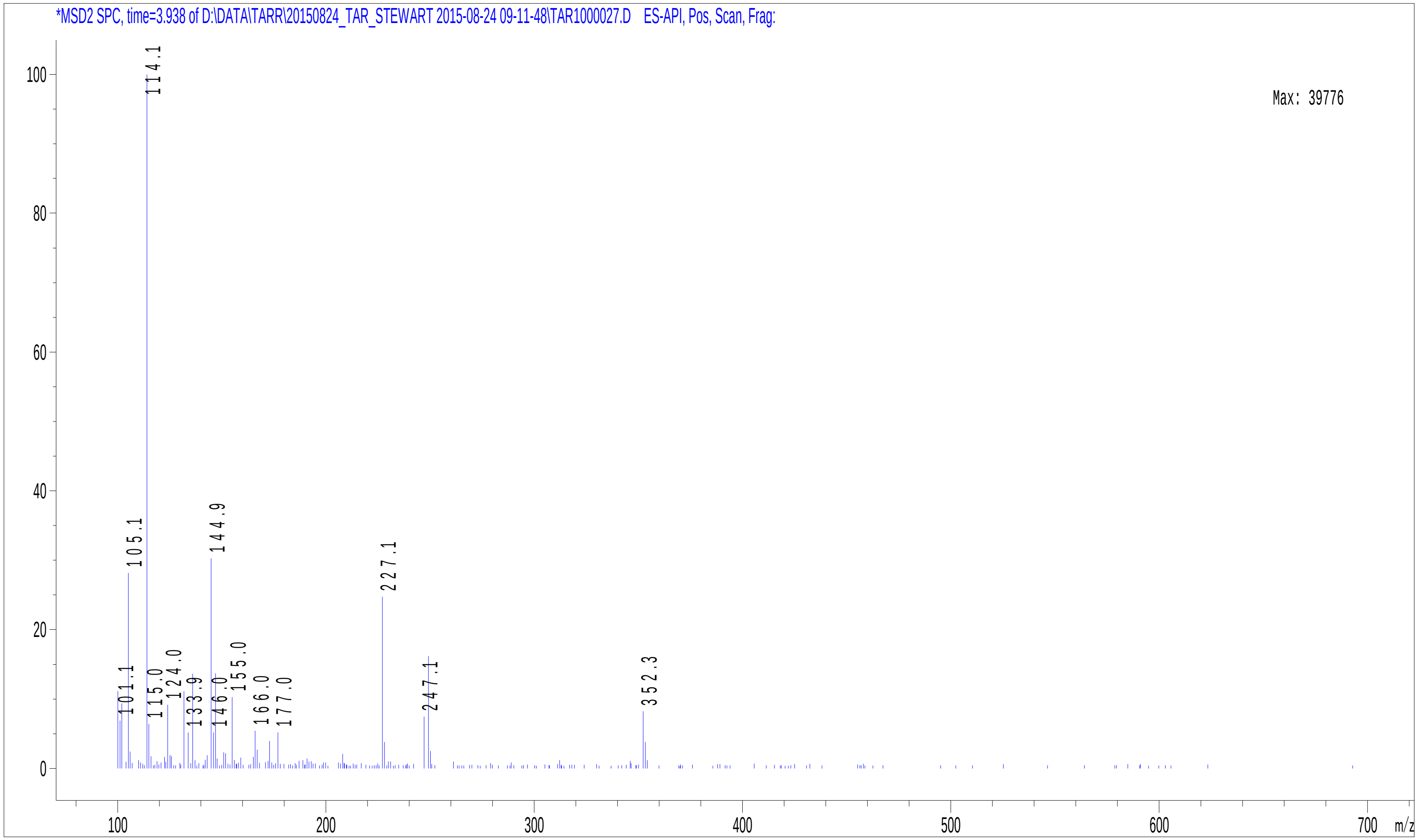

*MSD2 SPC, time=3.106 of D:\DATA\TARR\20150824_TAR_STEWART 2015-08-24 09-11-48\TAR1000027.D ES-API, Pos, Scan, Frag:
Max: 134720
105.0
106.1
132.0
144.9
0
20
40
60
80
100
100
200
300
400
500
600
700
m/z

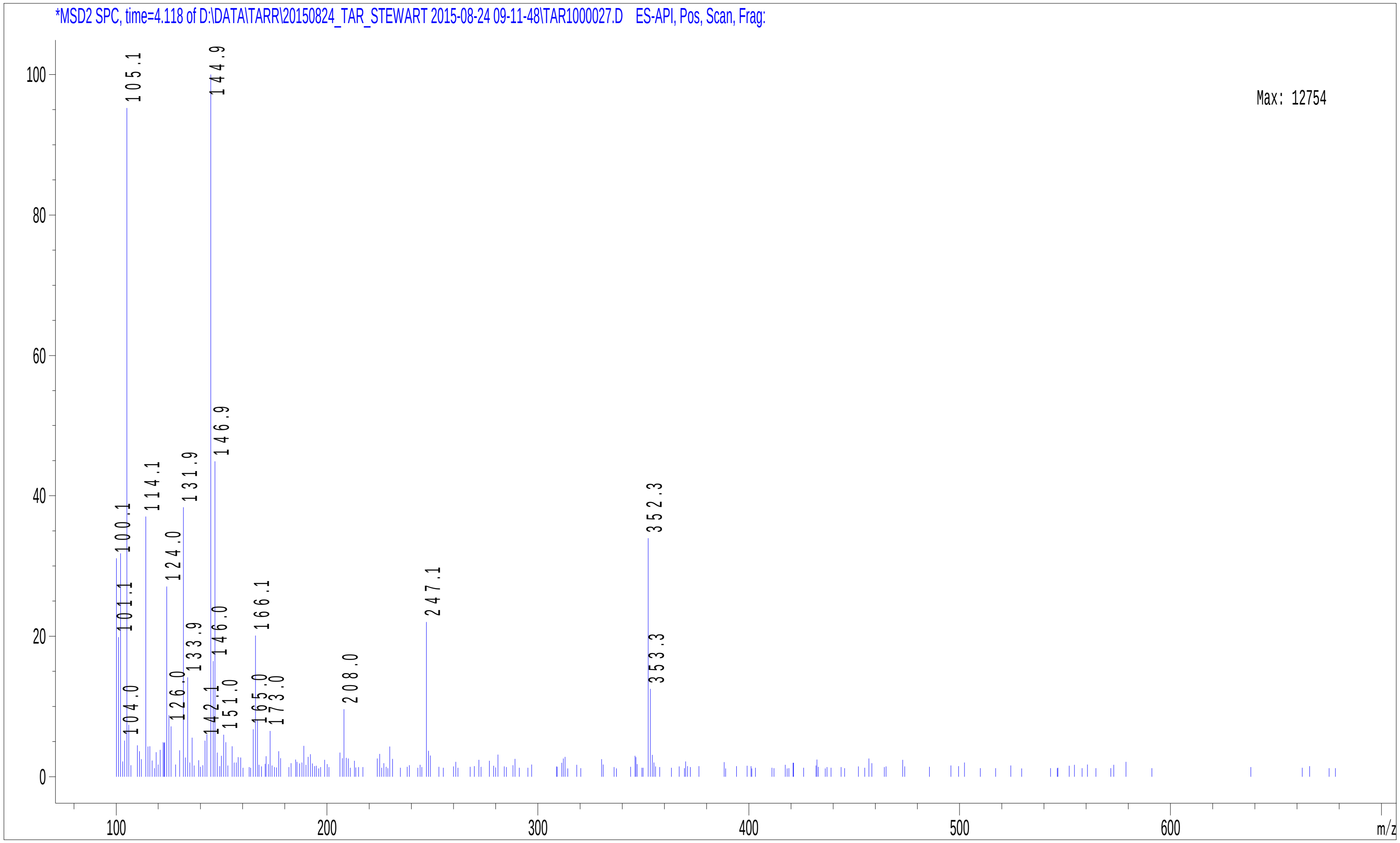

*MSD2 SPC, time=3.269 of D:\DATA\TARR\20150824_TAR_STEWART 2015-08-24 09-11-48\TAR1000027.D ES-API, Pos, Scan, Frag:
Max: 30384
105.0
106.0
124.0
131.9
147.0
166.0
247.1
352.3
0
20
40
60
80
100
100
200
300
400
500
600
m/z


*MSD2 SPC, time=3.595 of D:\DATA\TARR\20150824_TAR_STEWART 2015-08-24 09-11-48\TAR1000027.D ES-API, Pos, Scan, Frag:
Max: 16027
105.0
100.1
101.1
106.0
122.5
124.0
134.0
145.0
151.0
165.1
166.0
189.1
207.9
247.1
352.3
0
20
40
60
80
100
100
200
300
400
500
600
700
m/z


*MSD2 SPC, time=3.661 of D:\DATA\TARR\20150824_TAR_STEWART 2015-08-24 09-11-48\TAR1000027.D   ES-API, Pos, Scan, Frag:
Max: 14124
105.0
102.0
106.1
122.5
124.0
132.0
133.9
143.1
145.0
147.0
150.9
165.1
166.0
173.0
189.0
208.0
247.1
352.2
353.3
0
20
40
60
80
100
100
200
300
400
500
600
m/z


*MSD2 SPC, time=3.759 of D:\DATA\TARR\20150824_TAR_STEWART 2015-08-24 09-11-48\TAR1000027.D ES-API, Pos, Scan, Frag:
Max: 13049
105.0
144.9
147.0
131.9
124.0
102.0
133.9
166.1
106.0
116.1
126.0
142.9
151.1
165.0
208.0
247.2
352.3
353.2
0
20
40
60
80
100
100
200
300
400
500
600
m/z

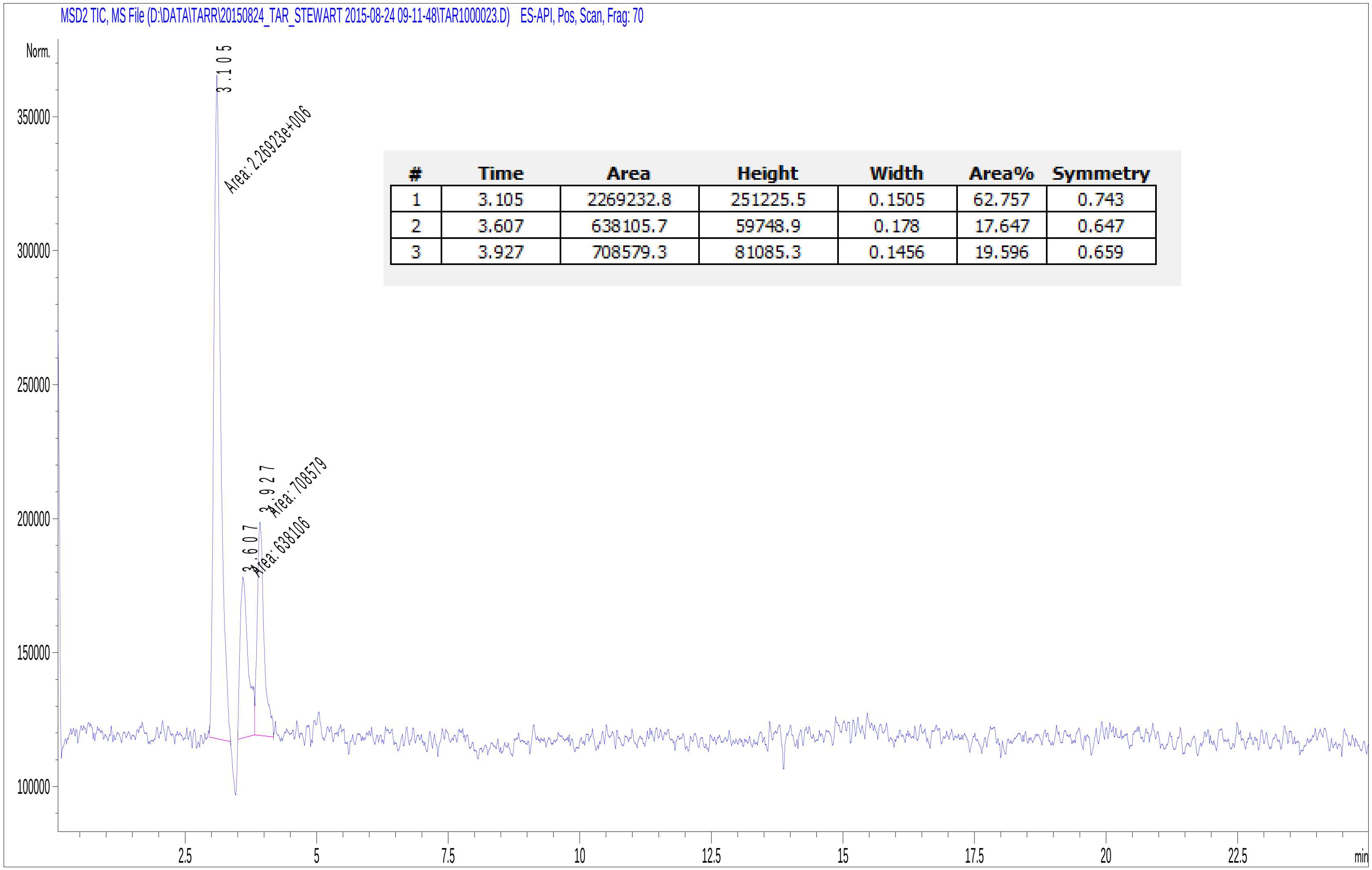

*MSD2 SPC, time=3.938 of D:\DATA\TARR\20150824_TAR_STEWART 2015-08-24 09-11-48\TAR1000027.D ES-API, Pos, Scan, Frag:
Max: 39776
114.1
105.1
144.9
227.1
101.1
115.0
124.0
133.9
146.0
155.0
166.0
177.0
247.1
352.3
0
20
40
60
80
100
100
200
300
400
500
600
700
m/z


*MSD2 SPC, time=4.118 of D:\DATA\TARR\20150824_TAR_STEWART 2015-08-24 09-11-48\TAR1000027.D ES-API, Pos, Scan, Frag:
Max: 12754
105.1
144.9
146.9
131.9
114.1
100.1
352.3
124.0
101.1
247.1
166.1
146.0
133.9
353.3
208.0
126.0
104.0
142.1
151.0
165.0
173.0
100
80
60
40
20
0
100
200
300
400
500
600
m/z

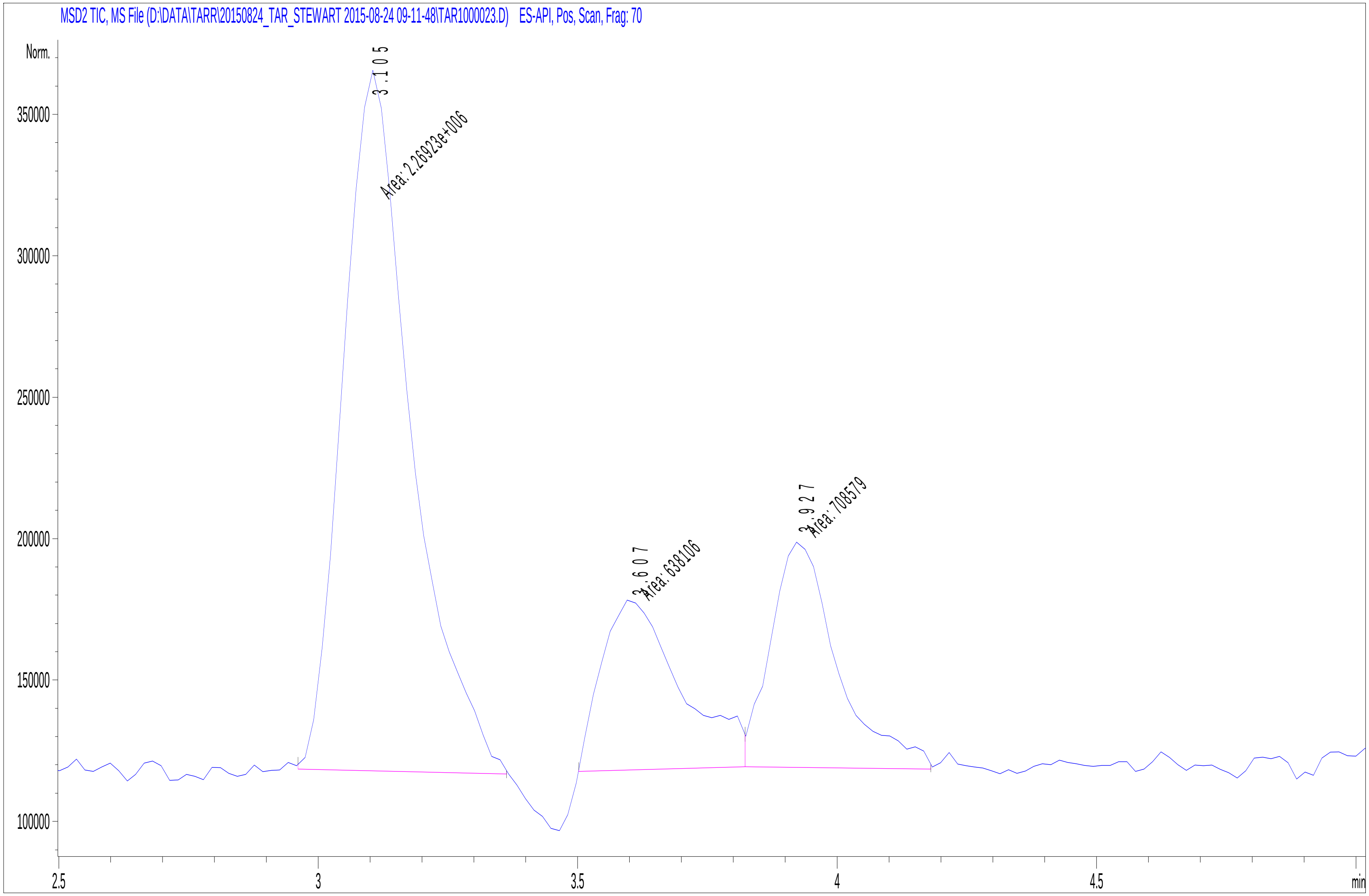
6-Jul-15

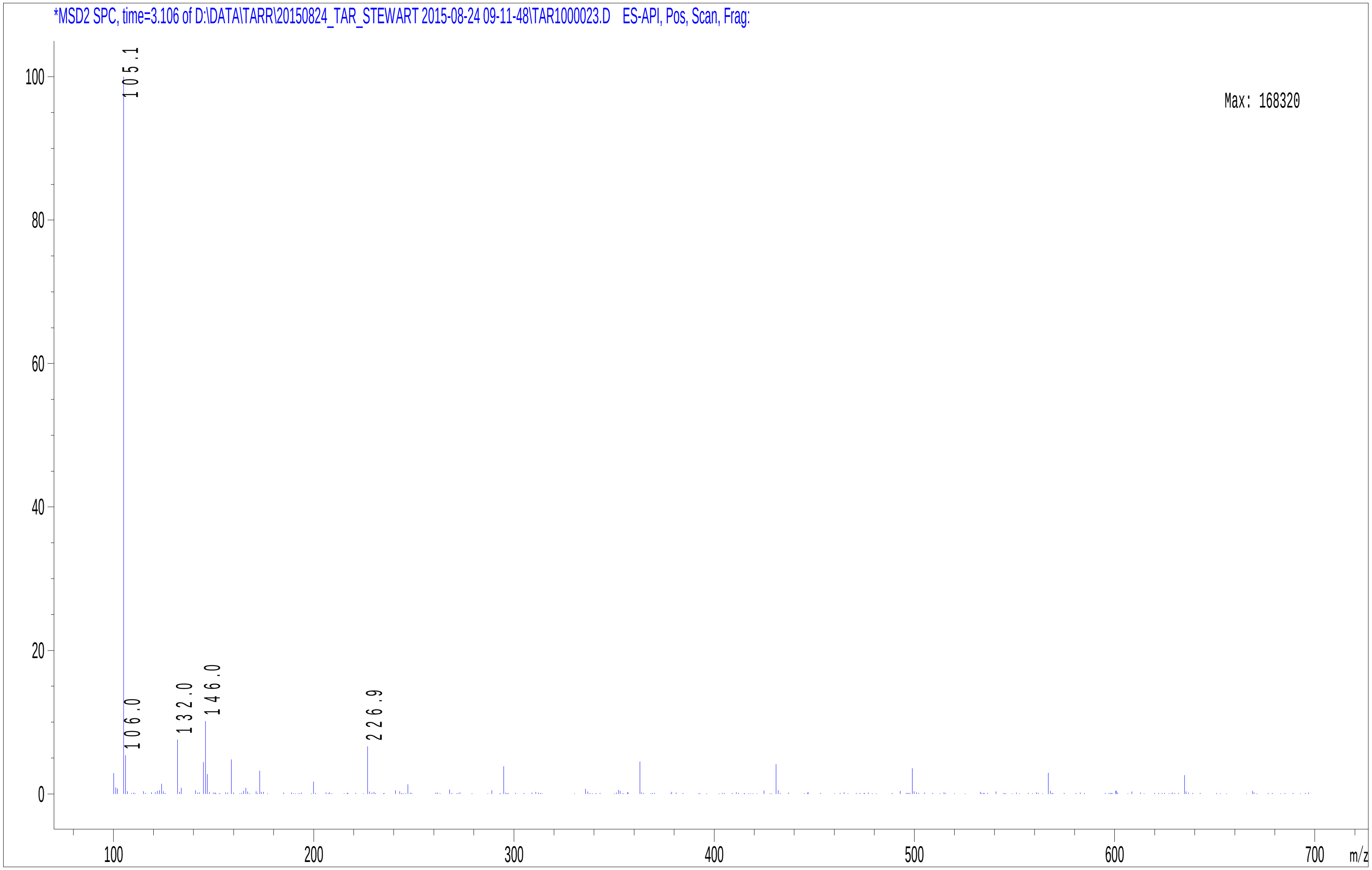
100 DC

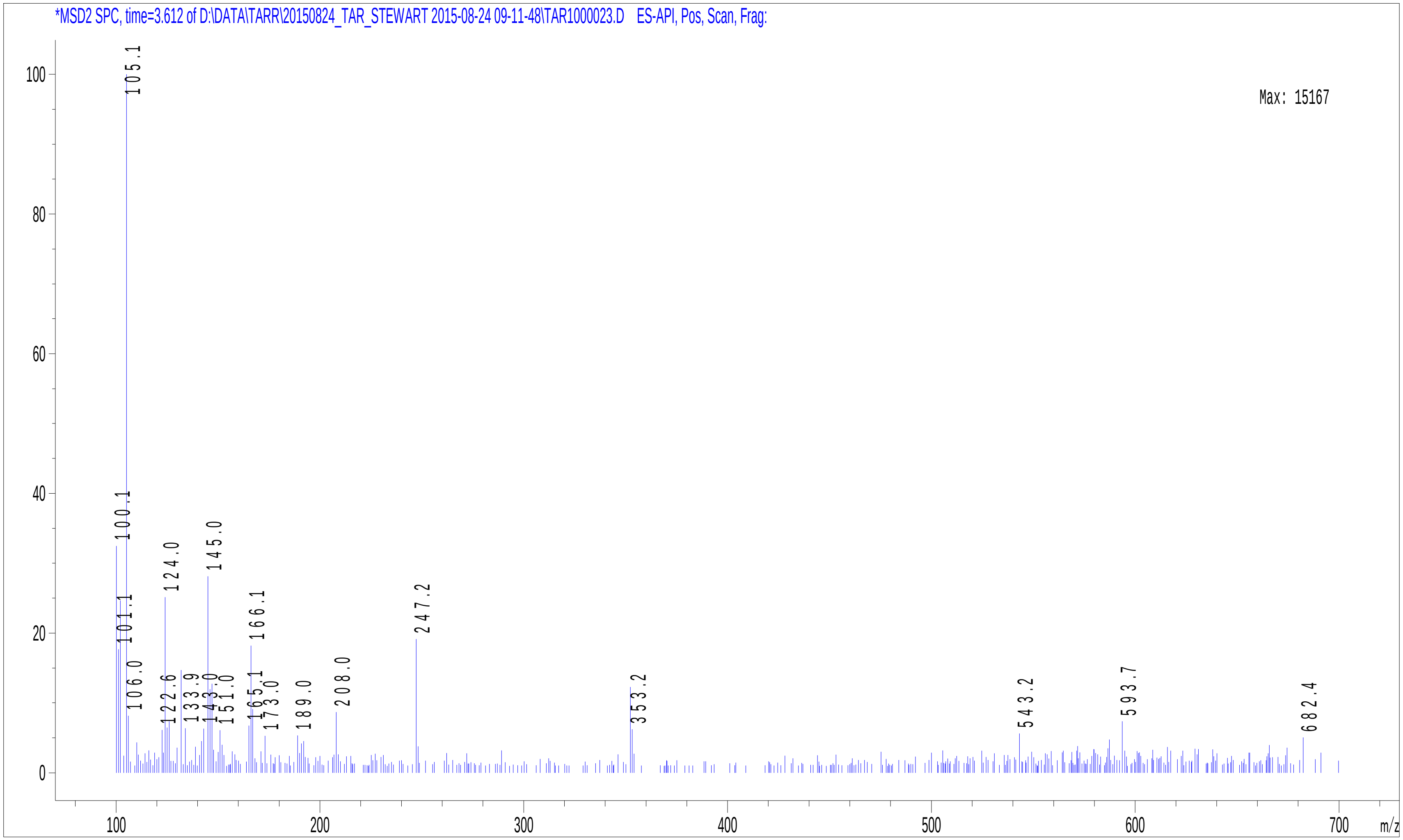
P2-C-05

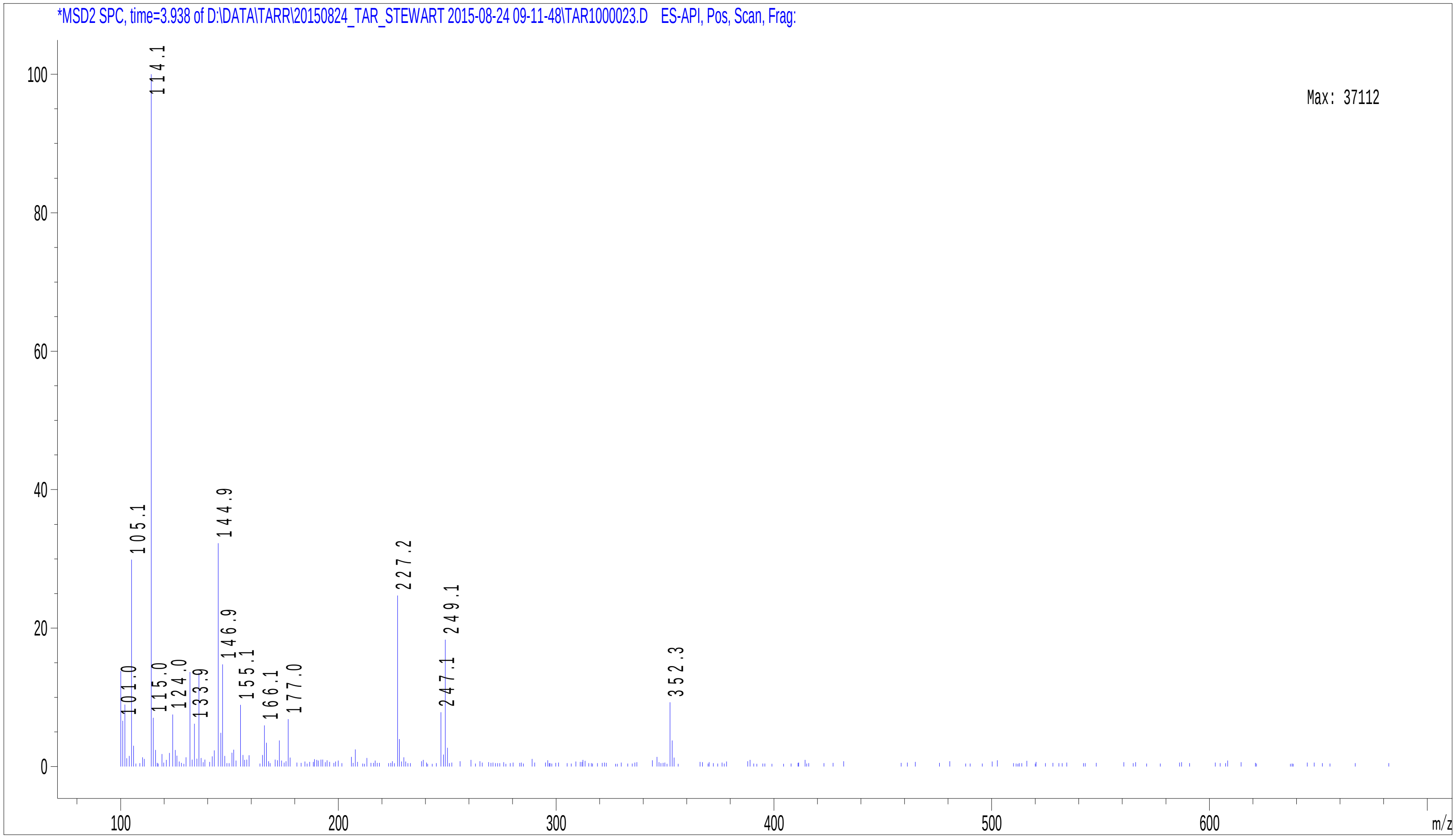


#	Time	Area	Height	Width	Area%	Symmetry
1	3.105	2269232.8	251225.5	0.1505	62.757	0.743
2	3.607	638105.7	59748.9	0.178	17.647	0.647
3	3.927	708579.3	81085.3	0.1456	19.596	0.659


MSD2 TIC, MS File (D:\DATA\TARR\20150824_TAR_STEWART 2015-08-24 09-11-48\TAR1000023.D)   ES-API, Pos, Scan, Frag: 70
Norm.
350000
300000
250000
200000
150000
100000
3.105
Area: 2.26923e+006
3.607
Area: 638106
3.927
Area: 708579
2.5
3
3.5
4
4.5
min


*MSD2 SPC, time=3.106 of D:\DATA\TARR\20150824_TAR_STEWART 2015-08-24 09-11-48\TAR1000023.D   ES-API, Pos, Scan, Frag:
Max: 168320
105.1
106.0
132.0
146.0
226.9
100
80
60
40
20
0
100
200
300
400
500
600
700
m/z

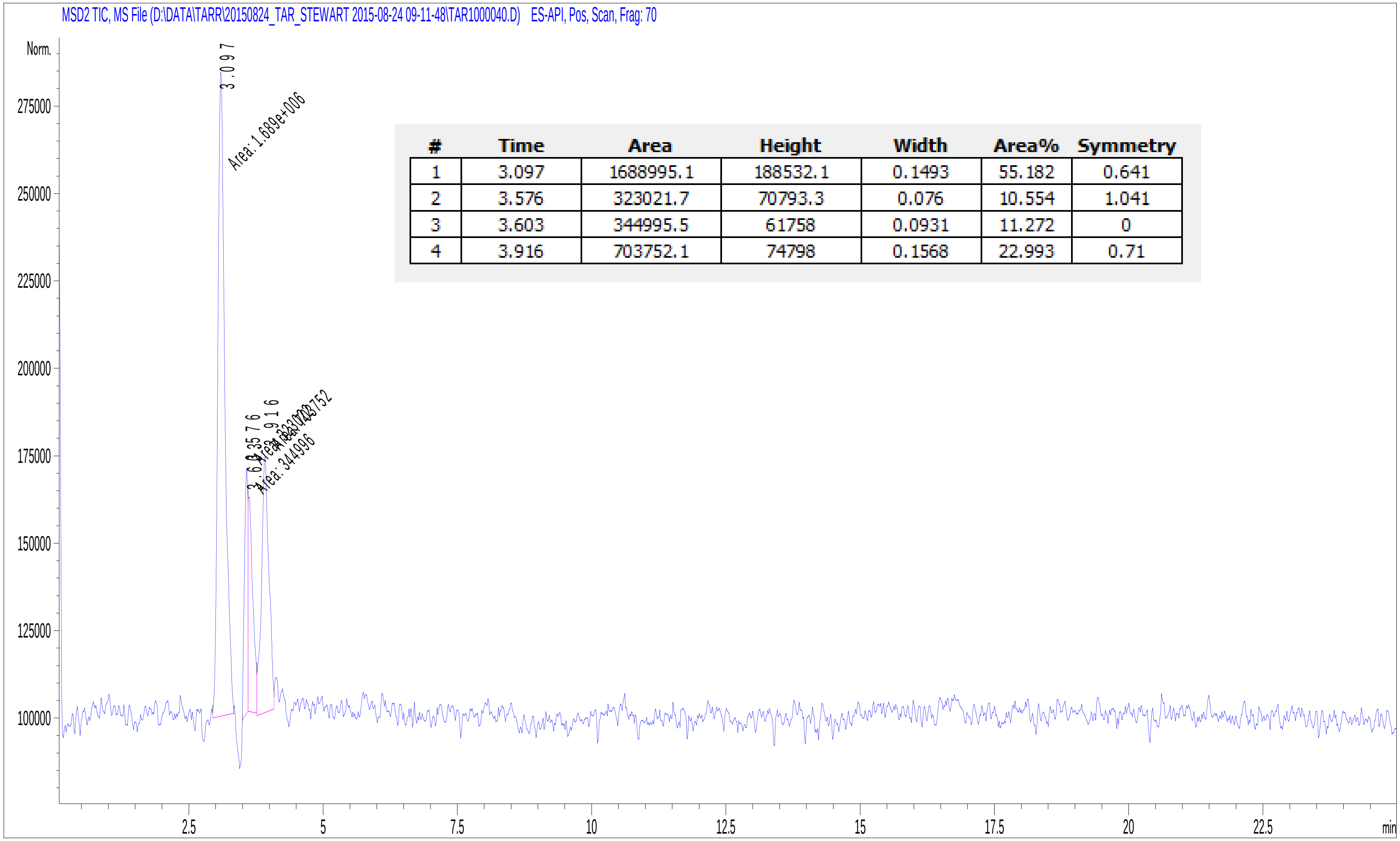

*MSD2 SPC, time=3.612 of D:\DATA\TARR\20150824_TAR_STEWART 2015-08-24 09-11-48\TAR1000023.D ES-API, Pos, Scan, Frag:
Max: 15167
105.1
100.1
101.1
106.0
122.6
124.0
133.9
143.0
145.0
151.0
165.1
166.1
173.0
189.0
208.0
247.2
353.2
543.2
593.7
682.4
0
20
40
60
80
100
100
200
300
400
500
600
700
m/z


*MSD2 SPC, time=3.938 of D:\DATA\TARR\20150824_TAR_STEWART 2015-08-24 09-11-48\TAR1000023.D ES-API, Pos, Scan, Frag:
Max: 37112
114.1
105.1
101.0
115.0
124.0
133.9
144.9
146.9
155.1
166.1
177.0
227.2
247.1
249.1
352.3
0
20
40
60
80
100
100
200
300
400
500
600
m/z

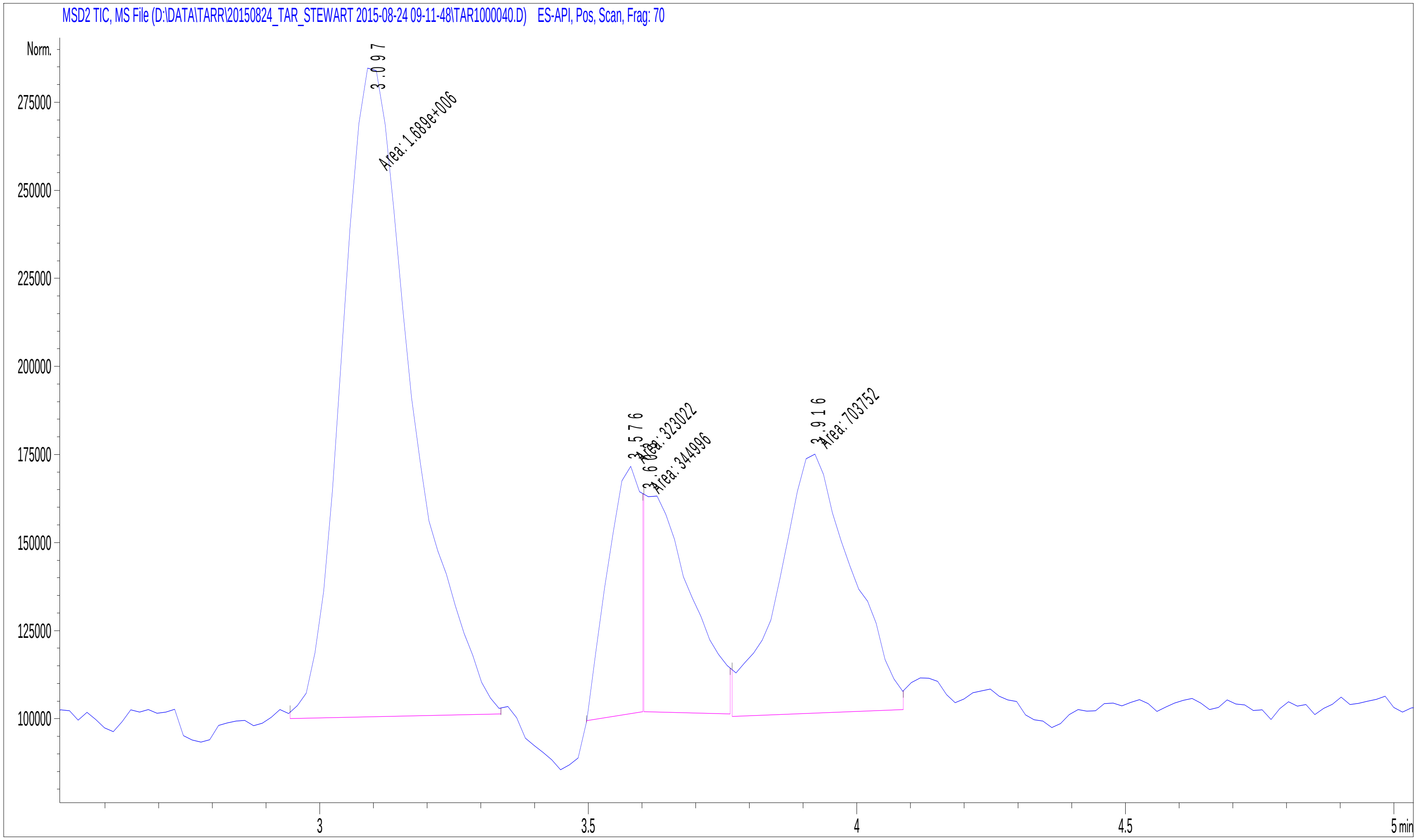
13-Aug-15

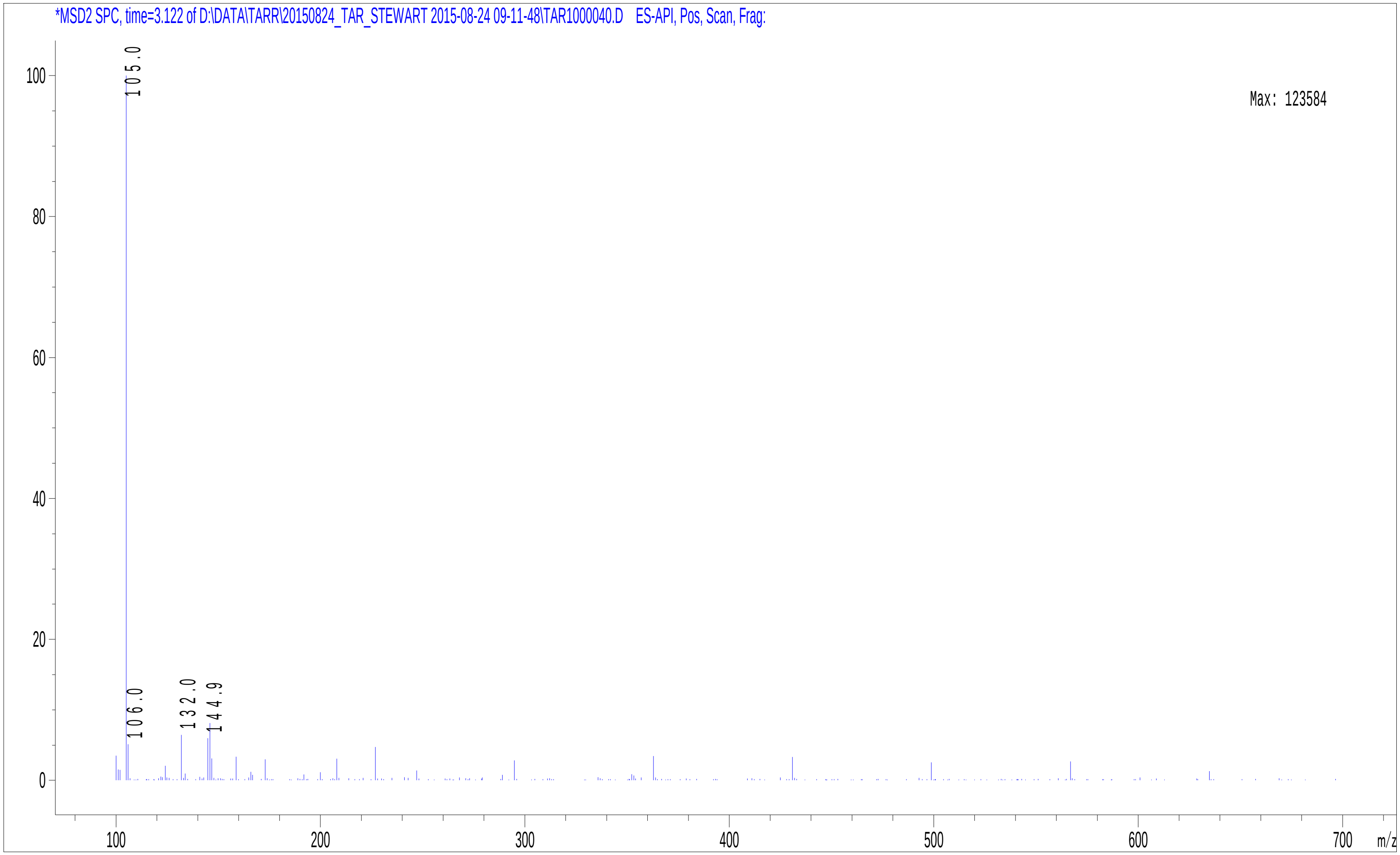
100 DC Repeat

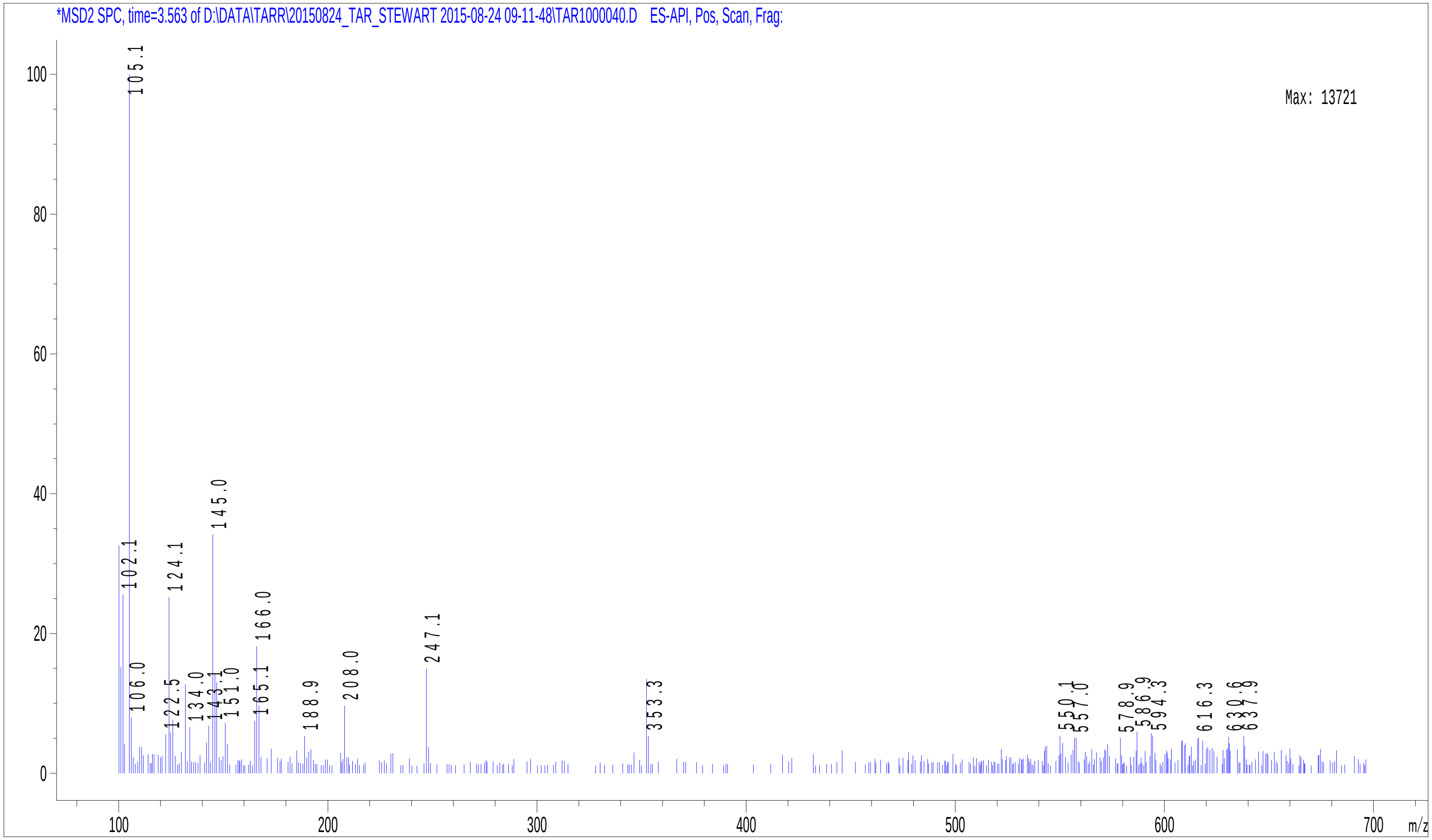
P2-E-04

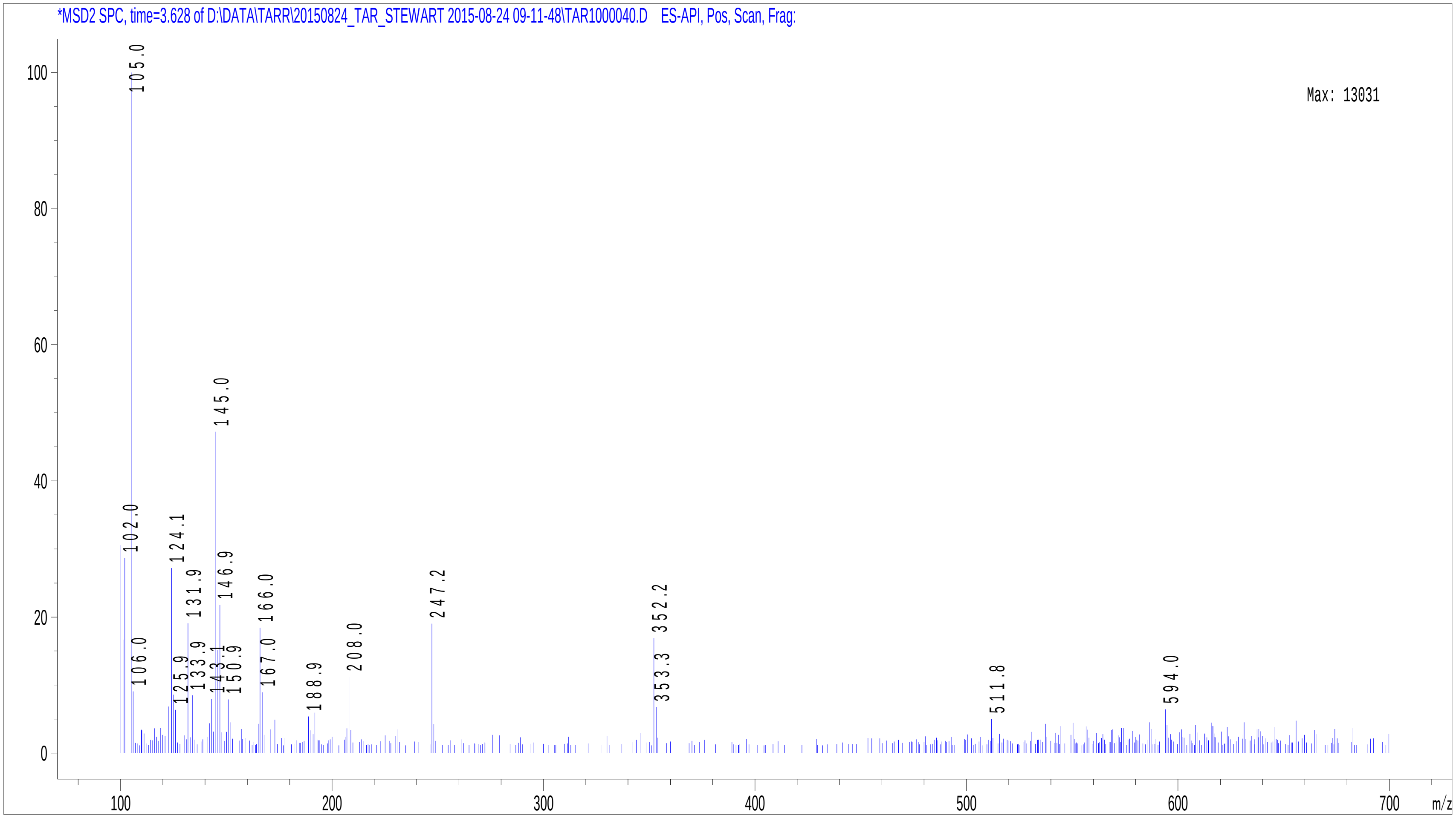


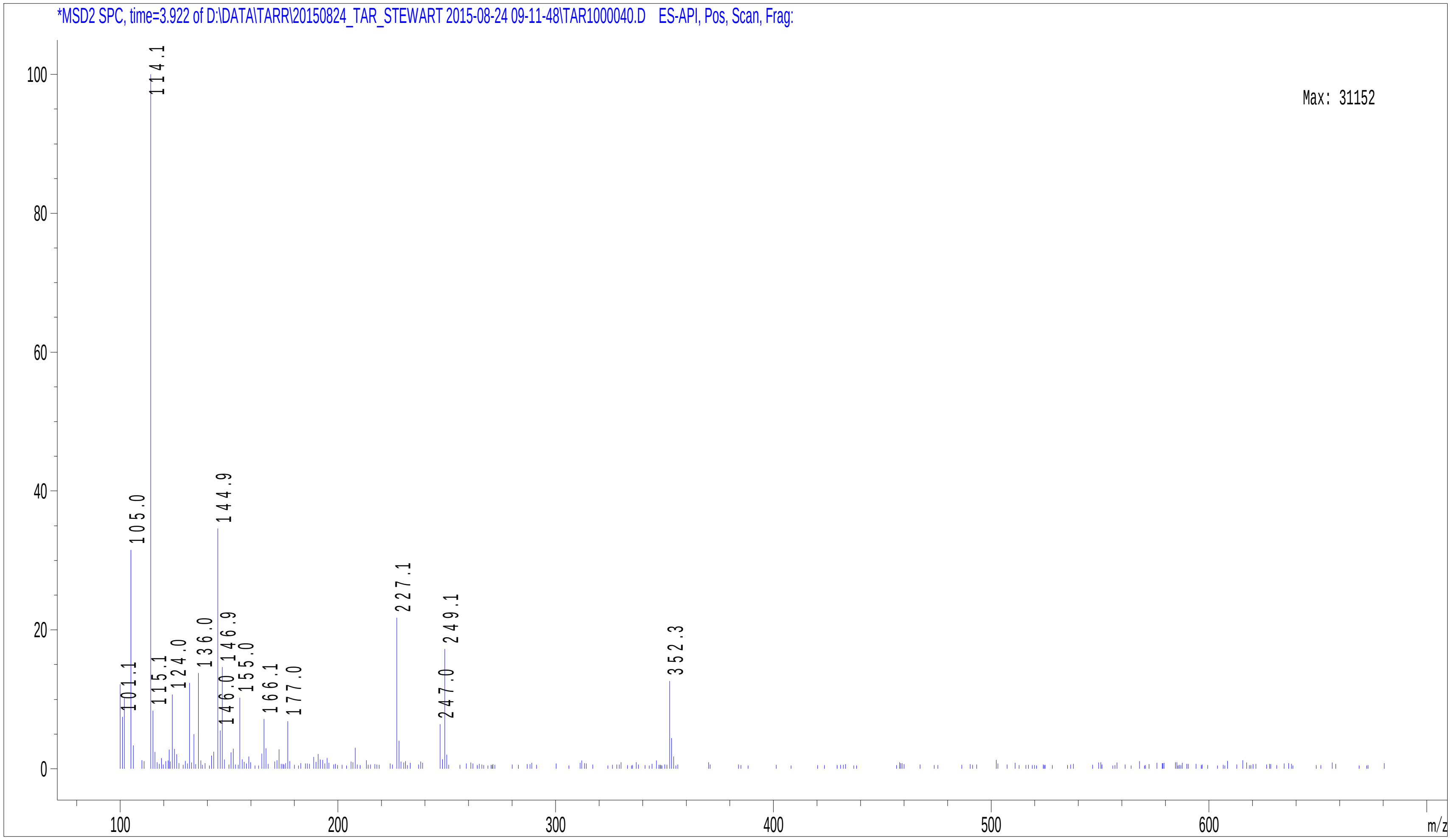
#	Time	Area	Height	Width	Area%	Symmetry
1	3.097	1688995.1	188532.1	0.1493	55.182	0.641
2	3.576	323021.7	70793.3	0.076	10.554	1.041
3	3.603	344995.5	61758	0.0931	11.272	0
4	3.916	703752.1	74798	0.1568	22.993	0.71


MSD2 TIC, MS File (D:\DATA\TARR\20150824_TAR_STEWART 2015-08-24 09-11-48\TAR1000040.D) ES-API, Pos, Scan, Frag: 70
Norm.
275000
250000
225000
200000
175000
150000
125000
100000
3.097
Area: 1.689e+006
3.576
Area: 323022
3.603
Area: 344996
3.916
Area: 703752
3
3.5
4
4.5
5 min


*MSD2 SPC, time=3.122 of D:\DATA\TARR\20150824_TAR_STEWART 2015-08-24 09-11-48\TAR1000040.D ES-API, Pos, Scan, Frag:
Max: 123584
105.0
106.0
132.0
144.9
100
80
60
40
20
0
100
200
300
400
500
600
700
m/z

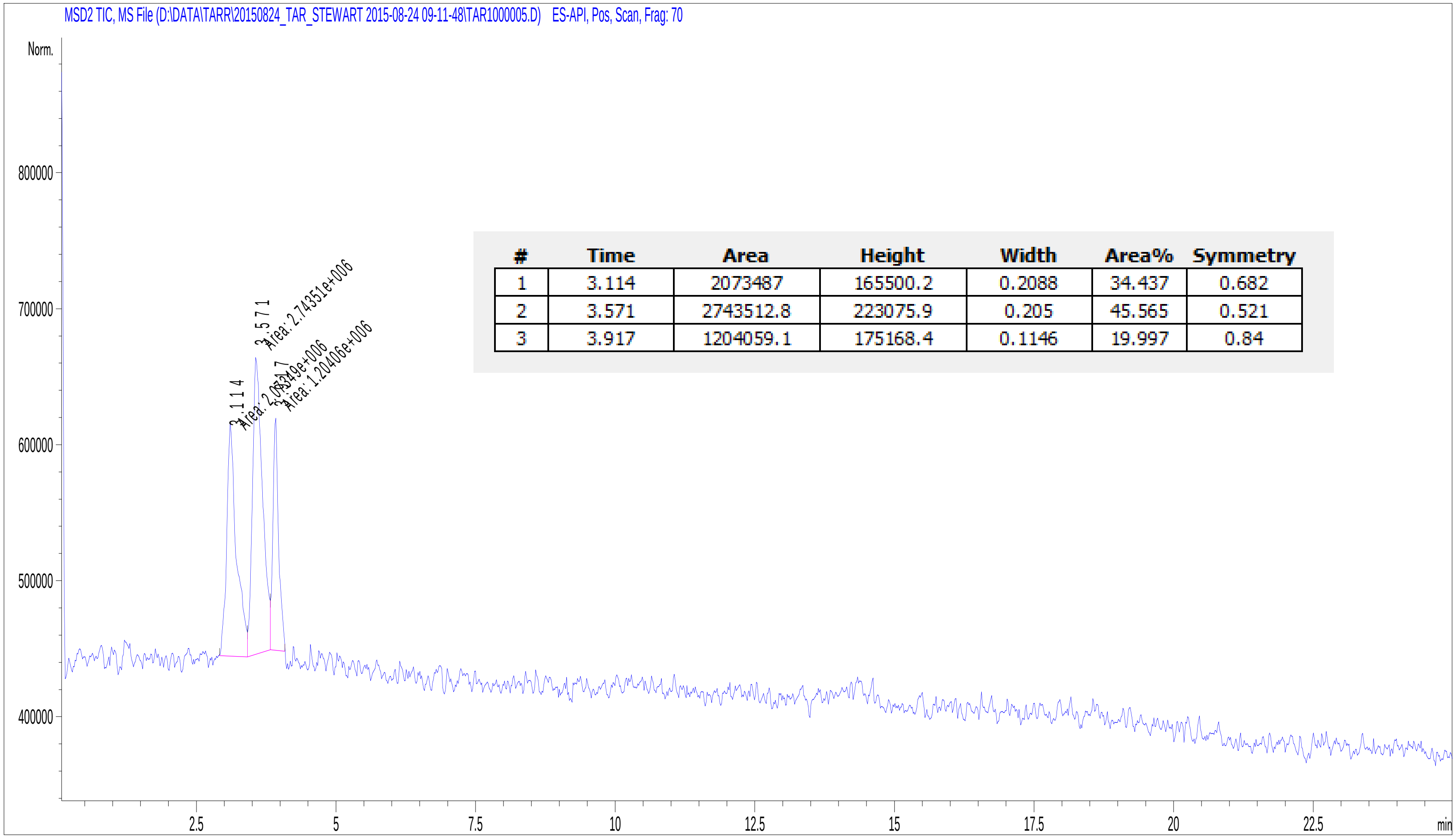

*MSD2 SPC, time=3.563 of D:\DATA\TARR\20150824_TAR_STEWART 2015-08-24 09-11-48\TAR1000040.D ES-API, Pos, Scan, Frag:
Max: 13721
105.1
102.1
124.1
145.0
166.0
106.0
122.5
134.0
143.1
151.0
165.1
188.9
208.0
247.1
353.3
550.1
557.0
578.9
586.9
594.3
616.3
630.6
637.9
0
20
40
60
80
100
100
200
300
400
500
600
700
m/z


*MSD2 SPC, time=3.628 of D:\DATA\TARR\20150824_TAR_STEWART 2015-08-24 09-11-48\TAR1000040.D ES-API, Pos, Scan, Frag:
Max: 13031
105.0
102.0
106.0
124.1
125.9
131.9
133.9
143.1
145.0
146.9
150.9
166.0
167.0
188.9
208.0
247.2
352.2
353.3
511.8
594.0
0
20
40
60
80
100
100
200
300
400
500
600
700
m/z

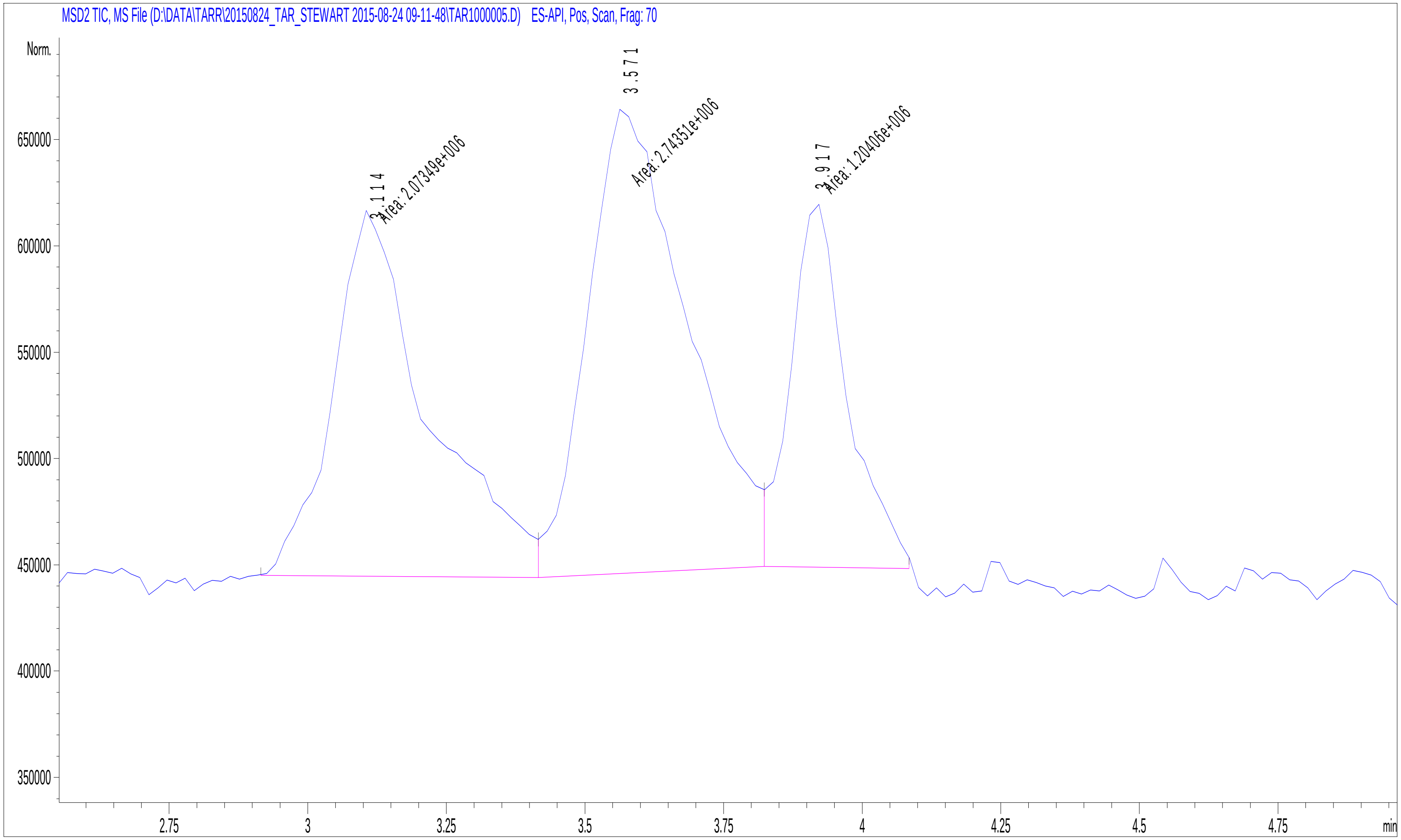

*MSD2 SPC, time=3.922 of D:\DATA\TARR\20150824_TAR_STEWART 2015-08-24 09-11-48\TAR1000040.D   ES-API, Pos, Scan, Frag:
Max: 31152
114.1
105.0
144.9
227.1
249.1
352.3
101.1
115.1
124.0
136.0
146.0
146.9
155.0
166.1
177.0
247.0
0
20
40
60
80
100
200
300
400
500
600
m/z

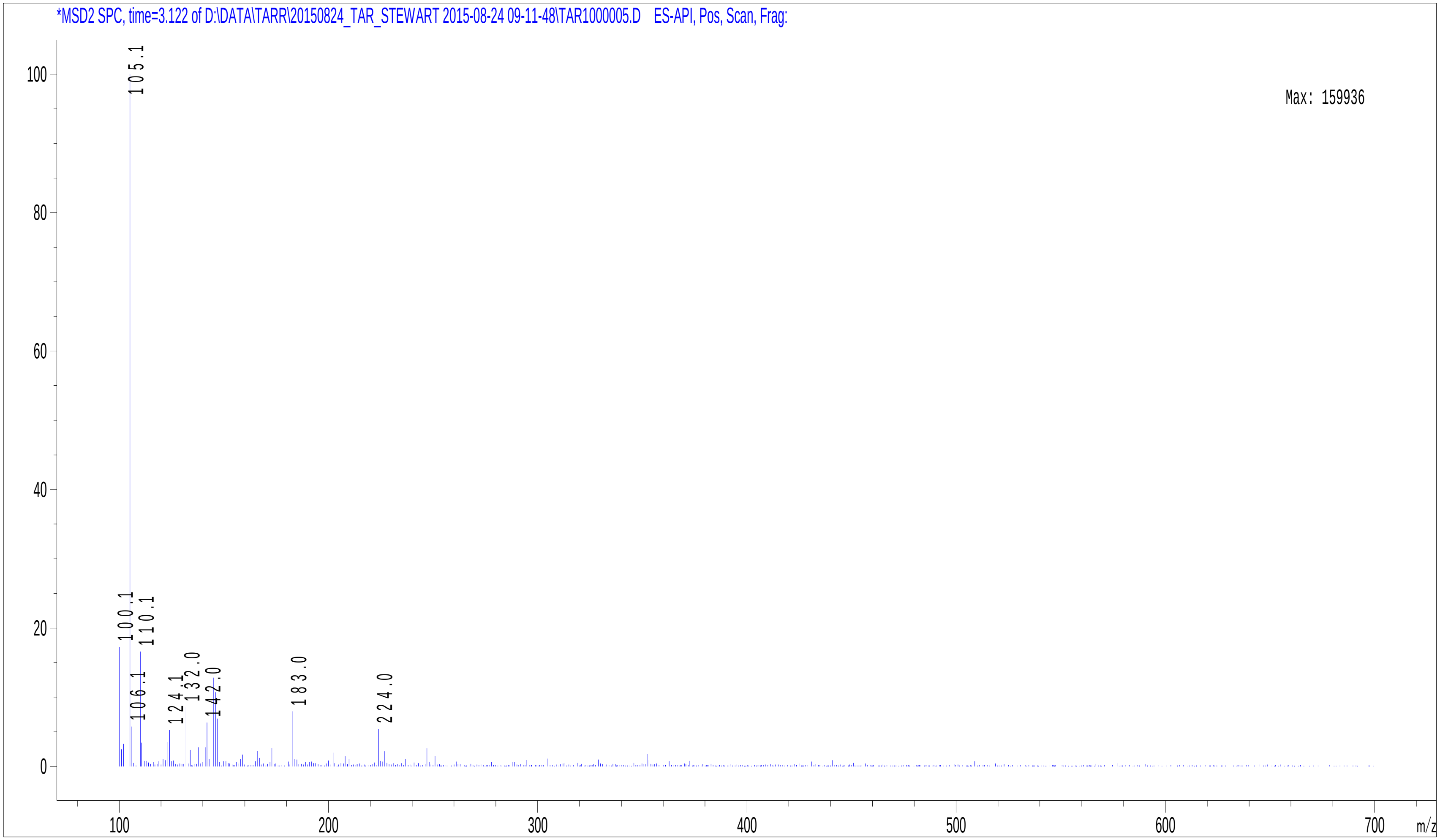
pH 9

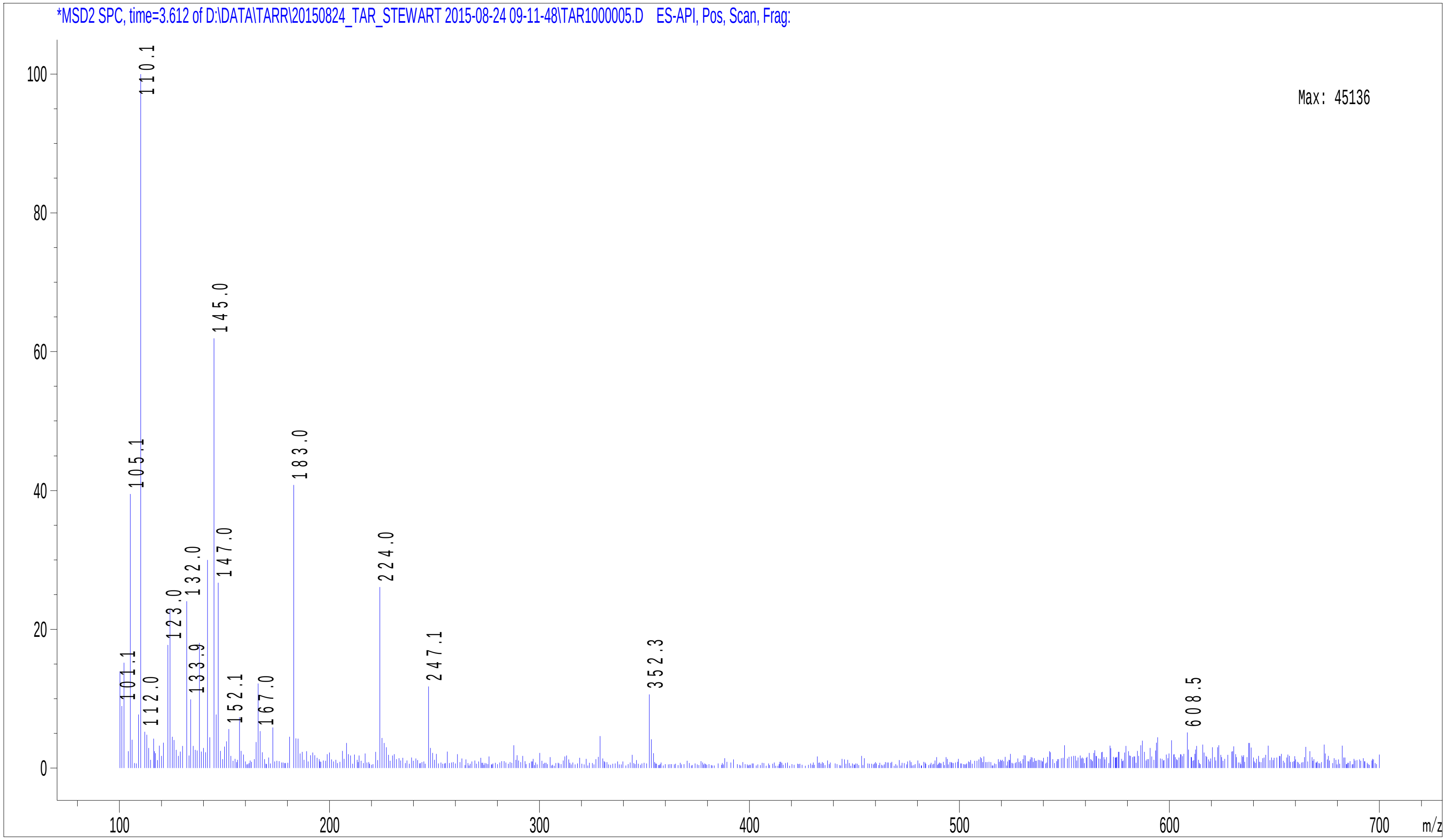
8-Apr-15
H2O2 Ctrl
P2-A-05

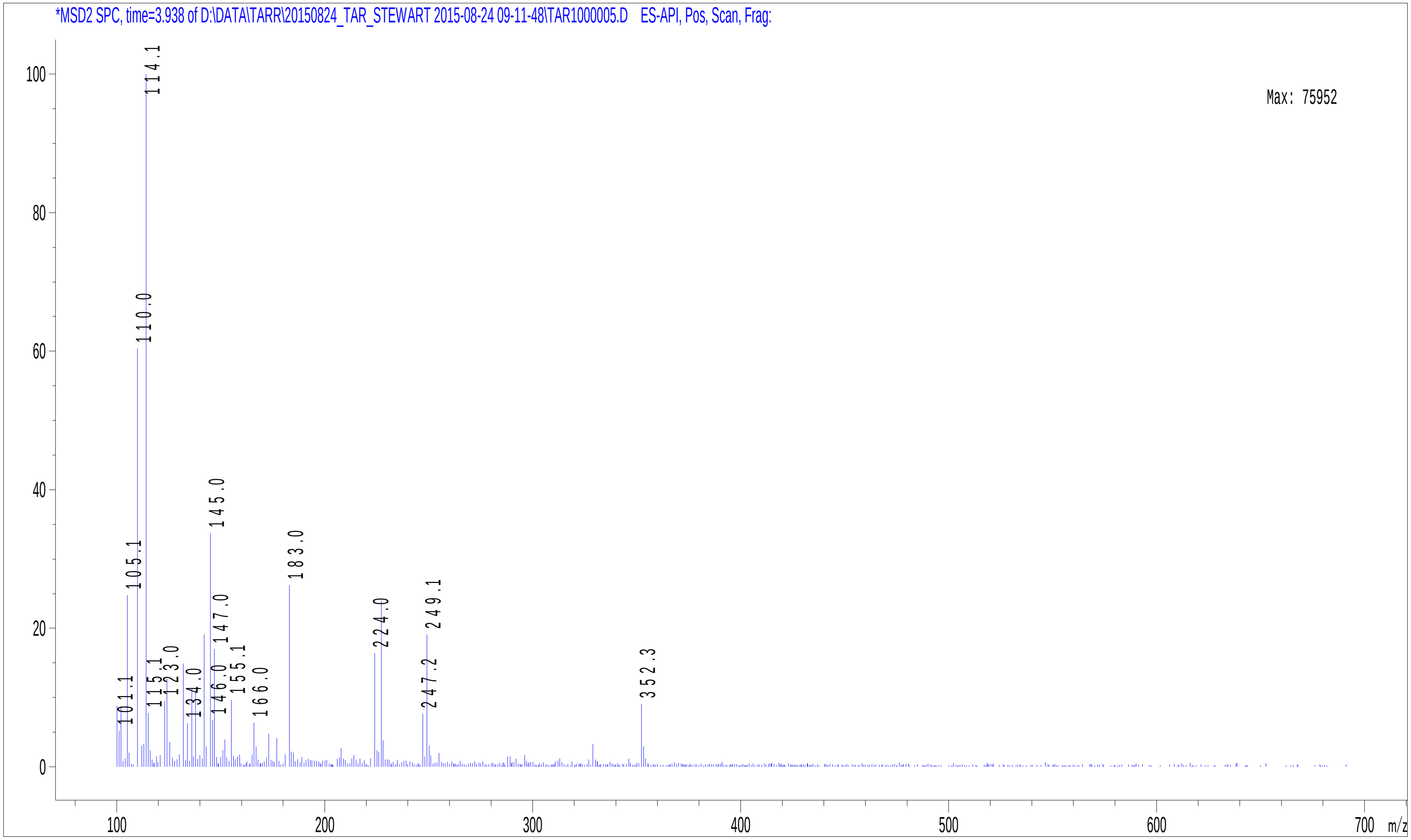


#	Time	Area	Height	Width	Area%	Symmetry
1	3.114	2073487	165500.2	0.2088	34.437	0.682
2	3.571	2743512.8	223075.9	0.205	45.565	0.521
3	3.917	1204059.1	175168.4	0.1146	19.997	0.84


MSD2 TIC, MS File (D:\DATA\TARR\20150824_TAR_STEWART 2015-08-24 09-11-48\TAR1000005.D) ES-API, Pos, Scan, Frag: 70
Norm.
650000
600000
550000
500000
450000
400000
350000
3.114
Area: 2.07349e+006
3.571
Area: 2.74351e+006
3.917
Area: 1.20406e+006
2.75
3
3.25
3.5
3.75
4
4.25
4.5
4.75
min


*MSD2 SPC, time=3.122 of D:\DATA\TARR\20150824_TAR_STEWART 2015-08-24 09-11-48\TAR1000005.D ES-API, Pos, Scan, Frag:
Max: 159936
105.1
100.1
110.1
106.1
124.1
132.0
142.0
183.0
224.0
100
80
60
40
20
0
100
200
300
400
500
600
700
m/z

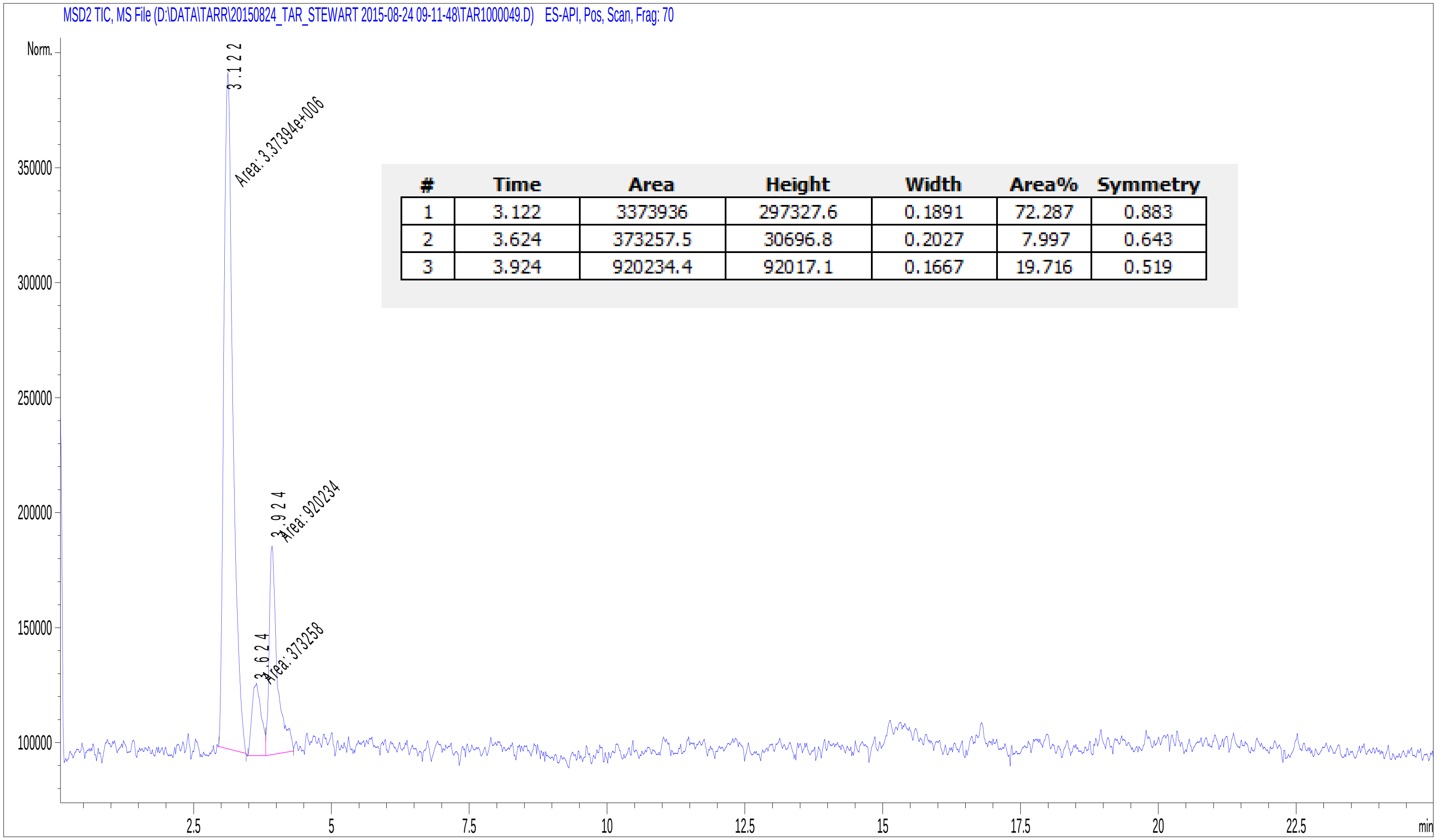

*MSD2 SPC, time=3.612 of D:\DATA\TARR\20150824_TAR_STEWART 2015-08-24 09-11-48\TAR1000005.D ES-API, Pos, Scan, Frag:
Max: 45136
110.1
145.0
105.1
183.0
147.0
132.0
224.0
123.0
133.9
101.1
247.1
352.3
112.0
152.1
167.0
608.5
0
20
40
60
80
100
100
200
300
400
500
600
700
m/z


*MSD2 SPC, time=3.938 of D:\DATA\TARR\20150824_TAR_STEWART 2015-08-24 09-11-48\TAR1000005.D ES-API, Pos, Scan, Frag:
Max: 75952
114.1
110.0
105.1
101.1
115.1
123.0
134.0
145.0
146.0
147.0
155.1
166.0
183.0
224.0
247.2
249.1
352.3
0
20
40
60
80
100
100
200
300
400
500
600
700
m/z

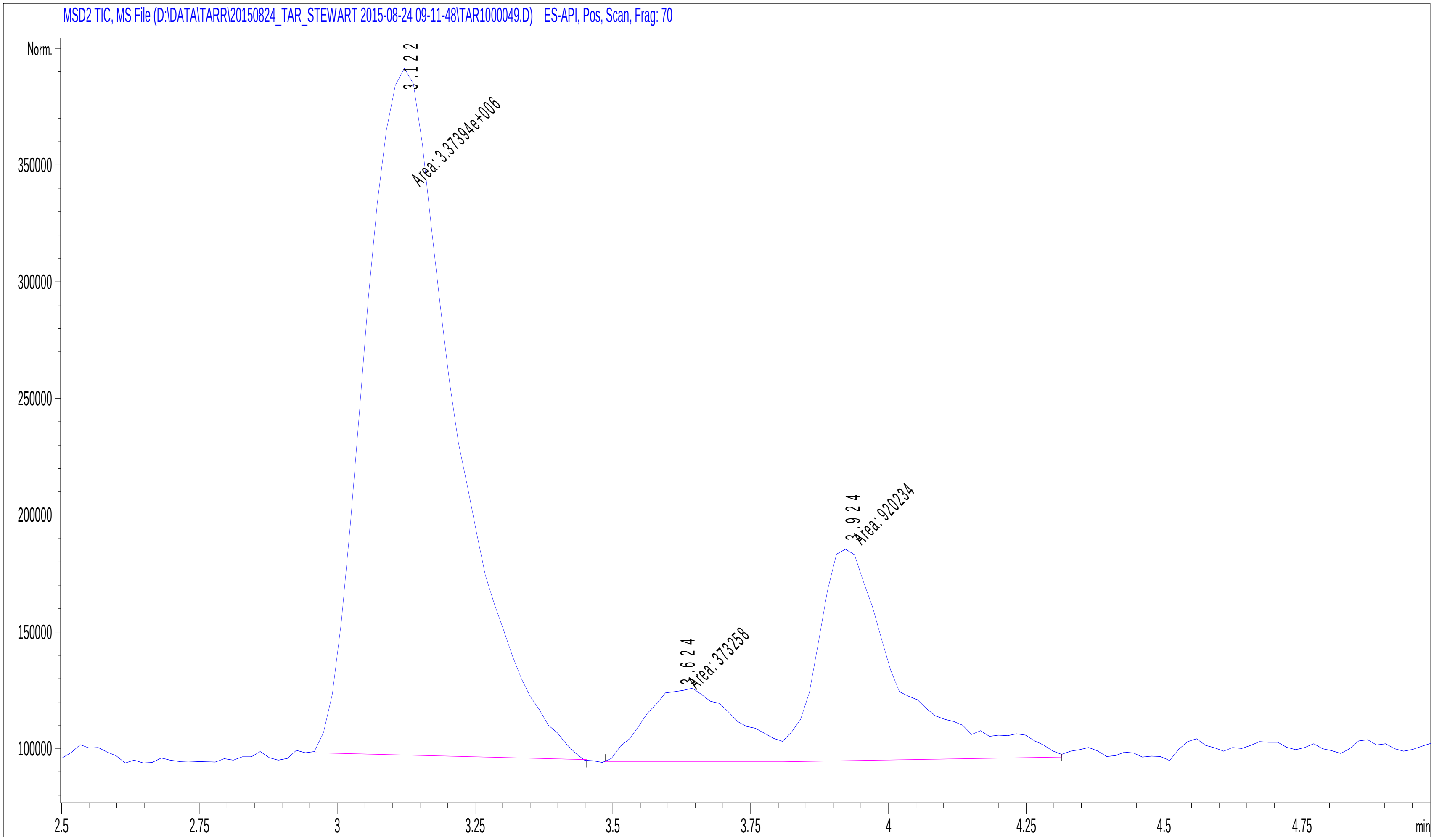
16-Mar-15

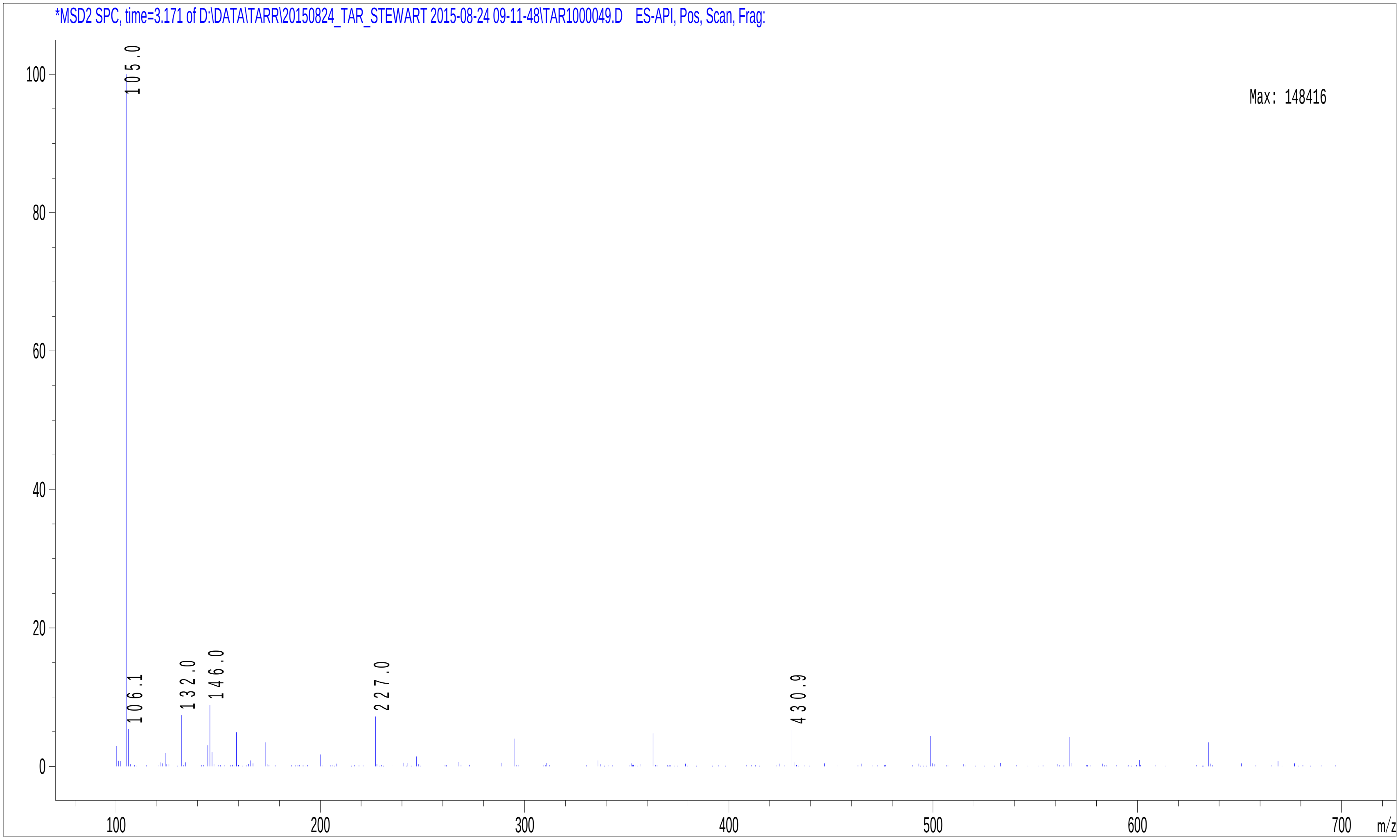
0 DC

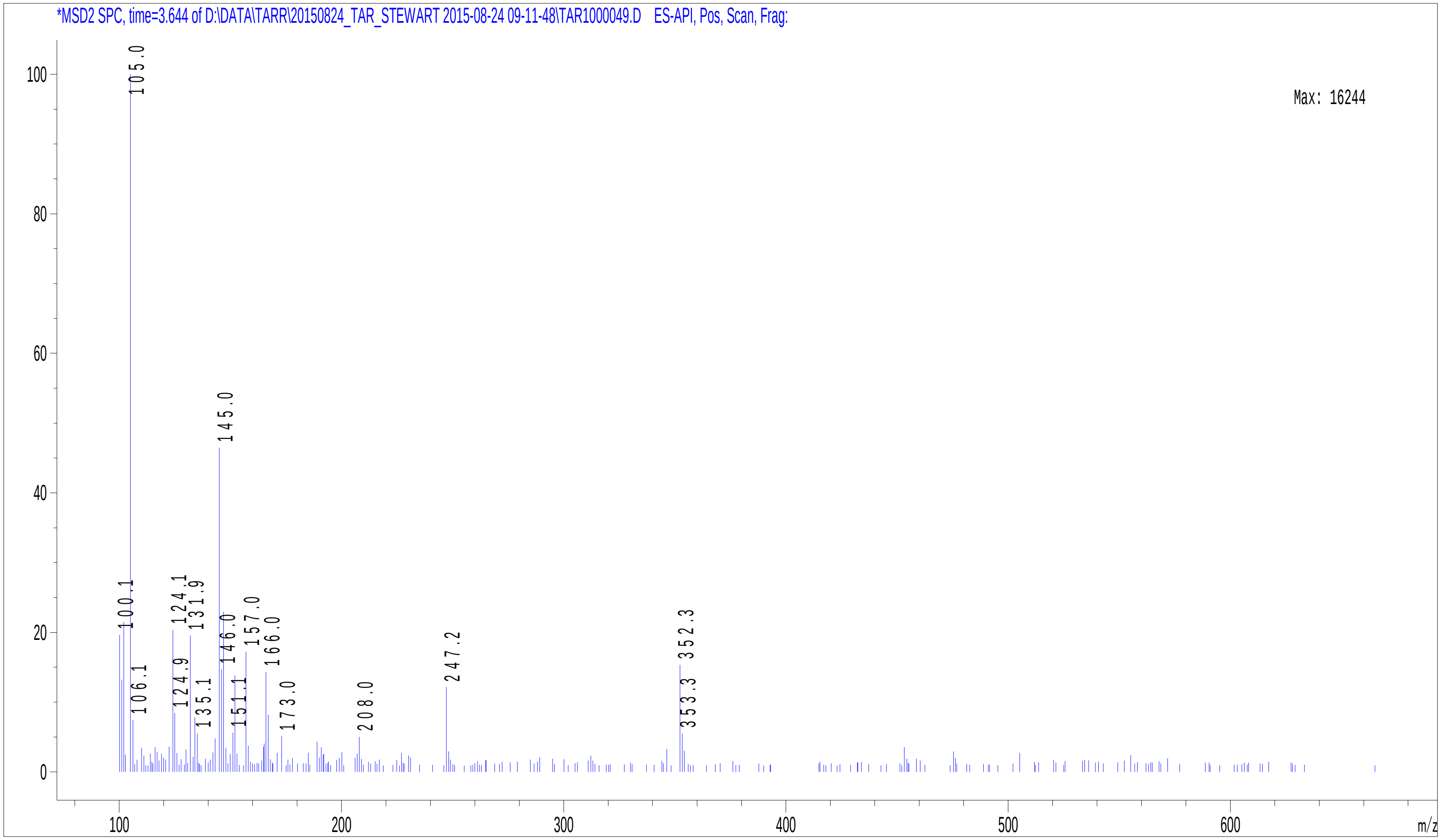
P2-A-04

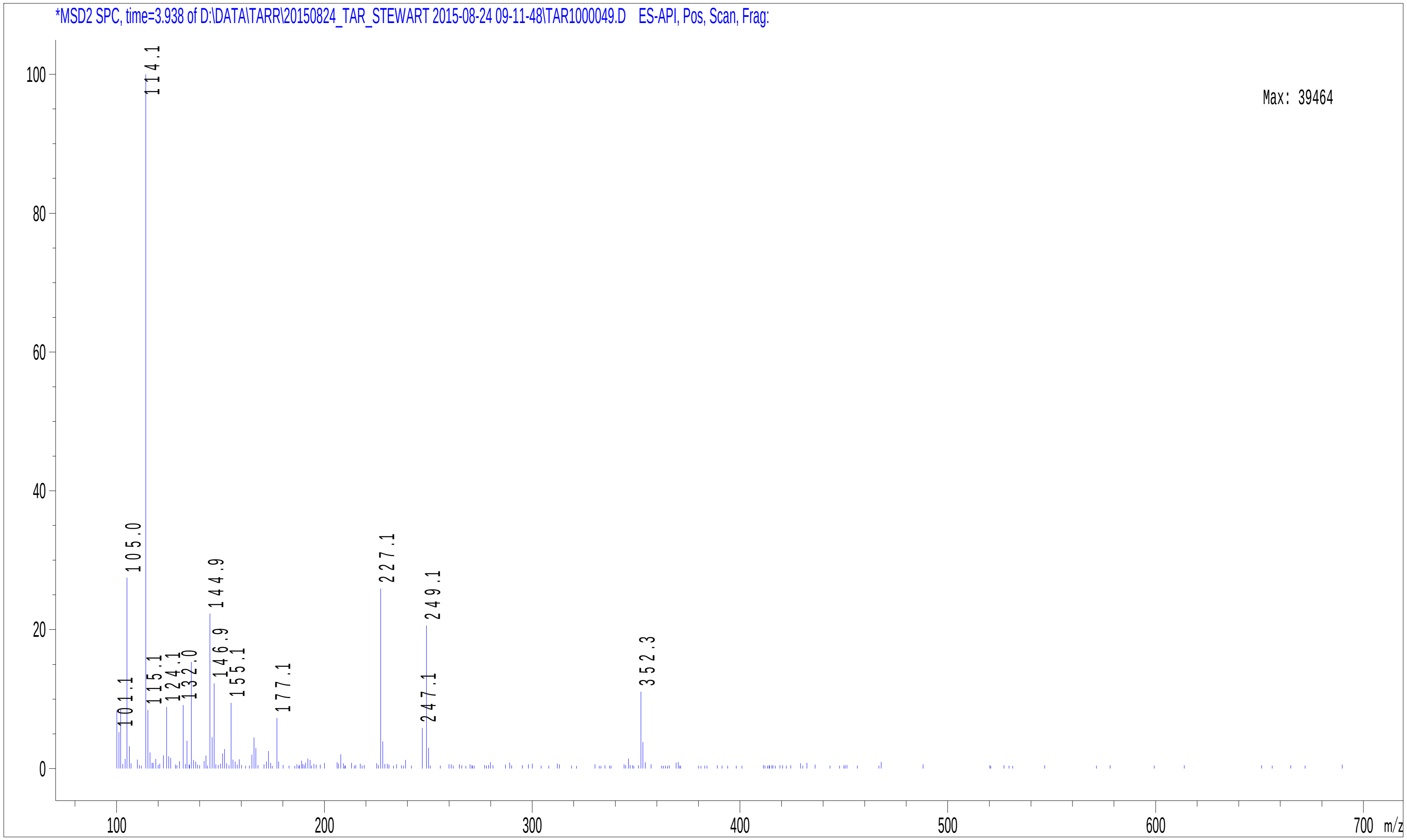


#	Time	Area	Height	Width	Area%	Symmetry
1	3.122	3373936	297327.6	0.1891	72.287	0.883
2	3.624	373257.5	30696.8	0.2027	7.997	0.643
3	3.924	920234.4	92017.1	0.1667	19.716	0.519


MSD2 TIC, MS File (D:\DATA\TARR\20150824_TAR_STEWART 2015-08-24 09-11-48\TAR1000049.D)   ES-API, Pos, Scan, Frag: 70
Norm.
350000
300000
250000
200000
150000
100000
3.122
Area: 3.37394e+006
3.624
Area: 373258
3.924
Area: 920234
2.5
2.75
3
3.25
3.5
3.75
4
4.25
4.5
4.75
min


*MSD2 SPC, time=3.171 of D:\DATA\TARR\20150824_TAR_STEWART 2015-08-24 09-11-48\TAR1000049.D ES-API, Pos, Scan, Frag:
Max: 148416
105.0
106.1
132.0
146.0
227.0
430.9
100
80
60
40
20
0
100
200
300
400
500
600
700
m/z

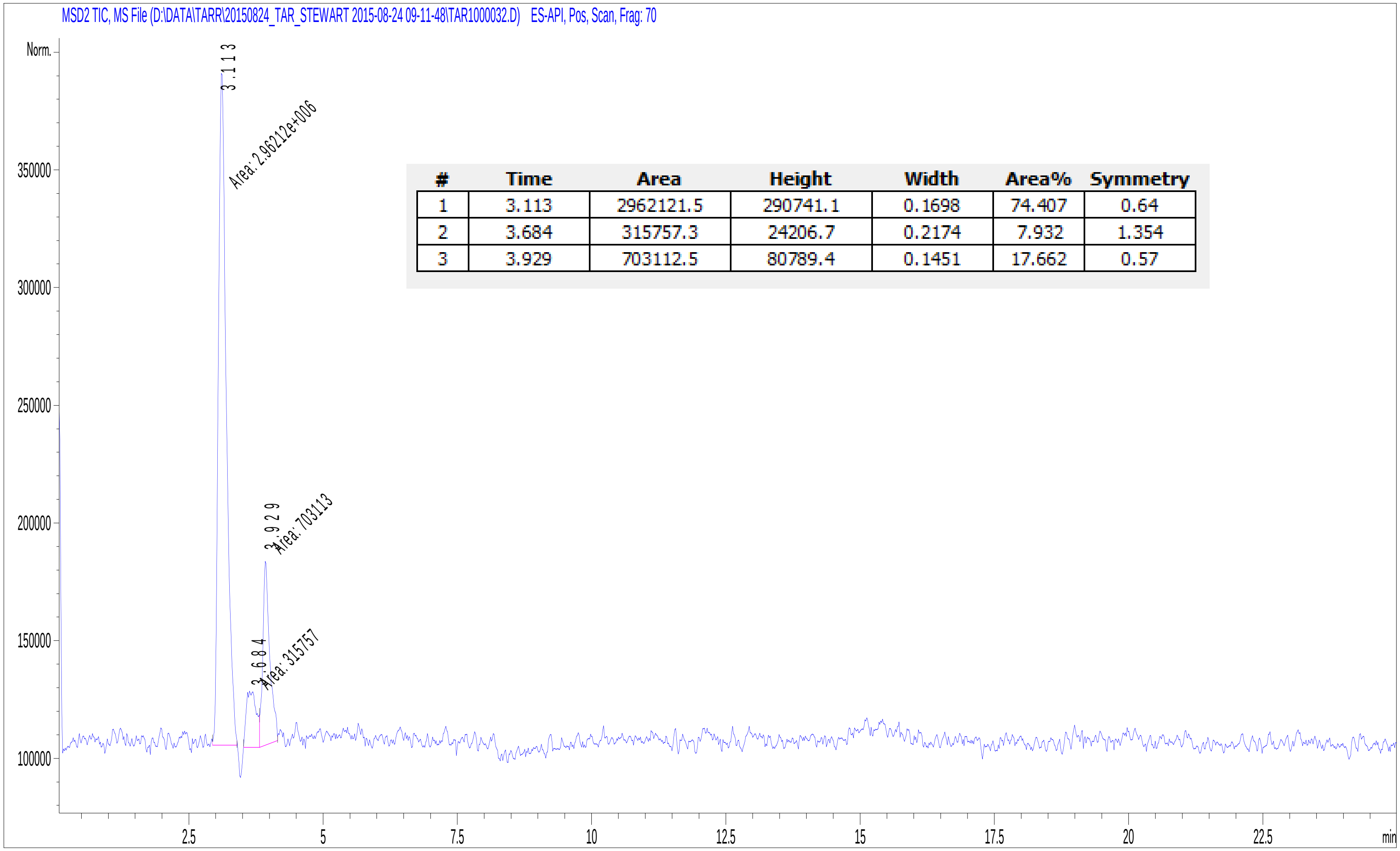

*MSD2 SPC, time=3.644 of D:\DATA\TARR\20150824_TAR_STEWART 2015-08-24 09-11-48\TAR1000049.D ES-API, Pos, Scan, Frag:
Max: 16244
105.0
100.1
106.1
124.1
124.9
131.9
135.1
145.0
146.0
151.1
157.0
166.0
173.0
208.0
247.2
352.3
353.3
100
80
60
40
20
0
100
200
300
400
500
600
m/z


*MSD2 SPC, time=3.938 of D:\DATA\TARR\20150824_TAR_STEWART 2015-08-24 09-11-48\TAR1000049.D ES-API, Pos, Scan, Frag:
Max: 39464
114.1
105.0
101.1
115.1
124.1
132.0
144.9
146.9
155.1
177.1
227.1
249.1
247.1
352.3
100
80
60
40
20
0
100
200
300
400
500
600
700
m/z

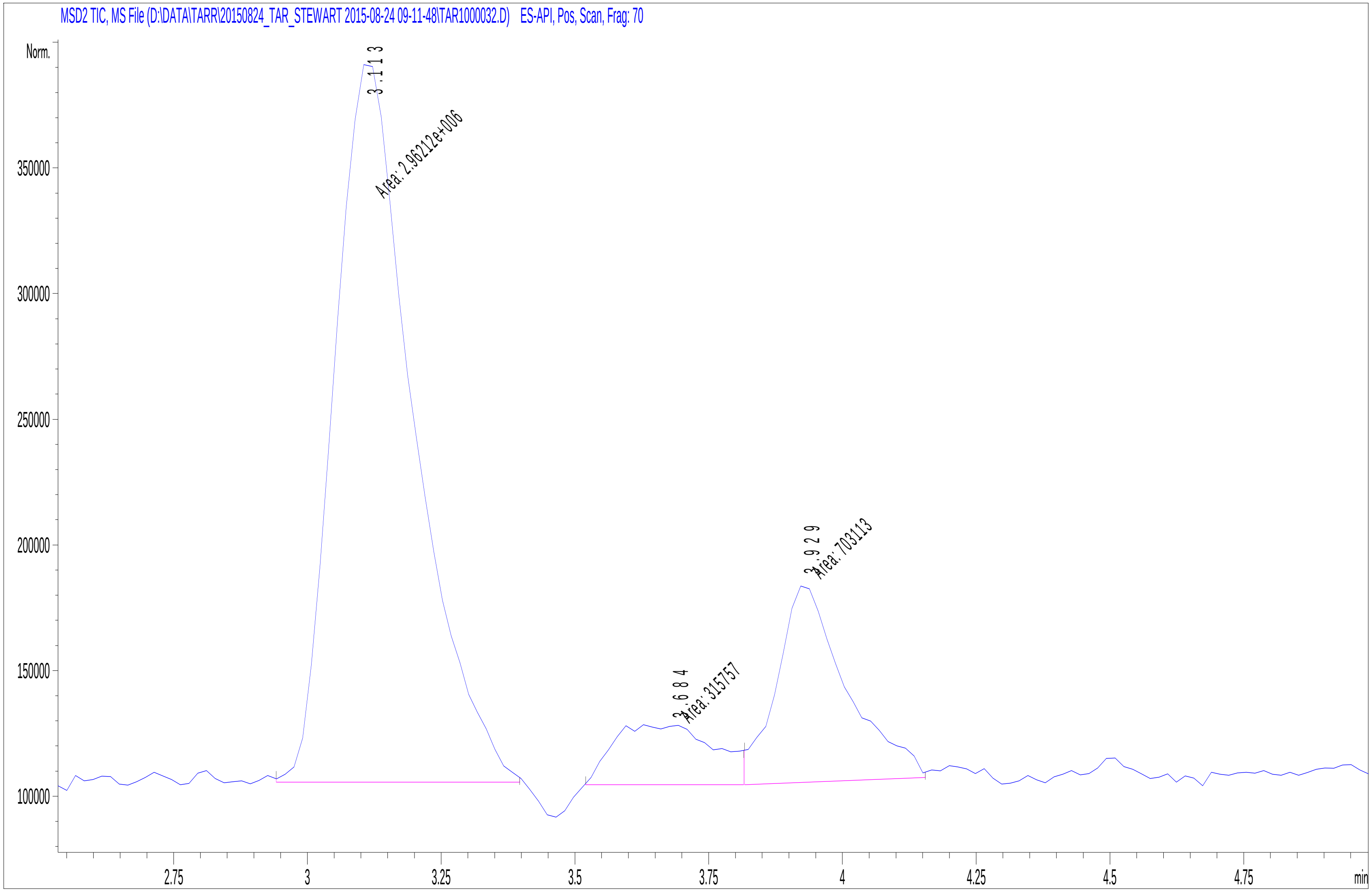
28-Jul-15

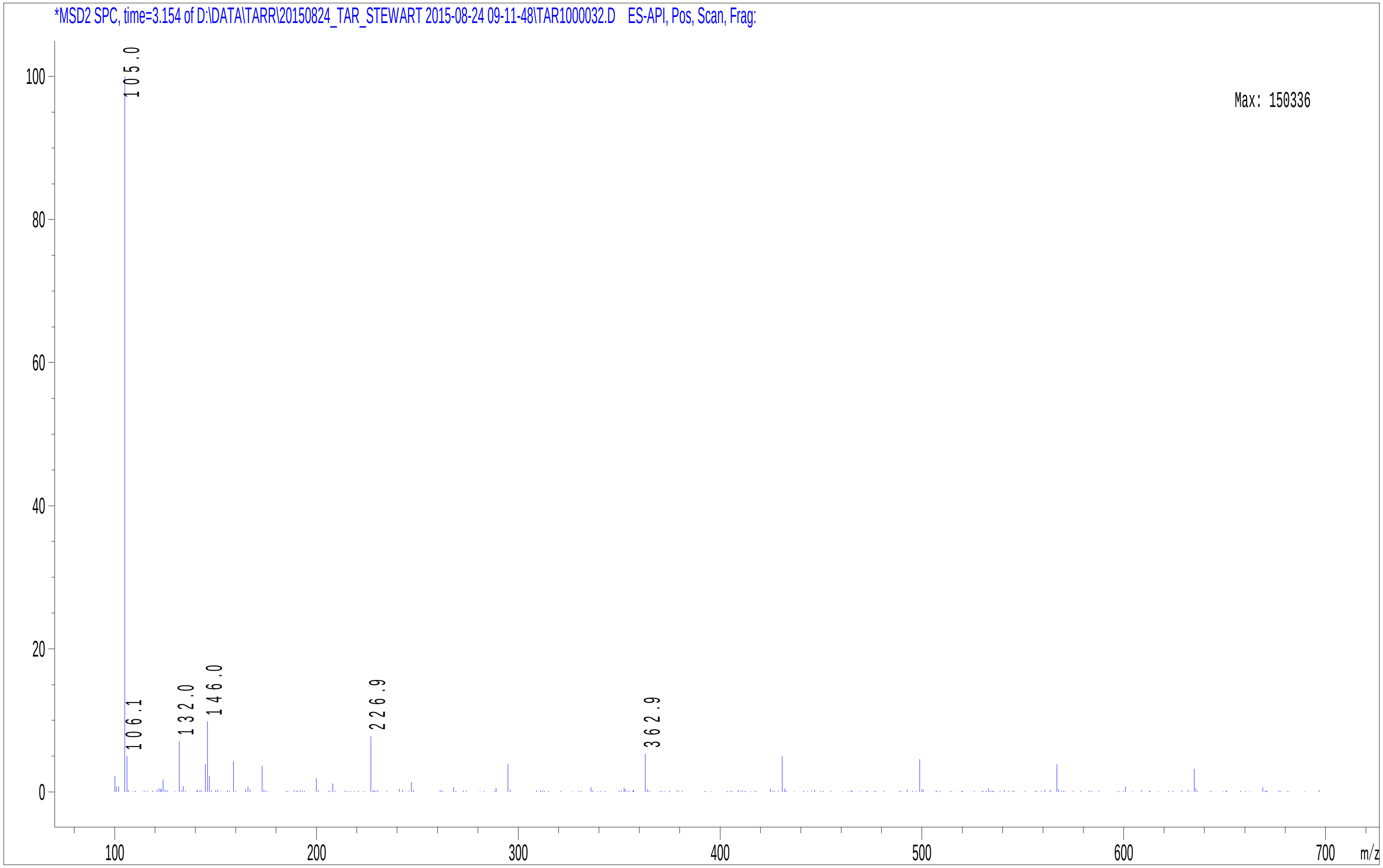
5 DC

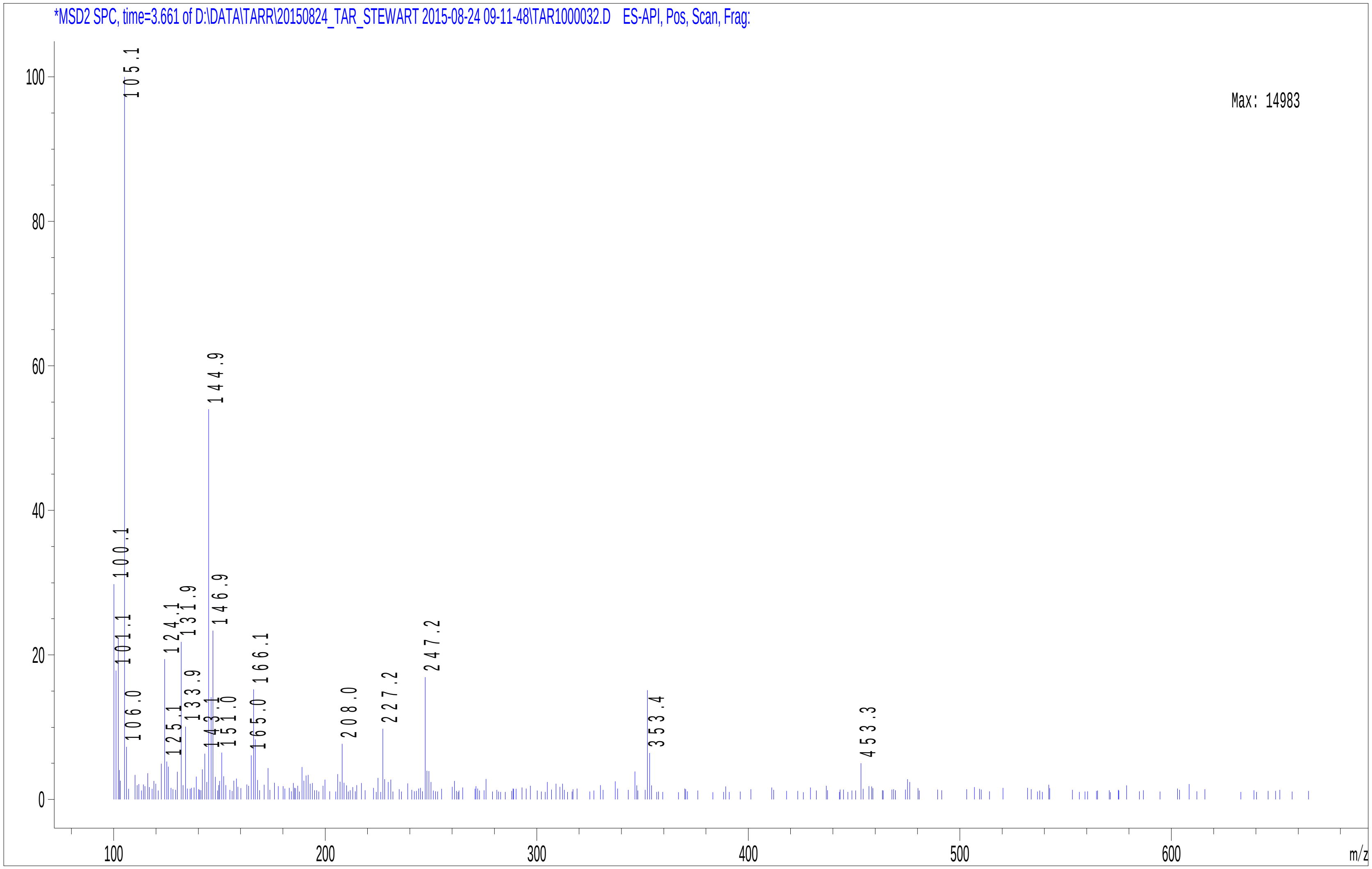
P2-D-05

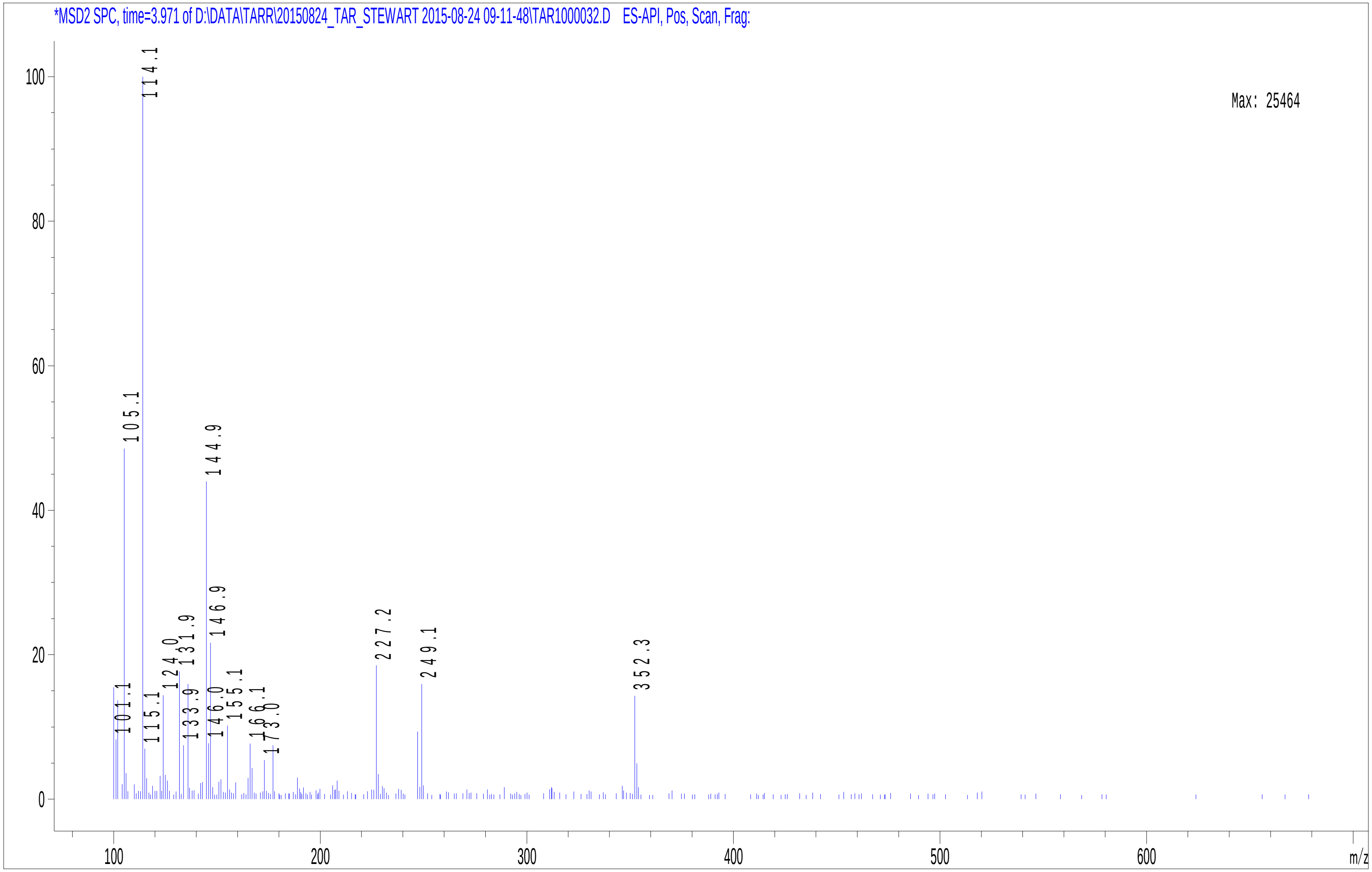


#	Time	Area	Height	Width	Area%	Symmetry
1	3.113	2962121.5	290741.1	0.1698	74.407	0.64
2	3.684	315757.3	24206.7	0.2174	7.932	1.354
3	3.929	703112.5	80789.4	0.1451	17.662	0.57


MSD2 TIC, MS File (D:\DATA\TARR\20150824_TAR_STEWART 2015-08-24 09-11-48\TAR1000032.D)   ES-API, Pos, Scan, Frag: 70
Norm.
350000
300000
250000
200000
150000
100000
3.113
Area: 2.96212e+006
3.684
Area: 315757
3.929
Area: 703113
2.75
3
3.25
3.5
3.75
4
4.25
4.5
4.75
min


*MSD2 SPC, time=3.154 of D:\DATA\TARR\20150824_TAR_STEWART 2015-08-24 09-11-48\TAR1000032.D ES-API, Pos, Scan, Frag:
Max: 150336
105.0
106.1
132.0
146.0
226.9
362.9
100
80
60
40
20
0
100
200
300
400
500
600
700
m/z

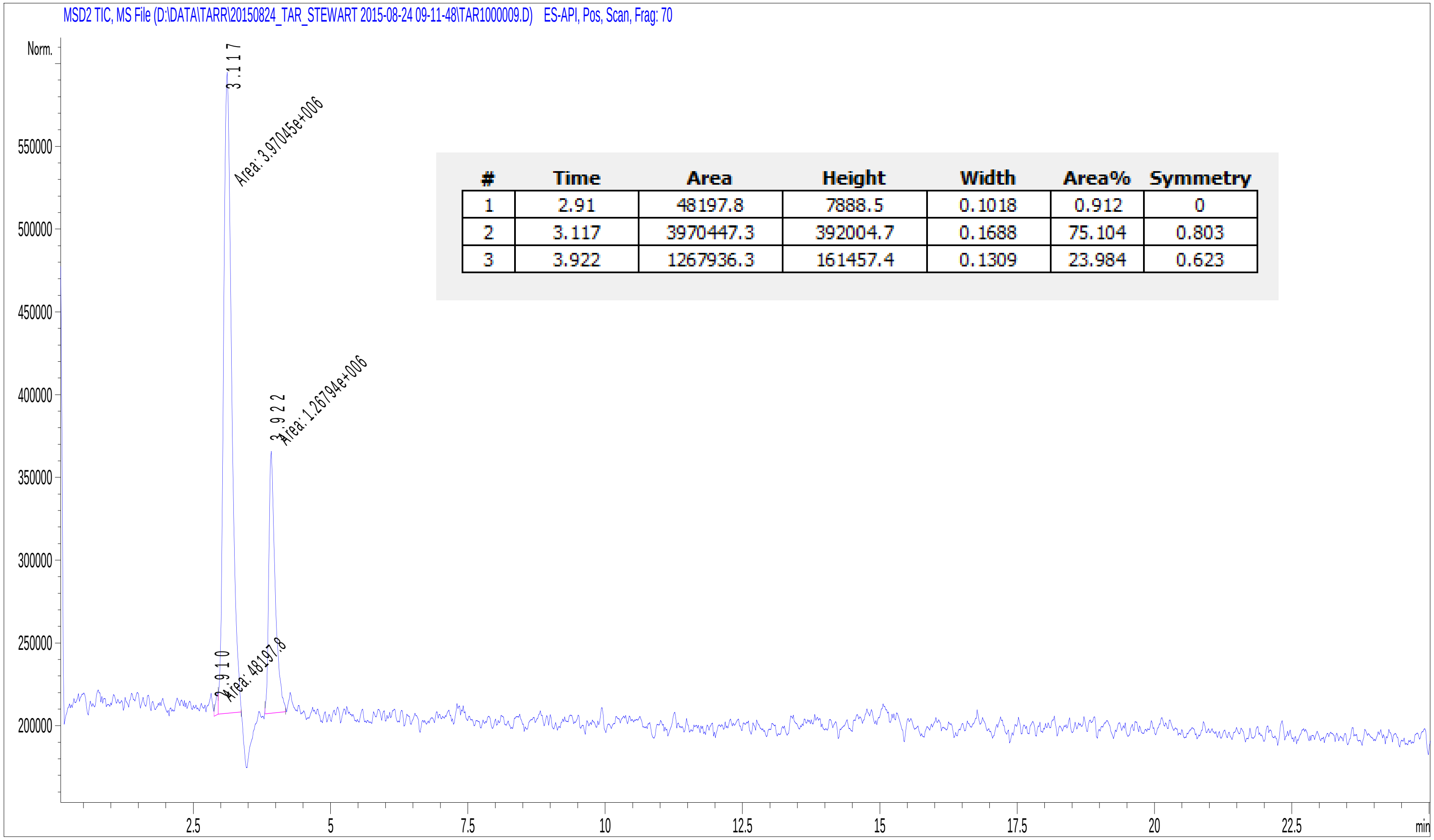

*MSD2 SPC, time=3.661 of D:\DATA\TARR\20150824_TAR_STEWART 2015-08-24 09-11-48\TAR1000032.D ES-API, Pos, Scan, Frag:
Max: 14983
105.1
144.9
100.1
101.1
106.0
124.1
125.1
131.9
133.9
143.1
146.9
151.0
165.0
166.1
208.0
227.2
247.2
353.4
453.3
0
20
40
60
80
100
200
300
400
500
600
m/z


*MSD2 SPC, time=3.971 of D:\DATA\TARR\20150824_TAR_STEWART 2015-08-24 09-11-48\TAR1000032.D ES-API, Pos, Scan, Frag:
Max: 25464
114.1
105.1
144.9
146.9
131.9
124.0
227.2
249.1
352.3
101.1
115.1
133.9
146.0
155.1
166.1
173.0
0
20
40
60
80
100
100
200
300
400
500
600
m/z

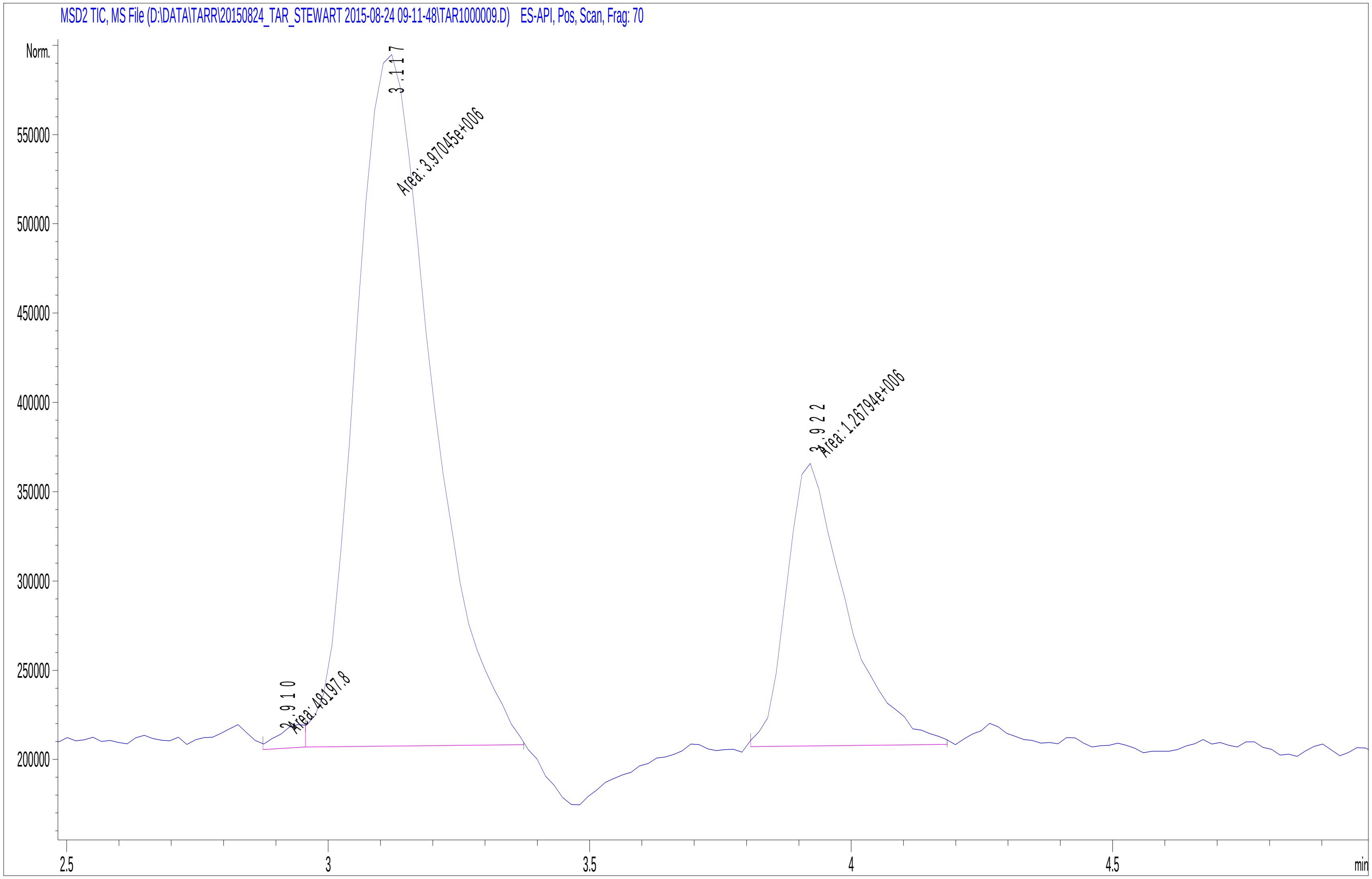
30-Apr-15

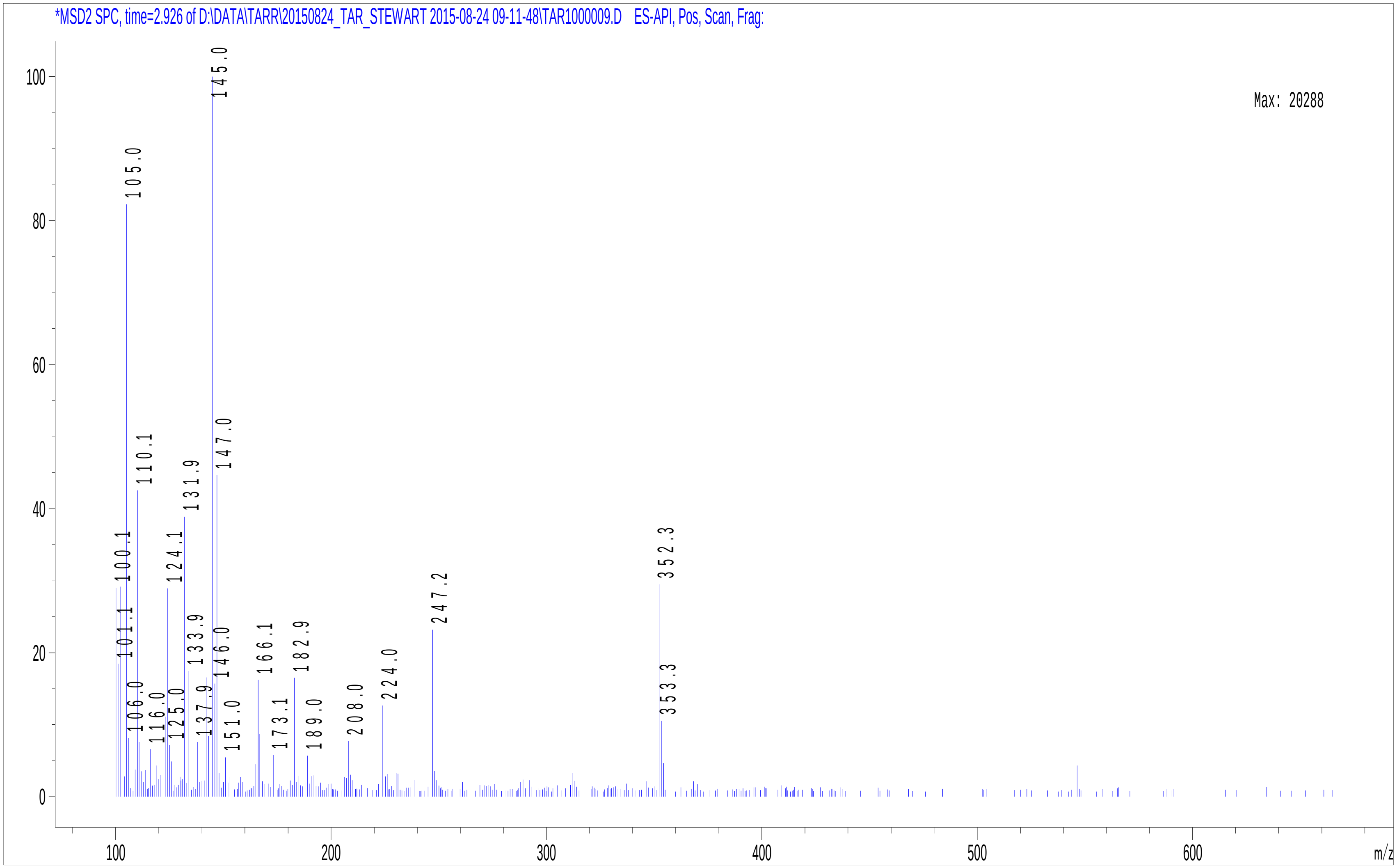
10 DC

P2-A-09

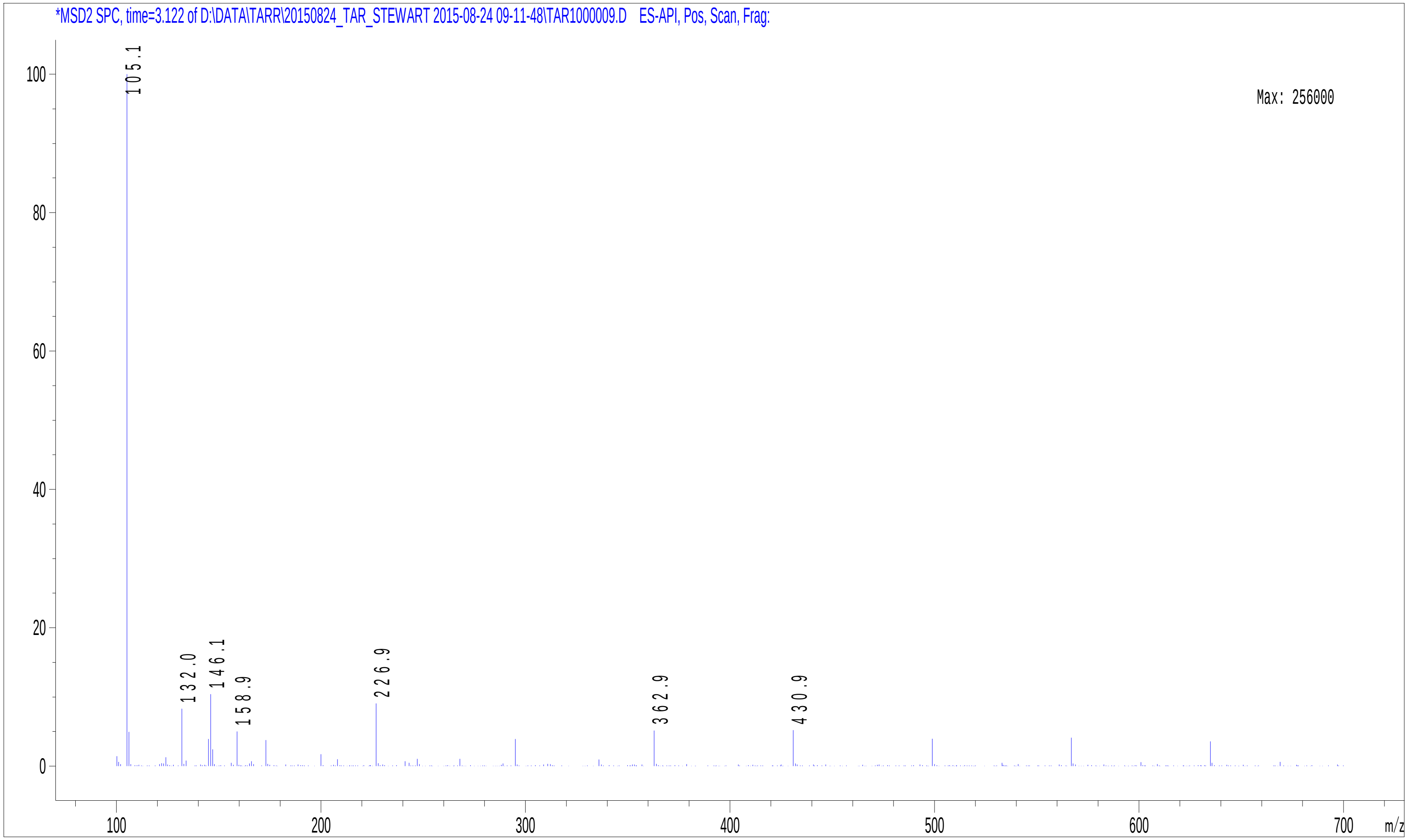


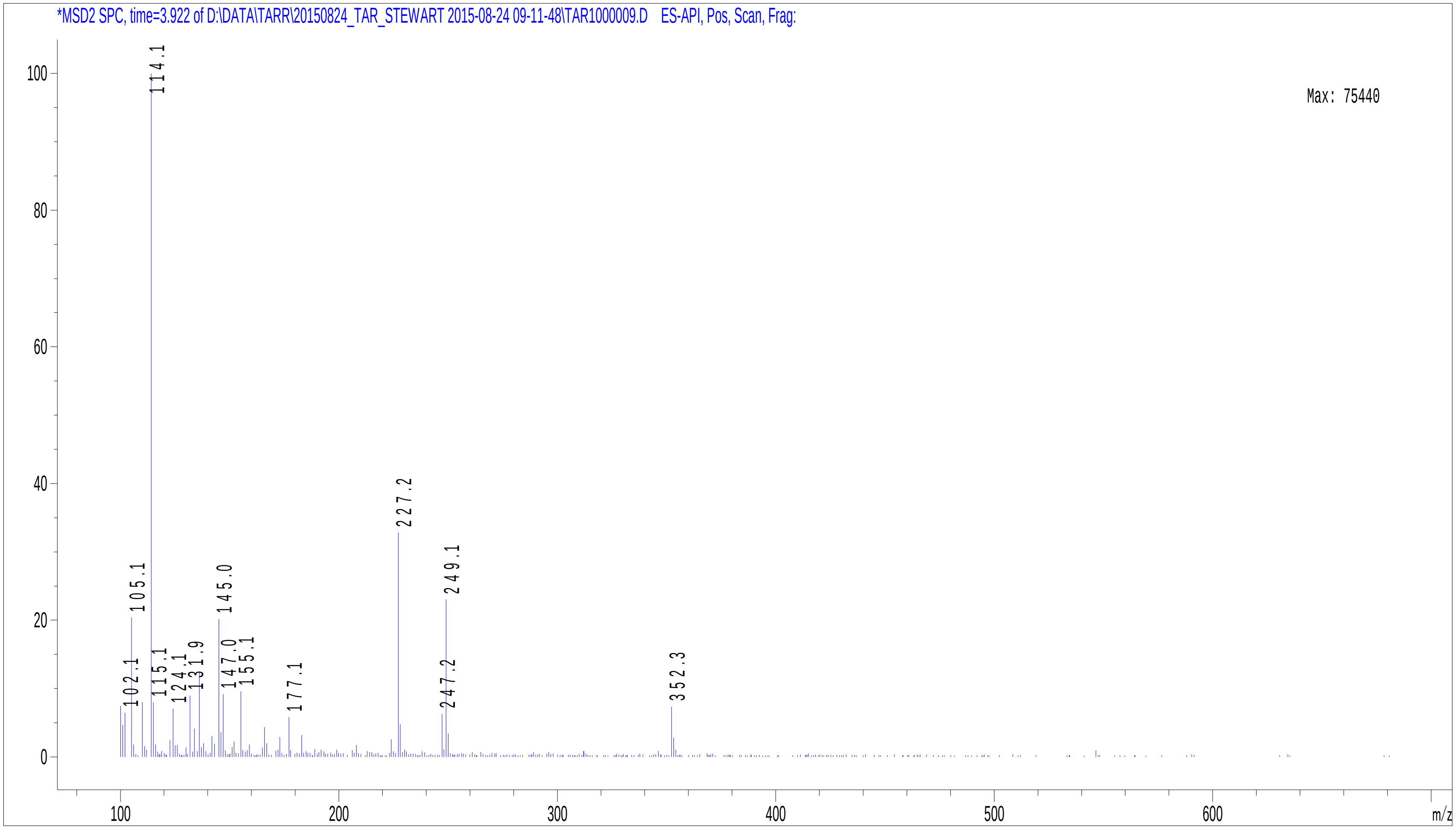
#	Time	Area	Height	Width	Area%	Symmetry
1	2.91	48197.8	7888.5	0.1018	0.912	0
2	3.117	3970447.3	392004.7	0.1688	75.104	0.803
3	3.922	1267936.3	161457.4	0.1309	23.984	0.623


MSD2 TIC, MS File (D:\DATA\TARR\20150824_TAR_STEWART 2015-08-24 09-11-48\TAR1000009.D)   ES-API, Pos, Scan, Frag: 70
Norm.
550000
500000
450000
400000
350000
300000
250000
200000
3.117
Area: 3.97045e+006
2.910
Area: 48197.8
3.922
Area: 1.26794e+006
2.5
3
3.5
4
4.5
min



*MSD2 SPC, time=2.926 of D:\DATA\TARR\20150824_TAR_STEWART 2015-08-24 09-11-48\TAR1000009.D ES-API, Pos, Scan, Frag:
Max: 20288
100
80
60
40
20
0
100.1
101.1
105.0
106.0
110.1
116.0
124.1
125.0
131.9
133.9
137.9
145.0
146.0
147.0
151.0
166.1
173.1
182.9
189.0
208.0
224.0
247.2
352.3
353.3
100
200
300
400
500
600
m/z

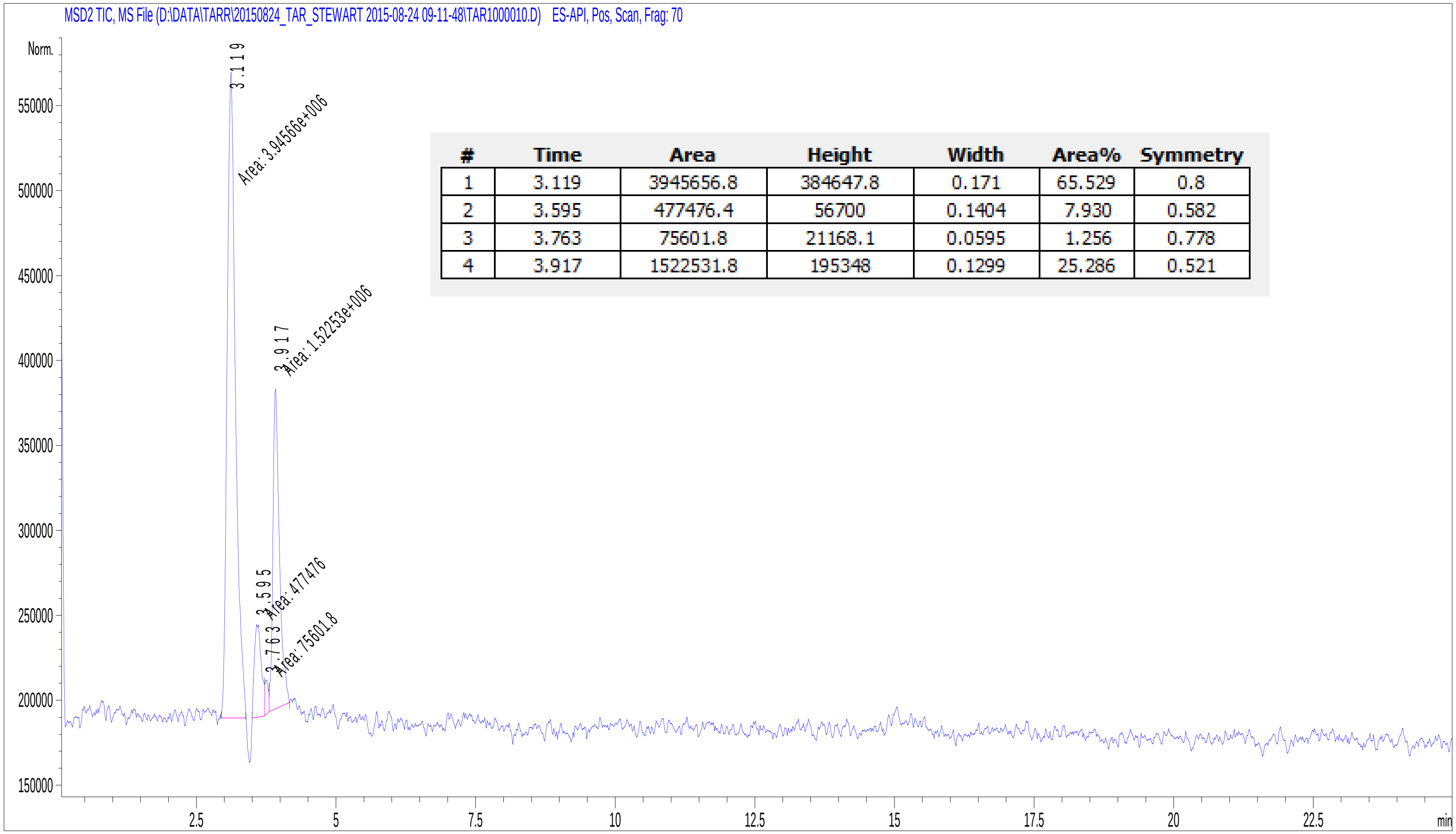

*MSD2 SPC, time=3.122 of D:\DATA\TARR\20150824_TAR_STEWART 2015-08-24 09-11-48\TAR1000009.D   ES-API, Pos, Scan, Frag:
Max: 256000
105.1
132.0
146.1
158.9
226.9
362.9
430.9
100
80
60
40
20
0
100
200
300
400
500
600
700
m/z


*MSD2 SPC, time=3.922 of D:\DATA\TARR\20150824_TAR_STEWART 2015-08-24 09-11-48\TAR1000009.D ES-API, Pos, Scan, Frag:
Max: 75440
114.1
105.1
102.1
115.1
124.1
131.9
145.0
147.0
155.1
177.1
227.2
249.1
247.2
352.3
100
80
60
40
20
0
100
200
300
400
500
600
m/z

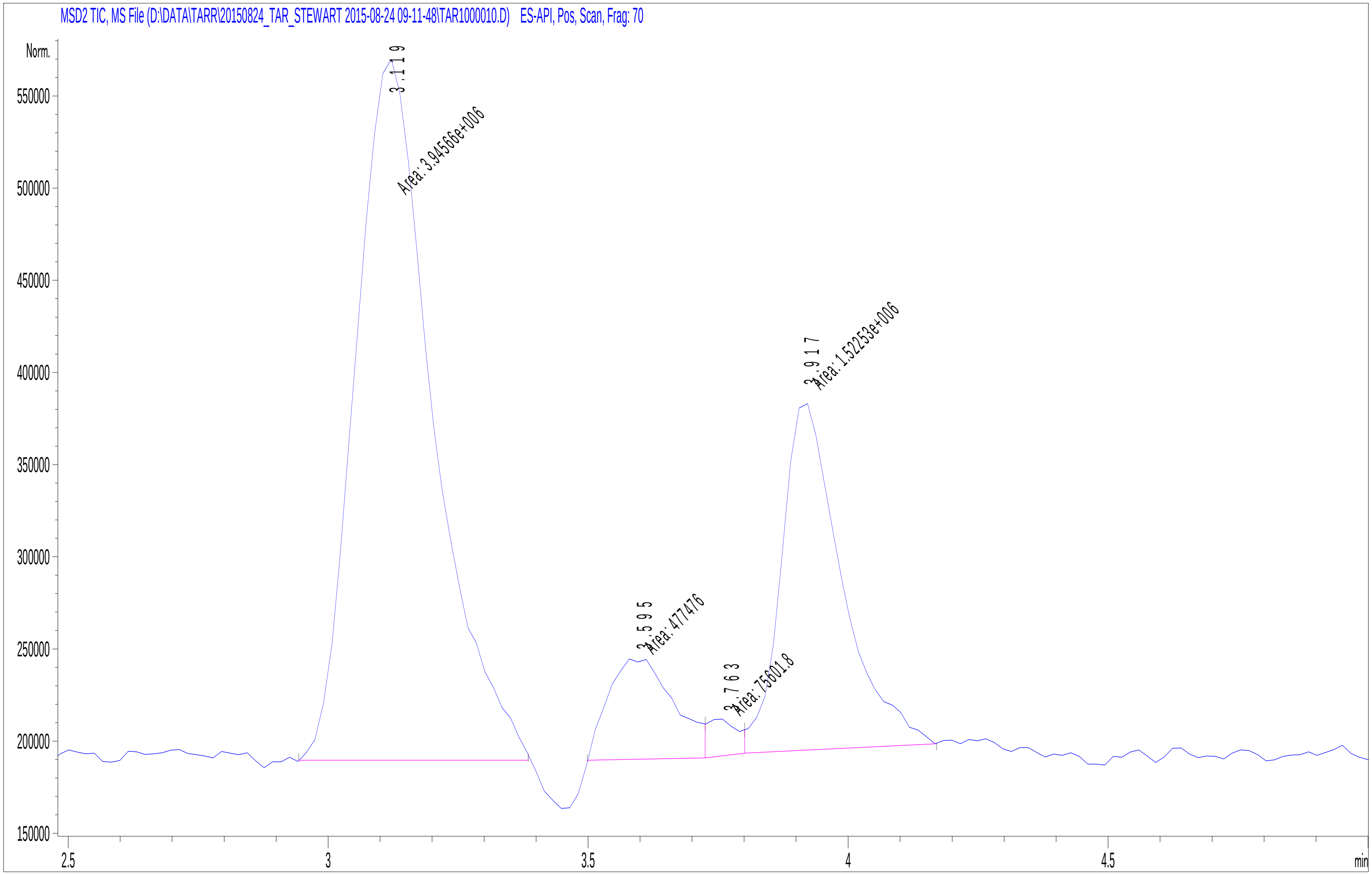
22-Jun-15

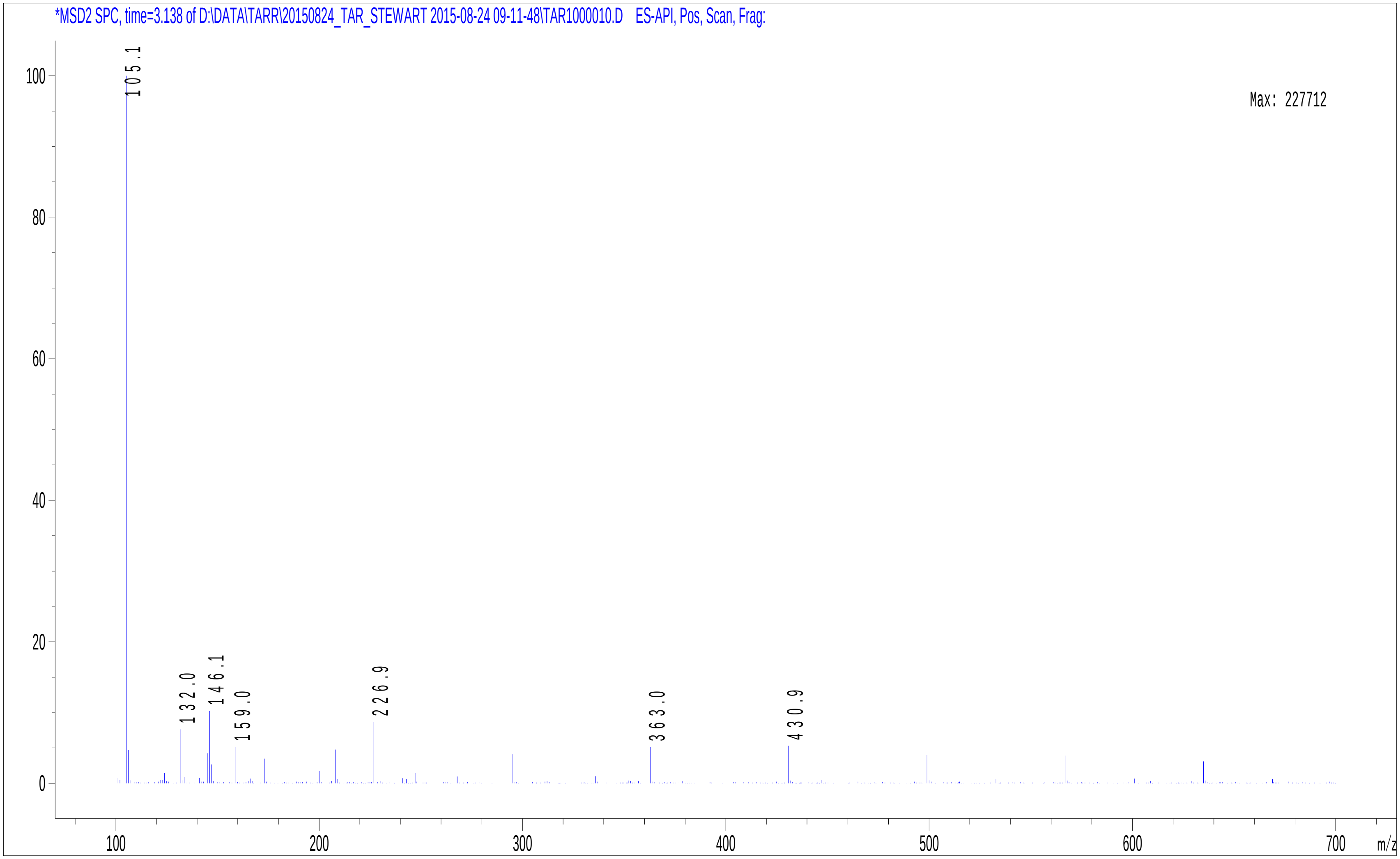
20 DC

P2-B-09

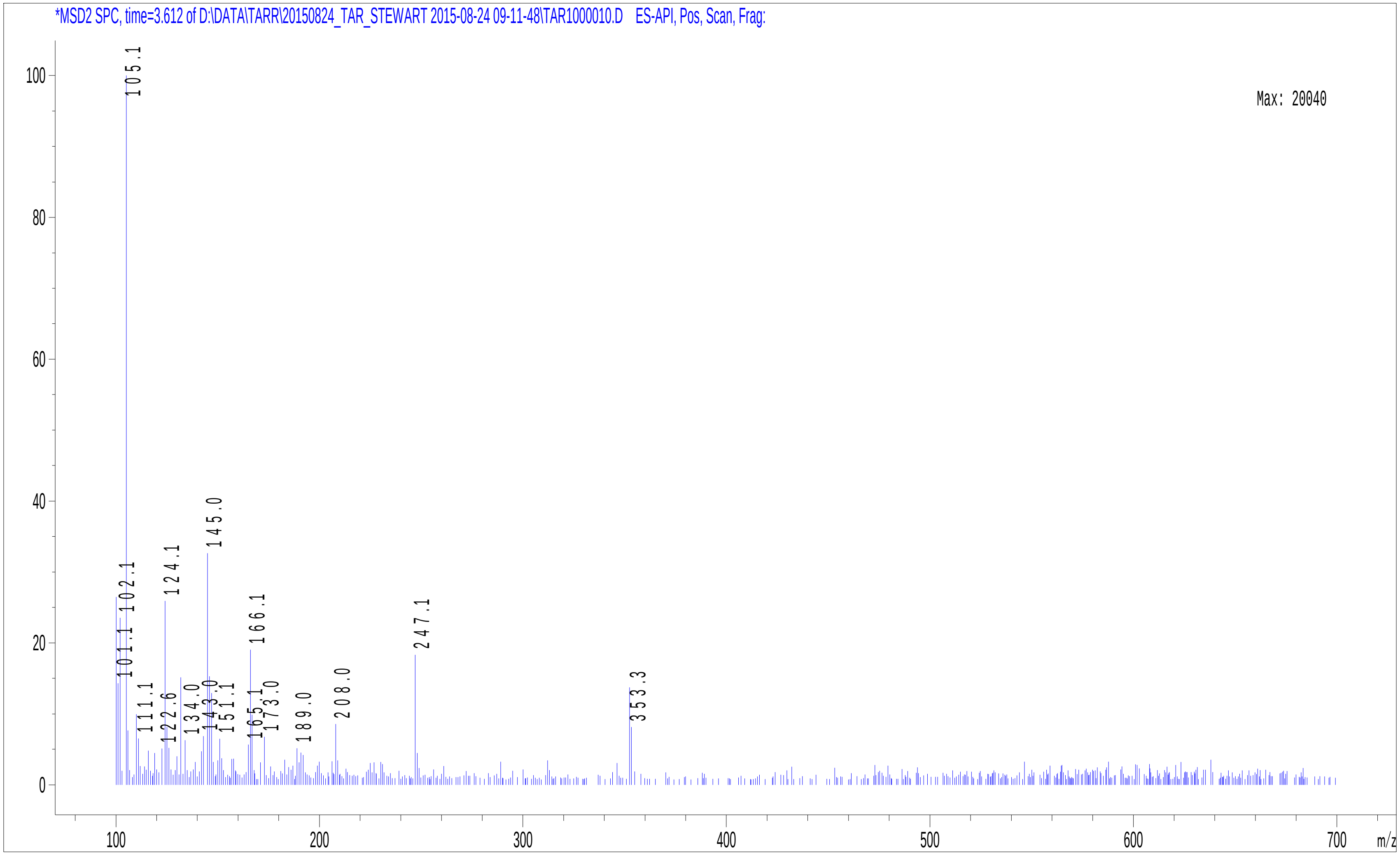


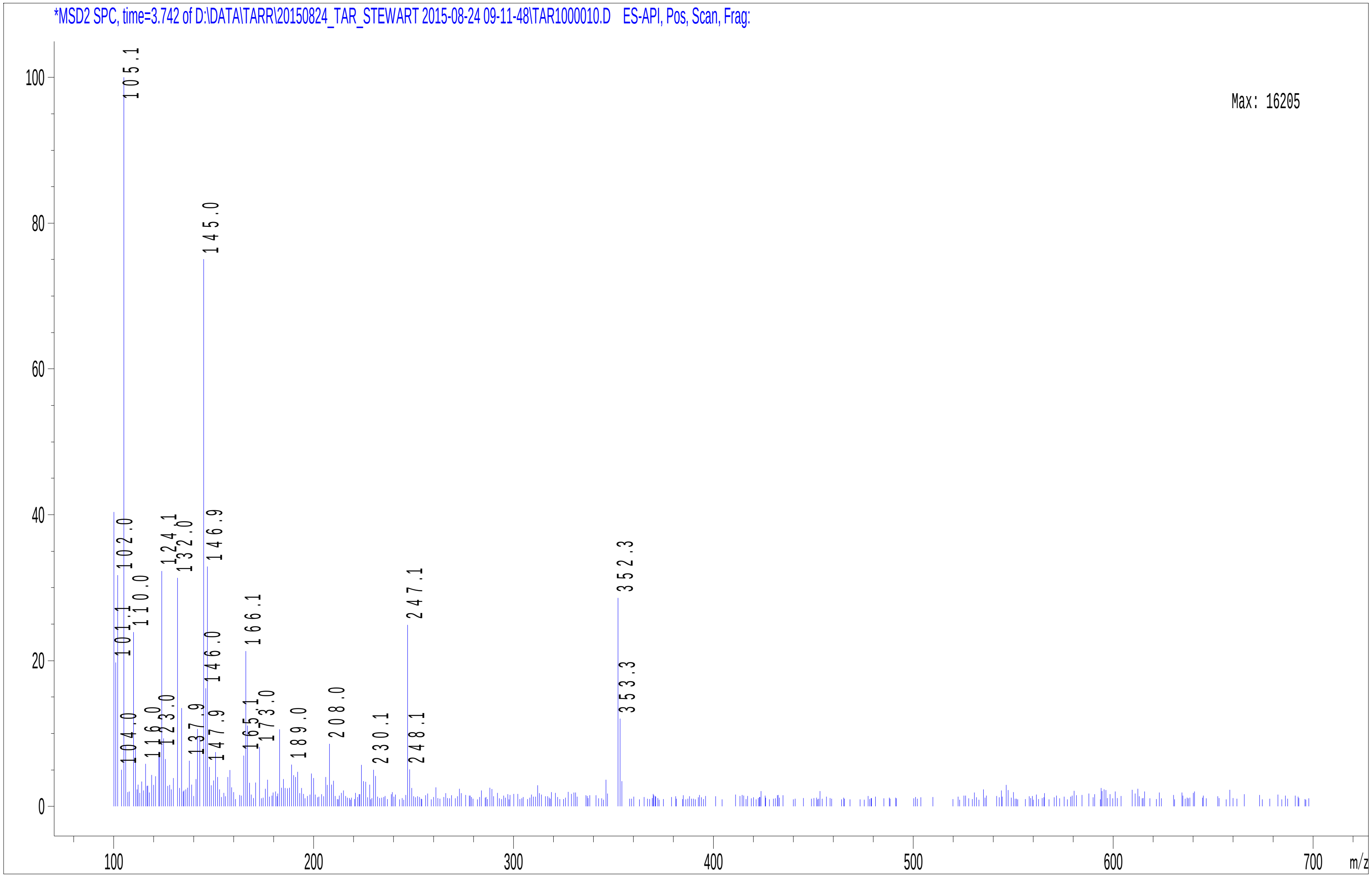
#	Time	Area	Height	Width	Area%	Symmetry
1	3.119	3945656.8	384647.8	0.171	65.529	0.8
2	3.595	477476.4	56700	0.1404	7.930	0.582
3	3.763	75601.8	21168.1	0.0595	1.256	0.778
4	3.917	1522531.8	195348	0.1299	25.286	0.521

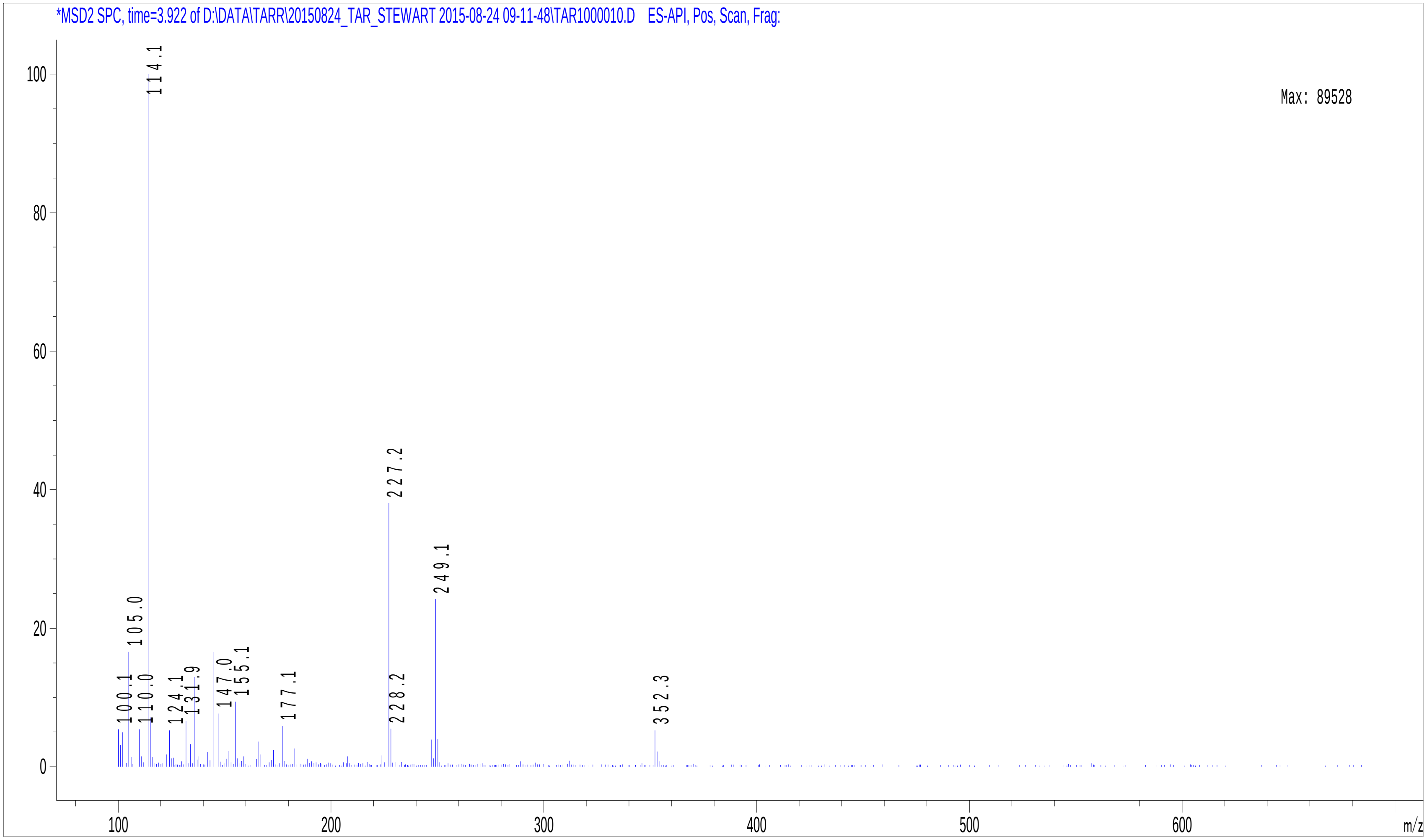

MSD2 TIC, MS File (D:\DATA\TARR\20150824_TAR_STEWART 2015-08-24 09-11-48\TAR1000010.D)   ES-API, Pos, Scan, Frag: 70
Norm.
550000
500000
450000
400000
350000
300000
250000
200000
150000
3.119
Area: 3.94566e+006
3.595
Area: 477476
3.763
Area: 75601.8
3.917
Area: 1.52253e+006
2.5
3
3.5
4
4.5
min



*MSD2 SPC, time=3.138 of D:\DATA\TARR\20150824_TAR_STEWART 2015-08-24 09-11-48\TAR1000010.D ES-API, Pos, Scan, Frag:
Max: 227712
105.1
132.0
146.1
159.0
226.9
363.0
430.9
100
80
60
40
20
0
100
200
300
400
500
600
700
m/z


*MSD2 SPC, time=3.612 of D:\DATA\TARR\20150824_TAR_STEWART 2015-08-24 09-11-48\TAR1000010.D ES-API, Pos, Scan, Frag:
Max: 20040
105.1
145.0
124.1
102.1
166.1
101.1
247.1
111.1
122.6
134.0
143.0
151.1
165.1
173.0
189.0
208.0
353.3
0
20
40
60
80
100
100
200
300
400
500
600
700
m/z


*MSD2 SPC, time=3.742 of D:\DATA\TARR\20150824_TAR_STEWART 2015-08-24 09-11-48\TAR1000010.D ES-API, Pos, Scan, Frag:
Max: 16205
105.1
145.0
102.0
124.1
132.0
146.9
110.0
101.1
166.1
146.0
104.0
116.0
123.0
137.9
147.9
165.1
173.0
189.0
208.0
230.1
247.1
248.1
352.3
353.3
0
20
40
60
80
100
100
200
300
400
500
600
700
m/z

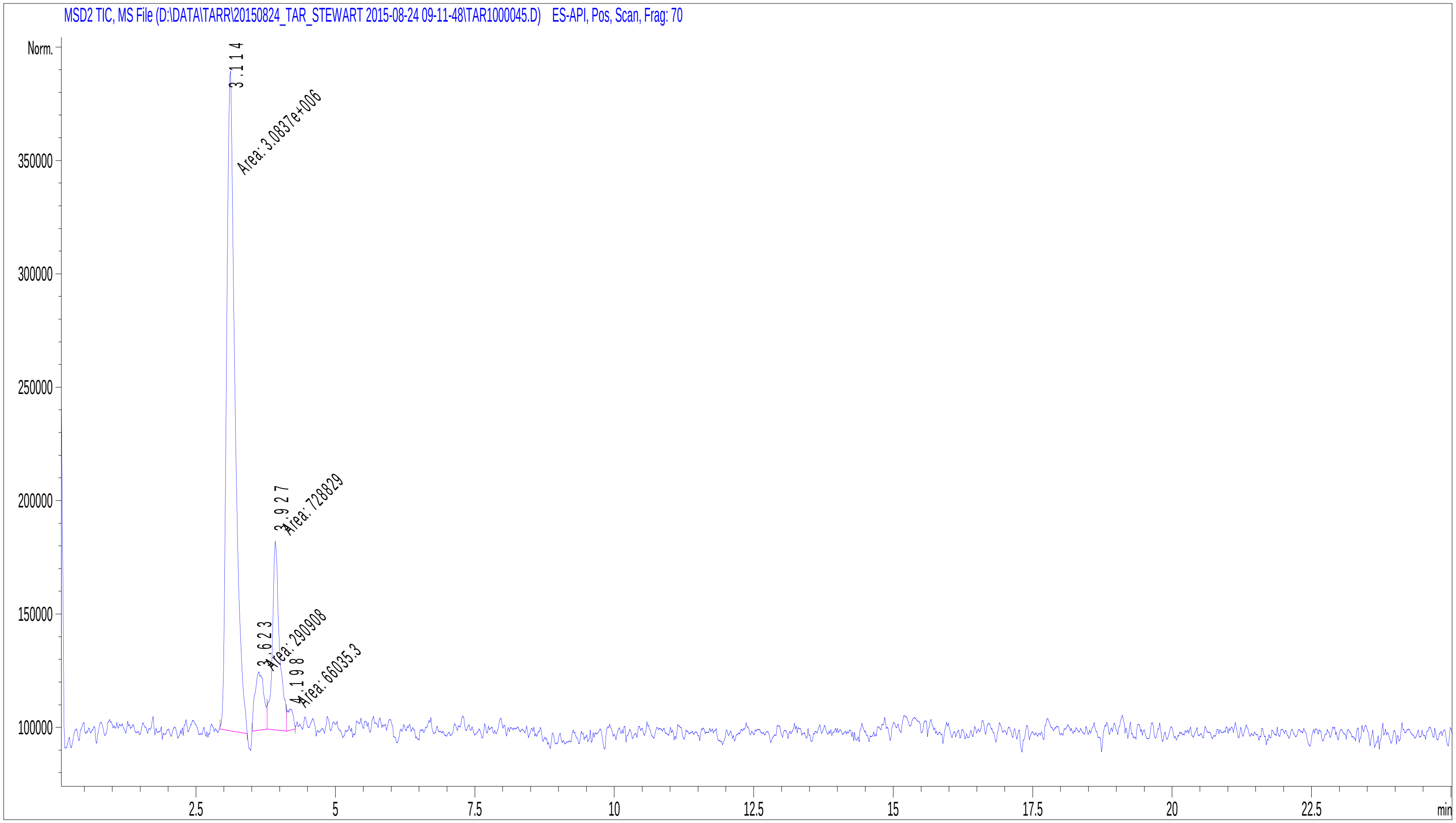


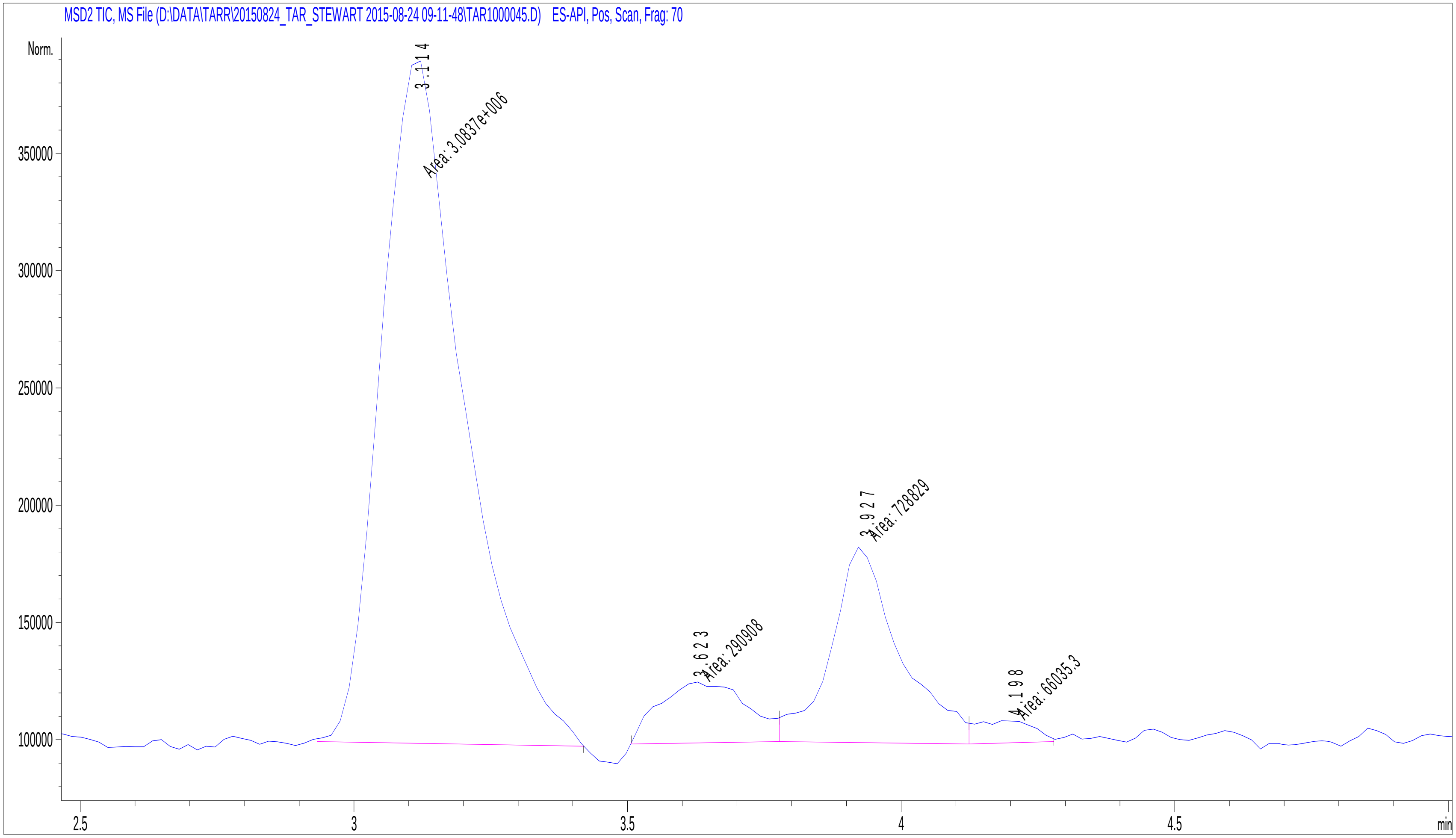
*MSD2 SPC, time=3.922 of D:\DATA\TARR\20150824_TAR_STEWART 2015-08-24 09-11-48\TAR1000010.D ES-API, Pos, Scan, Frag:
Max: 89528
114.1
105.0
100.1
110.0
124.1
131.9
147.0
155.1
177.1
227.2
228.2
249.1
352.3
0
20
40
60
80
100
100
200
300
400
500
600
m/z

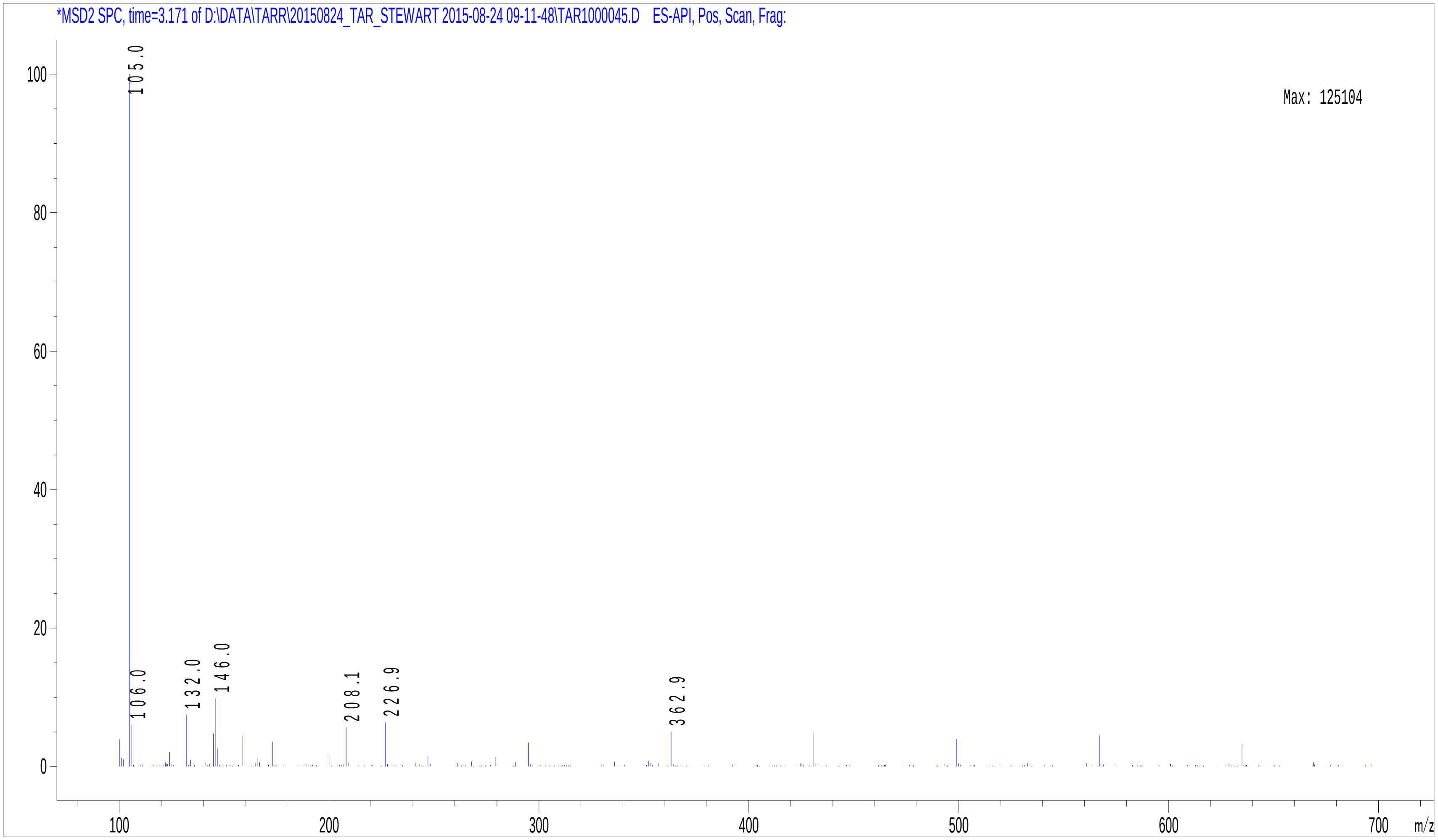
5-Aug-15

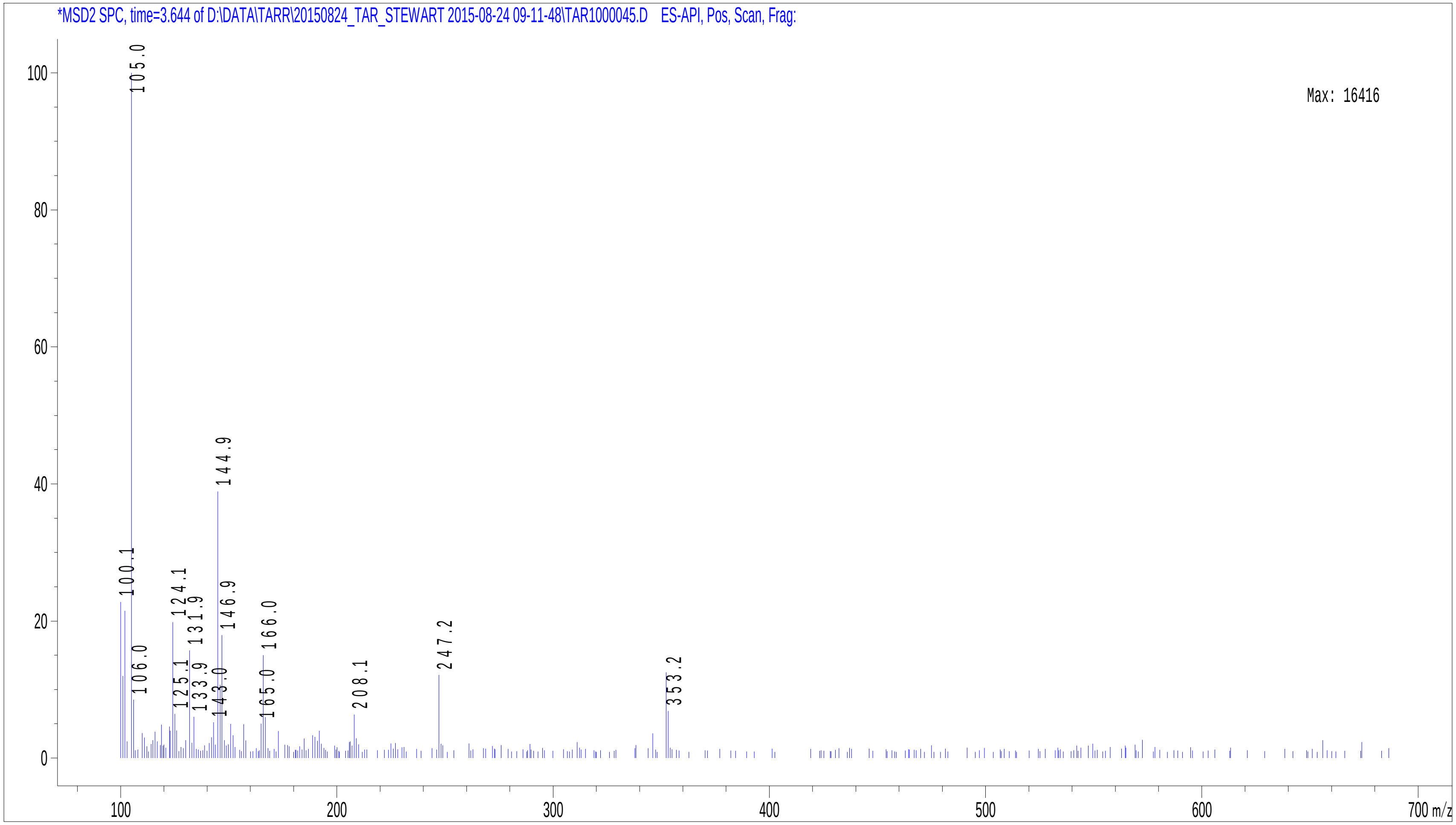
30 DC

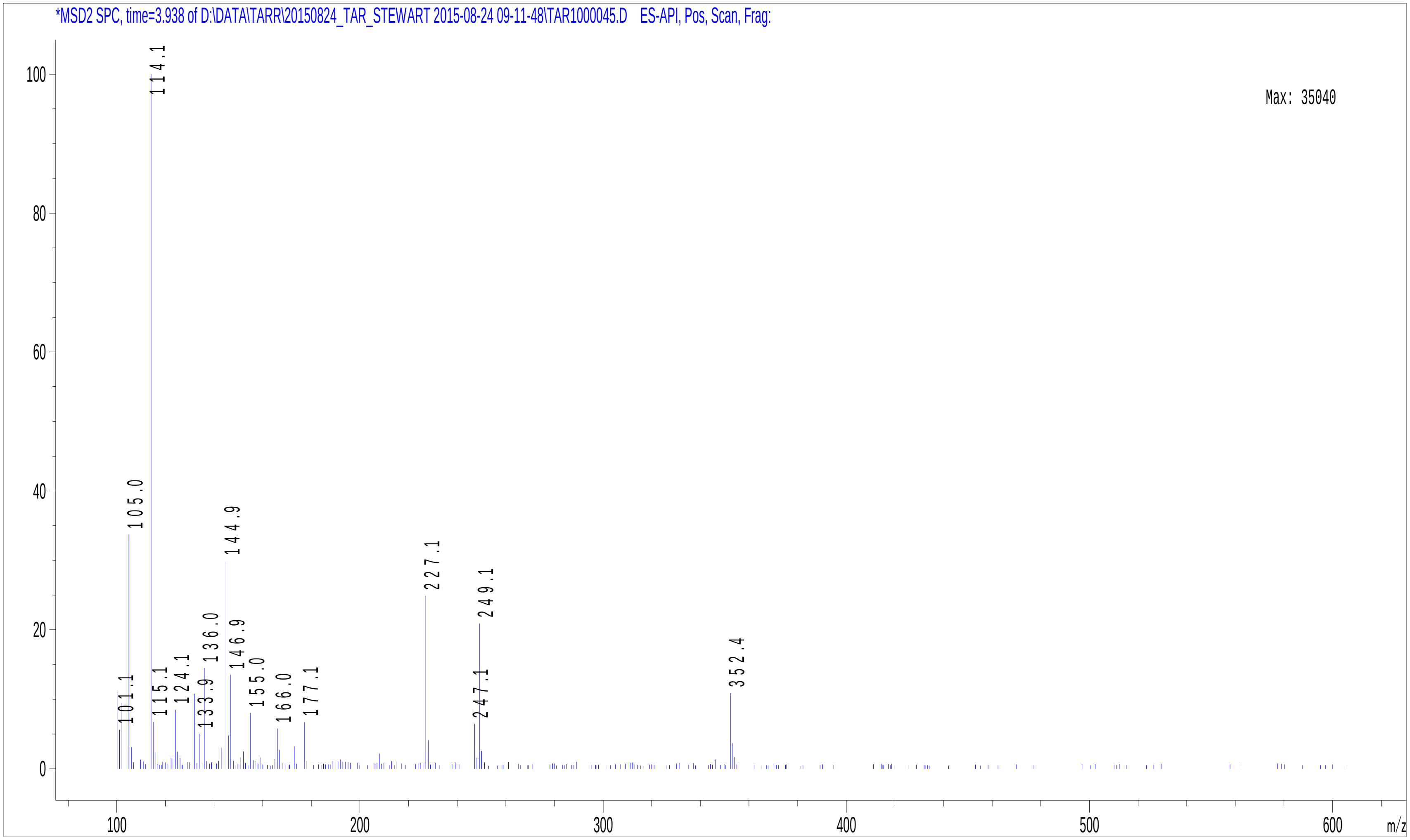
P2-E-09

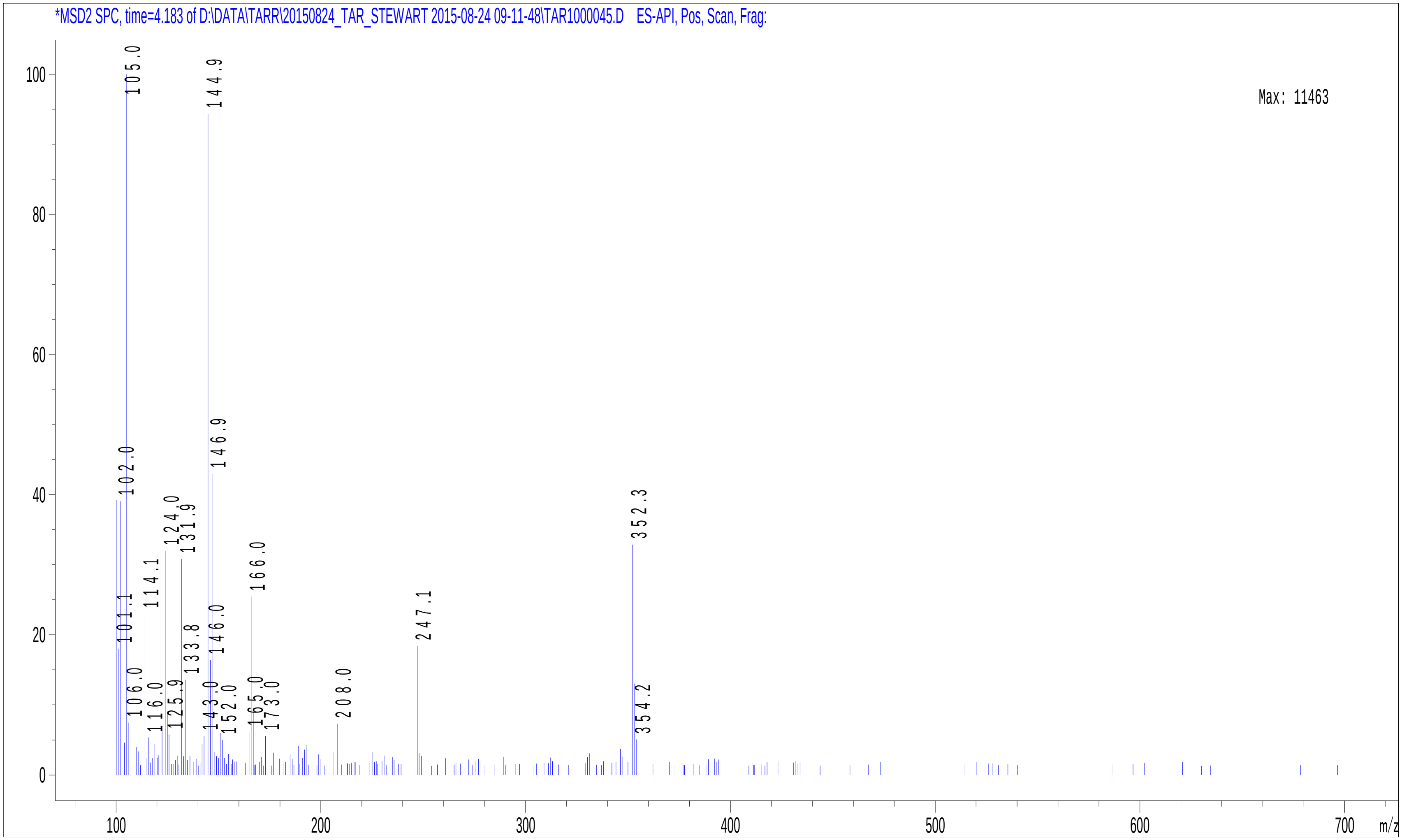



MSD2 TIC, MS File (D:\DATA\TARR\20150824_TAR_STEWART 2015-08-24 09-11-48\TAR1000045.D) ES-API, Pos, Scan, Frag: 70
Norm.
350000
300000
250000
200000
150000
100000
3.114
Area: 3.0837e+006
3.623
Area: 290908
3.927
Area: 728829
4.198
Area: 66035.3
2.5
3
3.5
4
4.5
min


*MSD2 SPC, time=3.171 of D:\DATA\TARR\20150824_TAR_STEWART 2015-08-24 09-11-48\TAR1000045.D ES-API, Pos, Scan, Frag:
Max: 125104
105.0
106.0
132.0
146.0
208.1
226.9
362.9
0
20
40
60
80
100
100
200
300
400
500
600
700
m/z


*MSD2 SPC, time=3.644 of D:\DATA\TARR\20150824_TAR_STEWART 2015-08-24 09-11-48\TAR1000045.D ES-API, Pos, Scan, Frag:
Max: 16416
105.0
144.9
100.1
124.1
146.9
131.9
166.0
106.0
125.1
133.9
143.0
165.0
208.1
247.2
353.2
0
20
40
60
80
100
100
200
300
400
500
600
700 m/z

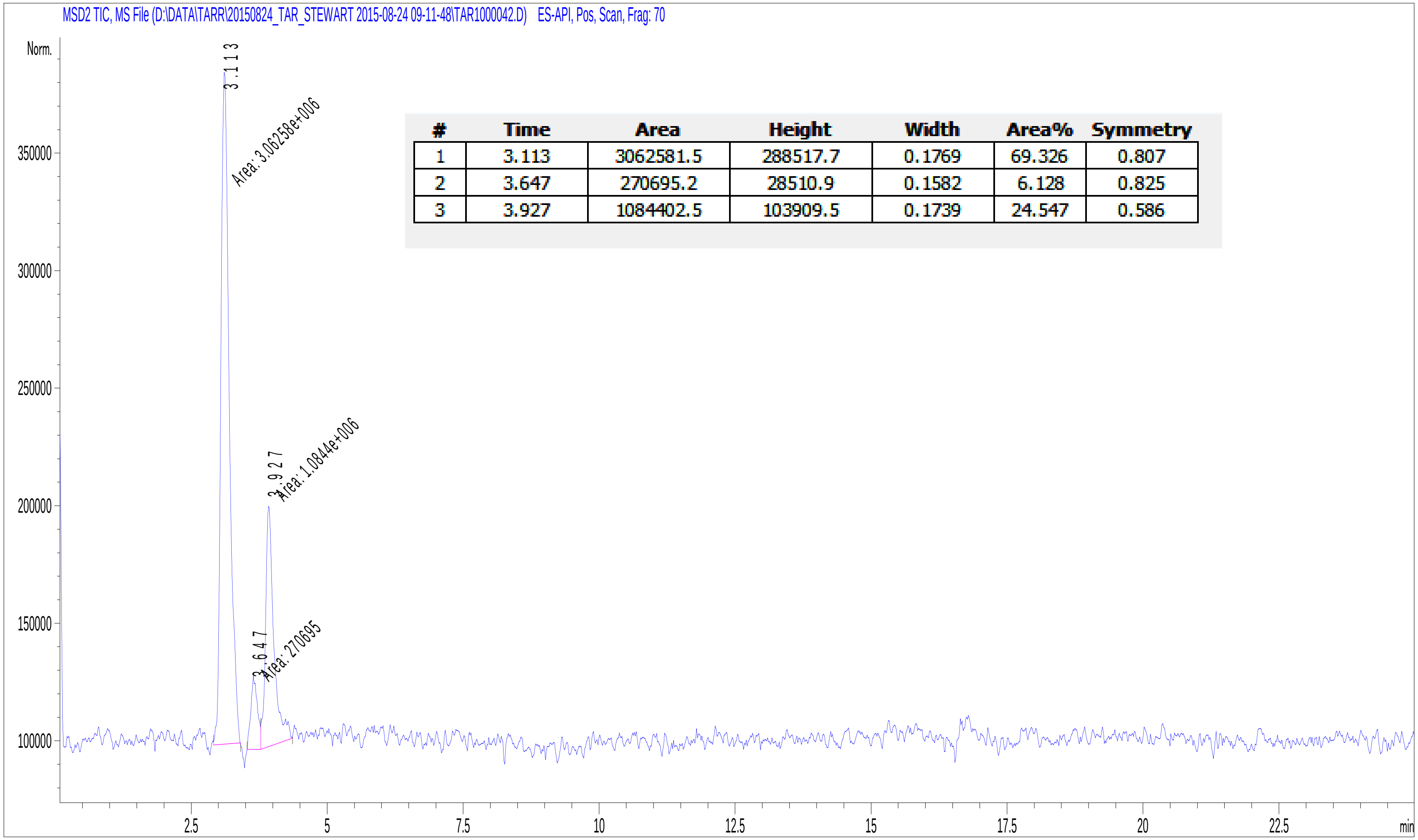

*MSD2 SPC, time=3.938 of D:\DATA\TARR\20150824_TAR_STEWART 2015-08-24 09-11-48\TAR1000045.D ES-API, Pos, Scan, Frag:
Max: 35040
114.1
105.0
144.9
227.1
249.1
136.0
146.9
352.4
101.1
115.1
124.1
133.9
155.0
166.0
177.1
247.1
100
80
60
40
20
0
100
200
300
400
500
600
m/z


*MSD2 SPC, time=4.183 of D:\DATA\TARR\20150824_TAR_STEWART 2015-08-24 09-11-48\TAR1000045.D ES-API, Pos, Scan, Frag:
Max: 11463
100
80
60
40
20
0
105.0
144.9
146.9
102.0
124.0
131.9
114.1
101.1
166.0
146.0
133.8
106.0
116.0
125.9
143.0
152.0
165.0
173.0
208.0
247.1
352.3
354.2
100
200
300
400
500
600
700
m/z

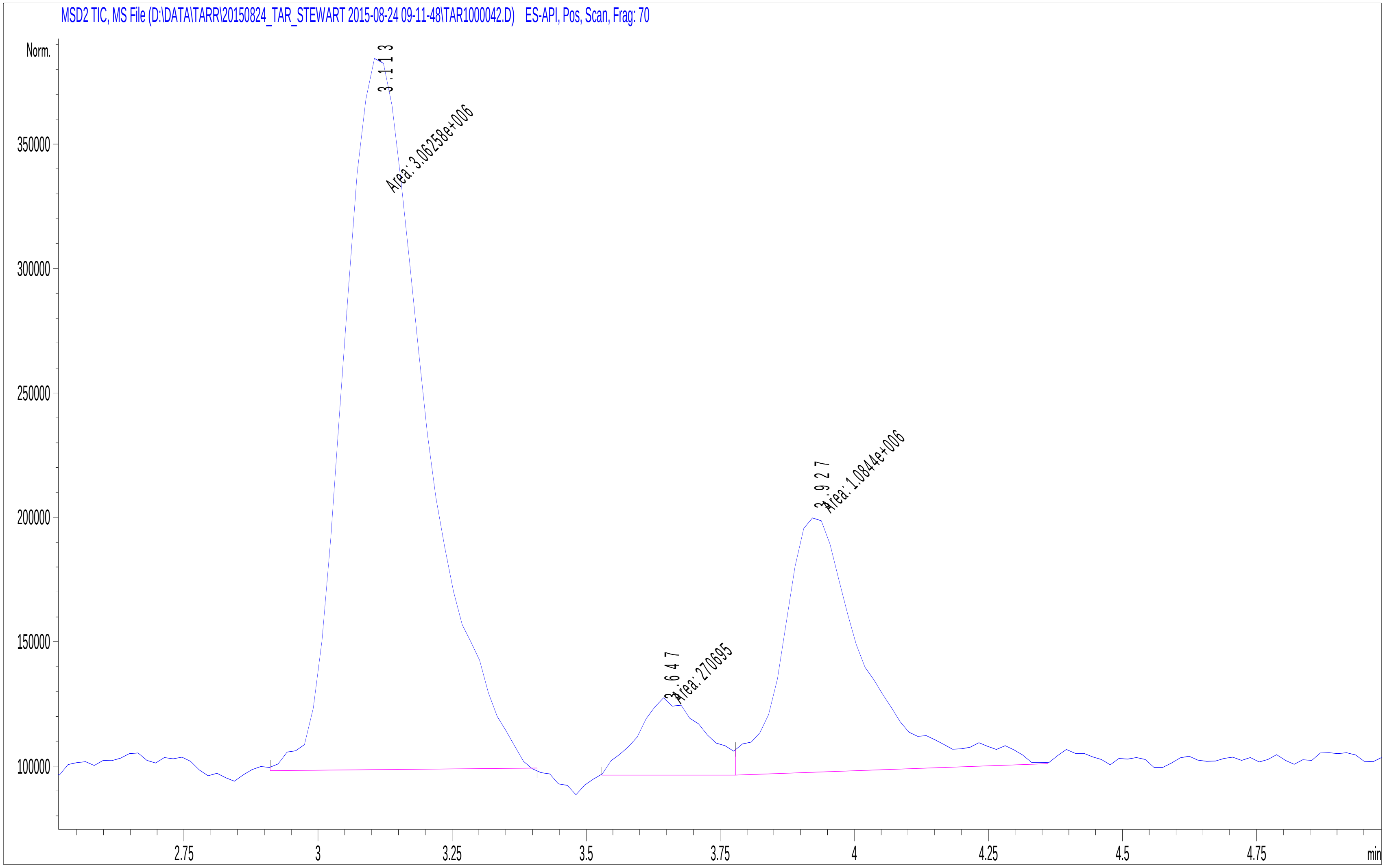
7-May-15

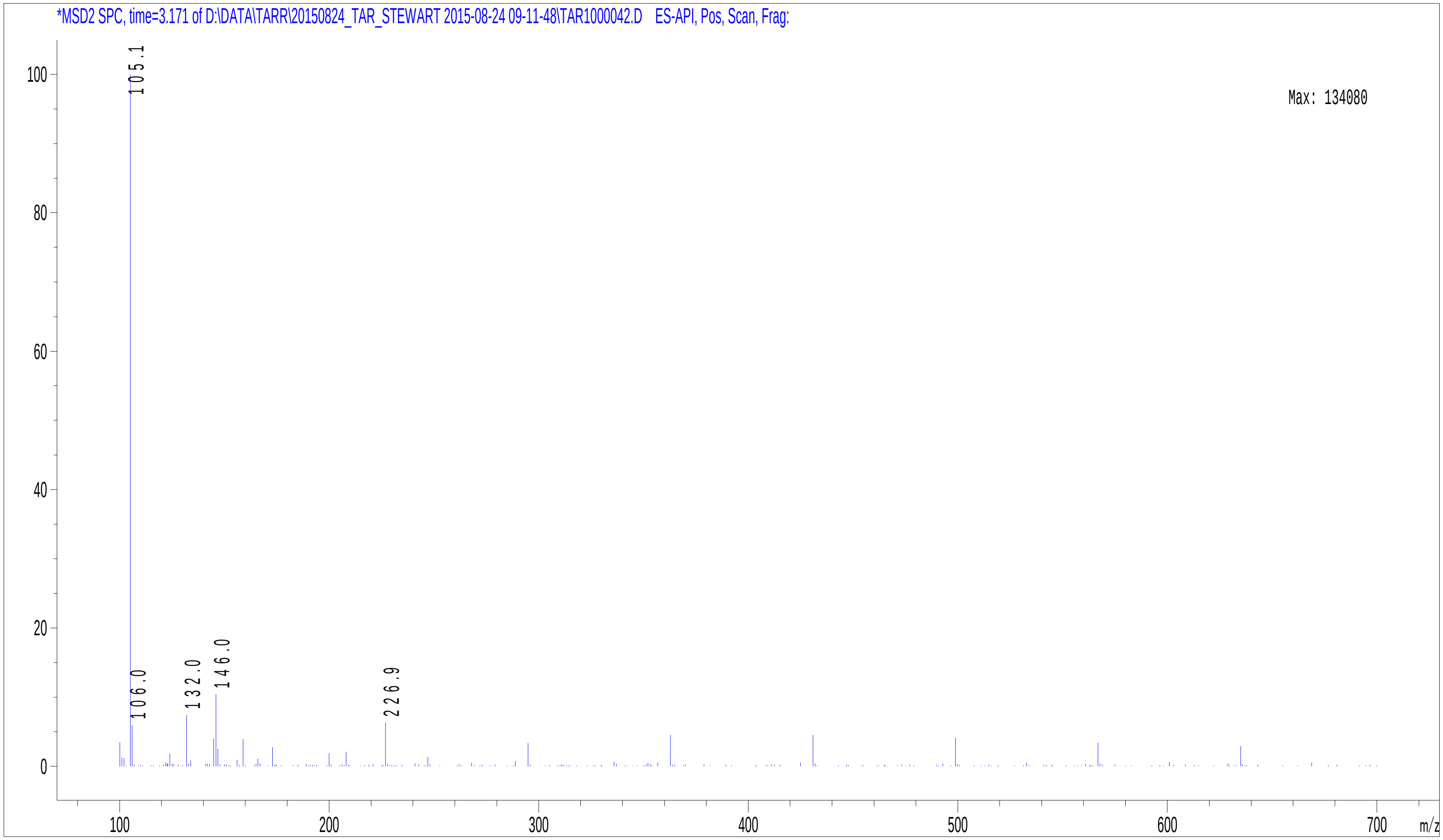
50 DC

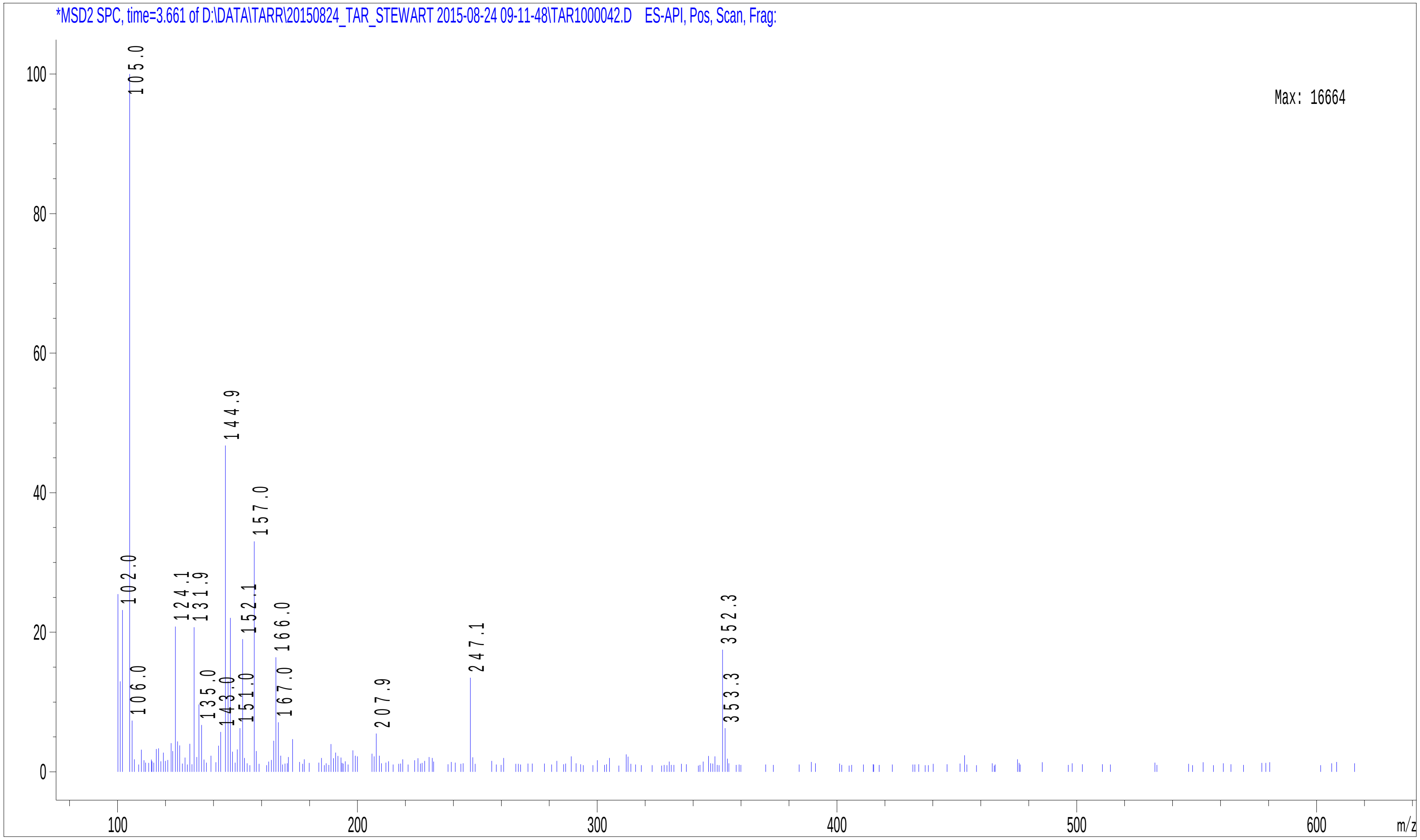
P2-E-06

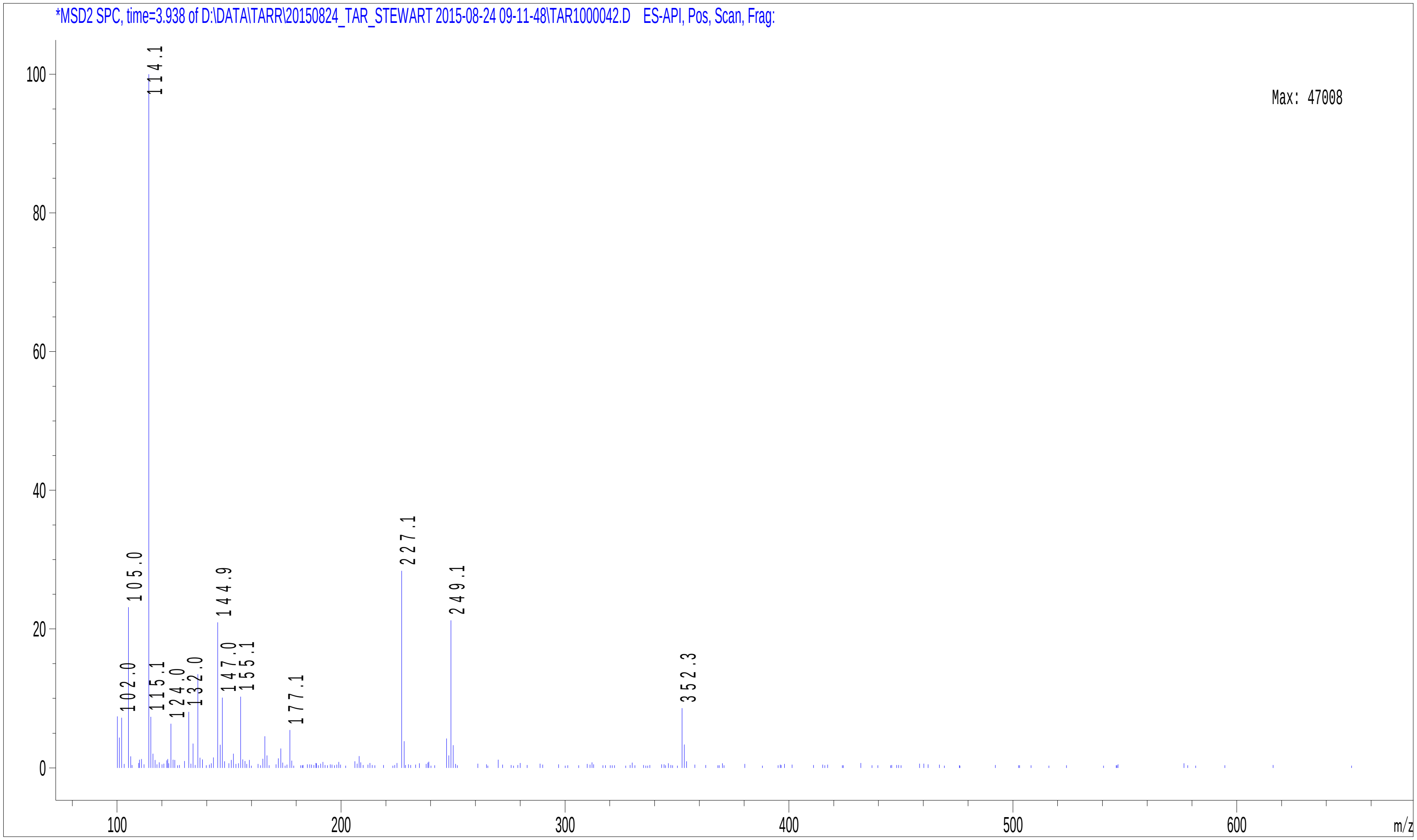


#	Time	Area	Height	Width	Area%	Symmetry
1	3.113	3062581.5	288517.7	0.1769	69.326	0.807
2	3.647	270695.2	28510.9	0.1582	6.128	0.825
3	3.927	1084402.5	103909.5	0.1739	24.547	0.586


MSD2 TIC, MS File (D:\DATA\TARR\20150824_TAR_STEWART 2015-08-24 09-11-48\TAR1000042.D) ES-API, Pos, Scan, Frag: 70
Norm.
350000
300000
250000
200000
150000
100000
3.113
Area: 3.06258e+006
3.647
Area: 270695
3.927
Area: 1.0844e+006
2.75
3
3.25
3.5
3.75
4
4.25
4.5
4.75
min


*MSD2 SPC, time=3.171 of D:\DATA\TARR\20150824_TAR_STEWART 2015-08-24 09-11-48\TAR1000042.D ES-API, Pos, Scan, Frag:
Max: 134080
105.1
106.0
132.0
146.0
226.9
100
80
60
40
20
0
100
200
300
400
500
600
700
m/z

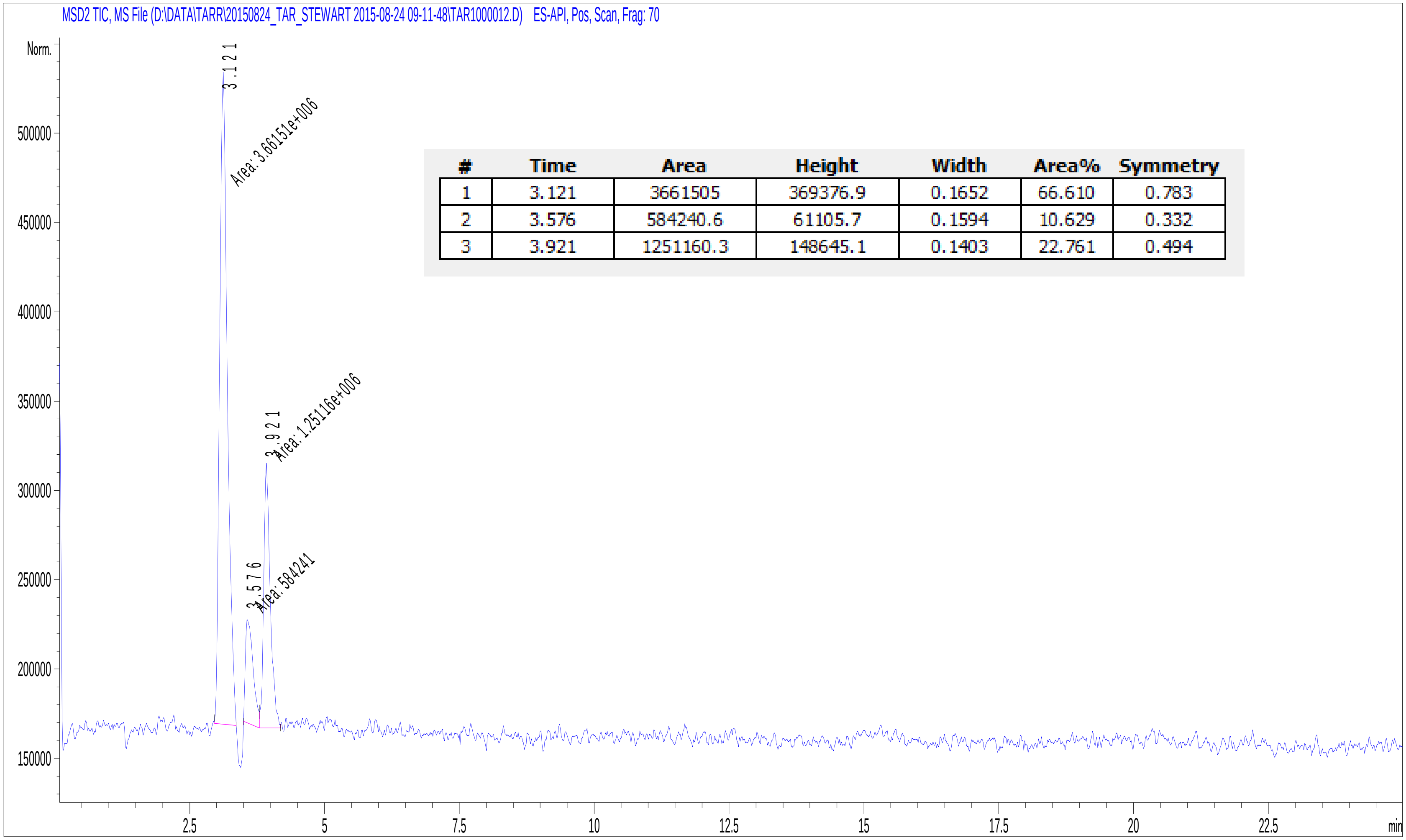

*MSD2 SPC, time=3.661 of D:\DATA\TARR\20150824_TAR_STEWART 2015-08-24 09-11-48\TAR1000042.D ES-API, Pos, Scan, Frag:
Max: 16664
105.0
102.0
106.0
124.1
131.9
135.0
143.0
144.9
151.0
152.1
157.0
166.0
167.0
207.9
247.1
352.3
353.3
0
20
40
60
80
100
100
200
300
400
500
600
m/z


*MSD2 SPC, time=3.938 of D:\DATA\TARR\20150824_TAR_STEWART 2015-08-24 09-11-48\TAR1000042.D ES-API, Pos, Scan, Frag:
Max: 47008
100
80
60
40
20
0
114.1
105.0
102.0
115.1
124.0
132.0
144.9
147.0
155.1
177.1
227.1
249.1
352.3
100
200
300
400
500
600
m/z

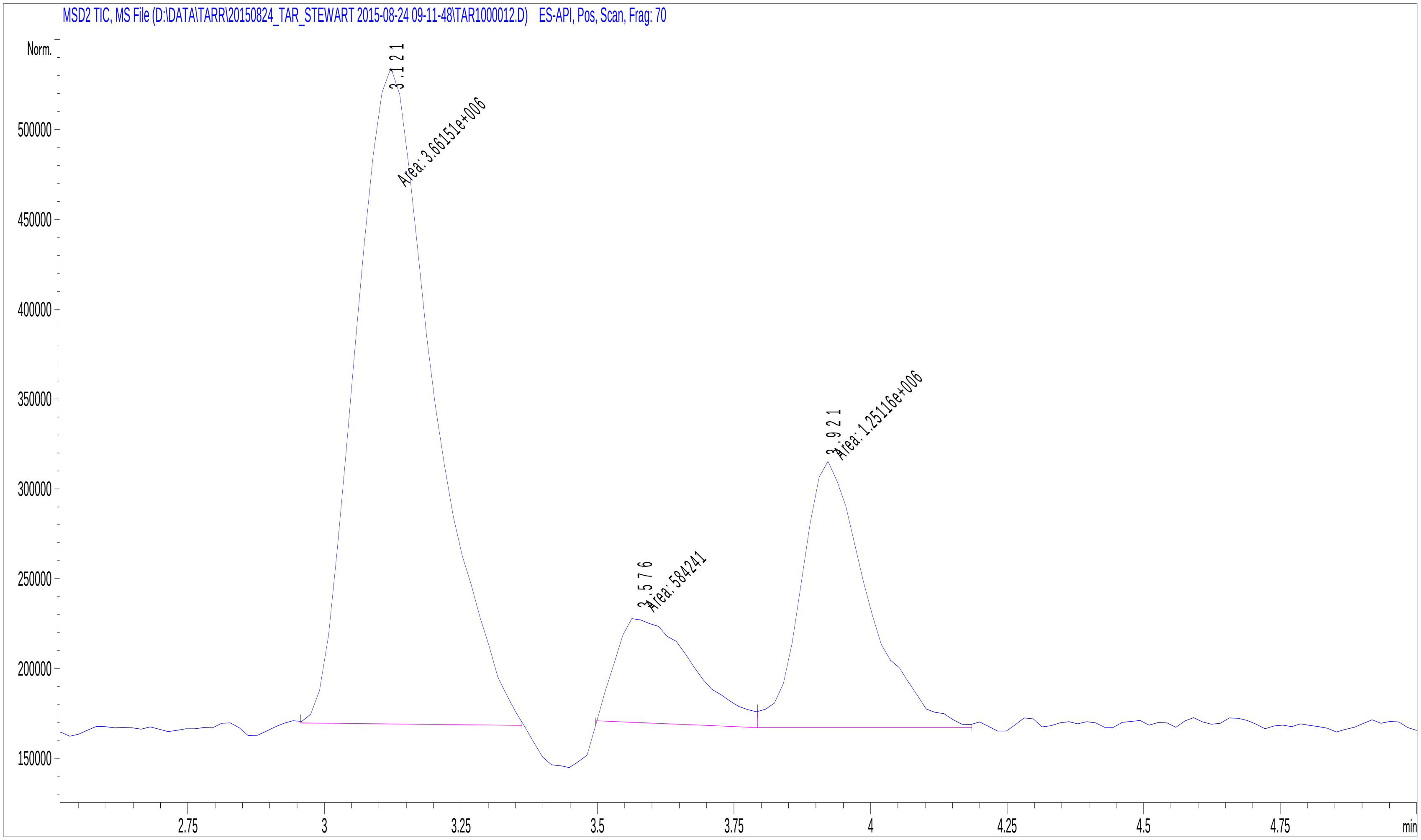
15-Jun-15

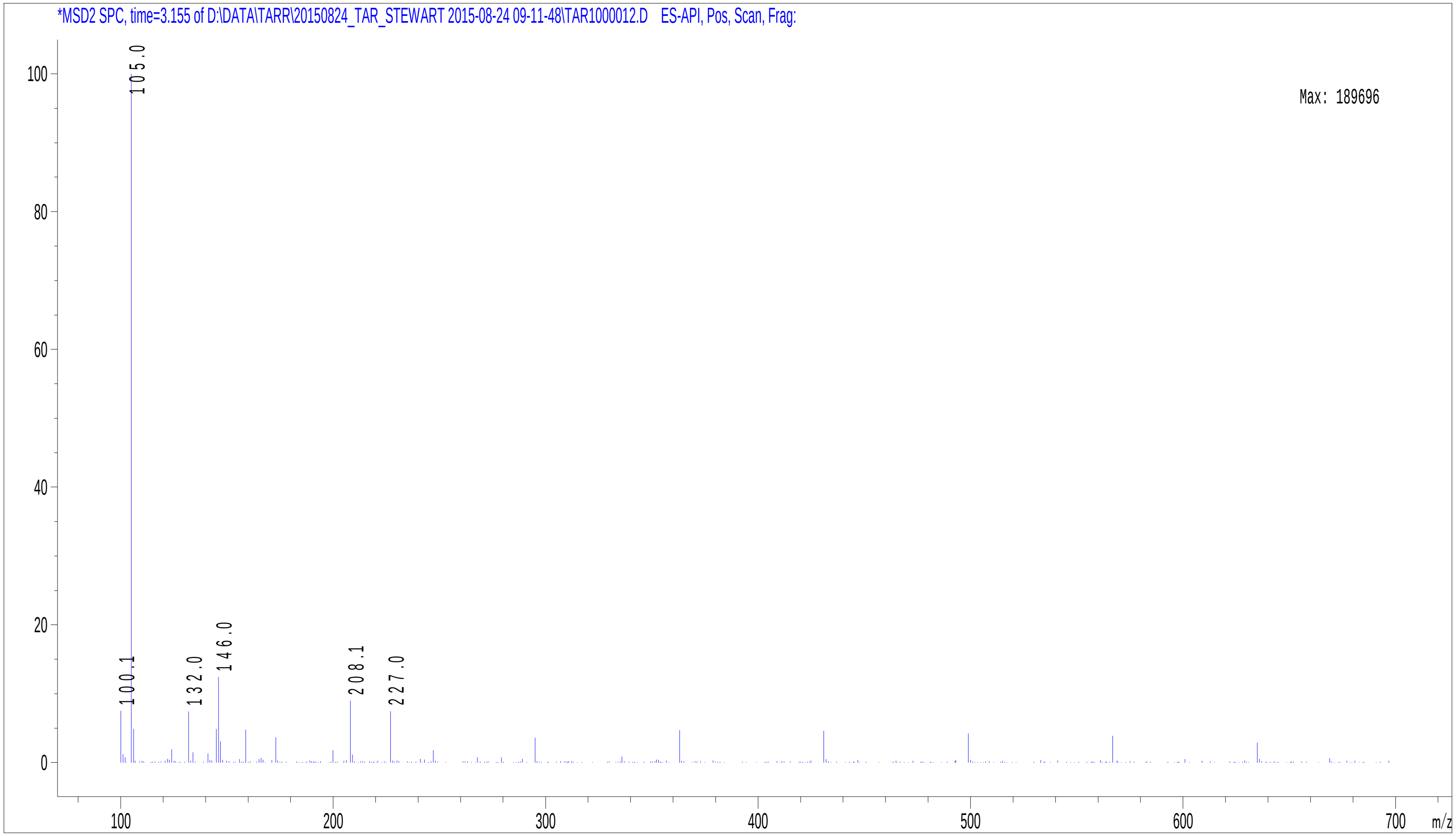
50 DC Repeat

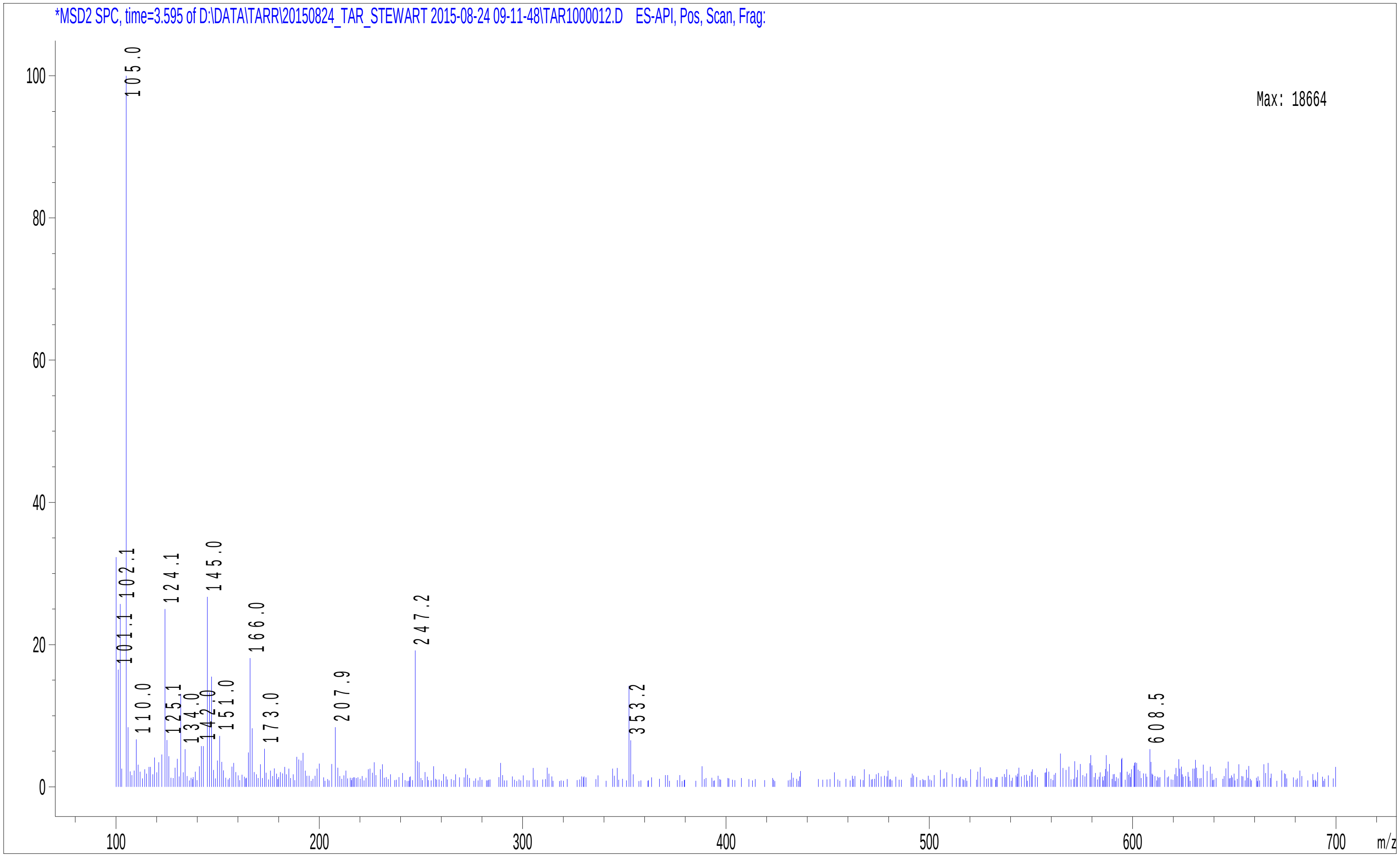
P2-B-07

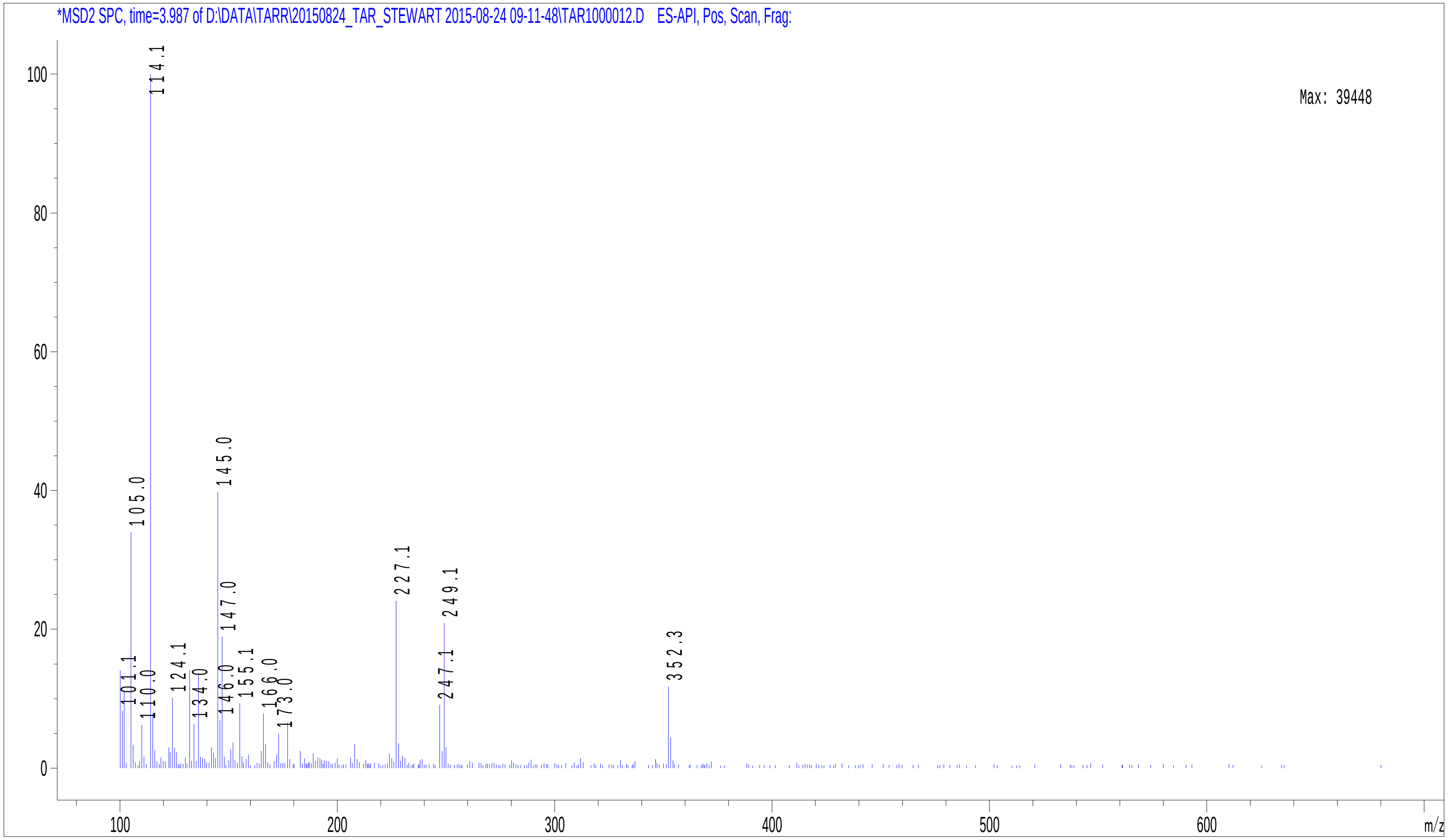


#	Time	Area	Height	Width	Area%	Symmetry
1	3.121	3661505	369376.9	0.1652	66.610	0.783
2	3.576	584240.6	61105.7	0.1594	10.629	0.332
3	3.921	1251160.3	148645.1	0.1403	22.761	0.494


MSD2 TIC, MS File (D:\DATA\TARR\20150824_TAR_STEWART 2015-08-24 09-11-48\TAR1000012.D) ES-API, Pos, Scan, Frag: 70
Norm.
500000
450000
400000
350000
300000
250000
200000
150000
3.121
Area: 3.66151e+006
3.576
Area: 584241
3.921
Area: 1.25116e+006
2.75
3
3.25
3.5
3.75
4
4.25
4.5
4.75
min


*MSD2 SPC, time=3.155 of D:\DATA\TARR\20150824_TAR_STEWART 2015-08-24 09-11-48\TAR1000012.D ES-API, Pos, Scan, Frag:
Max: 189696
105.0
100.1
132.0
146.0
208.1
227.0
100
80
60
40
20
0
100
200
300
400
500
600
700
m/z

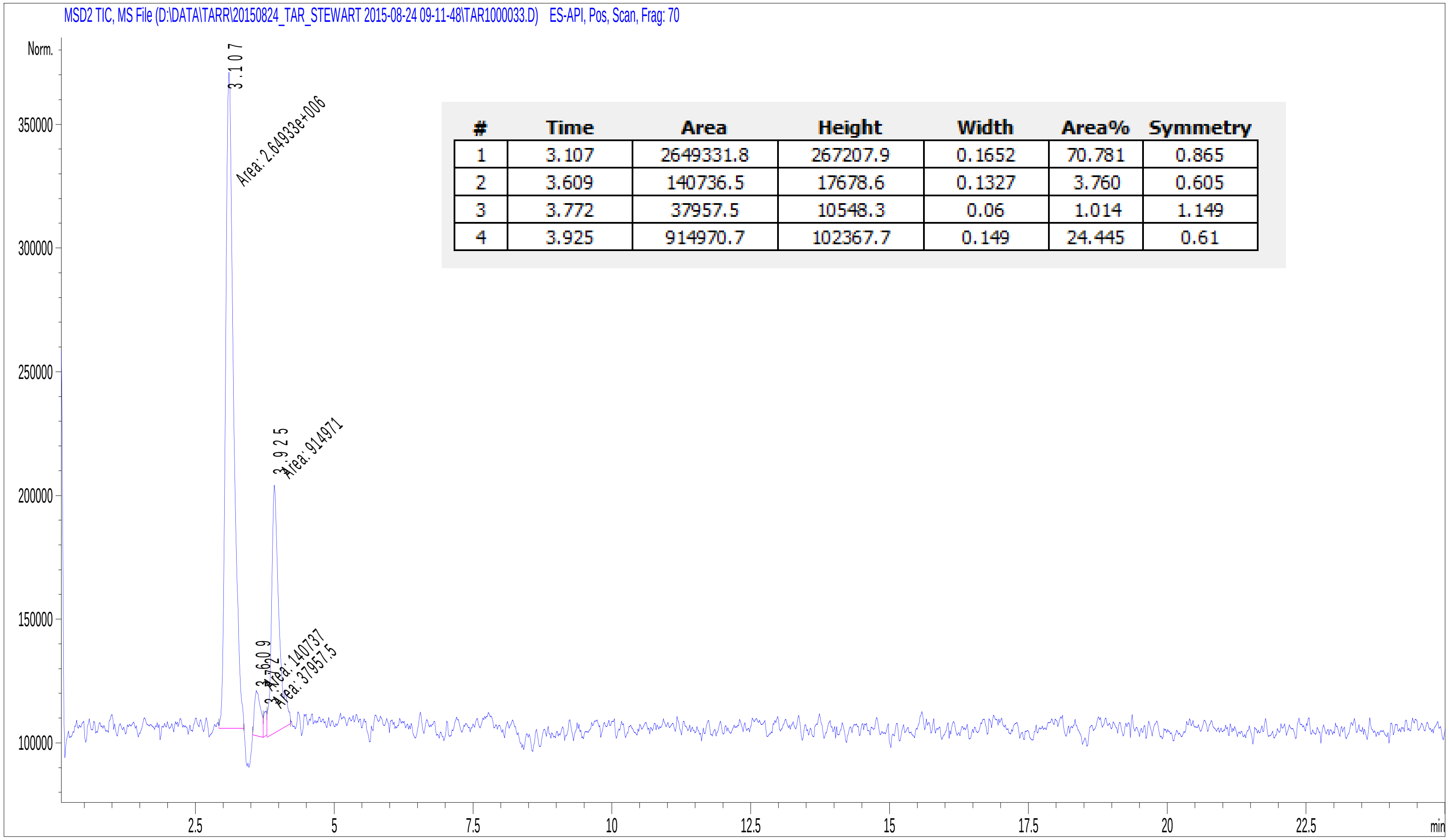

*MSD2 SPC, time=3.595 of D:\DATA\TARR\20150824_TAR_STEWART 2015-08-24 09-11-48\TAR1000012.D ES-API, Pos, Scan, Frag:
Max: 18664
105.0
102.1
101.1
110.0
124.1
125.1
134.0
142.0
145.0
151.0
166.0
173.0
207.9
247.2
353.2
608.5
0
20
40
60
80
100
100
200
300
400
500
600
700
m/z


*MSD2 SPC, time=3.987 of D:\DATA\TARR\20150824_TAR_STEWART 2015-08-24 09-11-48\TAR1000012.D ES-API, Pos, Scan, Frag:
Max: 39448
114.1
105.0
145.0
147.0
227.1
249.1
101.1
110.0
124.1
134.0
146.0
155.1
166.0
173.0
247.1
352.3
0
20
40
60
80
100
200
300
400
500
600
m/z

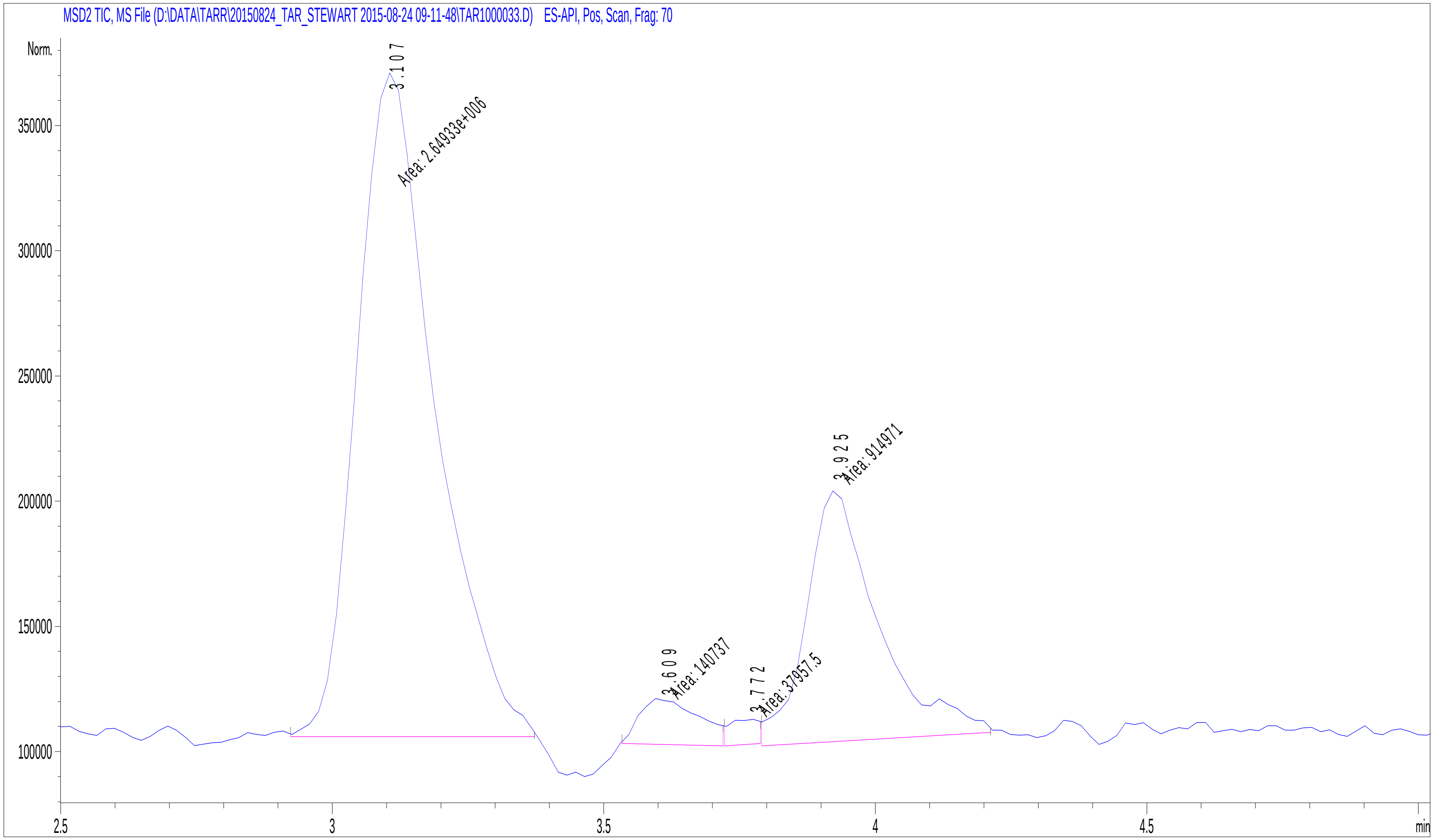
23-Jul-15

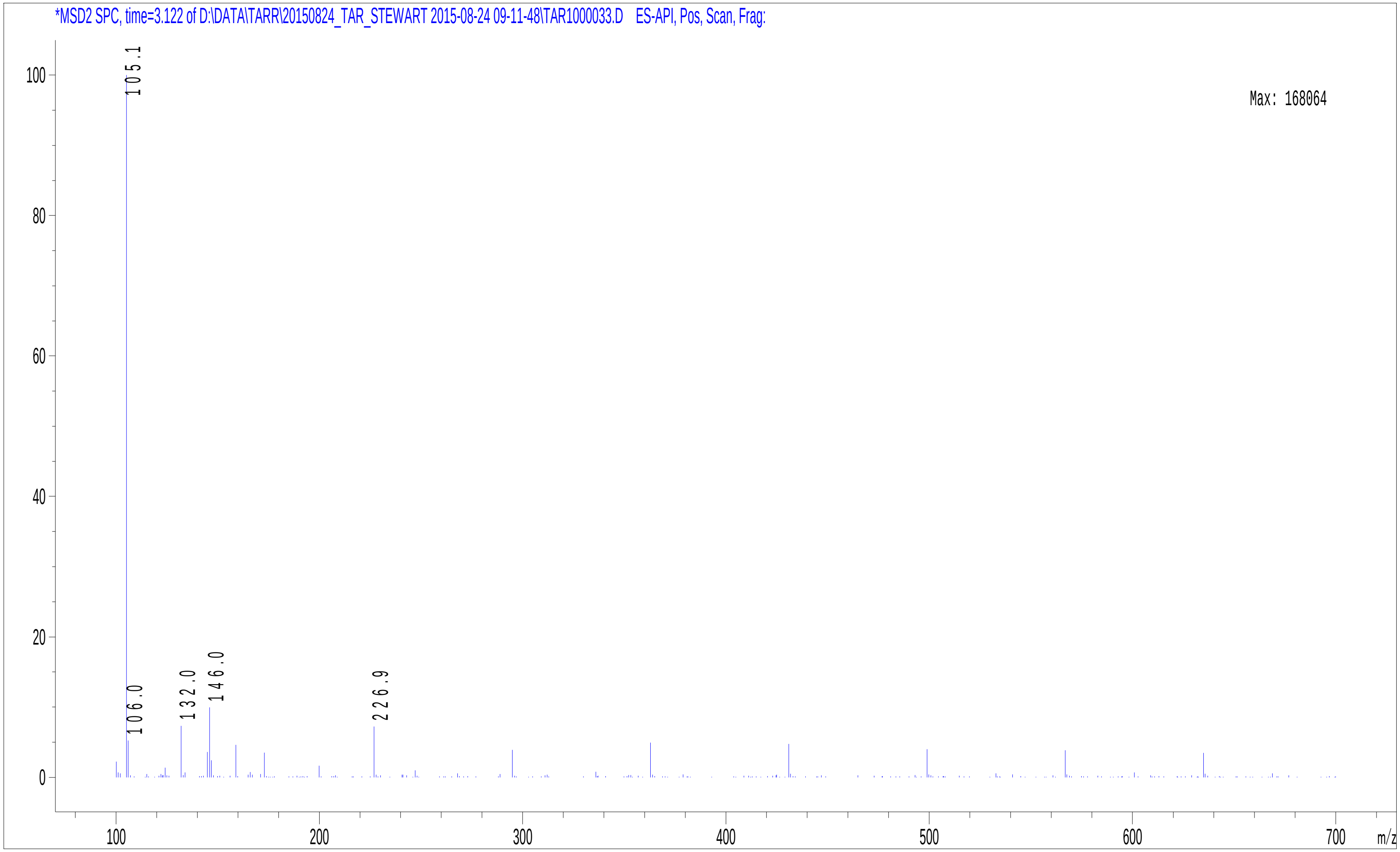
70 DC

P2-D-04

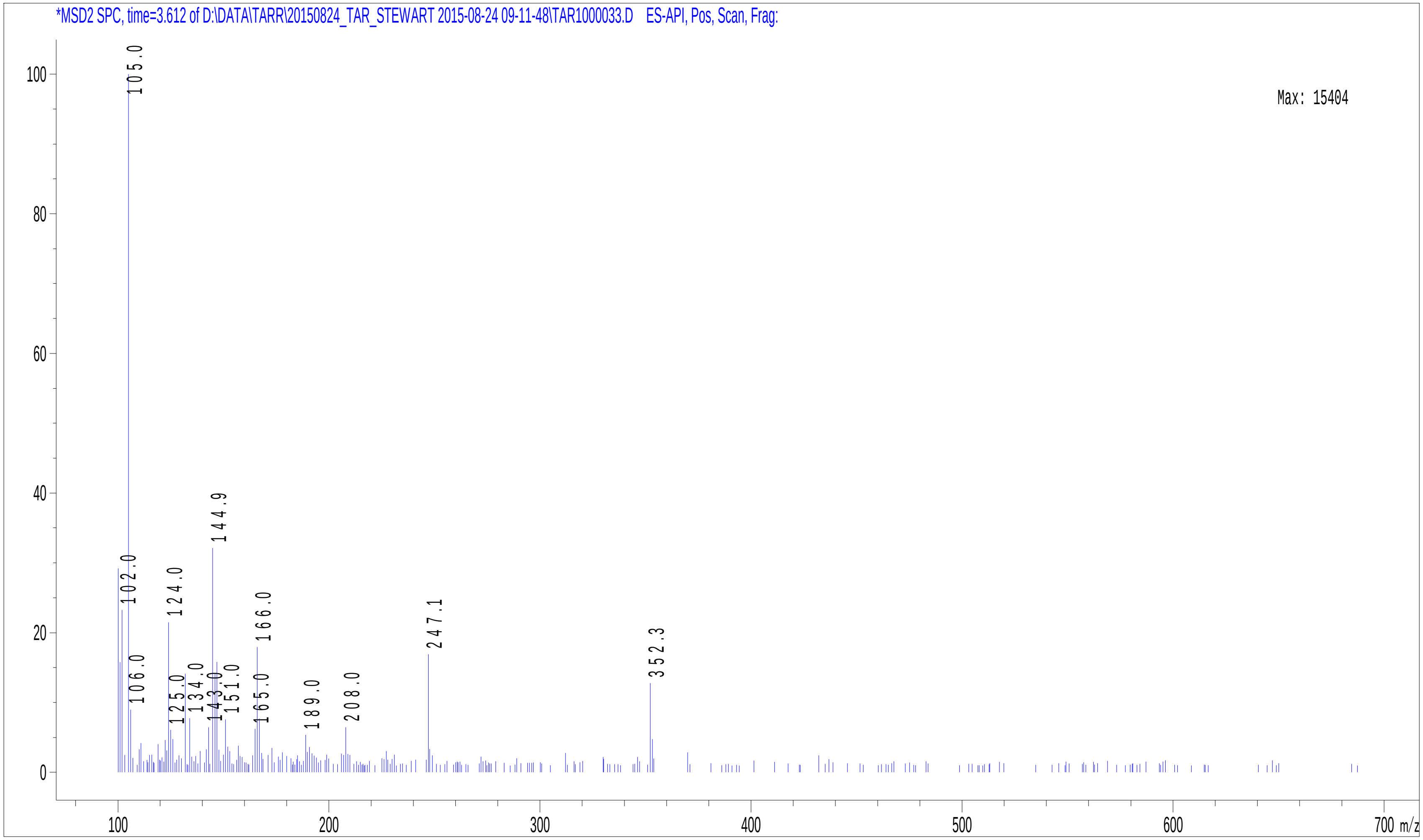


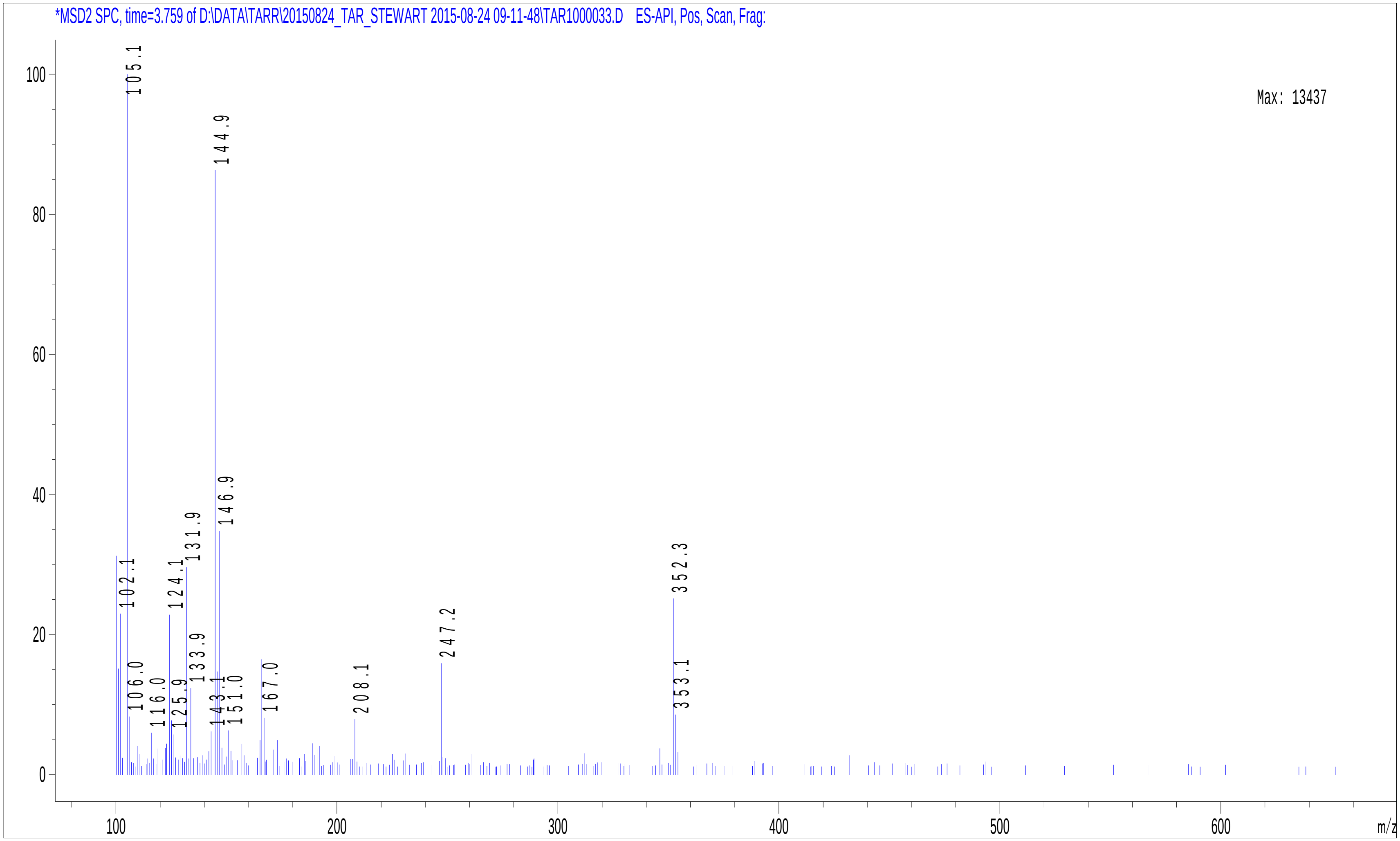
#	Time	Area	Height	Width	Area%	Symmetry
1	3.107	2649331.8	267207.9	0.1652	70.781	0.865
2	3.609	140736.5	17678.6	0.1327	3.760	0.605
3	3.772	37957.5	10548.3	0.06	1.014	1.149
4	3.925	914970.7	102367.7	0.149	24.445	0.61

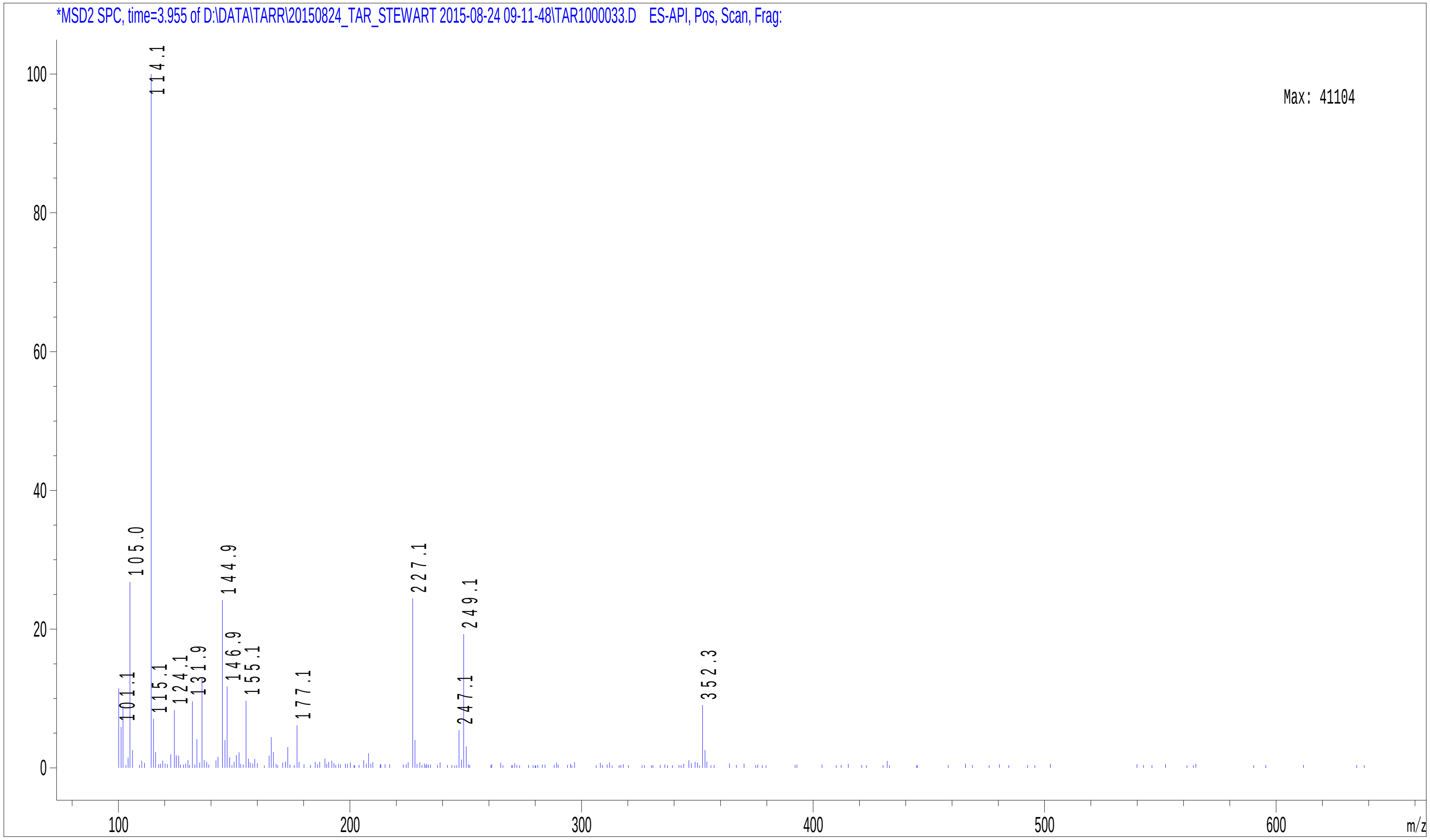

MSD2 TIC, MS File (D:\DATA\TARR\20150824_TAR_STEWART 2015-08-24 09-11-48\TAR1000033.D) ES-API, Pos, Scan, Frag: 70
Norm.
350000
300000
250000
200000
150000
100000
3.107
Area: 2.64933e+006
3.609
Area: 140737
3.772
Area: 37957.5
3.925
Area: 914971
2.5
3
3.5
4
4.5
min

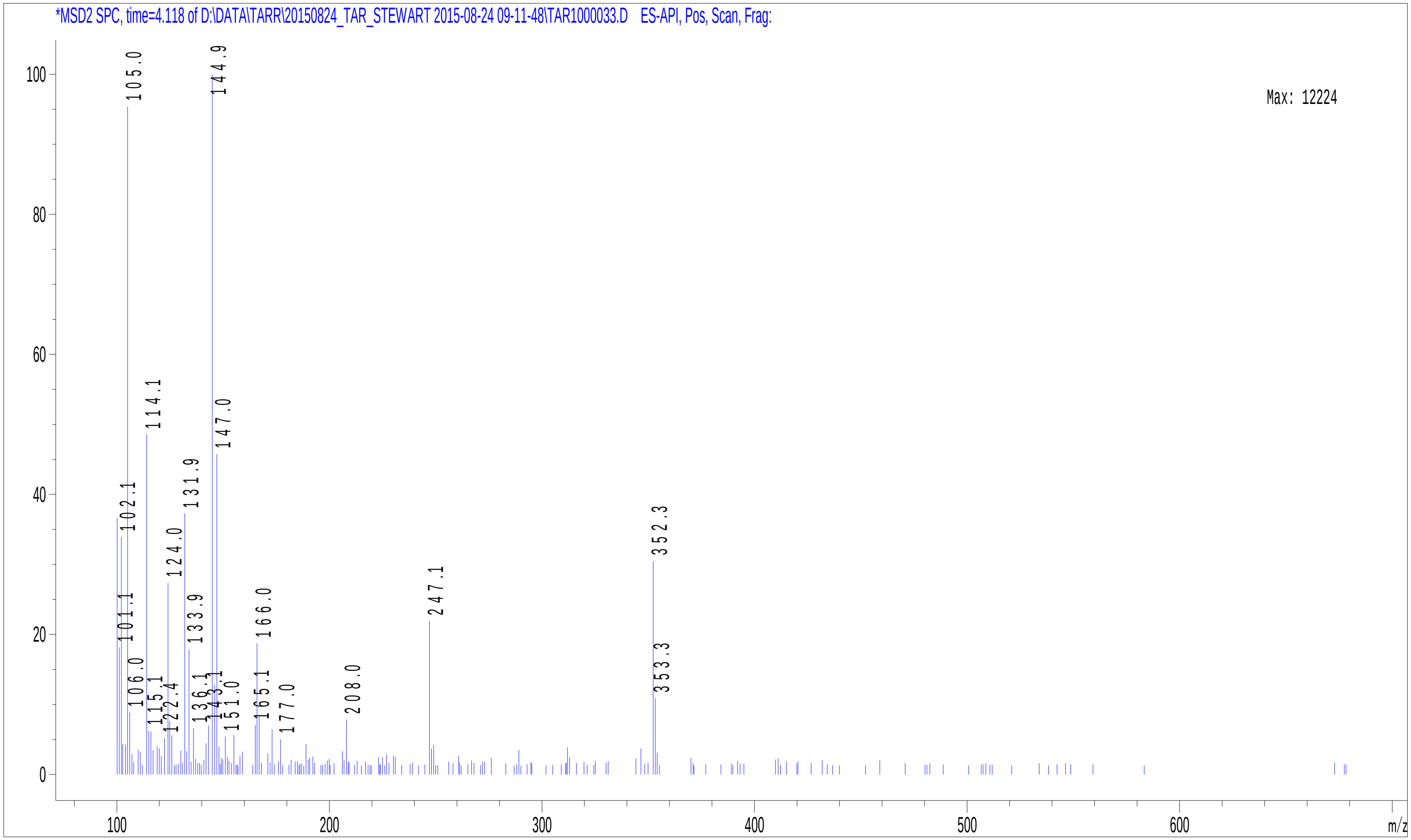


*MSD2 SPC, time=3.122 of D:\DATA\TARR\20150824_TAR_STEWART 2015-08-24 09-11-48\TAR1000033.D ES-API, Pos, Scan, Frag:
Max: 168064
105.1
106.0
132.0
146.0
226.9
100
80
60
40
20
0
100
200
300
400
500
600
700
m/z


*MSD2 SPC, time=3.612 of D:\DATA\TARR\20150824_TAR_STEWART 2015-08-24 09-11-48\TAR1000033.D ES-API, Pos, Scan, Frag:
Max: 15404
105.0
102.0
106.0
124.0
125.0
134.0
143.0
144.9
151.0
165.0
166.0
189.0
208.0
247.1
352.3
0
20
40
60
80
100
100
200
300
400
500
600
700 m/z


*MSD2 SPC, time=3.759 of D:\DATA\TARR\20150824_TAR_STEWART 2015-08-24 09-11-48\TAR1000033.D ES-API, Pos, Scan, Frag:
Max: 13437
105.1
144.9
146.9
131.9
124.1
102.1
133.9
106.0
116.0
125.9
143.1
151.0
167.0
208.1
247.2
352.3
353.1
0
20
40
60
80
100
100
200
300
400
500
600
m/z

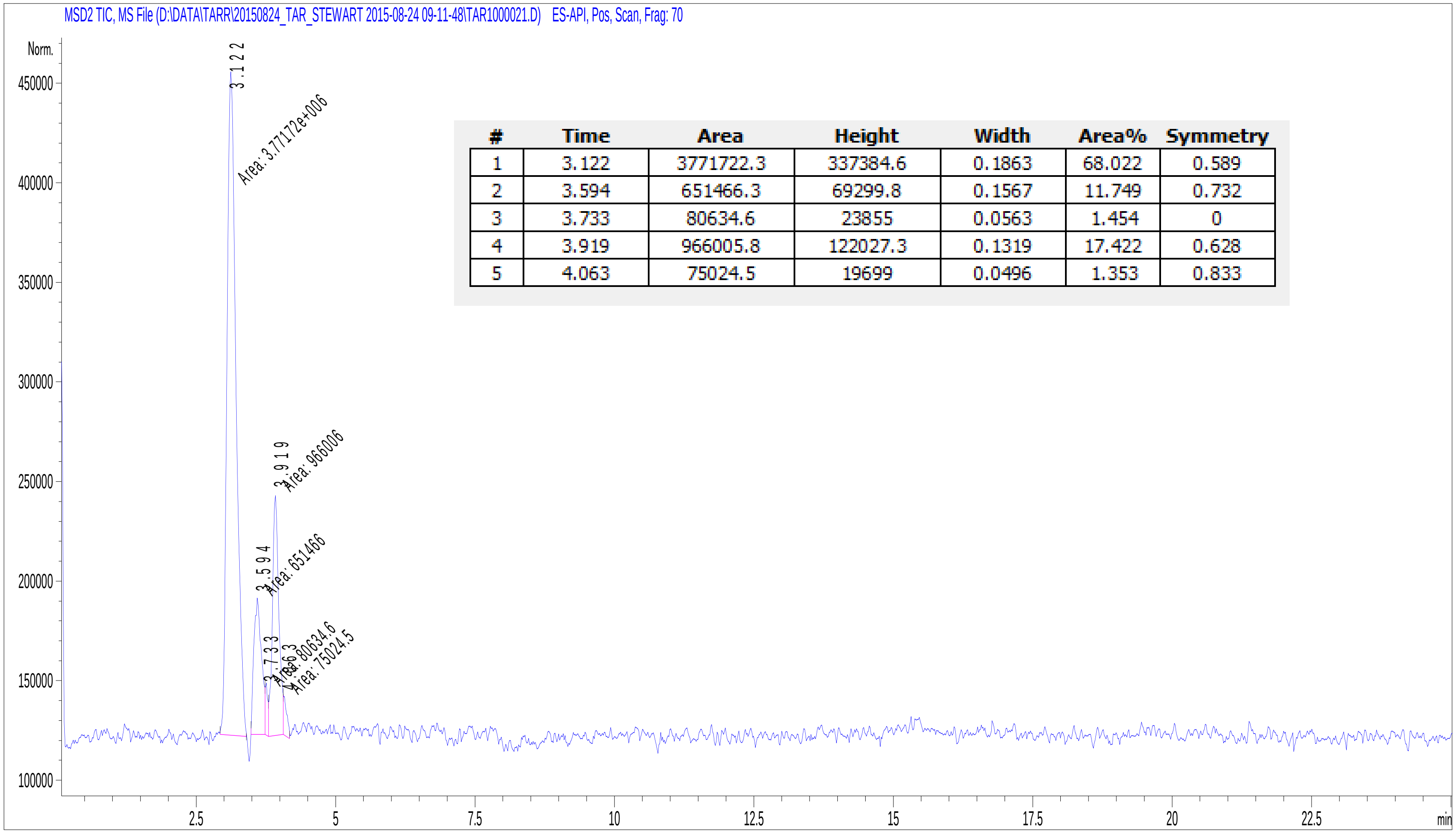

*MSD2 SPC, time=3.955 of D:\DATA\TARR\20150824_TAR_STEWART 2015-08-24 09-11-48\TAR1000033.D ES-API, Pos, Scan, Frag:
Max: 41104
114.1
105.0
101.1
115.1
124.1
131.9
144.9
146.9
155.1
177.1
227.1
247.1
249.1
352.3
0
20
40
60
80
100
100
200
300
400
500
600
m/z


*MSD2 SPC, time=4.118 of D:\DATA\TARR\20150824_TAR_STEWART 2015-08-24 09-11-48\TAR1000033.D ES-API, Pos, Scan, Frag:
Max: 12224
0
20
40
60
80
100
100
200
300
400
500
600
m/z
105.0
144.9
114.1
147.0
131.9
102.1
124.0
352.3
247.1
101.1
166.0
133.9
353.3
208.0
106.0
115.1
122.4
136.1
143.1
151.0
165.1
177.0

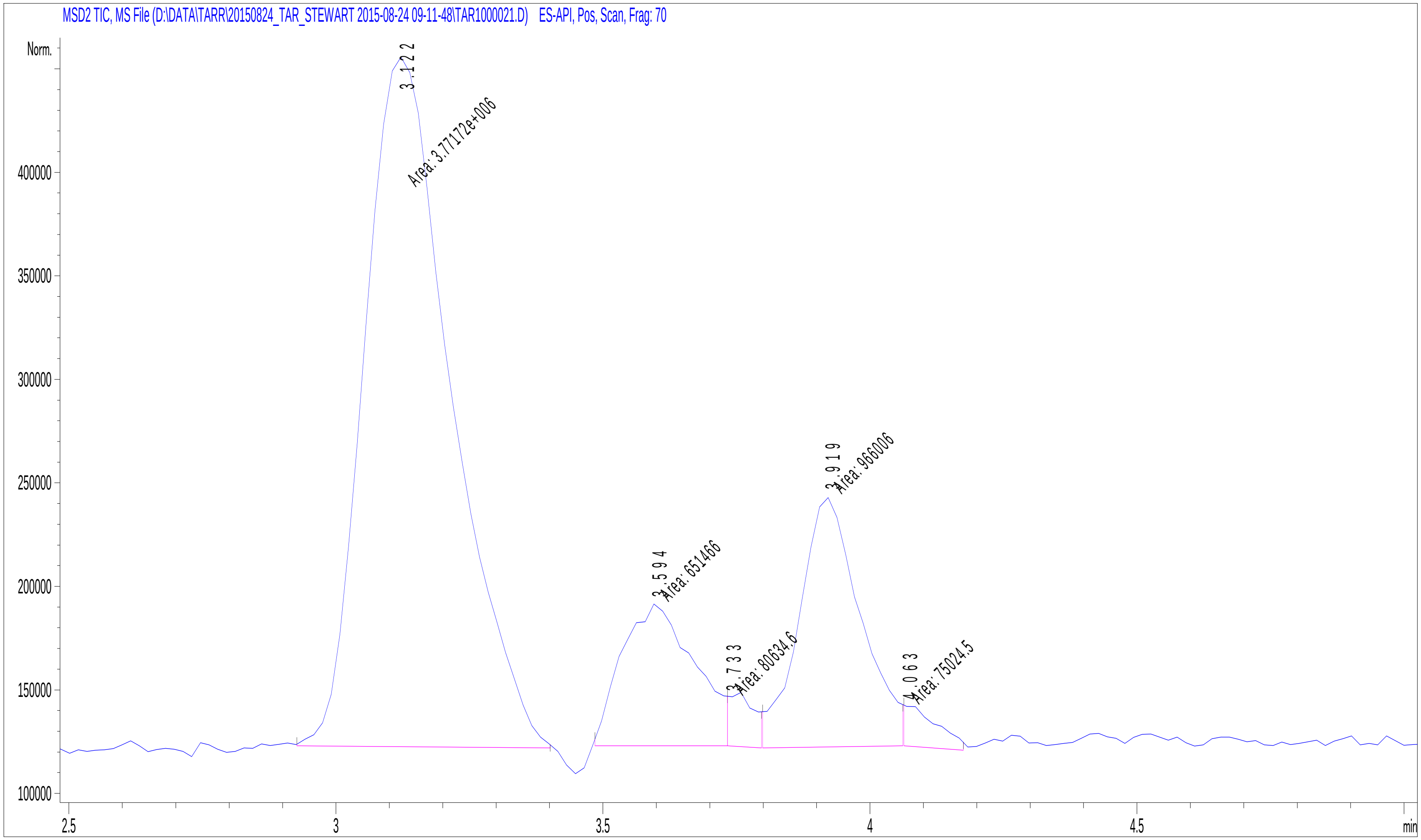
1-Jul-15

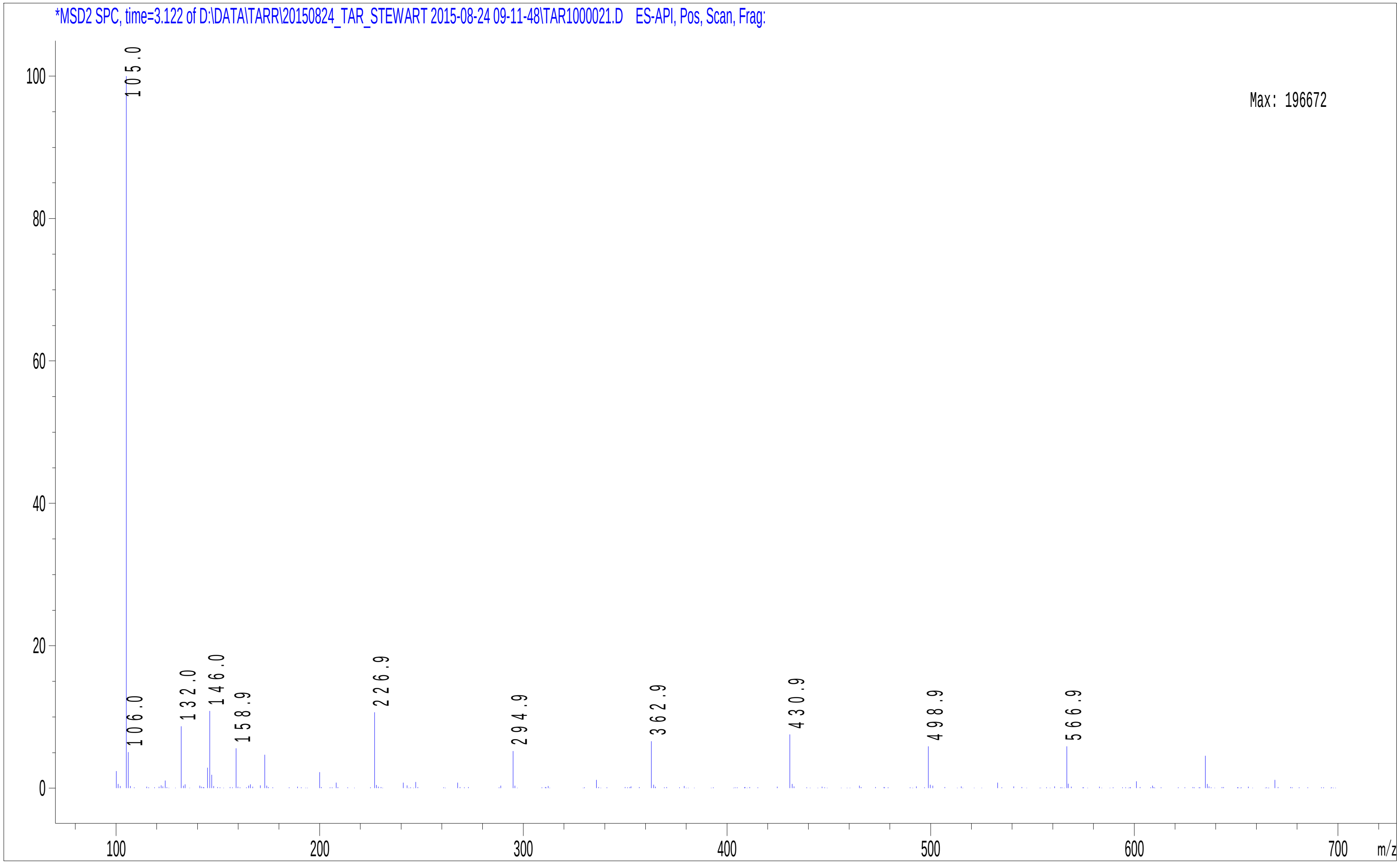
100 DC

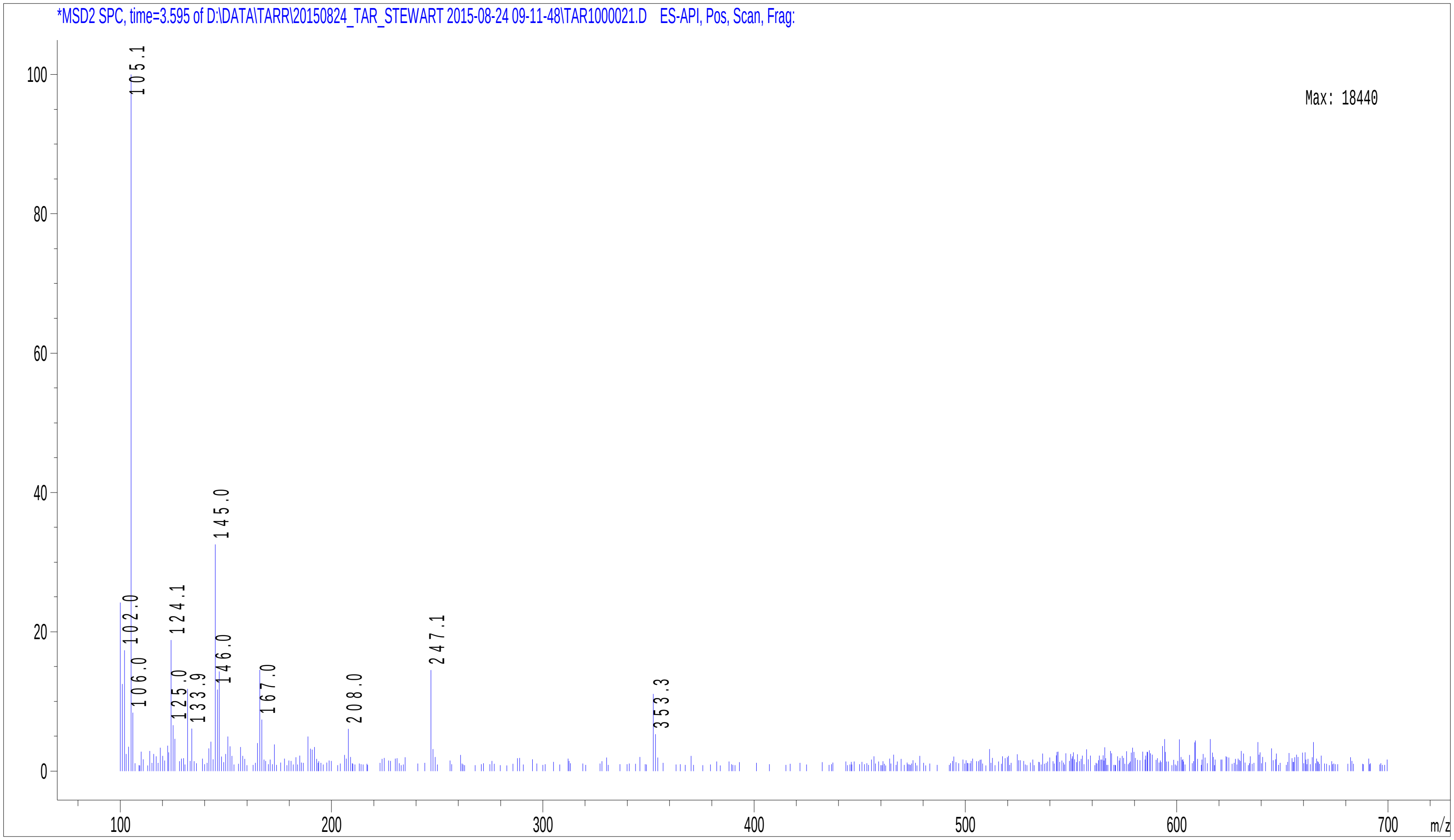
P2-C-03

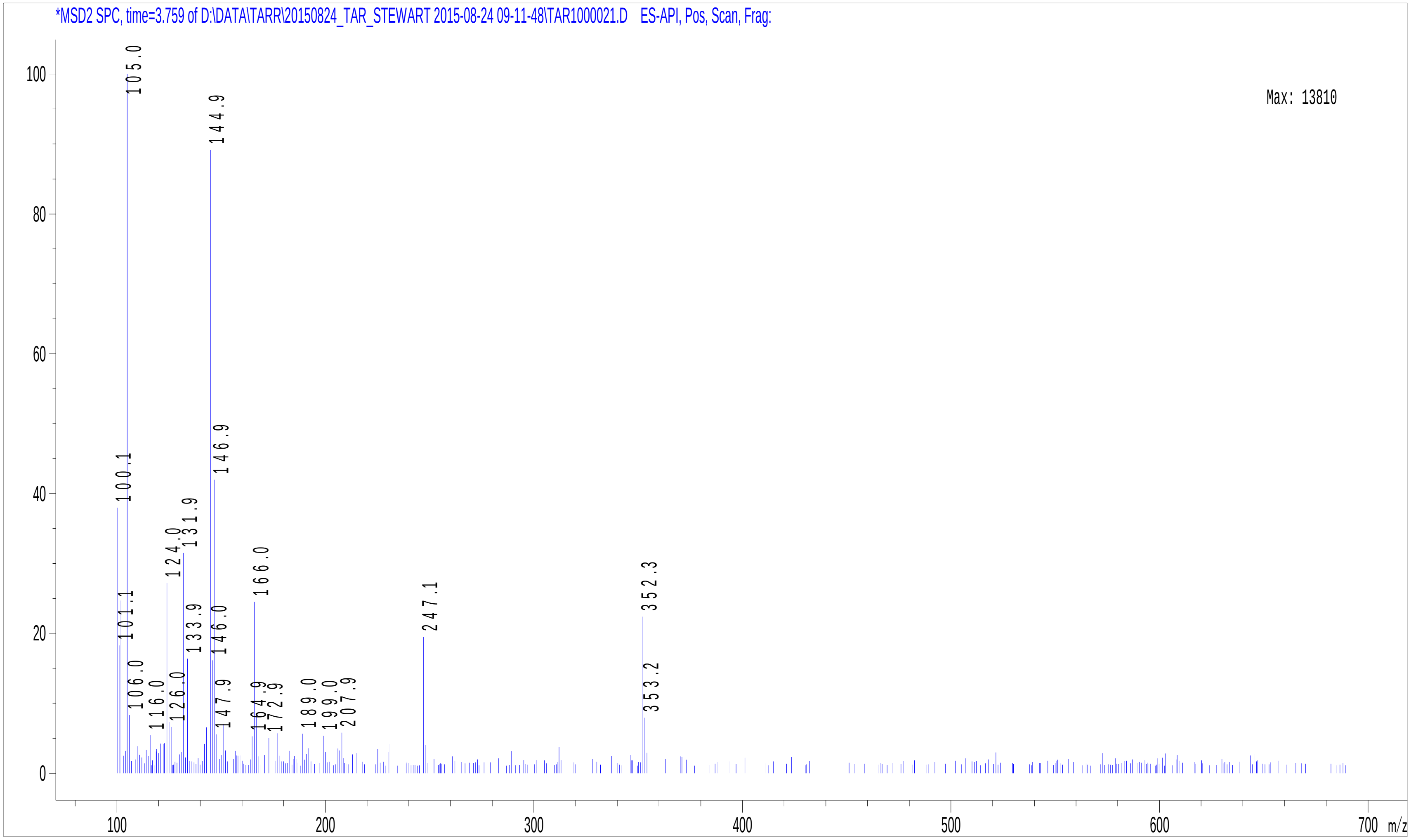


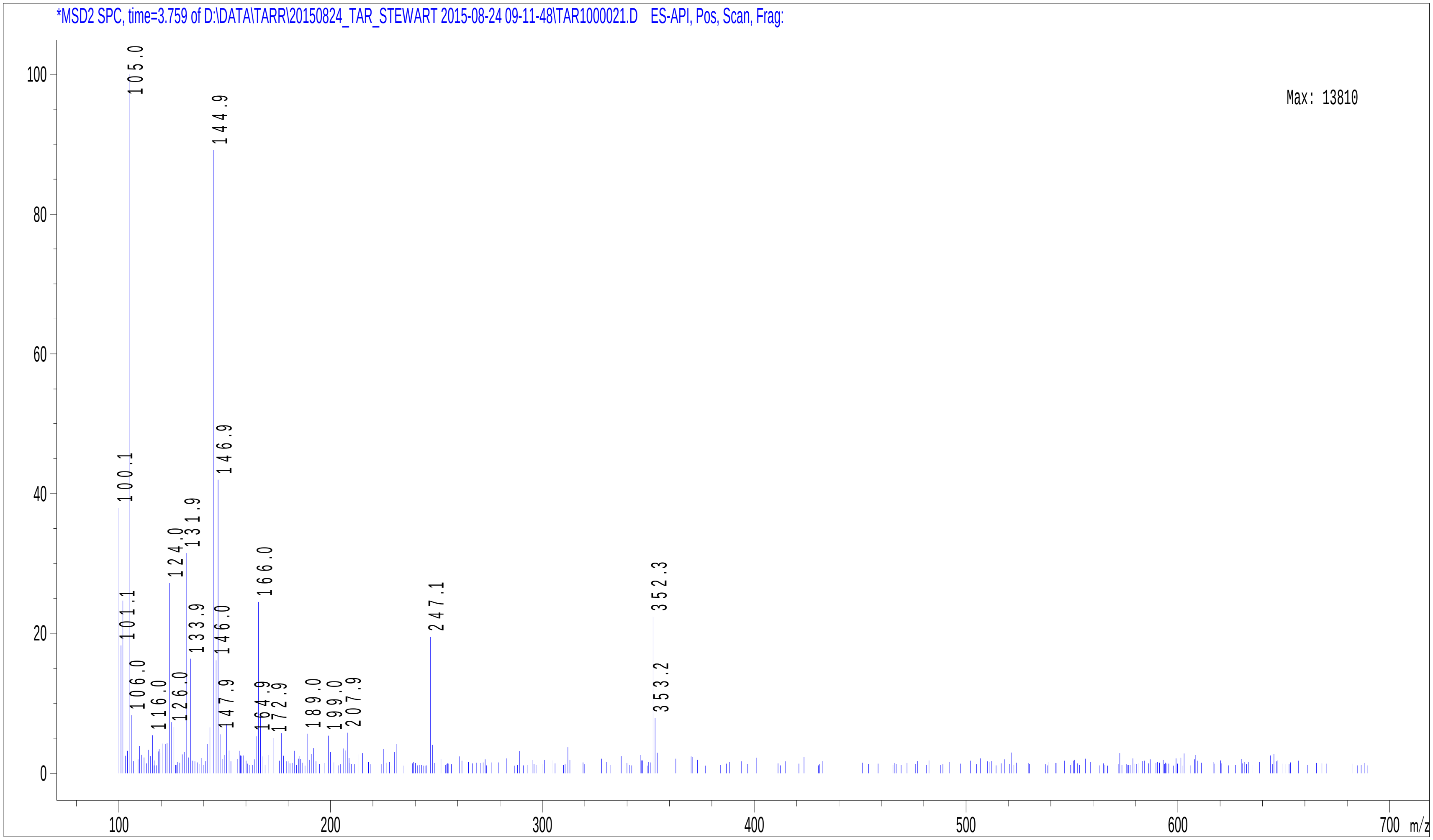
#	Time	Area	Height	Width	Area%	Symmetry
1	3.122	3771722.3	337384.6	0.1863	68.022	0.589
2	3.594	651466.3	69299.8	0.1567	11.749	0.732
3	3.733	80634.6	23855	0.0563	1.454	0
4	3.919	966005.8	122027.3	0.1319	17.422	0.628
5	4.063	75024.5	19699	0.0496	1.353	0.833

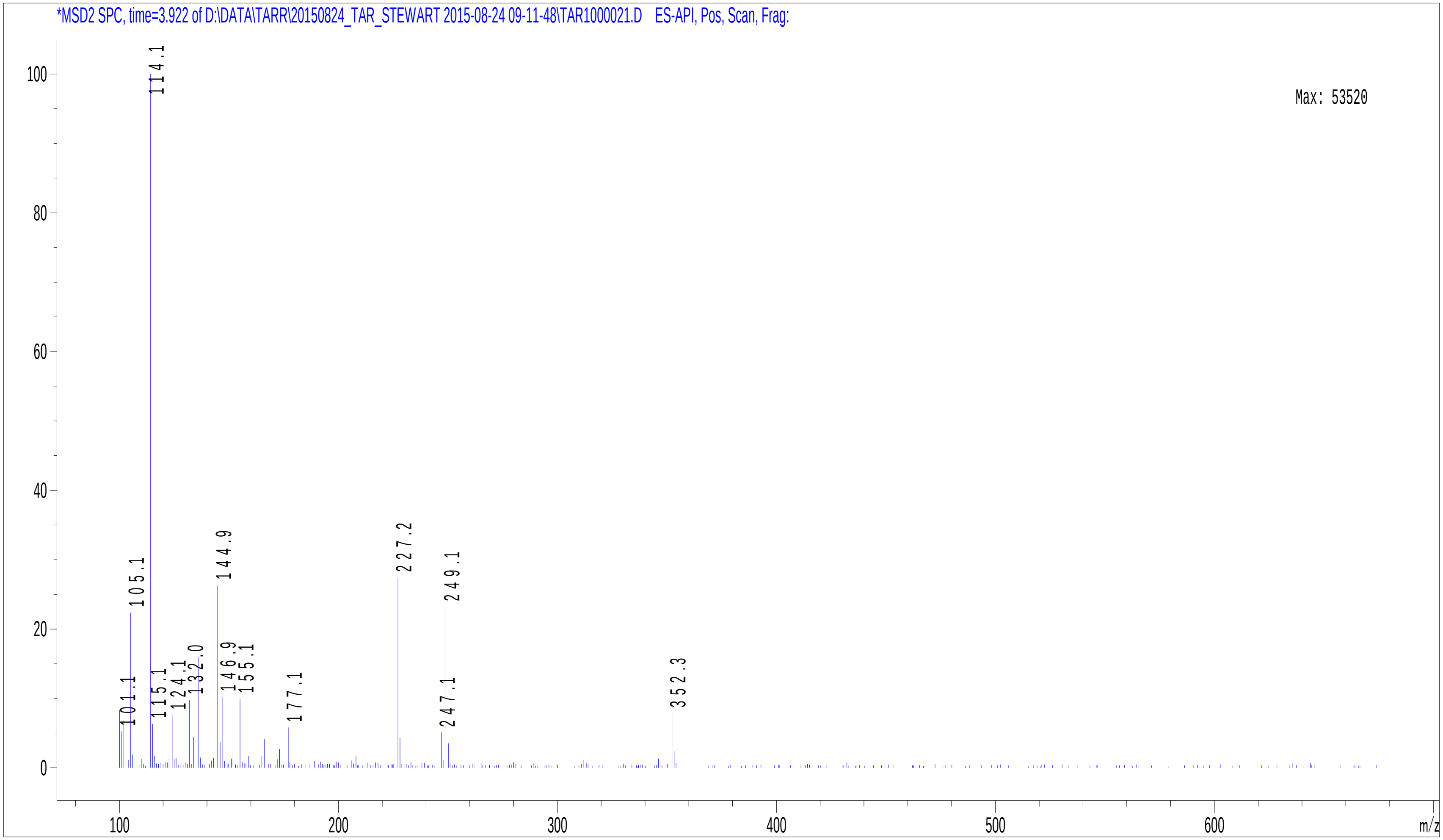

MSD2 TIC, MS File (D:\DATA\TARR\20150824_TAR_STEWART 2015-08-24 09-11-48\TAR1000021.D) ES-API, Pos, Scan, Frag: 70
Norm.
400000
350000
300000
250000
200000
150000
100000
2.5
3
3.5
4
4.5
min
3.122
Area: 3.77172e+006
3.594
Area: 651466
3.733
Area: 80634.6
3.919
Area: 966006
4.063
Area: 75024.5


*MSD2 SPC, time=3.122 of D:\DATA\TARR\20150824_TAR_STEWART 2015-08-24 09-11-48\TAR1000021.D ES-API, Pos, Scan, Frag:
Max: 196672
105.0
106.0
132.0
146.0
158.9
226.9
294.9
362.9
430.9
498.9
566.9
0
20
40
60
80
100
100
200
300
400
500
600
700
m/z

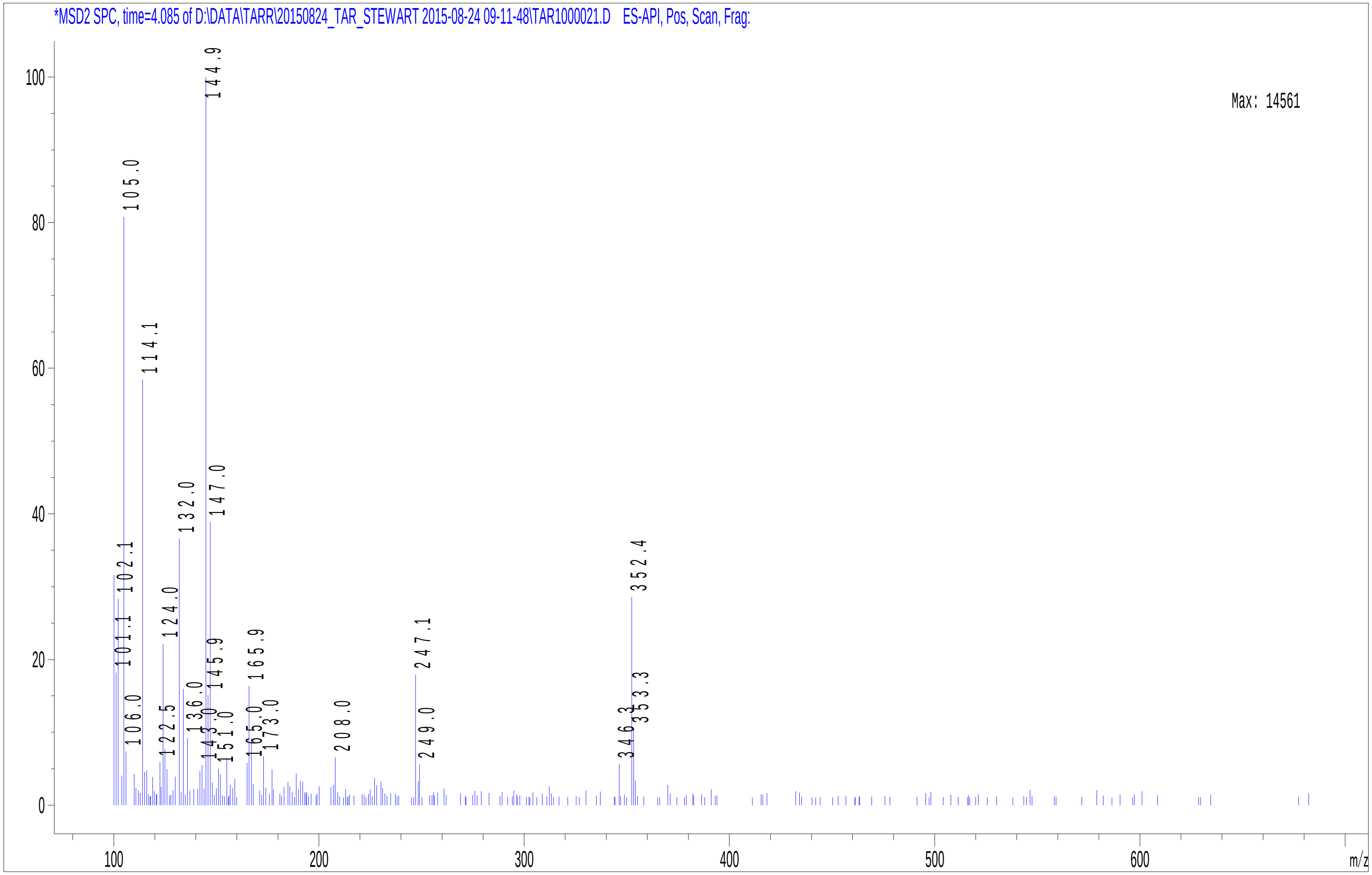

*MSD2 SPC, time=3.595 of D:\DATA\TARR\20150824_TAR_STEWART 2015-08-24 09-11-48\TAR1000021.D   ES-API, Pos, Scan, Frag:
Max: 18440
105.1
102.0
106.0
124.1
125.0
133.9
145.0
146.0
167.0
208.0
247.1
353.3
0
20
40
60
80
100
100
200
300
400
500
600
700
m/z


*MSD2 SPC, time=3.759 of D:\DATA\TARR\20150824_TAR_STEWART 2015-08-24 09-11-48\TAR1000021.D   ES-API, Pos, Scan, Frag:
Max: 13810
100
80
60
40
20
0
105.0
144.9
146.9
100.1
131.9
124.0
166.0
101.1
133.9
146.0
247.1
352.3
106.0
116.0
126.0
147.9
164.9
172.9
189.0
199.0
207.9
353.2
100
200
300
400
500
600
700
m/z


*MSD2 SPC, time=3.759 of D:\DATA\TARR\20150824_TAR_STEWART 2015-08-24 09-11-48\TAR1000021.D ES-API, Pos, Scan, Frag:
Max: 13810
105.0
144.9
146.9
100.1
131.9
124.0
166.0
101.1
133.9
146.0
247.1
352.3
106.0
116.0
126.0
147.9
164.9
172.9
189.0
199.0
207.9
353.2
0
20
40
60
80
100
100
200
300
400
500
600
700
m/z

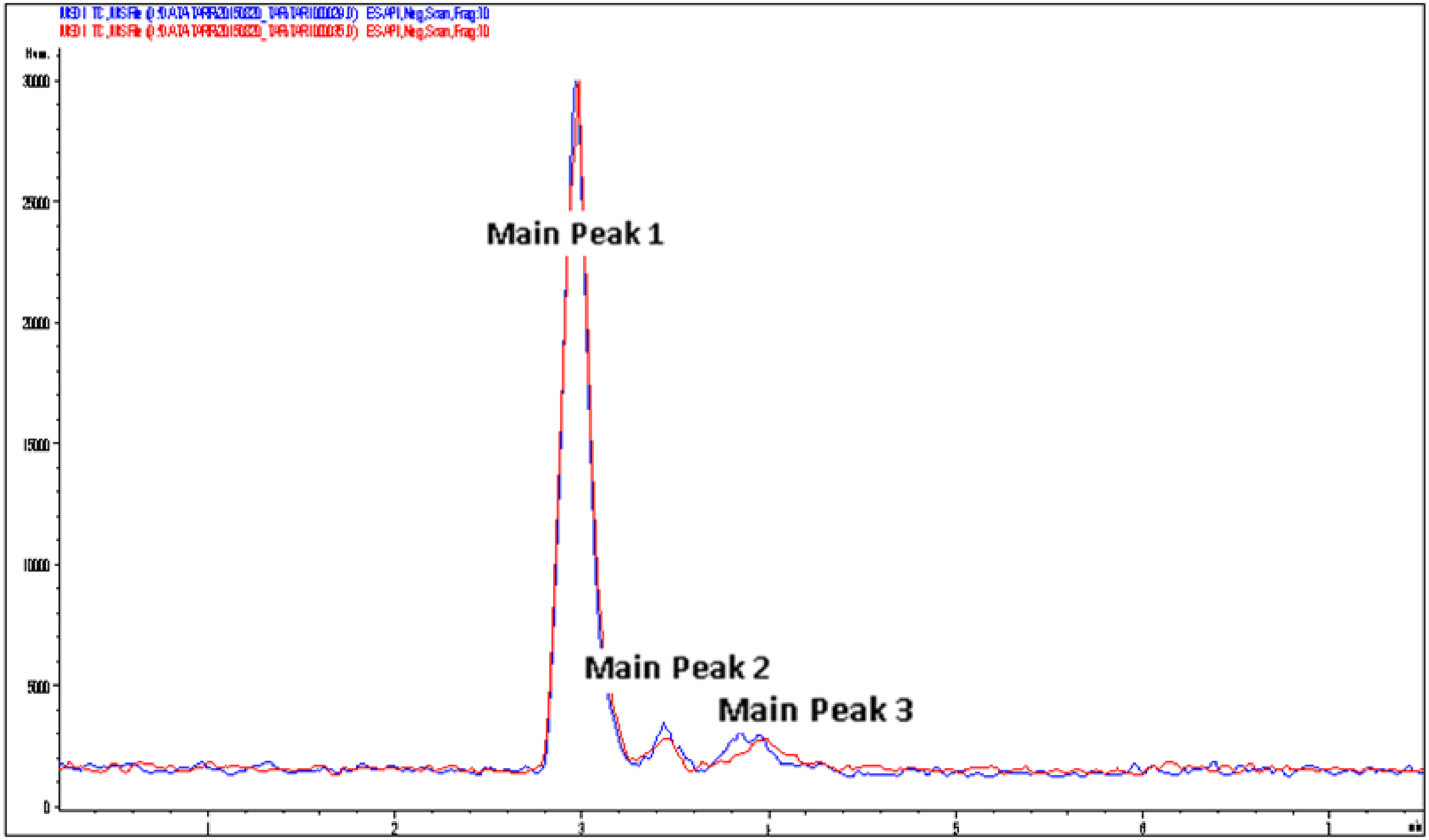


*MSD2 SPC, time=3.922 of D:\DATA\TARR\20150824_TAR_STEWART 2015-08-24 09-11-48\TAR1000021.D ES-API, Pos, Scan, Frag:


*MSD2 SPC, time=4.085 of D:\DATA\TARR\20150824_TAR_STEWART 2015-08-24 09-11-48\TAR1000021.D ES-API, Pos, Scan, Frag:
Max: 14561
100
80
60
40
20
0
144.9
105.0
114.1
147.0
132.0
102.1
124.0
101.1
106.0
122.5
136.0
143.0
145.9
151.0
165.9
165.0
173.0
208.0
247.1
249.0
352.4
353.3
346.3
100
200
300
400
500
600
m/z

Appendix K: Negative Ionization HPLC Chromatograms and Mass Spectroscopy

Example Negative Chromatogram

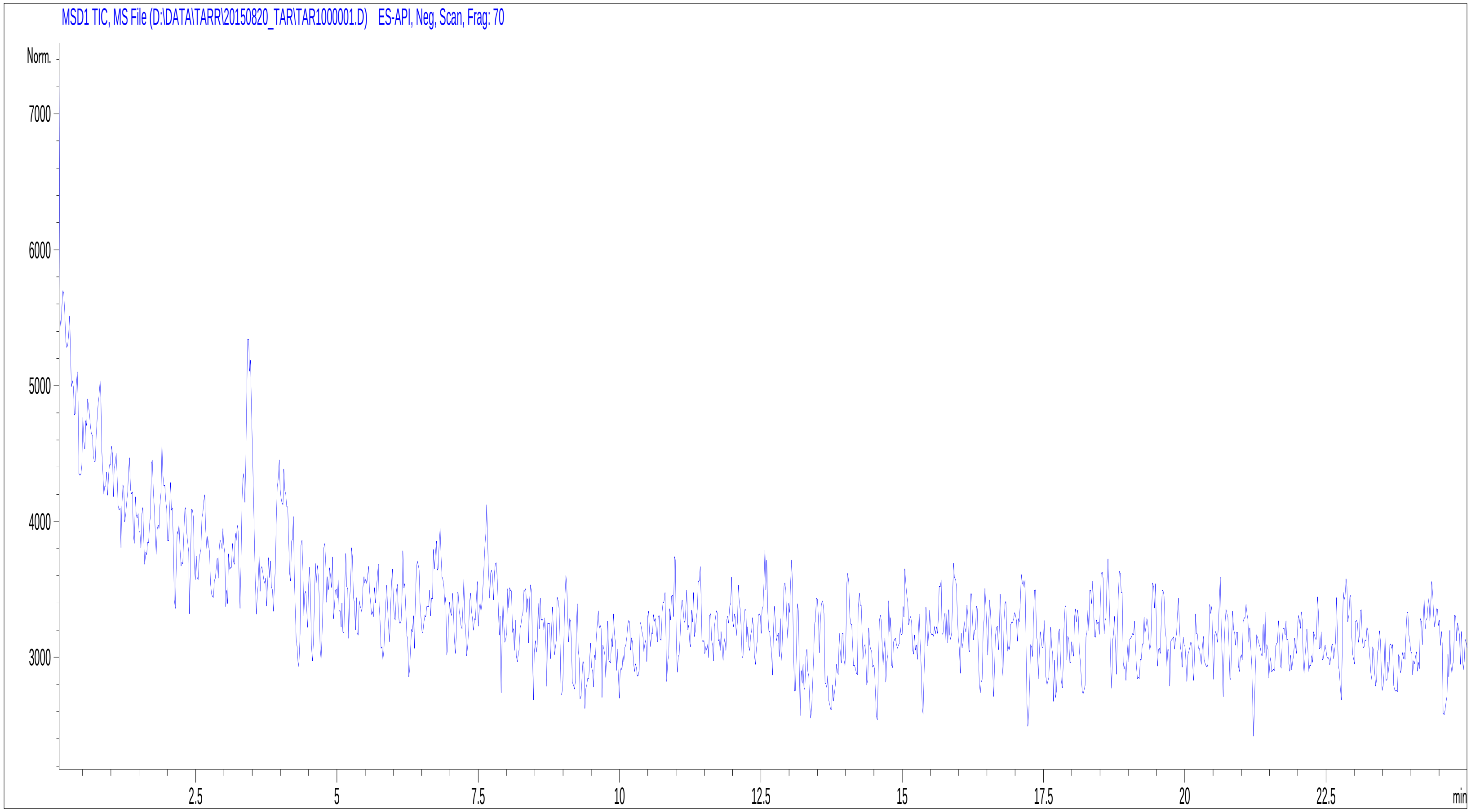


Baselines, Standards, Misc.

20-Aug-15

Baseline - DI Water

P2-A-01

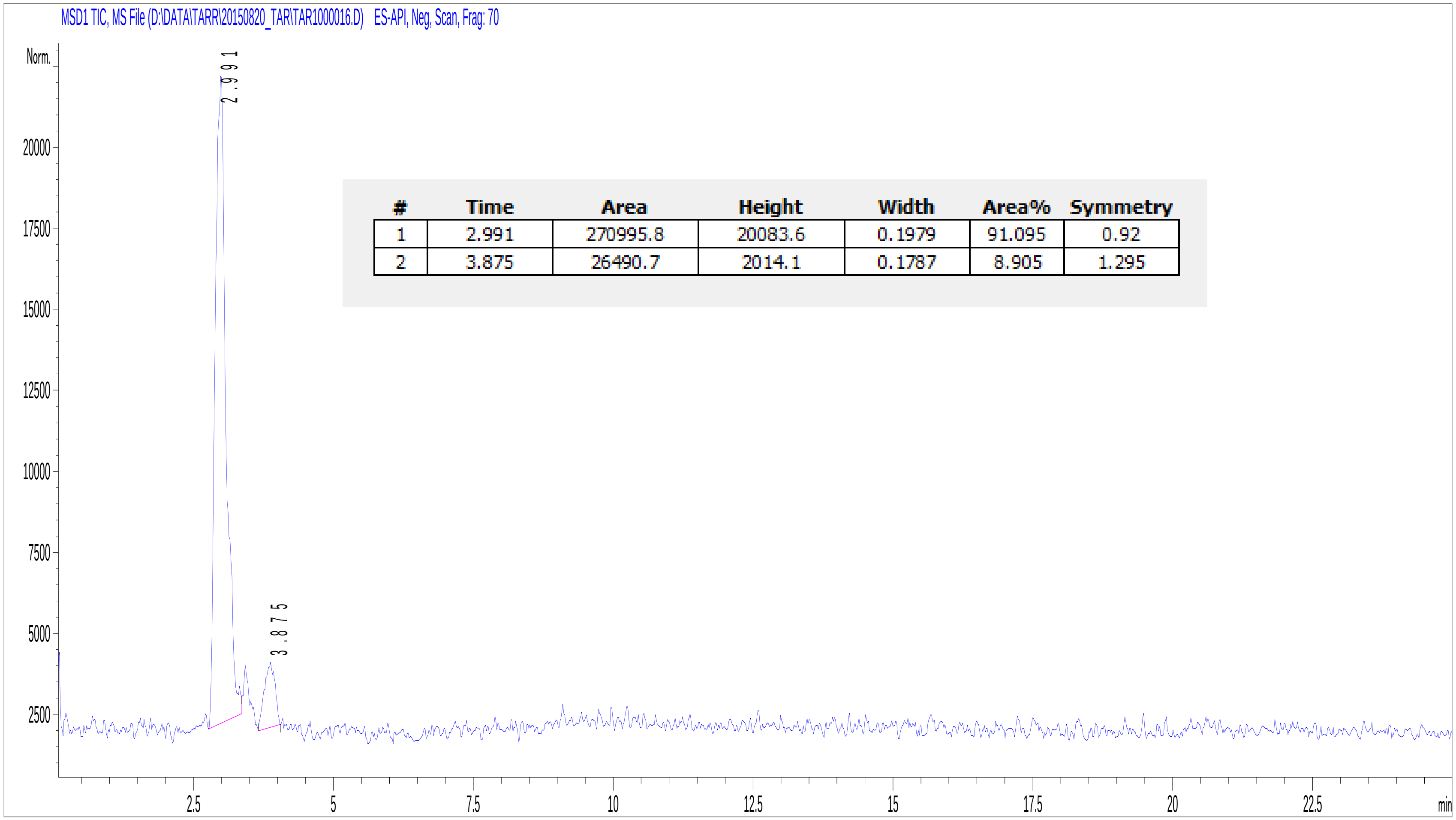


29-May-15

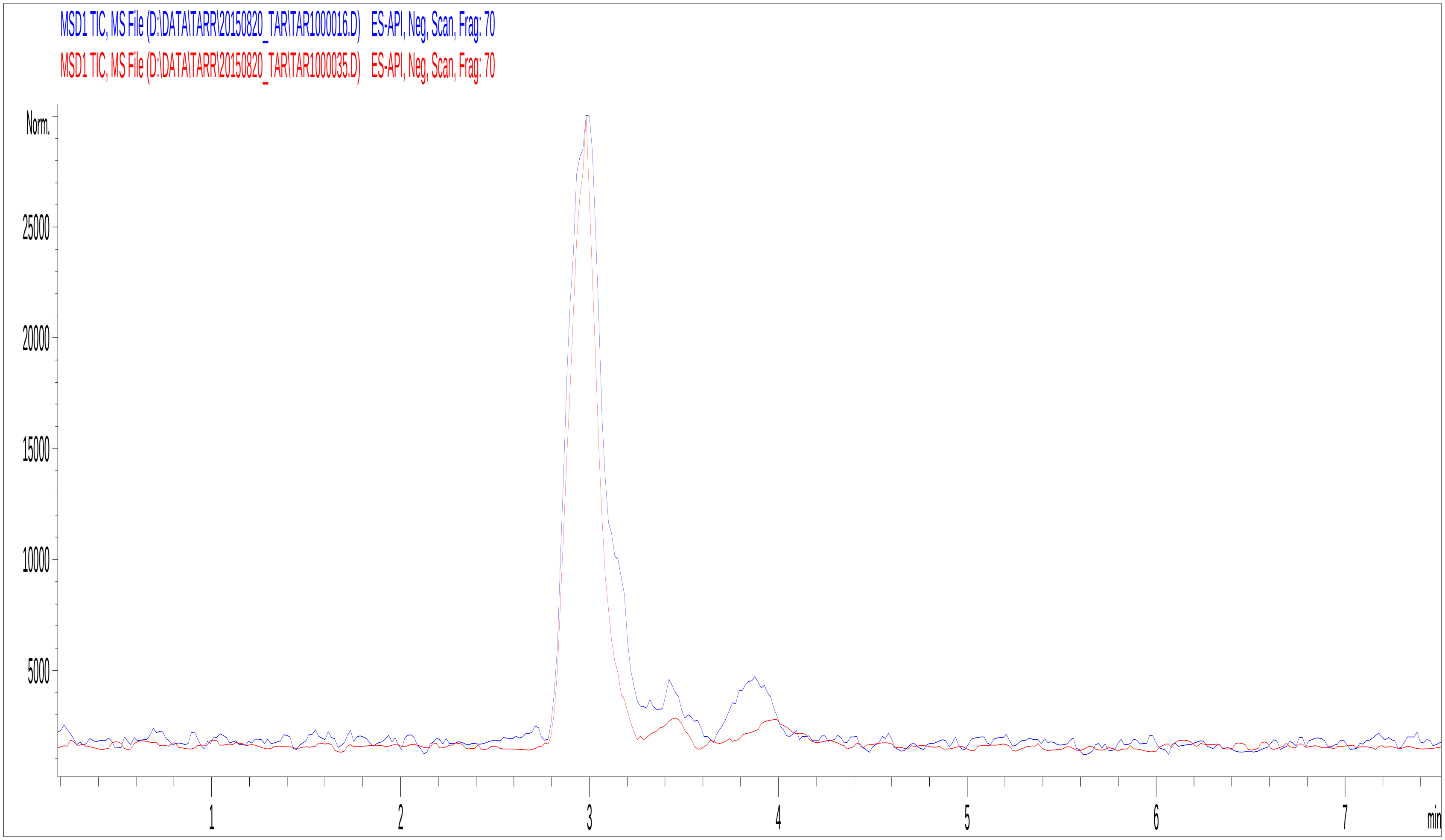
70

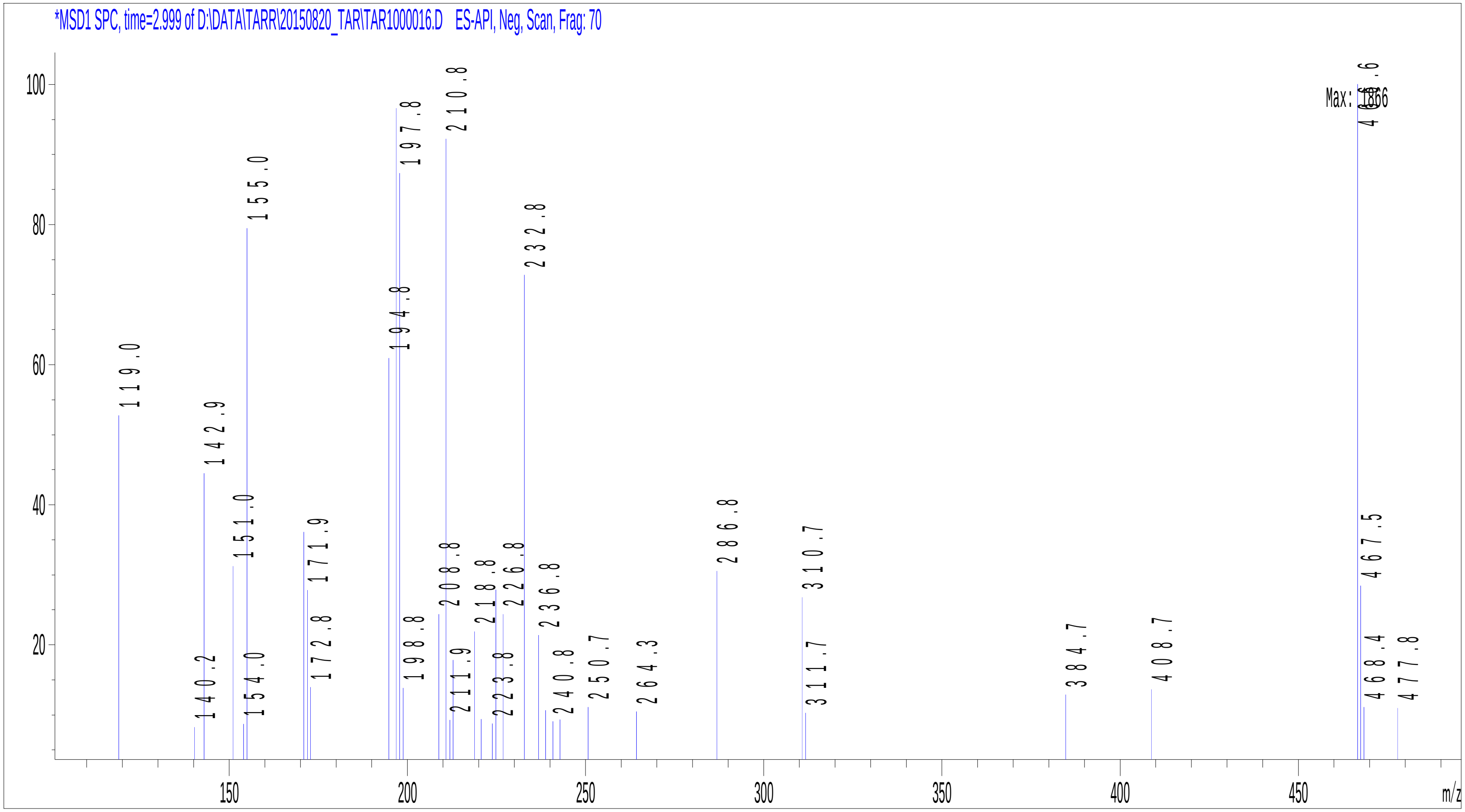
5

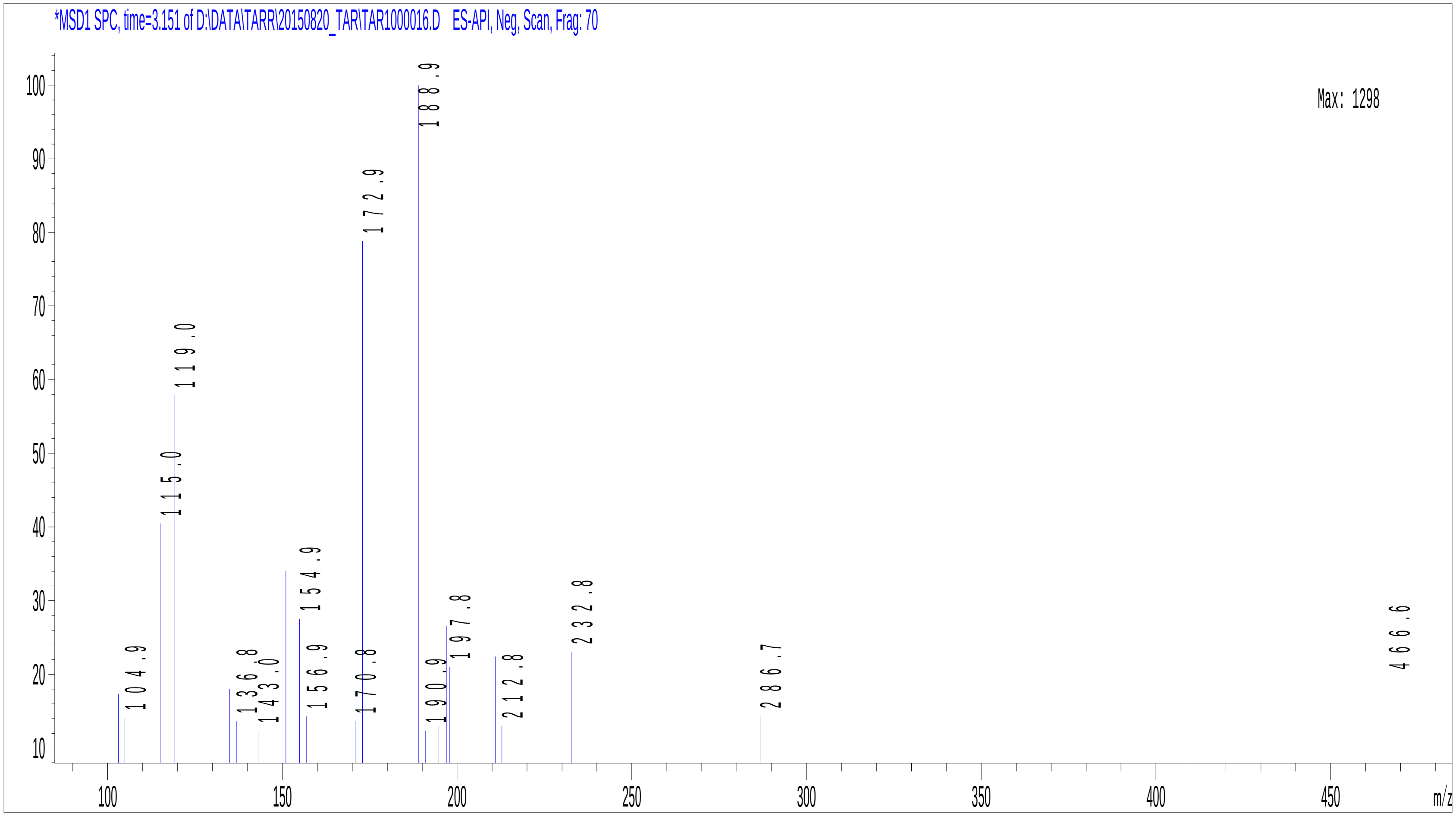
P2-B-03

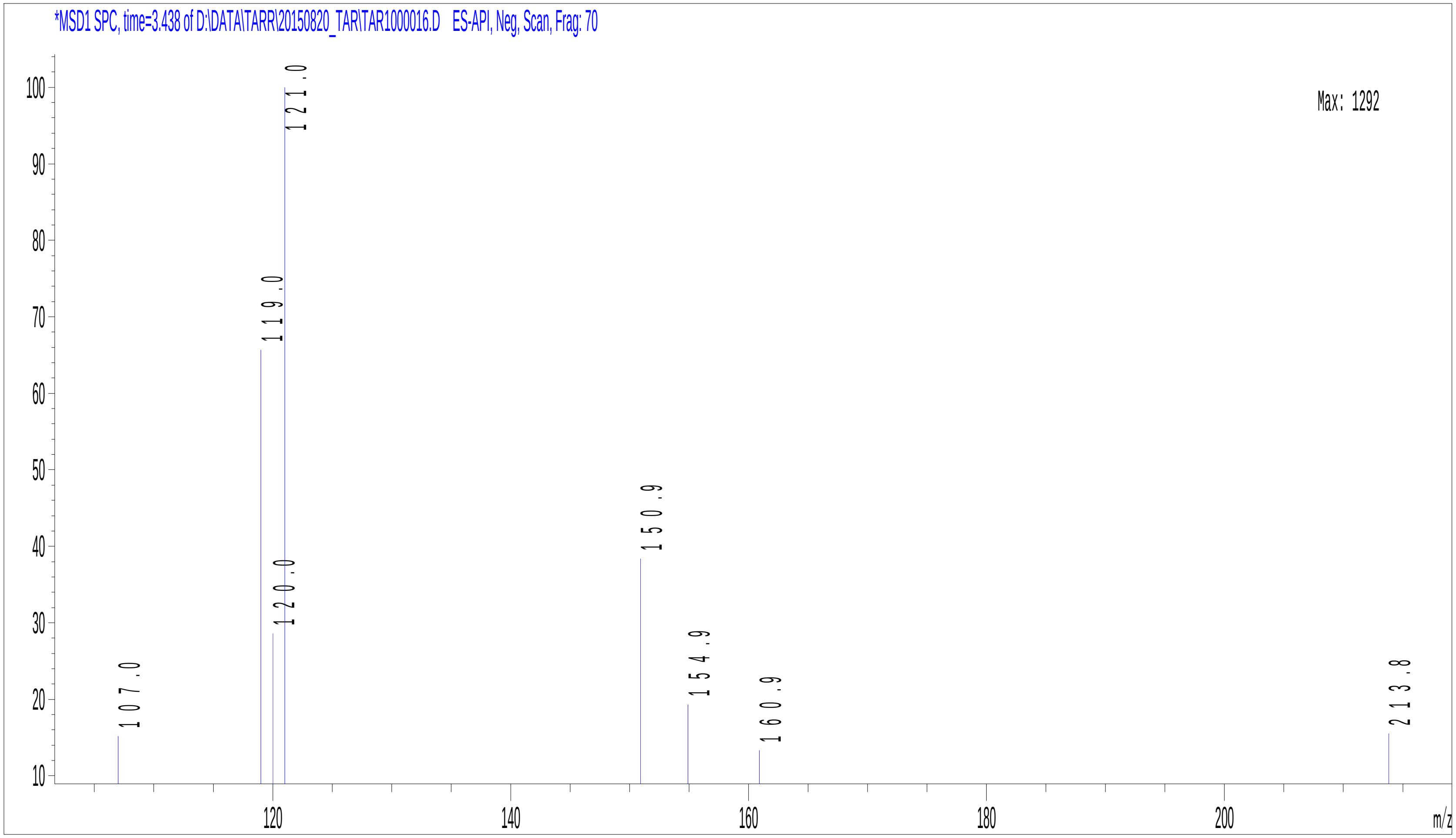


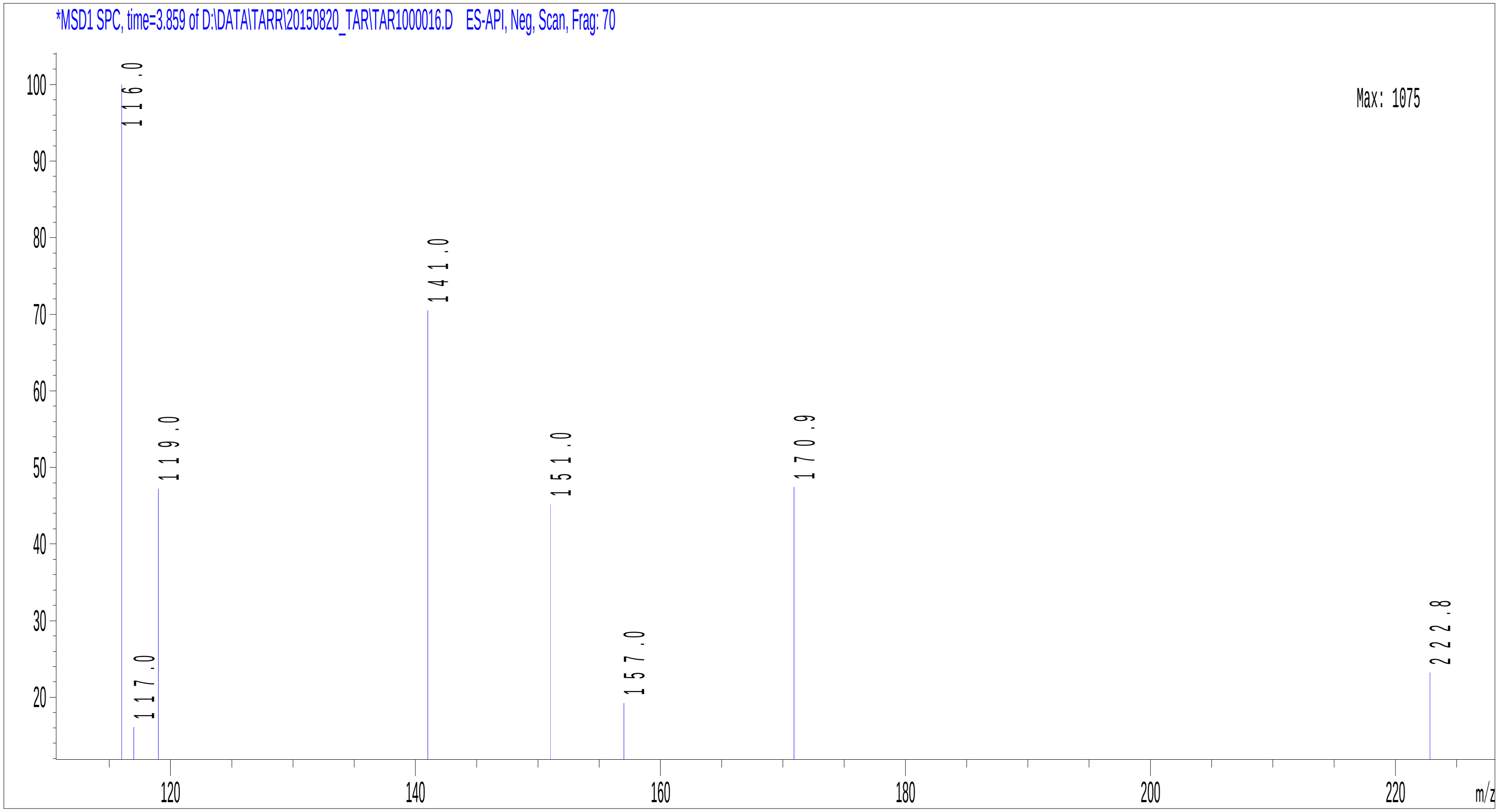
#	Time	Area	Height	Width	Area%	Symmetry
1	2.991	270995.8	20083.6	0.1979	91.095	0.92
2	3.875	26490.7	2014.1	0.1787	8.905	1.295


MSD1 TIC, MS File (D:\DATA\TARR\20150820_TAR\TAR1000016.D) ES-API, Neg, Scan, Frag: 70
MSD1 TIC, MS File (D:\DATA\TARR\20150820_TAR\TAR1000035.D) ES-API, Neg, Scan, Frag: 70
Norm.
25000
20000
15000
10000
5000
1
2
3
4
5
6
7
min

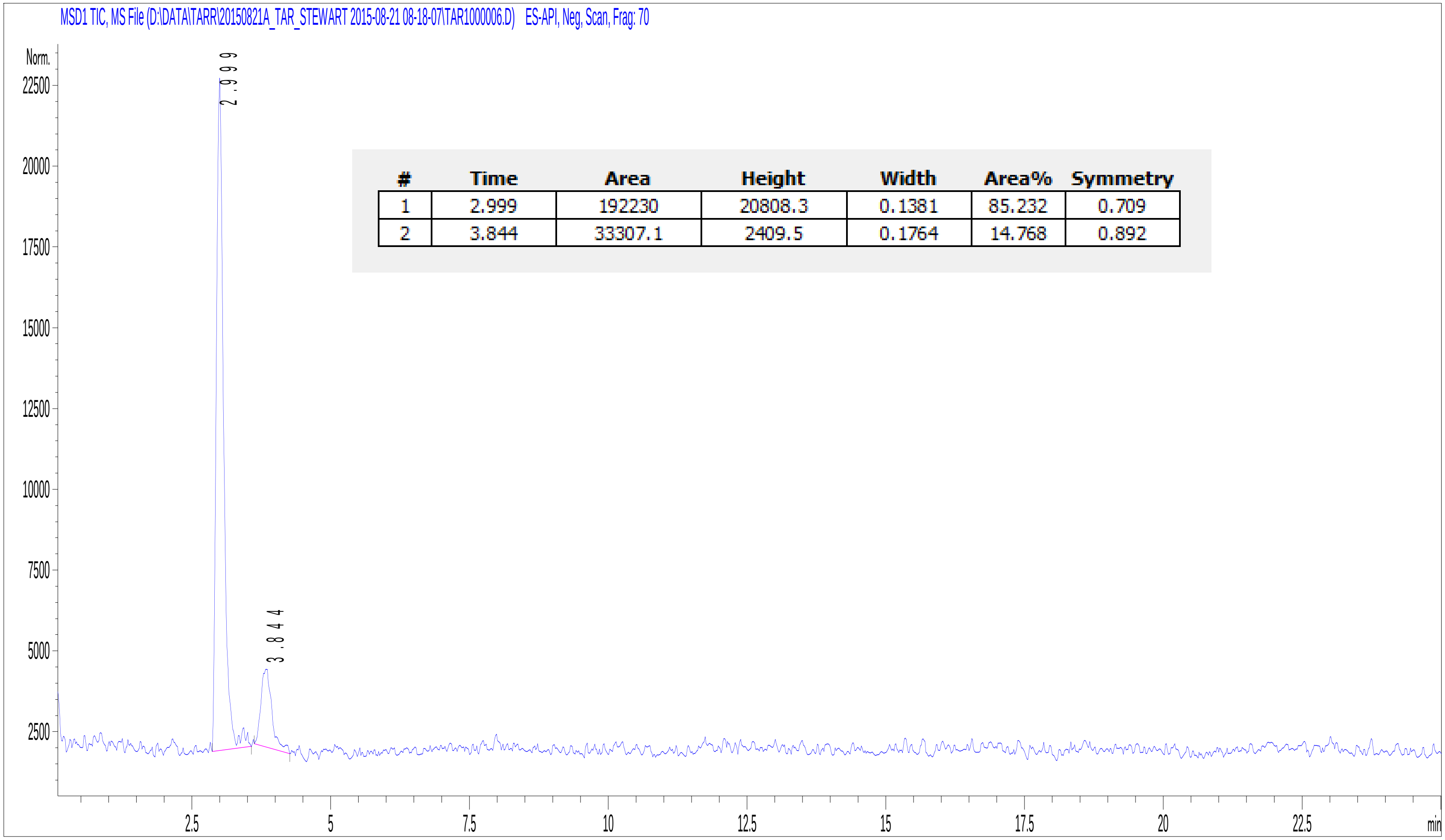

*MSD1 SPC, time=2.999 of D:\DATA\TARR\20150820_TAR\TAR1000016.D ES-API, Neg, Scan, Frag: 70
Max: 1866
100
80
60
40
20
150
200
250
300
350
400
450
m/z
119.0
140.2
142.9
151.0
154.0
155.0
171.9
172.8
194.8
197.8
198.8
208.8
210.8
211.9
218.8
223.8
226.8
232.8
236.8
240.8
250.7
264.3
286.8
310.7
311.7
384.7
408.7
466.6
467.5
468.4
477.8


*MSD1 SPC, time=3.151 of D:\DATA\TARR\20150820_TAR\TAR1000016.D ES-API, Neg, Scan, Frag: 70
Max: 1298
188.9
172.9
119.0
115.0
154.9
232.8
197.8
466.6
104.9
136.8
143.0
156.9
170.8
190.9
212.8
286.7
100
90
80
70
60
50
40
30
20
10
100
150
200
250
300
350
400
450
m/z

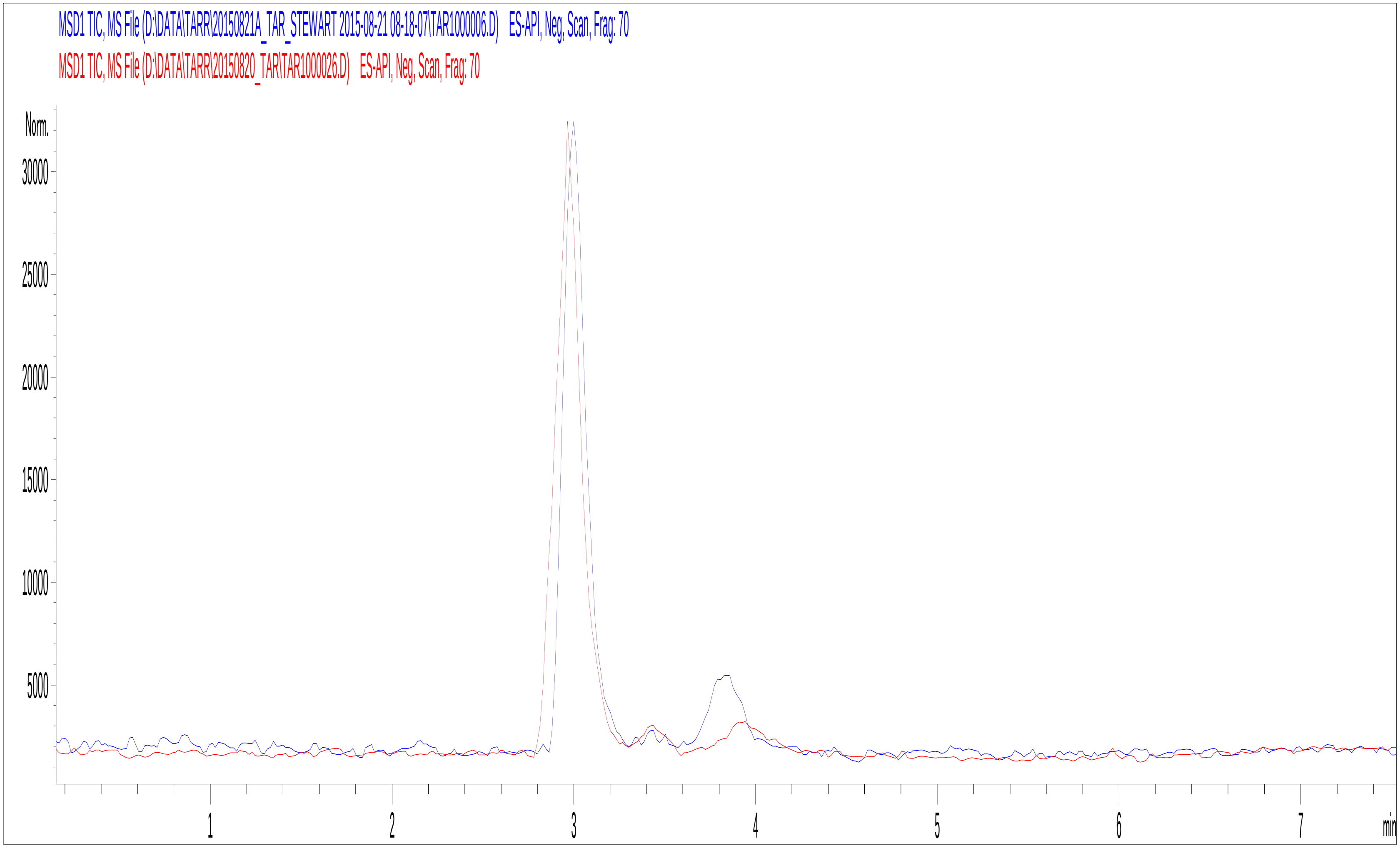

*MSD1 SPC, time=3.438 of D:\DATA\TARR\20150820_TAR\TAR1000016.D ES-API, Neg, Scan, Frag: 70
Max: 1292
100
90
80
70
60
50
40
30
20
10
120
140
160
180
200
m/z
121.0
119.0
120.0
107.0
150.9
154.9
160.9
213.8

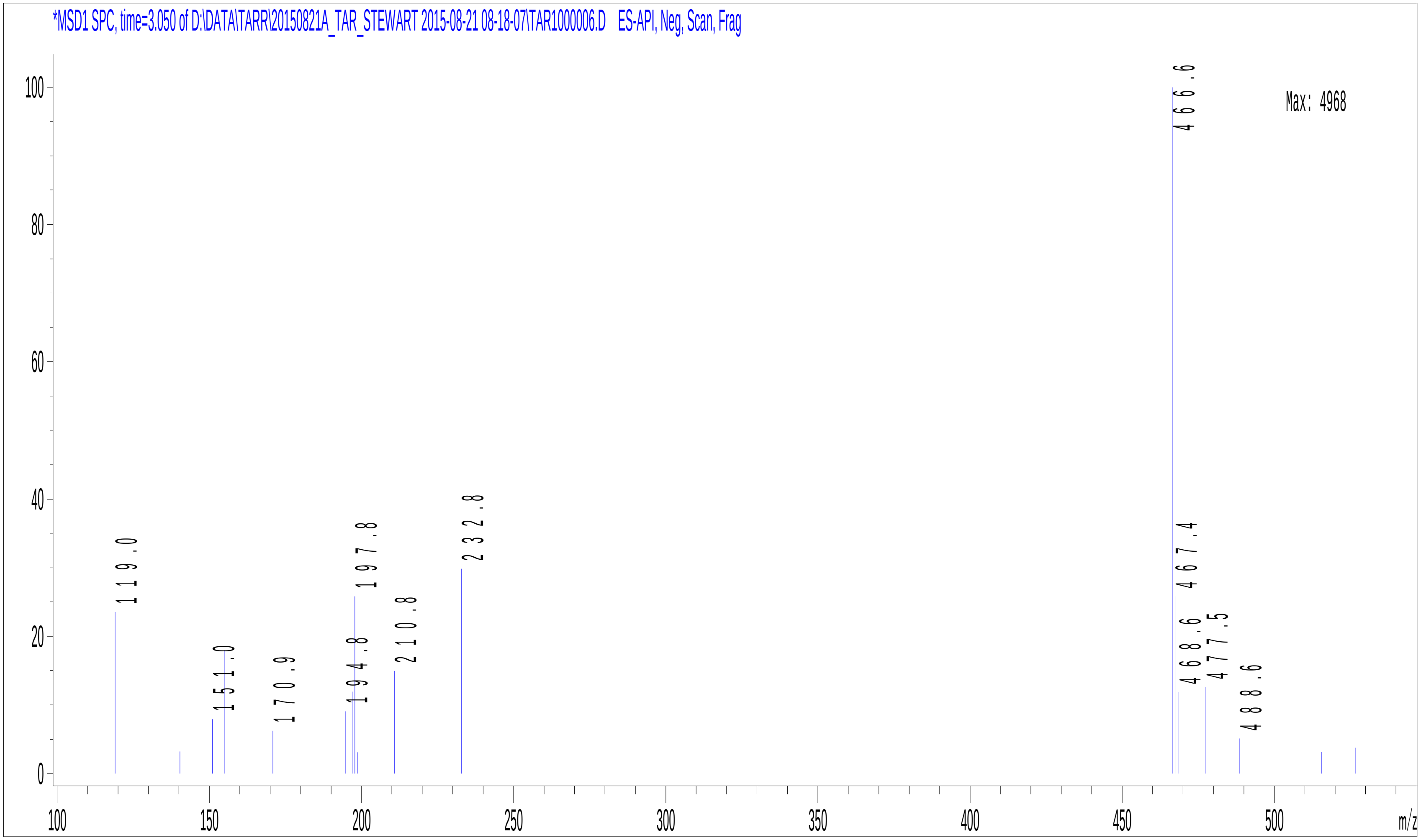

*MSD1 SPC, time=3.859 of D:\DATA\TARR\20150820_TAR\TAR1000016.D ES-API, Neg, Scan, Frag: 70
Max: 1075
116.0
117.0
119.0
141.0
151.0
157.0
170.9
222.8
100
90
80
70
60
50
40
30
20
120
140
160
180
200
220
m/z

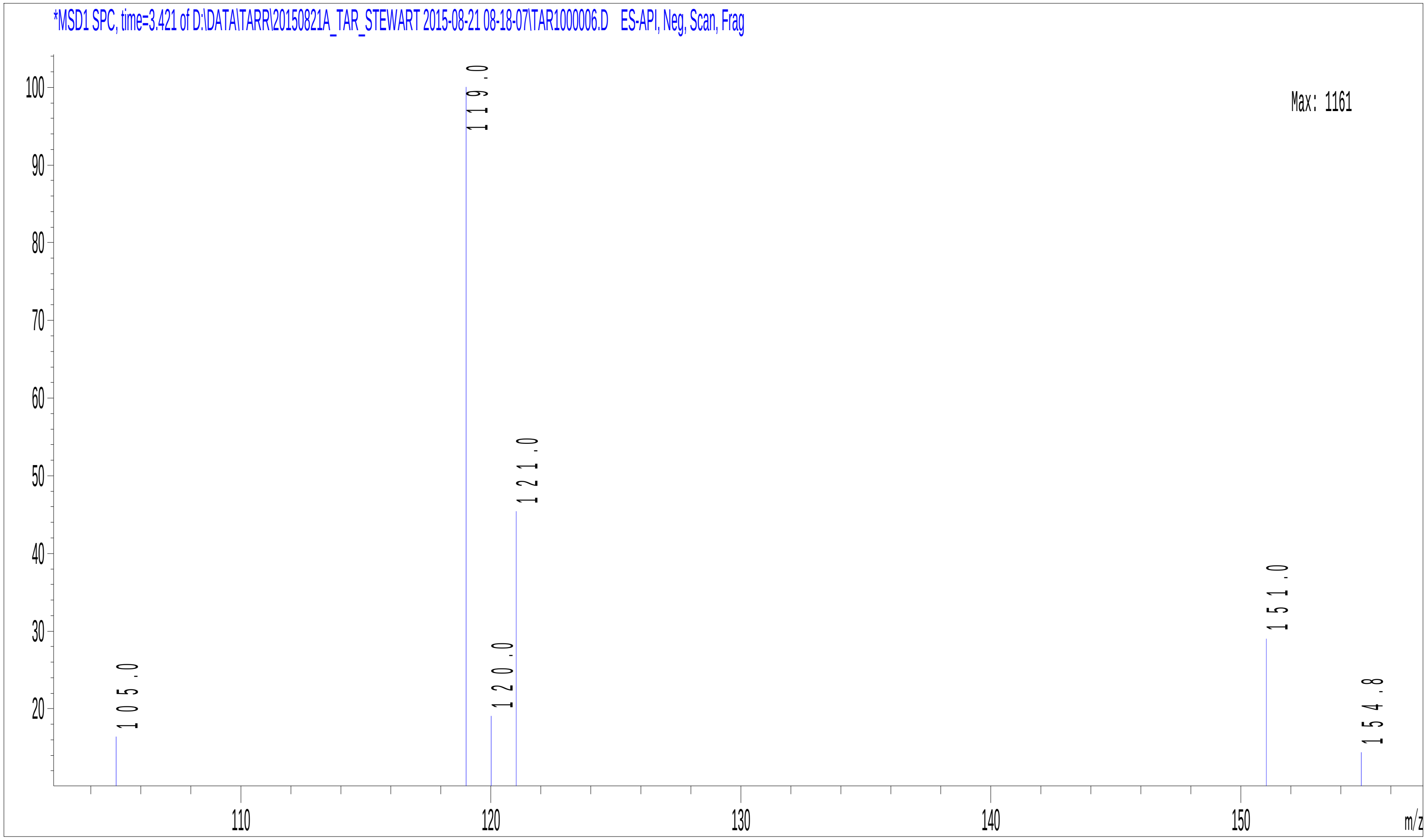
11-Aug-15
UNTREATED SOLUTION
7
P2-E-05

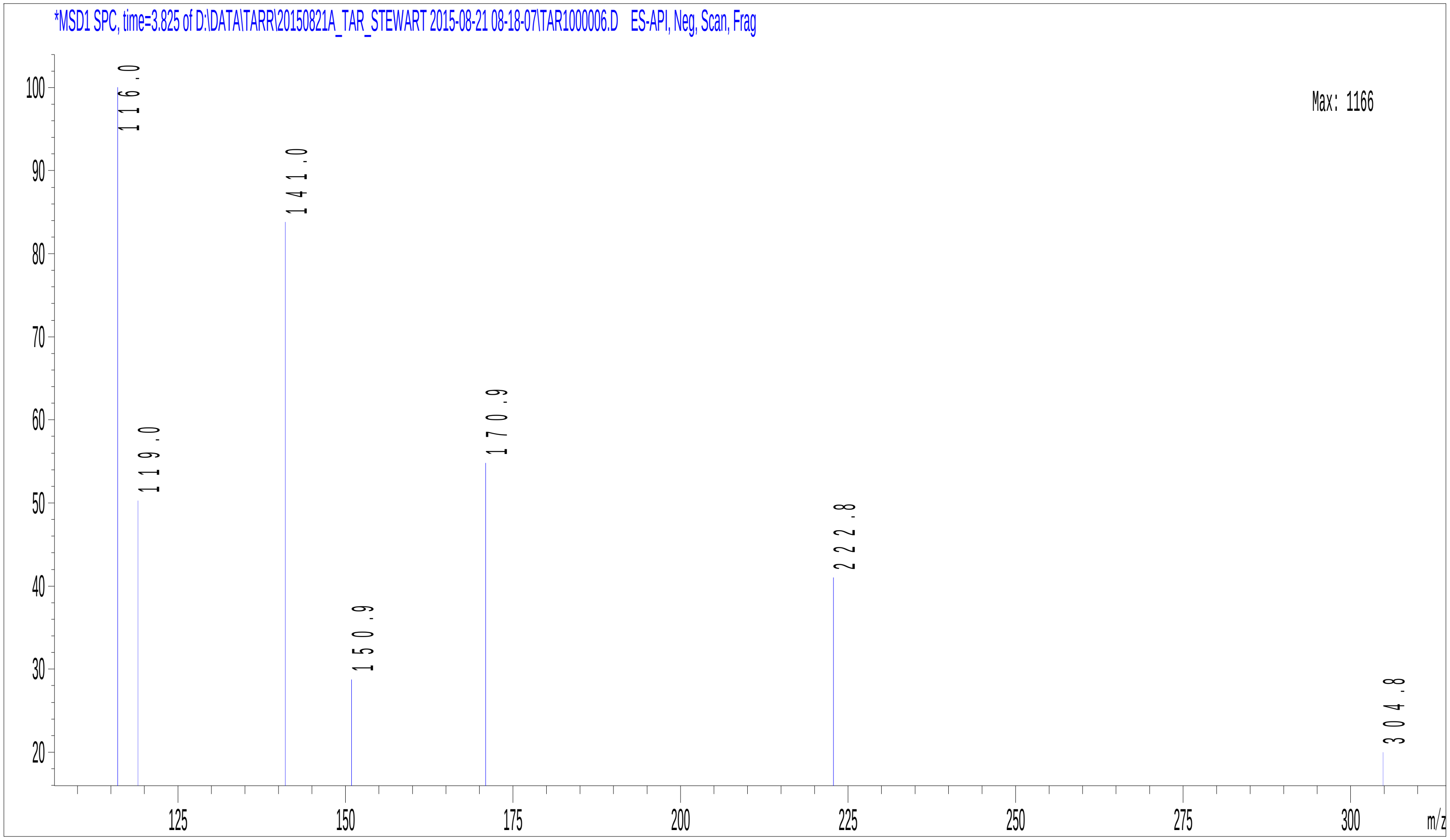


#	Time	Area	Height	Width	Area%	Symmetry
1	2.999	192230	20808.3	0.1381	85.232	0.709
2	3.844	33307.1	2409.5	0.1764	14.768	0.892


MSD1 TIC, MS File (D:\DATA\TARR\20150821A_TAR_STEWART 2015-08-21 08-18-07\TAR1000006.D) ES-API, Neg, Scan, Frag: 70
MSD1 TIC, MS File (D:\DATA\TARR\20150820_TAR\TAR1000026.D) ES-API, Neg, Scan, Frag: 70
Norm.
30000
25000
20000
15000
10000
5000
1
2
3
4
5
6
7
min


*MSD1 SPC, time=3.050 of D:\DATA\TARR\20150821A_TAR_STEWART 2015-08-21 08-18-07\TAR1000006.D ES-API, Neg, Scan, Frag
Max: 4968
466.6
467.4
468.6
477.5
488.6
119.0
151.0
170.9
194.8
197.8
210.8
232.8
0
20
40
60
80
100
100
150
200
250
300
350
400
450
500
m/z


*MSD1 SPC, time=3.421 of D:\DATA\TARR\20150821A_TAR_STEWART 2015-08-21 08-18-07\TAR1000006.D ES-API, Neg, Scan, Frag
Max: 1161
100
90
80
70
60
50
40
30
20
105.0
119.0
120.0
121.0
151.0
154.8
110
120
130
140
150
m/z


*MSD1 SPC, time=3.825 of D:\DATA\TARR\20150821A_TAR_STEWART 2015-08-21 08-18-07\TAR1000006.D ES-API, Neg, Scan, Frag
Max: 1166
116.0
119.0
141.0
150.9
170.9
222.8
304.8
100
90
80
70
60
50
40
30
20
125
150
175
200
225
250
275
300
m/z

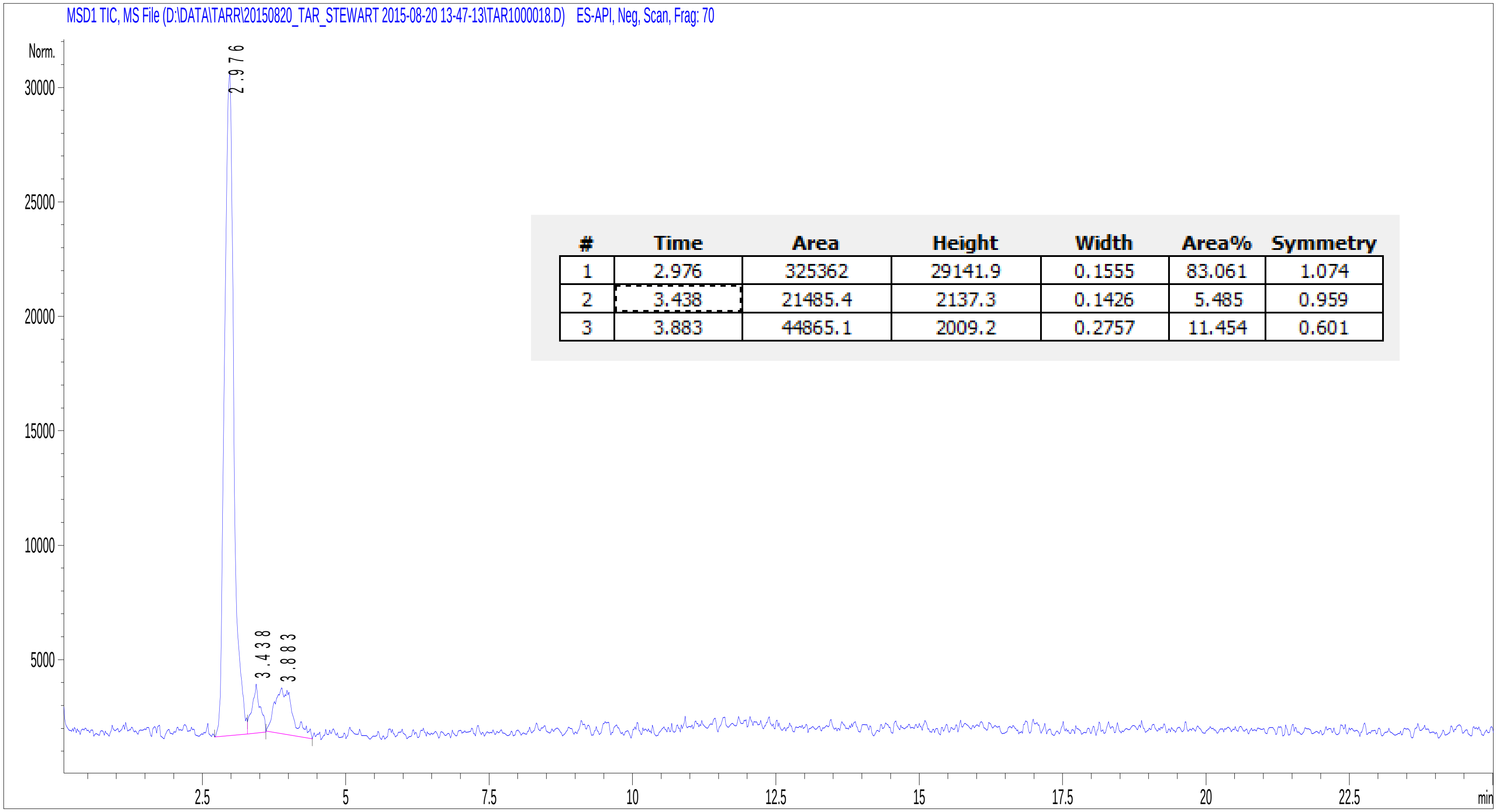
pH 6

14-May-15

0 DC

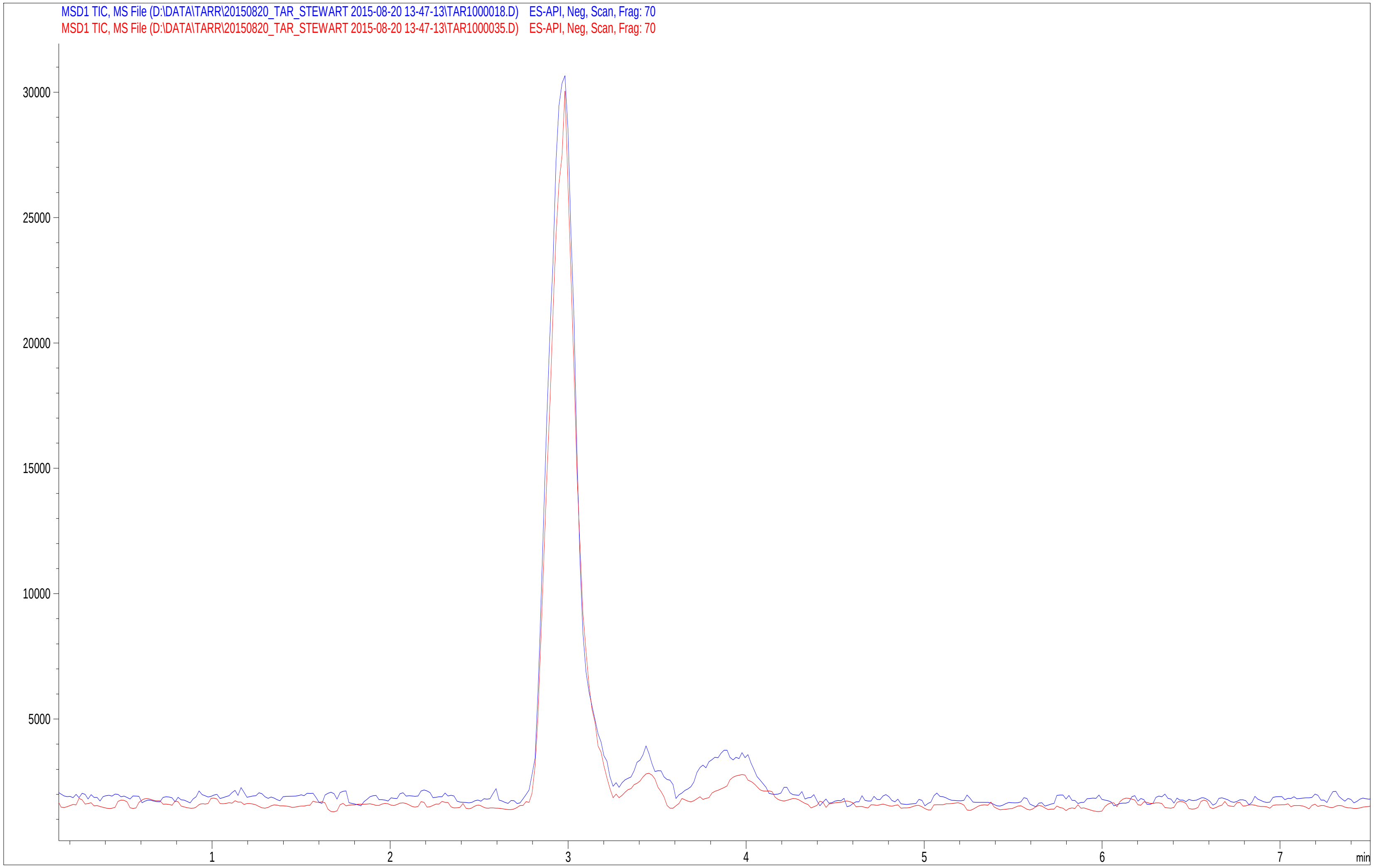
6

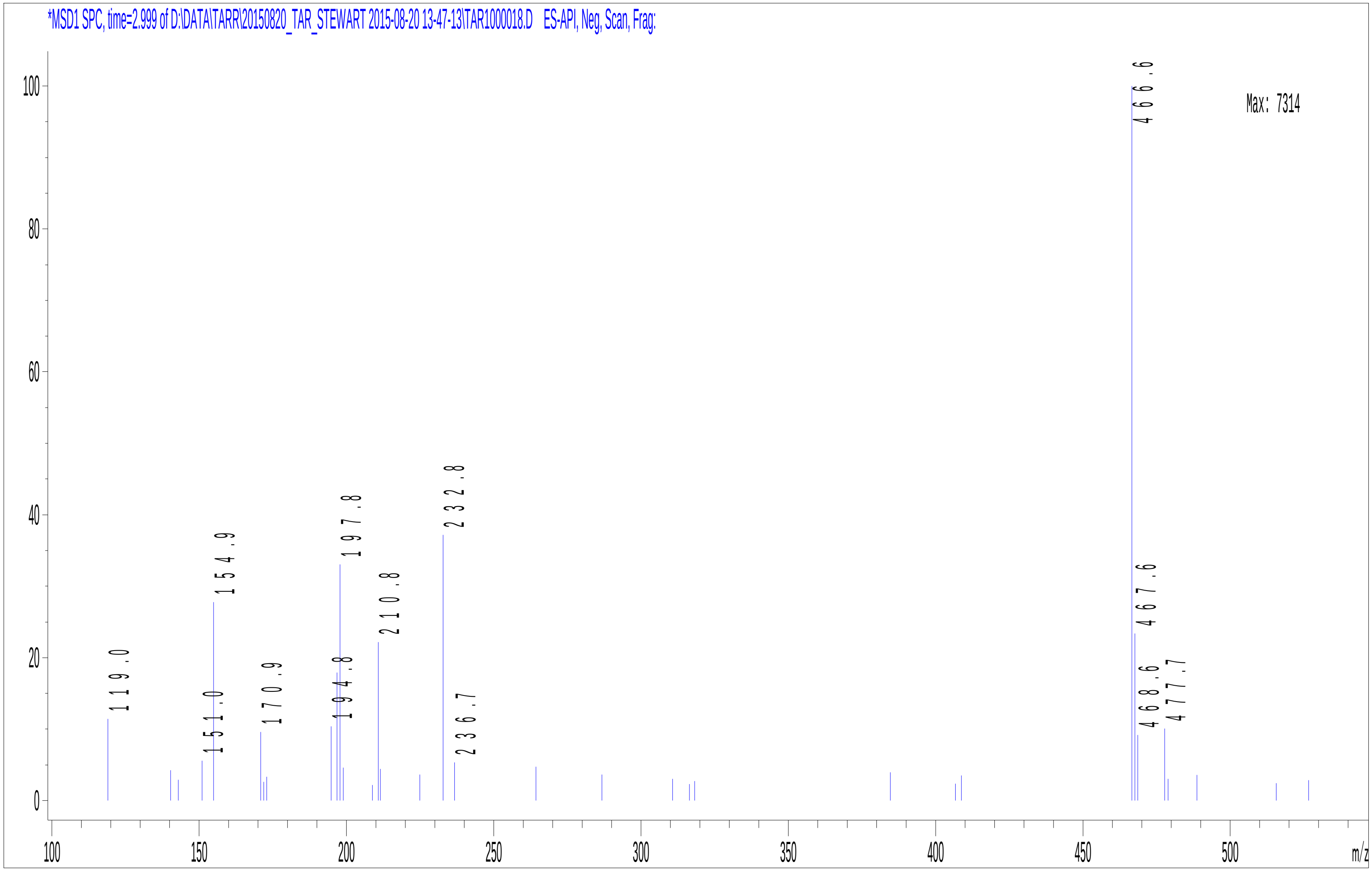
P2-B-01

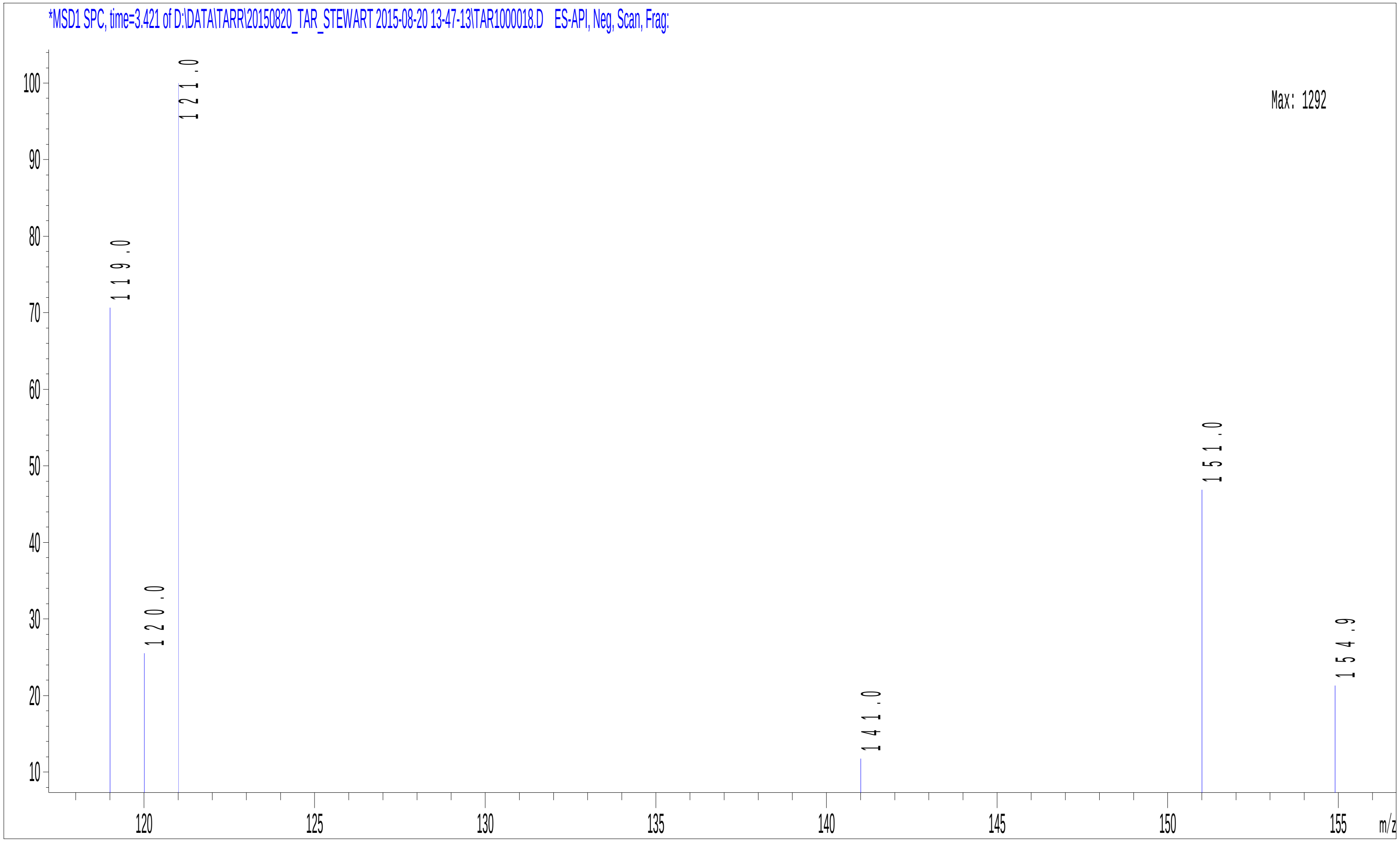


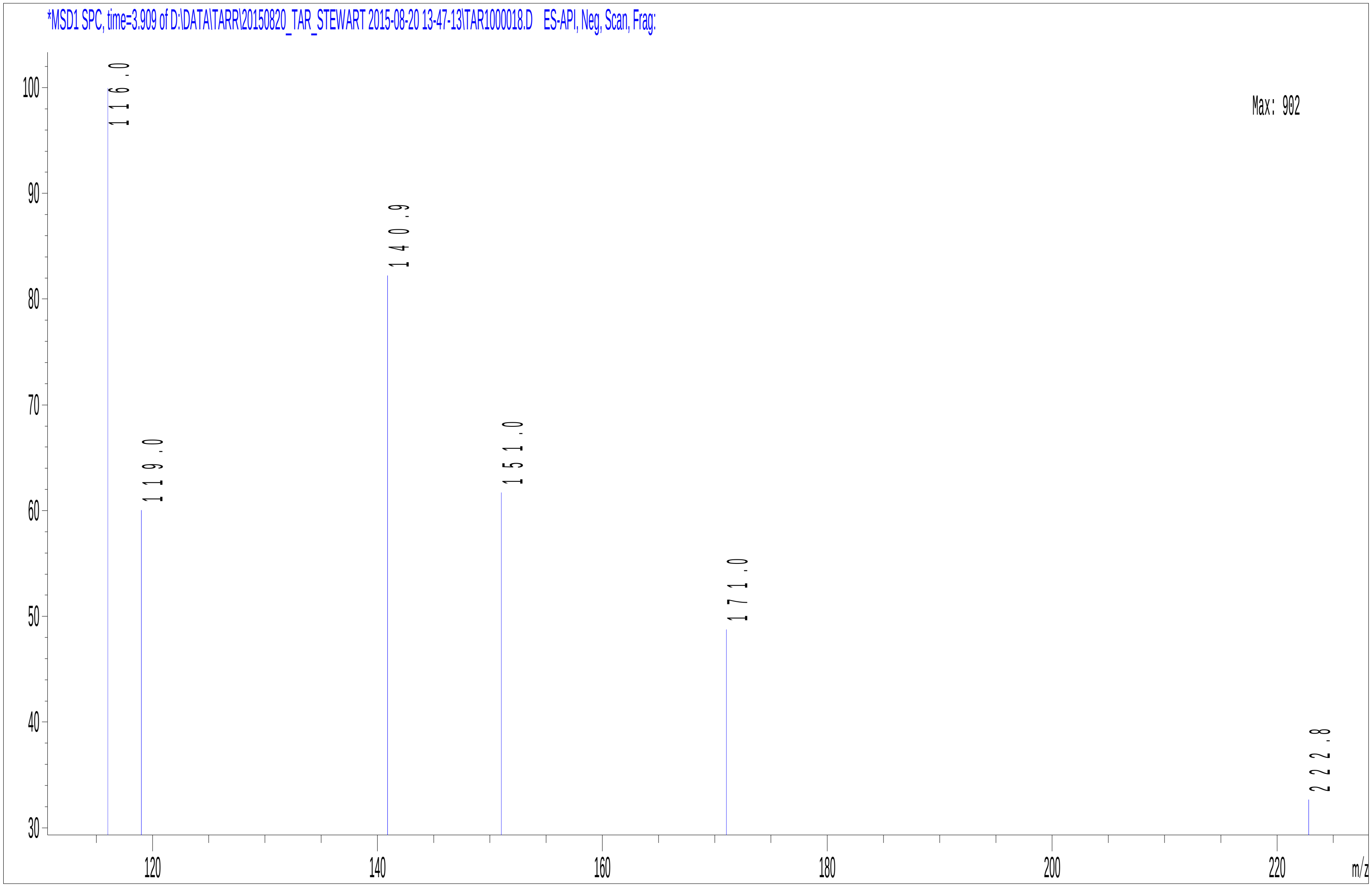
MSD1 TIC, MS File (D:\DATA\TARR\20150820_TAR_STEWART 2015-08-20 13-47-13\TAR1000018.D) ES-API, Neg, Scan, Frag: 70

#	Time	Area	Height	Width	Area%	Symmetry
1	2.976	325362	29141.9	0.1555	83.061	1.074
2	3.438	21485.4	2137.3	0.1426	5.485	0.959
3	3.883	44865.1	2009.2	0.2757	11.454	0.601


MSD1 TIC, MS File (D:\DATA\TARR\20150820_TAR_STEWART 2015-08-20 13-47-13\TAR1000018.D) ES-API, Neg, Scan, Frag: 70
MSD1 TIC, MS File (D:\DATA\TARR\20150820_TAR_STEWART 2015-08-20 13-47-13\TAR1000035.D) ES-API, Neg, Scan, Frag: 70
30000
25000
20000
15000
10000
5000
1
2
3
4
5
6
7
min


*MSD1 SPC, time=2.999 of D:\DATA\TARR\20150820_TAR_STEWART 2015-08-20 13-47-13\TAR1000018.D ES-API, Neg, Scan, Frag:
Max: 7314
466.6
467.6
468.6
477.7
119.0
151.0
154.9
170.9
194.8
197.8
210.8
232.8
236.7
0
20
40
60
80
100
100
150
200
250
300
350
400
450
500
m/z


*MSD1 SPC, time=3.421 of D:\DATA\TARR\20150820_TAR_STEWART 2015-08-20 13-47-13\TAR1000018.D ES-API, Neg, Scan, Frag:
Max: 1292
100
90
80
70
60
50
40
30
20
10
119.0
120.0
121.0
141.0
151.0
154.9
120
125
130
135
140
145
150
155
m/z

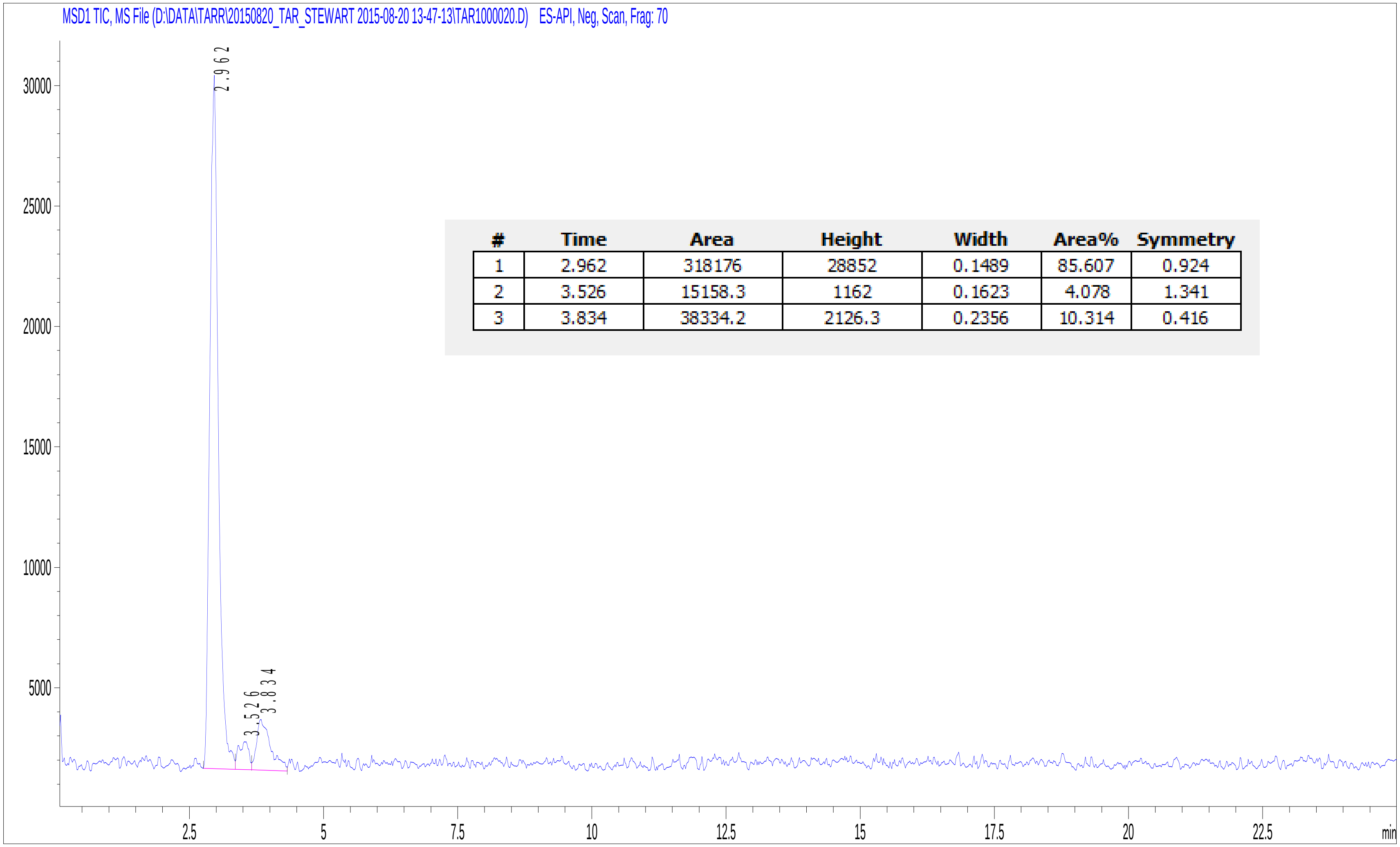

*MSD1 SPC, time=3.909 of D:\DATA\TARR\20150820_TAR_STEWART 2015-08-20 13-47-13\TAR1000018.D   ES-API, Neg, Scan, Frag:
Max: 902
116.0
119.0
140.9
151.0
171.0
222.8
100
90
80
70
60
50
40
30
120
140
160
180
200
220
m/z

29-Jun-15

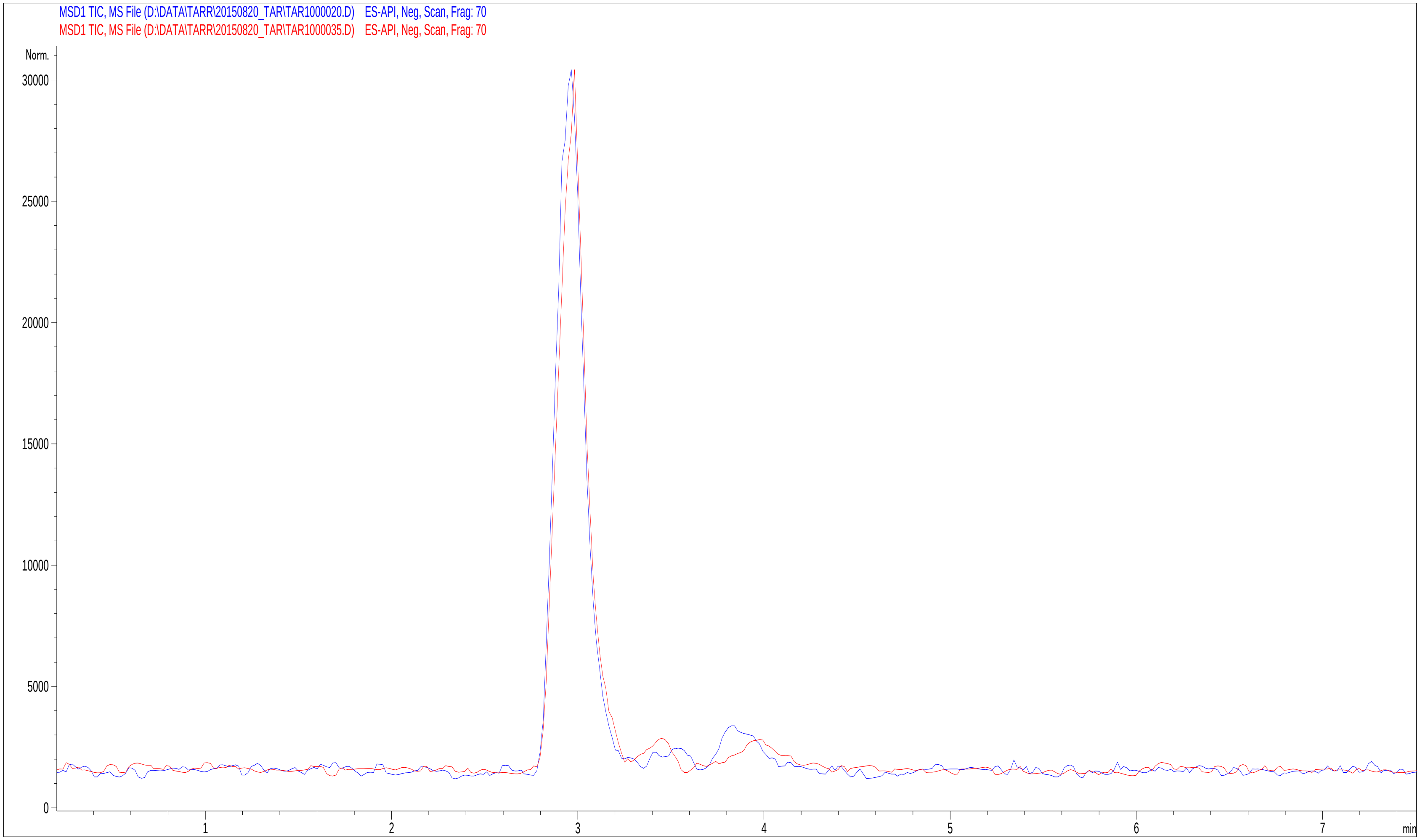
5 DC

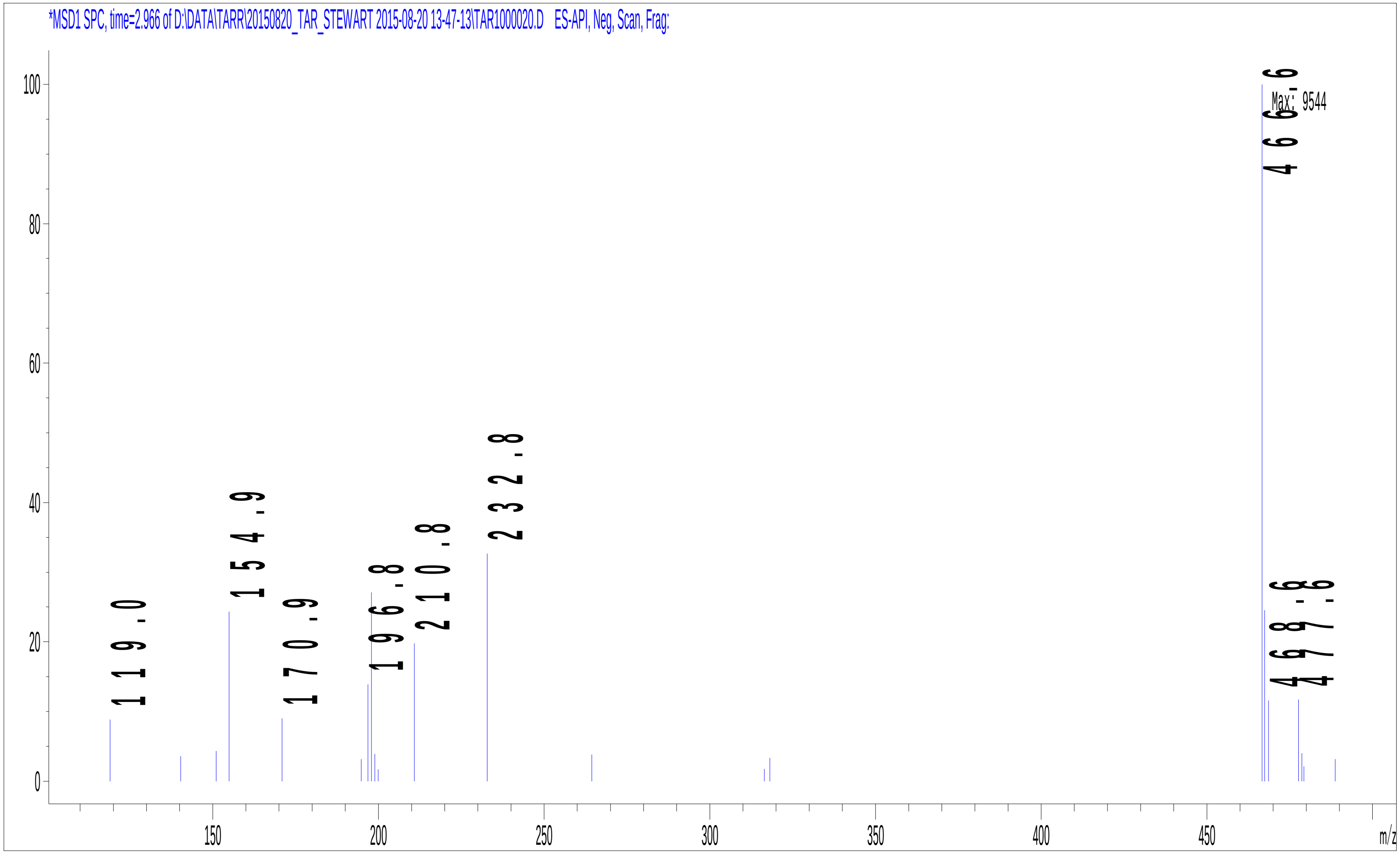
6

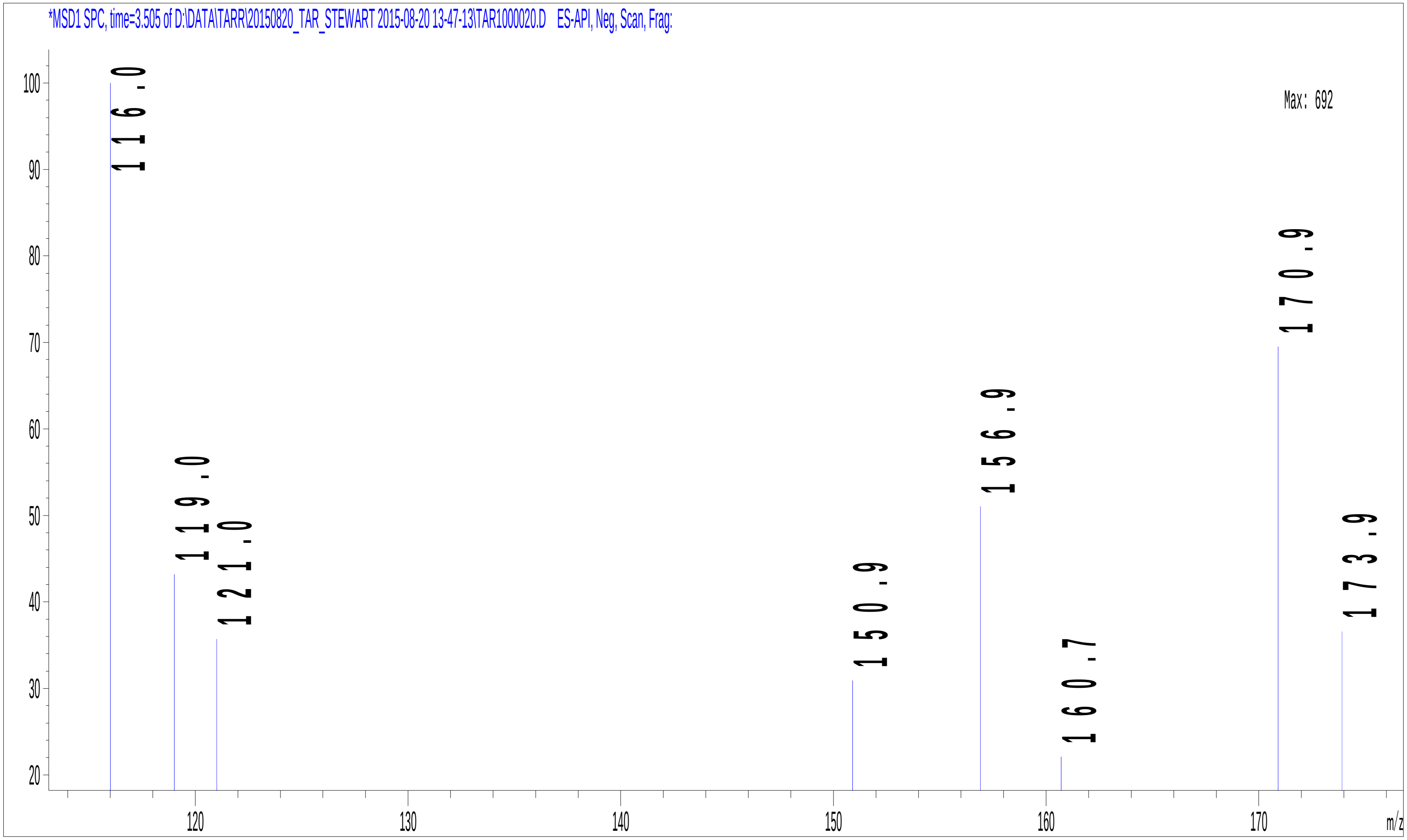
P2-C-02

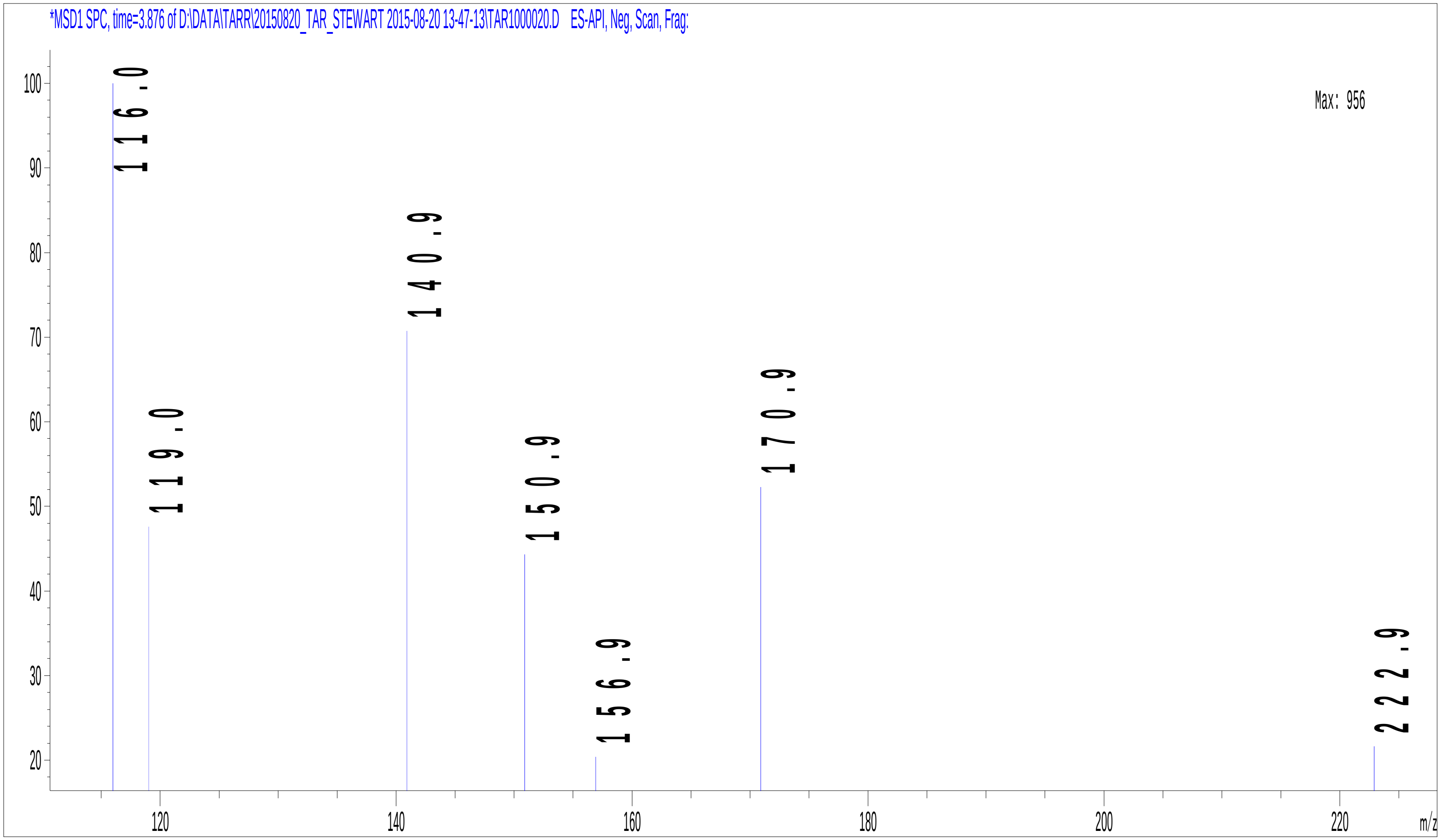


#	Time	Area	Height	Width	Area%	Symmetry
1	2.962	318176	28852	0.1489	85.607	0.924
2	3.526	15158.3	1162	0.1623	4.078	1.341
3	3.834	38334.2	2126.3	0.2356	10.314	0.416


MSD1 TIC, MS File (D:\DATA\TARR\20150820_TAR\TAR1000020.D) ES-API, Neg, Scan, Frag: 70
MSD1 TIC, MS File (D:\DATA\TARR\20150820_TAR\TAR1000035.D) ES-API, Neg, Scan, Frag: 70
Norm.
30000
25000
20000
15000
10000
5000
0
1
2
3
4
5
6
7
min


*MSD1 SPC, time=2.966 of D:\DATA\TARR\20150820_TAR_STEWART 2015-08-20 13-47-13\TAR1000020.D ES-API, Neg, Scan, Frag:
Max: 9544
466.6
468.6
477.6
119.0
154.9
170.9
196.8
210.8
232.8
100
80
60
40
20
0
150
200
250
300
350
400
450
m/z


*MSD1 SPC, time=3.505 of D:\DATA\TARR\20150820_TAR_STEWART 2015-08-20 13-47-13\TAR1000020.D ES-API, Neg, Scan, Frag:
Max: 692
116.0
119.0
121.0
150.9
156.9
160.7
170.9
173.9
100
90
80
70
60
50
40
30
20
120
130
140
150
160
170
m/z

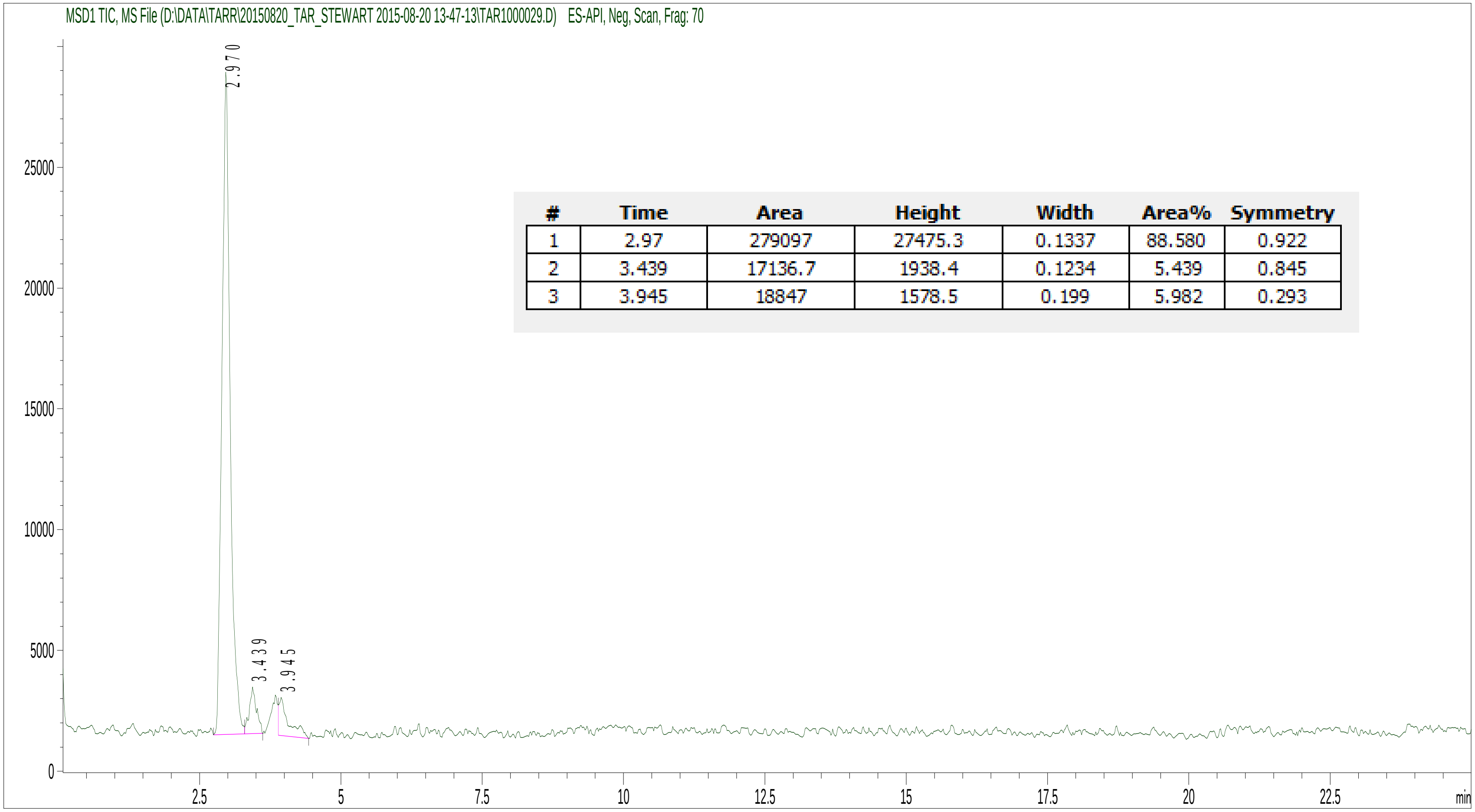

*MSD1 SPC, time=3.876 of D:\DATA\TARR\20150820_TAR_STEWART 2015-08-20 13-47-13\TAR1000020.D ES-API, Neg, Scan, Frag:
Max: 956
116.0
119.0
140.9
150.9
156.9
170.9
222.9
100
90
80
70
60
50
40
30
20
120
140
160
180
200
220
m/z

7-Aug-15

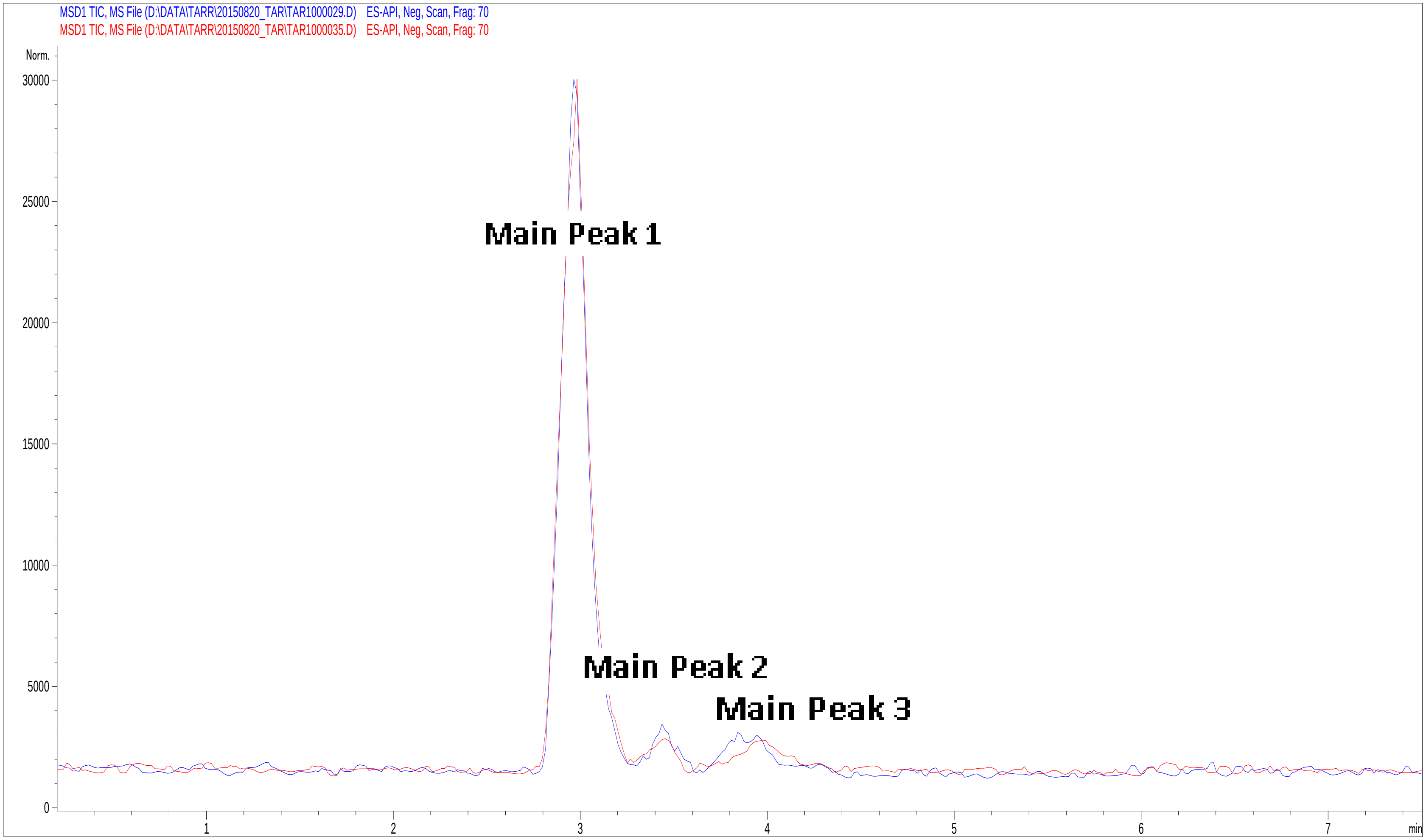
10 DC

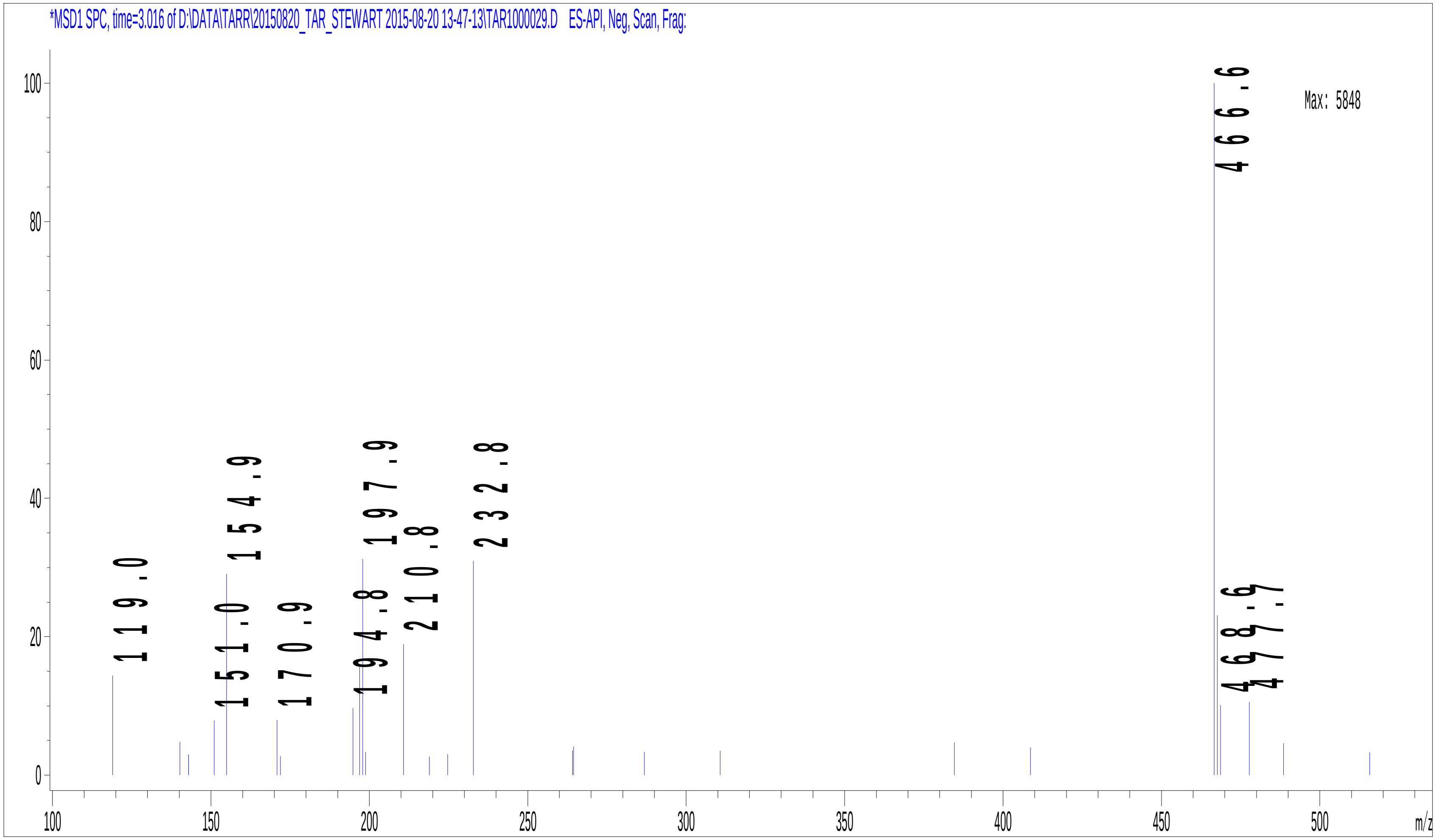
6

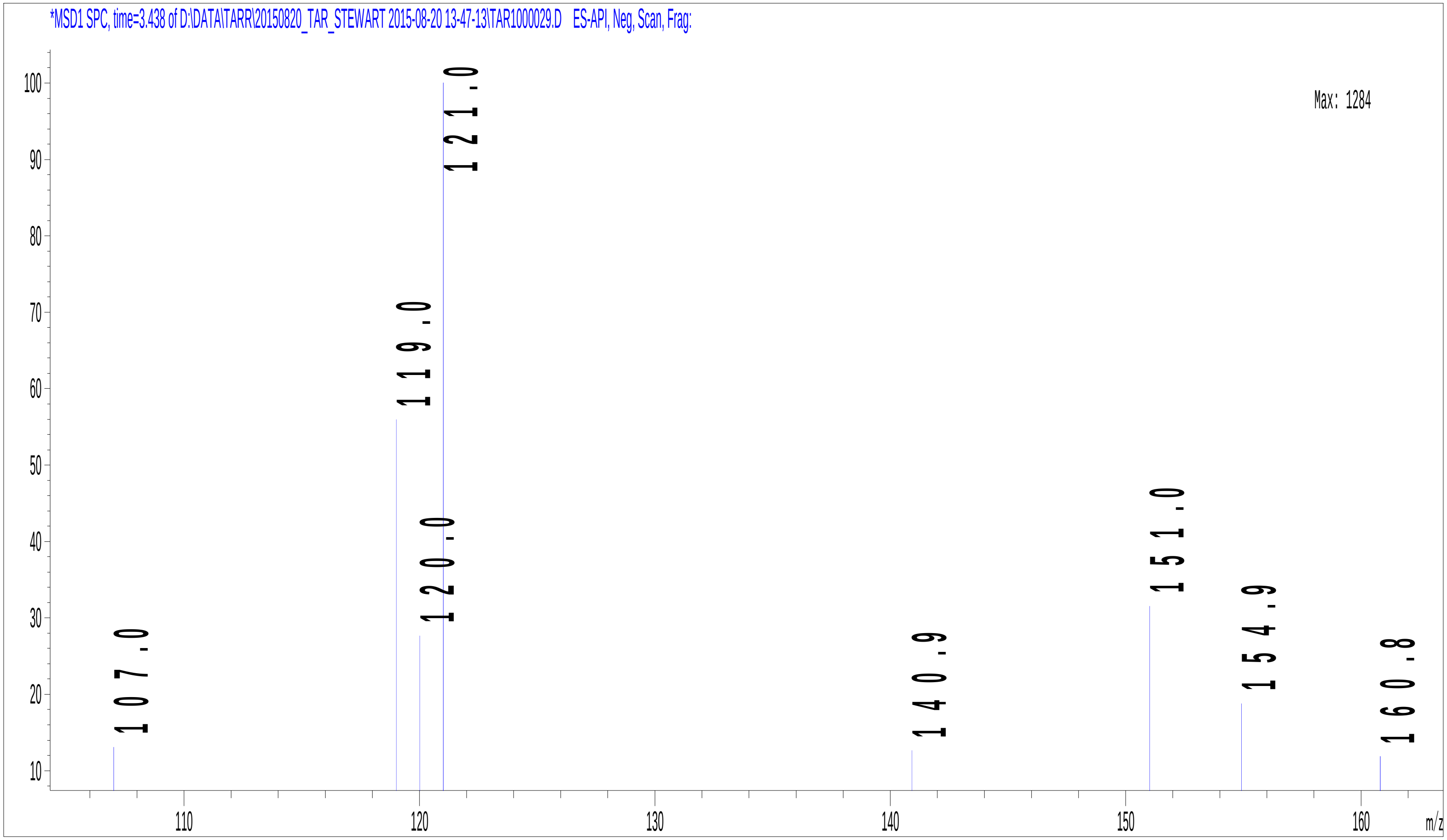
P2-D-08

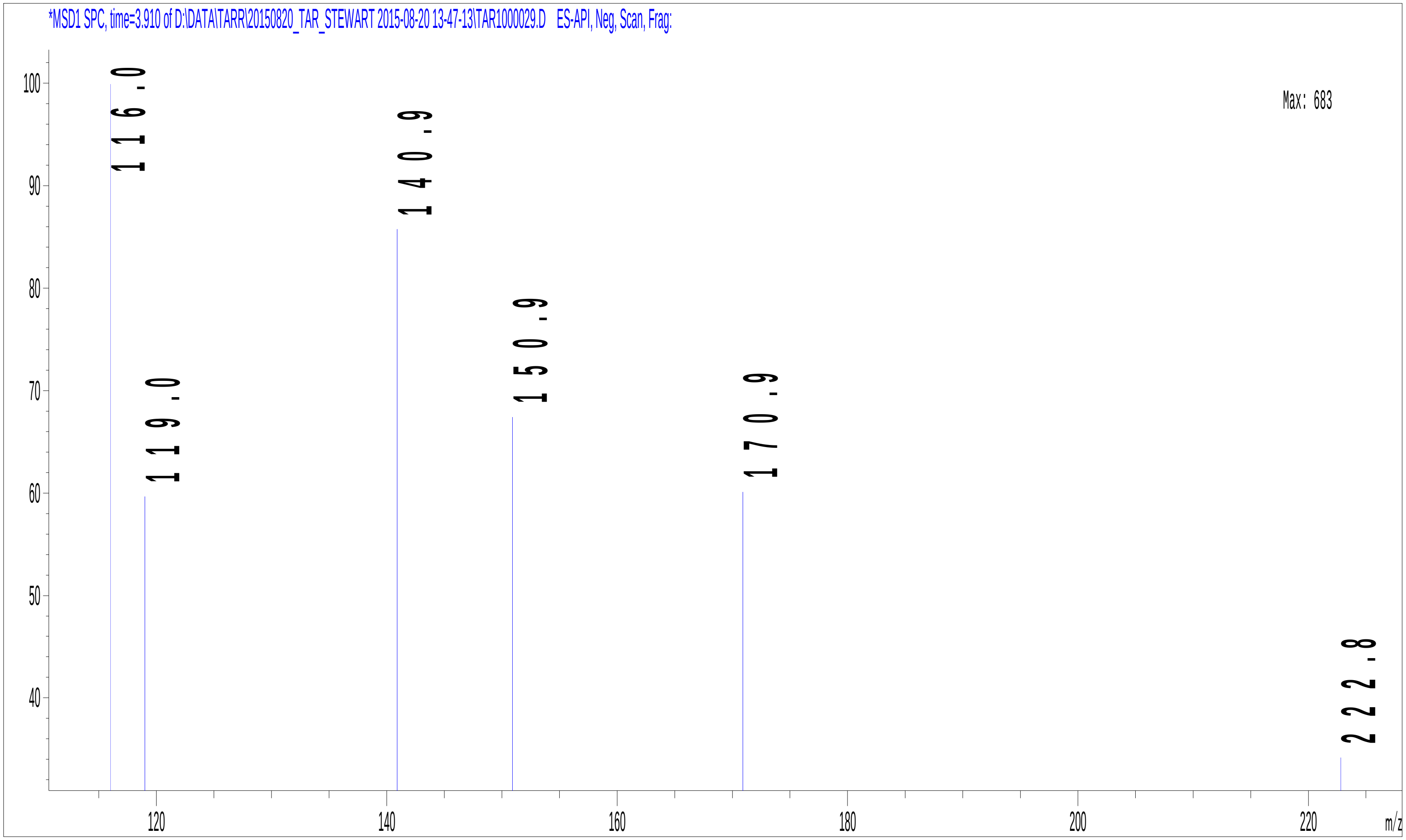


#	Time	Area	Height	Width	Area%	Symmetry
1	2.97	279097	27475.3	0.1337	88.580	0.922
2	3.439	17136.7	1938.4	0.1234	5.439	0.845
3	3.945	18847	1578.5	0.199	5.982	0.293


MSD1 TIC, MS File (D:\DATA\TARR\20150820_TAR\TAR1000029.D) ES-API, Neg, Scan, Frag: 70
MSD1 TIC, MS File (D:\DATA\TARR\20150820_TAR\TAR1000035.D) ES-API, Neg, Scan, Frag: 70
Norm.
30000
25000
20000
15000
10000
5000
0
Main Peak 1
Main Peak 2
Main Peak 3
1
2
3
4
5
6
7
min


*MSD1 SPC, time=3.016 of D:\DATA\TARR\20150820_TAR_STEWART 2015-08-20 13-47-13\TAR1000029.D ES-API, Neg, Scan, Frag:
Max: 5848
466.6
468.6
477.7
119.0
151.0
154.9
170.9
194.8
197.9
210.8
232.8
0
20
40
60
80
100
100
150
200
250
300
350
400
450
500
m/z


*MSD1 SPC, time=3.438 of D:\DATA\TARR\20150820_TAR_STEWART 2015-08-20 13-47-13\TAR1000029.D ES-API, Neg, Scan, Frag:
Max: 1284
100
90
80
70
60
50
40
30
20
10
110
120
130
140
150
160
m/z
107.0
119.0
120.0
121.0
140.9
151.0
154.9
160.8

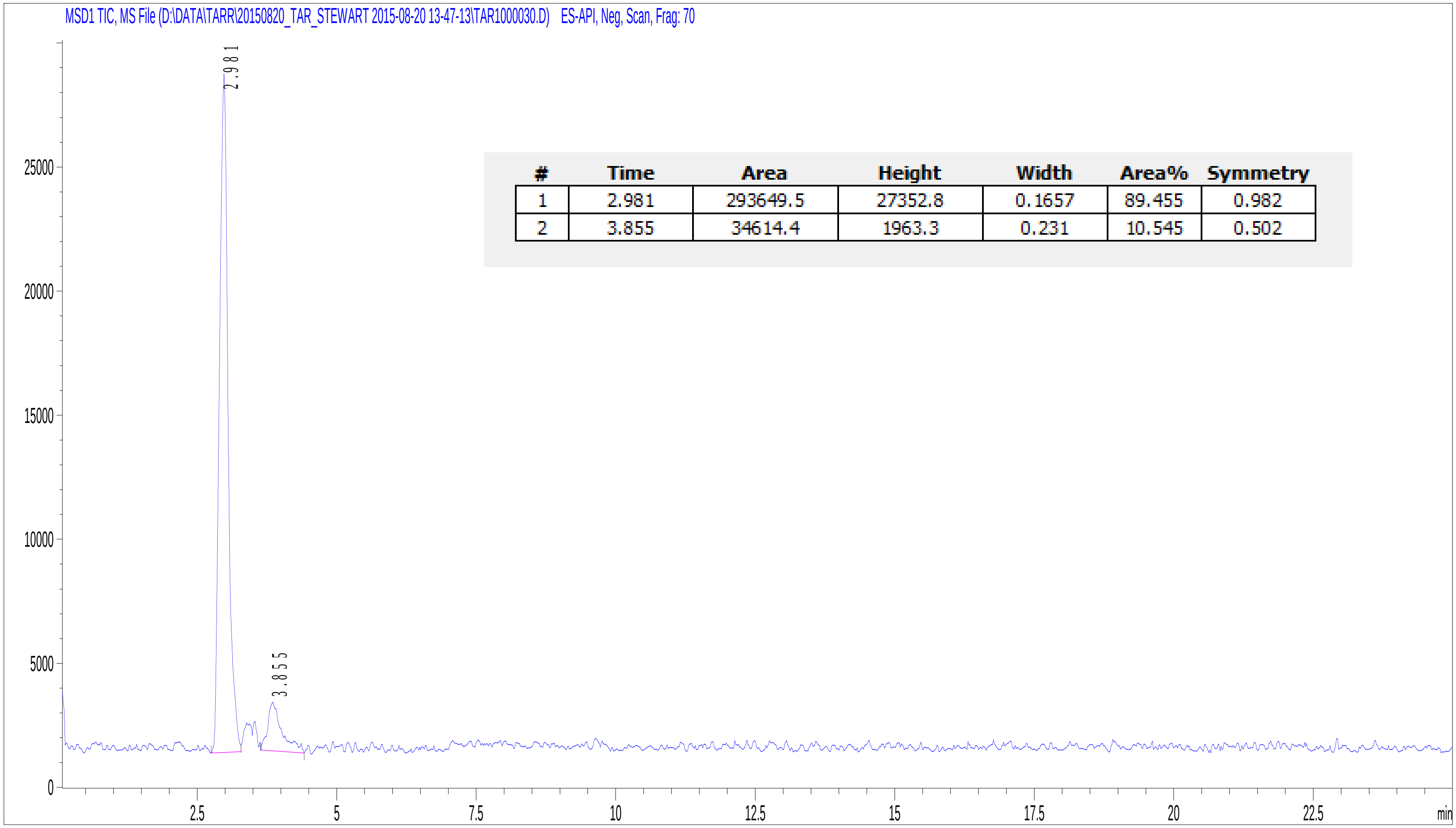

*MSD1 SPC, time=3.910 of D:\DATA\TARR\20150820_TAR_STEWART 2015-08-20 13-47-13\TAR1000029.D ES-API, Neg, Scan, Frag:
Max: 683
116.0
119.0
140.9
150.9
170.9
222.8
100
90
80
70
60
50
40
120
140
160
180
200
220
m/z

31-Jul-15

10 DC Problem (removal went up)

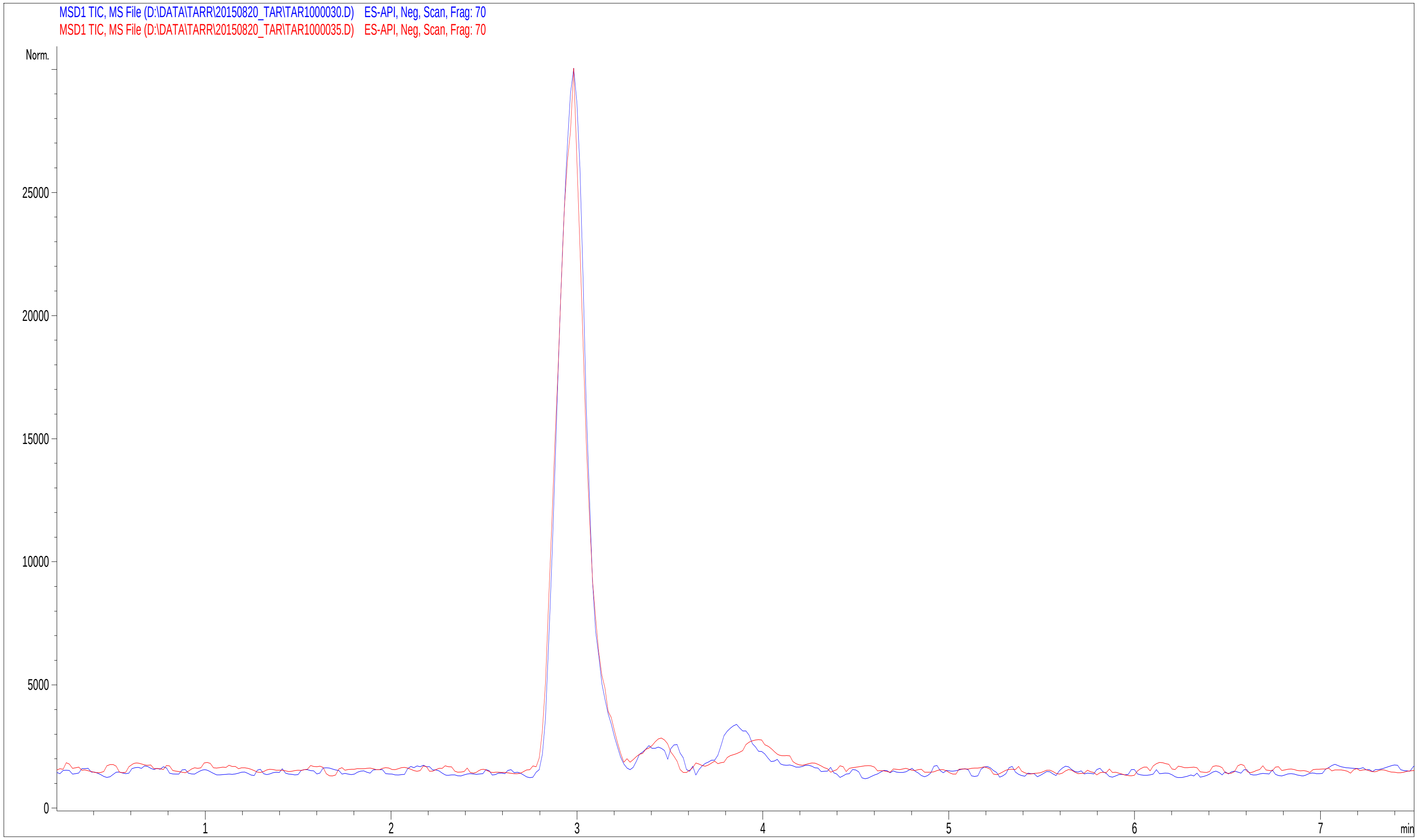
6

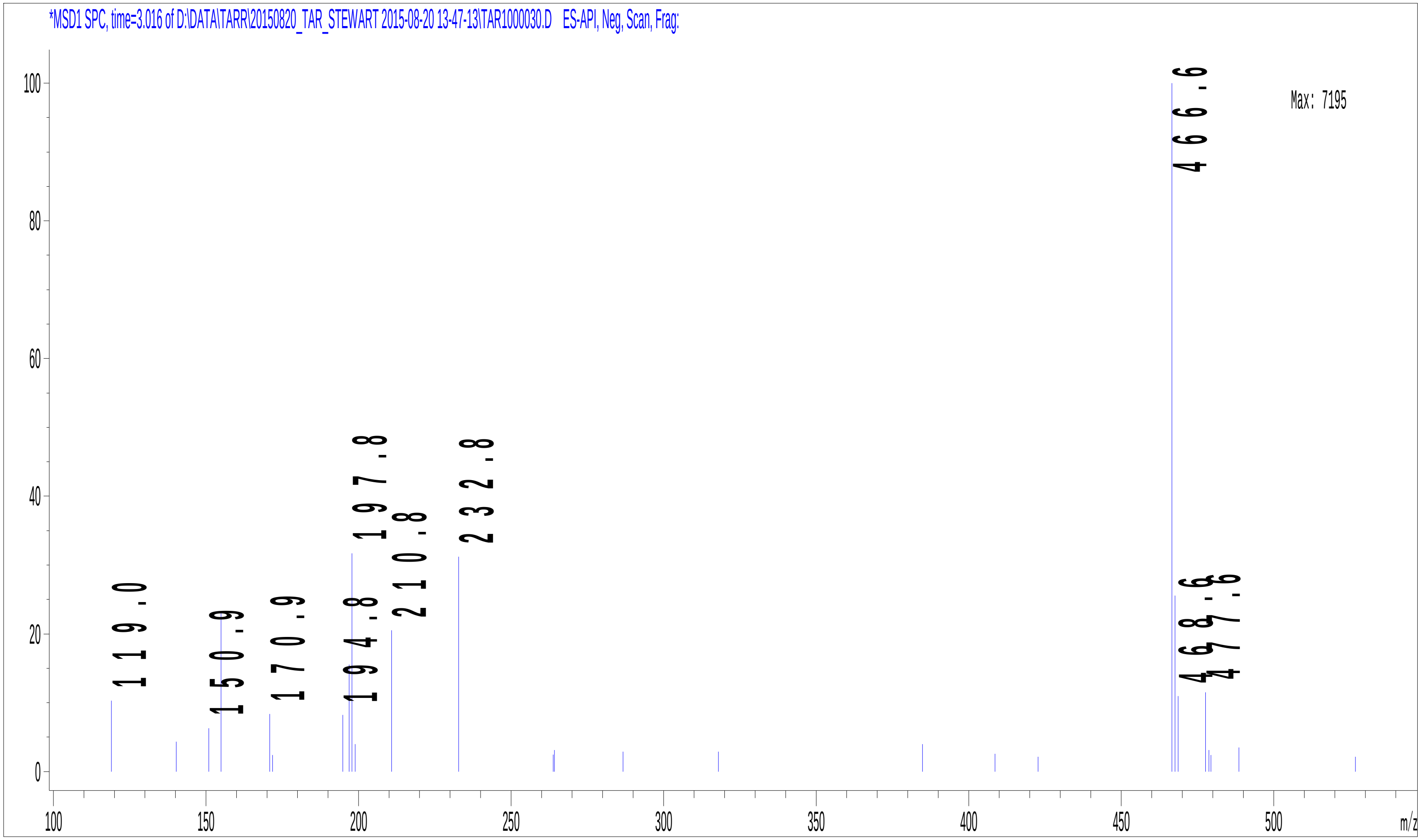
P2-D-07



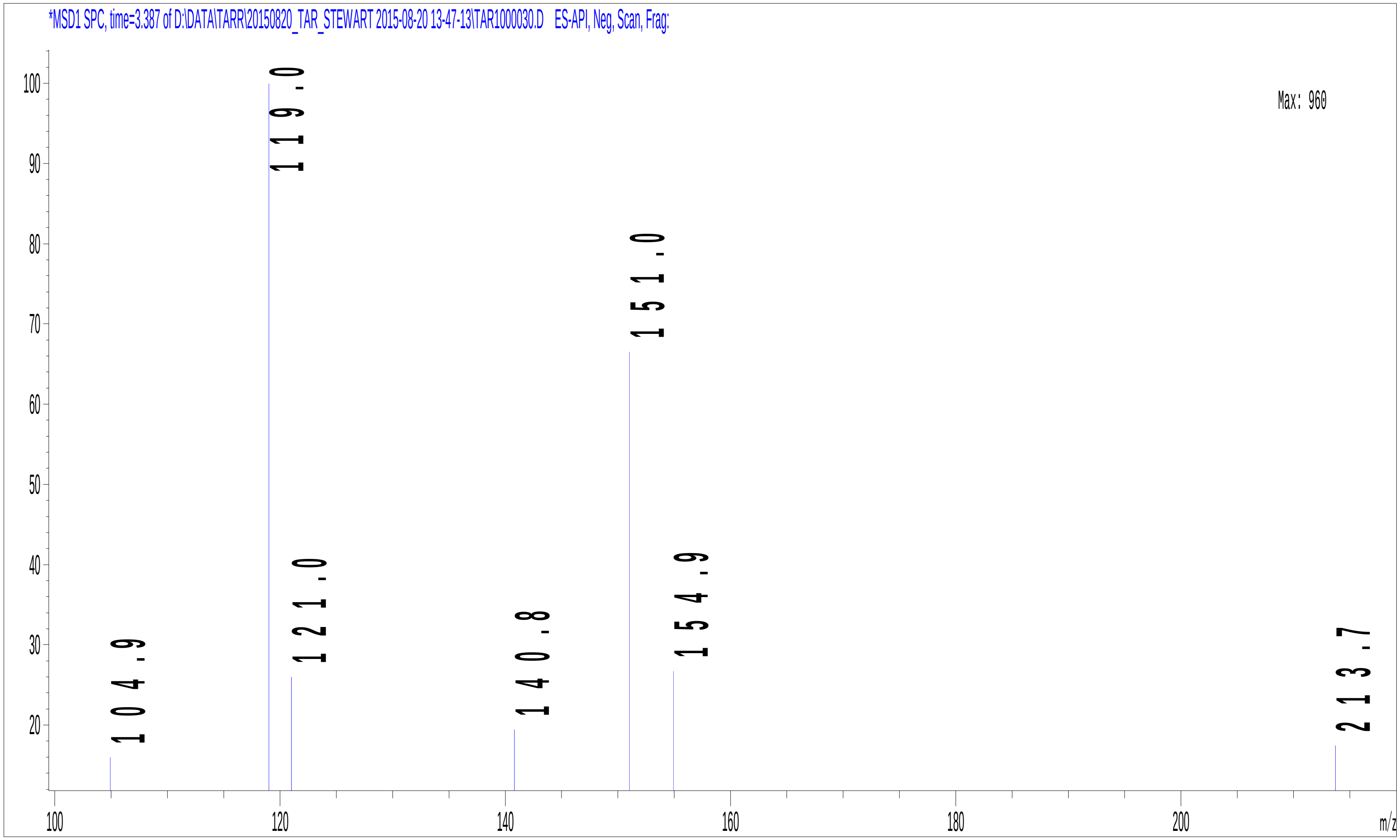
MSD1 TIC, MS File (D:\DATA\TARR\20150820_TAR_STEWART 2015-08-20 13-47-13\TAR1000030.D)   ES-API, Neg, Scan, Frag: 70

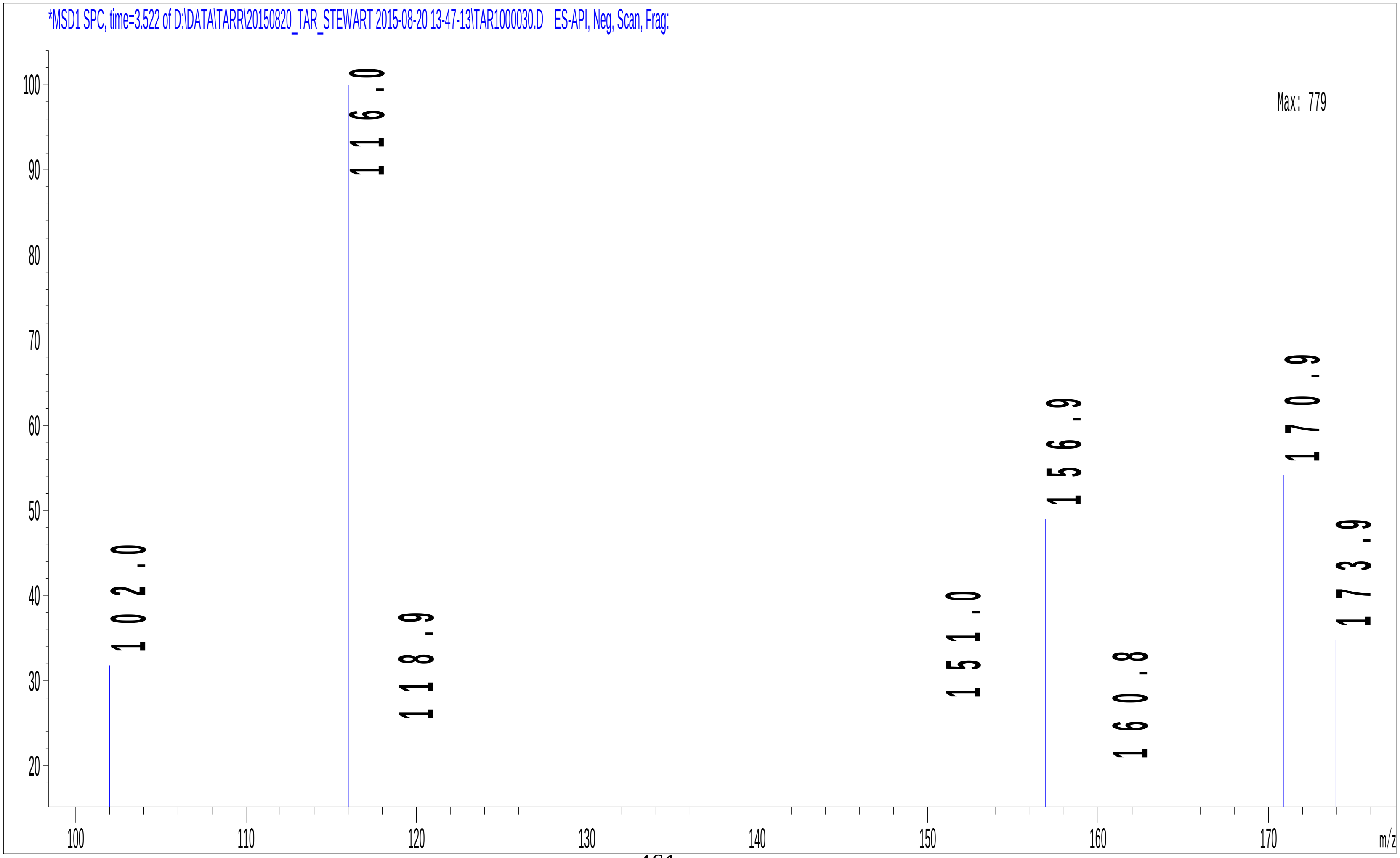
#	Time	Area	Height	Width	Area%	Symmetry
1	2.981	293649.5	27352.8	0.1657	89.455	0.982
2	3.855	34614.4	1963.3	0.231	10.545	0.502

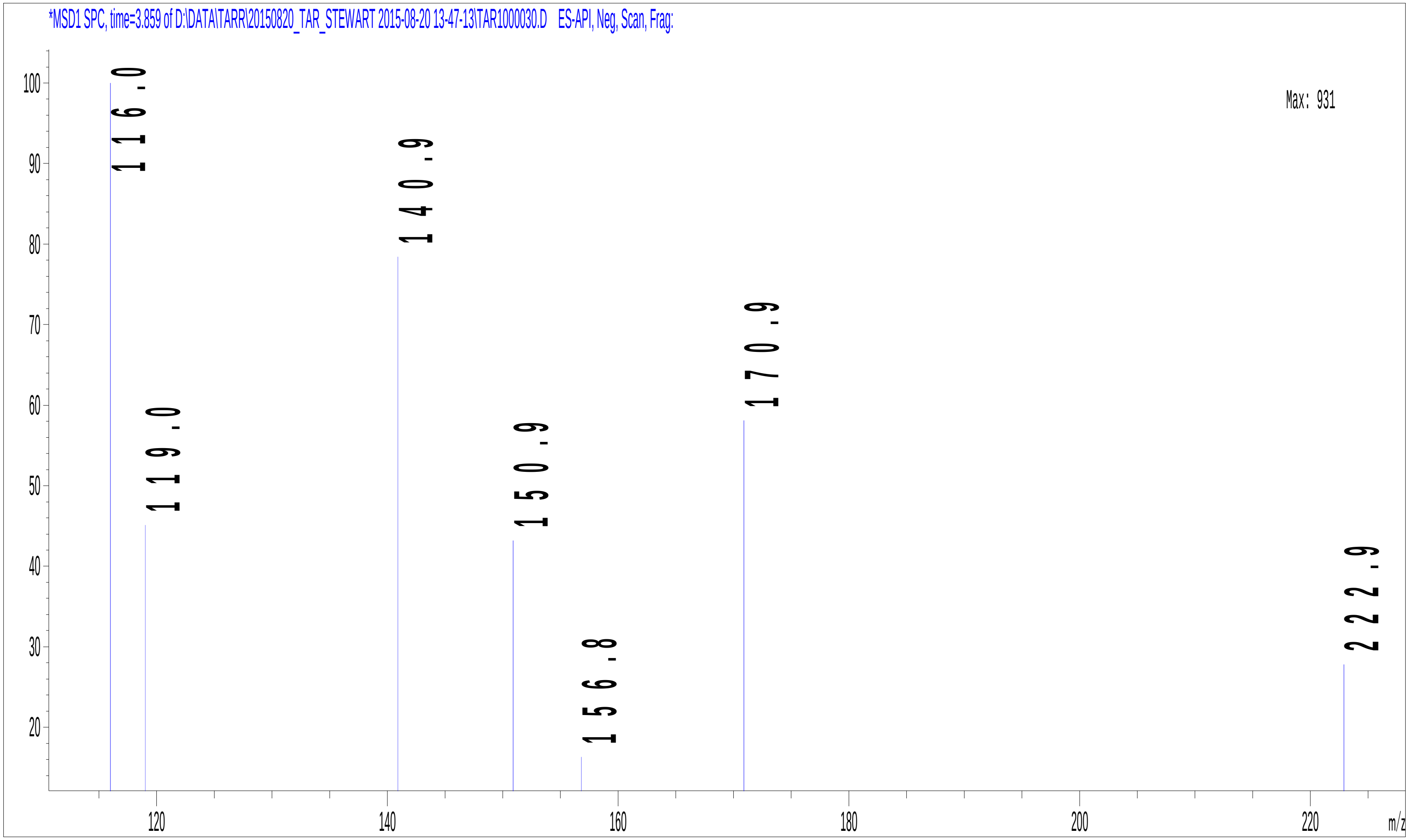

MSD1 TIC, MS File (D:\DATA\TARR\20150820_TAR\TAR1000030.D) ES-API, Neg, Scan, Frag: 70
MSD1 TIC, MS File (D:\DATA\TARR\20150820_TAR\TAR1000035.D) ES-API, Neg, Scan, Frag: 70
Norm.
25000
20000
15000
10000
5000
0
1
2
3
4
5
6
7
min



*MSD1 SPC, time=3.016 of D:\DATA\TARR\20150820_TAR_STEWART 2015-08-20 13-47-13\TAR1000030.D ES-API, Neg, Scan, Frag:
Max: 7195
466.6
468.6
477.6
119.0
150.9
170.9
194.8
197.8
210.8
232.8
100
80
60
40
20
0
100
150
200
250
300
350
400
450
500
m/z


*MSD1 SPC, time=3.387 of D:\DATA\TARR\20150820_TAR_STEWART 2015-08-20 13-47-13\TAR1000030.D ES-API, Neg, Scan, Frag:
Max: 960
100
90
80
70
60
50
40
30
20
100
120
140
160
180
200
m/z
104.9
119.0
121.0
140.8
151.0
154.9
213.7


*MSD1 SPC, time=3.522 of D:\DATA\TARR\20150820_TAR_STEWART 2015-08-20 13-47-13\TAR1000030.D ES-API, Neg, Scan, Frag:
Max: 779
100
90
80
70
60
50
40
30
20
102.0
116.0
118.9
151.0
156.9
160.8
170.9
173.9
100
110
120
130
140
150
160
170
m/z

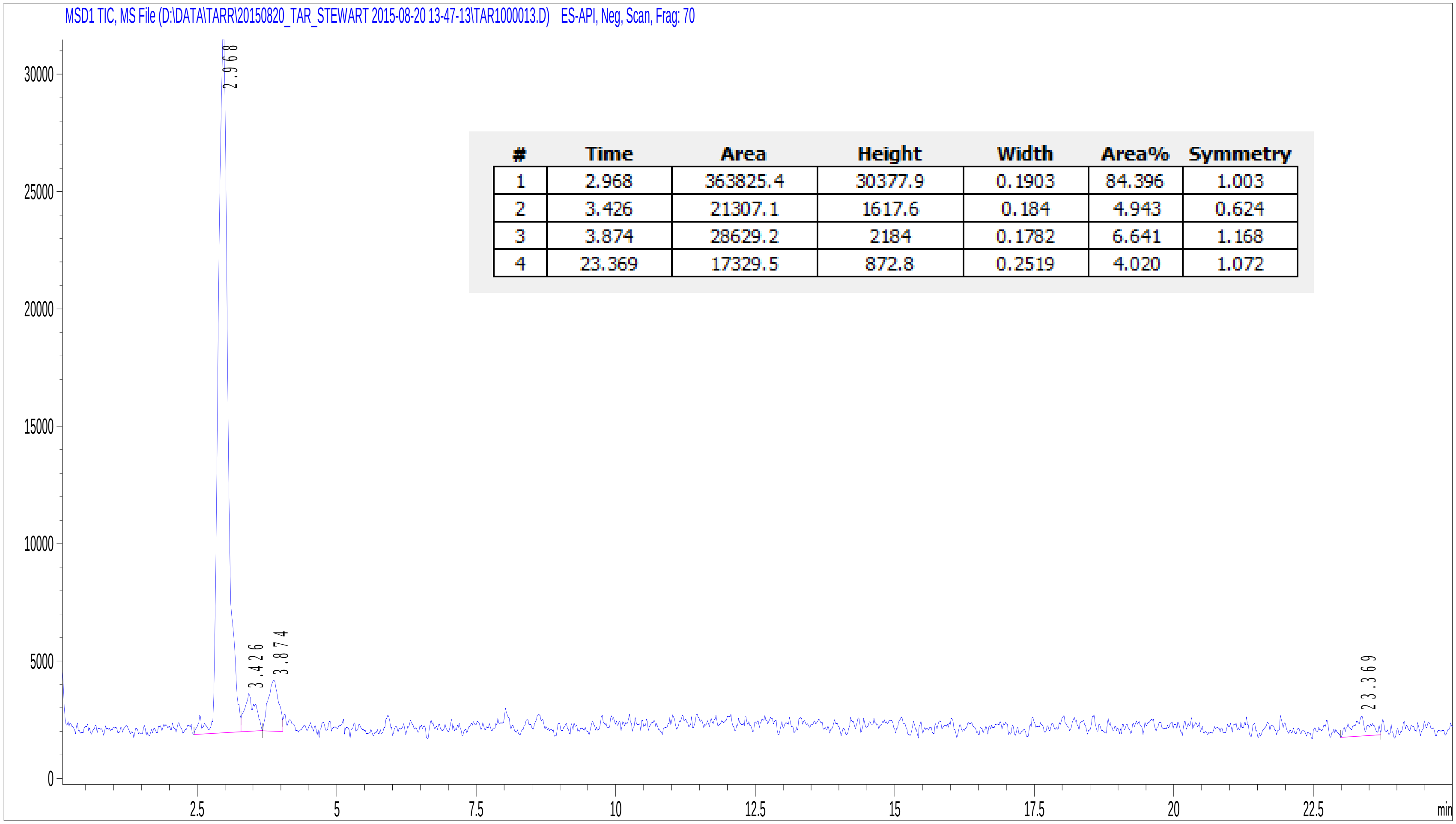

*MSD1 SPC, time=3.859 of D:\DATA\TARR\20150820_TAR_STEWART 2015-08-20 13-47-13\TAR1000030.D ES-API, Neg, Scan, Frag:
Max: 931
116.0
119.0
140.9
150.9
156.8
170.9
222.9
100
90
80
70
60
50
40
30
20
120
140
160
180
200
220
m/z

9-Jun-15

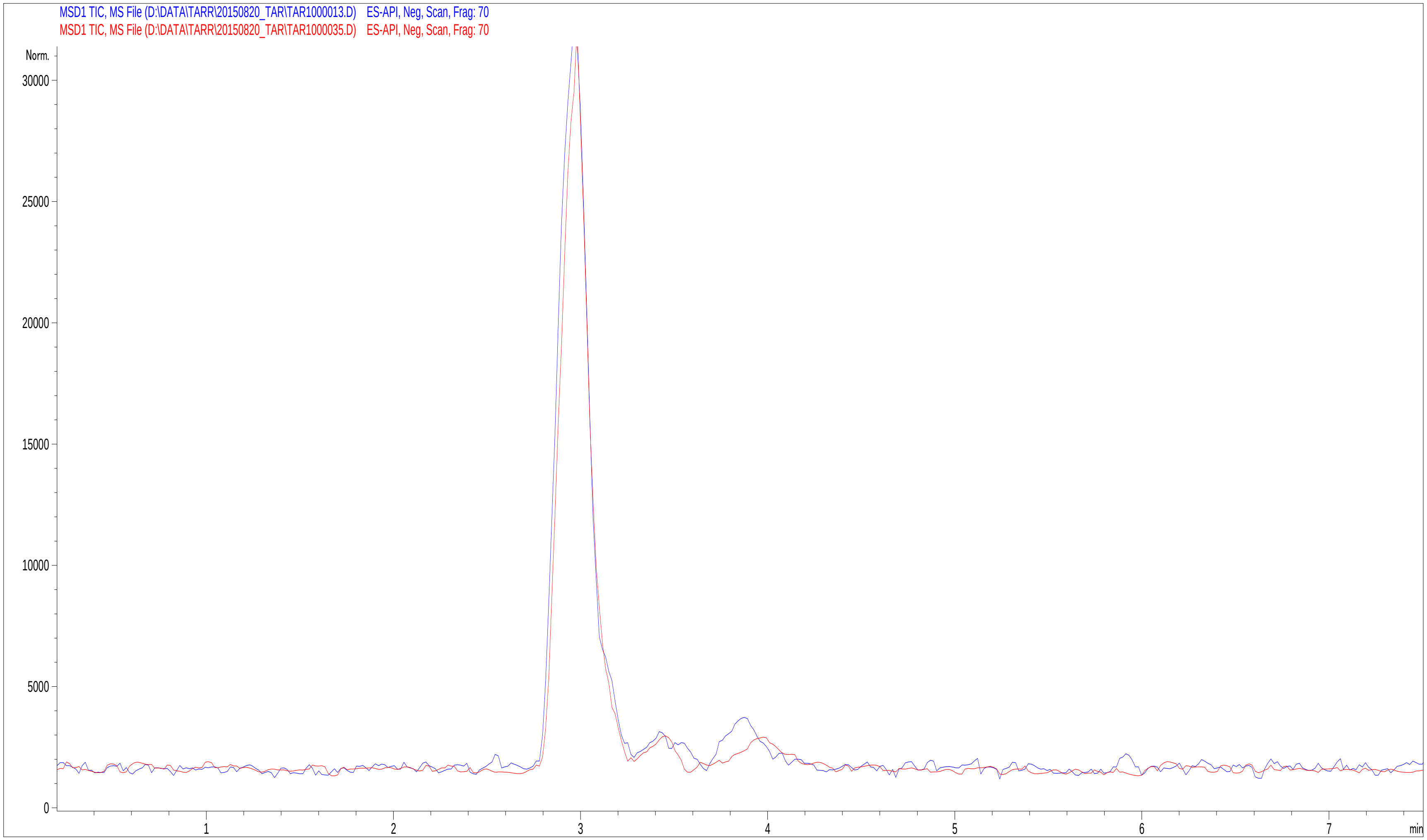
20 DC

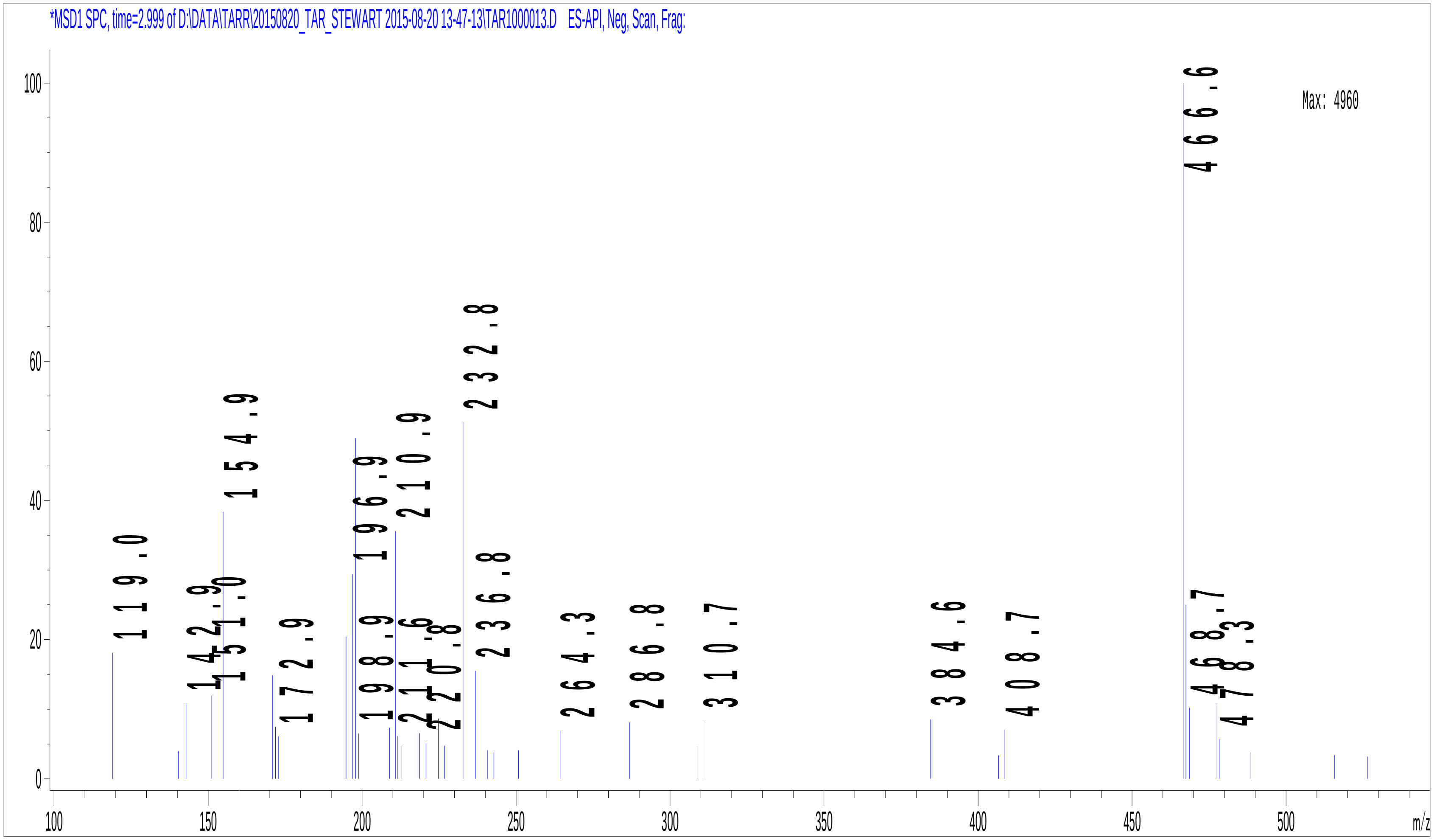
6

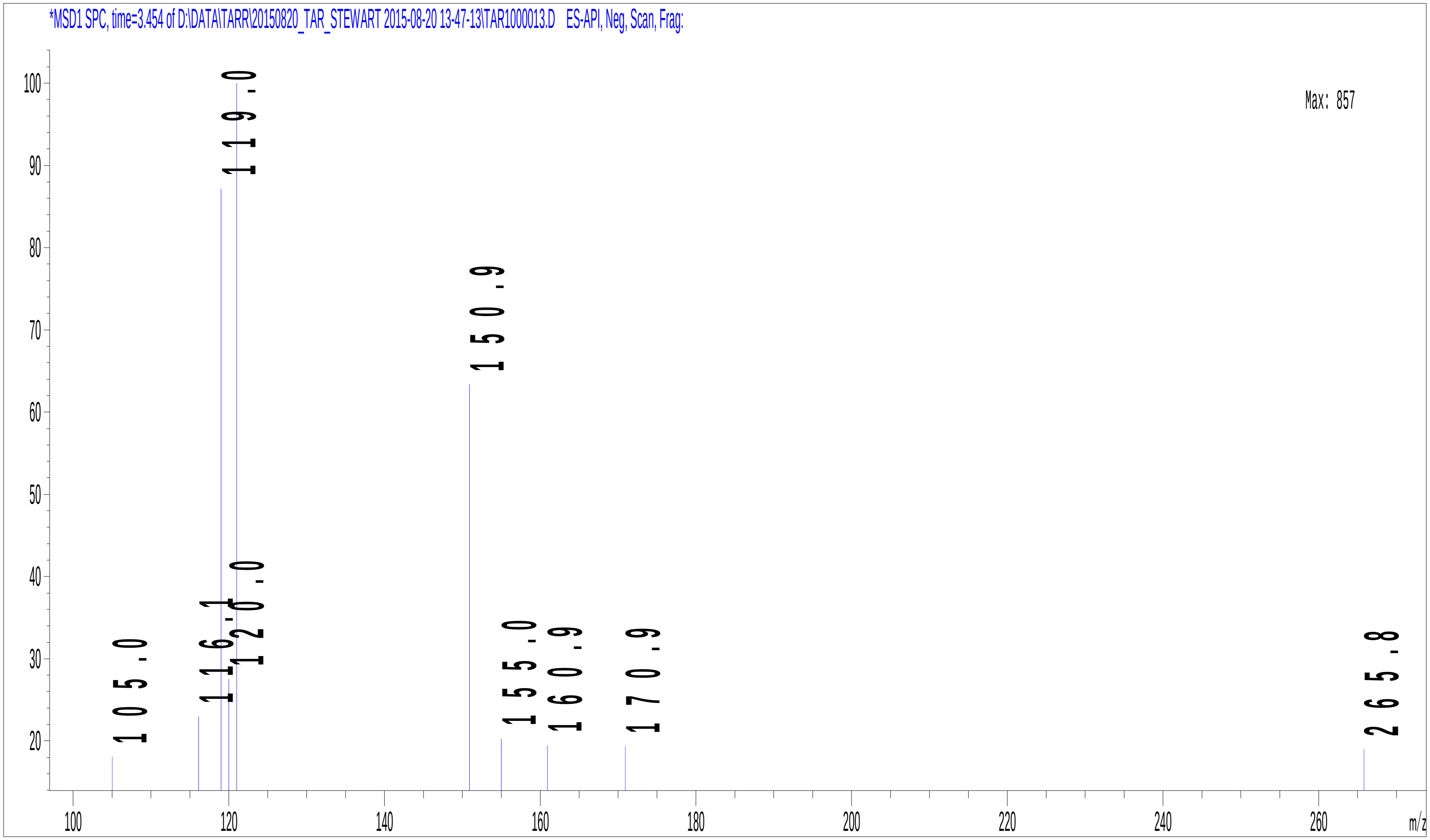
P2-B-06

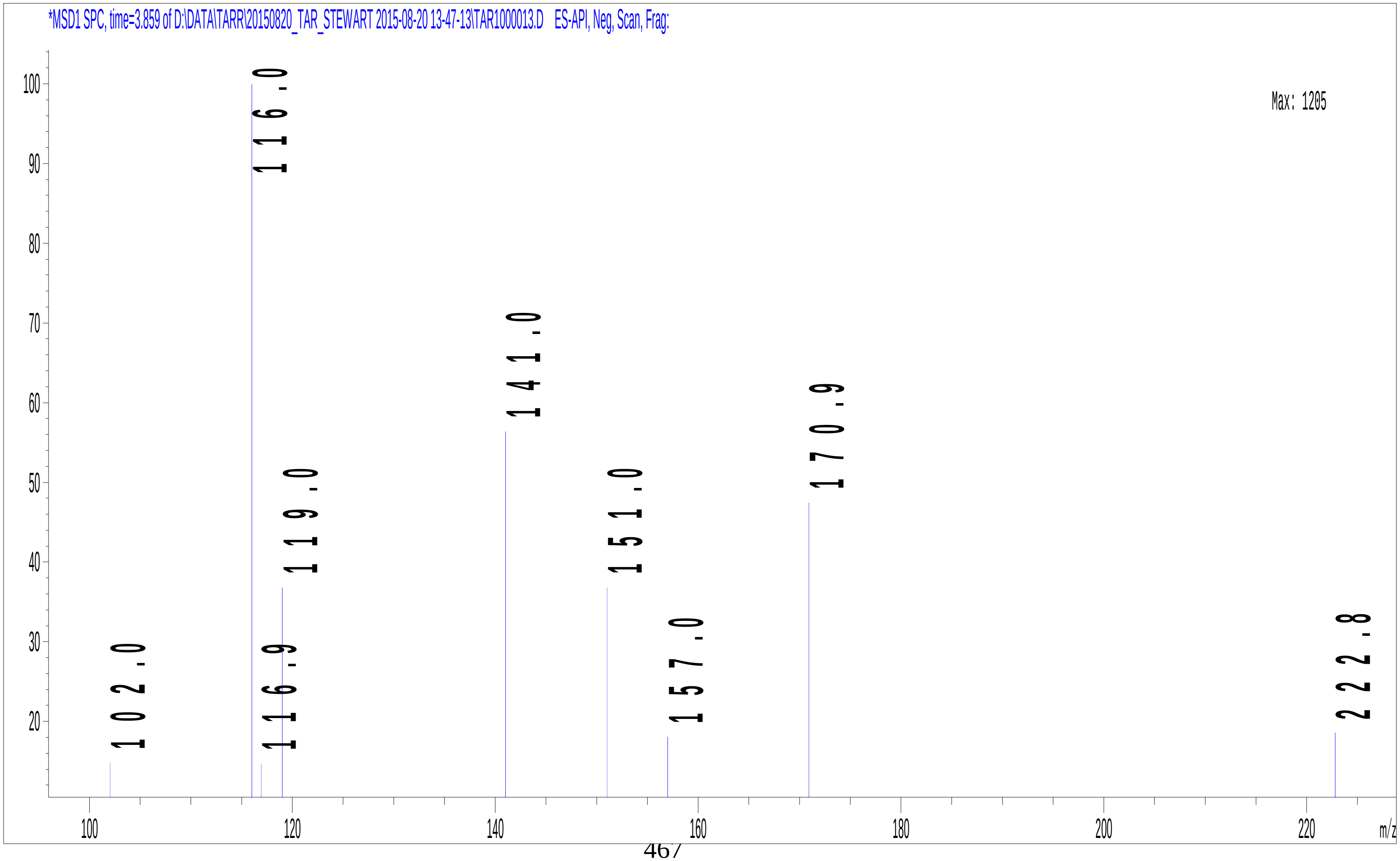


#	Time	Area	Height	Width	Area%	Symmetry
1	2.968	363825.4	30377.9	0.1903	84.396	1.003
2	3.426	21307.1	1617.6	0.184	4.943	0.624
3	3.874	28629.2	2184	0.1782	6.641	1.168
4	23.369	17329.5	872.8	0.2519	4.020	1.072


MSD1 TIC, MS File (D:\DATA\TARR\20150820_TAR\TAR1000013.D) ES-API, Neg, Scan, Frag: 70
MSD1 TIC, MS File (D:\DATA\TARR\20150820_TAR\TAR1000035.D) ES-API, Neg, Scan, Frag: 70
Norm.
30000
25000
20000
15000
10000
5000
0
1
2
3
4
5
6
7
min


*MSD1 SPC, time=2.999 of D:\DATA\TARR\20150820_TAR_STEWART 2015-08-20 13-47-13\TAR1000013.D ES-API, Neg, Scan, Frag:
Max: 4960
466.6
232.8
154.9
210.9
196.9
119.0
142.9
151.0
172.9
198.9
211.6
220.8
236.8
264.3
286.8
310.7
384.6
408.7
468.7
478.3
0
20
40
60
80
100
100
150
200
250
300
350
400
450
500
m/z


*MSD1 SPC, time=3.454 of D:\DATA\TARR\20150820_TAR_STEWART 2015-08-20 13-47-13\TAR1000013.D ES-API, Neg, Scan, Frag:
Max: 857
119.0
150.9
120.0
116.1
105.0
155.0
160.9
170.9
265.8
100
90
80
70
60
50
40
30
20
100
120
140
160
180
200
220
240
260
m/z

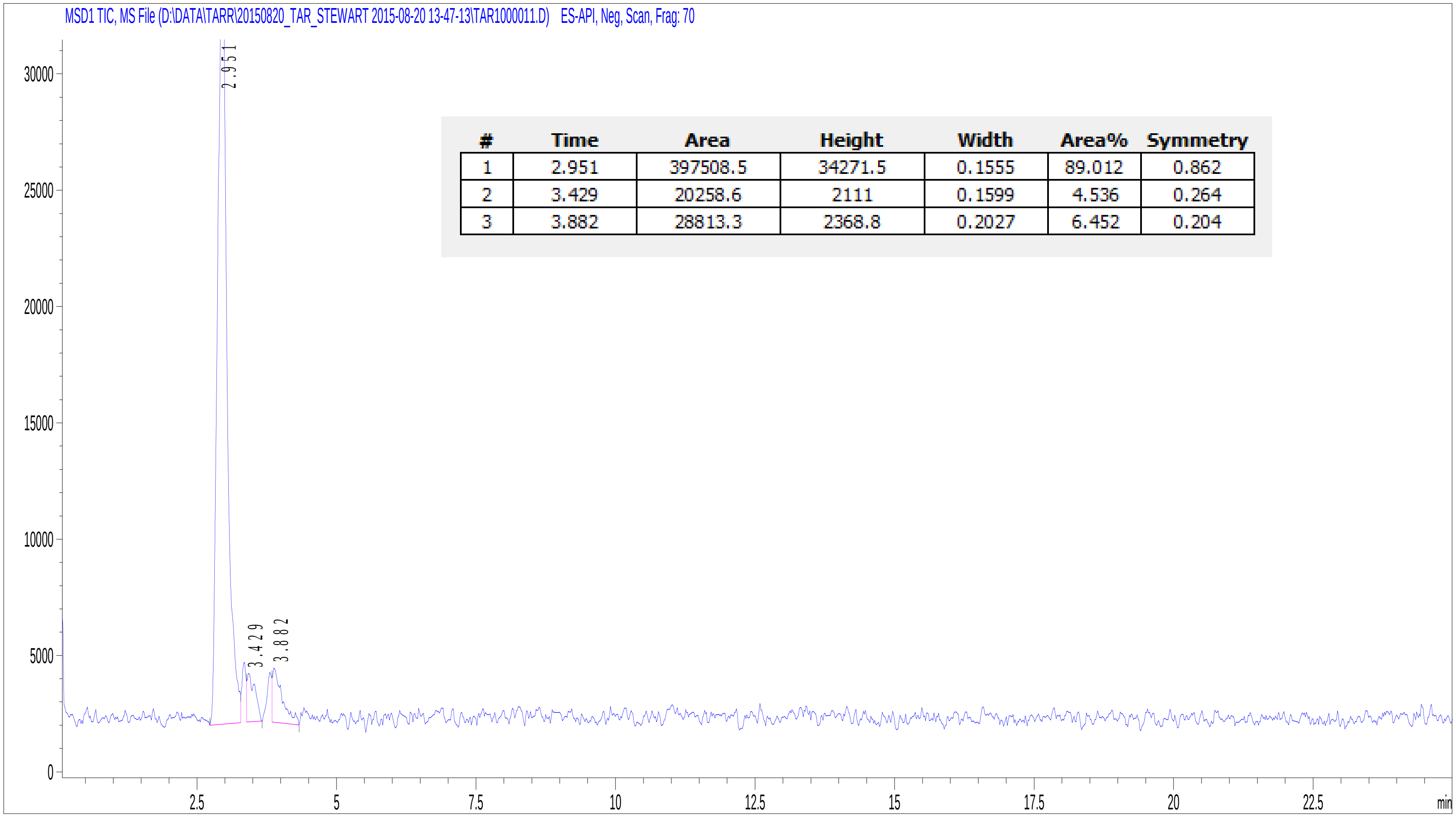

*MSD1 SPC, time=3.859 of D:\DATA\TARR\20150820_TAR_STEWART 2015-08-20 13-47-13\TAR1000013.D ES-API, Neg, Scan, Frag:
Max: 1205
116.0
141.0
170.9
119.0
151.0
102.0
116.9
157.0
222.8
100
90
80
70
60
50
40
30
20
100
120
140
160
180
200
220
m/z

17-Jun-15

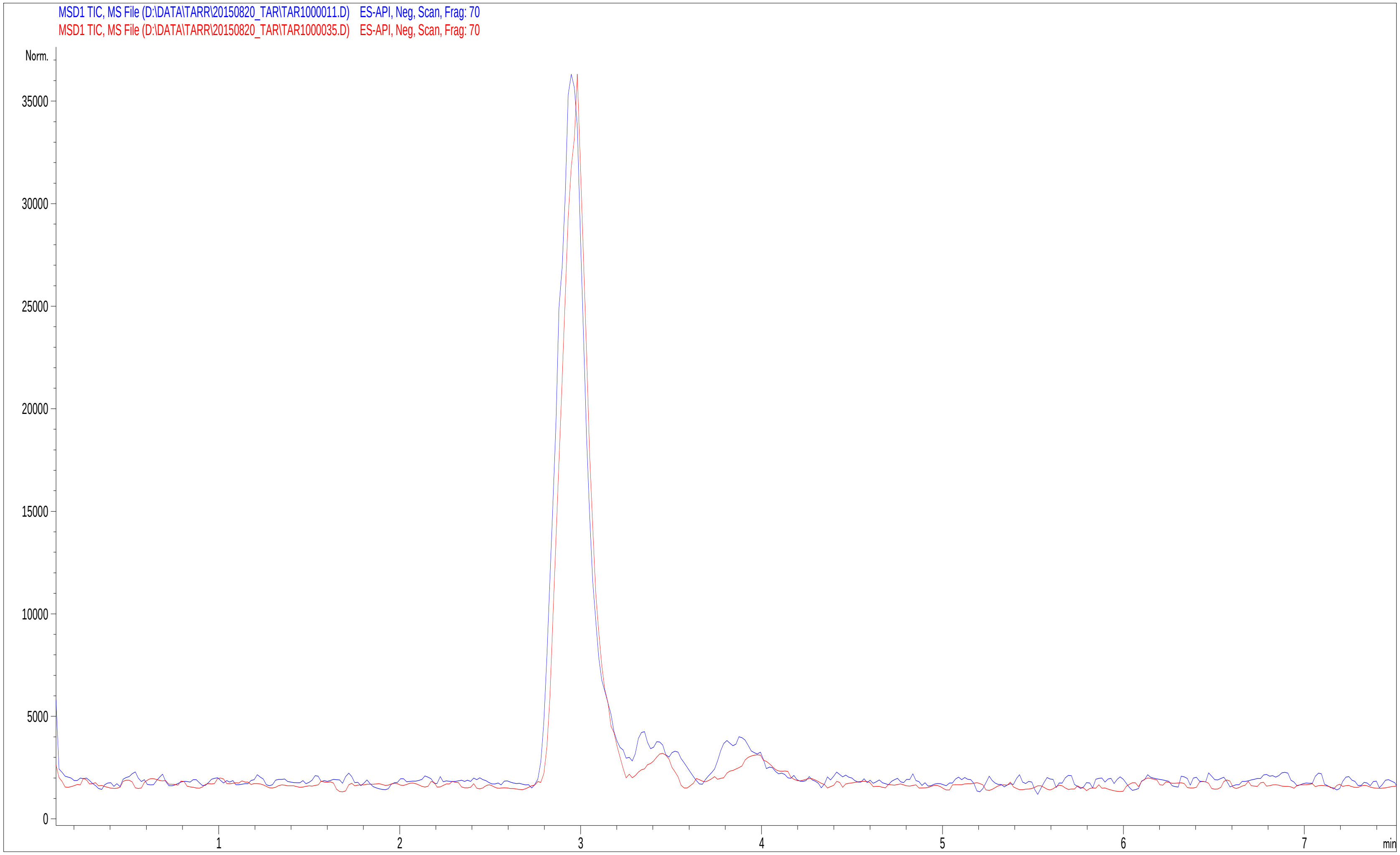
30 DC

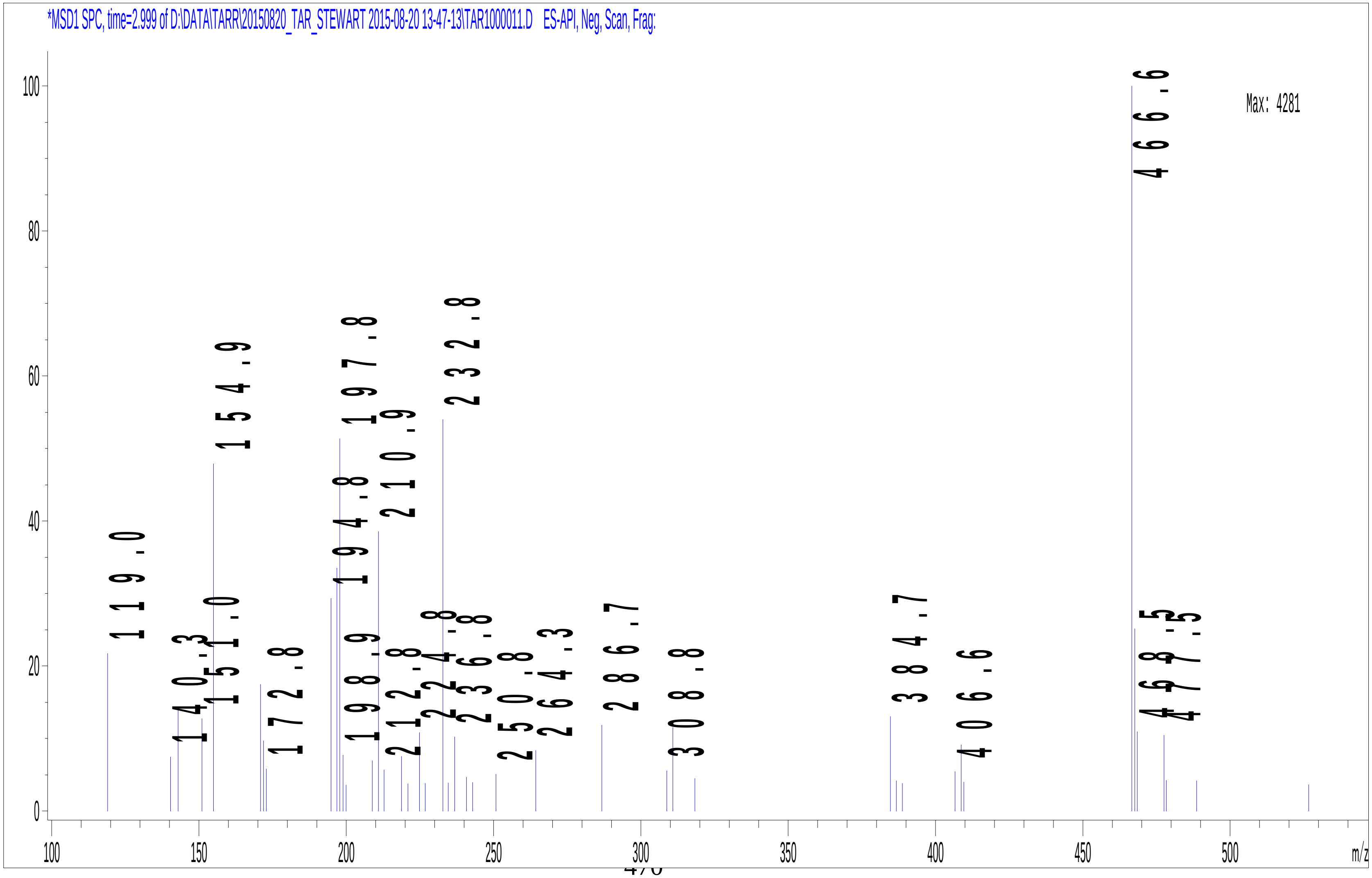
6

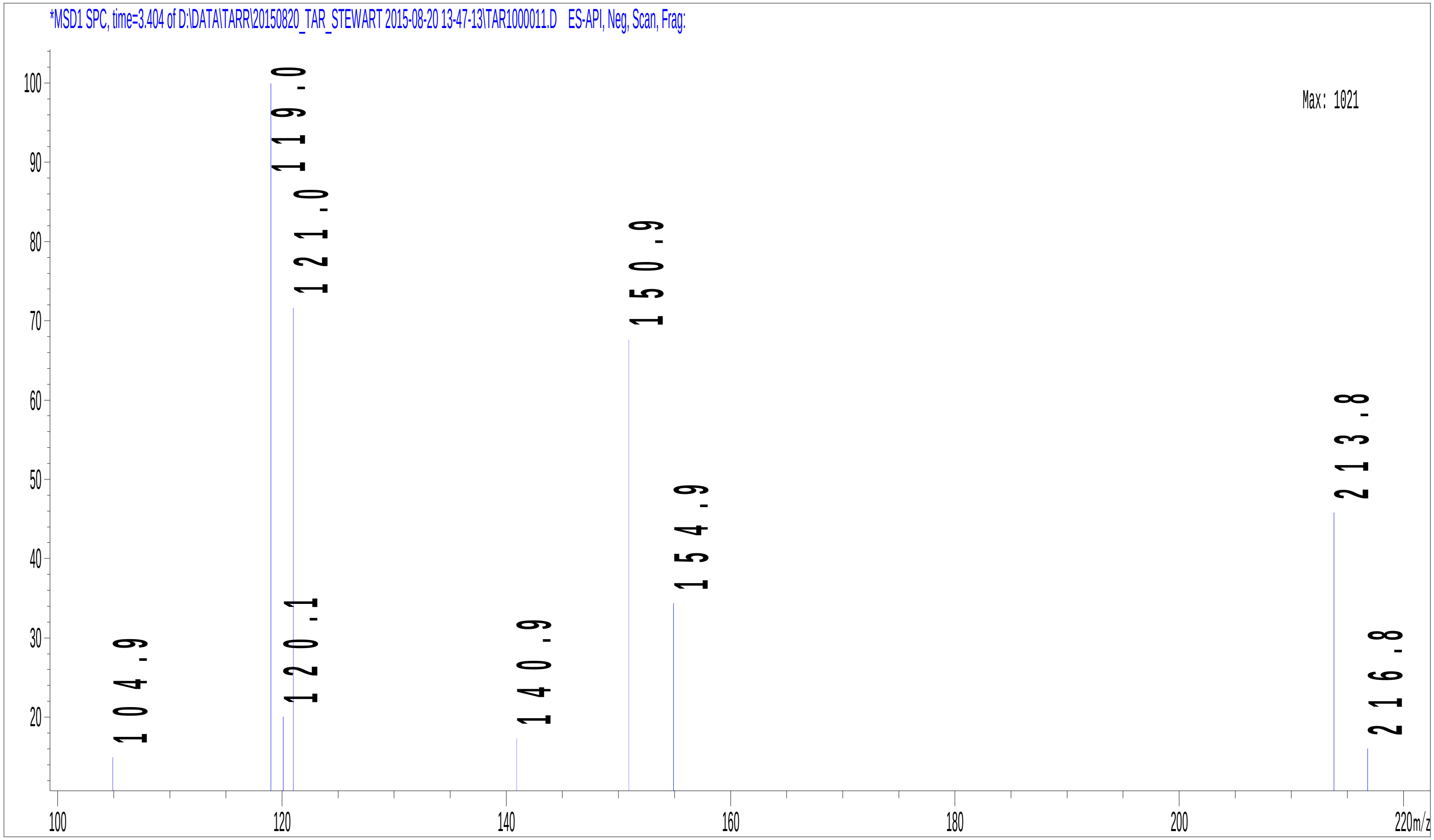
P2-B-08

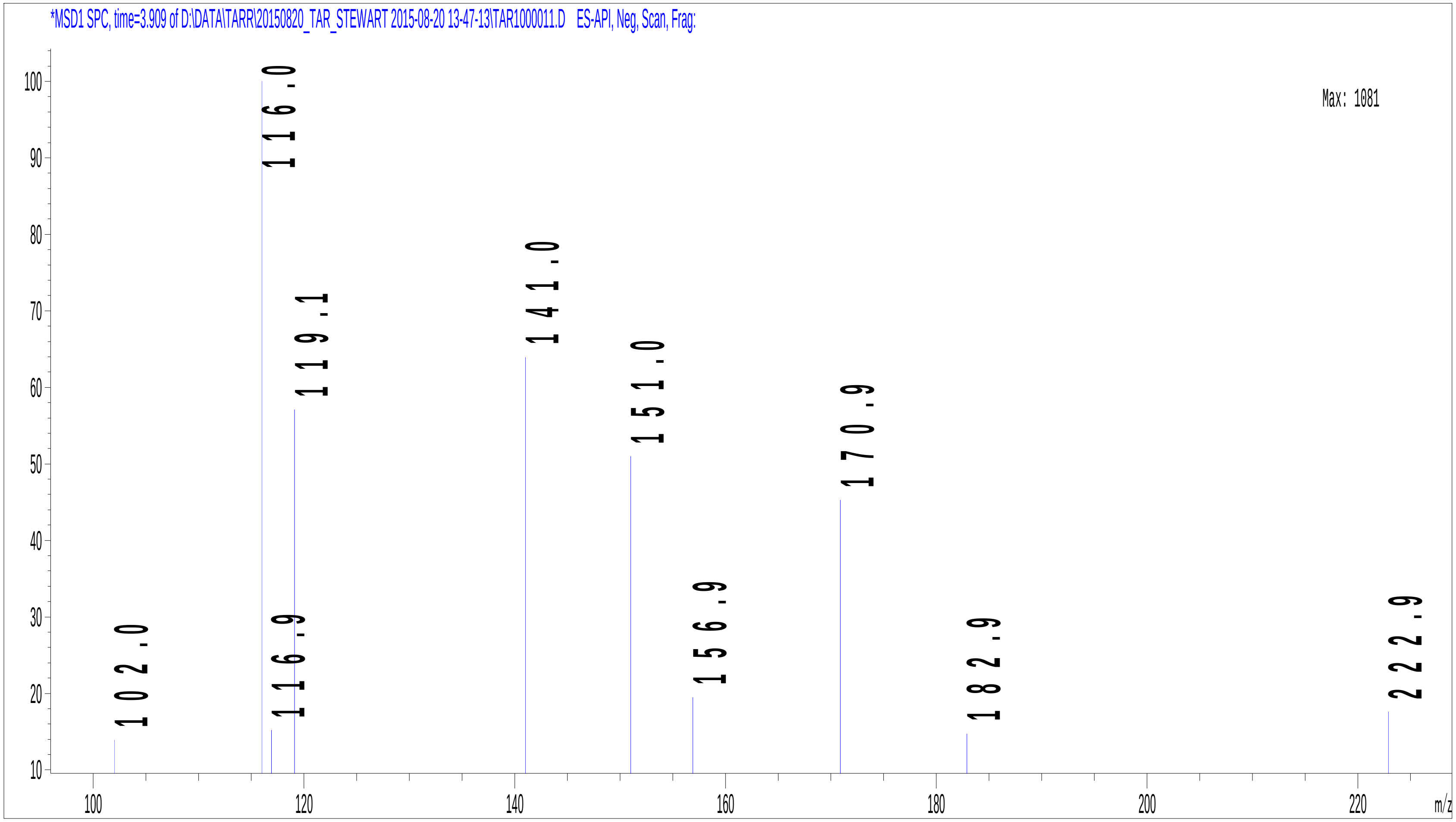


#	Time	Area	Height	Width	Area%	Symmetry
1	2.951	397508.5	34271.5	0.1555	89.012	0.862
2	3.429	20258.6	2111	0.1599	4.536	0.264
3	3.882	28813.3	2368.8	0.2027	6.452	0.204


MSD1 TIC, MS File (D:\DATA\TARR\20150820_TAR\TAR1000011.D) ES-API, Neg, Scan, Frag: 70
MSD1 TIC, MS File (D:\DATA\TARR\20150820_TAR\TAR1000035.D) ES-API, Neg, Scan, Frag: 70
Norm.
35000
30000
25000
20000
15000
10000
5000
0
1
2
3
4
5
6
7
min


*MSD1 SPC, time=2.999 of D:\DATA\TARR\20150820_TAR_STEWART 2015-08-20 13-47-13\TAR1000011.D ES-API, Neg, Scan, Frag:
Max: 4281
100
80
60
40
20
0
100
150
200
250
300
350
400
450
500
m/z
119.0
140.3
151.0
154.9
172.8
194.8
197.8
198.9
210.9
212.8
224.8
236.8
232.8
250.8
264.3
286.7
308.8
384.7
406.6
466.6
468.5
477.5


*MSD1 SPC, time=3.404 of D:\DATA\TARR\20150820_TAR_STEWART 2015-08-20 13-47-13\TAR1000011.D ES-API, Neg, Scan, Frag:
Max: 1021
100
90
80
70
60
50
40
30
20
104.9
119.0
120.1
121.0
140.9
150.9
154.9
213.8
216.8
100
120
140
160
180
200
220
m/z

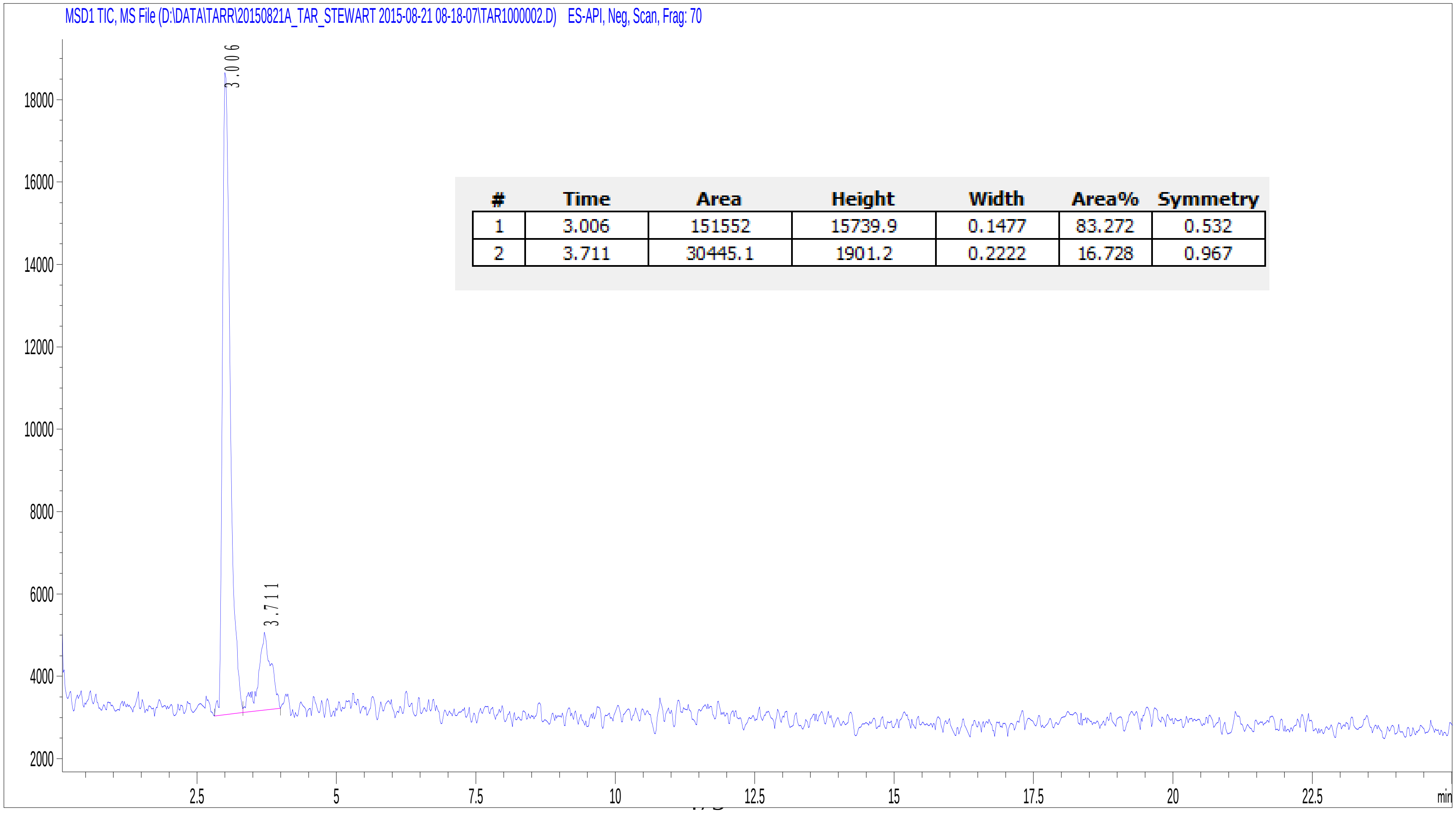

*MSD1 SPC, time=3.909 of D:\DATA\TARR\20150820_TAR_STEWART 2015-08-20 13-47-13\TAR1000011.D ES-API, Neg, Scan, Frag:
Max: 1081
100
90
80
70
60
50
40
30
20
10
102.0
116.0
116.9
119.1
141.0
151.0
156.9
170.9
182.9
222.9
100
120
140
160
180
200
220
m/z

4-Aug-15

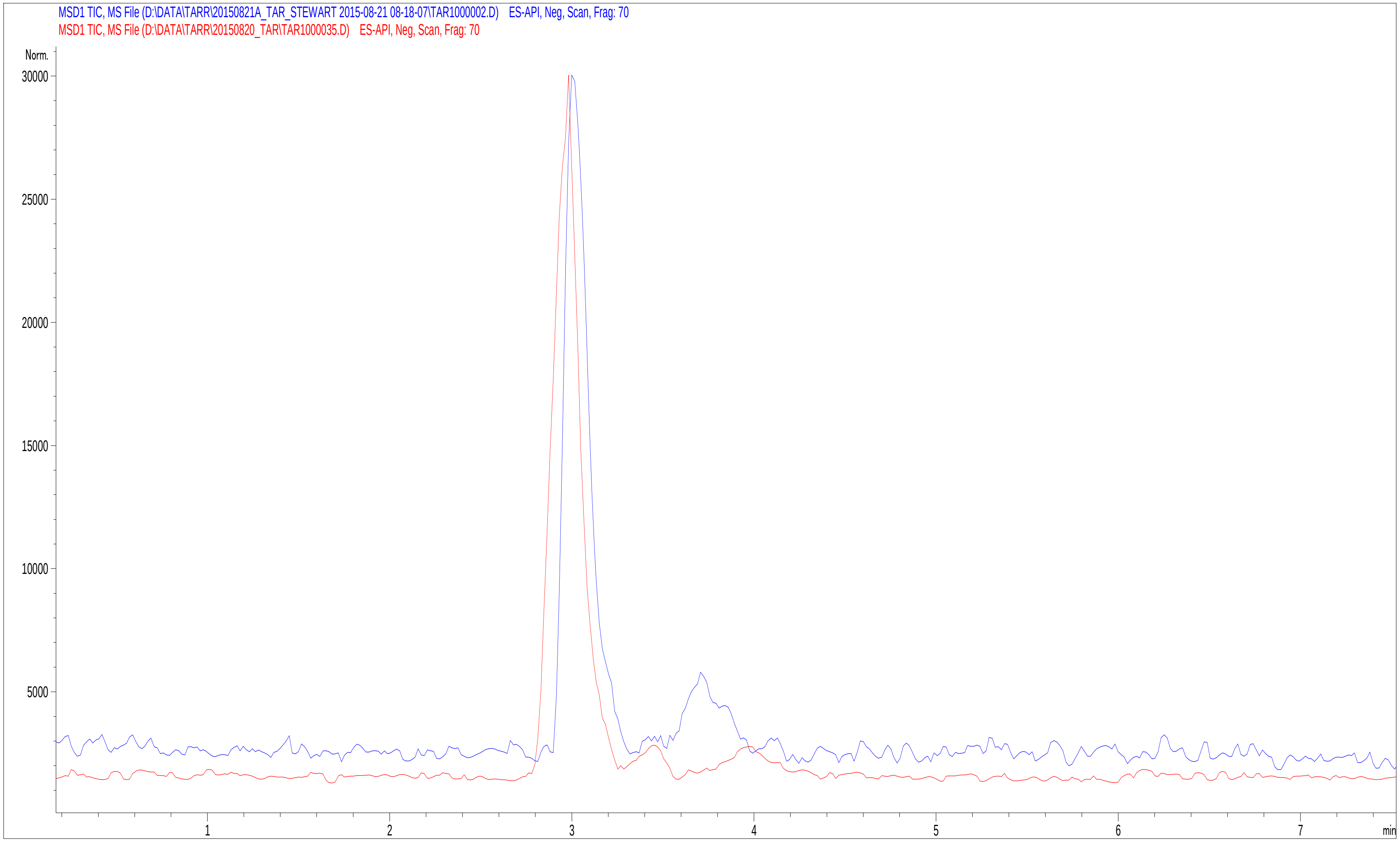
50 DC

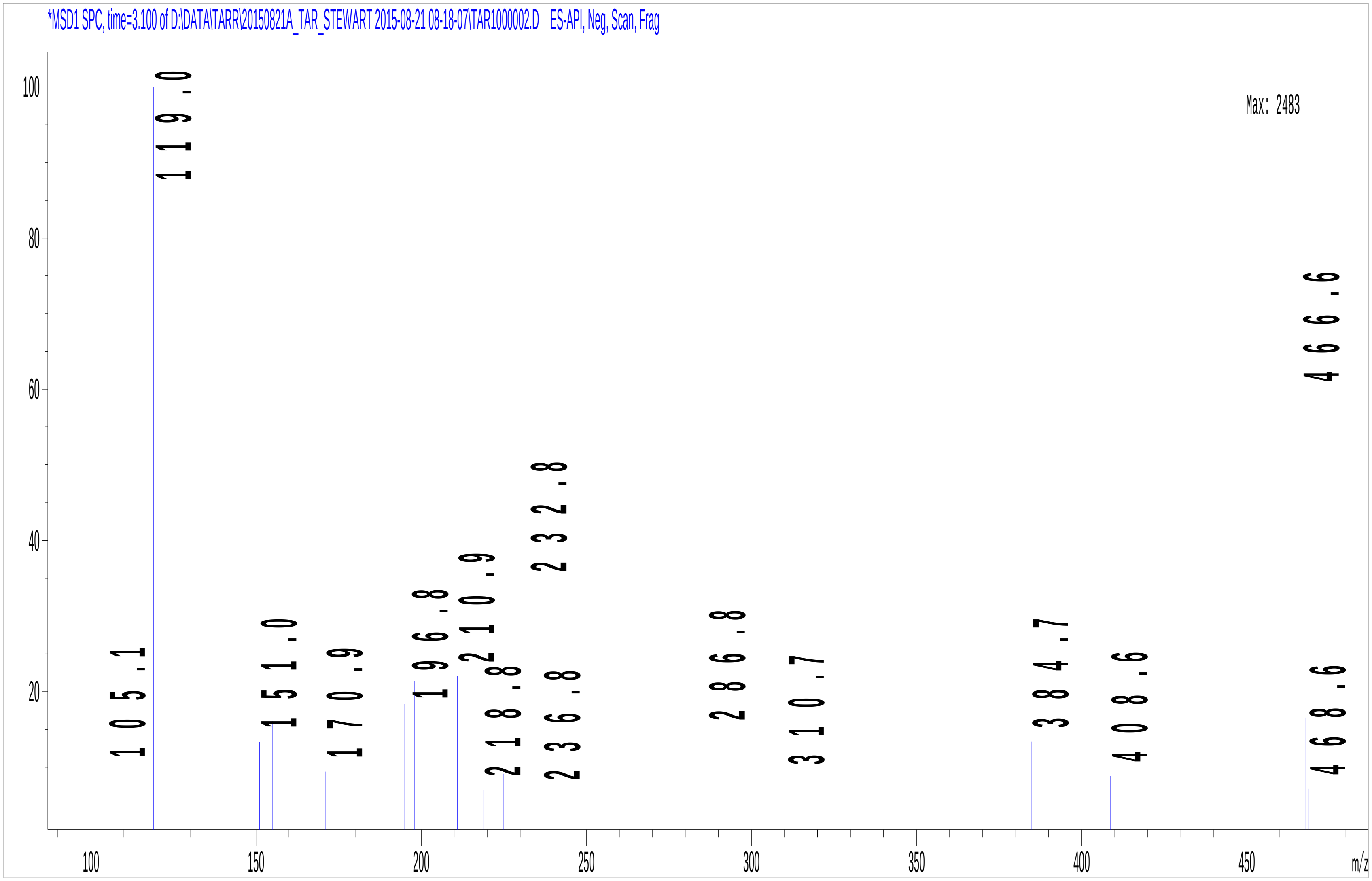
6

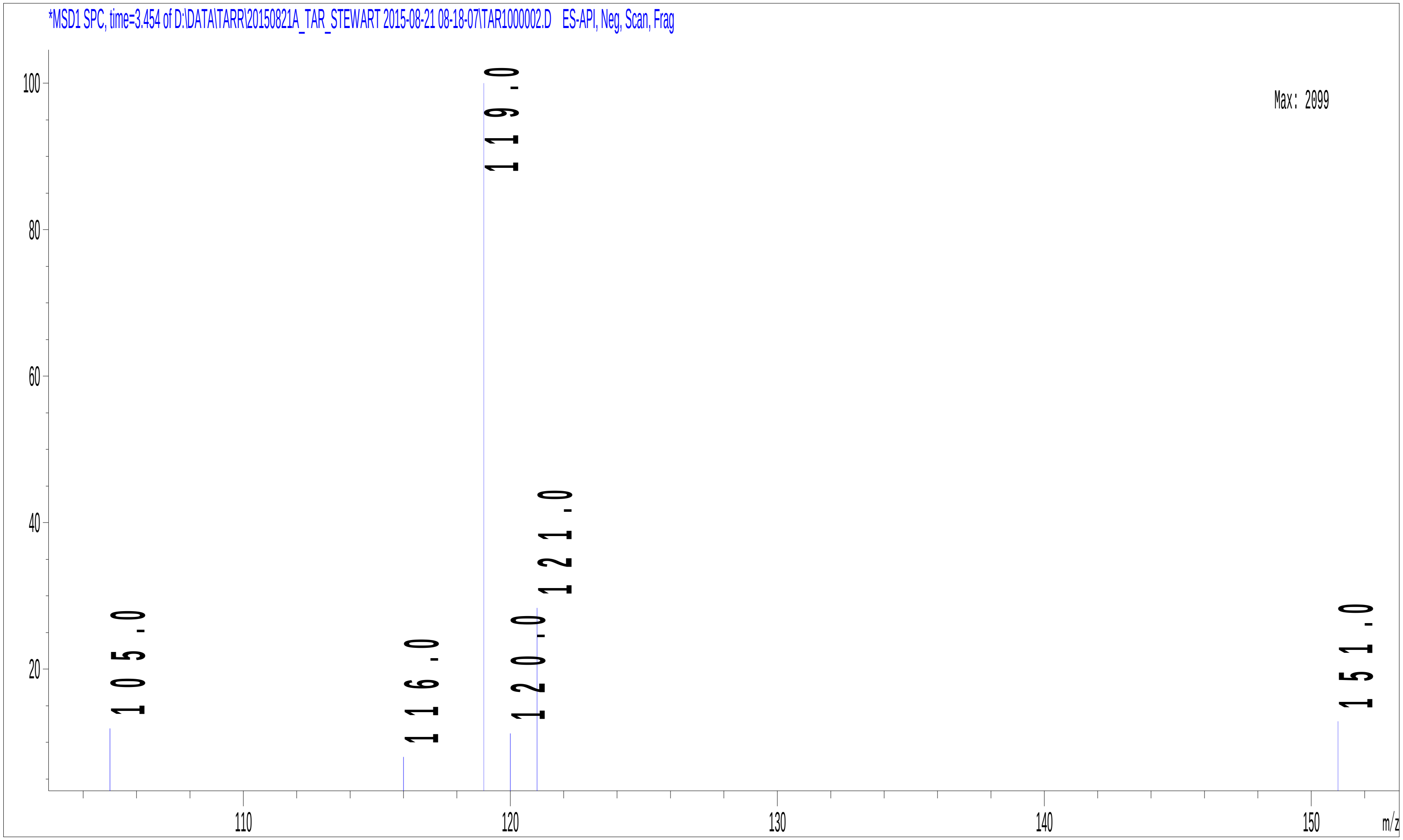
P2-E-01

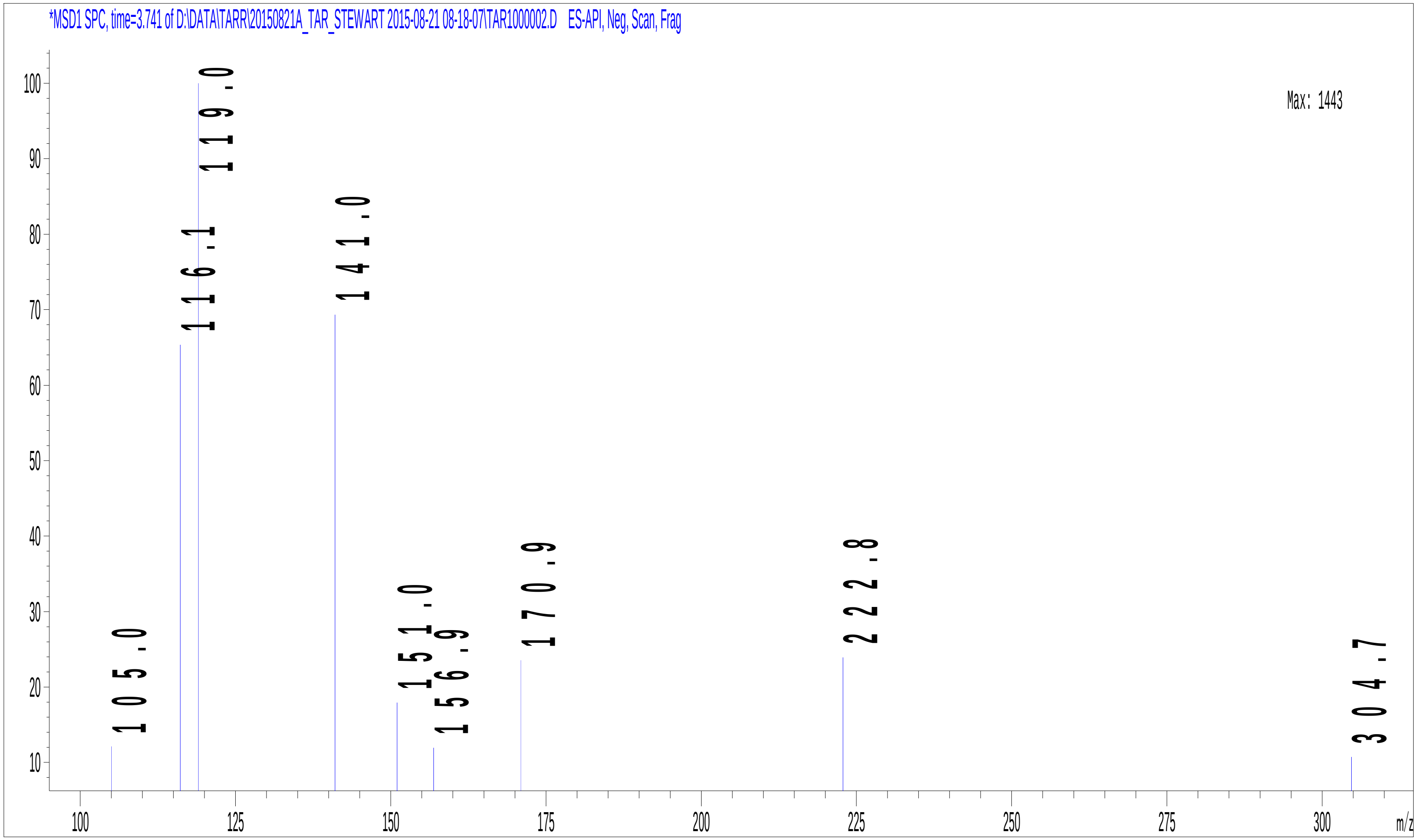


#	Time	Area	Height	Width	Area%	Symmetry
1	3.006	151552	15739.9	0.1477	83.272	0.532
2	3.711	30445.1	1901.2	0.2222	16.728	0.967


MSD1 TIC, MS File (D:\DATA\TARR\20150821A_TAR_STEWART 2015-08-21 08-18-07\TAR1000002.D) ES-API, Neg, Scan, Frag: 70
MSD1 TIC, MS File (D:\DATA\TARR\20150820_TAR\TAR1000035.D) ES-API, Neg, Scan, Frag: 70
Norm.
30000
25000
20000
15000
10000
5000
1
2
3
4
5
6
7
min


*MSD1 SPC, time=3.100 of D:\DATA\TARR\20150821A_TAR_STEWART 2015-08-21 08-18-07\TAR1000002.D ES-API, Neg, Scan, Frag
Max: 2483
100
80
60
40
20
100
150
200
250
300
350
400
450
m/z
105.1
119.0
151.0
170.9
196.8
210.9
218.8
232.8
236.8
286.8
310.7
384.7
408.6
466.6
468.6


*MSD1 SPC, time=3.454 of D:\DATA\TARR\20150821A_TAR_STEWART 2015-08-21 08-18-07\TAR1000002.D ES-API, Neg, Scan, Frag
Max: 2099
100
80
60
40
20
105.0
116.0
119.0
120.0
121.0
151.0
110
120
130
140
150
m/z

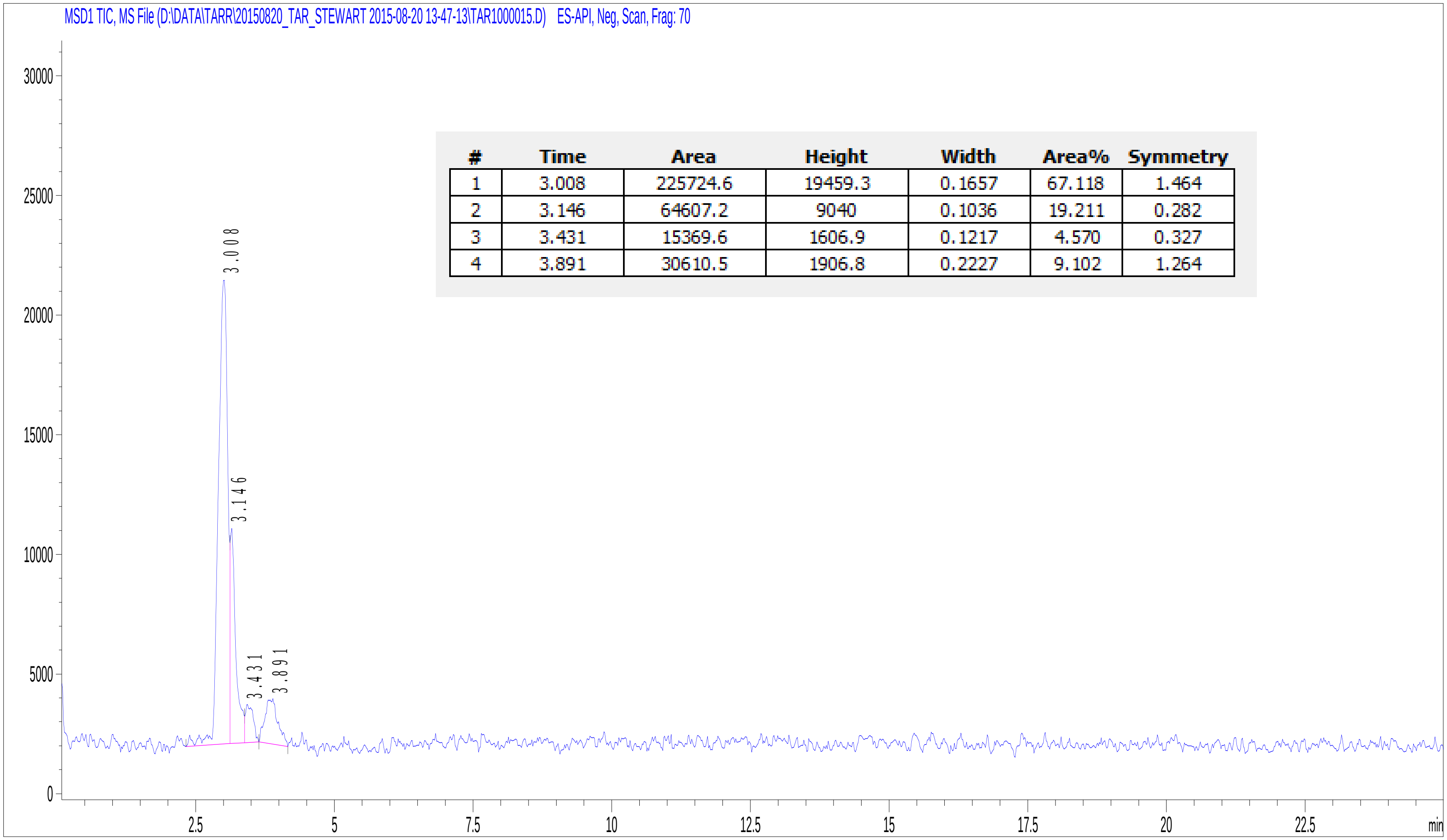

*MSD1 SPC, time=3.741 of D:\DATA\TARR\20150821A_TAR_STEWART 2015-08-21 08-18-07\TAR1000002.D ES-API, Neg, Scan, Frag
Max: 1443
105.0
116.1
119.0
141.0
151.0
156.9
170.9
222.8
304.7
100
90
80
70
60
50
40
30
20
10
100
125
150
175
200
225
250
275
300
m/z

1-Jun-15

70 DC

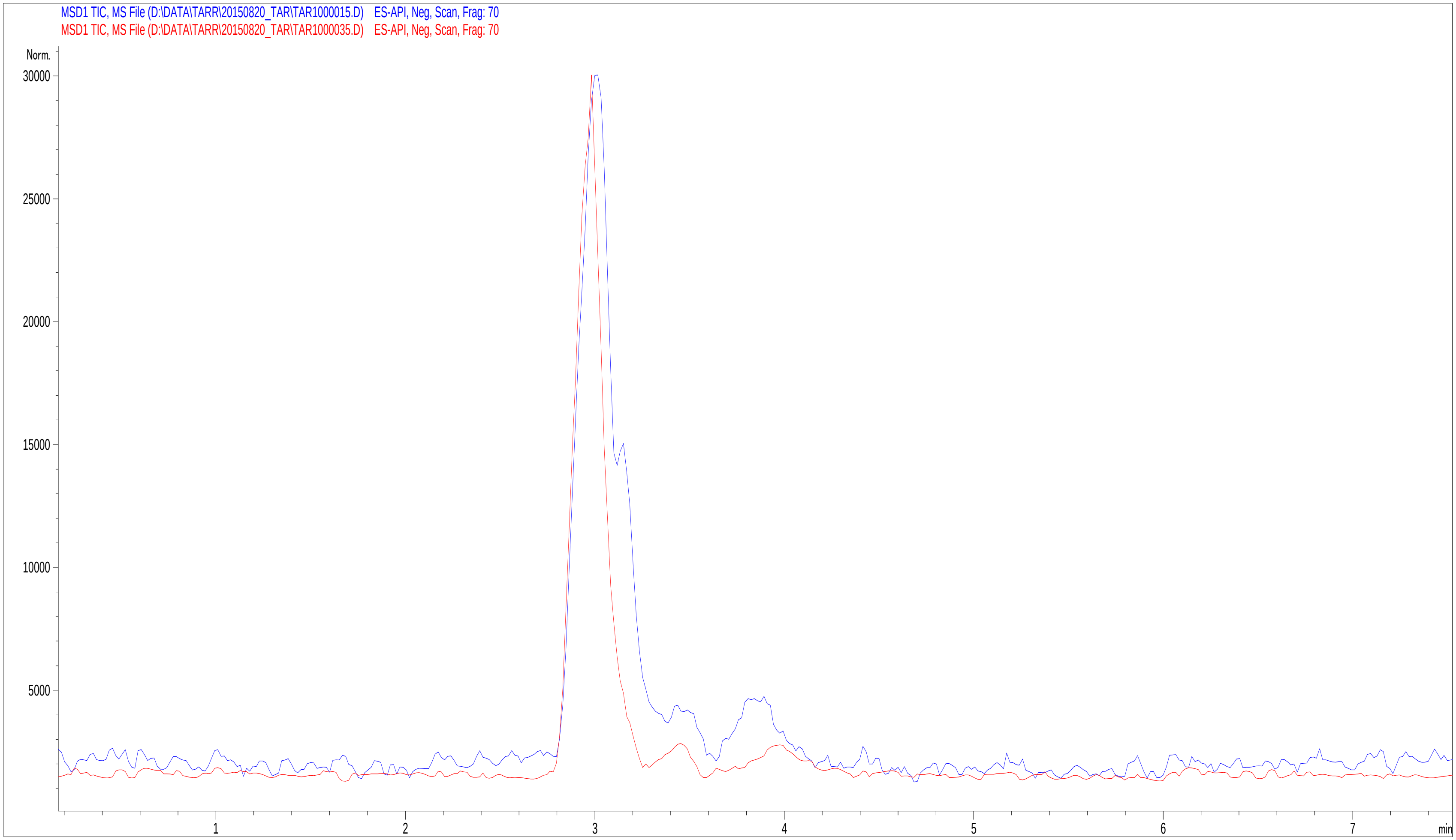
6

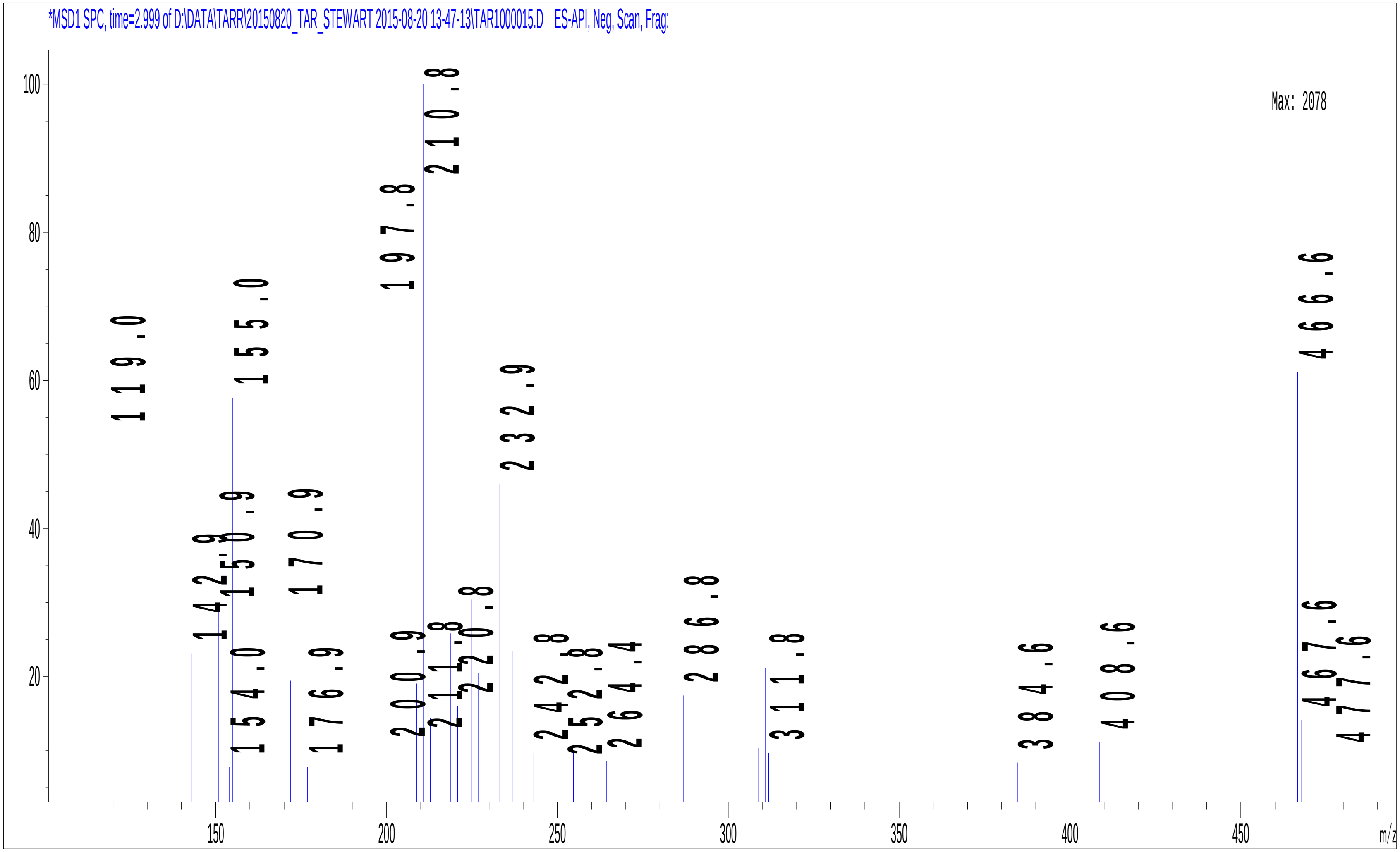
P2-B-04

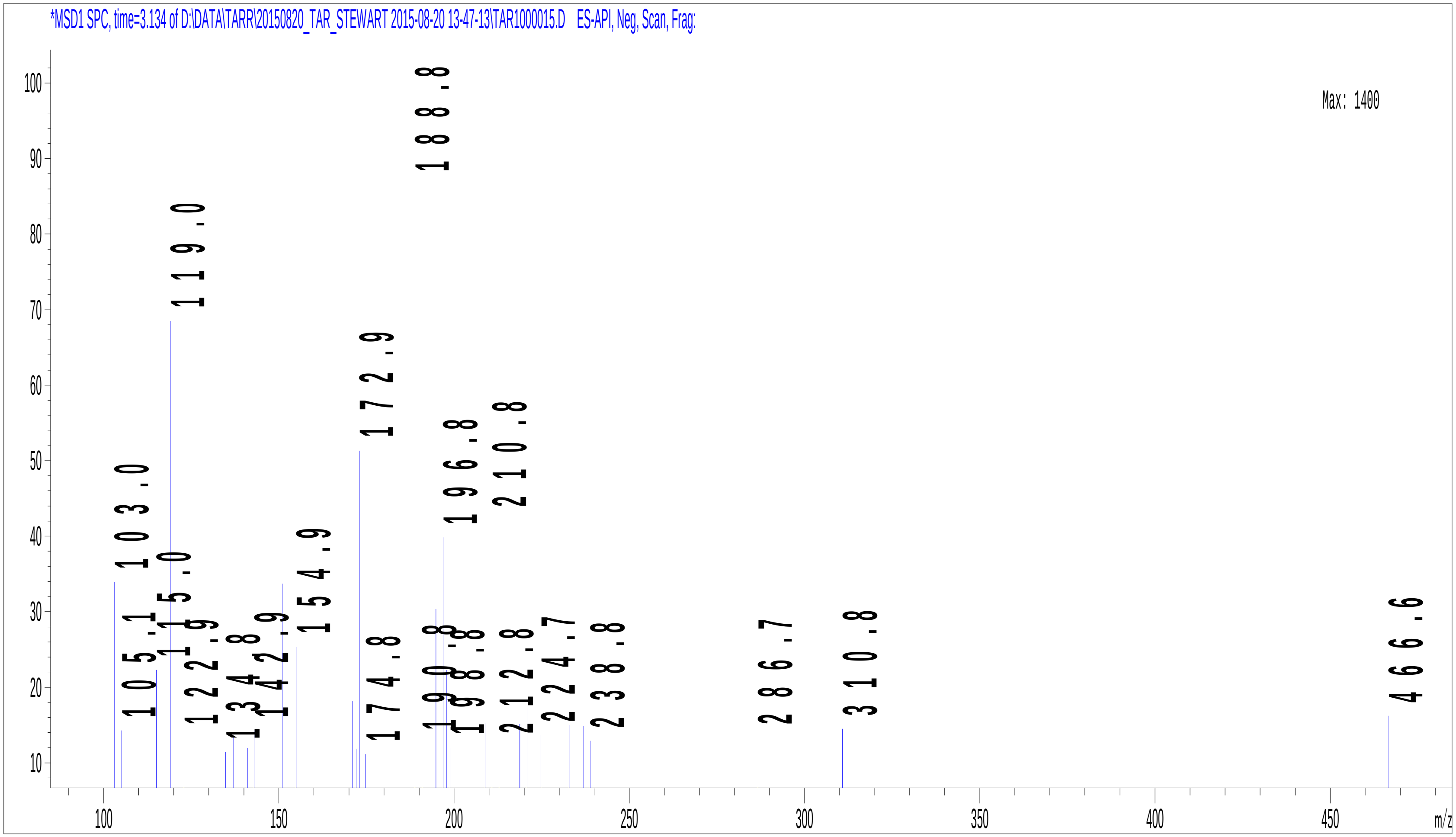


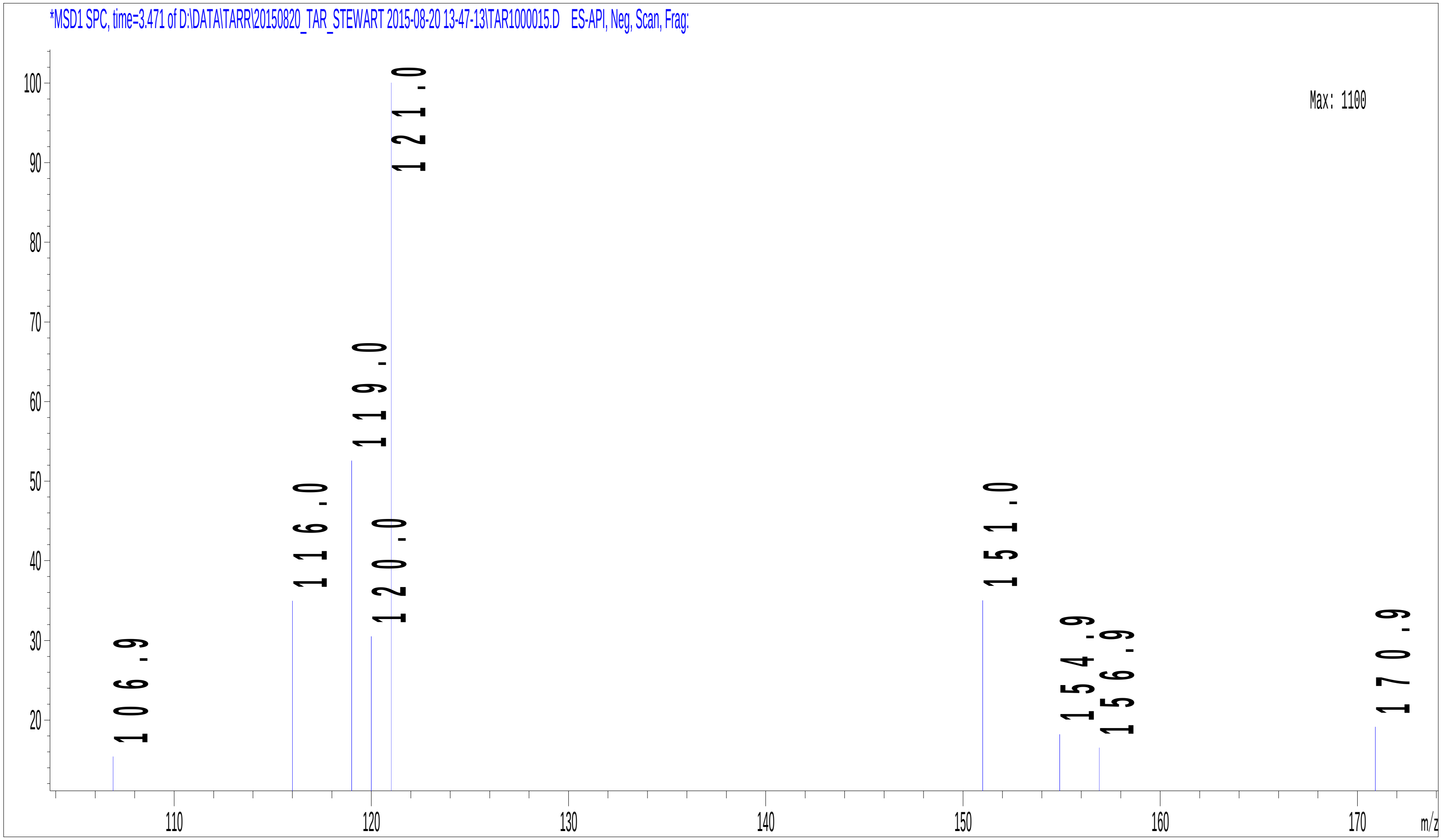
MSD1 TIC, MS File (D:\DATA\TARR\20150820_TAR_STEWART 2015-08-20 13-47-13\TAR1000015.D)   ES-API, Neg, Scan, Frag: 70

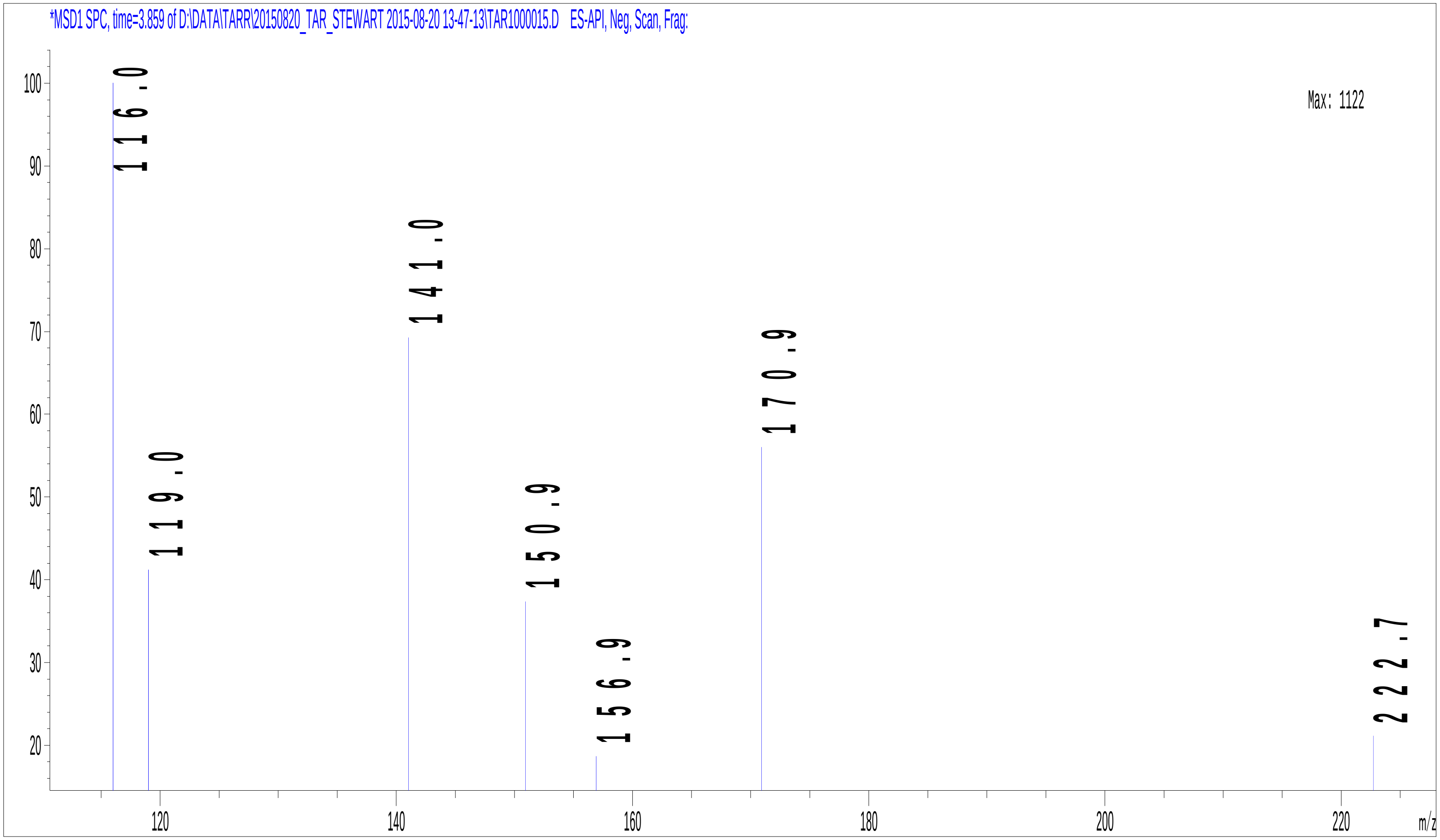
#	Time	Area	Height	Width	Area%	Symmetry
1	3.008	225724.6	19459.3	0.1657	67.118	1.464
2	3.146	64607.2	9040	0.1036	19.211	0.282
3	3.431	15369.6	1606.9	0.1217	4.570	0.327
4	3.891	30610.5	1906.8	0.2227	9.102	1.264


MSD1 TIC, MS File (D:\DATA\TARR\20150820_TAR\TAR1000015.D) ES-API, Neg, Scan, Frag: 70
MSD1 TIC, MS File (D:\DATA\TARR\20150820_TAR\TAR1000035.D) ES-API, Neg, Scan, Frag: 70
Norm.
30000
25000
20000
15000
10000
5000
1
2
3
4
5
6
7
min


*MSD1 SPC, time=2.999 of D:\DATA\TARR\20150820_TAR_STEWART 2015-08-20 13-47-13\TAR1000015.D ES-API, Neg, Scan, Frag:
Max: 2078
100
80
60
40
20
150
200
250
300
350
400
450
m/z
119.0
142.9
150.9
155.0
154.0
170.9
176.9
197.8
200.9
210.8
211.8
220.8
232.9
242.8
252.8
264.4
286.8
311.8
384.6
408.6
466.6
467.6
477.6


*MSD1 SPC, time=3.134 of D:\DATA\TARR\20150820_TAR_STEWART 2015-08-20 13-47-13\TAR1000015.D   ES-API, Neg, Scan, Frag:
Max: 1400
188.8
119.0
172.9
210.8
196.8
103.0
115.0
154.9
105.1
122.9
134.8
142.9
174.8
190.8
198.8
212.8
224.7
238.8
286.7
310.8
466.6
100
90
80
70
60
50
40
30
20
10
100
150
200
250
300
350
400
450
m/z


*MSD1 SPC, time=3.471 of D:\DATA\TARR\20150820_TAR_STEWART 2015-08-20 13-47-13\TAR1000015.D ES-API, Neg, Scan, Frag:
Max: 1100
100
90
80
70
60
50
40
30
20
106.9
116.0
119.0
120.0
121.0
151.0
154.9
156.9
170.9
110
120
130
140
150
160
170
m/z

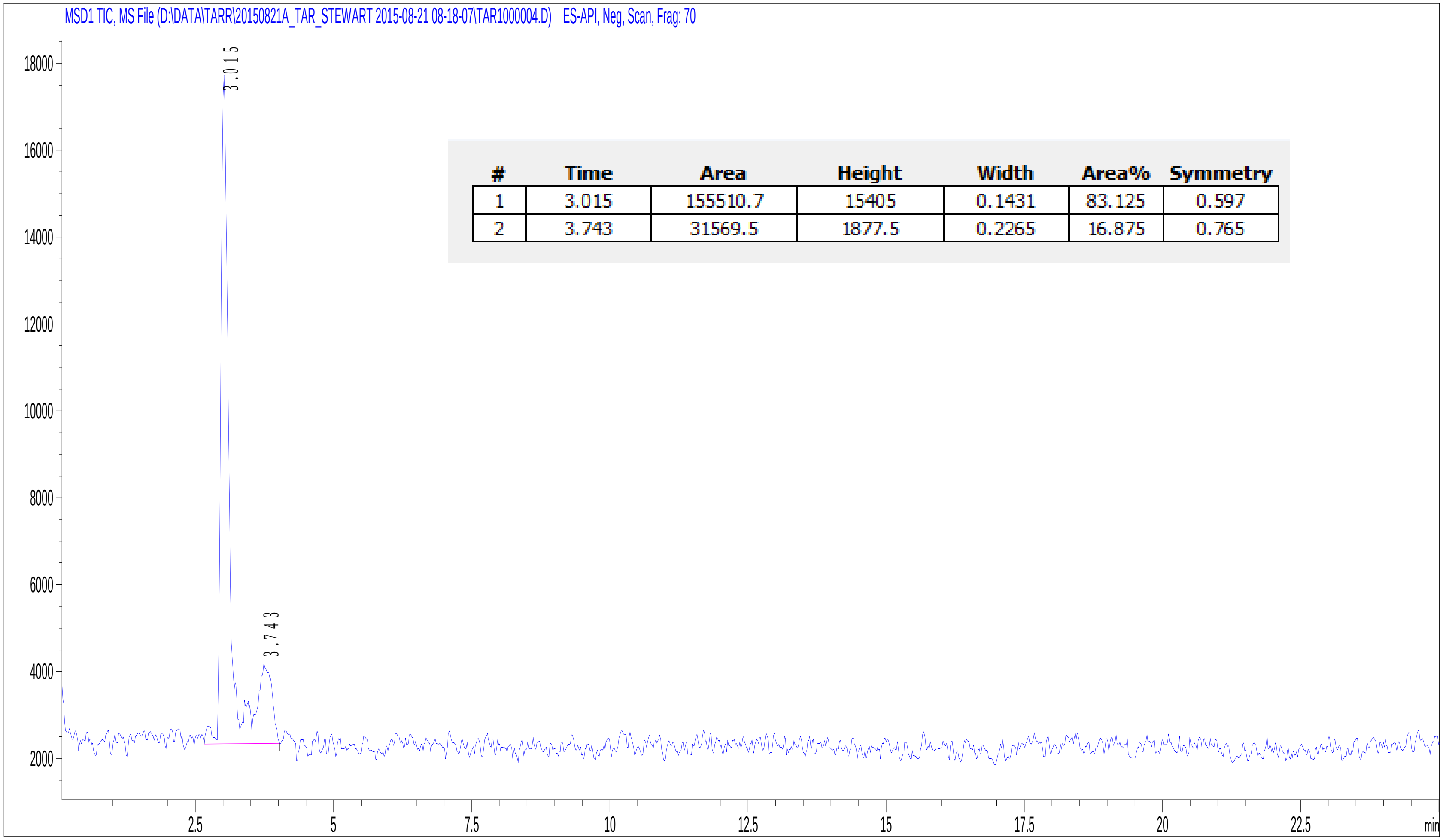

*MSD1 SPC, time=3.859 of D:\DATA\TARR\20150820_TAR_STEWART 2015-08-20 13-47-13\TAR1000015.D ES-API, Neg, Scan, Frag:
Max: 1122
116.0
119.0
141.0
150.9
156.9
170.9
222.7
100
90
80
70
60
50
40
30
20
120
140
160
180
200
220
m/z

12-Aug-15

70 DC repeat

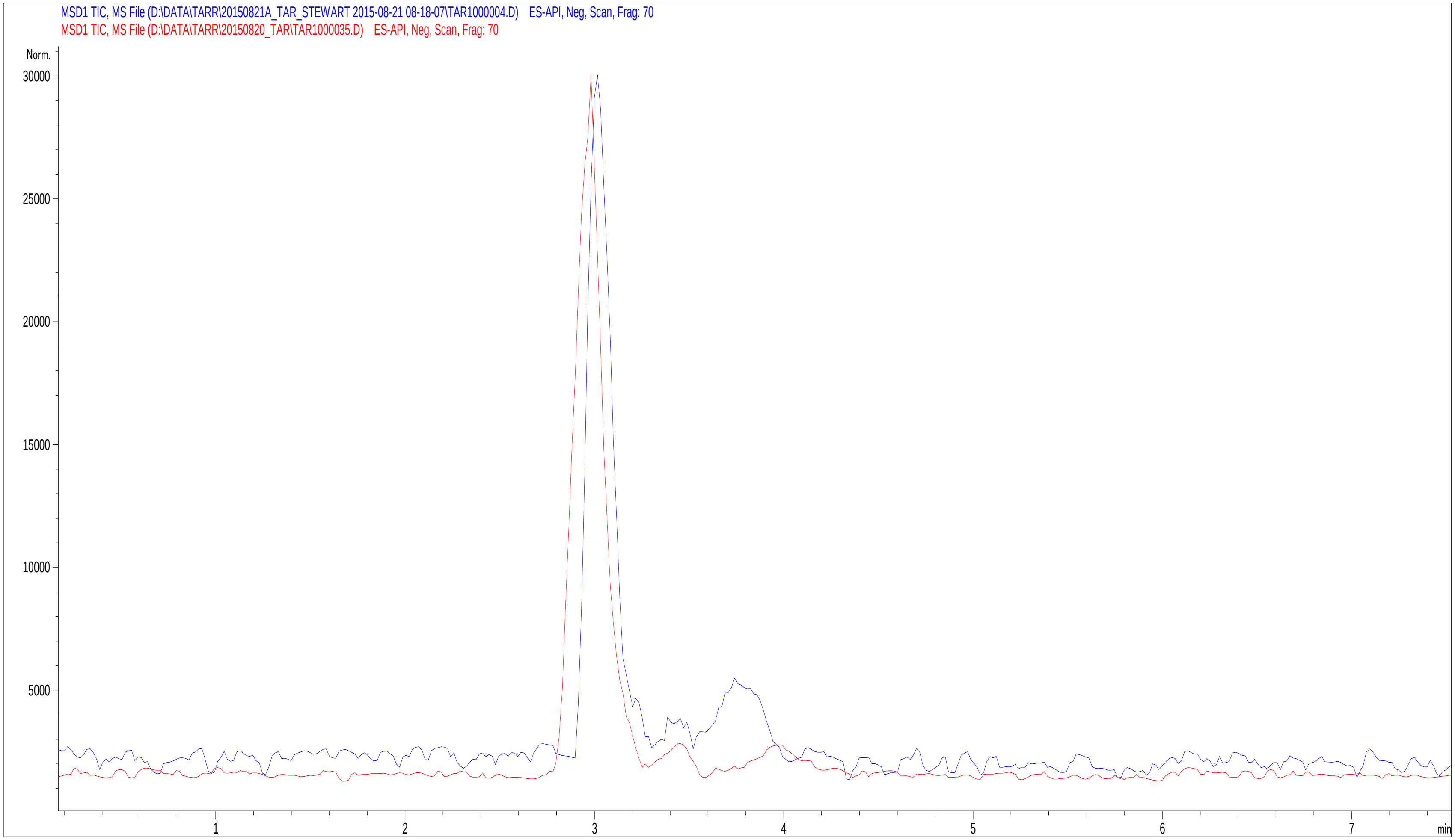
6

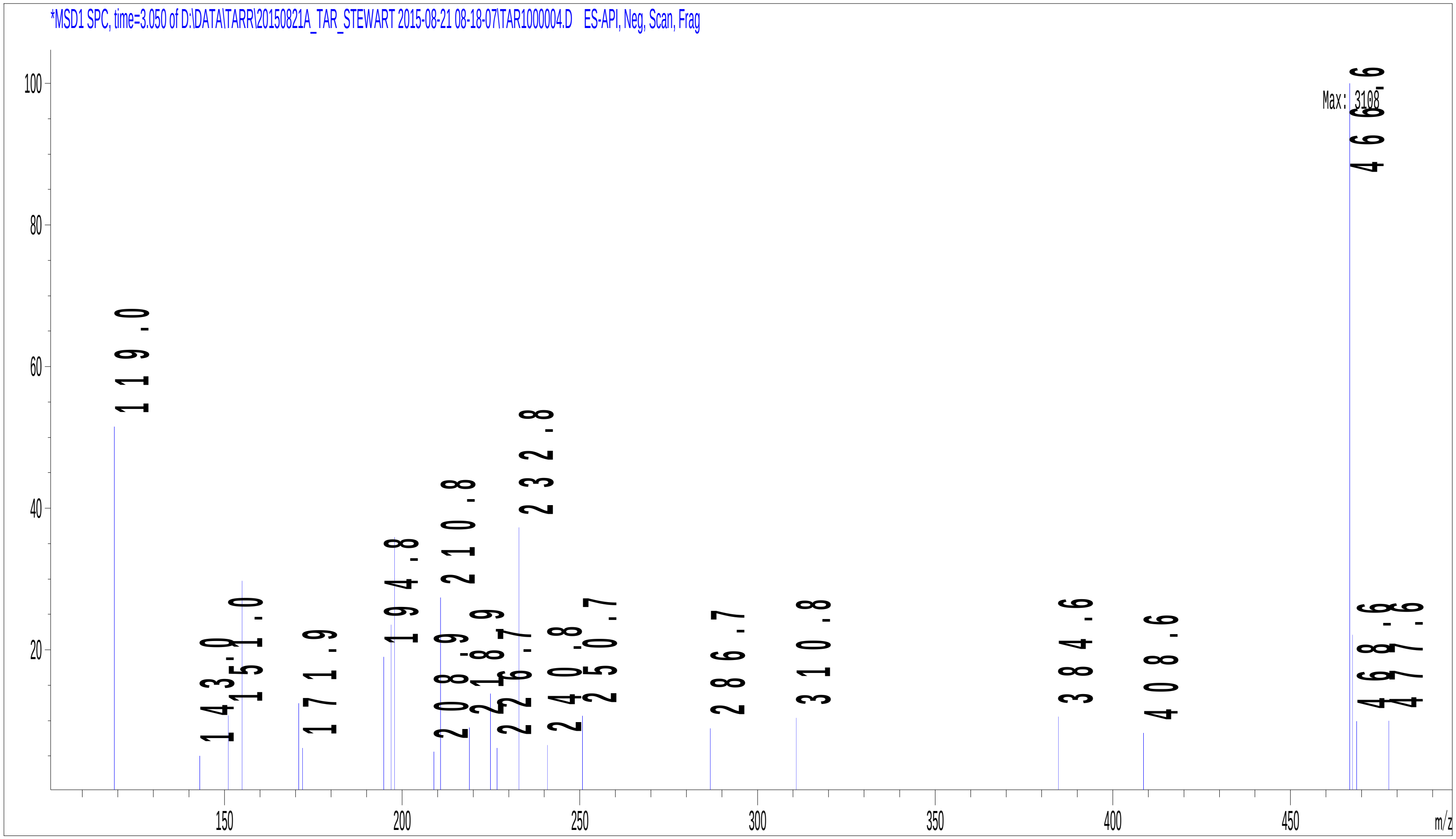
P2-E-03

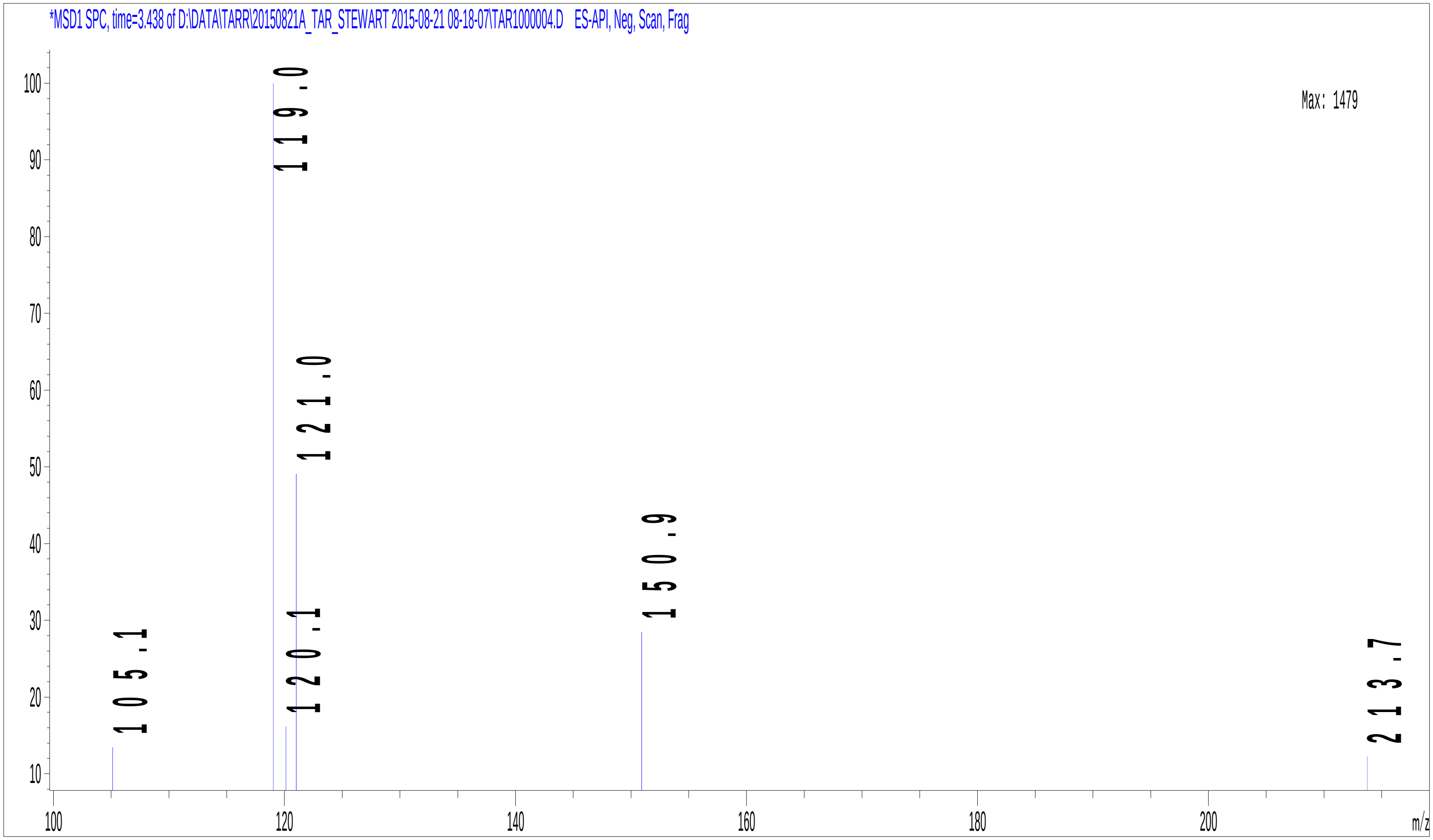


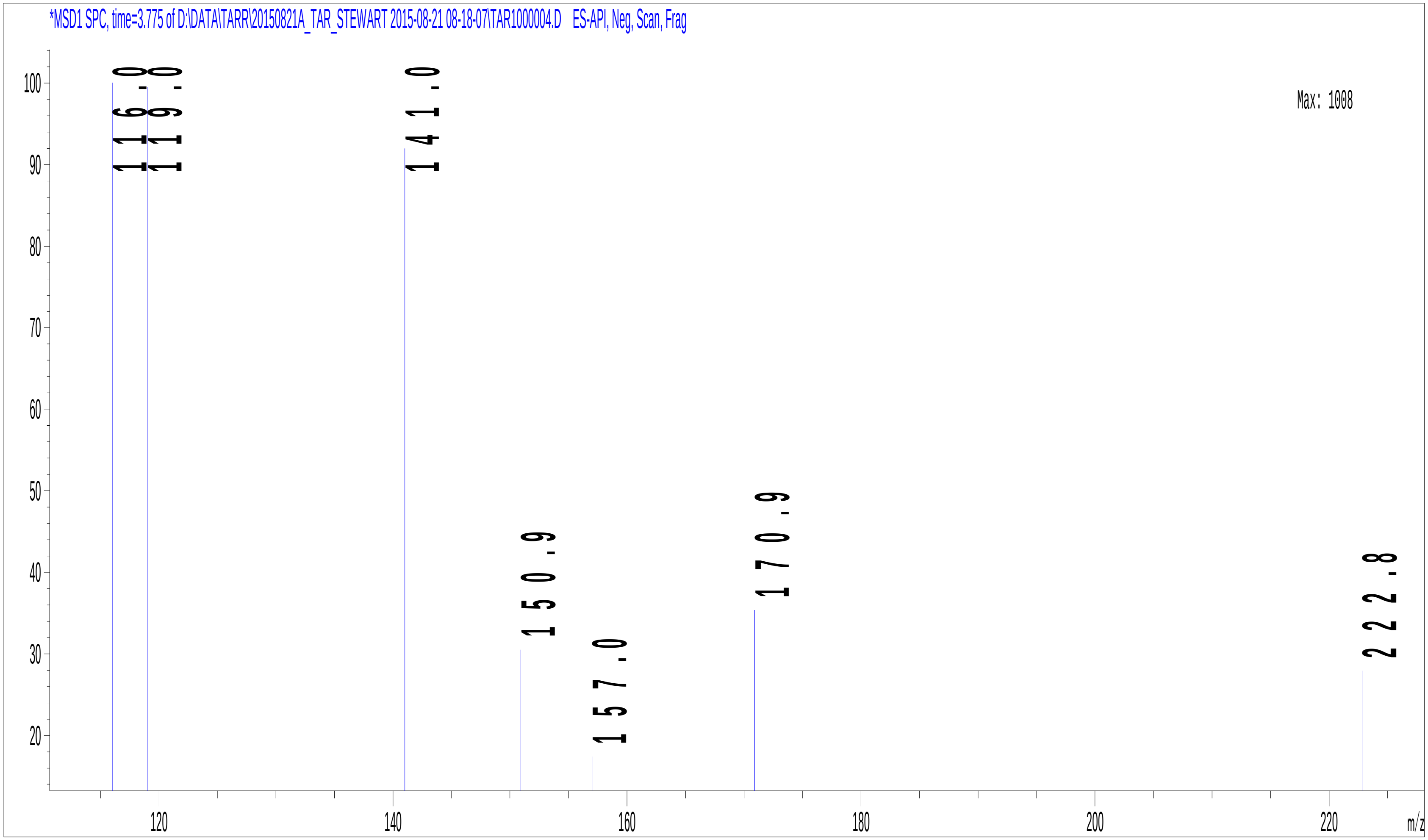
MSD1 TIC, MS File (D:\DATA\TARR\20150821A_TAR_STEWART 2015-08-21 08-18-07\TAR1000004.D) ES-API, Neg, Scan, Frag: 70

#	Time	Area	Height	Width	Area%	Symmetry
1	3.015	155510.7	15405	0.1431	83.125	0.597
2	3.743	31569.5	1877.5	0.2265	16.875	0.765


MSD1 TIC, MS File (D:\DATA\TARR\20150821A_TAR_STEWART 2015-08-21 08-18-07\TAR1000004.D) ES-API, Neg, Scan, Frag: 70
MSD1 TIC, MS File (D:\DATA\TARR\20150820_TAR\TAR1000035.D) ES-API, Neg, Scan, Frag: 70
Norm.
30000
25000
20000
15000
10000
5000
1
2
3
4
5
6
7
min


*MSD1 SPC, time=3.050 of D:\DATA\TARR\20150821A_TAR_STEWART 2015-08-21 08-18-07\TAR1000004.D ES-API, Neg, Scan, Frag
Max: 3108
466.6
119.0
232.8
210.8
194.8
151.0
143.0
171.9
208.9
218.9
226.7
240.8
250.7
286.7
310.8
384.6
408.6
468.6
477.6
100
80
60
40
20
150
200
250
300
350
400
450
m/z


*MSD1 SPC, time=3.438 of D:\DATA\TARR\20150821A_TAR_STEWART 2015-08-21 08-18-07\TAR1000004.D   ES-API, Neg, Scan, Frag
Max: 1479
100
90
80
70
60
50
40
30
20
10
105.1
119.0
120.1
121.0
150.9
213.7
100
120
140
160
180
200
m/z

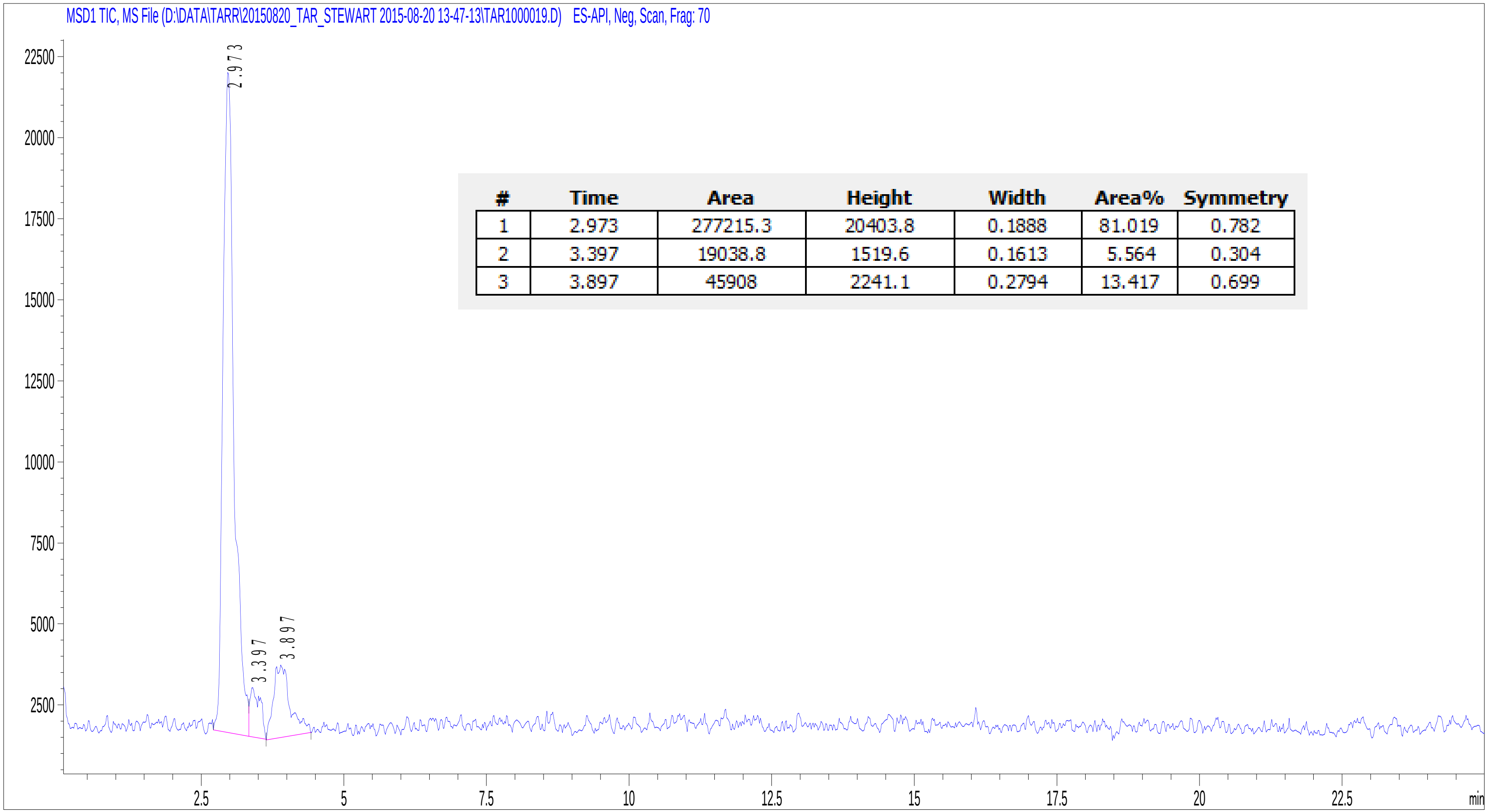

*MSD1 SPC, time=3.775 of D:\DATA\TARR\20150821A_TAR_STEWART 2015-08-21 08-18-07\TAR1000004.D ES-API, Neg, Scan, Frag
Max: 1008
116.0
119.0
141.0
150.9
157.0
170.9
222.8
100
90
80
70
60
50
40
30
20
120
140
160
180
200
220
m/z

26-Jun-15

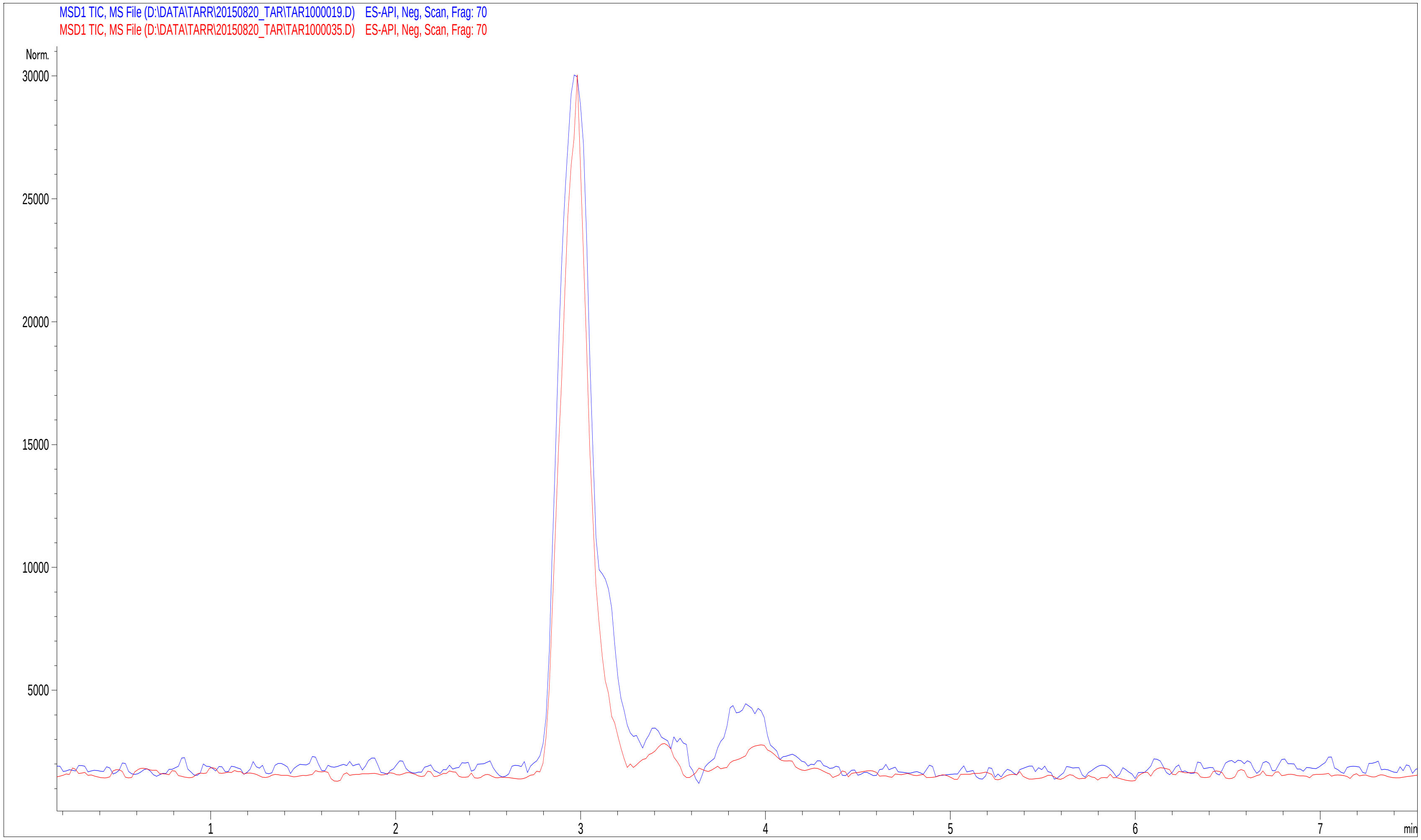
100 DC

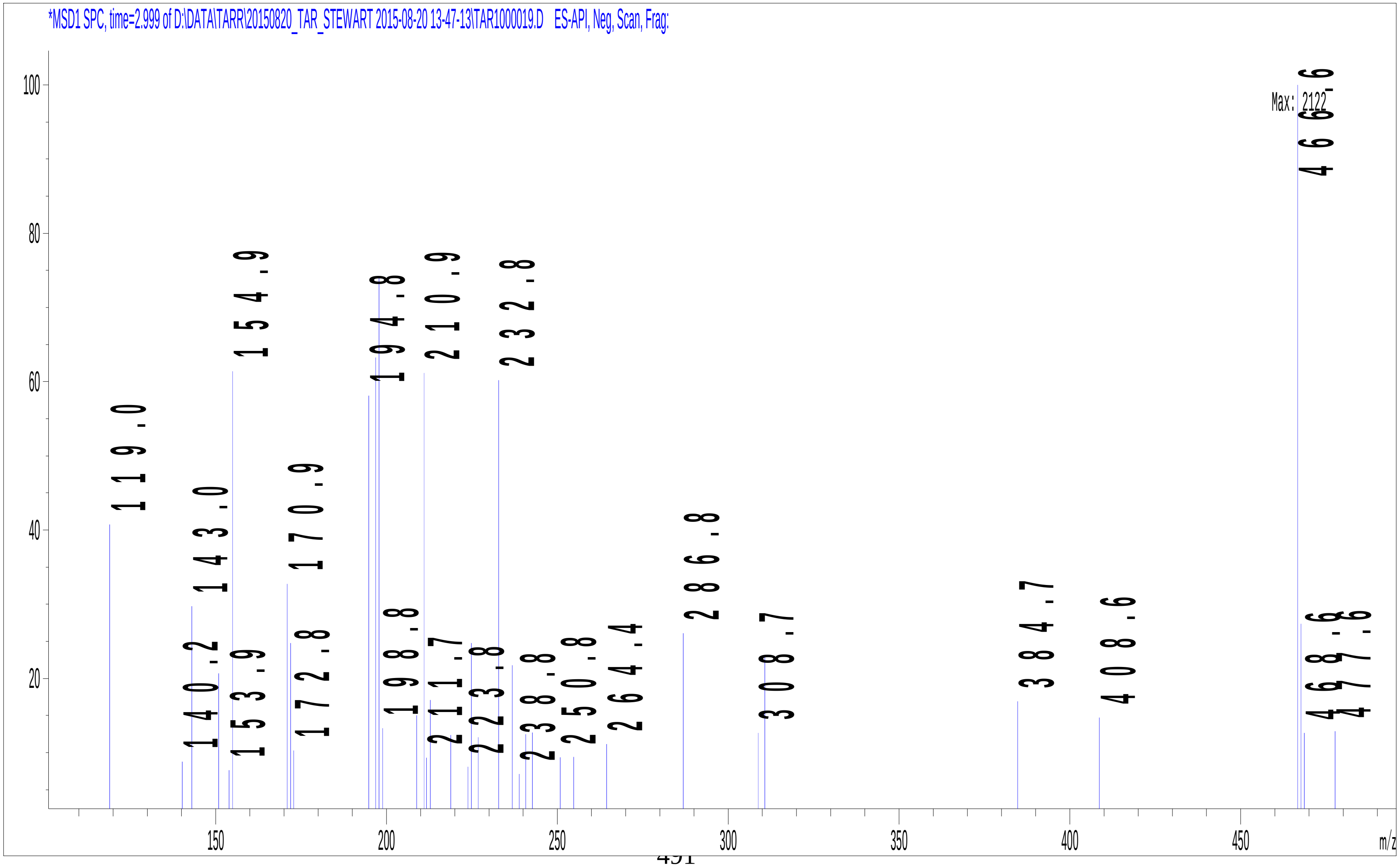
6

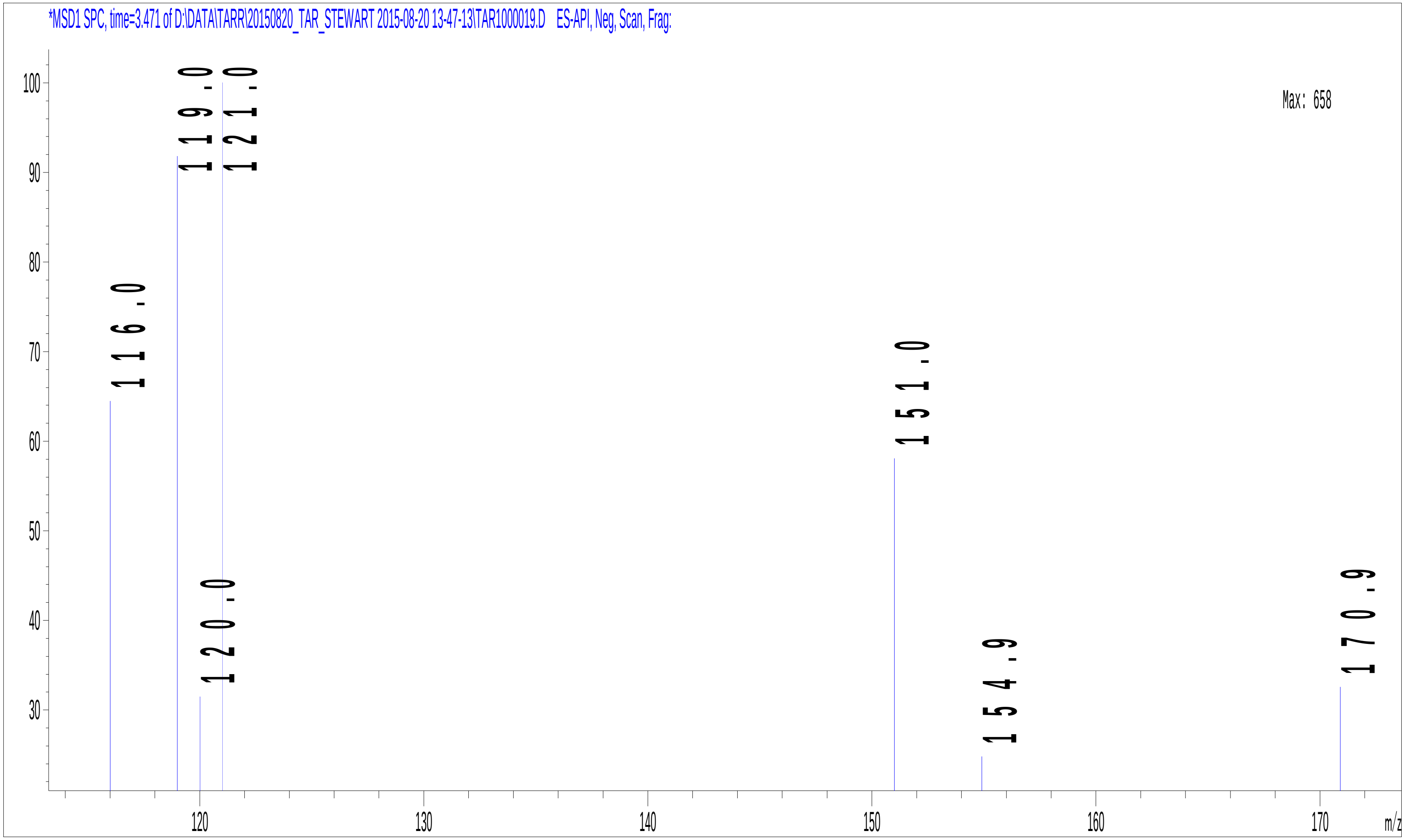
P2-C-01

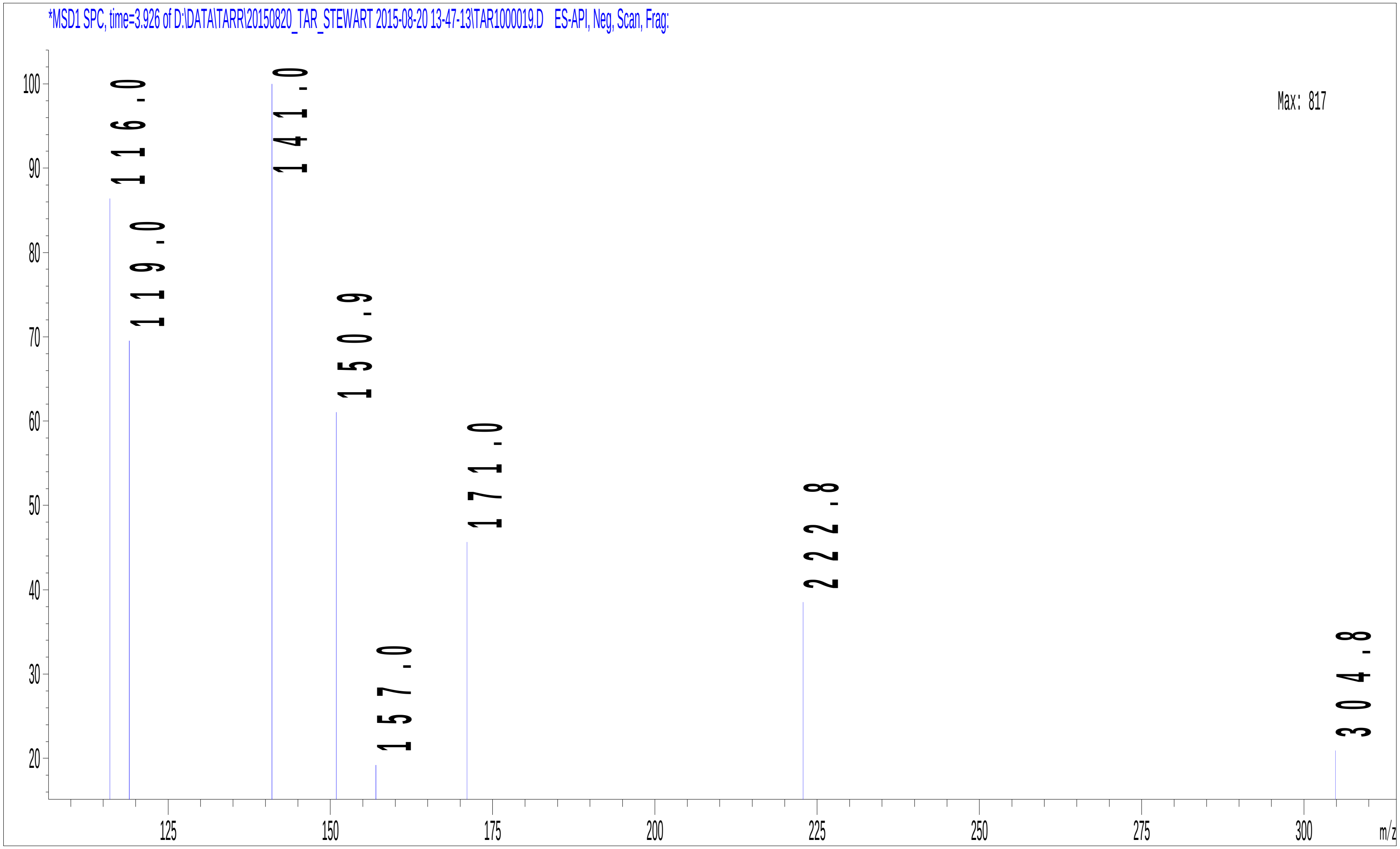


#	Time	Area	Height	Width	Area%	Symmetry
1	2.973	277215.3	20403.8	0.1888	81.019	0.782
2	3.397	19038.8	1519.6	0.1613	5.564	0.304
3	3.897	45908	2241.1	0.2794	13.417	0.699


MSD1 TIC, MS File (D:\DATA\TARR\20150820_TAR\TAR1000019.D) ES-API, Neg, Scan, Frag: 70
MSD1 TIC, MS File (D:\DATA\TARR\20150820_TAR\TAR1000035.D) ES-API, Neg, Scan, Frag: 70
Norm.
30000
25000
20000
15000
10000
5000
1
2
3
4
5
6
7
min


*MSD1 SPC, time=2.999 of D:\DATA\TARR\20150820_TAR_STEWART 2015-08-20 13-47-13\TAR1000019.D ES-API, Neg, Scan, Frag:
Max: 2122
100
80
60
40
20
119.0
140.2
143.0
153.9
154.9
170.9
172.8
194.8
198.8
210.9
211.7
223.8
232.8
238.8
250.8
264.4
286.8
308.7
384.7
408.6
466.6
468.6
477.6
150
200
250
300
350
400
450
m/z


*MSD1 SPC, time=3.471 of D:\DATA\TARR\20150820_TAR_STEWART 2015-08-20 13-47-13\TAR1000019.D   ES-API, Neg, Scan, Frag:
Max: 658
116.0
119.0
121.0
120.0
151.0
154.9
170.9
100
90
80
70
60
50
40
30
120
130
140
150
160
170
m/z

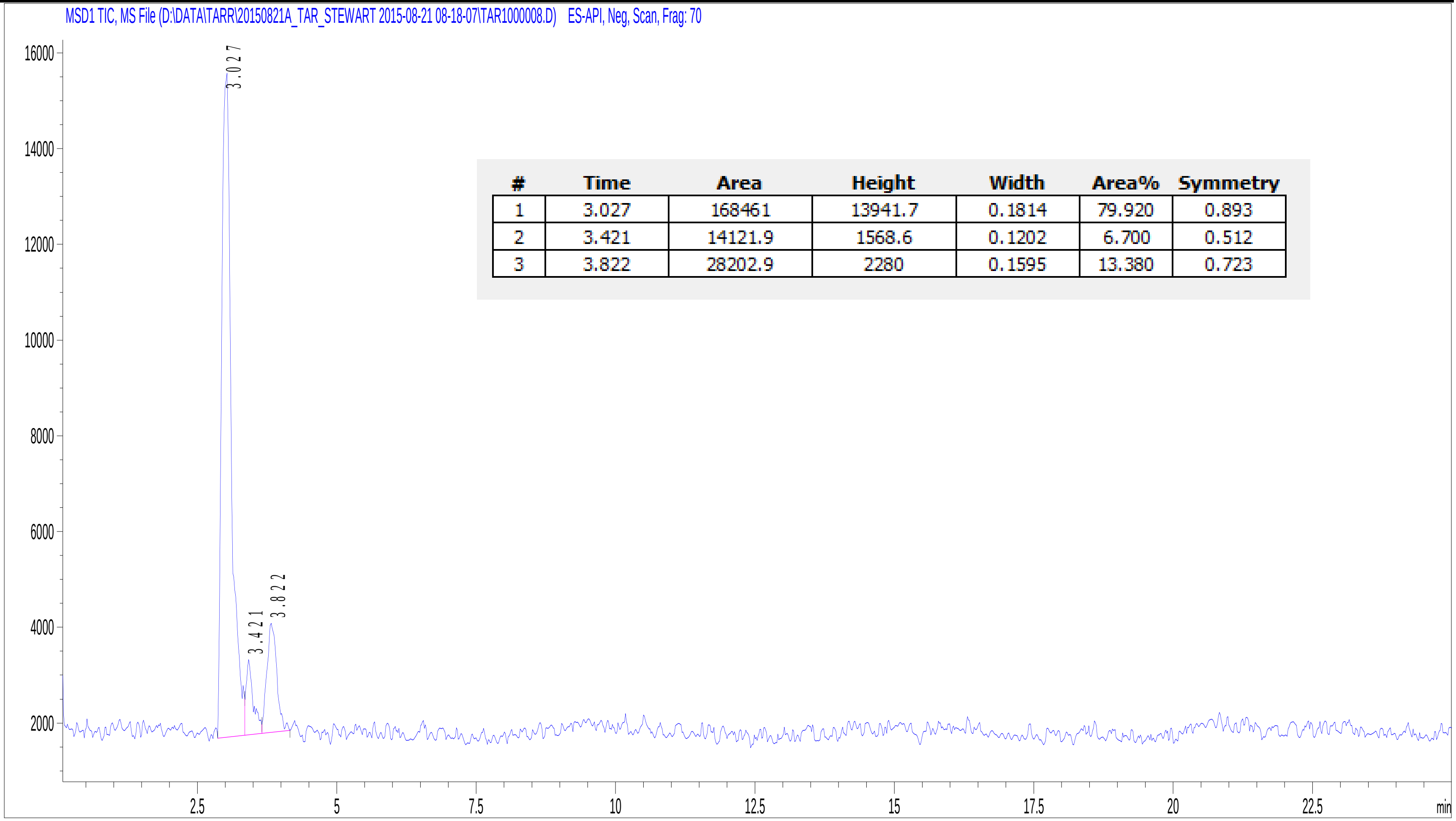

*MSD1 SPC, time=3.926 of D:\DATA\TARR\20150820_TAR_STEWART 2015-08-20 13-47-13\TAR1000019.D ES-API, Neg, Scan, Frag:
Max: 817
116.0
119.0
141.0
150.9
157.0
171.0
222.8
304.8
100
90
80
70
60
50
40
30
20
125
150
175
200
225
250
275
300
m/z

24-Jun-15

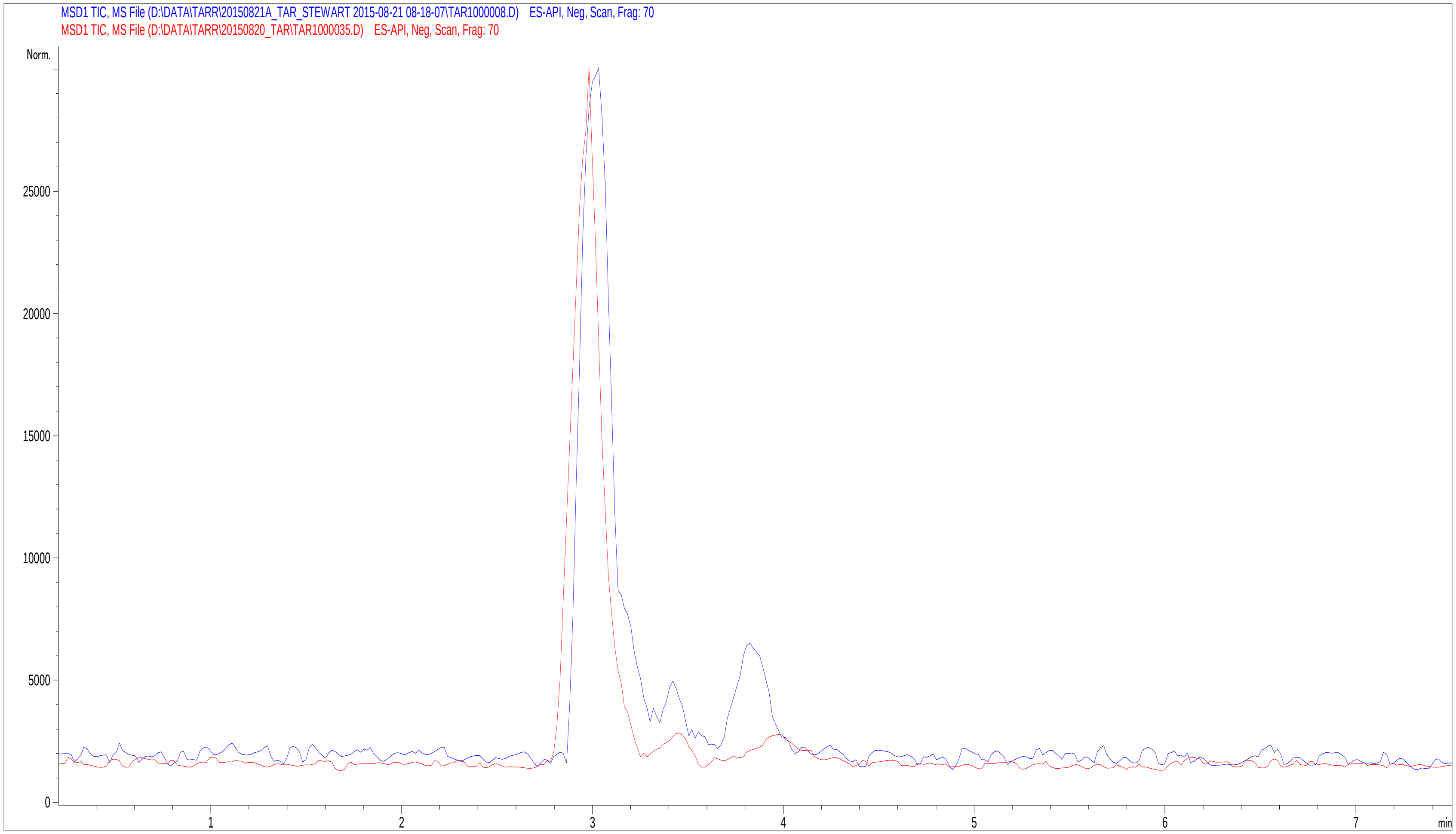
100 DC problem (no romoval)

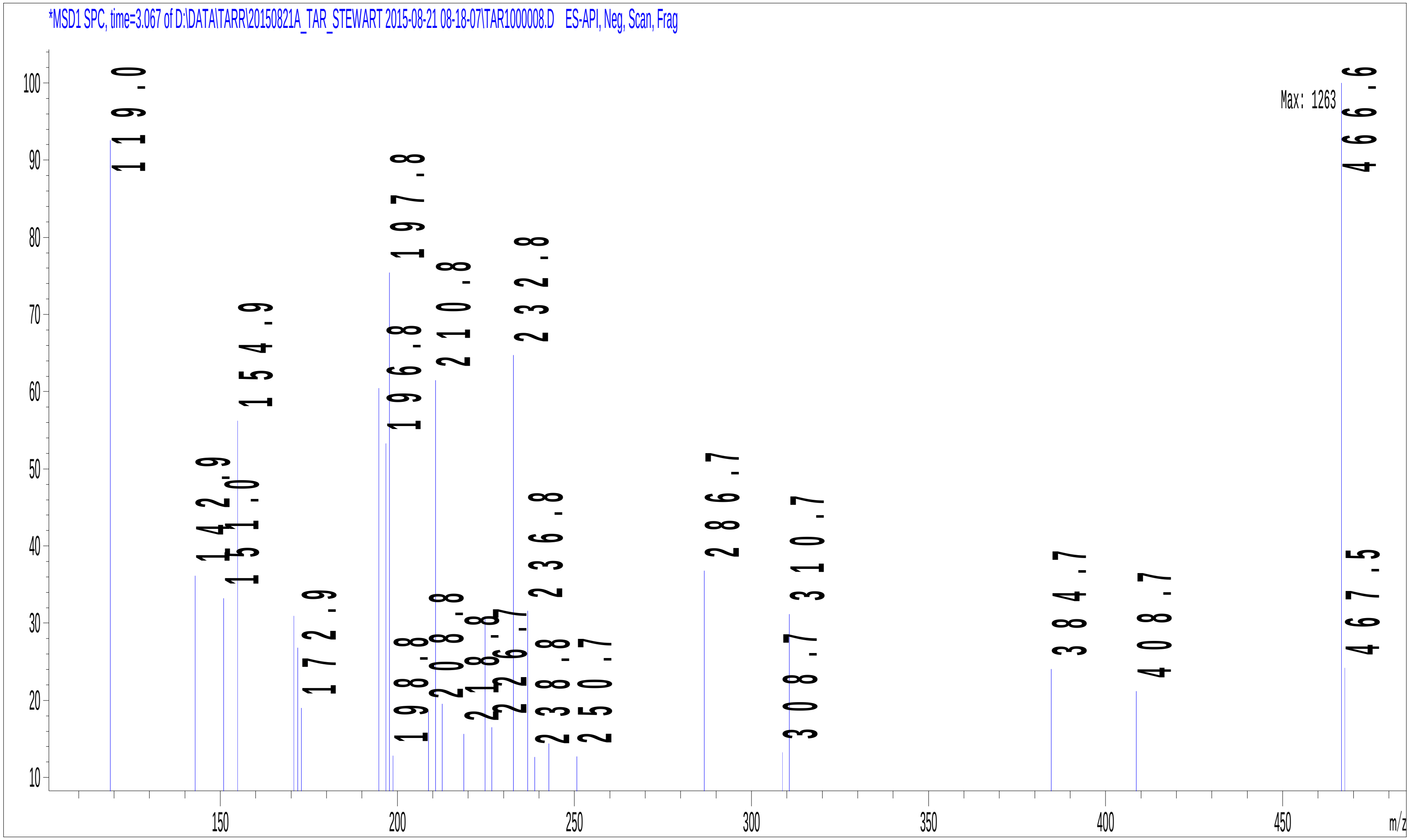
6

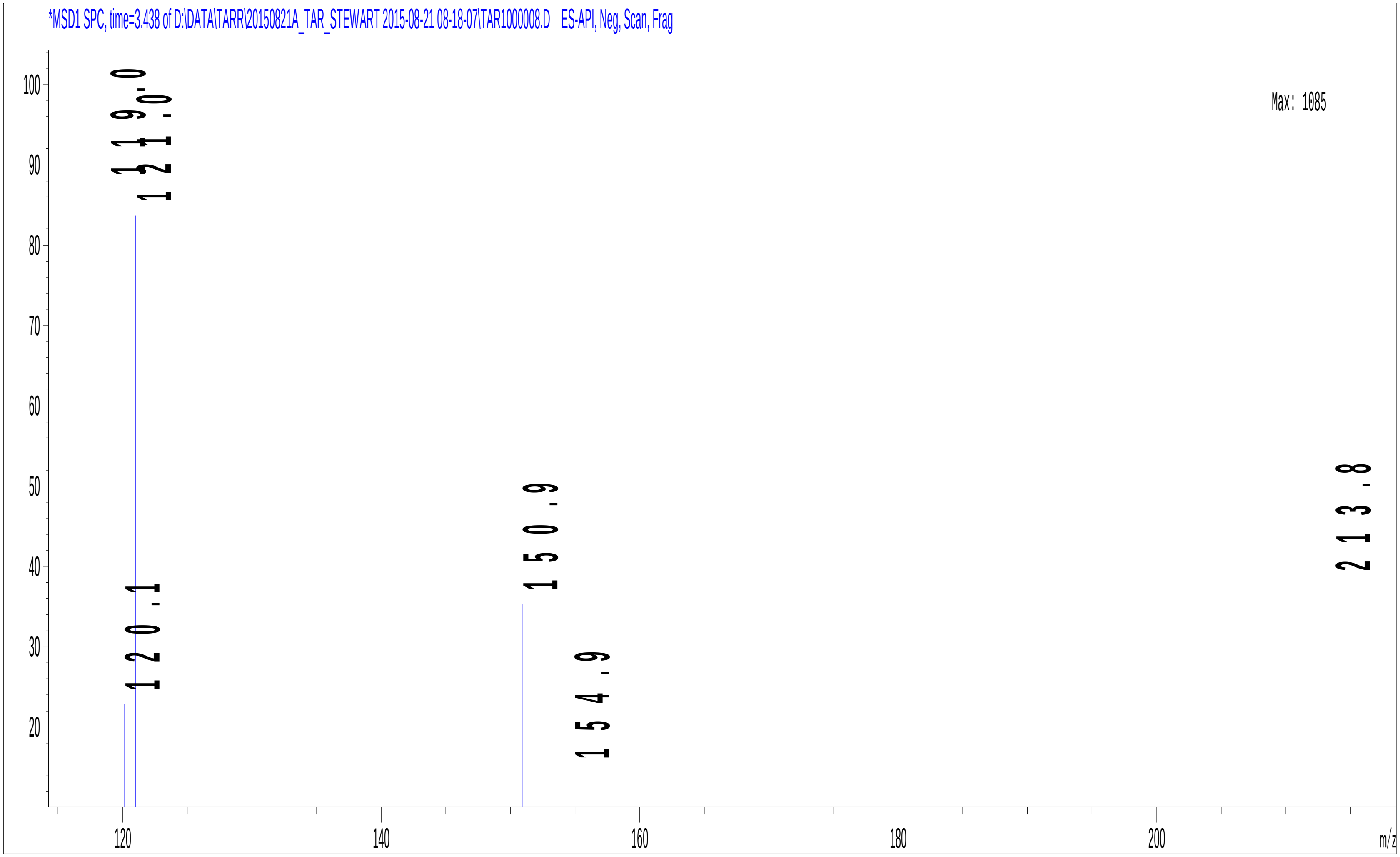
P2-E-07

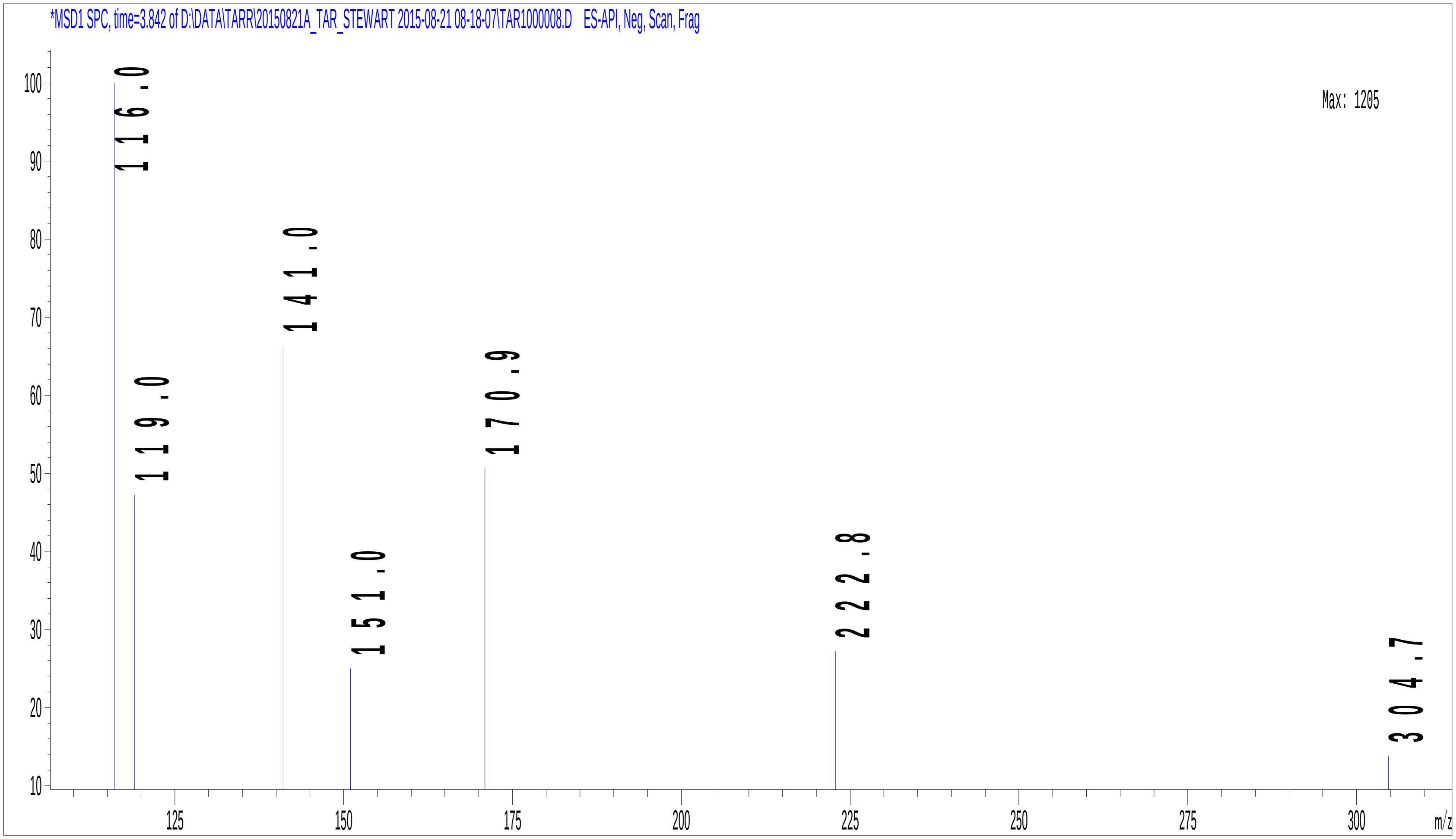


#	Time	Area	Height	Width	Area%	Symmetry
1	3.027	168461	13941.7	0.1814	79.920	0.893
2	3.421	14121.9	1568.6	0.1202	6.700	0.512
3	3.822	28202.9	2280	0.1595	13.380	0.723


MSD1 TIC, MS File (D:\DATA\TARR\20150821A_TAR_STEWART 2015-08-21 08-18-07\TAR1000008.D) ES-API, Neg, Scan, Frag: 70
MSD1 TIC, MS File (D:\DATA\TARR\20150820_TAR\TAR1000035.D) ES-API, Neg, Scan, Frag: 70
Norm.
25000
20000
15000
10000
5000
0
1
2
3
4
5
6
7
min

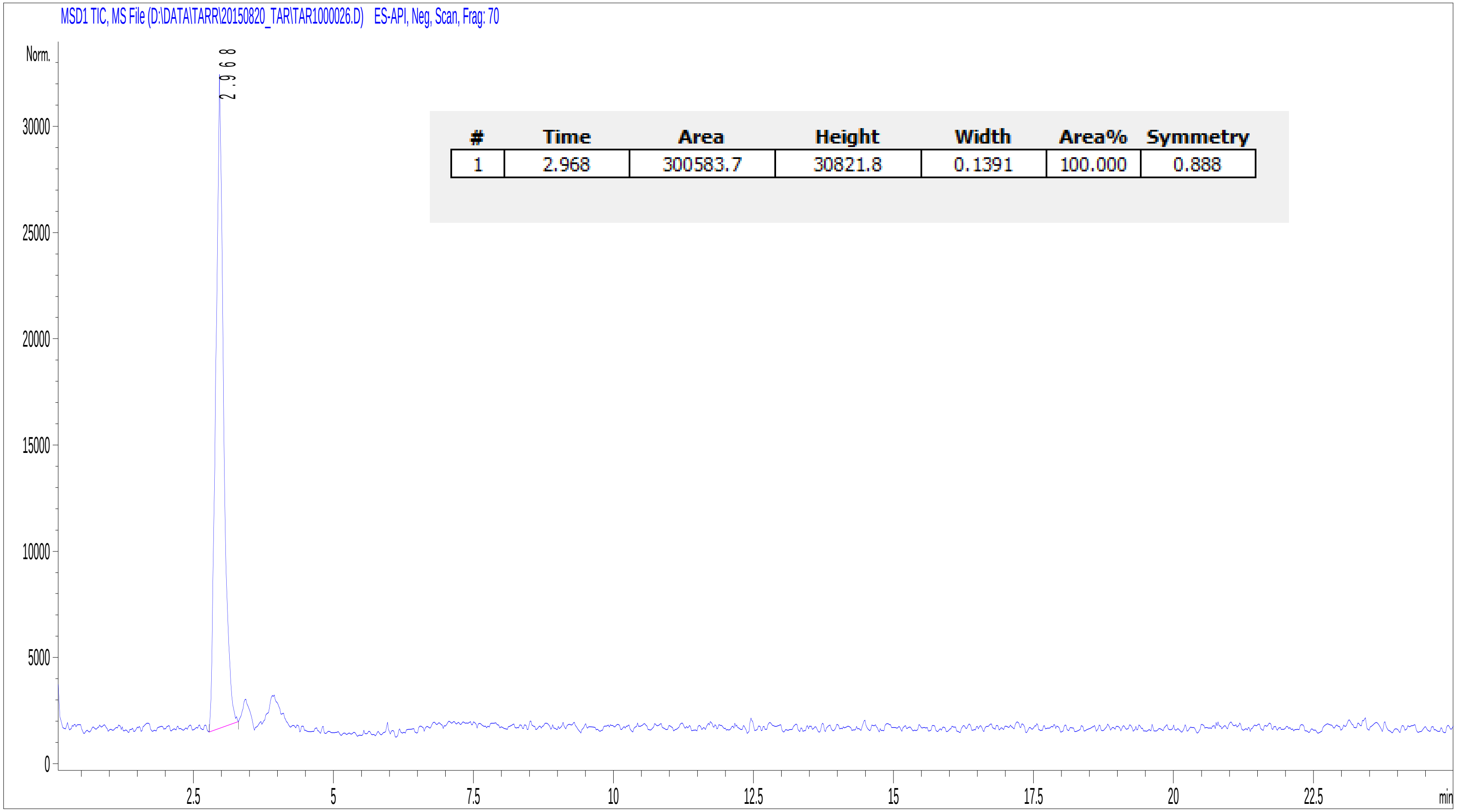

*MSD1 SPC, time=3.067 of D:\DATA\TARR\20150821A_TAR_STEWART 2015-08-21 08-18-07\TAR1000008.D ES-API, Neg, Scan, Frag
Max: 1263
100
90
80
70
60
50
40
30
20
10
150
200
250
300
350
400
450
m/z
119.0
142.9
151.0
154.9
172.9
196.8
197.8
198.8
208.8
210.8
218.8
226.7
232.8
236.8
238.8
250.7
286.7
308.7
310.7
384.7
408.7
466.6
467.5


*MSD1 SPC, time=3.438 of D:\DATA\TARR\20150821A_TAR_STEWART 2015-08-21 08-18-07\TAR1000008.D   ES-API, Neg, Scan, Frag
Max: 1085
119.0
121.0
120.1
150.9
154.9
213.8
100
90
80
70
60
50
40
30
20
120
140
160
180
200
m/z

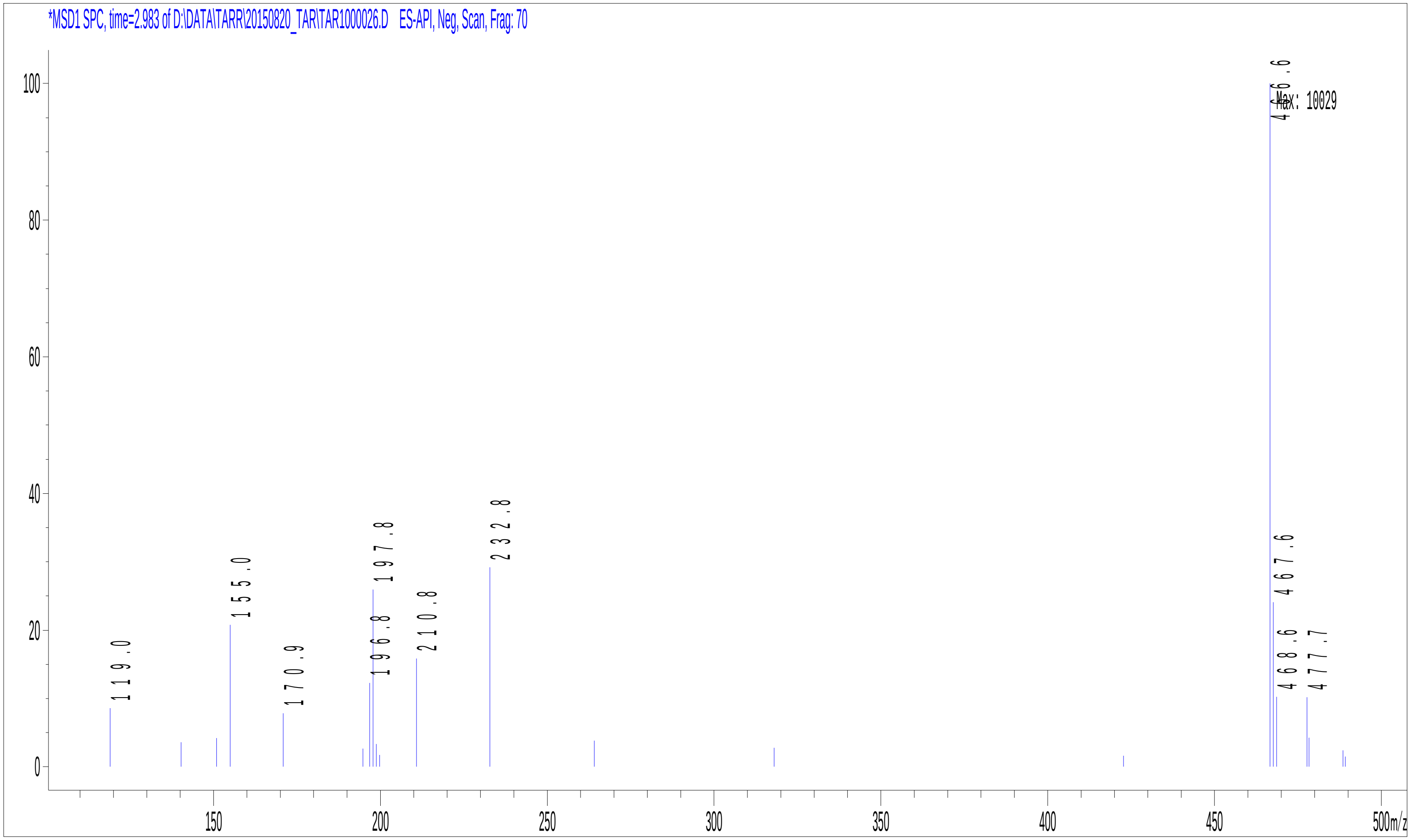
*MSD1 SPC, time=3.842 of D:\DATA\TARR\20150821A_TAR_STEWART 2015-08-21 08-18-07\TAR1000008.D   ES-API, Neg, Scan, Frag
Max: 1205
116.0
119.0
141.0
151.0
170.9
222.8
304.7
100
90
80
70
60
50
40
30
20
10
125
150
175
200
225
250
275
300
m/z

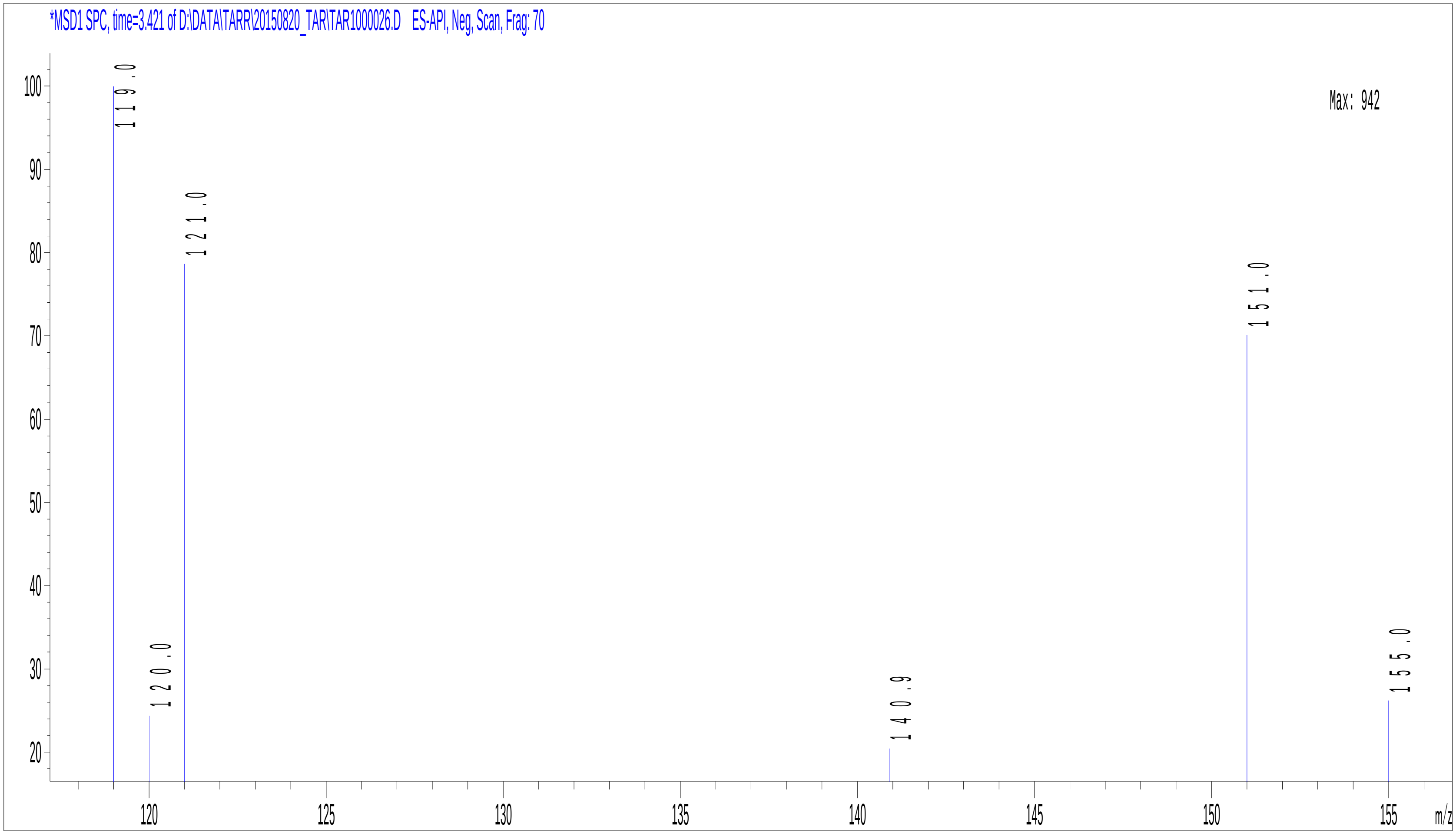
pH 7

14-Jul-15
H2O2 Ctrl
7
P2-C-08

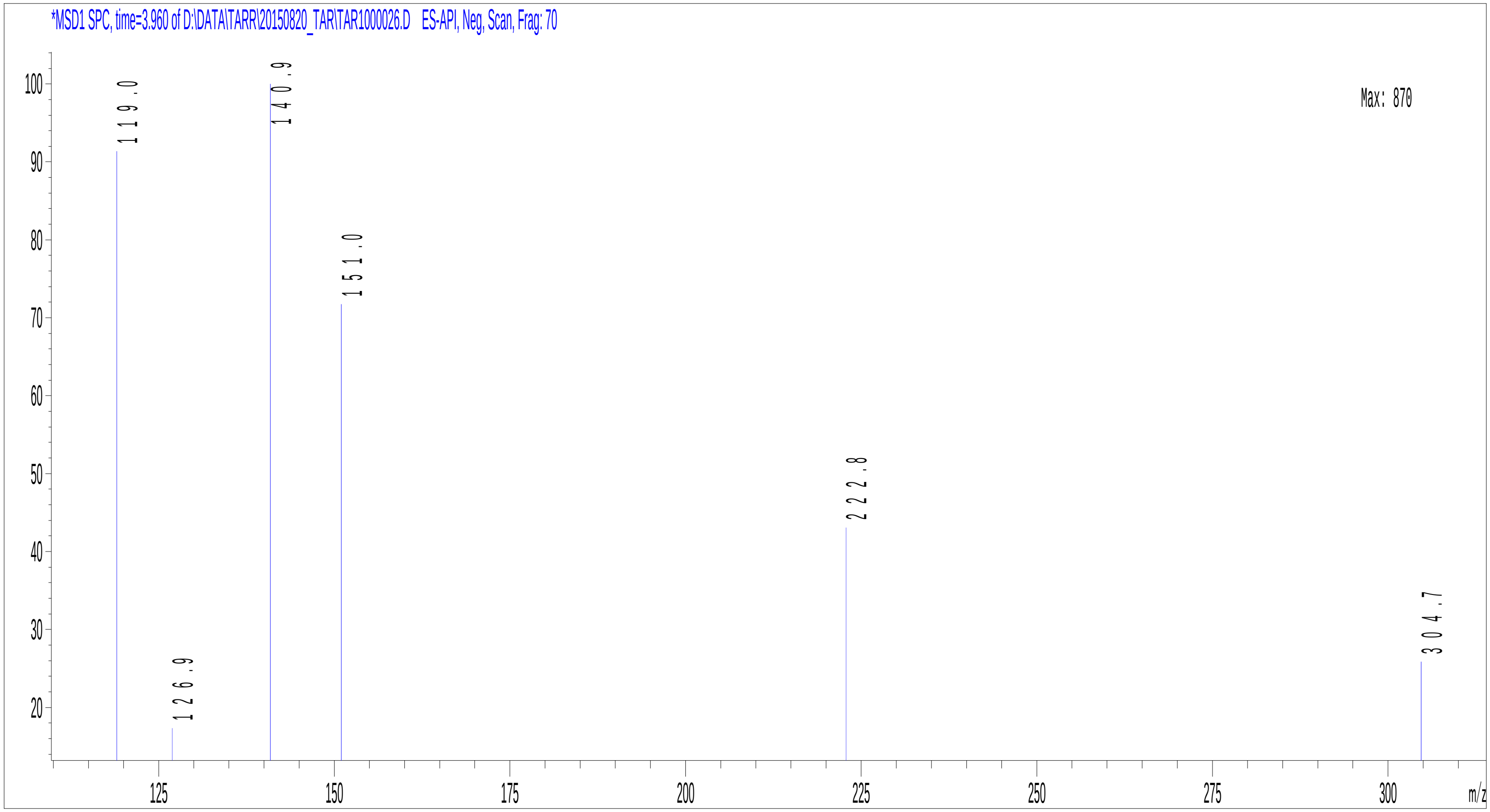


#	Time	Area	Height	Width	Area%	Symmetry
1	2.968	300583.7	30821.8	0.1391	100.000	0.888

*MSD1 SPC, time=2.983 of D:\DATA\TARR\20150820_TAR\TAR1000026.D ES-API, Neg, Scan, Frag: 70
Max: 10029
466.6
467.6
468.6
477.7
232.8
197.8
196.8
210.8
155.0
170.9
119.0
0
20
40
60
80
100
150
200
250
300
350
400
450
500m/z



*MSD1 SPC, time=3.421 of D:\DATA\TARR\20150820_TAR\TAR1000026.D ES-API, Neg, Scan, Frag: 70
Max: 942
119.0
120.0
121.0
140.9
151.0
155.0
100
90
80
70
60
50
40
30
20
120
125
130
135
140
145
150
155
m/z

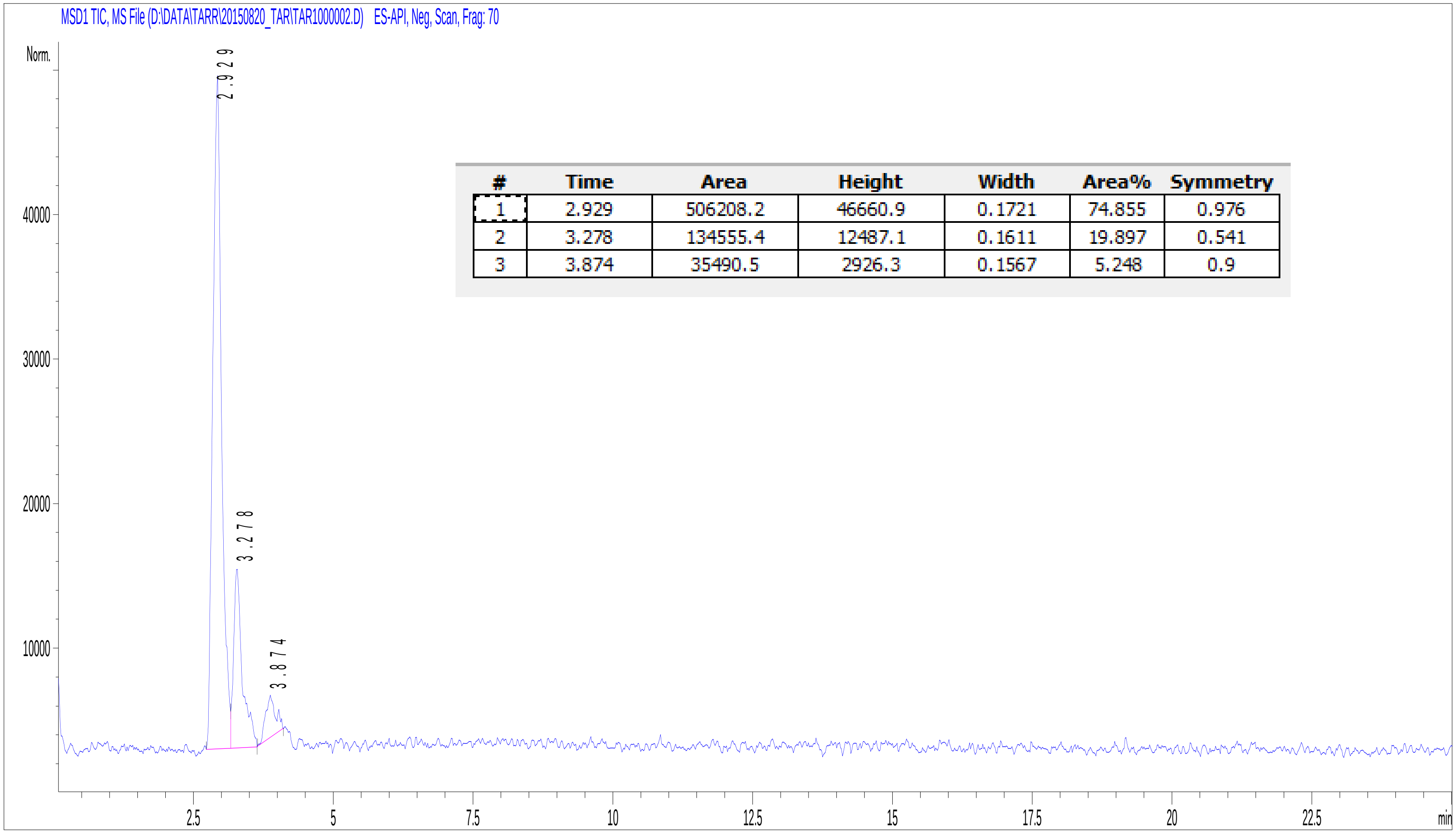

*MSD1 SPC, time=3.960 of D:\DATA\TARR\20150820_TAR\TAR1000026.D ES-API, Neg, Scan, Frag: 70
Max: 870
119.0
126.9
140.9
151.0
222.8
304.7
100
90
80
70
60
50
40
30
20
125
150
175
200
225
250
275
300
m/z

7-Mar-15

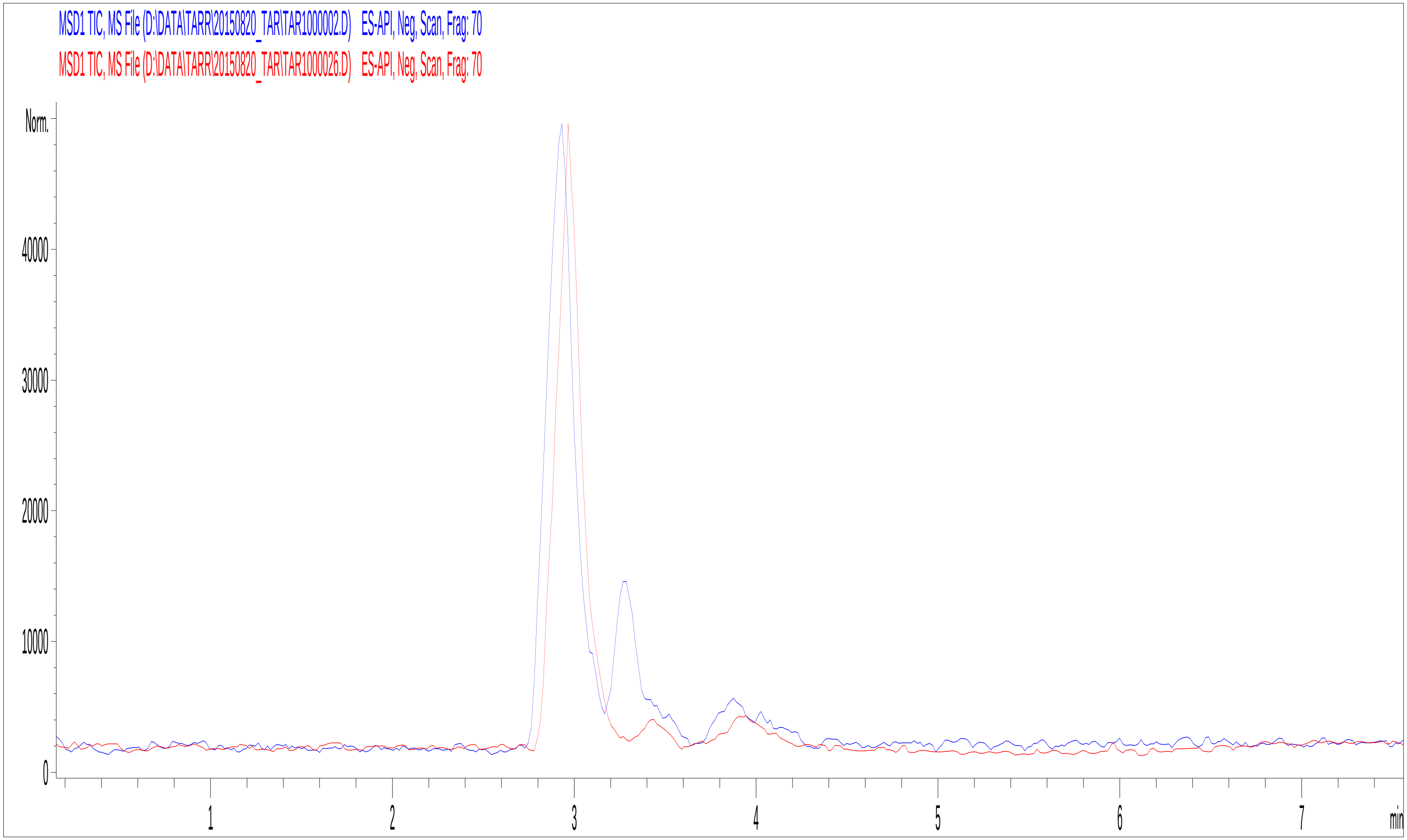
0 DC

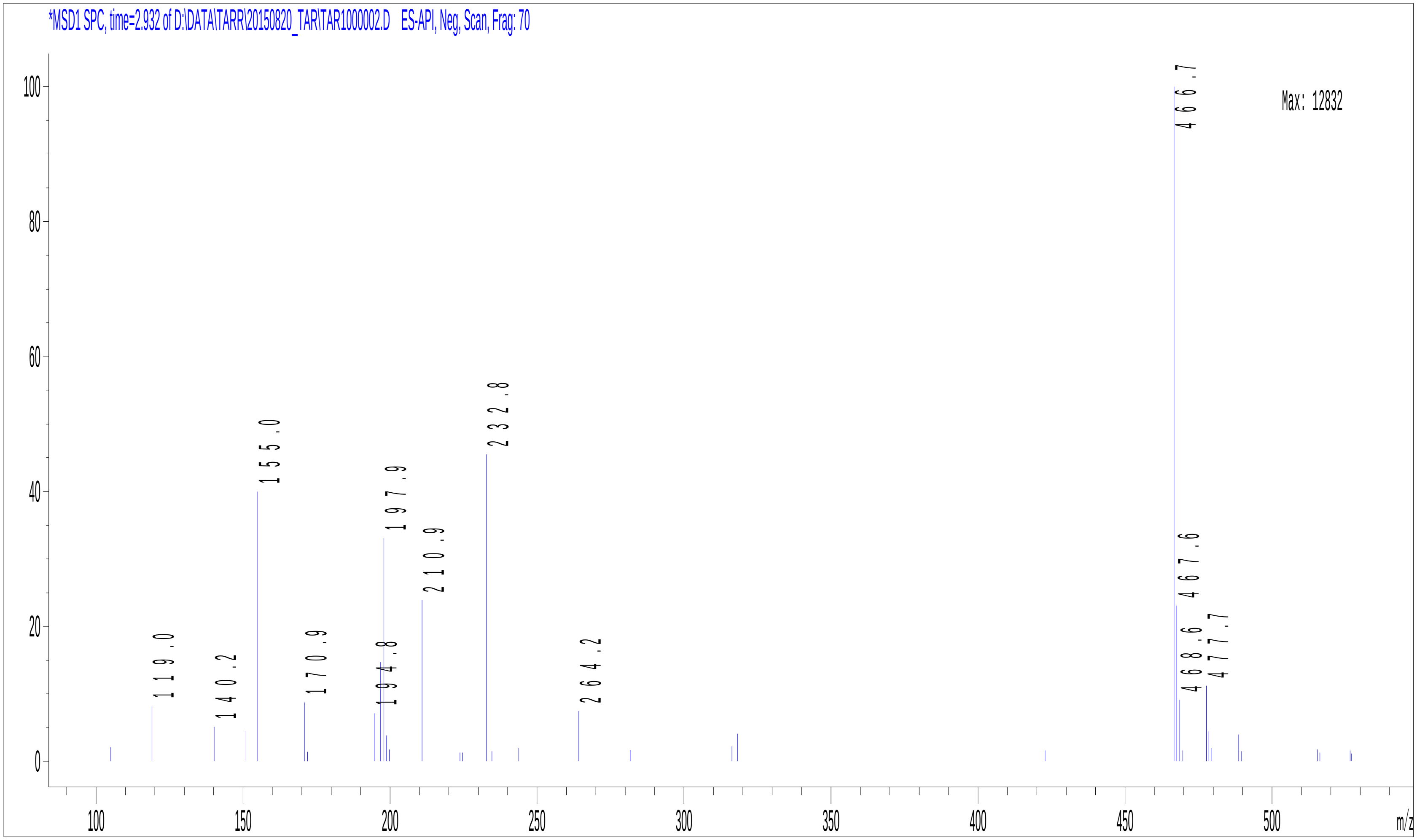
7

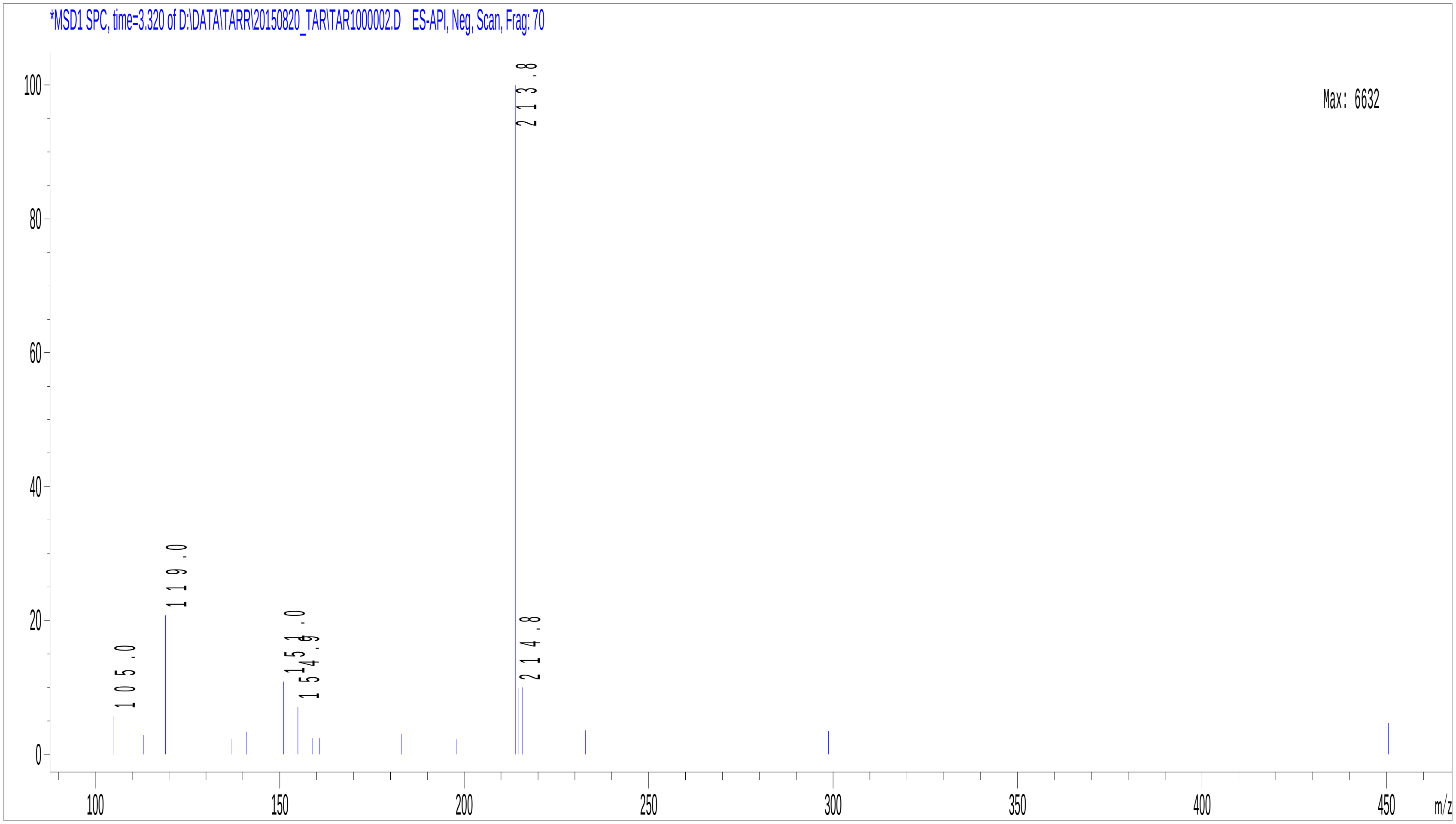
P2-A-02

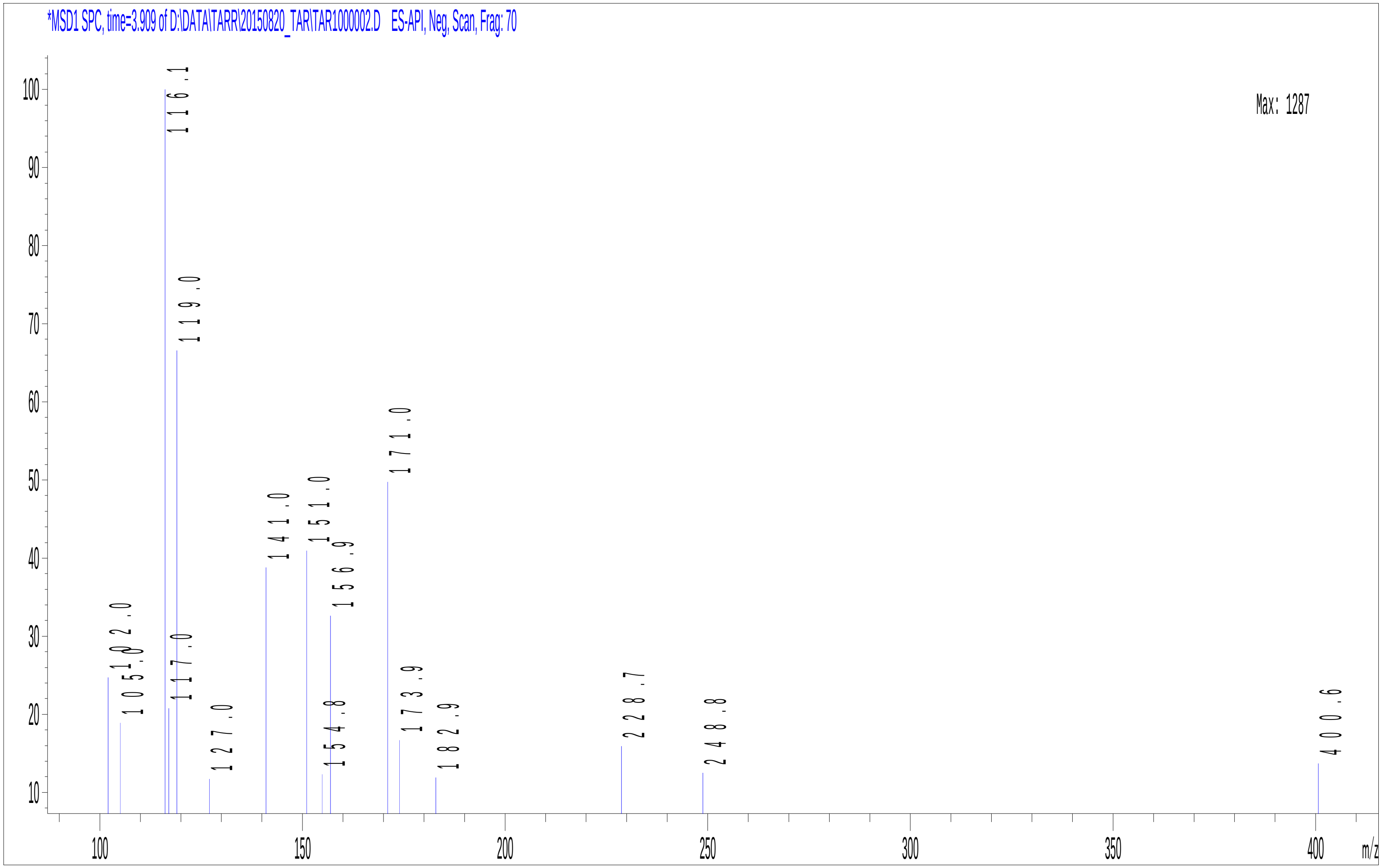


#	Time	Area	Height	Width	Area%	Symmetry
1	2.929	506208.2	46660.9	0.1721	74.855	0.976
2	3.278	134555.4	12487.1	0.1611	19.897	0.541
3	3.874	35490.5	2926.3	0.1567	5.248	0.9


MSD1 TIC, MS File (D:\DATA\TARR\20150820_TAR\TAR1000002.D) ES-API, Neg, Scan, Frag: 70
MSD1 TIC, MS File (D:\DATA\TARR\20150820_TAR\TAR1000026.D) ES-API, Neg, Scan, Frag: 70
Norm.
40000
30000
20000
10000
0
1
2
3
4
5
6
7
min


*MSD1 SPC, time=2.932 of D:\DATA\TARR\20150820_TAR\TAR1000002.D ES-API, Neg, Scan, Frag: 70
Max: 12832
466.7
467.6
468.6
477.7
232.8
155.0
197.9
210.9
194.8
170.9
140.2
119.0
264.2
0
20
40
60
80
100
100
150
200
250
300
350
400
450
500
m/z

*MSD1 SPC, time=3.320 of D:\DATA\TARR\20150820_TAR\TAR1000002.D ES-API, Neg, Scan, Frag: 70
Max: 6632
213.8
119.0
105.0
151.0
154.9
214.8
0
20
40
60
80
100
100
150
200
250
300
350
400
450
m/z

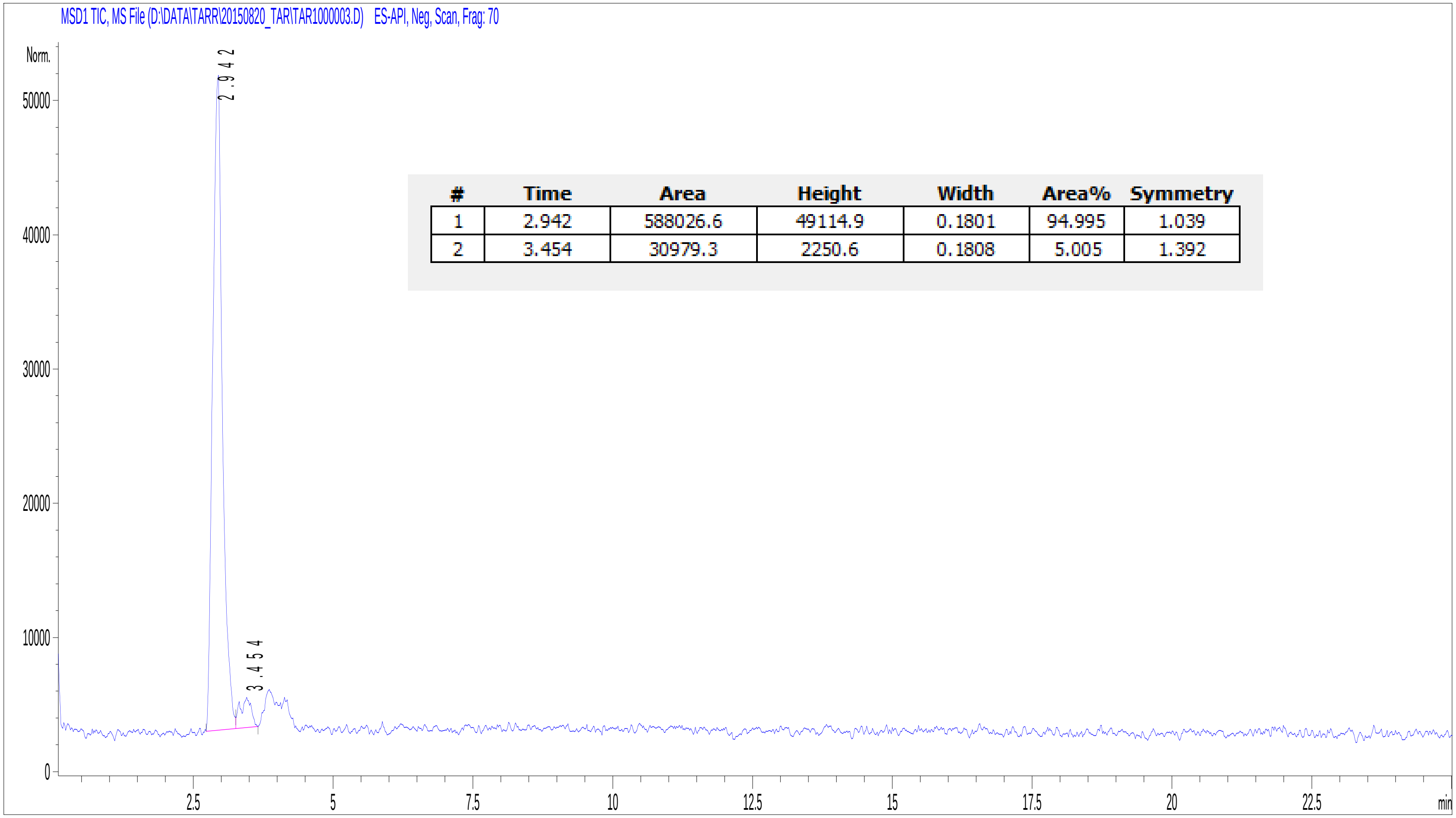

*MSD1 SPC, time=3.909 of D:\DATA\TARR\20150820_TAR\TAR1000002.D ES-API, Neg, Scan, Frag: 70
Max: 1287
100
90
80
70
60
50
40
30
20
10
102.0
105.0
116.1
117.0
119.0
127.0
141.0
151.0
154.8
156.9
171.0
173.9
182.9
228.7
248.8
400.6
100
150
200
250
300
350
400
m/z

13-Mar-15

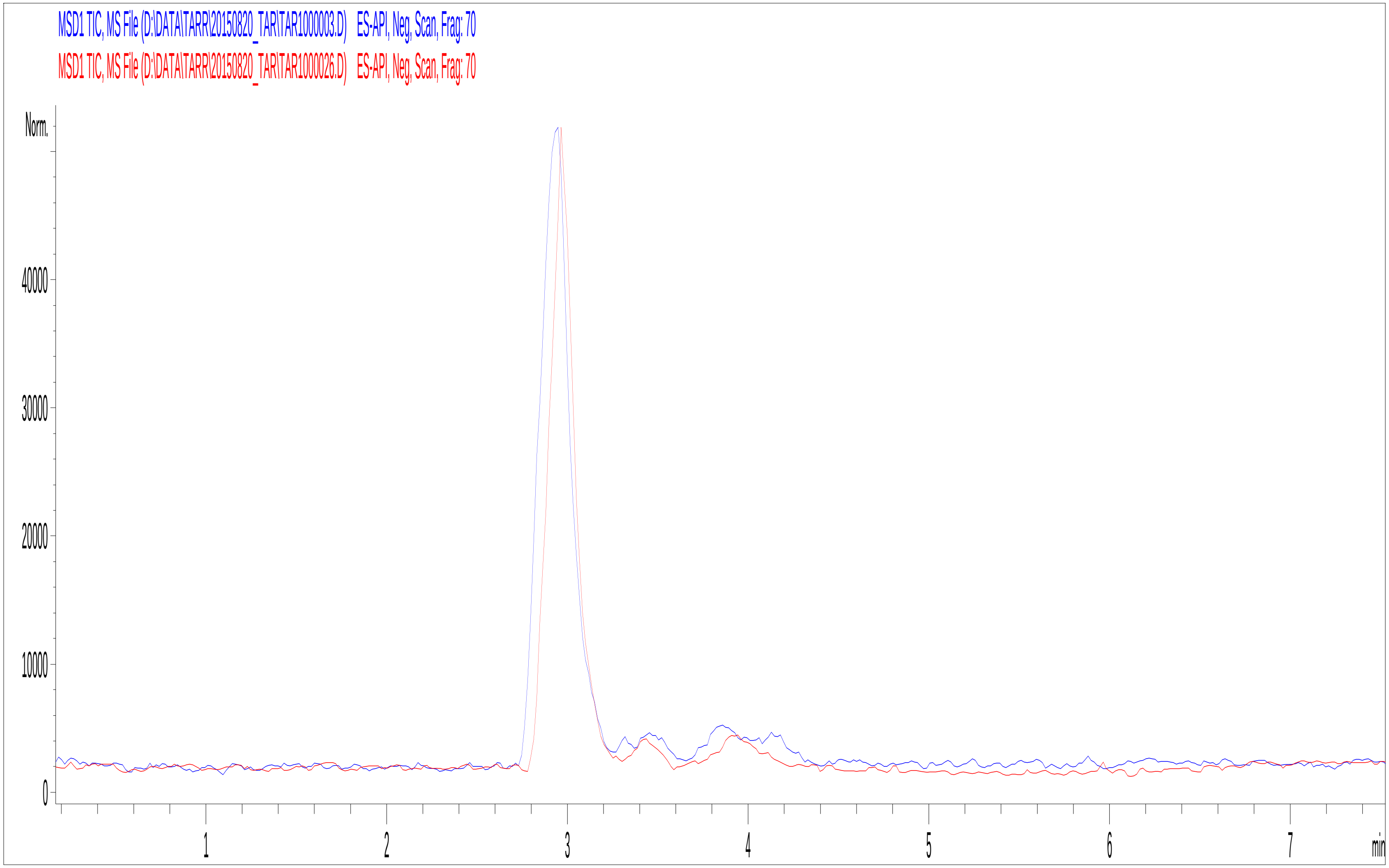
5 DC

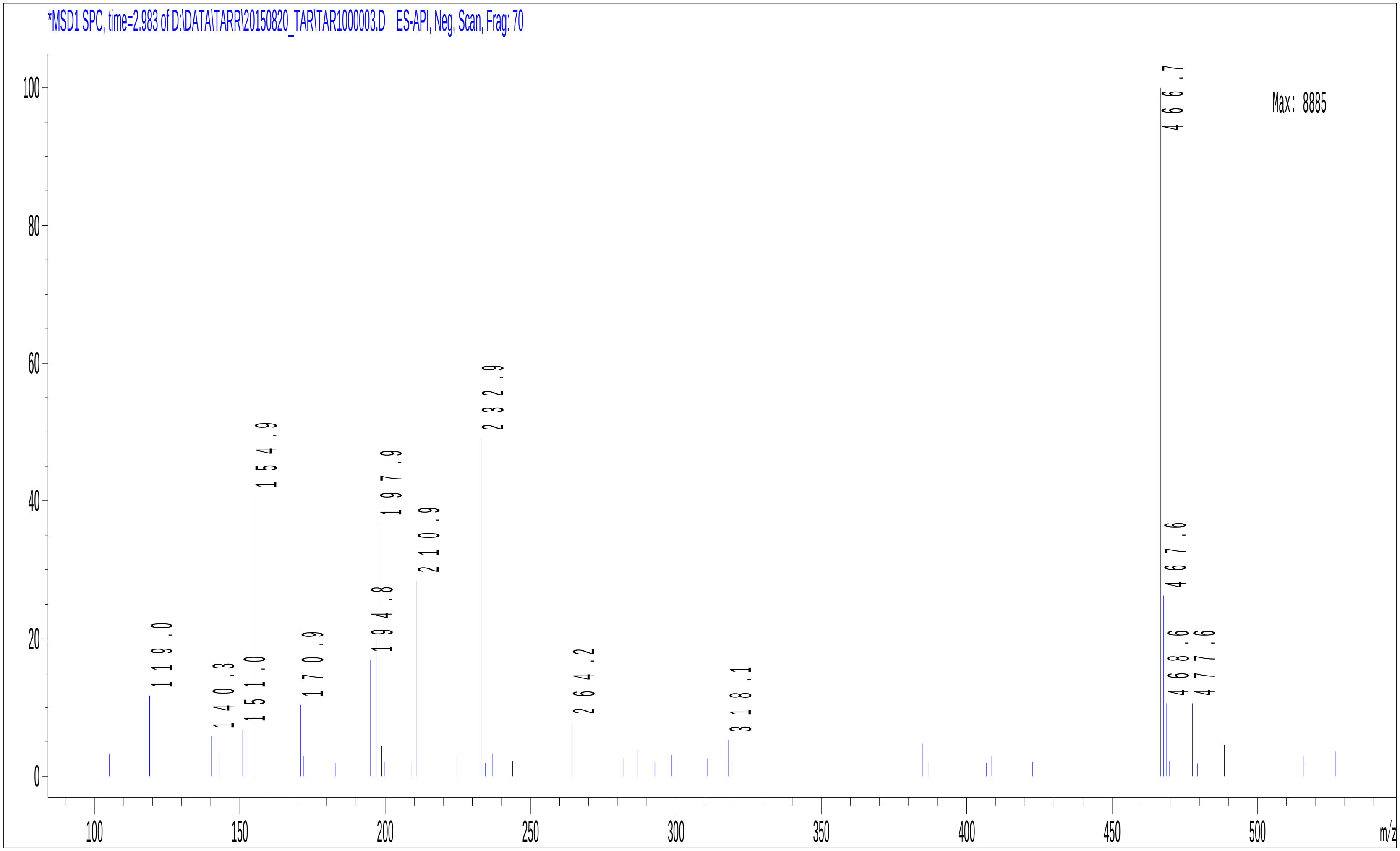
7

P2-A-03

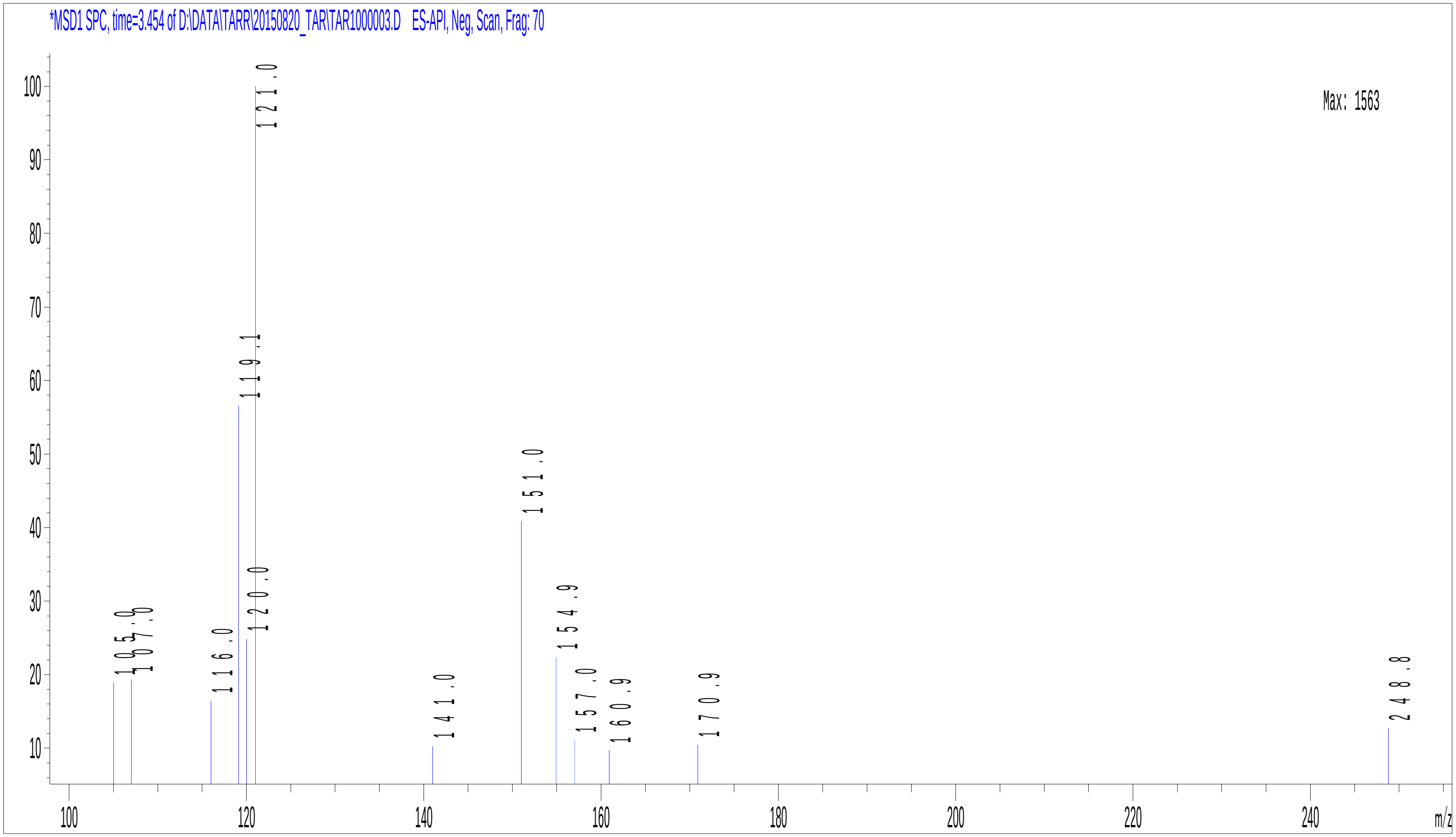


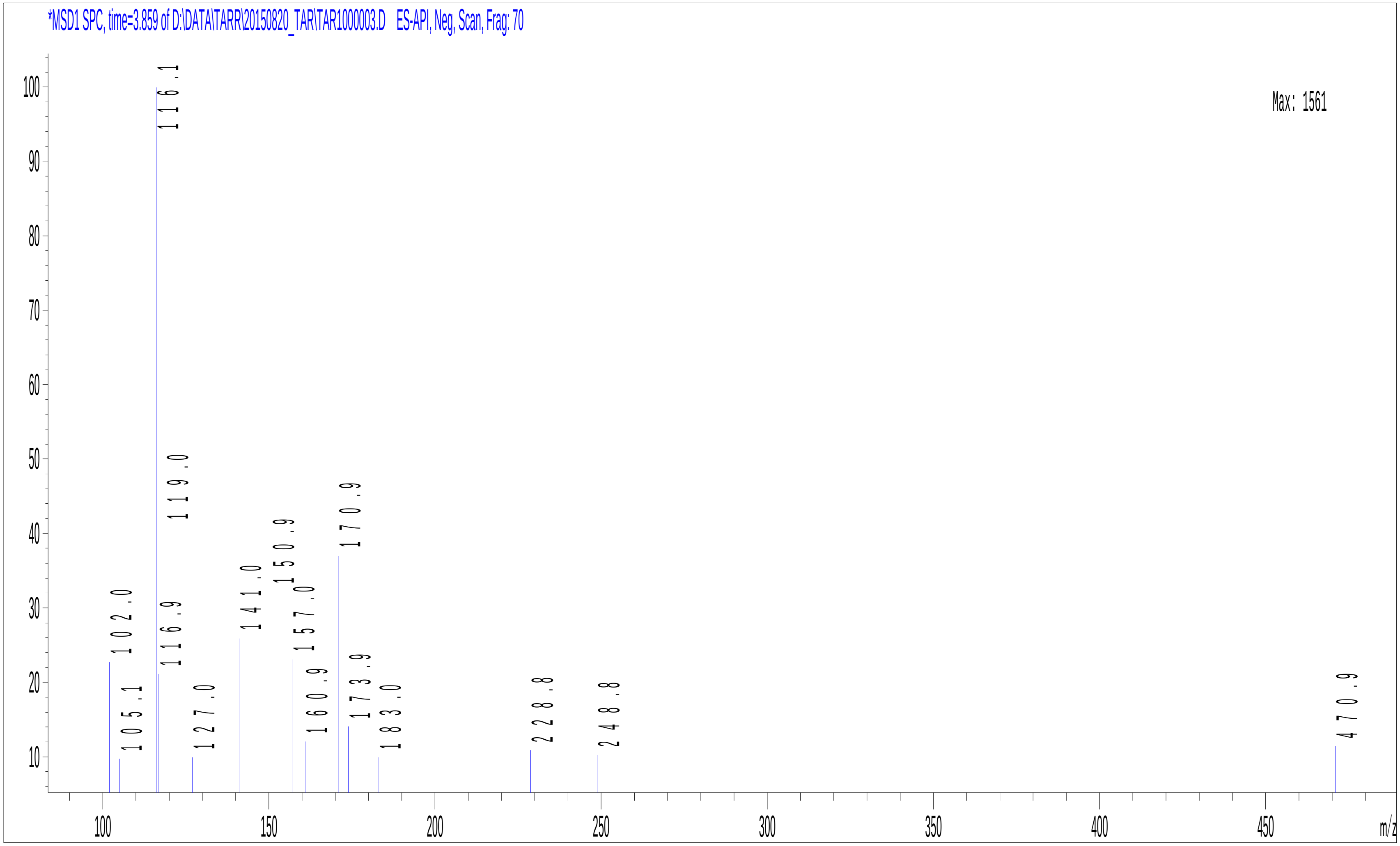
#	Time	Area	Height	Width	Area%	Symmetry
1	2.942	588026.6	49114.9	0.1801	94.995	1.039
2	3.454	30979.3	2250.6	0.1808	5.005	1.392

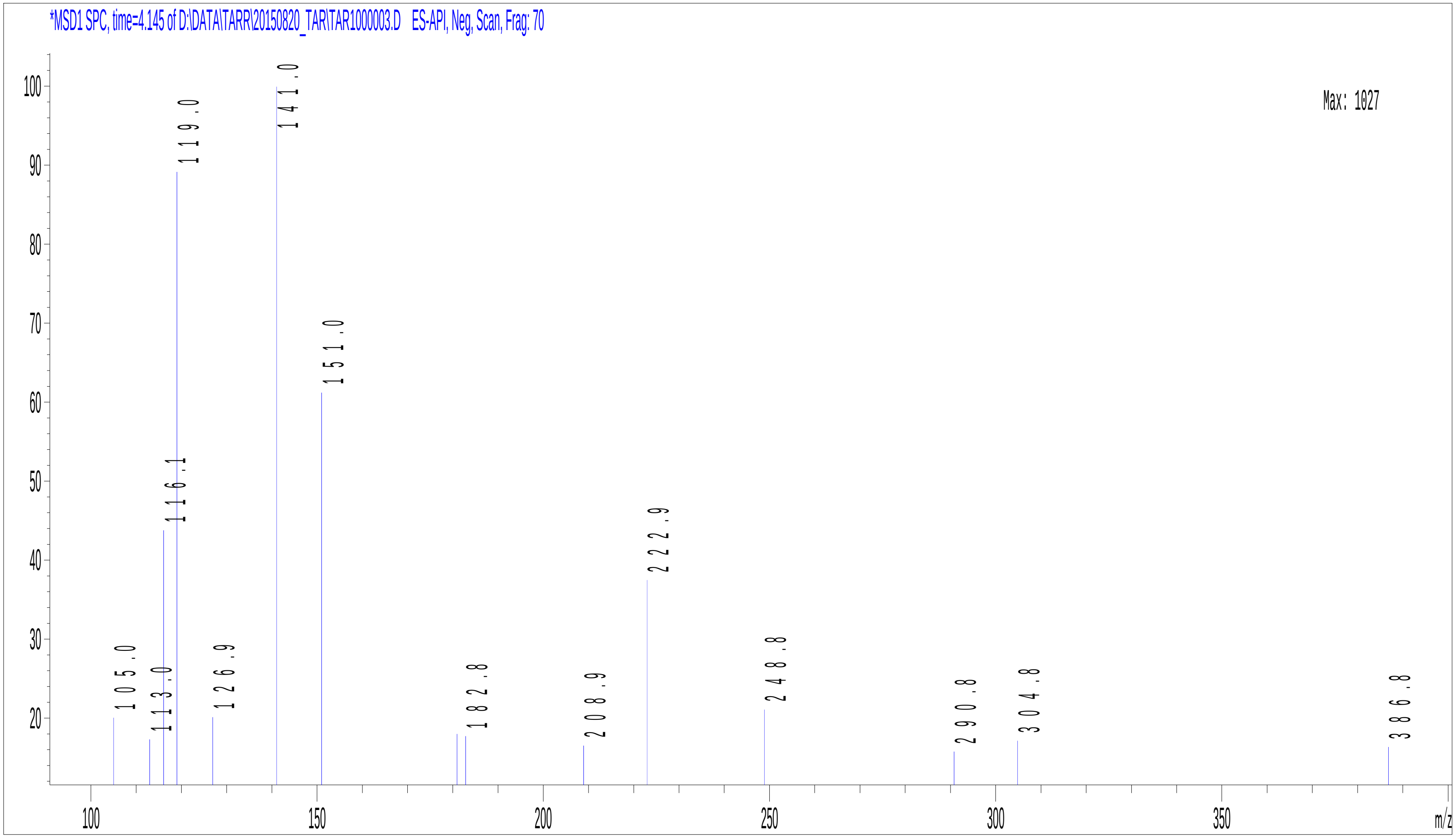

MSD1 TIC, MS File (D:\DATA\TARR\20150820_TAR\TAR1000003.D) ES-API, Neg, Scan, Frag: 70
MSD1 TIC, MS File (D:\DATA\TARR\20150820_TAR\TAR1000026.D) ES-API, Neg, Scan, Frag: 70
Norm.
40000
30000
20000
10000
0
1
2
3
4
5
6
7
min



*MSD1 SPC, time=2.983 of D:\DATA\TARR\20150820_TAR\TAR1000003.D ES-API, Neg, Scan, Frag: 70
Max: 8885
0
20
40
60
80
100
100
150
200
250
300
350
400
450
500
m/z
119.0
140.3
151.0
154.9
170.9
194.8
197.9
210.9
232.9
264.2
318.1
466.7
467.6
468.6
477.6


*MSD1 SPC, time=3.454 of D:\DATA\TARR\20150820_TAR\TAR1000003.D ES-API, Neg, Scan, Frag: 70
Max: 1563
121.0
119.1
151.0
120.0
154.9
105.0
107.0
116.0
141.0
157.0
160.9
170.9
248.8
100
90
80
70
60
50
40
30
20
10
100
120
140
160
180
200
220
240
m/z


*MSD1 SPC, time=3.859 of D:\DATA\TARR\20150820_TAR\TAR1000003.D ES-API, Neg, Scan, Frag: 70
Max: 1561
100
90
80
70
60
50
40
30
20
10
100
150
200
250
300
350
400
450
m/z
116.1
119.0
170.9
150.9
141.0
157.0
102.0
116.9
173.9
105.1
127.0
160.9
183.0
228.8
248.8
470.9

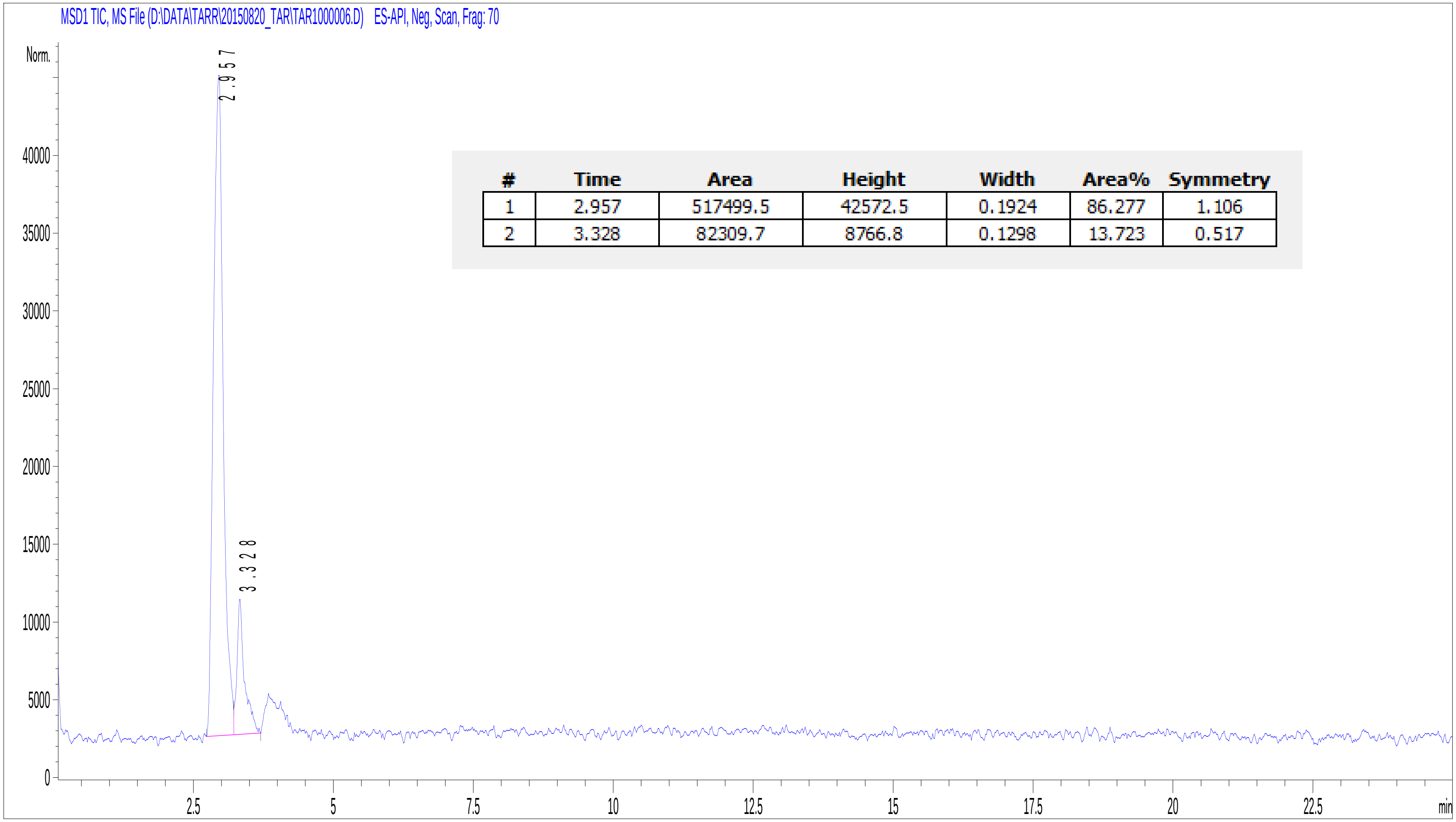

*MSD1 SPC, time=4.145 of D:\DATA\TARR\20150820_TAR\TAR1000003.D ES-API, Neg, Scan, Frag: 70
Max: 1027
105.0
113.0
116.1
119.0
126.9
141.0
151.0
182.8
208.9
222.9
248.8
290.8
304.8
386.8
100
90
80
70
60
50
40
30
20
100
150
200
250
300
350
m/z

9-Apr-15

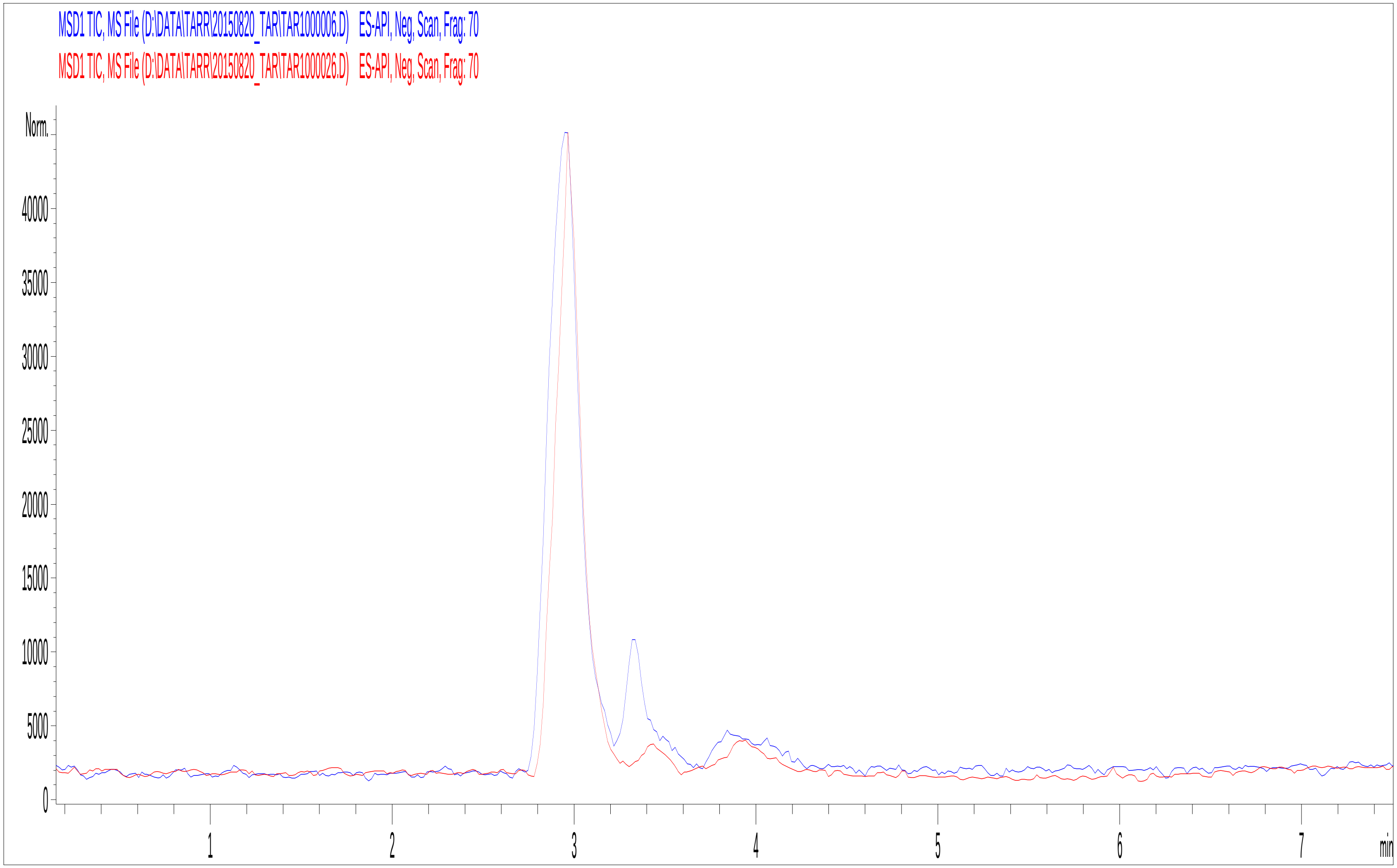
10 DC

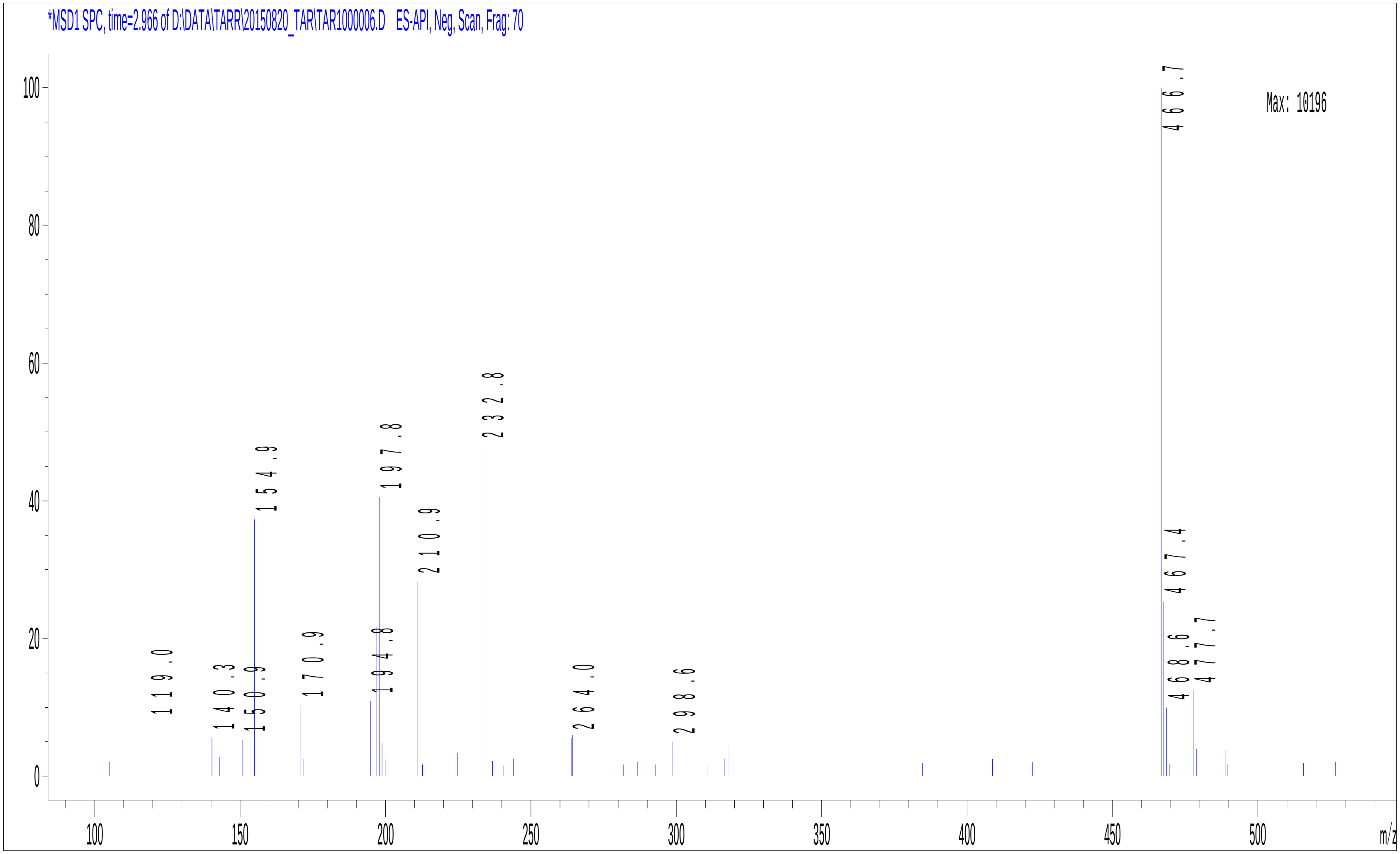
7

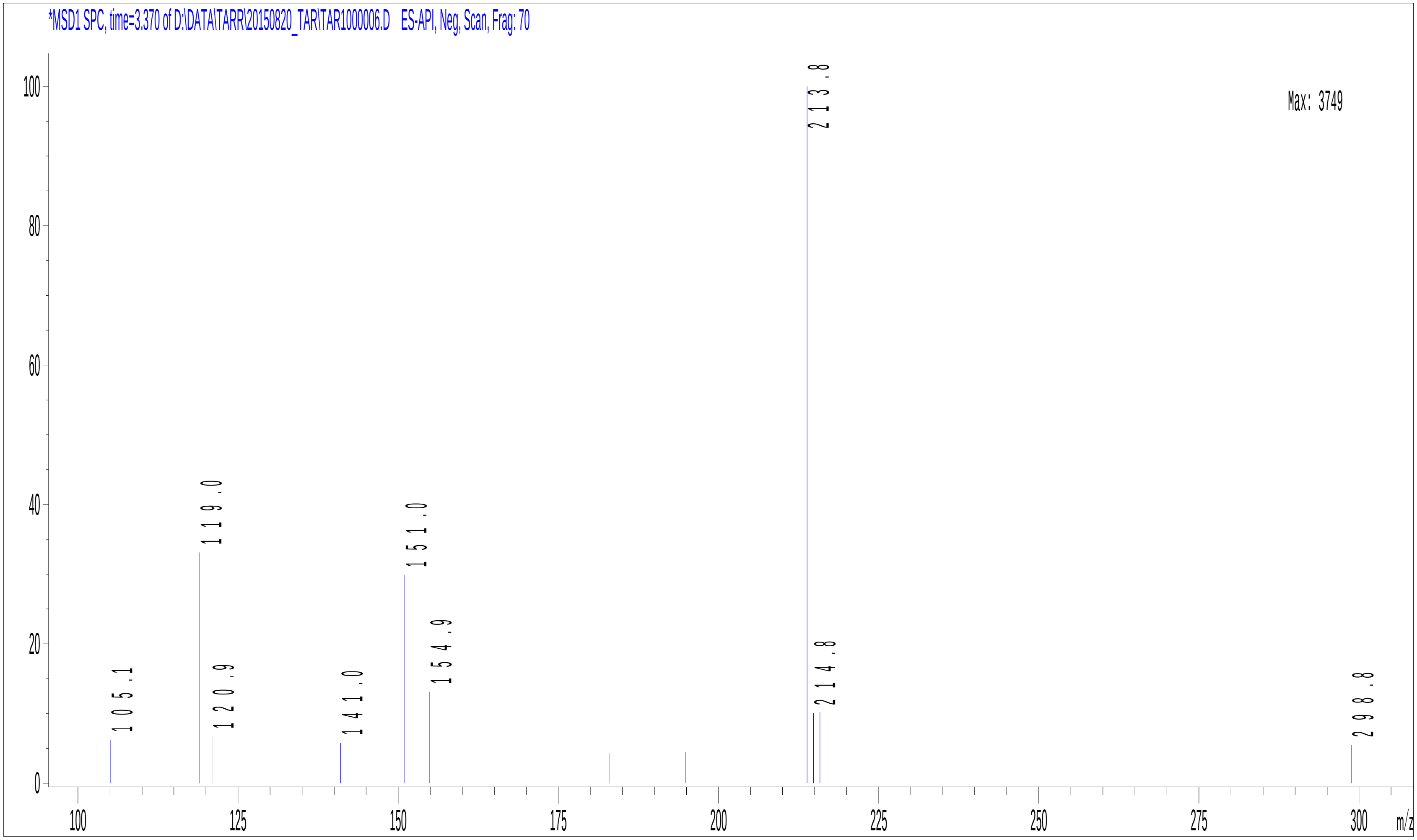
P2-A-06

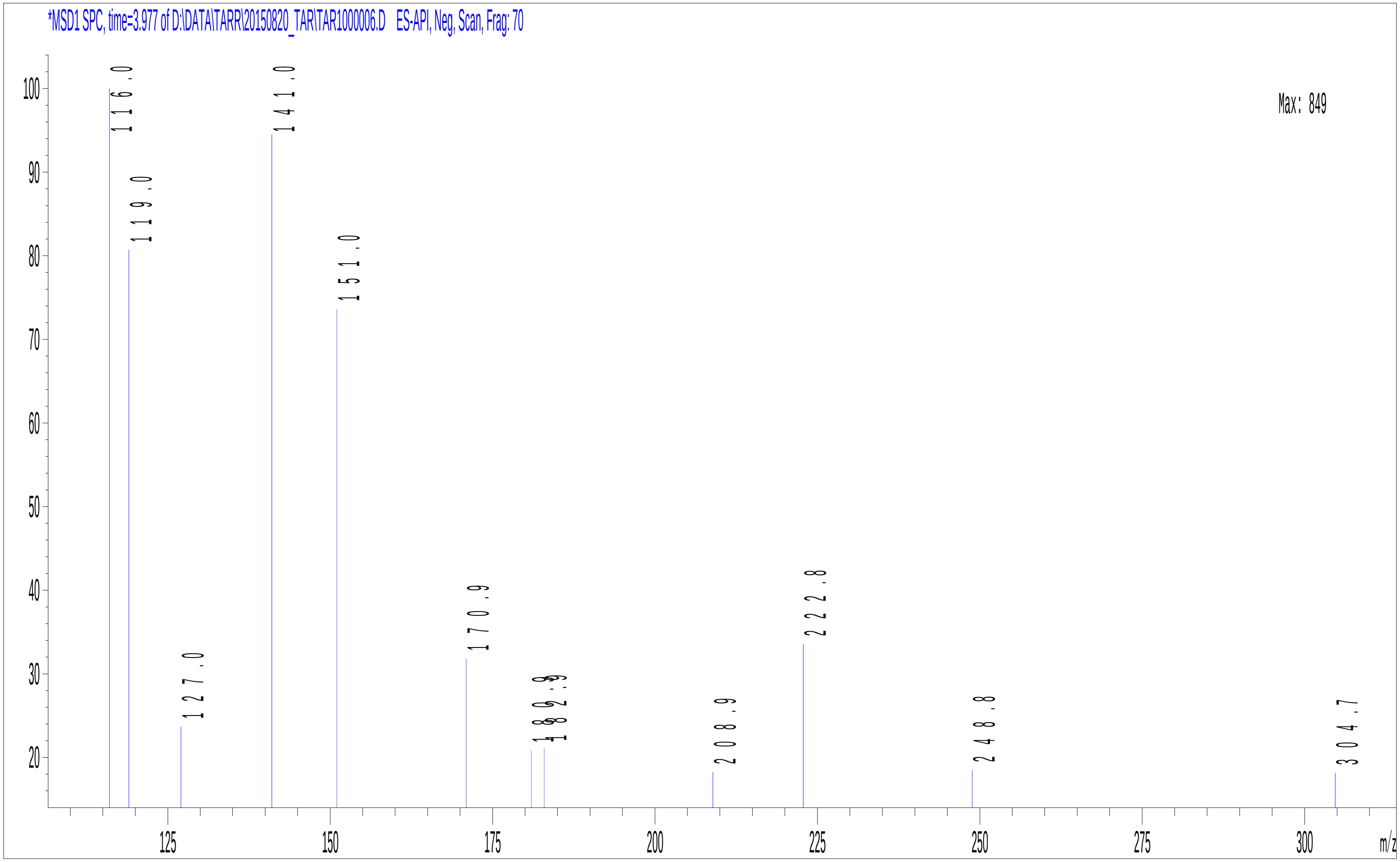


#	Time	Area	Height	Width	Area%	Symmetry
1	2.957	517499.5	42572.5	0.1924	86.277	1.106
2	3.328	82309.7	8766.8	0.1298	13.723	0.517


MSD1 TIC, MS File (D:\DATA\TARR\20150820_TAR\TAR1000006.D)   ES-API, Neg, Scan, Frag: 70
MSD1 TIC, MS File (D:\DATA\TARR\20150820_TAR\TAR1000026.D)   ES-API, Neg, Scan, Frag: 70
Norm.
40000
35000
30000
25000
20000
15000
10000
5000
0
1
2
3
4
5
6
7
min


*MSD1 SPC, time=2.966 of D:\DATA\TARR\20150820_TAR\TAR1000006.D ES-API, Neg, Scan, Frag: 70
Max: 10196
466.7
232.8
154.9
197.8
210.9
467.4
119.0
140.3
150.9
170.9
194.8
264.0
298.6
468.6
477.7
0
20
40
60
80
100
100
150
200
250
300
350
400
450
500
m/z


*MSD1 SPC, time=3.370 of D:\DATA\TARR\20150820_TAR\TAR1000006.D ES-API, Neg, Scan, Frag: 70
Max: 3749
213.8
119.0
151.0
154.9
105.1
120.9
141.0
214.8
298.8
0
20
40
60
80
100
100
125
150
175
200
225
250
275
300
m/z

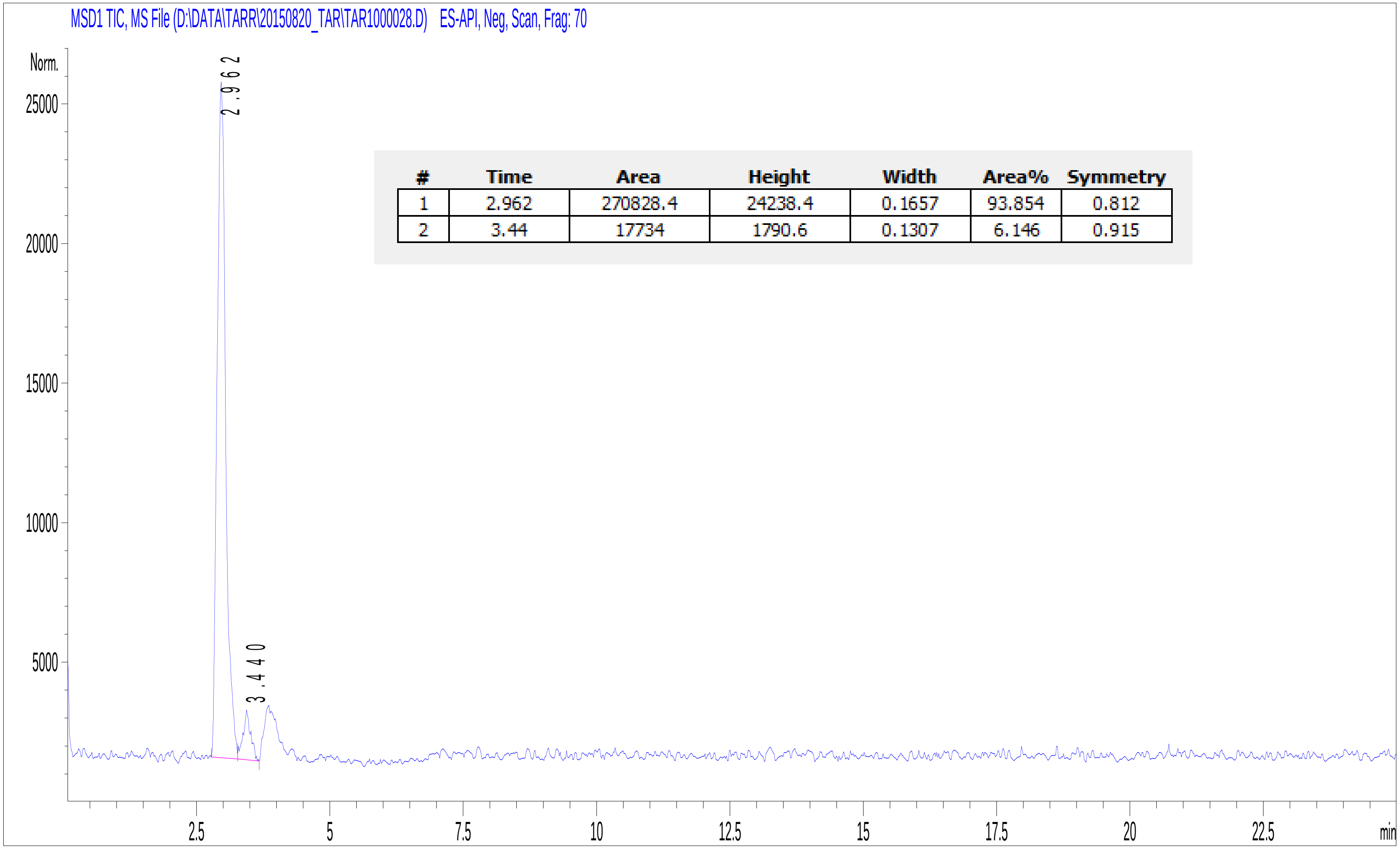

*MSD1 SPC, time=3.977 of D:\DATA\TARR\20150820_TAR\TAR1000006.D   ES-API, Neg, Scan, Frag: 70
Max: 849
116.0
119.0
127.0
141.0
151.0
170.9
180.9
182.9
208.9
222.8
248.8
304.7
100
90
80
70
60
50
40
30
20
125
150
175
200
225
250
275
300
m/z

6-Aug-15

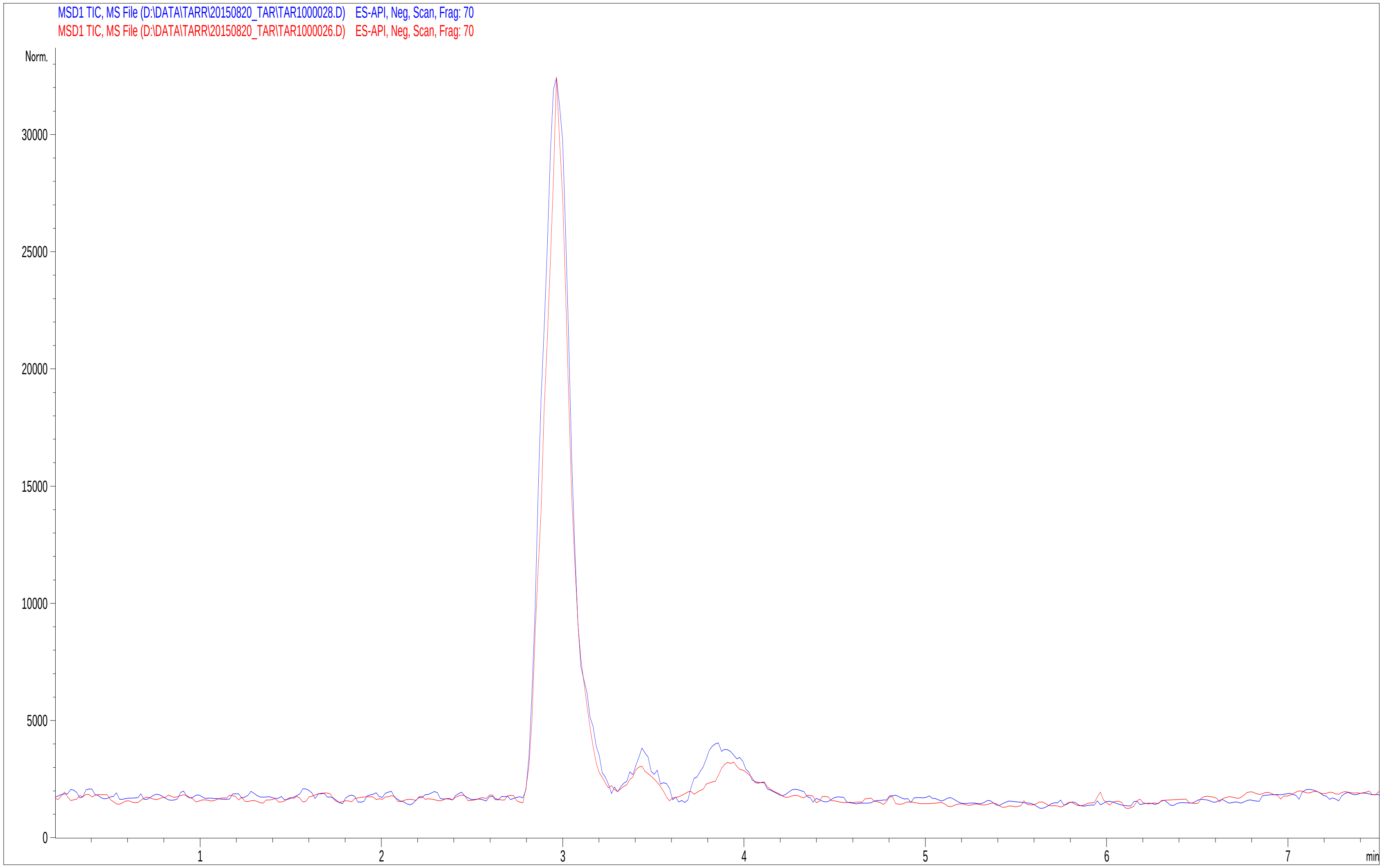
20 DC

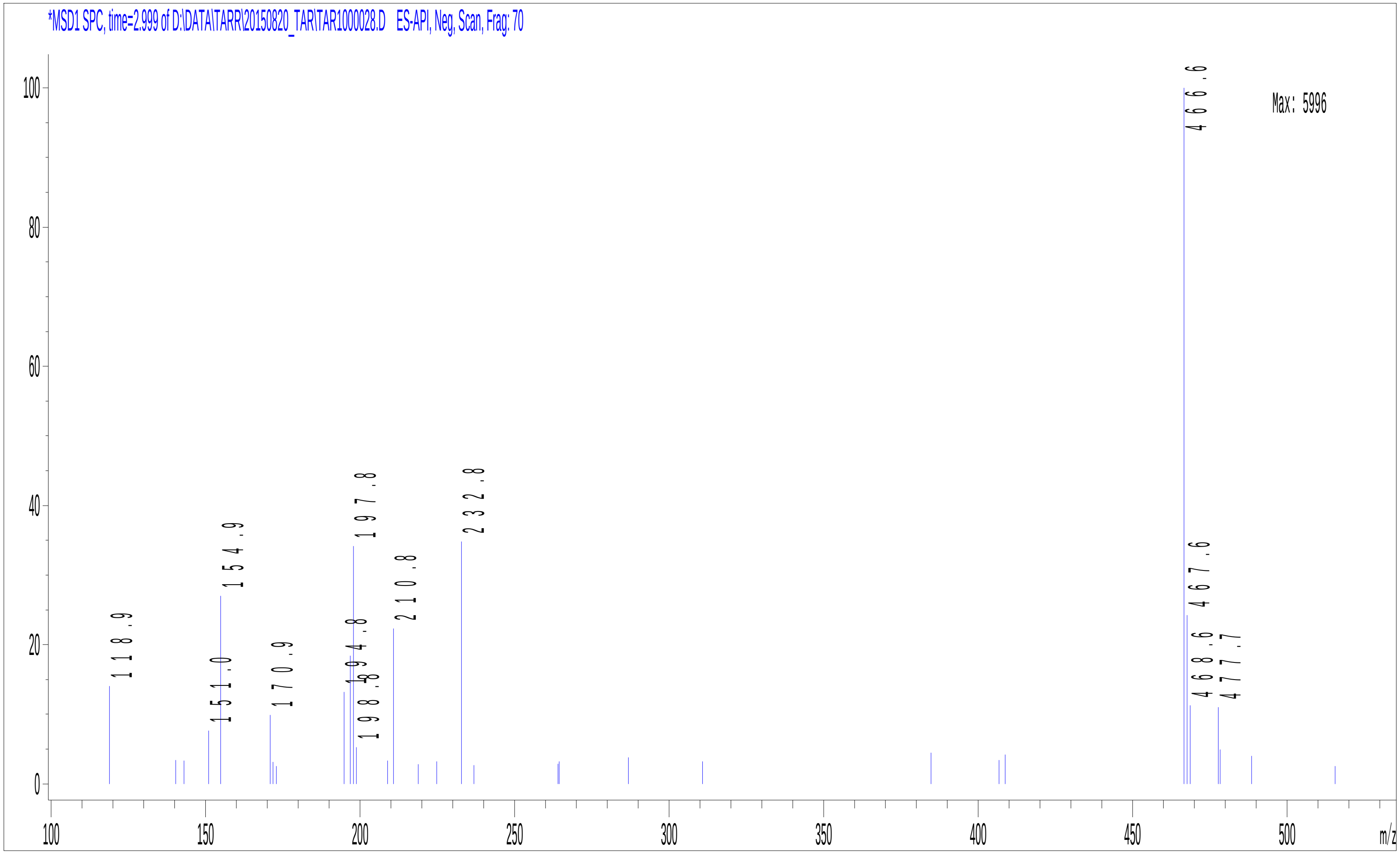
7

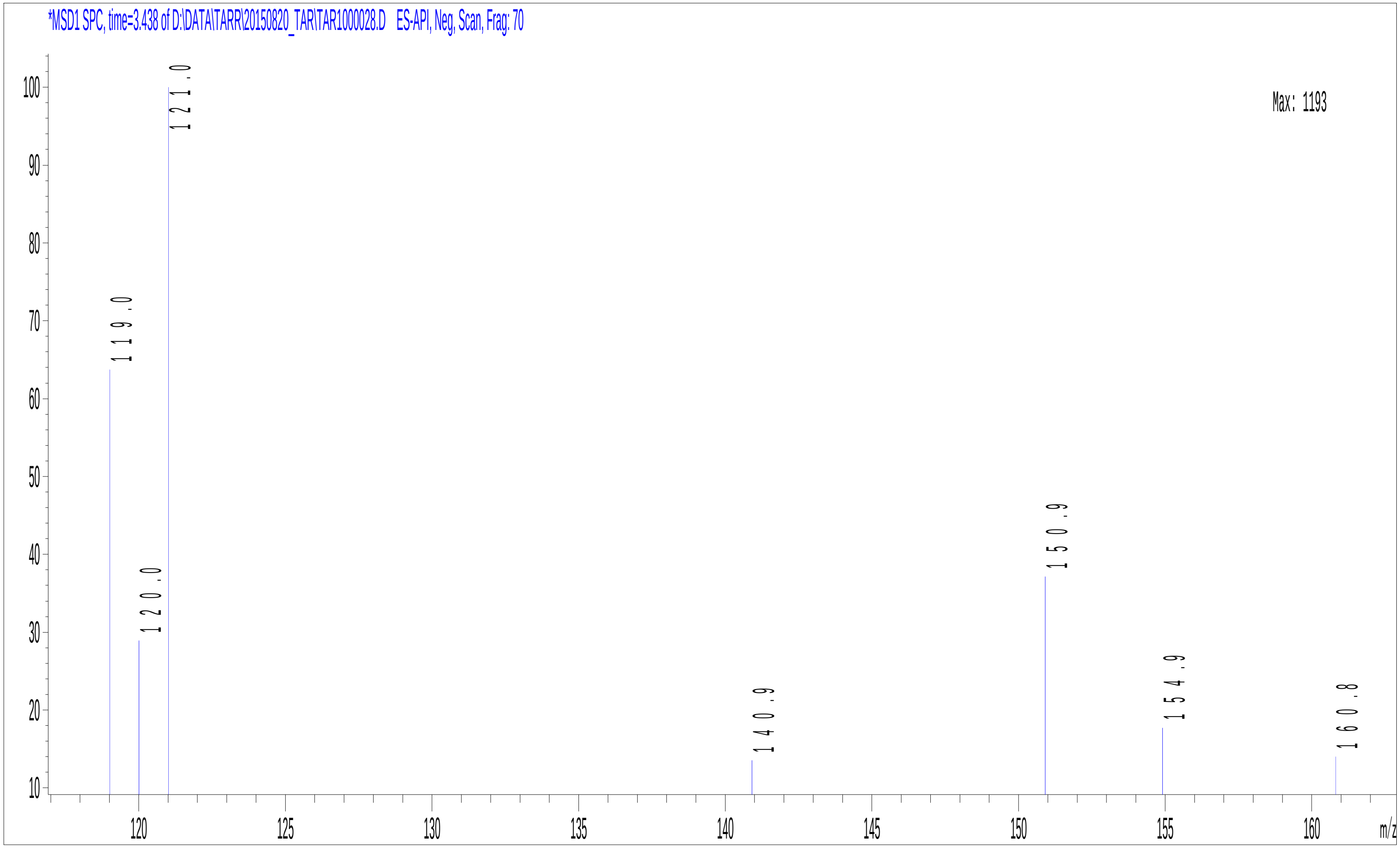
P2-D-09

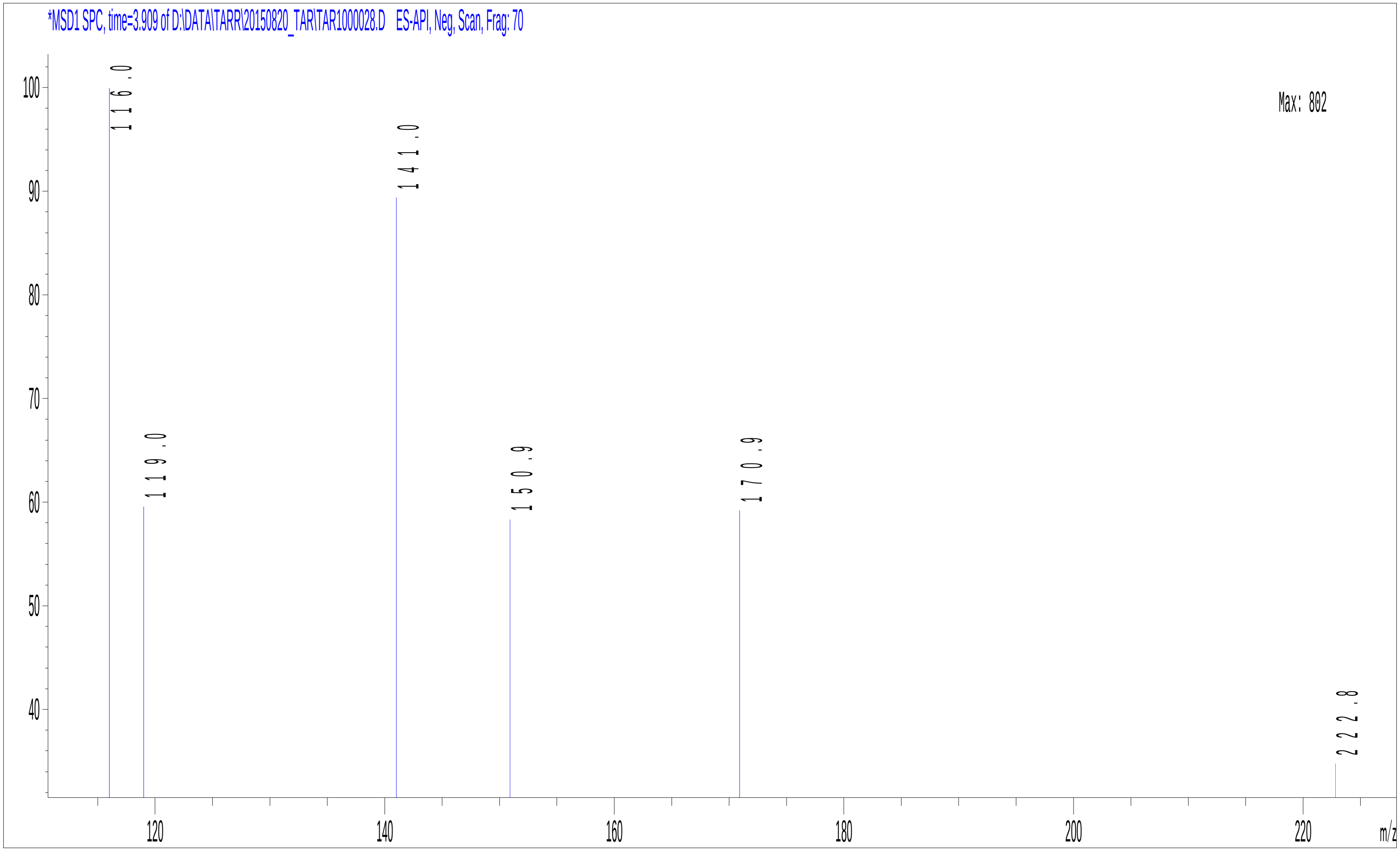


#	Time	Area	Height	Width	Area%	Symmetry
1	2.962	270828.4	24238.4	0.1657	93.854	0.812
2	3.44	17734	1790.6	0.1307	6.146	0.915


MSD1 TIC, MS File (D:\DATA\TARR\20150820_TAR\TAR1000028.D) ES-API, Neg, Scan, Frag: 70
MSD1 TIC, MS File (D:\DATA\TARR\20150820_TAR\TAR1000026.D) ES-API, Neg, Scan, Frag: 70
Norm.
30000
25000
20000
15000
10000
5000
0
1
2
3
4
5
6
7
min


*MSD1 SPC, time=2.999 of D:\DATA\TARR\20150820_TAR\TAR1000028.D ES-API, Neg, Scan, Frag: 70
Max: 5996
466.6
467.6
468.6
477.7
118.9
151.0
154.9
170.9
194.8
197.8
198.8
210.8
232.8
0
20
40
60
80
100
100
150
200
250
300
350
400
450
500
m/z


*MSD1 SPC, time=3.438 of D:\DATA\TARR\20150820_TAR\TAR1000028.D ES-API, Neg, Scan, Frag: 70
Max: 1193
100
90
80
70
60
50
40
30
20
10
119.0
120.0
121.0
140.9
150.9
154.9
160.8
120
125
130
135
140
145
150
155
160
m/z

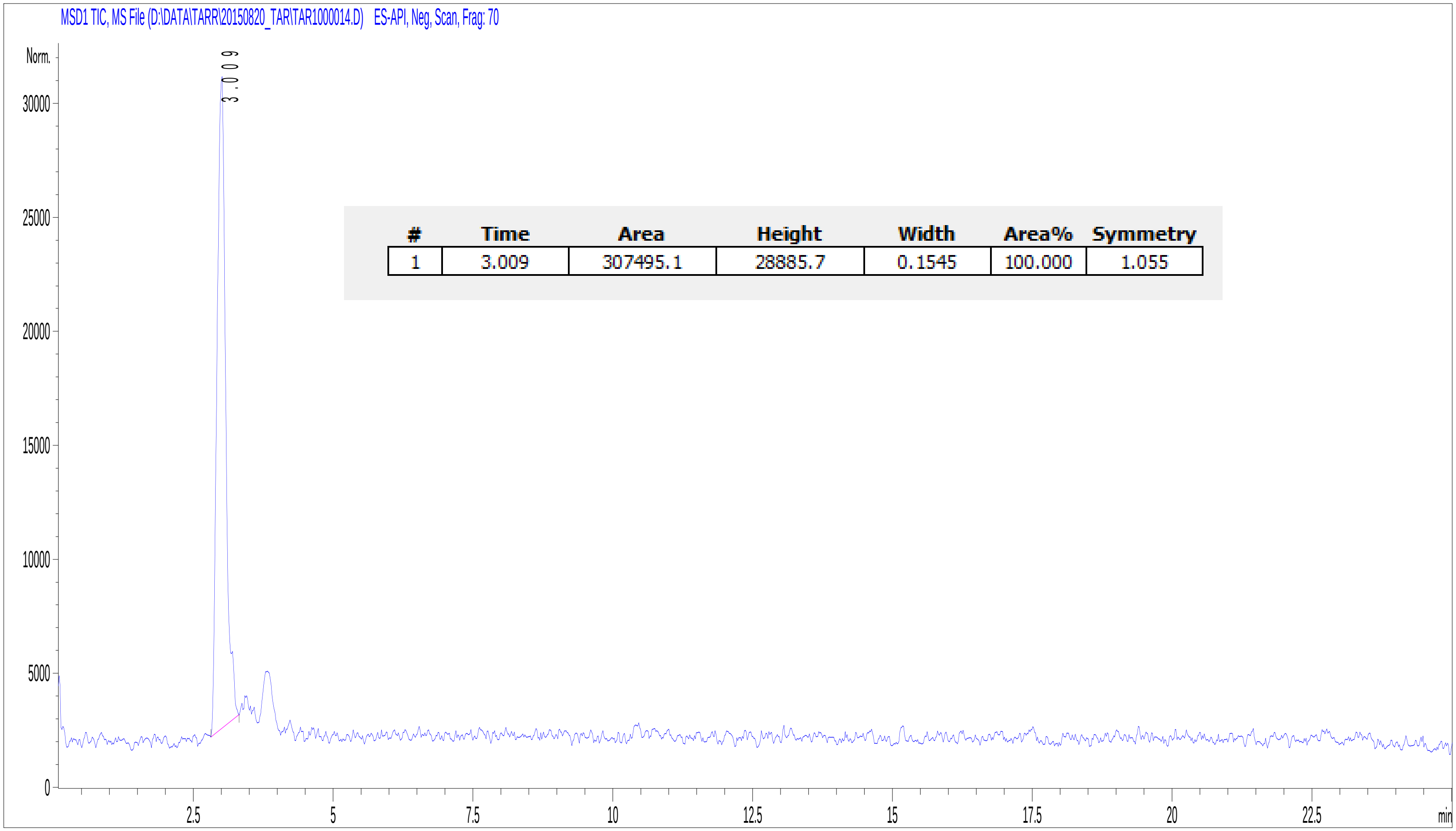

*MSD1 SPC, time=3.909 of D:\DATA\TARR\20150820_TAR\TAR1000028.D ES-API, Neg, Scan, Frag: 70
Max: 802
116.0
119.0
141.0
150.9
170.9
222.8
100
90
80
70
60
50
40
120
140
160
180
200
220
m/z

3-Jun-15

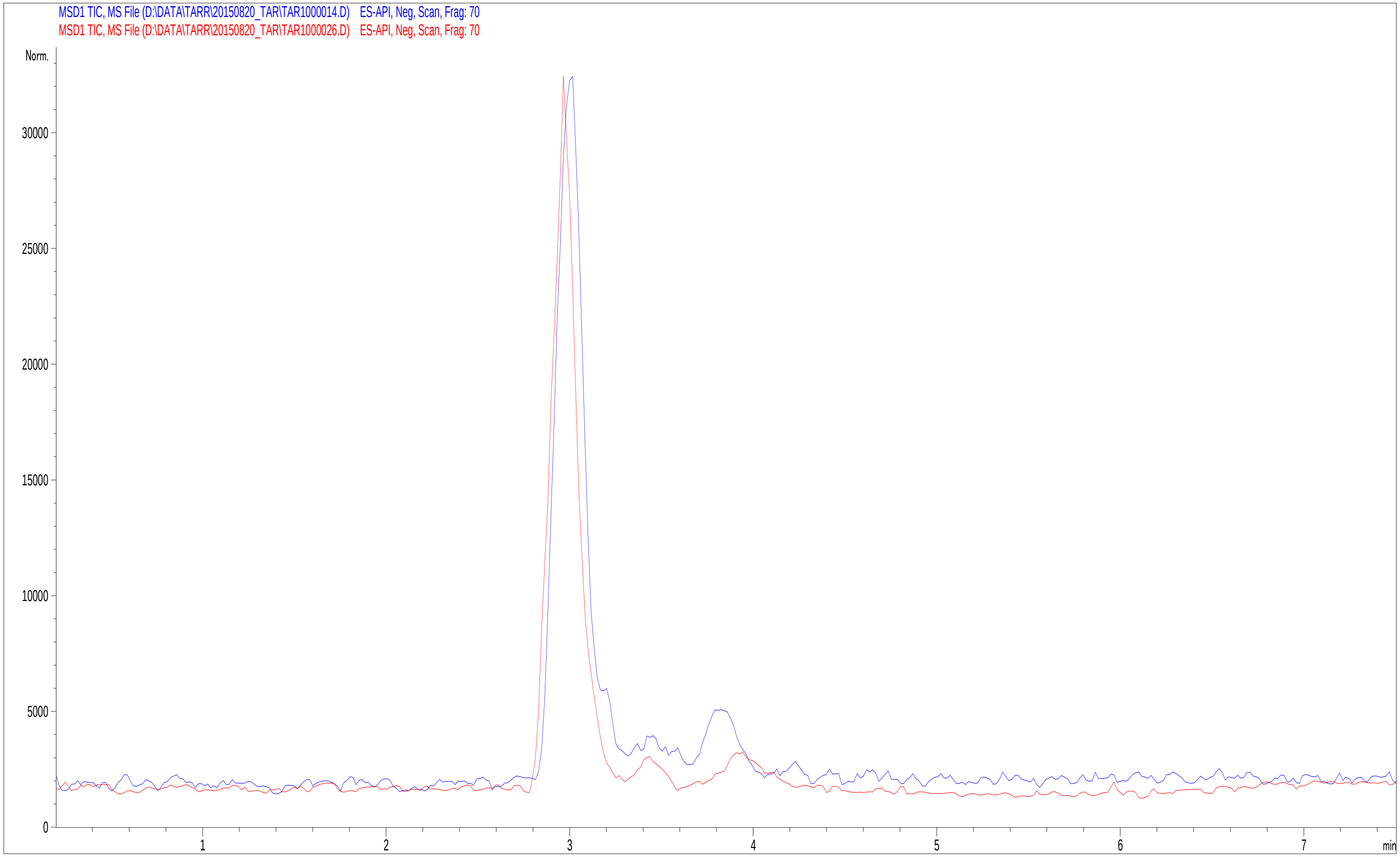
30 DC

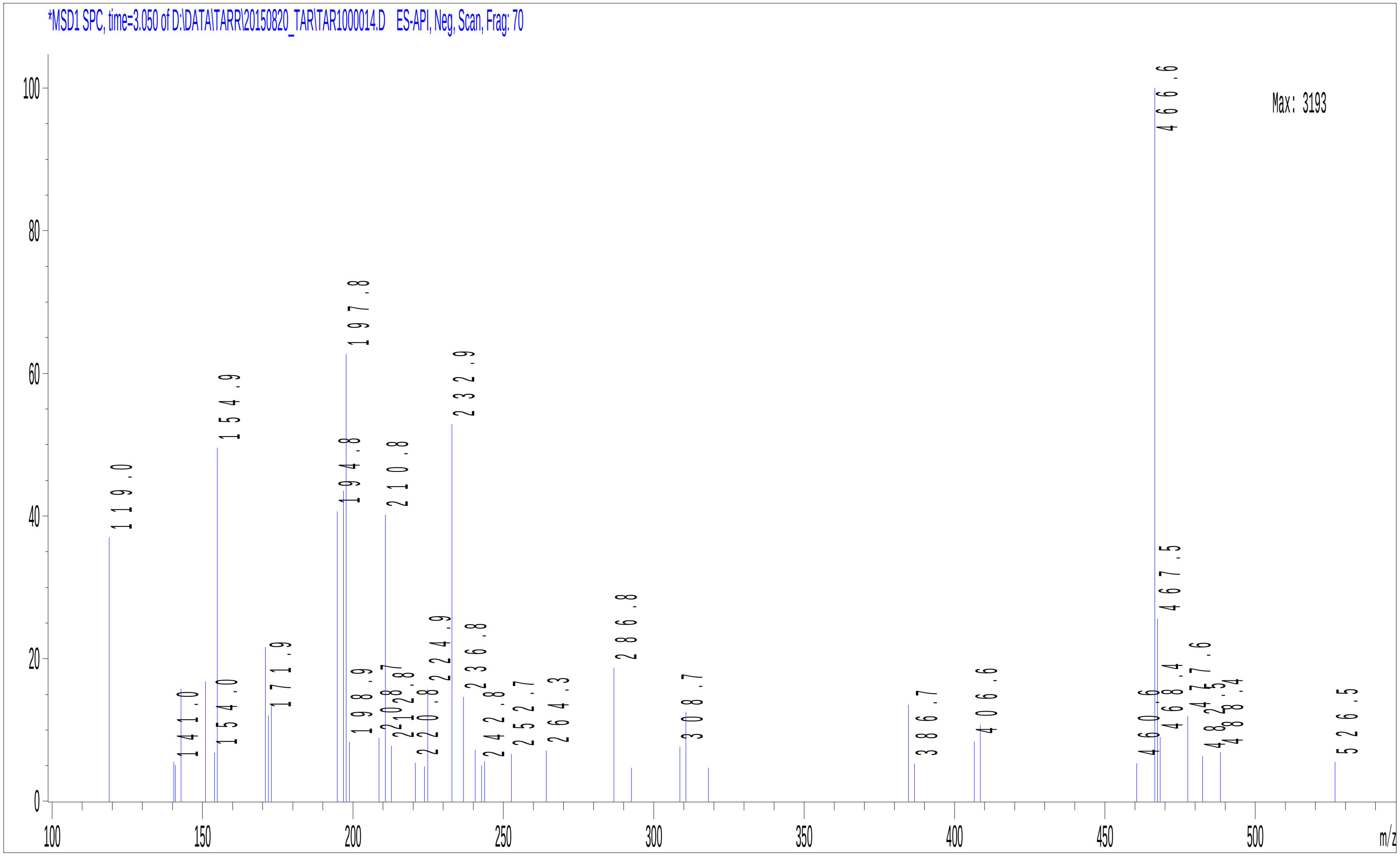
7

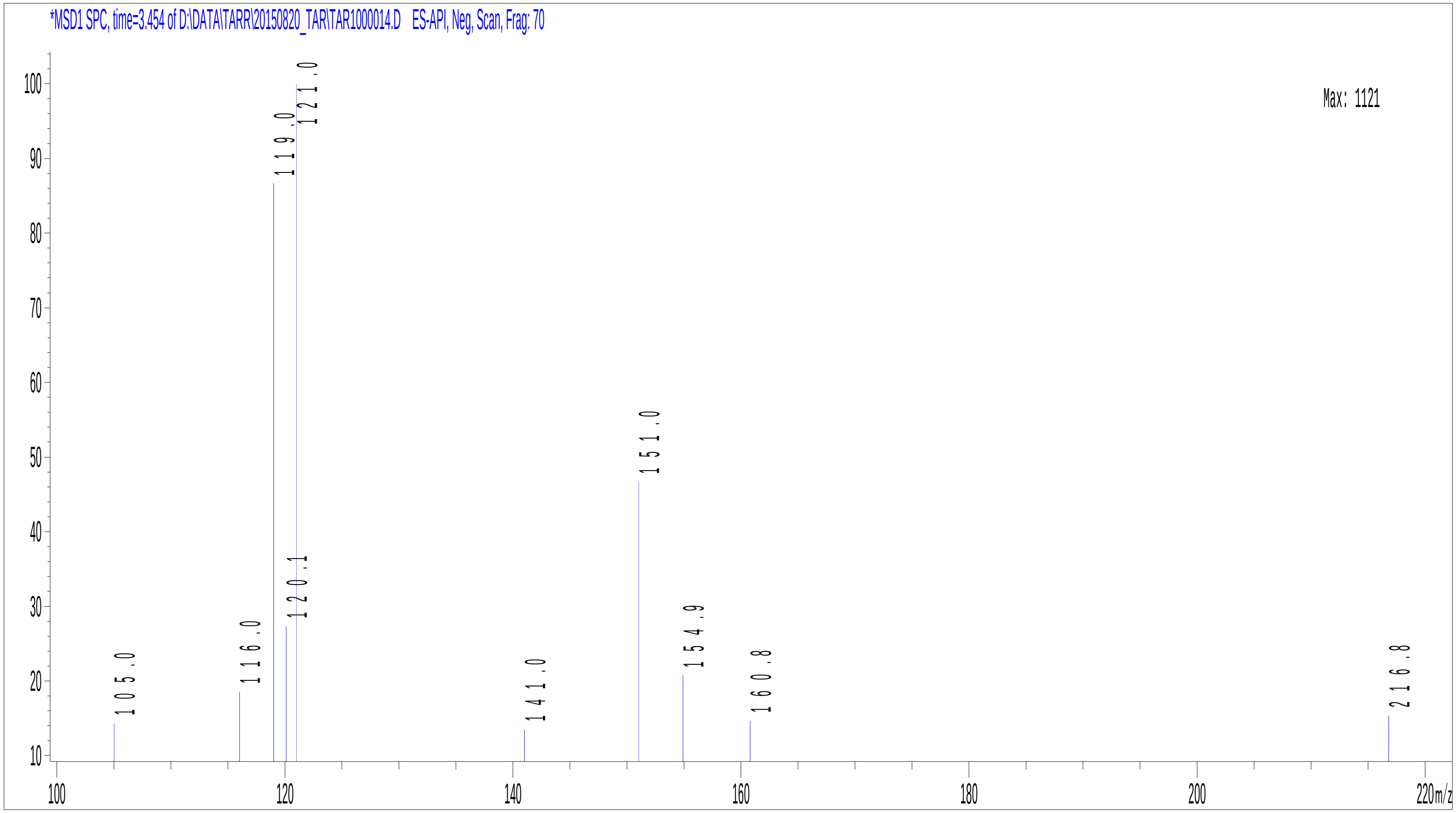
P2-B-05

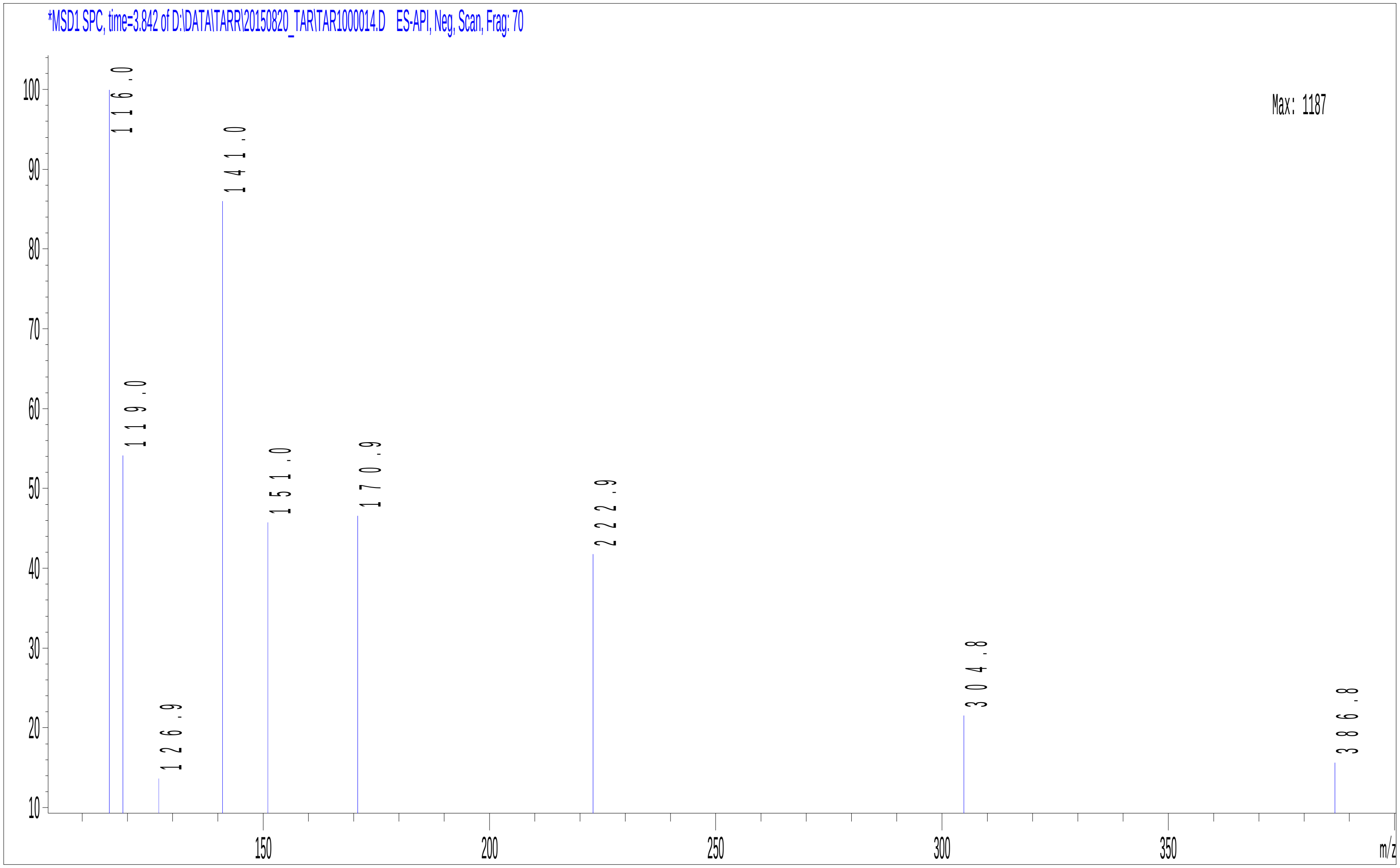


#	Time	Area	Height	Width	Area%	Symmetry
1	3.009	307495.1	28885.7	0.1545	100.000	1.055


MSD1 TIC, MS File (D:\DATA\TARR\20150820_TAR\TAR1000014.D) ES-API, Neg, Scan, Frag: 70
MSD1 TIC, MS File (D:\DATA\TARR\20150820_TAR\TAR1000026.D) ES-API, Neg, Scan, Frag: 70
Norm.
30000
25000
20000
15000
10000
5000
0
1
2
3
4
5
6
7
min


*MSD1 SPC, time=3.050 of D:\DATA\TARR\20150820_TAR\TAR1000014.D ES-API, Neg, Scan, Frag: 70
Max: 3193
466.6
197.8
154.9
232.9
119.0
194.8
210.8
467.5
286.8
224.9
236.8
171.9
141.0
154.0
198.9
208.7
212.8
220.8
242.8
252.7
264.3
308.7
386.7
406.6
460.6
468.4
477.6
482.5
488.4
526.5
0
20
40
60
80
100
100
150
200
250
300
350
400
450
500
m/z


*MSD1 SPC, time=3.454 of D:\DATA\TARR\20150820_TAR\TAR1000014.D ES-API, Neg, Scan, Frag: 70
Max: 1121
105.0
116.0
119.0
120.1
121.0
141.0
151.0
154.9
160.8
216.8
100
90
80
70
60
50
40
30
20
10
100
120
140
160
180
200
220
m/z

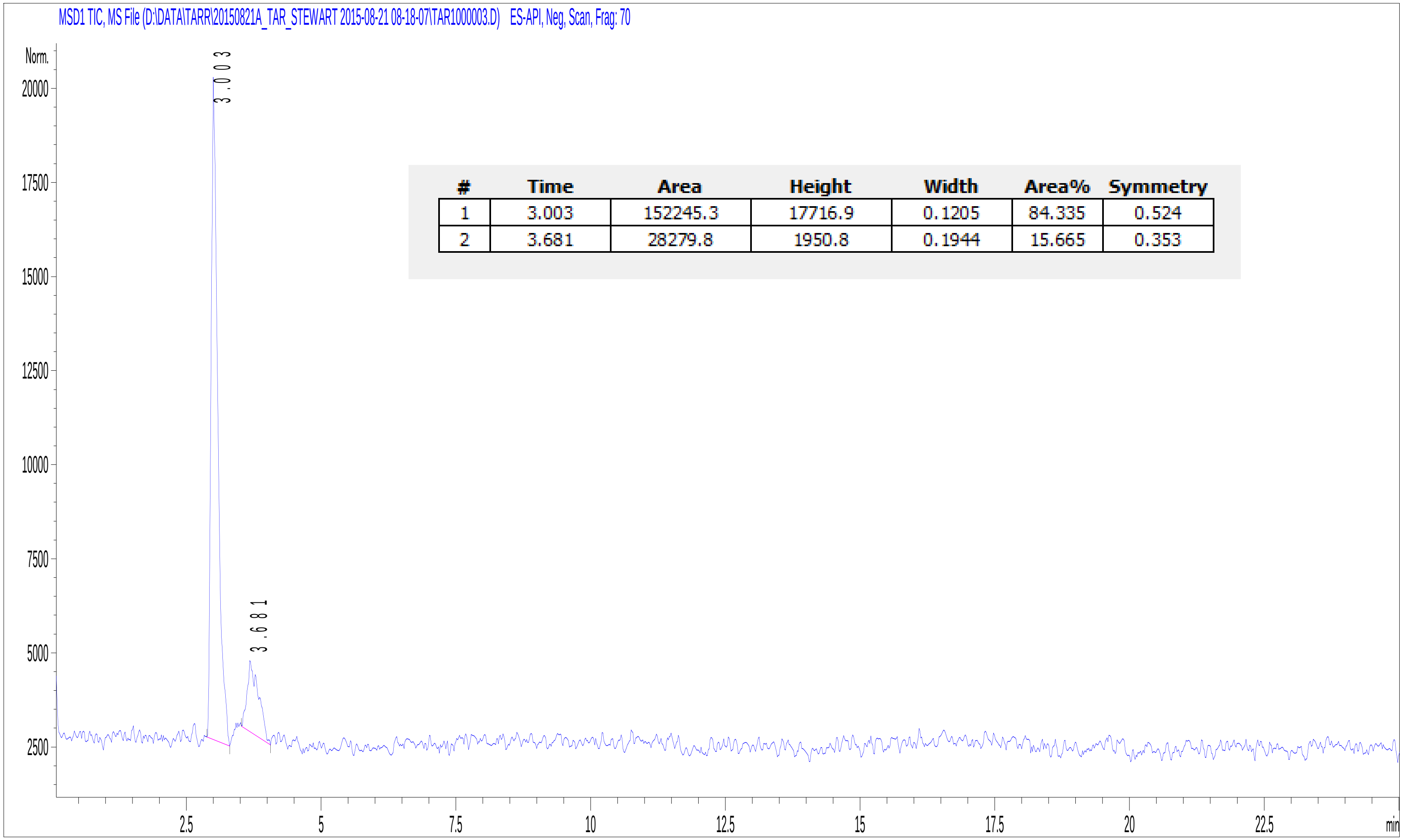
*MSD1 SPC, time=3.842 of D:\DATA\TARR\20150820_TAR\TAR1000014.D ES-API, Neg, Scan, Frag: 70
Max: 1187
116.0
119.0
126.9
141.0
151.0
170.9
222.9
304.8
386.8
100
90
80
70
60
50
40
30
20
10
150
200
250
300
350
m/z

11-Aug-15

50 DC

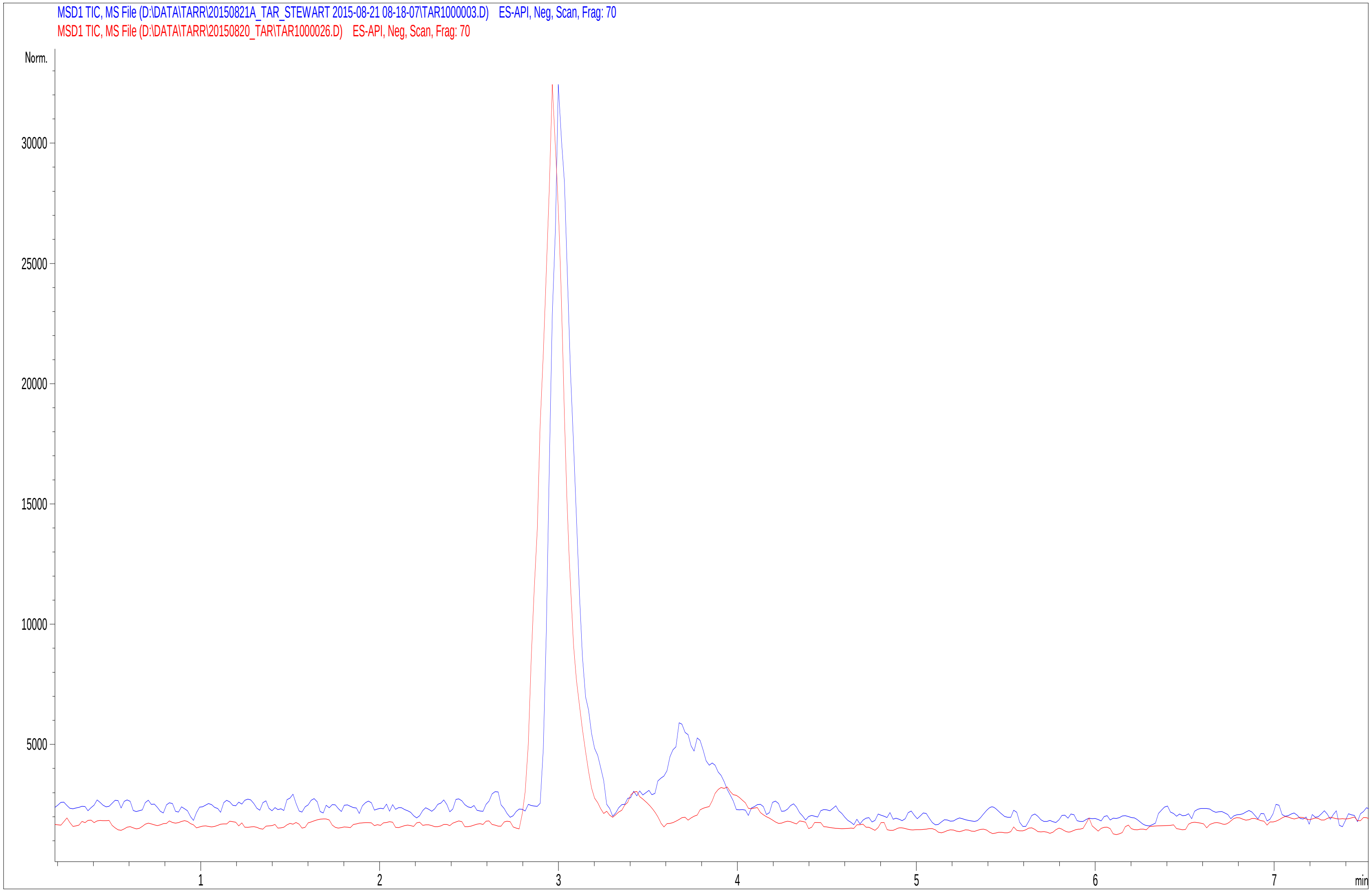
7

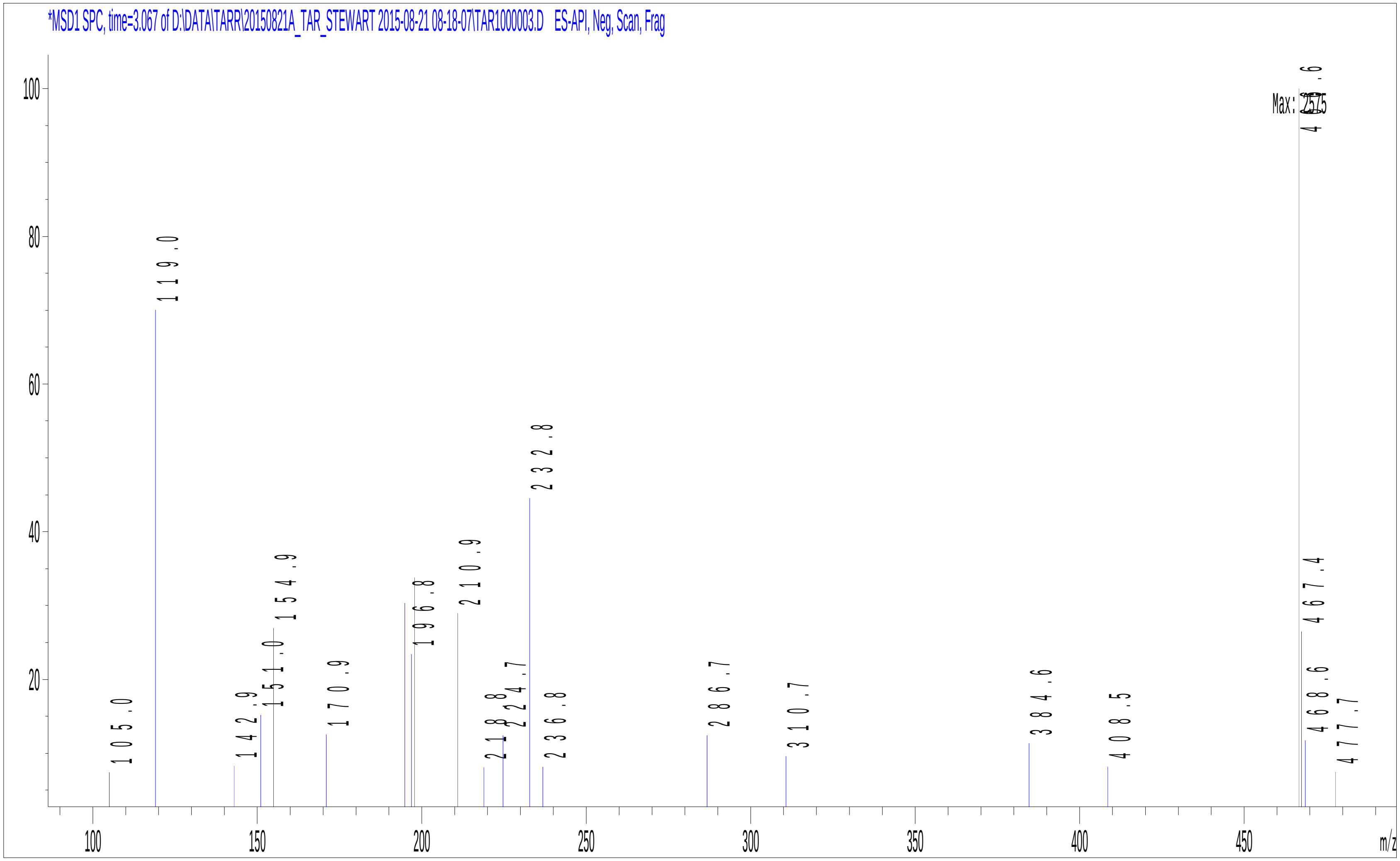
P2-E-02

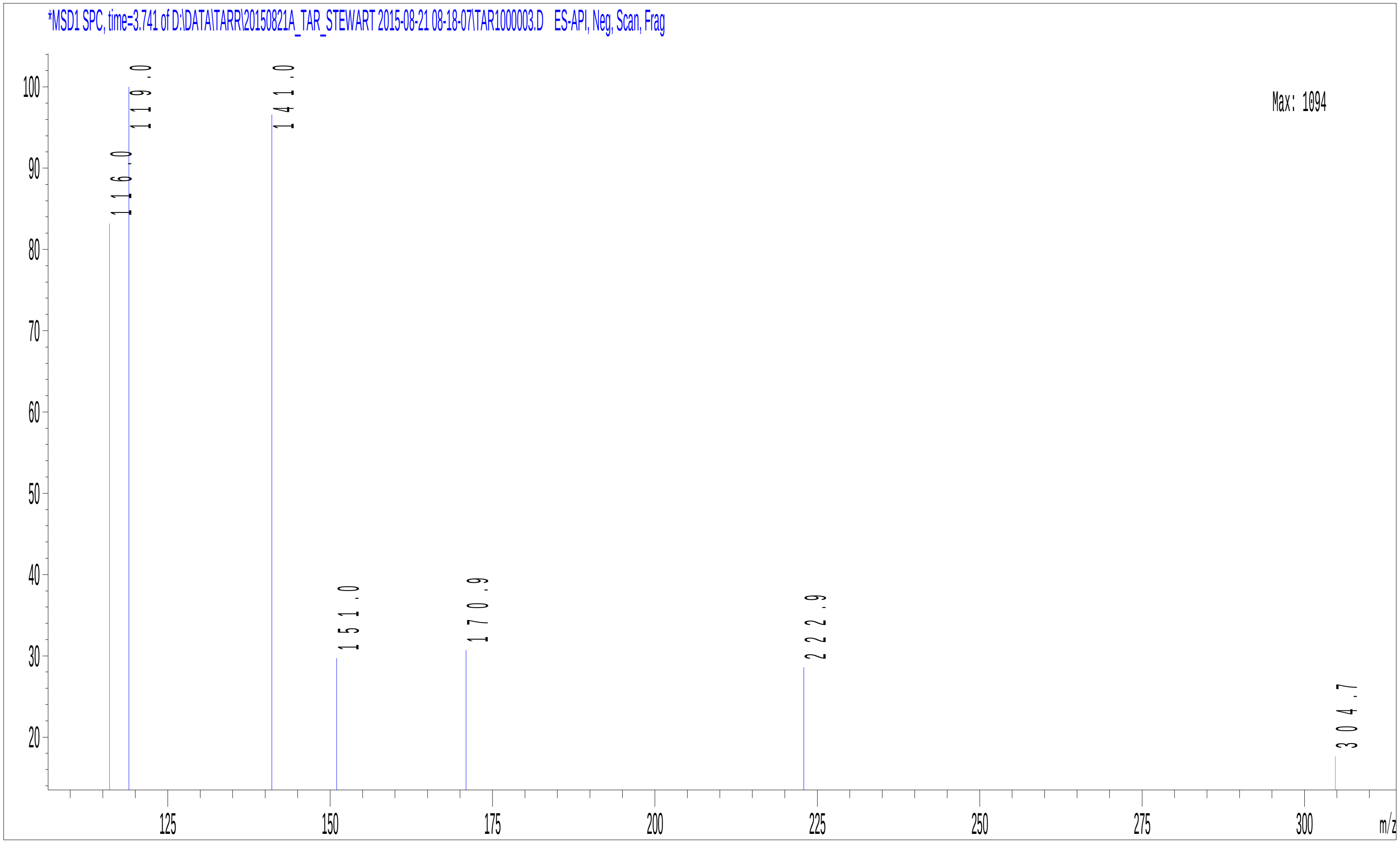


MSD1 TIC, MS File (D:\DATA\TARR\20150821A_TAR_STEWART 2015-08-21 08-18-07\TAR1000003.D) ES-API, Neg, Scan, Frag: 70

#	Time	Area	Height	Width	Area%	Symmetry
1	3.003	152245.3	17716.9	0.1205	84.335	0.524
2	3.681	28279.8	1950.8	0.1944	15.665	0.353


MSD1 TIC, MS File (D:\DATA\TARR\20150821A_TAR_STEWART 2015-08-21 08-18-07\TAR1000003.D)   ES-API, Neg, Scan, Frag: 70
MSD1 TIC, MS File (D:\DATA\TARR\20150820_TAR\TAR1000026.D)   ES-API, Neg, Scan, Frag: 70
Norm.
30000
25000
20000
15000
10000
5000
1
2
3
4
5
6
7
min


*MSD1 SPC, time=3.067 of D:\DATA\TARR\20150821A_TAR_STEWART 2015-08-21 08-18-07\TAR1000003.D   ES-API, Neg, Scan, Frag
Max: 2575
100
80
60
40
20
100
150
200
250
300
350
400
450
m/z
105.0
119.0
142.9
151.0
154.9
170.9
196.8
210.9
218.8
224.7
232.8
236.8
286.7
310.7
384.6
408.5
466.6
467.4
468.6
477.7

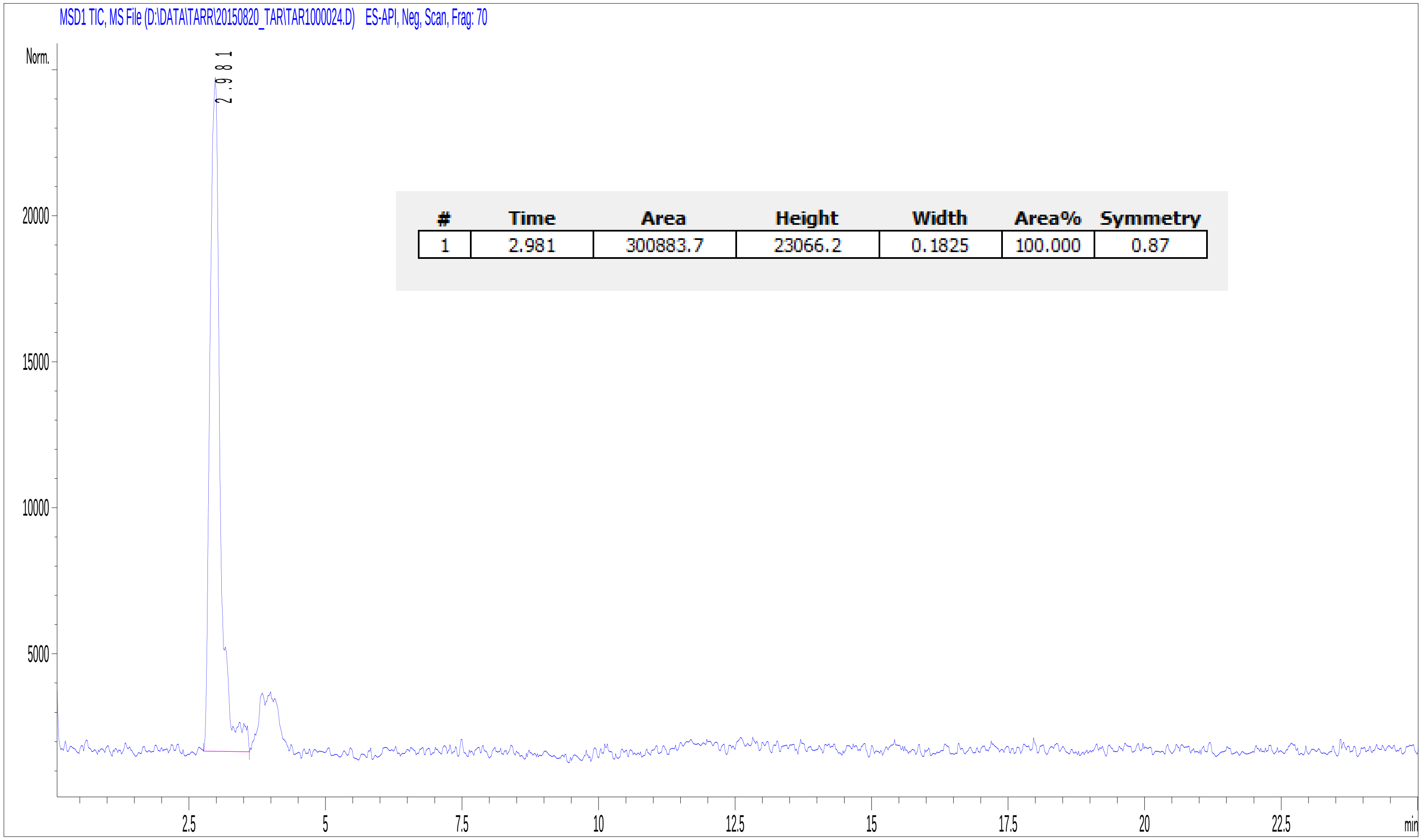

*MSD1 SPC, time=3.741 of D:\DATA\TARR\20150821A_TAR_STEWART 2015-08-21 08-18-07\TAR1000003.D   ES-API, Neg, Scan, Frag
Max: 1094
116.0
119.0
141.0
151.0
170.9
222.9
304.7
100
90
80
70
60
50
40
30
20
125
150
175
200
225
250
275
300
m/z

13-Jul-15

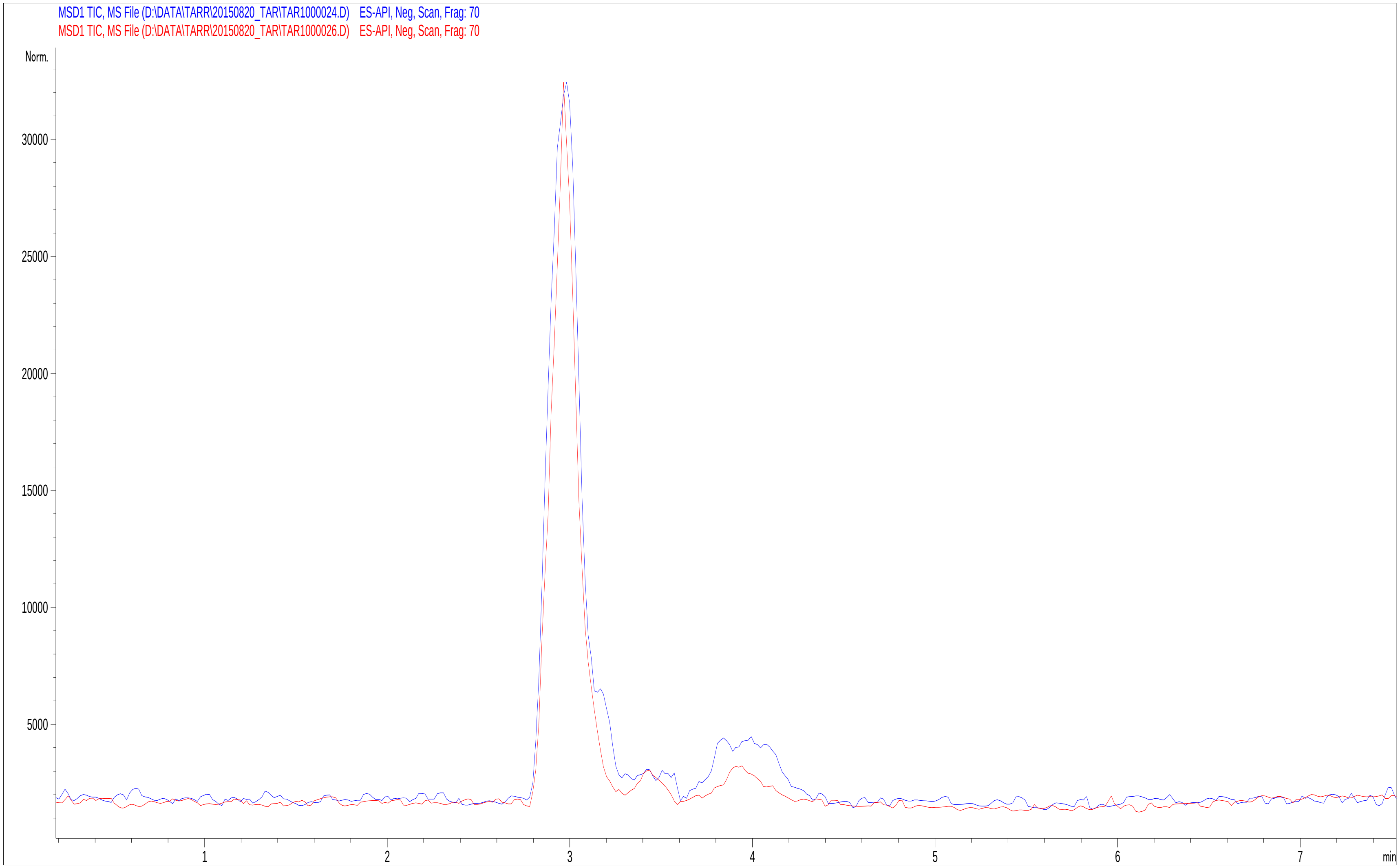
70 DC

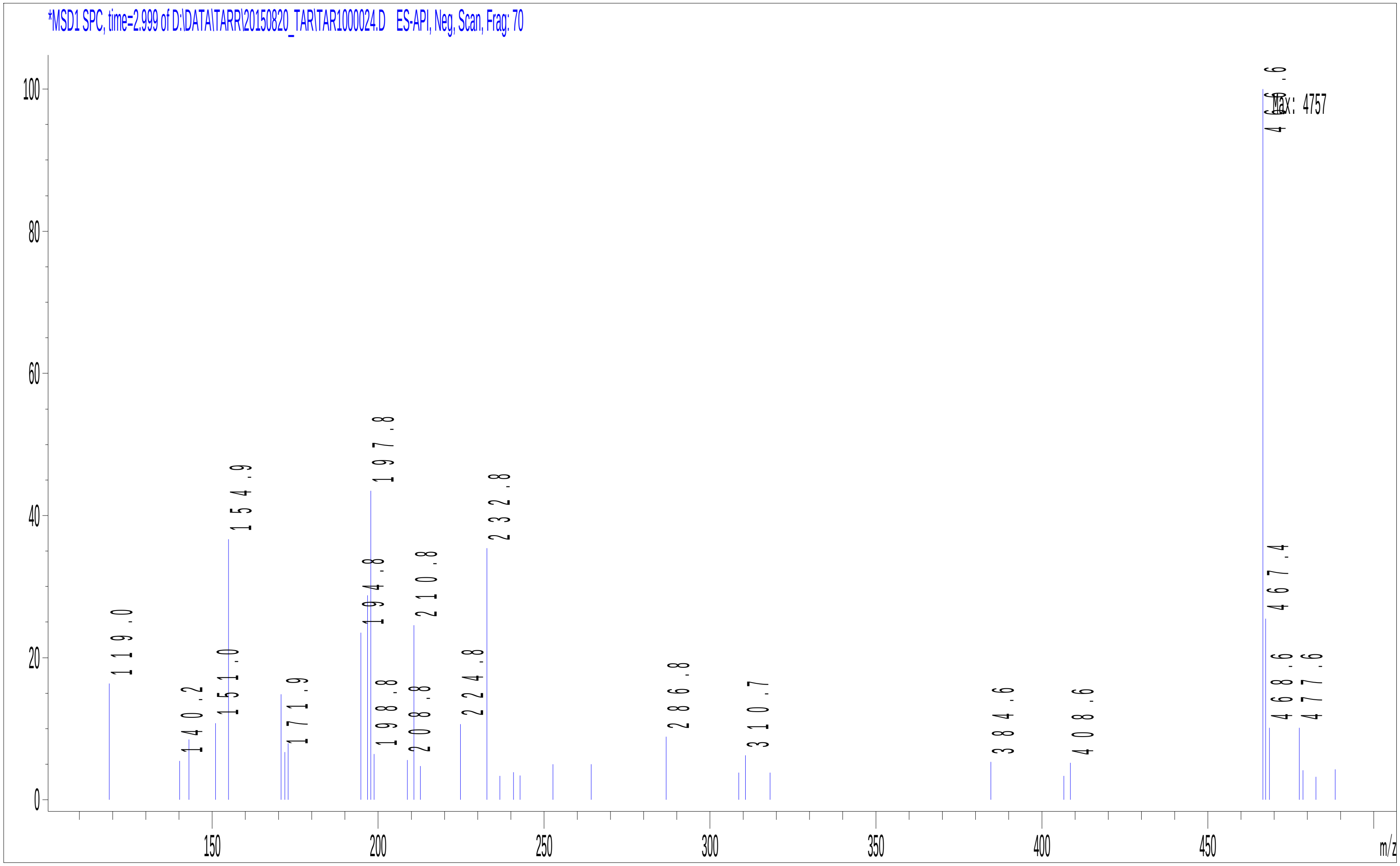
7

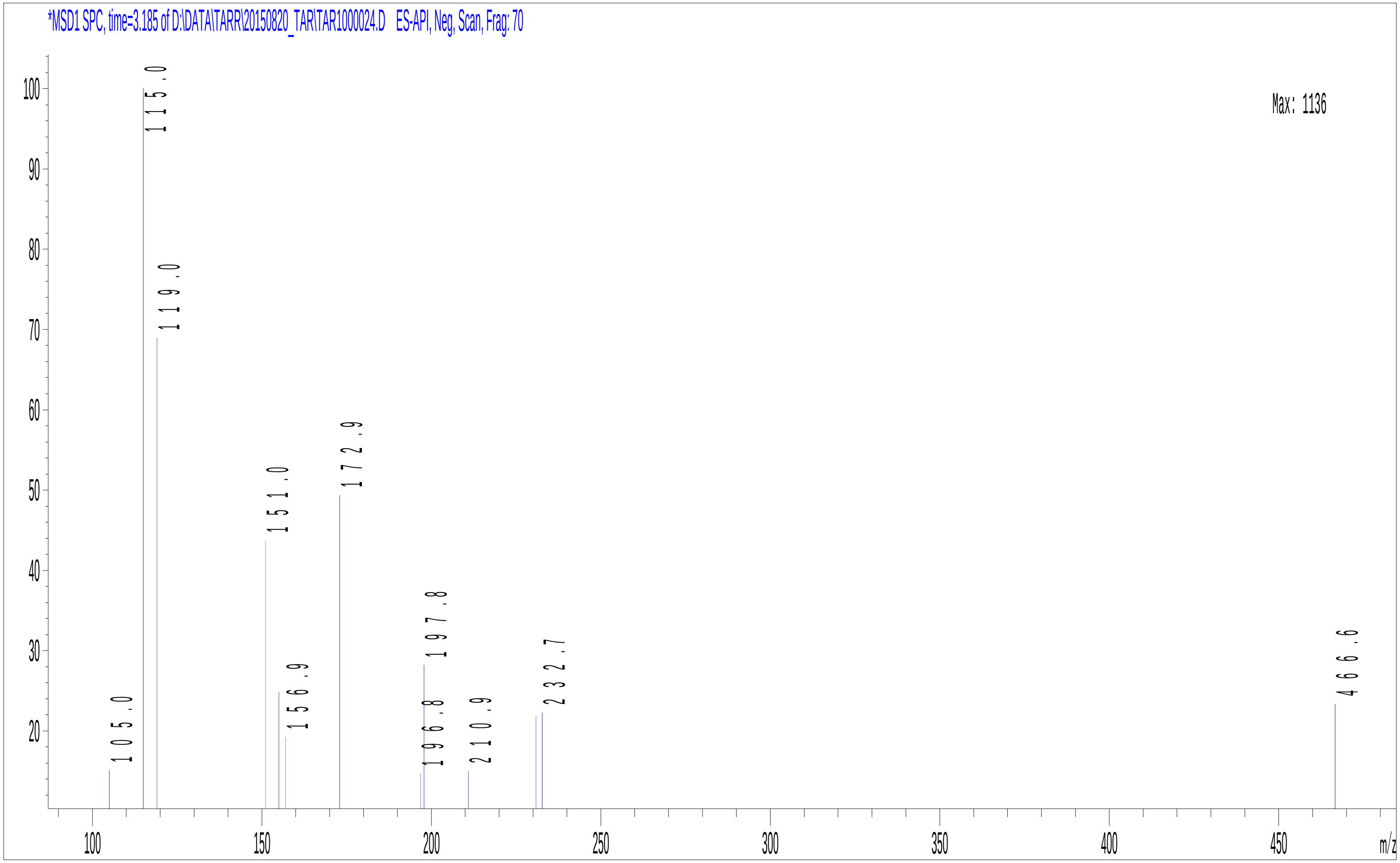
P2-C-06

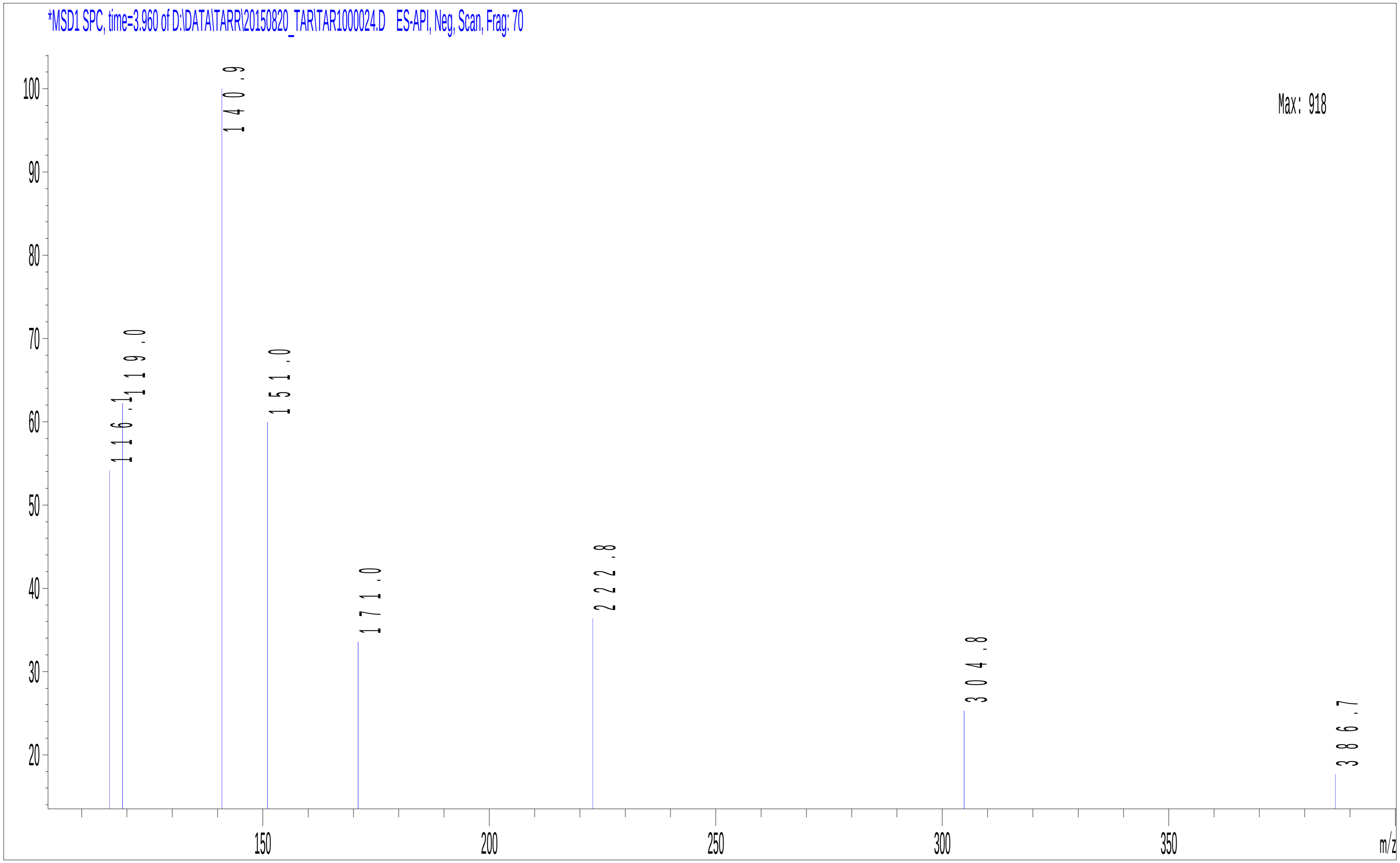


#	Time	Area	Height	Width	Area%	Symmetry
1	2.981	300883.7	23066.2	0.1825	100.000	0.87


MSD1 TIC, MS File (D:\DATA\TARR\20150820_TAR\TAR1000024.D) ES-API, Neg, Scan, Frag: 70
MSD1 TIC, MS File (D:\DATA\TARR\20150820_TAR\TAR1000026.D) ES-API, Neg, Scan, Frag: 70
Norm.
30000
25000
20000
15000
10000
5000
1
2
3
4
5
6
7
min


*MSD1 SPC, time=2.999 of D:\DATA\TARR\20150820_TAR\TAR1000024.D ES-API, Neg, Scan, Frag: 70
Max: 4757
119.0
140.2
151.0
154.9
171.9
194.8
197.8
198.8
208.8
210.8
224.8
232.8
286.8
310.7
384.6
408.6
466.6
467.4
468.6
477.6
0
20
40
60
80
100
150
200
250
300
350
400
450
m/z


*MSD1 SPC, time=3.185 of D:\DATA\TARR\20150820_TAR\TAR1000024.D ES-API, Neg, Scan, Frag: 70
Max: 1136
100
90
80
70
60
50
40
30
20
105.0
115.0
119.0
151.0
156.9
172.9
196.8
197.8
210.9
232.7
466.6
100
150
200
250
300
350
400
450
m/z

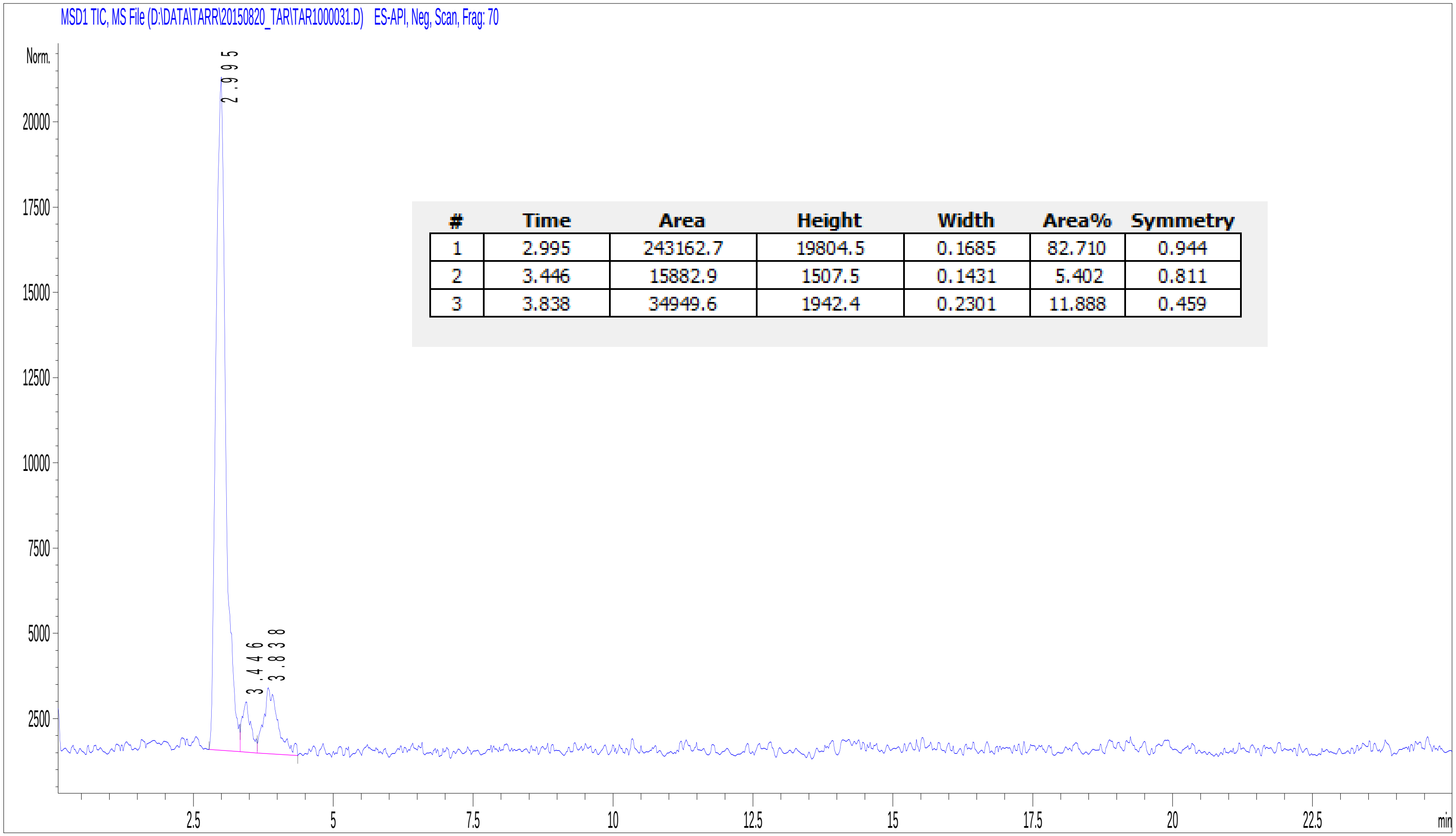

*MSD1 SPC, time=3.960 of D:\DATA\TARR\20150820_TAR\TAR1000024.D ES-API, Neg, Scan, Frag: 70
Max: 918
100
90
80
70
60
50
40
30
20
116.1
119.0
140.9
151.0
171.0
222.8
304.8
386.7
150
200
250
300
350
m/z

30-Jul-15

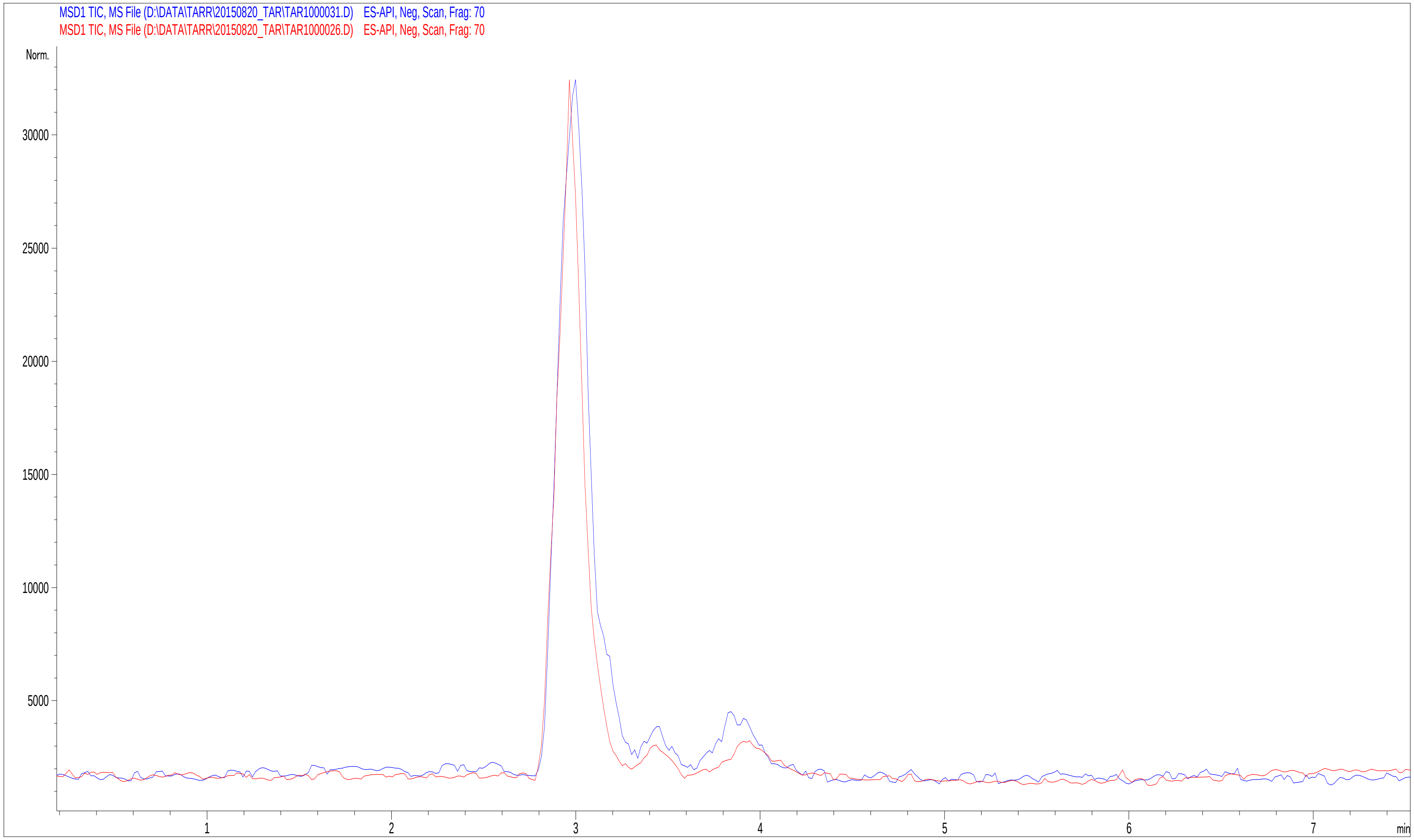
100 DC

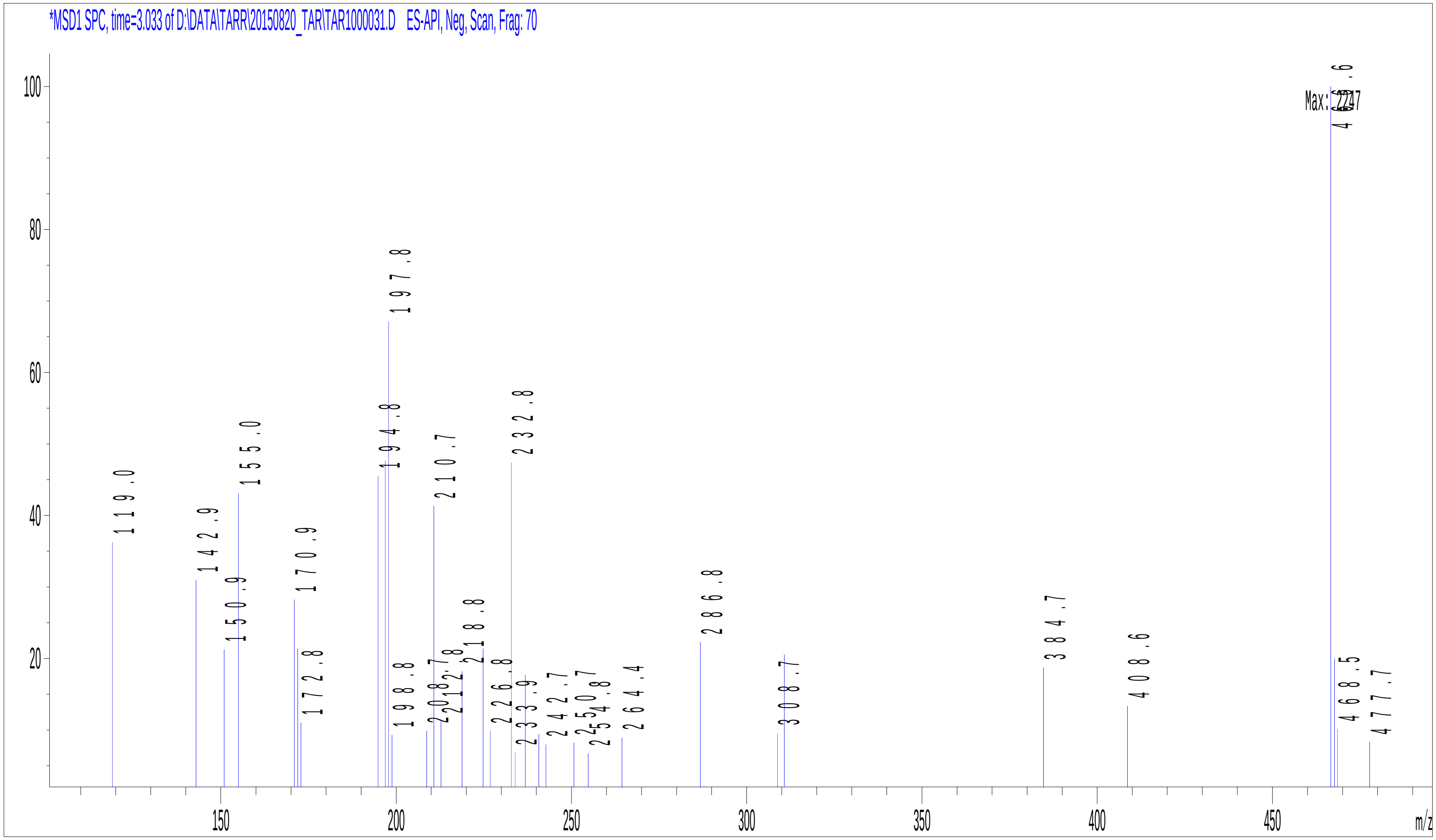
7

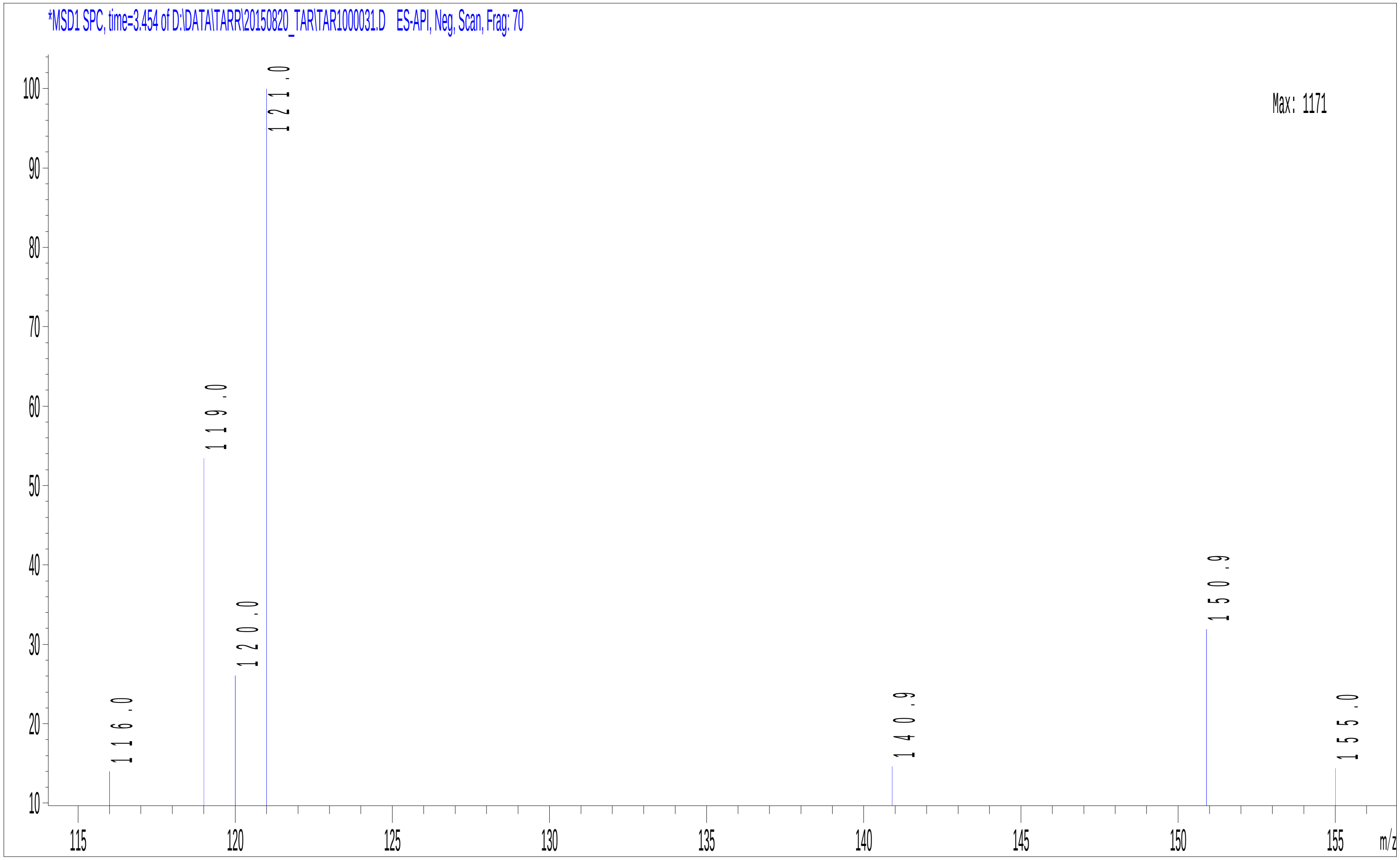
P2-D-06



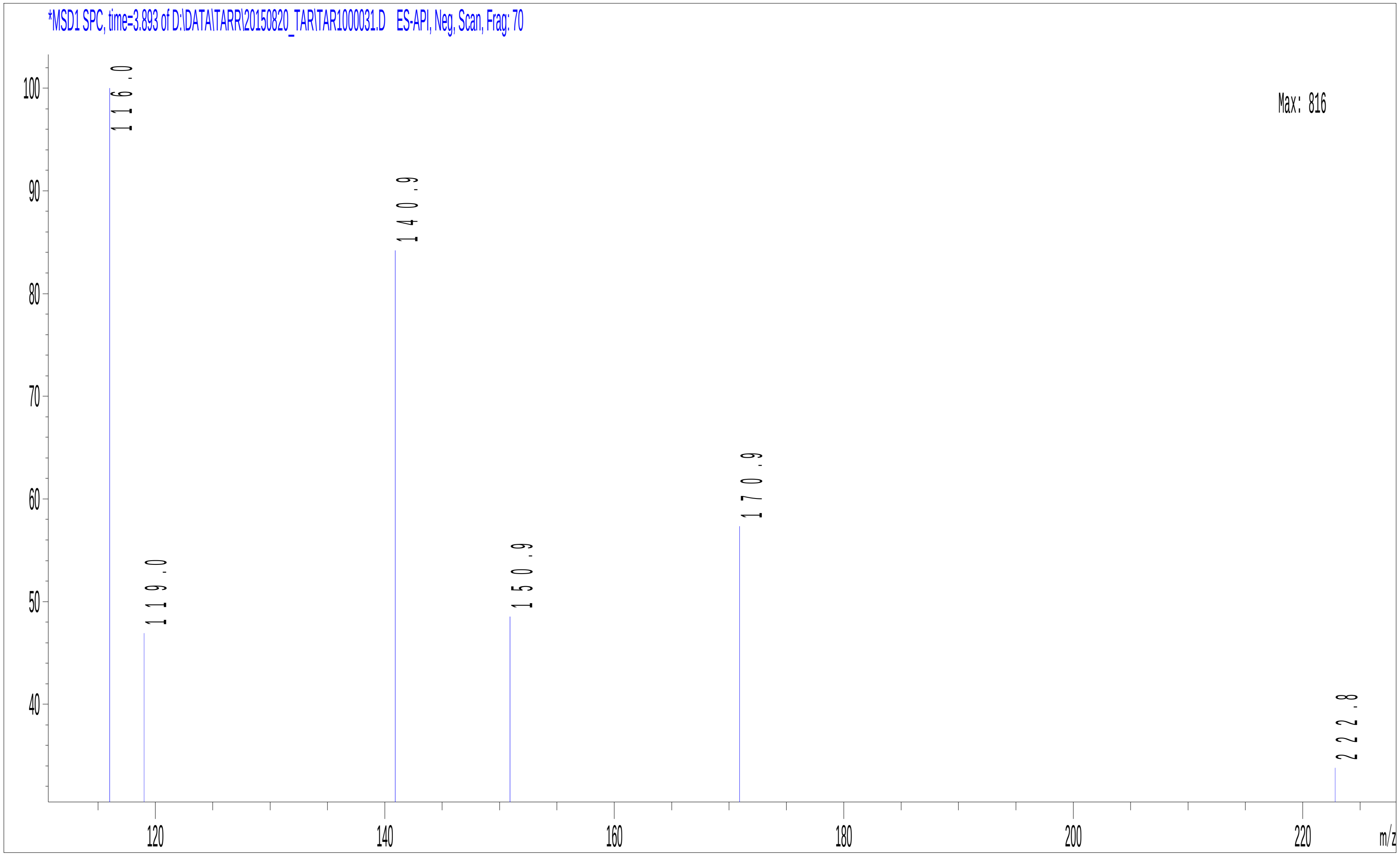
#	Time	Area	Height	Width	Area%	Symmetry
1	2.995	243162.7	19804.5	0.1685	82.710	0.944
2	3.446	15882.9	1507.5	0.1431	5.402	0.811
3	3.838	34949.6	1942.4	0.2301	11.888	0.459


MSD1 TIC, MS File (D:\DATA\TARR\20150820_TAR\TAR1000031.D) ES-API, Neg, Scan, Frag: 70
MSD1 TIC, MS File (D:\DATA\TARR\20150820_TAR\TAR1000026.D) ES-API, Neg, Scan, Frag: 70
Norm.
30000
25000
20000
15000
10000
5000
1
2
3
4
5
6
7
min


*MSD1 SPC, time=3.033 of D:\DATA\TARR\20150820_TAR\TAR1000031.D ES-API, Neg, Scan, Frag: 70
Max: 2247
100
80
60
40
20
150
200
250
300
350
400
450
m/z
119.0
142.9
150.9
155.0
170.9
172.8
194.8
197.8
198.8
208.7
210.7
212.8
218.8
226.8
232.8
233.9
242.7
250.7
254.8
264.4
286.8
308.7
384.7
408.6
466.6
468.5
477.7



*MSD1 SPC, time=3.454 of D:\DATA\TARR\20150820_TAR\TAR1000031.D ES-API, Neg, Scan, Frag: 70
Max: 1171
100
90
80
70
60
50
40
30
20
10
121.0
119.0
120.0
116.0
140.9
150.9
155.0
115
120
125
130
135
140
145
150
155
m/z

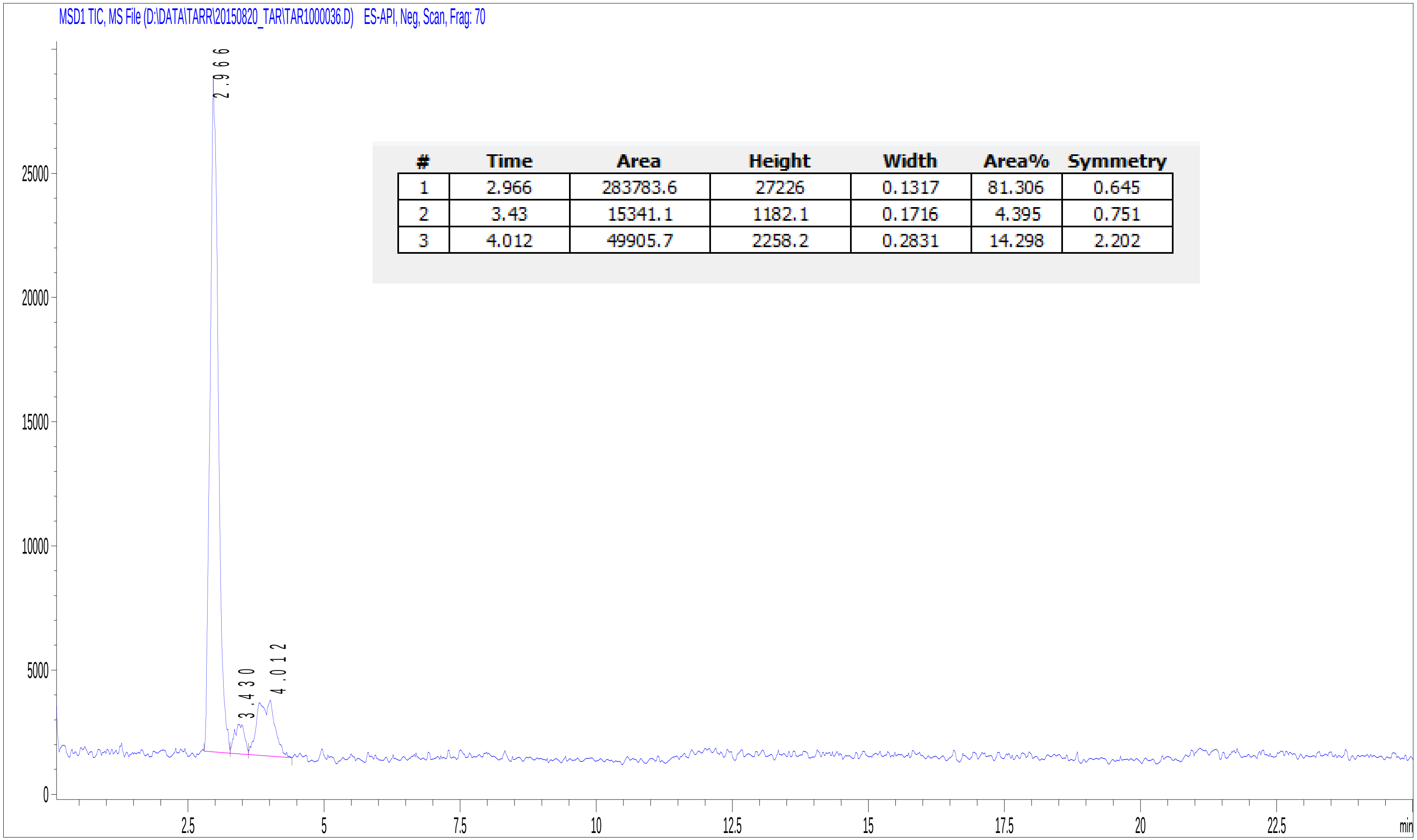

*MSD1 SPC, time=3.893 of D:\DATA\TARR\20150820_TAR\TAR1000031.D ES-API, Neg, Scan, Frag: 70
Max: 816
116.0
119.0
140.9
150.9
170.9
222.8
100
90
80
70
60
50
40
120
140
160
180
200
220
m/z

16-Jul-15

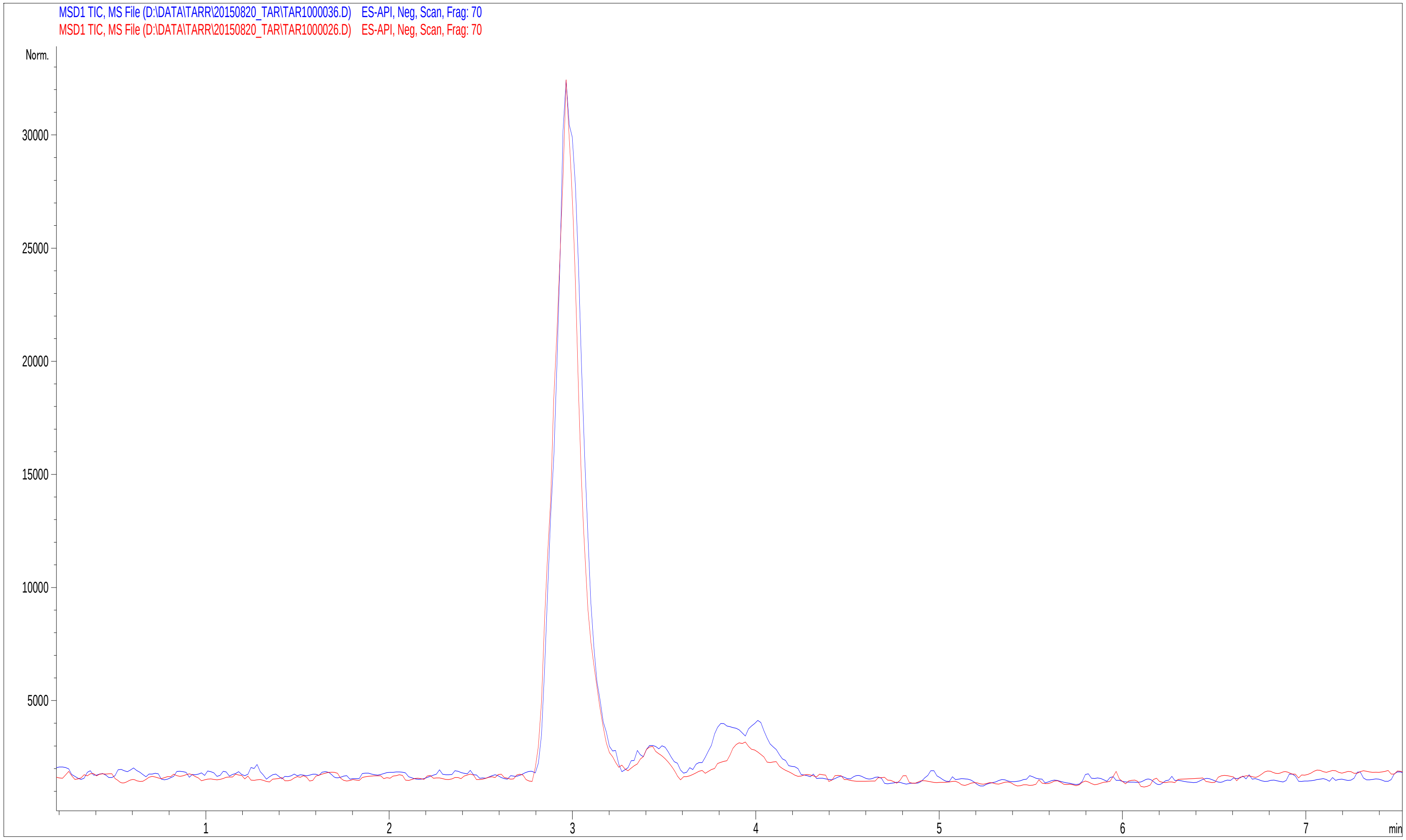
100 DC Problem no removal

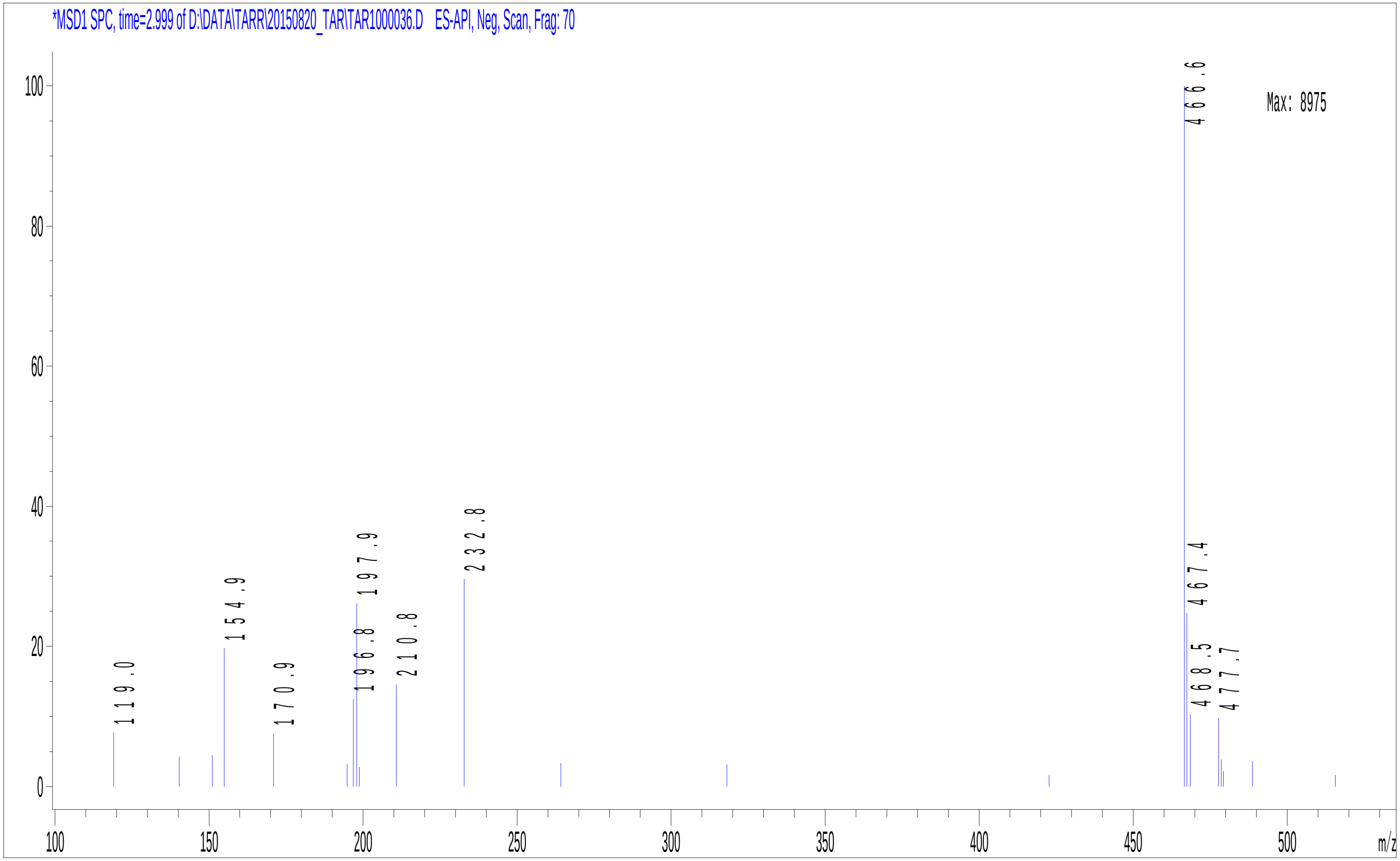
7

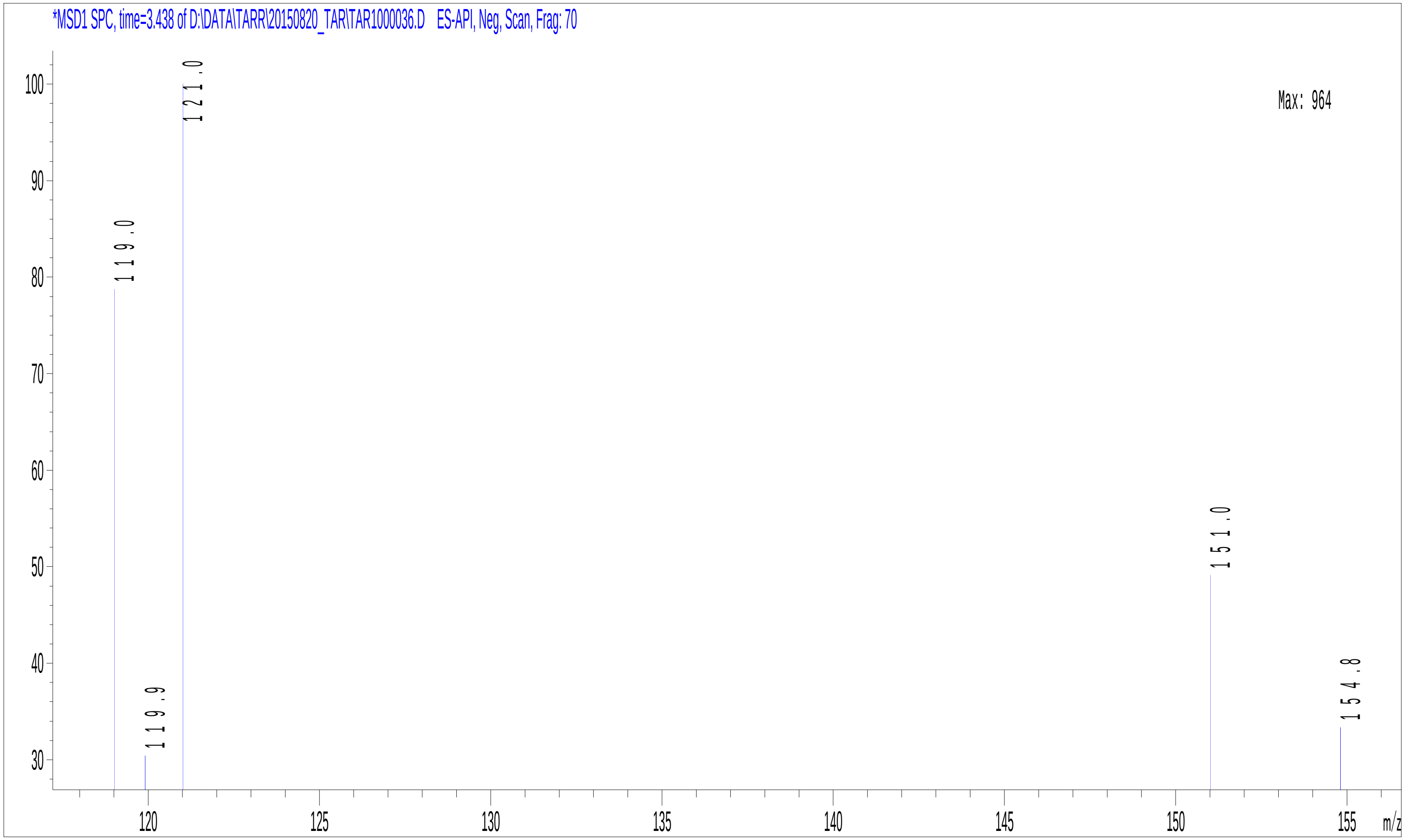
P2-D-01

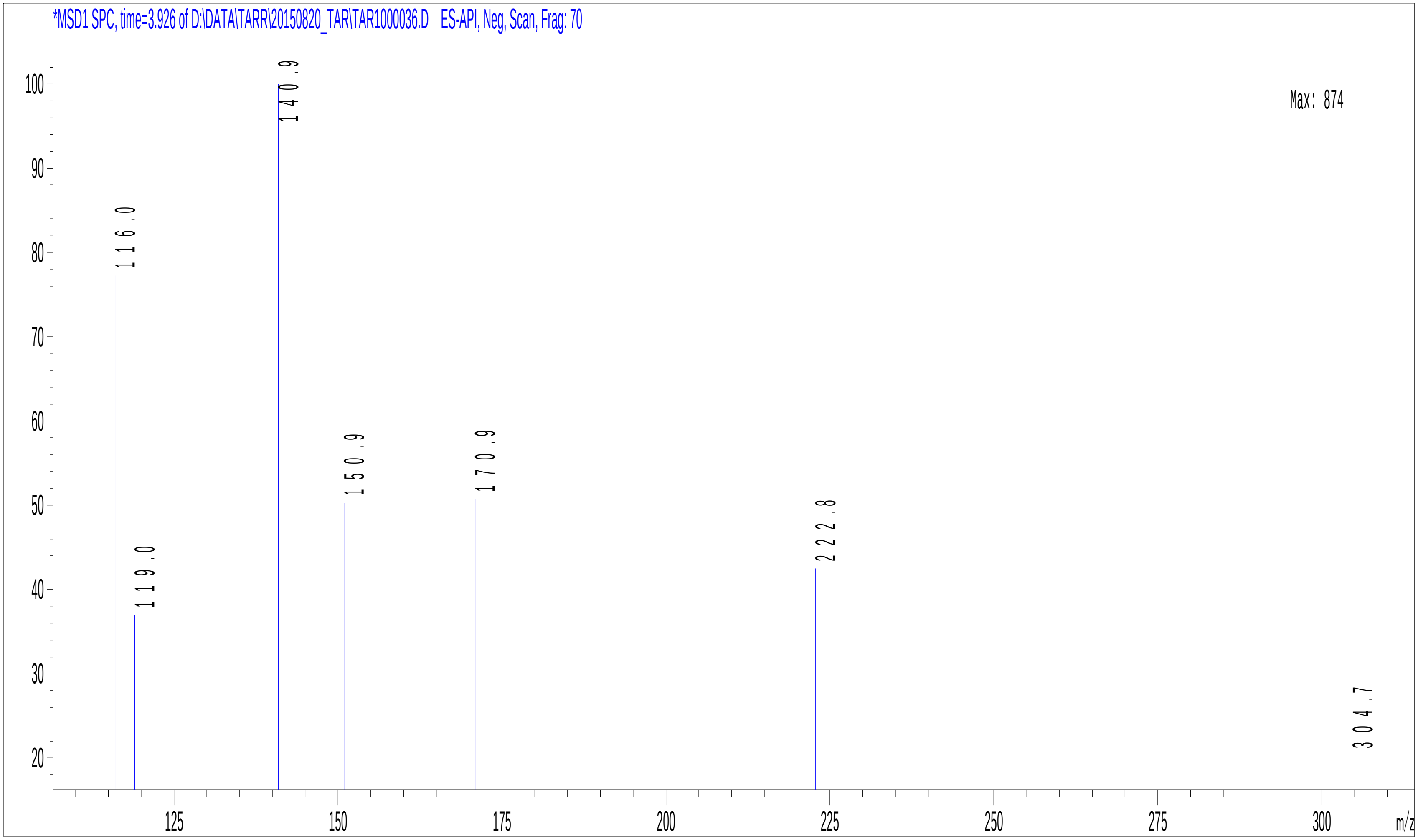


#	Time	Area	Height	Width	Area%	Symmetry
1	2.966	283783.6	27226	0.1317	81.306	0.645
2	3.43	15341.1	1182.1	0.1716	4.395	0.751
3	4.012	49905.7	2258.2	0.2831	14.298	2.202


MSD1 TIC, MS File (D:\DATA\TARR\20150820_TAR\TAR1000036.D) ES-API, Neg, Scan, Frag: 70
MSD1 TIC, MS File (D:\DATA\TARR\20150820_TAR\TAR1000026.D) ES-API, Neg, Scan, Frag: 70
Norm.
30000
25000
20000
15000
10000
5000
1
2
3
4
5
6
7
min

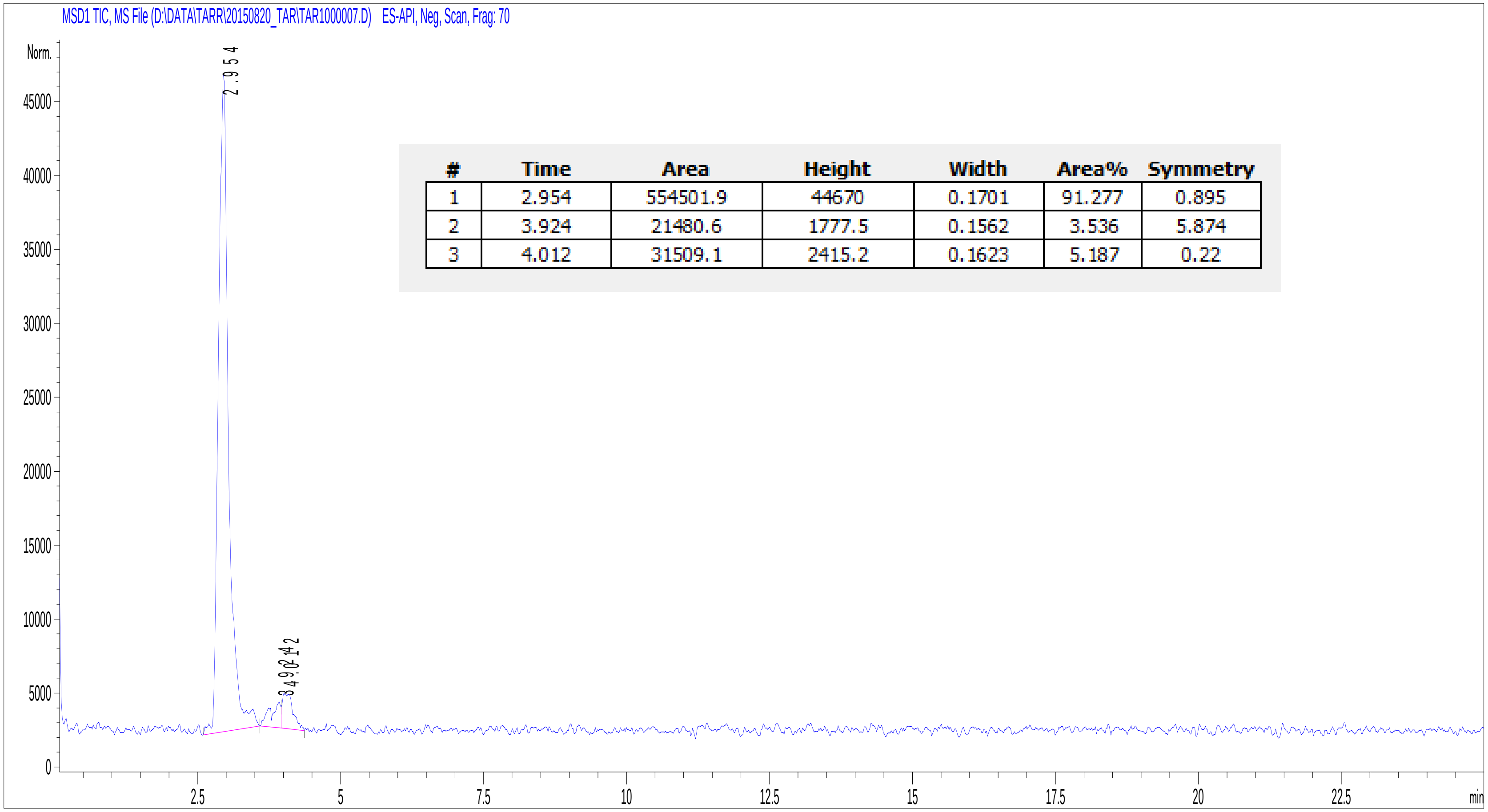

*MSD1 SPC, time=2.999 of D:\DATA\TARR\20150820_TAR\TAR1000036.D ES-API, Neg, Scan, Frag: 70
Max: 8975
466.6
467.4
468.5
477.7
232.8
197.9
196.8
210.8
154.9
170.9
119.0
0
20
40
60
80
100
100
150
200
250
300
350
400
450
500
m/z


*MSD1 SPC, time=3.438 of D:\DATA\TARR\20150820_TAR\TAR1000036.D ES-API, Neg, Scan, Frag: 70
Max: 964
119.0
119.9
121.0
151.0
154.8
100
90
80
70
60
50
40
30
120
125
130
135
140
145
150
155
m/z

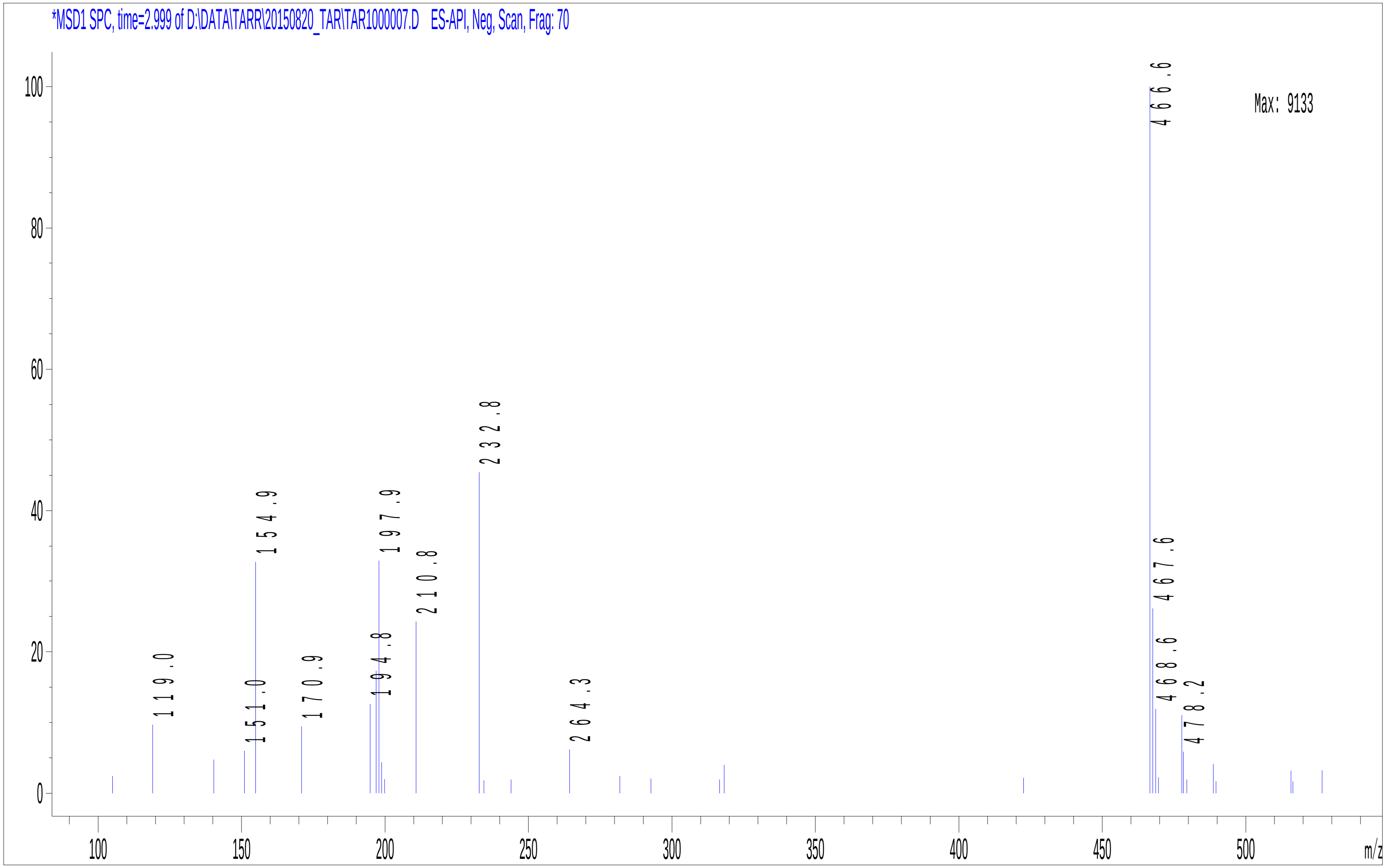

*MSD1 SPC, time=3.926 of D:\DATA\TARR\20150820_TAR\TAR1000036.D ES-API, Neg, Scan, Frag: 70
Max: 874
116.0
119.0
140.9
150.9
170.9
222.8
304.7
100
90
80
70
60
50
40
30
20
125
150
175
200
225
250
275
300
m/z

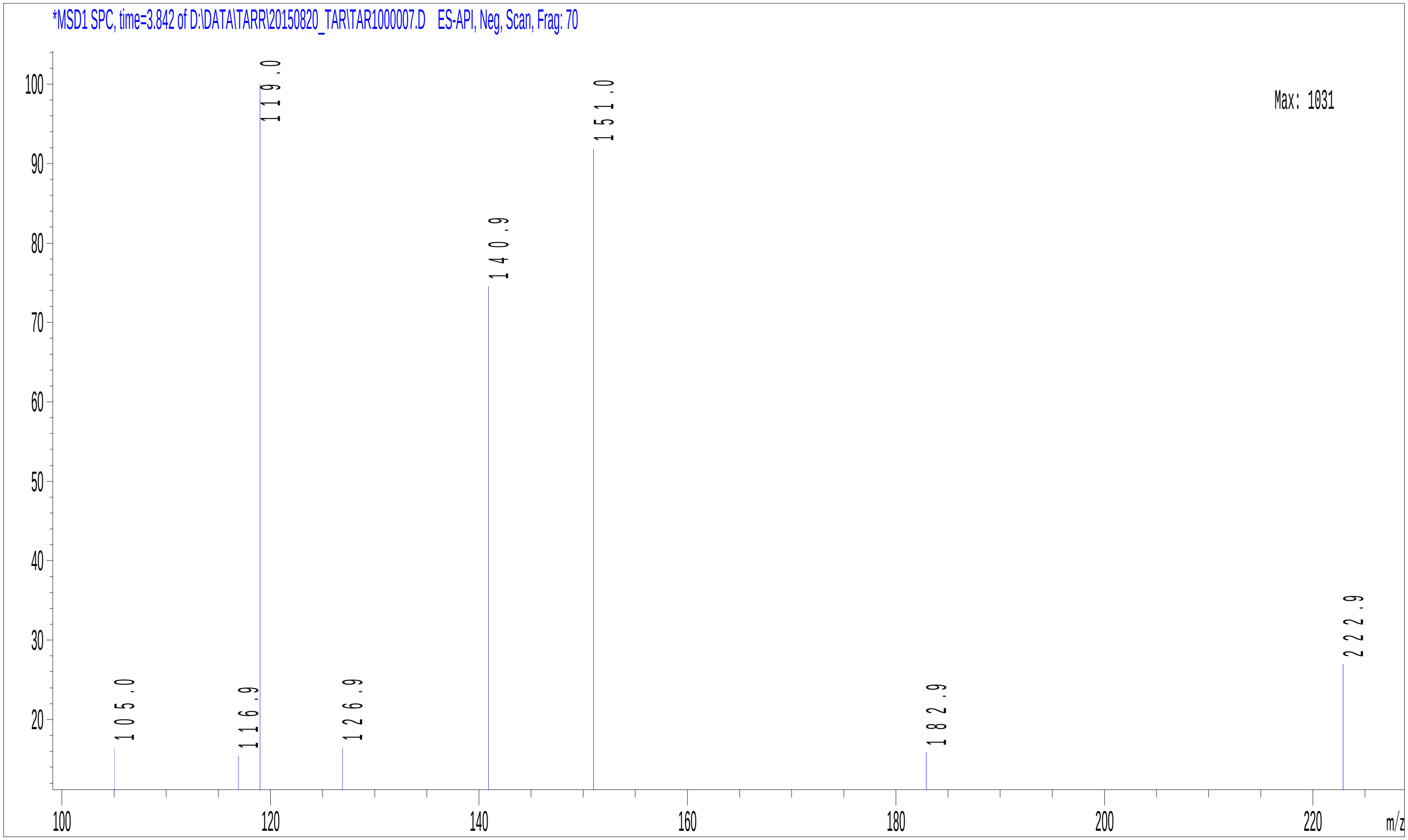
pH 8

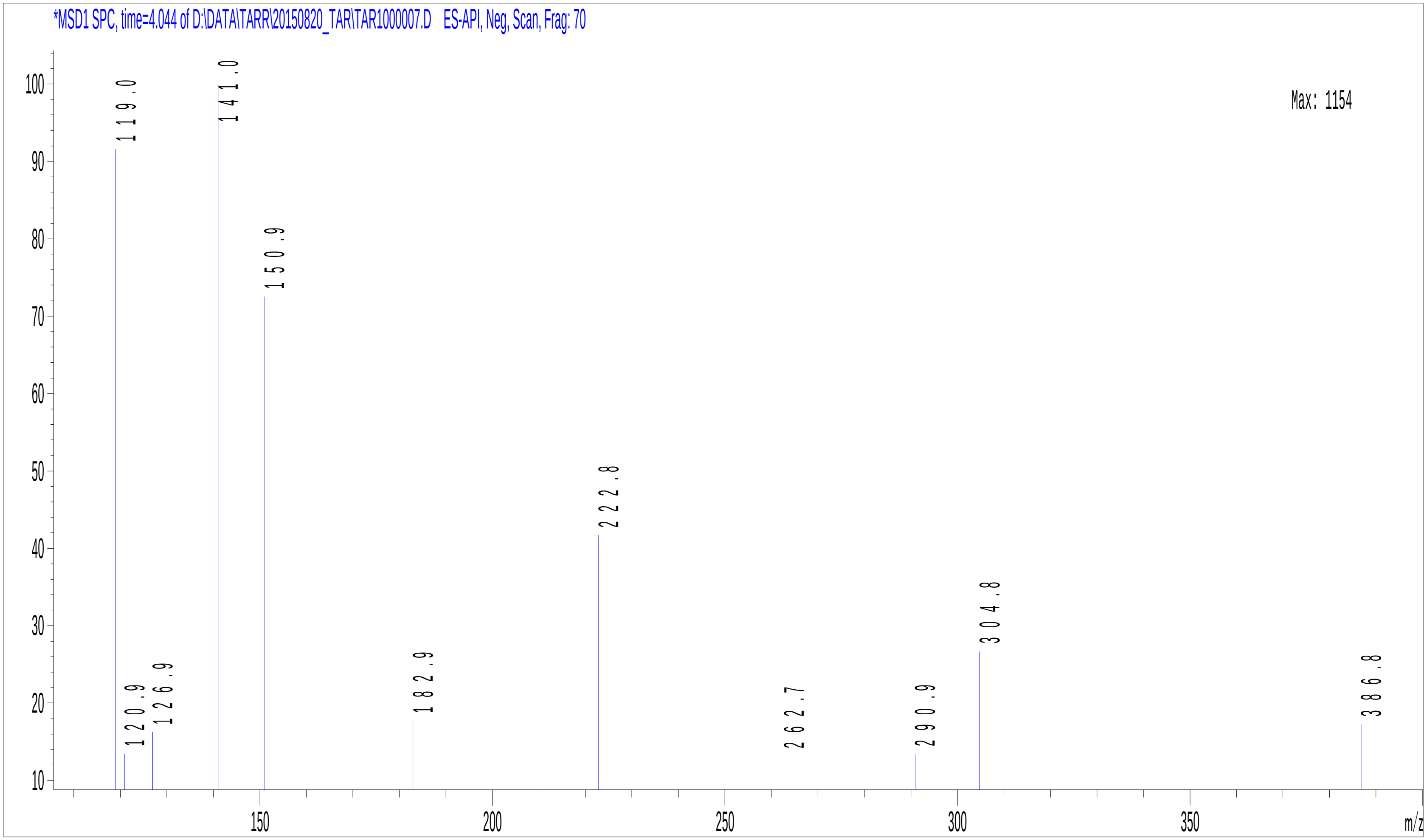
16-Apr-15
H2O2 Ctrl
8
P2-A-07



#	Time	Area	Height	Width	Area%	Symmetry
1	2.954	554501.9	44670	0.1701	91.277	0.895
2	3.924	21480.6	1777.5	0.1562	3.536	5.874
3	4.012	31509.1	2415.2	0.1623	5.187	0.22


*MSD1 SPC, time=2.999 of D:\DATA\TARR\20150820_TAR\TAR1000007.D   ES-API, Neg, Scan, Frag: 70
Max: 9133
0
20
40
60
80
100
100
150
200
250
300
350
400
450
500
m/z
119.0
151.0
154.9
170.9
194.8
197.9
210.8
232.8
264.3
466.6
467.6
468.6
478.2


*MSD1 SPC, time=3.842 of D:\DATA\TARR\20150820_TAR\TAR1000007.D ES-API, Neg, Scan, Frag: 70
Max: 1031
100
90
80
70
60
50
40
30
20
105.0
116.9
119.0
126.9
140.9
151.0
182.9
222.9
100
120
140
160
180
200
220
m/z

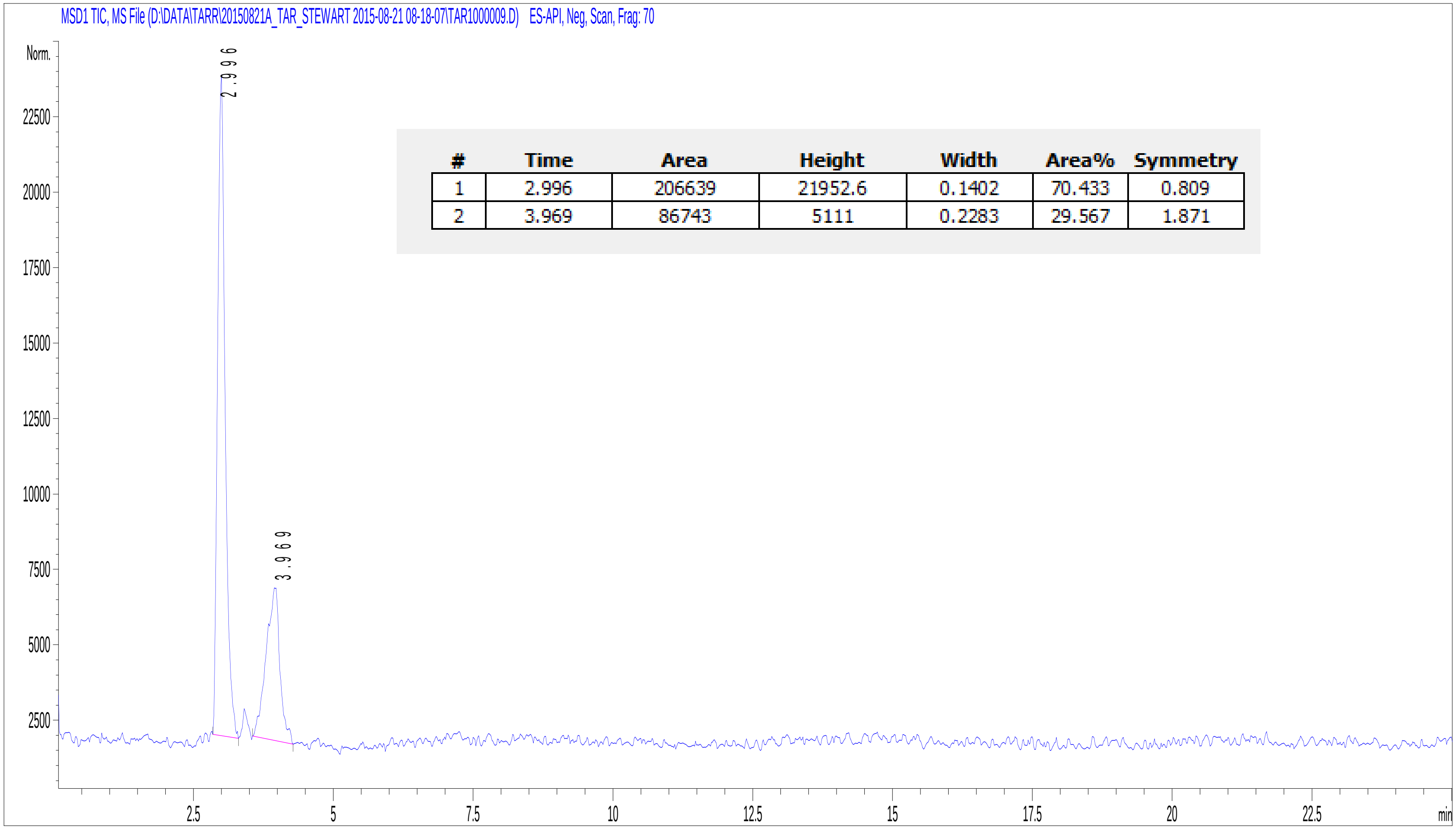
*MSD1 SPC, time=4.044 of D:\DATA\TARR\20150820_TAR\TAR1000007.D ES-API, Neg, Scan, Frag: 70
Max: 1154
119.0
120.9
126.9
141.0
150.9
182.9
222.8
262.7
290.9
304.8
386.8
100
90
80
70
60
50
40
30
20
10
150
200
250
300
350
m/z

15-Jul-15

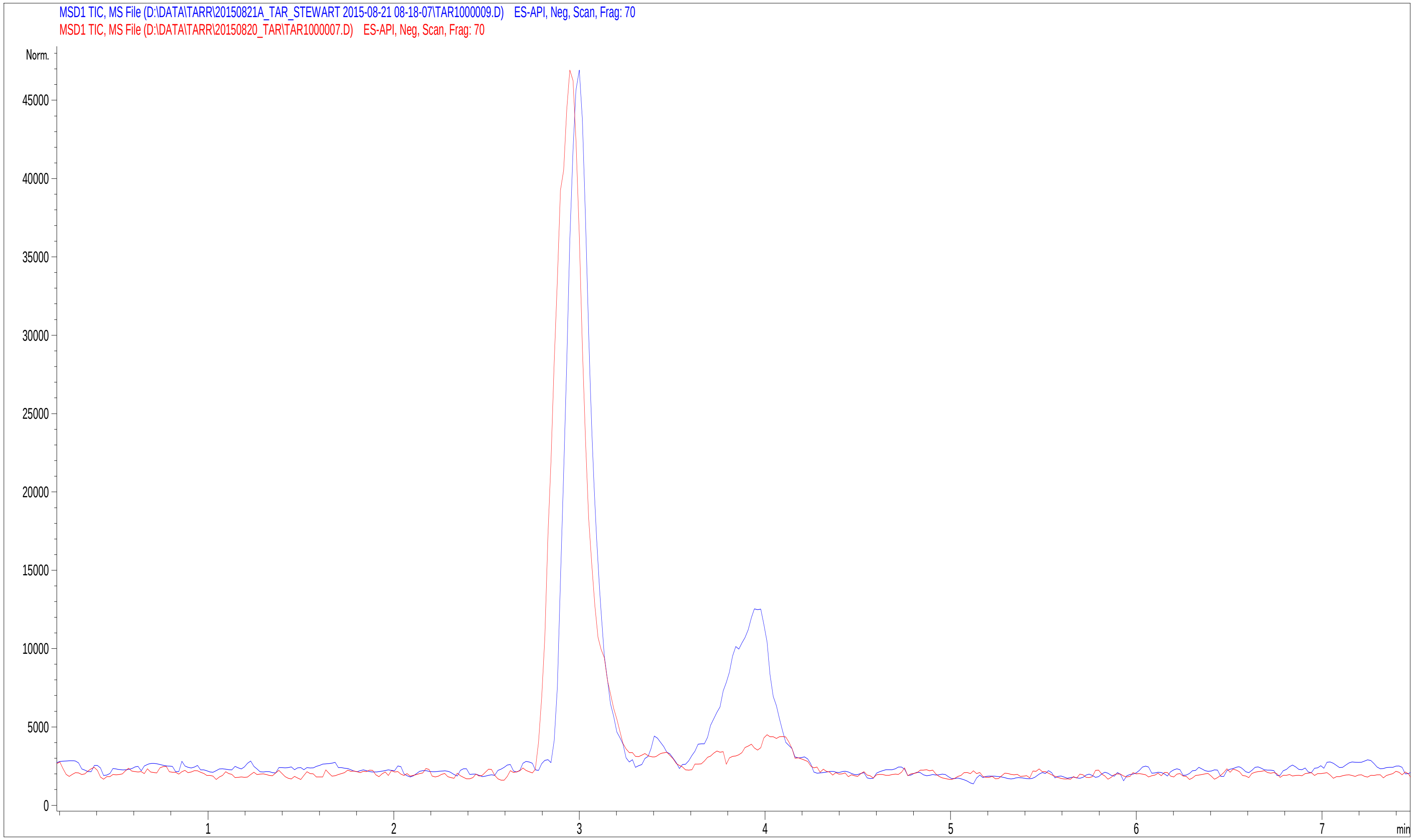
0 DC

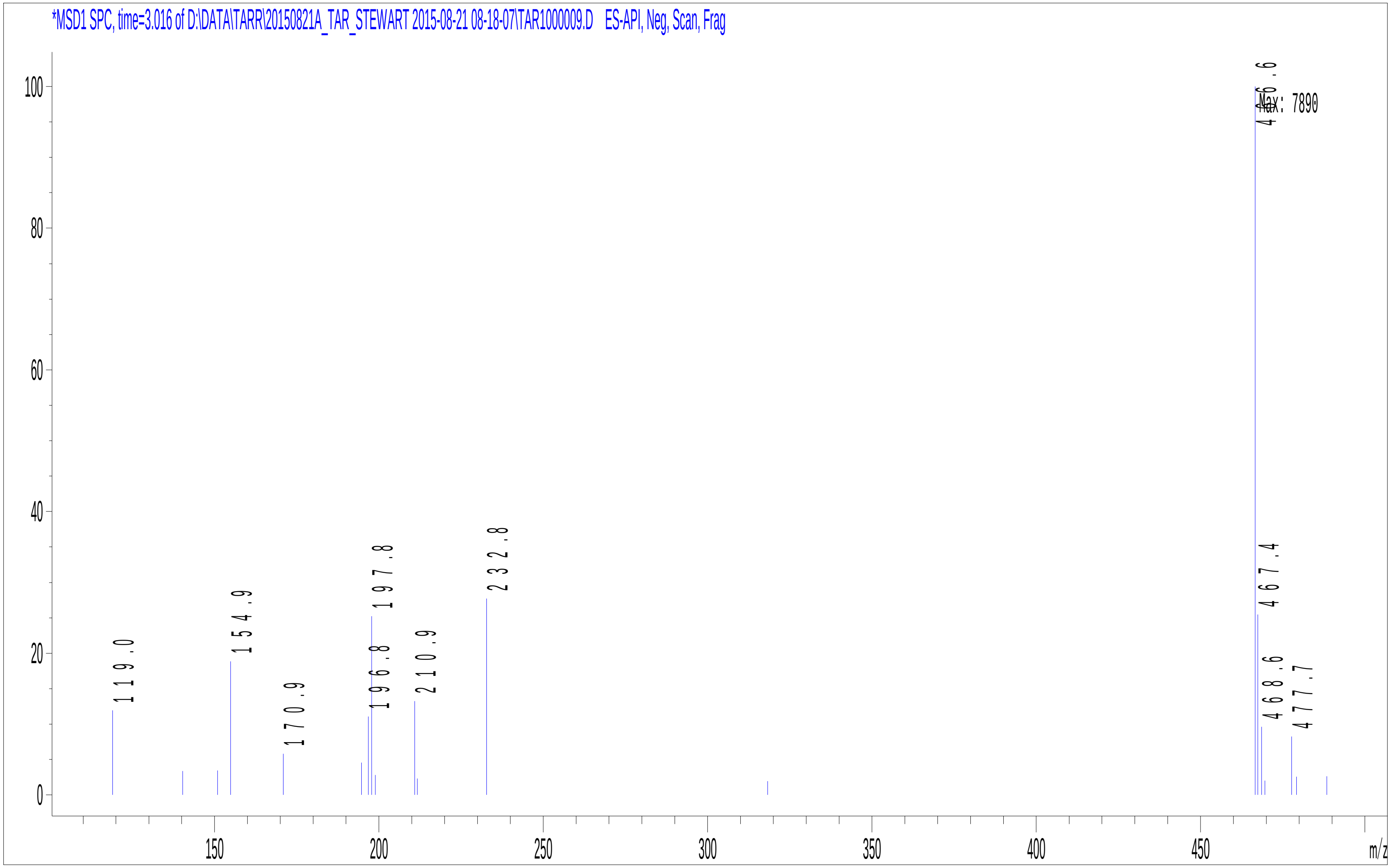
8

P2-E-08

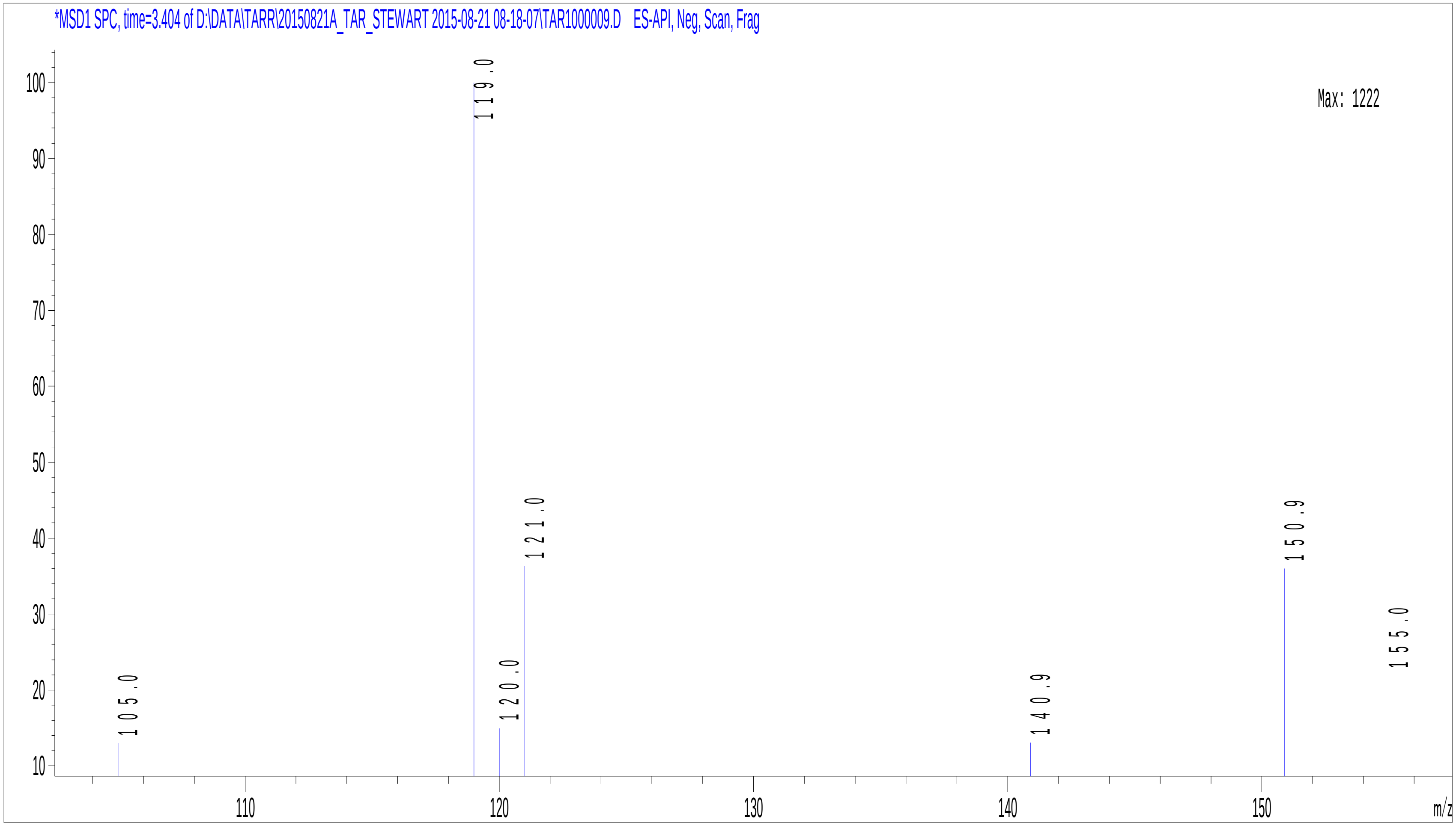


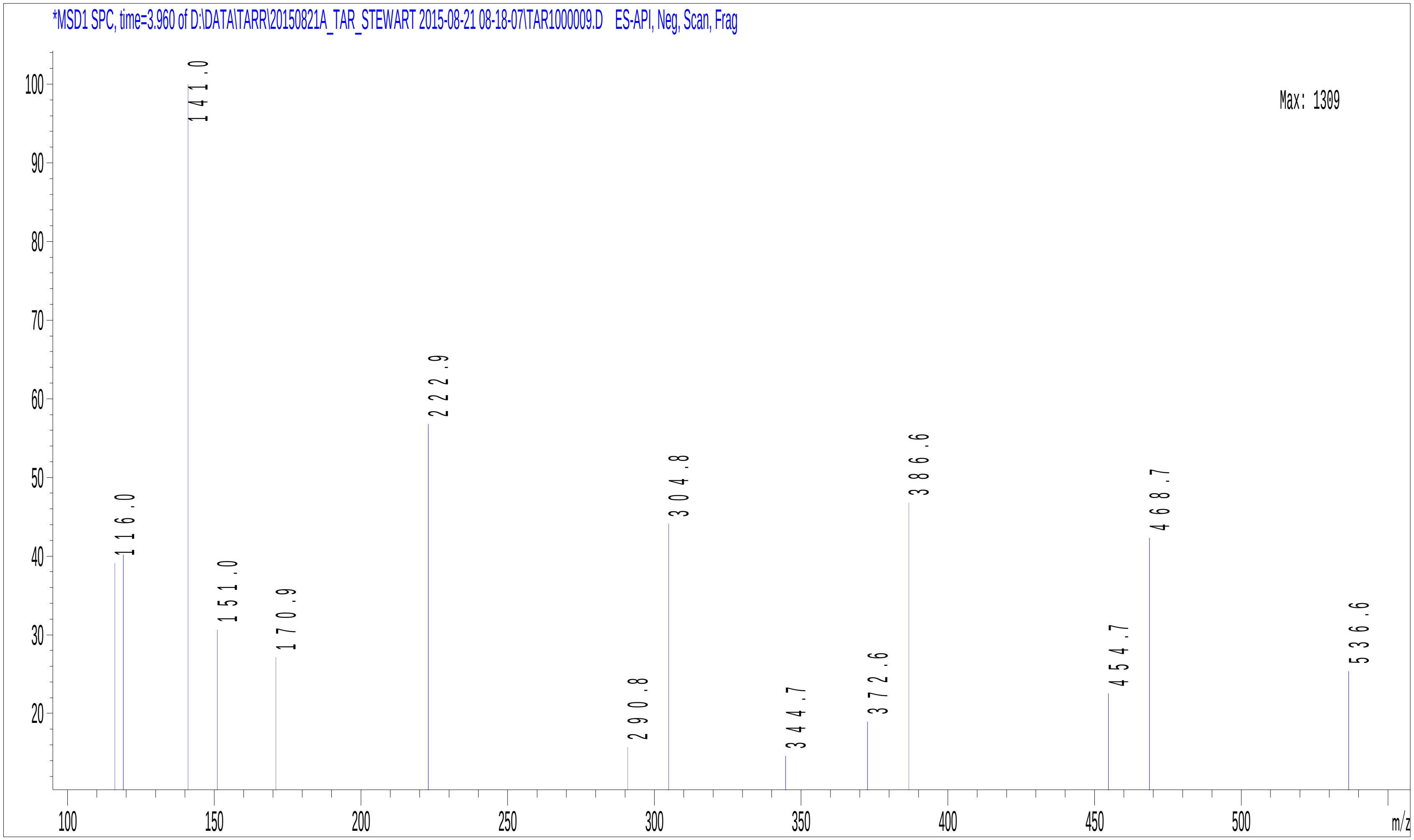
#	Time	Area	Height	Width	Area%	Symmetry
1	2.996	206639	21952.6	0.1402	70.433	0.809
2	3.969	86743	5111	0.2283	29.567	1.871


MSD1 TIC, MS File (D:\DATA\TARR\20150821A_TAR_STEWART 2015-08-21 08-18-07\TAR1000009.D) ES-API, Neg, Scan, Frag: 70
MSD1 TIC, MS File (D:\DATA\TARR\20150820_TAR\TAR1000007.D) ES-API, Neg, Scan, Frag: 70
Norm.
45000
40000
35000
30000
25000
20000
15000
10000
5000
0
1
2
3
4
5
6
7
min



*MSD1 SPC, time=3.016 of D:\DATA\TARR\20150821A_TAR_STEWART 2015-08-21 08-18-07\TAR1000009.D ES-API, Neg, Scan, Frag
Max: 7890
100
80
60
40
20
0
150
200
250
300
350
400
450
m/z
119.0
154.9
170.9
196.8
197.8
210.9
232.8
466.6
467.4
468.6
477.7


*MSD1 SPC, time=3.404 of D:\DATA\TARR\20150821A_TAR_STEWART 2015-08-21 08-18-07\TAR1000009.D ES-API, Neg, Scan, Frag
Max: 1222
100
90
80
70
60
50
40
30
20
10
105.0
119.0
120.0
121.0
140.9
150.9
155.0
110
120
130
140
150
m/z

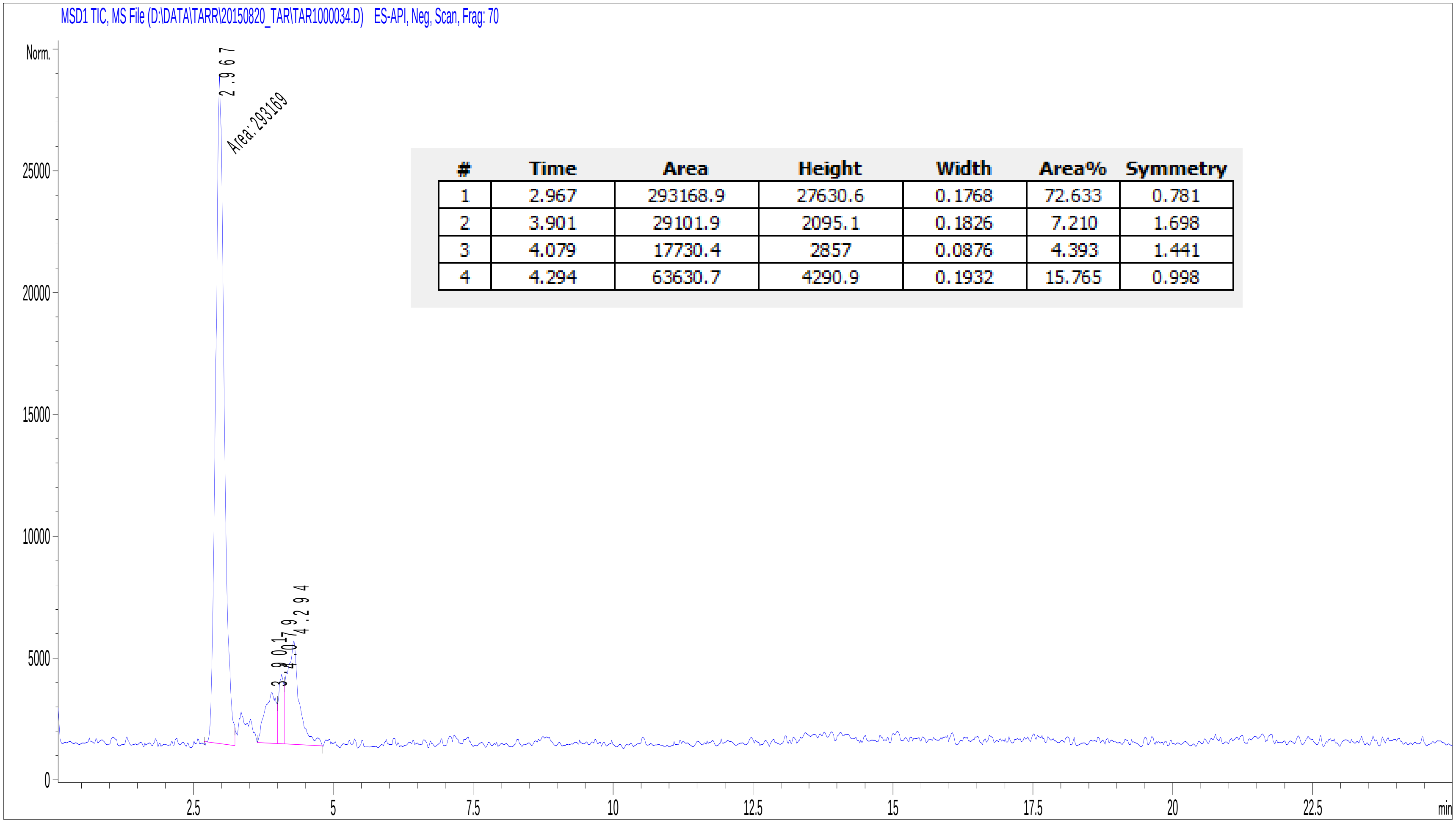
*MSD1 SPC, time=3.960 of D:\DATA\TARR\20150821A_TAR_STEWART 2015-08-21 08-18-07\TAR1000009.D ES-API, Neg, Scan, Frag
Max: 1309
100
90
80
70
60
50
40
30
20
116.0
141.0
151.0
170.9
222.9
290.8
304.8
344.7
372.6
386.6
454.7
468.7
536.6
100
150
200
250
300
350
400
450
500
m/z

21-Jul-15

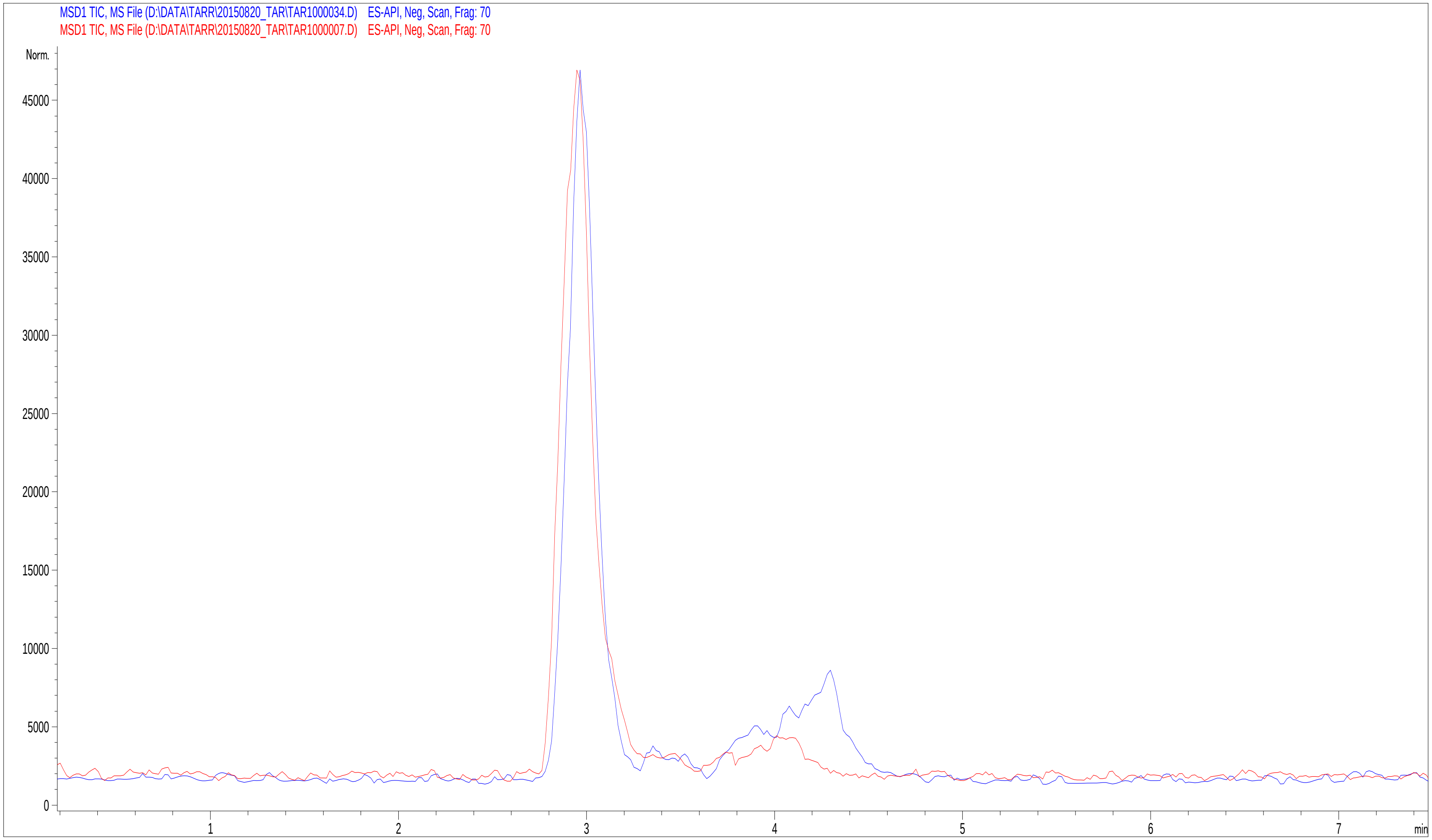
5 DC

8

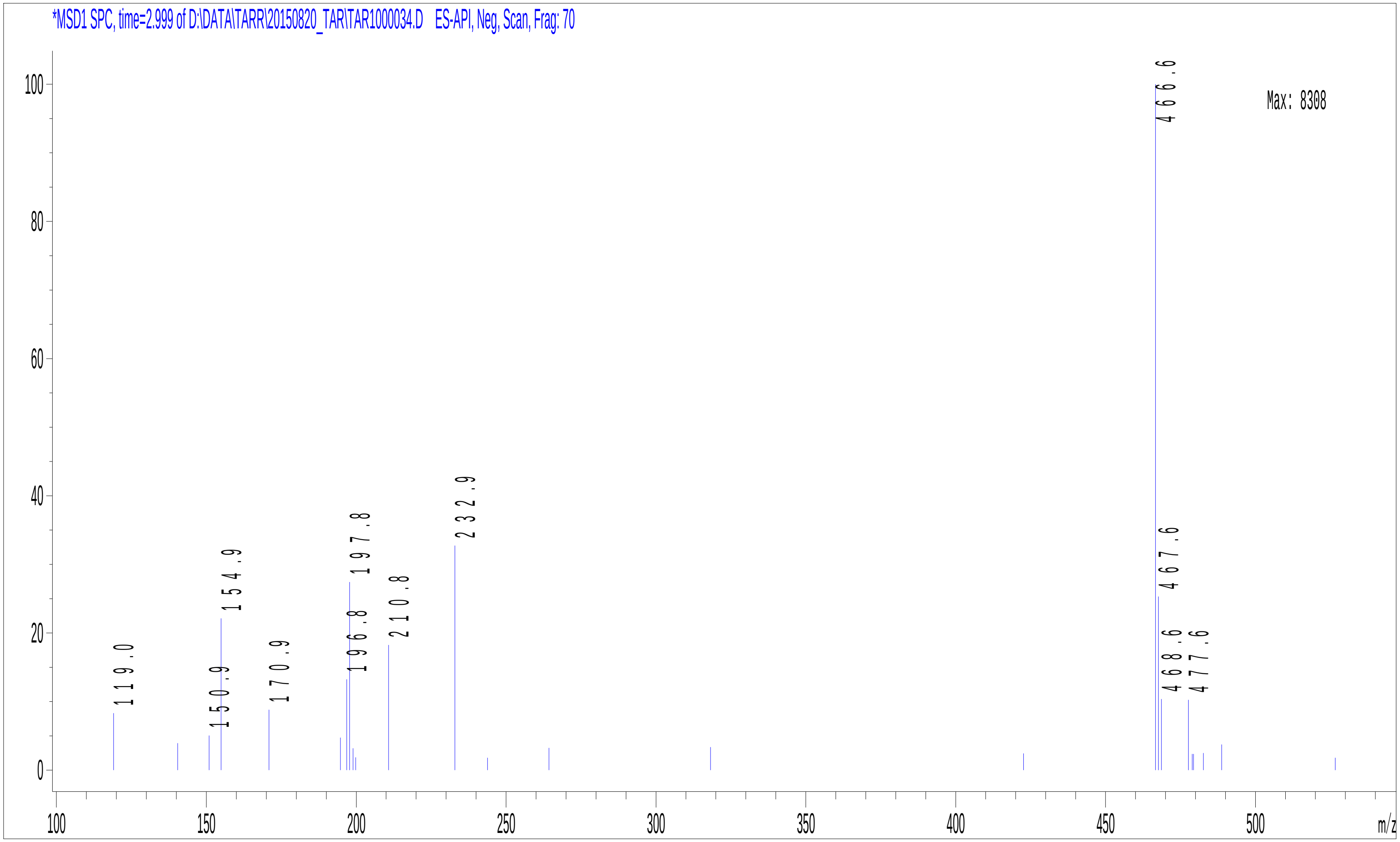
P2-D-03

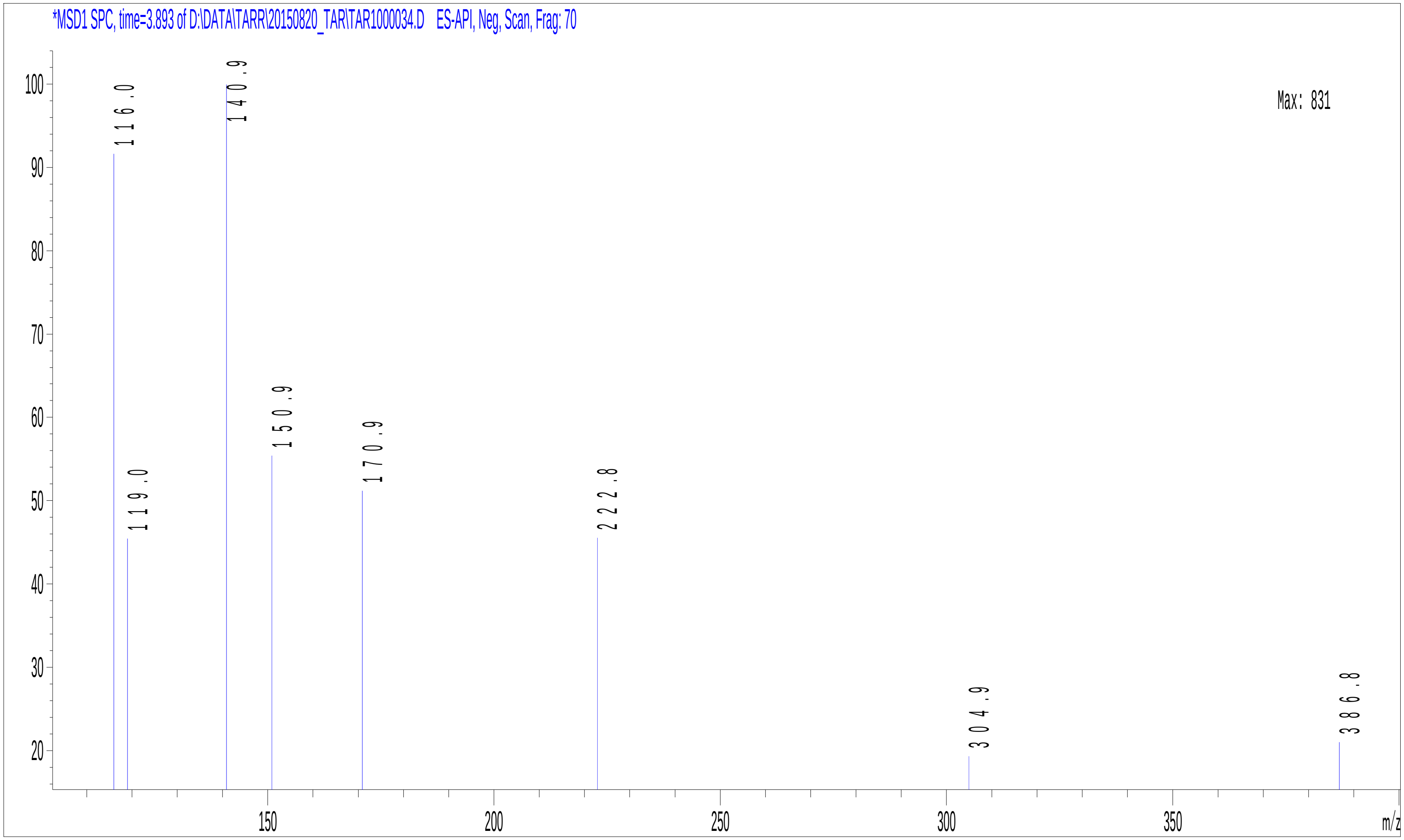


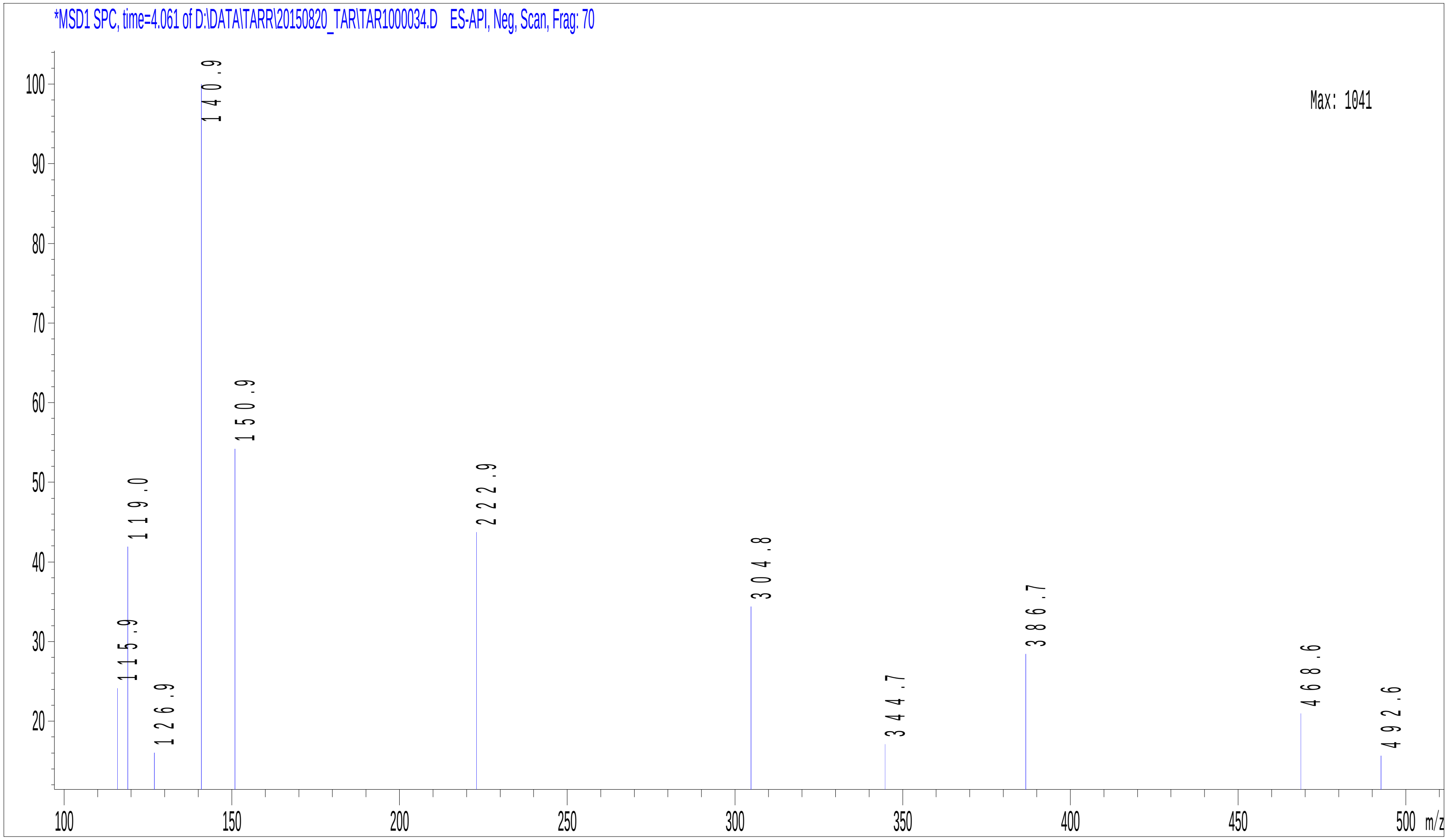
#	Time	Area	Height	Width	Area%	Symmetry
1	2.967	293168.9	27630.6	0.1768	72.633	0.781
2	3.901	29101.9	2095.1	0.1826	7.210	1.698
3	4.079	17730.4	2857	0.0876	4.393	1.441
4	4.294	63630.7	4290.9	0.1932	15.765	0.998

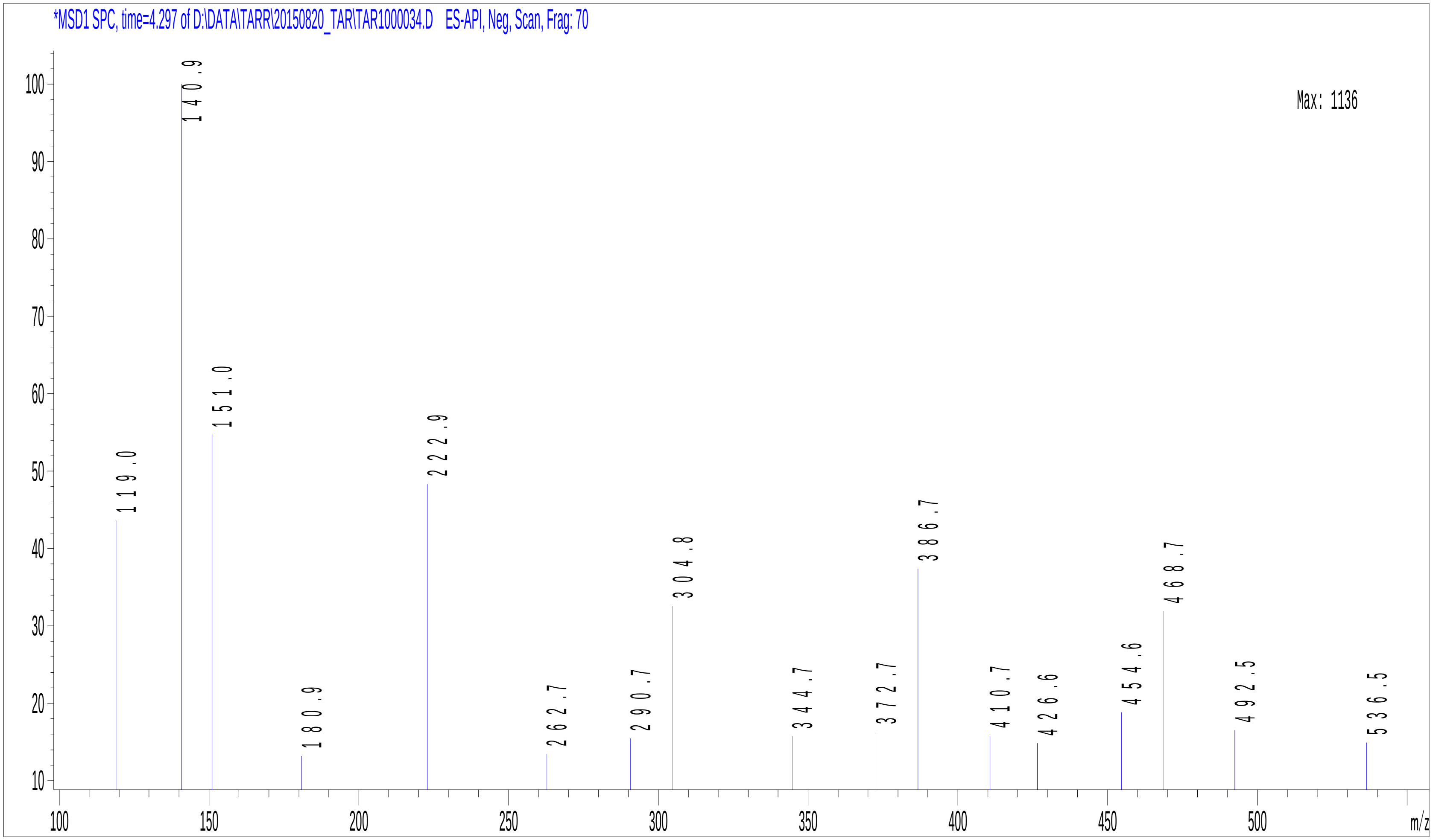


MSD1 TIC, MS File (D:\DATA\TARR\20150820_TAR\TAR1000034.D) ES-API, Neg, Scan, Frag: 70
MSD1 TIC, MS File (D:\DATA\TARR\20150820_TAR\TAR1000007.D) ES-API, Neg, Scan, Frag: 70
Norm.
45000
40000
35000
30000
25000
20000
15000
10000
5000
0
1
2
3
4
5
6
7
min


*MSD1 SPC, time=2.999 of D:\DATA\TARR\20150820_TAR\TAR1000034.D ES-API, Neg, Scan, Frag: 70
Max: 8308
100
80
60
40
20
0
100
150
200
250
300
350
400
450
500
m/z
119.0
150.9
154.9
170.9
196.8
197.8
210.8
232.9
466.6
467.6
468.6
477.6


*MSD1 SPC, time=3.893 of D:\DATA\TARR\20150820_TAR\TAR1000034.D ES-API, Neg, Scan, Frag: 70
Max: 831
116.0
119.0
140.9
150.9
170.9
222.8
304.9
386.8
100
90
80
70
60
50
40
30
20
150
200
250
300
350
m/z


*MSD1 SPC, time=4.061 of D:\DATA\TARR\20150820_TAR\TAR1000034.D ES-API, Neg, Scan, Frag: 70
Max: 1041
100
90
80
70
60
50
40
30
20
115.9
119.0
126.9
140.9
150.9
222.9
304.8
344.7
386.7
468.6
492.6
100
150
200
250
300
350
400
450
500
m/z

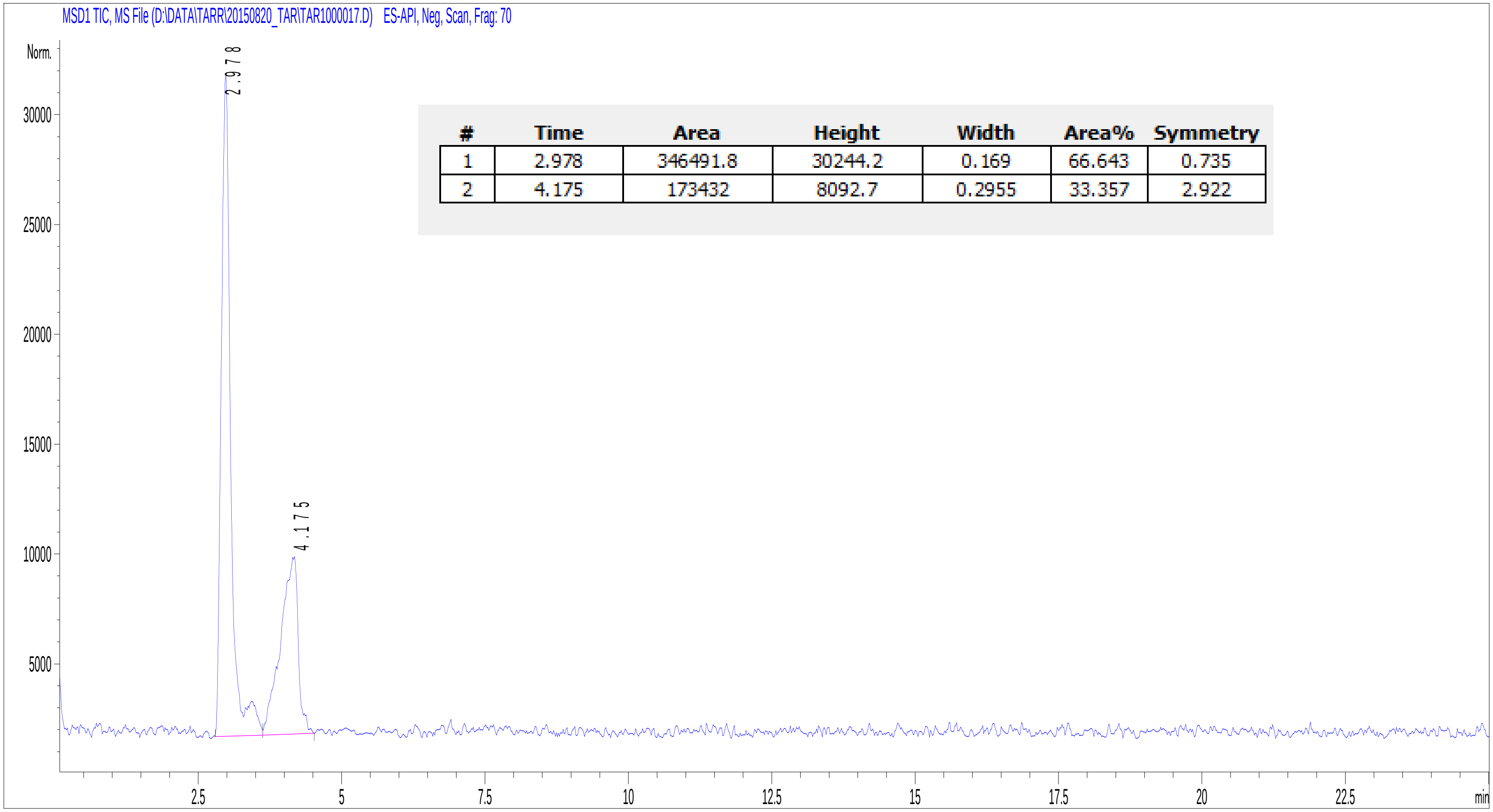

*MSD1 SPC, time=4.297 of D:\DATA\TARR\20150820_TAR\TAR1000034.D ES-API, Neg, Scan, Frag: 70
Max: 1136
100
90
80
70
60
50
40
30
20
10
119.0
140.9
151.0
180.9
222.9
262.7
290.7
304.8
344.7
372.7
386.7
410.7
426.6
454.6
468.7
492.5
536.5
100
150
200
250
300
350
400
450
500
m/z

27-May-15

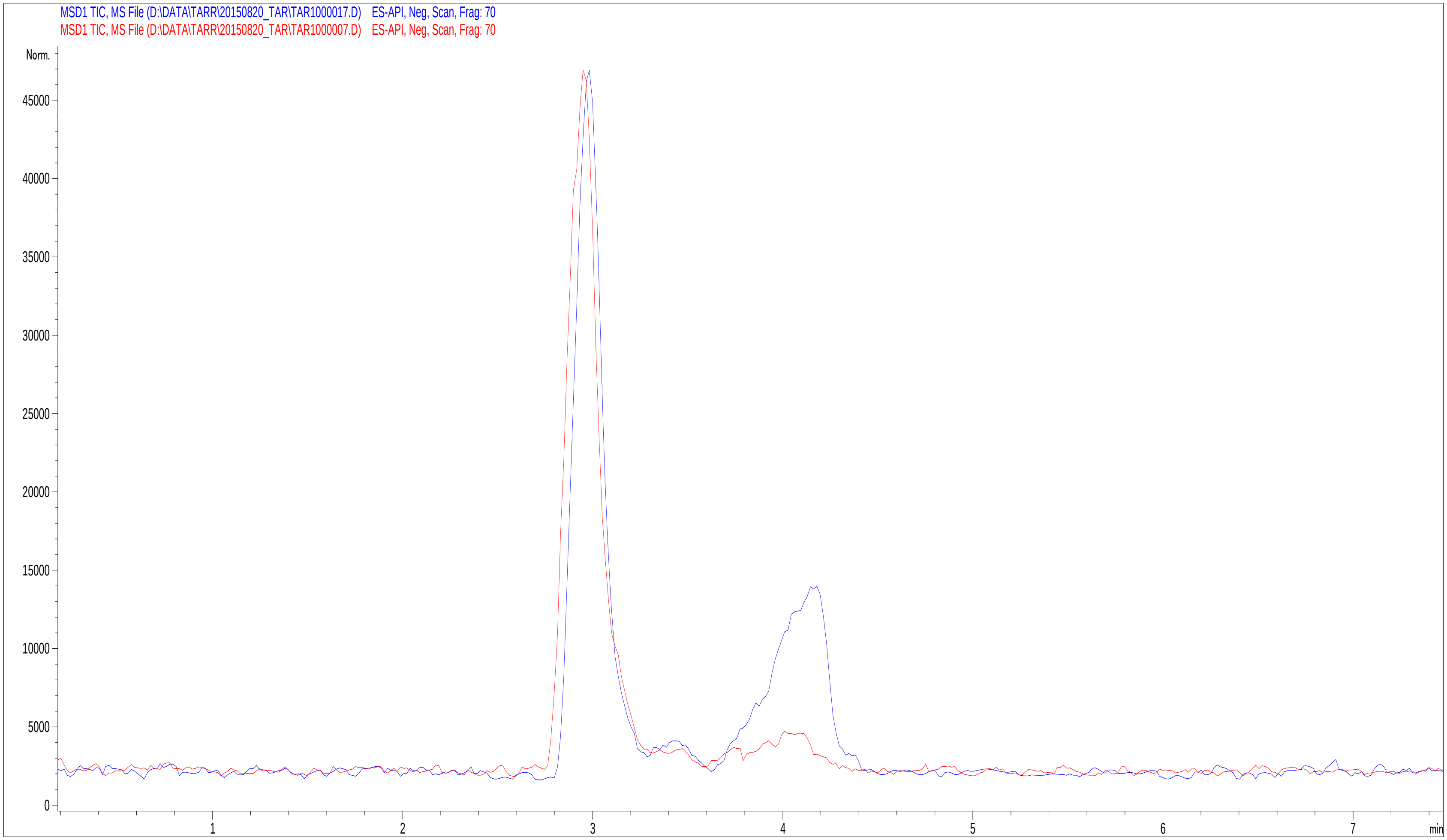
10 DC

8

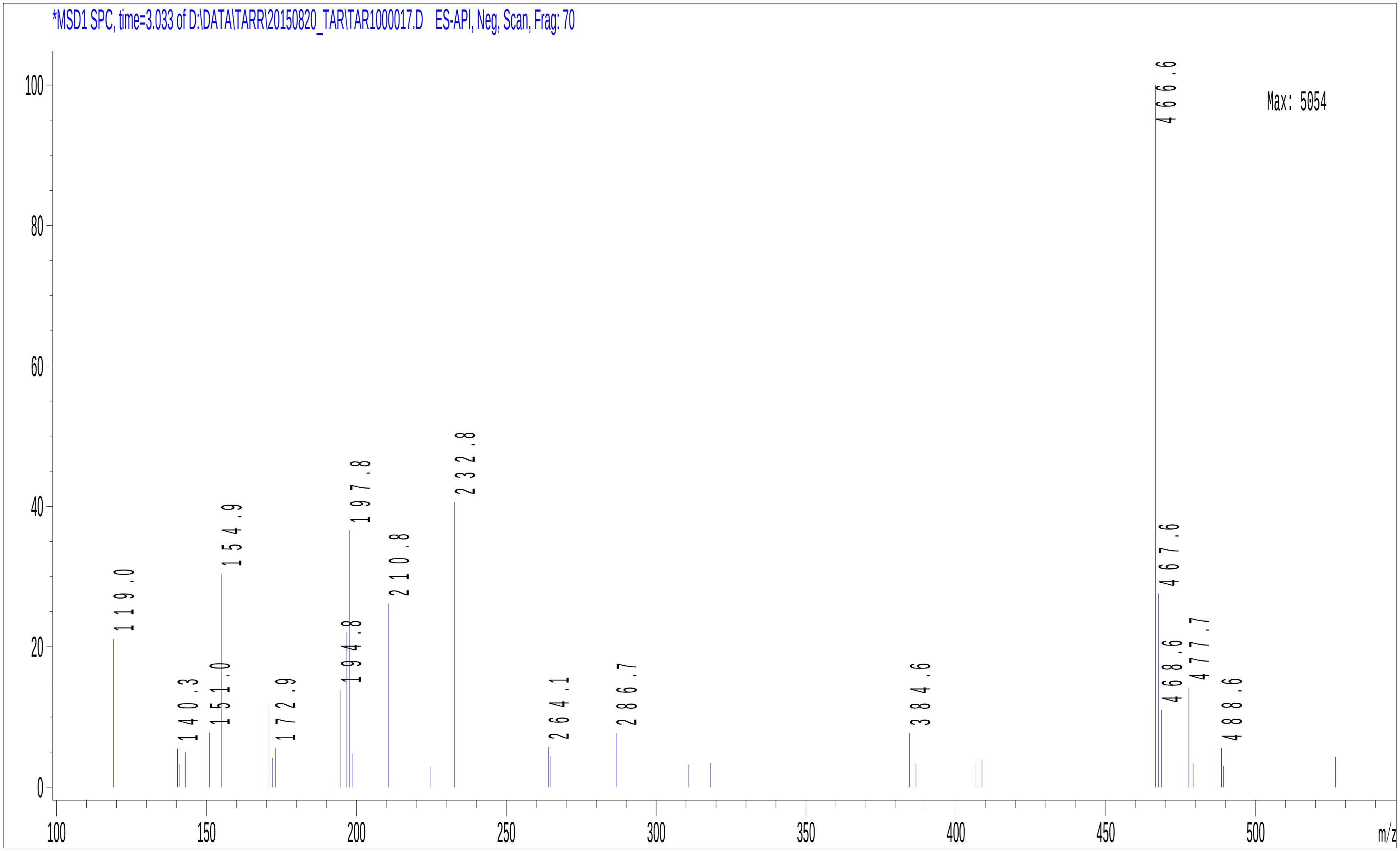
P2-B-02

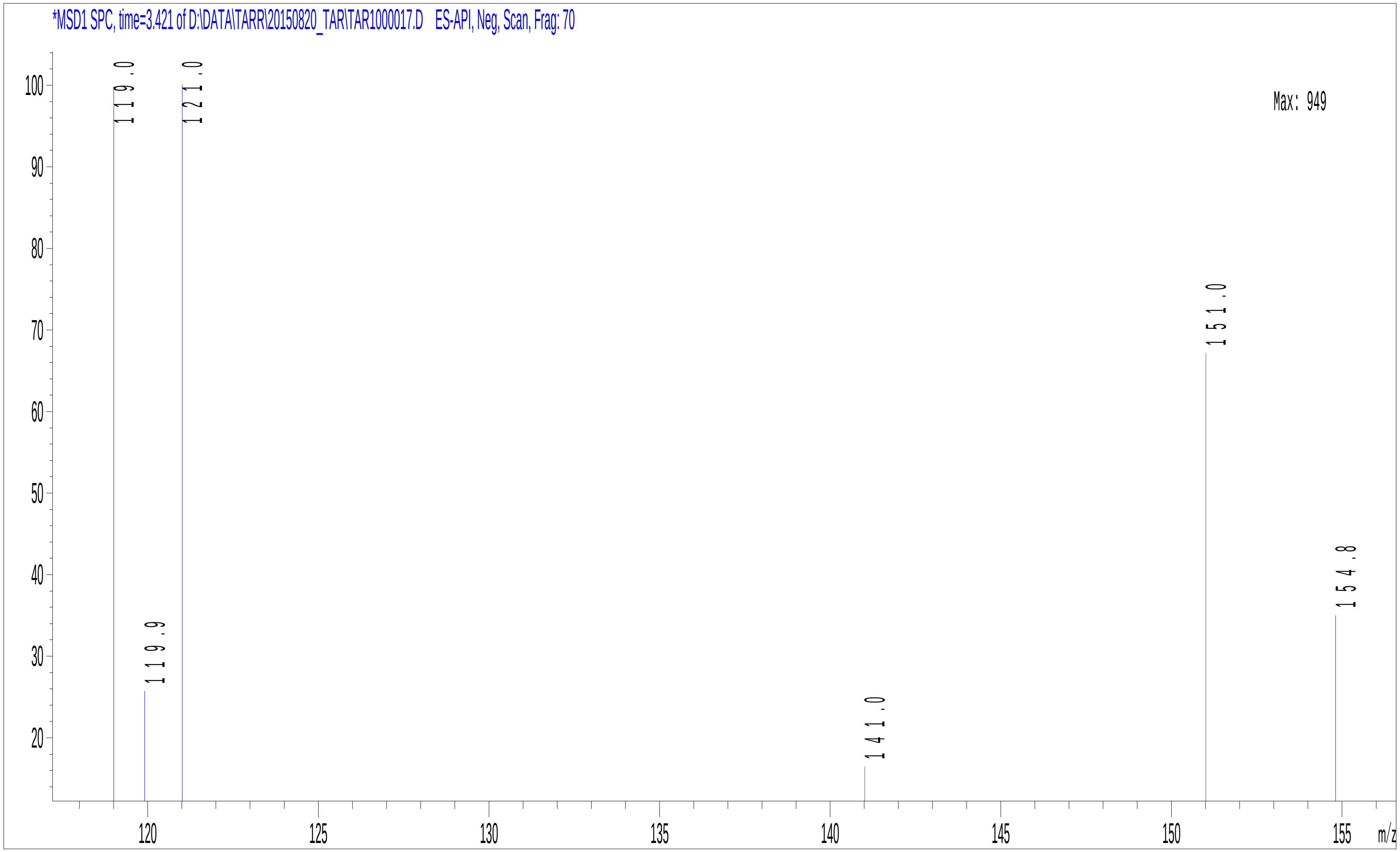


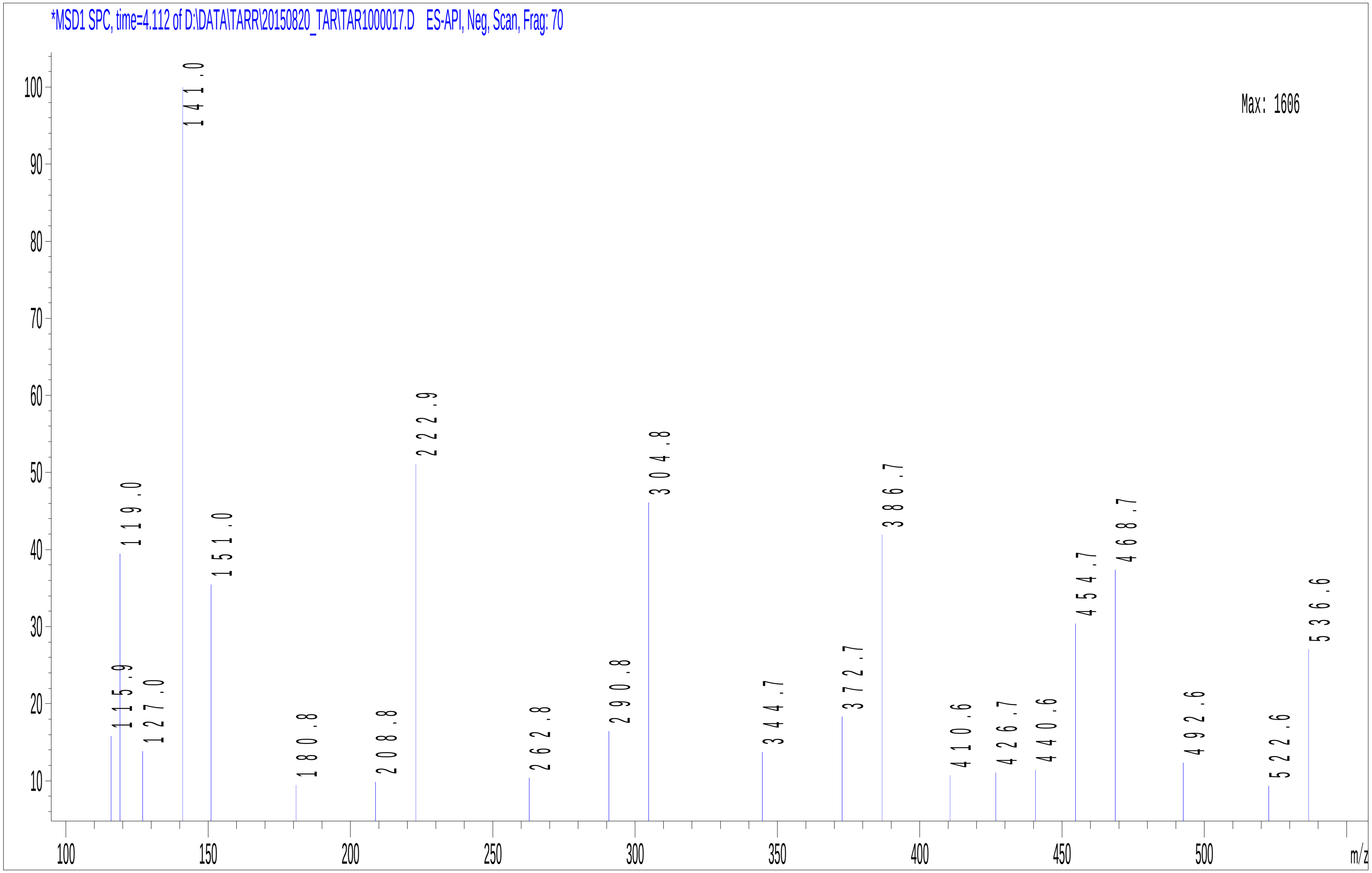
#	Time	Area	Height	Width	Area%	Symmetry
1	2.978	346491.8	30244.2	0.169	66.643	0.735
2	4.175	173432	8092.7	0.2955	33.357	2.922



MSD1 TIC, MS File (D:\DATA\TARR\20150820_TAR\TAR1000017.D) ES-API, Neg, Scan, Frag: 70
MSD1 TIC, MS File (D:\DATA\TARR\20150820_TAR\TAR1000007.D) ES-API, Neg, Scan, Frag: 70
Norm.
45000
40000
35000
30000
25000
20000
15000
10000
5000
0
1
2
3
4
5
6
7
min


*MSD1 SPC, time=3.033 of D:\DATA\TARR\20150820_TAR\TAR1000017.D ES-API, Neg, Scan, Frag: 70
Max: 5054
466.6
467.6
468.6
477.7
488.6
384.6
286.7
264.1
232.8
210.8
197.8
194.8
172.9
154.9
151.0
140.3
119.0
0
20
40
60
80
100
100
150
200
250
300
350
400
450
500
m/z


*MSD1 SPC, time=3.421 of D:\DATA\TARR\20150820_TAR\TAR1000017.D ES-API, Neg, Scan, Frag: 70
Max: 949
119.0
121.0
119.9
141.0
151.0
154.8
100
90
80
70
60
50
40
30
20
120
125
130
135
140
145
150
155
m/z

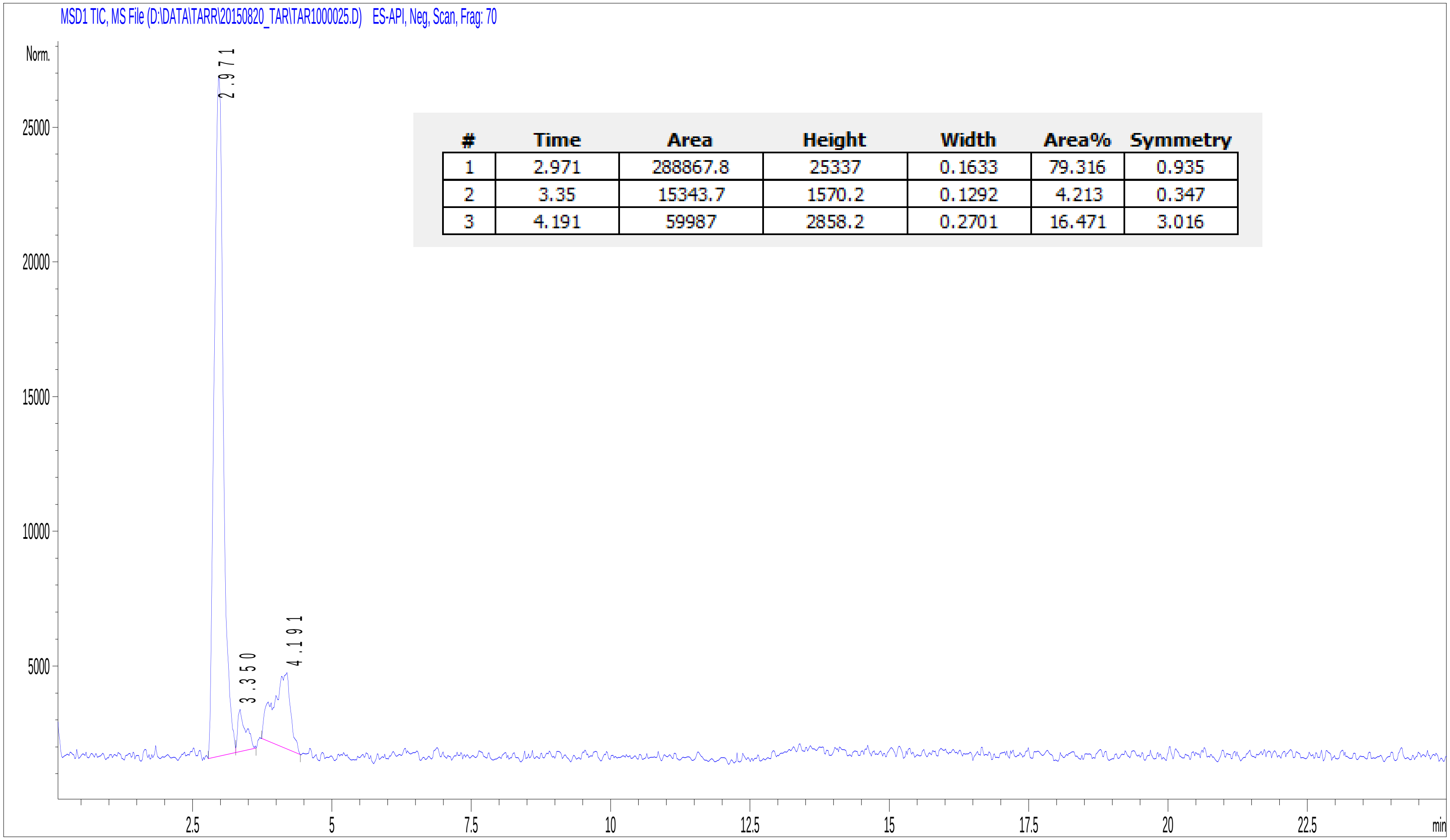

*MSD1 SPC, time=4.112 of D:\DATA\TARR\20150820_TAR\TAR1000017.D ES-API, Neg, Scan, Frag: 70
Max: 1606
100
90
80
70
60
50
40
30
20
10
100
150
200
250
300
350
400
450
500
m/z
115.9
119.0
127.0
141.0
151.0
180.8
208.8
222.9
262.8
290.8
304.8
344.7
372.7
386.7
410.6
426.7
440.6
454.7
468.7
492.6
522.6
536.6

10-Jul-15

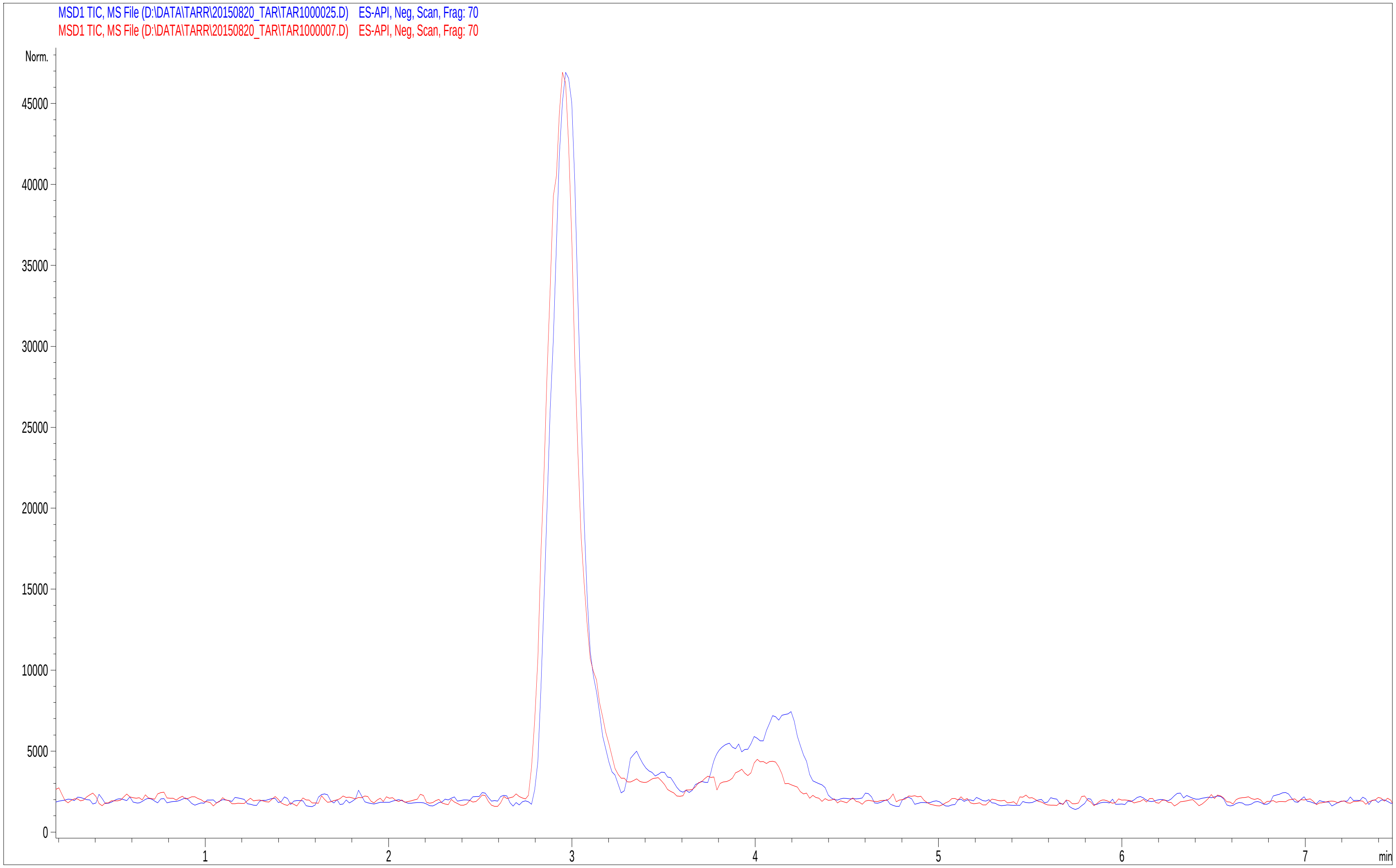
20 DC

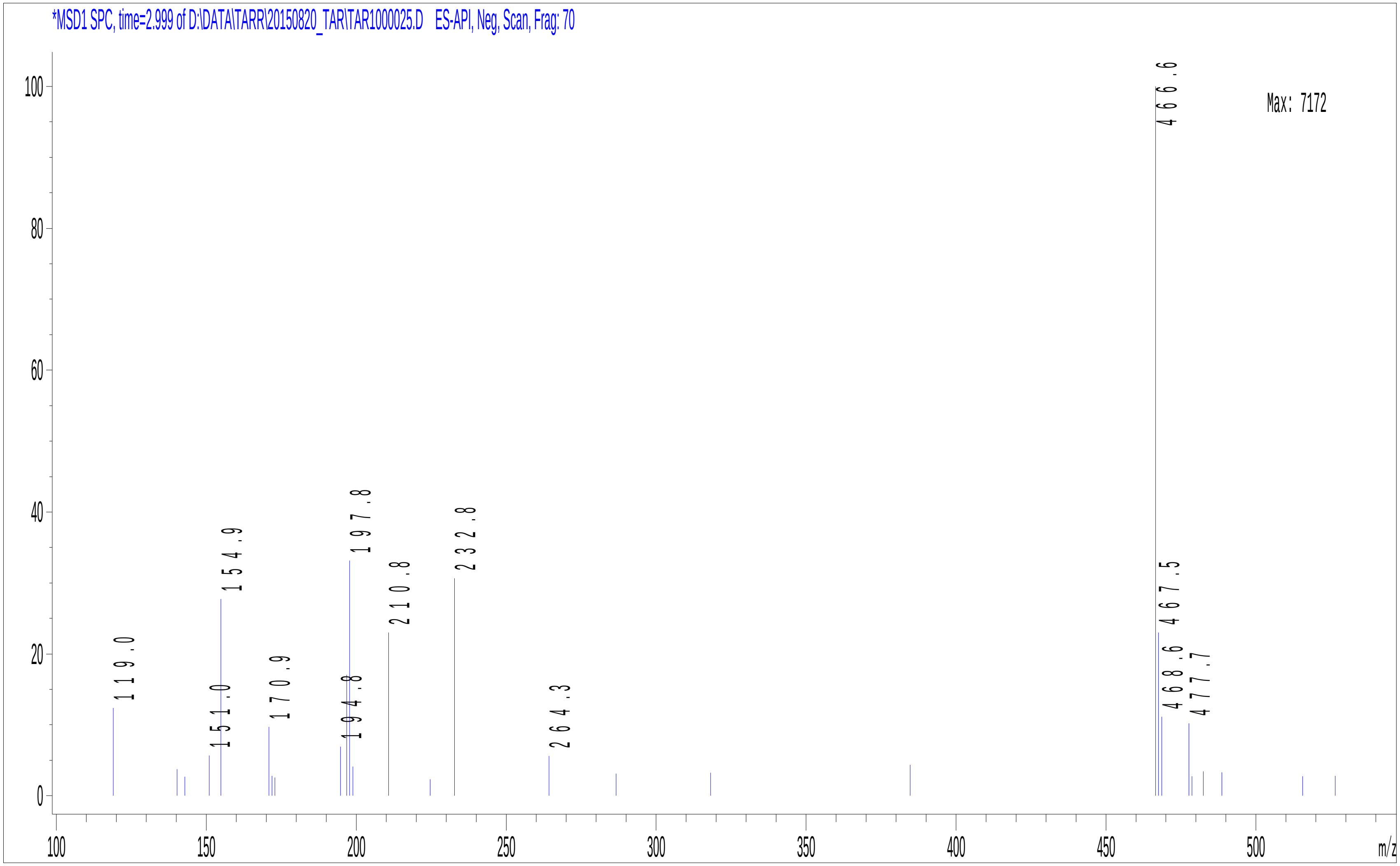
8

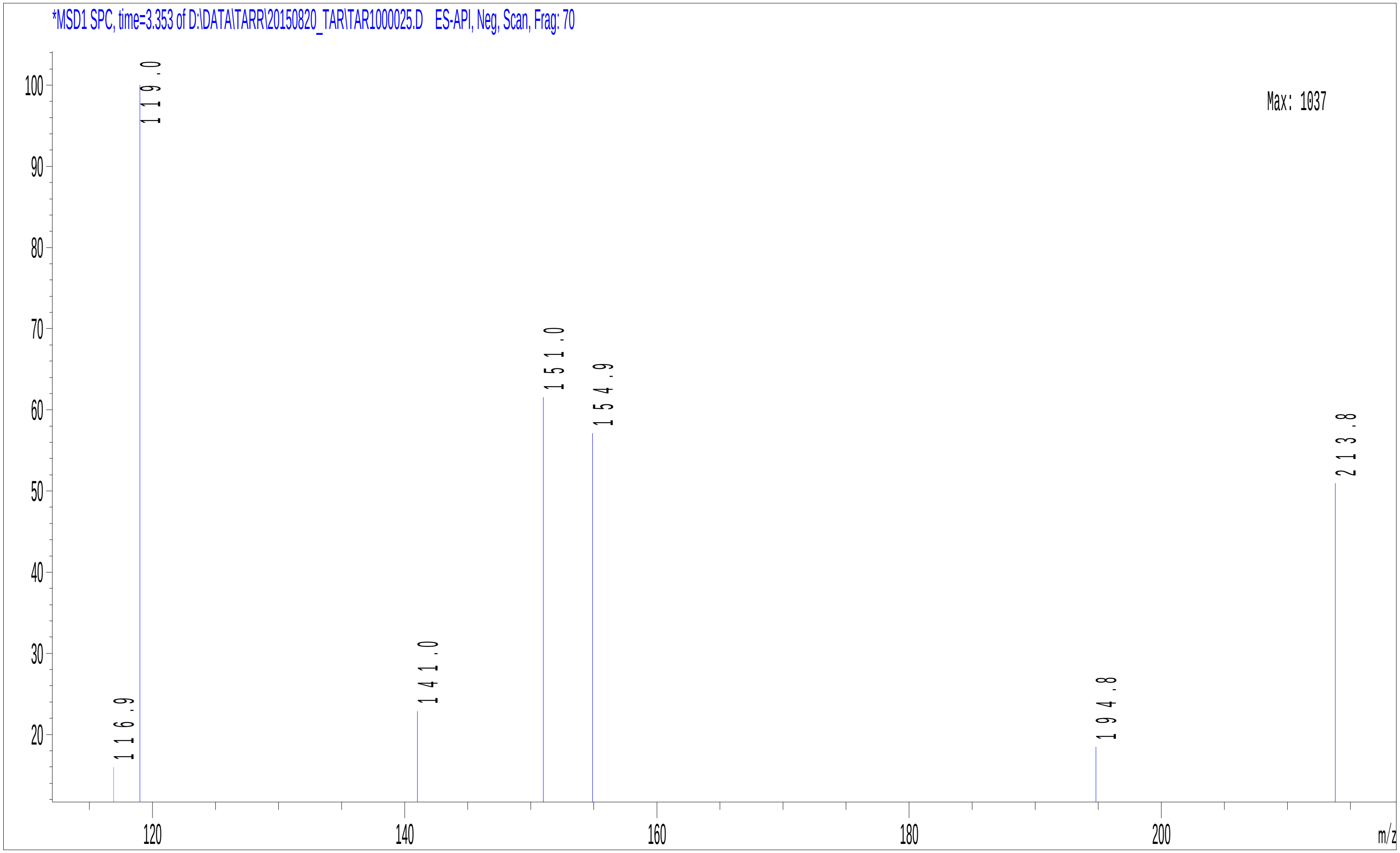
P2-C-07

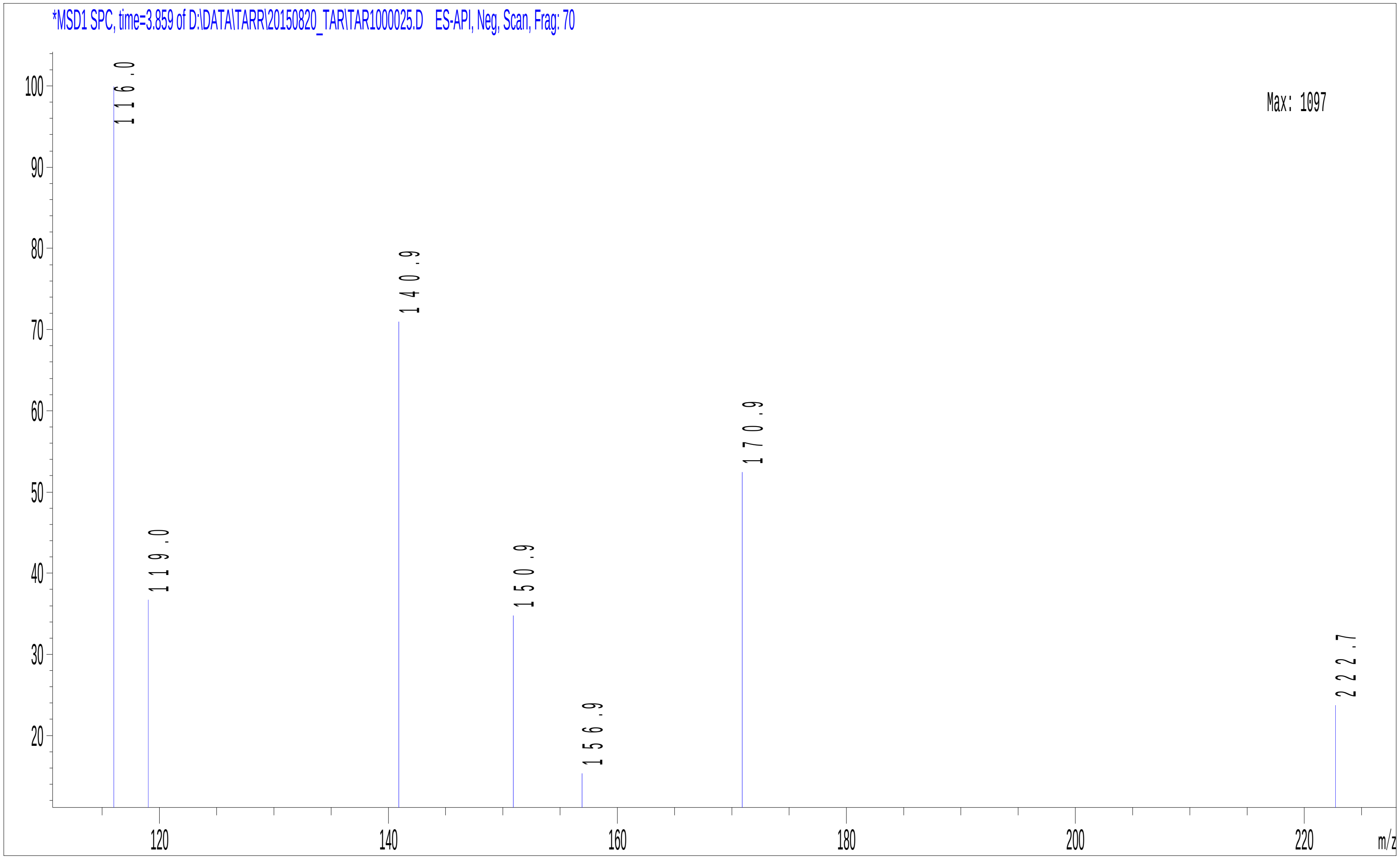


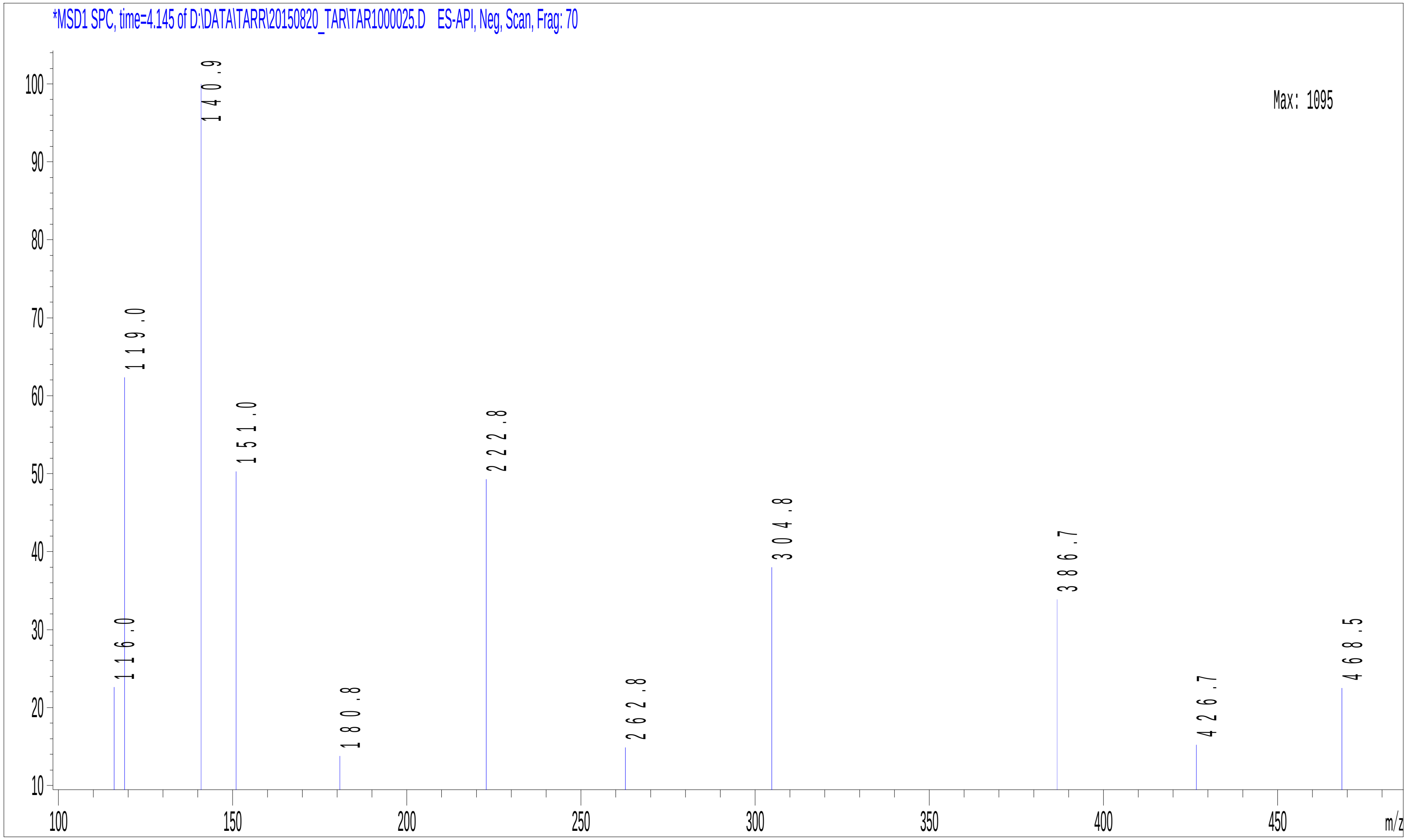
#	Time	Area	Height	Width	Area%	Symmetry
1	2.971	288867.8	25337	0.1633	79.316	0.935
2	3.35	15343.7	1570.2	0.1292	4.213	0.347
3	4.191	59987	2858.2	0.2701	16.471	3.016


MSD1 TIC, MS File (D:\DATA\TARR\20150820_TAR\TAR1000025.D) ES-API, Neg, Scan, Frag: 70
MSD1 TIC, MS File (D:\DATA\TARR\20150820_TAR\TAR1000007.D) ES-API, Neg, Scan, Frag: 70
Norm.
45000
40000
35000
30000
25000
20000
15000
10000
5000
0
1
2
3
4
5
6
7
min


*MSD1 SPC, time=2.999 of D:\DATA\TARR\20150820_TAR\TAR1000025.D ES-API, Neg, Scan, Frag: 70
Max: 7172
466.6
467.5
468.6
477.7
119.0
151.0
154.9
170.9
194.8
197.8
210.8
232.8
264.3
0
20
40
60
80
100
100
150
200
250
300
350
400
450
500
m/z


*MSD1 SPC, time=3.353 of D:\DATA\TARR\20150820_TAR\TAR1000025.D ES-API, Neg, Scan, Frag: 70
Max: 1037
100
90
80
70
60
50
40
30
20
116.9
119.0
141.0
151.0
154.9
194.8
213.8
120
140
160
180
200
m/z


*MSD1 SPC, time=3.859 of D:\DATA\TARR\20150820_TAR\TAR1000025.D ES-API, Neg, Scan, Frag: 70
Max: 1097
116.0
119.0
140.9
150.9
156.9
170.9
222.7
100
90
80
70
60
50
40
30
20
120
140
160
180
200
220
m/z

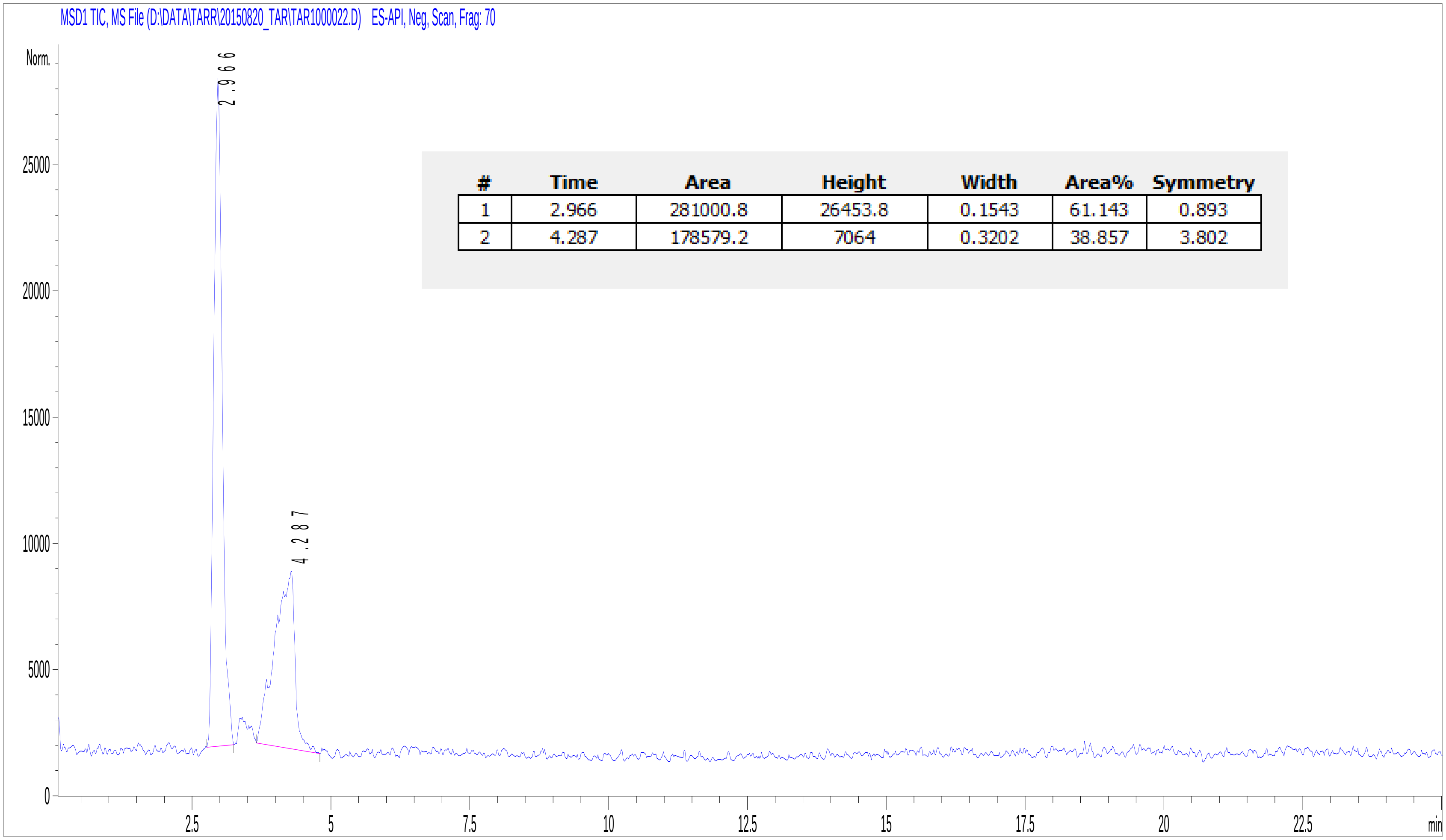

*MSD1 SPC, time=4.145 of D:\DATA\TARR\20150820_TAR\TAR1000025.D ES-API, Neg, Scan, Frag: 70
Max: 1095
100
90
80
70
60
50
40
30
20
10
140.9
119.0
151.0
222.8
304.8
386.7
116.0
468.5
180.8
262.8
426.7
100
150
200
250
300
350
400
450
m/z

2-Jul-15

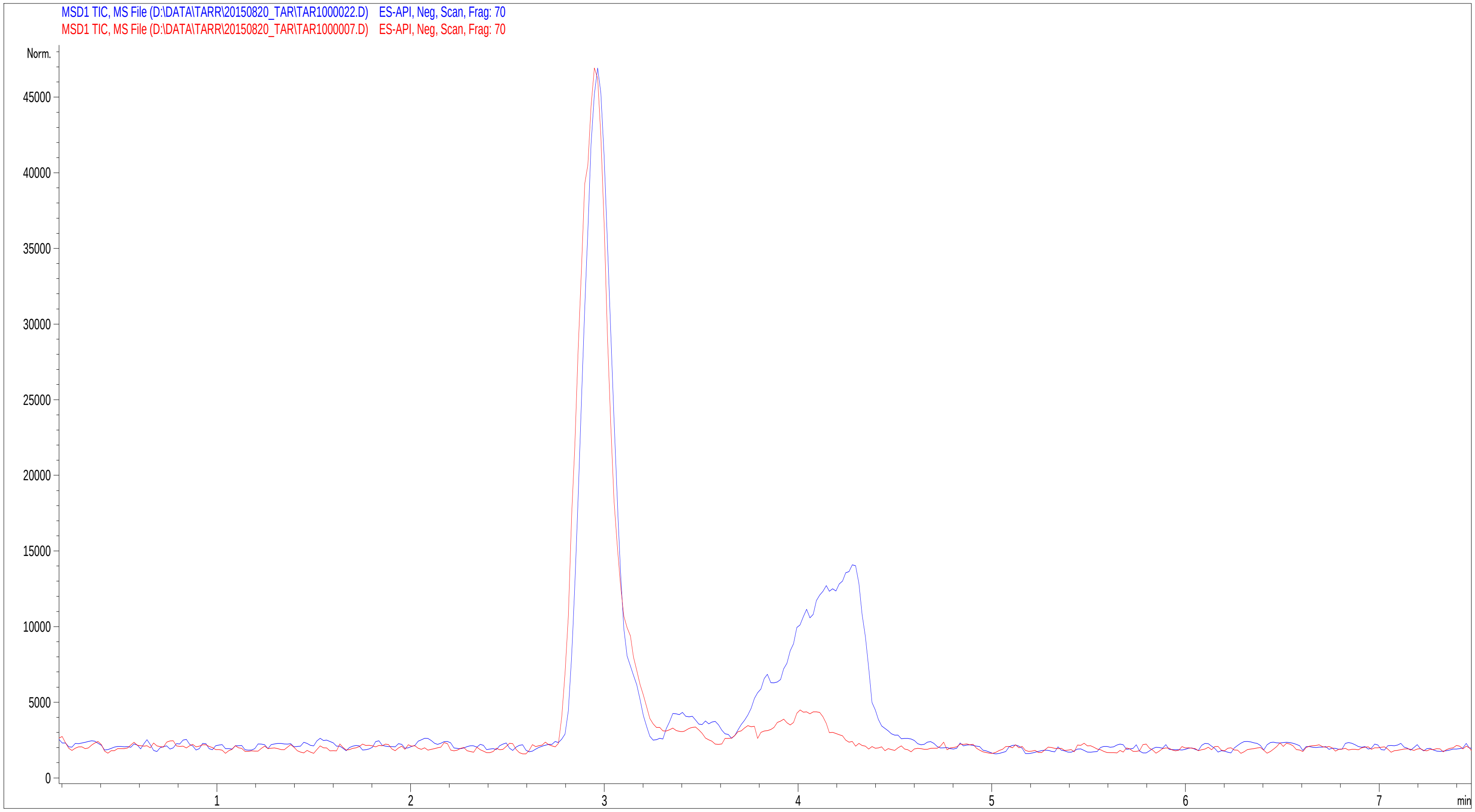
30 DC

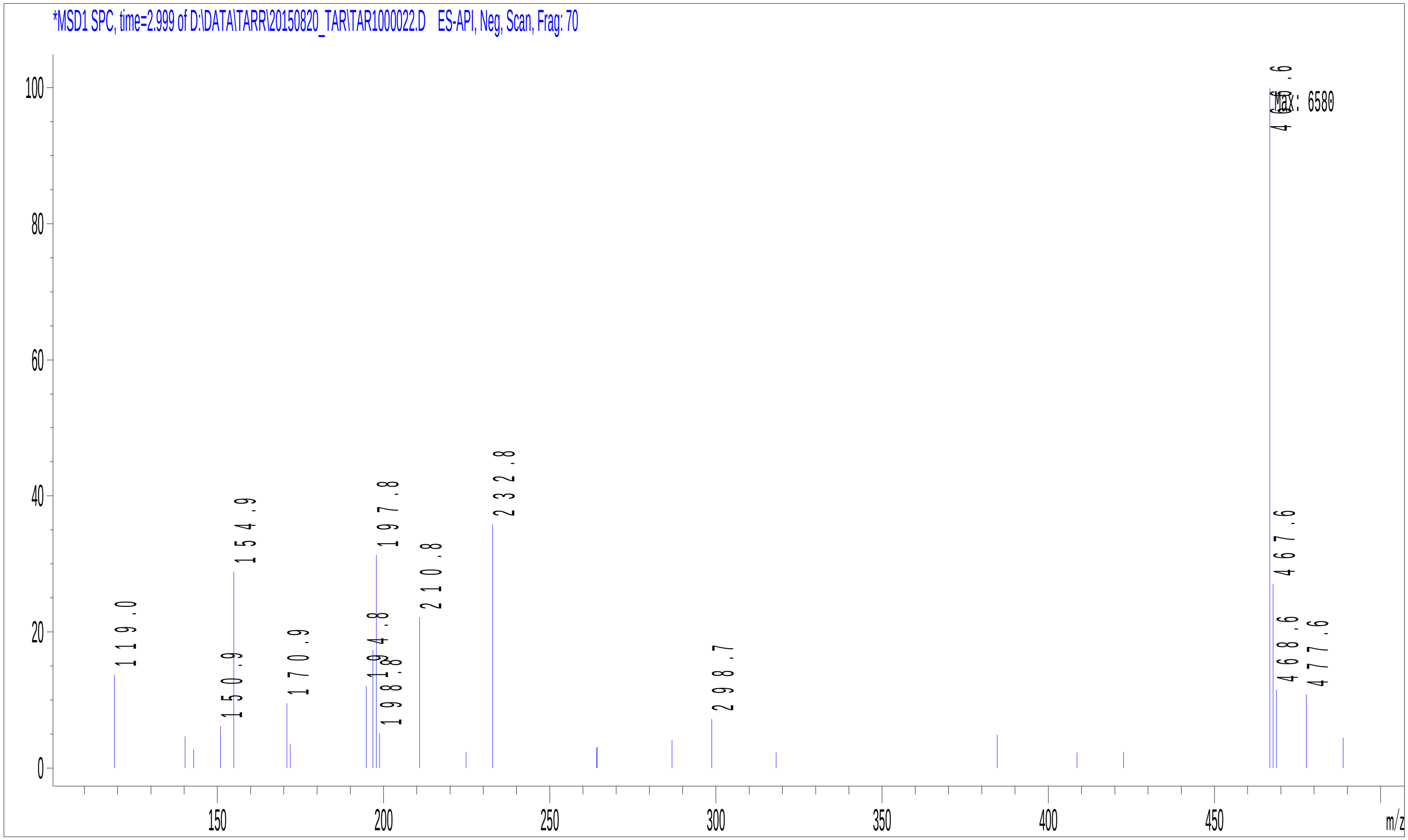
8

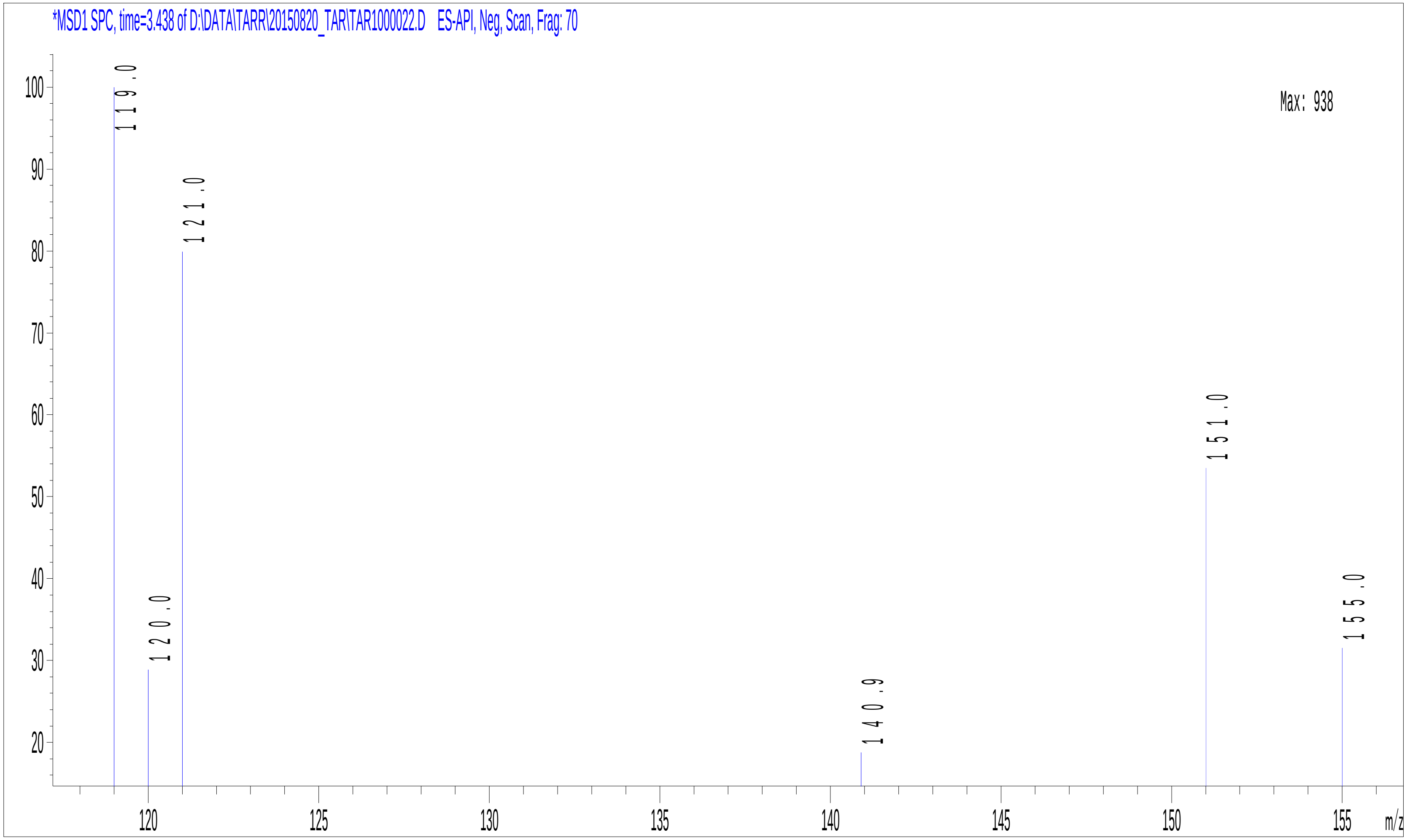
P2-C-04

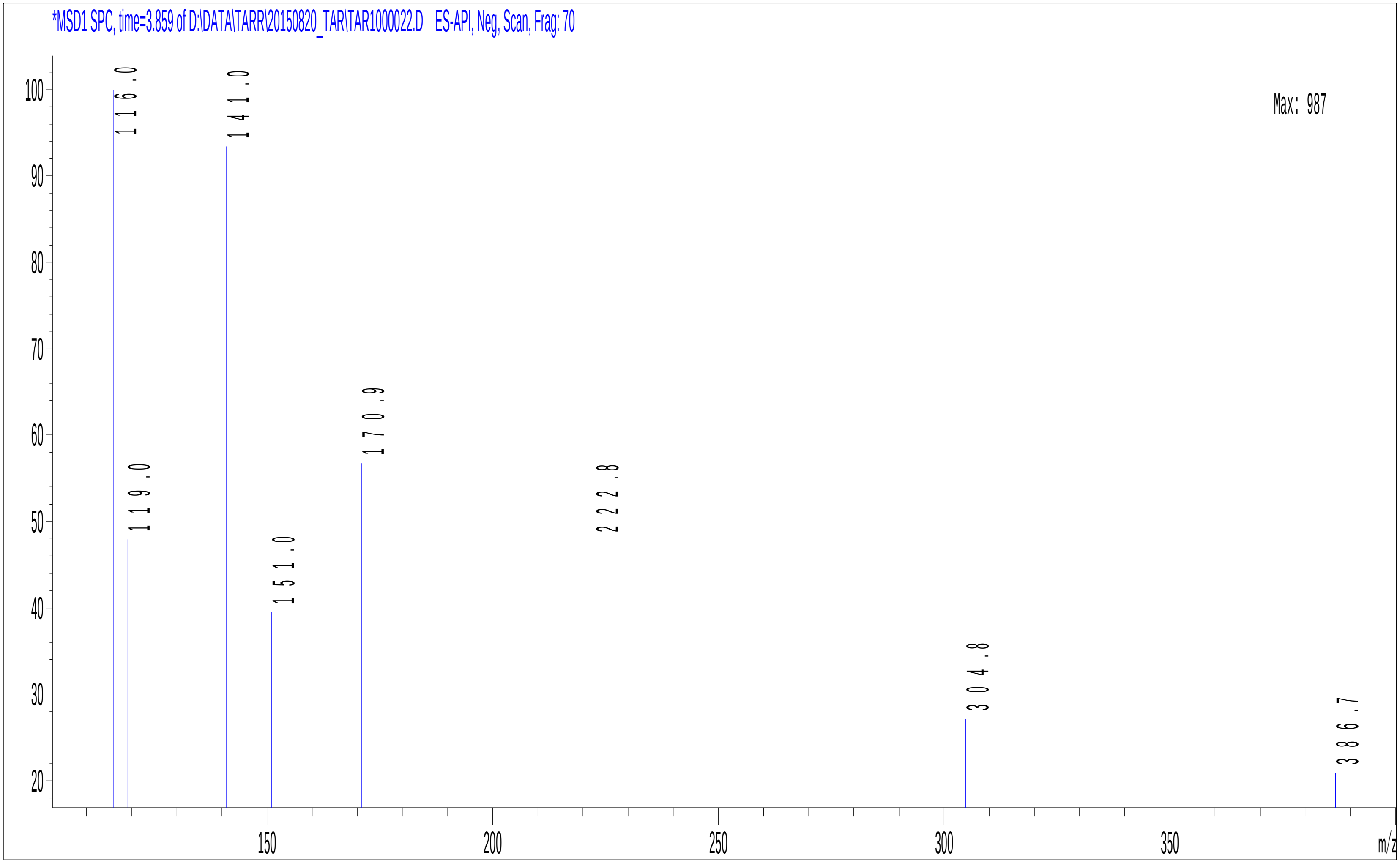


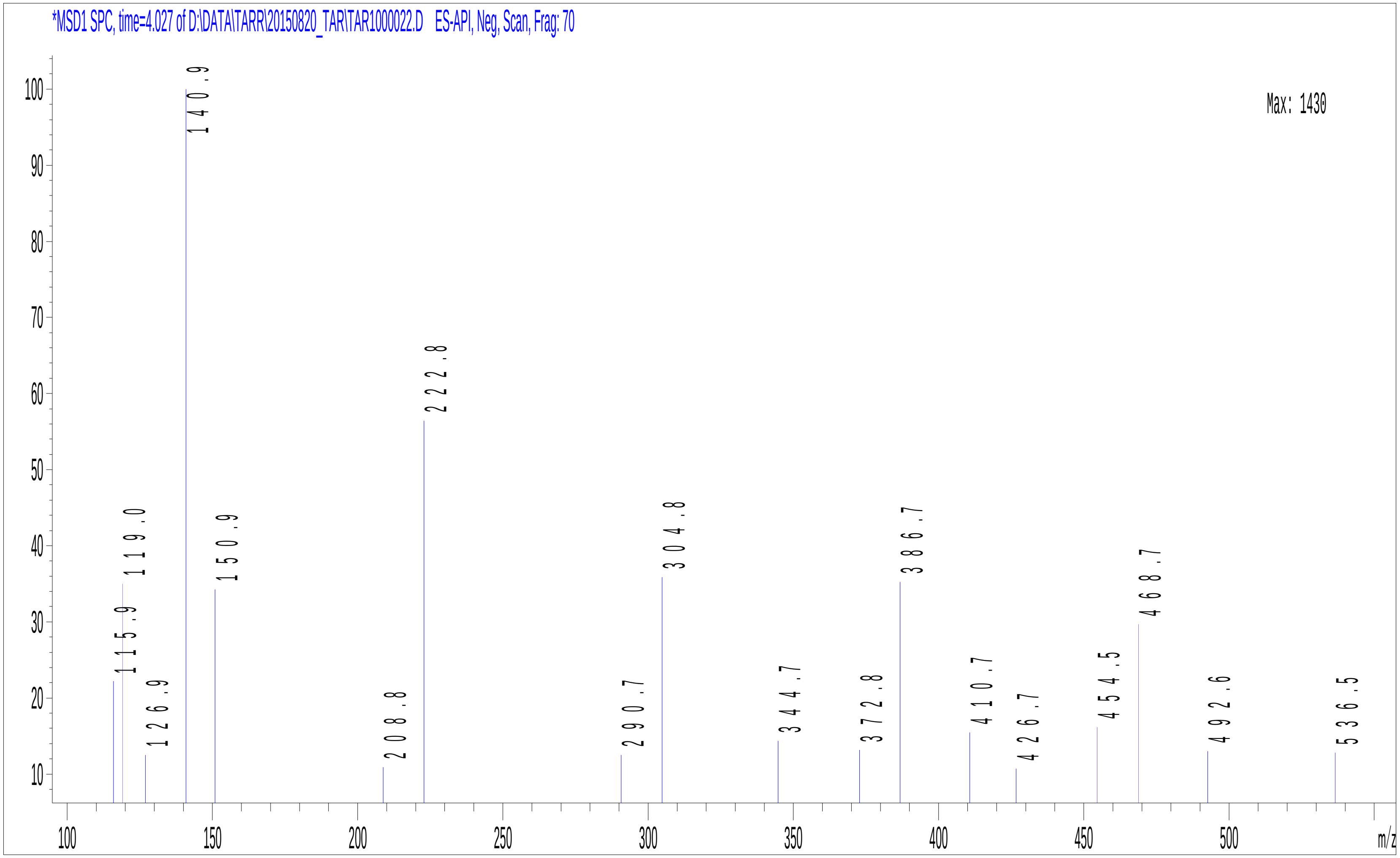
#	Time	Area	Height	Width	Area%	Symmetry
1	2.966	281000.8	26453.8	0.1543	61.143	0.893
2	4.287	178579.2	7064	0.3202	38.857	3.802

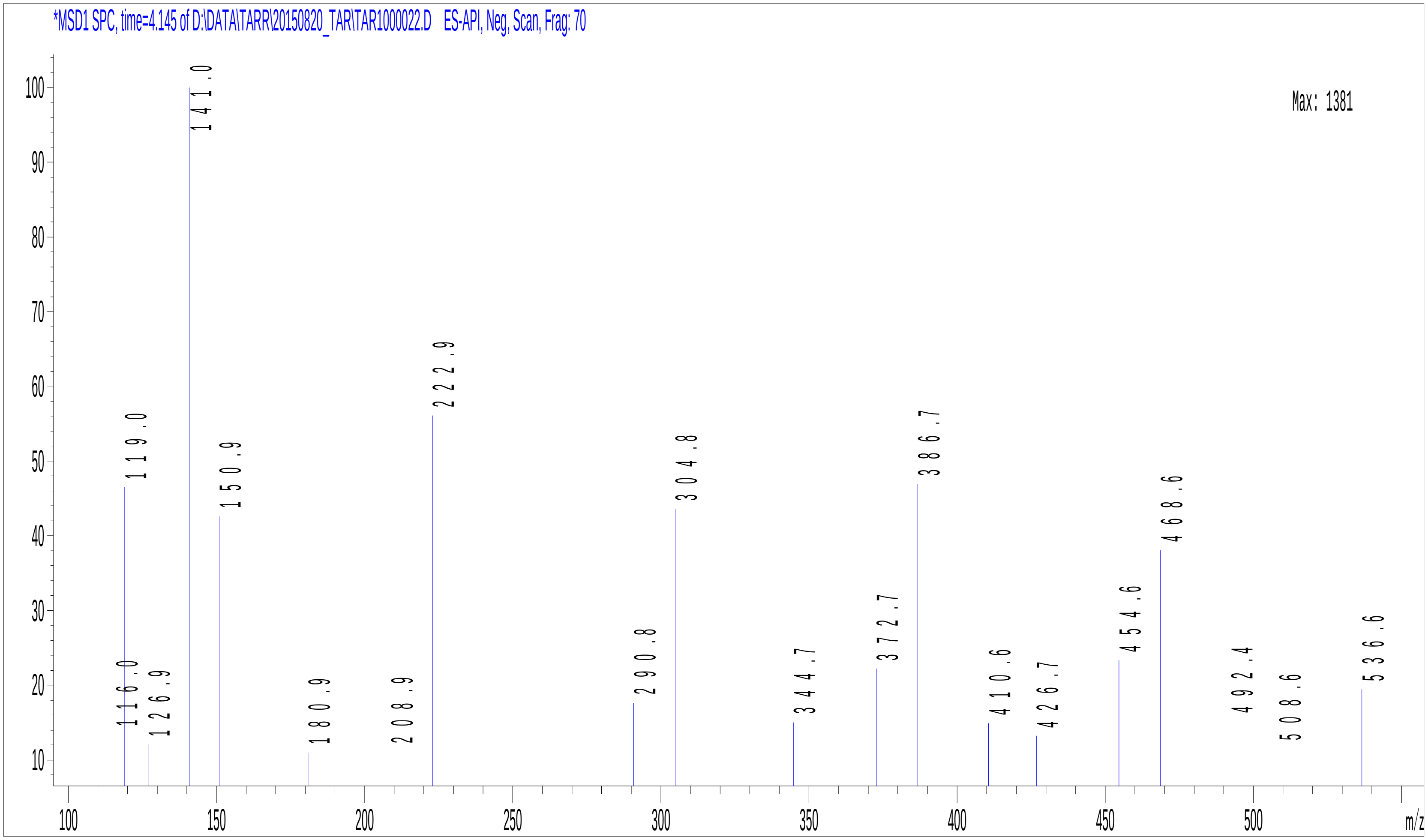

MSD1 TIC, MS File (D:\DATA\TARR\20150820_TAR\TAR1000022.D) ES-API, Neg, Scan, Frag: 70
MSD1 TIC, MS File (D:\DATA\TARR\20150820_TAR\TAR1000007.D) ES-API, Neg, Scan, Frag: 70
Norm.
45000
40000
35000
30000
25000
20000
15000
10000
5000
0
1
2
3
4
5
6
7
min

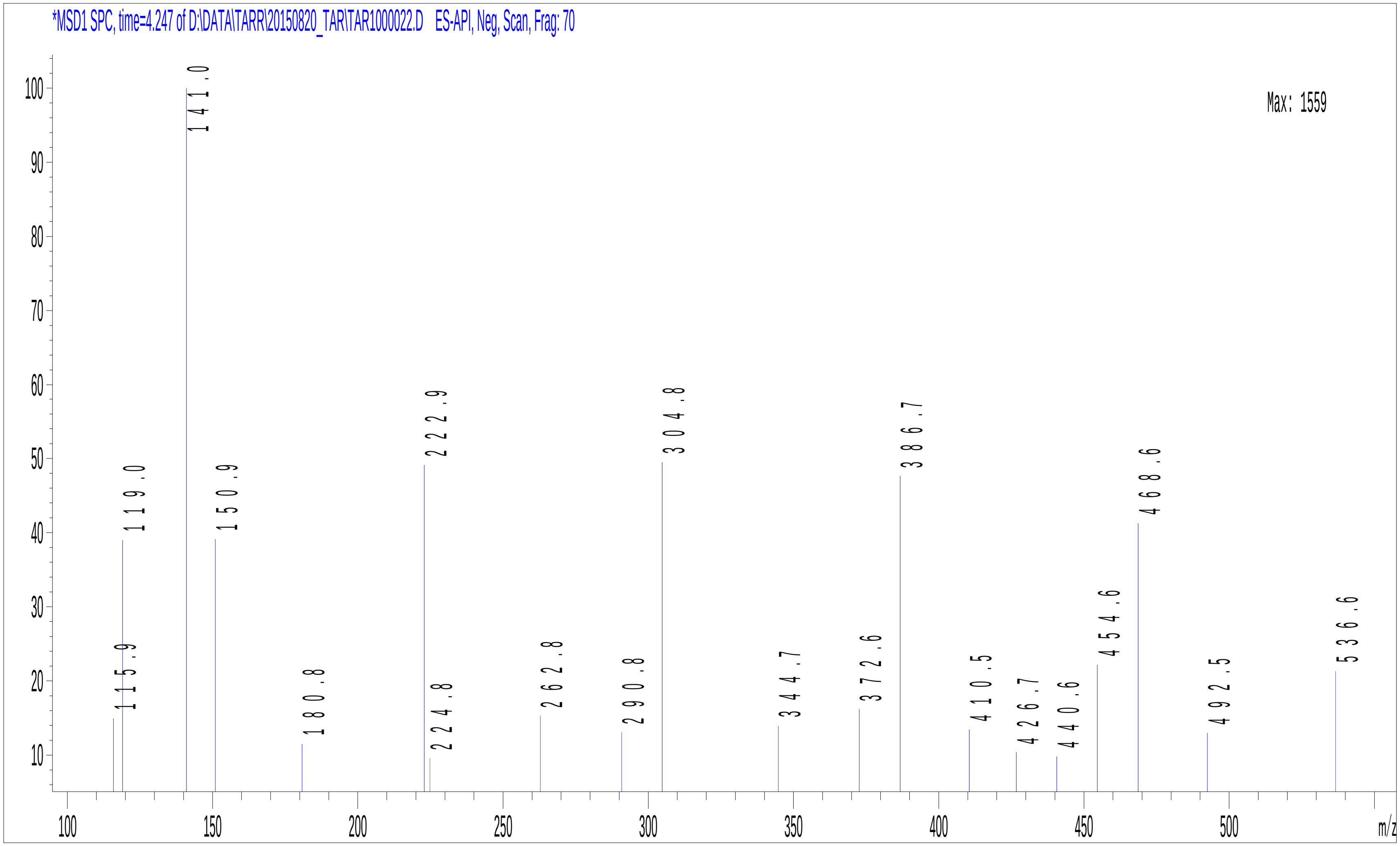

*MSD1 SPC, time=2.999 of D:\DATA\TARR\20150820_TAR\TAR1000022.D ES-API, Neg, Scan, Frag: 70
Max: 6580
0
20
40
60
80
100
150
200
250
300
350
400
450
m/z
119.0
150.9
154.9
170.9
194.8
197.8
198.8
210.8
232.8
298.7
466.6
467.6
468.6
477.6


*MSD1 SPC, time=3.438 of D:\DATA\TARR\20150820_TAR\TAR1000022.D ES-API, Neg, Scan, Frag: 70
Max: 938
119.0
120.0
121.0
140.9
151.0
155.0
100
90
80
70
60
50
40
30
20
120
125
130
135
140
145
150
155
m/z


*MSD1 SPC, time=3.859 of D:\DATA\TARR\20150820_TAR\TAR1000022.D ES-API, Neg, Scan, Frag: 70
Max: 987
116.0
119.0
141.0
151.0
170.9
222.8
304.8
386.7
100
90
80
70
60
50
40
30
20
150
200
250
300
350
m/z


*MSD1 SPC, time=4.027 of D:\DATA\TARR\20150820_TAR\TAR1000022.D ES-API, Neg, Scan, Frag: 70
Max: 1430
100
90
80
70
60
50
40
30
20
10
140.9
222.8
119.0
115.9
126.9
150.9
208.8
290.7
304.8
344.7
372.8
386.7
410.7
426.7
454.5
468.7
492.6
536.5
100
150
200
250
300
350
400
450
500
m/z


*MSD1 SPC, time=4.145 of D:\DATA\TARR\20150820_TAR\TAR1000022.D   ES-API, Neg, Scan, Frag: 70
Max: 1381
100
90
80
70
60
50
40
30
20
10
116.0
119.0
126.9
141.0
150.9
180.9
208.9
222.9
290.8
304.8
344.7
372.7
386.7
410.6
426.7
454.6
468.6
492.4
508.6
536.6
100
150
200
250
300
350
400
450
500
m/z

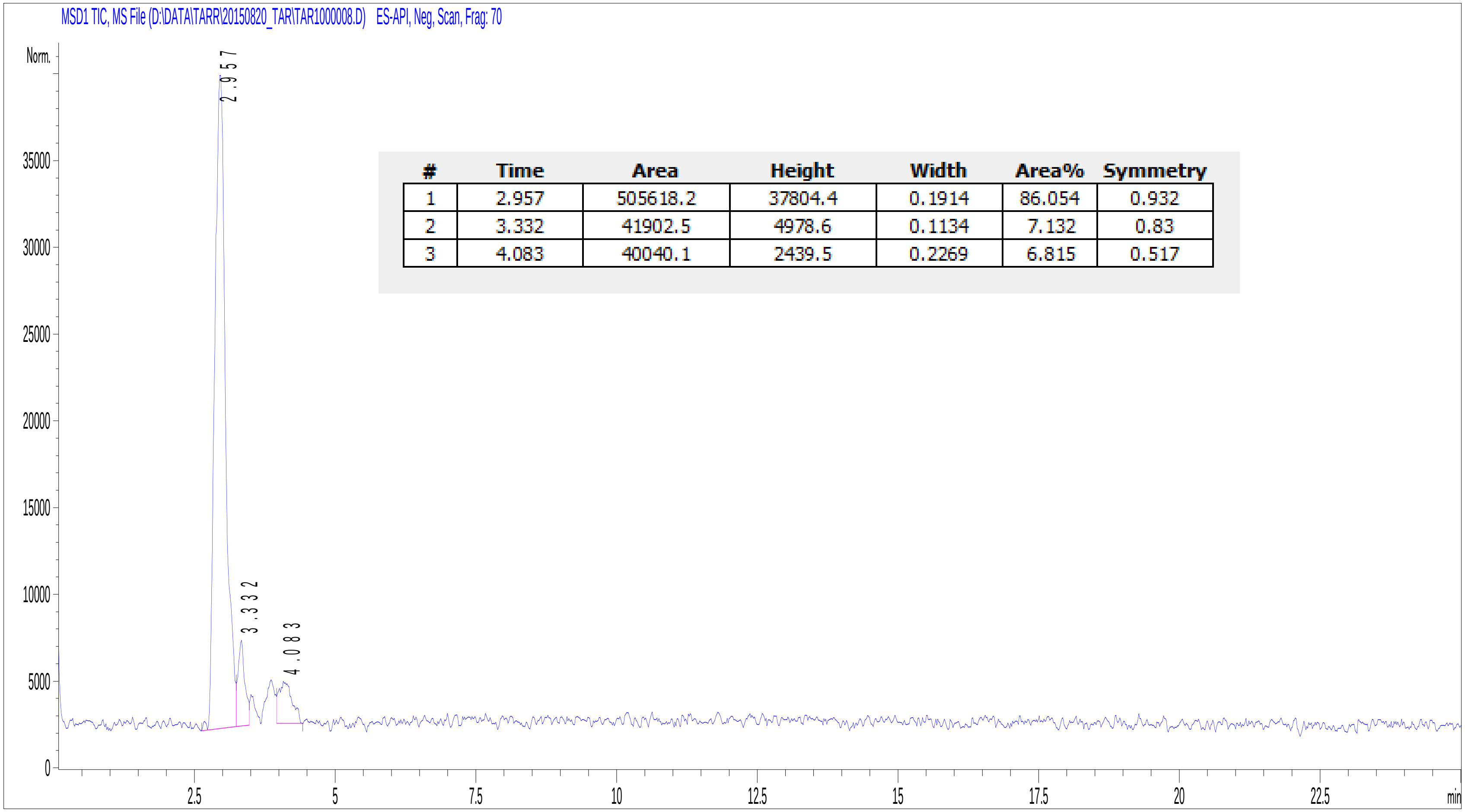

*MSD1 SPC, time=4.247 of D:\DATA\TARR\20150820_TAR\TAR1000022.D ES-API, Neg, Scan, Frag: 70
Max: 1559
100
90
80
70
60
50
40
30
20
10
115.9
119.0
141.0
150.9
180.8
222.9
224.8
262.8
290.8
304.8
344.7
372.6
386.7
410.5
426.7
440.6
454.6
468.6
492.5
536.6
100
150
200
250
300
350
400
450
500
m/z

23-Apr-15

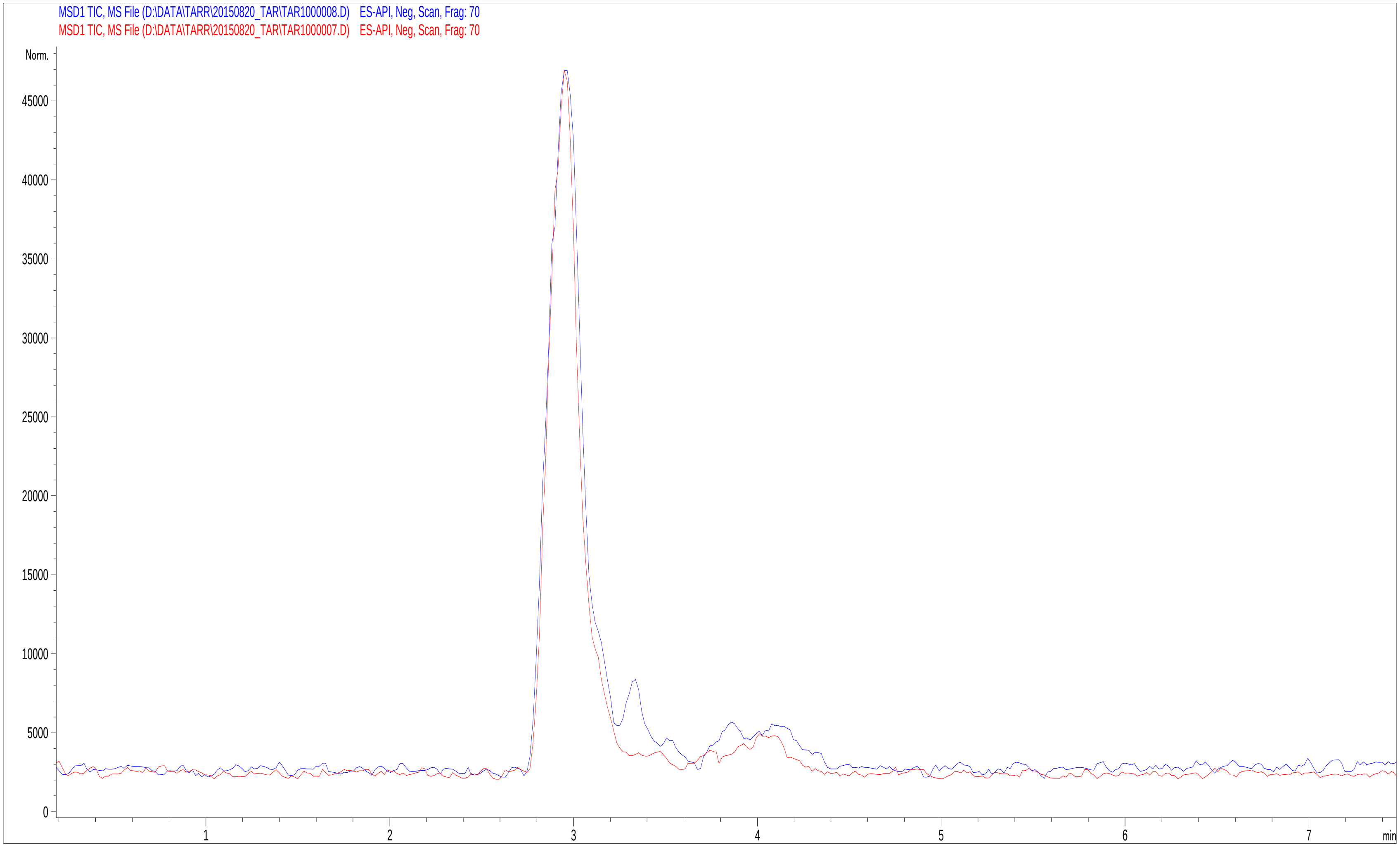
50 DC

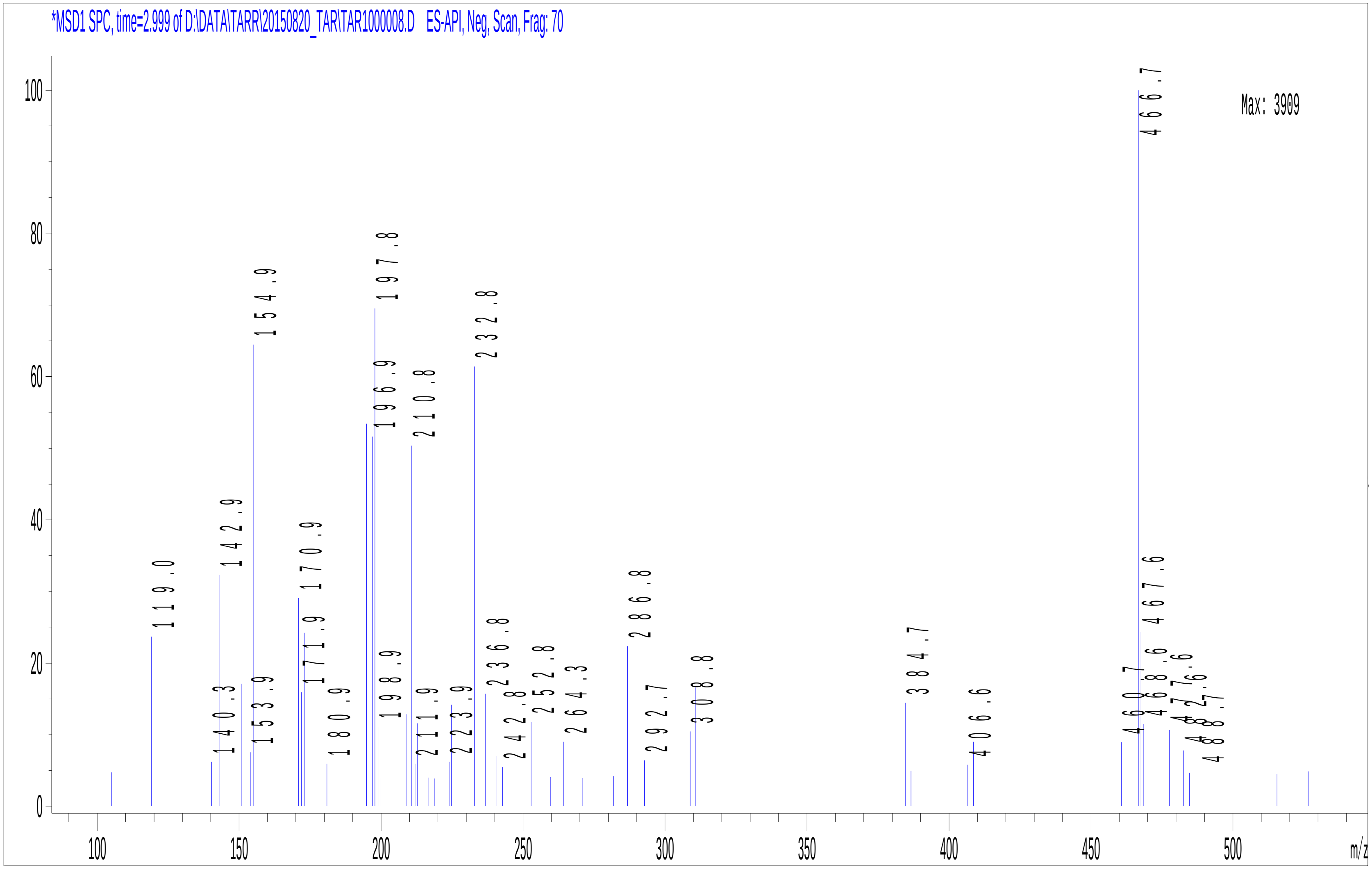
8

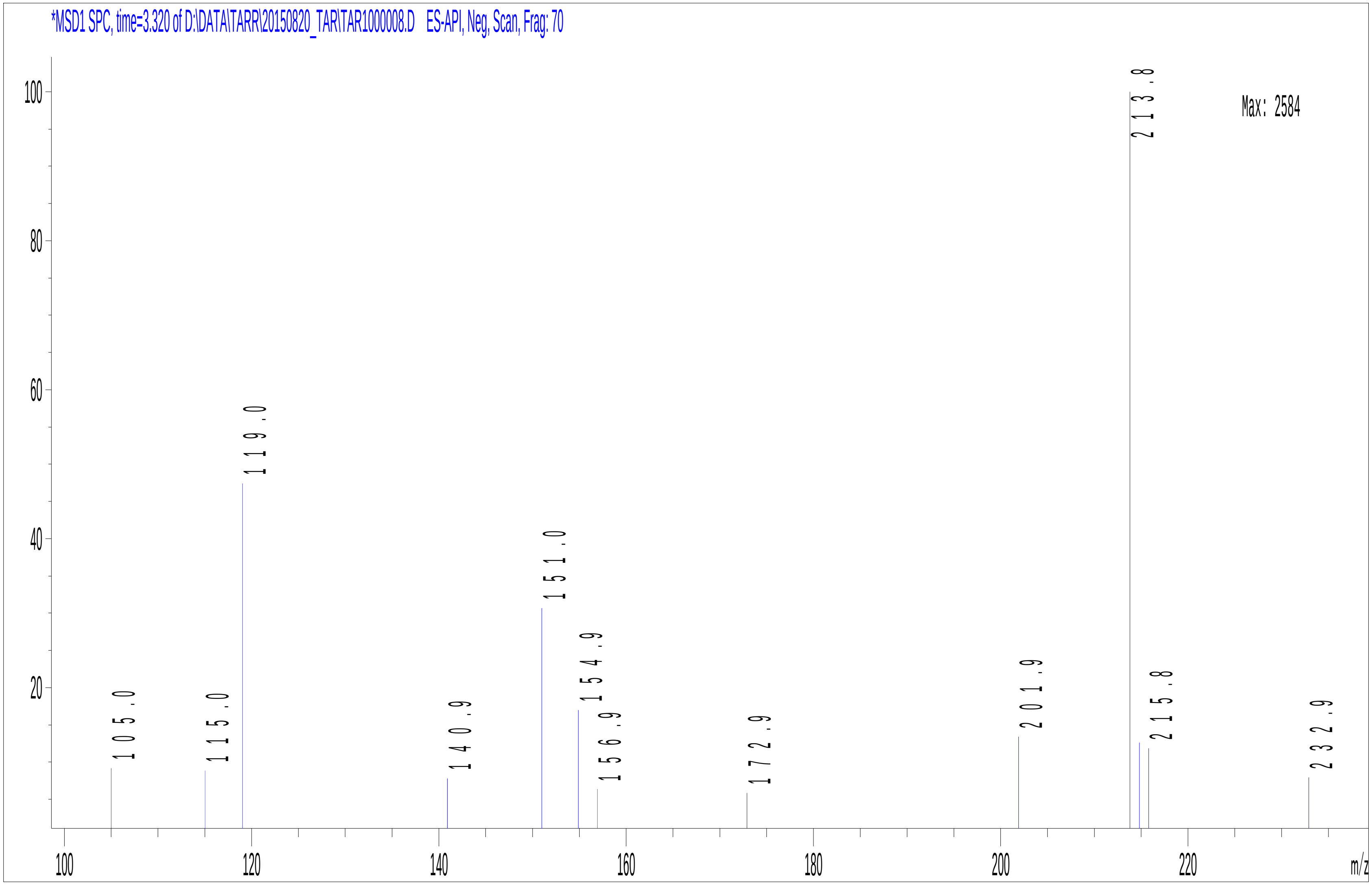
P2-A-08

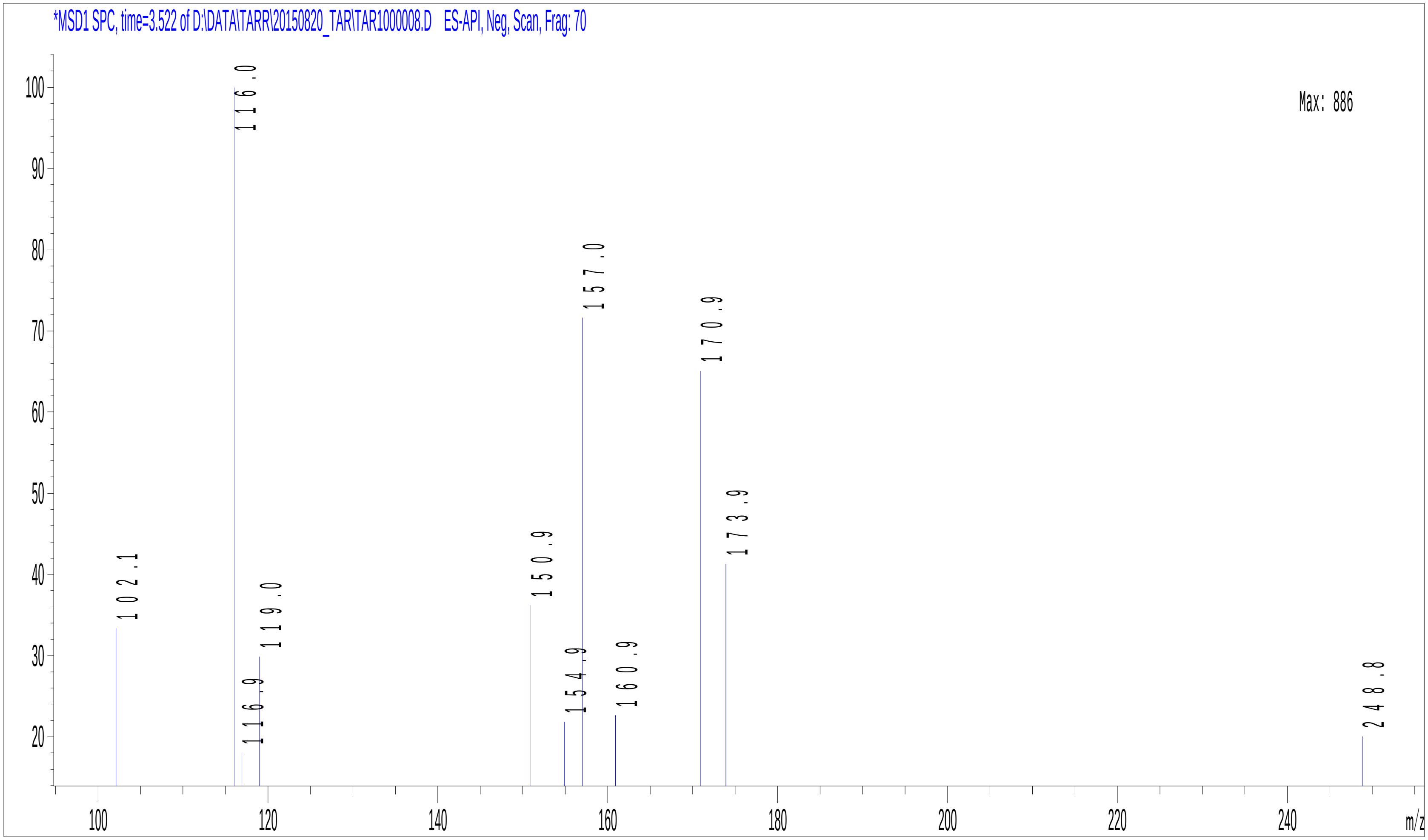


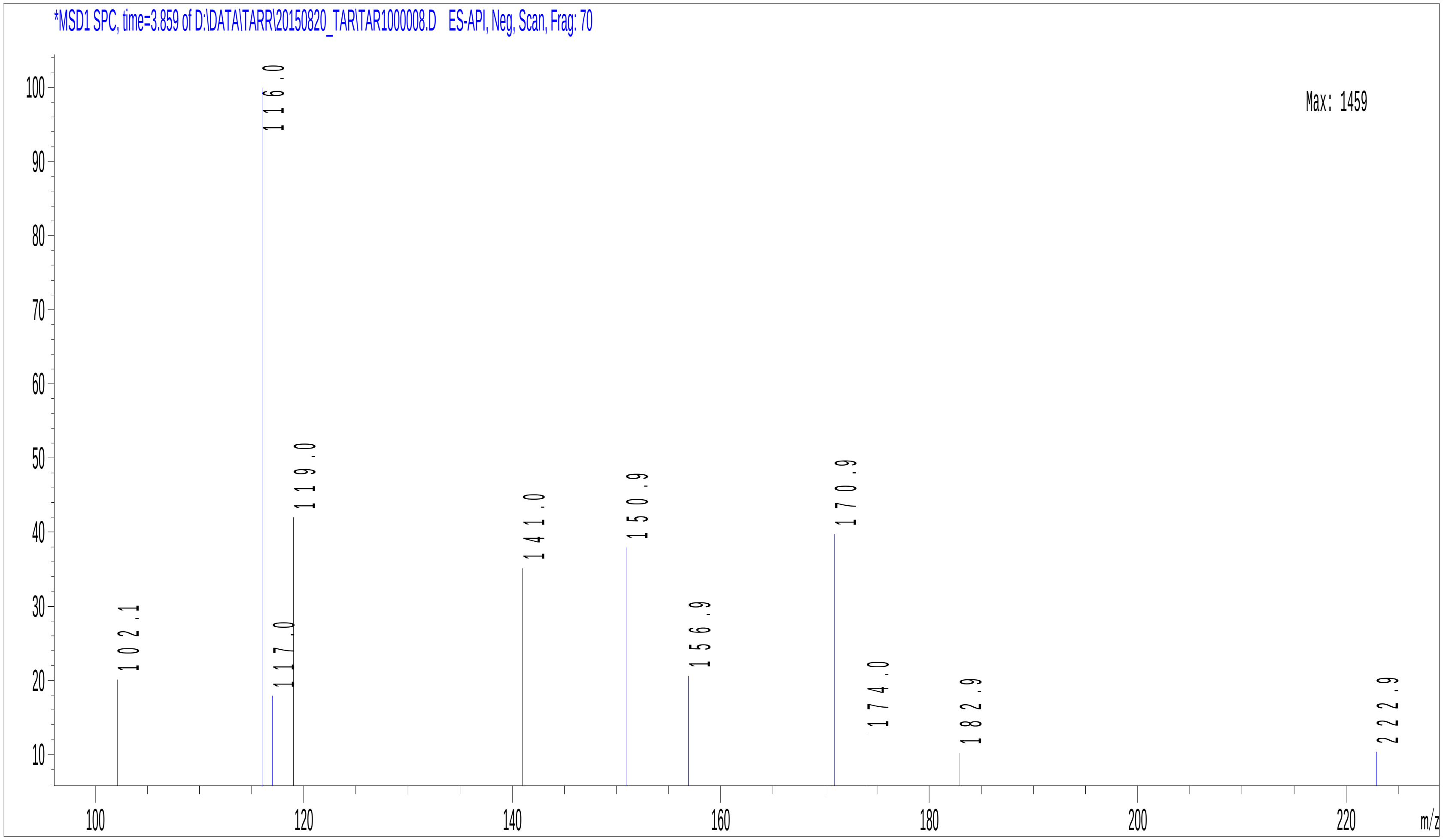
#	Time	Area	Height	Width	Area%	Symmetry
1	2.957	505618.2	37804.4	0.1914	86.054	0.932
2	3.332	41902.5	4978.6	0.1134	7.132	0.83
3	4.083	40040.1	2439.5	0.2269	6.815	0.517

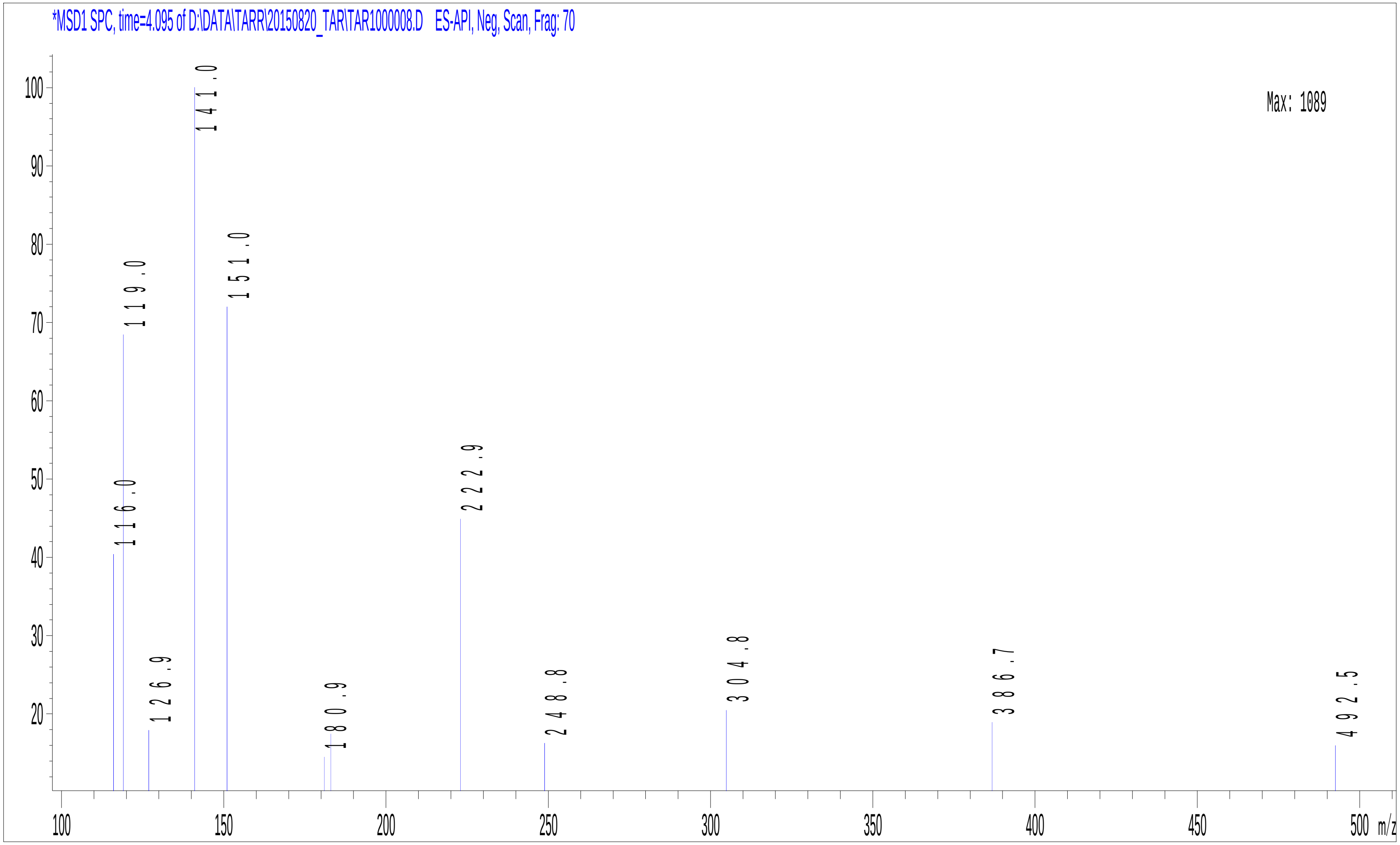

MSD1 TIC, MS File (D:\DATA\TARR\20150820_TAR\TAR1000008.D) ES-API, Neg, Scan, Frag: 70
MSD1 TIC, MS File (D:\DATA\TARR\20150820_TAR\TAR1000007.D) ES-API, Neg, Scan, Frag: 70
Norm.
45000
40000
35000
30000
25000
20000
15000
10000
5000
0
1
2
3
4
5
6
7
min


*MSD1 SPC, time=2.999 of D:\DATA\TARR\20150820_TAR\TAR1000008.D ES-API, Neg, Scan, Frag: 70
Max: 3909
0
20
40
60
80
100
100
150
200
250
300
350
400
450
500
m/z
119.0
140.3
142.9
153.9
154.9
170.9
171.9
180.9
196.9
197.8
198.9
210.8
211.9
223.9
232.8
236.8
242.8
252.8
264.3
286.8
292.7
308.8
384.7
406.6
460.7
466.7
467.6
468.6
477.6
482.6
488.7


*MSD1 SPC, time=3.320 of D:\DATA\TARR\20150820_TAR\TAR1000008.D ES-API, Neg, Scan, Frag: 70
Max: 2584
100
80
60
40
20
105.0
115.0
119.0
140.9
151.0
154.9
156.9
172.9
201.9
213.8
215.8
232.9
100
120
140
160
180
200
220
m/z


*MSD1 SPC, time=3.522 of D:\DATA\TARR\20150820_TAR\TAR1000008.D ES-API, Neg, Scan, Frag: 70
Max: 886
100
90
80
70
60
50
40
30
20
100
120
140
160
180
200
220
240
m/z
102.1
116.0
116.9
119.0
150.9
154.9
157.0
160.9
170.9
173.9
248.8


*MSD1 SPC, time=3.859 of D:\DATA\TARR\20150820_TAR\TAR1000008.D ES-API, Neg, Scan, Frag: 70
Max: 1459
100
90
80
70
60
50
40
30
20
10
100
120
140
160
180
200
220
m/z
102.1
116.0
117.0
119.0
141.0
150.9
156.9
170.9
174.0
182.9
222.9

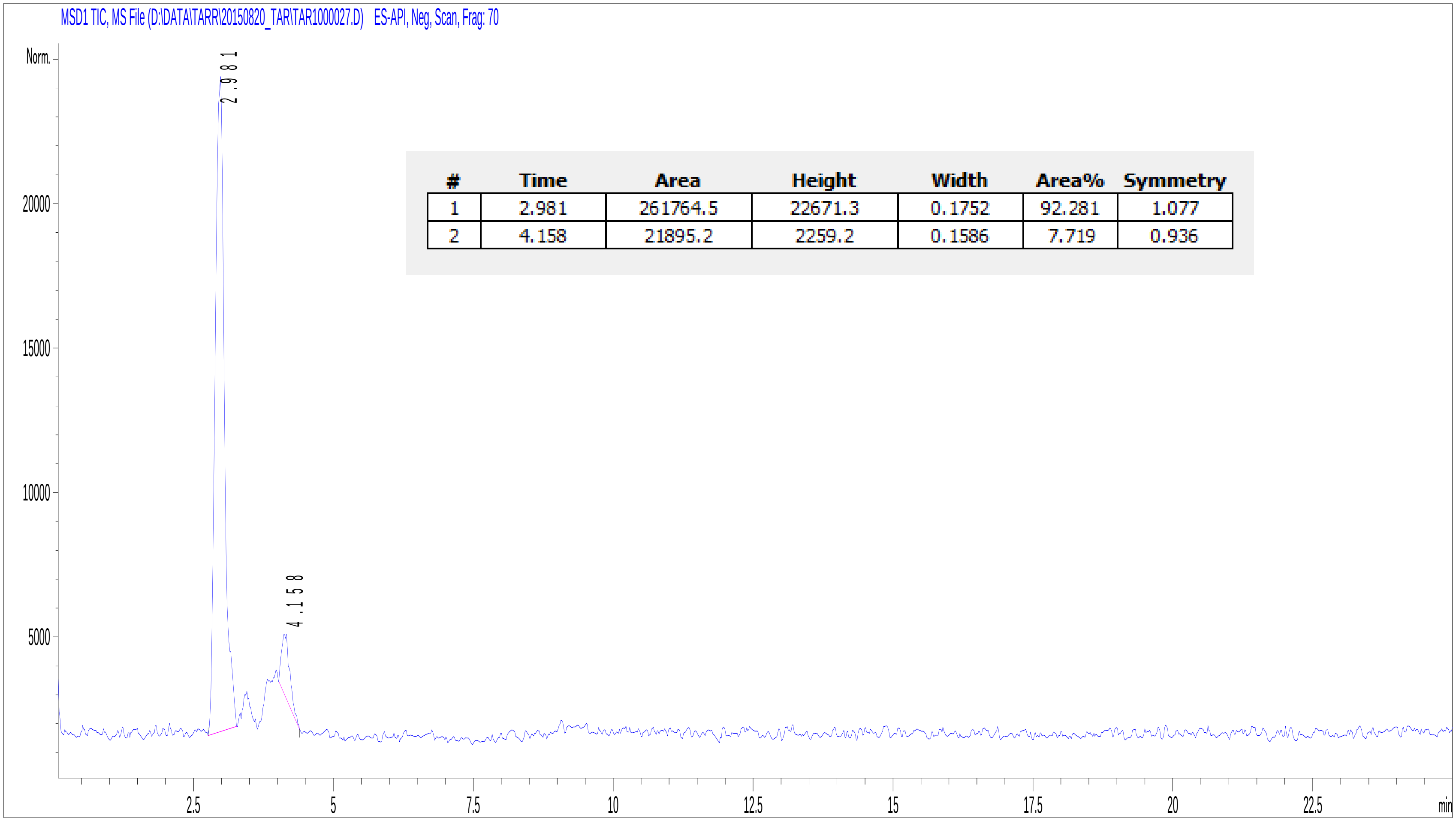

*MSD1 SPC, time=4.095 of D:\DATA\TARR\20150820_TAR\TAR1000008.D ES-API, Neg, Scan, Frag: 70
Max: 1089
116.0
119.0
126.9
141.0
151.0
180.9
222.9
248.8
304.8
386.7
492.5
100
90
80
70
60
50
40
30
20
100
150
200
250
300
350
400
450
500
m/z

9-Jul-15

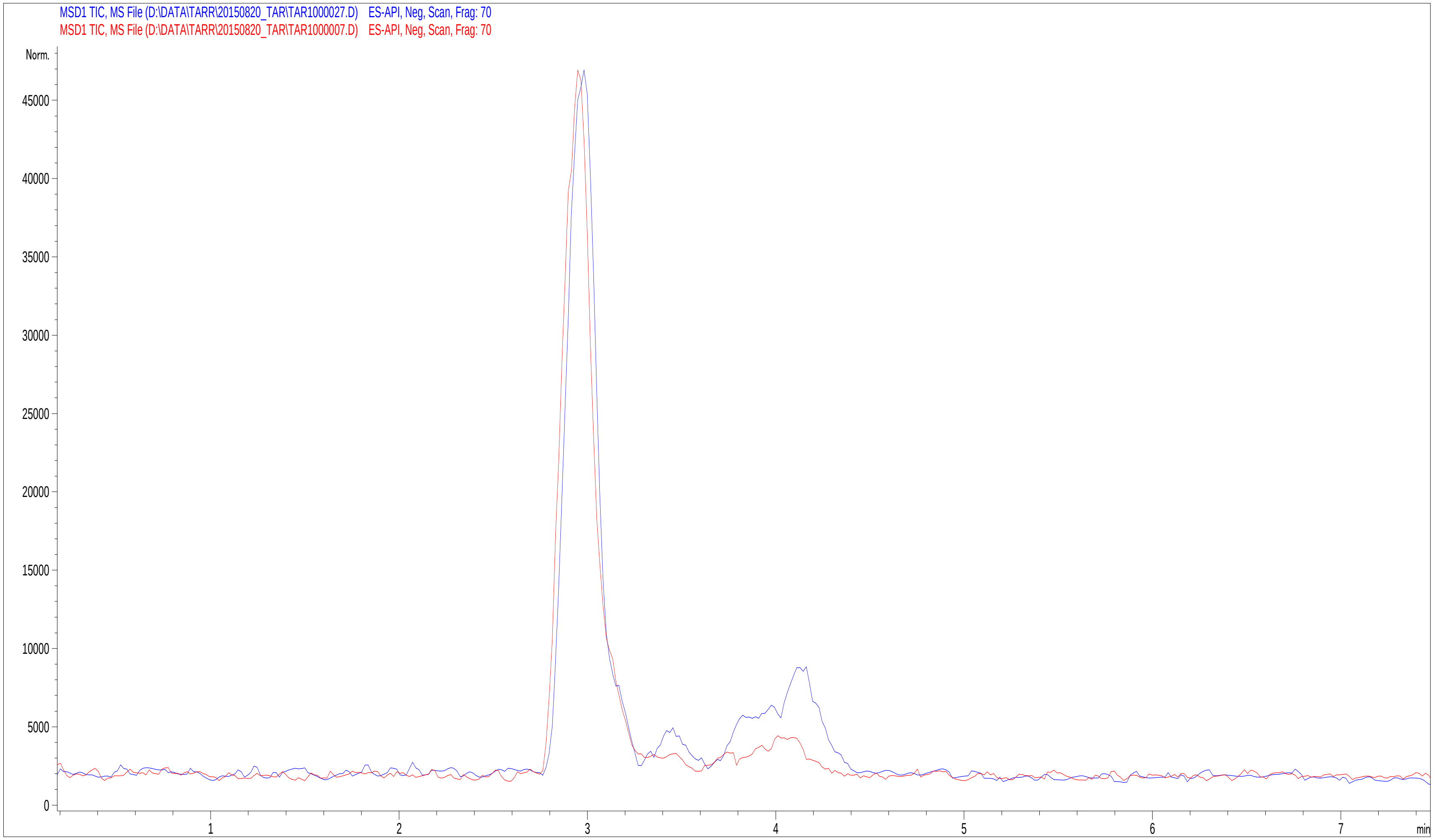
70 DC

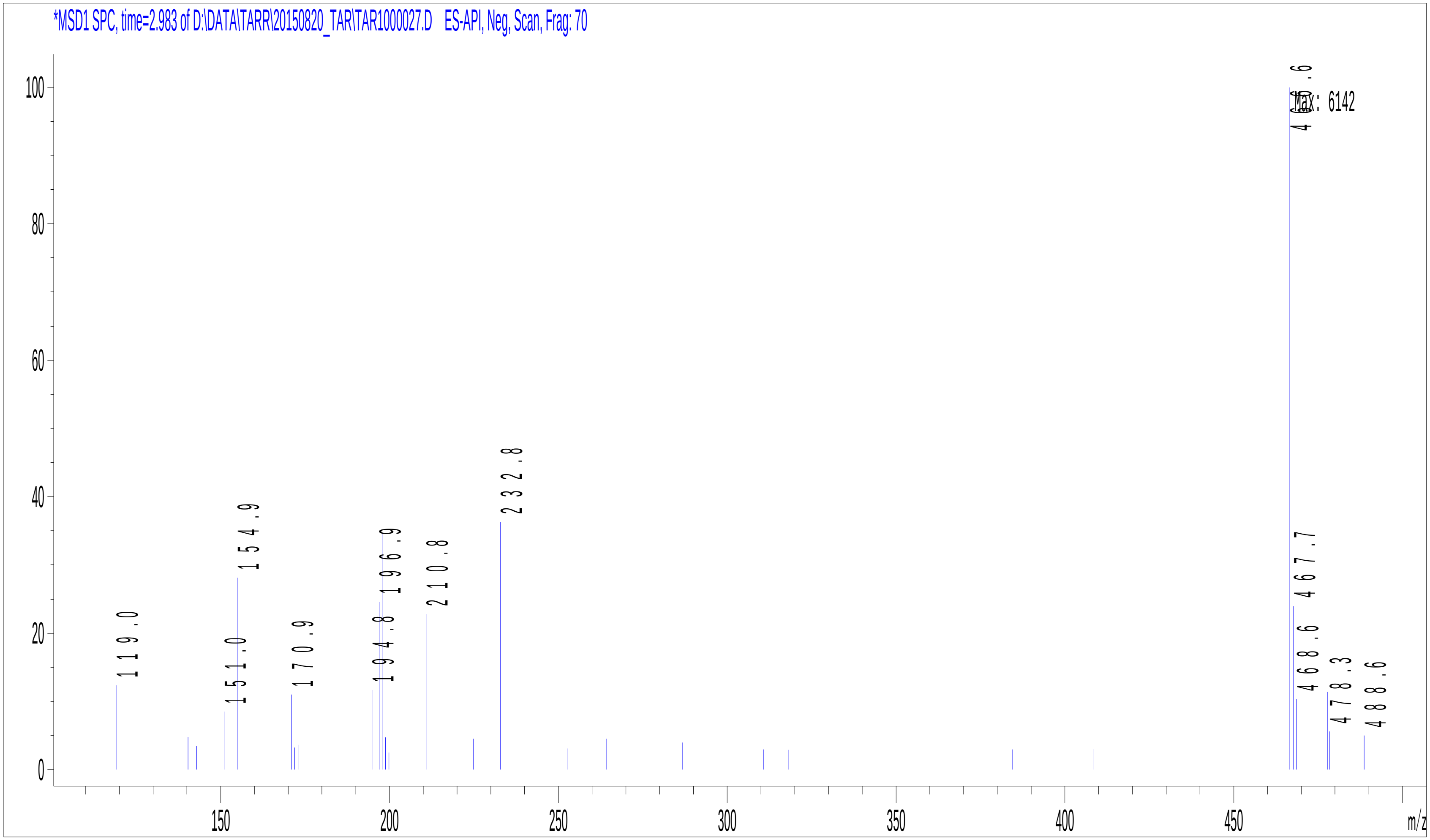
8

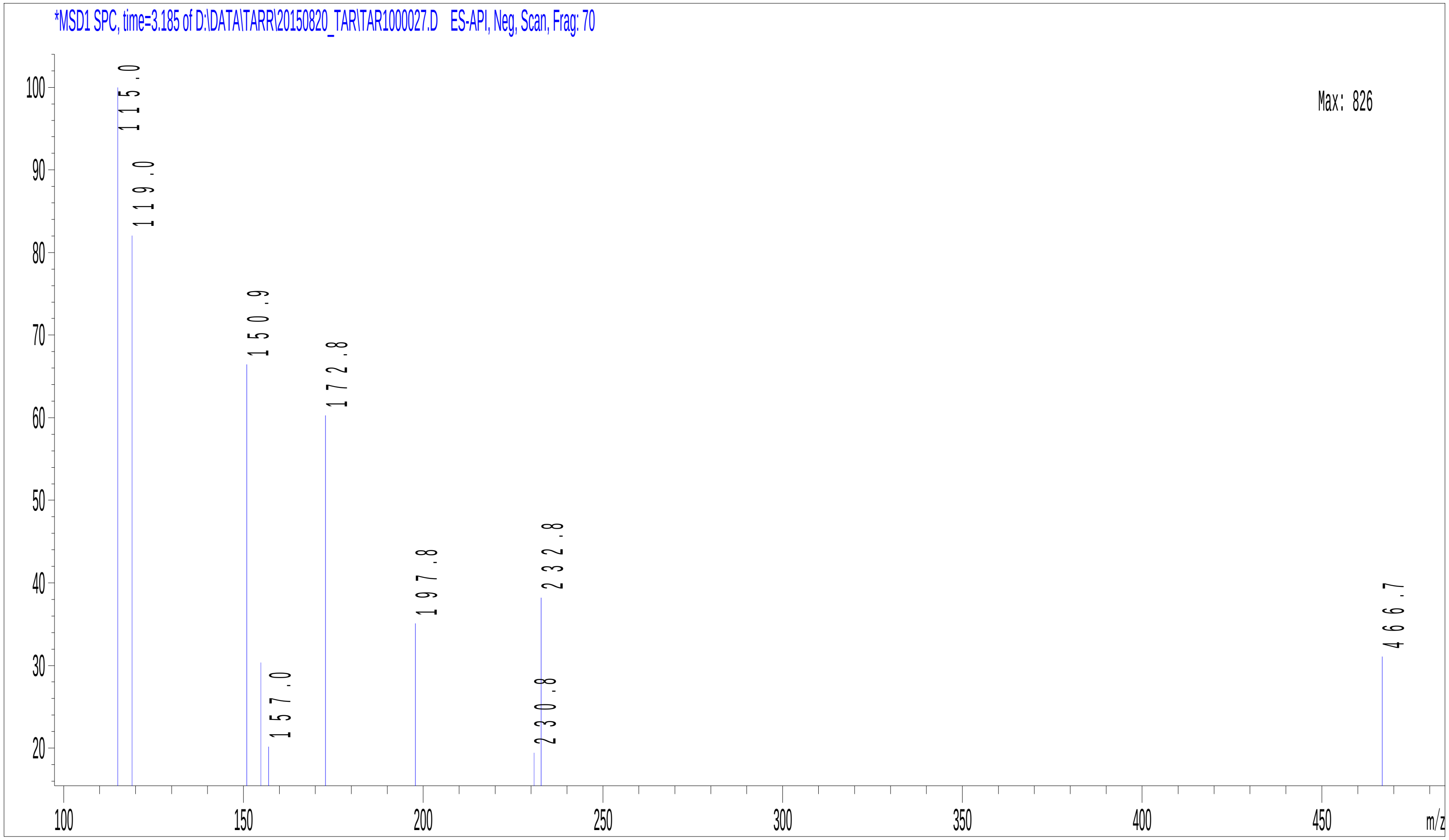
P2-C-09

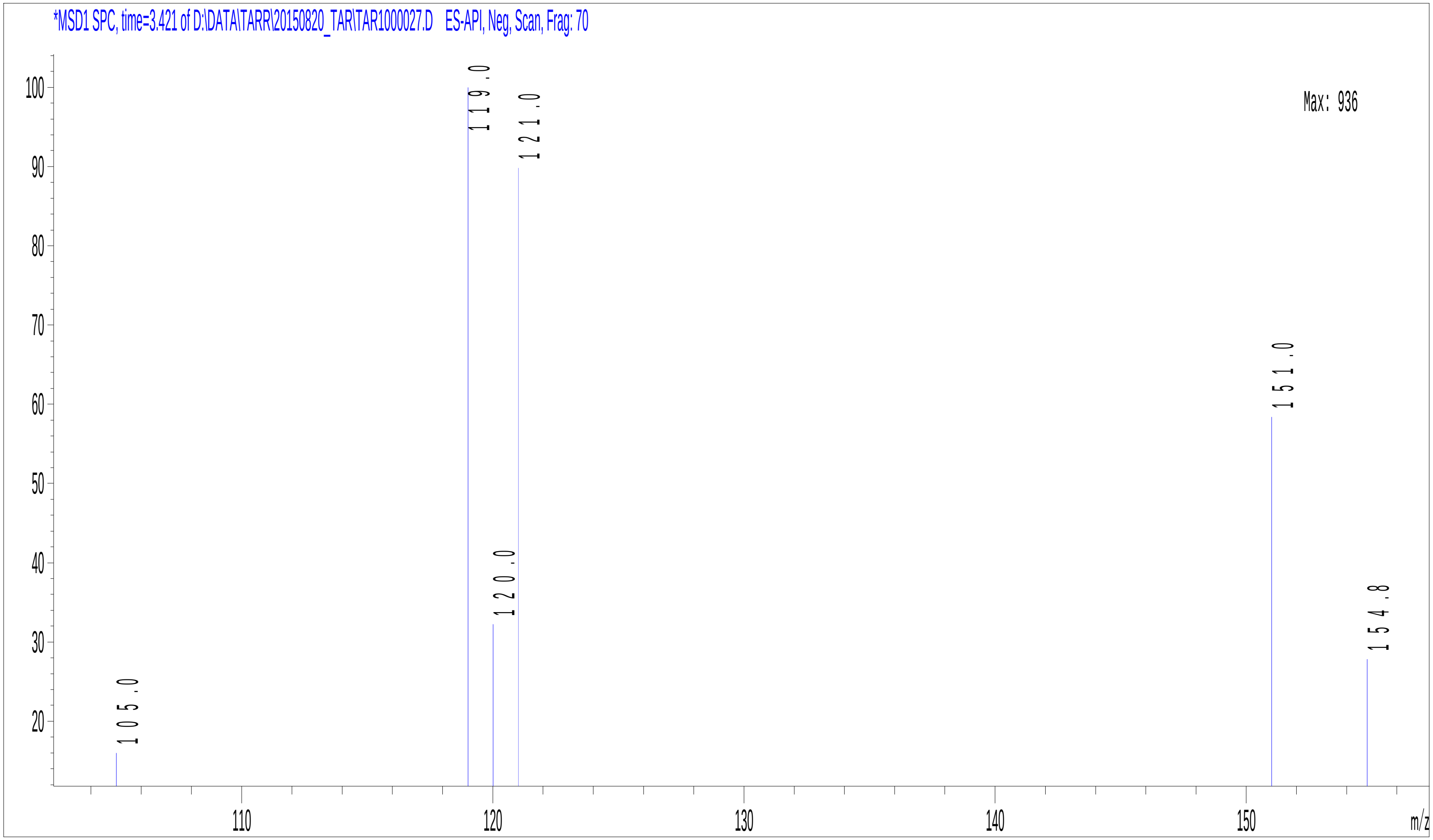


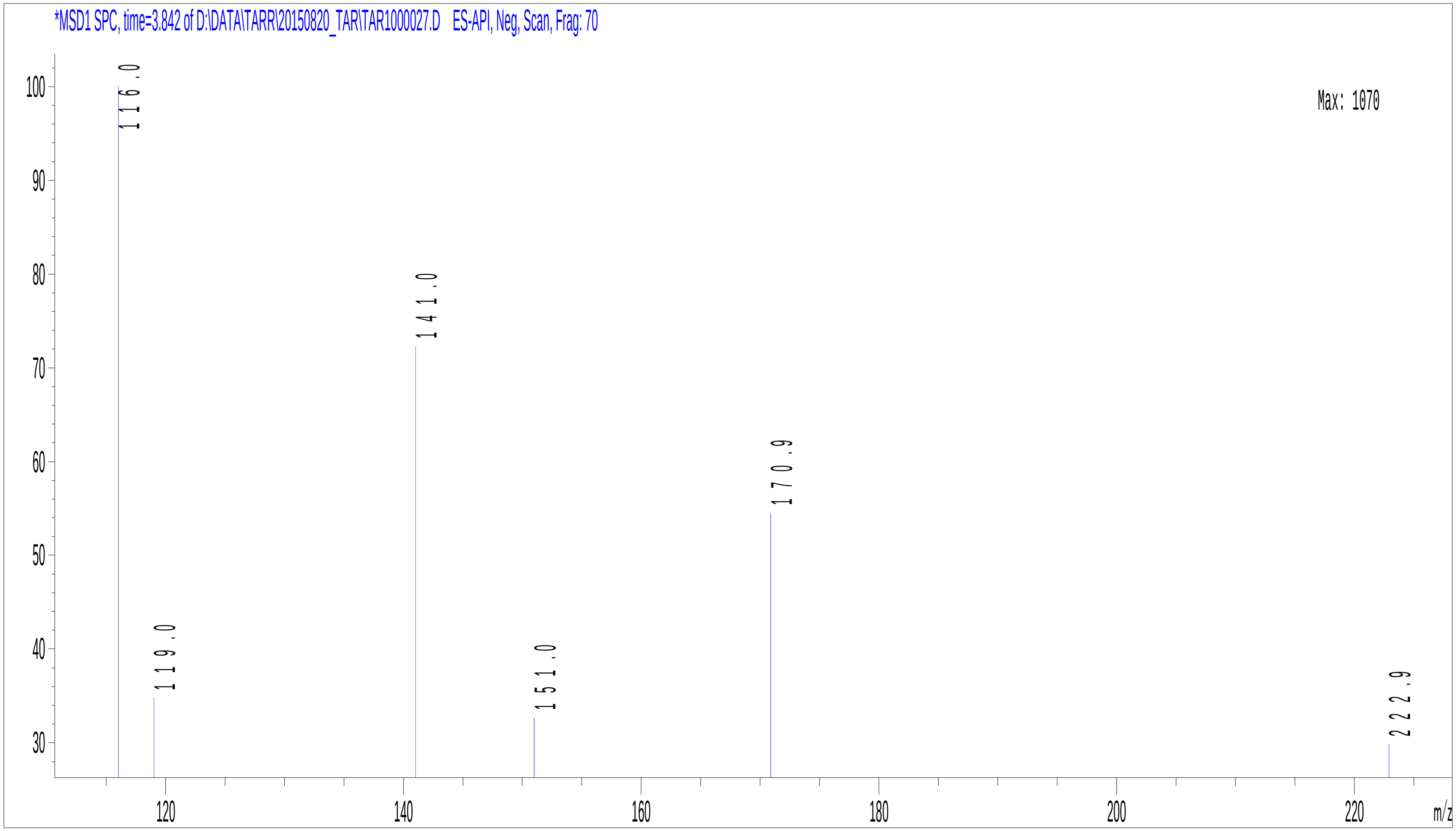
#	Time	Area	Height	Width	Area%	Symmetry
1	2.981	261764.5	22671.3	0.1752	92.281	1.077
2	4.158	21895.2	2259.2	0.1586	7.719	0.936

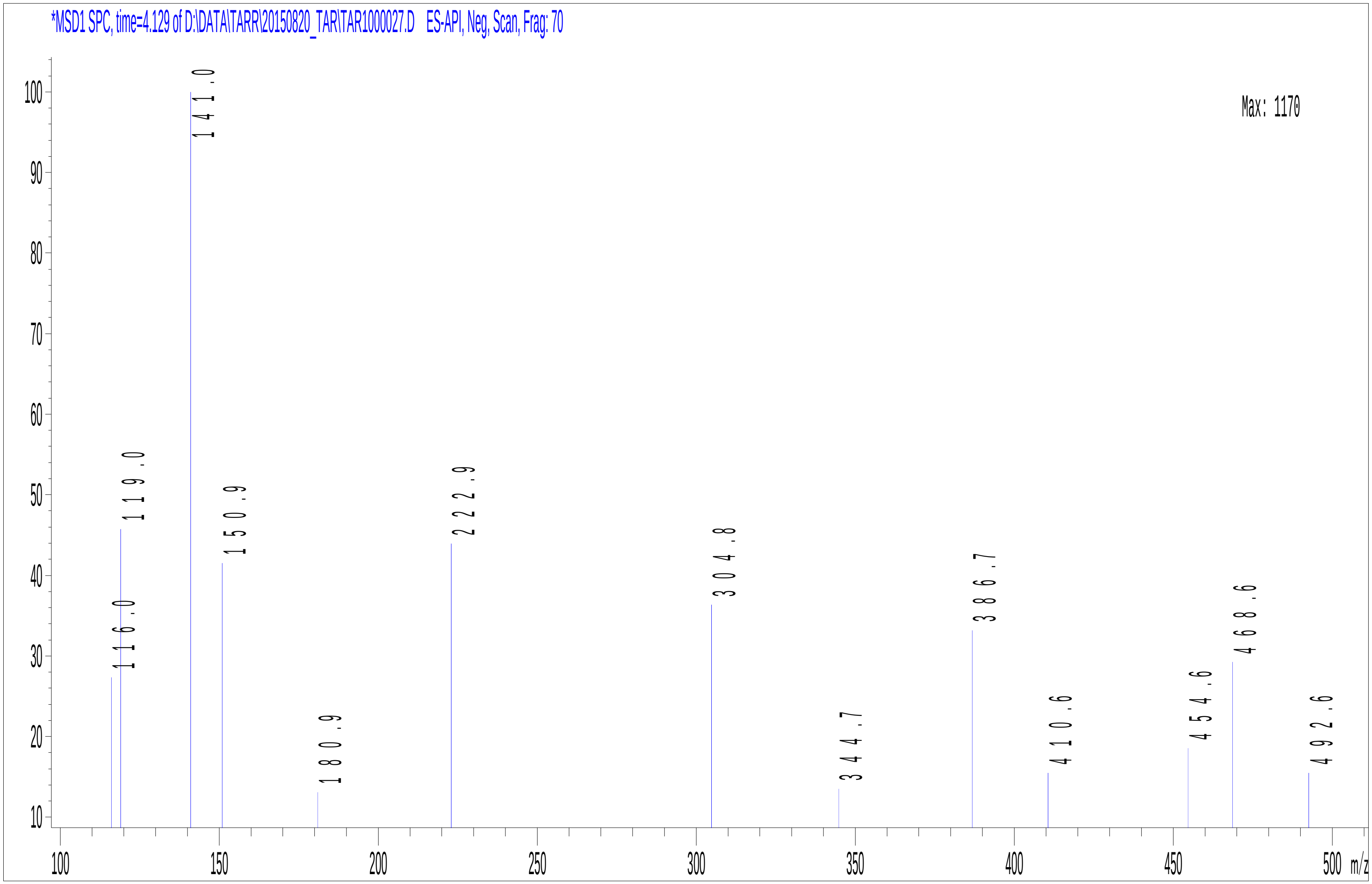

MSD1 TIC, MS File (D:\DATA\TARR\20150820_TAR\TAR1000027.D) ES-API, Neg, Scan, Frag: 70
MSD1 TIC, MS File (D:\DATA\TARR\20150820_TAR\TAR1000007.D) ES-API, Neg, Scan, Frag: 70
Norm.
45000
40000
35000
30000
25000
20000
15000
10000
5000
0
1
2
3
4
5
6
7
min


*MSD1 SPC, time=2.983 of D:\DATA\TARR\20150820_TAR\TAR1000027.D ES-API, Neg, Scan, Frag: 70
Max: 6142
466.6
467.7
468.6
478.3
488.6
232.8
154.9
196.9
210.8
119.0
151.0
170.9
194.8
100
80
60
40
20
0
150
200
250
300
350
400
450
m/z


*MSD1 SPC, time=3.185 of D:\DATA\TARR\20150820_TAR\TAR1000027.D ES-API, Neg, Scan, Frag: 70
Max: 826
115.0
119.0
150.9
157.0
172.8
197.8
230.8
232.8
466.7
100
90
80
70
60
50
40
30
20
100
150
200
250
300
350
400
450
m/z


*MSD1 SPC, time=3.421 of D:\DATA\TARR\20150820_TAR\TAR1000027.D ES-API, Neg, Scan, Frag: 70
Max: 936
100
90
80
70
60
50
40
30
20
110
120
130
140
150
m/z
105.0
119.0
120.0
121.0
151.0
154.8


*MSD1 SPC, time=3.842 of D:\DATA\TARR\20150820_TAR\TAR1000027.D ES-API, Neg, Scan, Frag: 70
Max: 1070
116.0
119.0
141.0
151.0
170.9
222.9
100
90
80
70
60
50
40
30
120
140
160
180
200
220
m/z

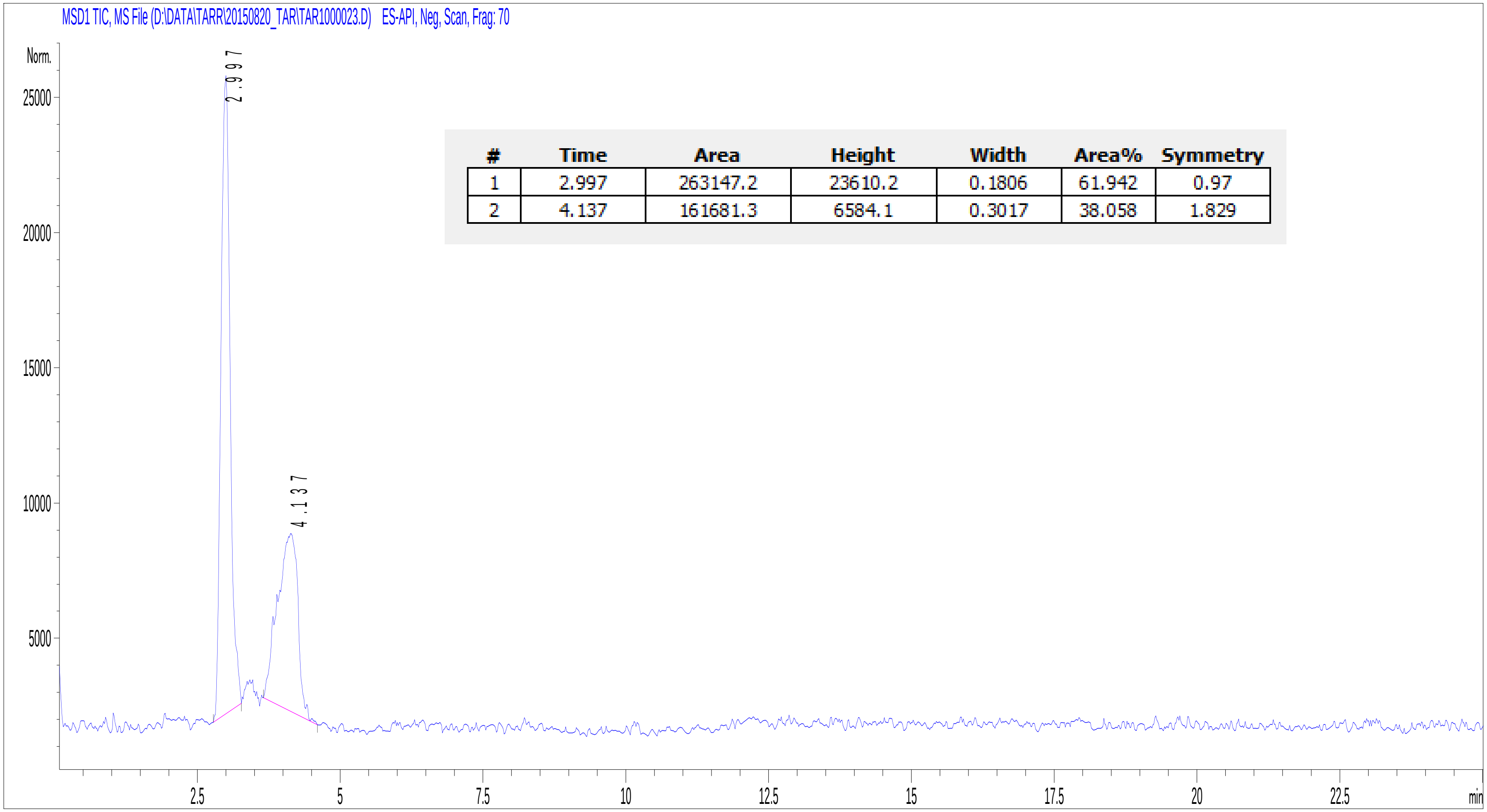

*MSD1 SPC, time=4.129 of D:\DATA\TARR\20150820_TAR\TAR1000027.D ES-API, Neg, Scan, Frag: 70
Max: 1170
116.0
119.0
141.0
150.9
180.9
222.9
304.8
344.7
386.7
410.6
454.6
468.6
492.6
100
90
80
70
60
50
40
30
20
10
100
150
200
250
300
350
400
450
500
m/z

6-Jul-15

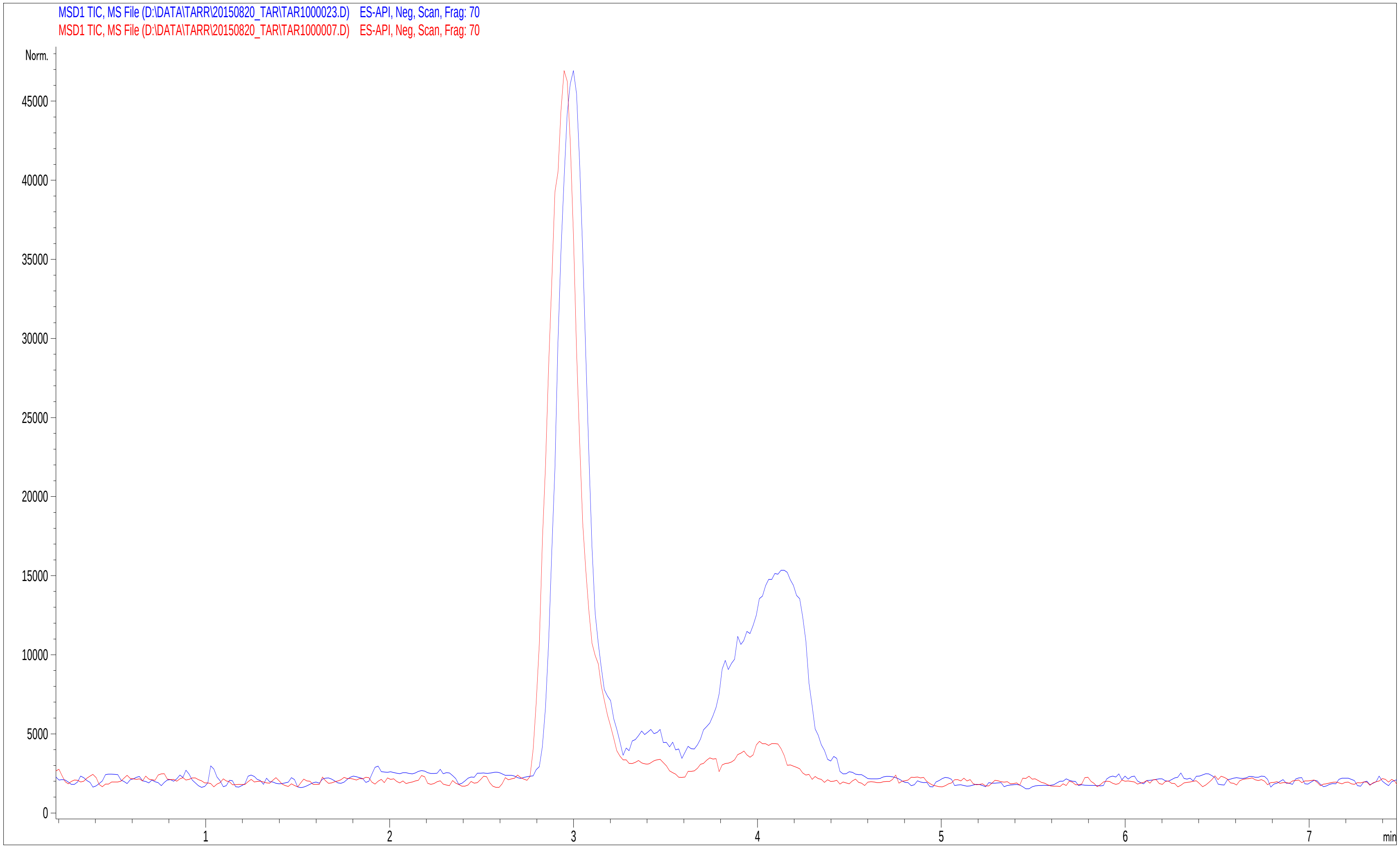
100 DC

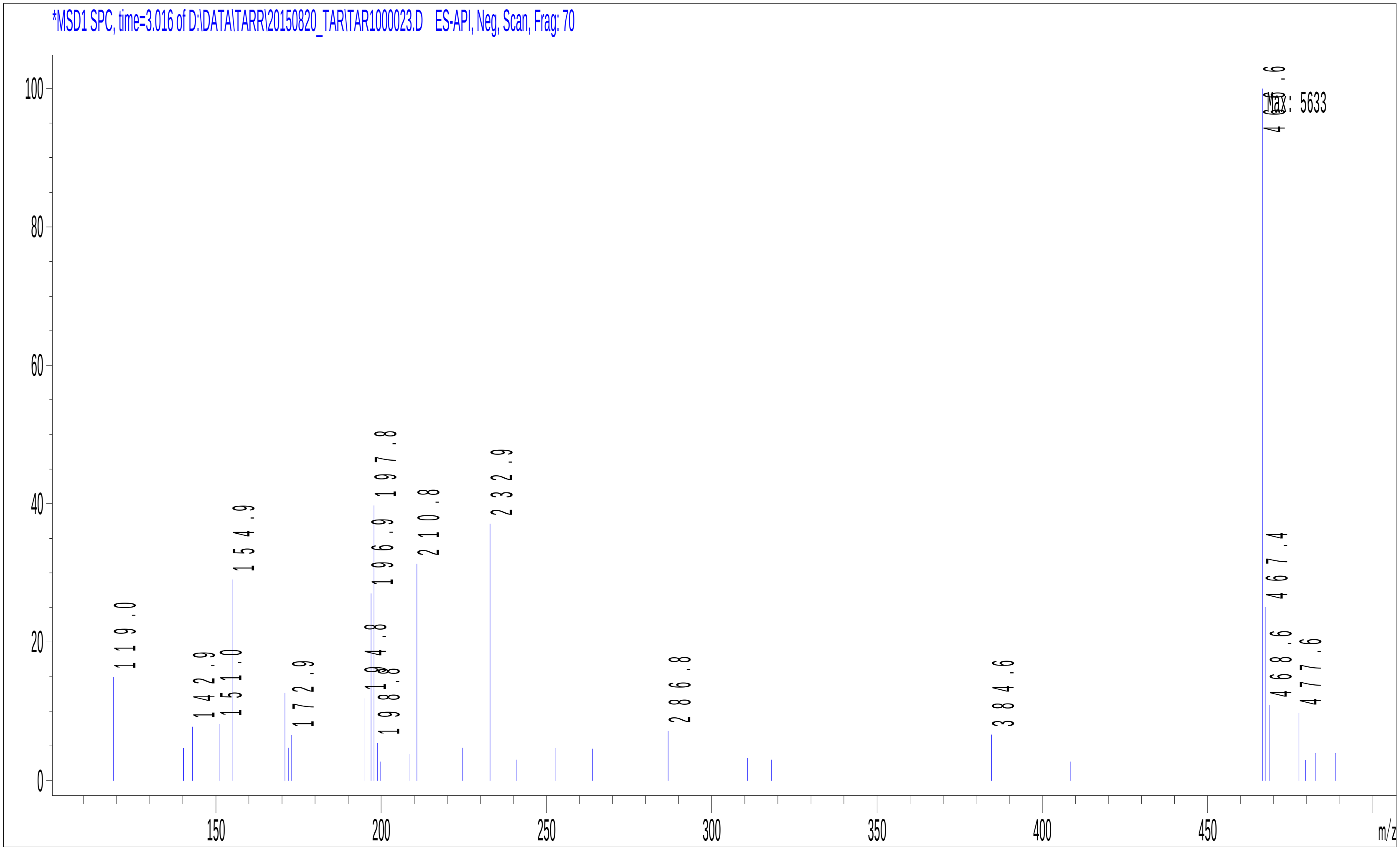
8

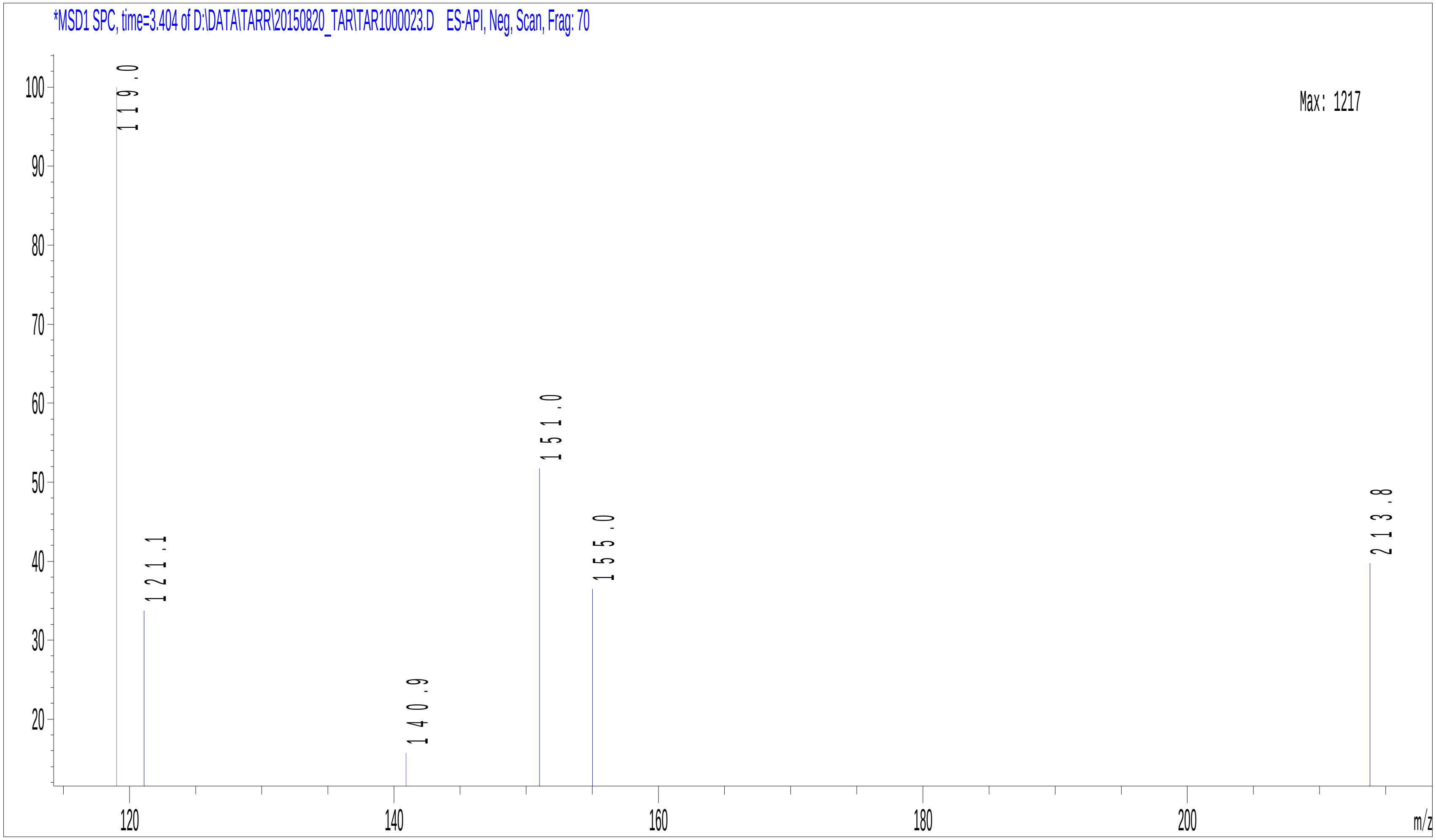
P2-C-05

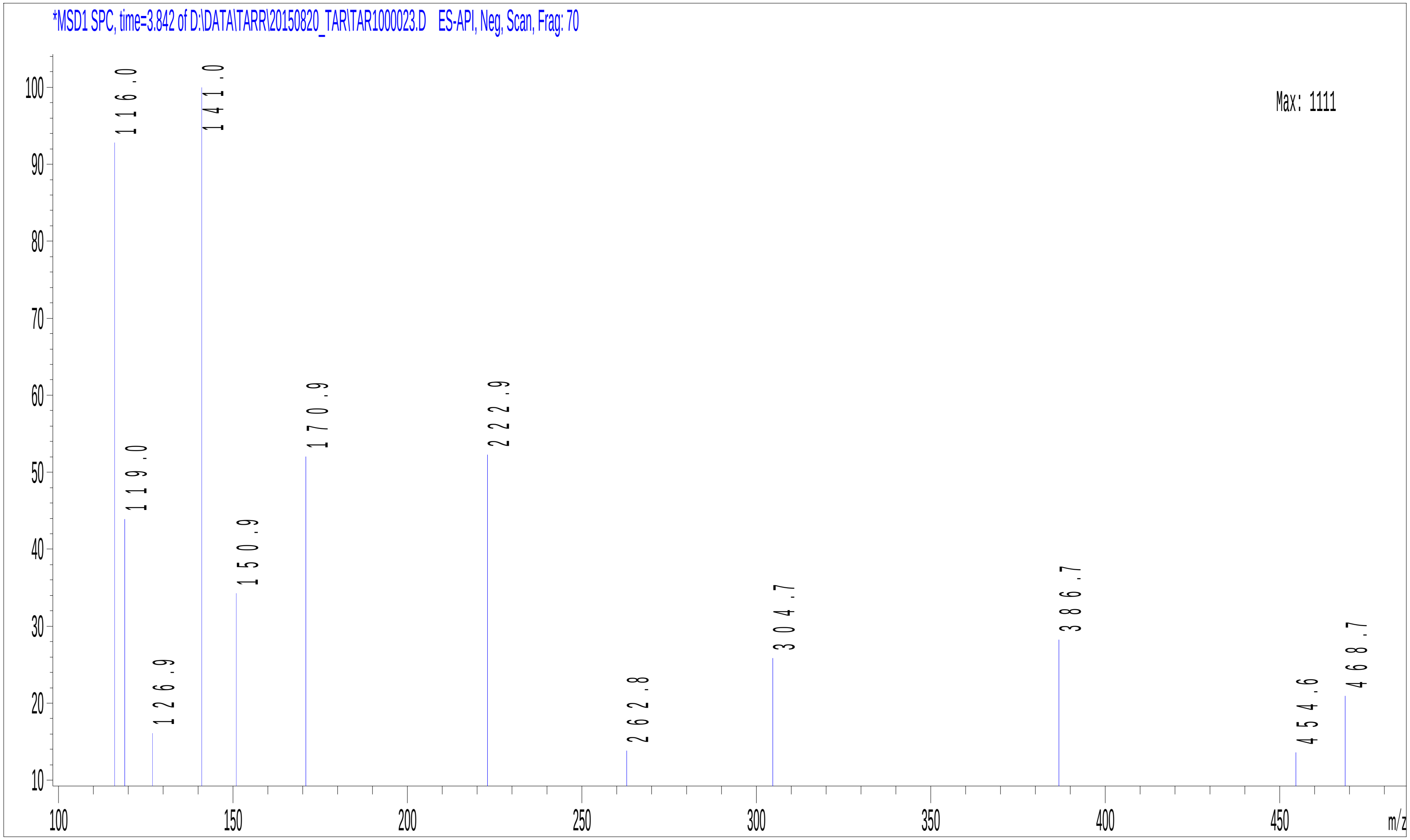


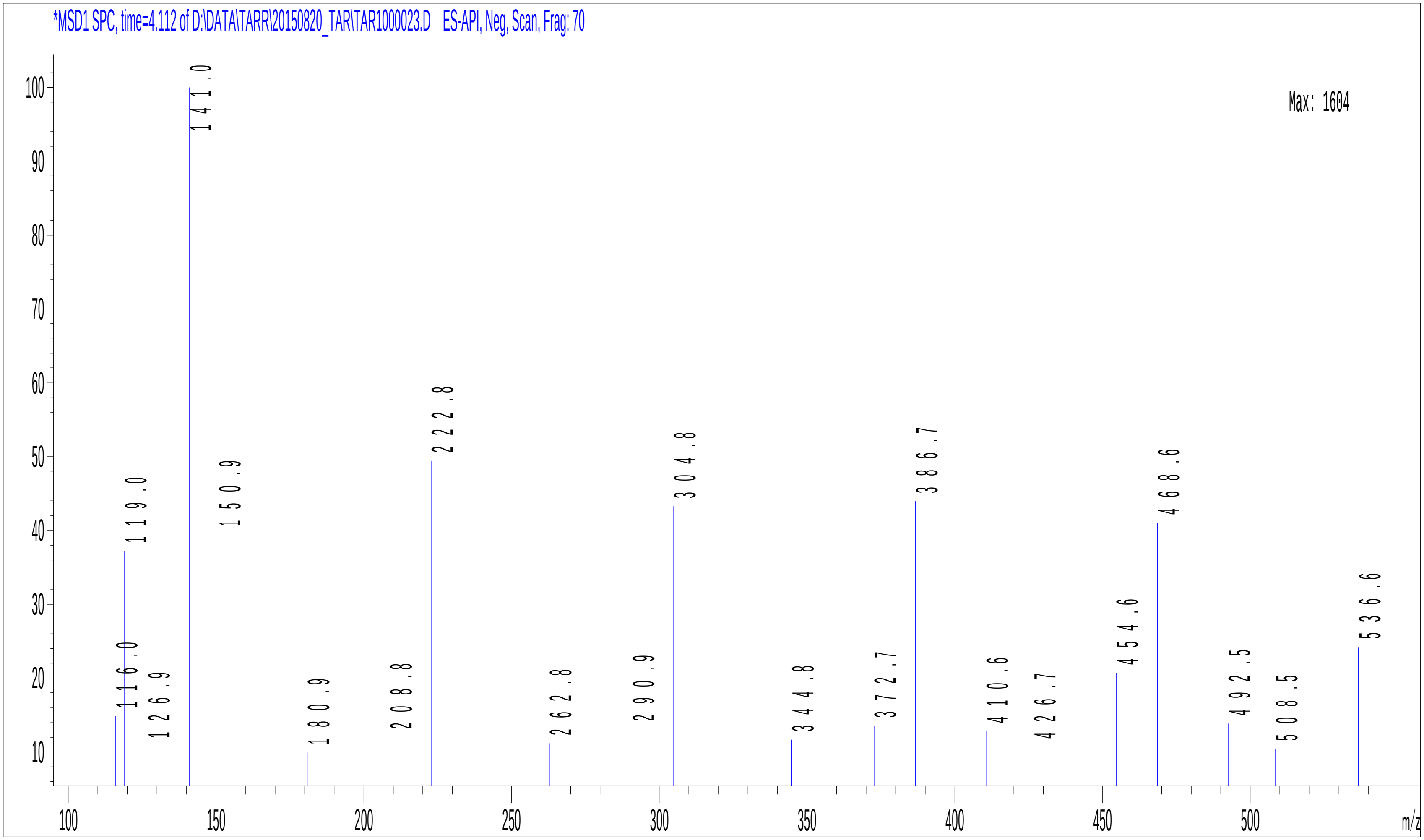
#	Time	Area	Height	Width	Area%	Symmetry
1	2.997	263147.2	23610.2	0.1806	61.942	0.97
2	4.137	161681.3	6584.1	0.3017	38.058	1.829

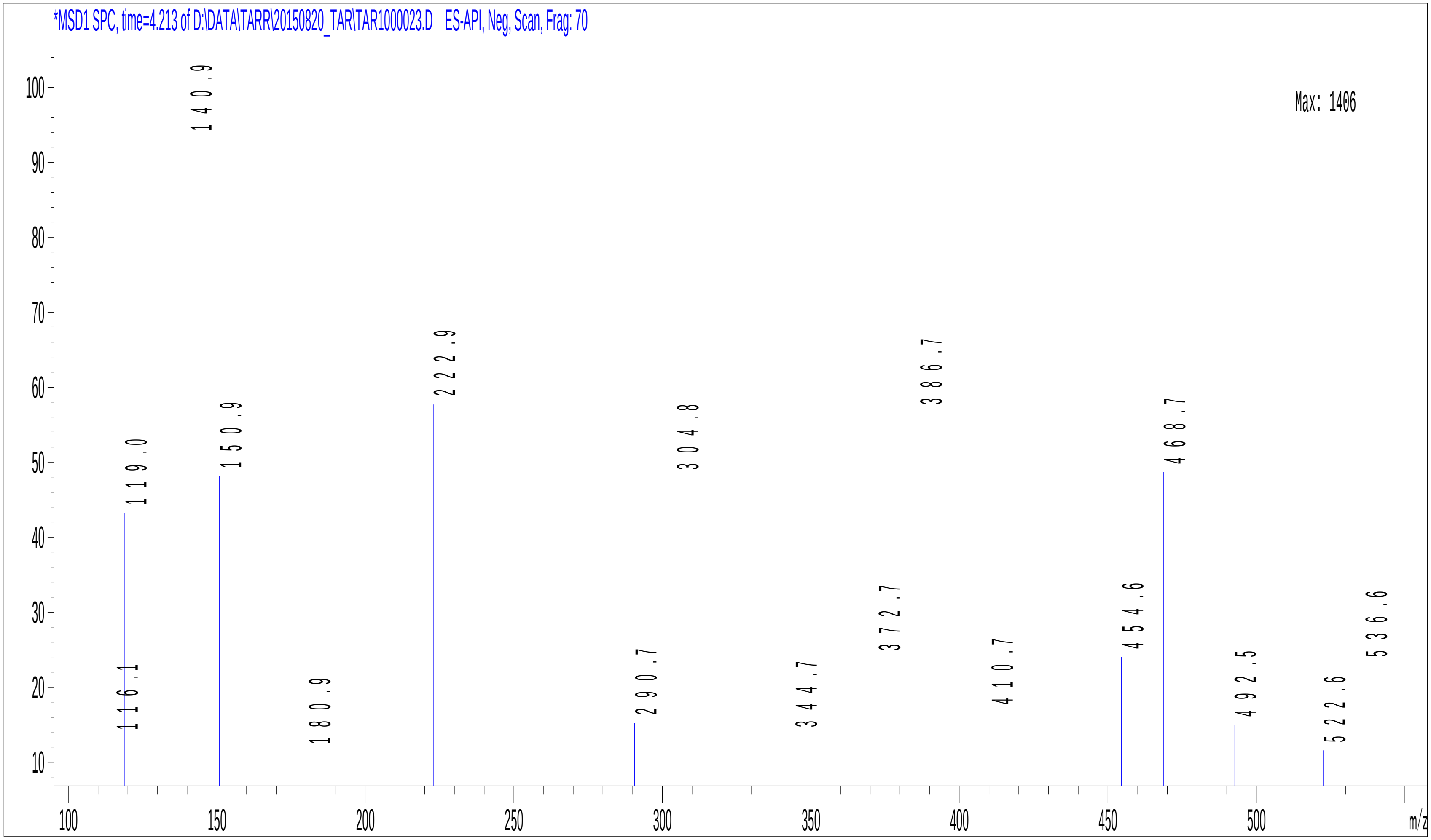

MSD1 TIC, MS File (D:\DATA\TARR\20150820_TAR\TAR1000023.D) ES-API, Neg, Scan, Frag: 70
MSD1 TIC, MS File (D:\DATA\TARR\20150820_TAR\TAR1000007.D) ES-API, Neg, Scan, Frag: 70
Norm.
45000
40000
35000
30000
25000
20000
15000
10000
5000
0
1
2
3
4
5
6
7
min


*MSD1 SPC, time=3.016 of D:\DATA\TARR\20150820_TAR\TAR1000023.D   ES-API, Neg, Scan, Frag: 70
Max: 5633
466.6
467.4
468.6
477.6
384.6
286.8
232.9
210.8
197.8
196.9
198.8
194.8
172.9
154.9
151.0
142.9
119.0
0
20
40
60
80
100
150
200
250
300
350
400
450
m/z


*MSD1 SPC, time=3.404 of D:\DATA\TARR\20150820_TAR\TAR1000023.D ES-API, Neg, Scan, Frag: 70
Max: 1217
119.0
121.1
140.9
151.0
155.0
213.8
100
90
80
70
60
50
40
30
20
120
140
160
180
200
m/z


*MSD1 SPC, time=3.842 of D:\DATA\TARR\20150820_TAR\TAR1000023.D ES-API, Neg, Scan, Frag: 70
Max: 1111
116.0
119.0
126.9
141.0
150.9
170.9
222.9
262.8
304.7
386.7
454.6
468.7
100
90
80
70
60
50
40
30
20
10
100
150
200
250
300
350
400
450
m/z


*MSD1 SPC, time=4.112 of D:\DATA\TARR\20150820_TAR\TAR1000023.D ES-API, Neg, Scan, Frag: 70
Max: 1604
100
90
80
70
60
50
40
30
20
10
100
150
200
250
300
350
400
450
500
m/z
116.0
119.0
126.9
141.0
150.9
180.9
208.8
222.8
262.8
290.9
304.8
344.8
372.7
386.7
410.6
426.7
454.6
468.6
492.5
508.5
536.6

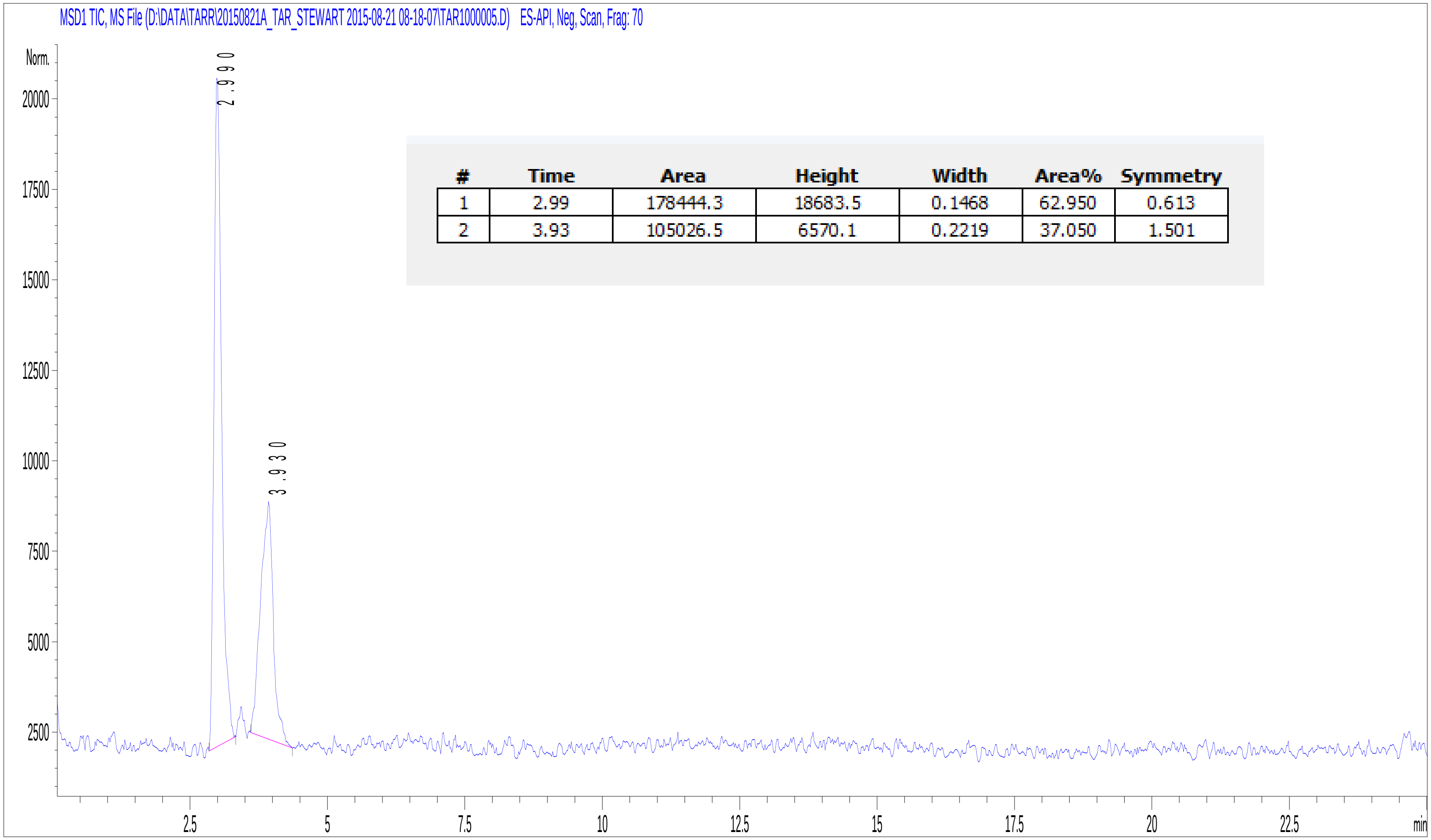

*MSD1 SPC, time=4.213 of D:\DATA\TARR\20150820_TAR\TAR1000023.D ES-API, Neg, Scan, Frag: 70
Max: 1406
100
90
80
70
60
50
40
30
20
10
116.1
119.0
140.9
150.9
180.9
222.9
290.7
304.8
344.7
372.7
386.7
410.7
454.6
468.7
492.5
522.6
536.6
100
150
200
250
300
350
400
450
500
m/z

13-Aug-15

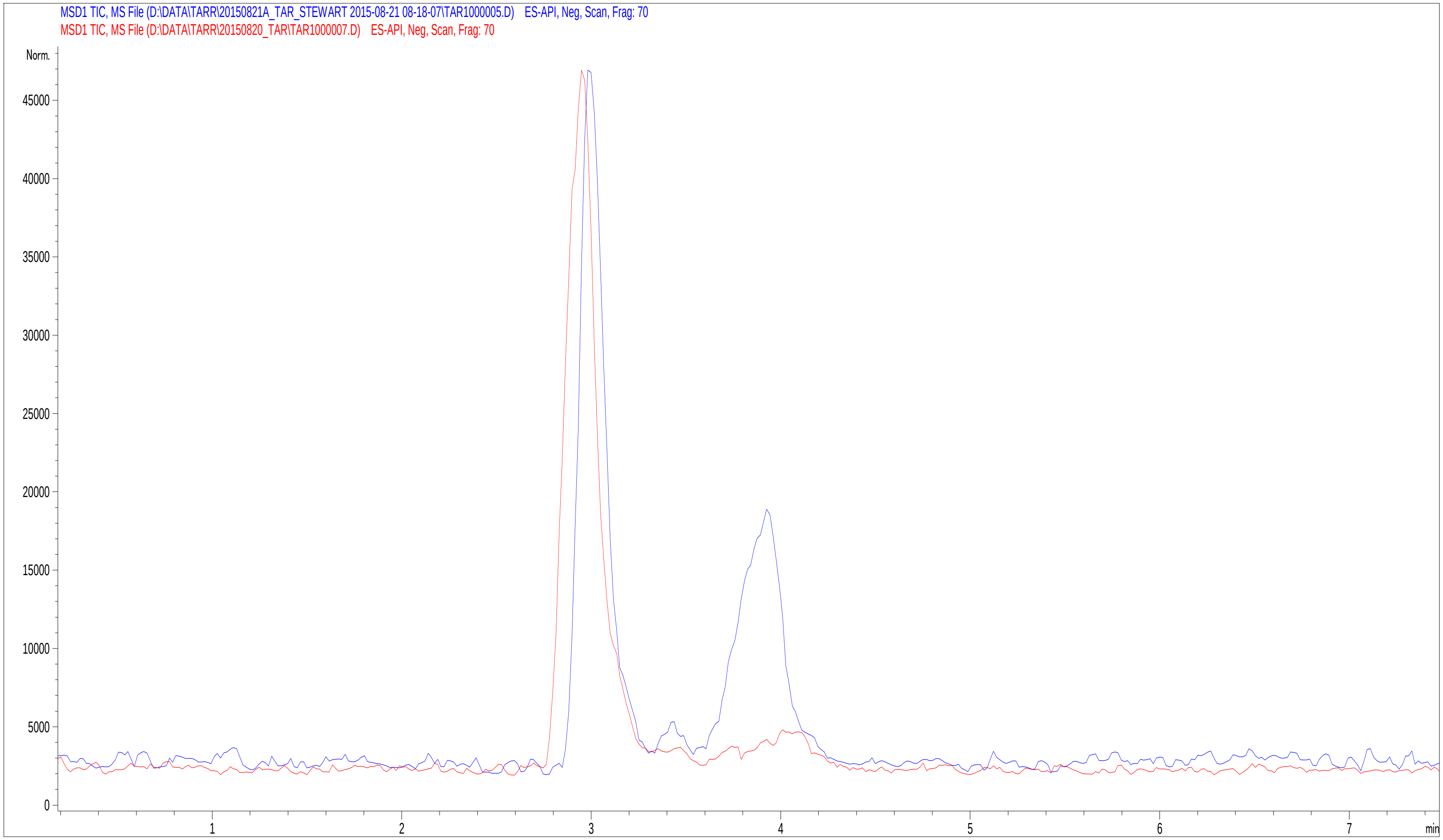
100 DC Repeat

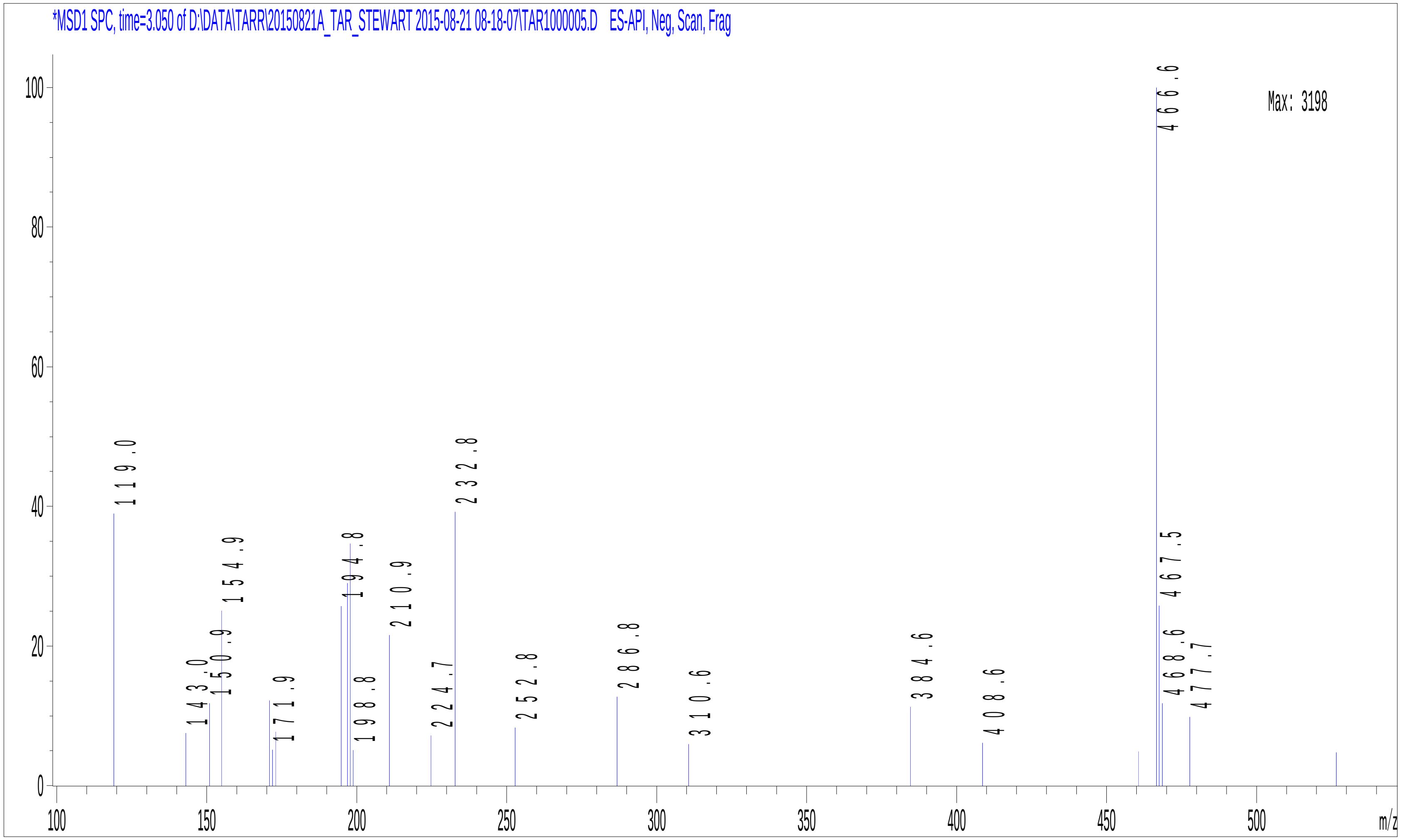
8

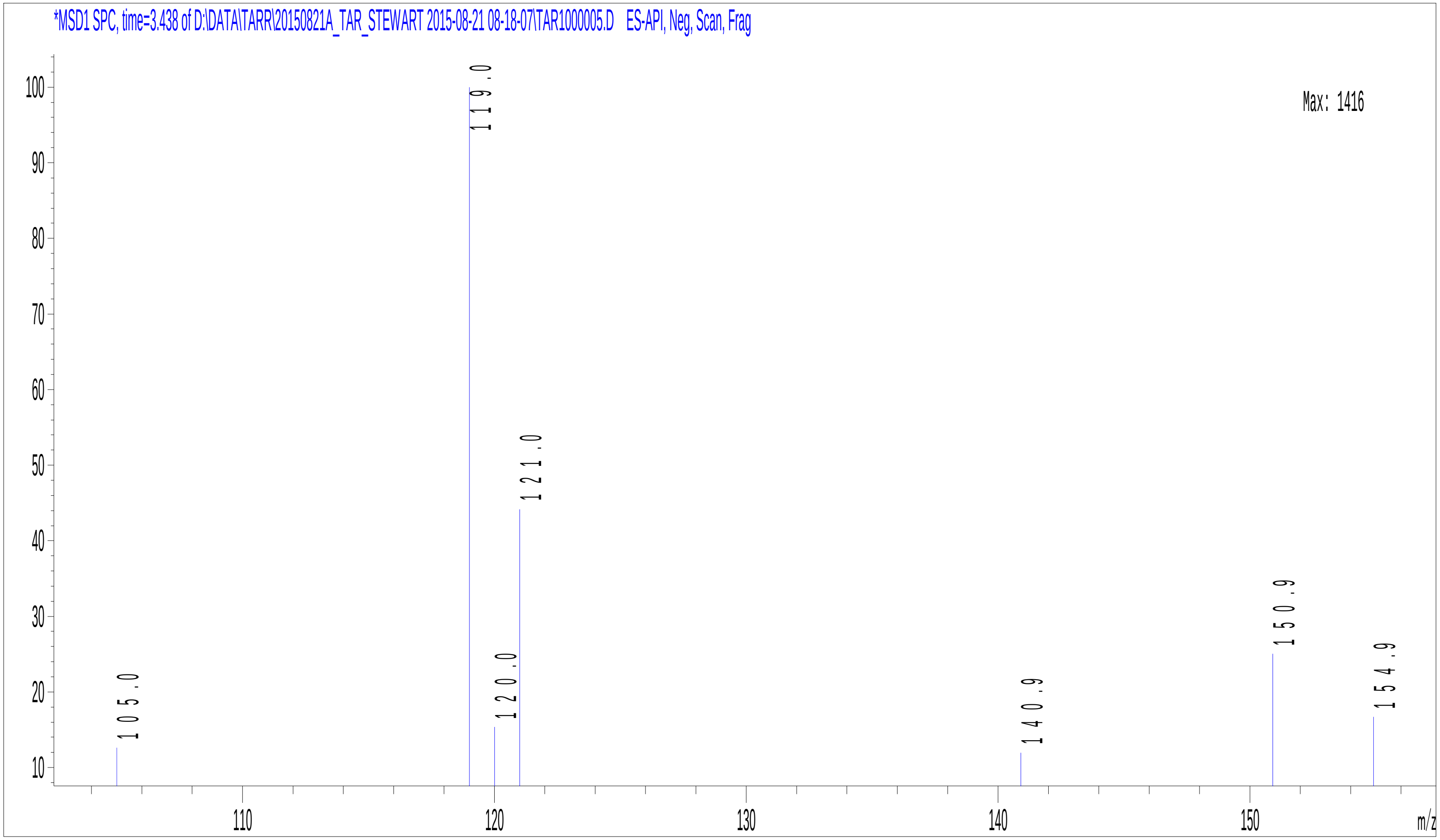
P2-E-04

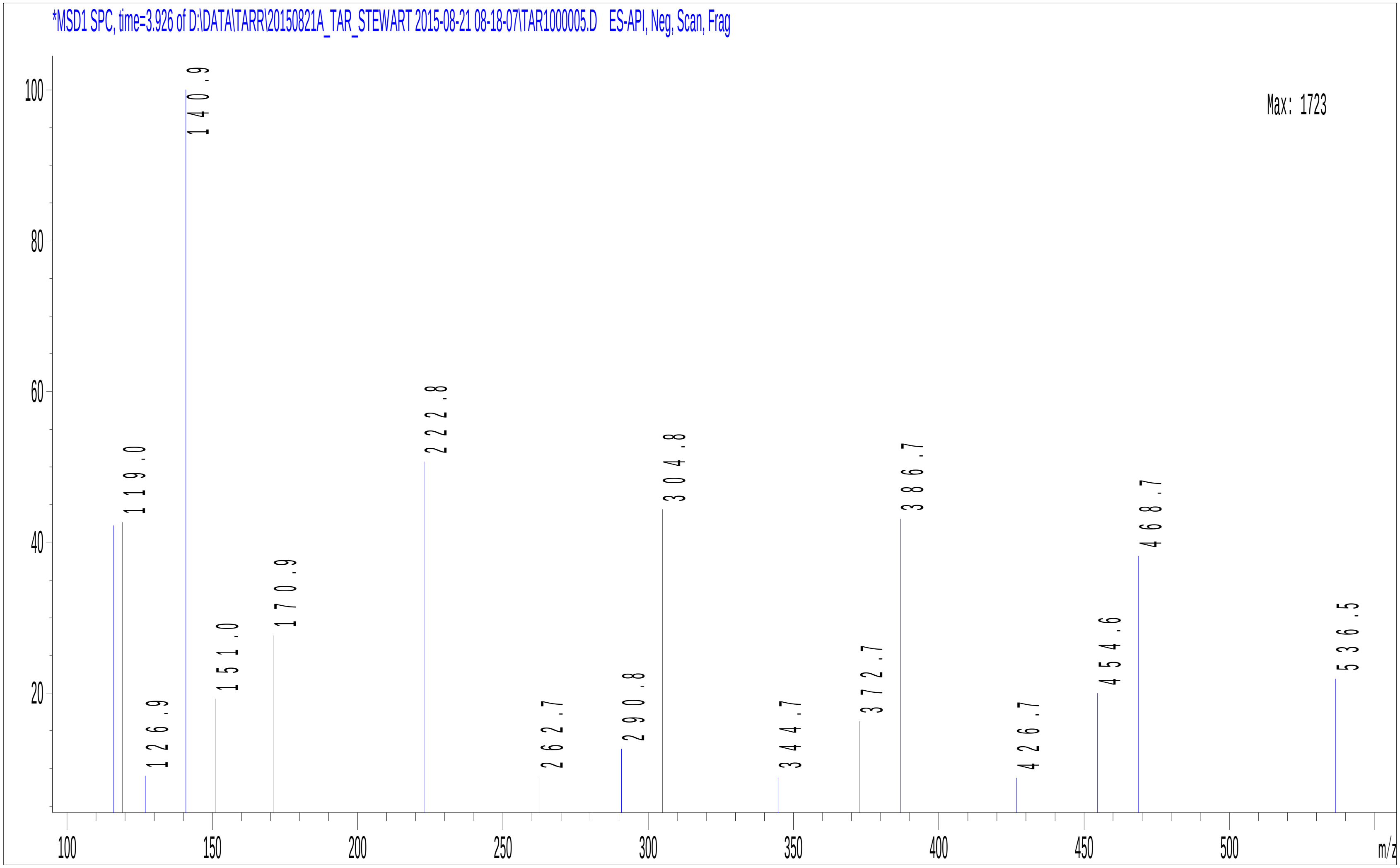


#	Time	Area	Height	Width	Area%	Symmetry
1	2.99	178444.3	18683.5	0.1468	62.950	0.613
2	3.93	105026.5	6570.1	0.2219	37.050	1.501


MSD1 TIC, MS File (D:\DATA\TARR\20150821A_TAR_STEWART 2015-08-21 08-18-07\TAR1000005.D)   ES-API, Neg, Scan, Frag: 70
MSD1 TIC, MS File (D:\DATA\TARR\20150820_TAR\TAR1000007.D)   ES-API, Neg, Scan, Frag: 70
Norm.
45000
40000
35000
30000
25000
20000
15000
10000
5000
0
1
2
3
4
5
6
7
min

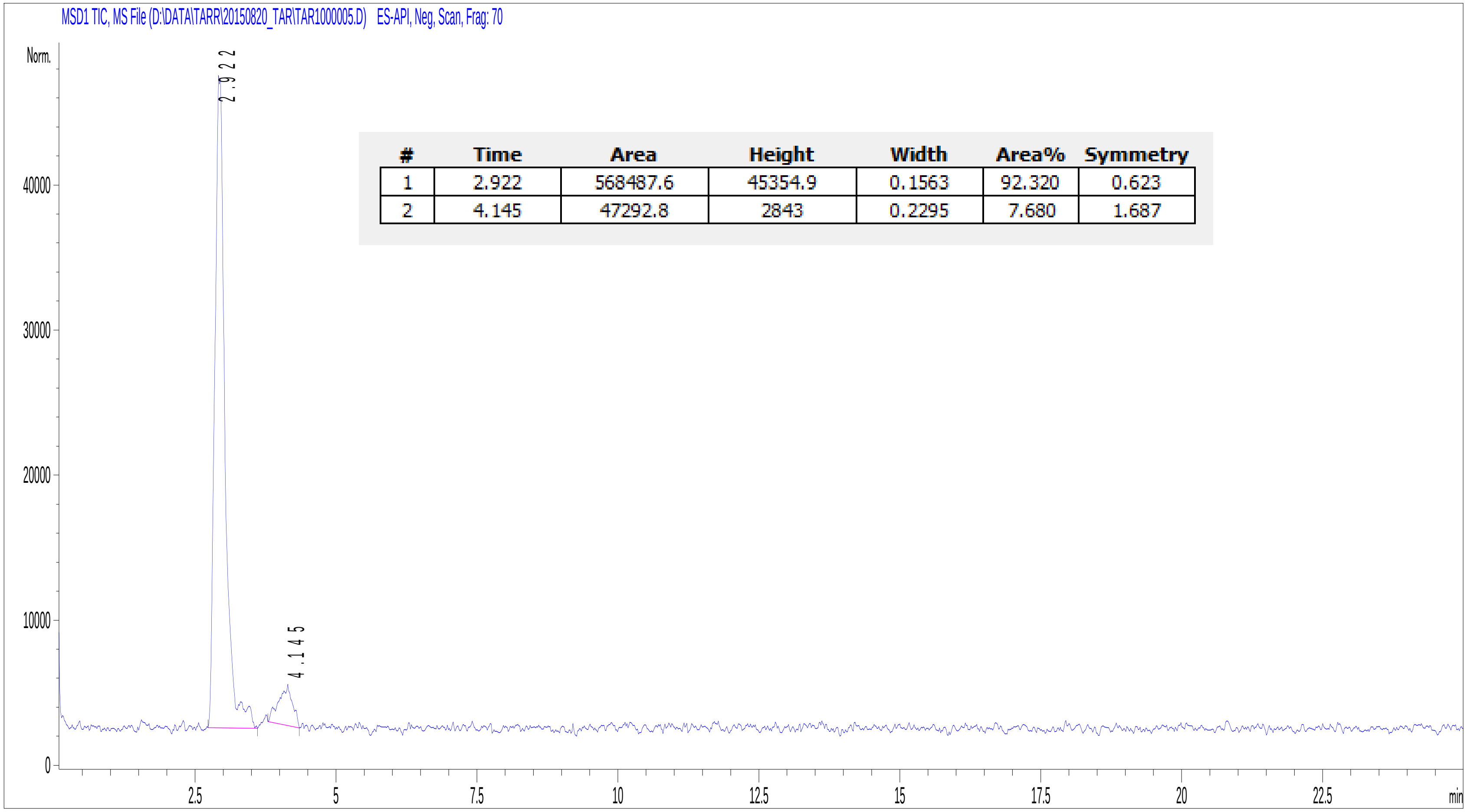

*MSD1 SPC, time=3.050 of D:\DATA\TARR\20150821A_TAR_STEWART 2015-08-21 08-18-07\TAR1000005.D ES-API, Neg, Scan, Frag
Max: 3198
100
80
60
40
20
0
119.0
143.0
150.9
154.9
171.9
194.8
198.8
210.9
224.7
232.8
252.8
286.8
310.6
384.6
408.6
466.6
467.5
468.6
477.7
100
150
200
250
300
350
400
450
500
m/z


*MSD1 SPC, time=3.438 of D:\DATA\TARR\20150821A_TAR_STEWART 2015-08-21 08-18-07\TAR1000005.D ES-API, Neg, Scan, Frag
Max: 1416
100
90
80
70
60
50
40
30
20
10
105.0
119.0
120.0
121.0
140.9
150.9
154.9
110
120
130
140
150
m/z

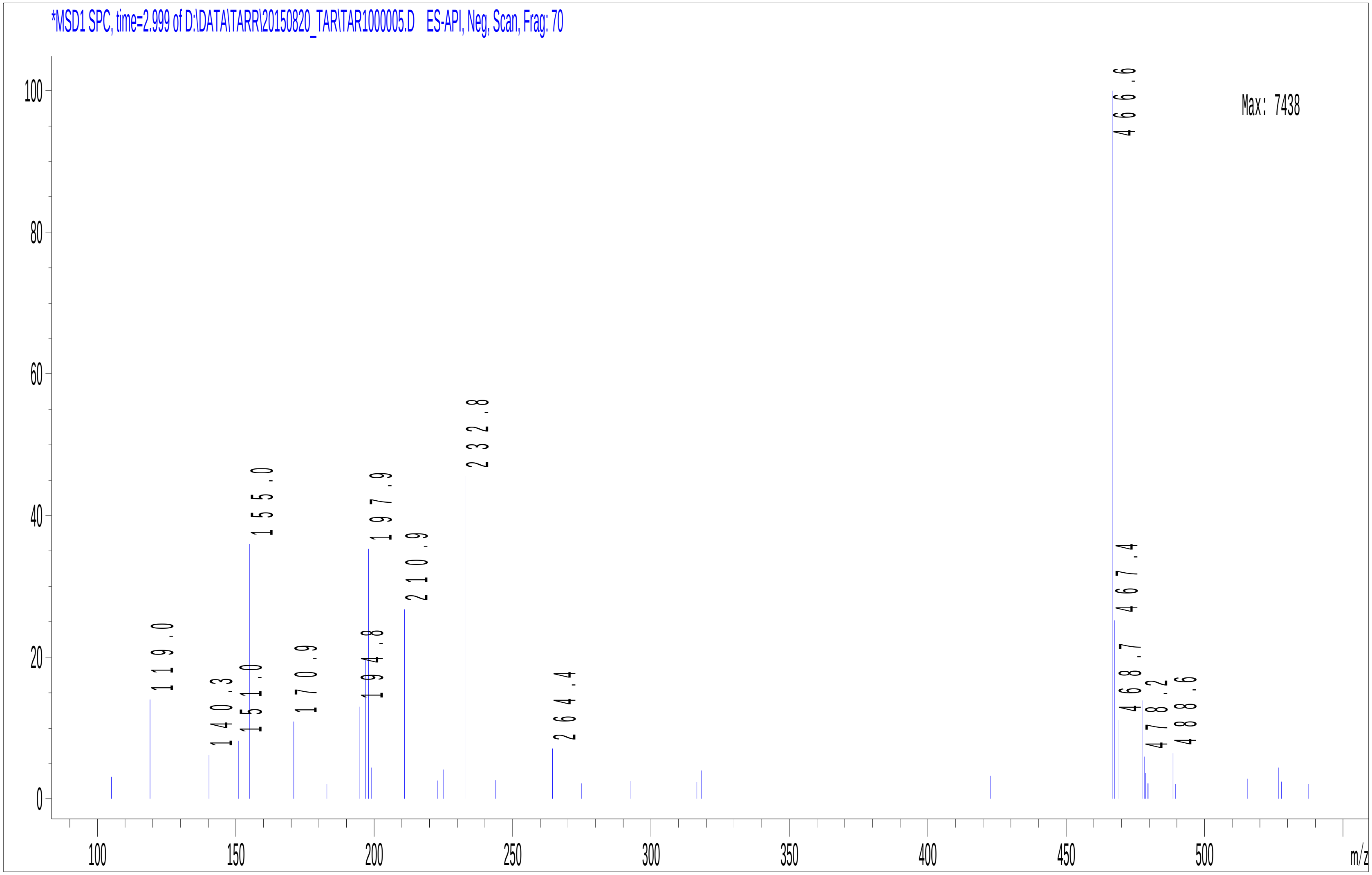

*MSD1 SPC, time=3.926 of D:\DATA\TARR\20150821A_TAR_STEWART 2015-08-21 08-18-07\TAR1000005.D   ES-API, Neg, Scan, Frag
Max: 1723
100
80
60
40
20
119.0
126.9
140.9
151.0
170.9
222.8
262.7
290.8
304.8
344.7
372.7
386.7
426.7
454.6
468.7
536.5
100
150
200
250
300
350
400
450
500
m/z

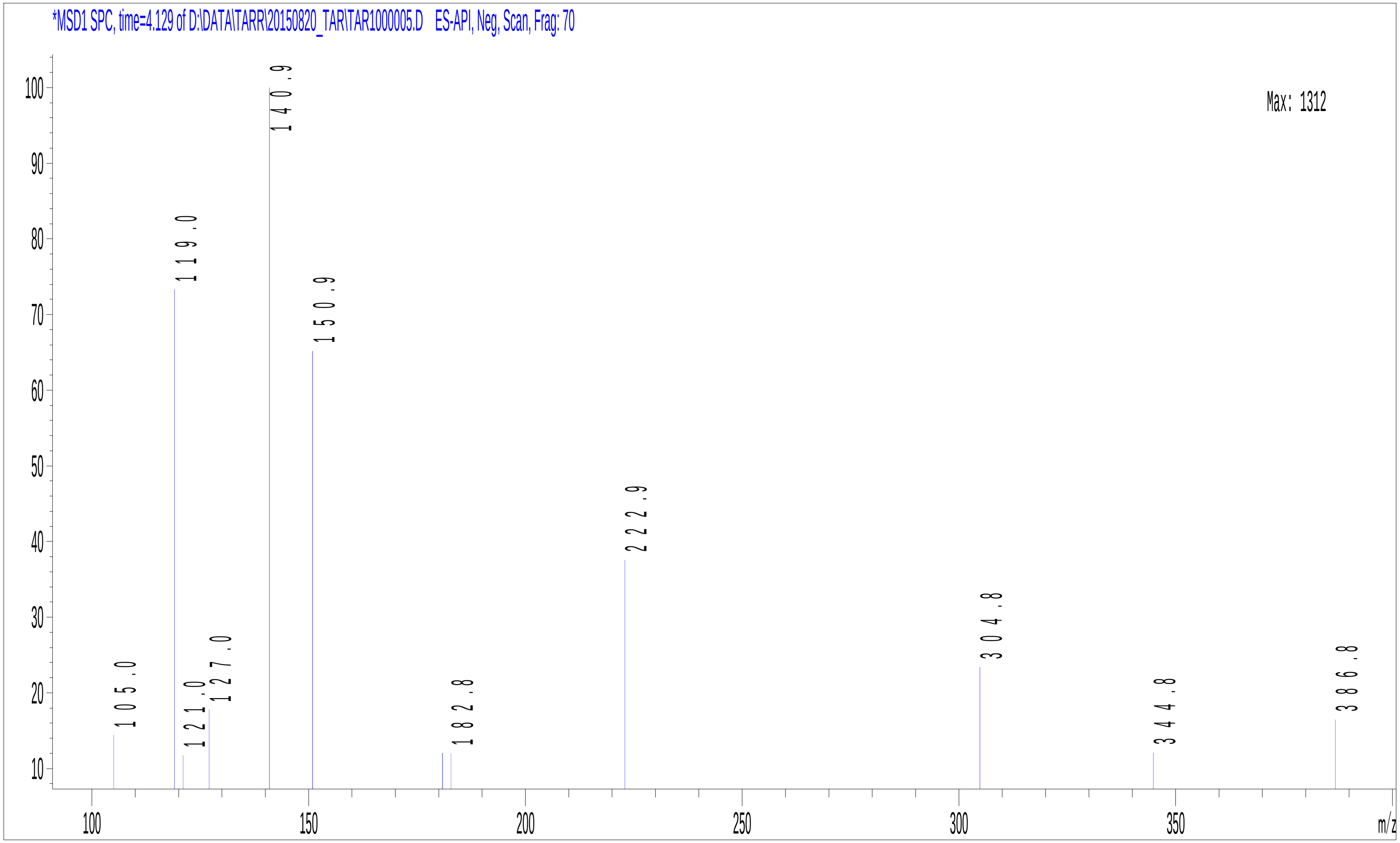
pH 9

8-Apr-15
H2O2 Ctrl
9
P2-A-05


MSD1 TIC, MS File (D:\DATA\TARR\20150820_TAR\TAR1000005.D) ES-API, Neg, Scan, Frag: 70

#	Time	Area	Height	Width	Area%	Symmetry
1	2.922	568487.6	45354.9	0.1563	92.320	0.623
2	4.145	47292.8	2843	0.2295	7.680	1.687


*MSD1 SPC, time=2.999 of D:\DATA\TARR\20150820_TAR\TAR1000005.D   ES-API, Neg, Scan, Frag: 70
Max: 7438
0
20
40
60
80
100
100
150
200
250
300
350
400
450
500
m/z
119.0
140.3
151.0
155.0
170.9
194.8
197.9
210.9
232.8
264.4
466.6
467.4
468.7
478.2
488.6

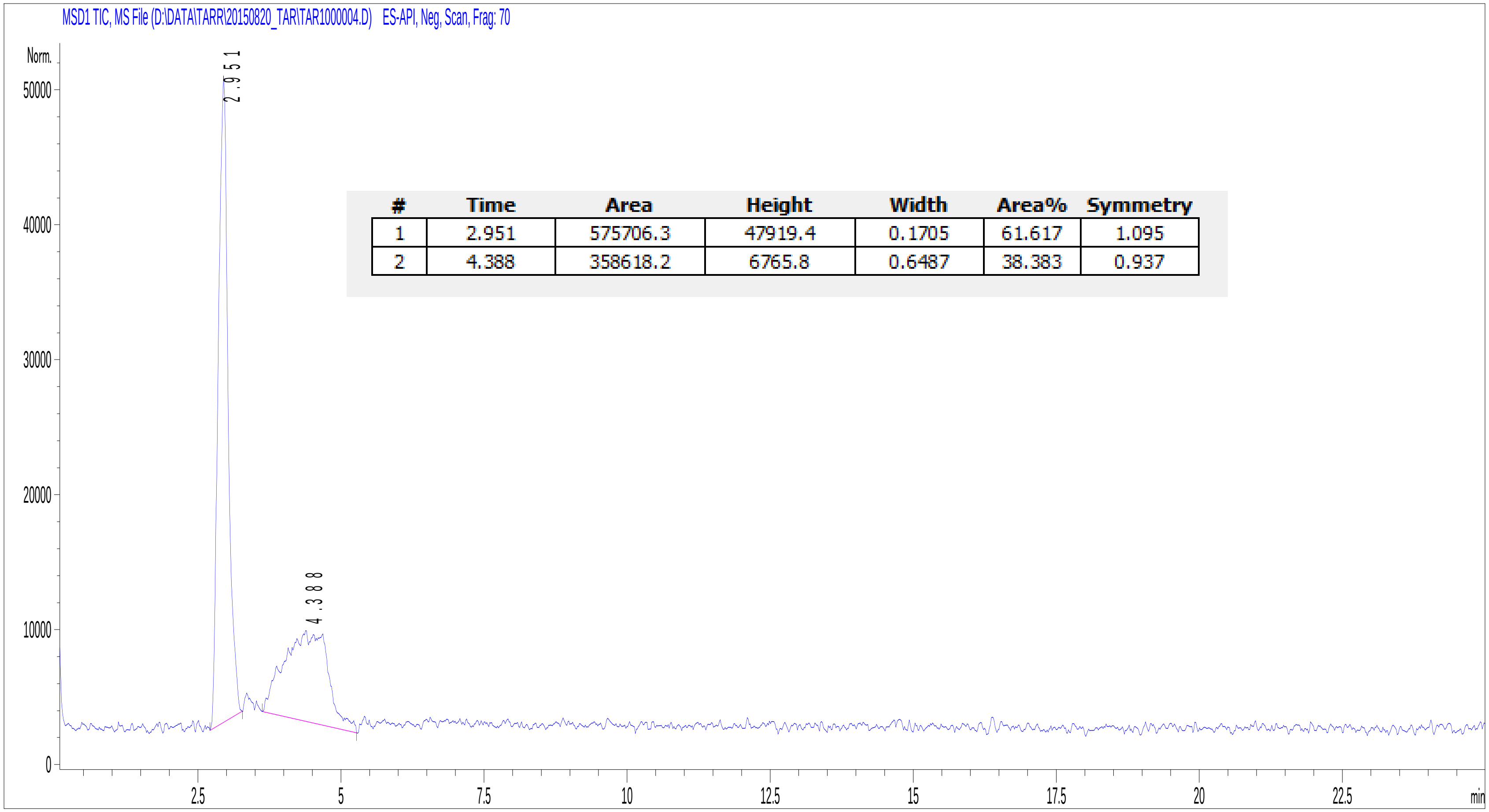

*MSD1 SPC, time=4.129 of D:\DATA\TARR\20150820_TAR\TAR1000005.D ES-API, Neg, Scan, Frag: 70
Max: 1312
105.0
119.0
121.0
127.0
140.9
150.9
182.8
222.9
304.8
344.8
386.8
100
90
80
70
60
50
40
30
20
10
100
150
200
250
300
350
m/z

16-Mar-15

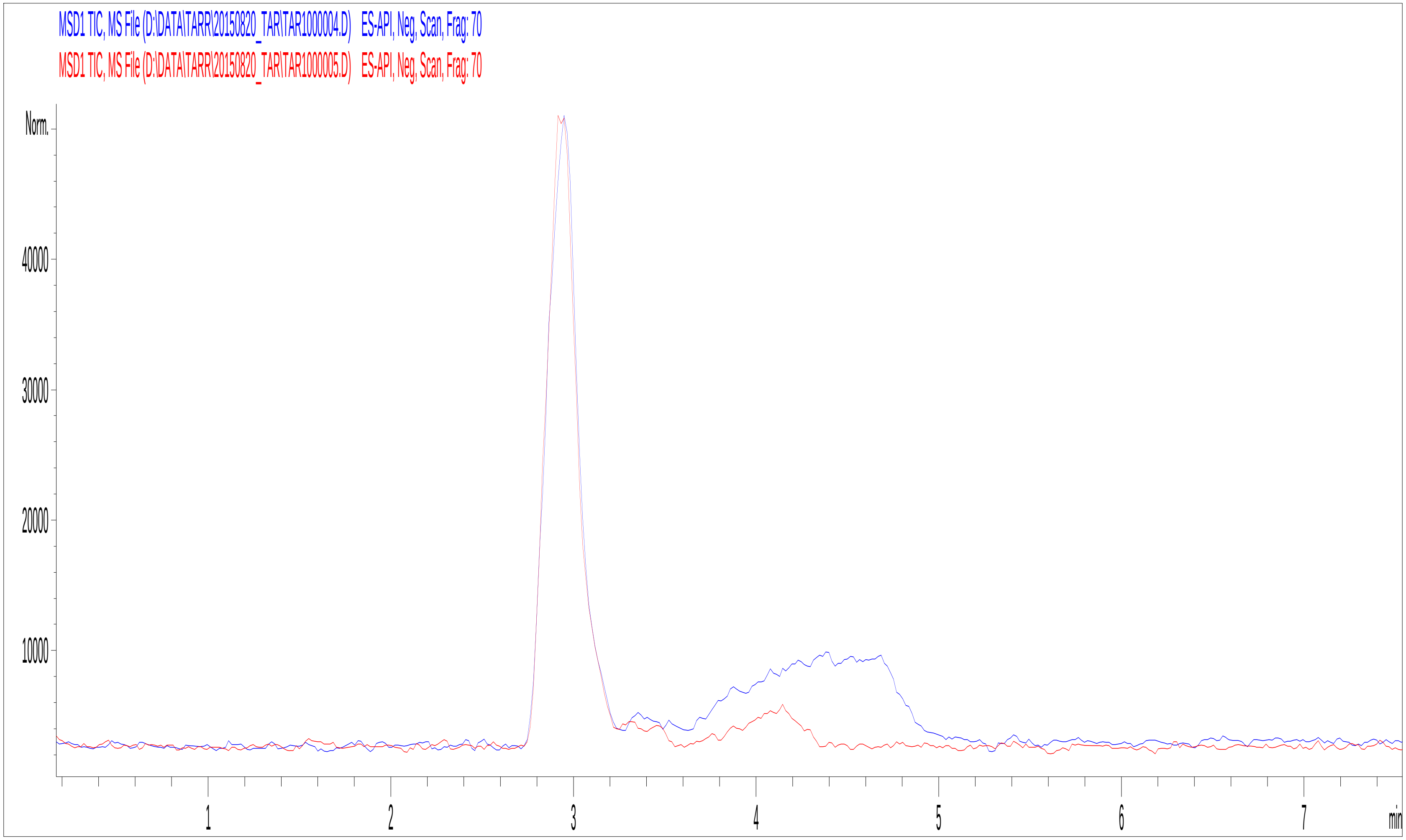
0 DC

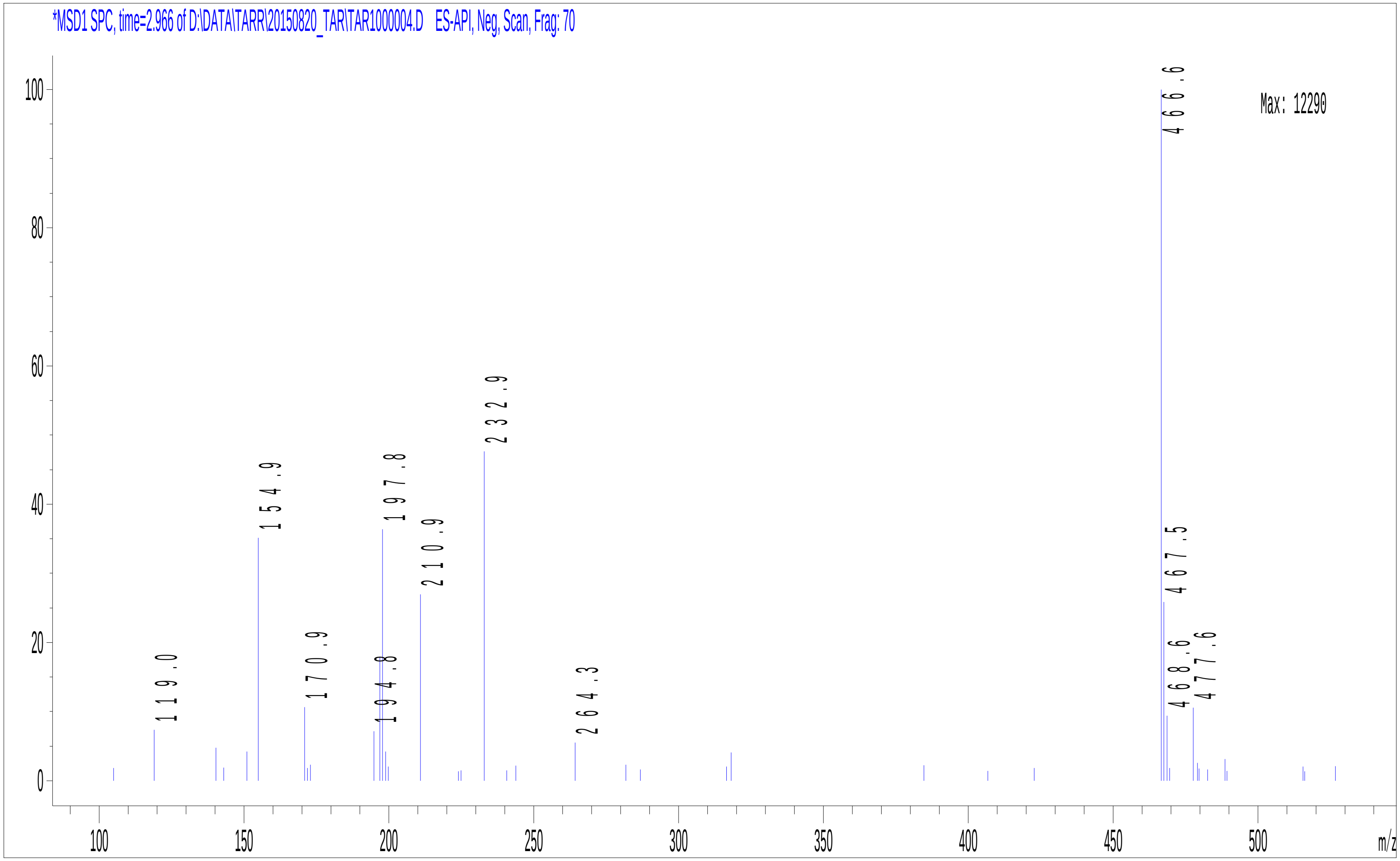
9

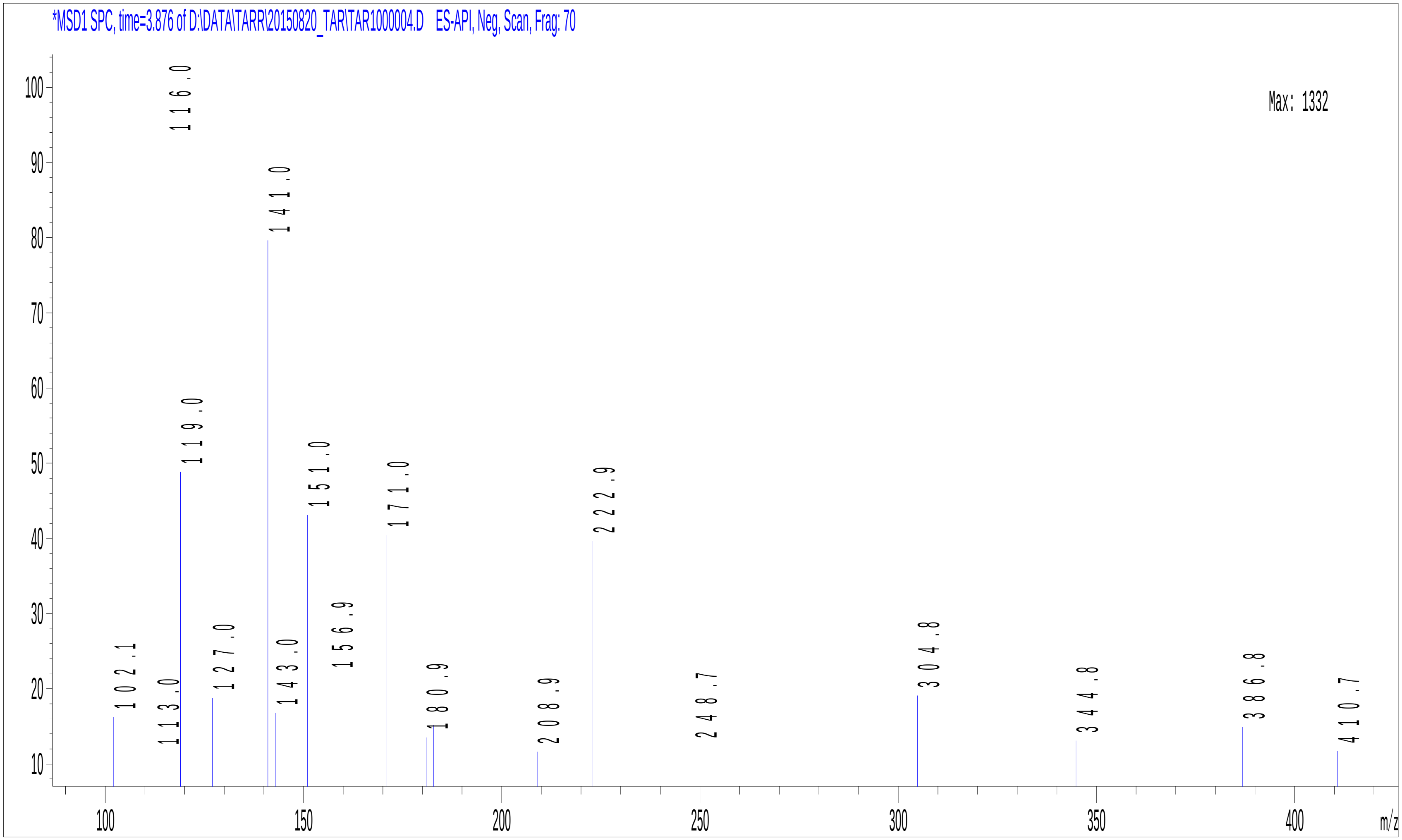
P2-A-04

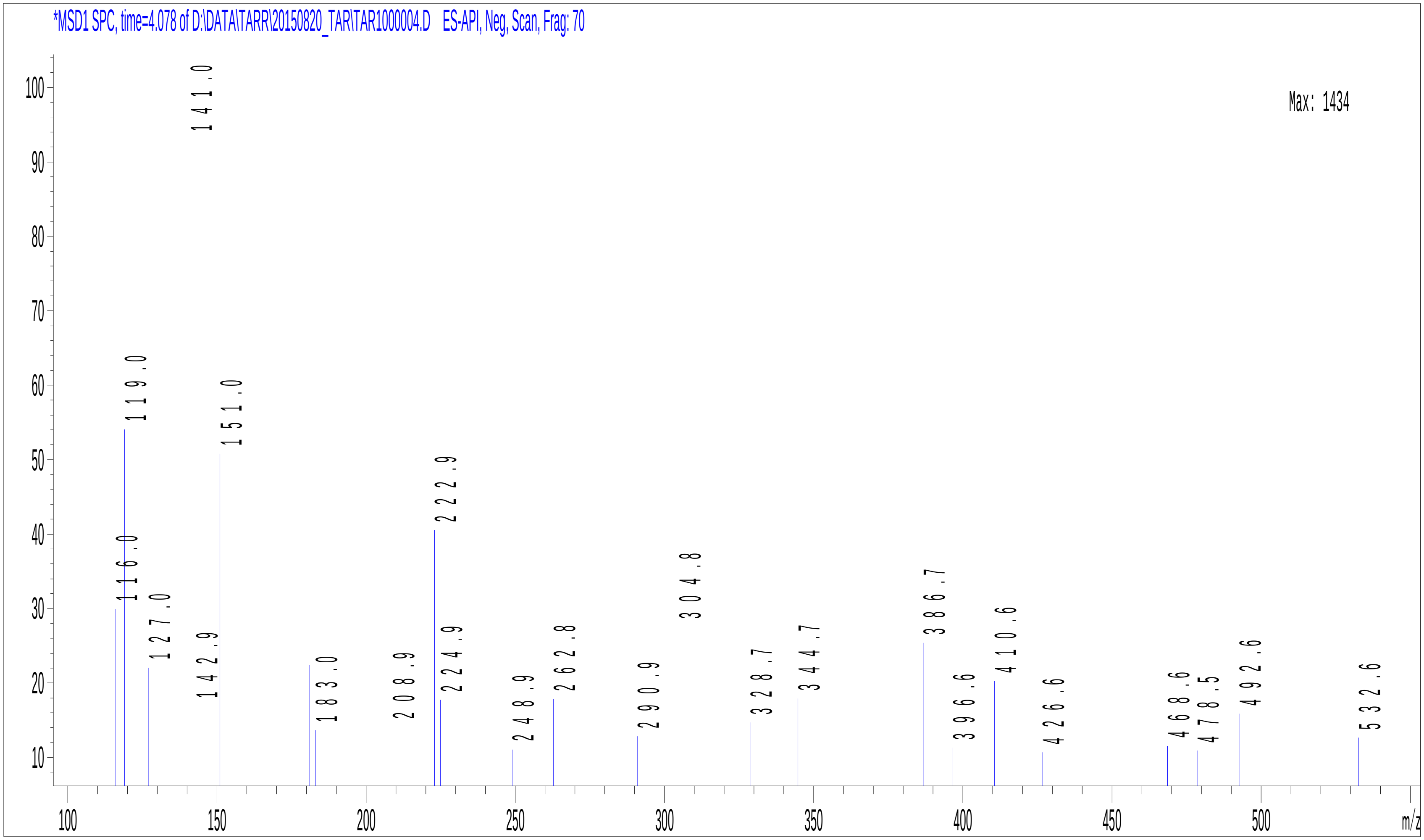


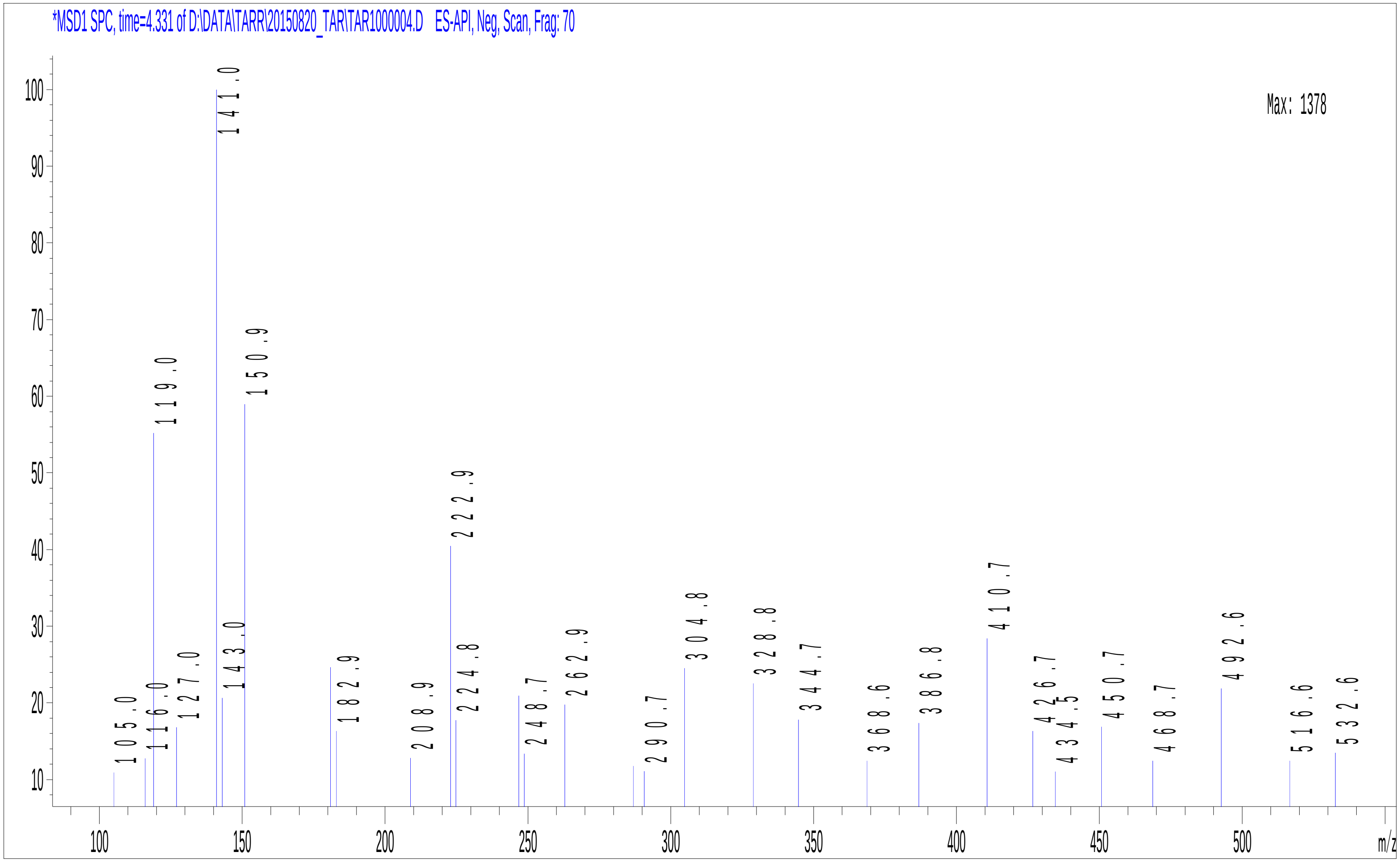
#	Time	Area	Height	Width	Area%	Symmetry
1	2.951	575706.3	47919.4	0.1705	61.617	1.095
2	4.388	358618.2	6765.8	0.6487	38.383	0.937

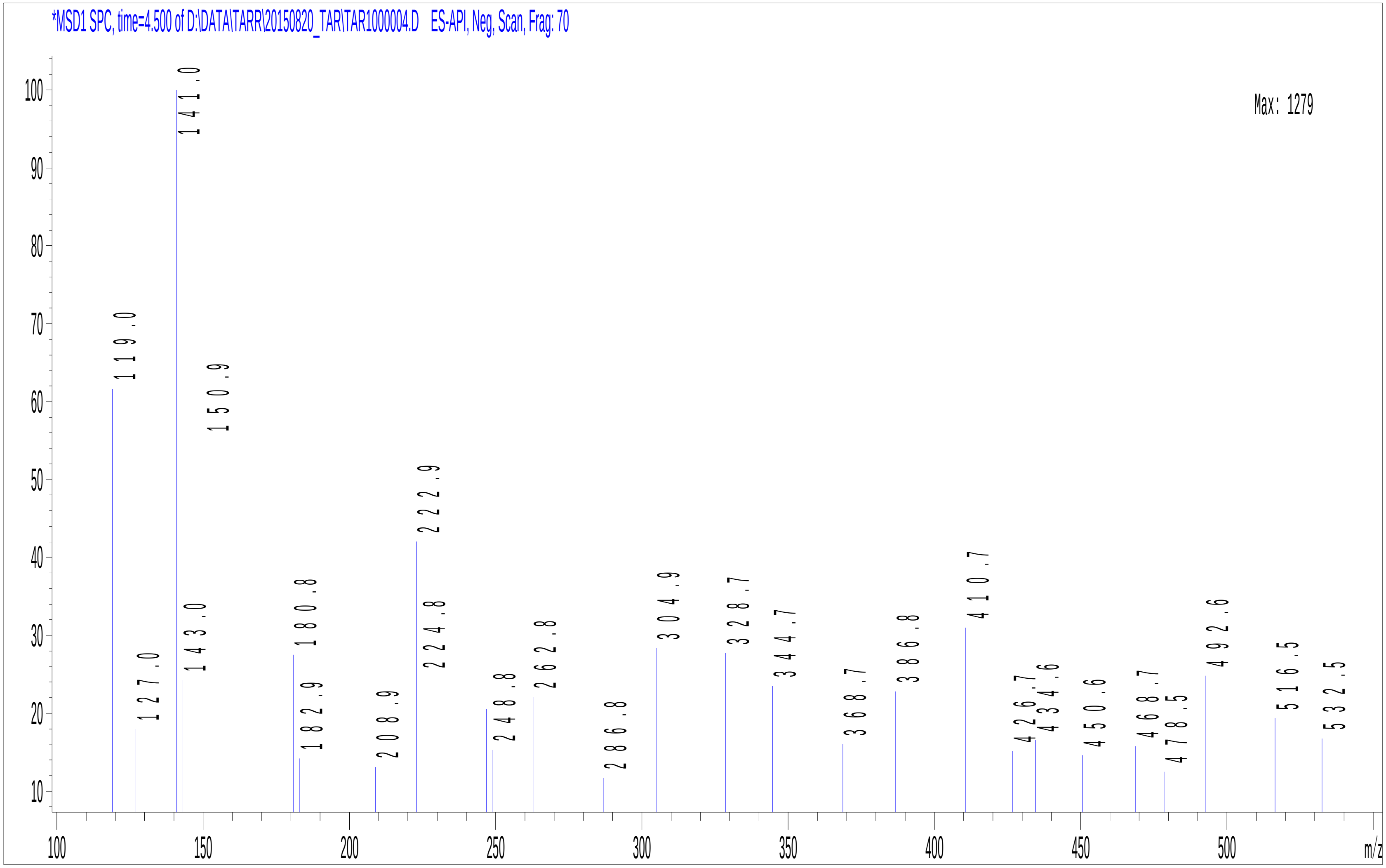

MSD1 TIC, MS File (D:\DATA\TARR\20150820_TAR\TAR1000004.D)   ES-API, Neg, Scan, Frag: 70
MSD1 TIC, MS File (D:\DATA\TARR\20150820_TAR\TAR1000005.D)   ES-API, Neg, Scan, Frag: 70
Norm.
40000
30000
20000
10000
1
2
3
4
5
6
7
min

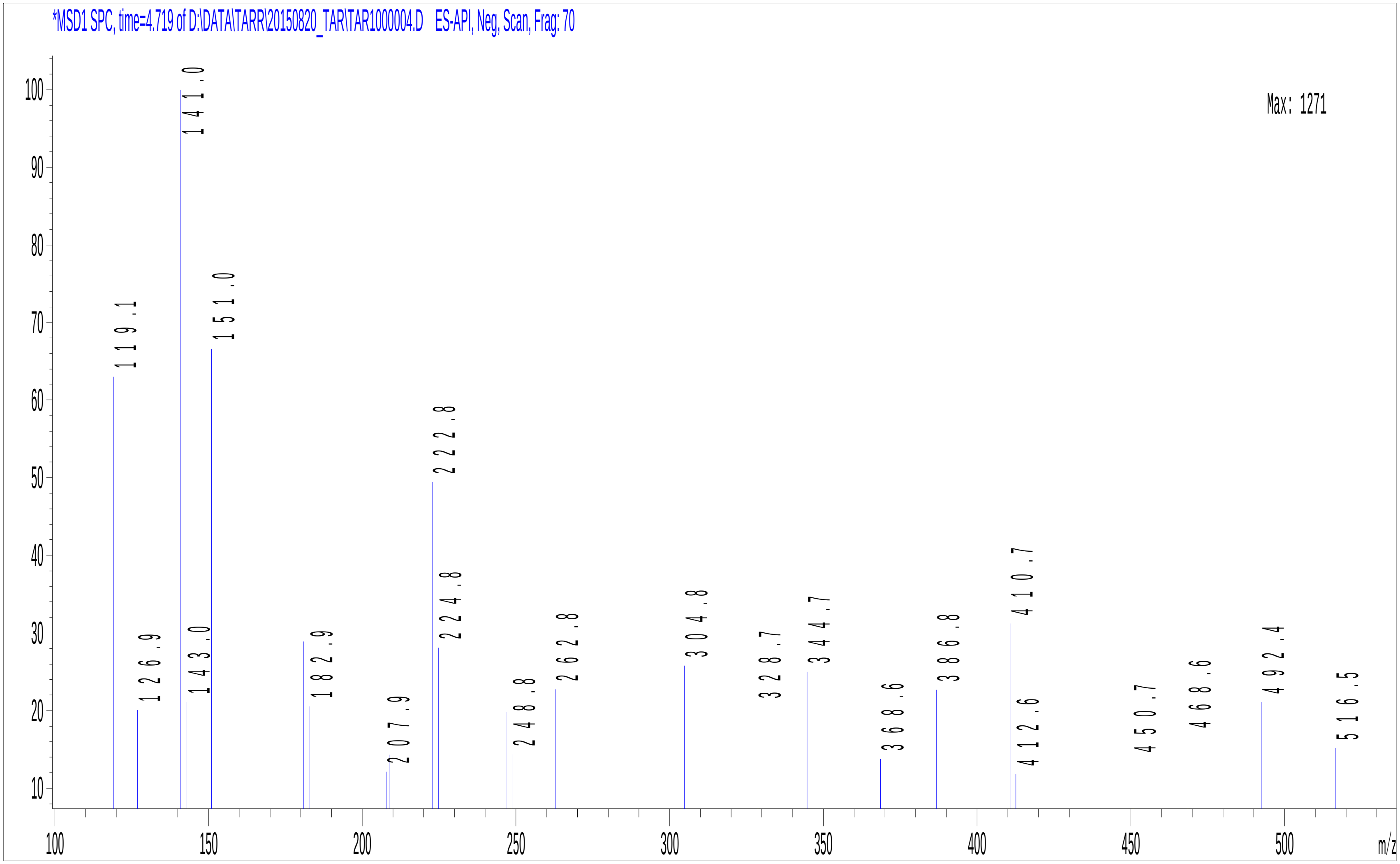

*MSD1 SPC, time=2.966 of D:\DATA\TARR\20150820_TAR\TAR1000004.D ES-API, Neg, Scan, Frag: 70
Max: 12290
466.6
467.5
468.6
477.6
232.9
154.9
197.8
210.9
170.9
194.8
119.0
264.3
0
20
40
60
80
100
100
150
200
250
300
350
400
450
500
m/z


*MSD1 SPC, time=3.876 of D:\DATA\TARR\20150820_TAR\TAR1000004.D ES-API, Neg, Scan, Frag: 70
Max: 1332
102.1
113.0
116.0
119.0
127.0
141.0
143.0
151.0
156.9
171.0
180.9
208.9
222.9
248.7
304.8
344.8
386.8
410.7
100
90
80
70
60
50
40
30
20
10
100
150
200
250
300
350
400
m/z


*MSD1 SPC, time=4.078 of D:\DATA\TARR\20150820_TAR\TAR1000004.D ES-API, Neg, Scan, Frag: 70
Max: 1434
100
90
80
70
60
50
40
30
20
10
100
150
200
250
300
350
400
450
500
m/z
116.0
119.0
127.0
141.0
142.9
151.0
183.0
208.9
222.9
224.9
248.9
262.8
290.9
304.8
328.7
344.7
386.7
396.6
410.6
426.6
468.6
478.5
492.6
532.6


*MSD1 SPC, time=4.331 of D:\DATA\TARR\20150820_TAR\TAR1000004.D ES-API, Neg, Scan, Frag: 70
Max: 1378
100
90
80
70
60
50
40
30
20
10
100
150
200
250
300
350
400
450
500
m/z
105.0
116.0
119.0
127.0
141.0
143.0
150.9
182.9
208.9
222.9
224.8
248.7
262.9
290.7
304.8
328.8
344.7
368.6
386.8
410.7
426.7
434.5
450.7
468.7
492.6
516.6
532.6


*MSD1 SPC, time=4.500 of D:\DATA\TARR\20150820_TAR\TAR1000004.D ES-API, Neg, Scan, Frag: 70
Max: 1279
100
90
80
70
60
50
40
30
20
10
119.0
127.0
141.0
143.0
150.9
180.8
182.9
208.9
222.9
224.8
248.8
262.8
286.8
304.9
328.7
344.7
368.7
386.8
410.7
426.7
434.6
450.6
468.7
478.5
492.6
516.5
532.5
100
150
200
250
300
350
400
450
500
m/z


*MSD1 SPC, time=4.719 of D:\DATA\TARR\20150820_TAR\TAR1000004.D ES-API, Neg, Scan, Frag: 70
Max: 1271
119.1
126.9
141.0
143.0
151.0
182.9
207.9
222.8
224.8
248.8
262.8
304.8
328.7
344.7
368.6
386.8
410.7
412.6
450.7
468.6
492.4
516.5
100
90
80
70
60
50
40
30
20
10
100
150
200
250
300
350
400
450
500
m/z

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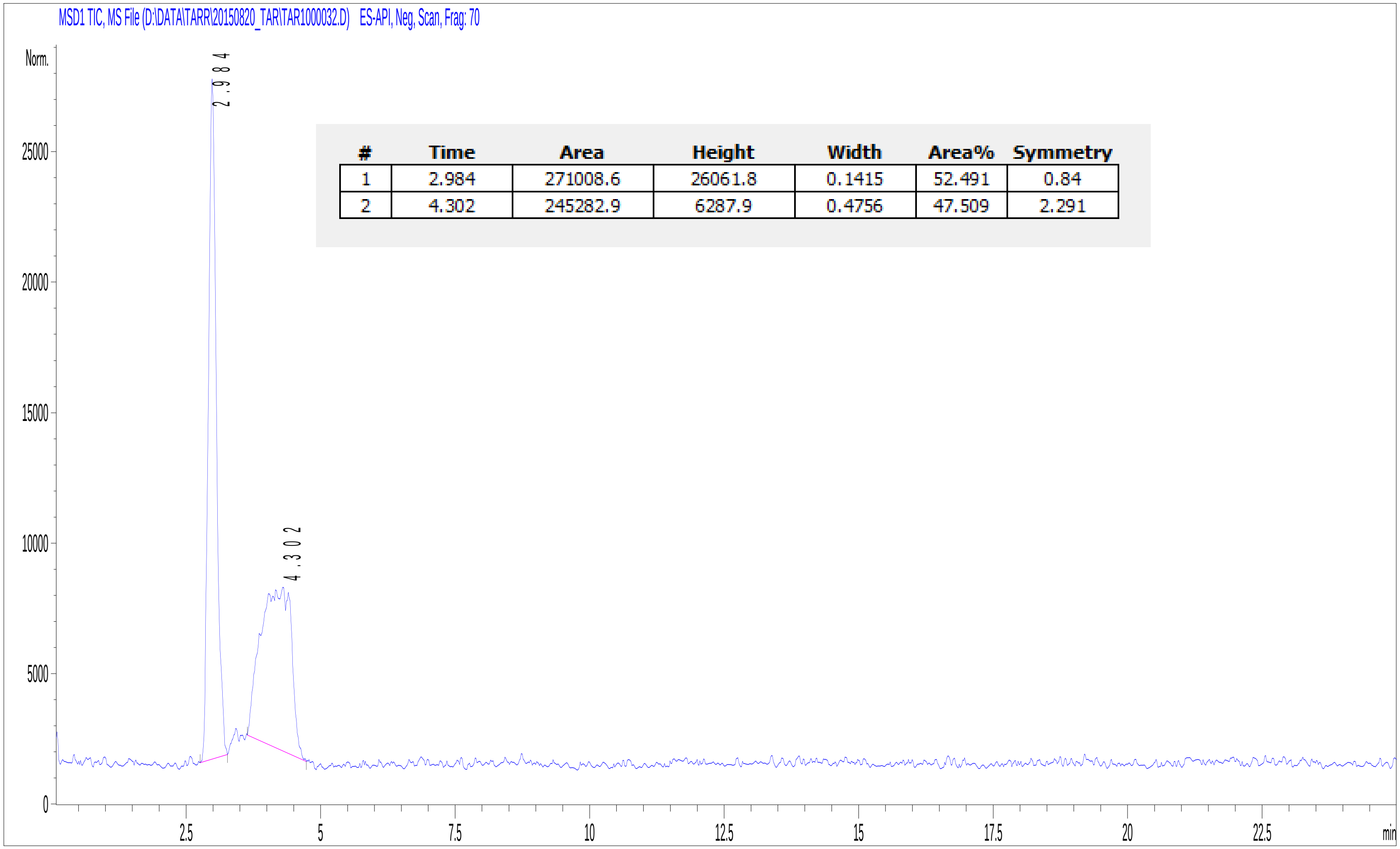
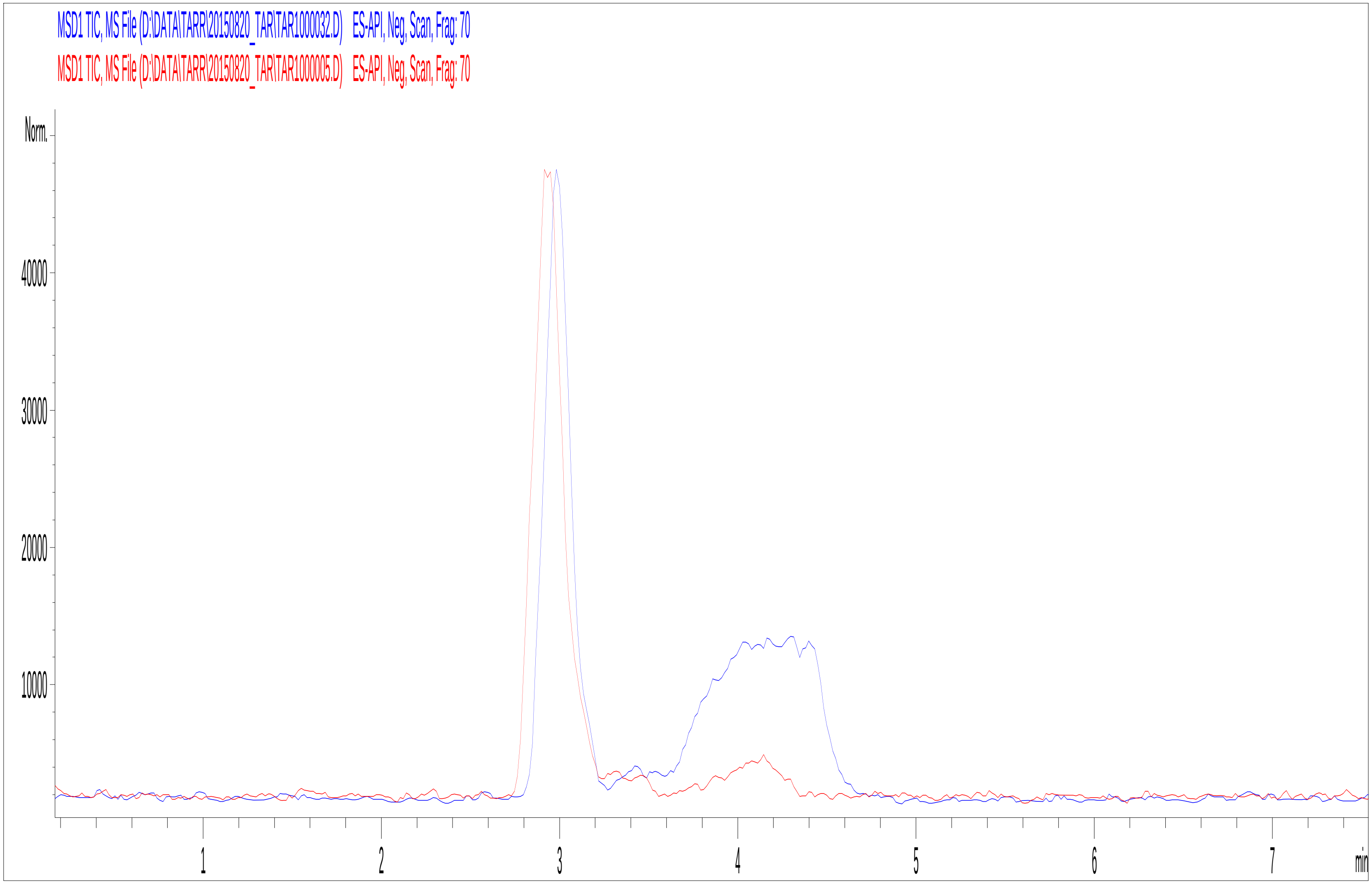
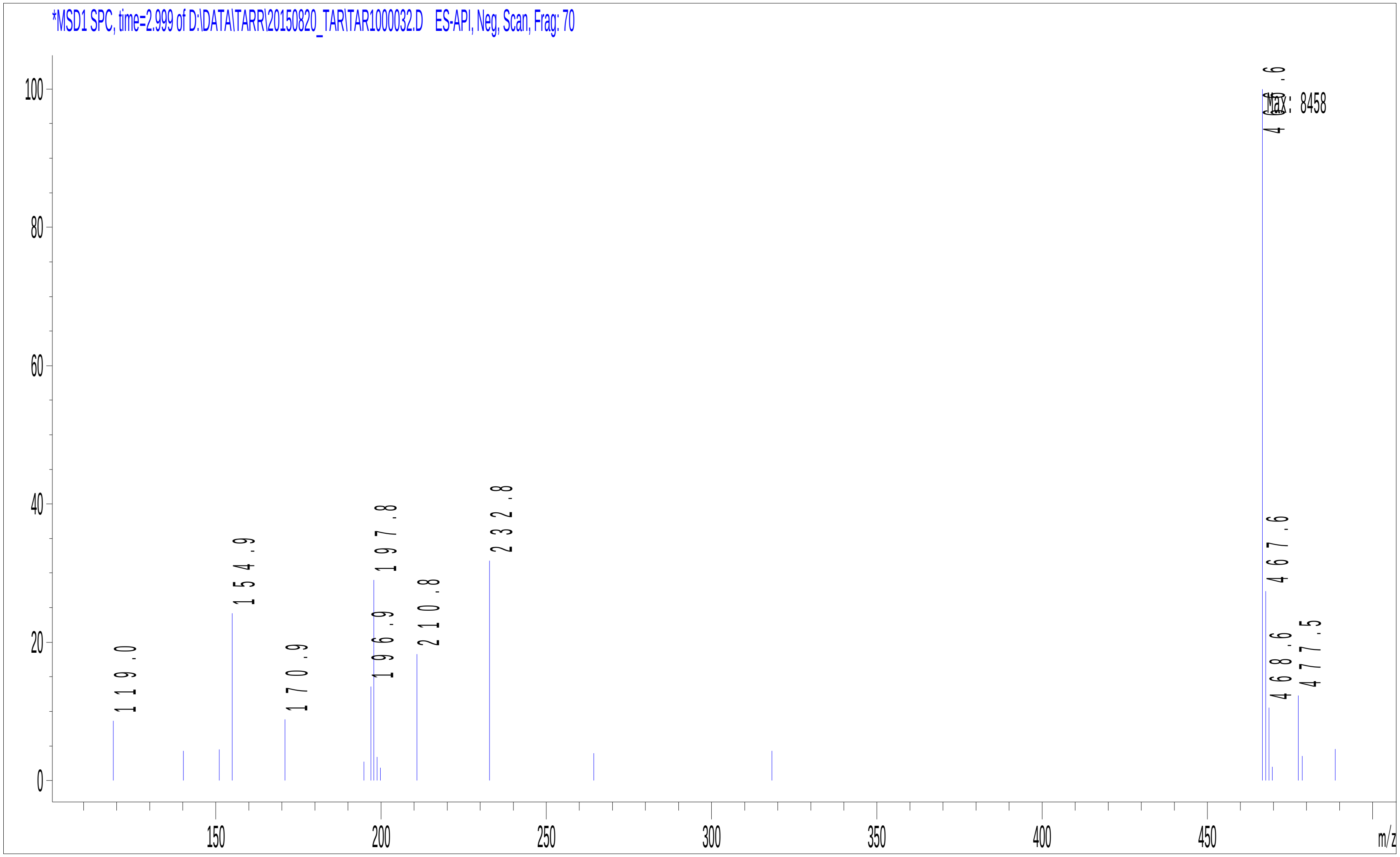
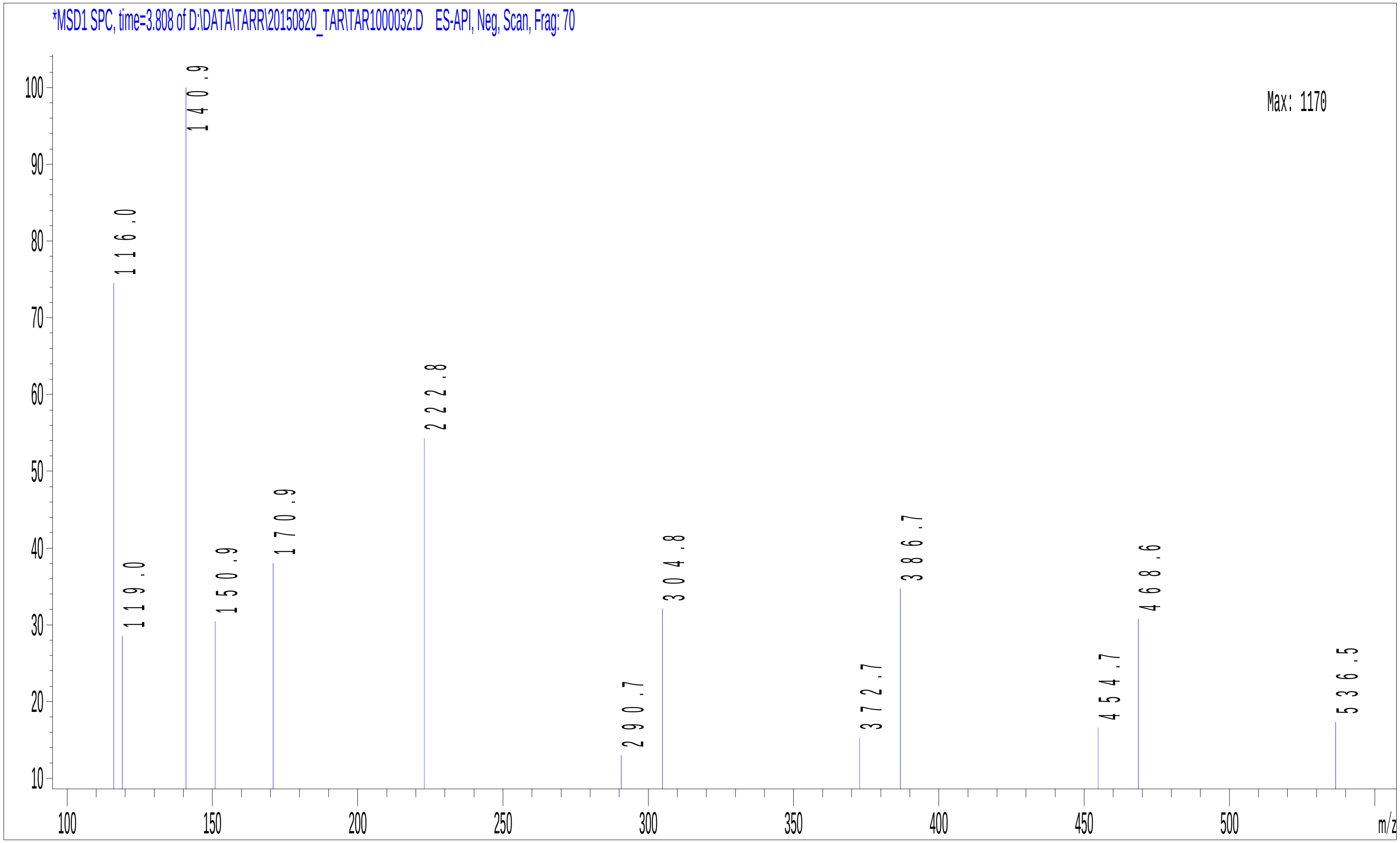
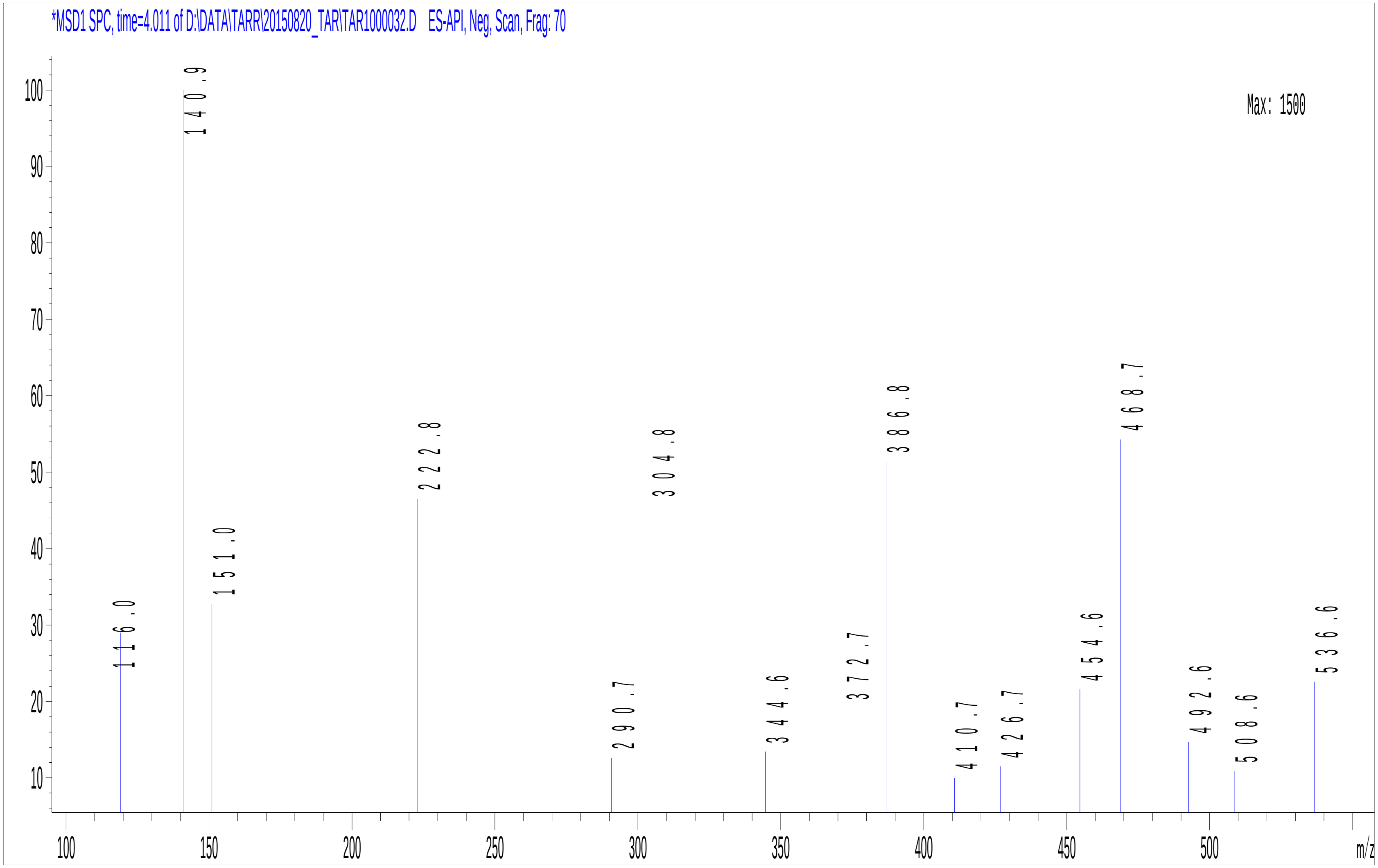


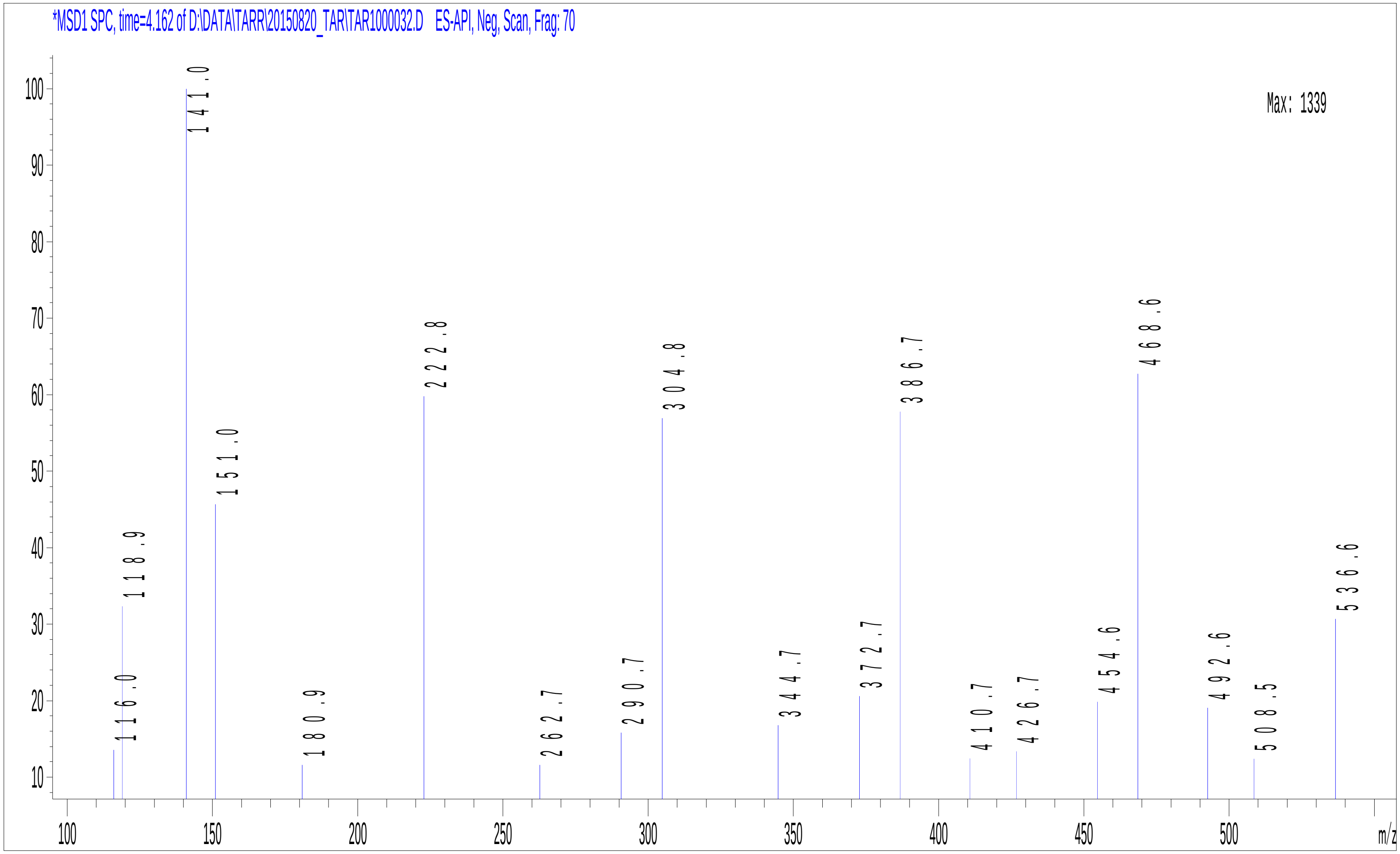
#	Time	Area	Height	Width	Area%	Symmetry
1	2.984	271008.6	26061.8	0.1415	52.491	0.84
2	4.302	245282.9	6287.9	0.4756	47.509	2.291

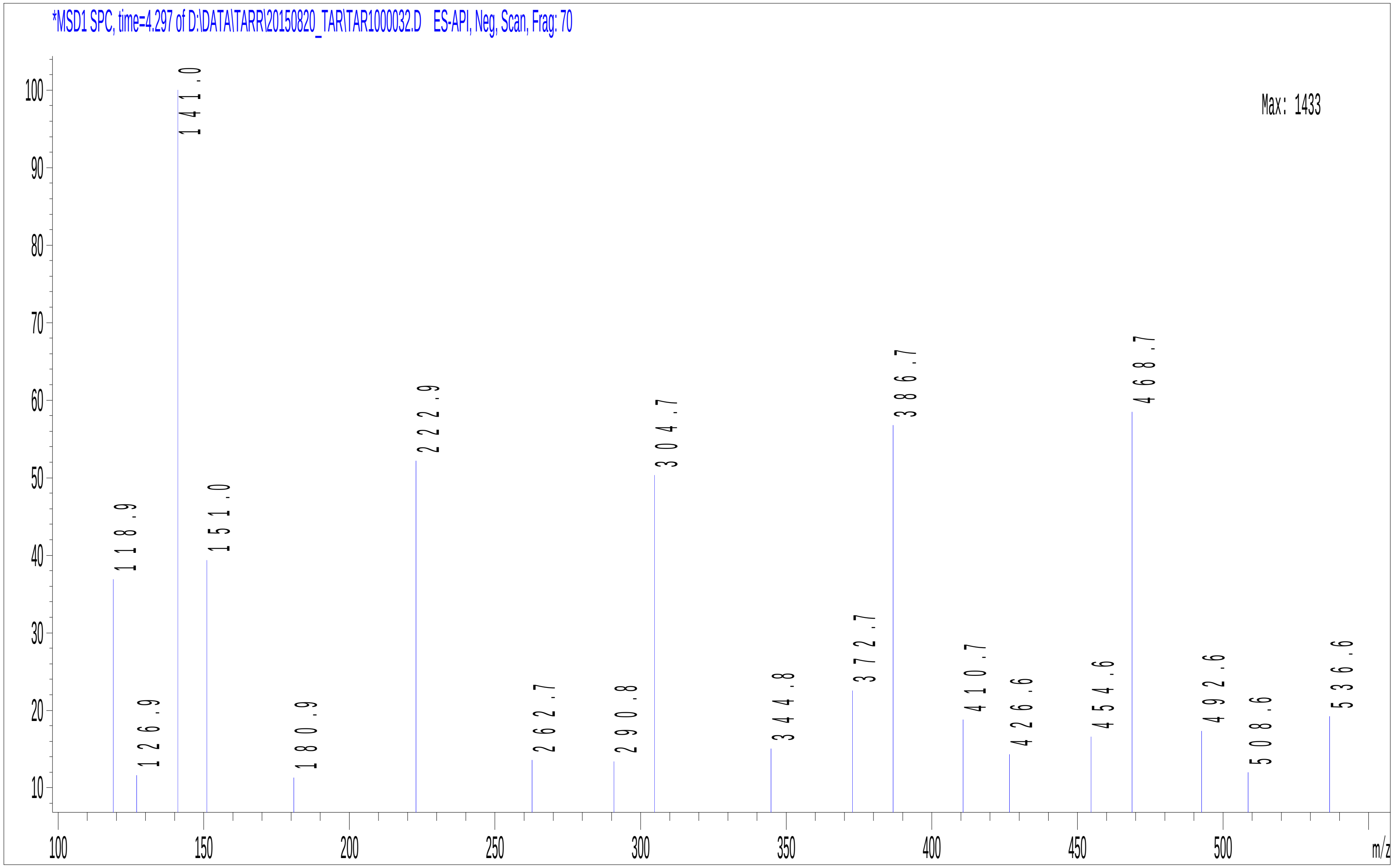

MSD1 TIC, MS File (D:\DATA\TARR\20150820_TAR\TAR1000032.D) ES-API, Neg, Scan, Frag: 70
MSD1 TIC, MS File (D:\DATA\TARR\20150820_TAR\TAR1000005.D) ES-API, Neg, Scan, Frag: 70
Norm.
40000
30000
20000
10000
1
2
3
4
5
6
7
min

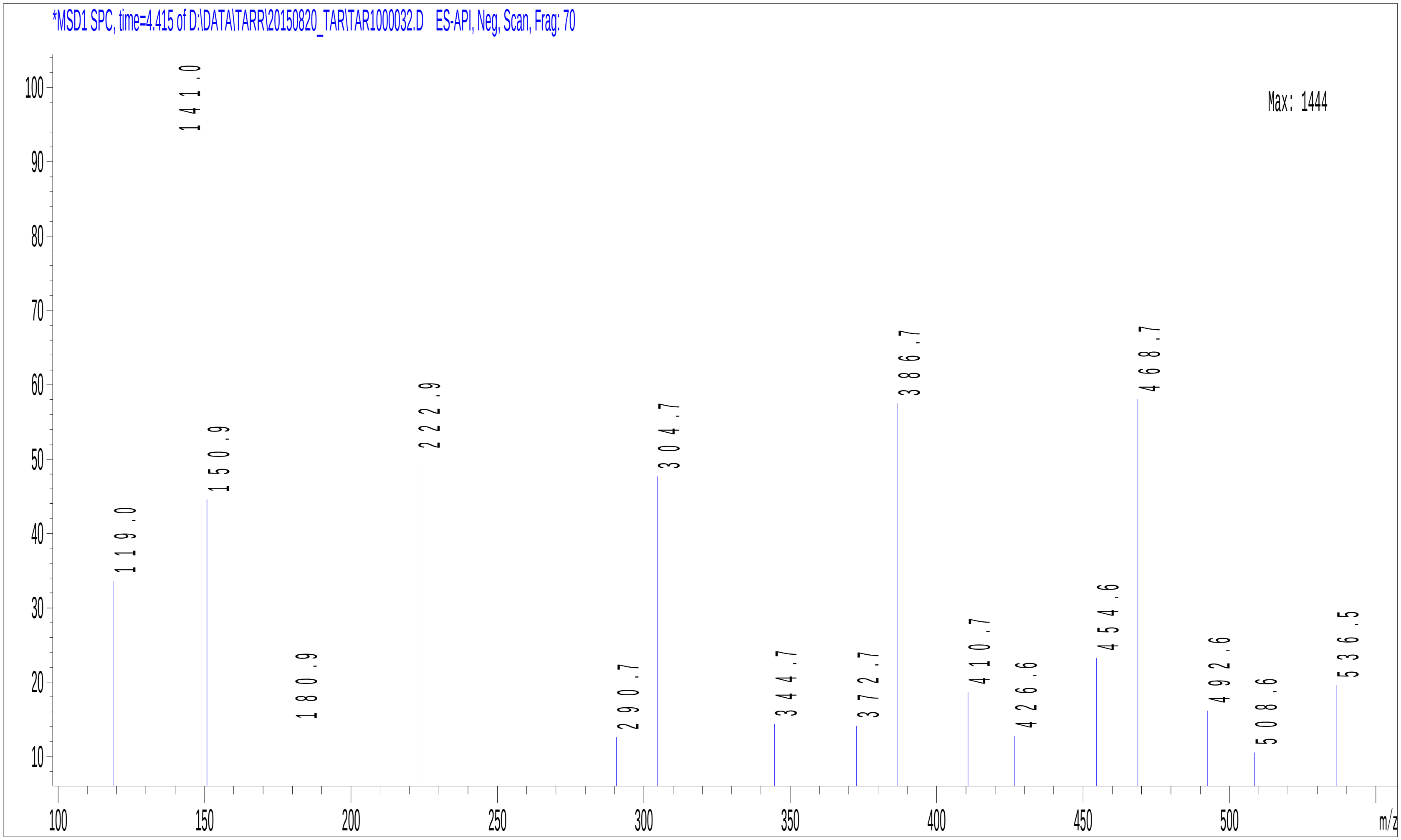
*MSD1 SPC, time=2.999 of D:\DATA\TARR\20150820_TAR\TAR1000032.D   ES-API, Neg, Scan, Frag: 70
Max: 8458
466.6
467.6
468.6
477.5
232.8
197.8
196.9
210.8
154.9
170.9
119.0
100
80
60
40
20
0
150
200
250
300
350
400
450
m/z


*MSD1 SPC, time=3.808 of D:\DATA\TARR\20150820_TAR\TAR1000032.D ES-API, Neg, Scan, Frag: 70
Max: 1170
116.0
119.0
140.9
150.9
170.9
222.8
290.7
304.8
372.7
386.7
454.7
468.6
536.5
100
90
80
70
60
50
40
30
20
10
100
150
200
250
300
350
400
450
500
m/z


*MSD1 SPC, time=4.011 of D:\DATA\TARR\20150820_TAR\TAR1000032.D ES-API, Neg, Scan, Frag: 70
Max: 1500
100
90
80
70
60
50
40
30
20
10
116.0
140.9
151.0
222.8
290.7
304.8
344.6
372.7
386.8
410.7
426.7
454.6
468.7
492.6
508.6
536.6
100
150
200
250
300
350
400
450
500
m/z


*MSD1 SPC, time=4.162 of D:\DATA\TARR\20150820_TAR\TAR1000032.D ES-API, Neg, Scan, Frag: 70
Max: 1339
100
90
80
70
60
50
40
30
20
10
116.0
118.9
141.0
151.0
180.9
222.8
262.7
290.7
304.8
344.7
372.7
386.7
410.7
426.7
454.6
468.6
492.6
508.5
536.6
100
150
200
250
300
350
400
450
500
m/z


*MSD1 SPC, time=4.297 of D:\DATA\TARR\20150820_TAR\TAR1000032.D ES-API, Neg, Scan, Frag: 70
Max: 1433
100
90
80
70
60
50
40
30
20
10
118.9
126.9
141.0
151.0
180.9
222.9
262.7
290.8
304.7
344.8
372.7
386.7
410.7
426.6
454.6
468.7
492.6
508.6
536.6
100
150
200
250
300
350
400
450
500
m/z


*MSD1 SPC, time=4.415 of D:\DATA\TARR\20150820_TAR\TAR1000032.D ES-API, Neg, Scan, Frag: 70
Max: 1444
100
90
80
70
60
50
40
30
20
10
119.0
141.0
150.9
180.9
222.9
290.7
304.7
344.7
372.7
386.7
410.7
426.6
454.6
468.7
492.6
508.6
536.5
100
150
200
250
300
350
400
450
500
m/z

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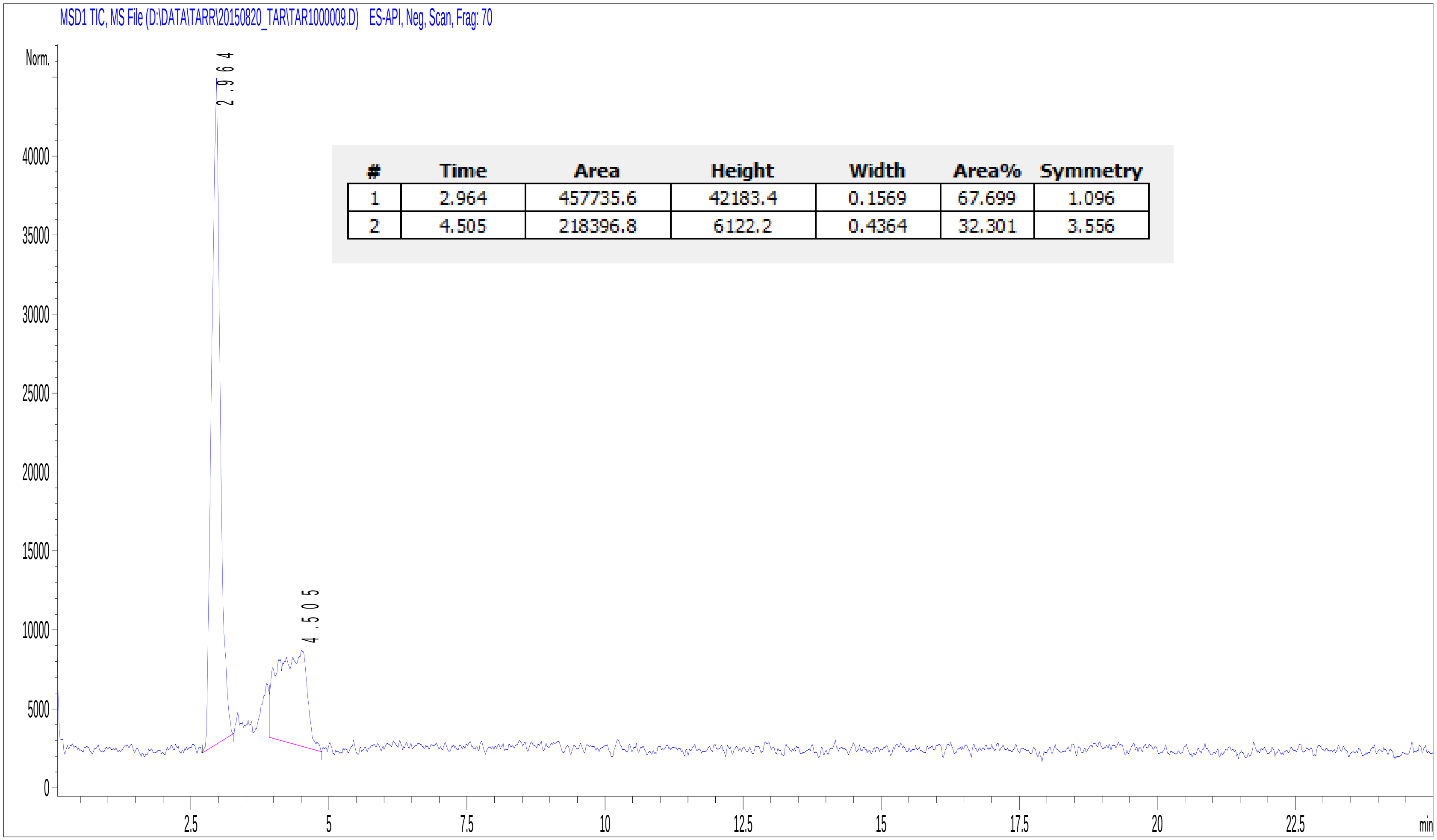
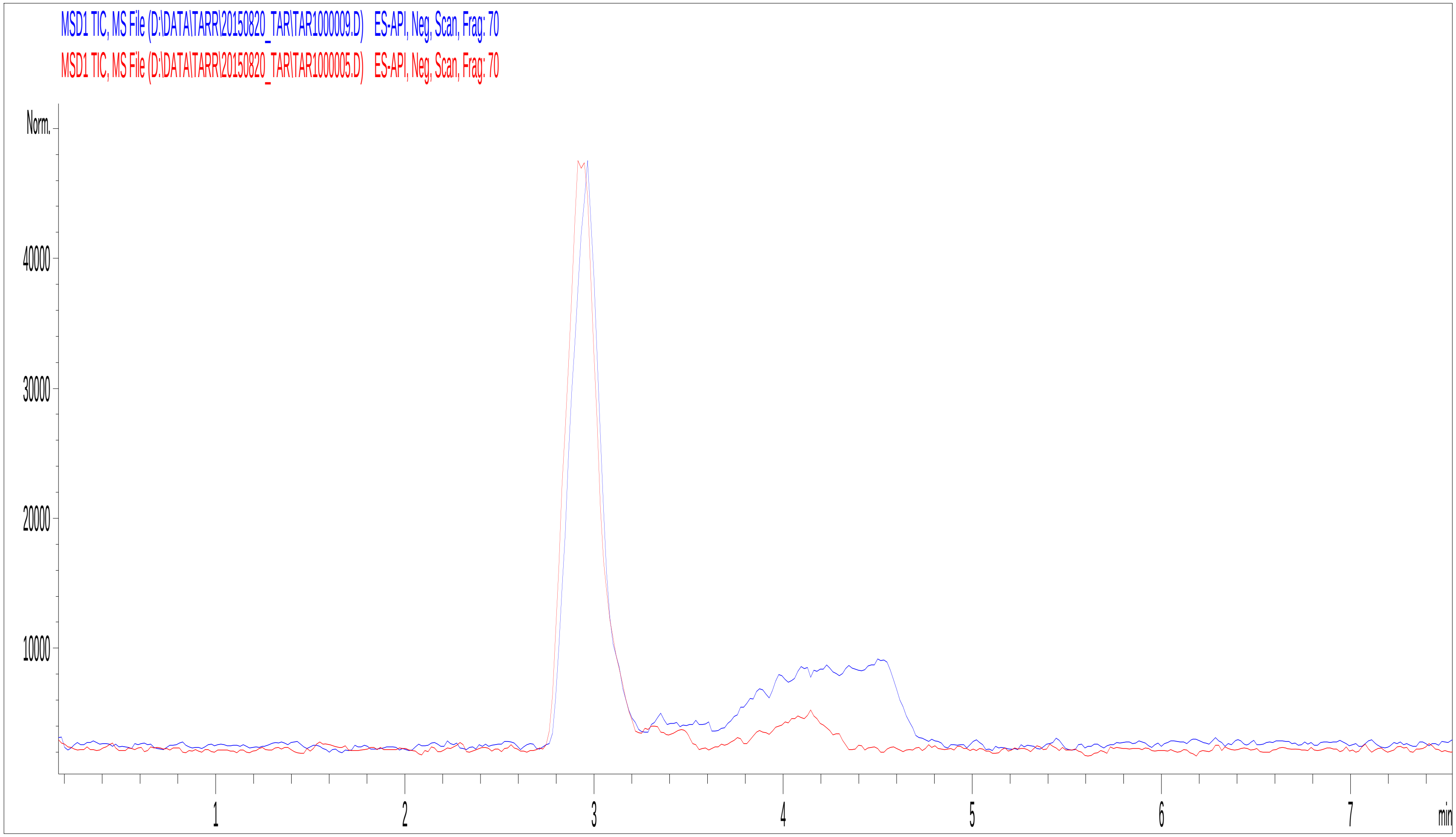
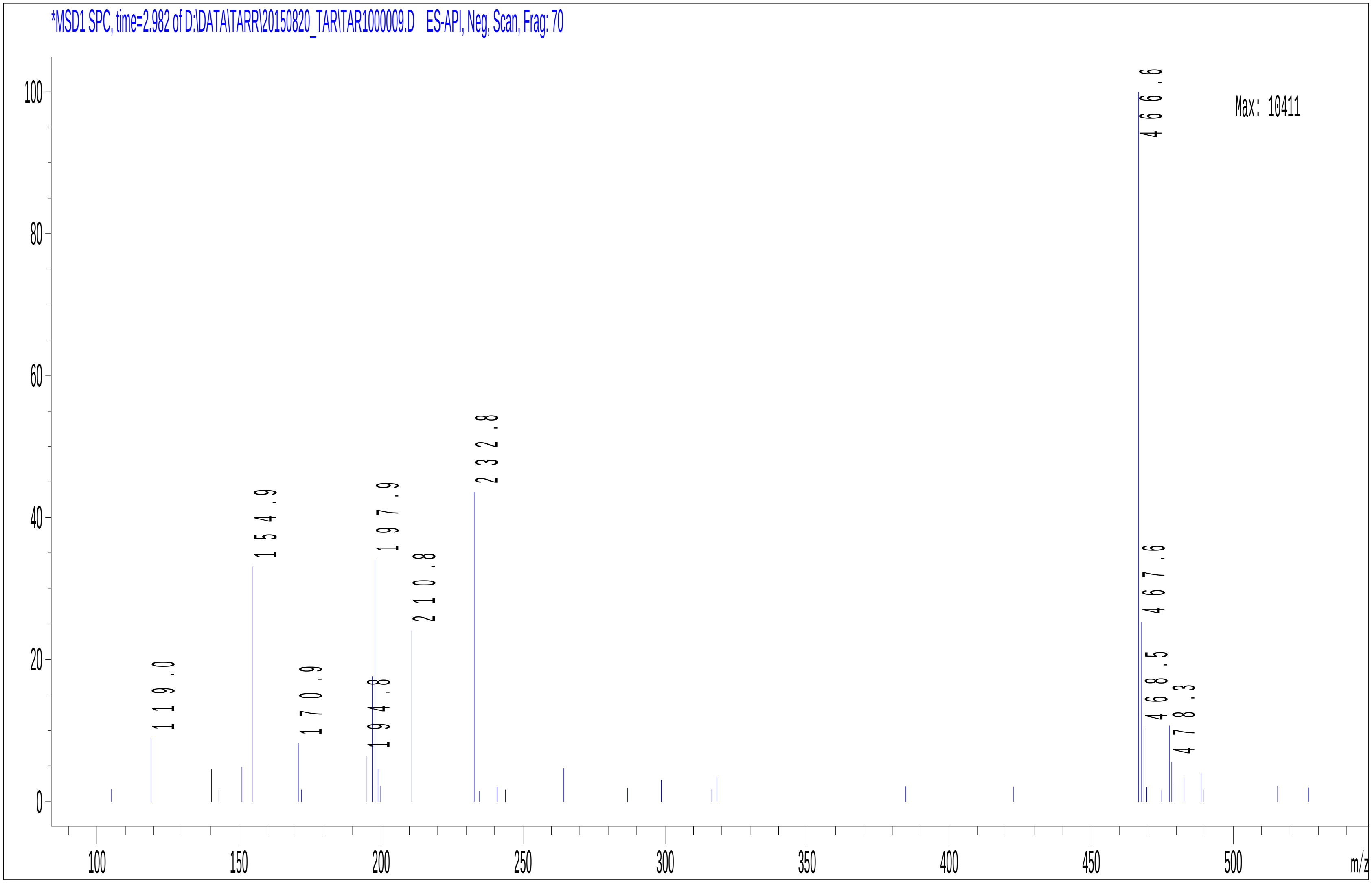
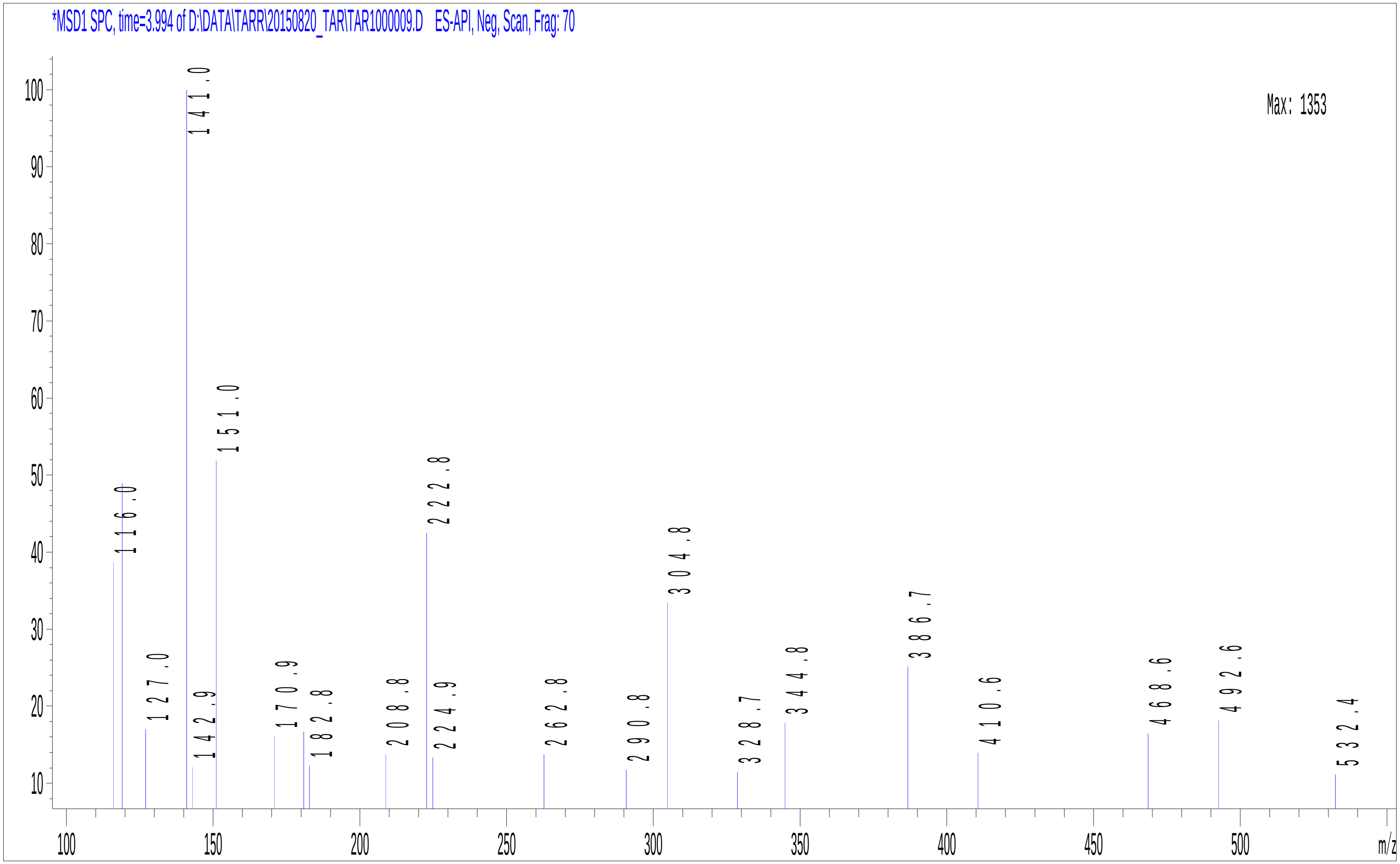


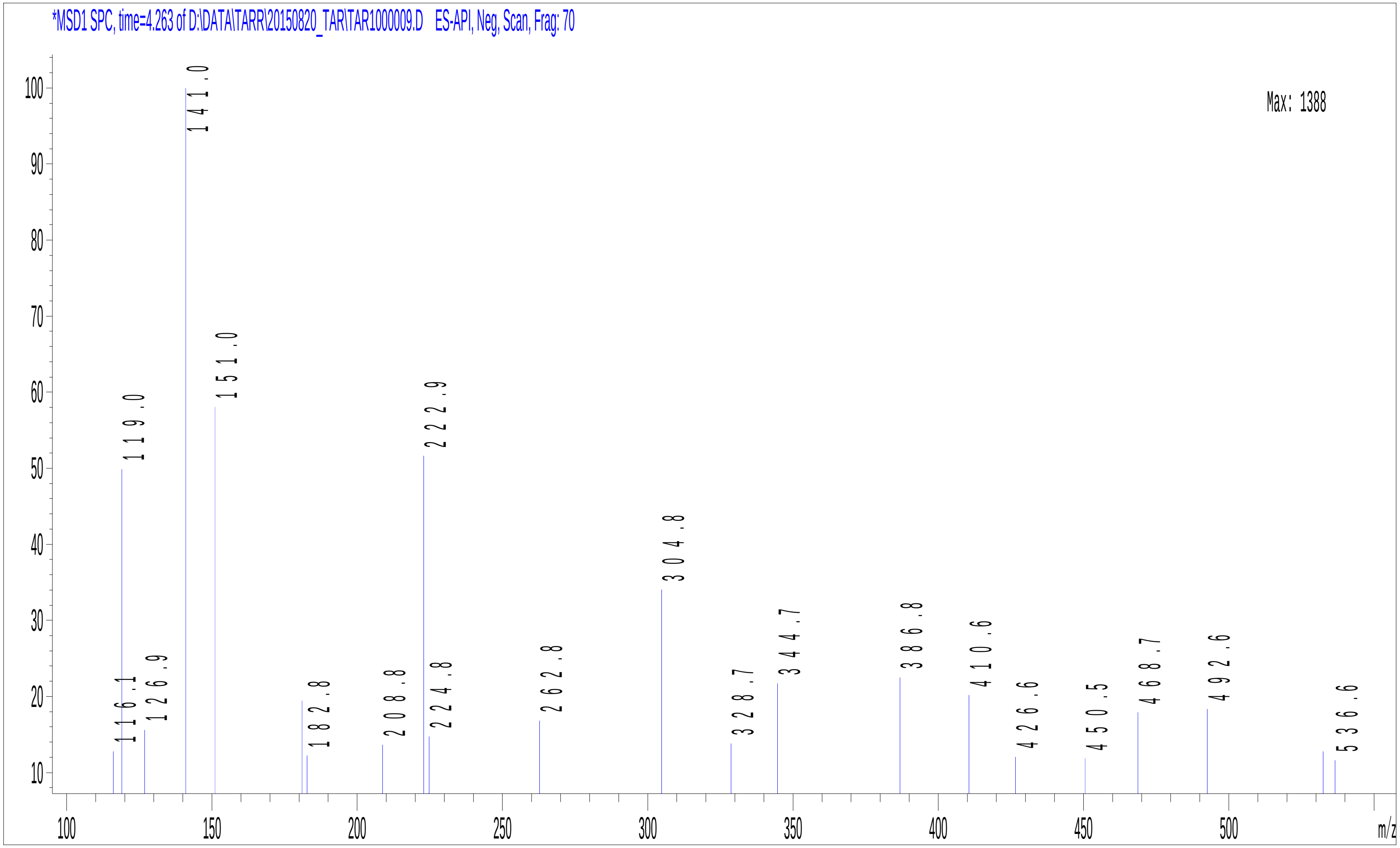
#	Time	Area	Height	Width	Area%	Symmetry
1	2.964	457735.6	42183.4	0.1569	67.699	1.096
2	4.505	218396.8	6122.2	0.4364	32.301	3.556

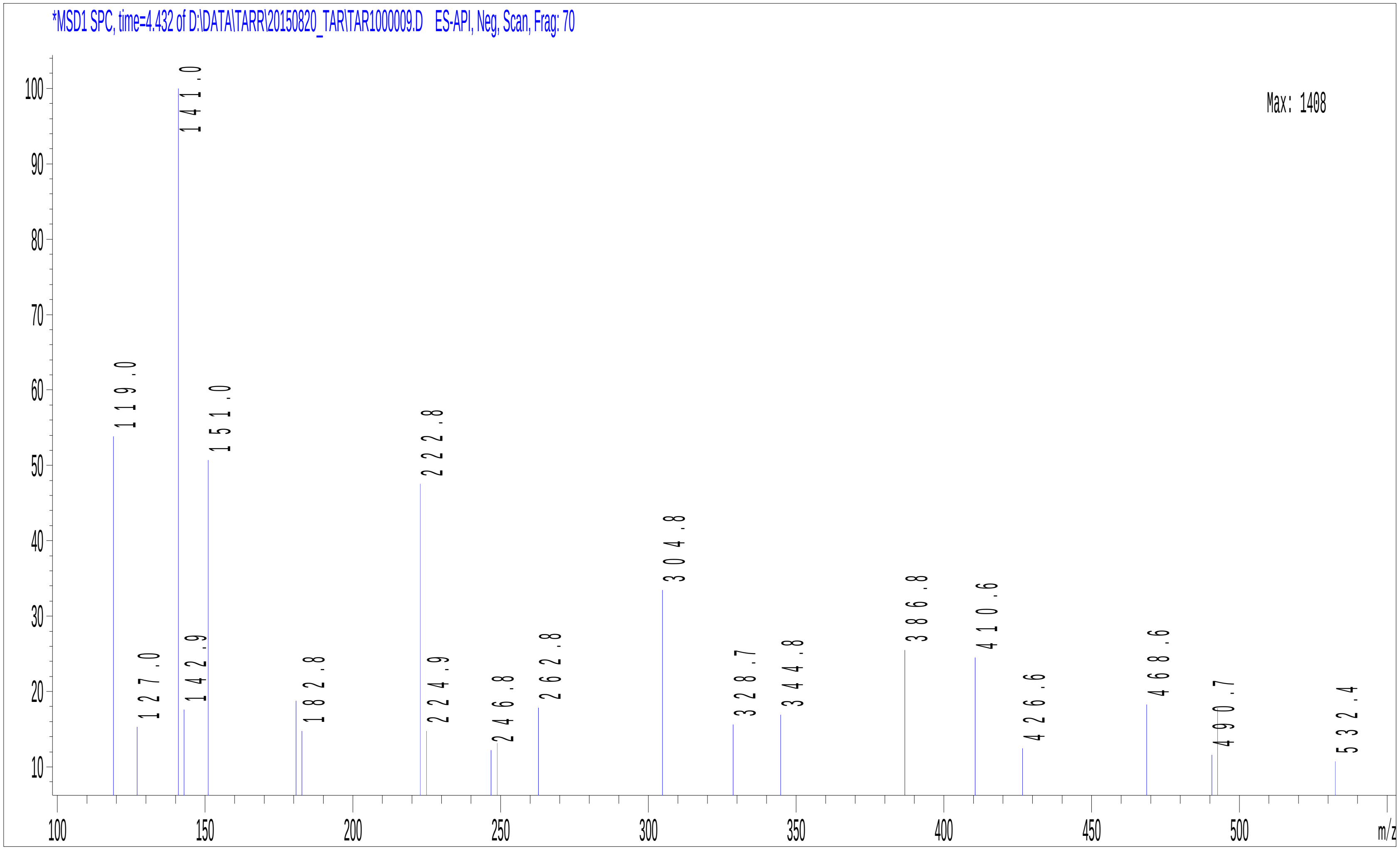

MSD1 TIC, MS File (D:\DATA\TARR\20150820_TAR\TAR1000009.D) ES-API, Neg, Scan, Frag: 70
MSD1 TIC, MS File (D:\DATA\TARR\20150820_TAR\TAR1000005.D) ES-API, Neg, Scan, Frag: 70
Norm.
40000
30000
20000
10000
1
2
3
4
5
6
7
min

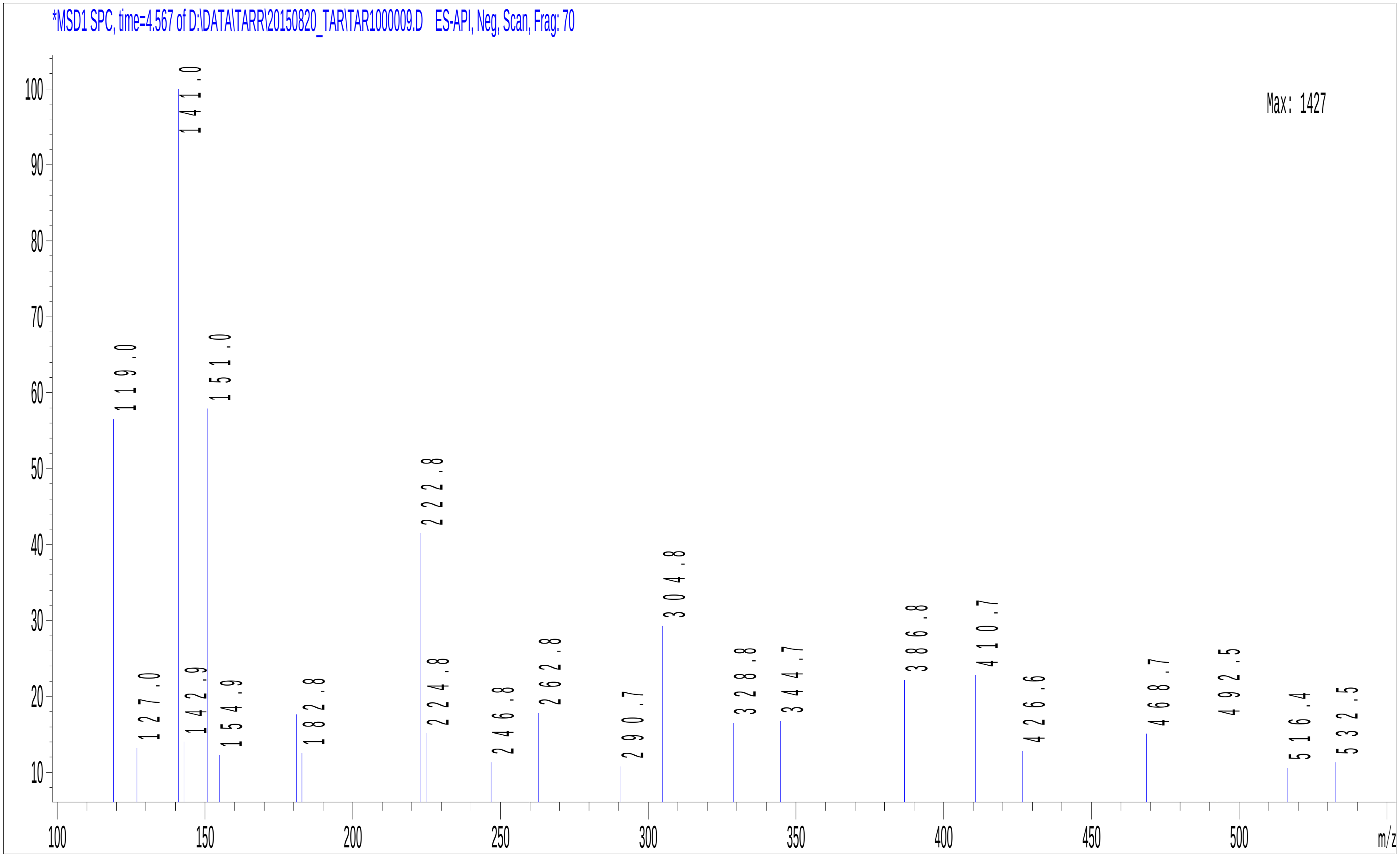


*MSD1 SPC, time=2.982 of D:\DATA\TARR\20150820_TAR\TAR1000009.D ES-API, Neg, Scan, Frag: 70
Max: 10411
466.6
232.8
154.9
197.9
210.8
467.6
119.0
170.9
194.8
468.5
478.3
0
20
40
60
80
100
100
150
200
250
300
350
400
450
500
m/z


*MSD1 SPC, time=3.994 of D:\DATA\TARR\20150820_TAR\TAR1000009.D ES-API, Neg, Scan, Frag: 70
Max: 1353
100
90
80
70
60
50
40
30
20
10
116.0
127.0
141.0
142.9
151.0
170.9
182.8
208.8
222.8
224.9
262.8
290.8
304.8
328.7
344.8
386.7
410.6
468.6
492.6
532.4
100
150
200
250
300
350
400
450
500
m/z


*MSD1 SPC, time=4.263 of D:\DATA\TARR\20150820_TAR\TAR1000009.D ES-API, Neg, Scan, Frag: 70
Max: 1388
100
90
80
70
60
50
40
30
20
10
141.0
151.0
119.0
222.9
304.8
344.7
386.8
410.6
492.6
468.7
262.8
224.8
116.1
126.9
182.8
208.8
328.7
426.6
450.5
536.6
100
150
200
250
300
350
400
450
500
m/z


*MSD1 SPC, time=4.432 of D:\DATA\TARR\20150820_TAR\TAR1000009.D ES-API, Neg, Scan, Frag: 70
Max: 1408
100
90
80
70
60
50
40
30
20
10
119.0
127.0
141.0
142.9
151.0
182.8
222.8
224.9
246.8
262.8
304.8
328.7
344.8
386.8
410.6
426.6
468.6
490.7
532.4
100
150
200
250
300
350
400
450
500
m/z


*MSD1 SPC, time=4.567 of D:\DATA\TARR\20150820_TAR\TAR1000009.D ES-API, Neg, Scan, Frag: 70
Max: 1427
119.0
127.0
141.0
142.9
151.0
154.9
182.8
222.8
224.8
246.8
262.8
290.7
304.8
328.8
344.7
386.8
410.7
426.6
468.7
492.5
516.4
532.5
100
90
80
70
60
50
40
30
20
10
100
150
200
250
300
350
400
450
500
m/z

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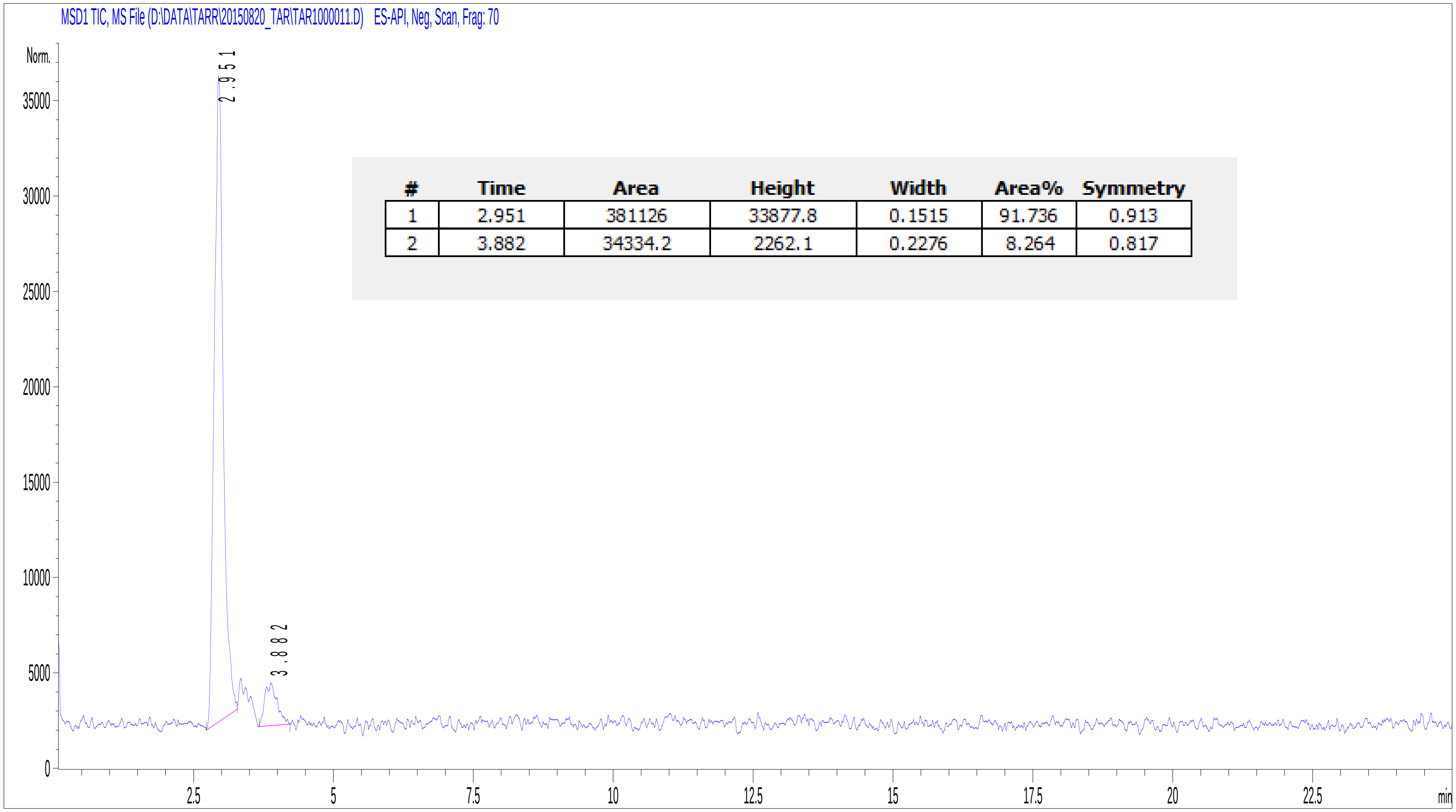
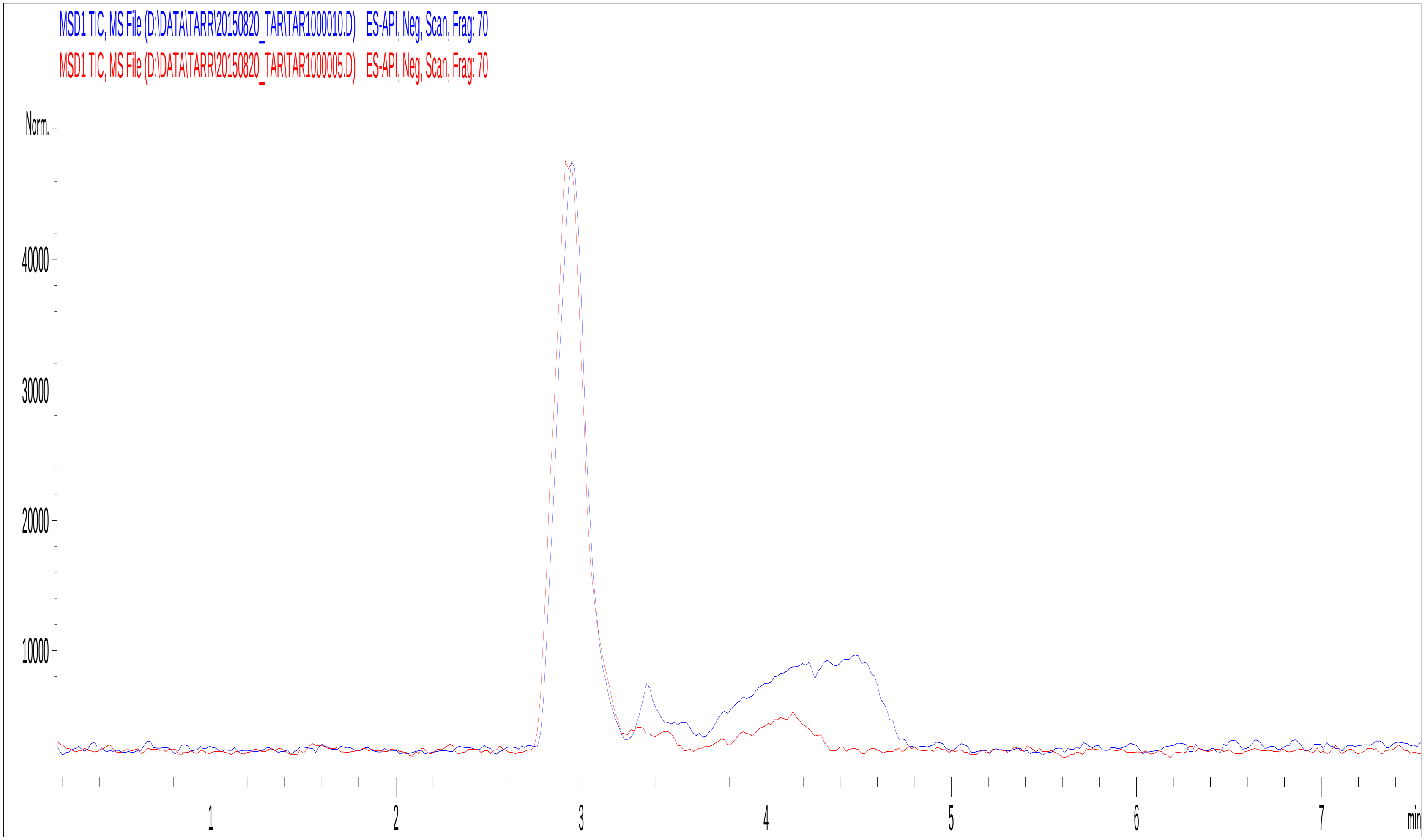
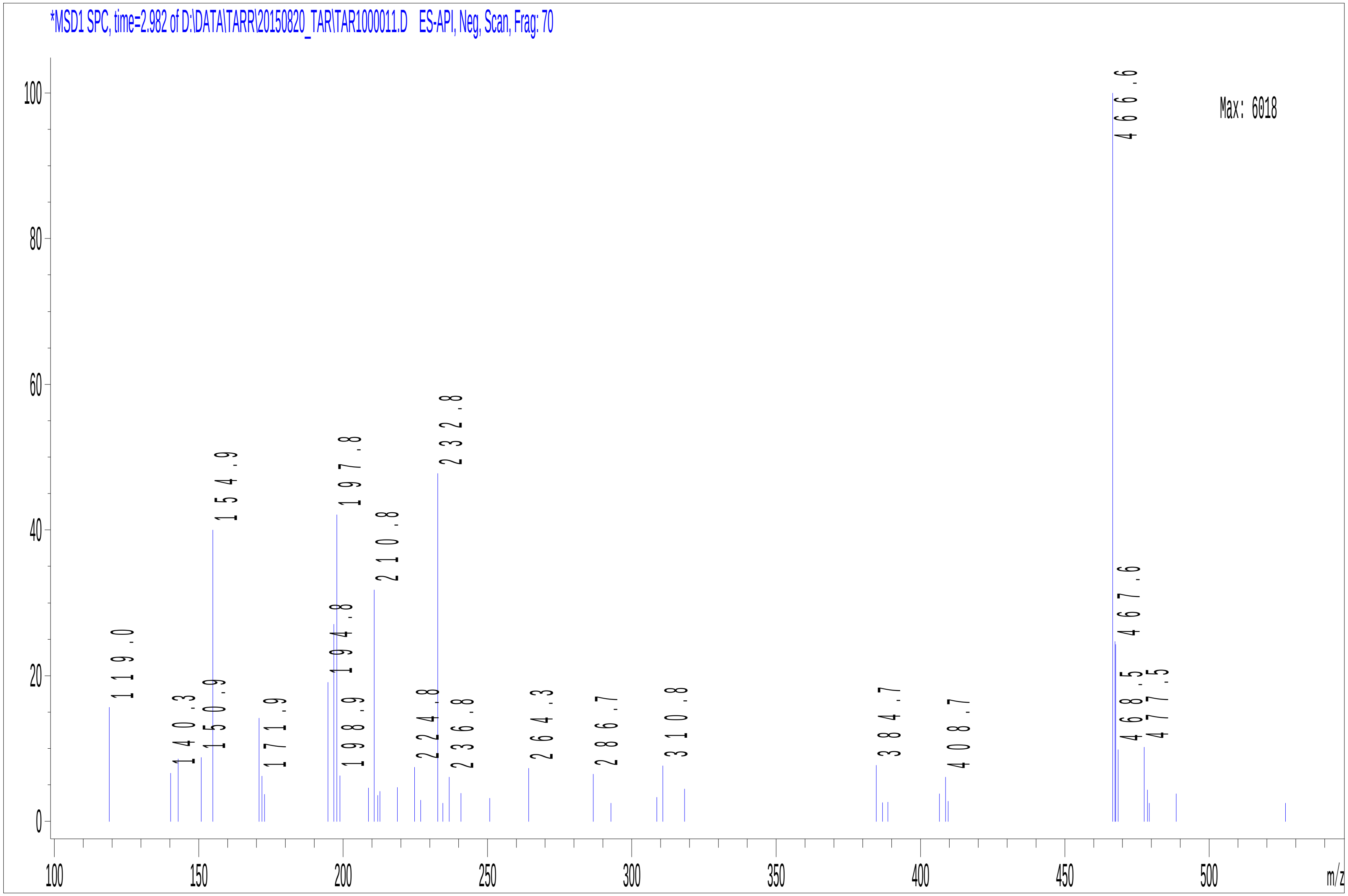
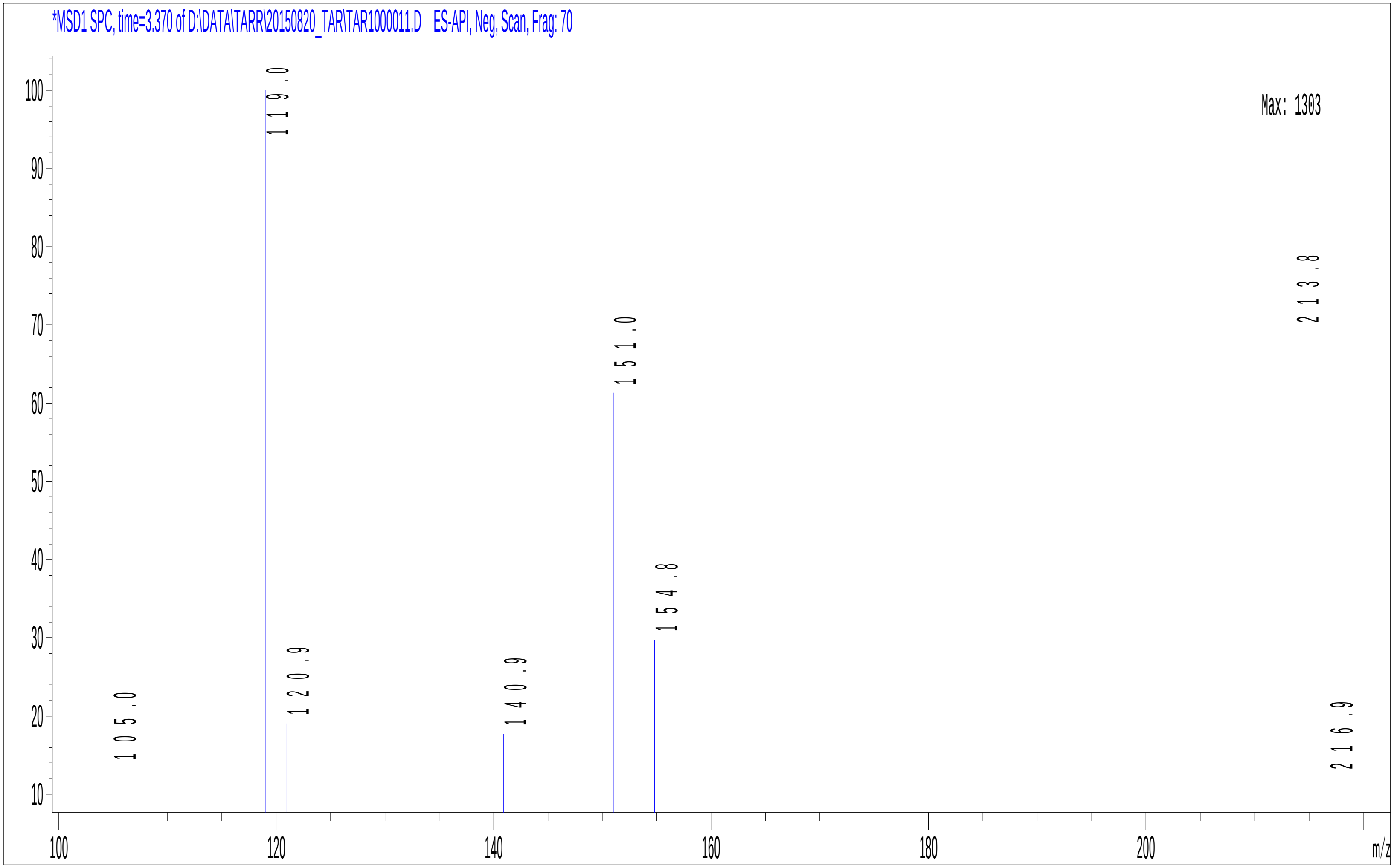
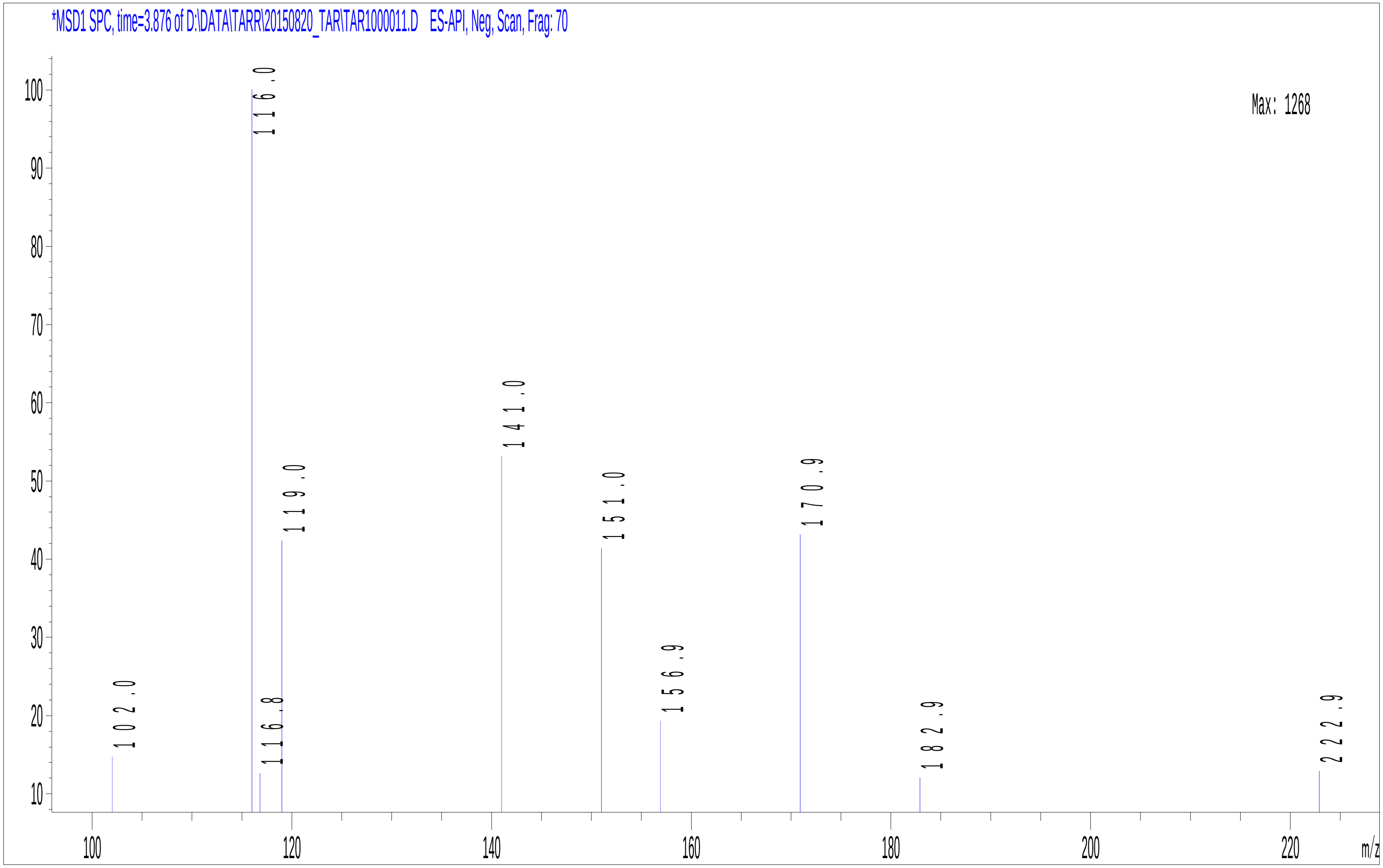


#	Time	Area	Height	Width	Area%	Symmetry
1	2.951	381126	33877.8	0.1515	91.736	0.913
2	3.882	34334.2	2262.1	0.2276	8.264	0.817


MSD1 TIC, MS File (D:\DATA\TARR\20150820_TAR\TAR1000010.D) ES-API, Neg, Scan, Frag: 70
MSD1 TIC, MS File (D:\DATA\TARR\20150820_TAR\TAR1000005.D) ES-API, Neg, Scan, Frag: 70
Norm.
40000
30000
20000
10000
1
2
3
4
5
6
7
min


*MSD1 SPC, time=2.982 of D:\DATA\TARR\20150820_TAR\TAR1000011.D ES-API, Neg, Scan, Frag: 70
Max: 6018
0
20
40
60
80
100
100
150
200
250
300
350
400
450
500
m/z
119.0
140.3
150.9
154.9
171.9
194.8
197.8
198.9
210.8
224.8
232.8
236.8
264.3
286.7
310.8
384.7
408.7
466.6
467.6
468.5
477.5


*MSD1 SPC, time=3.370 of D:\DATA\TARR\20150820_TAR\TAR1000011.D ES-API, Neg, Scan, Frag: 70
Max: 1303
119.0
213.8
151.0
154.8
120.9
140.9
105.0
216.9
100
90
80
70
60
50
40
30
20
10
100
120
140
160
180
200
m/z



*MSD1 SPC, time=3.876 of D:\DATA\TARR\20150820_TAR\TAR1000011.D ES-API, Neg, Scan, Frag: 70
Max: 1268
100
90
80
70
60
50
40
30
20
10
100
120
140
160
180
200
220
m/z
102.0
116.0
116.8
119.0
141.0
151.0
156.9
170.9
182.9
222.9

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30 DC

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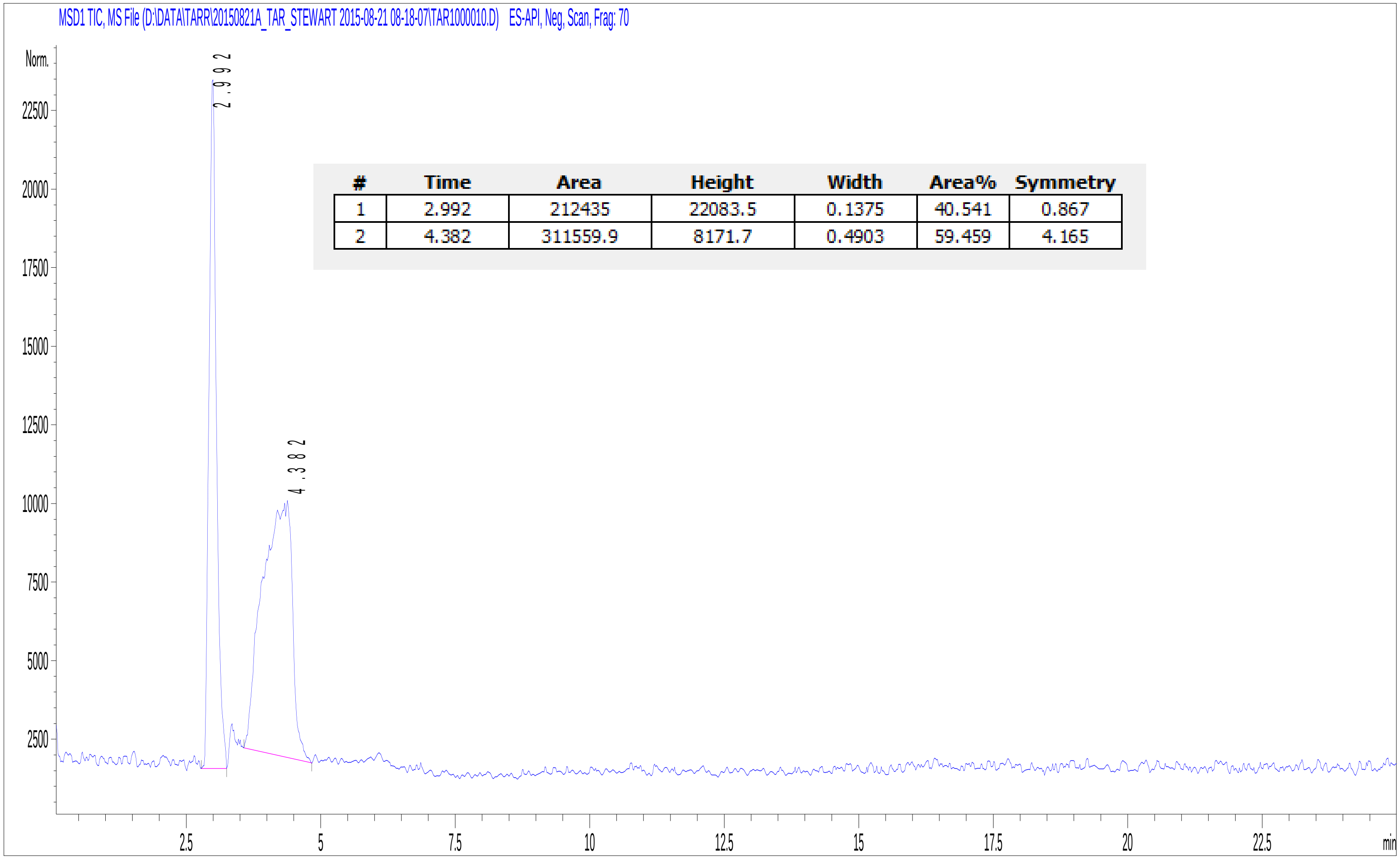
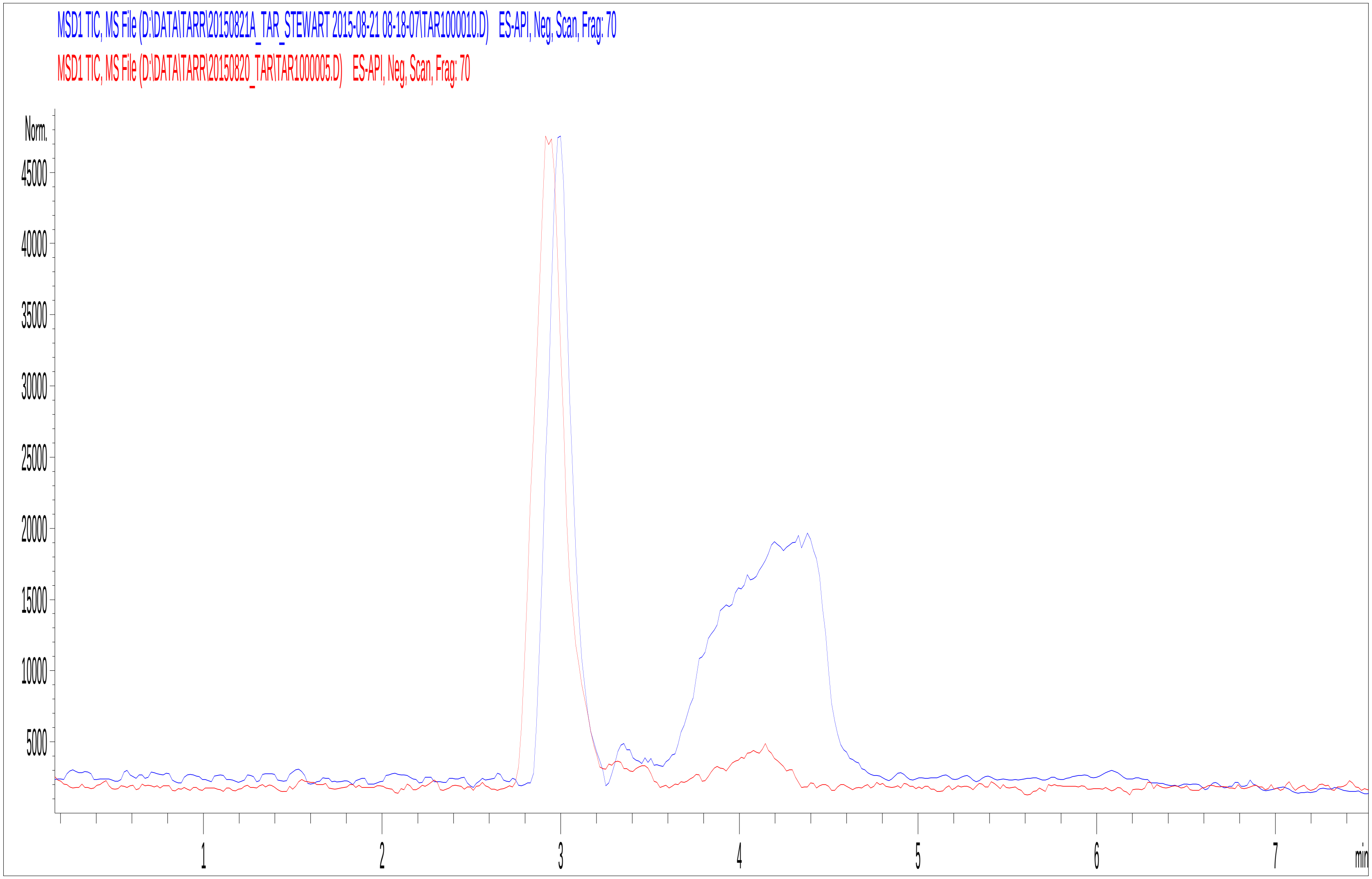
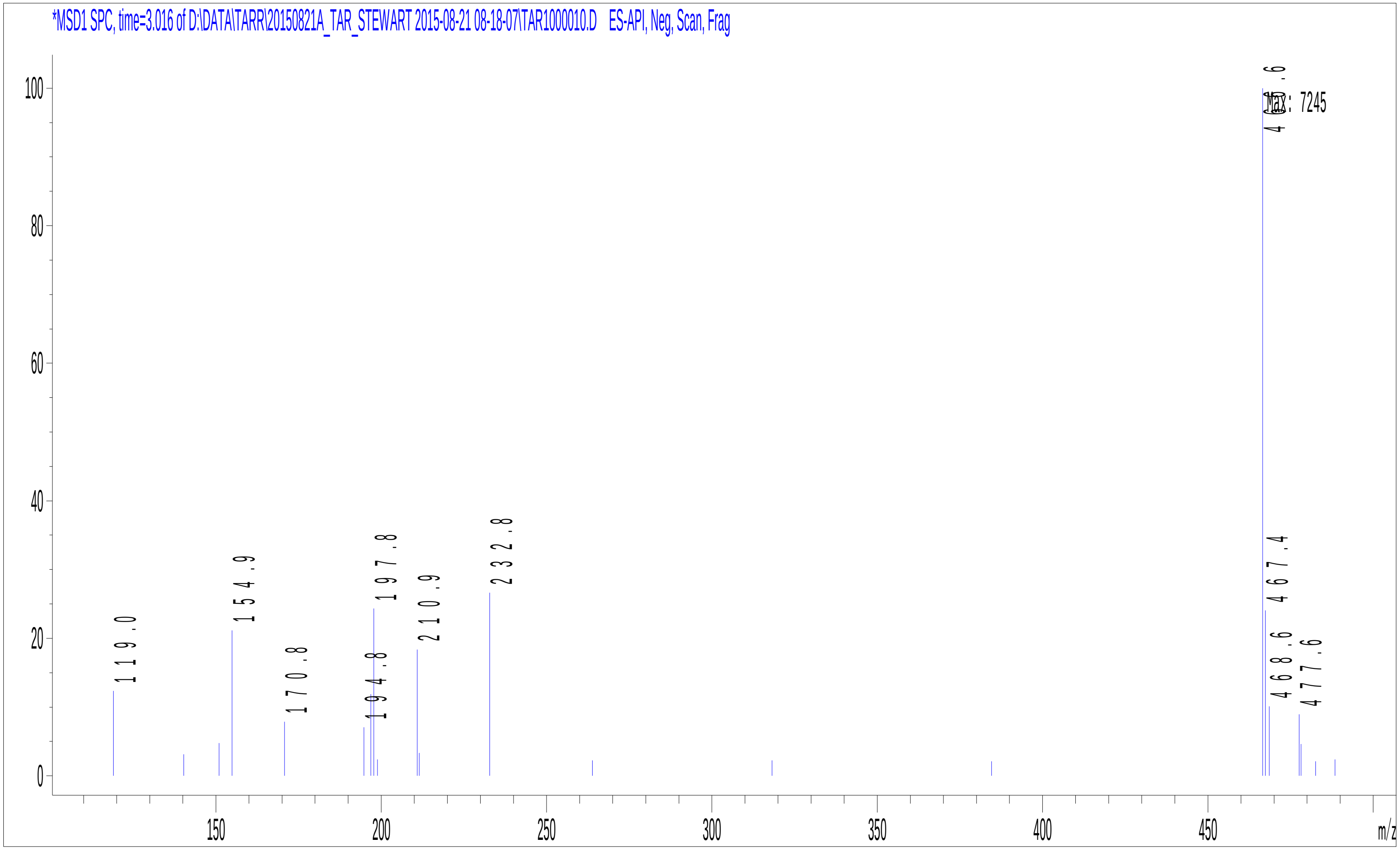
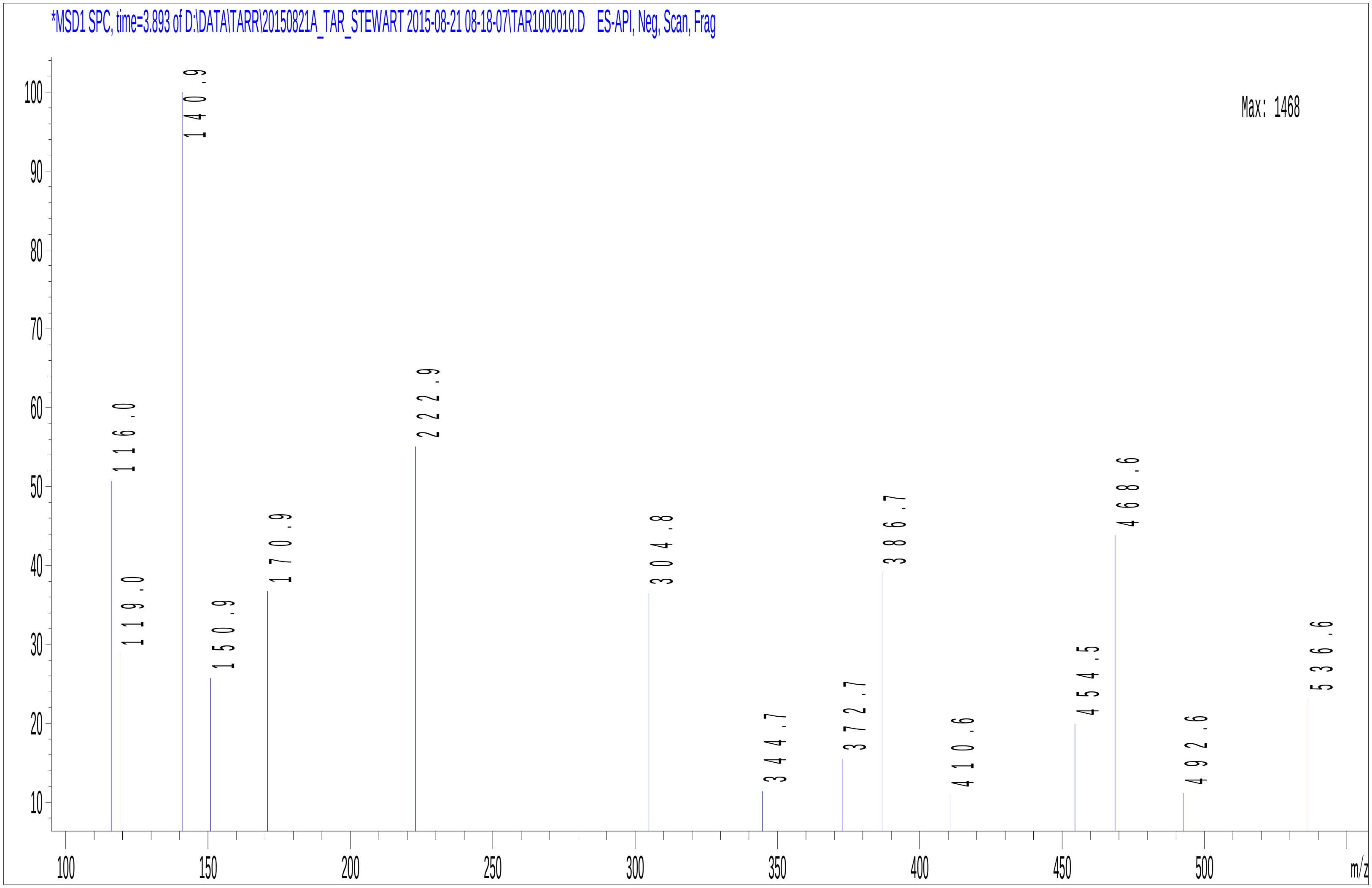


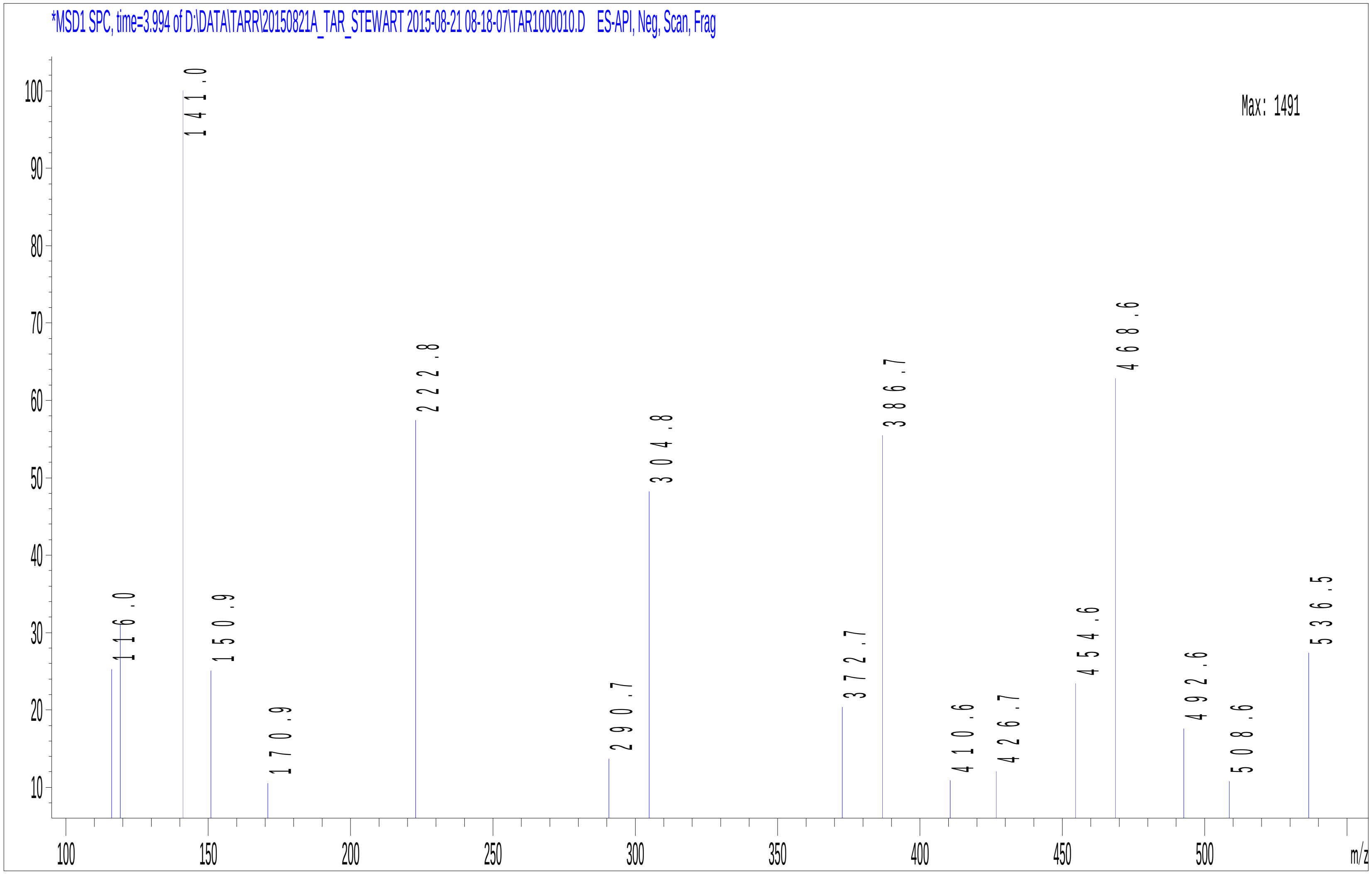
MSD1 TIC, MS File (D:\DATA\TARR\20150821A_TAR_STEWART 2015-08-21 08-18-07\TAR1000010.D) ES-API, Neg, Scan, Frag: 70

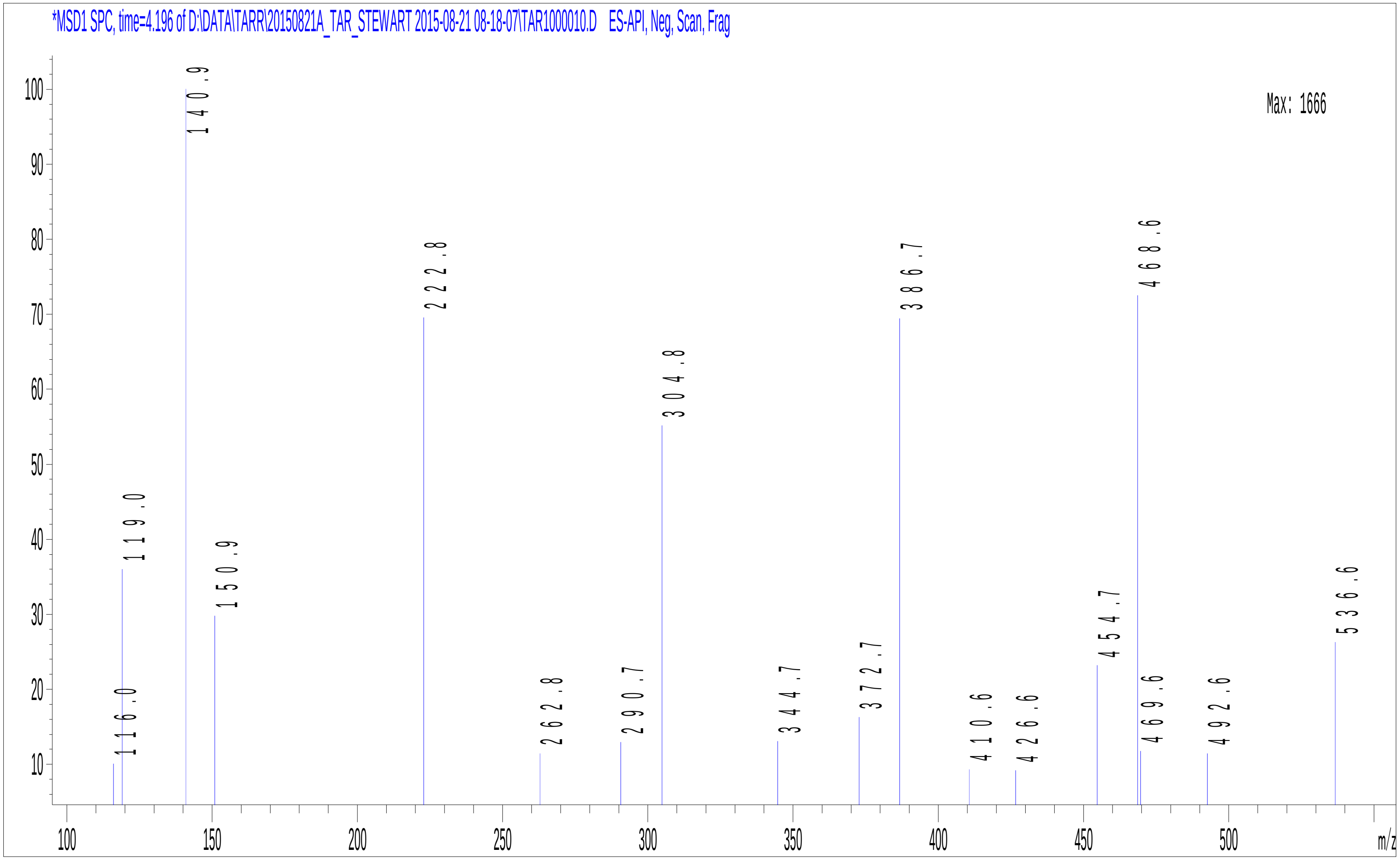
#	Time	Area	Height	Width	Area%	Symmetry
1	2.992	212435	22083.5	0.1375	40.541	0.867
2	4.382	311559.9	8171.7	0.4903	59.459	4.165

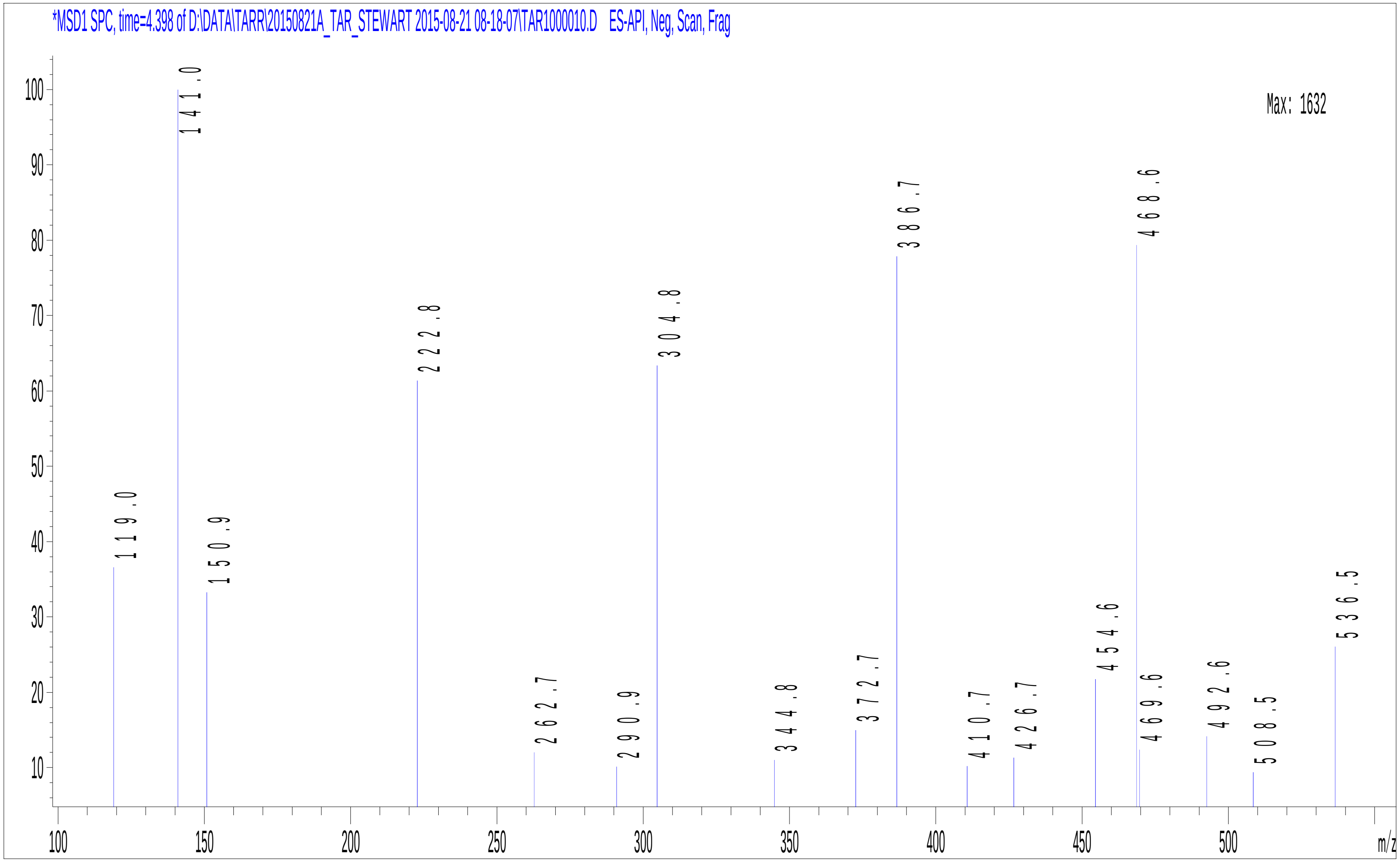

MSD1 TIC, MS File (D:\DATA\TARR\20150821A_TAR_STEWART 2015-08-21 08-18-07\TAR1000010.D)   ES-API, Neg, Scan, Frag: 70
MSD1 TIC, MS File (D:\DATA\TARR\20150820_TAR\TAR1000005.D)   ES-API, Neg, Scan, Frag: 70
Norm.
45000
40000
35000
30000
25000
20000
15000
10000
5000
1
2
3
4
5
6
7
min

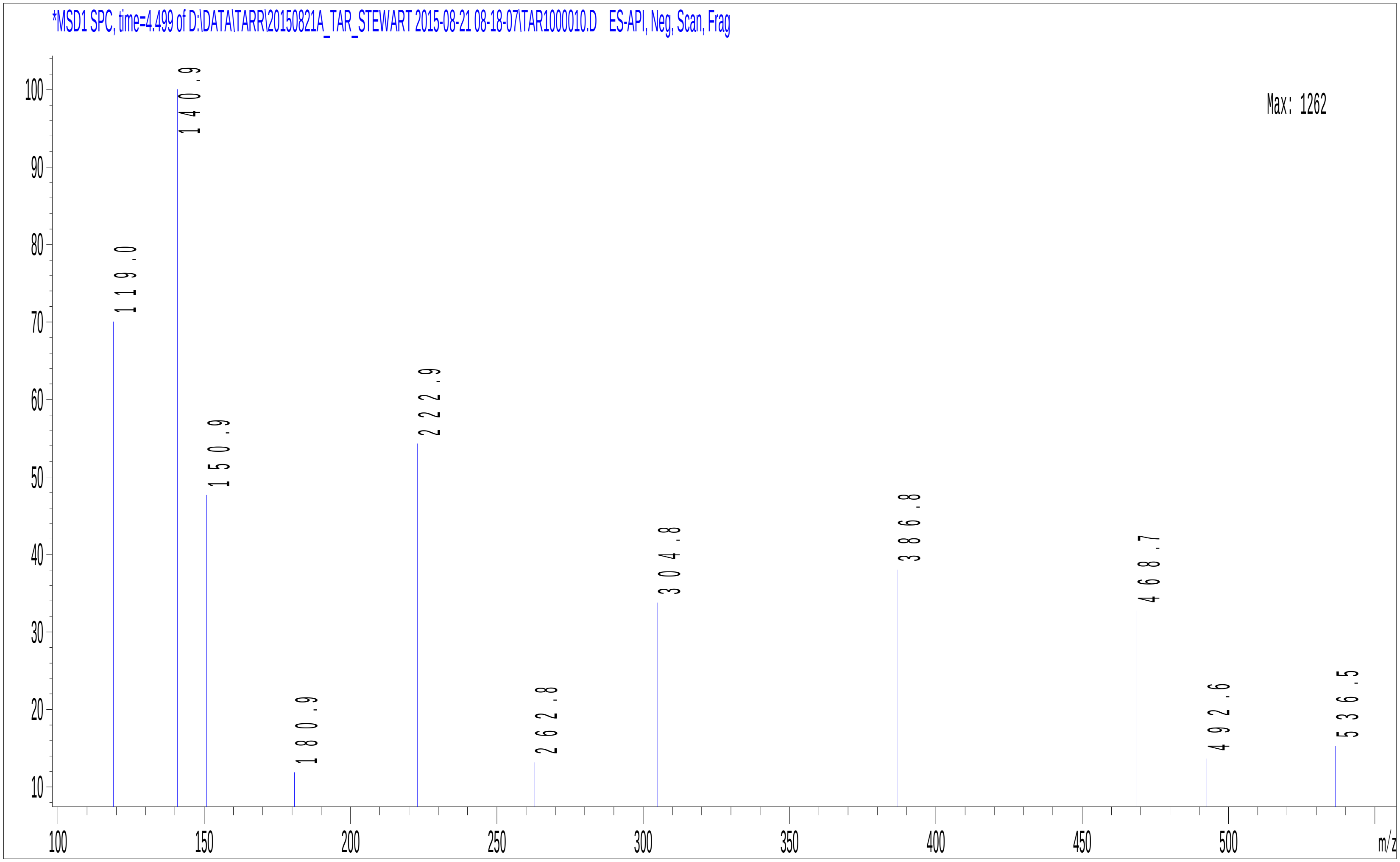

*MSD1 SPC, time=3.016 of D:\DATA\TARR\20150821A_TAR_STEWART 2015-08-21 08-18-07\TAR1000010.D   ES-API, Neg, Scan, Frag
Max: 7245
466.6
467.4
468.6
477.6
119.0
154.9
170.8
194.8
197.8
210.9
232.8
100
80
60
40
20
0
150
200
250
300
350
400
450
m/z


*MSD1 SPC, time=3.893 of D:\DATA\TARR\20150821A_TAR_STEWART 2015-08-21 08-18-07\TAR1000010.D ES-API, Neg, Scan, Frag
Max: 1468
116.0
119.0
140.9
150.9
170.9
222.9
304.8
344.7
372.7
386.7
410.6
454.5
468.6
492.6
536.6
100
90
80
70
60
50
40
30
20
10
100
150
200
250
300
350
400
450
500
m/z


*MSD1 SPC, time=3.994 of D:\DATA\TARR\20150821A_TAR_STEWART 2015-08-21 08-18-07\TAR1000010.D ES-API, Neg, Scan, Frag
Max: 1491
116.0
141.0
150.9
170.9
222.8
290.7
304.8
372.7
386.7
410.6
426.7
454.6
468.6
492.6
508.6
536.5
100
90
80
70
60
50
40
30
20
10
100
150
200
250
300
350
400
450
500
m/z


*MSD1 SPC, time=4.196 of D:\DATA\TARR\20150821A_TAR_STEWART 2015-08-21 08-18-07\TAR1000010.D ES-API, Neg, Scan, Frag
Max: 1666
100
90
80
70
60
50
40
30
20
10
100
150
200
250
300
350
400
450
500
m/z
116.0
119.0
140.9
150.9
222.8
262.8
290.7
304.8
344.7
372.7
386.7
410.6
426.6
454.7
468.6
469.6
492.6
536.6


*MSD1 SPC, time=4.398 of D:\DATA\TARR\20150821A_TAR_STEWART 2015-08-21 08-18-07\TAR1000010.D ES-API, Neg, Scan, Frag
Max: 1632
100
90
80
70
60
50
40
30
20
10
119.0
141.0
150.9
222.8
262.7
290.9
304.8
344.8
372.7
386.7
410.7
426.7
454.6
468.6
469.6
492.6
508.5
536.5
100
150
200
250
300
350
400
450
500
m/z

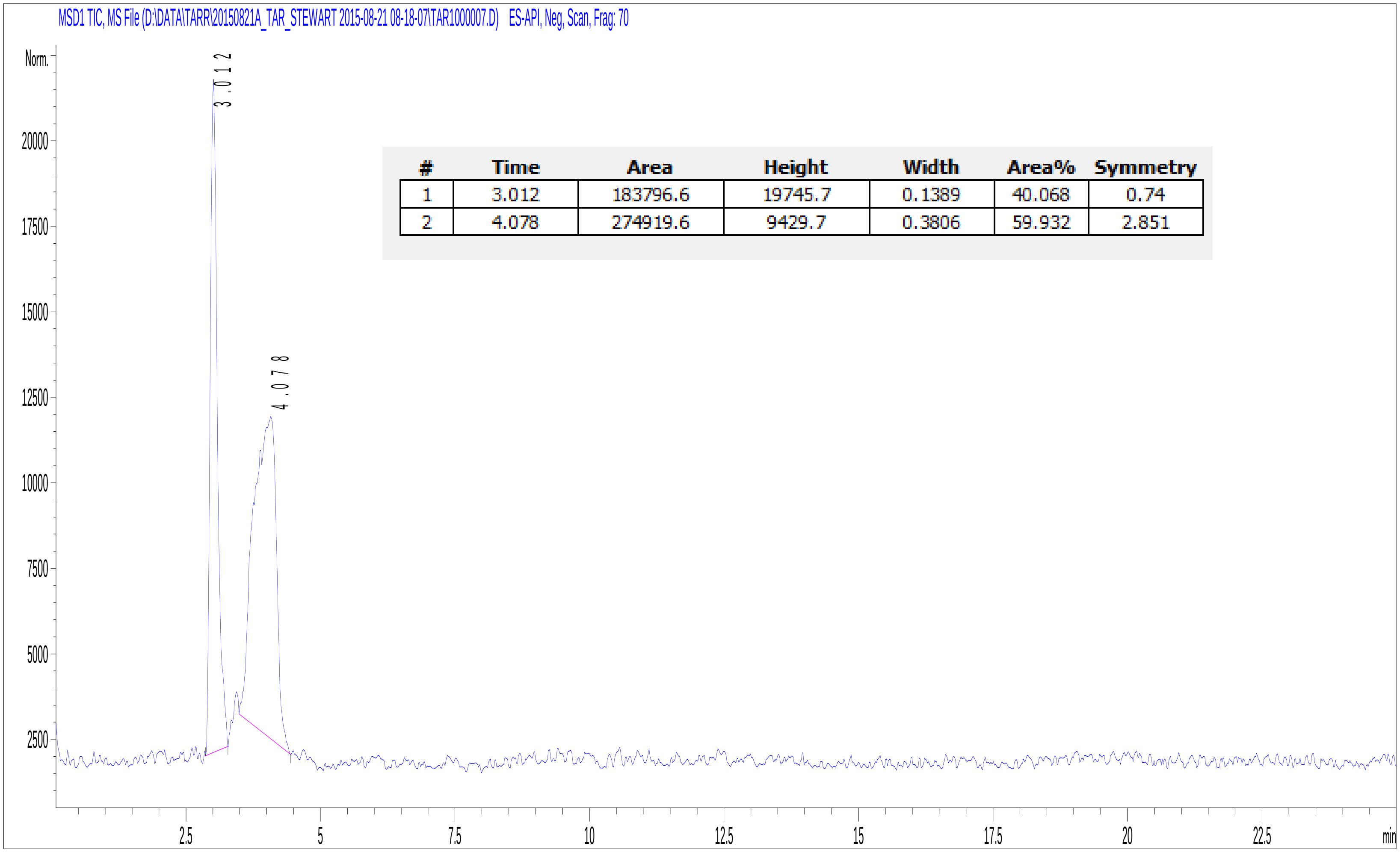

*MSD1 SPC, time=4.499 of D:\DATA\TARR\20150821A_TAR_STEWART 2015-08-21 08-18-07\TAR1000010.D ES-API, Neg, Scan, Frag
Max: 1262
100
90
80
70
60
50
40
30
20
10
119.0
140.9
150.9
180.9
222.9
262.8
304.8
386.8
468.7
492.6
536.5
100
150
200
250
300
350
400
450
500
m/z

7-May-15

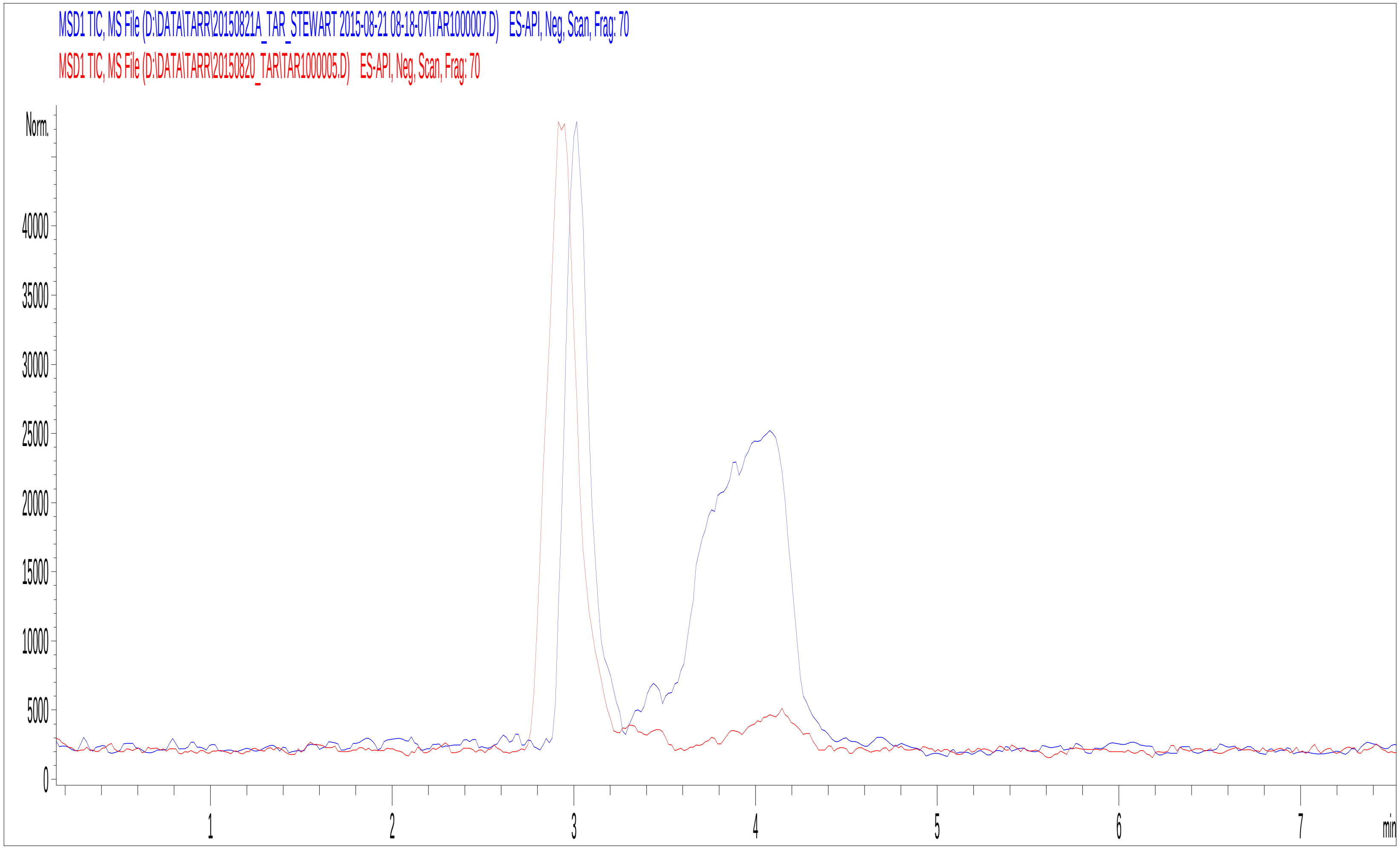
50 DC

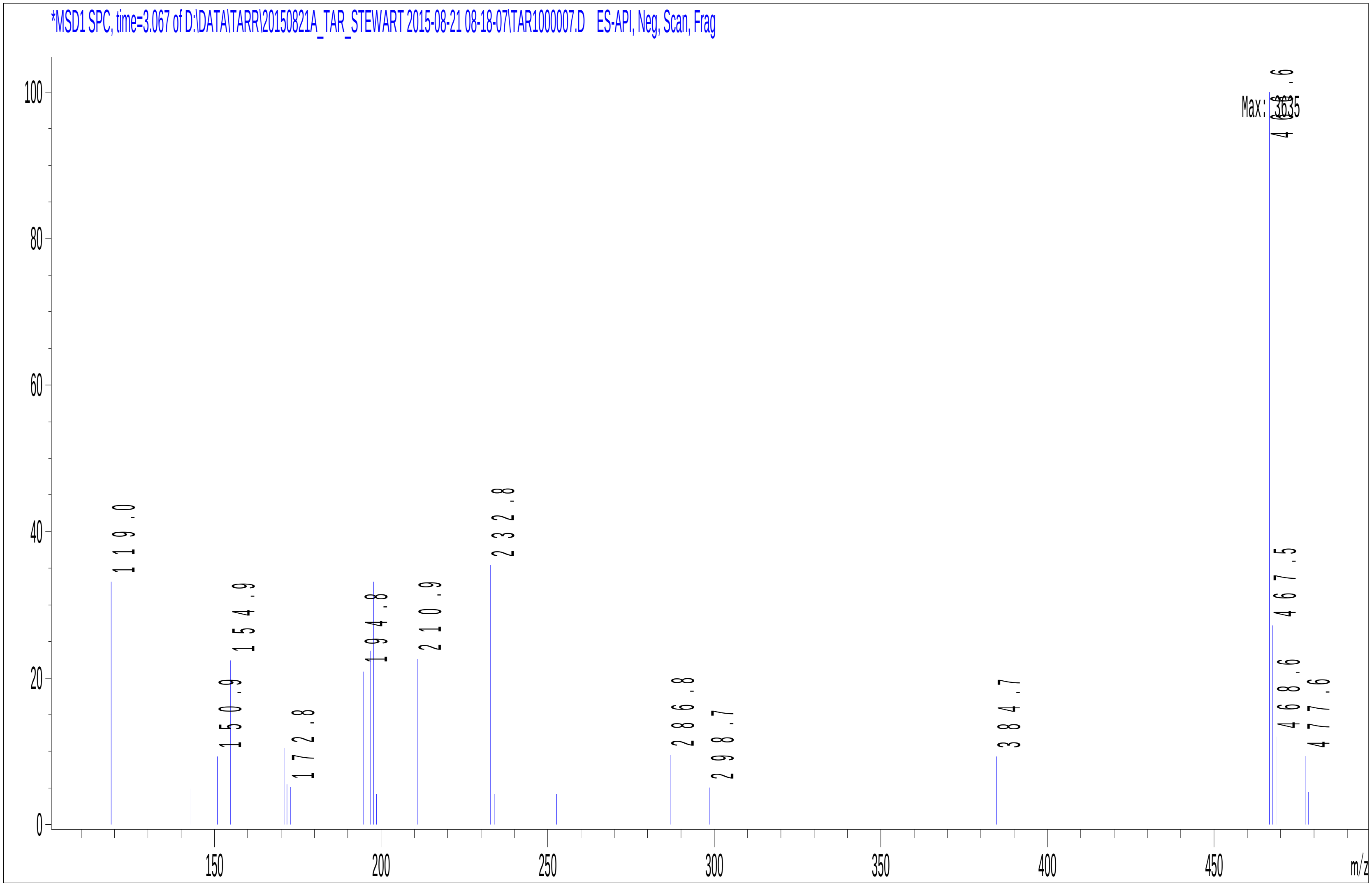
9

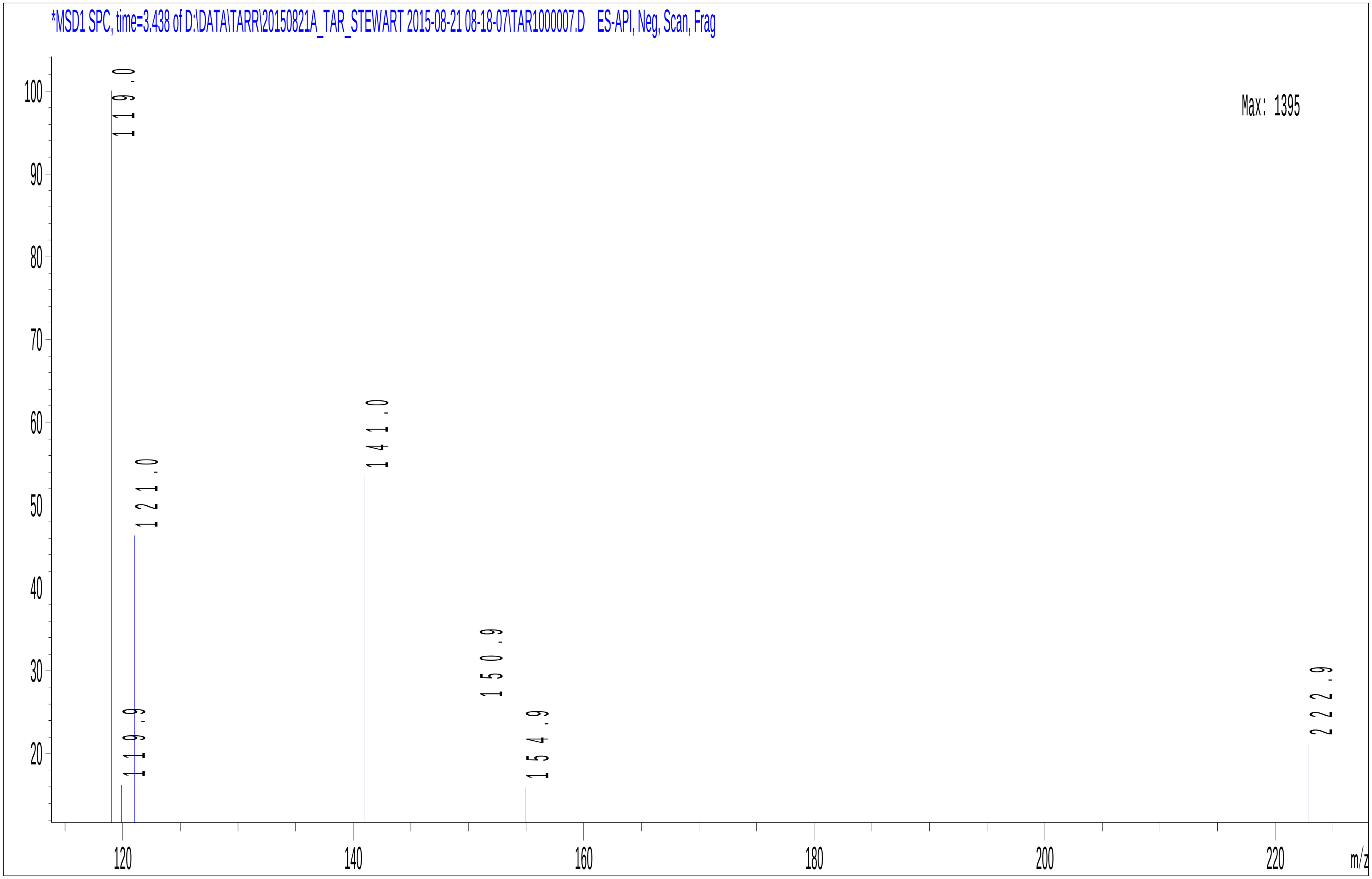
P2-E-06

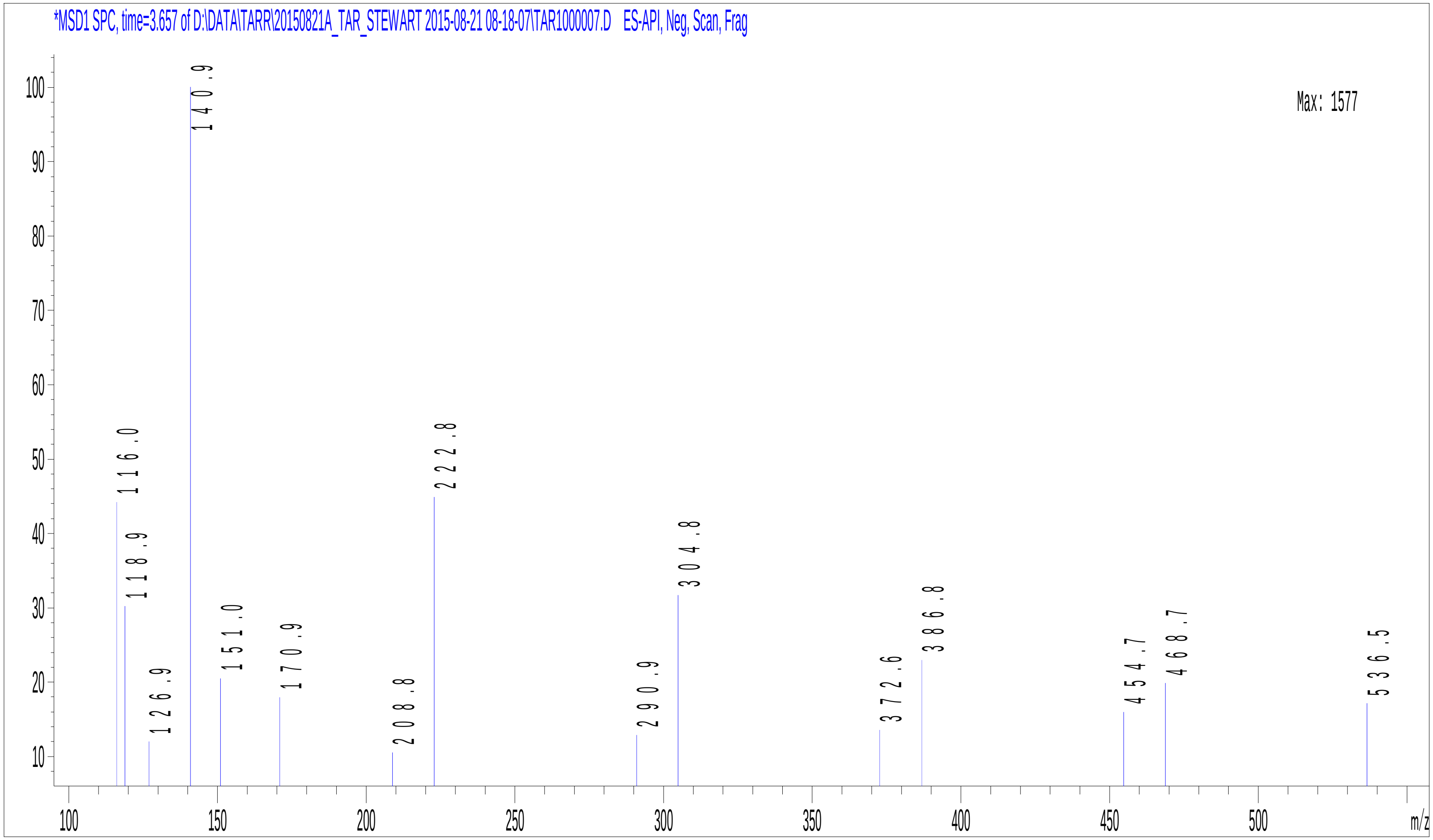


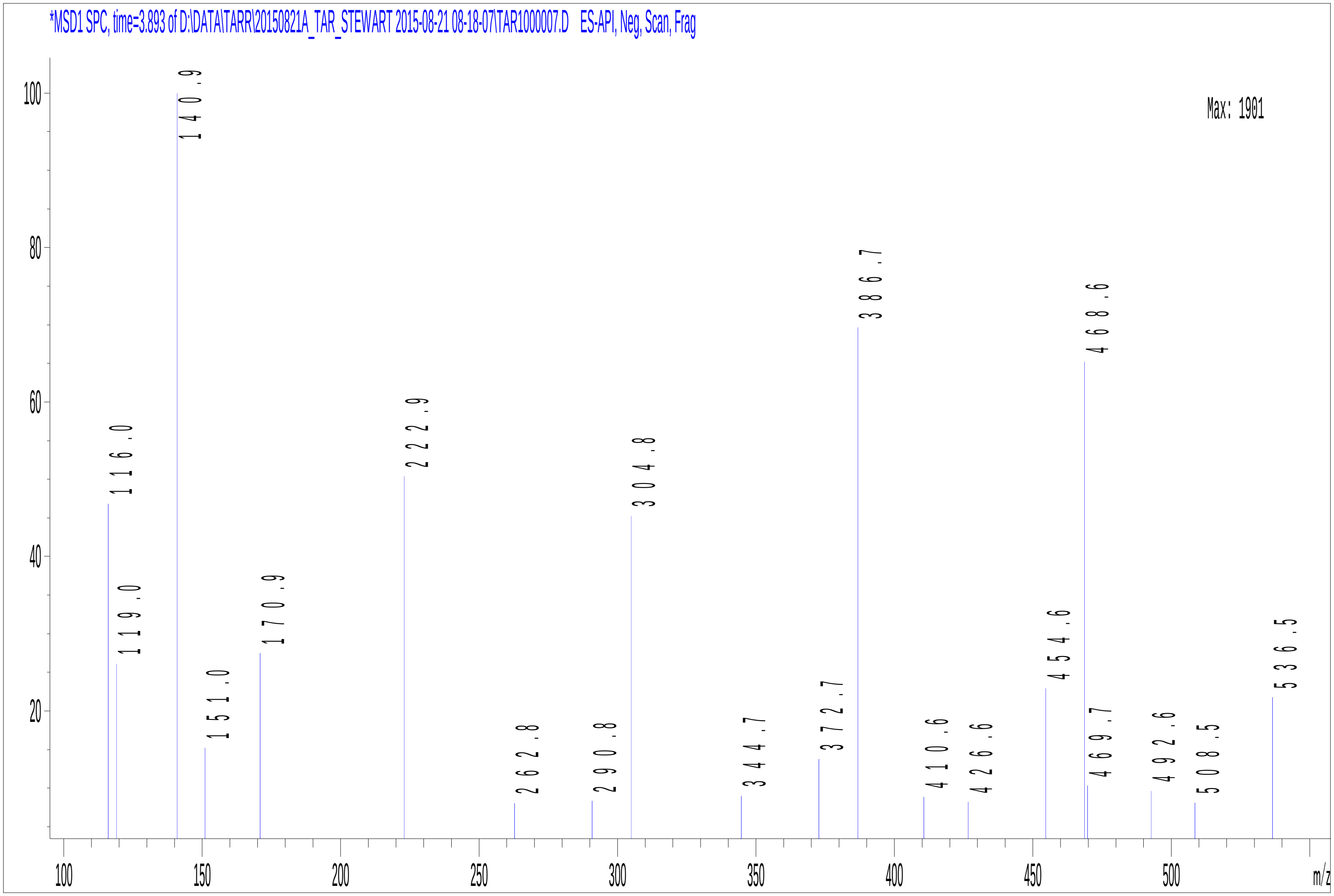
#	Time	Area	Height	Width	Area%	Symmetry
1	3.012	183796.6	19745.7	0.1389	40.068	0.74
2	4.078	274919.6	9429.7	0.3806	59.932	2.851

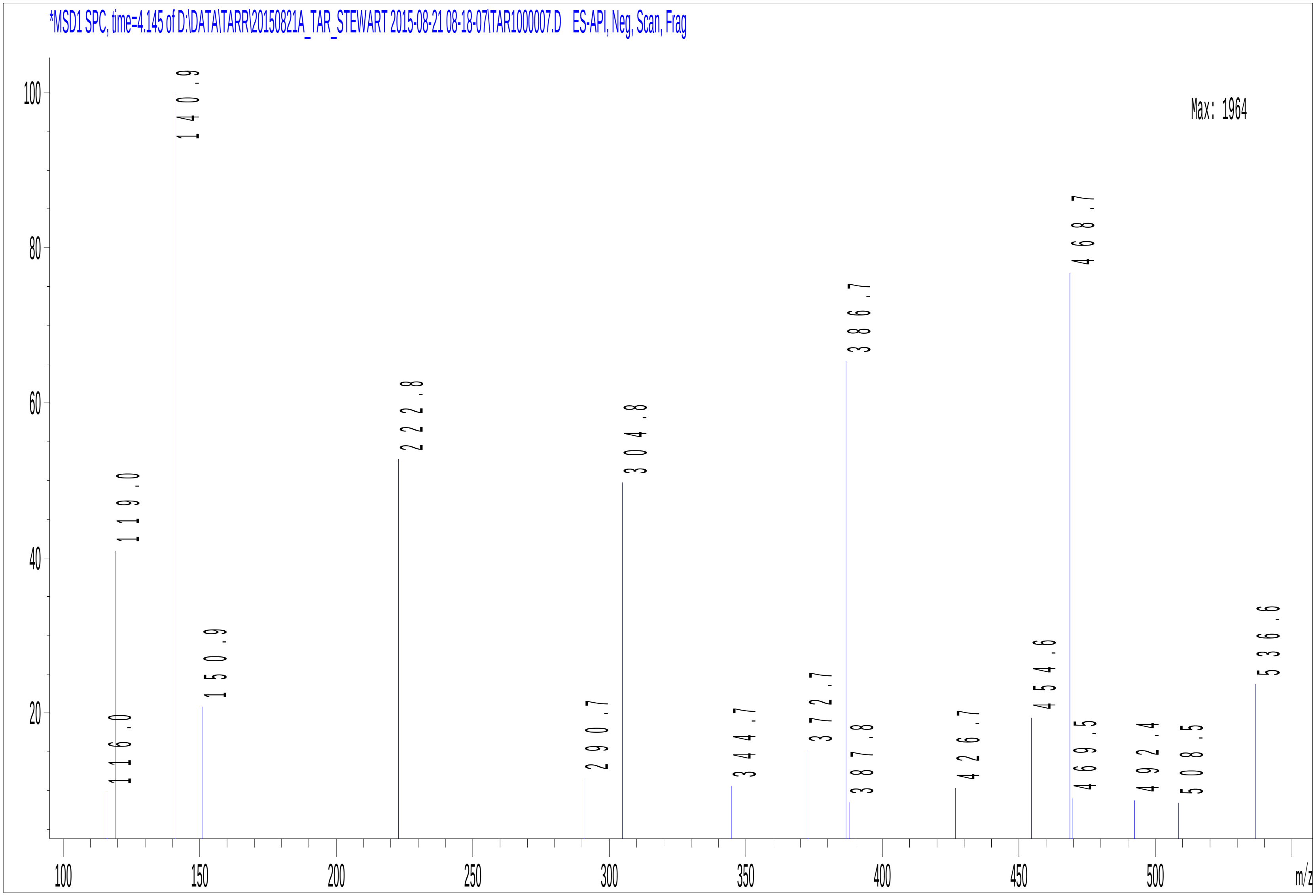

MSD1 TIC, MS File (D:\DATA\TARR\20150821A_TAR_STEWART 2015-08-21 08-18-07\TAR1000007.D)   ES-API, Neg, Scan, Frag: 70
MSD1 TIC, MS File (D:\DATA\TARR\20150820_TAR\TAR1000005.D)   ES-API, Neg, Scan, Frag: 70
Norm.
40000
35000
30000
25000
20000
15000
10000
5000
0
1
2
3
4
5
6
7
min


*MSD1 SPC, time=3.067 of D:\DATA\TARR\20150821A_TAR_STEWART 2015-08-21 08-18-07\TAR1000007.D   ES-API, Neg, Scan, Frag
Max: 3635
466.6
119.0
150.9
154.9
172.8
194.8
210.9
232.8
286.8
298.7
384.7
467.5
468.6
477.6
0
20
40
60
80
100
150
200
250
300
350
400
450
m/z


*MSD1 SPC, time=3.438 of D:\DATA\TARR\20150821A_TAR_STEWART 2015-08-21 08-18-07\TAR1000007.D   ES-API, Neg, Scan, Frag
Max: 1395
119.0
119.9
121.0
141.0
150.9
154.9
222.9
100
90
80
70
60
50
40
30
20
120
140
160
180
200
220
m/z


*MSD1 SPC, time=3.657 of D:\DATA\TARR\20150821A_TAR_STEWART 2015-08-21 08-18-07\TAR1000007.D ES-API, Neg, Scan, Frag
Max: 1577
100
90
80
70
60
50
40
30
20
10
116.0
118.9
126.9
140.9
151.0
170.9
208.8
222.8
290.9
304.8
372.6
386.8
454.7
468.7
536.5
100
150
200
250
300
350
400
450
500
m/z


*MSD1 SPC, time=3.893 of D:\DATA\TARR\20150821A_TAR_STEWART 2015-08-21 08-18-07\TAR1000007.D ES-API, Neg, Scan, Frag
Max: 1901
100
80
60
40
20
100
150
200
250
300
350
400
450
500
m/z
116.0
119.0
140.9
151.0
170.9
222.9
262.8
290.8
304.8
344.7
372.7
386.7
410.6
426.6
454.6
468.6
469.7
492.6
508.5
536.5

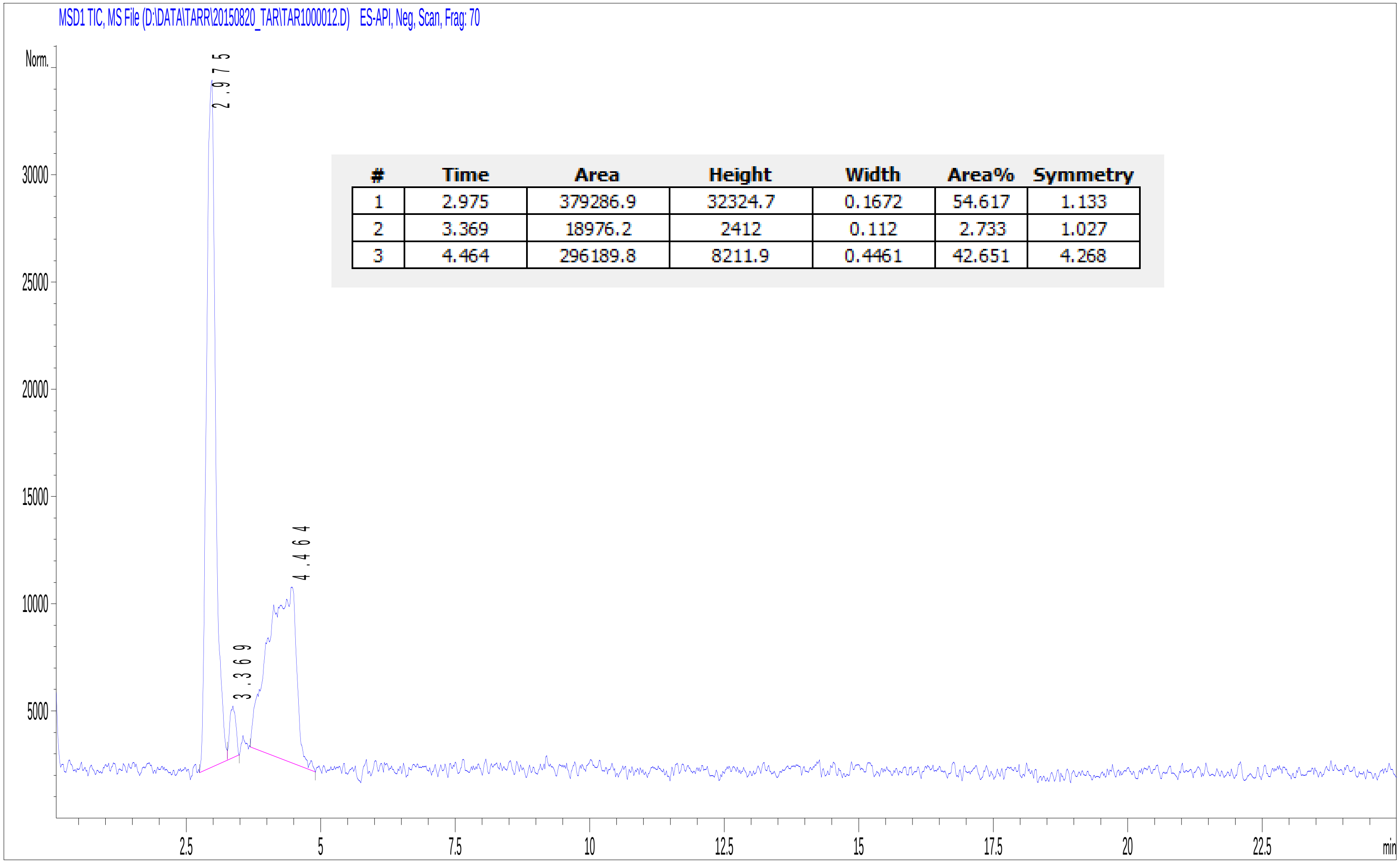

*MSD1 SPC, time=4.145 of D:\DATA\TARR\20150821A_TAR_STEWART 2015-08-21 08-18-07\TAR1000007.D ES-API, Neg, Scan, Frag
Max: 1964
100
80
60
40
20
100
150
200
250
300
350
400
450
500
m/z
116.0
119.0
140.9
150.9
222.8
290.7
304.8
344.7
372.7
386.7
387.8
426.7
454.6
468.7
469.5
492.4
508.5
536.6

15-Jun-15

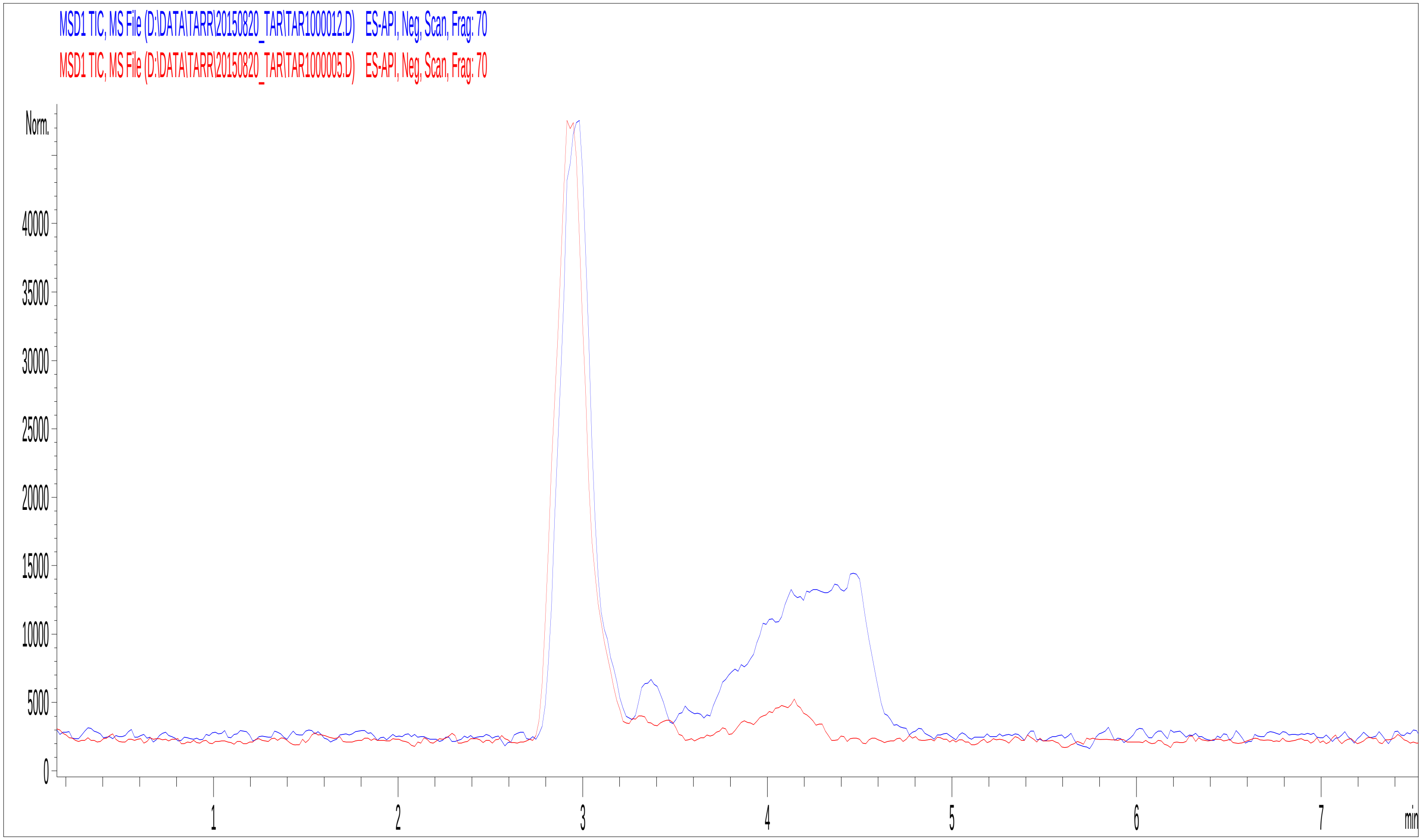
50 DC Repeat

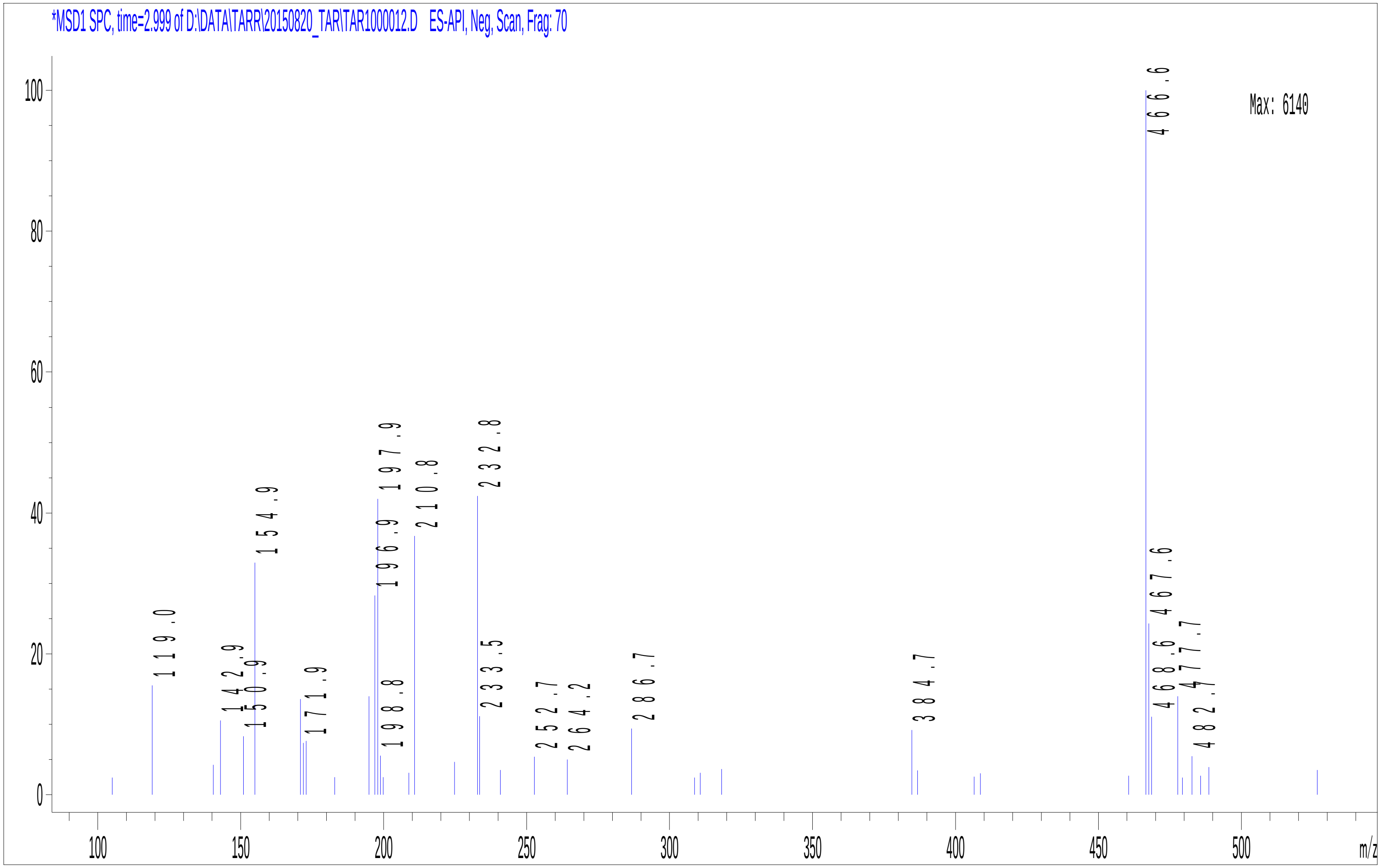
9

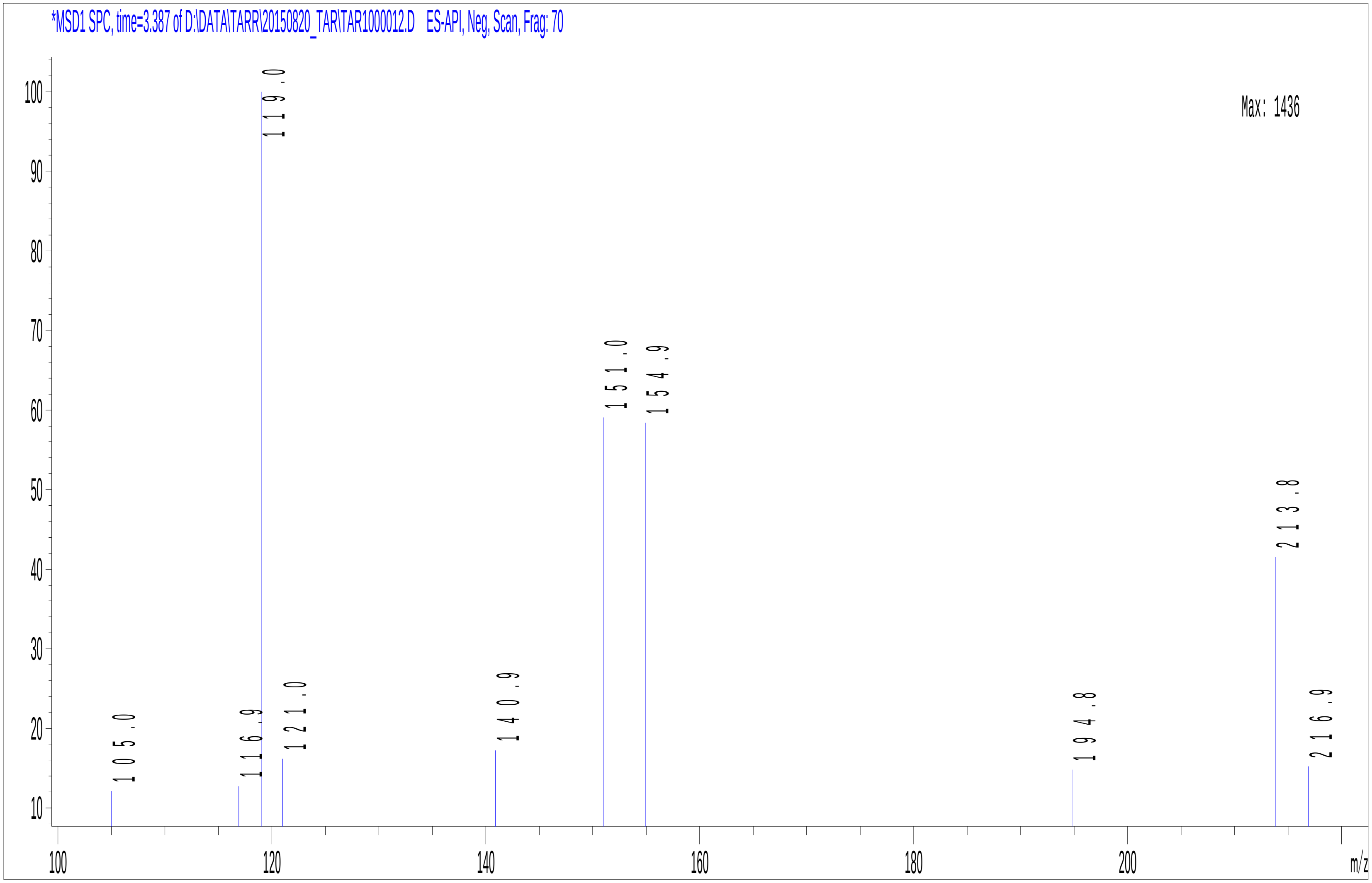
P2-B-07

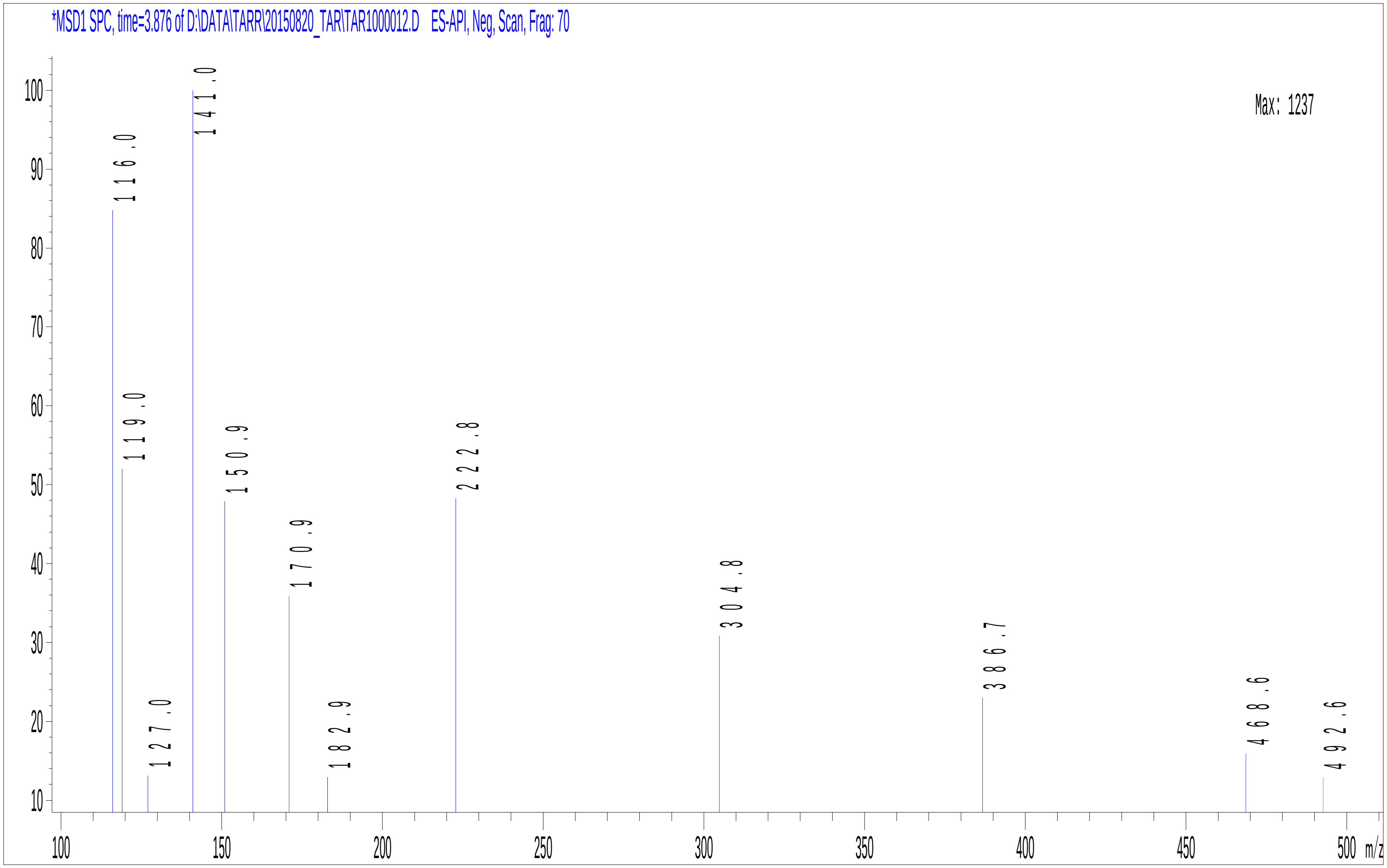


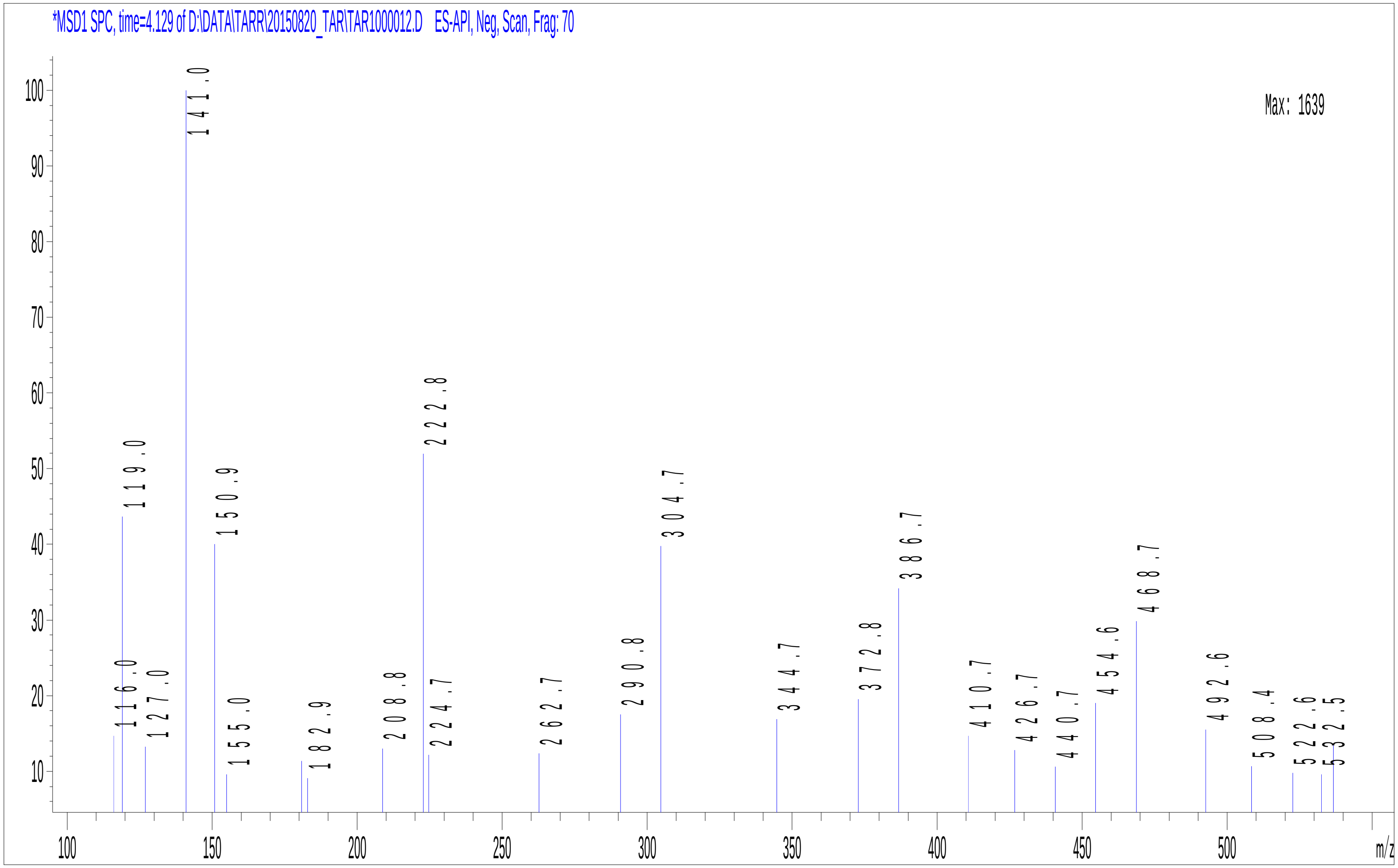
#	Time	Area	Height	Width	Area%	Symmetry
1	2.975	379286.9	32324.7	0.1672	54.617	1.133
2	3.369	18976.2	2412	0.112	2.733	1.027
3	4.464	296189.8	8211.9	0.4461	42.651	4.268

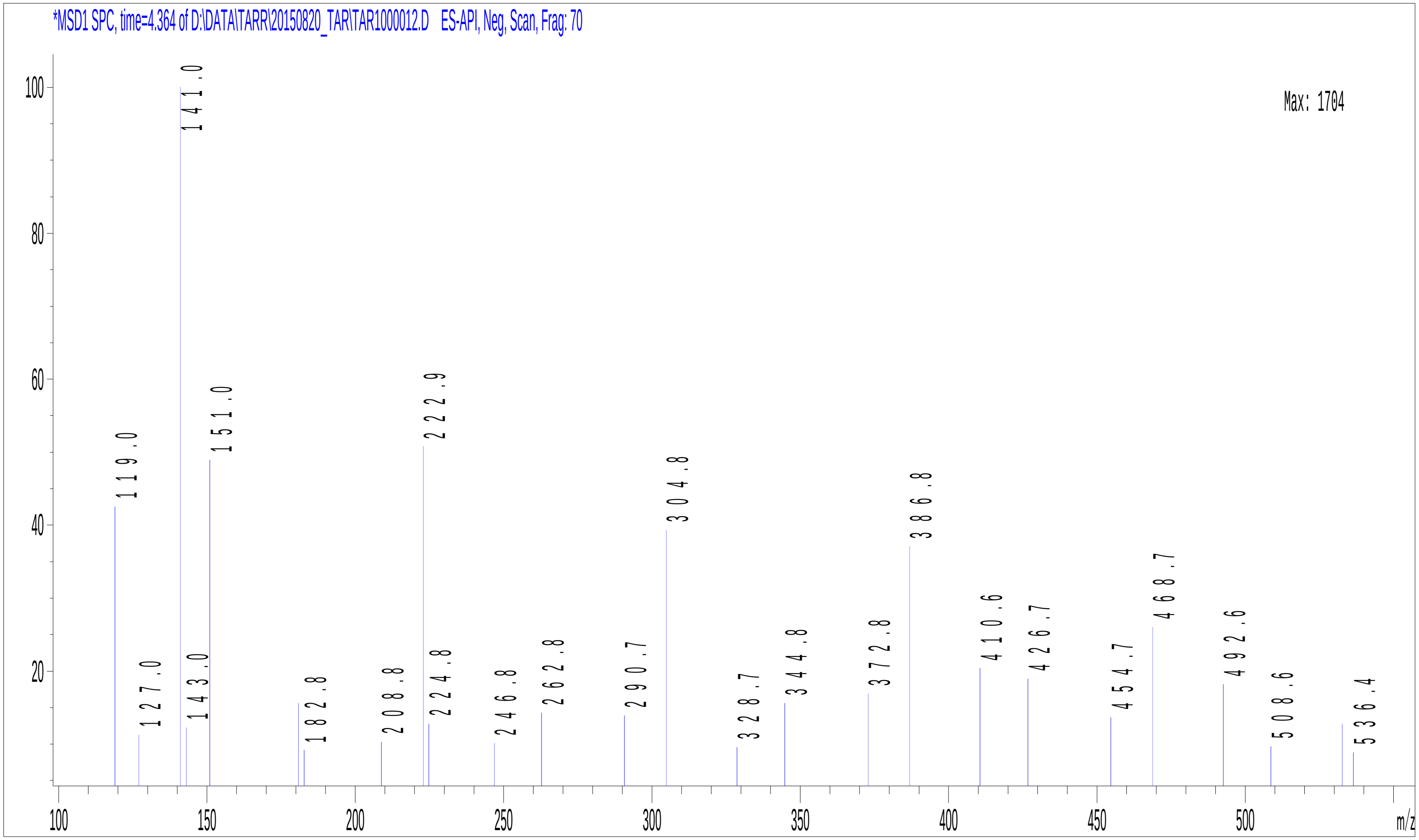

MSD1 TIC, MS File (D:\DATA\TARR\20150820_TAR\TAR1000012.D) ES-API, Neg, Scan, Frag: 70
MSD1 TIC, MS File (D:\DATA\TARR\20150820_TAR\TAR1000005.D) ES-API, Neg, Scan, Frag: 70
Norm.
40000
35000
30000
25000
20000
15000
10000
5000
0
1
2
3
4
5
6
7
min

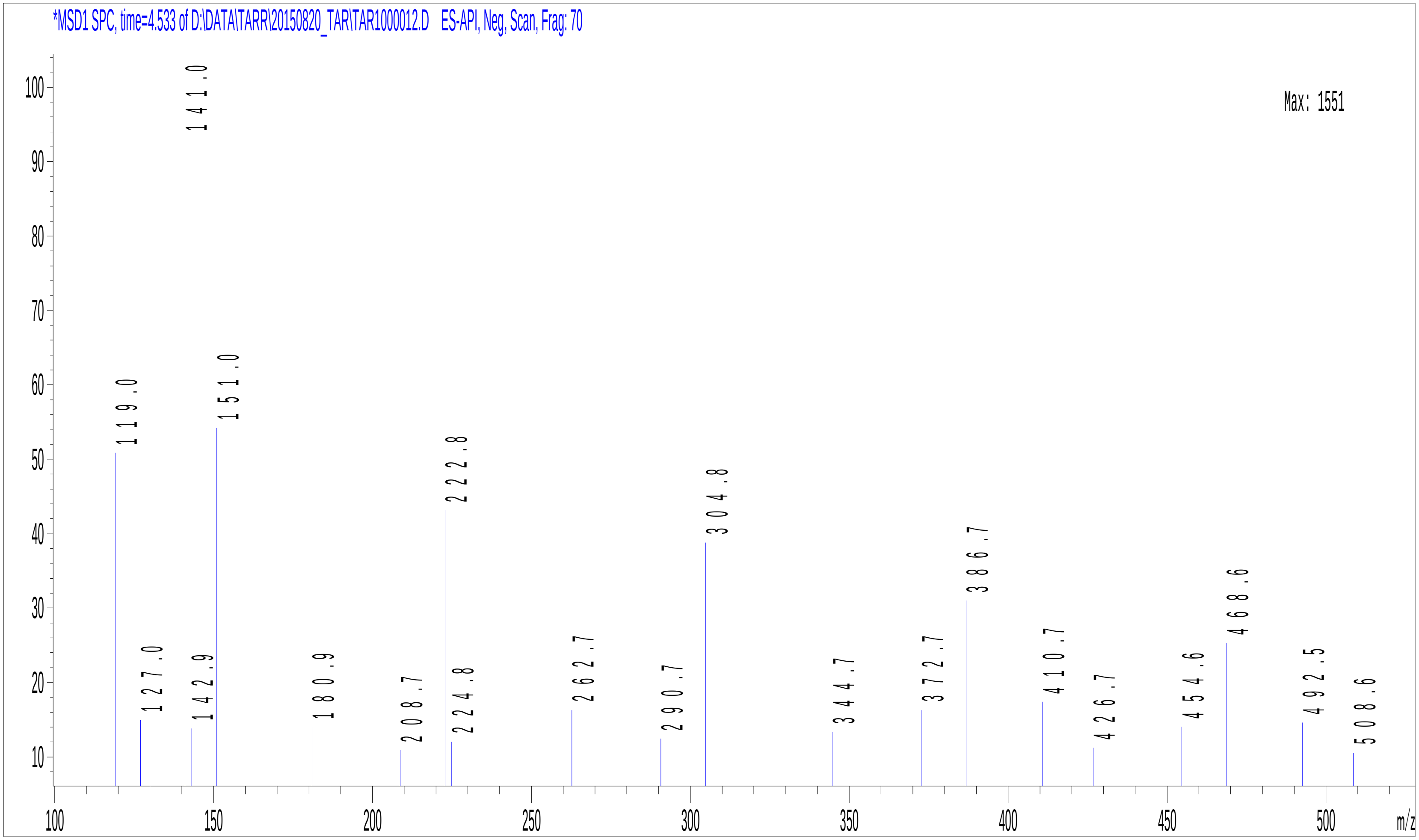

*MSD1 SPC, time=2.999 of D:\DATA\TARR\20150820_TAR\TAR1000012.D ES-API, Neg, Scan, Frag: 70
Max: 6140
0
20
40
60
80
100
100
150
200
250
300
350
400
450
500
m/z
119.0
142.9
150.9
154.9
171.9
196.9
197.9
198.8
210.8
232.8
233.5
252.7
264.2
286.7
384.7
466.6
467.6
468.6
477.7
482.7


*MSD1 SPC, time=3.387 of D:\DATA\TARR\20150820_TAR\TAR1000012.D ES-API, Neg, Scan, Frag: 70
Max: 1436
105.0
116.9
119.0
121.0
140.9
151.0
154.9
194.8
213.8
216.9
100
90
80
70
60
50
40
30
20
10
100
120
140
160
180
200
m/z


*MSD1 SPC, time=3.876 of D:\DATA\TARR\20150820_TAR\TAR1000012.D ES-API, Neg, Scan, Frag: 70
Max: 1237
116.0
119.0
127.0
141.0
150.9
170.9
182.9
222.8
304.8
386.7
468.6
492.6
100
90
80
70
60
50
40
30
20
10
100
150
200
250
300
350
400
450
500
m/z


*MSD1 SPC, time=4.129 of D:\DATA\TARR\20150820_TAR\TAR1000012.D ES-API, Neg, Scan, Frag: 70
Max: 1639
100
90
80
70
60
50
40
30
20
10
116.0
119.0
127.0
141.0
150.9
155.0
182.9
208.8
222.8
224.7
262.7
290.8
304.7
344.7
372.8
386.7
410.7
426.7
440.7
454.6
468.7
492.6
508.4
522.6
532.5
100
150
200
250
300
350
400
450
500
m/z


*MSD1 SPC, time=4.364 of D:\DATA\TARR\20150820_TAR\TAR1000012.D ES-API, Neg, Scan, Frag: 70
Max: 1704
100
80
60
40
20
119.0
127.0
141.0
143.0
151.0
182.8
208.8
222.9
224.8
246.8
262.8
290.7
304.8
328.7
344.8
372.8
386.8
410.6
426.7
454.7
468.7
492.6
508.6
536.4
100
150
200
250
300
350
400
450
500
m/z

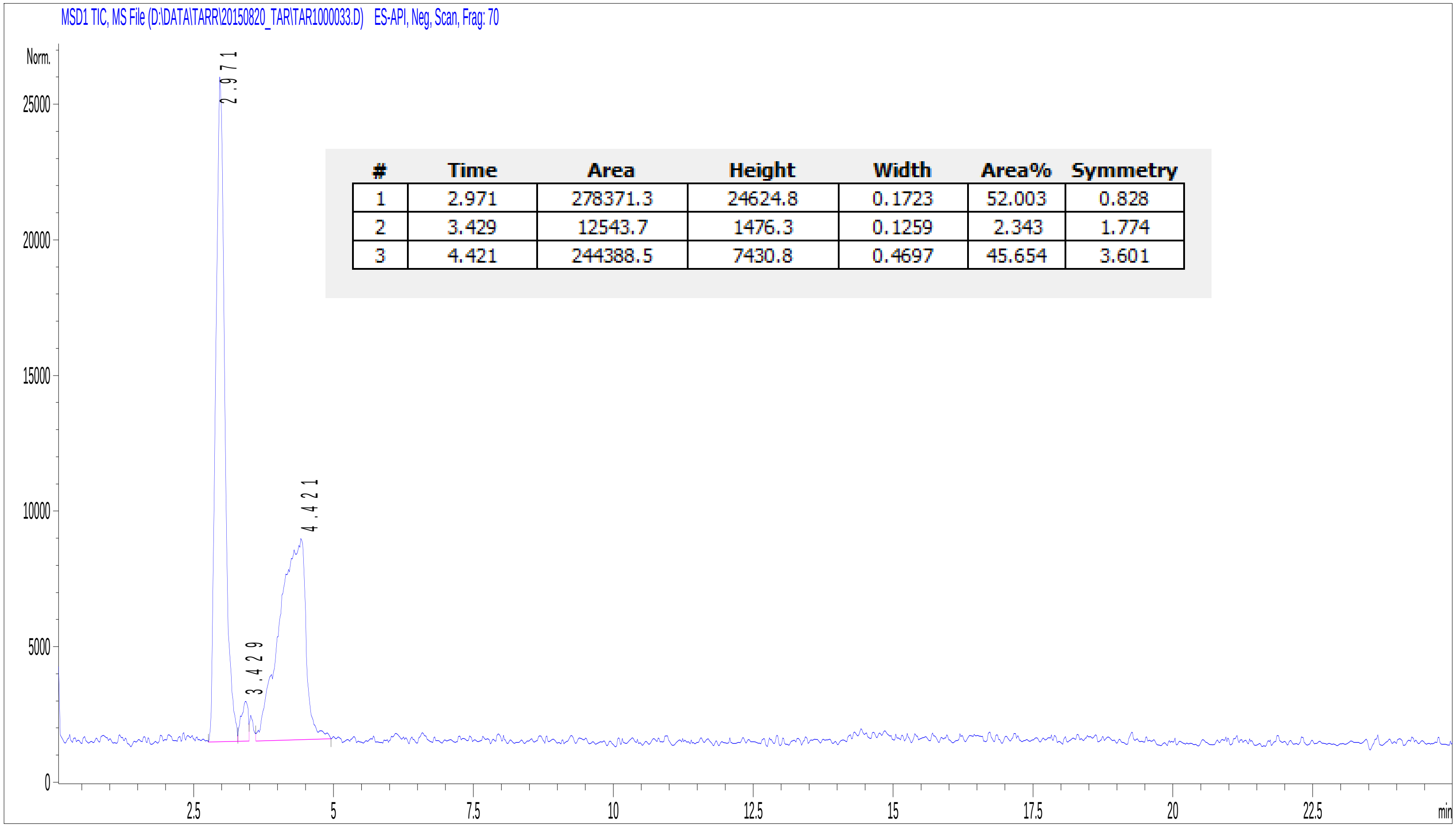

*MSD1 SPC, time=4.533 of D:\DATA\TARR\20150820_TAR\TAR1000012.D ES-API, Neg, Scan, Frag: 70
Max: 1551
100
90
80
70
60
50
40
30
20
10
119.0
127.0
141.0
142.9
151.0
180.9
208.7
222.8
224.8
262.7
290.7
304.8
344.7
372.7
386.7
410.7
426.7
454.6
468.6
492.5
508.6
100
150
200
250
300
350
400
450
500
m/z

23-Jul-15

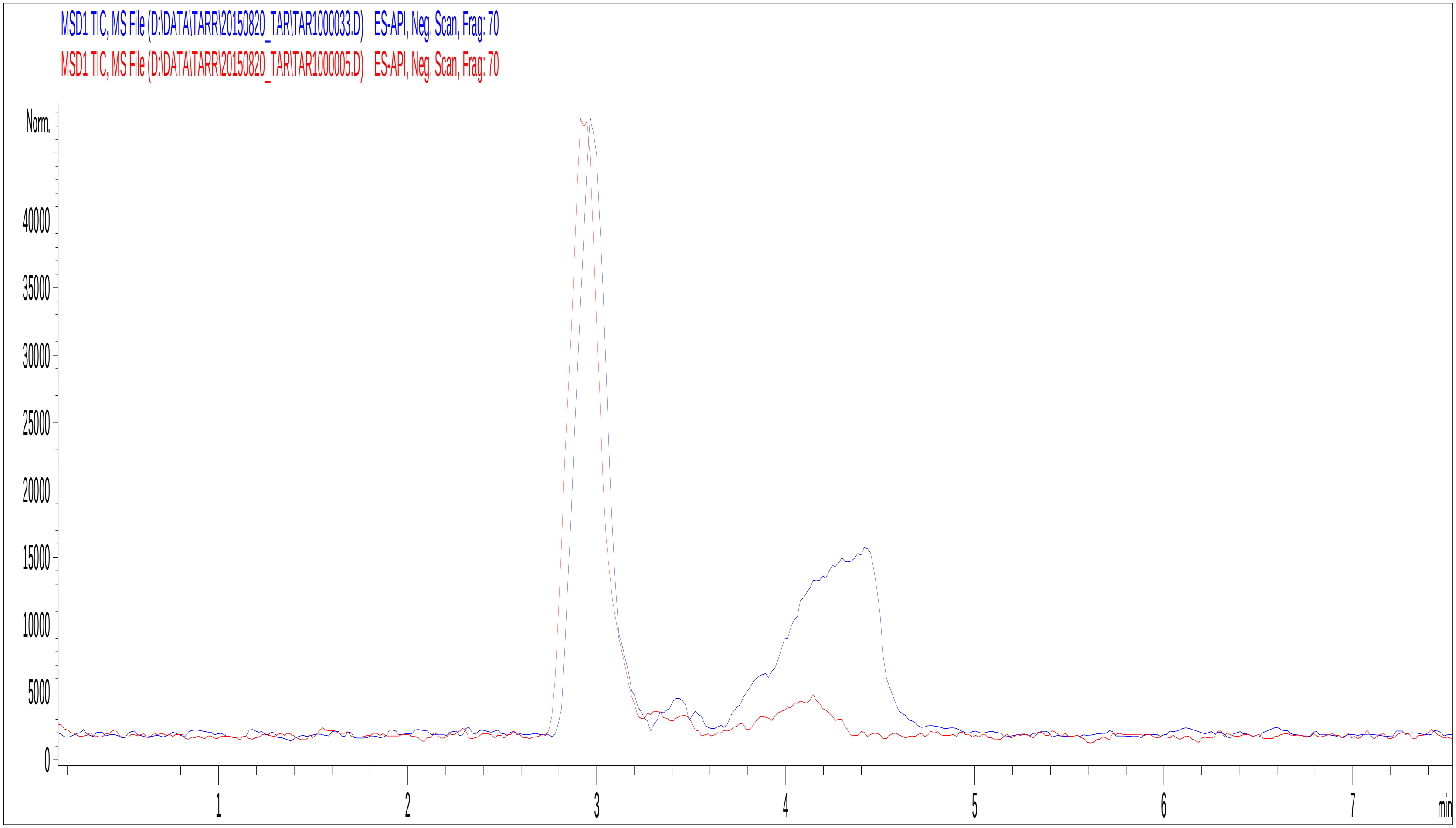
70 DC

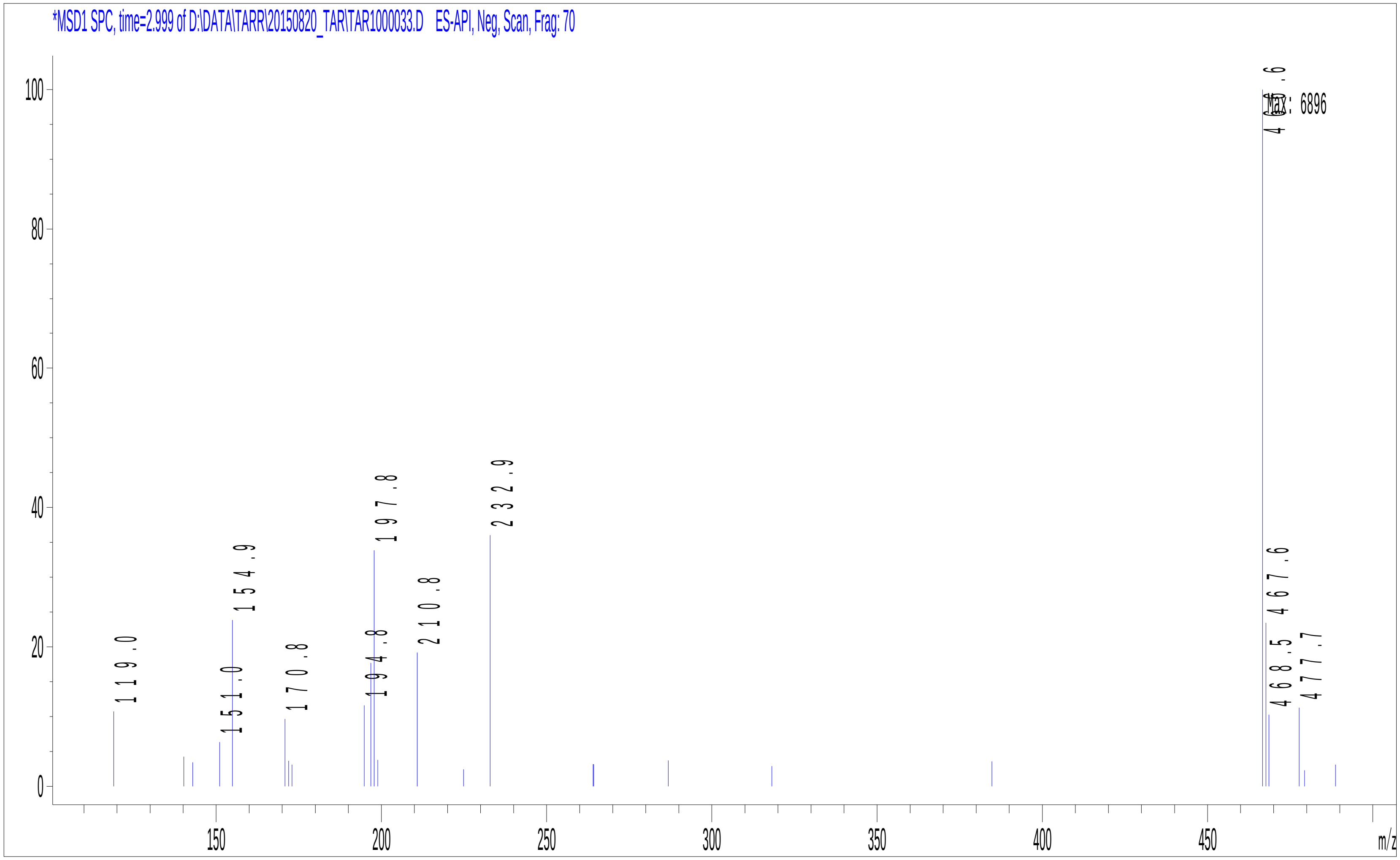
9

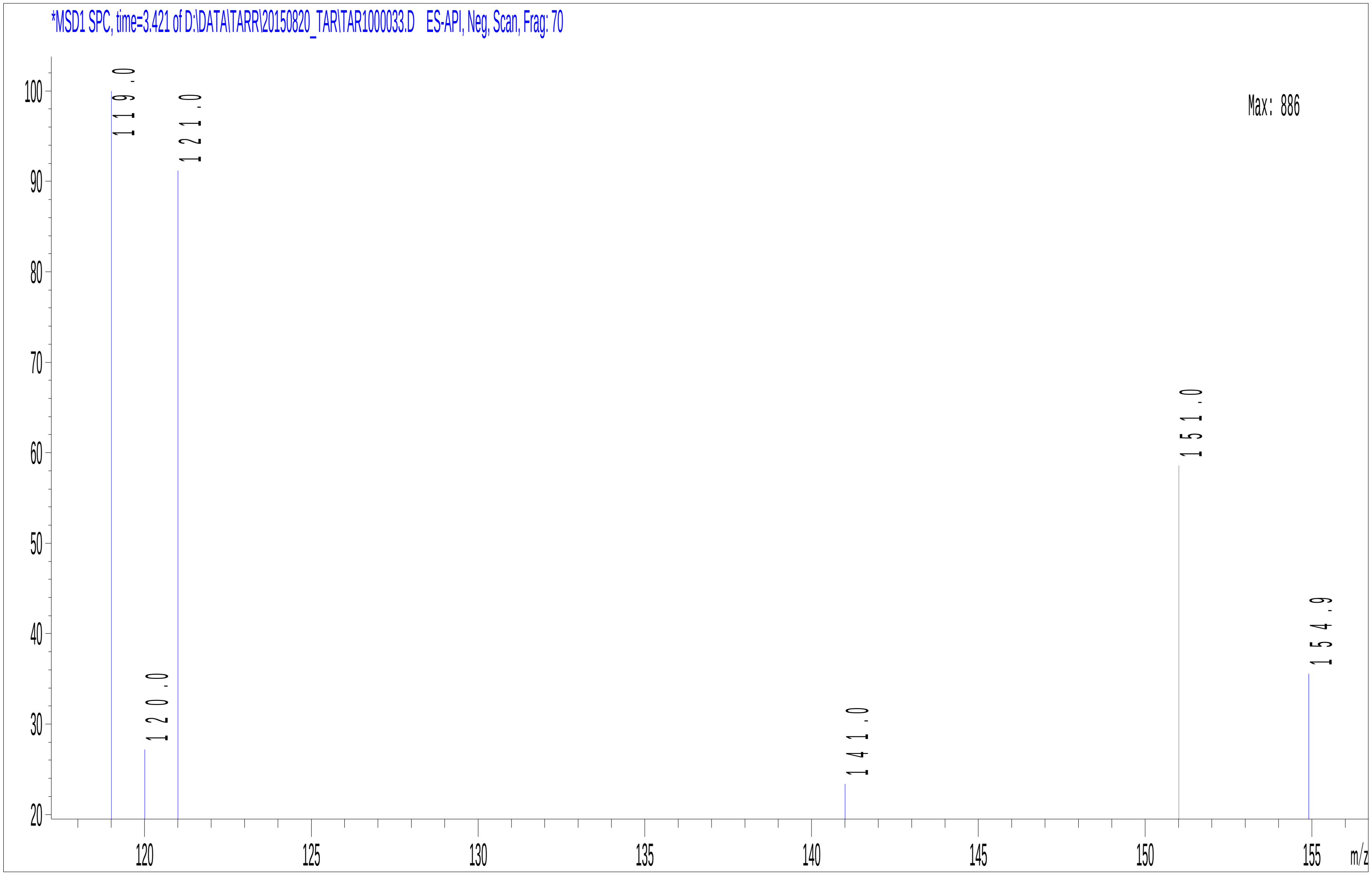
P2-D-04

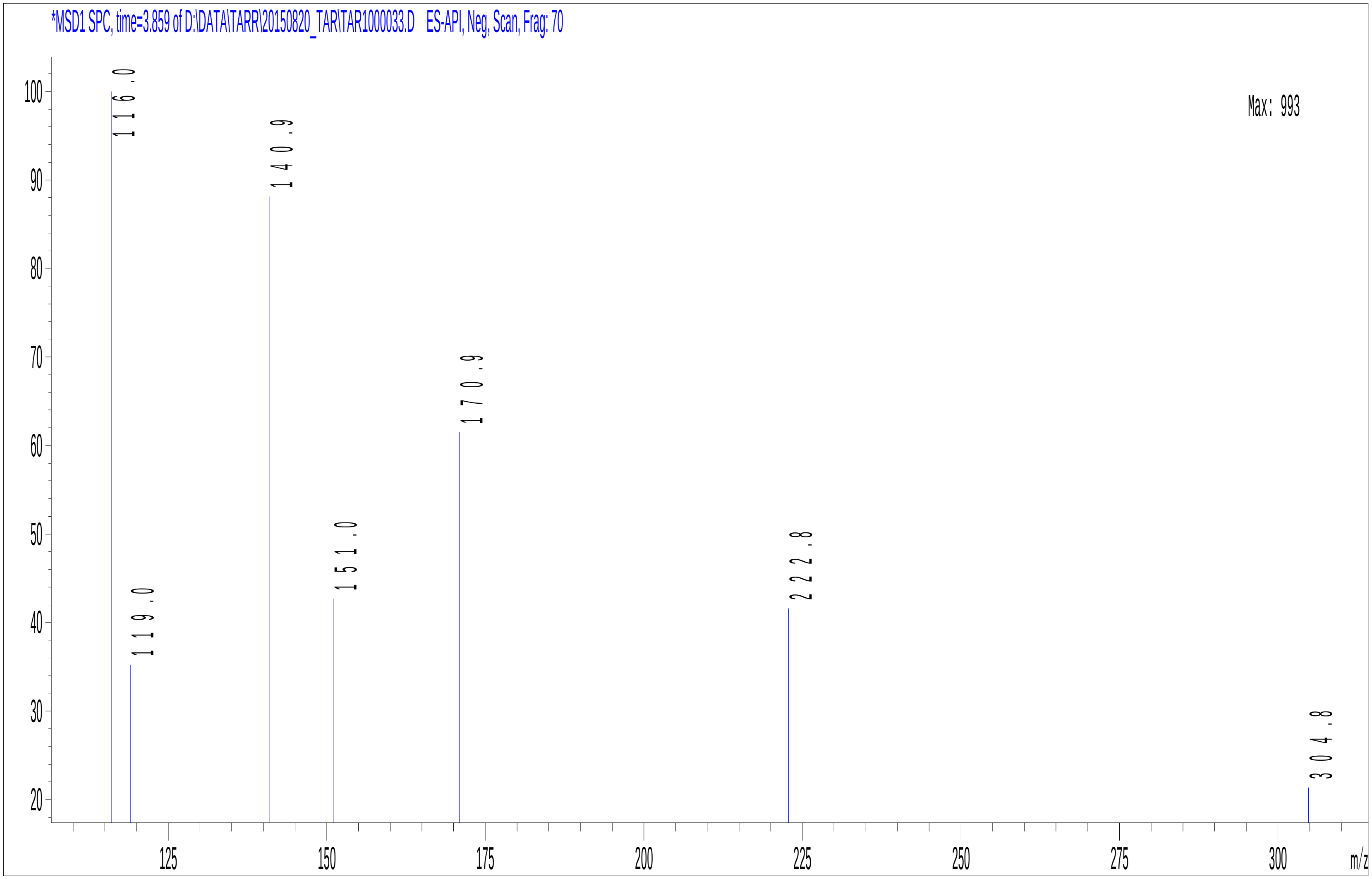


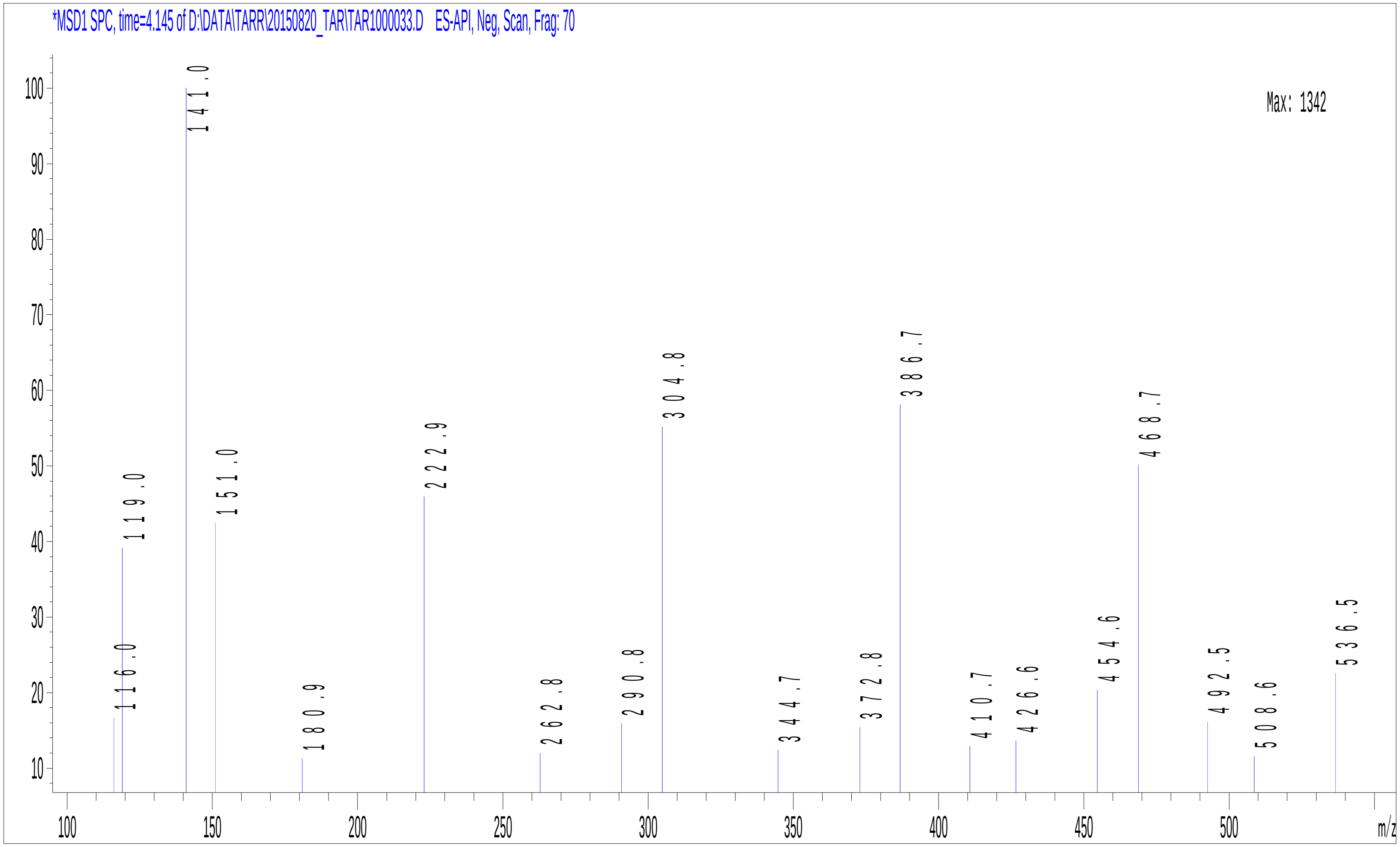
#	Time	Area	Height	Width	Area%	Symmetry
1	2.971	278371.3	24624.8	0.1723	52.003	0.828
2	3.429	12543.7	1476.3	0.1259	2.343	1.774
3	4.421	244388.5	7430.8	0.4697	45.654	3.601

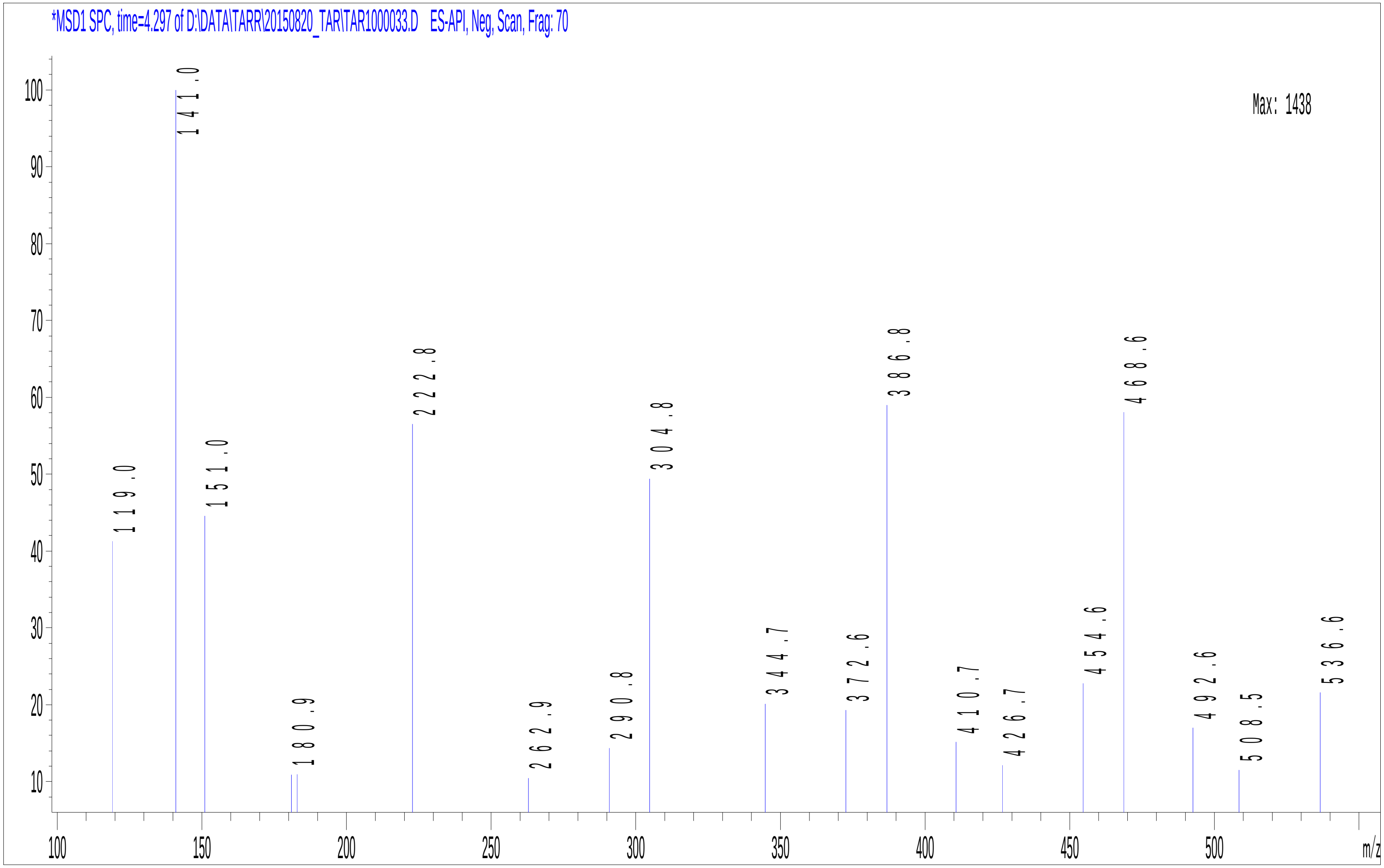

MSD1 TIC, MS File (D:\DATA\TARR\20150820_TAR\TAR1000033.D) ES-API, Neg, Scan, Frag: 70
MSD1 TIC, MS File (D:\DATA\TARR\20150820_TAR\TAR1000005.D) ES-API, Neg, Scan, Frag: 70
Norm.
40000
35000
30000
25000
20000
15000
10000
5000
0
1
2
3
4
5
6
7
min

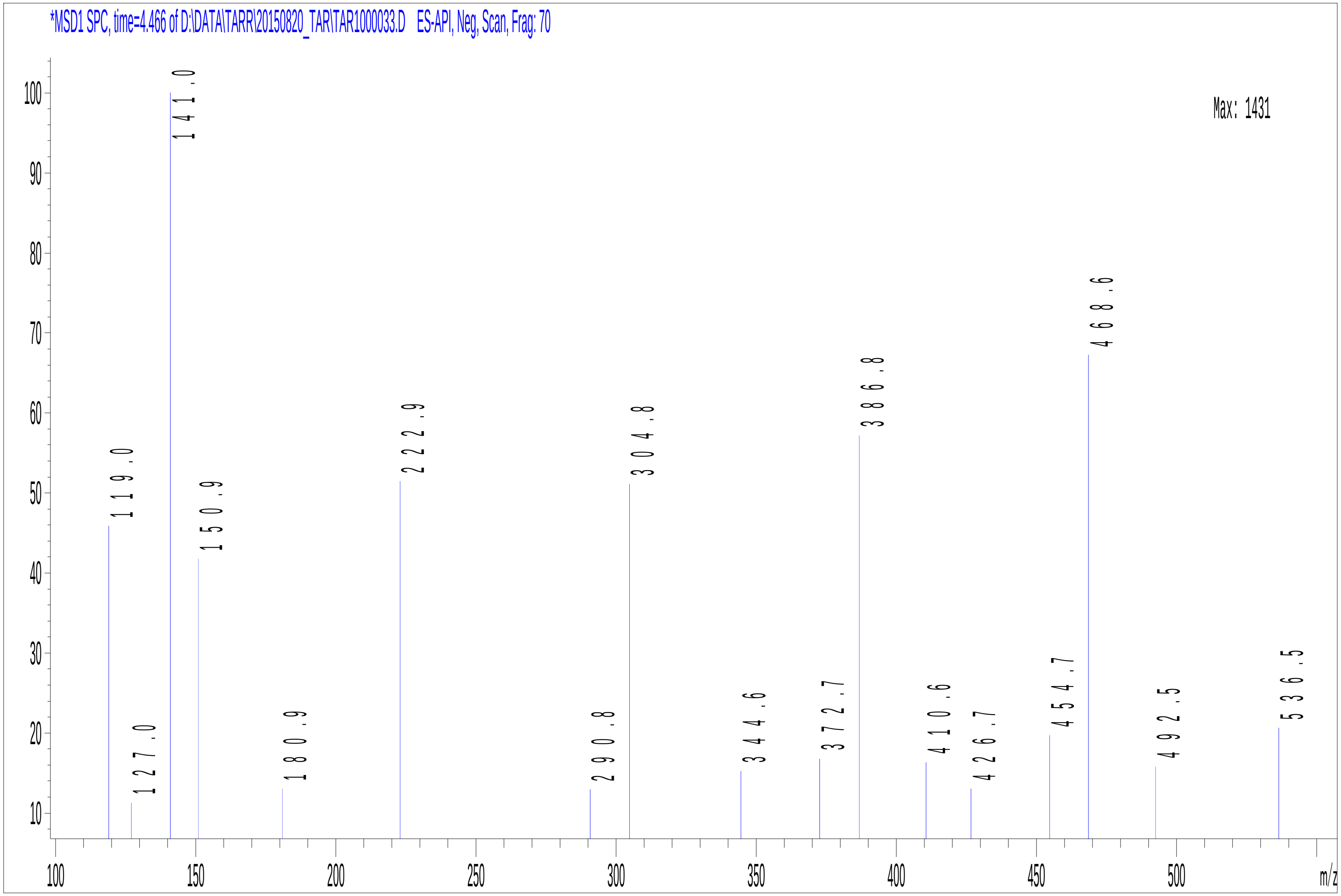

*MSD1 SPC, time=2.999 of D:\DATA\TARR\20150820_TAR\TAR1000033.D ES-API, Neg, Scan, Frag: 70
Max: 6896
100
80
60
40
20
0
150
200
250
300
350
400
450
m/z
119.0
151.0
154.9
170.8
194.8
197.8
210.8
232.9
466.6
467.6
468.5
477.7


*MSD1 SPC, time=3.421 of D:\DATA\TARR\20150820_TAR\TAR1000033.D ES-API, Neg, Scan, Frag: 70
Max: 886
119.0
120.0
121.0
141.0
151.0
154.9
100
90
80
70
60
50
40
30
20
120
125
130
135
140
145
150
155
m/z


*MSD1 SPC, time=3.859 of D:\DATA\TARR\20150820_TAR\TAR1000033.D ES-API, Neg, Scan, Frag: 70
Max: 993
116.0
119.0
140.9
151.0
170.9
222.8
304.8
100
90
80
70
60
50
40
30
20
125
150
175
200
225
250
275
300
m/z


*MSD1 SPC, time=4.145 of D:\DATA\TARR\20150820_TAR\TAR1000033.D ES-API, Neg, Scan, Frag: 70
Max: 1342
116.0
119.0
141.0
151.0
180.9
222.9
262.8
290.8
304.8
344.7
372.8
386.7
410.7
426.6
454.6
468.7
492.5
508.6
536.5
100
90
80
70
60
50
40
30
20
10
100
150
200
250
300
350
400
450
500
m/z


*MSD1 SPC, time=4.297 of D:\DATA\TARR\20150820_TAR\TAR1000033.D ES-API, Neg, Scan, Frag: 70
Max: 1438
119.0
141.0
151.0
180.9
222.8
262.9
290.8
304.8
344.7
372.6
386.8
410.7
426.7
454.6
468.6
492.6
508.5
536.6
100
90
80
70
60
50
40
30
20
10
100
150
200
250
300
350
400
450
500
m/z

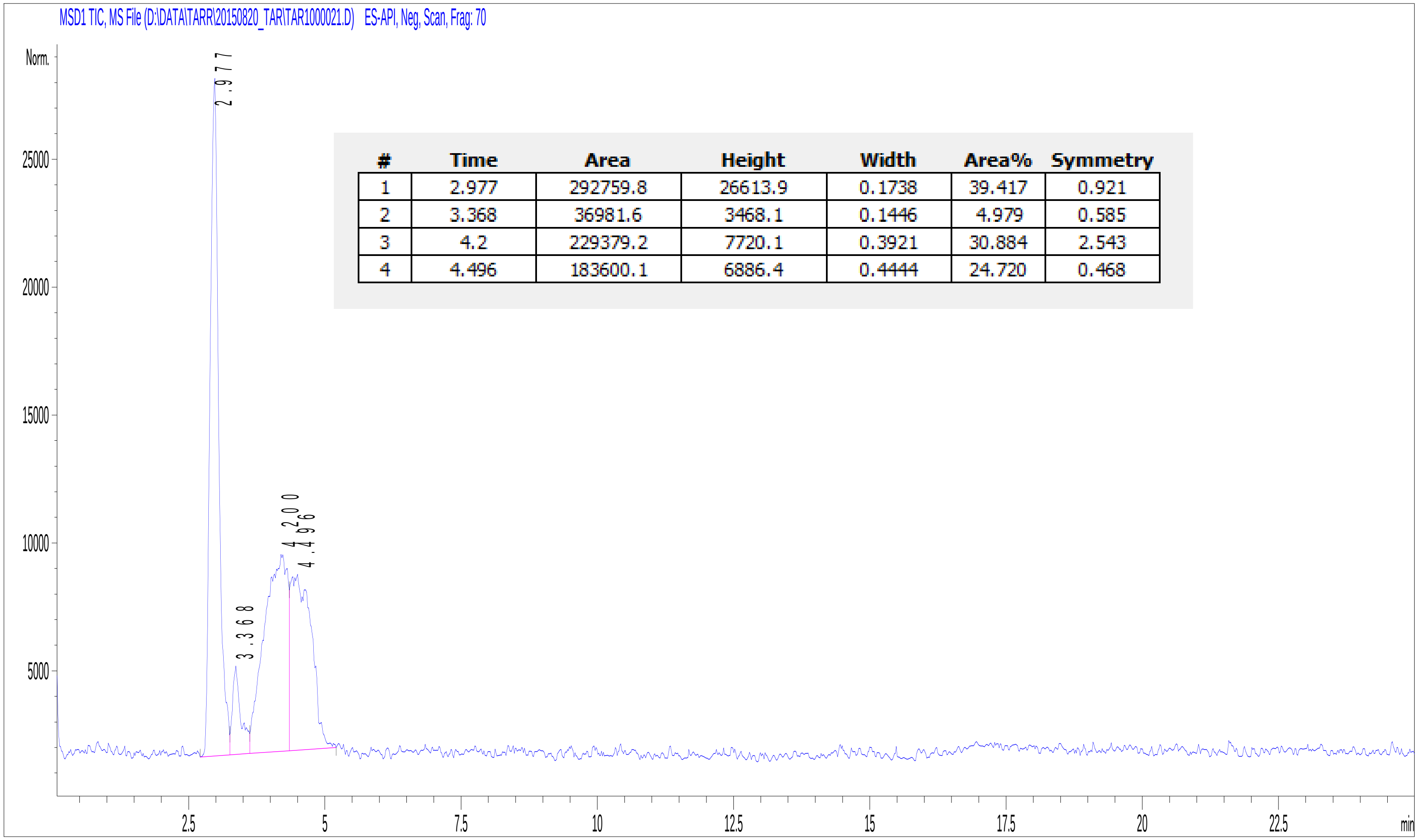

*MSD1 SPC, time=4.466 of D:\DATA\TARR\20150820_TAR\TAR1000033.D ES-API, Neg, Scan, Frag: 70
Max: 1431
100
90
80
70
60
50
40
30
20
10
119.0
127.0
141.0
150.9
180.9
222.9
290.8
304.8
344.6
372.7
386.8
410.6
426.7
454.7
468.6
492.5
536.5
100
150
200
250
300
350
400
450
500
m/z

1-Jul-15

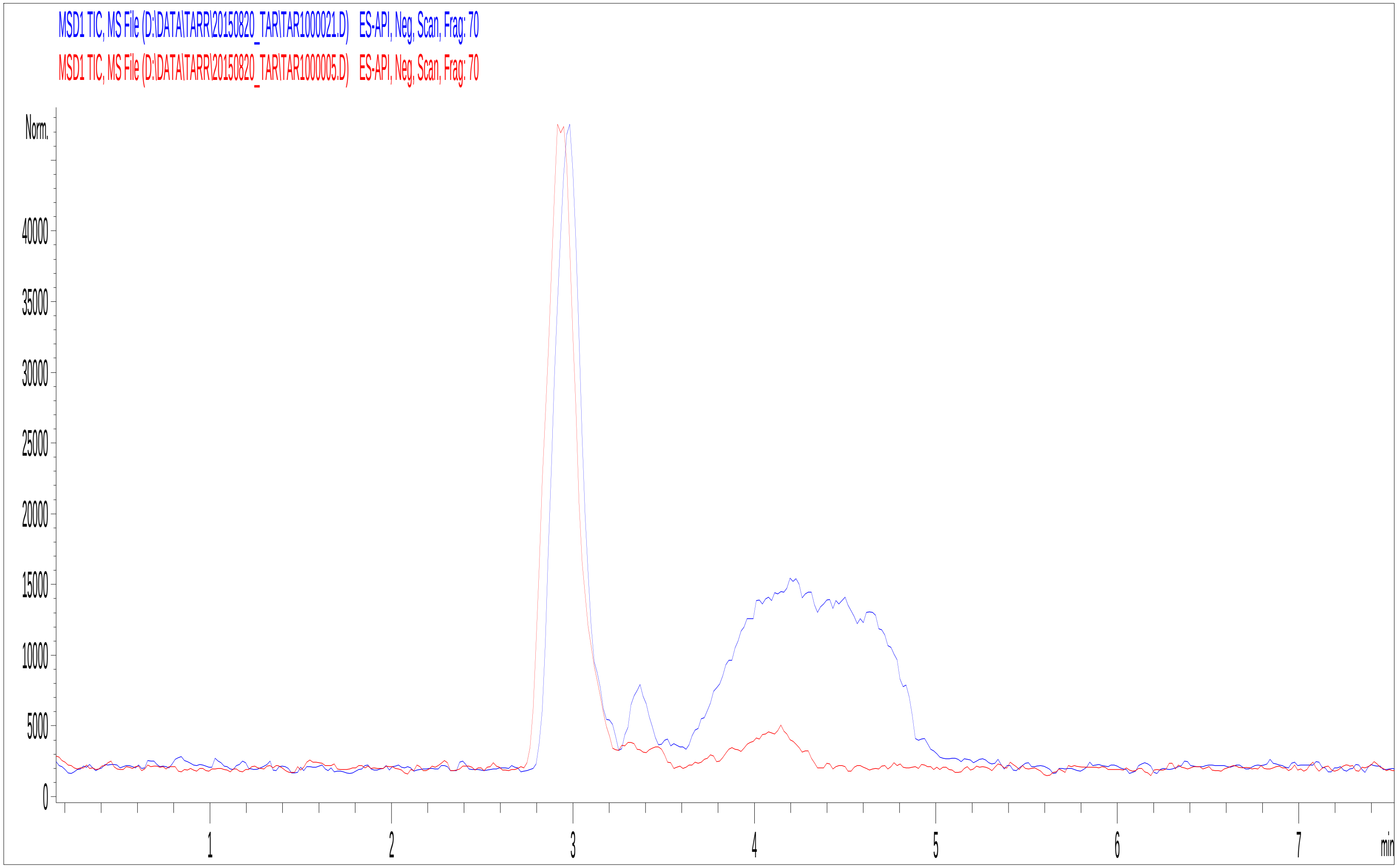
100 DC

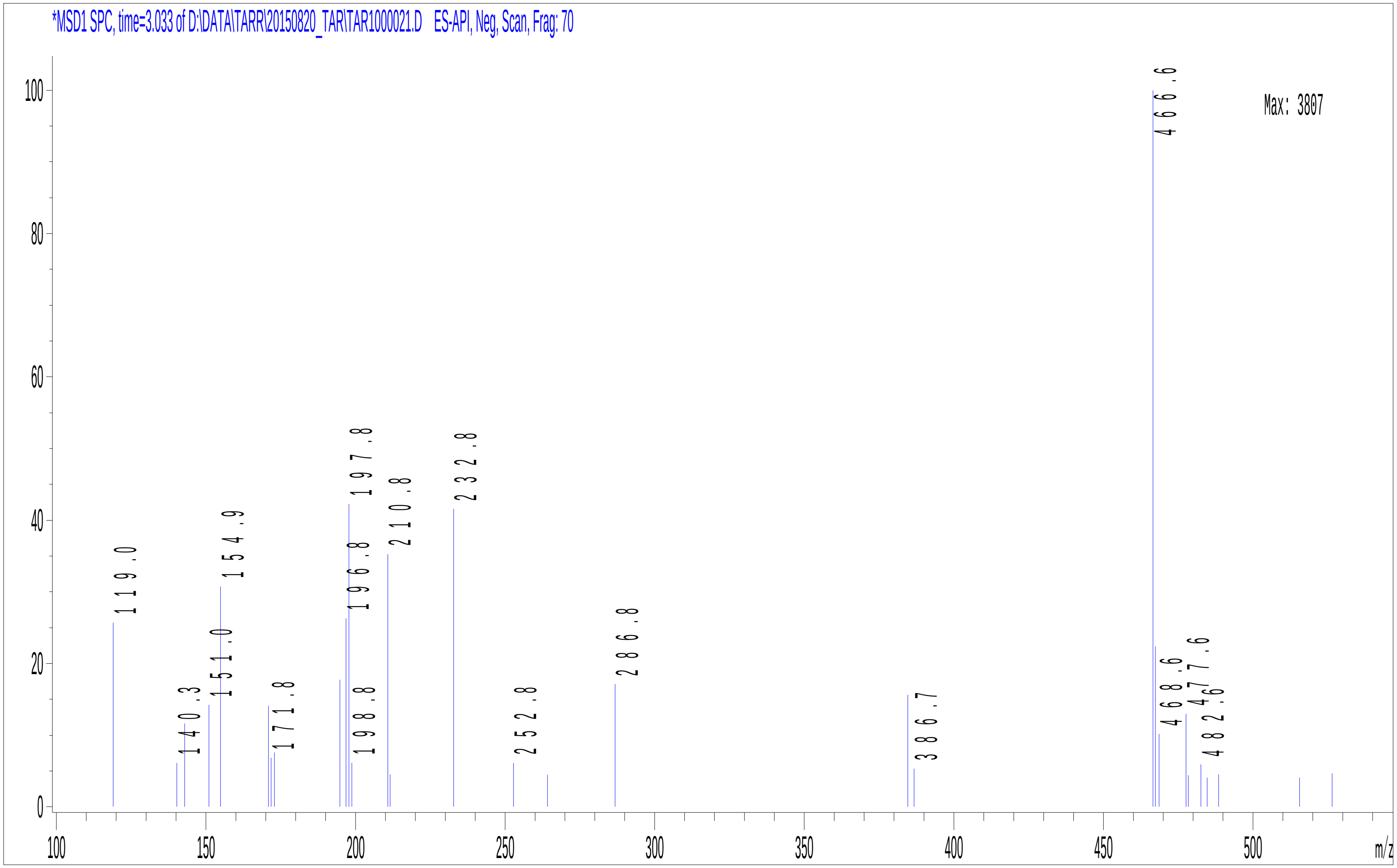
9

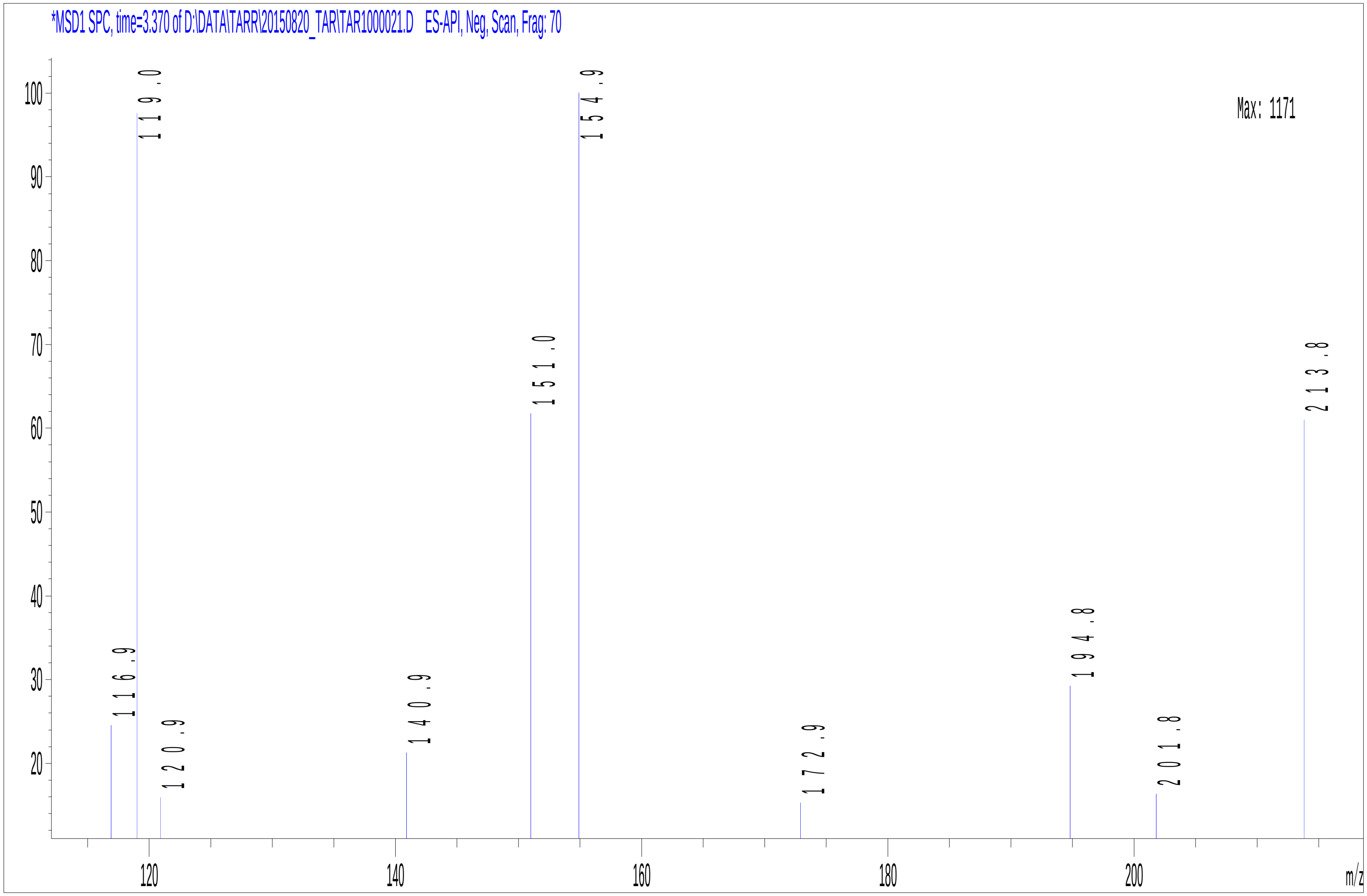
P2-C-03

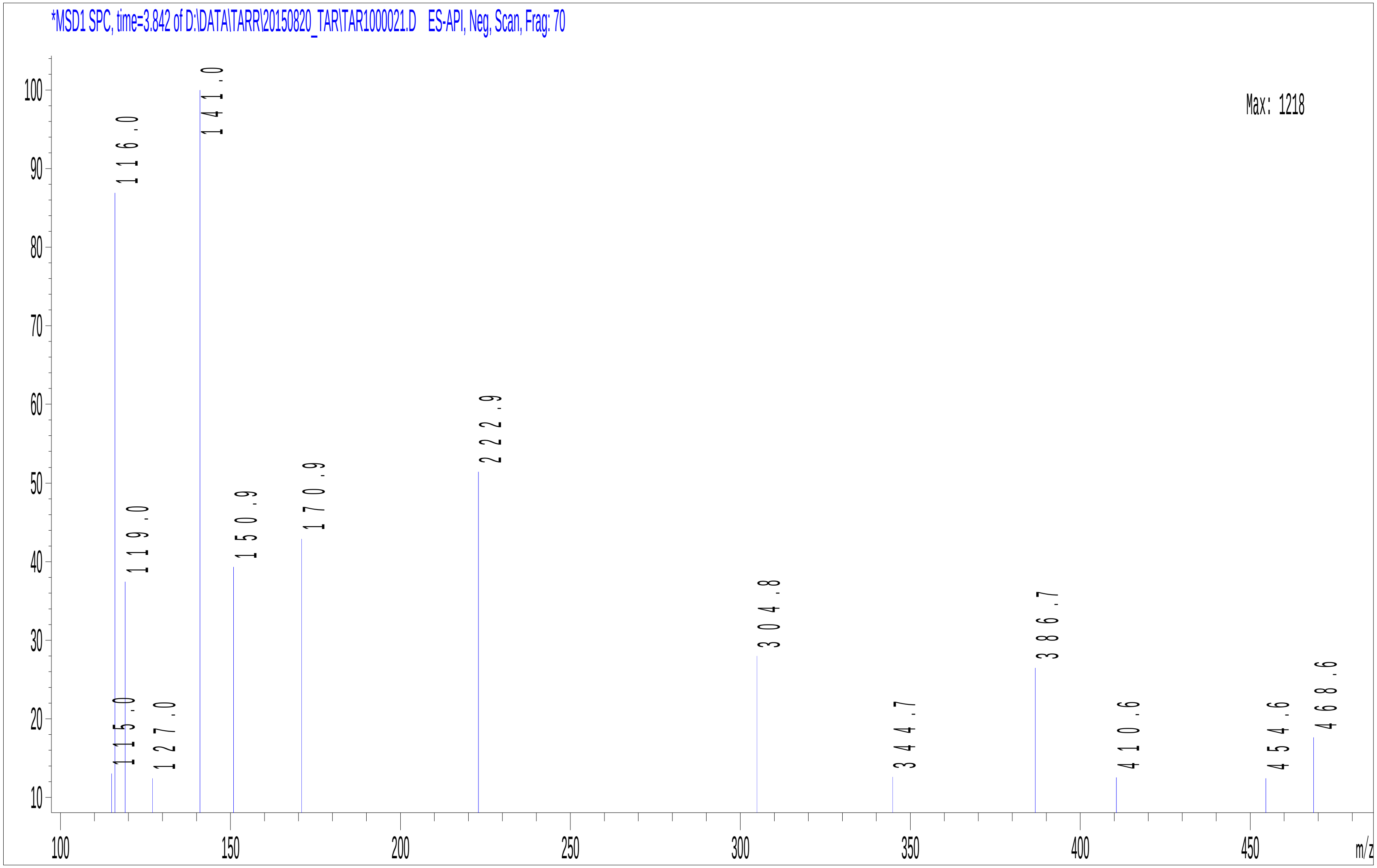


#	Time	Area	Height	Width	Area%	Symmetry
1	2.977	292759.8	26613.9	0.1738	39.417	0.921
2	3.368	36981.6	3468.1	0.1446	4.979	0.585
3	4.2	229379.2	7720.1	0.3921	30.884	2.543
4	4.496	183600.1	6886.4	0.4444	24.720	0.468


MSD1 TIC, MS File (D:\DATA\TARR\20150820_TAR\TAR1000021.D) ES-API, Neg, Scan, Frag: 70
MSD1 TIC, MS File (D:\DATA\TARR\20150820_TAR\TAR1000005.D) ES-API, Neg, Scan, Frag: 70
Norm.
40000
35000
30000
25000
20000
15000
10000
5000
0
1
2
3
4
5
6
7
min


*MSD1 SPC, time=3.033 of D:\DATA\TARR\20150820_TAR\TAR1000021.D ES-API, Neg, Scan, Frag: 70
Max: 3807
119.0
140.3
151.0
154.9
171.8
196.8
197.8
198.8
210.8
232.8
252.8
286.8
386.7
466.6
468.6
477.6
482.6
0
20
40
60
80
100
100
150
200
250
300
350
400
450
500
m/z


*MSD1 SPC, time=3.370 of D:\DATA\TARR\20150820_TAR\TAR1000021.D ES-API, Neg, Scan, Frag: 70
Max: 1171
100
90
80
70
60
50
40
30
20
116.9
119.0
120.9
140.9
151.0
154.9
172.9
194.8
201.8
213.8
120
140
160
180
200
m/z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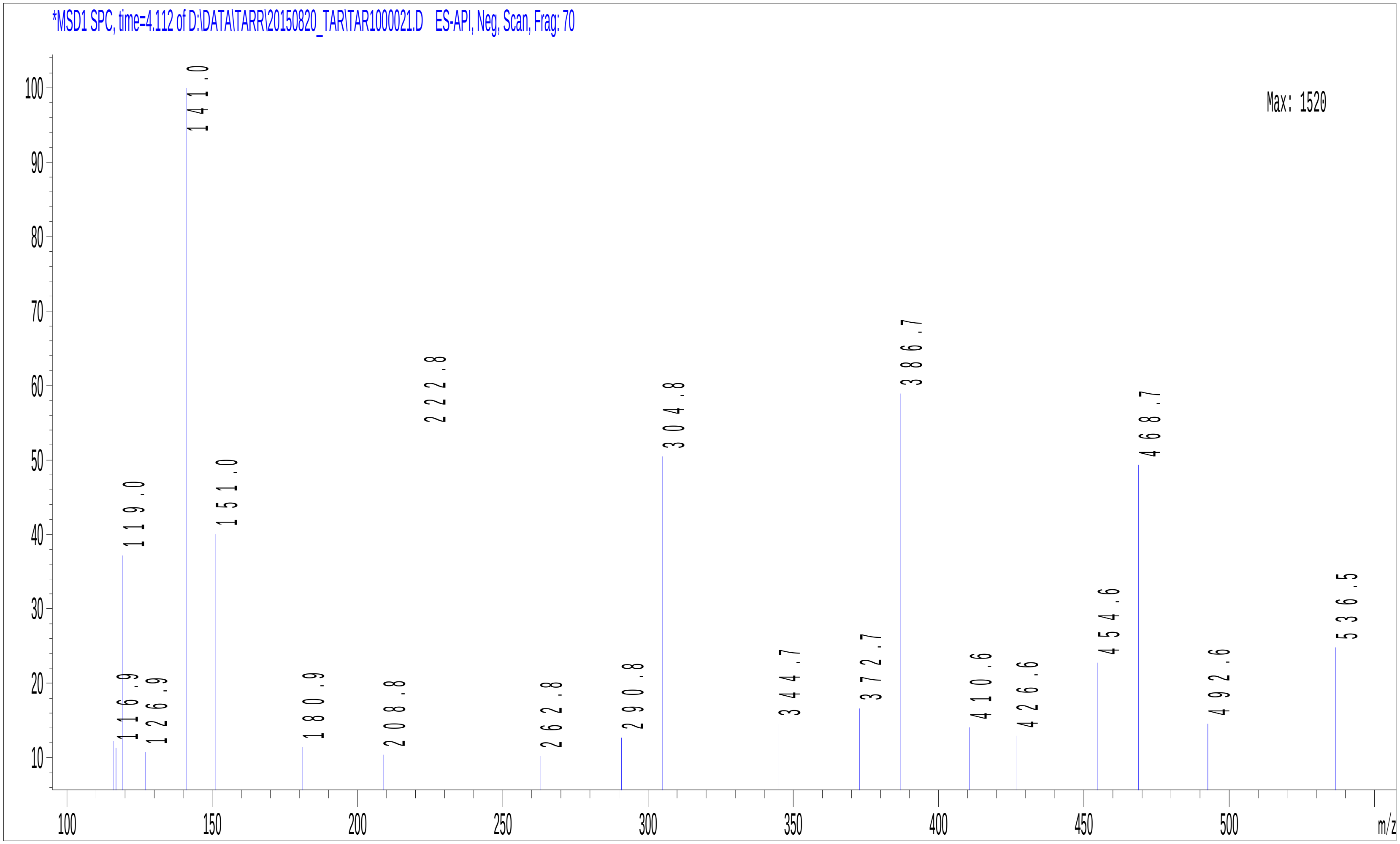
119.0
115.0
127.0
150.9
170.9
222.9
304.8
344.7
386.7
410.6
454.6
468.6
100
90
80
70
60
50
40
30
20
10
100
150
200
250
300
350
400
450
m/z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80
70
60
50
40
30
20
10
100
150
200
250
300
350
400
450
500
m/z
116.9
119.0
126.9
141.0
151.0
180.9
208.8
222.8
262.8
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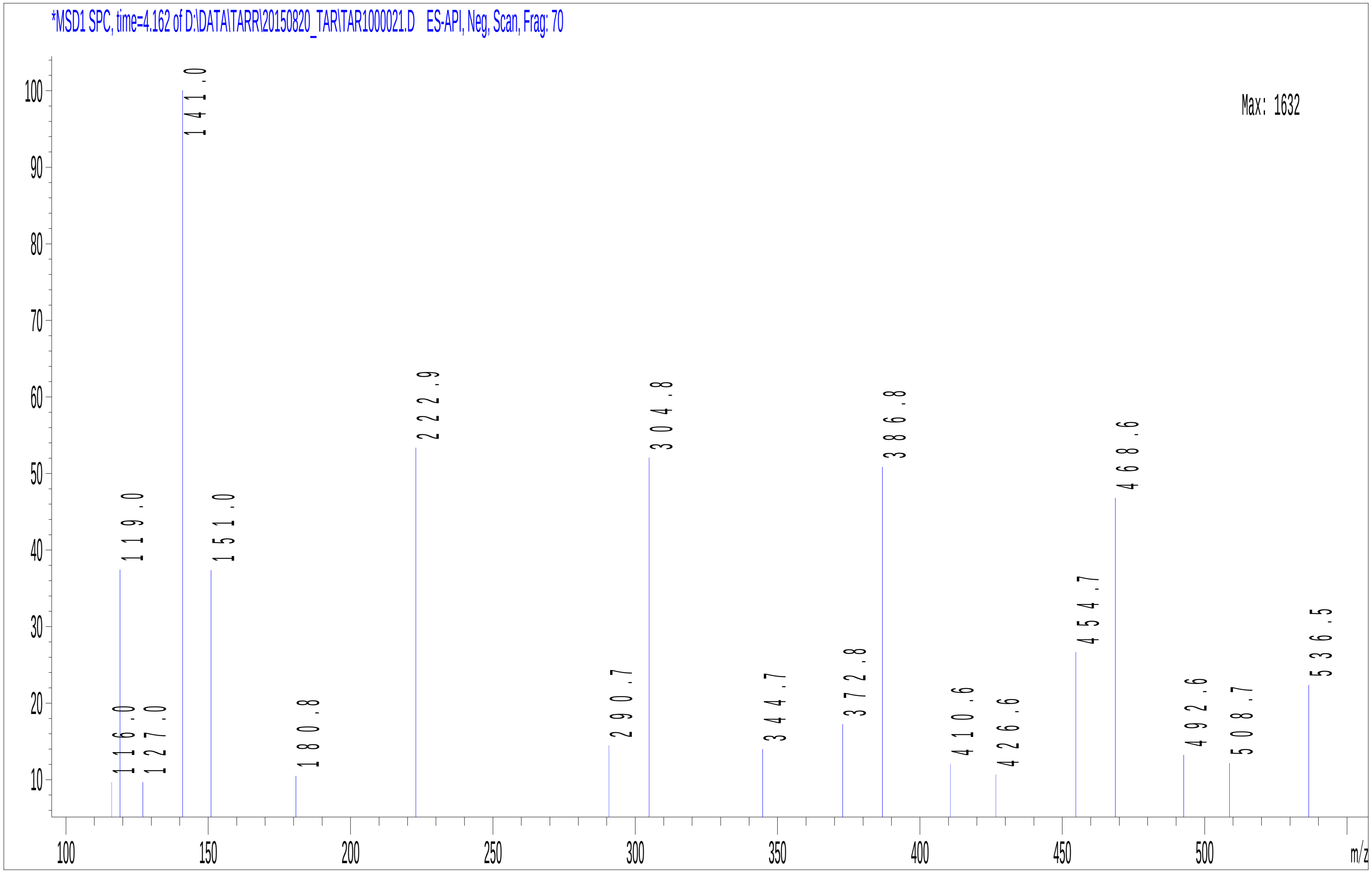
304.8
344.7
372.7
386.7
410.6
426.6
454.6
468.7
492.6
536.5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30
20
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151.0
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304.8
344.7
372.8
386.8
410.6
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400
450
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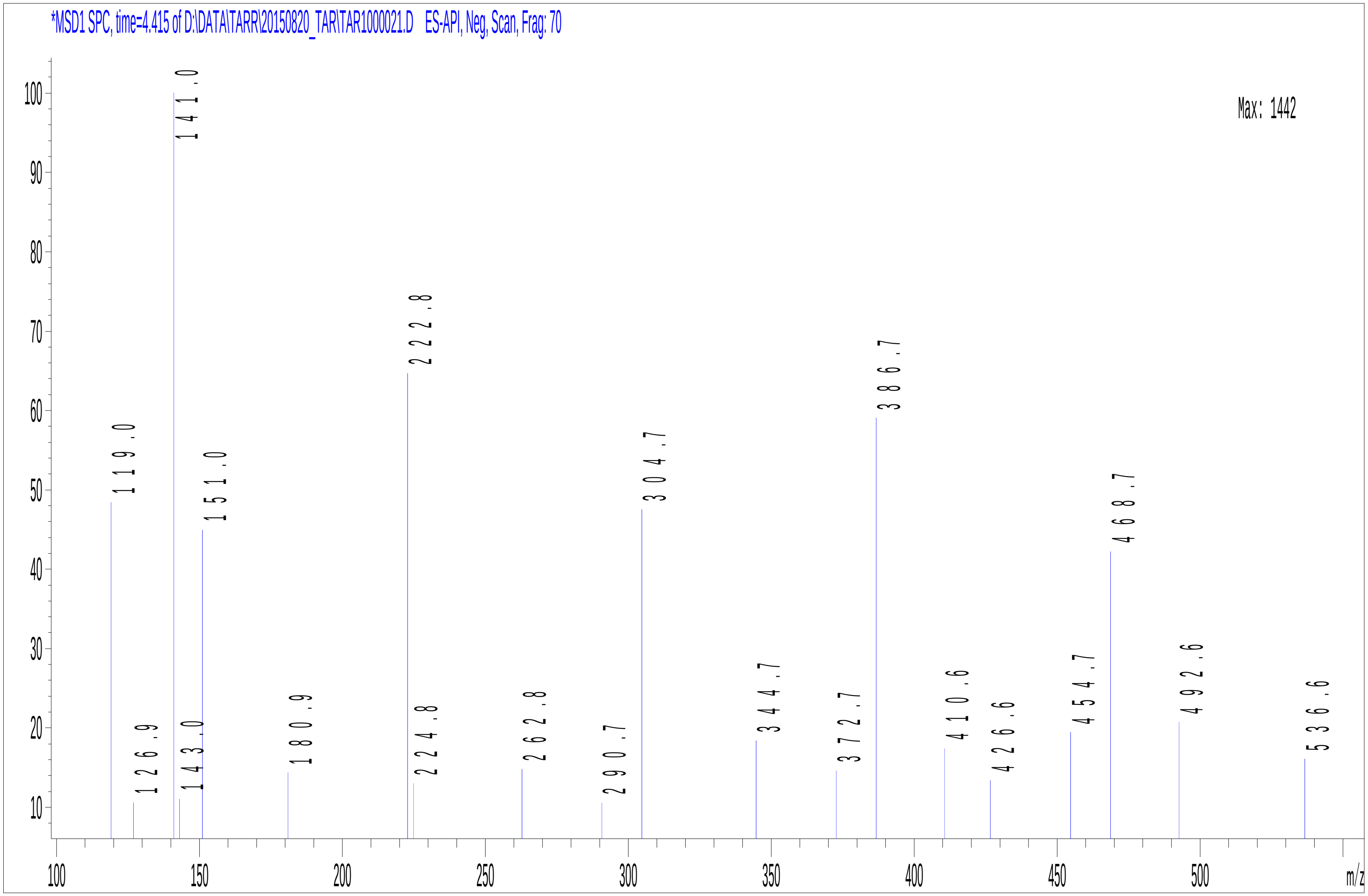
m/z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30
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10
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143.0
151.0
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224.8
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290.7
304.7
344.7
372.7
386.7
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426.6
454.7
468.7
492.6
536.6
100
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200
250
300
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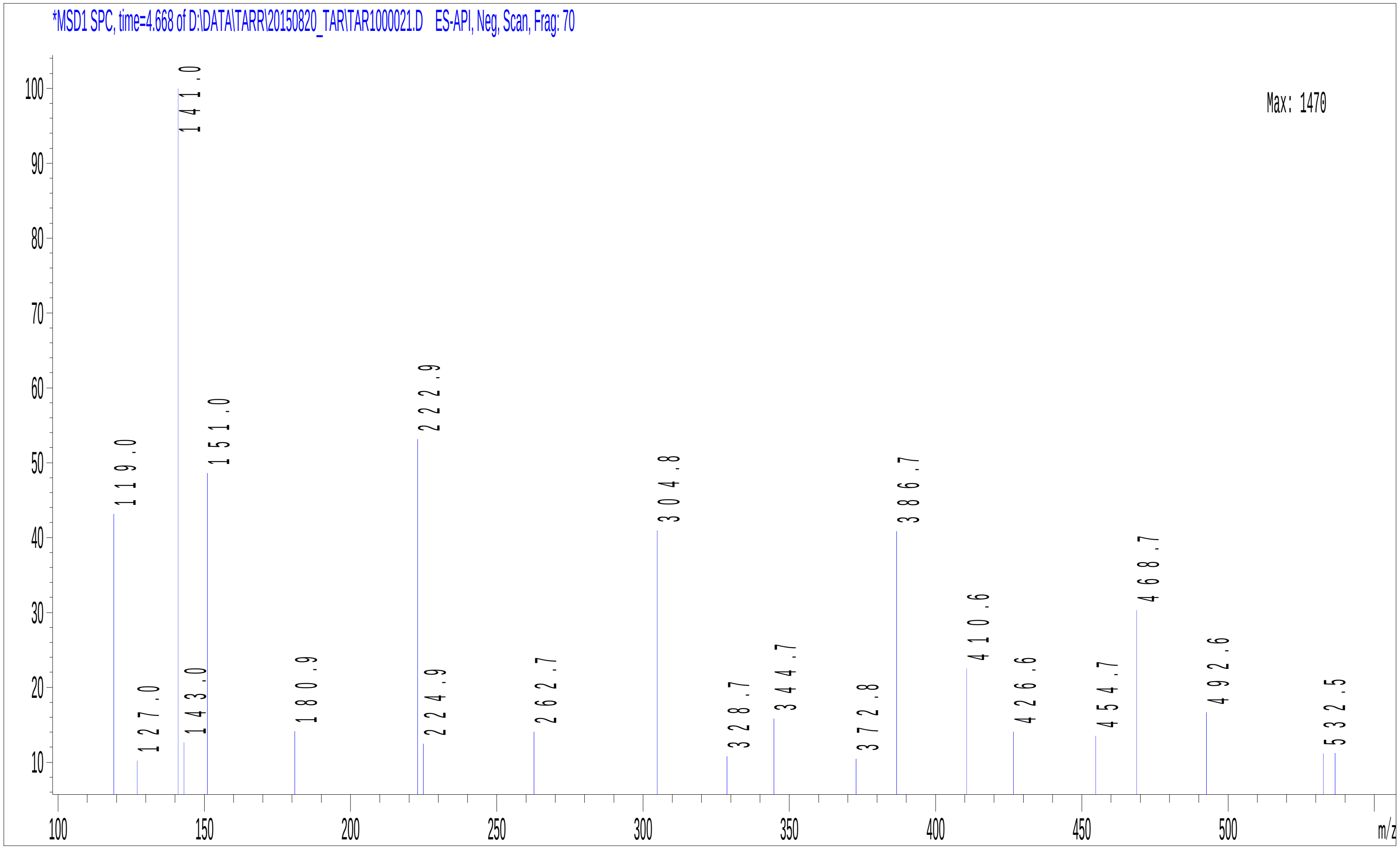
500
m/z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20
10
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143.0
151.0
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222.9
224.9
262.7
304.8
328.7
344.7
372.8
386.7
410.6
426.6
454.7
468.7
492.6
532.5
100
150
200
250
300
350
400
450
500
m/z

Appendix L: Chromatographic Contrast Angle Summaries

Positive

0% DC	Theta (Deg) Whole	Theta (Deg) 2.5-4.5
pH6 Comp w pH8	3.375918422	6.723188691
pH6 Comp w pH9	3.42610567	7.907831248
pH8 Comp w pH9	5.245054624	11.18602854
pH6 Comp w pH7	11.48356239	24.03847461
pH7 Comp w pH8	11.06561411	24.66379254
pH7 Comp w pH9	12.22613449	24.92113008

H_2O_2 Ctrl	Theta (Deg)	Theta (Deg) 2.5-4.5
pH8 Comp w pH9	1.780189654	2.894453995
pH6 Comp w pH8	3.783486646	5.159573841
pH6 Comp w pH9	3.872725509	6.913180549
pH6 Comp w pH7	3.043401804	7.078502639
pH7 Comp w pH8	4.692746649	9.244153793
pH7 Comp w pH9	4.305227895	9.407799531

	Duty Cycle	pH 6	pH 7	pH 8	pH 9
0 DC Comp w H2O2 Ctrl	H2O2 Ctrl	19.84760124	30.06175819	23.32015516	21.96194288
0 DC Comp w 5 DC	5	1.506501447	23.96279159	3.056264052	16.44890953
0 DC Comp w 10 DC	10	5.639061308	14.57841327	2.701092136	11.41825989
0 DC Comp w 20 DC	20	2.44069513	21.24374485	6.73941897	11.94213319
0 DC Comp w 30 DC	30	7.508182612	24.2961799	4.97775981	17.87267424
0 DC Comp w 50 DC	50	4.038199613	10.85555459	12.55758574	17.37739471
0 DC Comp w 70 DC	70	14.23321809	23.80256933	3.379406247	15.41170405
0 DC Comp w 100 DC	100	1.506501447	21.23052869	6.852131469	17.03485288
0 DC Comp w 70 DC (2)	Repeat 70	14.23321809			
0 DC Comp w 100 DC (2)	Repeat 100			7.09280342	

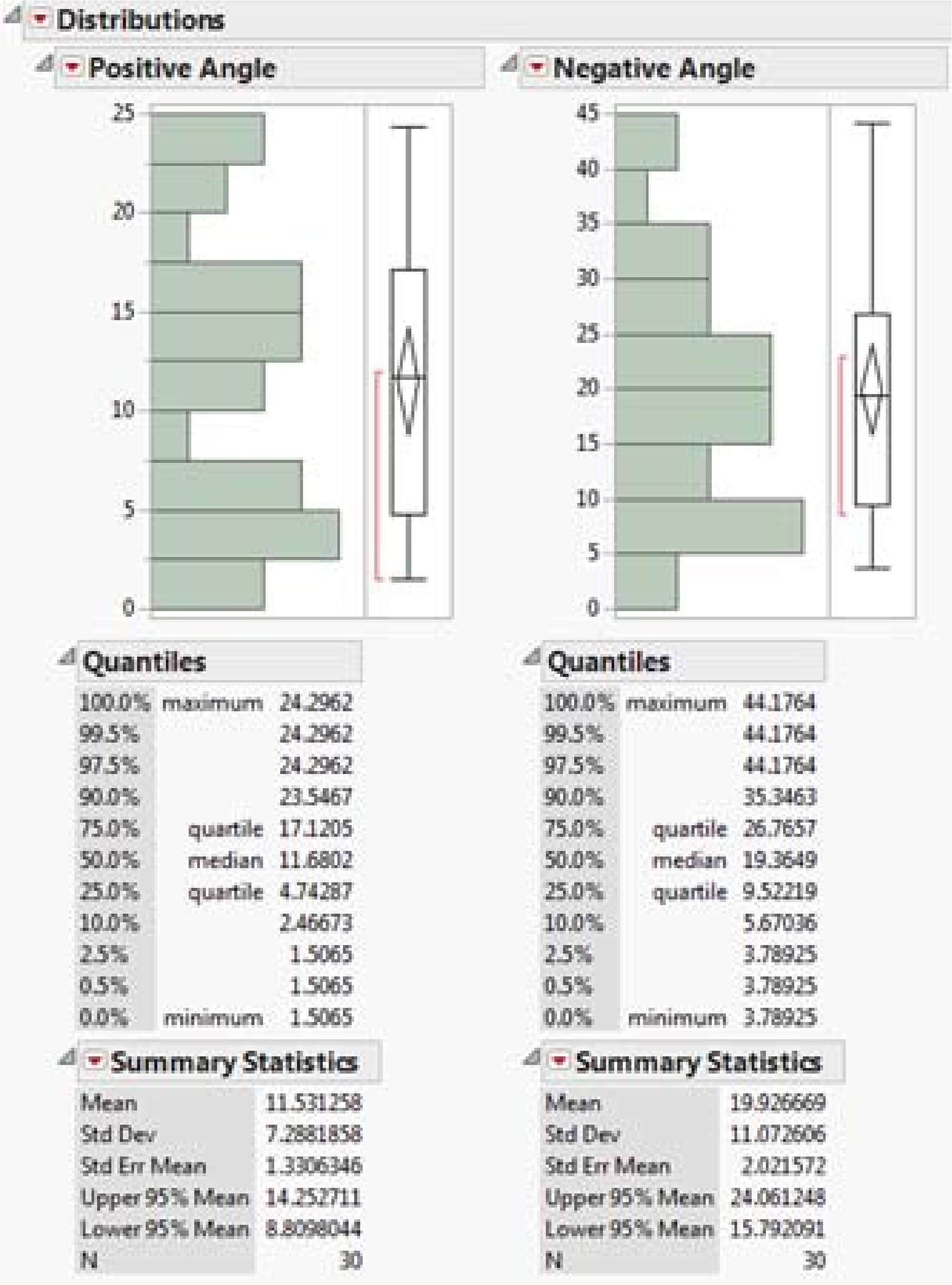
Negative

0% DC	Theta (Deg) 2.5-4.5
pH7 Comp w pH9	16.57104377
pH6 Comp w pH9	16.72608901
pH6 Comp w pH8	20.61519241
pH6 Comp w pH7	23.09971409
pH8 Comp w pH9	30.19031693
pH7 Comp w pH8	37.8272853

H_2O_2 Ctrl	Theta (Deg) 2.5-4.5
pH6 Comp w pH7	3.574156638
pH8 Comp w pH9	6.27061759
pH6 Comp w pH8	12.11077217
pH7 Comp w pH8	12.49426866
pH6 Comp w pH9	17.47102257
pH7 Comp w pH9	17.9140816

	Duty Cycle	pH 6	pH 7	pH 8	pH 9
0 DC Comp w H2O2 Ctrl	H_2O_2 Ctrl	4.287375869	25.39208308	29.21614692	13.98393889
0 DC Comp w 5 DC	5	5.435667548	11.60653237	18.27342076	25.3374457
0 DC Comp w 10 DC	10	3.789254145	12.06138548	17.3084023	8.906979859
0 DC Comp w 20 DC	20	4.236908762	22.6824843	18.94669199	7.782610468
0 DC Comp w 30 DC	30	8.60704675	35.62249185	22.66396489	31.55611185
0 DC Comp w 50 DC	50	32.84861223	44.17639494	26.04684018	43.38847849
0 DC Comp w 70 DC	70	20.80601967	22.9937655	18.44558516	19.78317349
0 DC Comp w 100 DC	100	8.098637143	28.92238094	14.75679853	20.12767796
0 DC Comp w 70 DC (2)	Repeat 70	32.86106106			
0 DC Comp w 100 DC (2)	Repeat 100			9.727257579	

Appendix M: CCA Summary Statistics, ANOVA, and Tukey Analyses



Positive Angle

Quantiles

100.0%	maximum	24.2962
99.5%		24.2962
97.5%		24.2962
90.0%		23.5467
75.0%	quartile	17.1205
50.0%	median	11.6802
25.0%	quartile	4.74287
10.0%		2.46673
2.5%		1.5065
0.5%		1.5065
0.0%	minimum	1.5065

Summary Statistics

Mean	11.531258
Std Dev	7.2881858
Std Err Mean	1.3306346
Upper 95% Mean	14.252711
Lower 95% Mean	8.8098044
N	30

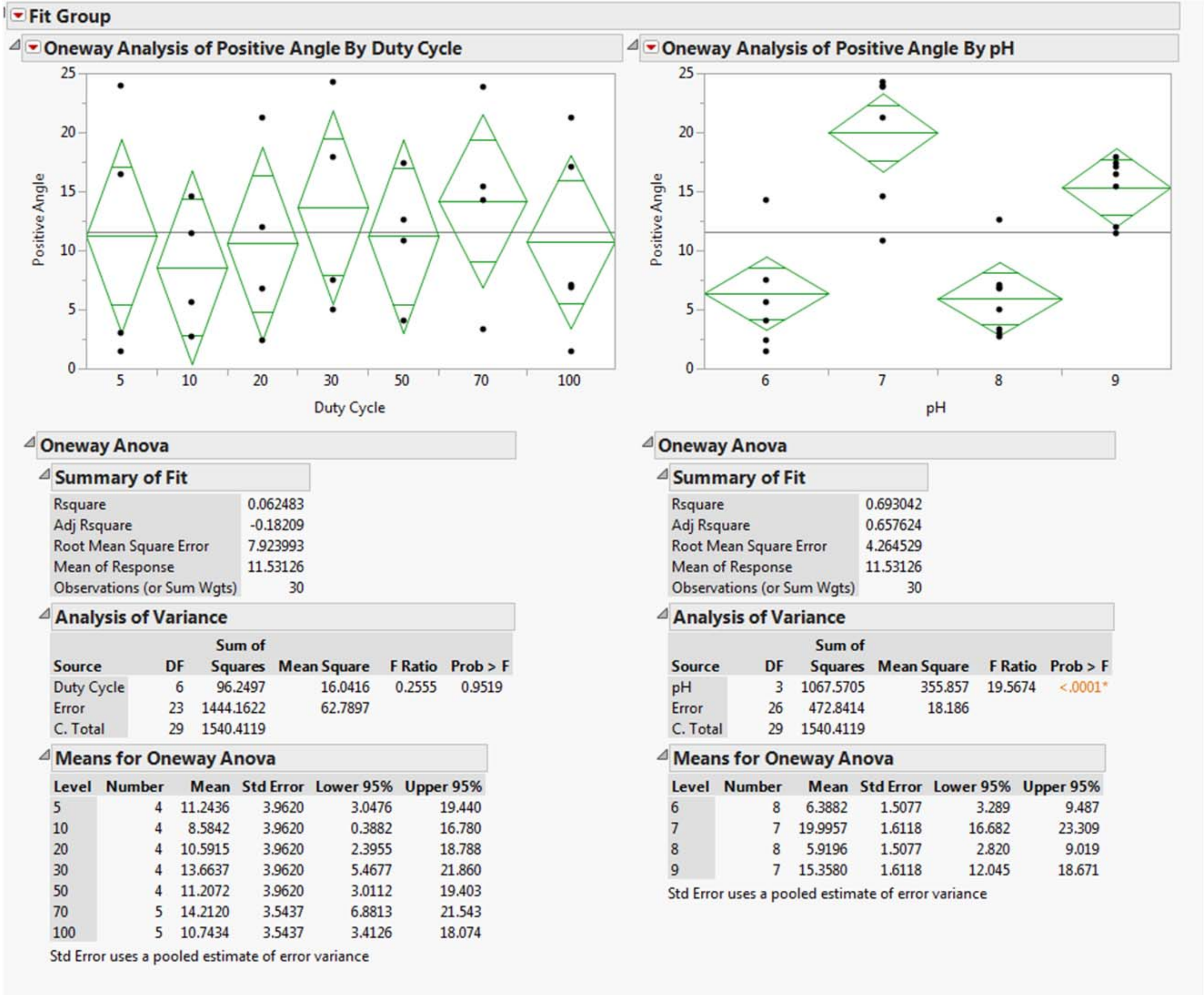
Negative Angle

Quantiles

100.0%	maximum	44.1764
99.5%		44.1764
97.5%		44.1764
90.0%		35.3463
75.0%	quartile	26.7657
50.0%	median	19.3649
25.0%	quartile	9.52219
10.0%		5.67036
2.5%		3.78925
0.5%		3.78925
0.0%	minimum	3.78925

Summary Statistics

Mean	19.926669
Std Dev	11.072606
Std Err Mean	2.021572
Upper 95% Mean	24.061248
Lower 95% Mean	15.792091
N	30



Oneway Anova

Summary of Fit

Rsquare	0.062483
Adj Rsquare	-0.18209
Root Mean Square Error	7.923993
Mean of Response	11.53126
Observations (or Sum Wgts)	30

Analysis of Variance

Source	DF	Sum of Squares	Mean Square	F Ratio	Prob > F
Duty Cycle	6	96.2497	16.0416	0.2555	0.9519
Error	23	1444.1622	62.7897		
C. Total	29	1540.4119			

Means for Oneway Anova

Level	Number	Mean	Std Error	Lower 95%	Upper 95%
5	4	11.2436	3.9620	3.0476	19.440
10	4	8.5842	3.9620	0.3882	16.780
20	4	10.5915	3.9620	2.3955	18.788
30	4	13.6637	3.9620	5.4677	21.860
50	4	11.2072	3.9620	3.0112	19.403
70	5	14.2120	3.5437	6.8813	21.543
100	5	10.7434	3.5437	3.4126	18.074

Std Error uses a pooled estimate of error variance

Oneway Anova

Summary of Fit

Rsquare	0.693042
Adj Rsquare	0.657624
Root Mean Square Error	4.264529
Mean of Response	11.53126
Observations (or Sum Wgts)	30

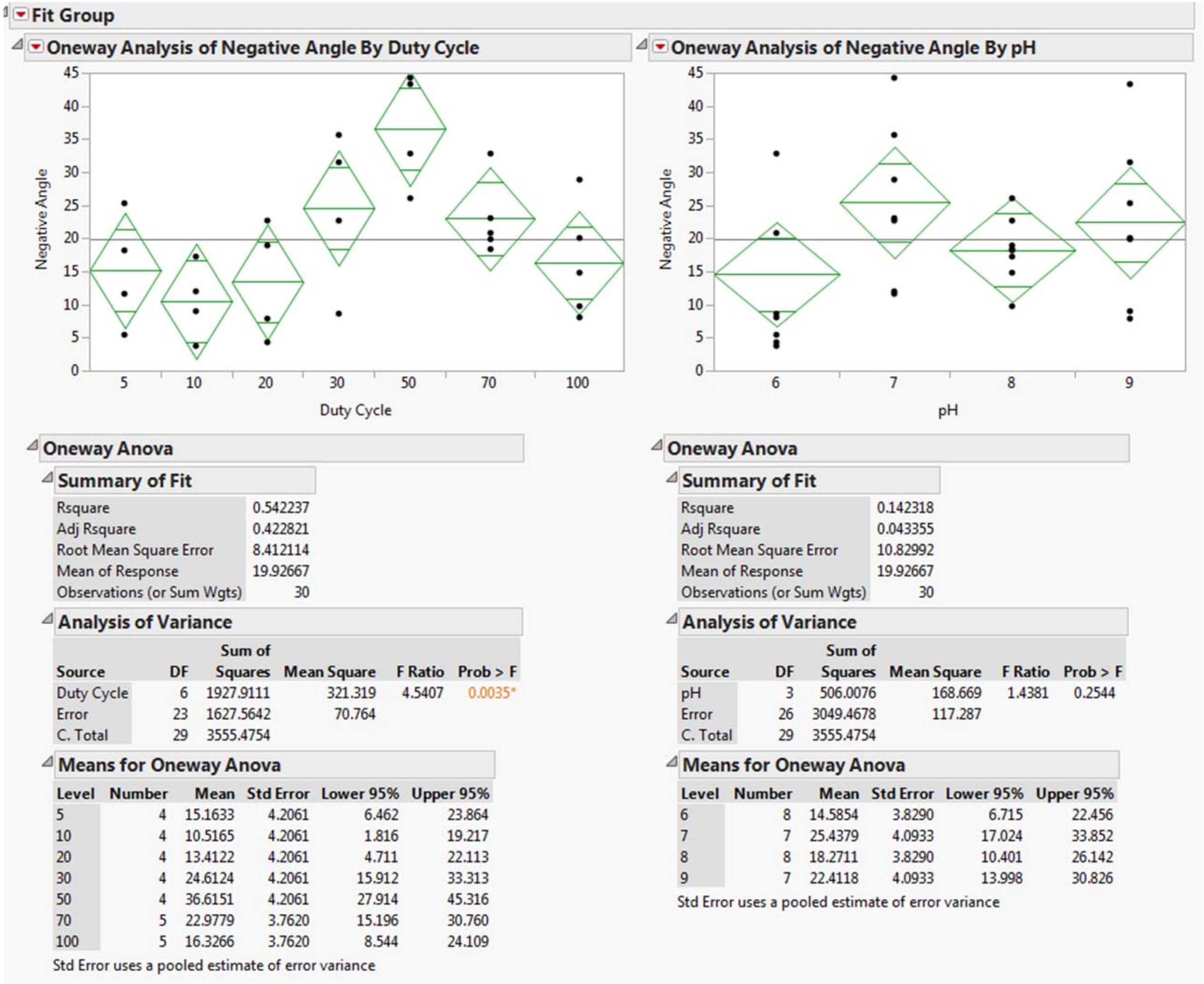
Analysis of Variance

Source	DF	Sum of Squares	Mean Square	F Ratio	Prob > F
pH	3	1067.5705	355.857	19.5674	<.0001*
Error	26	472.8414	18.186		
C. Total	29	1540.4119			

Means for Oneway Anova

Level	Number	Mean	Std Error	Lower 95%	Upper 95%
6	8	6.3882	1.5077	3.289	9.487
7	7	19.9957	1.6118	16.682	23.309
8	8	5.9196	1.5077	2.820	9.019
9	7	15.3580	1.6118	12.045	18.671

Std Error uses a pooled estimate of error variance



Fit Group

Oneway Analysis of Negative Angle By Duty Cycle

Oneway Anova

Summary of Fit

Rsquare	0.542237
Adj Rsquare	0.422821
Root Mean Square Error	8.412114
Mean of Response	19.92667
Observations (or Sum Wgts)	30

Analysis of Variance

Source	DF	Sum of Squares	Mean Square	F Ratio	Prob > F
Duty Cycle	6	1927.9111	321.319	4.5407	0.0035*
Error	23	1627.5642	70.764		
C. Total	29	3555.4754			

Means for Oneway Anova

Level	Number	Mean	Std Error	Lower 95%	Upper 95%
5	4	15.1633	4.2061	6.462	23.864
10	4	10.5165	4.2061	1.816	19.217
20	4	13.4122	4.2061	4.711	22.113
30	4	24.6124	4.2061	15.912	33.313
50	4	36.6151	4.2061	27.914	45.316
70	5	22.9779	3.7620	15.196	30.760
100	5	16.3266	3.7620	8.544	24.109

Std Error uses a pooled estimate of error variance

Oneway Analysis of Negative Angle By pH

Oneway Anova

Summary of Fit

Rsquare	0.142318
Adj Rsquare	0.043355
Root Mean Square Error	10.82992
Mean of Response	19.92667
Observations (or Sum Wgts)	30

Analysis of Variance

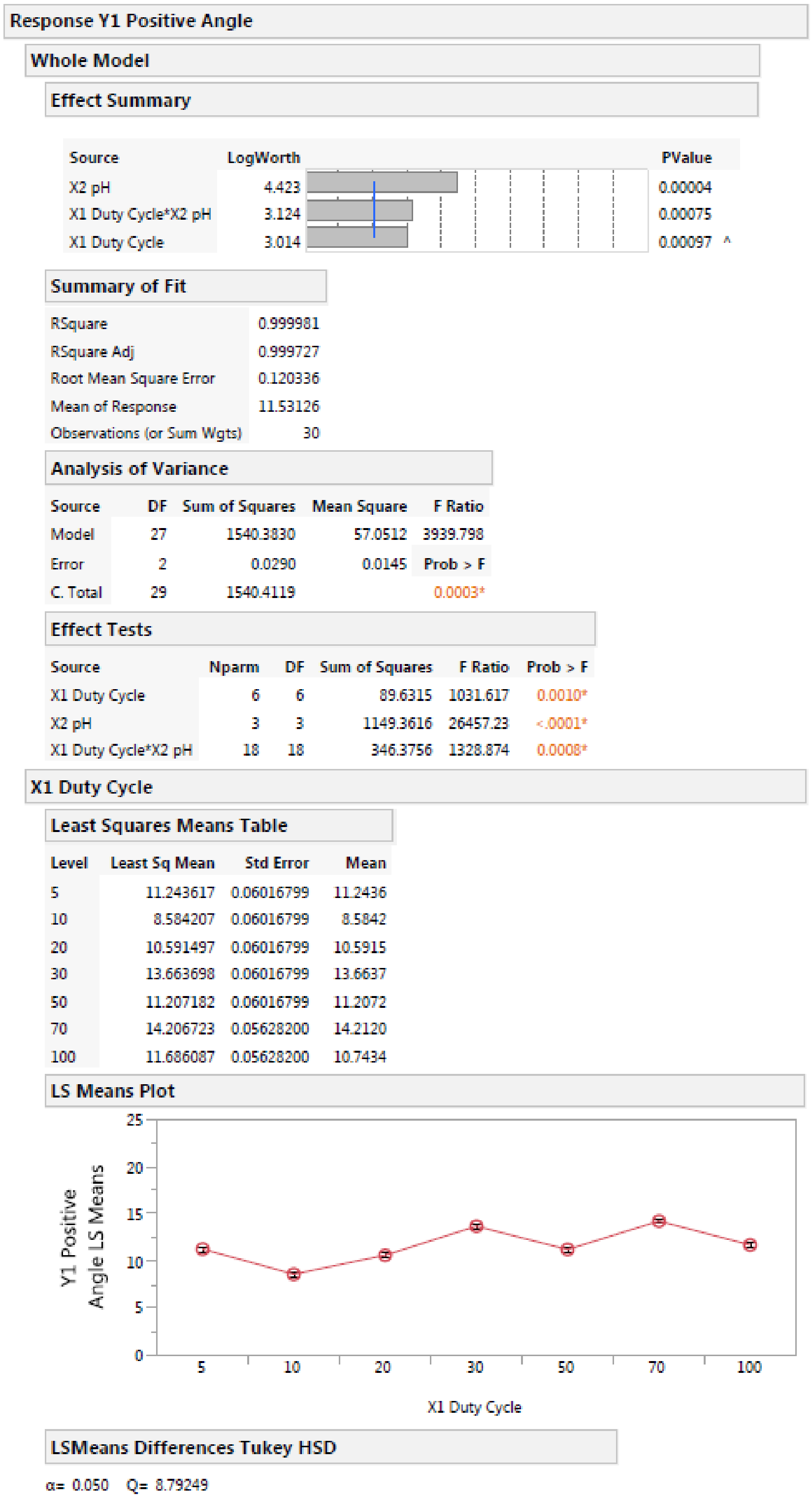
Source	DF	Sum of Squares	Mean Square	F Ratio	Prob > F
pH	3	506.0076	168.669	1.4381	0.2544
Error	26	3049.4678	117.287		
C. Total	29	3555.4754			

Means for Oneway Anova

Level	Number	Mean	Std Error	Lower 95%	Upper 95%
6	8	14.5854	3.8290	6.715	22.456
7	7	25.4379	4.0933	17.024	33.852
8	8	18.2711	3.8290	10.401	26.142
9	7	22.4118	4.0933	13.998	30.826

Std Error uses a pooled estimate of error variance

Positive Ionization CCA Tukey Analysis



Response Y1 Positive Angle

Whole Model

Effect Summary

Source	LogWorth	PValue
X2 pH	4.423	0.00004
X1 Duty Cycle*X2 pH	3.124	0.00075
X1 Duty Cycle	3.014	0.00097 ^

Summary of Fit

RSquare	0.999981
RSquare Adj	0.999727
Root Mean Square Error	0.120336
Mean of Response	11.53126
Observations (or Sum Wgts)	30

Analysis of Variance

Source	DF	Sum of Squares	Mean Square	F Ratio
Model	27	1540.3830	57.0512	3939.798
Error	2	0.0290	0.0145	Prob > F
C. Total	29	1540.4119		0.0003*

Effect Tests

Source	Nparm	DF	Sum of Squares	F Ratio	Prob > F
X1 Duty Cycle	6	6	89.6315	1031.617	0.0010*
X2 pH	3	3	1149.3616	26457.23	<.0001*
X1 Duty Cycle*X2 pH	18	18	346.3756	1328.874	0.0008*

X1 Duty Cycle

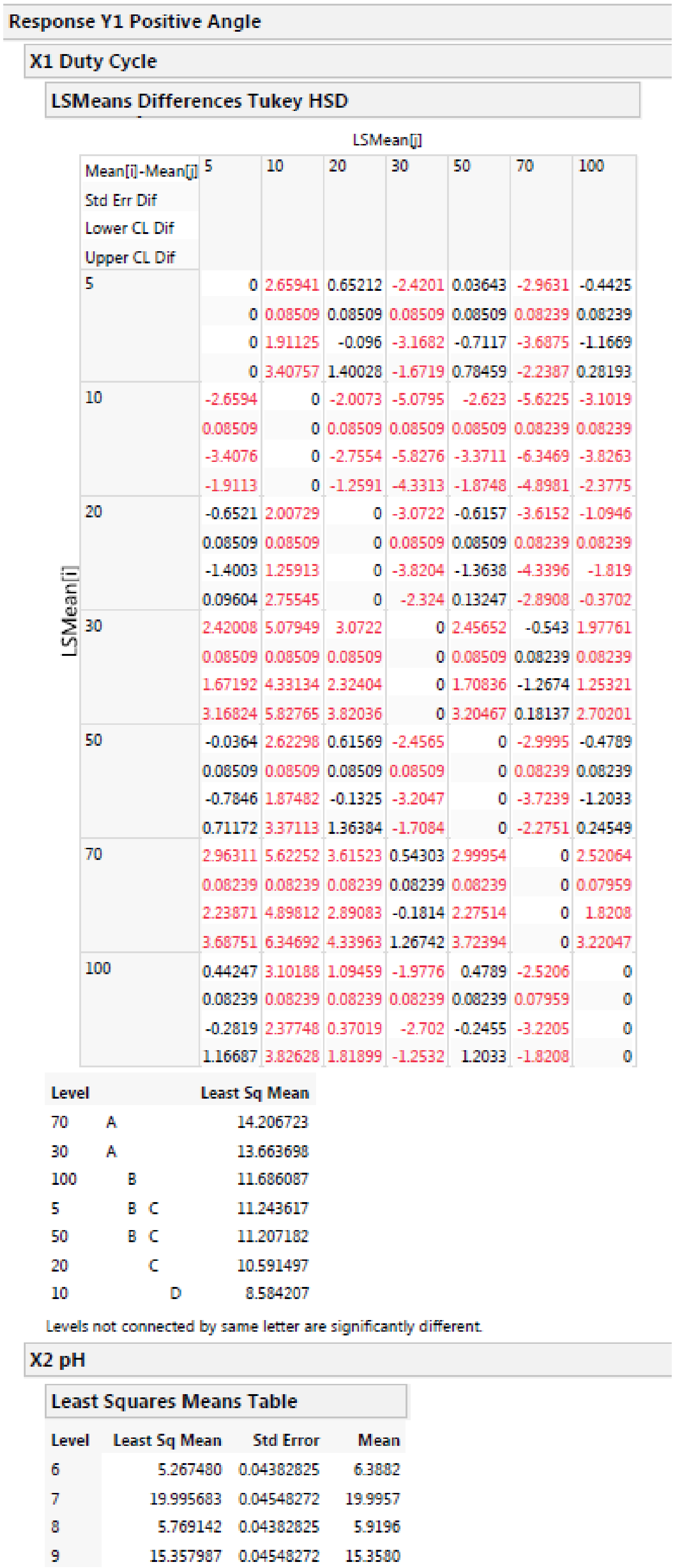
Least Squares Means Table

Level	Least Sq Mean	Std Error	Mean
5	11.243617	0.06016799	11.2436
10	8.584207	0.06016799	8.5842
20	10.591497	0.06016799	10.5915
30	13.663698	0.06016799	13.6637
50	11.207182	0.06016799	11.2072
70	14.206723	0.05628200	14.2120
100	11.686087	0.05628200	10.7434

LS Means Plot

LSMeans Differences Tukey HSD

α= 0.050 Q= 8.79249



Response Y1 Positive Angle

X1 Duty Cycle

LSMeans Differences Tukey HSD

LSMean[j]

	Mean[i]-Mean[j] Std Err Dif Lower CL Dif Upper CL Dif	5	10	20	30	50	70	100
LSMean[i]	5	0	2.65941	0.65212	-2.4201	0.03643	-2.9631	-0.4425
		0	0.08509	0.08509	0.08509	0.08509	0.08239	0.08239
		0	1.91125	-0.096	-3.1682	-0.7117	-3.6875	-1.1669
		0	3.40757	1.40028	-1.6719	0.78459	-2.2387	0.28193
	10	-2.6594	0	-2.0073	-5.0795	-2.623	-5.6225	-3.1019
		0.08509	0	0.08509	0.08509	0.08509	0.08239	0.08239
		-3.4076	0	-2.7554	-5.8276	-3.3711	-6.3469	-3.8263
		-1.9113	0	-1.2591	-4.3313	-1.8748	-4.8981	-2.3775
	20	-0.6521	2.00729	0	-3.0722	-0.6157	-3.6152	-1.0946
		0.08509	0.08509	0	0.08509	0.08509	0.08239	0.08239
		-1.4003	1.25913	0	-3.8204	-1.3638	-4.3396	-1.819
		0.09604	2.75545	0	-2.324	0.13247	-2.8908	-0.3702
	30	2.42008	5.07949	3.0722	0	2.45652	-0.543	1.97761
		0.08509	0.08509	0.08509	0	0.08509	0.08239	0.08239
		1.67192	4.33134	2.32404	0	1.70836	-1.2674	1.25321
		3.16824	5.82765	3.82036	0	3.20467	0.18137	2.70201
	50	-0.0364	2.62298	0.61569	-2.4565	0	-2.9995	-0.4789
		0.08509	0.08509	0.08509	0.08509	0	0.08239	0.08239
		-0.7846	1.87482	-0.1325	-3.2047	0	-3.7239	-1.2033
		0.71172	3.37113	1.36384	-1.7084	0	-2.2751	0.24549
	70	2.96311	5.62252	3.61523	0.54303	2.99954	0	2.52064
		0.08239	0.08239	0.08239	0.08239	0.08239	0	0.07959
		2.23871	4.89812	2.89083	-0.1814	2.27514	0	1.8208
		3.68751	6.34692	4.33963	1.26742	3.72394	0	3.22047
	100	0.44247	3.10188	1.09459	-1.9776	0.4789	-2.5206	0
		0.08239	0.08239	0.08239	0.08239	0.08239	0.07959	0
		-0.2819	2.37748	0.37019	-2.702	-0.2455	-3.2205	0
		1.16687	3.82628	1.81899	-1.2532	1.2033	-1.8208	0

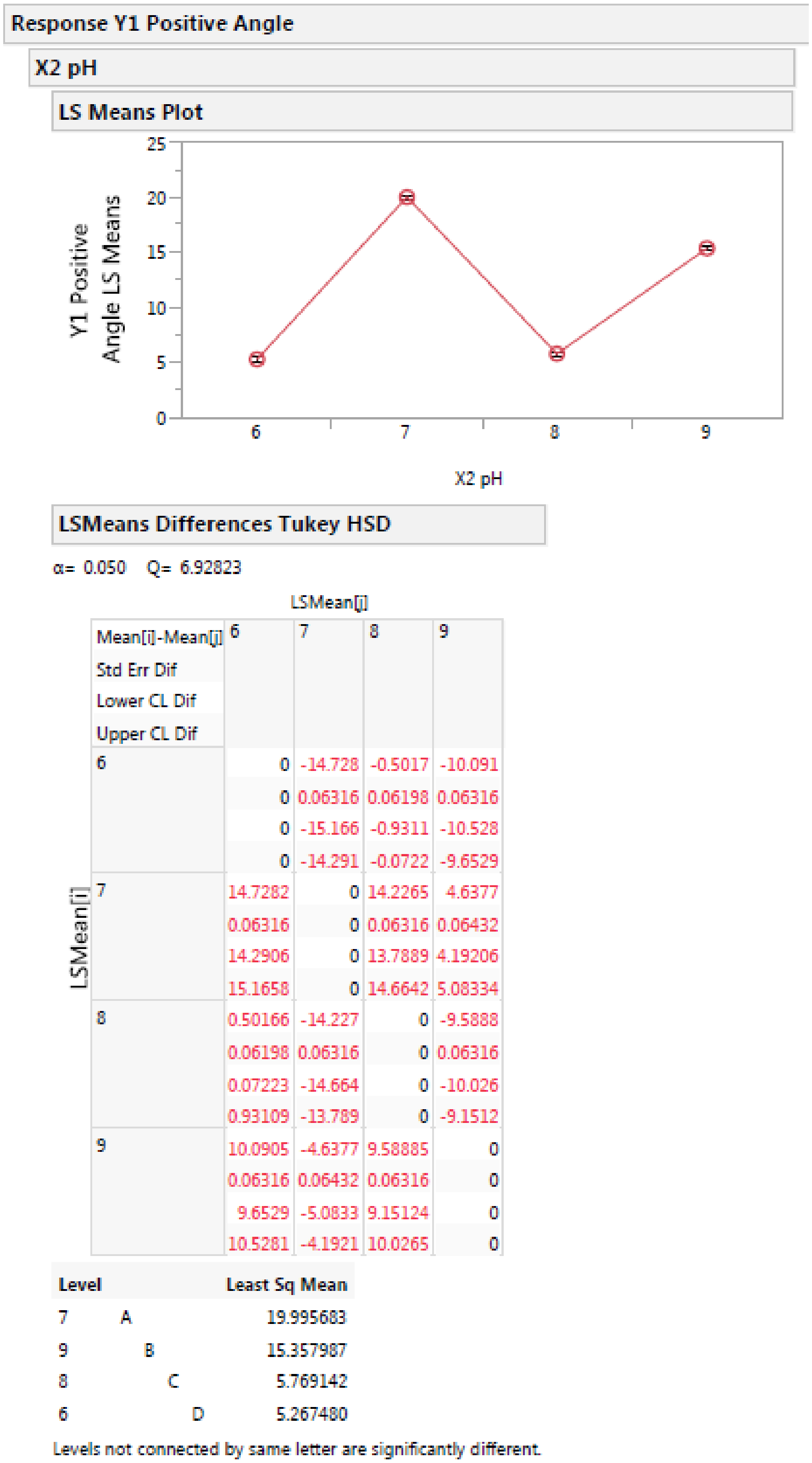
Level					Least Sq Mean
70	A				14.206723
30	A				13.663698
100		B			11.686087
5		B	C		11.243617
50		B	C		11.207182
20			C		10.591497
10				D	8.584207

Levels not connected by same letter are significantly different.

X2 pH

Least Squares Means Table

Level	Least Sq Mean	Std Error	Mean
6	5.267480	0.04382825	6.3882
7	19.995683	0.04548272	19.9957
8	5.769142	0.04382825	5.9196
9	15.357987	0.04548272	15.3580



Response Y1 Positive Angle

X2 pH

LS Means Plot

LSMeans Differences Tukey HSD

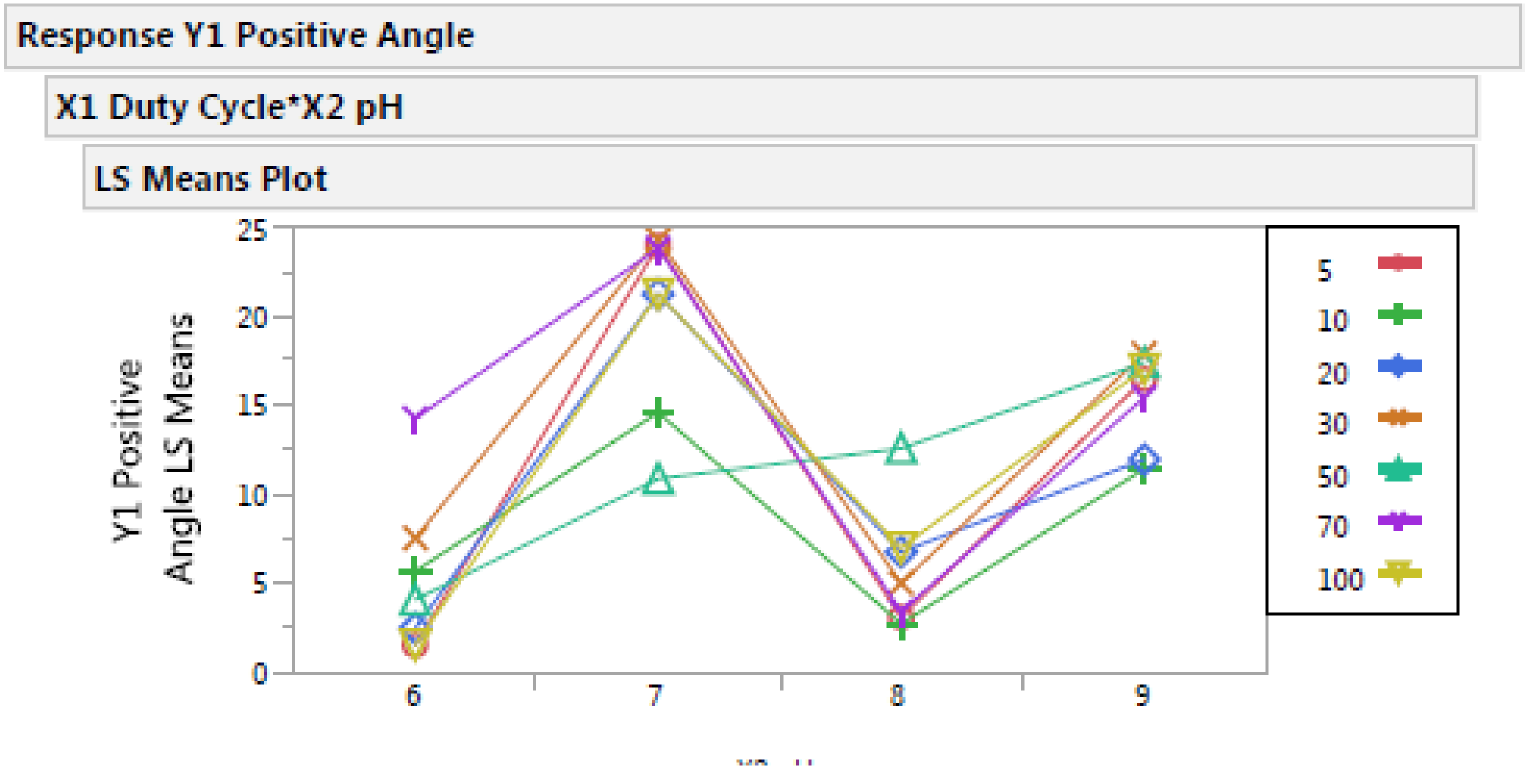
α= 0.050 Q= 6.92823

LSMean[j]

LSMean[i]	Mean[i]-Mean[j] Std Err Dif Lower CL Dif Upper CL Dif	6	7	8	9
	6	0 0 0 0	-14.728 0.06316 -15.166 -14.291	-0.5017 0.06198 -0.9311 -0.0722	-10.091 0.06316 -10.528 -9.6529
	7	14.7282 0.06316 14.2906 15.1658	0 0 0 0	14.2265 0.06316 13.7889 14.6642	4.6377 0.06432 4.19206 5.08334
	8	0.50166 0.06198 0.07223 0.93109	-14.227 0.06316 -14.664 -13.789	0 0 0 0	-9.5888 0.06316 -10.026 -9.1512
	9	10.0905 0.06316 9.6529 10.5281	-4.6377 0.06432 -5.0833 -4.1921	9.58885 0.06316 9.15124 10.0265	0 0 0 0

Level					Least Sq Mean
7	A				19.995683
9		B			15.357987
8			C		5.769142
6				D	5.267480

Levels not connected by same letter are significantly different.

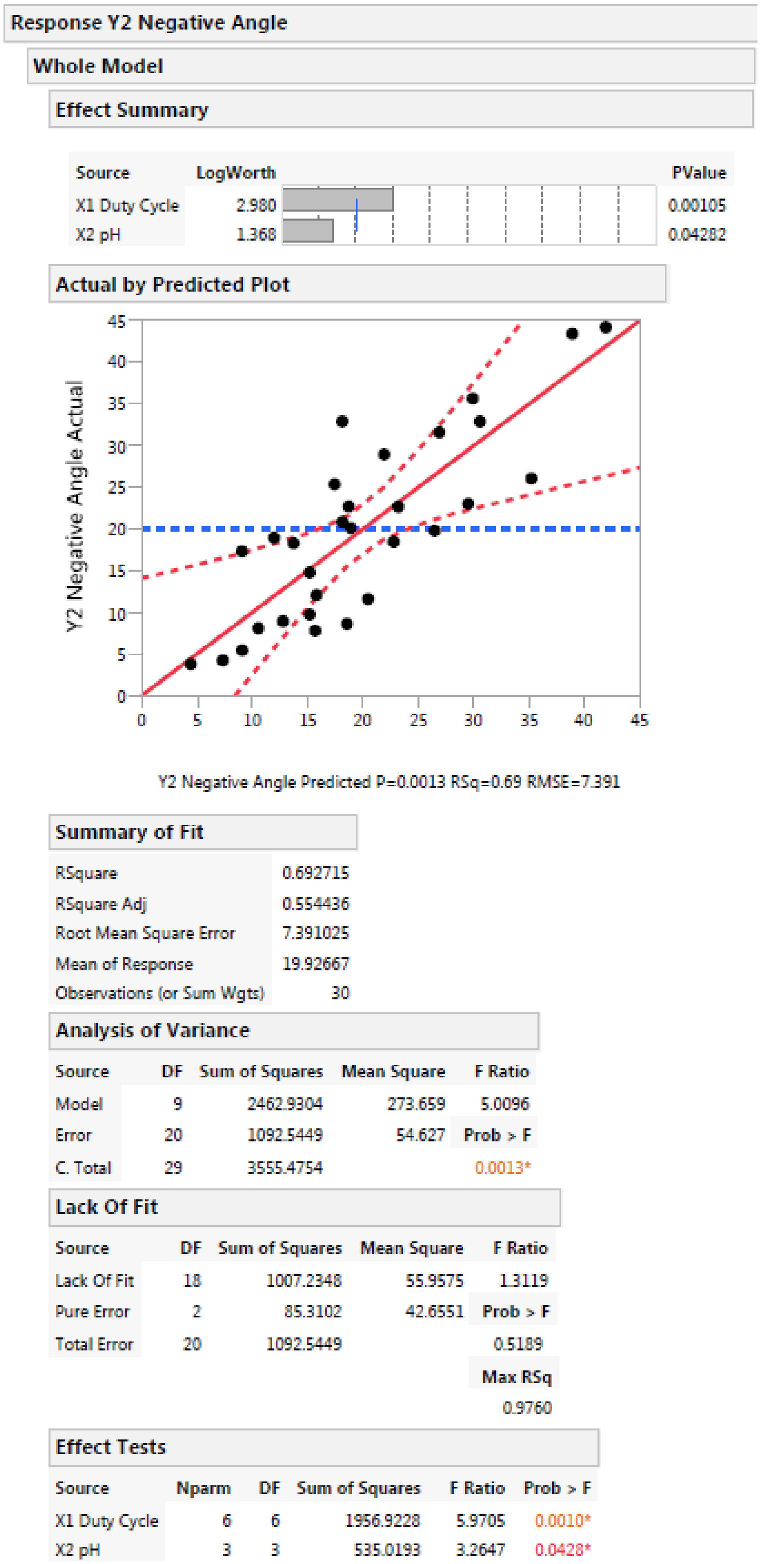


Response Y1 Positive Angle

X1 Duty Cycle*X2 pH

LS Means Plot

Negative Ionization CCA Tukey Analysis



Response Y2 Negative Angle

Whole Model

Effect Summary

Source	LogWorth	PValue
X1 Duty Cycle	2.980	0.00105
X2 pH	1.368	0.04282

Actual by Predicted Plot

Y2 Negative Angle Predicted P=0.0013 RSq=0.69 RMSE=7.391

Summary of Fit

RSquare	0.692715
RSquare Adj	0.554436
Root Mean Square Error	7.391025
Mean of Response	19.92667
Observations (or Sum Wgts)	30

Analysis of Variance

Source	DF	Sum of Squares	Mean Square	F Ratio
Model	9	2462.9304	273.659	5.0096
Error	20	1092.5449	54.627	Prob > F
C. Total	29	3555.4754		0.0013*

Lack Of Fit

Source	DF	Sum of Squares	Mean Square	F Ratio
Lack Of Fit	18	1007.2348	55.9575	1.3119
Pure Error	2	85.3102	42.6551	Prob > F
Total Error	20	1092.5449		0.5189
				Max RSq
				0.9760

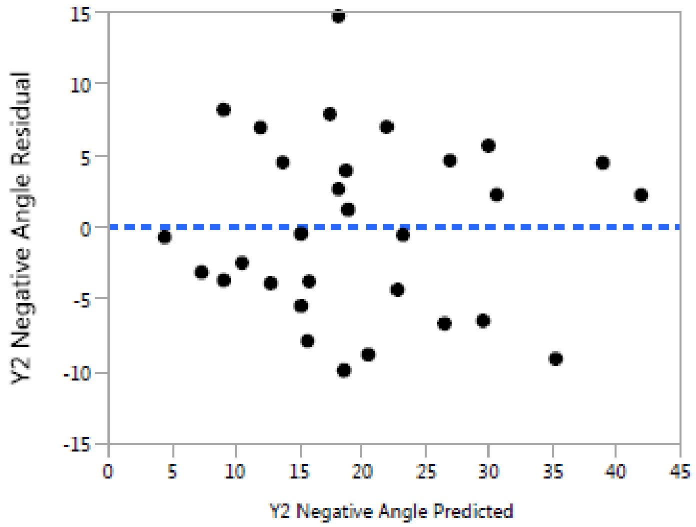
Effect Tests

Source	Nparm	DF	Sum of Squares	F Ratio	Prob > F
X1 Duty Cycle	6	6	1956.9228	5.9705	0.0010*
X2 pH	3	3	535.0193	3.2647	0.0428*

Response Y2 Negative Angle

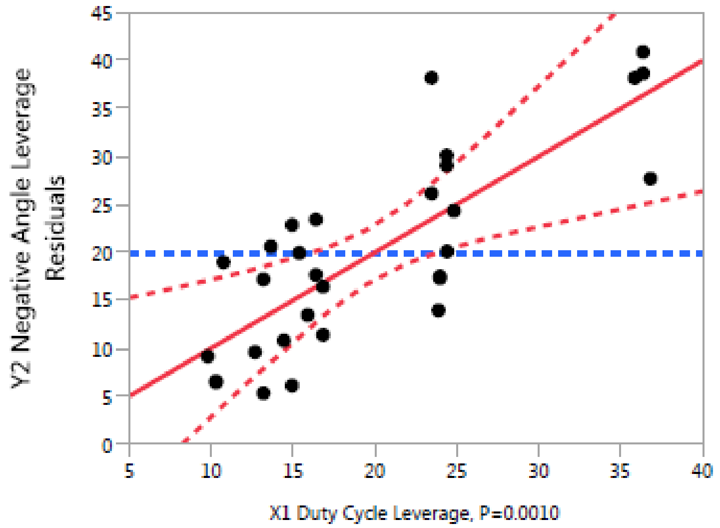
Whole Model

Residual by Predicted Plot



X1 Duty Cycle

Leverage Plot



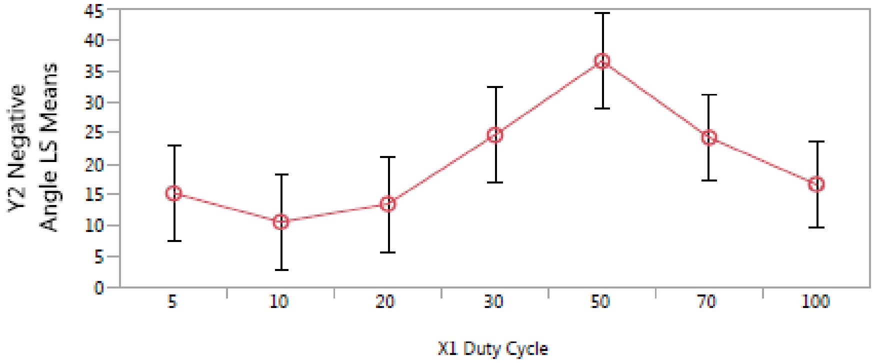
Least Squares Means Table

Level	Least Sq Mean	Std Error	Mean
5	15.163268	3.6955124	15.1633
10	10.516505	3.6955124	10.5165
20	13.412174	3.6955124	13.4122
30	24.612403	3.6955124	24.6124
50	36.615082	3.6955124	36.6151
70	24.193921	3.3375650	22.9779
100	16.615959	3.3375650	16.3266

Response Y2 Negative Angle

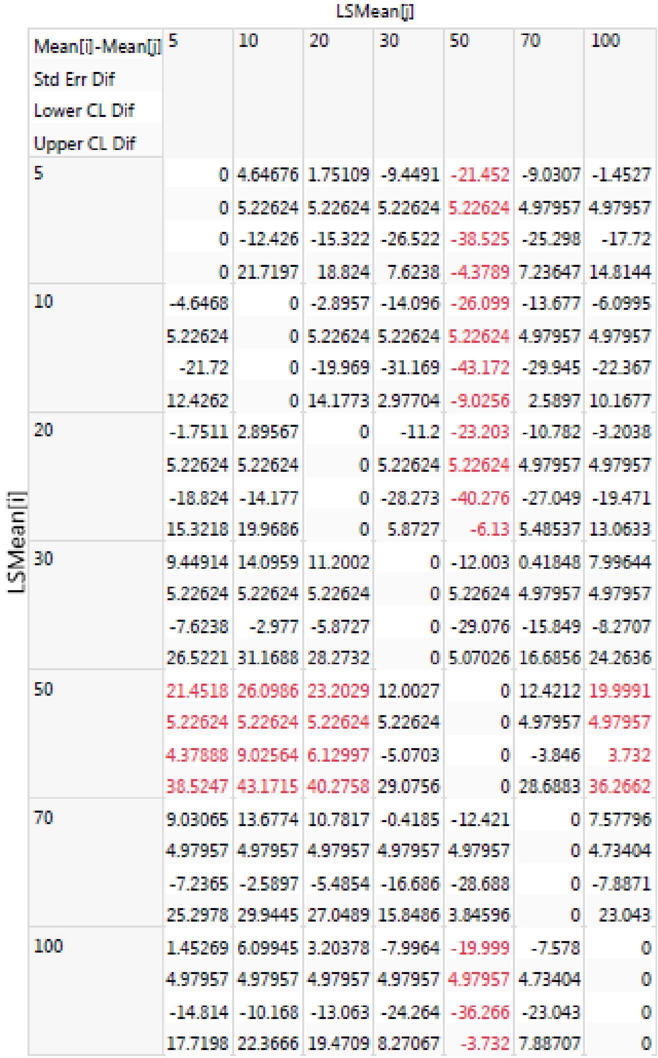
X1 Duty Cycle

LS Means Plot



LSMeans Differences Tukey HSD

α= 0.050 Q= 3.26677



LSMean[j]

LSMean[i]

Mean[i]-Mean[j] Std Err Dif Lower CL Dif Upper CL Dif	5	10	20	30	50	70	100
5	0	4.64676	1.75109	-9.4491	-21.452	-9.0307	-1.4527
	0	5.22624	5.22624	5.22624	5.22624	4.97957	4.97957
	0	-12.426	-15.322	-26.522	-38.525	-25.298	-17.72
	0	21.7197	18.824	7.6238	-4.3789	7.23647	14.8144
10	-4.6468	0	-2.8957	-14.096	-26.099	-13.677	-6.0995
	5.22624	0	5.22624	5.22624	5.22624	4.97957	4.97957
	-21.72	0	-19.969	-31.169	-43.172	-29.945	-22.367
	12.4262	0	14.1773	2.97704	-9.0256	2.5897	10.1677
20	-1.7511	2.89567	0	-11.2	-23.203	-10.782	-3.2038
	5.22624	5.22624	0	5.22624	5.22624	4.97957	4.97957
	-18.824	-14.177	0	-28.273	-40.276	-27.049	-19.471
	15.3218	19.9686	0	5.8727	-6.13	5.48537	13.0633
30	9.44914	14.0959	11.2002	0	-12.003	0.41848	7.99644
	5.22624	5.22624	5.22624	0	5.22624	4.97957	4.97957
	-7.6238	-2.977	-5.8727	0	-29.076	-15.849	-8.2707
	26.5221	31.1688	28.2732	0	5.07026	16.6856	24.2636
50	21.4518	26.0986	23.2029	12.0027	0	12.4212	19.9991
	5.22624	5.22624	5.22624	5.22624	0	4.97957	4.97957
	4.37888	9.02564	6.12997	-5.0703	0	-3.846	3.732
	38.5247	43.1715	40.2758	29.0756	0	28.6883	36.2662
70	9.03065	13.6774	10.7817	-0.4185	-12.421	0	7.57796
	4.97957	4.97957	4.97957	4.97957	4.97957	0	4.73404
	-7.2365	-2.5897	-5.4854	-16.686	-28.688	0	-7.8871
	25.2978	29.9445	27.0489	15.8486	3.84596	0	23.043
100	1.45269	6.09945	3.20378	-7.9964	-19.999	-7.578	0
	4.97957	4.97957	4.97957	4.97957	4.97957	4.73404	0
	-14.814	-10.168	-13.063	-24.264	-36.266	-23.043	0
	17.7198	22.3666	19.4709	8.27067	-3.732	7.88707	0

Response Y2 Negative Angle

X1 Duty Cycle

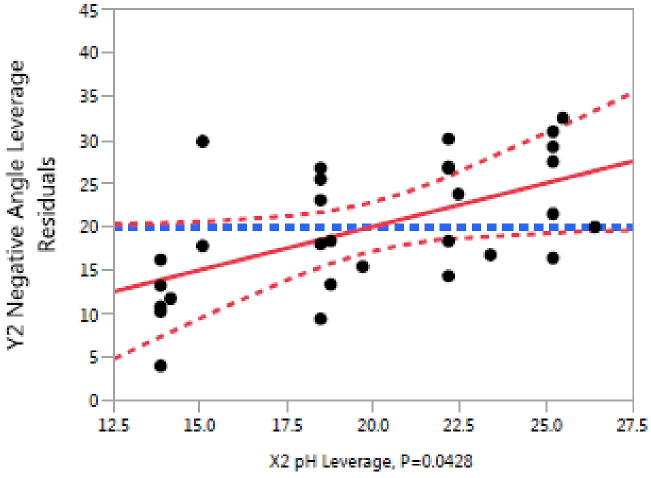
LSMeans Differences Tukey HSD

Level			Least Sq Mean
50	A		36.615082
30	A	B	24.612403
70	A	B	24.193921
100		B	16.615959
5		B	15.163268
20		B	13.412174
10		B	10.516505

Levels not connected by same letter are significantly different.

X2 pH

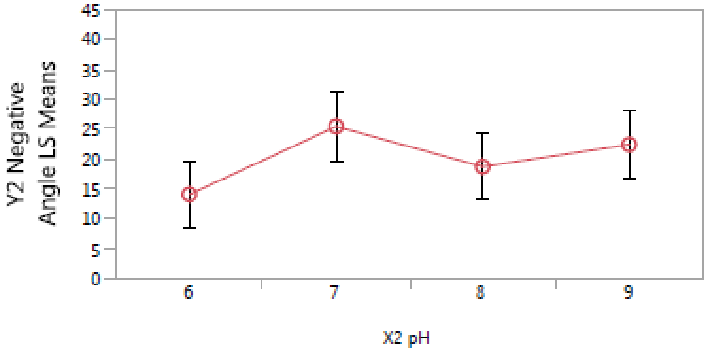
Leverage Plot



Least Squares Means Table

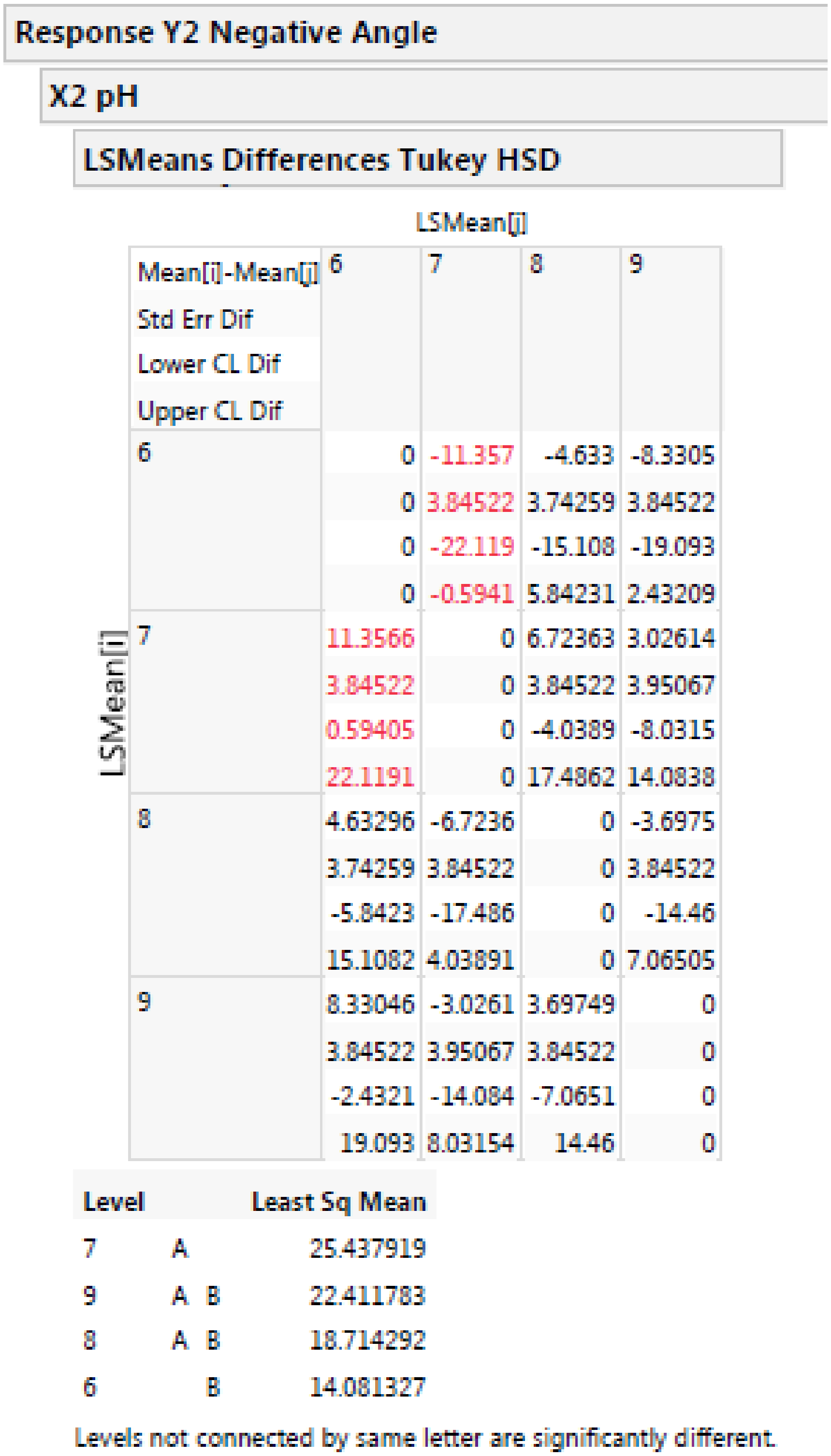
Level	Least Sq Mean	Std Error	Mean
6	14.081327	2.6423211	14.5854
7	25.437919	2.7935448	25.4379
8	18.714292	2.6423211	18.2711
9	22.411783	2.7935448	22.4118

LS Means Plot



LSMeans Differences Tukey HSD

α= 0.050 Q= 2.79894



Response Y2 Negative Angle

X2 pH

LSMeans Differences Tukey HSD

LSMean[i]	Mean[i]-Mean[j] Std Err Dif Lower CL Dif Upper CL Dif	LSMean[j] 6	7	8	9
LSMean[i]	6	0 0 0 0	-11.357 3.84522 -22.119 -0.5941	-4.633 3.74259 -15.108 5.84231	-8.3305 3.84522 -19.093 2.43209
LSMean[i]	7	11.3566 3.84522 0.59405 22.1191	0 0 0 0	6.72363 3.84522 -4.0389 17.4862	3.02614 3.95067 -8.0315 14.0838
LSMean[i]	8	4.63296 3.74259 -5.8423 15.1082	-6.7236 3.84522 -17.486 4.03891	0 0 0 0	-3.6975 3.84522 -14.46 7.06505
LSMean[i]	9	8.33046 3.84522 -2.4321 19.093	-3.0261 3.95067 -14.084 8.03154	3.69749 3.84522 -7.0651 14.46	0 0 0 0

Level			Least Sq Mean
7	A		25.437919
9	A	B	22.411783
8	A	B	18.714292
6		B	14.081327

Levels not connected by same letter are significantly different.

Appendix N: Positive Ionization Chromatographic Contrast Angle Regression Report

Upholds SW, DW, BP

Y1: Positive Angle

X1: DV pH6

X2: DV pH7

X3: DV pH8

X4: DV DC 70

X5: DV DC 70*DV pH6

R Squared: .8000

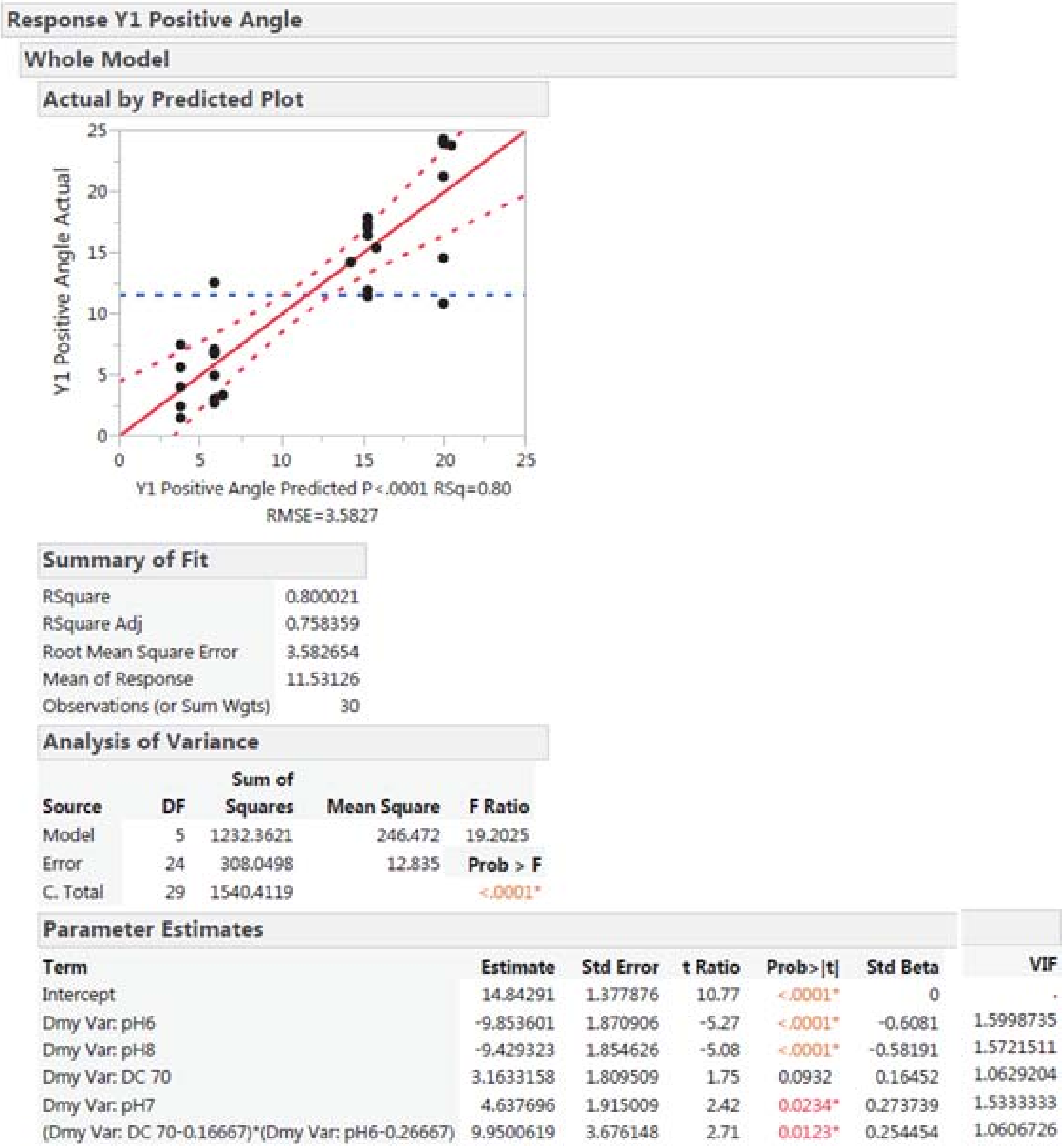
R Squared, Adj: .7584

	percent	degrees			
Max Error	150.50%	9.07°	between 0 and 9 degrees		4.533645
Mean Error	38.30%	2.51°	Error:	±4.53°	
Median Error	17.50%	2.18°			

stdev 2.02 degrees

All VIF Scores below 2.0

Durbin Watson assumption of Independence upheld



Response Y1 Positive Angle

Whole Model

Actual by Predicted Plot

Summary of Fit

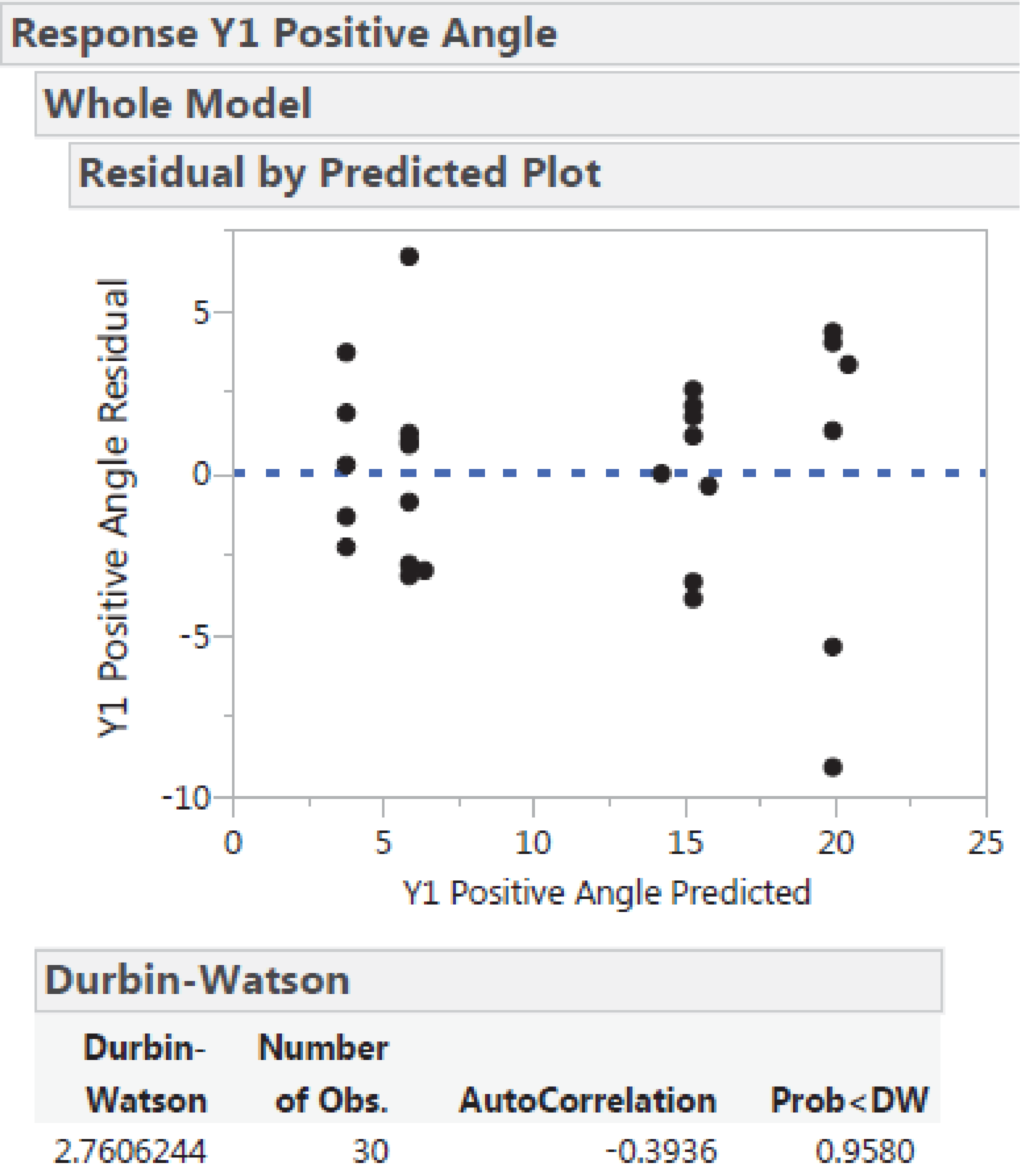
RSquare	0.800021
RSquare Adj	0.758359
Root Mean Square Error	3.582654
Mean of Response	11.53126
Observations (or Sum Wgts)	30

Analysis of Variance

Source	DF	Sum of Squares	Mean Square	F Ratio
Model	5	1232.3621	246.472	19.2025
Error	24	308.0498	12.835	**Prob > F**
C. Total	29	1540.4119		<.0001*

Parameter Estimates

Term	Estimate	Std Error	t Ratio	Prob>|t|	Std Beta	VIF
Intercept	14.84291	1.377876	10.77	<.0001*	0	.
Dmy Var: pH6	-9.853601	1.870906	-5.27	<.0001*	-0.6081	1.5998735
Dmy Var: pH8	-9.429323	1.854626	-5.08	<.0001*	-0.58191	1.5721511
Dmy Var: DC 70	3.1633158	1.809509	1.75	0.0932	0.16452	1.0629204
Dmy Var: pH7	4.637696	1.915009	2.42	0.0234*	0.273739	1.5333333
(Dmy Var: DC 70-0.16667)*(Dmy Var: pH6-0.26667)	9.9500619	3.676148	2.71	0.0123*	0.254454	1.0606726



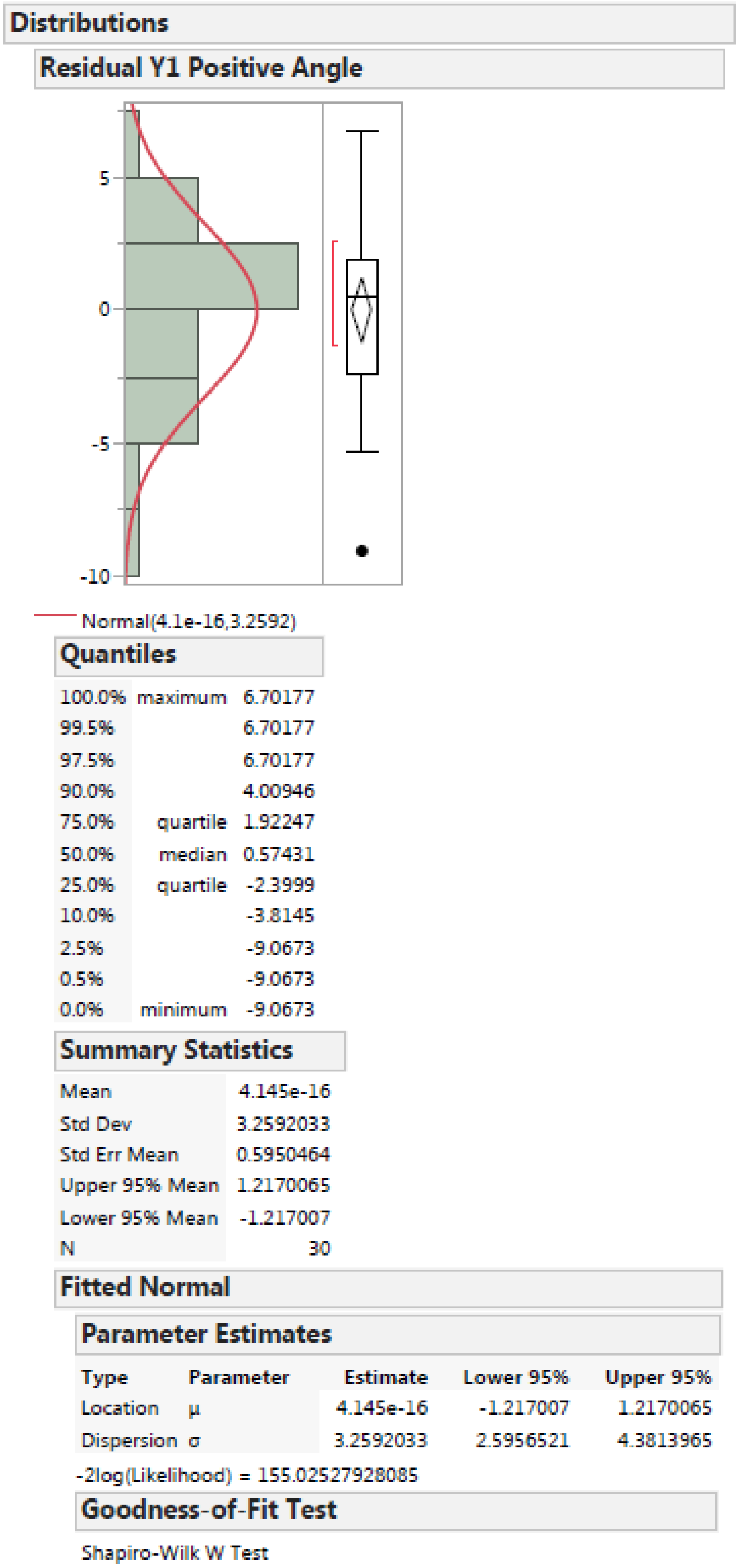
Response Y1 Positive Angle

Whole Model

Residual by Predicted Plot

Durbin-Watson

Durbin-Watson	Number of Obs.	AutoCorrelation	Prob<DW
2.7606244	30	-0.3936	0.9580



Distributions

Residual Y1 Positive Angle

Normal(4.1e-16,3.2592)

Quantiles

100.0%	maximum	6.70177
99.5%		6.70177
97.5%		6.70177
90.0%		4.00946
75.0%	quartile	1.92247
50.0%	median	0.57431
25.0%	quartile	-2.3999
10.0%		-3.8145
2.5%		-9.0673
0.5%		-9.0673
0.0%	minimum	-9.0673

Summary Statistics

Mean	4.145e-16
Std Dev	3.2592033
Std Err Mean	0.5950464
Upper 95% Mean	1.2170065
Lower 95% Mean	-1.217007
N	30

Fitted Normal

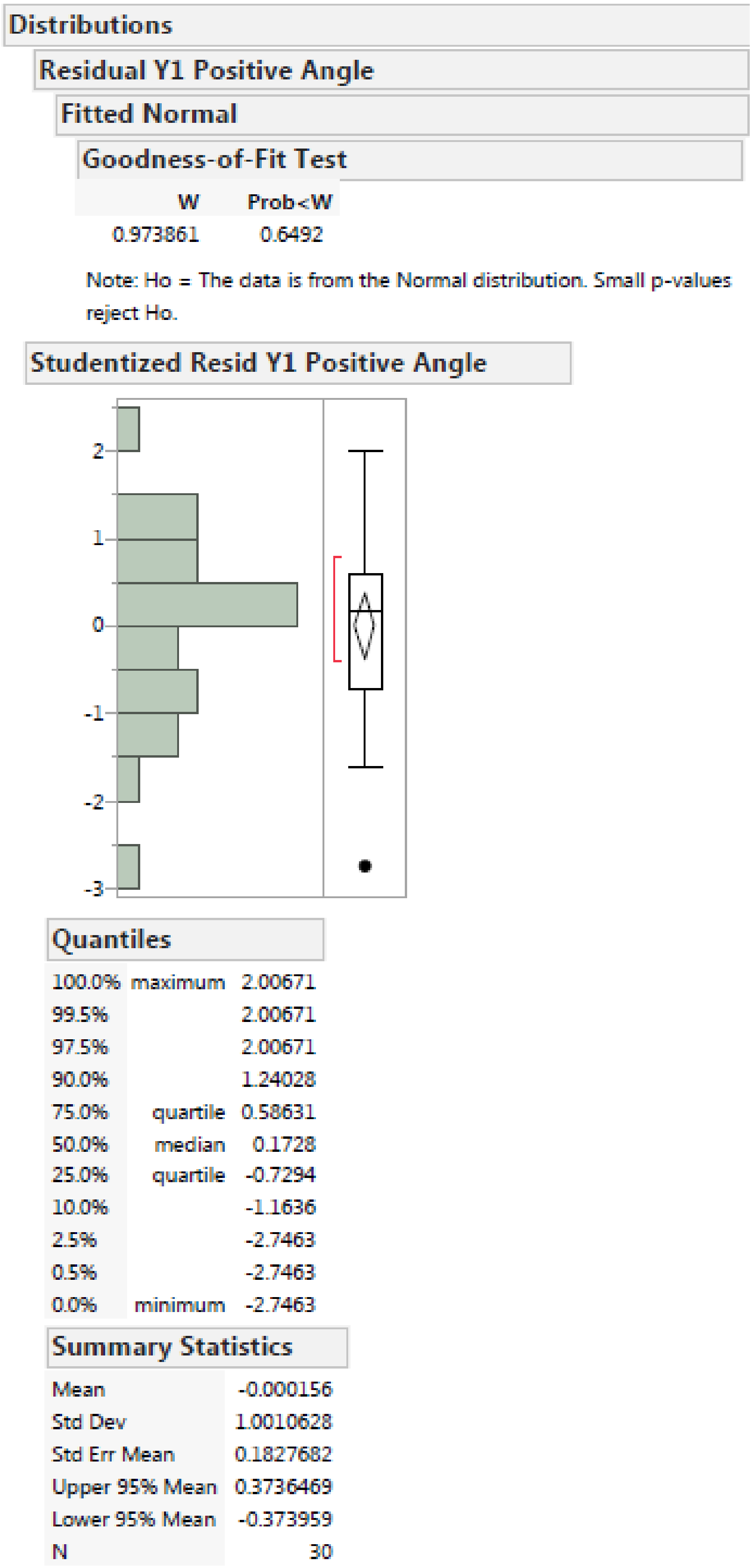
Parameter Estimates

Type	Parameter	Estimate	Lower 95%	Upper 95%
Location	μ	4.145e-16	-1.217007	1.2170065
Dispersion	σ	3.2592033	2.5956521	4.3813965

-2log(Likelihood) = 155.02527928085

Goodness-of-Fit Test

Shapiro-Wilk W Test



Distributions

Residual Y1 Positive Angle

Fitted Normal

Goodness-of-Fit Test

W	Prob<W
0.973861	0.6492

Note: Ho = The data is from the Normal distribution. Small p-values reject Ho.

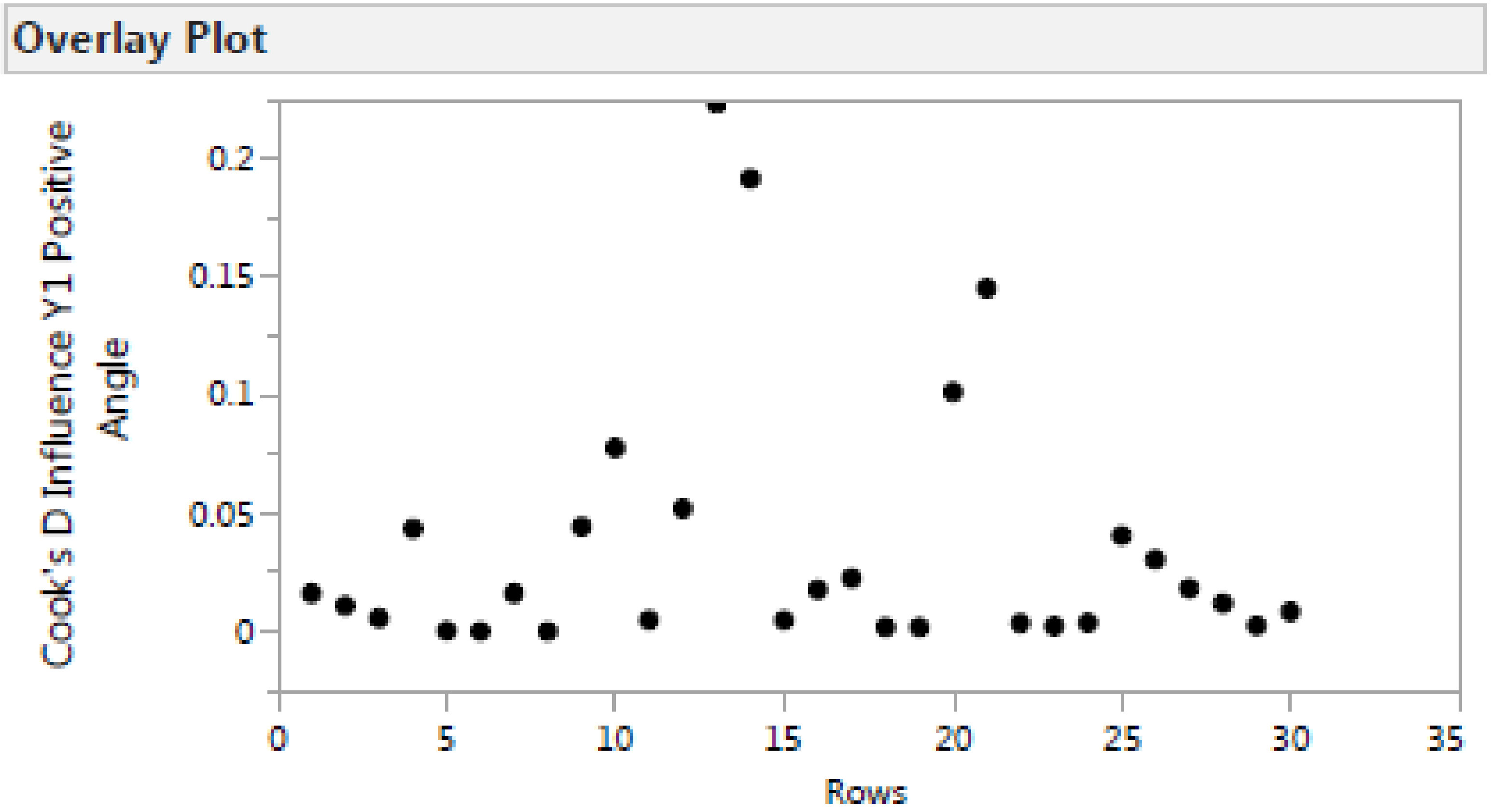
Studentized Resid Y1 Positive Angle

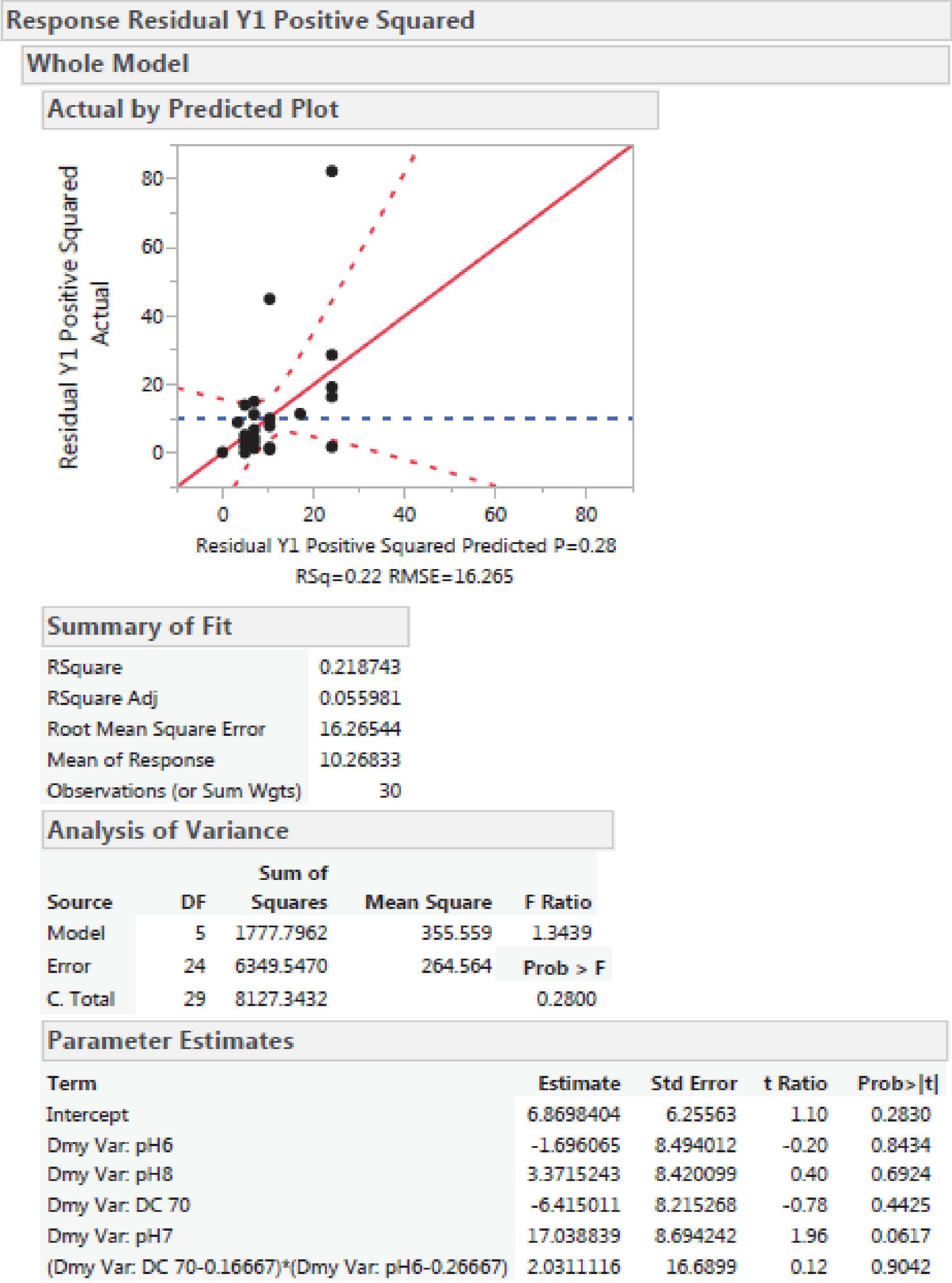
Quantiles

100.0%	maximum	2.00671
99.5%		2.00671
97.5%		2.00671
90.0%		1.24028
75.0%	quartile	0.58631
50.0%	median	0.1728
25.0%	quartile	-0.7294
10.0%		-1.1636
2.5%		-2.7463
0.5%		-2.7463
0.0%	minimum	-2.7463

Summary Statistics

Mean	-0.000156
Std Dev	1.0010628
Std Err Mean	0.1827682
Upper 95% Mean	0.3736469
Lower 95% Mean	-0.373959
N	30


Overlay Plot
Cook's D Influence Y1 Positive Angle
0.2
0.15
0.1
0.05
0
0
5
10
15
20
25
30
35
Rows



Response Residual Y1 Positive Squared

Whole Model

Actual by Predicted Plot

Summary of Fit

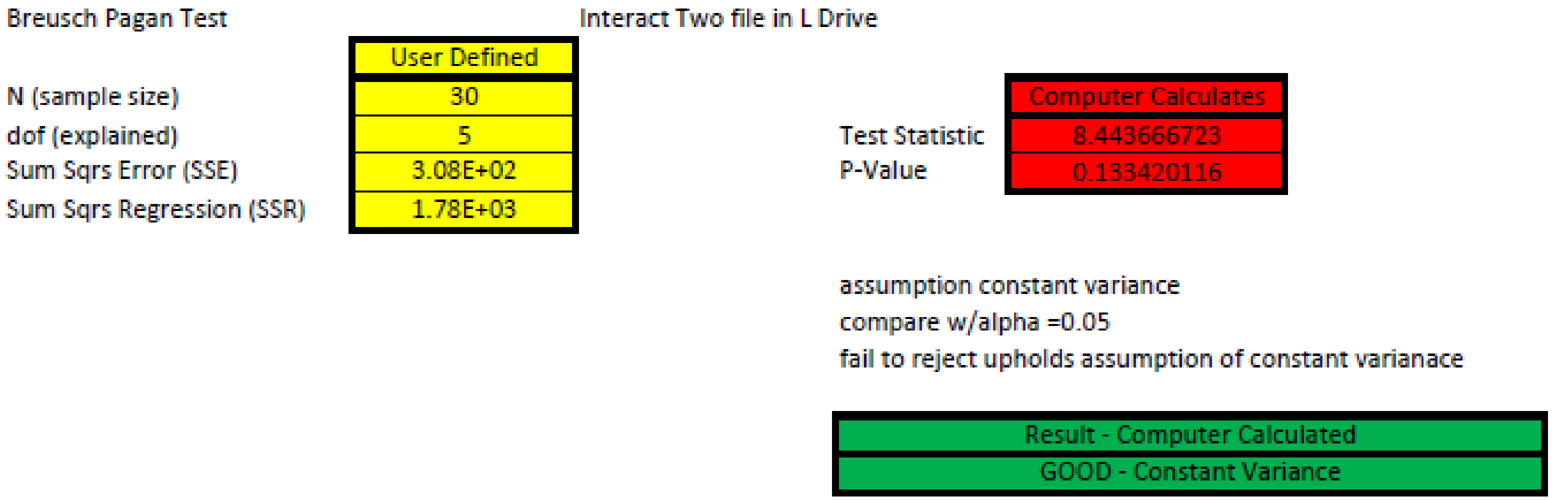
RSquare	0.218743
RSquare Adj	0.055981
Root Mean Square Error	16.26544
Mean of Response	10.26833
Observations (or Sum Wgts)	30

Analysis of Variance

Source	DF	Sum of Squares	Mean Square	F Ratio
Model	5	1777.7962	355.559	1.3439
Error	24	6349.5470	264.564	Prob > F
C. Total	29	8127.3432		0.2800

Parameter Estimates

Term	Estimate	Std Error	t Ratio	Prob>|t|
Intercept	6.8698404	6.25563	1.10	0.2830
Dmy Var: pH6	-1.696065	8.494012	-0.20	0.8434
Dmy Var: pH8	3.3715243	8.420099	0.40	0.6924
Dmy Var: DC 70	-6.415011	8.215268	-0.78	0.4425
Dmy Var: pH7	17.038839	8.694242	1.96	0.0617
(Dmy Var: DC 70-0.16667)*(Dmy Var: pH6-0.26667)	2.0311116	16.6899	0.12	0.9042



Breusch Pagan Test

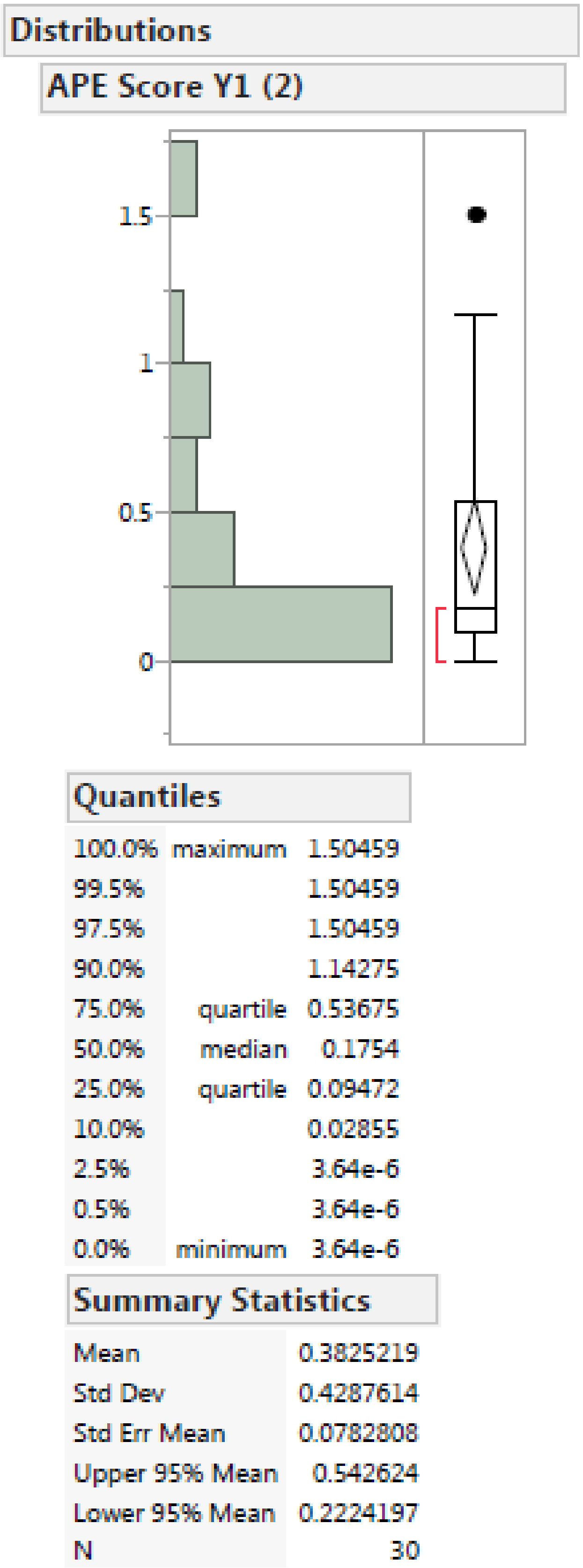
Interact Two file in L Drive

	User Defined
N (sample size)	30
dof (explained)	5
Sum Sqrs Error (SSE)	3.08E+02
Sum Sqrs Regression (SSR)	1.78E+03

	Computer Calculates
Test Statistic	8.443666723
P-Value	0.133420116

assumption constant variance
compare w/alpha =0.05
fail to reject upholds assumption of constant varianace

Result - Computer Calculated
GOOD - Constant Variance



Distributions

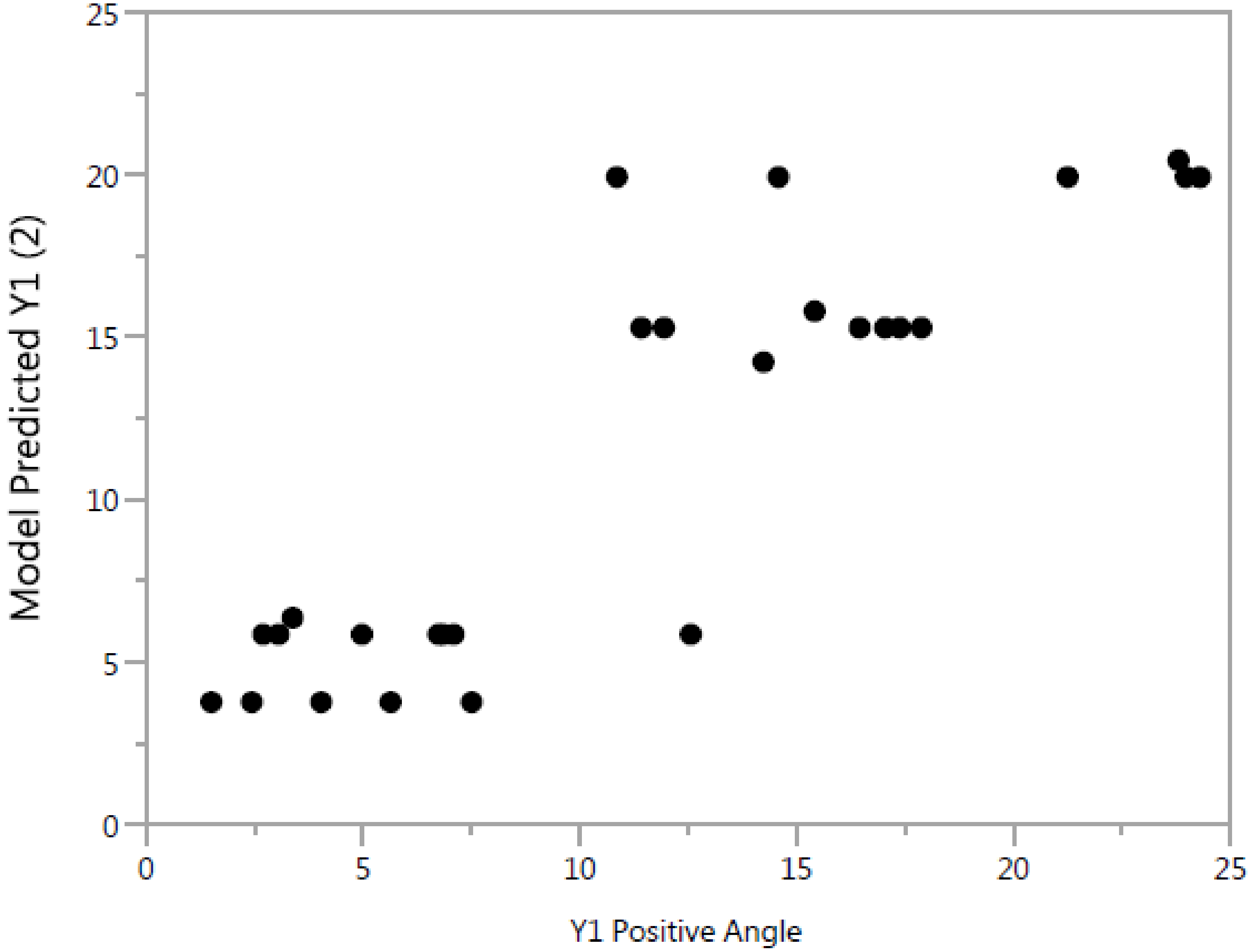
APE Score Y1 (2)

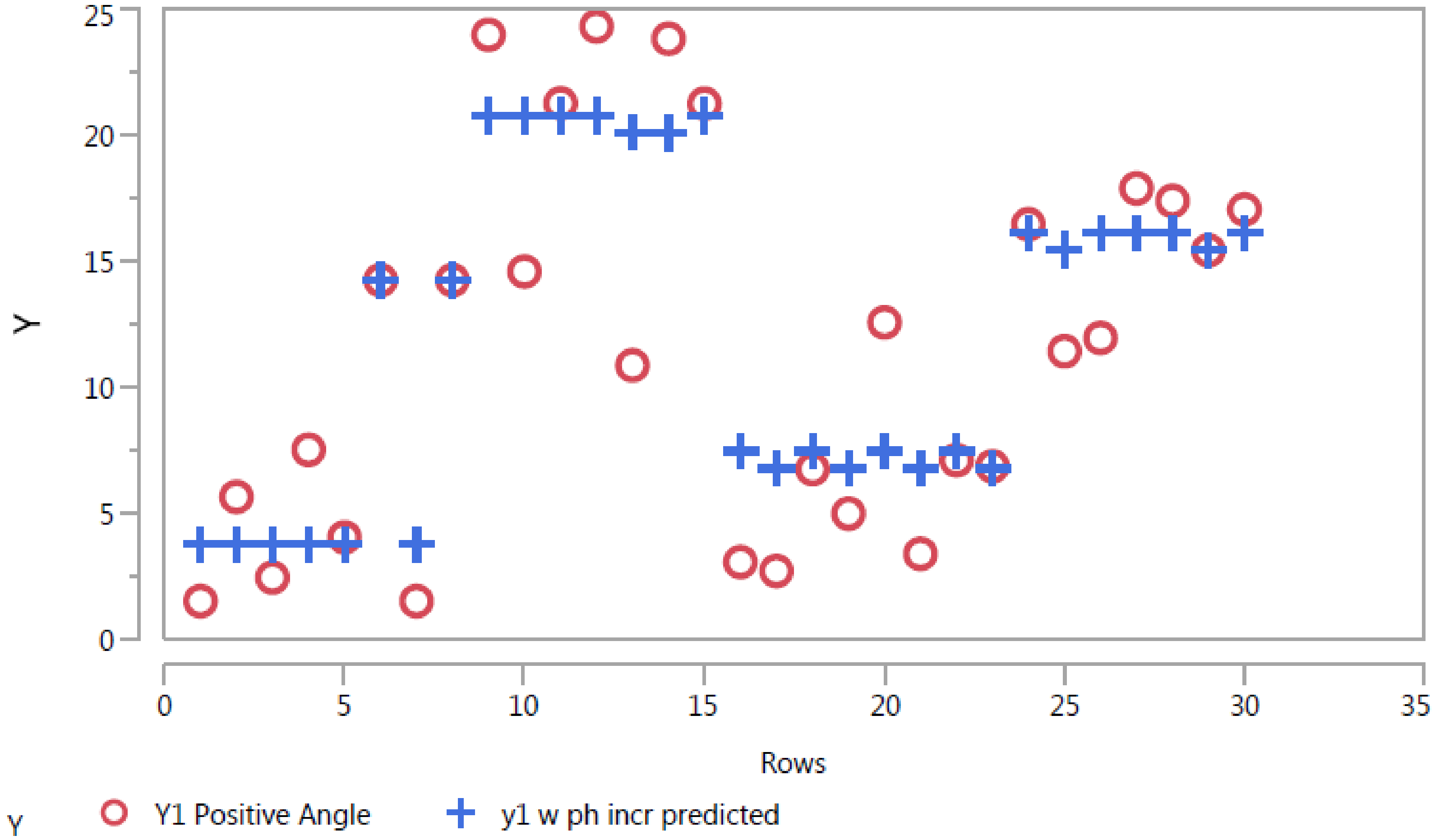
Quantiles

100.0%	maximum	1.50459
99.5%		1.50459
97.5%		1.50459
90.0%		1.14275
75.0%	quartile	0.53675
50.0%	median	0.1754
25.0%	quartile	0.09472
10.0%		0.02855
2.5%		3.64e-6
0.5%		3.64e-6
0.0%	minimum	3.64e-6

Summary Statistics

Mean	0.3825219
Std Dev	0.4287614
Std Err Mean	0.0782808
Upper 95% Mean	0.542624
Lower 95% Mean	0.2224197
N	30


Model Predicted Y1 (2)
0
5
10
15
20
25
Y1 Positive Angle
0
5
10
15
20
25



25
20
15
10
5
0
Y
0
5
10
15
20
25
30
35
Rows
Y
○ Y1 Positive Angle
+ y1 w ph incr predicted

Appendix O: Negative Ionization Chromatographic Contrast Angle Regression Report

Upholds SW, DW, BP
Y1: Negative Angle
X1: DV pH6
X2: DV pH8
X3: DV DC 30
X4: DV DC 70
X5: DV DC 50
X6: DV DV70*pH6
R Squared: .7500
R Squared, Adj: .6848

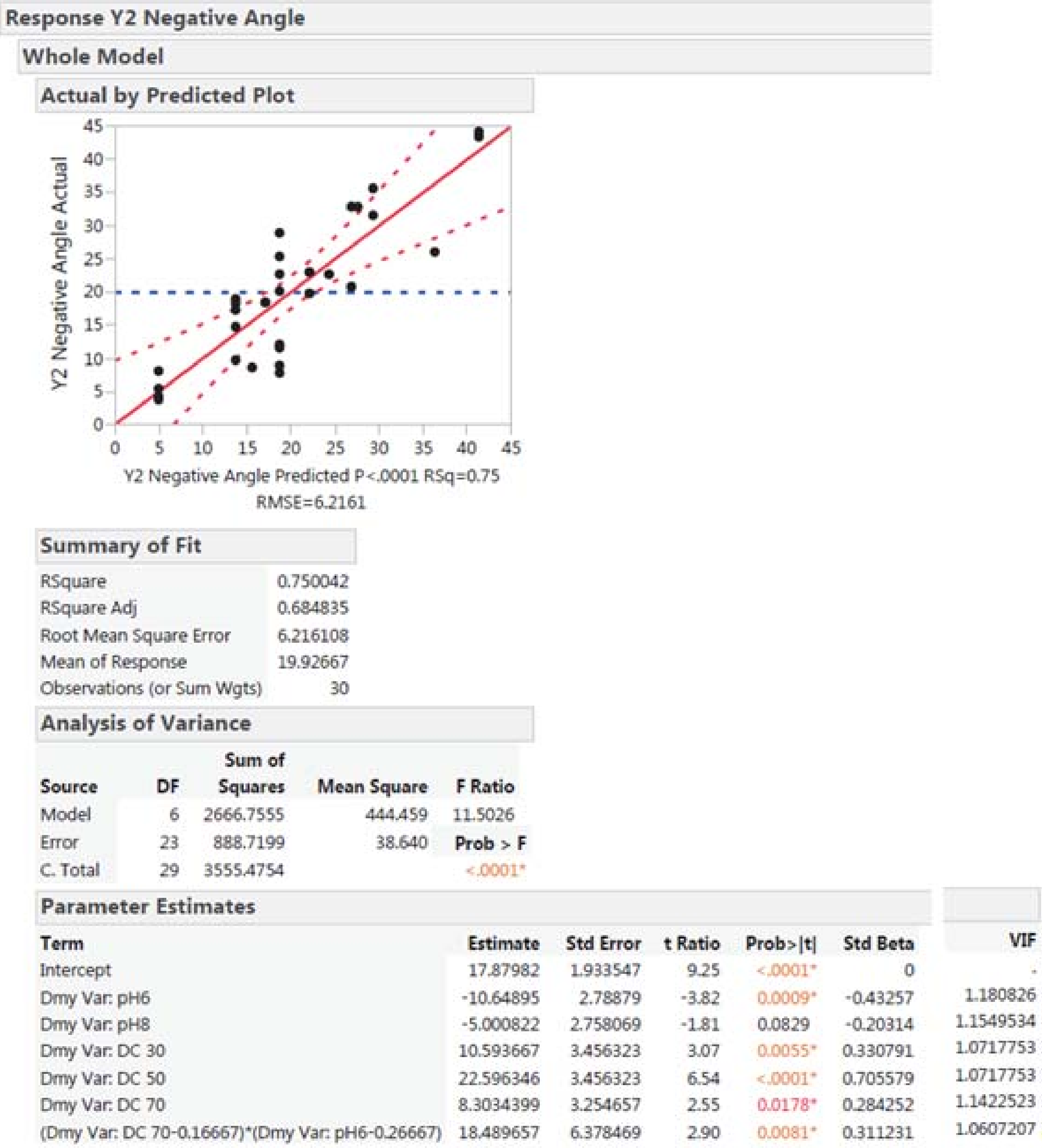
All VIF Scores below 2.0
Durbin Watson assumption of Independence upheld

	Y2	APE	Degrees
Mean	19.9267	0.30664	6.110323
Median	19.3649	0.19593	3.794165

Mean Error ±6.11°
Median Error ±3.79°

	percent	degrees			
Max Error	140.30%	10.9°	between 0 and 10 degrees		5.4595
Mean Error	30.66%	4.50°	Error:	±5.46°	
Median Error	19.59%	3.97°			

stdev error 3.11 degrees



Response Y2 Negative Angle

Whole Model

Actual by Predicted Plot

Y2 Negative Angle Predicted P<.0001 RSq=0.75
RMSE=6.2161

Summary of Fit

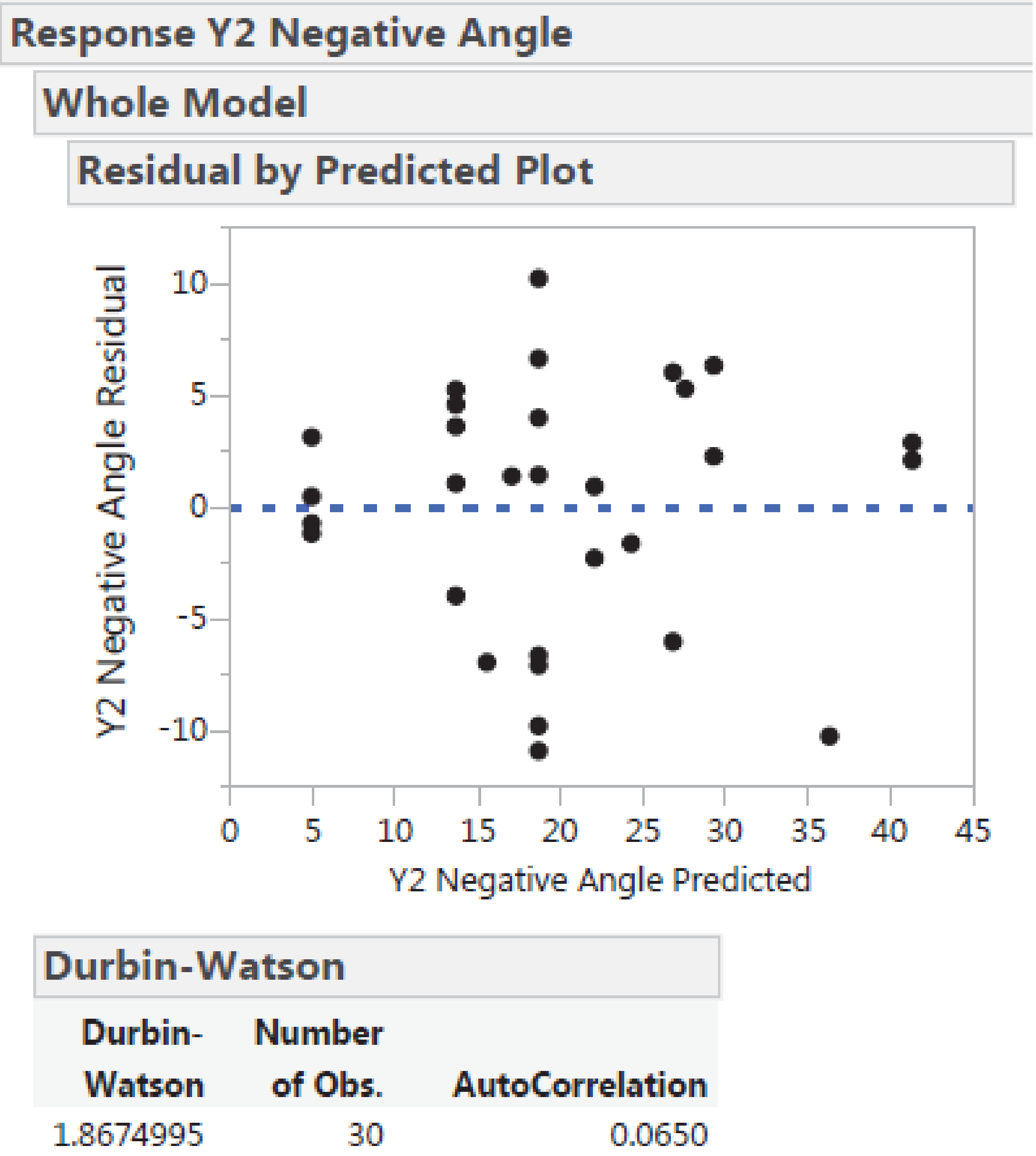
RSquare	0.750042
RSquare Adj	0.684835
Root Mean Square Error	6.216108
Mean of Response	19.92667
Observations (or Sum Wgts)	30

Analysis of Variance

Source	DF	Sum of Squares	Mean Square	F Ratio
Model	6	2666.7555	444.459	11.5026
Error	23	888.7199	38.640	**Prob > F**
C. Total	29	3555.4754		<.0001*

Parameter Estimates

Term	Estimate	Std Error	t Ratio	Prob>|t|	Std Beta	VIF
Intercept	17.87982	1.933547	9.25	<.0001*	0	.
Dmy Var: pH6	-10.64895	2.78879	-3.82	0.0009*	-0.43257	1.180826
Dmy Var: pH8	-5.000822	2.758069	-1.81	0.0829	-0.20314	1.1549534
Dmy Var: DC 30	10.593667	3.456323	3.07	0.0055*	0.330791	1.0717753
Dmy Var: DC 50	22.596346	3.456323	6.54	<.0001*	0.705579	1.0717753
Dmy Var: DC 70	8.3034399	3.254657	2.55	0.0178*	0.284252	1.1422523
(Dmy Var: DC 70-0.16667)*(Dmy Var: pH6-0.26667)	18.489657	6.378469	2.90	0.0081*	0.311231	1.0607207



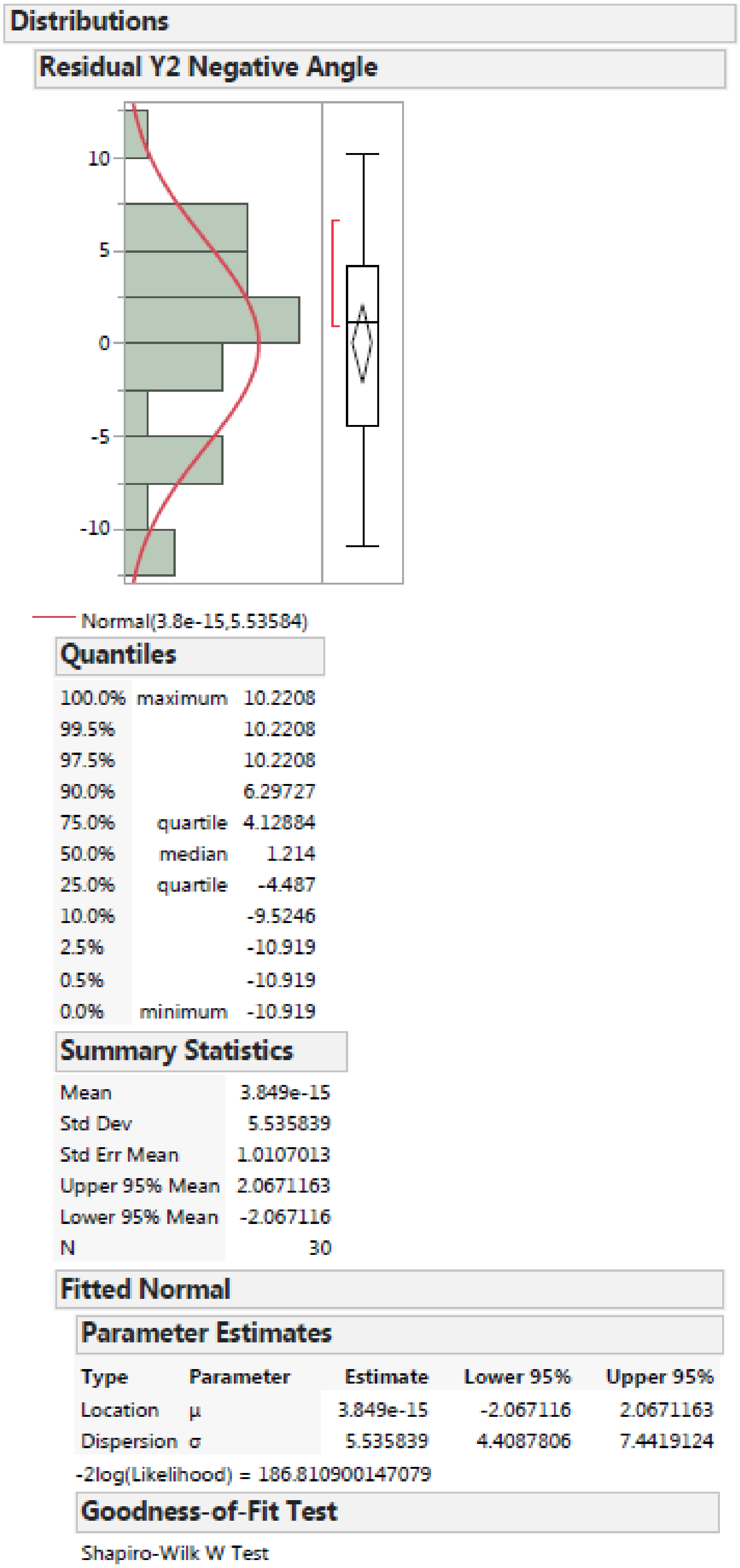
Response Y2 Negative Angle

Whole Model

Residual by Predicted Plot

Durbin-Watson

Durbin-Watson	Number of Obs.	AutoCorrelation
1.8674995	30	0.0650



Distributions

Residual Y2 Negative Angle

Quantiles

100.0%	maximum	10.2208
99.5%		10.2208
97.5%		10.2208
90.0%		6.29727
75.0%	quartile	4.12884
50.0%	median	1.214
25.0%	quartile	-4.487
10.0%		-9.5246
2.5%		-10.919
0.5%		-10.919
0.0%	minimum	-10.919

Summary Statistics

Mean	3.849e-15
Std Dev	5.535839
Std Err Mean	1.0107013
Upper 95% Mean	2.0671163
Lower 95% Mean	-2.067116
N	30

Fitted Normal

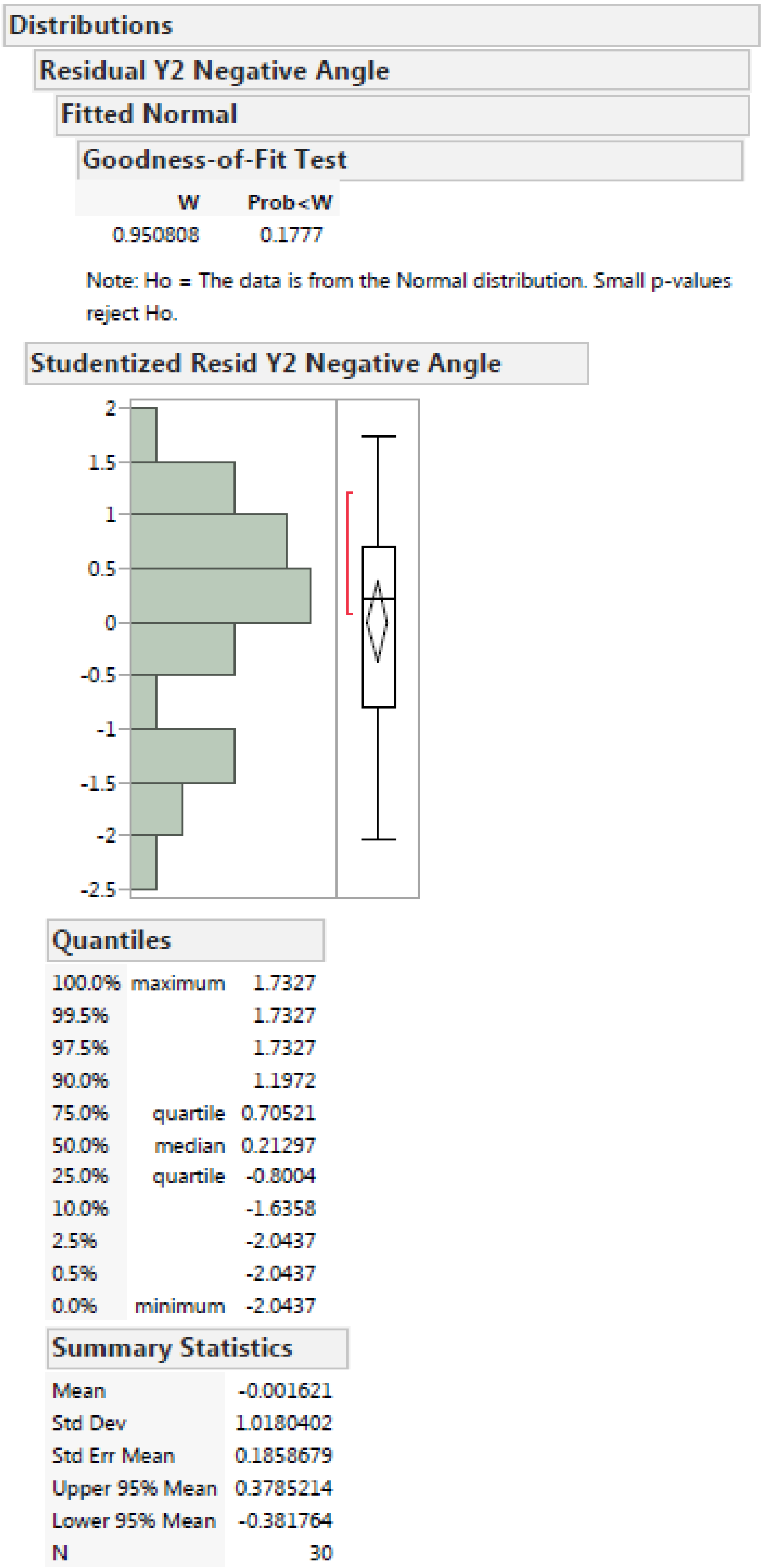
Parameter Estimates

Type	Parameter	Estimate	Lower 95%	Upper 95%
Location	μ	3.849e-15	-2.067116	2.0671163
Dispersion	σ	5.535839	4.4087806	7.4419124

-2log(Likelihood) = 186.810900147079

Goodness-of-Fit Test

Shapiro-Wilk W Test



Distributions

Residual Y2 Negative Angle

Fitted Normal

Goodness-of-Fit Test

W	Prob<W
0.950808	0.1777

Note: Ho = The data is from the Normal distribution. Small p-values reject Ho.

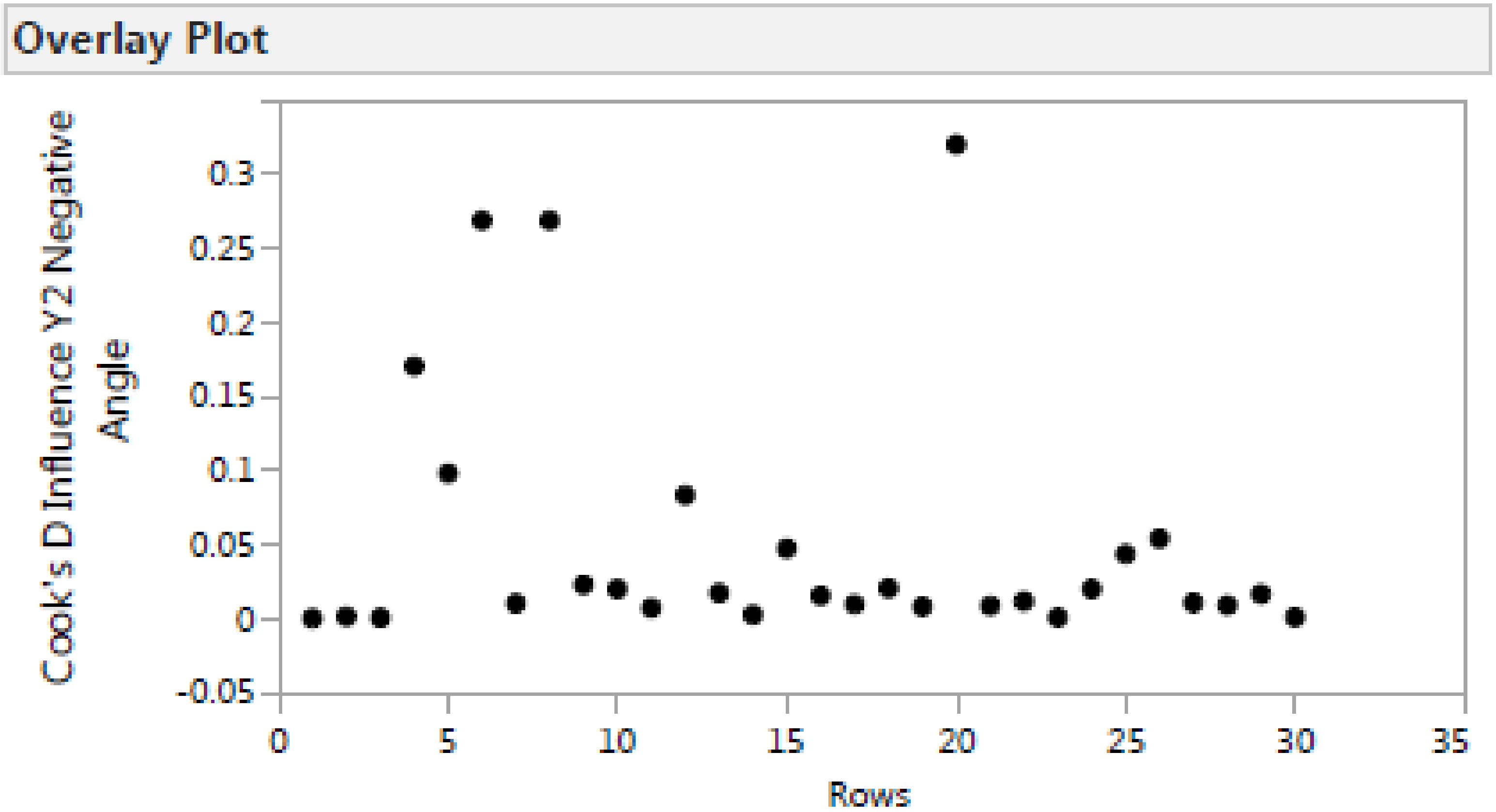
Studentized Resid Y2 Negative Angle

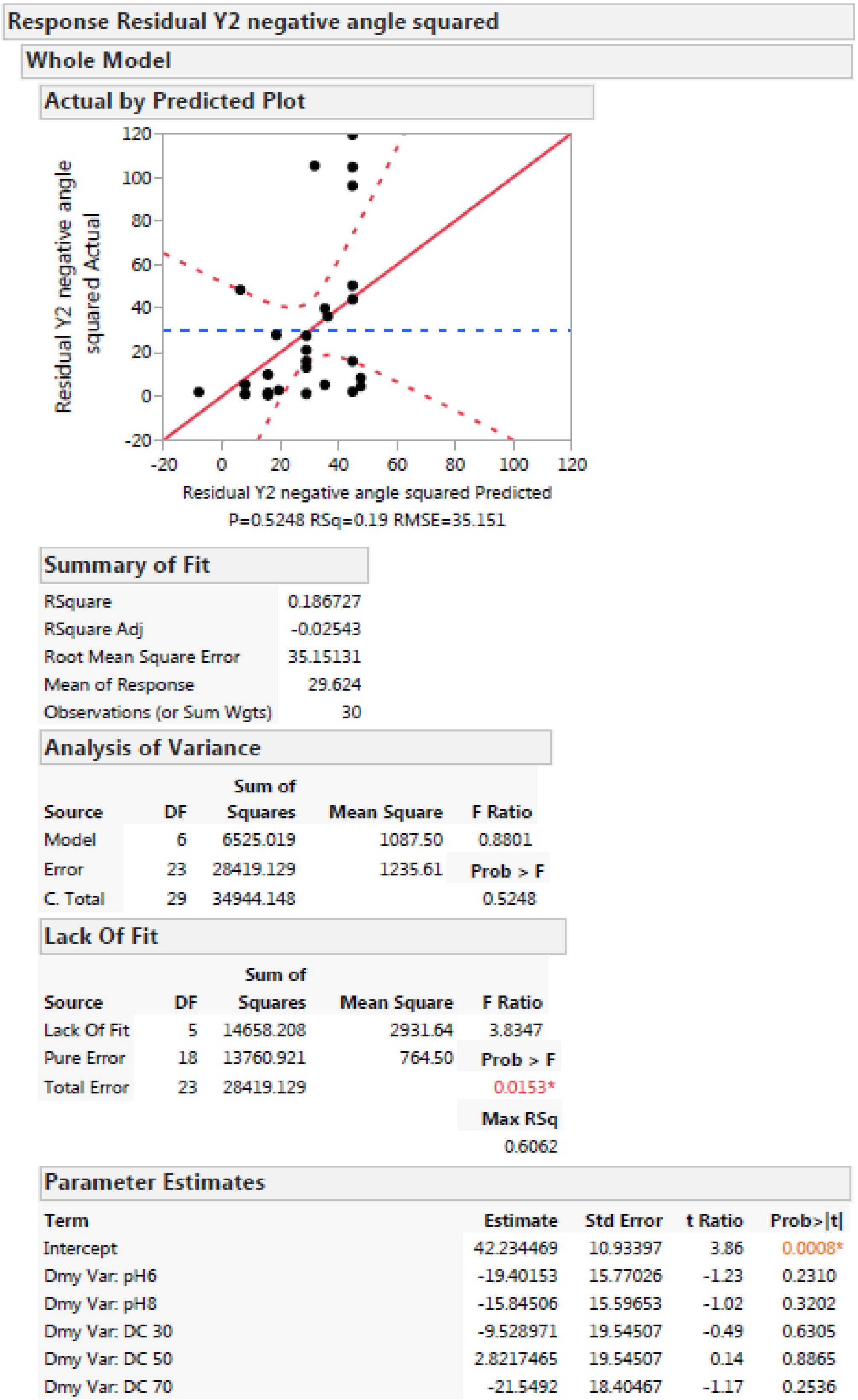
Quantiles

100.0%	maximum	1.7327
99.5%		1.7327
97.5%		1.7327
90.0%		1.1972
75.0%	quartile	0.70521
50.0%	median	0.21297
25.0%	quartile	-0.8004
10.0%		-1.6358
2.5%		-2.0437
0.5%		-2.0437
0.0%	minimum	-2.0437

Summary Statistics

Mean	-0.001621
Std Dev	1.0180402
Std Err Mean	0.1858679
Upper 95% Mean	0.3785214
Lower 95% Mean	-0.381764
N	30


Overlay Plot
Cook's D Influence Y2 Negative Angle
0.3
0.25
0.2
0.15
0.1
0.05
0
-0.05
0
5
10
15
20
25
30
35
Rows



Response Residual Y2 negative angle squared

Whole Model

Actual by Predicted Plot

Summary of Fit

RSquare	0.186727
RSquare Adj	-0.02543
Root Mean Square Error	35.15131
Mean of Response	29.624
Observations (or Sum Wgts)	30

Analysis of Variance

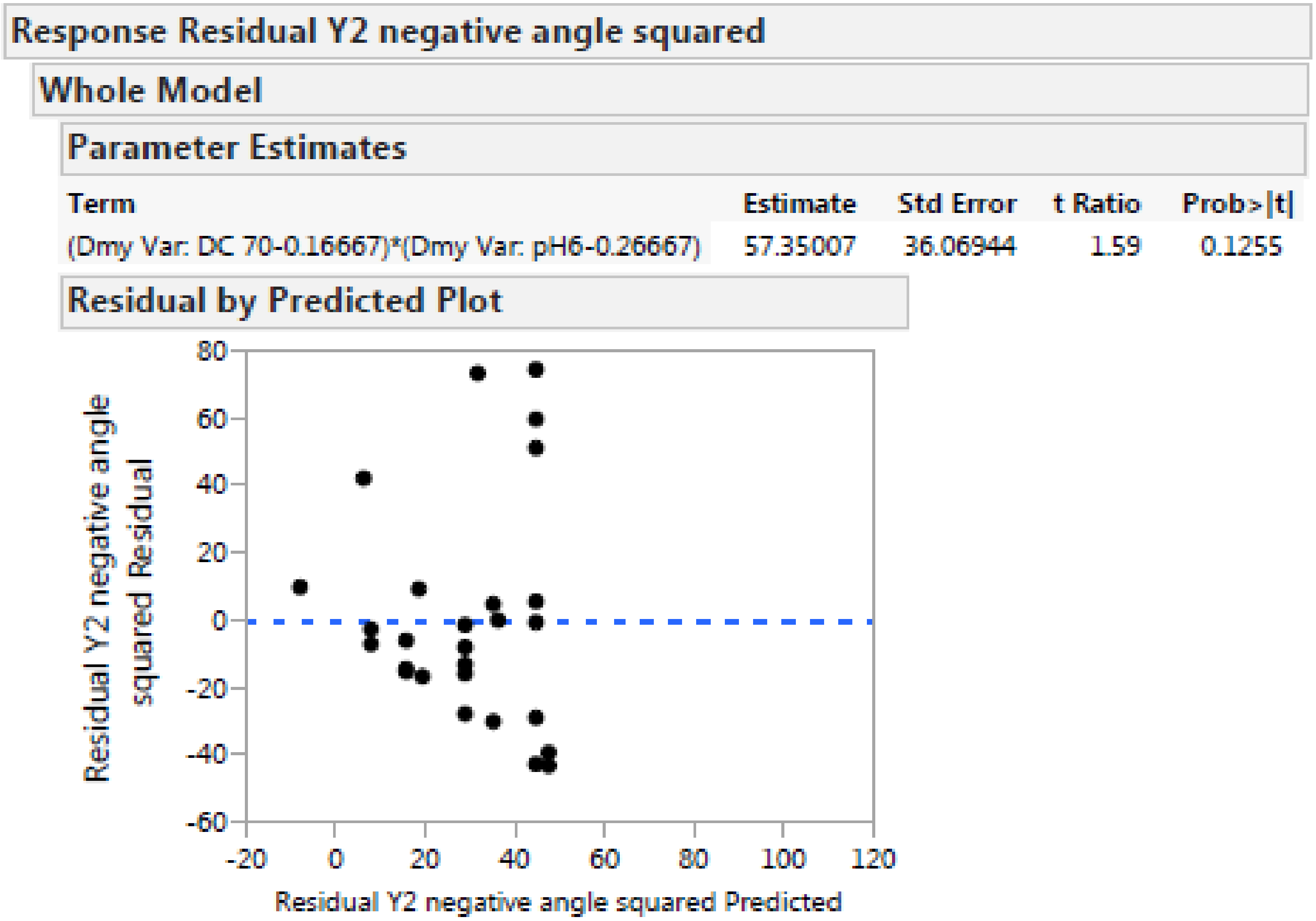
Source	DF	Sum of Squares	Mean Square	F Ratio
Model	6	6525.019	1087.50	0.8801
Error	23	28419.129	1235.61	Prob > F
C. Total	29	34944.148		0.5248

Lack Of Fit

Source	DF	Sum of Squares	Mean Square	F Ratio
Lack Of Fit	5	14658.208	2931.64	3.8347
Pure Error	18	13760.921	764.50	Prob > F
Total Error	23	28419.129		0.0153*
				Max RSq
				0.6062

Parameter Estimates

Term	Estimate	Std Error	t Ratio	Prob>|t|
Intercept	42.234469	10.93397	3.86	0.0008*
Dmy Var: pH6	-19.40153	15.77026	-1.23	0.2310
Dmy Var: pH8	-15.84506	15.59653	-1.02	0.3202
Dmy Var: DC 30	-9.528971	19.54507	-0.49	0.6305
Dmy Var: DC 50	2.8217465	19.54507	0.14	0.8865
Dmy Var: DC 70	-21.5492	18.40467	-1.17	0.2536



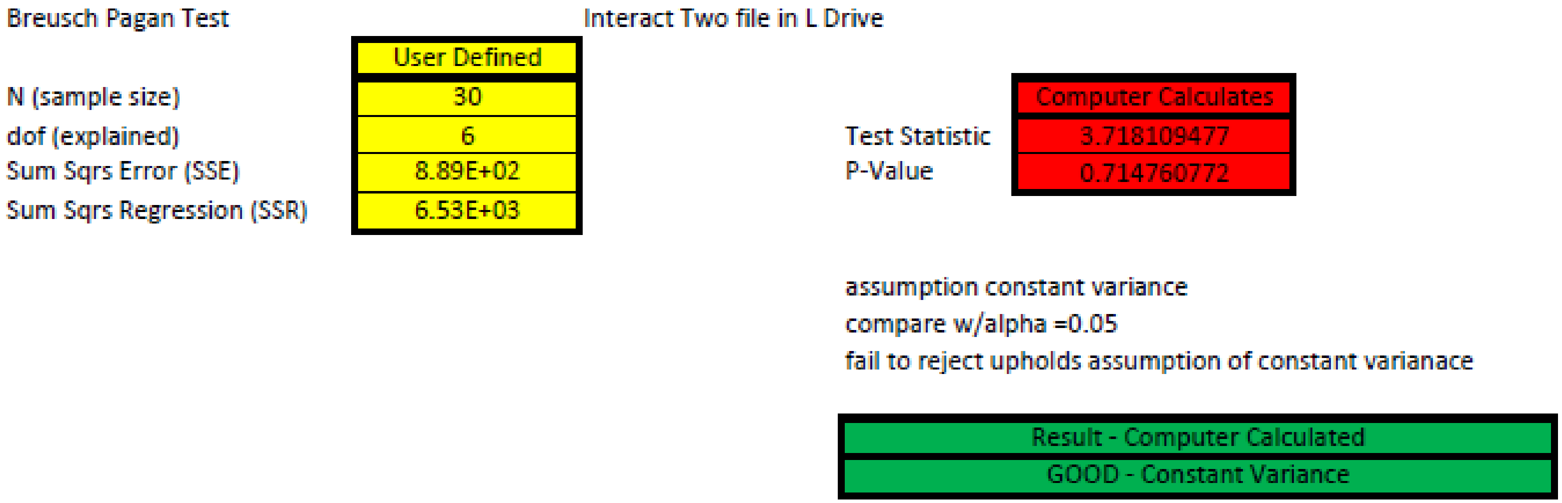
Response Residual Y2 negative angle squared

Whole Model

Parameter Estimates

Term	Estimate	Std Error	t Ratio	Prob>|t|
(Dmy Var: DC 70-0.16667)*(Dmy Var: pH6-0.26667)	57.35007	36.06944	1.59	0.1255

Residual by Predicted Plot



Breusch Pagan Test

Interact Two file in L Drive

	User Defined
N (sample size)	30
dof (explained)	6
Sum Sqrs Error (SSE)	8.89E+02
Sum Sqrs Regression (SSR)	6.53E+03

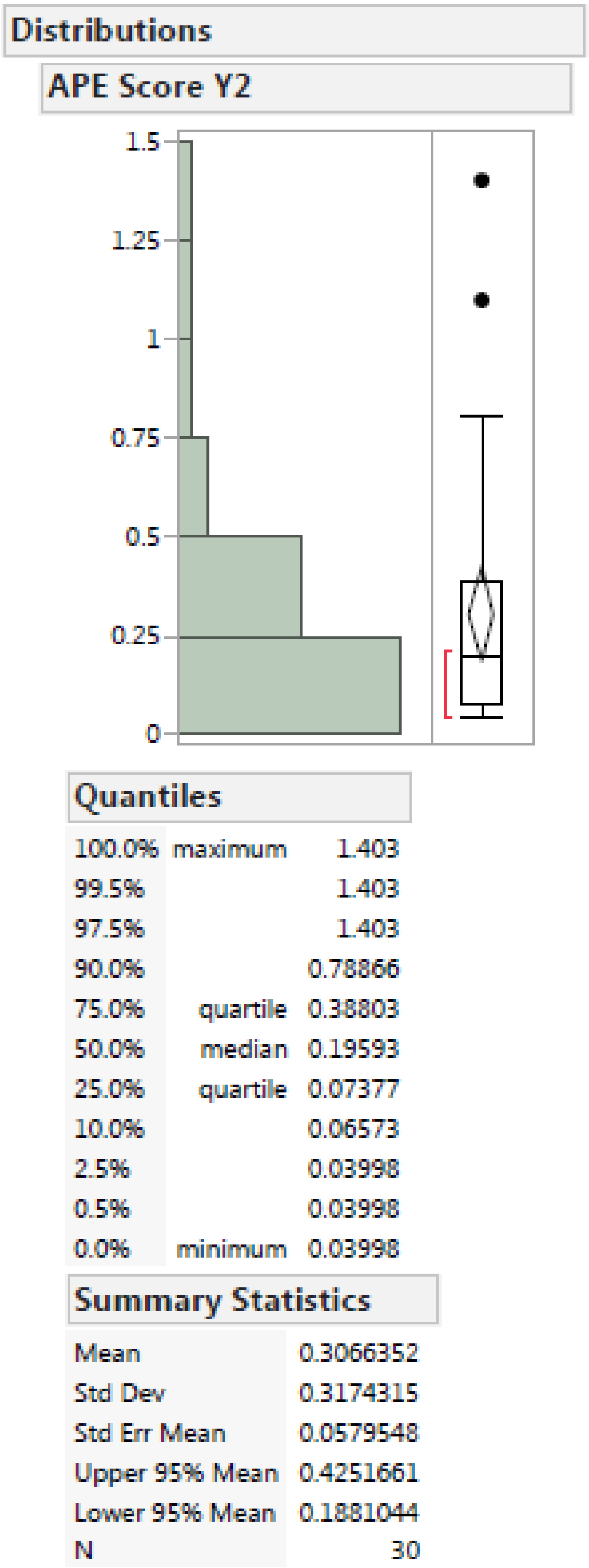
	Computer Calculates
Test Statistic	3.718109477
P-Value	0.714760772

assumption constant variance

compare w/alpha =0.05

fail to reject upholds assumption of constant varianace

Result - Computer Calculated
GOOD - Constant Variance



Distributions

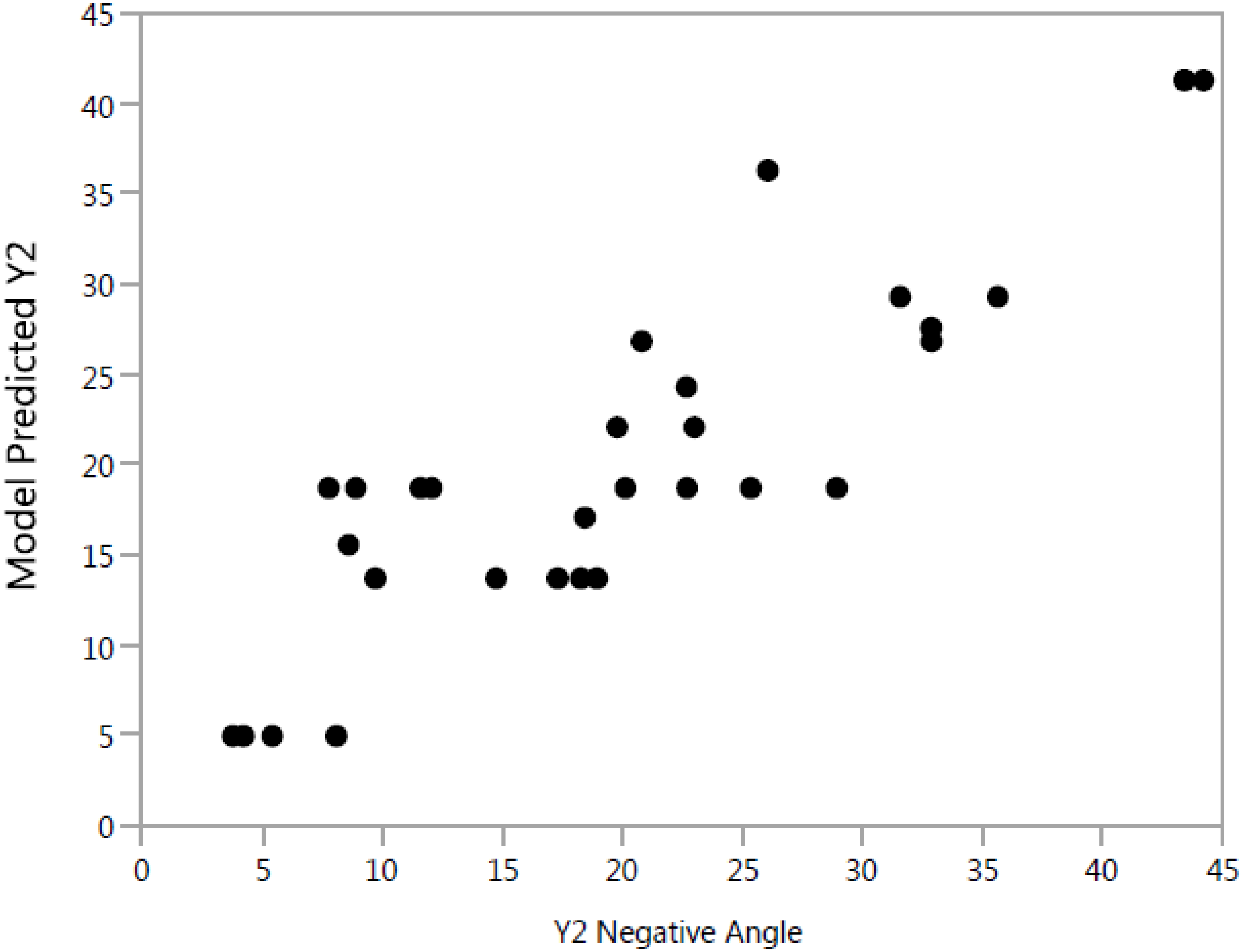
APE Score Y2

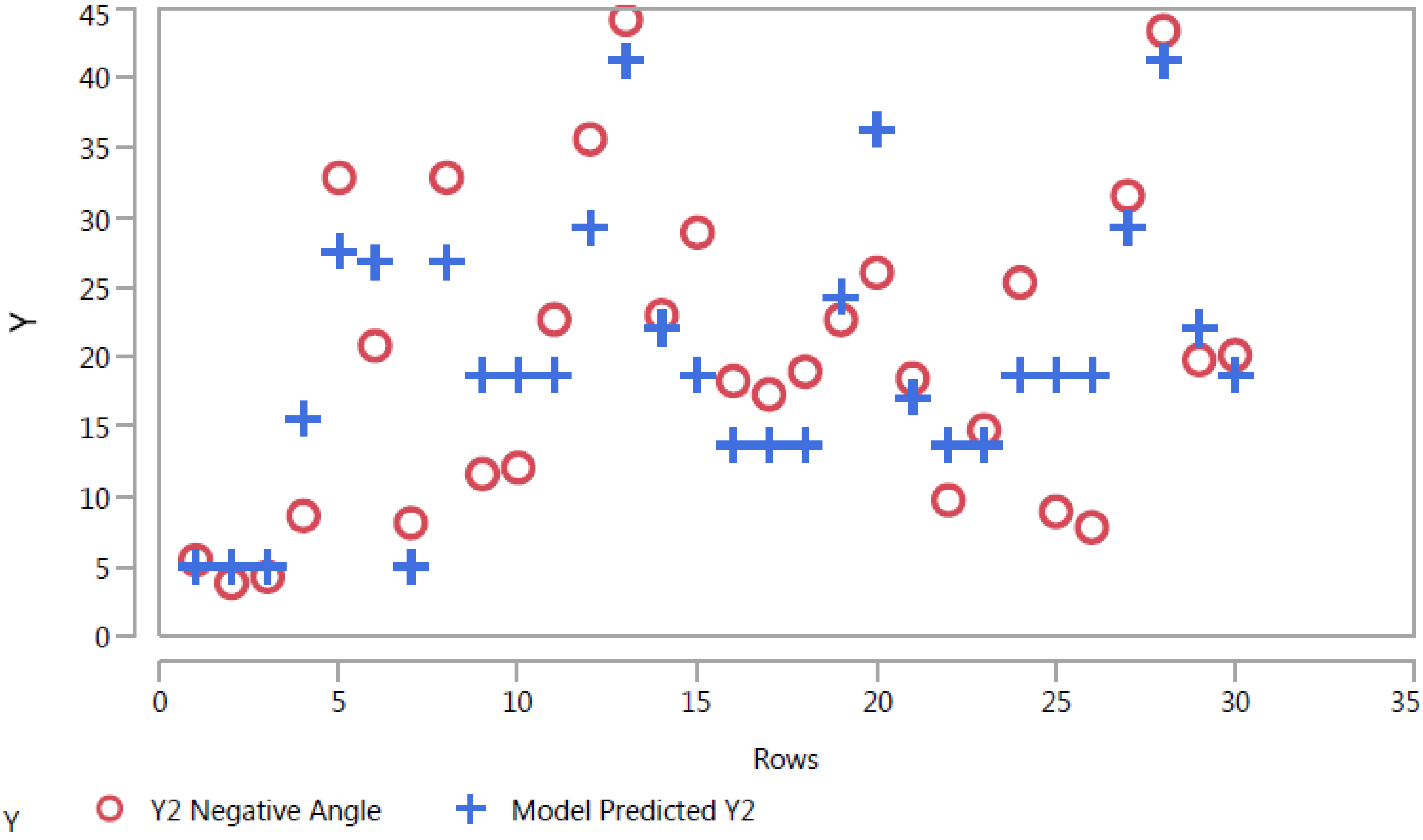
Quantiles

100.0%	maximum	1.403
99.5%		1.403
97.5%		1.403
90.0%		0.78866
75.0%	quartile	0.38803
50.0%	median	0.19593
25.0%	quartile	0.07377
10.0%		0.06573
2.5%		0.03998
0.5%		0.03998
0.0%	minimum	0.03998

Summary Statistics

Mean	0.3066352
Std Dev	0.3174315
Std Err Mean	0.0579548
Upper 95% Mean	0.4251661
Lower 95% Mean	0.1881044
N	30


Model Predicted Y2
45
40
35
30
25
20
15
10
5
0
0
5
10
15
20
25
30
35
40
45
Y2 Negative Angle


Y
45
40
35
30
25
20
15
10
5
0
0
5
10
15
20
25
30
35
Rows
Y
○ Y2 Negative Angle
+ Model Predicted Y2

Appendix P: Byproduct Mass Calculations

	Atomic Weight	Sulfonic Acid Group	Sulfonic Acid Group'	Tar - Sulf	A (Tar)	A' (Tar - Na)	A'' (Tar - 2Na)	A''' (Tar - 3Na)
C	12.01	6	6	10	16	16	16	16
H	1.008	4	4	5	9	9	9	9
N	14.01	0	0	4	4	4	4	4
Na	22.99	1	0	2	3	2	1	0
O	16	3	3	6	9	9	9	9
S	32.06	1	1	1	2	2	2	2
	Mass	**179.142**	**156.152**	**355.22**	**534.362**	**511.372**	**488.382**	**465.392**

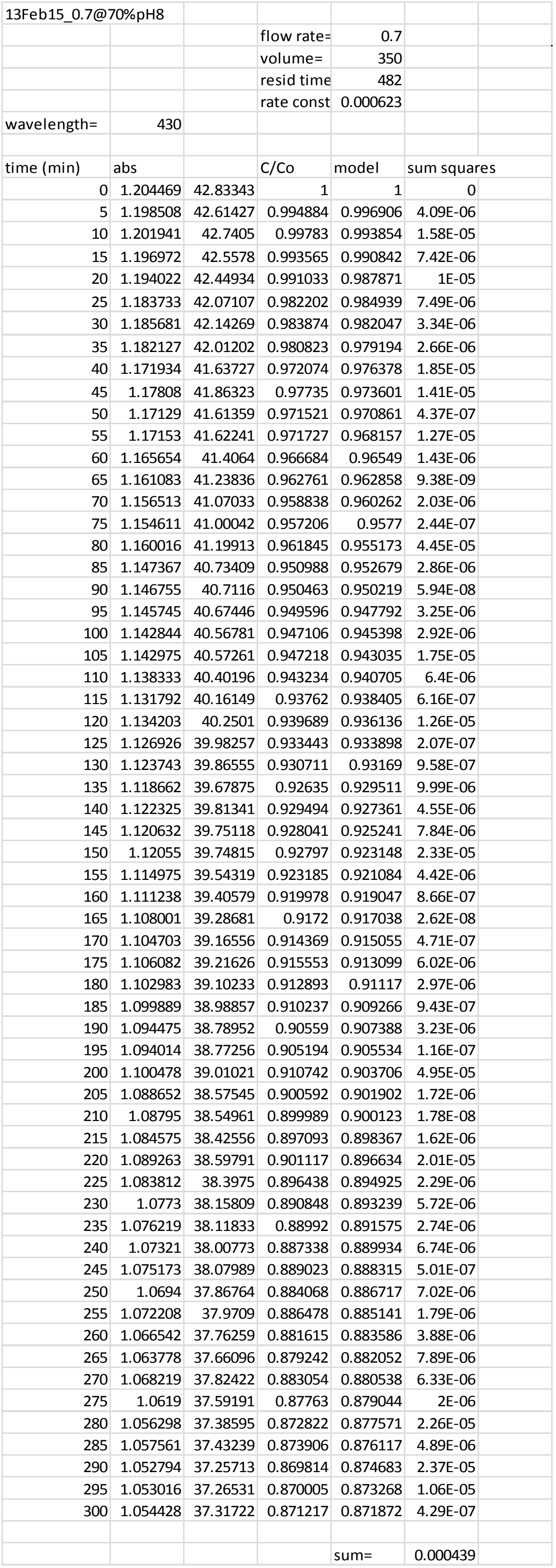
Mass	A	B	C	D	E	F
- 0Na (Product)	534.362	551.37	474.352	536.378	328.218	371.22
- 1Na (Product')	511.372	528.38	451.362	513.388	305.228	348.23
- 2Na (Product'')	488.382	505.39	428.372	490.398	282.238	325.24
- 3Na (Product''')	465.392	482.4	405.382	467.408	-	-

B (Tar + OH)	B' (Tar + OH)	B'' (Tar + OH)	B''' (Tar + OH)	C (Tar - O - CO2)	C' (Tar - O - CO2)	C'' (Tar - O - CO2)	C''' (Tar - O - CO2)
16	16	16	16	15	15	15	15
10	10	10	10	9	9	9	9
4	4	4	4	4	4	4	4
3	2	1	0	3	2	1	0
10	10	10	10	6	6	6	6
2	2	2	2	2	2	2	2
551.37	**528.38**	**505.39**	**482.4**	**474.352**	**451.362**	**428.372**	**405.382**

D (Tar + 2H)	D' (Tar + 2H)	D'' (Tar + 2H)	D''' (Tar + 2H)	E (Tar - Sulf - CO2 + OH)	E' (Tar - Sulf - CO2 + OH)	E'' (Tar - Sulf - CO2 + OH)
16	16	16	16	9	9	9
11	11	11	11	6	6	6
4	4	4	4	4	4	4
3	2	1	0	2	1	0
9	9	9	9	5	5	5
2	2	2	2	1	1	1
536.378	**513.388**	**490.398**	**467.408**	**328.218**	**305.228**	**282.238**

F (Tar - Sulf + O)	F' (Tar - Sulf + O)	F'' (Tar - Sulf + O)
10	10	10
5	5	5
4	4	4
2	1	0
7	7	7
1	1	1
371.22	**348.23**	**325.24**

Appendix Q: AOP Original Data and Calibration Curves



13Feb15_0.7@70%pH8						
			flow rate=	0.7		
			volume=	350		
			resid time	482		
			rate const	0.000623		
wavelength=	430					
time (min)	abs		C/Co	model	sum squares	
0	1.204469	42.83343	1	1	0	
5	1.198508	42.61427	0.994884	0.996906	4.09E-06	
10	1.201941	42.7405	0.99783	0.993854	1.58E-05	
15	1.196972	42.5578	0.993565	0.990842	7.42E-06	
20	1.194022	42.44934	0.991033	0.987871	1E-05	
25	1.183733	42.07107	0.982202	0.984939	7.49E-06	
30	1.185681	42.14269	0.983874	0.982047	3.34E-06	
35	1.182127	42.01202	0.980823	0.979194	2.66E-06	
40	1.171934	41.63727	0.972074	0.976378	1.85E-05	
45	1.17808	41.86323	0.97735	0.973601	1.41E-05	
50	1.17129	41.61359	0.971521	0.970861	4.37E-07	
55	1.17153	41.62241	0.971727	0.968157	1.27E-05	
60	1.165654	41.4064	0.966684	0.96549	1.43E-06	
65	1.161083	41.23836	0.962761	0.962858	9.38E-09	
70	1.156513	41.07033	0.958838	0.960262	2.03E-06	
75	1.154611	41.00042	0.957206	0.9577	2.44E-07	
80	1.160016	41.19913	0.961845	0.955173	4.45E-05	
85	1.147367	40.73409	0.950988	0.952679	2.86E-06	
90	1.146755	40.7116	0.950463	0.950219	5.94E-08	
95	1.145745	40.67446	0.949596	0.947792	3.25E-06	
100	1.142844	40.56781	0.947106	0.945398	2.92E-06	
105	1.142975	40.57261	0.947218	0.943035	1.75E-05	
110	1.138333	40.40196	0.943234	0.940705	6.4E-06	
115	1.131792	40.16149	0.93762	0.938405	6.16E-07	
120	1.134203	40.2501	0.939689	0.936136	1.26E-05	
125	1.126926	39.98257	0.933443	0.933898	2.07E-07	
130	1.123743	39.86555	0.930711	0.93169	9.58E-07	
135	1.118662	39.67875	0.92635	0.929511	9.99E-06	
140	1.122325	39.81341	0.929494	0.927361	4.55E-06	
145	1.120632	39.75118	0.928041	0.925241	7.84E-06	
150	1.12055	39.74815	0.92797	0.923148	2.33E-05	
155	1.114975	39.54319	0.923185	0.921084	4.42E-06	
160	1.111238	39.40579	0.919978	0.919047	8.66E-07	
165	1.108001	39.28681	0.9172	0.917038	2.62E-08	
170	1.104703	39.16556	0.914369	0.915055	4.71E-07	
175	1.106082	39.21626	0.915553	0.913099	6.02E-06	
180	1.102983	39.10233	0.912893	0.91117	2.97E-06	
185	1.099889	38.98857	0.910237	0.909266	9.43E-07	
190	1.094475	38.78952	0.90559	0.907388	3.23E-06	
195	1.094014	38.77256	0.905194	0.905534	1.16E-07	
200	1.100478	39.01021	0.910742	0.903706	4.95E-05	
205	1.088652	38.57545	0.900592	0.901902	1.72E-06	
210	1.08795	38.54961	0.899989	0.900123	1.78E-08	
215	1.084575	38.42556	0.897093	0.898367	1.62E-06	
220	1.089263	38.59791	0.901117	0.896634	2.01E-05	
225	1.083812	38.3975	0.896438	0.894925	2.29E-06	
230	1.0773	38.15809	0.890848	0.893239	5.72E-06	
235	1.076219	38.11833	0.88992	0.891575	2.74E-06	
240	1.07321	38.00773	0.887338	0.889934	6.74E-06	
245	1.075173	38.07989	0.889023	0.888315	5.01E-07	
250	1.0694	37.86764	0.884068	0.886717	7.02E-06	
255	1.072208	37.9709	0.886478	0.885141	1.79E-06	
260	1.066542	37.76259	0.881615	0.883586	3.88E-06	
265	1.063778	37.66096	0.879242	0.882052	7.89E-06	
270	1.068219	37.82422	0.883054	0.880538	6.33E-06	
275	1.0619	37.59191	0.87763	0.879044	2E-06	
280	1.056298	37.38595	0.872822	0.877571	2.26E-05	
285	1.057561	37.43239	0.873906	0.876117	4.89E-06	
290	1.052794	37.25713	0.869814	0.874683	2.37E-05	
295	1.053016	37.26531	0.870005	0.873268	1.06E-05	
300	1.054428	37.31722	0.871217	0.871872	4.29E-07	
				sum=	0.000439	

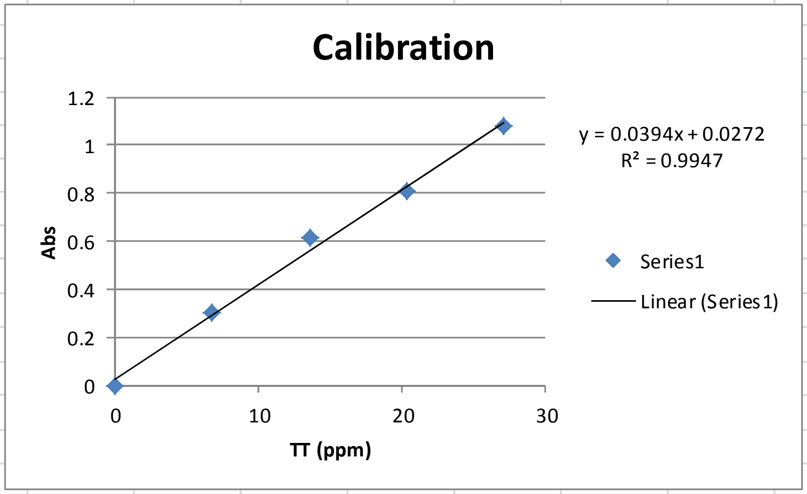
Calibratio Curve

a=	0.0394
b=	0.0272

%	TT (ppm)	abs
0	0	0.0008
0.25	6.7775	0.3019
0.5	13.555	0.6121
0.75	20.3325	0.8113
1	27.11	1.0825

pH Before	8
pH After	

R	0.99782
Rsquard	0.995645



7Mar15_0.7@0%pH7					
			flow rate=	0.7	
			volume=	350	
			resid time	482	
			rate const	1.97E-05	
wavelength=	430				
time (min)	abs		C/Co	model	sum squares
0	1.347136	23.50424	1	1	0
5	1.350849	23.57102	1.002841	0.999902	8.64E-06
10	1.348934	23.53658	1.001376	0.999805	2.47E-06
15	1.348248	23.52424	1.000851	0.999708	1.3E-06
20	1.3499	23.55396	1.002115	0.999613	6.26E-06
25	1.342373	23.41857	0.996355	0.999519	1E-05
30	1.340749	23.38938	0.995113	0.999426	1.86E-05
35	1.344021	23.44821	0.997616	0.999334	2.95E-06
40	1.349348	23.54403	1.001693	0.999243	6E-06
45	1.343877	23.44564	0.997507	0.999152	2.71E-06
50	1.350504	23.56482	1.002578	0.999063	1.24E-05
55	1.351606	23.58465	1.003421	0.998974	1.98E-05
60	1.342429	23.41959	0.996398	0.998887	6.19E-06
65	1.336644	23.31554	0.991972	0.9988	4.66E-05
70	1.348672	23.53188	1.001176	0.998715	6.06E-06
75	1.350174	23.55889	1.002325	0.99863	1.37E-05
80	1.344847	23.46307	0.998248	0.998546	8.85E-08
85	1.350204	23.55943	1.002348	0.998463	1.51E-05
90	1.347413	23.50923	1.000212	0.998381	3.35E-06
95	1.343704	23.44252	0.997374	0.998299	8.56E-07
100	1.343469	23.43829	0.997194	0.998219	1.05E-06
105	1.348678	23.53199	1.001181	0.998139	9.25E-06
110	1.349594	23.54844	1.001881	0.99806	1.46E-05
115	1.351111	23.57574	1.003042	0.997982	2.56E-05
120	1.335763	23.2997	0.991298	0.997905	4.37E-05
125	1.343258	23.4345	0.997033	0.997829	6.33E-07
130	1.339791	23.37214	0.99438	0.997753	1.14E-05
135	1.340201	23.37951	0.994694	0.997679	8.91E-06
140	1.343414	23.4373	0.997152	0.997605	2.05E-07
145	1.341348	23.40015	0.995571	0.997531	3.84E-06
150	1.351436	23.58159	1.003291	0.997459	3.4E-05
155	1.34084	23.39101	0.995183	0.997387	4.86E-06
160	1.340608	23.38683	0.995005	0.997316	5.34E-06
165	1.349836	23.55281	1.002066	0.997246	2.32E-05
170	1.337726	23.335	0.9928	0.997176	1.92E-05
175	1.336776	23.31792	0.992073	0.997108	2.53E-05
180	1.340186	23.37924	0.994682	0.99704	5.56E-06
185	1.341591	23.40452	0.995758	0.996972	1.48E-06
190	1.339185	23.36125	0.993916	0.996906	8.93E-06
195	1.34869	23.5322	1.00119	0.99684	1.89E-05
200	1.341588	23.40447	0.995755	0.996774	1.04E-06
205	1.346927	23.50049	0.99984	0.99671	9.8E-06
210	1.349863	23.55329	1.002087	0.996646	2.96E-05
215	1.342975	23.4294	0.996816	0.996583	5.44E-08
220	1.337947	23.33897	0.992969	0.99652	1.26E-05
225	1.348032	23.52036	1.000686	0.996458	1.79E-05
230	1.344025	23.4483	0.99762	0.996397	1.5E-06
235	1.3375	23.33093	0.992627	0.996336	1.38E-05
240	1.348585	23.53031	1.001109	0.996276	2.34E-05
245	1.339528	23.36741	0.994179	0.996217	4.15E-06
250	1.343466	23.43823	0.997192	0.996158	1.07E-06
255	1.343612	23.44087	0.997304	0.9961	1.45E-06
260	1.337768	23.33575	0.992832	0.996042	1.03E-05
265	1.344269	23.45268	0.997807	0.995985	3.32E-06
270	1.347889	23.51779	1.000577	0.995929	2.16E-05
275	1.341426	23.40154	0.995631	0.995873	5.88E-08
280	1.350573	23.56606	1.00263	0.995818	4.64E-05
285	1.337829	23.33684	0.992878	0.995763	8.32E-06
290	1.33766	23.33382	0.992749	0.995709	8.76E-06
295	1.335	23.28597	0.990714	0.995656	2.44E-05
300	1.338162	23.34285	0.993134	0.995603	6.1E-06
				sum=	0.000695

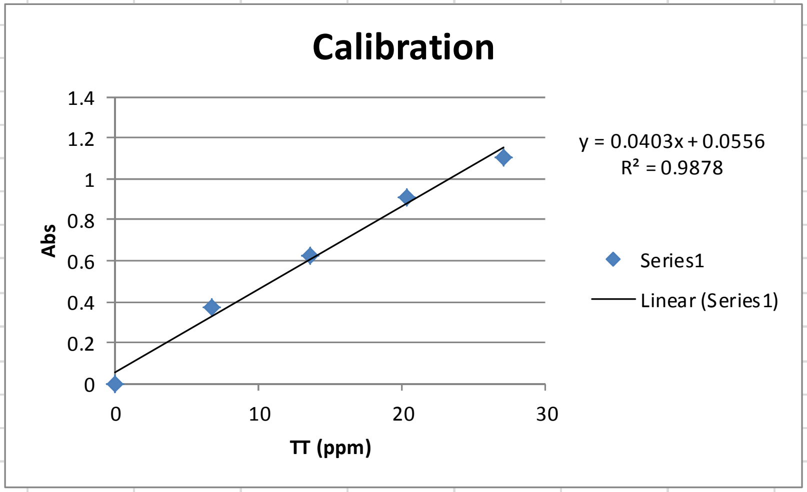
Calibratio Curve

a= 0.0403

b= 0.0556

%	TT (ppm)	abs
0	0	0.0013
0.25	6.7775	0.3765
0.5	13.555	0.6217
0.75	20.3325	0.912
1	27.11	1.1008

pH Before	7
pH After	



13Mar15_0.7@5%pH7					
			flow rate=	0.7	
			volume=	350	
			resid time	482	
			rate const	9.07E-05	
wavelength=	430				
time (min)	abs		C/Co	model	sum squares
0	1.23038	110.9981	1	1	0
5	1.222567	110.268	0.993422	0.999549	3.75E-05
10	1.234194	111.3546	1.003211	0.999103	1.69E-05
15	1.226878	110.6709	0.997052	0.998661	2.59E-06
20	1.225585	110.55	0.995963	0.998225	5.12E-06
25	1.232246	111.1725	1.001571	0.997793	1.43E-05
30	1.227749	110.7522	0.997785	0.997366	1.76E-07
35	1.226388	110.625	0.996639	0.996943	9.26E-08
40	1.223906	110.3931	0.99455	0.996525	3.9E-06
45	1.230713	111.0293	1.000281	0.996111	1.74E-05
50	1.226309	110.6176	0.996572	0.995702	7.57E-07
55	1.227442	110.7235	0.997526	0.995298	4.97E-06
60	1.222023	110.2171	0.992964	0.994897	3.74E-06
65	1.224014	110.4031	0.99464	0.994501	1.92E-08
70	1.220963	110.118	0.992071	0.994109	4.15E-06
75	1.218882	109.9235	0.990319	0.993722	1.16E-05
80	1.219184	109.9518	0.990573	0.993338	7.65E-06
85	1.226177	110.6053	0.996461	0.992959	1.23E-05
90	1.222691	110.2796	0.993526	0.992584	8.88E-07
95	1.214266	109.4921	0.986432	0.992213	3.34E-05
100	1.21531	109.5897	0.987312	0.991846	2.06E-05
105	1.213807	109.4492	0.986046	0.991482	2.96E-05
110	1.213169	109.3896	0.985509	0.991123	3.15E-05
115	1.213494	109.42	0.985783	0.990768	2.49E-05
120	1.221479	110.1663	0.992506	0.990416	4.37E-06
125	1.215341	109.5926	0.987337	0.990068	7.46E-06
130	1.219137	109.9474	0.990534	0.989724	6.55E-07
135	1.211527	109.2362	0.984126	0.989384	2.76E-05
140	1.218657	109.9025	0.99013	0.989047	1.17E-06
145	1.21438	109.5028	0.986529	0.988714	4.78E-06
150	1.216062	109.66	0.987945	0.988385	1.94E-07
155	1.210601	109.1497	0.983347	0.988059	2.22E-05
160	1.213534	109.4237	0.985816	0.987736	3.69E-06
165	1.221324	110.1518	0.992375	0.987417	2.46E-05
170	1.214742	109.5366	0.986833	0.987102	7.22E-08
175	1.21019	109.1112	0.983001	0.98679	1.44E-05
180	1.214652	109.5282	0.986757	0.986481	7.64E-08
185	1.213058	109.3792	0.985415	0.986176	5.78E-07
190	1.211967	109.2772	0.984496	0.985873	1.9E-06
195	1.214663	109.5293	0.986767	0.985575	1.42E-06
200	1.21959	109.9897	0.990915	0.985279	3.18E-05
205	1.211616	109.2445	0.984201	0.984986	6.17E-07
210	1.220786	110.1015	0.991922	0.984697	5.22E-05
215	1.211623	109.2452	0.984208	0.984411	4.14E-08
220	1.205627	108.6848	0.979159	0.984128	2.47E-05
225	1.218551	109.8926	0.990041	0.983848	3.84E-05
230	1.206918	108.8055	0.980246	0.983571	1.11E-05
235	1.216765	109.7257	0.988537	0.983297	2.75E-05
240	1.213016	109.3753	0.98538	0.983025	5.54E-06
245	1.213948	109.4624	0.986165	0.982757	1.16E-05
250	1.218909	109.9261	0.990342	0.982492	6.16E-05
255	1.206083	108.7274	0.979543	0.982229	7.22E-06
260	1.214847	109.5464	0.986921	0.98197	2.45E-05
265	1.206509	108.7672	0.979902	0.981713	3.28E-06
270	1.213019	109.3756	0.985382	0.981459	1.54E-05
275	1.213614	109.4312	0.985883	0.981207	2.19E-05
280	1.206276	108.7455	0.979705	0.980959	1.57E-06
285	1.205132	108.6385	0.978742	0.980713	3.88E-06
290	1.203713	108.5059	0.977547	0.98047	8.54E-06
295	1.200695	108.2238	0.975006	0.980229	2.73E-05
300	1.20452	108.5814	0.978227	0.979991	3.11E-06
				sum=	0.000781

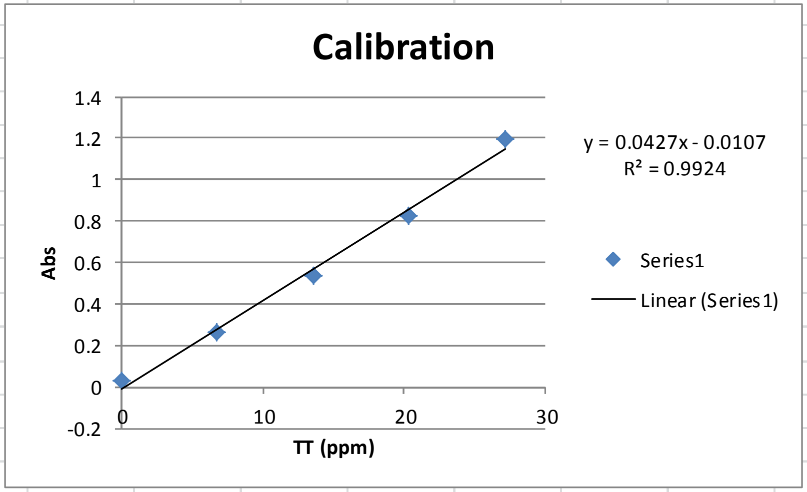
Calibratio Curve

a= 0.0427

b= 0.0107

%	TT (ppm)	abs
0	0	0.0298
0.25	6.7775	0.2589
0.5	13.555	0.5334
0.75	20.3325	0.826
1	27.11	1.1939

pH Before	7
pH After	6

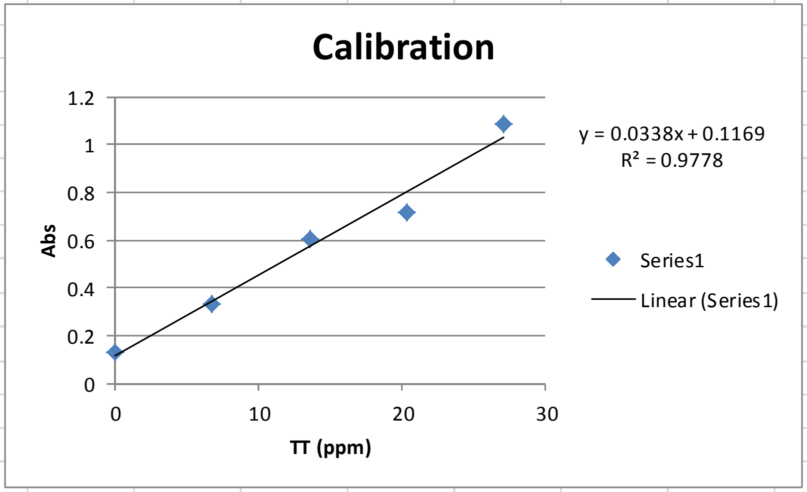


16Mar15_0.7@0%pH9					
			flow rate=	0.7	
			volume=	350	
			resid time	482	
			rate const	-1.6E-05	
wavelength=	430				
time (min)	abs		C/Co	model	sum squares
0	1.089044	9.026898	1	1	0
5	1.097648	9.100496	1.008153	1.000077	6.52E-05
10	1.094525	9.073781	1.005194	1.000154	2.54E-05
15	1.092652	9.057755	1.003418	1.000229	1.02E-05
20	1.091003	9.043651	1.001856	1.000304	2.41E-06
25	1.096163	9.087791	1.006746	1.000378	4.05E-05
30	1.093745	9.067112	1.004455	1.000452	1.6E-05
35	1.094047	9.06969	1.00474	1.000524	1.78E-05
40	1.100506	9.124945	1.010862	1.000596	0.000105
45	1.099427	9.115712	1.009839	1.000667	8.41E-05
50	1.093896	9.068397	1.004597	1.000738	1.49E-05
55	1.102695	9.143674	1.012936	1.000807	0.000147
60	1.097598	9.100072	1.008106	1.000876	5.23E-05
65	1.097597	9.100064	1.008105	1.000945	5.13E-05
70	1.094955	9.077459	1.005601	1.001012	2.11E-05
75	1.09943	9.115742	1.009842	1.001079	7.68E-05
80	1.092563	9.057	1.003335	1.001145	4.79E-06
85	1.090992	9.043558	1.001846	1.001211	4.03E-07
90	1.099896	9.119723	1.010283	1.001276	8.11E-05
95	1.094018	9.069441	1.004713	1.00134	1.14E-05
100	1.092546	9.056852	1.003318	1.001403	3.67E-06
105	1.09182	9.050645	1.002631	1.001466	1.36E-06
110	1.092992	9.060668	1.003741	1.001528	4.9E-06
115	1.092684	9.058035	1.003449	1.00159	3.46E-06
120	1.091814	9.050589	1.002624	1.001651	9.48E-07
125	1.091535	9.048204	1.00236	1.001711	4.22E-07
130	1.095445	9.081654	1.006066	1.001771	1.84E-05
135	1.092384	9.055468	1.003165	1.00183	1.78E-06
140	1.090872	9.042529	1.001732	1.001888	2.46E-08
145	1.092664	9.057857	1.00343	1.001946	2.2E-06
150	1.092723	9.05837	1.003487	1.002004	2.2E-06
155	1.089581	9.031486	1.000508	1.00206	2.41E-06
160	1.093762	9.067256	1.004471	1.002116	5.54E-06
165	1.089883	9.034076	1.000795	1.002172	1.9E-06
170	1.092827	9.059256	1.003585	1.002227	1.84E-06
175	1.086721	9.007025	0.997798	1.002281	2.01E-05
180	1.091185	9.045208	1.002028	1.002335	9.41E-08
185	1.093033	9.061019	1.00378	1.002389	1.94E-06
190	1.088751	9.024387	0.999722	1.002441	7.4E-06
195	1.089519	9.030961	1.00045	1.002494	4.18E-06
200	1.089049	9.026937	1.000004	1.002545	6.46E-06
205	1.088885	9.025533	0.999849	1.002596	7.55E-06
210	1.092084	9.052902	1.002881	1.002647	5.46E-08
215	1.098274	9.105855	1.008747	1.002697	3.66E-05
220	1.09094	9.043111	1.001796	1.002747	9.04E-07
225	1.089637	9.031969	1.000562	1.002796	4.99E-06
230	1.095751	9.084266	1.006355	1.002844	1.23E-05
235	1.08757	9.014283	0.998603	1.002893	1.84E-05
240	1.085639	8.997767	0.996773	1.00294	3.8E-05
245	1.089055	9.026987	1.00001	1.002987	8.86E-06
250	1.087058	9.009905	0.998118	1.003034	2.42E-05
255	1.088977	9.026326	0.999937	1.00308	9.88E-06
260	1.092321	9.054924	1.003105	1.003126	4.44E-10
265	1.090817	9.042059	1.00168	1.003171	2.22E-06
270	1.088707	9.024013	0.99968	1.003216	1.25E-05
275	1.090337	9.037959	1.001225	1.00326	4.14E-06
280	1.090565	9.039905	1.001441	1.003304	3.47E-06
285	1.091601	9.048764	1.002422	1.003347	8.55E-07
290	1.091923	9.051523	1.002728	1.00339	4.39E-07
295	1.090315	9.037766	1.001204	1.003433	4.97E-06
300	1.095662	9.083506	1.006271	1.003475	7.82E-06
				sum=	0.001118

Calibratio Curve

a=	0.0338		%	TT (ppm)	abs
b=	0.1169		0	0	0.1337
			0.25	6.7775	0.3321
			0.5	13.555	0.6054
			0.75	20.3325	0.7164
			1	27.11	1.0861

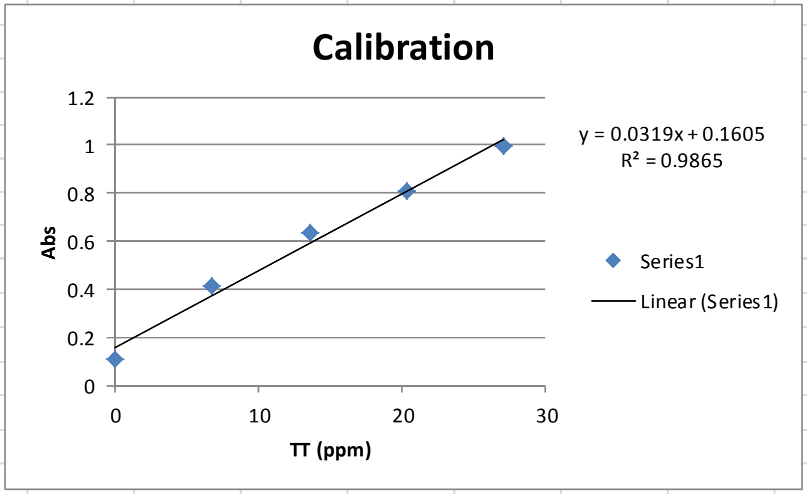
pH Before	9
pH After	9



8Apr15_0.7@100%pH9H2O2Ctrl					
			flow rate=	0.7	
			volume=	350	
			resid time	482	
			rate const	4.34E-05	
wavelength=	430				
time (min)	abs		C/Co	model	sum squares
0	0.932205	5.609379	1	1	0
5	0.942214	5.67174	1.011117	0.999784	0.000128
10	0.934182	5.621696	1.002196	0.999571	6.89E-06
15	0.935651	5.63085	1.003828	0.999359	2E-05
20	0.936384	5.635414	1.004641	0.99915	3.02E-05
25	0.930519	5.59887	0.998127	0.998944	6.67E-07
30	0.933189	5.615508	1.001093	0.998739	5.54E-06
35	0.941072	5.664621	1.009848	0.998536	0.000128
40	0.927239	5.578434	0.994483	0.998336	1.48E-05
45	0.932213	5.609429	1.000009	0.998138	3.5E-06
50	0.930038	5.595873	0.997592	0.997942	1.22E-07
55	0.929404	5.591924	0.996888	0.997747	7.38E-07
60	0.931739	5.606473	0.999482	0.997555	3.71E-06
65	0.930879	5.601114	0.998527	0.997365	1.35E-06
70	0.93959	5.655386	1.008202	0.997177	0.000122
75	0.928589	5.58685	0.995984	0.996991	1.01E-06
80	0.933122	5.615092	1.001019	0.996807	1.77E-05
85	0.929218	5.590769	0.996682	0.996625	3.31E-09
90	0.932583	5.611732	1.000419	0.996445	1.58E-05
95	0.925239	5.565977	0.992263	0.996266	1.6E-05
100	0.927472	5.579886	0.994742	0.99609	1.82E-06
105	0.925332	5.566553	0.992365	0.995915	1.26E-05
110	0.92742	5.579561	0.994684	0.995743	1.12E-06
115	0.933001	5.614335	1.000884	0.995572	2.82E-05
120	0.92743	5.579629	0.994696	0.995402	4.98E-07
125	0.925467	5.567395	0.992515	0.995235	7.4E-06
130	0.923117	5.552755	0.989906	0.995069	2.67E-05
135	0.924275	5.559971	0.991192	0.994906	1.38E-05
140	0.925489	5.56753	0.99254	0.994743	4.86E-06
145	0.929579	5.593016	0.997083	0.994583	6.25E-06
150	0.929729	5.593952	0.99725	0.994424	7.98E-06
155	0.922473	5.548744	0.989191	0.994267	2.58E-05
160	0.928174	5.584264	0.995523	0.994112	1.99E-06
165	0.923094	5.552612	0.98988	0.993958	1.66E-05
170	0.928122	5.583939	0.995465	0.993806	2.75E-06
175	0.927673	5.581139	0.994966	0.993655	1.72E-06
180	0.926343	5.572854	0.993489	0.993506	3.18E-10
185	0.927574	5.58052	0.994855	0.993359	2.24E-06
190	0.921681	5.54381	0.988311	0.993213	2.4E-05
195	0.921884	5.545071	0.988536	0.993069	2.06E-05
200	0.917002	5.514651	0.983113	0.992926	9.63E-05
205	0.919723	5.531608	0.986136	0.992785	4.42E-05
210	0.921918	5.545282	0.988573	0.992645	1.66E-05
215	0.922173	5.546869	0.988856	0.992507	1.33E-05
220	0.919115	5.527822	0.985461	0.99237	4.77E-05
225	0.923572	5.555589	0.990411	0.992234	3.33E-06
230	0.920168	5.534383	0.98663	0.992101	2.99E-05
235	0.930028	5.595811	0.997581	0.991968	3.15E-05
240	0.918019	5.520991	0.984243	0.991837	5.77E-05
245	0.920589	5.537001	0.987097	0.991707	2.13E-05
250	0.924369	5.560554	0.991296	0.991579	7.99E-08
255	0.92658	5.574328	0.993751	0.991451	5.29E-06
260	0.930785	5.600532	0.998423	0.991326	5.04E-05
265	0.924951	5.56418	0.991942	0.991201	5.49E-07
270	0.926369	5.573013	0.993517	0.991078	5.95E-06
275	0.927791	5.581876	0.995097	0.990956	1.71E-05
280	0.936193	5.634222	1.004429	0.990836	0.000185
285	0.923098	5.552638	0.989885	0.990717	6.92E-07
290	0.927071	5.577388	0.994297	0.990599	1.37E-05
295	0.92644	5.573457	0.993596	0.990482	9.7E-06
300	0.929785	5.594299	0.997312	0.990366	4.82E-05
				sum=	0.001421

Calibratio Curve

a=	0.0319	%	TT (ppm)	abs
b=	0.1605	0	0	0.1116
		0.25	6.7775	0.4145
		0.5	13.555	0.6338
		0.75	20.3325	0.8081
		1	27.11	0.9953



H2O2 Control

pH Before	9
pH After	8.5

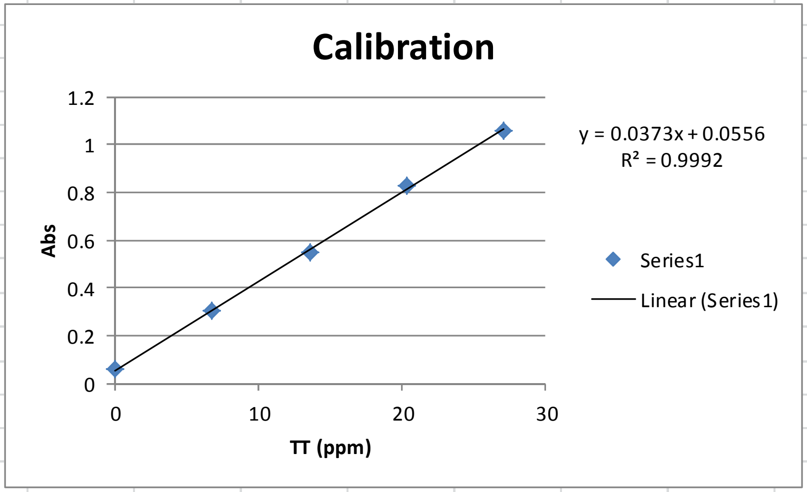
R	0.608253
Rsquard	0.369972

9Apr15_0.7@10%pH7					
			flow rate=	0.7	
			volume=	350	
			resid time	482	
			rate const	0.00016	
wavelength=	430				
time (min)	abs		C/Co	model	sum squares
0	1.16541	20.28974	1	1	0
5	1.167143	20.32092	1.001537	0.999206	5.43E-06
10	1.165206	20.28608	0.99982	0.998421	1.96E-06
15	1.16667	20.31241	1.001117	0.997645	1.21E-05
20	1.162	20.22842	0.996978	0.996877	1E-08
25	1.165599	20.29314	1.000167	0.996118	1.64E-05
30	1.169795	20.36862	1.003887	0.995368	7.26E-05
35	1.160384	20.19935	0.995545	0.994625	8.46E-07
40	1.168191	20.33976	1.002465	0.993891	7.35E-05
45	1.155349	20.1088	0.991082	0.993165	4.34E-06
50	1.161528	20.21993	0.996559	0.992448	1.69E-05
55	1.155834	20.11751	0.991511	0.991738	5.12E-08
60	1.155432	20.11028	0.991155	0.991036	1.42E-08
65	1.153369	20.07318	0.989327	0.990342	1.03E-06
70	1.155217	20.10642	0.990965	0.989655	1.72E-06
75	1.155183	20.10581	0.990935	0.988976	3.84E-06
80	1.152546	20.05839	0.988598	0.988305	8.57E-08
85	1.155679	20.11473	0.991374	0.987641	1.39E-05
90	1.153079	20.06797	0.98907	0.986985	4.35E-06
95	1.147578	19.96904	0.984194	0.986335	4.59E-06
100	1.151601	20.04139	0.98776	0.985693	4.27E-06
105	1.147191	19.96207	0.983851	0.985059	1.46E-06
110	1.147445	19.96663	0.984075	0.984431	1.26E-07
115	1.146816	19.95532	0.983518	0.98381	8.54E-08
120	1.153031	20.0671	0.989027	0.983196	3.4E-05
125	1.140669	19.84477	0.978069	0.982589	2.04E-05
130	1.138873	19.81246	0.976477	0.981989	3.04E-05
135	1.150136	20.01504	0.986461	0.981395	2.57E-05
140	1.141989	19.86851	0.979239	0.980808	2.46E-06
145	1.151769	20.04441	0.987909	0.980227	5.9E-05
150	1.140806	19.84723	0.97819	0.979653	2.14E-06
155	1.146226	19.94471	0.982995	0.979086	1.53E-05
160	1.13883	19.81169	0.976439	0.978524	4.35E-06
165	1.141436	19.85856	0.978749	0.977969	6.08E-07
170	1.137207	19.7825	0.975	0.97742	5.85E-06
175	1.14017	19.83579	0.977627	0.976877	5.62E-07
180	1.137428	19.78647	0.975196	0.97634	1.31E-06
185	1.139001	19.81476	0.97659	0.975809	6.1E-07
190	1.139704	19.82741	0.977214	0.975284	3.72E-06
195	1.135321	19.74859	0.973329	0.974765	2.06E-06
200	1.13453	19.73436	0.972627	0.974252	2.64E-06
205	1.137133	19.78118	0.974935	0.973744	1.42E-06
210	1.133244	19.71123	0.971487	0.973242	3.08E-06
215	1.133356	19.71325	0.971587	0.972745	1.34E-06
220	1.130719	19.66581	0.969249	0.972254	9.03E-06
225	1.141598	19.86147	0.978892	0.971769	5.07E-05
230	1.128199	19.62048	0.967015	0.971289	1.83E-05
235	1.14049	19.84154	0.97791	0.970814	5.04E-05
240	1.126791	19.59517	0.965767	0.970344	2.09E-05
245	1.130763	19.6666	0.969288	0.96988	3.51E-07
250	1.136717	19.77369	0.974566	0.969421	2.65E-05
255	1.128552	19.62683	0.967328	0.968967	2.69E-06
260	1.127759	19.61257	0.966625	0.968518	3.58E-06
265	1.12366	19.53885	0.962992	0.968074	2.58E-05
270	1.127643	19.61049	0.966522	0.967635	1.24E-06
275	1.125492	19.5718	0.964615	0.9672	6.68E-06
280	1.128413	19.62434	0.967205	0.966771	1.89E-07
285	1.122943	19.52595	0.962356	0.966346	1.59E-05
290	1.122578	19.51939	0.962032	0.965926	1.52E-05
295	1.133249	19.71131	0.971491	0.965511	3.58E-05
300	1.125296	19.56827	0.964442	0.965101	4.34E-07
				sum=	0.00074

Calibratio Curve

a=	0.0373		%	TT (ppm)	abs
b=	0.0556		0	0	0.0582
			0.25	6.7775	0.3086
			0.5	13.555	0.5475
			0.75	20.3325	0.8299
			1	27.11	1.0611

pH Before	7.8
pH After	7.4



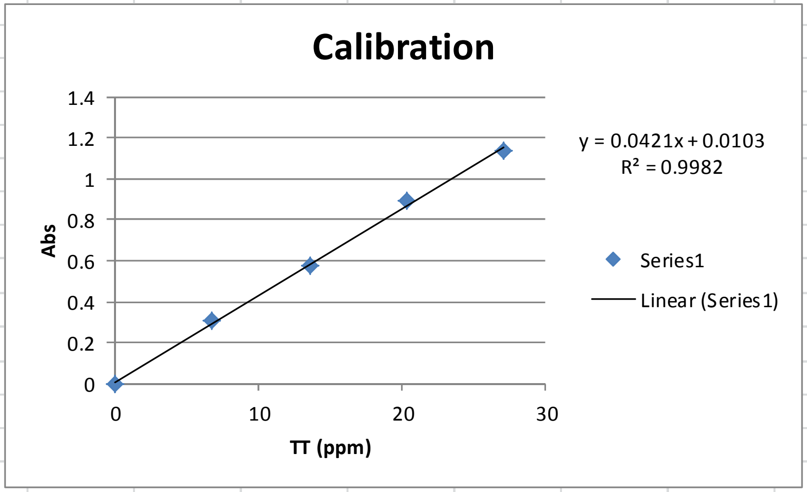
16Apr15 0.7@100%pH8H2O2Ctrl					
			flow rate=	0.7	
			volume=	350	
			resid time	482	
			rate const	9.41E-07	
wavelength=	430				
time (min)	abs		C/Co	model	sum squares
0	1.181593	110.6304	1	1	0
5	1.180632	110.5371	0.999157	0.999995	7.03E-07
10	1.181702	110.641	1.000096	0.999991	1.11E-08
15	1.183201	110.7865	1.001412	0.999986	2.03E-06
20	1.176988	110.1833	0.995959	0.999982	1.62E-05
25	1.188059	111.2581	1.005674	0.999977	3.25E-05
30	1.175248	110.0144	0.994432	0.999973	3.07E-05
35	1.177969	110.2786	0.99682	0.999968	9.91E-06
40	1.178779	110.3572	0.997531	0.999964	5.92E-06
45	1.175979	110.0854	0.995074	0.99996	2.39E-05
50	1.175632	110.0516	0.994769	0.999955	2.69E-05
55	1.178662	110.3459	0.997428	0.999951	6.36E-06
60	1.171872	109.6866	0.991469	0.999947	7.19E-05
65	1.174713	109.9625	0.993963	0.999943	3.58E-05
70	1.176388	110.1251	0.995433	0.999939	2.03E-05
75	1.175156	110.0055	0.994351	0.999935	3.12E-05
80	1.175789	110.0669	0.994907	0.999931	2.52E-05
85	1.180648	110.5387	0.999171	0.999927	5.71E-07
90	1.174901	109.9807	0.994128	0.999923	3.36E-05
95	1.174226	109.9152	0.993535	0.999919	4.08E-05
100	1.174946	109.985	0.994167	0.999915	3.3E-05
105	1.179317	110.4095	0.998003	0.999911	3.64E-06
110	1.178542	110.3342	0.997323	0.999907	6.68E-06
115	1.18413	110.8767	1.002227	0.999904	5.4E-06
120	1.176342	110.1206	0.995392	0.9999	2.03E-05
125	1.178303	110.311	0.997113	0.999896	7.75E-06
130	1.177618	110.2445	0.996512	0.999893	1.14E-05
135	1.184078	110.8717	1.002181	0.999889	5.25E-06
140	1.173139	109.8096	0.992581	0.999886	5.34E-05
145	1.17789	110.2708	0.99675	0.999882	9.81E-06
150	1.177909	110.2727	0.996767	0.999879	9.68E-06
155	1.176552	110.141	0.995576	0.999875	1.85E-05
160	1.186253	111.0828	1.00409	0.999872	1.78E-05
165	1.176188	110.1056	0.995257	0.999868	2.13E-05
170	1.180074	110.483	0.998668	0.999865	1.43E-06
175	1.182863	110.7537	1.001115	0.999862	1.57E-06
180	1.178446	110.3249	0.997239	0.999859	6.86E-06
185	1.175982	110.0857	0.995076	0.999855	2.28E-05
190	1.178735	110.353	0.997493	0.999852	5.57E-06
195	1.179872	110.4633	0.99849	0.999849	1.85E-06
200	1.182931	110.7603	1.001174	0.999846	1.76E-06
205	1.185531	111.0128	1.003457	0.999843	1.31E-05
210	1.182026	110.6724	1.00038	0.99984	2.92E-07
215	1.183977	110.8619	1.002093	0.999837	5.09E-06
220	1.182024	110.6722	1.000378	0.999834	2.96E-07
225	1.17636	110.1224	0.995408	0.999831	1.96E-05
230	1.177909	110.2727	0.996767	0.999828	9.37E-06
235	1.182387	110.7075	1.000697	0.999825	7.61E-07
240	1.179727	110.4492	0.998362	0.999822	2.13E-06
245	1.183571	110.8225	1.001736	0.999819	3.68E-06
250	1.183943	110.8585	1.002062	0.999816	5.04E-06
255	1.19078	111.5223	1.008063	0.999814	6.8E-05
260	1.192421	111.6816	1.009502	0.999811	9.39E-05
265	1.180769	110.5504	0.999277	0.999808	2.82E-07
270	1.183078	110.7746	1.001304	0.999805	2.24E-06
275	1.183793	110.844	1.001931	0.999803	4.53E-06
280	1.184114	110.8752	1.002213	0.9998	5.82E-06
285	1.182479	110.7164	1.000778	0.999798	9.61E-07
290	1.1899	111.4369	1.007291	0.999795	5.62E-05
295	1.183729	110.8378	1.001875	0.999792	4.34E-06
300	1.190069	111.4533	1.007439	0.99979	5.85E-05
				sum=	0.001034

Calibratio Curve

a=	0.0421	%	TT (ppm)	abs
b=	0.0103	0	0	0
		0.25	6.7775	0.3061
		0.5	13.555	0.5724
		0.75	20.3325	0.8947
		1	27.11	1.1331

H2O2 Control

pH Before	7.8
pH After	7

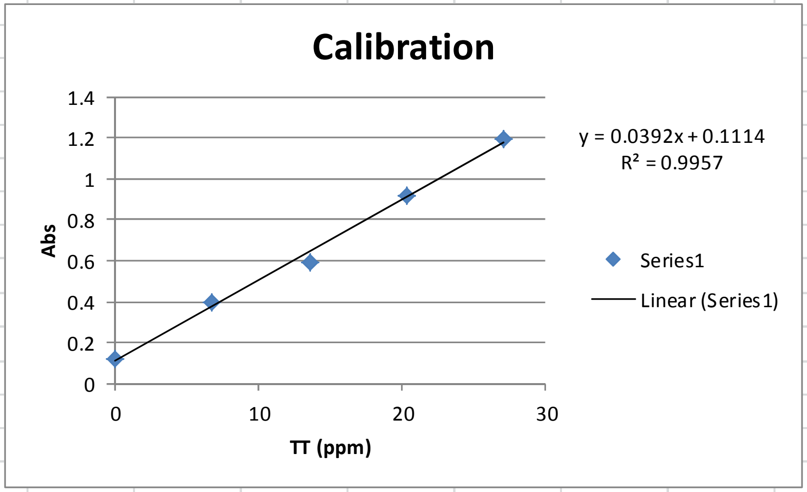


23Apr15_0.7@50%pH8					
			flow rate=	0.7	
			volume=	350	
			resid time	482	
			rate const	0.000749	
wavelength=	430				
time (min)	abs		C/Co	model	sum squares
0	1.163441	10.09193	1	1	0
5	1.157367	10.0374	0.994597	0.996282	2.84E-06
10	1.15644	10.02909	0.993773	0.992616	1.34E-06
15	1.152344	9.992314	0.990129	0.989002	1.27E-06
20	1.148051	9.953775	0.986311	0.985439	7.6E-07
25	1.145089	9.927192	0.983676	0.981925	3.07E-06
30	1.142747	9.906164	0.981593	0.97846	9.81E-06
35	1.139098	9.873414	0.978348	0.975045	1.09E-05
40	1.134523	9.832343	0.974278	0.971677	6.77E-06
45	1.129933	9.791144	0.970196	0.968356	3.38E-06
50	1.128852	9.78144	0.969234	0.965082	1.72E-05
55	1.124342	9.740953	0.965222	0.961853	1.13E-05
60	1.121271	9.713382	0.96249	0.95867	1.46E-05
65	1.117776	9.682013	0.959382	0.955532	1.48E-05
70	1.11552	9.661764	0.957375	0.952437	2.44E-05
75	1.111232	9.62327	0.953561	0.949386	1.74E-05
80	1.106211	9.578196	0.949095	0.946378	7.38E-06
85	1.103579	9.55457	0.946754	0.943412	1.12E-05
90	1.100689	9.528626	0.944183	0.940487	1.37E-05
95	1.098174	9.50605	0.941946	0.937604	1.89E-05
100	1.095854	9.485224	0.939882	0.934761	2.62E-05
105	1.091	9.441656	0.935565	0.931957	1.3E-05
110	1.086711	9.403147	0.931749	0.929193	6.53E-06
115	1.08444	9.382762	0.929729	0.926468	1.06E-05
120	1.081766	9.358759	0.927351	0.923781	1.27E-05
125	1.080595	9.348246	0.926309	0.921132	2.68E-05
130	1.074224	9.291056	0.920642	0.91852	4.51E-06
135	1.07242	9.274862	0.919038	0.915944	9.57E-06
140	1.069026	9.2444	0.916019	0.913405	6.84E-06
145	1.067921	9.234483	0.915037	0.910901	1.71E-05
150	1.062841	9.188875	0.910517	0.908432	4.35E-06
155	1.058944	9.153899	0.907052	0.905998	1.11E-06
160	1.059781	9.161412	0.907796	0.903598	1.76E-05
165	1.053022	9.100738	0.901784	0.901231	3.05E-07
170	1.05118	9.084197	0.900145	0.898898	1.55E-06
175	1.048702	9.061959	0.897941	0.896597	1.81E-06
180	1.045862	9.036466	0.895415	0.894329	1.18E-06
185	1.041926	9.001131	0.891914	0.892093	3.2E-08
190	1.039385	8.978321	0.889654	0.889888	5.47E-08
195	1.036104	8.948871	0.886735	0.887713	9.56E-07
200	1.03468	8.936087	0.885469	0.88557	1.02E-08
205	1.032759	8.918843	0.88376	0.883456	9.24E-08
210	1.030625	8.899687	0.881862	0.881372	2.4E-07
215	1.028037	8.876452	0.87956	0.879317	5.88E-08
220	1.023058	8.831761	0.875131	0.877291	4.67E-06
225	1.021992	8.82219	0.874183	0.875293	1.23E-06
230	1.019747	8.802035	0.872186	0.873324	1.3E-06
235	1.017038	8.777721	0.869776	0.871382	2.58E-06
240	1.013902	8.749565	0.866986	0.869467	6.15E-06
245	1.012704	8.738811	0.865921	0.867579	2.75E-06
250	1.008778	8.70357	0.862429	0.865718	1.08E-05
255	1.007712	8.694004	0.861481	0.863882	5.77E-06
260	1.006333	8.681626	0.860254	0.862072	3.31E-06
265	1.002012	8.642839	0.856411	0.860288	1.5E-05
270	1.001165	8.635236	0.855658	0.858529	8.24E-06
275	0.998898	8.61488	0.853641	0.856794	9.95E-06
280	0.996724	8.595372	0.851708	0.855084	1.14E-05
285	0.996181	8.59049	0.851224	0.853398	4.73E-06
290	0.993748	8.568655	0.84906	0.851735	7.15E-06
295	0.989932	8.534402	0.845666	0.850096	1.96E-05
300	0.987548	8.513001	0.843546	0.848479	2.43E-05
				sum=	0.000493

Calibratio Curve

a=	0.0392	%	TT (ppm)	abs
b=	0.1114	0	0	0.1221
		0.25	6.7775	0.3939
		0.5	13.555	0.5945
		0.75	20.3325	0.9135
		1	27.11	1.1918

pH Before	7.8
pH After	7.8



30Apr15_0.7@10%pH9					
			flow rate=	0.7	
			volume=	350	
			resid time	482	
			rate const	0.000102	
wavelength=	430				
time (min)	abs		C/Co	model	sum squares
0	0.917999	17.2315	1	1	0
5	0.91093	17.09397	0.992019	0.999494	5.59E-05
10	0.915517	17.18321	0.997198	0.998993	3.22E-06
15	0.917883	17.22925	0.999869	0.998497	1.88E-06
20	0.914883	17.17087	0.996481	0.998007	2.33E-06
25	0.911525	17.10555	0.992691	0.997523	2.33E-05
30	0.912456	17.12366	0.993741	0.997043	1.09E-05
35	0.91135	17.10215	0.992493	0.996569	1.66E-05
40	0.912496	17.12444	0.993786	0.9961	5.35E-06
45	0.912323	17.12108	0.993592	0.995636	4.18E-06
50	0.919087	17.25267	1.001228	0.995176	3.66E-05
55	0.912346	17.12152	0.993617	0.994722	1.22E-06
60	0.911024	17.09579	0.992124	0.994273	4.62E-06
65	0.909952	17.07495	0.990915	0.993829	8.49E-06
70	0.91444	17.16227	0.995982	0.993389	6.72E-06
75	0.916056	17.1937	0.997806	0.992955	2.35E-05
80	0.913786	17.14954	0.995243	0.992525	7.39E-06
85	0.908811	17.05275	0.989626	0.992099	6.11E-06
90	0.919094	17.2528	1.001236	0.991678	9.13E-05
95	0.911878	17.11241	0.993088	0.991262	3.34E-06
100	0.914829	17.16982	0.99642	0.99085	3.1E-05
105	0.916524	17.2028	0.998334	0.990443	6.23E-05
110	0.907497	17.02718	0.988142	0.99004	3.6E-06
115	0.914149	17.1566	0.995653	0.989642	3.61E-05
120	0.902724	16.93432	0.982753	0.989247	4.22E-05
125	0.907532	17.02785	0.988181	0.988858	4.57E-07
130	0.89766	16.83579	0.977036	0.988472	0.000131
135	0.906788	17.01338	0.987341	0.98809	5.61E-07
140	0.90436	16.96615	0.984601	0.987713	9.69E-06
145	0.901439	16.90932	0.981303	0.98734	3.64E-05
150	0.903564	16.95066	0.983702	0.98697	1.07E-05
155	0.903146	16.94252	0.983229	0.986605	1.14E-05
160	0.903619	16.95173	0.983764	0.986244	6.15E-06
165	0.903204	16.94365	0.983295	0.985886	6.71E-06
170	0.910728	17.09003	0.99179	0.985533	3.92E-05
175	0.91021	17.07995	0.991205	0.985183	3.63E-05
180	0.900486	16.89077	0.980226	0.984837	2.13E-05
185	0.903788	16.95502	0.983955	0.984495	2.92E-07
190	0.902815	16.93609	0.982856	0.984156	1.69E-06
195	0.902958	16.93888	0.983018	0.983821	6.46E-07
200	0.902247	16.92504	0.982215	0.98349	1.63E-06
205	0.909699	17.07002	0.990629	0.983163	5.57E-05
210	0.910978	17.09491	0.992073	0.982839	8.53E-05
215	0.90113	16.90331	0.980954	0.982518	2.45E-06
220	0.909079	17.05796	0.989928	0.982201	5.97E-05
225	0.90572	16.9926	0.986136	0.981887	1.8E-05
230	0.905792	16.994	0.986217	0.981577	2.15E-05
235	0.89817	16.84572	0.977612	0.98127	1.34E-05
240	0.898757	16.85714	0.978275	0.980966	7.25E-06
245	0.903272	16.94498	0.983372	0.980666	7.32E-06
250	0.89654	16.814	0.975771	0.980369	2.11E-05
255	0.897415	16.83103	0.976759	0.980075	1.1E-05
260	0.899652	16.87455	0.979285	0.979785	2.5E-07
265	0.904291	16.9648	0.984522	0.979497	2.53E-05
270	0.897824	16.83899	0.977221	0.979213	3.97E-06
275	0.899576	16.87307	0.979199	0.978931	7.15E-08
280	0.897826	16.83902	0.977223	0.978653	2.05E-06
285	0.897286	16.82852	0.976614	0.978378	3.11E-06
290	0.895888	16.80131	0.975035	0.978106	9.43E-06
295	0.897405	16.83083	0.976748	0.977836	1.19E-06
300	0.896698	16.81708	0.97595	0.97757	2.62E-06
				sum=	0.001153

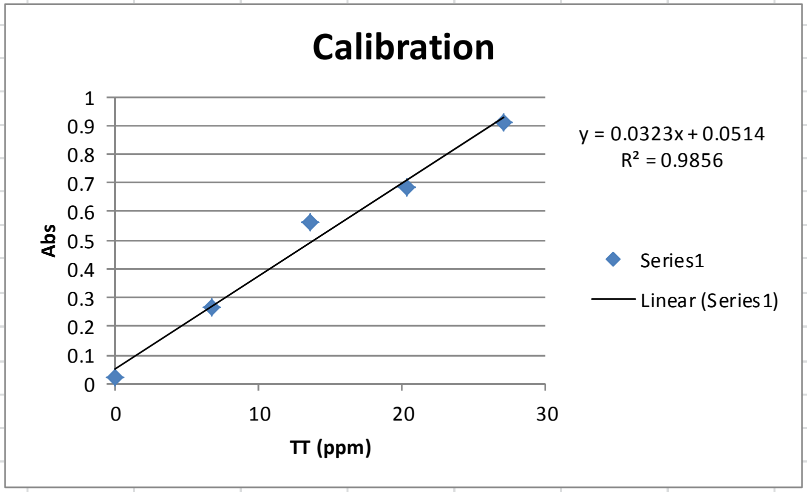
Calibratio Curve

a= 0.0323

b= 0.0514

%	TT (ppm)	abs
0	0	0.0249
0.25	6.7775	0.2646
0.5	13.555	0.562
0.75	20.3325	0.6831
1	27.11	0.909

pH Before	9
pH After	9.3



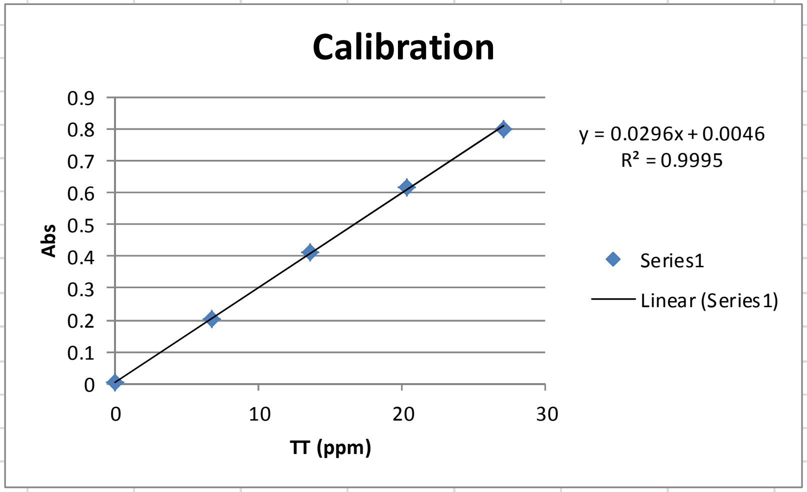
7May15_0.7@50%pH9					
			flow rate=	0.7	
			volume=	350	
			resid time	482	
			rate const	0.000338	
wavelength=	430				
time (min)	abs		C/Co	model	sum squares
0	0.831617	174.3514	1	1	0
5	0.84202	176.613	1.012971	0.99832	0.000215
10	0.842645	176.7488	1.01375	0.99666	0.000292
15	0.832887	174.6276	1.001584	0.99502	4.31E-05
20	0.832964	174.6443	1.001679	0.9934	6.85E-05
25	0.838111	175.7632	1.008097	0.9918	0.000266
30	0.829065	173.7967	0.996818	0.990218	4.36E-05
35	0.828973	173.7768	0.996704	0.988655	6.48E-05
40	0.83472	175.0261	1.00387	0.987111	0.000281
45	0.826132	173.1591	0.993161	0.985586	5.74E-05
50	0.826396	173.2164	0.99349	0.984079	8.86E-05
55	0.820385	171.9098	0.985996	0.98259	1.16E-05
60	0.815865	170.9272	0.98036	0.981119	5.76E-07
65	0.813493	170.4116	0.977403	0.979665	5.12E-06
70	0.808753	169.381	0.971492	0.978229	4.54E-05
75	0.80711	169.0239	0.969443	0.976811	5.43E-05
80	0.806122	168.8091	0.968211	0.975409	5.18E-05
85	0.805845	168.749	0.967867	0.974024	3.79E-05
90	0.801495	167.8033	0.962443	0.972655	0.000104
95	0.802055	167.9251	0.963141	0.971303	6.66E-05
100	0.80406	168.3608	0.96564	0.969967	1.87E-05
105	0.796428	166.7018	0.956125	0.968648	0.000157
110	0.798641	167.1828	0.958884	0.967344	7.16E-05
115	0.789287	165.1493	0.94722	0.966055	0.000355
120	0.789447	165.1841	0.947421	0.964782	0.000301
125	0.79586	166.5783	0.955417	0.963525	6.57E-05
130	0.789275	165.1467	0.947206	0.962282	0.000227
135	0.78418	164.0392	0.940854	0.961055	0.000408
140	0.778392	162.7809	0.933637	0.959842	0.000687
145	0.778819	162.8737	0.934169	0.958643	0.000599
150	0.780135	163.1597	0.935809	0.957459	0.000469
155	0.780351	163.2068	0.93608	0.95629	0.000408
160	0.786902	164.6308	0.944247	0.955134	0.000119
165	0.789195	165.1294	0.947107	0.953992	4.74E-05
170	0.786163	164.4703	0.943326	0.952864	9.1E-05
175	0.792375	165.8206	0.951071	0.951749	4.6E-07
180	0.787412	164.7418	0.944883	0.950648	3.32E-05
185	0.790023	165.3094	0.948139	0.94956	2.02E-06
190	0.789488	165.1932	0.947472	0.948485	1.02E-06
195	0.78637	164.5152	0.943584	0.947422	1.47E-05
200	0.782832	163.7462	0.939173	0.946373	5.18E-05
205	0.785397	164.3037	0.942371	0.945336	8.79E-06
210	0.777221	162.5264	0.932177	0.944312	0.000147
215	0.781429	163.4412	0.937424	0.9433	3.45E-05
220	0.782526	163.6796	0.938791	0.942299	1.23E-05
225	0.776754	162.4247	0.931594	0.941311	9.44E-05
230	0.787476	164.7556	0.944962	0.940335	2.14E-05
235	0.781087	163.3666	0.936996	0.939371	5.64E-06
240	0.781366	163.4273	0.937344	0.938418	1.15E-06
245	0.778688	162.8452	0.934006	0.937476	1.2E-05
250	0.786374	164.5161	0.943589	0.936546	4.96E-05
255	0.789409	165.1759	0.947373	0.935627	0.000138
260	0.78613	164.4631	0.943285	0.934719	7.34E-05
265	0.784553	164.1203	0.941319	0.933822	5.62E-05
270	0.780011	163.1329	0.935655	0.932936	7.4E-06
275	0.784596	164.1296	0.941372	0.93206	8.67E-05
280	0.777181	162.5177	0.932127	0.931195	8.69E-07
285	0.77647	162.363	0.93124	0.93034	8.09E-07
290	0.811274	169.9292	0.974636	0.929495	0.002038
295	0.807501	169.109	0.969931	0.928661	0.001703
300	0.807986	169.2143	0.970536	0.927836	0.001823
				sum=	0.012239

Calibratio Curve

a=	0.0296
b=	0.0046

%	TT (ppm)	abs
0	0	0.0028
0.25	6.7775	0.2006
0.5	13.555	0.4128
0.75	20.3325	0.6157
1	27.11	0.7995

pH Before	8.9
pH After	9.1



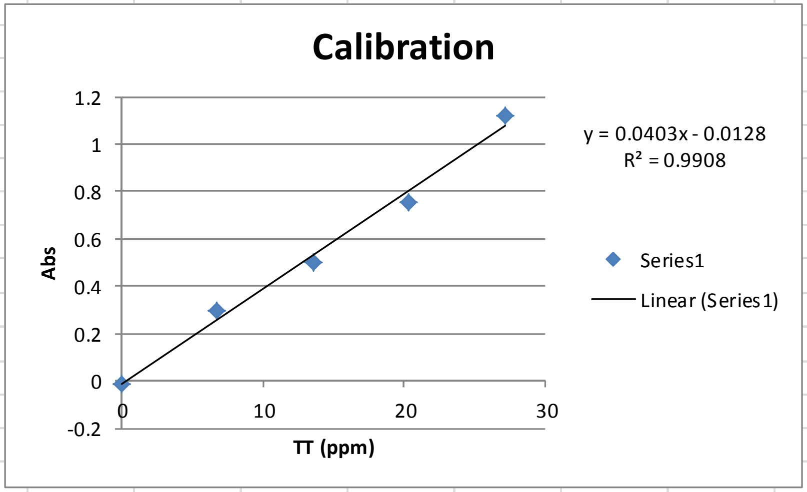
14May15_0.7@0%pH6					
			flow rate=	0.7	
			volume=	350	
			resid time	482	
			rate const	-3.5E-05	
wavelength=	430				
time (min)	abs		C/Co	model	sum squares
0	1.067307	-80.2349	1	1	0
5	1.075663	-80.8877	1.008136	1.000175	6.34E-05
10	1.06854	-80.3313	1.001201	1.000348	7.28E-07
15	1.071965	-80.5988	1.004536	1.000519	1.61E-05
20	1.070237	-80.4639	1.002854	1.000689	4.69E-06
25	1.069017	-80.3685	1.001666	1.000857	6.55E-07
30	1.068715	-80.3449	1.001371	1.001023	1.22E-07
35	1.067133	-80.2213	0.999831	1.001187	1.84E-06
40	1.069244	-80.3862	1.001886	1.00135	2.88E-07
45	1.063183	-79.9128	0.995985	1.001511	3.05E-05
50	1.068229	-80.307	1.000898	1.00167	5.96E-07
55	1.06805	-80.293	1.000724	1.001828	1.22E-06
60	1.066193	-80.1479	0.998915	1.001985	9.42E-06
65	1.070647	-80.4958	1.003252	1.002139	1.24E-06
70	1.068957	-80.3639	1.001608	1.002292	4.69E-07
75	1.071978	-80.5998	1.004548	1.002444	4.43E-06
80	1.0742	-80.7734	1.006712	1.002594	1.7E-05
85	1.076112	-80.9228	1.008574	1.002742	3.4E-05
90	1.068495	-80.3277	1.001157	1.002889	3E-06
95	1.068788	-80.3506	1.001442	1.003035	2.54E-06
100	1.06985	-80.4336	1.002476	1.003179	4.94E-07
105	1.068962	-80.3642	1.001612	1.003321	2.92E-06
110	1.068697	-80.3435	1.001354	1.003463	4.45E-06
115	1.070105	-80.4535	1.002725	1.003602	7.7E-07
120	1.068427	-80.3224	1.001091	1.003741	7.02E-06
125	1.075668	-80.8881	1.008141	1.003877	1.82E-05
130	1.070995	-80.523	1.003591	1.004013	1.78E-07
135	1.06969	-80.4211	1.002321	1.004147	3.33E-06
140	1.072817	-80.6654	1.005366	1.00428	1.18E-06
145	1.078577	-81.1154	1.010974	1.004411	4.31E-05
150	1.07001	-80.4461	1.002633	1.004541	3.64E-06
155	1.072011	-80.6024	1.004581	1.00467	7.96E-09
160	1.067944	-80.2847	1.000621	1.004797	1.74E-05
165	1.072309	-80.6257	1.004871	1.004923	2.72E-09
170	1.06957	-80.4117	1.002204	1.005048	8.09E-06
175	1.068949	-80.3632	1.001599	1.005172	1.28E-05
180	1.074089	-80.7648	1.006604	1.005294	1.72E-06
185	1.074581	-80.8032	1.007084	1.005415	2.78E-06
190	1.072225	-80.6191	1.004789	1.005535	5.57E-07
195	1.072863	-80.669	1.00541	1.005654	5.92E-08
200	1.079654	-81.1995	1.012023	1.005771	3.91E-05
205	1.070155	-80.4574	1.002773	1.005888	9.7E-06
210	1.073519	-80.7202	1.006049	1.006003	2.14E-09
215	1.073367	-80.7084	1.005902	1.006117	4.62E-08
220	1.073239	-80.6984	1.005777	1.006229	2.05E-07
225	1.07298	-80.6781	1.005524	1.006341	6.67E-07
230	1.078627	-81.1193	1.011022	1.006451	2.09E-05
235	1.072991	-80.679	1.005535	1.006561	1.05E-06
240	1.076036	-80.9169	1.0085	1.006669	3.35E-06
245	1.073729	-80.7367	1.006254	1.006776	2.73E-07
250	1.075669	-80.8882	1.008143	1.006882	1.59E-06
255	1.075588	-80.8818	1.008063	1.006987	1.16E-06
260	1.076295	-80.9371	1.008752	1.007091	2.76E-06
265	1.073183	-80.694	1.005722	1.007194	2.17E-06
270	1.075346	-80.8629	1.007828	1.007296	2.83E-07
275	1.075895	-80.9058	1.008362	1.007397	9.32E-07
280	1.073749	-80.7382	1.006273	1.007496	1.5E-06
285	1.073213	-80.6963	1.005751	1.007595	3.4E-06
290	1.074675	-80.8106	1.007175	1.007693	2.68E-07
295	1.074801	-80.8204	1.007298	1.00779	2.42E-07
300	1.074252	-80.7775	1.006763	1.007885	1.26E-06
				sum=	0.000412

Calibratio Curve

a=	0.0403
b=	-0.0128

%	TT (ppm)	abs
0	0	-0.0152
0.25	6.7775	0.2998
0.5	13.555	0.5036
0.75	20.3325	0.7549
1	27.11	1.1216

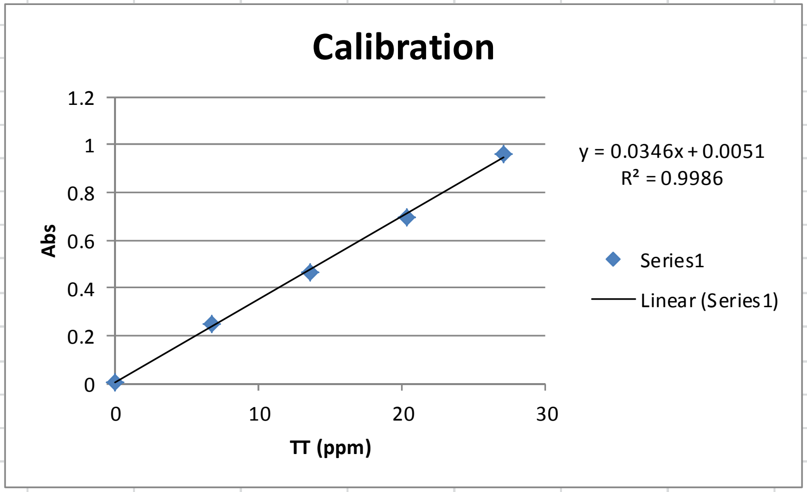
pH Before	6.73
pH After	6.55



27May15_0.7@10%pH8					
			flow rate=	0.7	
			volume=	350	
			resid time	482	
			rate const	8.85E-05	
wavelength=	430				
time (min)	abs		C/Co	model	sum squares
0	0.954391	180.3512	1	1	0
5	0.960247	181.4995	1.006367	0.99956	4.63E-05
10	0.951523	179.7889	0.996882	0.999125	5.03E-06
15	0.951064	179.6988	0.996383	0.998694	5.34E-06
20	0.956796	180.8227	1.002614	0.998268	1.89E-05
25	0.947339	178.9684	0.992333	0.997847	3.04E-05
30	0.95117	179.7195	0.996498	0.99743	8.69E-07
35	0.948684	179.2321	0.993795	0.997018	1.04E-05
40	0.949842	179.4592	0.995054	0.99661	2.42E-06
45	0.955585	180.5853	1.001298	0.996206	2.59E-05
50	0.955684	180.6047	1.001406	0.995807	3.13E-05
55	0.948242	179.1455	0.993315	0.995412	4.4E-06
60	0.945163	178.5417	0.989967	0.995022	2.55E-05
65	0.945949	178.696	0.990822	0.994635	1.45E-05
70	0.946747	178.8523	0.991689	0.994253	6.57E-06
75	0.951341	179.7532	0.996684	0.993875	7.89E-06
80	0.948099	179.1174	0.993159	0.993501	1.17E-07
85	0.948485	179.1932	0.993579	0.993131	2.01E-07
90	0.946424	178.7891	0.991339	0.992765	2.03E-06
95	0.950032	179.4964	0.995261	0.992403	8.17E-06
100	0.946313	178.7672	0.991217	0.992044	6.84E-07
105	0.949449	179.3823	0.994628	0.99169	8.63E-06
110	0.943716	178.2579	0.988394	0.991339	8.68E-06
115	0.945153	178.5399	0.989957	0.990993	1.07E-06
120	0.94555	178.6176	0.990388	0.990649	6.85E-08
125	0.946674	178.838	0.99161	0.99031	1.69E-06
130	0.946914	178.885	0.991871	0.989974	3.6E-06
135	0.948797	179.2543	0.993918	0.989642	1.83E-05
140	0.941533	177.83	0.986021	0.989314	1.08E-05
145	0.942777	178.0738	0.987373	0.988989	2.61E-06
150	0.941898	177.9016	0.986418	0.988667	5.06E-06
155	0.940724	177.6713	0.985141	0.988349	1.03E-05
160	0.948396	179.1758	0.993483	0.988034	2.97E-05
165	0.94922	179.3372	0.994378	0.987723	4.43E-05
170	0.940928	177.7114	0.985363	0.987415	4.21E-06
175	0.948106	179.1188	0.993167	0.987111	3.67E-05
180	0.944371	178.3864	0.989106	0.986809	5.27E-06
185	0.940503	177.628	0.984901	0.986511	2.59E-06
190	0.947555	179.0107	0.992567	0.986216	4.03E-05
195	0.948292	179.1553	0.993369	0.985925	5.54E-05
200	0.938785	177.2912	0.983033	0.985636	6.77E-06
205	0.93964	177.4588	0.983963	0.985351	1.93E-06
210	0.936241	176.7924	0.980268	0.985068	2.3E-05
215	0.936272	176.7984	0.980301	0.984789	2.01E-05
220	0.93988	177.5059	0.984224	0.984513	8.35E-08
225	0.936241	176.7923	0.980267	0.984239	1.58E-05
230	0.936244	176.7929	0.98027	0.983969	1.37E-05
235	0.936132	176.771	0.980149	0.983701	1.26E-05
240	0.937732	177.0847	0.981888	0.983437	2.4E-06
245	0.935742	176.6945	0.979725	0.983175	1.19E-05
250	0.935584	176.6635	0.979553	0.982916	1.13E-05
255	0.939603	177.4516	0.983923	0.98266	1.6E-06
260	0.941106	177.7463	0.985557	0.982406	9.93E-06
265	0.941196	177.7639	0.985654	0.982156	1.22E-05
270	0.938645	177.2637	0.982881	0.981908	9.48E-07
275	0.938668	177.2682	0.982906	0.981662	1.55E-06
280	0.935474	176.6419	0.979433	0.98142	3.95E-06
285	0.939529	177.4371	0.983842	0.981179	7.09E-06
290	0.936802	176.9024	0.980878	0.980942	4.12E-09
295	0.930882	175.7416	0.974441	0.980707	3.93E-05
300	0.942672	178.0533	0.987259	0.980475	4.6E-05
				sum=	0.000779

Calibratio Curve					
a=	0.0346		%	TT (ppm)	abs
b=	0.0051		0	0	0.0079
			0.25	6.7775	0.2491
			0.5	13.555	0.4629
			0.75	20.3325	0.6922
			1	27.11	0.9593

pH Before	8.227
pH After	8.261



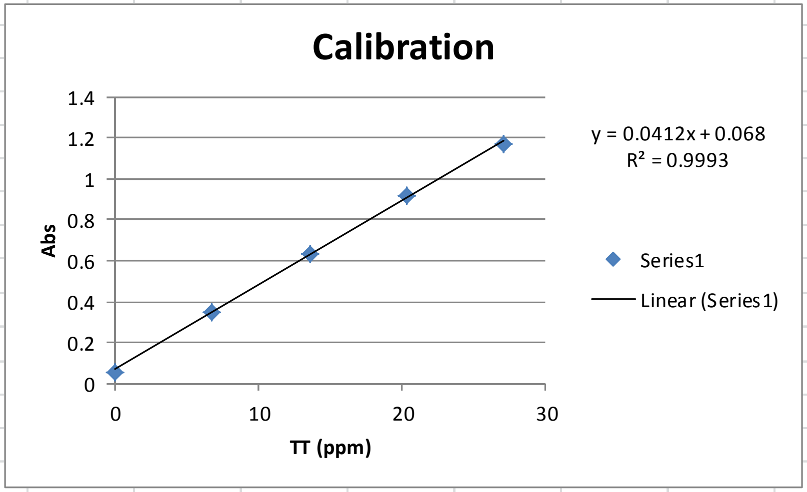
29May15_0.7@70%pH5						
			flow rate=	0.7		
			volume=	350		
			resid time	482		
			rate const	0.001262		
wavelength=	430					
time (min)	abs		C/Co	model	sum squares	
0	1.160983	220.8594	1	1	0	
5	1.154205	219.5305	0.993983	0.99374	5.88E-08	
10	1.145808	217.8838	0.986527	0.987585	1.12E-06	
15	1.140991	216.9395	0.982251	0.98153	5.2E-07	
20	1.131695	215.1167	0.973998	0.975577	2.49E-06	
25	1.128502	214.4906	0.971164	0.969721	2.08E-06	
30	1.120145	212.852	0.963745	0.963963	4.76E-08	
35	1.114923	211.828	0.959108	0.958299	6.53E-07	
40	1.111939	211.2429	0.956459	0.95273	1.39E-05	
45	1.102673	209.4261	0.948233	0.947253	9.6E-07	
50	1.098922	208.6905	0.944902	0.941866	9.22E-06	
55	1.098939	208.694	0.944918	0.936568	6.97E-05	
60	1.09135	207.2058	0.93818	0.931358	4.65E-05	
65	1.083879	205.741	0.931548	0.926235	2.82E-05	
70	1.076443	204.2829	0.924946	0.921196	1.41E-05	
75	1.072543	203.5183	0.921483	0.91624	2.75E-05	
80	1.07262	203.5334	0.921552	0.911367	0.000104	
85	1.061137	201.2818	0.911357	0.906574	2.29E-05	
90	1.060725	201.2011	0.910992	0.90186	8.34E-05	
95	1.053288	199.7427	0.904388	0.897225	5.13E-05	
100	1.04365	197.8529	0.895832	0.892666	1E-05	
105	1.044113	197.9438	0.896243	0.888182	6.5E-05	
110	1.034765	196.1107	0.887944	0.883773	1.74E-05	
115	1.032909	195.7469	0.886297	0.879437	4.71E-05	
120	1.028372	194.8572	0.882268	0.875172	5.04E-05	
125	1.024557	194.1091	0.878881	0.870978	6.25E-05	
130	1.020765	193.3657	0.875515	0.866853	7.5E-05	
135	1.014196	192.0776	0.869683	0.862797	4.74E-05	
140	1.007951	190.853	0.864138	0.858808	2.84E-05	
145	1.000481	189.3884	0.857507	0.854885	6.88E-06	
150	0.998651	189.0296	0.855882	0.851026	2.36E-05	
155	0.994341	188.1845	0.852056	0.847232	2.33E-05	
160	0.990566	187.4443	0.848704	0.8435	2.71E-05	
165	0.984463	186.2476	0.843286	0.83983	1.19E-05	
170	0.979942	185.3611	0.839272	0.836221	9.31E-06	
175	0.976622	184.7102	0.836325	0.832672	1.33E-05	
180	0.972282	183.8591	0.832471	0.829181	1.08E-05	
185	0.971034	183.6145	0.831364	0.825748	3.15E-05	
190	0.961597	181.7641	0.822985	0.822372	3.77E-07	
195	0.960708	181.5897	0.822196	0.819051	9.89E-06	
200	0.954243	180.3221	0.816456	0.815786	4.5E-07	
205	0.956462	180.7573	0.818427	0.812575	3.43E-05	
210	0.94575	178.6568	0.808916	0.809416	2.5E-07	
215	0.940967	177.7189	0.80467	0.80631	2.69E-06	
220	0.93884	177.302	0.802782	0.803256	2.24E-07	
225	0.933369	176.2293	0.797925	0.800252	5.41E-06	
230	0.930589	175.6841	0.795457	0.797298	3.39E-06	
235	0.930522	175.6711	0.795398	0.794392	1.01E-06	
240	0.922535	174.1049	0.788307	0.791535	1.04E-05	
245	0.917738	173.1643	0.784048	0.788725	2.19E-05	
250	0.913876	172.4071	0.780619	0.785961	2.85E-05	
255	0.910071	171.6611	0.777241	0.783243	3.6E-05	
260	0.909049	171.4606	0.776334	0.78057	1.79E-05	
265	0.900861	169.855	0.769064	0.777942	7.88E-05	
270	0.898508	169.3937	0.766975	0.775357	7.02E-05	
275	0.89489	168.6843	0.763763	0.772814	8.19E-05	
280	0.894082	168.5259	0.763046	0.770314	5.28E-05	
285	0.888591	167.4493	0.758172	0.767855	9.38E-05	
290	0.886469	167.0332	0.756287	0.765437	8.37E-05	
295	0.884531	166.6532	0.754567	0.763059	7.21E-05	
300	0.881258	166.0113	0.751661	0.76072	8.21E-05	
				sum=	0.001828	

Calibratio Curve

a=	0.0346
b=	0.0051

%	TT (ppm)	abs
0	0	0.0572
0.25	6.7775	0.3521
0.5	13.555	0.636
0.75	20.3325	0.918
1	27.11	1.172

pH Before	4.925
pH After	4.012



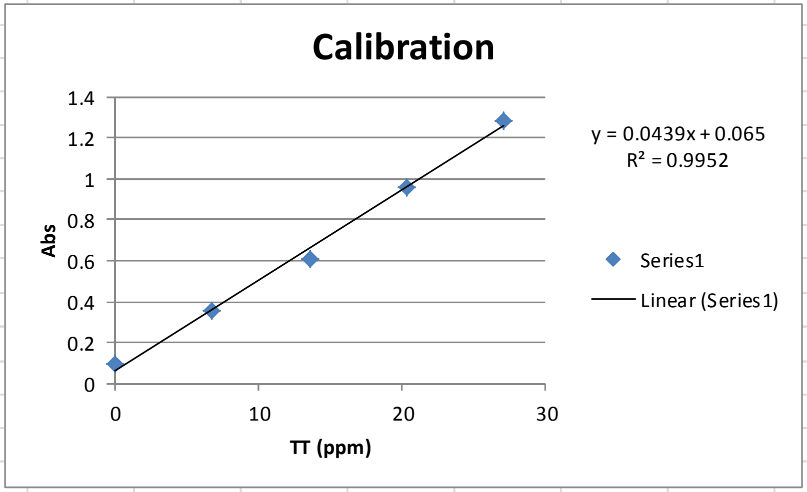
1Jun15_0.7@70%pH6					
			flow rate=	0.7	
			volume=	350	
			resid time	482	
			rate const	0.001235	
wavelength=	430				
time (min)	abs		C/Co	model	sum squares
0	1.266443	18.80835	1	1	0
5	1.259549	18.7023	0.994361	0.993878	2.34E-07
10	1.254731	18.62817	0.99042	0.987856	6.57E-06
15	1.239044	18.38683	0.977589	0.981933	1.89E-05
20	1.228587	18.22595	0.969035	0.976107	5E-05
25	1.219862	18.09172	0.961899	0.970377	7.19E-05
30	1.225991	18.18602	0.966912	0.964741	4.71E-06
35	1.21754	18.05599	0.959999	0.959197	6.42E-07
40	1.207736	17.90517	0.95198	0.953745	3.12E-06
45	1.202866	17.83025	0.947996	0.948382	1.49E-07
50	1.19635	17.73	0.942667	0.943107	1.94E-07
55	1.189701	17.62771	0.937228	0.937918	4.76E-07
60	1.183463	17.53173	0.932125	0.932815	4.76E-07
65	1.183312	17.52941	0.932002	0.927795	1.77E-05
70	1.174539	17.39445	0.924826	0.922858	3.87E-06
75	1.172568	17.36412	0.923213	0.918001	2.72E-05
80	1.16328	17.22122	0.915616	0.913225	5.72E-06
85	1.155836	17.10671	0.909528	0.908526	1E-06
90	1.156321	17.11416	0.909924	0.903905	3.62E-05
95	1.154088	17.07982	0.908098	0.89936	7.63E-05
100	1.149046	17.00224	0.903973	0.894889	8.25E-05
105	1.135931	16.80047	0.893245	0.890492	7.58E-06
110	1.130963	16.72405	0.889182	0.886167	9.09E-06
115	1.128831	16.69125	0.887438	0.881913	3.05E-05
120	1.122548	16.59458	0.882298	0.877728	2.09E-05
125	1.123443	16.60836	0.883031	0.873613	8.87E-05
130	1.114004	16.46315	0.87531	0.869564	3.3E-05
135	1.107829	16.36814	0.870259	0.865583	2.19E-05
140	1.110062	16.40249	0.872085	0.861666	0.000109
145	1.098321	16.22186	0.862482	0.857814	2.18E-05
150	1.096442	16.19295	0.860945	0.854025	4.79E-05
155	1.089032	16.07896	0.854884	0.850299	2.1E-05
160	1.089471	16.0857	0.855243	0.846633	7.41E-05
165	1.081205	15.95855	0.848482	0.843028	2.98E-05
170	1.077924	15.90807	0.845798	0.839481	3.99E-05
175	1.070823	15.79881	0.839989	0.835993	1.6E-05
180	1.064751	15.7054	0.835023	0.832562	6.05E-06
185	1.067039	15.74061	0.836895	0.829188	5.94E-05
190	1.057501	15.59386	0.829092	0.825869	1.04E-05
195	1.051362	15.49941	0.824071	0.822604	2.15E-06
200	1.04591	15.41553	0.819611	0.819393	4.76E-08
205	1.048769	15.45953	0.82195	0.816235	3.27E-05
210	1.036677	15.27349	0.812059	0.813128	1.14E-06
215	1.040371	15.33032	0.81508	0.810072	2.51E-05
220	1.034436	15.23902	0.810226	0.807067	9.98E-06
225	1.025826	15.10655	0.803183	0.804111	8.61E-07
230	1.019902	15.01541	0.798338	0.801203	8.21E-06
235	1.022951	15.06233	0.800832	0.798343	6.19E-06
240	1.018177	14.98887	0.796926	0.79553	1.95E-06
245	1.006435	14.80823	0.787322	0.792764	2.96E-05
250	1.008077	14.83349	0.788665	0.790042	1.9E-06
255	1.003735	14.76669	0.785114	0.787365	5.07E-06
260	0.998358	14.68396	0.780715	0.784733	1.61E-05
265	0.988277	14.52887	0.772469	0.782143	9.36E-05
270	0.987639	14.51907	0.771948	0.779596	5.85E-05
275	0.980316	14.4064	0.765958	0.777091	0.000124
280	0.982002	14.43233	0.767336	0.774626	5.31E-05
285	0.971037	14.26364	0.758368	0.772203	0.000191
290	0.971818	14.27567	0.759007	0.769819	0.000117
295	0.968982	14.23202	0.756686	0.767474	0.000116
300	0.965056	14.17163	0.753476	0.765167	0.000137
				sum=	0.002086

Calibratio Curve

a=	0.0439
b=	0.065

%	TT (ppm)	abs
0	0	0.0947
0.25	6.7775	0.3577
0.5	13.555	0.6098
0.75	20.3325	0.9559
1	27.11	1.2843

pH Before	6.372
pH After	4.276



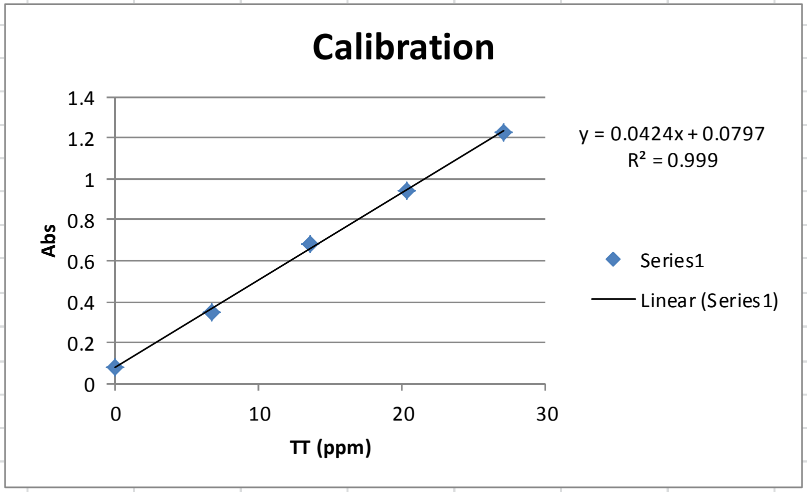
3Jun15_0.7@30%pH7					
			flow rate=	0.7	
			volume=	350	
			resid time	482	
			rate const	0.000423	
wavelength=	430				
time (min)	abs		C/Co	model	sum squares
0	1.261515	15.2963	1	1	0
5	1.268404	15.38274	1.005651	0.9979	6.01E-05
10	1.260961	15.28935	0.999546	0.995827	1.38E-05
15	1.259369	15.26937	0.998239	0.993779	1.99E-05
20	1.253829	15.19986	0.993695	0.991756	3.76E-06
25	1.260094	15.27847	0.998834	0.989759	8.24E-05
30	1.249113	15.14069	0.989827	0.987786	4.16E-06
35	1.247889	15.12533	0.988823	0.985838	8.91E-06
40	1.24284	15.06198	0.984681	0.983914	5.88E-07
45	1.240308	15.03021	0.982604	0.982014	3.48E-07
50	1.238479	15.00726	0.981104	0.980137	9.34E-07
55	1.237374	14.9934	0.980197	0.978284	3.66E-06
60	1.232355	14.93043	0.976081	0.976454	1.39E-07
65	1.234287	14.95466	0.977665	0.974646	9.11E-06
70	1.227262	14.86652	0.971903	0.972861	9.18E-07
75	1.227919	14.87477	0.972442	0.971098	1.81E-06
80	1.225893	14.84935	0.97078	0.969357	2.03E-06
85	1.229008	14.88844	0.973336	0.967638	3.25E-05
90	1.222734	14.80971	0.968189	0.96594	5.06E-06
95	1.221057	14.78867	0.966813	0.964263	6.51E-06
100	1.220366	14.78	0.966247	0.962606	1.33E-05
105	1.215819	14.72295	0.962517	0.960971	2.39E-06
110	1.208148	14.6267	0.956224	0.959355	9.8E-06
115	1.214183	14.70243	0.961175	0.95776	1.17E-05
120	1.214224	14.70294	0.961209	0.956184	2.52E-05
125	1.20431	14.57854	0.953076	0.954628	2.41E-06
130	1.202985	14.56192	0.951989	0.953092	1.21E-06
135	1.201988	14.54941	0.951171	0.951574	1.62E-07
140	1.198615	14.50708	0.948405	0.950075	2.79E-06
145	1.205065	14.58801	0.953695	0.948595	2.6E-05
150	1.19796	14.49887	0.947867	0.947133	5.39E-07
155	1.193979	14.44892	0.944602	0.945689	1.18E-06
160	1.200062	14.52525	0.949592	0.944264	2.84E-05
165	1.190423	14.40431	0.941685	0.942855	1.37E-06
170	1.193357	14.44112	0.944092	0.941465	6.9E-06
175	1.187998	14.37387	0.939696	0.940091	1.57E-07
180	1.182836	14.30911	0.935462	0.938735	1.07E-05
185	1.191449	14.41718	0.942527	0.937396	2.63E-05
190	1.182214	14.3013	0.934952	0.936073	1.26E-06
195	1.178614	14.25613	0.931998	0.934766	7.66E-06
200	1.17855	14.25534	0.931947	0.933476	2.34E-06
205	1.182685	14.30721	0.935338	0.932202	9.83E-06
210	1.175522	14.21734	0.929463	0.930943	2.19E-06
215	1.175078	14.21177	0.929098	0.929701	3.63E-07
220	1.172473	14.17908	0.926961	0.928473	2.29E-06
225	1.169183	14.1378	0.924262	0.927261	8.99E-06
230	1.171029	14.16096	0.925777	0.926064	8.25E-08
235	1.173138	14.18743	0.927507	0.924882	6.89E-06
240	1.17416	14.20026	0.928346	0.923714	2.15E-05
245	1.172227	14.17599	0.92676	0.922561	1.76E-05
250	1.165011	14.08546	0.920841	0.921422	3.38E-07
255	1.165853	14.09603	0.921532	0.920297	1.52E-06
260	1.157064	13.98575	0.914322	0.919187	2.37E-05
265	1.154284	13.95086	0.912041	0.91809	3.66E-05
270	1.156654	13.9806	0.913986	0.917007	9.12E-06
275	1.152421	13.92749	0.910513	0.915937	2.94E-05
280	1.15929	14.01368	0.916148	0.91488	1.61E-06
285	1.150468	13.90299	0.908912	0.913837	2.43E-05
290	1.158249	14.00061	0.915294	0.912806	6.19E-06
295	1.147096	13.86068	0.906146	0.911788	3.18E-05
300	1.154363	13.95186	0.912107	0.910783	1.75E-06
				sum=	0.000674

Calibratio Curve

a=	0.0424		%	TT (ppm)	abs
b=	0.0797		0	0	0.0803
			0.25	6.7775	0.3513
			0.5	13.555	0.6779
			0.75	20.3325	0.9423
			1	27.11	1.223

pH Before	7.144
pH After	7.017

Notes: Took averages b/c better R^2, pH aren't exact, rough estimate because I can't remember the exact numbers right now.



9Jun15_0.7@20%pH6					
			flow rate=	0.7	
			volume=	350	
			resid time	482	
			rate const	0.000356	
wavelength=	430				
time (min)	abs		C/Co	model	sum squares
0	1.177414	18.97682	1	1	0
5	1.175257	18.94075	0.998099	0.998228	1.67E-08
10	1.17346	18.9107	0.996516	0.996478	1.42E-09
15	1.173255	18.90728	0.996336	0.994749	2.52E-06
20	1.168647	18.83022	0.992275	0.993041	5.87E-07
25	1.169631	18.84667	0.993142	0.991353	3.2E-06
30	1.168131	18.82158	0.99182	0.989686	4.55E-06
35	1.169237	18.84008	0.992795	0.988039	2.26E-05
40	1.16988	18.85084	0.993361	0.986412	4.83E-05
45	1.160781	18.69868	0.985343	0.984804	2.91E-07
50	1.160818	18.6993	0.985376	0.983216	4.66E-06
55	1.158585	18.66195	0.983408	0.981647	3.1E-06
60	1.155749	18.61453	0.980909	0.980097	6.58E-07
65	1.162072	18.72027	0.986481	0.978566	6.26E-05
70	1.154804	18.59873	0.980076	0.977054	9.14E-06
75	1.152028	18.55231	0.97763	0.975559	4.29E-06
80	1.150214	18.52198	0.976032	0.974083	3.8E-06
85	1.147971	18.48447	0.974055	0.972624	2.05E-06
90	1.144944	18.43385	0.971388	0.971183	4.18E-08
95	1.142822	18.39837	0.969518	0.96976	5.85E-08
100	1.141644	18.37866	0.96848	0.968354	1.59E-08
105	1.14277	18.3975	0.969472	0.966964	6.29E-06
110	1.138524	18.32649	0.96573	0.965592	1.92E-08
115	1.138337	18.32336	0.965565	0.964236	1.77E-06
120	1.136058	18.28524	0.963557	0.962896	4.36E-07
125	1.133991	18.25069	0.961736	0.961573	2.65E-08
130	1.132048	18.21819	0.960024	0.960266	5.86E-08
135	1.13169	18.21221	0.959708	0.958974	5.39E-07
140	1.130828	18.19779	0.958948	0.957698	1.56E-06
145	1.129858	18.18158	0.958094	0.956437	2.74E-06
150	1.126851	18.13129	0.955444	0.955192	6.33E-08
155	1.12735	18.13963	0.955884	0.953962	3.69E-06
160	1.12455	18.09281	0.953417	0.952746	4.49E-07
165	1.122416	18.05712	0.951536	0.951546	9.92E-11
170	1.122586	18.05996	0.951685	0.950359	1.76E-06
175	1.121398	18.04011	0.950639	0.949188	2.11E-06
180	1.119646	18.01081	0.949095	0.94803	1.13E-06
185	1.117607	17.97671	0.947299	0.946886	1.7E-07
190	1.115129	17.93527	0.945115	0.945756	4.11E-07
195	1.117739	17.97891	0.947415	0.94464	7.7E-06
200	1.114904	17.93151	0.944916	0.943537	1.9E-06
205	1.118797	17.99661	0.948347	0.942448	3.48E-05
210	1.111693	17.87782	0.942087	0.941371	5.12E-07
215	1.108884	17.83083	0.939611	0.940308	4.86E-07
220	1.107949	17.81521	0.938788	0.939258	2.21E-07
225	1.1048	17.76254	0.936013	0.93822	4.87E-06
230	1.105686	17.77736	0.936793	0.937195	1.61E-07
235	1.103771	17.74533	0.935106	0.936182	1.16E-06
240	1.103526	17.74124	0.93489	0.935181	8.47E-08
245	1.099412	17.67244	0.931265	0.934193	8.57E-06
250	1.101416	17.70596	0.933031	0.933216	3.44E-08
255	1.097542	17.64117	0.929617	0.932251	6.94E-06
260	1.098345	17.6546	0.930324	0.931298	9.49E-07
265	1.095728	17.61084	0.928019	0.930357	5.47E-06
270	1.092557	17.5578	0.925224	0.929427	1.77E-05
275	1.100282	17.68699	0.932031	0.928508	1.24E-05
280	1.089122	17.50037	0.922197	0.9276	2.92E-05
285	1.089899	17.51336	0.922882	0.926703	1.46E-05
290	1.094135	17.5842	0.926614	0.925817	6.36E-07
295	1.09164	17.54247	0.924416	0.924941	2.77E-07
300	1.086544	17.45725	0.919925	0.924077	1.72E-05
				sum=	0.000362

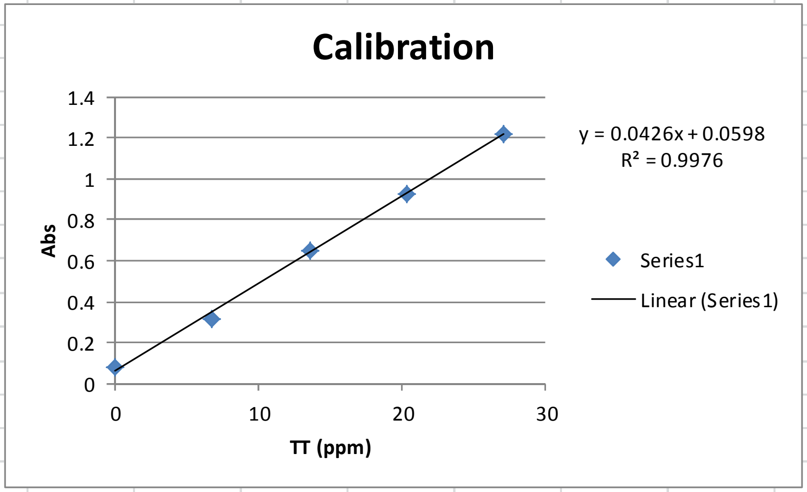
Calibratio Curve

a=	0.0426
b=	0.0598

%	TT (ppm)	abs
0	0	0.0834
0.25	6.7775	0.3122
0.5	13.555	0.6457
0.75	20.3325	0.9269
1	27.11	1.2213

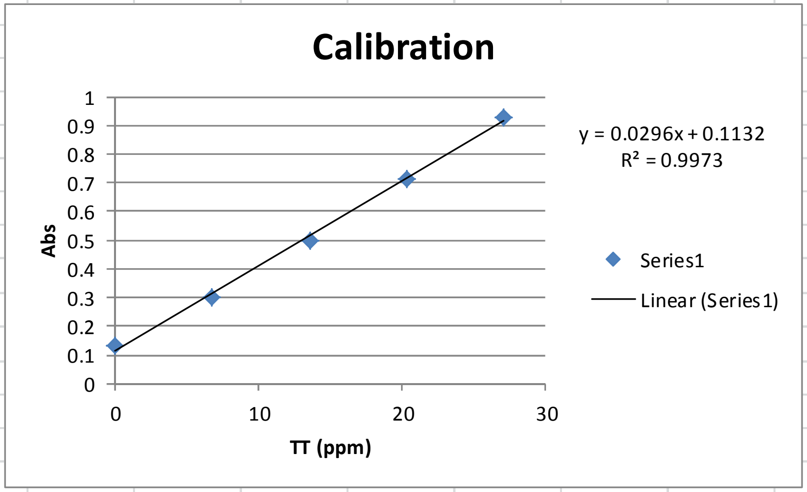
pH Before	6.433
pH After	5.55

Note: Both Avg and 1st abs values gave same R^2 value



15Jun15_0.7@50%pH9						
			flow rate=	0.7		
			volume=	350		
			resid time	482		
			rate const	0.000283		
wavelength=	430					
time (min)	abs		C/Co	model	sum squares	
0	0.859851	7.334377	1	1	0	
5	0.855267	7.293875	0.994478	0.998593	1.69E-05	
10	0.857092	7.310002	0.996677	0.997203	2.77E-07	
15	0.855225	7.293506	0.994428	0.995829	1.96E-06	
20	0.856037	7.300683	0.995406	0.994471	8.74E-07	
25	0.853232	7.275904	0.992028	0.993129	1.21E-06	
30	0.849618	7.243972	0.987674	0.991803	1.71E-05	
35	0.848448	7.233637	0.986265	0.990493	1.79E-05	
40	0.847485	7.225137	0.985106	0.989197	1.67E-05	
45	0.851972	7.264769	0.990509	0.987917	6.72E-06	
50	0.846437	7.215874	0.983843	0.986652	7.89E-06	
55	0.848282	7.232174	0.986065	0.985402	4.4E-07	
60	0.846378	7.215354	0.983772	0.984166	1.56E-07	
65	0.846509	7.216506	0.983929	0.982945	9.68E-07	
70	0.842216	7.178582	0.978758	0.981738	8.88E-06	
75	0.842216	7.178584	0.978759	0.980546	3.19E-06	
80	0.843433	7.18934	0.980225	0.979367	7.36E-07	
85	0.840137	7.160218	0.976255	0.978202	3.79E-06	
90	0.840649	7.164748	0.976872	0.977051	3.2E-08	
95	0.838149	7.142661	0.973861	0.975913	4.21E-06	
100	0.83988	7.157949	0.975945	0.974789	1.34E-06	
105	0.836907	7.13169	0.972365	0.973677	1.72E-06	
110	0.836429	7.127467	0.971789	0.972579	6.24E-07	
115	0.834809	7.113157	0.969838	0.971494	2.74E-06	
120	0.832747	7.09494	0.967354	0.970421	9.41E-06	
125	0.833953	7.105588	0.968806	0.969361	3.08E-07	
130	0.833057	7.097677	0.967727	0.968314	3.44E-07	
135	0.831084	7.080247	0.965351	0.967278	3.71E-06	
140	0.831846	7.086977	0.966268	0.966255	1.8E-10	
145	0.828683	7.059039	0.962459	0.965244	7.75E-06	
150	0.829133	7.063012	0.963001	0.964244	1.55E-06	
155	0.830323	7.073527	0.964435	0.963257	1.39E-06	
160	0.825872	7.034204	0.959073	0.962281	1.03E-05	
165	0.830267	7.073026	0.964366	0.961316	9.3E-06	
170	0.825149	7.027815	0.958202	0.960363	4.67E-06	
175	0.826283	7.037837	0.959568	0.959421	2.19E-08	
180	0.824388	7.021095	0.957286	0.958489	1.45E-06	
185	0.825625	7.032027	0.958776	0.957569	1.46E-06	
190	0.824904	7.025657	0.957908	0.95666	1.56E-06	
195	0.826297	7.037961	0.959585	0.955761	1.46E-05	
200	0.823198	7.010587	0.955853	0.954873	9.61E-07	
205	0.823239	7.010942	0.955902	0.953995	3.64E-06	
210	0.819759	6.980202	0.95171	0.953127	2.01E-06	
215	0.819757	6.980181	0.951708	0.95227	3.16E-07	
220	0.820974	6.990937	0.953174	0.951423	3.07E-06	
225	0.820432	6.986147	0.952521	0.950585	3.75E-06	
230	0.817326	6.958708	0.94878	0.949758	9.56E-07	
235	0.818974	6.973264	0.950764	0.94894	3.33E-06	
240	0.818159	6.96607	0.949784	0.948131	2.73E-06	
245	0.816822	6.954258	0.948173	0.947333	7.06E-07	
250	0.816029	6.947256	0.947218	0.946543	4.56E-07	
255	0.816356	6.950138	0.947611	0.945763	3.42E-06	
260	0.816669	6.952903	0.947988	0.944992	8.98E-06	
265	0.8124	6.915193	0.942847	0.94423	1.91E-06	
270	0.814029	6.929585	0.944809	0.943477	1.77E-06	
275	0.811539	6.907586	0.94181	0.942732	8.52E-07	
280	0.811109	6.903789	0.941292	0.941997	4.97E-07	
285	0.810371	6.897267	0.940403	0.94127	7.52E-07	
290	0.810306	6.896699	0.940325	0.940551	5.12E-08	
295	0.809964	6.893678	0.939913	0.939841	5.16E-09	
300	0.80902	6.885333	0.938775	0.93914	1.33E-07	
				sum=	0.000225	

Calibratio Curve					
a=	0.0296		%	TT (ppm)	abs
b=	0.1132		0	0	0.1333
			0.25	6.7775	0.2985
			0.5	13.555	0.496
			0.75	20.3325	0.716
			1	27.11	0.9267
	pH Before	9.085			
	pH After	9.071	8.841		



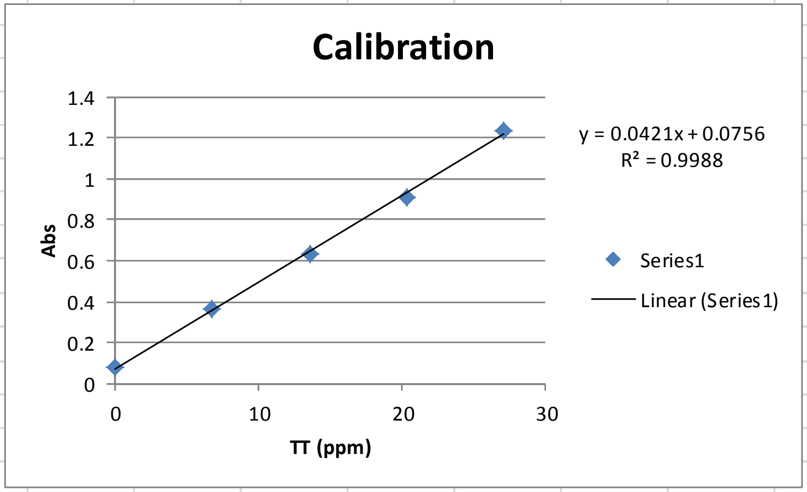
17Jun15_0.7@30%pH6					
			flow rate=	0.7	
			volume=	350	
			resid time	482	
			rate const	0.000458	
wavelength=	430				
time (min)	abs		C/Co	model	sum squares
0	1.165817	14.86398	1	1	0
5	1.170727	14.92892	1.004369	0.997724	4.42E-05
10	1.164987	14.853	0.999261	0.995477	1.43E-05
15	1.158279	14.76427	0.993292	0.993258	1.12E-09
20	1.160089	14.78822	0.994903	0.991067	1.47E-05
25	1.155557	14.72826	0.990869	0.988904	3.86E-06
30	1.151658	14.67669	0.987399	0.986768	3.99E-07
35	1.150276	14.65841	0.98617	0.984658	2.28E-06
40	1.14844	14.63413	0.984536	0.982575	3.84E-06
45	1.144869	14.58689	0.981358	0.980519	7.05E-07
50	1.143944	14.57465	0.980535	0.978488	4.19E-06
55	1.13987	14.52077	0.97691	0.976483	1.82E-07
60	1.139212	14.51207	0.976324	0.974503	3.32E-06
65	1.134824	14.45402	0.972419	0.972548	1.68E-08
70	1.133254	14.43326	0.971022	0.970618	1.64E-07
75	1.132266	14.42019	0.970143	0.968712	2.05E-06
80	1.127833	14.36155	0.966198	0.96683	3.99E-07
85	1.127928	14.36281	0.966283	0.964971	1.72E-06
90	1.130731	14.39988	0.968777	0.963136	3.18E-05
95	1.121513	14.27795	0.960574	0.961324	5.63E-07
100	1.124387	14.31596	0.963131	0.959535	1.29E-05
105	1.120132	14.25969	0.959345	0.957769	2.48E-06
110	1.115178	14.19415	0.954936	0.956024	1.18E-06
115	1.120301	14.26192	0.959495	0.954302	2.7E-05
120	1.112203	14.15481	0.952289	0.952601	9.75E-08
125	1.117983	14.23125	0.957432	0.950922	4.24E-05
130	1.111615	14.14702	0.951765	0.949264	6.26E-06
135	1.106639	14.08121	0.947337	0.947626	8.34E-08
140	1.105383	14.06459	0.946219	0.946009	4.4E-08
145	1.10563	14.06786	0.946439	0.944413	4.11E-06
150	1.102756	14.02984	0.943882	0.942837	1.09E-06
155	1.098779	13.97723	0.940342	0.94128	8.8E-07
160	1.099489	13.98663	0.940975	0.939743	1.52E-06
165	1.097015	13.9539	0.938773	0.938226	2.99E-07
170	1.099873	13.9917	0.941316	0.936727	2.11E-05
175	1.09626	13.94392	0.938101	0.935248	8.14E-06
180	1.09693	13.95277	0.938697	0.933787	2.41E-05
185	1.09047	13.86732	0.932948	0.932344	3.65E-07
190	1.090749	13.87102	0.933197	0.93092	5.19E-06
195	1.093419	13.90633	0.935572	0.929513	3.67E-05
200	1.086762	13.81828	0.929648	0.928124	2.32E-06
205	1.082092	13.75651	0.925493	0.926753	1.59E-06
210	1.084137	13.78356	0.927312	0.925399	3.66E-06
215	1.081786	13.75246	0.925221	0.924062	1.34E-06
220	1.081377	13.74705	0.924857	0.922742	4.47E-06
225	1.077765	13.69927	0.921642	0.921438	4.17E-08
230	1.076004	13.67598	0.920075	0.920151	5.79E-09
235	1.072248	13.6263	0.916733	0.91888	4.61E-06
240	1.076615	13.68407	0.920619	0.917625	8.97E-06
245	1.074134	13.65124	0.91841	0.916386	4.1E-06
250	1.067405	13.56224	0.912423	0.915162	7.5E-06
255	1.067438	13.56267	0.912452	0.913954	2.26E-06
260	1.062486	13.49716	0.908045	0.912761	2.22E-05
265	1.061839	13.48861	0.907469	0.911583	1.69E-05
270	1.062082	13.49183	0.907686	0.91042	7.47E-06
275	1.060832	13.47529	0.906573	0.909271	7.28E-06
280	1.05631	13.41548	0.902549	0.908137	3.12E-05
285	1.055687	13.40724	0.901995	0.907017	2.52E-05
290	1.059826	13.46198	0.905678	0.905911	5.45E-08
295	1.053313	13.37583	0.899882	0.90482	2.44E-05
300	1.049913	13.33086	0.896856	0.903741	4.74E-05
				sum=	0.000548

Calibratio Curve

a=	0.0421
b=	0.0756

%	TT (ppm)	abs
0	0	0.0806
0.25	6.7775	0.3684
0.5	13.555	0.6353
0.75	20.3325	0.9109
1	27.11	1.2357

pH Before	6.812
pH After	5.024



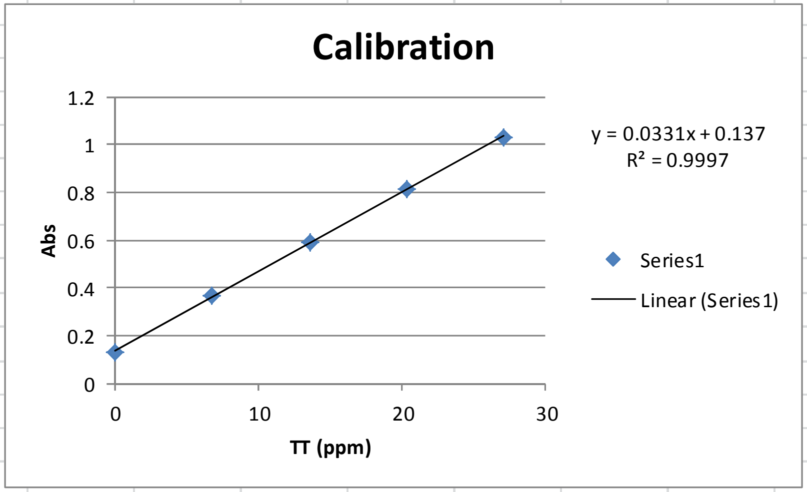
22Jun15_0.7@20%pH9					
			flow rate=	0.7	
			volume=	350	
			resid time	482	
			rate const	5.96E-05	
wavelength=	430				
time (min)	abs		C/Co	model	sum squares
0	0.93345	6.571896	1	1	0
5	0.94425	6.650732	1.011996	0.999703	0.000151
10	0.935591	6.587529	1.002379	0.99941	8.81E-06
15	0.936495	6.594122	1.003382	0.99912	1.82E-05
20	0.935765	6.588795	1.002571	0.998833	1.4E-05
25	0.936381	6.593294	1.003256	0.998548	2.22E-05
30	0.937102	6.598558	1.004057	0.998267	3.35E-05
35	0.931894	6.560538	0.998272	0.997989	7.98E-08
40	0.943152	6.642717	1.010776	0.997714	0.000171
45	0.935137	6.584212	1.001874	0.997442	1.96E-05
50	0.935403	6.586152	1.002169	0.997172	2.5E-05
55	0.9372	6.599269	1.004165	0.996906	5.27E-05
60	0.932829	6.567368	0.999311	0.996642	7.12E-06
65	0.931023	6.554184	0.997305	0.996381	8.53E-07
70	0.932822	6.567313	0.999303	0.996123	1.01E-05
75	0.933937	6.575454	1.000541	0.995868	2.18E-05
80	0.934861	6.582197	1.001567	0.995615	3.54E-05
85	0.931265	6.555951	0.997574	0.995365	4.88E-06
90	0.928376	6.534859	0.994364	0.995117	5.67E-07
95	0.92935	6.541969	0.995446	0.994873	3.29E-07
100	0.929217	6.540998	0.995298	0.994631	4.46E-07
105	0.931195	6.555436	0.997495	0.994391	9.64E-06
110	0.928509	6.535829	0.994512	0.994154	1.28E-07
115	0.928915	6.538799	0.994964	0.99392	1.09E-06
120	0.93069	6.551752	0.996935	0.993688	1.05E-05
125	0.928058	6.532539	0.994011	0.993458	3.06E-07
130	0.928674	6.537039	0.994696	0.993231	2.15E-06
135	0.934819	6.581887	1.00152	0.993006	7.25E-05
140	0.927916	6.531507	0.993854	0.992784	1.15E-06
145	0.931165	6.555218	0.997462	0.992564	2.4E-05
150	0.926259	6.519406	0.992013	0.992346	1.11E-07
155	0.933452	6.571914	1.000003	0.992131	6.2E-05
160	0.928166	6.53333	0.994132	0.991918	4.9E-06
165	0.925356	6.512816	0.99101	0.991707	4.86E-07
170	0.928139	6.533132	0.994101	0.991499	6.77E-06
175	0.93007	6.547229	0.996247	0.991292	2.45E-05
180	0.925813	6.51615	0.991518	0.991088	1.84E-07
185	0.924327	6.505307	0.989868	0.990886	1.04E-06
190	0.924228	6.504583	0.989757	0.990687	8.63E-07
195	0.920645	6.478433	0.985778	0.990489	2.22E-05
200	0.919201	6.467894	0.984175	0.990293	3.74E-05
205	0.924819	6.508898	0.990414	0.9901	9.87E-08
210	0.921127	6.481946	0.986313	0.989908	1.29E-05
215	0.921819	6.486998	0.987082	0.989719	6.95E-06
220	0.921435	6.484194	0.986655	0.989531	8.27E-06
225	0.921708	6.486189	0.986959	0.989346	5.7E-06
230	0.926016	6.517638	0.991744	0.989163	6.66E-06
235	0.925673	6.51513	0.991362	0.988981	5.67E-06
240	0.921096	6.481722	0.986279	0.988801	6.36E-06
245	0.919832	6.472496	0.984875	0.988624	1.41E-05
250	0.921281	6.483076	0.986485	0.988448	3.85E-06
255	0.919354	6.469004	0.984344	0.988274	1.54E-05
260	0.928222	6.533739	0.994194	0.988102	3.71E-05
265	0.917578	6.456046	0.982372	0.987932	3.09E-05
270	0.918887	6.465601	0.983826	0.987763	1.55E-05
275	0.92288	6.494747	0.988261	0.987597	4.41E-07
280	0.921591	6.485335	0.986829	0.987432	3.64E-07
285	0.923842	6.501767	0.989329	0.987269	4.24E-06
290	0.914252	6.431766	0.978677	0.987107	7.11E-05
295	0.921107	6.481803	0.986291	0.986947	4.31E-07
300	0.918746	6.464571	0.983669	0.986789	9.74E-06
				sum=	0.001135

Calibratio Curve

a=	0.0331
b=	0.137

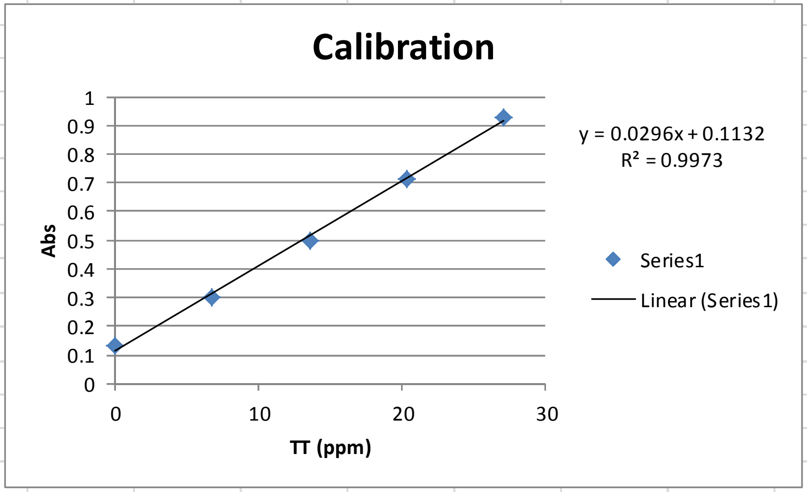
%	TT (ppm)	abs
0	0	0.1293
0.25	6.7775	0.3668
0.5	13.555	0.5929
0.75	20.3325	0.8129
1	27.11	1.0293

pH Before	9.243
pH After	9.188



24Jun15_0.7@100%pH6 Throwout					
			flow rate=	0.7	
			volume=	350	
			resid time	482	
			rate const	0.001199	
wavelength=	430				
time (min)	abs		C/Co	model	sum squares
0	1.237493	10.67043	1	1	0
5	1.229578	10.60051	0.993447	0.994052	3.66E-07
10	1.226262	10.57122	0.990702	0.988201	6.26E-06
15	1.216127	10.48169	0.982311	0.982444	1.78E-08
20	1.21564	10.47739	0.981908	0.976782	2.63E-05
25	1.206952	10.40064	0.974716	0.971211	1.23E-05
30	1.197791	10.31971	0.967131	0.96573	1.96E-06
35	1.19698	10.31254	0.96646	0.960339	3.75E-05
40	1.186696	10.22169	0.957945	0.955035	8.47E-06
45	1.178789	10.15185	0.9514	0.949817	2.5E-06
50	1.172988	10.1006	0.946597	0.944684	3.66E-06
55	1.171241	10.08517	0.945151	0.939634	3.04E-05
60	1.169725	10.07177	0.943895	0.934666	8.52E-05
65	1.162458	10.00758	0.937879	0.929779	6.56E-05
70	1.152499	9.9196	0.929634	0.924971	2.17E-05
75	1.147615	9.876455	0.925591	0.920242	2.86E-05
80	1.14359	9.8409	0.922259	0.915589	4.45E-05
85	1.137164	9.784133	0.916939	0.911012	3.51E-05
90	1.137999	9.79151	0.91763	0.906509	0.000124
95	1.129887	9.719848	0.910914	0.902079	7.81E-05
100	1.123968	9.66756	0.906014	0.897721	6.88E-05
105	1.116936	9.605446	0.900193	0.893433	4.57E-05
110	1.112112	9.562825	0.896198	0.889216	4.88E-05
115	1.104816	9.498374	0.890158	0.885067	2.59E-05
120	1.100966	9.46436	0.886971	0.880985	3.58E-05
125	1.093409	9.397602	0.880714	0.876969	1.4E-05
130	1.089509	9.363156	0.877486	0.873019	2E-05
135	1.086225	9.334141	0.874767	0.869133	3.17E-05
140	1.080285	9.281671	0.86985	0.86531	2.06E-05
145	1.078293	9.264076	0.868201	0.861549	4.42E-05
150	1.070276	9.193247	0.861563	0.857849	1.38E-05
155	1.066459	9.159534	0.858403	0.854209	1.76E-05
160	1.0623	9.122788	0.854959	0.850629	1.88E-05
165	1.056654	9.072915	0.850286	0.847106	1.01E-05
170	1.056486	9.071428	0.850146	0.843641	4.23E-05
175	1.046213	8.980682	0.841642	0.840232	1.99E-06
180	1.044108	8.962081	0.839899	0.836878	9.13E-06
185	1.03925	8.919172	0.835877	0.833578	5.28E-06
190	1.039777	8.923828	0.836314	0.830333	3.58E-05
195	1.028854	8.827336	0.827271	0.82714	1.72E-08
200	1.025082	8.794013	0.824148	0.823998	2.23E-08
205	1.019959	8.748754	0.819906	0.820908	1E-06
210	1.016042	8.714151	0.816663	0.817868	1.45E-06
215	1.01181	8.676763	0.813159	0.814878	2.95E-06
220	1.006184	8.627068	0.808502	0.811935	1.18E-05
225	1.004644	8.613466	0.807227	0.809041	3.29E-06
230	0.999937	8.571885	0.803331	0.806194	8.2E-06
235	0.994537	8.524179	0.79886	0.803393	2.05E-05
240	0.991102	8.493831	0.796016	0.800637	2.14E-05
245	0.987617	8.463044	0.79313	0.797926	2.3E-05
250	0.985851	8.447446	0.791669	0.795259	1.29E-05
255	0.977787	8.376215	0.784993	0.792636	5.84E-05
260	0.977226	8.37125	0.784528	0.790055	3.05E-05
265	0.974406	8.346345	0.782194	0.787516	2.83E-05
270	0.967829	8.288239	0.776748	0.785018	6.84E-05
275	0.97097	8.315991	0.779349	0.782561	1.03E-05
280	0.961828	8.235229	0.77178	0.780143	6.99E-05
285	0.963588	8.250774	0.773237	0.777765	2.05E-05
290	0.958313	8.204174	0.76887	0.775426	4.3E-05
295	0.957546	8.197406	0.768236	0.773124	2.39E-05
300	0.947788	8.111201	0.760157	0.77086	0.000115
				sum=	0.001697

Calibratio Curve					
a=	0.0296		%	TT (ppm)	abs
b=	0.1132		0	0	0.1333
			0.25	6.7775	0.2985
			0.5	13.555	0.496
			0.75	20.3325	0.716
			1	27.11	0.9267
	pH Before	9.085			
	pH After	9.071	8.841		



26Jun15_0.7@100%pH6					
			flow rate=	0.7	
			volume=	350	
			resid time	482	
			rate const	0.001224	
wavelength=	430				
time (min)	abs		C/Co	model	sum squares
0	1.236743	8.396371	1	1	0
5	1.227521	8.33161	0.992287	0.993933	2.71E-06
10	1.223997	8.306859	0.989339	0.987964	1.89E-06
15	1.215212	8.245167	0.981992	0.982094	1.04E-08
20	1.208181	8.19579	0.976111	0.976319	4.33E-08
25	1.200593	8.142504	0.969765	0.970639	7.64E-07
30	1.199269	8.133209	0.968658	0.965052	1.3E-05
35	1.187557	8.050959	0.958862	0.959556	4.82E-07
40	1.18941	8.063975	0.960412	0.95415	3.92E-05
45	1.181836	8.010783	0.954077	0.948832	2.75E-05
50	1.169094	7.921308	0.943421	0.943602	3.29E-08
55	1.167182	7.907882	0.941821	0.938457	1.13E-05
60	1.155692	7.827192	0.932211	0.933396	1.4E-06
65	1.155273	7.824246	0.93186	0.928418	1.19E-05
70	1.146178	7.76038	0.924254	0.923521	5.37E-07
75	1.140834	7.722851	0.919784	0.918705	1.17E-06
80	1.134842	7.680772	0.914773	0.913967	6.5E-07
85	1.134603	7.679091	0.914573	0.909306	2.77E-05
90	1.124961	7.611384	0.906509	0.904722	3.19E-06
95	1.120932	7.583093	0.903139	0.900213	8.56E-06
100	1.11216	7.521489	0.895802	0.895778	6.01E-10
105	1.107879	7.491428	0.892222	0.891415	6.51E-07
110	1.095025	7.40116	0.881471	0.887124	3.19E-05
115	1.103301	7.459277	0.888393	0.882902	3.01E-05
120	1.089516	7.362469	0.876863	0.87875	3.56E-06
125	1.087412	7.3477	0.875104	0.874666	1.92E-07
130	1.08594	7.337363	0.873873	0.870648	1.04E-05
135	1.083695	7.321593	0.871995	0.866696	2.81E-05
140	1.081671	7.307384	0.870303	0.862809	5.62E-05
145	1.071827	7.238254	0.862069	0.858986	9.51E-06
150	1.069559	7.222322	0.860172	0.855225	2.45E-05
155	1.058546	7.144985	0.850961	0.851525	3.18E-07
160	1.054079	7.113615	0.847225	0.847886	4.37E-07
165	1.057174	7.135353	0.849814	0.844307	3.03E-05
170	1.051629	7.096414	0.845176	0.840786	1.93E-05
175	1.042933	7.035347	0.837903	0.837322	3.38E-07
180	1.047667	7.068591	0.841863	0.833916	6.32E-05
185	1.036657	6.991272	0.832654	0.830565	4.37E-06
190	1.033443	6.968703	0.829966	0.827268	7.28E-06
195	1.032678	6.963327	0.829326	0.824026	2.81E-05
200	1.027649	6.928014	0.82512	0.820837	1.83E-05
205	1.018309	6.862426	0.817309	0.8177	1.53E-07
210	1.018005	6.860291	0.817054	0.814614	5.96E-06
215	1.010478	6.807431	0.810759	0.811579	6.72E-07
220	1.008011	6.790102	0.808695	0.808593	1.04E-08
225	1.009963	6.803813	0.810328	0.805656	2.18E-05
230	0.999766	6.732206	0.801799	0.802767	9.37E-07
235	0.995897	6.705036	0.798564	0.799926	1.86E-06
240	0.995564	6.702699	0.798285	0.797131	1.33E-06
245	0.988937	6.656156	0.792742	0.794381	2.69E-06
250	0.983293	6.616525	0.788022	0.791677	1.34E-05
255	0.979177	6.587619	0.784579	0.789017	1.97E-05
260	0.975001	6.558294	0.781087	0.7864	2.82E-05
265	0.972813	6.542929	0.779257	0.783826	2.09E-05
270	0.970348	6.525615	0.777195	0.781294	1.68E-05
275	0.967067	6.502581	0.774451	0.778804	1.89E-05
280	0.962899	6.473309	0.770965	0.776355	2.9E-05
285	0.960206	6.454393	0.768712	0.773945	2.74E-05
290	0.954588	6.414945	0.764014	0.771575	5.72E-05
295	0.958274	6.440832	0.767097	0.769243	4.61E-06
300	0.949053	6.376076	0.759385	0.76695	5.72E-05
				sum=	0.000848

Calibratio Curve

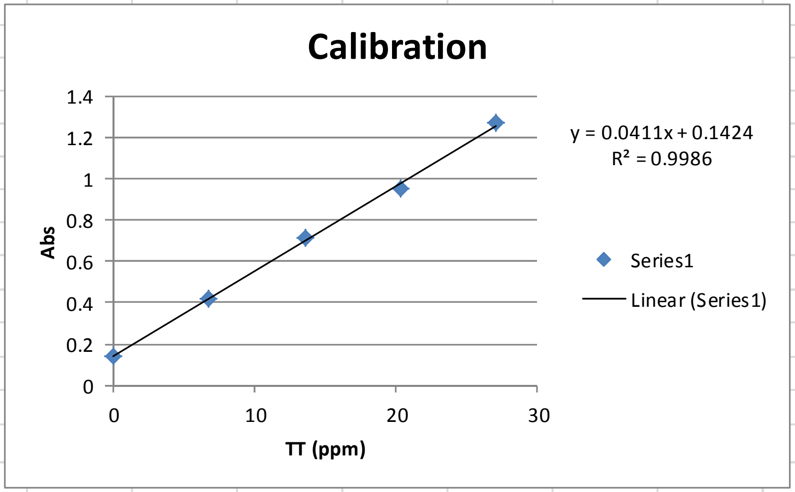
a=	0.0411
b=	0.1424

%	TT (ppm)	abs
0	0	0.1407
0.25	6.7775	0.4231
0.5	13.555	0.7141
0.75	20.3325	0.9516
1	27.11	1.2706

pH Before	6.696
pH After	5.35

Correlation Coefficient
0.998768713

R^2 of Module
0.997538943



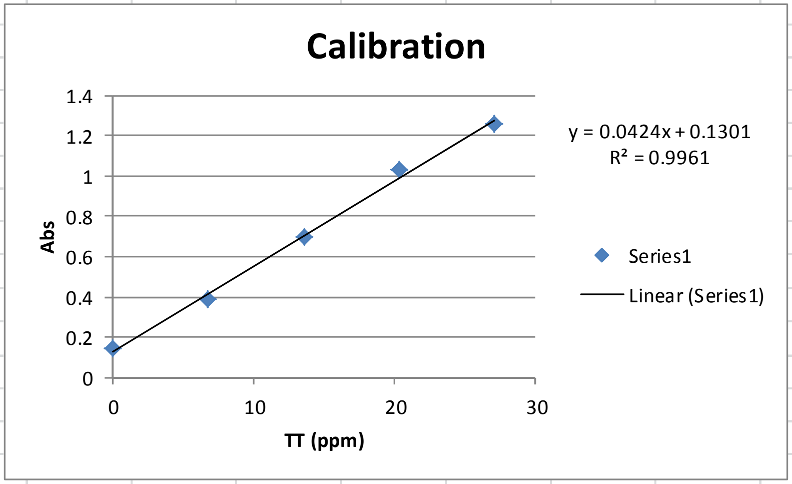
29Jun15_0.7@5%pH6						
			flow rate=	0.7		
			volume=	350		
			resid time	482		
			rate const	9.69E-05		
wavelength=	430					
time (min)	abs		C/Co	model	sum squares	
0	1.210083	11.93201	1	1	0	
5	1.207514	11.90601	0.997821	0.999518	2.88E-06	
10	1.203953	11.86997	0.994801	0.999041	1.8E-05	
15	1.205359	11.8842	0.995993	0.99857	6.64E-06	
20	1.203867	11.8691	0.994728	0.998103	1.14E-05	
25	1.203846	11.86889	0.99471	0.997642	8.6E-06	
30	1.205705	11.88771	0.996287	0.997186	8.08E-07	
35	1.203731	11.86773	0.994612	0.996734	4.5E-06	
40	1.203103	11.86137	0.994079	0.996287	4.88E-06	
45	1.204514	11.87564	0.995276	0.995846	3.24E-07	
50	1.201609	11.84624	0.992812	0.995409	6.74E-06	
55	1.201632	11.84648	0.992832	0.994976	4.6E-06	
60	1.198273	11.81248	0.989983	0.994549	2.08E-05	
65	1.199479	11.82469	0.991005	0.994126	9.74E-06	
70	1.202693	11.85721	0.993731	0.993707	5.8E-10	
75	1.199519	11.82509	0.991039	0.993293	5.08E-06	
80	1.196347	11.79298	0.988348	0.992884	2.06E-05	
85	1.200211	11.83209	0.991626	0.992479	7.27E-07	
90	1.2039	11.86943	0.994755	0.992078	7.17E-06	
95	1.198488	11.81465	0.990165	0.991682	2.3E-06	
100	1.199037	11.82022	0.990631	0.99129	4.34E-07	
105	1.197168	11.80129	0.989045	0.990902	3.45E-06	
110	1.201932	11.84952	0.993086	0.990518	6.6E-06	
115	1.197947	11.80918	0.989706	0.990139	1.87E-07	
120	1.202286	11.8531	0.993386	0.989763	1.31E-05	
125	1.194916	11.7785	0.987135	0.989392	5.09E-06	
130	1.195022	11.77957	0.987225	0.989025	3.24E-06	
135	1.195559	11.78501	0.98768	0.988661	9.62E-07	
140	1.198287	11.81262	0.989994	0.988302	2.86E-06	
145	1.195995	11.78943	0.98805	0.987946	1.08E-08	
150	1.193137	11.7605	0.985626	0.987595	3.88E-06	
155	1.192179	11.7508	0.984813	0.987247	5.92E-06	
160	1.191782	11.74678	0.984476	0.986903	5.89E-06	
165	1.191055	11.73942	0.98386	0.986562	7.3E-06	
170	1.189499	11.72368	0.98254	0.986225	1.36E-05	
175	1.198409	11.81385	0.990097	0.985892	1.77E-05	
180	1.189457	11.72325	0.982504	0.985563	9.35E-06	
185	1.190276	11.73154	0.983199	0.985237	4.15E-06	
190	1.192251	11.75152	0.984874	0.984914	1.63E-09	
195	1.191204	11.74093	0.983986	0.984595	3.71E-07	
200	1.18841	11.71265	0.981616	0.98428	7.1E-06	
205	1.194491	11.7742	0.986774	0.983968	7.88E-06	
210	1.191036	11.73923	0.983843	0.983659	3.41E-08	
215	1.192284	11.75187	0.984902	0.983353	2.4E-06	
220	1.189992	11.72866	0.982958	0.983051	8.71E-09	
225	1.191913	11.7481	0.984587	0.982752	3.37E-06	
230	1.192839	11.75748	0.985373	0.982457	8.5E-06	
235	1.188999	11.71861	0.982116	0.982164	2.38E-09	
240	1.190983	11.73869	0.983799	0.981875	3.7E-06	
245	1.186759	11.69594	0.980215	0.981589	1.89E-06	
250	1.184216	11.6702	0.978058	0.981306	1.05E-05	
255	1.185755	11.68578	0.979364	0.981026	2.76E-06	
260	1.1862	11.69028	0.979741	0.980749	1.02E-06	
265	1.186179	11.69007	0.979723	0.980475	5.65E-07	
270	1.191548	11.74441	0.984278	0.980204	1.66E-05	
275	1.187257	11.70098	0.980638	0.979936	4.93E-07	
280	1.187351	11.70194	0.980718	0.979671	1.1E-06	
285	1.192489	11.75393	0.985076	0.979408	3.21E-05	
290	1.187218	11.70059	0.980605	0.979149	2.12E-06	
295	1.187313	11.70155	0.980686	0.978892	3.22E-06	
300	1.188058	11.70909	0.981318	0.978638	7.18E-06	
				sum=	0.000352	

Calibratio Curve

a=	0.0312
b=	0.0988

%	TT (ppm)	abs
0	0	0.1485
0.25	6.7775	0.3852
0.5	13.555	0.6963
0.75	20.3325	1.0308
1	27.11	1.2615

pH Before	6.789
pH After	6.625



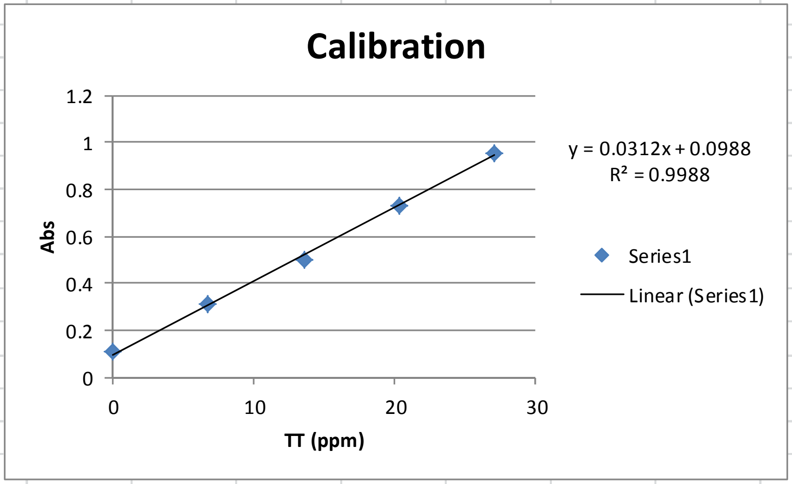
1Jul15_0.7@100%pH9						
			flow rate=	0.7		
			volume=	350		
			resid time	482		
			rate const	0.000242		
wavelength=	430					
time (min)	abs		C/Co	model	sum squares	
0	0.901425	8.807942	1	1	0	
5	0.900986	8.8035	0.999496	0.998796	4.9E-07	
10	0.908873	8.88333	1.008559	0.997606	0.00012	
15	0.908235	8.876872	1.007826	0.996429	0.00013	
20	0.907171	8.866108	1.006604	0.995266	0.000129	
25	0.903385	8.827782	1.002253	0.994116	6.62E-05	
30	0.901005	8.803697	0.999518	0.99298	4.27E-05	
35	0.900706	8.800664	0.999174	0.991857	5.35E-05	
40	0.901136	8.805021	0.999668	0.990746	7.96E-05	
45	0.897292	8.76611	0.995251	0.989649	3.14E-05	
50	0.894711	8.739985	0.992285	0.988564	1.38E-05	
55	0.899757	8.791067	0.998084	0.987492	0.000112	
60	0.895738	8.750386	0.993465	0.986432	4.95E-05	
65	0.894342	8.736255	0.991861	0.985384	4.2E-05	
70	0.891649	8.709	0.988767	0.984348	1.95E-05	
75	0.89825	8.775807	0.996352	0.983324	0.00017	
80	0.895874	8.751763	0.993622	0.982312	0.000128	
85	0.890439	8.696751	0.987376	0.981312	3.68E-05	
90	0.887278	8.66476	0.983744	0.980323	1.17E-05	
95	0.884914	8.64083	0.981027	0.979345	2.83E-06	
100	0.884503	8.636665	0.980554	0.978379	4.73E-06	
105	0.884317	8.634786	0.980341	0.977424	8.51E-06	
110	0.881993	8.611268	0.977671	0.97648	1.42E-06	
115	0.884845	8.640131	0.980948	0.975546	2.92E-05	
120	0.879261	8.583618	0.974532	0.974624	8.54E-09	
125	0.880336	8.594493	0.975766	0.973712	4.22E-06	
130	0.877738	8.568198	0.972781	0.972811	8.88E-10	
135	0.878762	8.578564	0.973958	0.97192	4.15E-06	
140	0.879805	8.589119	0.975156	0.971039	1.7E-05	
145	0.878122	8.572085	0.973222	0.970169	9.33E-06	
150	0.873984	8.530199	0.968467	0.969308	7.08E-07	
155	0.882223	8.613594	0.977935	0.968457	8.98E-05	
160	0.873079	8.521038	0.967427	0.967617	3.61E-08	
165	0.871736	8.50745	0.965884	0.966785	8.13E-07	
170	0.872509	8.515274	0.966772	0.965964	6.54E-07	
175	0.878254	8.573426	0.973374	0.965152	6.76E-05	
180	0.872496	8.515144	0.966758	0.964349	5.8E-06	
185	0.868964	8.479396	0.962699	0.963555	7.34E-07	
190	0.868911	8.478856	0.962638	0.962771	1.78E-08	
195	0.874875	8.539221	0.969491	0.961996	5.62E-05	
200	0.866475	8.454195	0.959838	0.961229	1.94E-06	
205	0.866543	8.45489	0.959917	0.960472	3.08E-07	
210	0.869059	8.480357	0.962808	0.959723	9.52E-06	
215	0.86267	8.415686	0.955466	0.958983	1.24E-05	
220	0.863839	8.427521	0.956809	0.958251	2.08E-06	
225	0.868353	8.473212	0.961997	0.957528	2E-05	
230	0.863772	8.426844	0.956732	0.956813	6.44E-09	
235	0.857593	8.364306	0.949632	0.956106	4.19E-05	
240	0.861403	8.402862	0.95401	0.955407	1.95E-06	
245	0.859964	8.388302	0.952357	0.954717	5.57E-06	
250	0.855614	8.344271	0.947358	0.954034	4.46E-05	
255	0.856734	8.355606	0.948645	0.95336	2.22E-05	
260	0.859743	8.386058	0.952102	0.952693	3.49E-07	
265	0.854748	8.335501	0.946362	0.952033	3.22E-05	
270	0.857415	8.362499	0.949427	0.951382	3.82E-06	
275	0.853336	8.321211	0.94474	0.950738	3.6E-05	
280	0.851216	8.299758	0.942304	0.950101	6.08E-05	
285	0.859198	8.380549	0.951476	0.949471	4.02E-06	
290	0.850508	8.29259	0.94149	0.948849	5.42E-05	
295	0.85208	8.308505	0.943297	0.948234	2.44E-05	
300	0.848349	8.270737	0.939009	0.947626	7.43E-05	
				sum=	0.001992	

Calibratio Curve

a=	0.0312
b=	0.0988

%	TT (ppm)	abs	
0	0	0.108	0.108
0.25	6.7775	0.3107	0.3107
0.5	13.555	0.5038	0.5038
0.75	20.3325	0.7315	0.7315
1	27.11	0.9551	0.9551

pH Before	9.89
pH After	9.527



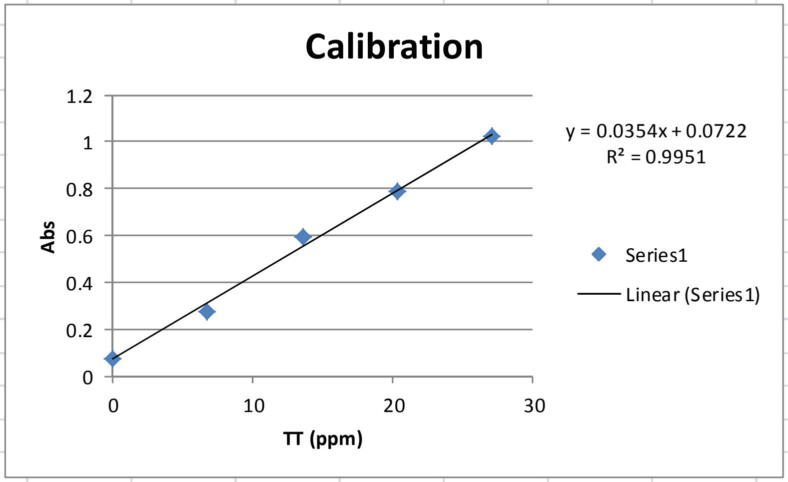
2Jul15 0.7@30%pH8						
			flow rate=	0.7		
			volume=	350		
			resid time	482		
			rate const	0.000184		
wavelength=	430					
time (min)	abs		C/Co	model	sum squares	
0	0.964623	12.87012	1	1	0	
5	0.958008	12.77851	0.992882	0.999087	3.85E-05	
10	0.962411	12.83949	0.99762	0.998183	3.18E-07	
15	0.961793	12.83093	0.996955	0.997291	1.13E-07	
20	0.963399	12.85317	0.998683	0.996408	5.18E-06	
25	0.958179	12.78088	0.993066	0.995534	6.09E-06	
30	0.962604	12.84216	0.997828	0.994671	9.96E-06	
35	0.957762	12.7751	0.992617	0.993818	1.44E-06	
40	0.960506	12.8131	0.995569	0.992974	6.74E-06	
45	0.955501	12.74378	0.990183	0.992139	3.82E-06	
50	0.95366	12.71829	0.988203	0.991314	9.68E-06	
55	0.954978	12.73654	0.989621	0.990498	7.7E-07	
60	0.957829	12.77603	0.992689	0.989692	8.99E-06	
65	0.956815	12.76198	0.991598	0.988894	7.31E-06	
70	0.951458	12.68778	0.985832	0.988105	5.17E-06	
75	0.95115	12.68351	0.985501	0.987325	3.33E-06	
80	0.951836	12.69302	0.98624	0.986554	9.9E-08	
85	0.948637	12.64872	0.982797	0.985792	8.97E-06	
90	0.949825	12.66516	0.984075	0.985038	9.28E-07	
95	0.947888	12.63833	0.98199	0.984293	5.3E-06	
100	0.94874	12.65015	0.982908	0.983556	4.19E-07	
105	0.947672	12.63534	0.981758	0.982827	1.14E-06	
110	0.945591	12.60652	0.979519	0.982106	6.7E-06	
115	0.94539	12.60374	0.979302	0.981394	4.38E-06	
120	0.944683	12.59395	0.978542	0.980689	4.61E-06	
125	0.945991	12.61207	0.979949	0.979993	1.89E-09	
130	0.949064	12.65463	0.983257	0.979304	1.56E-05	
135	0.942704	12.56654	0.976412	0.978623	4.89E-06	
140	0.949036	12.65423	0.983226	0.97795	2.78E-05	
145	0.945737	12.60855	0.979676	0.977284	5.72E-06	
150	0.946864	12.62415	0.980888	0.976626	1.82E-05	
155	0.946933	12.62511	0.980963	0.975975	2.49E-05	
160	0.943201	12.57343	0.976947	0.975331	2.61E-06	
165	0.945544	12.60587	0.979468	0.974695	2.28E-05	
170	0.944979	12.59804	0.97886	0.974066	2.3E-05	
175	0.941854	12.55477	0.975498	0.973443	4.22E-06	
180	0.938791	12.51235	0.972201	0.972828	3.93E-07	
185	0.938602	12.50973	0.971998	0.97222	4.93E-08	
190	0.935392	12.46527	0.968543	0.971618	9.46E-06	
195	0.935435	12.46585	0.968589	0.971024	5.93E-06	
200	0.941252	12.54643	0.974849	0.970436	1.95E-05	
205	0.936946	12.48679	0.970215	0.969854	1.3E-07	
210	0.933011	12.43228	0.96598	0.969279	1.09E-05	
215	0.932804	12.42942	0.965758	0.968711	8.72E-06	
220	0.932876	12.43041	0.965835	0.968149	5.35E-06	
225	0.933721	12.44212	0.966744	0.967593	7.2E-07	
230	0.930844	12.40227	0.963649	0.967044	1.15E-05	
235	0.932258	12.42186	0.965171	0.9665	1.77E-06	
240	0.933271	12.43588	0.96626	0.965963	8.81E-08	
245	0.930553	12.39824	0.963335	0.965432	4.4E-06	
250	0.933707	12.44193	0.96673	0.964907	3.32E-06	
255	0.934052	12.4467	0.9671	0.964387	7.36E-06	
260	0.928939	12.37589	0.961598	0.963874	5.18E-06	
265	0.929708	12.38653	0.962426	0.963366	8.84E-07	
270	0.930041	12.39115	0.962784	0.962864	6.38E-09	
275	0.927041	12.34959	0.959556	0.962368	7.91E-06	
280	0.928864	12.37485	0.961518	0.961877	1.29E-07	
285	0.928815	12.37417	0.961465	0.961391	5.38E-09	
290	0.927786	12.35992	0.960358	0.960912	3.07E-07	
295	0.930702	12.40031	0.963496	0.960437	9.36E-06	
300	0.928385	12.36822	0.961002	0.959968	1.07E-06	
				sum=	0.000404	

Calibratio Curve

a=	0.0354
b=	0.0722

%	TT (ppm)	abs
0	0	0.0784
0.25	6.7775	0.2785
0.5	13.555	0.5922
0.75	20.3325	0.7903
1	27.11	1.0235

pH Before	8.444
pH After	8.699



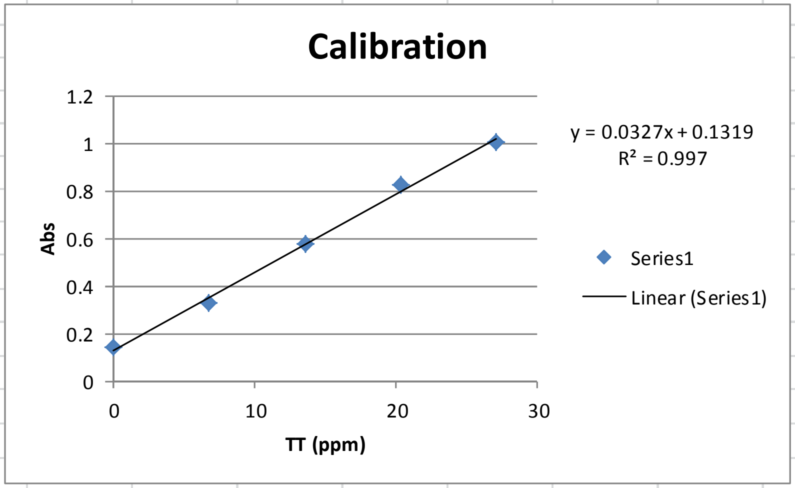
6Jul15_0.7@100%pH8						
			flow rate=	0.7		
			volume=	350		
			resid time	482		
			rate const	0.000472		
wavelength=	430					
time (min)	abs		C/Co	model	sum squares	
0	0.926073	6.77311	1	1	1.23E-32	
5	0.923546	6.753946	0.997171	0.997653	2.33E-07	
10	0.923245	6.751671	0.996835	0.995337	2.24E-06	
15	0.919688	6.724697	0.992852	0.993049	3.87E-08	
20	0.917768	6.710141	0.990703	0.99079	7.62E-09	
25	0.917023	6.704497	0.98987	0.98856	1.71E-06	
30	0.915572	6.693493	0.988245	0.986359	3.56E-06	
35	0.915245	6.691015	0.987879	0.984185	1.37E-05	
40	0.91051	6.655121	0.98258	0.982038	2.93E-07	
45	0.910952	6.658467	0.983074	0.979919	9.95E-06	
50	0.910098	6.651994	0.982118	0.977827	1.84E-05	
55	0.908409	6.639187	0.980227	0.975761	2E-05	
60	0.906301	6.623206	0.977868	0.973721	1.72E-05	
65	0.906002	6.620938	0.977533	0.971707	3.39E-05	
70	0.900989	6.582937	0.971922	0.969718	4.86E-06	
75	0.898614	6.564927	0.969263	0.967755	2.28E-06	
80	0.898954	6.567508	0.969644	0.965816	1.47E-05	
85	0.89735	6.555344	0.967848	0.963902	1.56E-05	
90	0.893342	6.52496	0.963362	0.962013	1.82E-06	
95	0.894073	6.530497	0.96418	0.960147	1.63E-05	
100	0.893484	6.526031	0.963521	0.958305	2.72E-05	
105	0.888544	6.48858	0.957991	0.956486	2.27E-06	
110	0.888985	6.491926	0.958485	0.95469	1.44E-05	
115	0.887667	6.48193	0.957009	0.952917	1.68E-05	
120	0.886524	6.473271	0.955731	0.951166	2.08E-05	
125	0.88421	6.455721	0.95314	0.949437	1.37E-05	
130	0.881677	6.436523	0.950305	0.947731	6.63E-06	
135	0.879099	6.416977	0.94742	0.946045	1.89E-06	
140	0.876026	6.393676	0.943979	0.944382	1.62E-07	
145	0.8767	6.398786	0.944734	0.942739	3.98E-06	
150	0.876949	6.400675	0.945013	0.941117	1.52E-05	
155	0.875605	6.390482	0.943508	0.939515	1.59E-05	
160	0.872623	6.367875	0.94017	0.937934	5E-06	
165	0.871917	6.362528	0.939381	0.936373	9.05E-06	
170	0.867673	6.330347	0.934629	0.934832	4.1E-08	
175	0.869165	6.341658	0.936299	0.93331	8.94E-06	
180	0.867022	6.325413	0.933901	0.931807	4.38E-06	
185	0.863003	6.294941	0.929402	0.930324	8.5E-07	
190	0.862477	6.290953	0.928813	0.928859	2.09E-09	
195	0.860064	6.272658	0.926112	0.927412	1.69E-06	
200	0.859326	6.267068	0.925287	0.925984	4.87E-07	
205	0.857527	6.253426	0.923272	0.924574	1.7E-06	
210	0.856671	6.246935	0.922314	0.923182	7.54E-07	
215	0.853033	6.219352	0.918242	0.921808	1.27E-05	
220	0.855027	6.234477	0.920475	0.920451	5.75E-10	
225	0.851664	6.208976	0.91671	0.919111	5.77E-06	
230	0.85106	6.204397	0.916034	0.917788	3.08E-06	
235	0.849822	6.195011	0.914648	0.916482	3.36E-06	
240	0.848141	6.18227	0.912767	0.915192	5.88E-06	
245	0.846559	6.170271	0.910995	0.913919	8.55E-06	
250	0.847323	6.176068	0.911851	0.912661	6.57E-07	
255	0.845445	6.161825	0.909748	0.91142	2.79E-06	
260	0.845169	6.159736	0.90944	0.910194	5.69E-07	
265	0.842026	6.135905	0.905921	0.908984	9.38E-06	
270	0.840774	6.126413	0.90452	0.907789	1.07E-05	
275	0.839904	6.119815	0.903546	0.90661	9.39E-06	
280	0.838825	6.11164	0.902339	0.905445	9.65E-06	
285	0.842222	6.137395	0.906141	0.904295	3.41E-06	
290	0.836544	6.094341	0.899785	0.903159	1.14E-05	
295	0.836388	6.093159	0.89961	0.902038	5.9E-06	
300	0.833828	6.073749	0.896745	0.900931	1.75E-05	
				sum=	0.000469	

Calibratio Curve

a=	0.0327	%	TT (ppm)	abs	
b=	0.1319	0	0	0.1413	0.1413
		0.25	6.7775	0.3323	0.3323
		0.5	13.555	0.5754	0.5754
		0.75	20.3325	0.8239	0.8239
		1	27.11	1.0046	1.0046

pH Before	8.512
pH After	8.493

Correlation Coefficient	R^2
0.997653123	0.995311755



9Jul15_0.7@70%pH8 Accidental Redo						
			flow rate=	0.7		
			volume=	350		
			resid time	482		
			rate const	0.00045		
wavelength=	430					
time (min)	abs		C/Co	model	sum squares	
0	1.071357	9.391269	1	1	1.23E-32	
5	1.076478	9.437699	1.004944	0.997764	5.16E-05	
10	1.064583	9.329852	0.99346	0.995556	4.39E-06	
15	1.07242	9.400907	1.001026	0.993376	5.85E-05	
20	1.061813	9.304744	0.990787	0.991223	1.91E-07	
25	1.061378	9.300795	0.990366	0.989097	1.61E-06	
30	1.058328	9.273148	0.987422	0.986998	1.8E-07	
35	1.064293	9.327229	0.993181	0.984925	6.82E-05	
40	1.059219	9.281227	0.988283	0.982878	2.92E-05	
45	1.052529	9.220572	0.981824	0.980857	9.34E-07	
50	1.046733	9.168025	0.976229	0.978862	6.93E-06	
55	1.057988	9.270064	0.987094	0.976891	0.000104	
60	1.048942	9.188052	0.978361	0.974945	1.17E-05	
65	1.048937	9.188004	0.978356	0.973023	2.84E-05	
70	1.040807	9.114294	0.970507	0.971126	3.82E-07	
75	1.039713	9.104382	0.969452	0.969252	4E-08	
80	1.043311	9.137003	0.972925	0.967402	3.05E-05	
85	1.039915	9.106212	0.969647	0.965575	1.66E-05	
90	1.037692	9.086055	0.9675	0.96377	1.39E-05	
95	1.036777	9.077758	0.966617	0.961989	2.14E-05	
100	1.029341	9.010345	0.959439	0.96023	6.26E-07	
105	1.039207	9.099789	0.968963	0.958493	0.00011	
110	1.02561	8.976519	0.955837	0.956778	8.85E-07	
115	1.026331	8.983055	0.956533	0.955084	2.1E-06	
120	1.027637	8.994891	0.957793	0.953411	1.92E-05	
125	1.024548	8.966894	0.954812	0.95176	9.31E-06	
130	1.02902	9.007431	0.959128	0.950129	8.1E-05	
135	1.01916	8.918038	0.949609	0.948519	1.19E-06	
140	1.028044	8.998581	0.958186	0.946929	0.000127	
145	1.016024	8.889611	0.946582	0.945358	1.5E-06	
150	1.009117	8.826992	0.939915	0.943808	1.52E-05	
155	1.010642	8.840814	0.941387	0.942277	7.93E-07	
160	1.010131	8.836187	0.940894	0.940765	1.66E-08	
165	1.012159	8.854565	0.942851	0.939272	1.28E-05	
170	1.01251	8.857754	0.94319	0.937798	2.91E-05	
175	1.009678	8.832081	0.940457	0.936342	1.69E-05	
180	1.001556	8.758442	0.932615	0.934905	5.24E-06	
185	1.004215	8.782548	0.935182	0.933486	2.88E-06	
190	0.997117	8.718192	0.928329	0.932084	1.41E-05	
195	0.997403	8.720793	0.928606	0.9307	4.38E-06	
200	0.996447	8.71212	0.927683	0.929333	2.72E-06	
205	0.998368	8.729541	0.929538	0.927984	2.41E-06	
210	0.990993	8.662676	0.922418	0.926651	1.79E-05	
215	0.990423	8.657506	0.921867	0.925335	1.2E-05	
220	0.989602	8.650062	0.921075	0.924036	8.77E-06	
225	0.99115	8.664097	0.922569	0.922753	3.38E-08	
230	0.985561	8.61343	0.917174	0.921486	1.86E-05	
235	0.994439	8.69392	0.925745	0.920235	3.04E-05	
240	0.988147	8.636868	0.91967	0.919	4.49E-07	
245	0.986135	8.618632	0.917728	0.91778	2.69E-09	
250	0.990653	8.659595	0.92209	0.916575	3.04E-05	
255	0.975881	8.525668	0.907829	0.915386	5.71E-05	
260	0.977707	8.542223	0.909592	0.914211	2.13E-05	
265	0.972777	8.497529	0.904833	0.913052	6.75E-05	
270	0.97915	8.555303	0.910985	0.911906	8.5E-07	
275	0.975167	8.519196	0.90714	0.910776	1.32E-05	
280	0.978898	8.553015	0.910741	0.909659	1.17E-06	
285	0.97162	8.487035	0.903715	0.908556	2.34E-05	
290	0.970248	8.474594	0.902391	0.907467	2.58E-05	
295	0.970296	8.475032	0.902437	0.906392	1.56E-05	
300	0.973651	8.505446	0.905676	0.90533	1.19E-07	
				sum=	0.001252	

Calibratio Curve

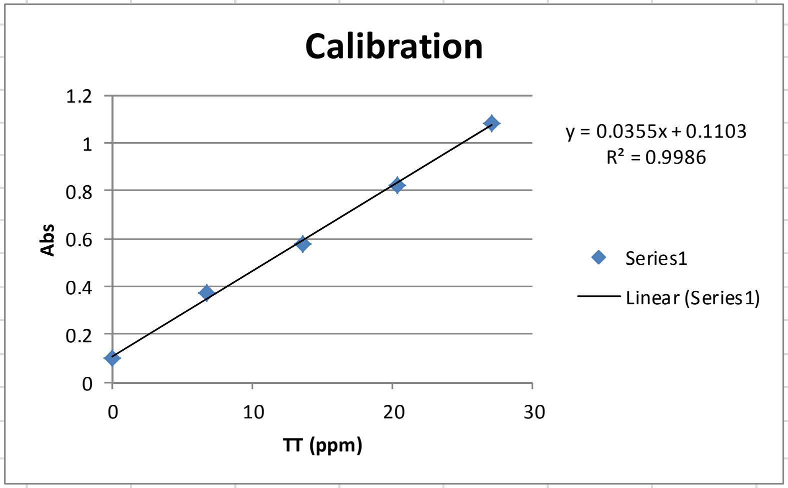
a=	0.0355
b=	0.1103

%	TT (ppm)	abs
0	0	0.1037
0.25	6.7775	0.3718
0.5	13.555	0.5763
0.75	20.3325	0.8238
1	27.11	1.0797

pH Before	8.053
pH After	7.911

Correlation Coefficent
0.991537087

R^2 of Module
0.983145795



10Jul15_0.7@20%pH8						
			flow rate=	0.7		
			volume=	350		
			resid time	482		
			rate const	0.000141		
wavelength=	430					
time (min)	abs		C/Co	model	sum squares	
0	1.066882	10.06832	1	1	0	
5	1.06745	10.07388	1.000552	0.999301	1.57E-06	
10	1.068568	10.08482	1.001639	0.998609	9.18E-06	
15	1.065758	10.05732	0.998908	0.997926	9.64E-07	
20	1.063806	10.03822	0.997011	0.997249	5.7E-08	
25	1.067263	10.07204	1.00037	0.996581	1.44E-05	
30	1.066126	10.06092	0.999265	0.995919	1.12E-05	
35	1.063746	10.03763	0.996952	0.995265	2.85E-06	
40	1.060081	10.00177	0.99339	0.994618	1.51E-06	
45	1.058192	9.983288	0.991555	0.993978	5.87E-06	
50	1.061567	10.01631	0.994835	0.993346	2.22E-06	
55	1.054999	9.952043	0.988451	0.99272	1.82E-05	
60	1.058162	9.982996	0.991526	0.992101	3.31E-07	
65	1.062397	10.02444	0.995642	0.991489	1.72E-05	
70	1.057306	9.974615	0.990693	0.990883	3.61E-08	
75	1.056249	9.964275	0.989666	0.990285	3.82E-07	
80	1.054746	9.949573	0.988206	0.989693	2.21E-06	
85	1.057308	9.974636	0.990695	0.989107	2.52E-06	
90	1.056111	9.962923	0.989532	0.988528	1.01E-06	
95	1.053642	9.938763	0.987132	0.987955	6.77E-07	
100	1.055239	9.954393	0.988685	0.987389	1.68E-06	
105	1.054242	9.944633	0.987715	0.986829	7.87E-07	
110	1.053548	9.937846	0.987041	0.986275	5.88E-07	
115	1.053658	9.93892	0.987148	0.985727	2.02E-06	
120	1.049527	9.898499	0.983133	0.985185	4.21E-06	
125	1.049985	9.902983	0.983579	0.984649	1.15E-06	
130	1.050172	9.90481	0.98376	0.984119	1.29E-07	
135	1.047819	9.881791	0.981474	0.983595	4.5E-06	
140	1.046309	9.867018	0.980007	0.983076	9.42E-06	
145	1.046329	9.867207	0.980025	0.982564	6.44E-06	
150	1.04582	9.862233	0.979531	0.982057	6.38E-06	
155	1.048581	9.889242	0.982214	0.981555	4.34E-07	
160	1.047534	9.878997	0.981196	0.981059	1.88E-08	
165	1.045772	9.86176	0.979484	0.980569	1.18E-06	
170	1.045481	9.85891	0.979201	0.980084	7.79E-07	
175	1.044647	9.850758	0.978392	0.979604	1.47E-06	
180	1.048079	9.884338	0.981727	0.979129	6.75E-06	
185	1.045959	9.863592	0.979666	0.97866	1.01E-06	
190	1.048072	9.884268	0.98172	0.978196	1.24E-05	
195	1.042875	9.833415	0.976669	0.977737	1.14E-06	
200	1.047896	9.882541	0.981548	0.977283	1.82E-05	
205	1.040434	9.809526	0.974296	0.976835	6.44E-06	
210	1.040753	9.812656	0.974607	0.976391	3.18E-06	
215	1.042036	9.825207	0.975854	0.975952	9.55E-09	
220	1.040158	9.806831	0.974029	0.975517	2.22E-06	
225	1.041812	9.82301	0.975636	0.975088	3E-07	
230	1.041647	9.821401	0.975476	0.974663	6.6E-07	
235	1.038681	9.79238	0.972593	0.974243	2.72E-06	
240	1.037735	9.783124	0.971674	0.973828	4.64E-06	
245	1.04106	9.81566	0.974906	0.973417	2.22E-06	
250	1.039045	9.795938	0.972947	0.973011	4.09E-09	
255	1.040993	9.814996	0.97484	0.972609	4.98E-06	
260	1.037223	9.778107	0.971176	0.972212	1.07E-06	
265	1.038103	9.786721	0.972031	0.971819	4.53E-08	
270	1.038829	9.793827	0.972737	0.97143	1.71E-06	
275	1.035323	9.759516	0.969329	0.971045	2.95E-06	
280	1.036628	9.772286	0.970598	0.970665	4.58E-09	
285	1.03469	9.753332	0.968715	0.970289	2.48E-06	
290	1.039991	9.805199	0.973867	0.969918	1.56E-05	
295	1.034408	9.750567	0.968441	0.96955	1.23E-06	
300	1.037601	9.781805	0.971543	0.969186	5.56E-06	
				sum=	0.000231	

Calibratio Curve

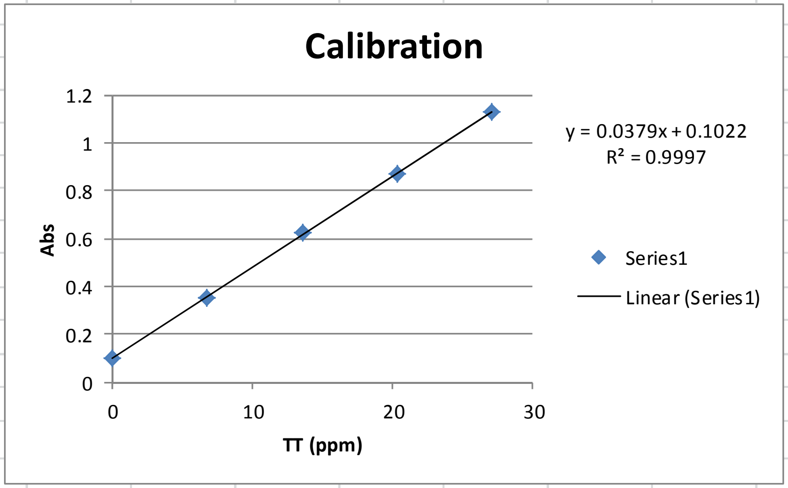
a=	0.0379
b=	0.1022

%	TT (ppm)	abs
0	0	0.1015
0.25	6.7775	0.3529
0.5	13.555	0.6283
0.75	20.3325	0.8678
1	27.11	1.1274

pH Before	8.15
pH After	7.984

Correlation Coefficent
0.978734332

R^2 of Module
0.957920892



13Jul15_0.7@70%pH7					
			flow rate=	0.7	
			volume=	350	
			resid time	482	
			rate const	0.000511	
wavelength=	430				
time (min)	abs		C/Co	model	sum squares
0	1.127297	8.358103	1	1	0
5	1.1266	8.352762	0.999361	0.997462	3.6E-06
10	1.123517	8.32912	0.996532	0.994958	2.48E-06
15	1.123365	8.327953	0.996393	0.992485	1.53E-05
20	1.120969	8.30958	0.994195	0.990044	1.72E-05
25	1.116045	8.271814	0.989676	0.987634	4.17E-06
30	1.118339	8.289413	0.991782	0.985256	4.26E-05
35	1.115987	8.271371	0.989623	0.982907	4.51E-05
40	1.105952	8.194419	0.980416	0.980589	3E-08
45	1.107973	8.209915	0.98227	0.978301	1.58E-05
50	1.097724	8.131319	0.972867	0.976042	1.01E-05
55	1.098435	8.13677	0.973519	0.973813	8.63E-08
60	1.09797	8.133203	0.973092	0.971611	2.19E-06
65	1.091843	8.086222	0.967471	0.969439	3.87E-06
70	1.091707	8.08518	0.967346	0.967294	2.78E-09
75	1.087633	8.053932	0.963608	0.965176	2.46E-06
80	1.091654	8.084768	0.967297	0.963086	1.77E-05
85	1.083282	8.020566	0.959616	0.961023	1.98E-06
90	1.079975	7.995204	0.956581	0.958986	5.78E-06
95	1.079214	7.989368	0.955883	0.956975	1.19E-06
100	1.076547	7.968917	0.953436	0.95499	2.41E-06
105	1.081324	8.005555	0.95782	0.953031	2.29E-05
110	1.07645	7.968174	0.953347	0.951097	5.07E-06
115	1.067415	7.898891	0.945058	0.949187	1.71E-05
120	1.072539	7.938183	0.949759	0.947302	6.04E-06
125	1.065826	7.886702	0.9436	0.945442	3.39E-06
130	1.062752	7.863126	0.940779	0.943605	7.99E-06
135	1.064926	7.879803	0.942774	0.941792	9.65E-07
140	1.056231	7.81312	0.934796	0.940002	2.71E-05
145	1.064671	7.877848	0.94254	0.938235	1.85E-05
150	1.056672	7.816507	0.935201	0.936491	1.66E-06
155	1.054234	7.797803	0.932963	0.934769	3.26E-06
160	1.053548	7.79255	0.932335	0.933069	5.4E-07
165	1.061103	7.850483	0.939266	0.931391	6.2E-05
170	1.051631	7.777847	0.930576	0.929735	7.06E-07
175	1.047657	7.74737	0.926929	0.9281	1.37E-06
180	1.046672	7.73982	0.926026	0.926486	2.12E-07
185	1.044408	7.722456	0.923948	0.924893	8.92E-07
190	1.039998	7.688634	0.919902	0.92332	1.17E-05
195	1.041833	7.70271	0.921586	0.921767	3.29E-08
200	1.03743	7.668938	0.917545	0.920235	7.23E-06
205	1.042751	7.709744	0.922428	0.918722	1.37E-05
210	1.037382	7.66857	0.917501	0.917228	7.46E-08
215	1.032413	7.630464	0.912942	0.915754	7.91E-06
220	1.031074	7.620202	0.911714	0.914298	6.68E-06
225	1.033664	7.640065	0.914091	0.912862	1.51E-06
230	1.026413	7.584455	0.907437	0.911443	1.6E-05
235	1.03648	7.661659	0.916674	0.910043	4.4E-05
240	1.025751	7.57938	0.90683	0.908661	3.35E-06
245	1.024019	7.566093	0.905241	0.907297	4.23E-06
250	1.024329	7.568471	0.905525	0.90595	1.81E-07
255	1.019777	7.533565	0.901349	0.904621	1.07E-05
260	1.021593	7.547493	0.903015	0.903308	8.58E-08
265	1.024349	7.568628	0.905544	0.902013	1.25E-05
270	1.018423	7.523183	0.900107	0.900734	3.93E-07
275	1.023699	7.563644	0.904947	0.899471	3E-05
280	1.014235	7.491069	0.896264	0.898225	3.84E-06
285	1.019441	7.530993	0.901041	0.896994	1.64E-05
290	1.013931	7.488738	0.895985	0.89578	4.22E-08
295	1.010089	7.459269	0.89246	0.894581	4.5E-06
300	1.009663	7.456001	0.892069	0.893398	1.77E-06
				sum=	0.000571

Calibratio Curve

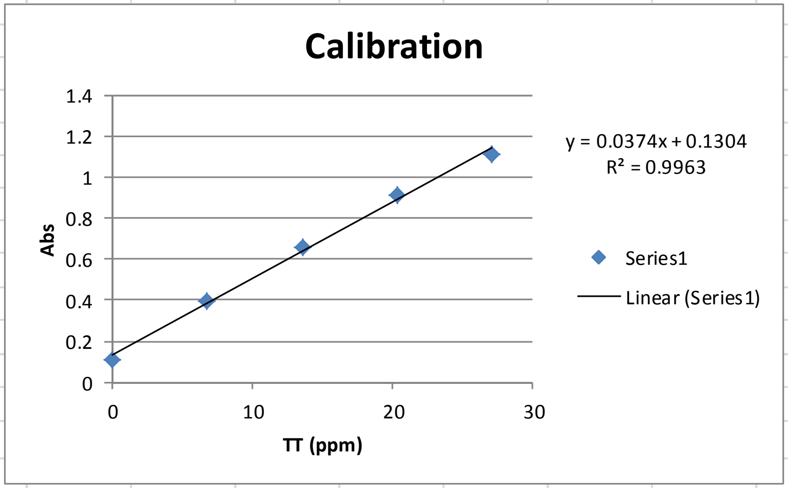
a= 0.0374
b= 0.1304

%	TT (ppm)	abs	
0	0	0.1074	0.1074
0.25	6.7775	0.3932	0.3932
0.5	13.555	0.6577	0.6577
0.75	20.3325	0.9116	0.9116
1	27.11	1.1144	1.1144

pH Before	7.778
pH After	7.264

Correlation Coefficent
0.995702567

R^2 of Module
0.991423603



14Jul15_0.7@100%pH7H2O2Ctrl					
			flow rate=	0.7	
			volume=	350	
			resid time	482	
			rate const	-4.8E-05	
wavelength=	430				
time (min)	abs		C/Co	model	sum squares
0	1.122369	9.240966	1	1	0
5	1.124769	9.2615	1.002222	1.000238	3.94E-06
10	1.124286	9.257364	1.001774	1.000473	1.69E-06
15	1.122663	9.243482	1.000272	1.000706	1.88E-07
20	1.122574	9.242719	1.00019	1.000937	5.59E-07
25	1.122326	9.240597	0.99996	1.001166	1.45E-06
30	1.128052	9.289578	1.00526	1.001392	1.5E-05
35	1.120137	9.221872	0.997934	1.001615	1.36E-05
40	1.127716	9.286707	1.00495	1.001837	9.69E-06
45	1.122494	9.242039	1.000116	1.002056	3.76E-06
50	1.126376	9.275242	1.003709	1.002273	2.06E-06
55	1.123865	9.253765	1.001385	1.002488	1.22E-06
60	1.124652	9.260499	1.002114	1.002701	3.45E-07
65	1.125034	9.263761	1.002467	1.002912	1.98E-07
70	1.126515	9.276431	1.003838	1.00312	5.15E-07
75	1.125133	9.264612	1.002559	1.003327	5.9E-07
80	1.125053	9.263925	1.002484	1.003531	1.1E-06
85	1.122693	9.243738	1.0003	1.003733	1.18E-05
90	1.126802	9.278885	1.004103	1.003933	2.89E-08
95	1.131019	9.314962	1.008007	1.004132	1.5E-05
100	1.124052	9.255362	1.001558	1.004328	7.67E-06
105	1.124213	9.256738	1.001707	1.004522	7.93E-06
110	1.125966	9.271736	1.00333	1.004714	1.92E-06
115	1.126138	9.273209	1.003489	1.004905	2E-06
120	1.125806	9.270367	1.003182	1.005093	3.65E-06
125	1.129217	9.299543	1.006339	1.005279	1.12E-06
130	1.124727	9.261142	1.002183	1.005464	1.08E-05
135	1.131463	9.31876	1.008418	1.005647	7.68E-06
140	1.1273	9.283151	1.004565	1.005828	1.59E-06
145	1.12937	9.300852	1.006481	1.006007	2.24E-07
150	1.129982	9.306091	1.007047	1.006184	7.45E-07
155	1.128404	9.292594	1.005587	1.00636	5.97E-07
160	1.134	9.340466	1.010767	1.006533	1.79E-05
165	1.124939	9.262949	1.002379	1.006705	1.87E-05
170	1.125991	9.271953	1.003353	1.006876	1.24E-05
175	1.127111	9.281532	1.00439	1.007044	7.05E-06
180	1.128644	9.294644	1.005809	1.007211	1.97E-06
185	1.12807	9.289734	1.005277	1.007376	4.4E-06
190	1.130624	9.311586	1.007642	1.00754	1.05E-08
195	1.13548	9.353125	1.012137	1.007701	1.97E-05
200	1.13126	9.317024	1.008231	1.007862	1.36E-07
205	1.12994	9.305729	1.007008	1.00802	1.02E-06
210	1.137203	9.367864	1.013732	1.008177	3.09E-05
215	1.134822	9.347493	1.011528	1.008333	1.02E-05
220	1.128847	9.296382	1.005997	1.008486	6.2E-06
225	1.131729	9.321039	1.008665	1.008639	6.95E-10
230	1.131298	9.317347	1.008265	1.008789	2.75E-07
235	1.131314	9.317488	1.008281	1.008939	4.33E-07
240	1.127706	9.286617	1.00494	1.009086	1.72E-05
245	1.133226	9.333844	1.010051	1.009233	6.69E-07
250	1.134227	9.342401	1.010977	1.009377	2.56E-06
255	1.134057	9.340948	1.010819	1.009521	1.69E-06
260	1.133604	9.337077	1.010401	1.009662	5.45E-07
265	1.133405	9.335374	1.010216	1.009803	1.71E-07
270	1.134779	9.34713	1.011488	1.009942	2.39E-06
275	1.132816	9.330337	1.009671	1.01008	1.67E-07
280	1.133189	9.333527	1.010016	1.010216	3.97E-08
285	1.136019	9.357731	1.012636	1.010351	5.22E-06
290	1.133089	9.33267	1.009924	1.010484	3.14E-07
295	1.135788	9.355758	1.012422	1.010616	3.26E-06
300	1.133579	9.336861	1.010377	1.010747	1.37E-07
				sum=	0.000294

Calibratio Curve

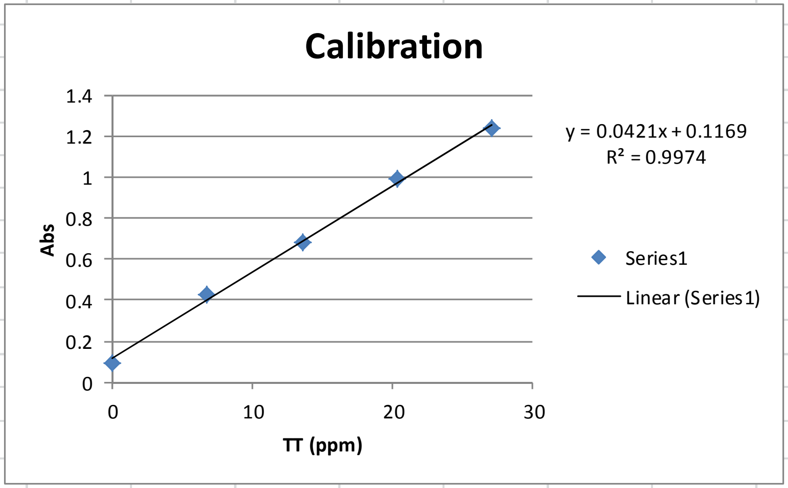
a=	0.0421
b=	0.1169

%	TT (ppm)	abs
0	0	0.0939
0.25	6.7775	0.4264
0.5	13.555	0.6853
0.75	20.3325	0.9945
1	27.11	1.2353

pH Before	7.451
pH After	6.52

Correlation Coefficent
0.8340118

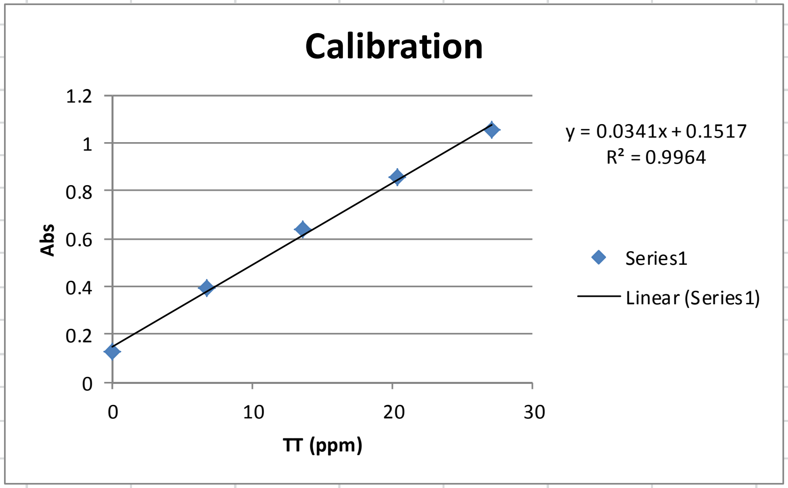
R^2 of Module
0.695575683



15Jul15 0.7@0%pH8						
			flow rate=	0.7		
			volume=	350		
			resid time	482		
			rate const	9.88E-06		
wavelength=	430					
time (min)	abs		C/Co	model	sum squares	
0	1.032964	6.584469	1	1	0	
5	1.027988	6.551666	0.995018	0.999951	2.43E-05	
10	1.027815	6.550527	0.994845	0.999902	2.56E-05	
15	1.029322	6.560464	0.996354	0.999854	1.22E-05	
20	1.029073	6.558818	0.996104	0.999806	1.37E-05	
25	1.030498	6.568213	0.997531	0.999759	4.96E-06	
30	1.030018	6.565047	0.99705	0.999713	7.09E-06	
35	1.030133	6.565807	0.997166	0.999666	6.25E-06	
40	1.031441	6.574428	0.998475	0.999621	1.31E-06	
45	1.030505	6.568259	0.997538	0.999576	4.15E-06	
50	1.028054	6.5521	0.995084	0.999531	1.98E-05	
55	1.034395	6.5939	1.001432	0.999487	3.79E-06	
60	1.035699	6.602495	1.002738	0.999443	1.09E-05	
65	1.031571	6.575289	0.998606	0.999399	6.3E-07	
70	1.030799	6.570198	0.997833	0.999356	2.32E-06	
75	1.030987	6.571434	0.99802	0.999314	1.67E-06	
80	1.032289	6.580018	0.999324	0.999272	2.71E-09	
85	1.028216	6.553174	0.995247	0.99923	1.59E-05	
90	1.028435	6.554614	0.995466	0.999189	1.39E-05	
95	1.027328	6.547319	0.994358	0.999148	2.29E-05	
100	1.029095	6.558962	0.996126	0.999108	8.89E-06	
105	1.031768	6.576584	0.998802	0.999068	7.06E-08	
110	1.030516	6.568332	0.997549	0.999029	2.19E-06	
115	1.028942	6.557955	0.995973	0.99899	9.1E-06	
120	1.030314	6.567001	0.997347	0.998951	2.57E-06	
125	1.03199	6.578049	0.999025	0.998913	1.26E-08	
130	1.030079	6.565448	0.997111	0.998875	3.11E-06	
135	1.031352	6.573842	0.998386	0.998837	2.04E-07	
140	1.030528	6.568409	0.997561	0.9988	1.54E-06	
145	1.035907	6.60387	1.002947	0.998763	1.75E-05	
150	1.030297	6.566889	0.99733	0.998727	1.95E-06	
155	1.028803	6.557041	0.995834	0.998691	8.16E-06	
160	1.02956	6.562028	0.996592	0.998656	4.26E-06	
165	1.031895	6.577421	0.99893	0.99862	9.56E-08	
170	1.032304	6.580117	0.999339	0.998586	5.68E-07	
175	1.034119	6.592082	1.001156	0.998551	6.79E-06	
180	1.028755	6.556727	0.995787	0.998517	7.45E-06	
185	1.030184	6.566145	0.997217	0.998483	1.6E-06	
190	1.028857	6.557393	0.995888	0.99845	6.56E-06	
195	1.032383	6.580642	0.999419	0.998417	1E-06	
200	1.029263	6.560073	0.996295	0.998384	4.36E-06	
205	1.033191	6.585965	1.000227	0.998351	3.52E-06	
210	1.02989	6.564206	0.996923	0.998319	1.95E-06	
215	1.029156	6.559365	0.996187	0.998288	4.41E-06	
220	1.03164	6.575741	0.998674	0.998256	1.75E-07	
225	1.03172	6.576267	0.998754	0.998225	2.8E-07	
230	1.030824	6.570361	0.997857	0.998194	1.14E-07	
235	1.030044	6.565218	0.997076	0.998164	1.18E-06	
240	1.032248	6.579747	0.999283	0.998134	1.32E-06	
245	1.031637	6.57572	0.998671	0.998104	3.22E-07	
250	1.030129	6.565778	0.997161	0.998075	8.34E-07	
255	1.031917	6.577567	0.998952	0.998045	8.21E-07	
260	1.032271	6.579899	0.999306	0.998017	1.66E-06	
265	1.032304	6.580117	0.999339	0.997988	1.83E-06	
270	1.034697	6.595895	1.001735	0.99796	1.43E-05	
275	1.034623	6.595405	1.001661	0.997932	1.39E-05	
280	1.032794	6.583349	0.99983	0.997904	3.71E-06	
285	1.033015	6.584806	1.000051	0.997877	4.73E-06	
290	1.032575	6.581903	0.99961	0.997849	3.1E-06	
295	1.034345	6.593573	1.001383	0.997823	1.27E-05	
300	1.03047	6.568031	0.997503	0.997796	8.56E-08	
				sum=	0.00035	

Calibratio Curve

a=	0.0341	%	TT (ppm)	abs	
b=	0.1517	0	0	0.1285	0.1285
		0.25	6.7775	0.3935	0.3935
		0.5	13.555	0.6383	0.6383
		0.75	20.3325	0.8542	0.8542
		1	27.11	1.0522	1.0522



pH Before	8.164
pH After	8.059

Correlation Coefficent
-0.342715353

R^2 of Module
0.117453813

16Jul15_0.7@100%pH7					
			flow rate=	0.7	
			volume=	350	
			resid time	482	
			rate const	9.88E-06	
wavelength=	430				
time (min)	abs		C/Co	model	sum squares
0	1.148655	36.44917	1	1	0
5	1.147227	36.40219	0.998711	0.999951	1.54E-06
10	1.147631	36.4155	0.999076	0.999902	6.82E-07
15	1.152025	36.56004	1.003042	0.999854	1.02E-05
20	1.152366	36.57126	1.00335	0.999806	1.26E-05
25	1.153865	36.62055	1.004702	0.999759	2.44E-05
30	1.151102	36.52966	1.002208	0.999713	6.23E-06
35	1.149988	36.49304	1.001204	0.999666	2.36E-06
40	1.150893	36.5228	1.00202	0.999621	5.76E-06
45	1.142974	36.2623	0.994873	0.999576	2.21E-05
50	1.144872	36.32474	0.996586	0.999531	8.67E-06
55	1.145516	36.34591	0.997167	0.999487	5.38E-06
60	1.15245	36.574	1.003425	0.999443	1.59E-05
65	1.145917	36.3591	0.997529	0.999399	3.5E-06
70	1.148742	36.45203	1.000079	0.999356	5.22E-07
75	1.14745	36.40954	0.998913	0.999314	1.61E-07
80	1.147005	36.39489	0.998511	0.999272	5.79E-07
85	1.145357	36.3407	0.997024	0.99923	4.87E-06
90	1.152532	36.57671	1.003499	0.999189	1.86E-05
95	1.150652	36.51486	1.001802	0.999148	7.04E-06
100	1.154567	36.64366	1.005336	0.999108	3.88E-05
105	1.147133	36.39913	0.998627	0.999068	1.94E-07
110	1.14633	36.3727	0.997902	0.999029	1.27E-06
115	1.150652	36.51487	1.001802	0.99899	7.91E-06
120	1.144896	36.32554	0.996608	0.998951	5.49E-06
125	1.147619	36.41509	0.999065	0.998913	2.33E-08
130	1.149819	36.48748	1.001051	0.998875	4.74E-06
135	1.14695	36.39308	0.998461	0.998837	1.41E-07
140	1.14482	36.32303	0.996539	0.9988	5.11E-06
145	1.147915	36.42482	0.999332	0.998763	3.23E-07
150	1.146639	36.38285	0.998181	0.998727	2.99E-07
155	1.151927	36.55682	1.002954	0.998691	1.82E-05
160	1.151135	36.53074	1.002238	0.998656	1.28E-05
165	1.149057	36.46241	1.000363	0.99862	3.04E-06
170	1.150913	36.52345	1.002038	0.998586	1.19E-05
175	1.146207	36.36864	0.997791	0.998551	5.78E-07
180	1.157181	36.72962	1.007694	0.998517	8.42E-05
185	1.149079	36.46312	1.000383	0.998483	3.61E-06
190	1.151374	36.53863	1.002454	0.99845	1.6E-05
195	1.146112	36.36554	0.997706	0.998417	5.05E-07
200	1.144924	36.32646	0.996633	0.998384	3.06E-06
205	1.149696	36.48343	1.00094	0.998351	6.7E-06
210	1.149293	36.47017	1.000576	0.998319	5.09E-06
215	1.150159	36.49865	1.001358	0.998288	9.42E-06
220	1.150695	36.51627	1.001841	0.998256	1.29E-05
225	1.148021	36.42833	0.999428	0.998225	1.45E-06
230	1.150843	36.52116	1.001975	0.998194	1.43E-05
235	1.147017	36.3953	0.998522	0.998164	1.28E-07
240	1.151239	36.53418	1.002332	0.998134	1.76E-05
245	1.15491	36.65493	1.005645	0.998104	5.69E-05
250	1.153899	36.62166	1.004733	0.998075	4.43E-05
255	1.146356	36.37356	0.997926	0.998045	1.44E-08
260	1.145887	36.35814	0.997503	0.998017	2.64E-07
265	1.154231	36.63259	1.005032	0.997988	4.96E-05
270	1.15017	36.49902	1.001368	0.99796	1.16E-05
275	1.149101	36.46385	1.000403	0.997932	6.11E-06
280	1.150671	36.51551	1.00182	0.997904	1.53E-05
285	1.153143	36.5968	1.00405	0.997877	3.81E-05
290	1.149215	36.46758	1.000505	0.997849	7.05E-06
295	1.150167	36.49893	1.001365	0.997823	1.25E-05
300	1.150449	36.50818	1.001619	0.997796	1.46E-05
				sum=	0.000693

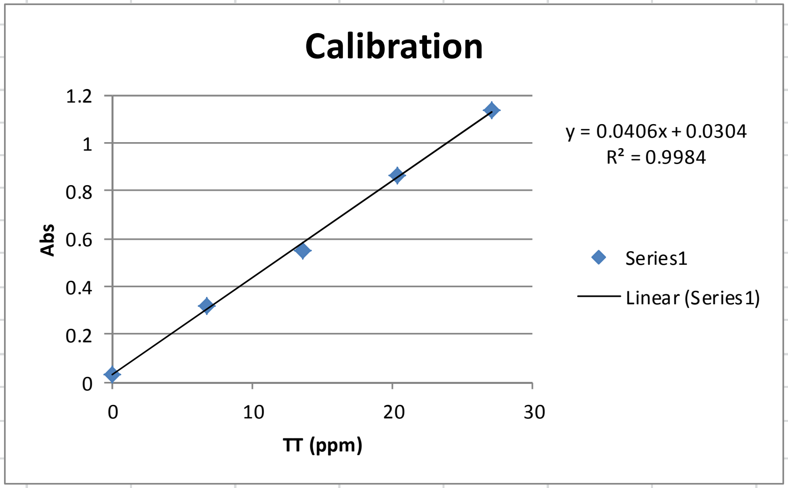
Calibratio Curve	
a=	0.0406
b=	0.0304

%	TT (ppm)	abs	
0	0	0.0329	0.0329
0.25	6.7775	0.3192	0.3192
0.5	13.555	0.5505	0.5505
0.75	20.3325	0.8662	0.8662
1	27.11	1.1354	1.1354

pH Before	7.896
pH After	7.684

Correlation Coefficent
-0.164422772

R^2 of Module
0.027034848



17Jul15_0.7@100%pH6H2O2Ctrl					
			flow rate=	0.7	
			volume=	350	
			resid time	482	
			rate const	-2.4E-05	
wavelength=	430				
time (min)	abs		C/Co	model	sum squares
0	1.219664	9.99544	1	1	0
5	1.220991	10.00672	1.001129	1.00012	1.02E-06
10	1.216736	9.970548	0.99751	1.000238	7.44E-06
15	1.22108	10.00749	1.001205	1.000355	7.23E-07
20	1.222512	10.01966	1.002423	1.000471	3.81E-06
25	1.224149	10.03358	1.003816	1.000586	1.04E-05
30	1.218693	9.987181	0.999174	1.000699	2.33E-06
35	1.224369	10.03545	1.004003	1.000812	1.02E-05
40	1.222574	10.02018	1.002475	1.000923	2.41E-06
45	1.223897	10.03144	1.003601	1.001033	6.6E-06
50	1.219209	9.991574	0.999613	1.001142	2.34E-06
55	1.221074	10.00744	1.0012	1.00125	2.48E-09
60	1.221347	10.00975	1.001432	1.001357	5.67E-09
65	1.220108	9.999218	1.000378	1.001462	1.18E-06
70	1.218392	9.984628	0.998918	1.001567	7.02E-06
75	1.220226	10.00022	1.000478	1.001671	1.42E-06
80	1.219218	9.991646	0.99962	1.001773	4.63E-06
85	1.222747	10.02166	1.002623	1.001875	5.6E-07
90	1.223442	10.02756	1.003214	1.001975	1.53E-06
95	1.220313	10.00096	1.000553	1.002074	2.32E-06
100	1.219841	9.996943	1.00015	1.002173	4.09E-06
105	1.219205	9.991539	0.99961	1.00227	7.08E-06
110	1.225183	10.04237	1.004695	1.002367	5.42E-06
115	1.217303	9.975369	0.997992	1.002462	2E-05
120	1.220792	10.00503	1.00096	1.002556	2.55E-06
125	1.223385	10.02708	1.003165	1.00265	2.66E-07
130	1.221247	10.0089	1.001347	1.002742	1.95E-06
135	1.219708	9.995817	1.000038	1.002834	7.82E-06
140	1.219231	9.991764	0.999632	1.002925	1.08E-05
145	1.221147	10.00805	1.001262	1.003014	3.07E-06
150	1.220875	10.00574	1.001031	1.003103	4.3E-06
155	1.226355	10.05234	1.005693	1.003191	6.26E-06
160	1.22249	10.01947	1.002405	1.003278	7.63E-07
165	1.221625	10.01212	1.001668	1.003364	2.88E-06
170	1.222907	10.02302	1.002759	1.003449	4.76E-07
175	1.220419	10.00186	1.000642	1.003534	8.36E-06
180	1.223402	10.02723	1.00318	1.003617	1.91E-07
185	1.222823	10.02231	1.002688	1.0037	1.02E-06
190	1.222456	10.01919	1.002376	1.003782	1.98E-06
195	1.22335	10.02679	1.003136	1.003863	5.28E-07
200	1.224047	10.03271	1.003729	1.003943	4.57E-08
205	1.227199	10.05952	1.006411	1.004022	5.71E-06
210	1.224787	10.039	1.004358	1.004101	6.63E-08
215	1.221443	10.01057	1.001514	1.004178	7.1E-06
220	1.223971	10.03207	1.003665	1.004255	3.49E-07
225	1.227032	10.0581	1.006269	1.004331	3.75E-06
230	1.226483	10.05343	1.005802	1.004407	1.95E-06
235	1.227157	10.05916	1.006375	1.004481	3.59E-06
240	1.230831	10.0904	1.009501	1.004555	2.45E-05
245	1.228028	10.06657	1.007116	1.004628	6.19E-06
250	1.225157	10.04215	1.004673	1.004701	7.57E-10
255	1.225779	10.04744	1.005202	1.004772	1.85E-07
260	1.228406	10.06978	1.007437	1.004843	6.73E-06
265	1.227172	10.05929	1.006388	1.004913	2.17E-06
270	1.222178	10.01682	1.002139	1.004983	8.09E-06
275	1.225338	10.04369	1.004827	1.005051	5.04E-08
280	1.225498	10.04505	1.004964	1.005119	2.43E-08
285	1.22537	10.04396	1.004854	1.005187	1.1E-07
290	1.229901	10.08249	1.008709	1.005253	1.19E-05
295	1.225596	10.04588	1.005047	1.005319	7.43E-08
300	1.227913	10.06559	1.007018	1.005385	2.67E-06
				sum=	0.000241

Calibratio Curve

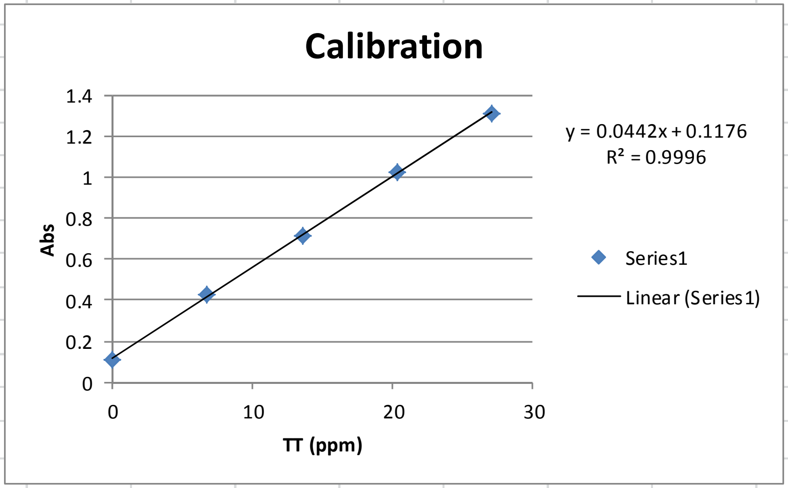
a=	0.0442
b=	0.1176

%	TT (ppm)	abs
0	0	0.1065
0.25	6.7775	0.4313
0.5	13.555	0.7165
0.75	20.3325	1.0199
1	27.11	1.3106

pH Before	6.559
pH After	6.49

Correlation Coefficent
0.671334548

R^2 of Module
0.450690076



21Jul15 0.7@5%pH8					
			flow rate=	0.7	
			volume=	350	
			resid time	482	
			rate const	-3.8E-06	
wavelength=	430				
time (min)	abs		C/Co	model	sum squares
0	0.919907	17.13141	1	1	0
5	0.919112	17.11607	0.999105	1.000019	8.36E-07
10	0.919111	17.11605	0.999103	1.000038	8.73E-07
15	0.918874	17.11147	0.998836	1.000056	1.49E-06
20	0.919696	17.12733	0.999762	1.000074	9.76E-08
25	0.919887	17.13102	0.999977	1.000093	1.33E-08
30	0.916442	17.06452	0.996095	1.000111	1.61E-05
35	0.919867	17.13064	0.999955	1.000128	2.99E-08
40	0.9191	17.11584	0.999091	1.000146	1.11E-06
45	0.919644	17.12633	0.999704	1.000163	2.11E-07
50	0.92049	17.14267	1.000657	1.00018	2.27E-07
55	0.918074	17.09602	0.997934	1.000198	5.12E-06
60	0.920312	17.13922	1.000456	1.000214	5.84E-08
65	0.919912	17.1315	1.000005	1.000231	5.1E-08
70	0.920966	17.15185	1.001193	1.000248	8.95E-07
75	0.918707	17.10825	0.998648	1.000264	2.61E-06
80	0.921348	17.15923	1.001624	1.00028	1.81E-06
85	0.91785	17.0917	0.997682	1.000296	6.83E-06
90	0.919277	17.11925	0.99929	1.000312	1.04E-06
95	0.917546	17.08583	0.997339	1.000328	8.93E-06
100	0.919092	17.11568	0.999082	1.000343	1.59E-06
105	0.923484	17.20047	1.004031	1.000359	1.35E-05
110	0.9219	17.16988	1.002246	1.000374	3.51E-06
115	0.921099	17.15443	1.001344	1.000389	9.12E-07
120	0.92163	17.16467	1.001942	1.000404	2.37E-06
125	0.920499	17.14284	1.000667	1.000418	6.19E-08
130	0.918659	17.10731	0.998594	1.000433	3.38E-06
135	0.919477	17.1231	0.999515	1.000447	8.69E-07
140	0.918395	17.10222	0.998296	1.000462	4.69E-06
145	0.918912	17.1122	0.998879	1.000476	2.55E-06
150	0.919503	17.12362	0.999545	1.00049	8.93E-07
155	0.919258	17.11889	0.999269	1.000504	1.52E-06
160	0.919876	17.1308	0.999965	1.000517	3.06E-07
165	0.91886	17.11119	0.99882	1.000531	2.93E-06
170	0.91968	17.12702	0.999744	1.000544	6.4E-07
175	0.918688	17.10787	0.998626	1.000558	3.73E-06
180	0.916786	17.07116	0.996483	1.000571	1.67E-05
185	0.923407	17.19899	1.003945	1.000584	1.13E-05
190	0.918687	17.10787	0.998626	1.000597	3.88E-06
195	0.923699	17.20461	1.004273	1.00061	1.34E-05
200	0.922243	17.17651	1.002633	1.000622	4.04E-06
205	0.918553	17.10528	0.998475	1.000635	4.67E-06
210	0.919148	17.11676	0.999145	1.000647	2.26E-06
215	0.920675	17.14624	1.000866	1.000659	4.26E-08
220	0.919341	17.12048	0.999362	1.000671	1.71E-06
225	0.920077	17.13469	1.000191	1.000683	2.42E-07
230	0.917944	17.09352	0.997788	1.000695	8.45E-06
235	0.920228	17.1376	1.000361	1.000707	1.19E-07
240	0.921788	17.16771	1.002119	1.000719	1.96E-06
245	0.924806	17.22599	1.005521	1.00073	2.3E-05
250	0.918449	17.10327	0.998357	1.000741	5.68E-06
255	0.917183	17.07883	0.996931	1.000753	1.46E-05
260	0.920958	17.1517	1.001185	1.000764	1.77E-07
265	0.920651	17.14577	1.000839	1.000775	4.07E-09
270	0.921141	17.15523	1.00139	1.000786	3.66E-07
275	0.922384	17.17923	1.002792	1.000797	3.98E-06
280	0.923795	17.20647	1.004382	1.000807	1.28E-05
285	0.921688	17.16579	1.002007	1.000818	1.41E-06
290	0.924598	17.22197	1.005286	1.000828	1.99E-05
295	0.920918	17.15093	1.00114	1.000839	9.06E-08
300	0.921532	17.16278	1.001831	1.000849	9.65E-07
				sum=	0.000243

Calibratio Curve

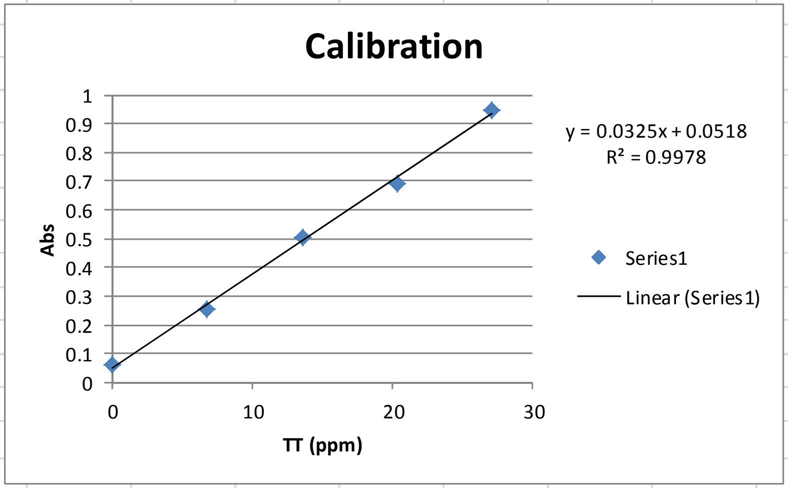
a=	0.0325
b=	0.0518

%	TT (ppm)	abs
0	0	0.0609
0.25	6.7775	0.2569
0.5	13.555	0.5068
0.75	20.3325	0.6921
1	27.11	0.9445

pH Before	8.796
pH After	8.301

Correlation Coefficent
0.35421266

R^2 of Module
0.125466608



21Jul15_0.7@70%pH9						
			flow rate=	0.7		
			volume=	350		
			resid time	482		
			rate const	0.000263		
wavelength=	430					
time (min)	abs		C/Co	model	sum squares	
0	0.908631	20.81308	1	1	0	
5	0.909805	20.84097	1.00134	0.998694	7E-06	
10	0.906645	20.76592	0.997734	0.997403	1.1E-07	
15	0.908959	20.82087	1.000374	0.996128	1.8E-05	
20	0.906432	20.76086	0.997491	0.994867	6.89E-06	
25	0.906279	20.75723	0.997317	0.993621	1.37E-05	
30	0.903117	20.68212	0.993708	0.992389	1.74E-06	
35	0.900532	20.6207	0.990757	0.991171	1.72E-07	
40	0.905263	20.73308	0.996156	0.989968	3.83E-05	
45	0.900422	20.61809	0.990632	0.988779	3.43E-06	
50	0.898675	20.57659	0.988638	0.987603	1.07E-06	
55	0.897854	20.55709	0.987701	0.986441	1.59E-06	
60	0.898898	20.58191	0.988893	0.985293	1.3E-05	
65	0.897537	20.54957	0.987339	0.984158	1.01E-05	
70	0.893284	20.44855	0.982486	0.983036	3.03E-07	
75	0.895073	20.49105	0.984528	0.981927	6.76E-06	
80	0.896427	20.5232	0.986072	0.980831	2.75E-05	
85	0.893811	20.46107	0.983087	0.979748	1.11E-05	
90	0.893771	20.46012	0.983042	0.978678	1.9E-05	
95	0.890278	20.37716	0.979056	0.977619	2.06E-06	
100	0.888563	20.33641	0.977098	0.976574	2.75E-07	
105	0.887028	20.29994	0.975346	0.97554	3.77E-08	
110	0.890295	20.37756	0.979075	0.974518	2.08E-05	
115	0.885664	20.26756	0.97379	0.973508	7.92E-08	
120	0.887024	20.29985	0.975341	0.97251	8.01E-06	
125	0.884284	20.23478	0.972215	0.971524	4.77E-07	
130	0.886953	20.29818	0.975261	0.970549	2.22E-05	
135	0.882287	20.18734	0.969935	0.969585	1.23E-07	
140	0.883399	20.21375	0.971205	0.968633	6.62E-06	
145	0.878521	20.09788	0.965637	0.967691	4.22E-06	
150	0.879859	20.12966	0.967164	0.966761	1.63E-07	
155	0.880304	20.14024	0.967672	0.965841	3.35E-06	
160	0.878055	20.08682	0.965106	0.964932	3.03E-08	
165	0.878038	20.08641	0.965086	0.964033	1.11E-06	
170	0.875997	20.03794	0.962757	0.963145	1.51E-07	
175	0.874457	20.00135	0.960999	0.962268	1.61E-06	
180	0.874876	20.01131	0.961478	0.9614	5.97E-09	
185	0.877131	20.06487	0.964051	0.960543	1.23E-05	
190	0.872262	19.94921	0.958494	0.959695	1.44E-06	
195	0.872968	19.96599	0.9593	0.958858	1.96E-07	
200	0.870661	19.91118	0.956667	0.95803	1.86E-06	
205	0.87056	19.90878	0.956552	0.957212	4.36E-07	
210	0.872261	19.94918	0.958493	0.956403	4.37E-06	
215	0.868608	19.86242	0.954324	0.955604	1.64E-06	
220	0.86851	19.8601	0.954213	0.954814	3.61E-07	
225	0.869756	19.88968	0.955634	0.954033	2.56E-06	
230	0.864986	19.77639	0.95019	0.953261	9.43E-06	
235	0.866487	19.81204	0.951903	0.952498	3.54E-07	
240	0.865188	19.7812	0.950422	0.951744	1.75E-06	
245	0.864756	19.77093	0.949928	0.950999	1.15E-06	
250	0.862065	19.707	0.946856	0.950262	1.16E-05	
255	0.859516	19.64647	0.943948	0.949534	3.12E-05	
260	0.86223	19.71093	0.947045	0.948815	3.13E-06	
265	0.864209	19.75794	0.949304	0.948104	1.44E-06	
270	0.863376	19.73814	0.948353	0.947401	9.07E-07	
275	0.860978	19.68119	0.945617	0.946706	1.19E-06	
280	0.857567	19.60016	0.941723	0.946019	1.85E-05	
285	0.859707	19.651	0.944166	0.945341	1.38E-06	
290	0.861253	19.68772	0.94593	0.94467	1.59E-06	
295	0.857208	19.59165	0.941314	0.944007	7.25E-06	
300	0.85842	19.62043	0.942697	0.943351	4.28E-07	
				sum=	0.000368	

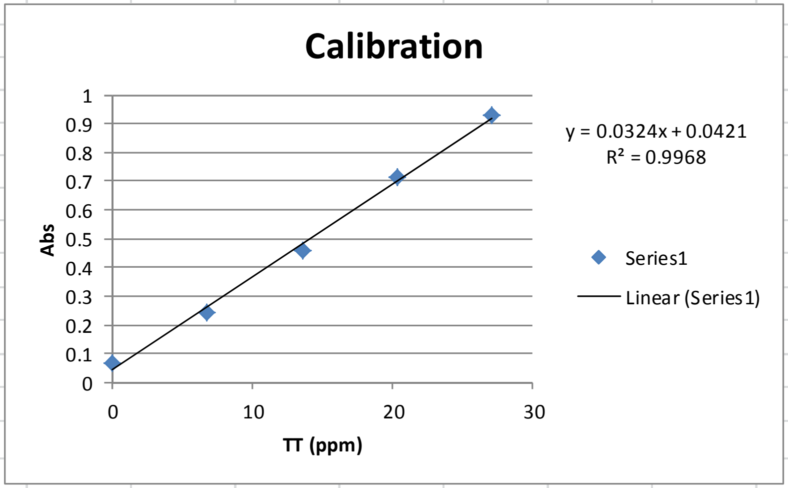
Calibratio Curve

a=	0.0324	%	TT (ppm)	abs	
b=	0.0421	0	0	0.065097	0.0652
		0.25	6.7775	0.2414	0.2415
		0.5	13.555	0.46	0.4601
		0.75	20.3325	0.712133	0.7124
		1	27.11	0.9276	0.9275

pH Before	8.796
pH After	8.301

Correlation Coefficent
0.994414947

R^2 of Module
0.988861087



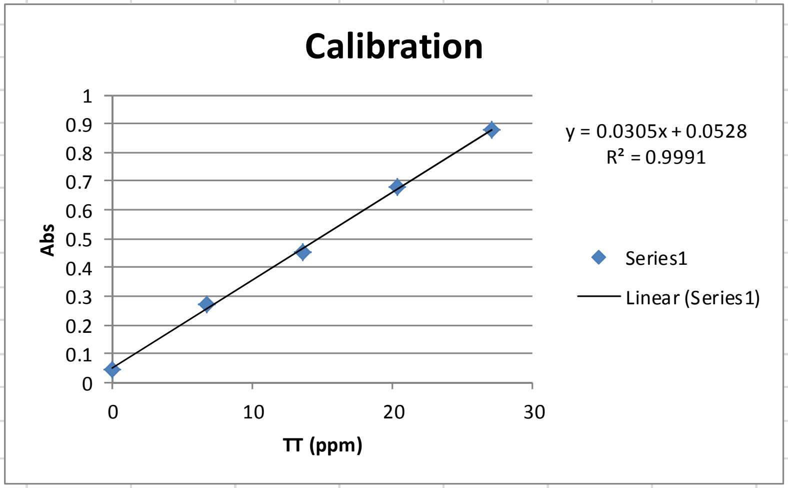
28Jul15_0.7@5%pH9					
			flow rate=	0.7	
			volume=	350	
			resid time	482	
			rate const	3.38E-05	
wavelength=	430				
time (min)	abs		C/Co	model	sum squares
0	0.894853	16.37033	1	1	0
5	0.893373	16.34229	0.998287	0.999832	2.38E-06
10	0.893825	16.35086	0.998811	0.999665	7.3E-07
15	0.892617	16.32798	0.997413	0.9995	4.36E-06
20	0.895918	16.39048	1.001231	0.999337	3.59E-06
25	0.89309	16.33694	0.99796	0.999176	1.48E-06
30	0.892219	16.32044	0.996953	0.999016	4.26E-06
35	0.891657	16.30978	0.996302	0.998858	6.54E-06
40	0.891846	16.31338	0.996521	0.998702	4.75E-06
45	0.891732	16.31121	0.996389	0.998547	4.66E-06
50	0.892946	16.33421	0.997794	0.998394	3.6E-07
55	0.895404	16.38076	1.000637	0.998243	5.73E-06
60	0.893377	16.34237	0.998292	0.998093	3.98E-08
65	0.893002	16.33527	0.997859	0.997945	7.38E-09
70	0.891549	16.30775	0.996178	0.997798	2.63E-06
75	0.891789	16.31229	0.996455	0.997653	1.43E-06
80	0.894578	16.36511	0.999681	0.997509	4.72E-06
85	0.891897	16.31434	0.99658	0.997367	6.2E-07
90	0.893233	16.33963	0.998125	0.997226	8.08E-07
95	0.891884	16.31408	0.996564	0.997087	2.73E-07
100	0.890363	16.28529	0.994806	0.996949	4.6E-06
105	0.89156	16.30795	0.99619	0.996813	3.89E-07
110	0.892712	16.32978	0.997523	0.996678	7.14E-07
115	0.891078	16.29882	0.995632	0.996545	8.33E-07
120	0.890886	16.29518	0.99541	0.996413	1.01E-06
125	0.889482	16.26859	0.993785	0.996282	6.23E-06
130	0.893055	16.33627	0.99792	0.996153	3.12E-06
135	0.891348	16.30394	0.995945	0.996025	6.34E-09
140	0.8919	16.31439	0.996583	0.995898	4.7E-07
145	0.889215	16.26355	0.993478	0.995773	5.27E-06
150	0.890512	16.2881	0.994977	0.995649	4.51E-07
155	0.891149	16.30017	0.995714	0.995526	3.54E-08
160	0.888227	16.24484	0.992334	0.995405	9.43E-06
165	0.891276	16.30258	0.995862	0.995285	3.33E-07
170	0.891513	16.30706	0.996135	0.995166	9.4E-07
175	0.895829	16.38881	1.001129	0.995048	3.7E-05
180	0.889517	16.26926	0.993826	0.994932	1.22E-06
185	0.891204	16.30122	0.995779	0.994817	9.25E-07
190	0.890926	16.29594	0.995456	0.994703	5.67E-07
195	0.890976	16.2969	0.995514	0.99459	8.55E-07
200	0.889738	16.27344	0.994082	0.994478	1.57E-07
205	0.890611	16.28998	0.995092	0.994368	5.24E-07
210	0.89097	16.29677	0.995507	0.994259	1.56E-06
215	0.890626	16.29026	0.995109	0.994151	9.19E-07
220	0.887776	16.23628	0.991812	0.994044	4.98E-06
225	0.889583	16.27051	0.993903	0.993938	1.24E-09
230	0.888578	16.25148	0.99274	0.993833	1.19E-06
235	0.88848	16.24961	0.992626	0.99373	1.22E-06
240	0.889887	16.27628	0.994255	0.993627	3.94E-07
245	0.8916	16.30872	0.996237	0.993526	7.35E-06
250	0.889584	16.27053	0.993904	0.993425	2.29E-07
255	0.889355	16.2662	0.993639	0.993326	9.81E-08
260	0.888481	16.24963	0.992627	0.993228	3.6E-07
265	0.887954	16.23966	0.992018	0.99313	1.24E-06
270	0.890225	16.28266	0.994645	0.993034	2.6E-06
275	0.886746	16.21678	0.99062	0.992939	5.37E-06
280	0.890508	16.28804	0.994973	0.992845	4.53E-06
285	0.888988	16.25924	0.993214	0.992751	2.14E-07
290	0.889292	16.265	0.993566	0.992659	8.22E-07
295	0.886796	16.21772	0.990678	0.992568	3.57E-06
300	0.887748	16.23576	0.99178	0.992477	4.87E-07
				sum=	0.000162

Calibratio Curve

a=	0.0305		%	TT (ppm)	abs
b=	0.0528		0	0	0.0469
			0.25	6.7775	0.2736
			0.5	13.555	0.4549
			0.75	20.3325	0.6796
			1	27.11	0.8787

pH Before	9.034
pH After	8.849

Correlation Coefficent	R^2 of Module
0.758952935	0.576009557



30Jul15_0.7@100%pH7					
			flow rate=	0.7	
			volume=	350	
			resid time	482	
			rate const	0.001025	
wavelength=	430				
time (min)	abs		C/Co	model	sum squares
0	1.149172	25.80354	1	1	0
5	1.143827	25.67895	0.995172	0.994916	6.52E-08
10	1.137243	25.52548	0.989224	0.989911	4.72E-07
15	1.131358	25.3883	0.983908	0.984982	1.15E-06
20	1.127556	25.29966	0.980472	0.980129	1.18E-07
25	1.121391	25.15597	0.974903	0.975351	2E-07
30	1.117589	25.06733	0.971469	0.970646	6.76E-07
35	1.109286	24.87381	0.963969	0.966014	4.18E-06
40	1.104321	24.75807	0.959483	0.961453	3.88E-06
45	1.101104	24.68307	0.956577	0.956962	1.48E-07
50	1.094831	24.53686	0.95091	0.95254	2.66E-06
55	1.090868	24.44447	0.94733	0.948186	7.33E-07
60	1.085204	24.31246	0.942214	0.943899	2.84E-06
65	1.080839	24.21069	0.93827	0.939678	1.98E-06
70	1.075463	24.08539	0.933414	0.935522	4.44E-06
75	1.06967	23.95034	0.92818	0.93143	1.06E-05
80	1.065019	23.84193	0.923979	0.9274	1.17E-05
85	1.061897	23.76916	0.921159	0.923433	5.17E-06
90	1.056443	23.64203	0.916232	0.919527	1.09E-05
95	1.051872	23.53547	0.912102	0.91568	1.28E-05
100	1.049933	23.49028	0.910351	0.911893	2.38E-06
105	1.043071	23.33032	0.904152	0.908164	1.61E-05
110	1.03904	23.23636	0.90051	0.904493	1.59E-05
115	1.035725	23.15909	0.897516	0.900878	1.13E-05
120	1.030211	23.03055	0.892534	0.897318	2.29E-05
125	1.026953	22.95461	0.889591	0.893814	1.78E-05
130	1.023207	22.8673	0.886208	0.890363	1.73E-05
135	1.019881	22.78976	0.883203	0.886965	1.42E-05
140	1.015515	22.688	0.879259	0.883619	1.9E-05
145	1.013225	22.63461	0.87719	0.880325	9.83E-06
150	1.01057	22.57273	0.874792	0.877082	5.24E-06
155	1.005995	22.46608	0.870659	0.873888	1.04E-05
160	1.002619	22.38738	0.867609	0.870744	9.83E-06
165	1.001338	22.35752	0.866452	0.867648	1.43E-06
170	0.997909	22.27761	0.863355	0.864599	1.55E-06
175	0.9949	22.20745	0.860636	0.861597	9.25E-07
180	0.990963	22.11568	0.857079	0.858642	2.44E-06
185	0.987957	22.04563	0.854364	0.855732	1.87E-06
190	0.984567	21.96659	0.851301	0.852867	2.45E-06
195	0.984042	21.95435	0.850827	0.850045	6.11E-07
200	0.979925	21.85839	0.847108	0.847268	2.54E-08
205	0.977954	21.81245	0.845328	0.844532	6.32E-07
210	0.973655	21.71224	0.841444	0.841839	1.56E-07
215	0.973458	21.70766	0.841266	0.839188	4.32E-06
220	0.96996	21.62611	0.838106	0.836577	2.34E-06
225	0.966974	21.5565	0.835408	0.834006	1.97E-06
230	0.964266	21.49338	0.832962	0.831475	2.21E-06
235	0.960611	21.40817	0.82966	0.828983	4.59E-07
240	0.960589	21.40766	0.82964	0.826529	9.68E-06
245	0.957655	21.33928	0.82699	0.824112	8.28E-06
250	0.955311	21.28465	0.824873	0.821733	9.86E-06
255	0.951846	21.20386	0.821742	0.819391	5.53E-06
260	0.950457	21.17148	0.820487	0.817084	1.16E-05
265	0.946606	21.08173	0.817009	0.814813	4.82E-06
270	0.945558	21.05731	0.816063	0.812577	1.21E-05
275	0.944271	21.02731	0.8149	0.810376	2.05E-05
280	0.939947	20.92651	0.810994	0.808208	7.76E-06
285	0.93703	20.8585	0.808358	0.806073	5.22E-06
290	0.937187	20.86216	0.8085	0.803972	2.05E-05
295	0.931171	20.72195	0.803066	0.801902	1.35E-06
300	0.930054	20.6959	0.802056	0.799865	4.8E-06
				sum=	0.000392

Calibratio Curve

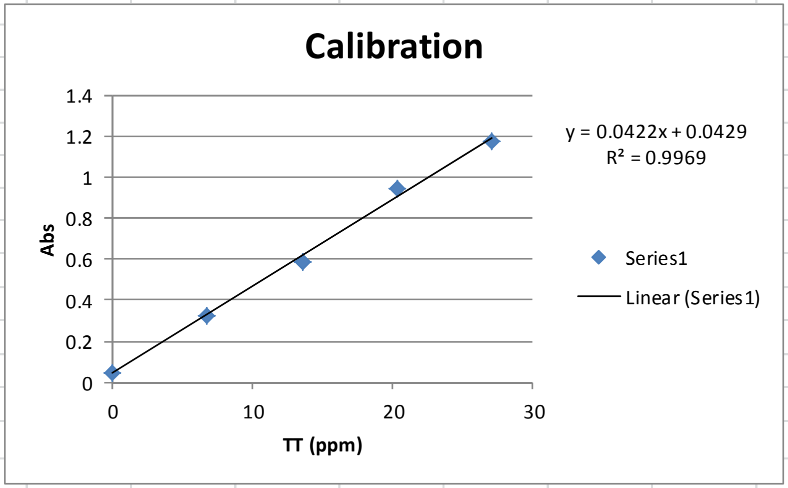
a=	0.0422
b=	0.0429

%	TT (ppm)	abs	
0	0	0.048767	0.0485
0.25	6.7775	0.3282	0.328
0.5	13.555	0.5862	0.586
0.75	20.3325	0.940167	0.9401
1	27.11	1.1743	1.1732

pH Before	7.006
pH After	5.356

Correlation Coefficent
0.999333692

R^2 of Module
0.998667827



31Jul15 0.7@10%pH6 removal increases throwout						
			flow rate=	0.7		
			volume=	350		
			resid time	482		
			rate const	-0.0003		
wavelength=	430					
time (min)	abs		C/Co	model	sum squares	
0	1.245828	28.05659	1	1	1.23E-32	
5	1.247947	28.10599	1.001761	1.001513	6.17E-08	
10	1.247502	28.09562	1.001391	1.003012	2.63E-06	
15	1.246327	28.06823	1.000415	1.004498	1.67E-05	
20	1.248333	28.11498	1.002081	1.005971	1.51E-05	
25	1.246422	28.07044	1.000494	1.007431	4.81E-05	
30	1.251022	28.17767	1.004316	1.008878	2.08E-05	
35	1.251163	28.18095	1.004433	1.010312	3.46E-05	
40	1.253246	28.22952	1.006164	1.011734	3.1E-05	
45	1.255379	28.27922	1.007935	1.013143	2.71E-05	
50	1.257795	28.33554	1.009943	1.01454	2.11E-05	
55	1.255595	28.28427	1.008115	1.015925	6.1E-05	
60	1.260154	28.39054	1.011903	1.017297	2.91E-05	
65	1.258026	28.34092	1.010134	1.018657	7.26E-05	
70	1.259218	28.36872	1.011125	1.020005	7.89E-05	
75	1.266387	28.53582	1.017081	1.021341	1.82E-05	
80	1.260949	28.40906	1.012563	1.022666	0.000102	
85	1.266868	28.54705	1.017481	1.023979	4.22E-05	
90	1.265781	28.5217	1.016578	1.02528	7.57E-05	
95	1.271334	28.65115	1.021191	1.02657	2.89E-05	
100	1.270806	28.63883	1.020752	1.027848	5.04E-05	
105	1.273727	28.70692	1.023179	1.029115	3.52E-05	
110	1.272436	28.67682	1.022107	1.030371	6.83E-05	
115	1.277927	28.80483	1.026669	1.031616	2.45E-05	
120	1.279031	28.83056	1.027586	1.03285	2.77E-05	
125	1.279032	28.83057	1.027587	1.034073	4.21E-05	
130	1.283125	28.926	1.030988	1.035286	1.85E-05	
135	1.287362	29.02475	1.034507	1.036487	3.92E-06	
140	1.287537	29.02883	1.034653	1.037678	9.15E-06	
145	1.287105	29.01876	1.034294	1.038859	2.08E-05	
150	1.299139	29.29928	1.044292	1.040029	1.82E-05	
155	1.288864	29.05976	1.035755	1.041189	2.95E-05	
160	1.29286	29.15291	1.039075	1.042338	1.06E-05	
165	1.299845	29.31574	1.044879	1.043477	1.96E-06	
170	1.304202	29.4173	1.048499	1.044607	1.51E-05	
175	1.305089	29.43798	1.049236	1.045726	1.23E-05	
180	1.300929	29.341	1.045779	1.046836	1.12E-06	
185	1.303498	29.40089	1.047914	1.047936	4.63E-10	
190	1.313288	29.6291	1.056048	1.049026	4.93E-05	
195	1.305132	29.43896	1.049271	1.050106	6.97E-07	
200	1.307536	29.49501	1.051269	1.051177	8.42E-09	
205	1.3117	29.59207	1.054728	1.052239	6.2E-06	
210	1.313217	29.62743	1.055988	1.053291	7.28E-06	
215	1.314878	29.66616	1.057369	1.054334	9.21E-06	
220	1.3128	29.61772	1.055642	1.055367	7.56E-08	
225	1.318178	29.74309	1.060111	1.056392	1.38E-05	
230	1.318038	29.73982	1.059994	1.057407	6.69E-06	
235	1.324108	29.88131	1.065037	1.058414	4.39E-05	
240	1.323262	29.86158	1.064334	1.059412	2.42E-05	
245	1.323209	29.86035	1.06429	1.060401	1.51E-05	
250	1.319734	29.77934	1.061403	1.061381	4.79E-10	
255	1.324654	29.89404	1.065491	1.062352	9.85E-06	
260	1.319022	29.76276	1.060812	1.063315	6.27E-06	
265	1.326054	29.92667	1.066654	1.06427	5.68E-06	
270	1.325879	29.9226	1.066509	1.065216	1.67E-06	
275	1.332235	30.07075	1.071789	1.066154	3.18E-05	
280	1.32455	29.89162	1.065405	1.067083	2.82E-06	
285	1.331146	30.04535	1.070884	1.068004	8.29E-06	
290	1.32619	29.92983	1.066767	1.068918	4.63E-06	
295	1.336945	30.18054	1.075703	1.069823	3.46E-05	
300	1.334853	30.13177	1.073964	1.07072	1.05E-05	
				sum=	0.001408	

Calibratio Curve

a= 0.0422

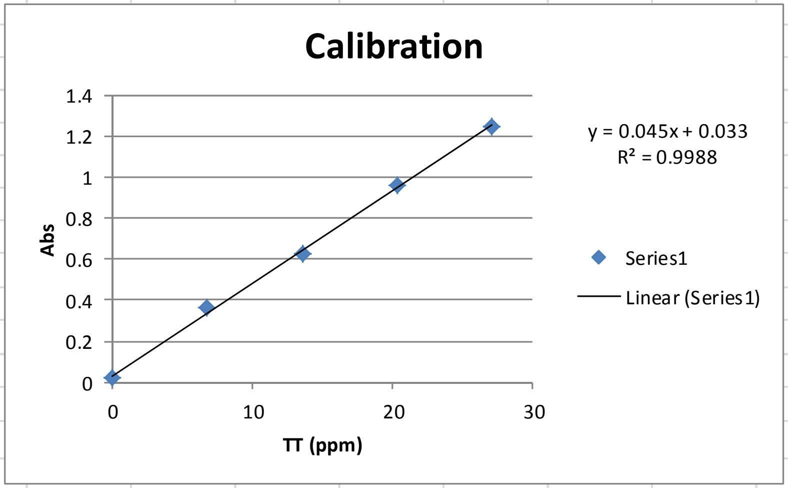
b= 0.0429

%	TT (ppm)	abs	
0	0	0.019467	0.0485
0.25	6.7775	0.361367	0.328
0.5	13.555	0.629833	0.586
0.75	20.3325	0.960667	0.9401
1	27.11	1.2458	1.1732

pH Before	7.006
pH After	5.356

Correlation Coefficent
0.99029733

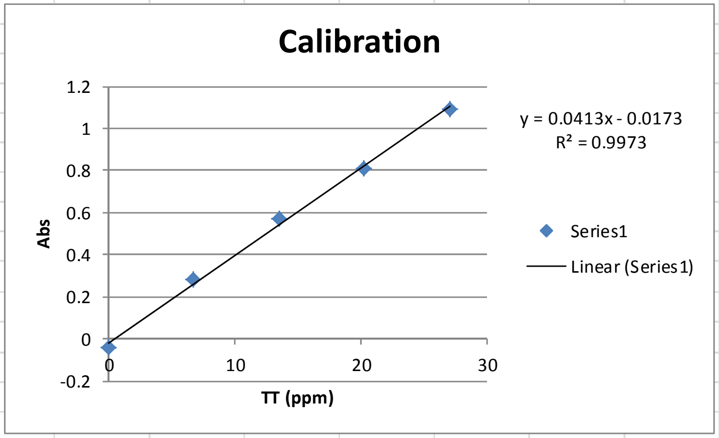
R^2 of Module
0.980688802



4Aug15_0.7@50%pH6						
			flow rate=	0.7		
			volume=	350		
			resid time	482		
			rate const	0.000641		
wavelength=	430					
time (min)	abs		C/Co	model	sum squares	
0	1.099795	7.786094	1	1	1.23E-32	
5	1.095667	7.755966	0.996131	0.996818	4.72E-07	
10	1.093898	7.743053	0.994472	0.993679	6.29E-07	
15	1.090264	7.716529	0.991065	0.990582	2.34E-07	
20	1.087877	7.6991	0.988827	0.987527	1.69E-06	
25	1.082084	7.656817	0.983396	0.984513	1.25E-06	
30	1.080311	7.643878	0.981735	0.98154	3.79E-08	
35	1.07819	7.628391	0.979746	0.978607	1.3E-06	
40	1.072035	7.583469	0.973976	0.975713	3.02E-06	
45	1.073144	7.591559	0.975015	0.972859	4.65E-06	
50	1.068037	7.554285	0.970228	0.970043	3.43E-08	
55	1.063766	7.523113	0.966224	0.967265	1.08E-06	
60	1.060382	7.498412	0.963052	0.964524	2.17E-06	
65	1.056723	7.471702	0.959621	0.96182	4.84E-06	
70	1.05321	7.446055	0.956327	0.959153	7.98E-06	
75	1.052098	7.437943	0.955286	0.956522	1.53E-06	
80	1.047845	7.406894	0.951298	0.953926	6.91E-06	
85	1.045092	7.386802	0.948717	0.951365	7.01E-06	
90	1.045832	7.392206	0.949411	0.948839	3.27E-07	
95	1.042096	7.364935	0.945909	0.946347	1.92E-07	
100	1.038032	7.335268	0.942099	0.943889	3.2E-06	
105	1.037477	7.331221	0.941579	0.941463	1.34E-08	
110	1.033578	7.302757	0.937923	0.939071	1.32E-06	
115	1.032161	7.292418	0.936595	0.93671	1.32E-08	
120	1.026889	7.253932	0.931652	0.934382	7.45E-06	
125	1.026496	7.251067	0.931284	0.932084	6.4E-07	
130	1.025924	7.246892	0.930748	0.929818	8.65E-07	
135	1.020337	7.206108	0.92551	0.927583	4.3E-06	
140	1.019834	7.202441	0.925039	0.925377	1.14E-07	
145	1.017562	7.185852	0.922908	0.923201	8.58E-08	
150	1.013886	7.159025	0.919463	0.921055	2.53E-06	
155	1.01317	7.153797	0.918791	0.918938	2.13E-08	
160	1.01049	7.134235	0.916279	0.916849	3.24E-07	
165	1.010395	7.133538	0.91619	0.914788	1.96E-06	
170	1.006296	7.103619	0.912347	0.912755	1.67E-07	
175	1.003437	7.082753	0.909667	0.910749	1.17E-06	
180	1.000739	7.063061	0.907138	0.908771	2.67E-06	
185	0.998802	7.048921	0.905322	0.906819	2.24E-06	
190	0.996331	7.030884	0.903005	0.904894	3.57E-06	
195	0.997191	7.037158	0.903811	0.902994	6.67E-07	
200	0.993554	7.010613	0.900402	0.90112	5.16E-07	
205	0.993152	7.00768	0.900025	0.899272	5.68E-07	
210	0.989787	6.983118	0.896871	0.897448	3.33E-07	
215	0.98841	6.973067	0.89558	0.895649	4.8E-09	
220	0.987998	6.970055	0.895193	0.893874	1.74E-06	
225	0.984573	6.945055	0.891982	0.892123	1.99E-08	
230	0.98534	6.950658	0.892702	0.890396	5.32E-06	
235	0.981085	6.919597	0.888712	0.888692	4.14E-10	
240	0.980103	6.912427	0.887791	0.887011	6.09E-07	
245	0.978944	6.903973	0.886706	0.885352	1.83E-06	
250	0.97574	6.880584	0.883702	0.883717	2.22E-10	
255	0.975224	6.876818	0.883218	0.882103	1.24E-06	
260	0.97374	6.865982	0.881826	0.88051	1.73E-06	
265	0.972471	6.856719	0.880637	0.87894	2.88E-06	
270	0.969605	6.835806	0.877951	0.87739	3.14E-07	
275	0.971403	6.848926	0.879636	0.875862	1.42E-05	
280	0.967181	6.818112	0.875678	0.874354	1.75E-06	
285	0.963882	6.79403	0.872585	0.872866	7.88E-08	
290	0.963531	6.791469	0.872256	0.871398	7.36E-07	
295	0.961524	6.776817	0.870374	0.869951	1.8E-07	
300	0.958136	6.752088	0.867198	0.868522	1.75E-06	
				sum=	0.000115	

Calibratio Curve								
a=	0.0331		%	TT (ppm)	abs	2	3	1
b=	0.137		0	0	-0.0429	-0.0429	-0.0429	-0.0429
			0.25	6.7775	0.2795	0.2791	0.279	0.2804
			0.5	13.555	0.574	0.5739	0.5746	0.5735
			0.75	20.3325	0.813167	0.8308	0.8046	0.8041
			1	27.11	1.091	1.0887	1.0893	1.095
								0.997

pH Before	6.742
pH After	5.509



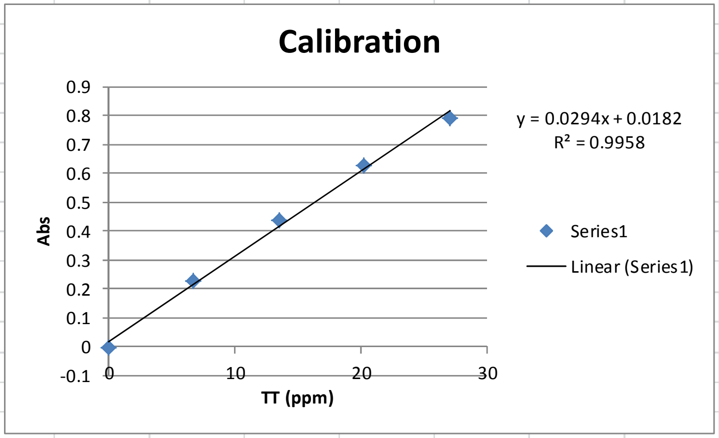
5Aug15_0.7@30%pH9					
			flow rate=	0.7	
			volume=	350	
			resid time	482	
			rate const	7.4676E-05	
wavelength=	430				
time (min)	abs		C/Co	model	sum squares
0	0.84115	44.60165	1	1	0
5	0.844218	44.77022	1.00378	0.999628619	1.72E-05
10	0.842179	44.65821	1.001268	0.999261208	4.03E-06
15	0.8417	44.63185	1.000677	0.998897725	3.17E-06
20	0.841584	44.62549	1.000534	0.998538127	3.99E-06
25	0.84005	44.54119	0.998644	0.998182373	2.14E-07
30	0.838787	44.47179	0.997088	0.997830421	5.51E-07
35	0.83789	44.42253	0.995984	0.997482232	2.24E-06
40	0.83754	44.4033	0.995553	0.997137764	2.51E-06
45	0.838417	44.45147	0.996633	0.996796979	2.7E-08
50	0.837853	44.42049	0.995938	0.996459836	2.72E-07
55	0.838834	44.47438	0.997146	0.996126297	1.04E-06
60	0.836597	44.35147	0.994391	0.995796324	1.98E-06
65	0.837618	44.40758	0.995649	0.995469877	3.2E-08
70	0.836134	44.32607	0.993821	0.99514692	1.76E-06
75	0.838091	44.43356	0.996231	0.994827416	1.97E-06
80	0.836478	44.34494	0.994244	0.994511326	7.13E-08
85	0.837826	44.419	0.995905	0.994198616	2.91E-06
90	0.836529	44.34775	0.994307	0.993889248	1.75E-07
95	0.836039	44.32085	0.993704	0.993583186	1.47E-08
100	0.837972	44.42703	0.996085	0.993280397	7.86E-06
105	0.834401	44.23084	0.991686	0.992980844	1.68E-06
110	0.838194	44.43922	0.996358	0.992684493	1.35E-05
115	0.832397	44.12074	0.989218	0.99239131	1.01E-05
120	0.832583	44.13094	0.989446	0.992101261	7.05E-06
125	0.835586	44.29596	0.993146	0.991814312	1.77E-06
130	0.833799	44.19773	0.990944	0.99153043	3.44E-07
135	0.834447	44.23336	0.991743	0.991249583	2.43E-07
140	0.835441	44.28799	0.992968	0.990971738	3.98E-06
145	0.833264	44.16834	0.990285	0.990696863	1.7E-07
150	0.836302	44.33529	0.994028	0.990424927	1.3E-05
155	0.83389	44.20276	0.991057	0.990155897	8.11E-07
160	0.832316	44.11625	0.989117	0.989889742	5.97E-07
165	0.834666	44.24538	0.992012	0.989626433	5.69E-06
170	0.831427	44.06743	0.988022	0.989365938	1.81E-06
175	0.834021	44.20995	0.991218	0.989108228	4.45E-06
180	0.835262	44.27813	0.992746	0.988853273	1.52E-05
185	0.833914	44.20404	0.991085	0.988601043	6.17E-06
190	0.831121	44.05061	0.987645	0.988351509	4.99E-07
195	0.833133	44.16118	0.990124	0.988104642	4.08E-06
200	0.831508	44.07189	0.988122	0.987860414	6.86E-08
205	0.831994	44.09857	0.988721	0.987618797	1.21E-06
210	0.829884	43.98263	0.986121	0.987379763	1.58E-06
215	0.833004	44.15408	0.989965	0.987143283	7.96E-06
220	0.827967	43.87733	0.98376	0.986909332	9.92E-06
225	0.828405	43.90139	0.9843	0.986677881	5.66E-06
230	0.830151	43.99734	0.986451	0.986448904	3.67E-12
235	0.829737	43.97456	0.98594	0.986222375	7.97E-08
240	0.829579	43.96587	0.985745	0.985998267	6.4E-08
245	0.831949	44.09611	0.988665	0.985776555	8.34E-06
250	0.828375	43.89975	0.984263	0.985557213	1.68E-06
255	0.827999	43.87909	0.9838	0.985340215	2.37E-06
260	0.829174	43.94362	0.985246	0.985125537	1.46E-08
265	0.826822	43.81441	0.982349	0.984913154	6.57E-06
270	0.828503	43.90675	0.98442	0.984703041	8.02E-08
275	0.825774	43.75683	0.981058	0.984495174	1.18E-05
280	0.827117	43.8306	0.982712	0.984289528	2.49E-06
285	0.828802	43.92321	0.984789	0.984086081	4.94E-07
290	0.828454	43.90408	0.98436	0.983884809	2.26E-07
295	0.828637	43.91411	0.984585	0.983685688	8.08E-07
300	0.825195	43.72501	0.980345	0.983488696	9.88E-06
				sum=	0.000214

Calibratio Curve

a=	0.0294
b=	0.0182

%	TT (ppm)	abs
0	0	-0.0036
0.25	6.7775	0.229
0.5	13.555	0.4351
0.75	20.3325	0.6281
1	27.11	0.7915

pH Before	9.003
pH After	8.937



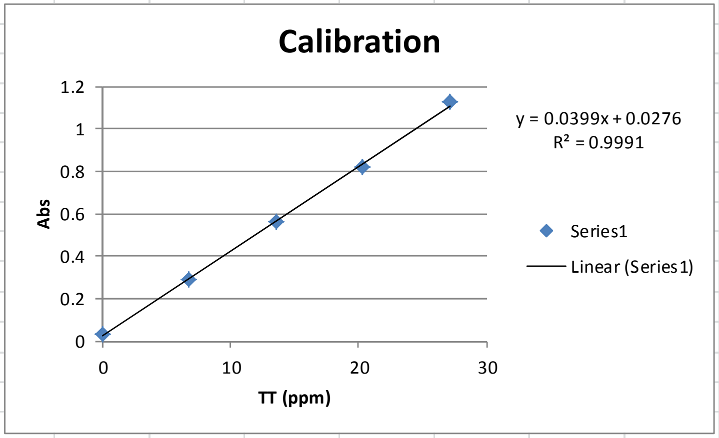
6Aug15_0.7@20%pH7					
			flow rate=	0.7	
			volume=	350	
			resid time	482	
			rate const	0.00022352	
wavelength=	430				
time (min)	abs		C/Co	model	sum squares
0	1.102808	38.51116	1	1	0
5	1.10477	38.58226	1.001846	0.998888795	8.75E-06
10	1.101777	38.47381	0.99903	0.997790287	1.54E-06
15	1.099396	38.38753	0.99679	0.996704329	7.29E-09
20	1.097544	38.32044	0.995048	0.995630778	3.4E-07
25	1.097384	38.31462	0.994897	0.994569493	1.07E-07
30	1.095621	38.25076	0.993238	0.993520333	7.95E-08
35	1.096327	38.27635	0.993903	0.992483161	2.02E-06
40	1.098011	38.33737	0.995487	0.991457838	1.62E-05
45	1.093195	38.16285	0.990956	0.99044423	2.61E-07
50	1.093173	38.16206	0.990935	0.989442202	2.23E-06
55	1.089864	38.04218	0.987822	0.988451624	3.96E-07
60	1.090741	38.07396	0.988648	0.987472362	1.38E-06
65	1.089353	38.02365	0.987341	0.986504289	7E-07
70	1.090674	38.07152	0.988584	0.985547277	9.22E-06
75	1.084924	37.86318	0.983174	0.984601199	2.04E-06
80	1.087068	37.94086	0.985191	0.98366593	2.33E-06
85	1.086145	37.90742	0.984323	0.982741346	2.5E-06
90	1.083868	37.82492	0.982181	0.981827327	1.25E-07
95	1.083027	37.79446	0.98139	0.98092375	2.17E-07
100	1.083019	37.79415	0.981382	0.980030496	1.83E-06
105	1.080959	37.71951	0.979444	0.979147449	8.78E-08
110	1.080215	37.69258	0.978744	0.97827449	2.21E-07
115	1.078404	37.62696	0.977041	0.977411506	1.38E-07
120	1.078599	37.63401	0.977223	0.976558381	4.42E-07
125	1.077904	37.60884	0.97657	0.975715003	7.31E-07
130	1.076482	37.55731	0.975232	0.974881261	1.23E-07
135	1.073513	37.44976	0.972439	0.974057045	2.62E-06
140	1.075512	37.52216	0.974319	0.973242246	1.16E-06
145	1.074311	37.47865	0.973189	0.972436756	5.66E-07
150	1.072029	37.39599	0.971043	0.971640469	3.57E-07
155	1.069417	37.30134	0.968585	0.97085328	5.14E-06
160	1.070954	37.35702	0.970031	0.970075085	1.93E-09
165	1.070525	37.34149	0.969628	0.96930578	1.04E-07
170	1.067369	37.22715	0.966659	0.968545266	3.56E-06
175	1.068736	37.27666	0.967944	0.96779344	2.28E-08
180	1.066163	37.18344	0.965524	0.967050204	2.33E-06
185	1.067062	37.21602	0.96637	0.96631546	2.96E-09
190	1.065182	37.14789	0.964601	0.965589111	9.77E-07
195	1.066268	37.18724	0.965622	0.96487106	5.65E-07
200	1.063927	37.10242	0.96342	0.964161213	5.5E-07
205	1.066074	37.18022	0.96544	0.963459476	3.92E-06
210	1.061557	37.01656	0.96119	0.962765757	2.48E-06
215	1.063061	37.07106	0.962606	0.962079964	2.76E-07
220	1.061937	37.03033	0.961548	0.961402006	2.14E-08
225	1.059763	36.95154	0.959502	0.960731795	1.51E-06
230	1.059663	36.94792	0.959408	0.96006924	4.37E-07
235	1.059779	36.95212	0.959517	0.959414255	1.06E-08
240	1.057437	36.8673	0.957315	0.958766754	2.11E-06
245	1.058681	36.91234	0.958484	0.958126651	1.28E-07
250	1.056533	36.83452	0.956464	0.95749386	1.06E-06
255	1.057446	36.86762	0.957323	0.9568683	2.07E-07
260	1.055735	36.80562	0.955713	0.956249887	2.88E-07
265	1.056613	36.83744	0.956539	0.95563854	8.12E-07
270	1.055643	36.80227	0.955626	0.955034177	3.5E-07
275	1.054335	36.7549	0.954396	0.954436719	1.66E-09
280	1.053887	36.73867	0.953975	0.953846088	1.65E-08
285	1.053348	36.71912	0.953467	0.953262204	4.19E-08
290	1.050883	36.62981	0.951148	0.952684992	2.36E-06
295	1.053858	36.7376	0.953947	0.952114374	3.36E-06
300	1.050697	36.62307	0.950973	0.951550276	3.33E-07
				sum=	9.17E-05

Calibratio Curve

a=	0.0399
b=	0.0276

%	TT (ppm)	abs
0	0	0.0368
0.25	6.7775	0.2932
0.5	13.555	0.5664
0.75	20.3325	0.8218
1	27.11	1.1253

pH Before	7.023
pH After	6.787



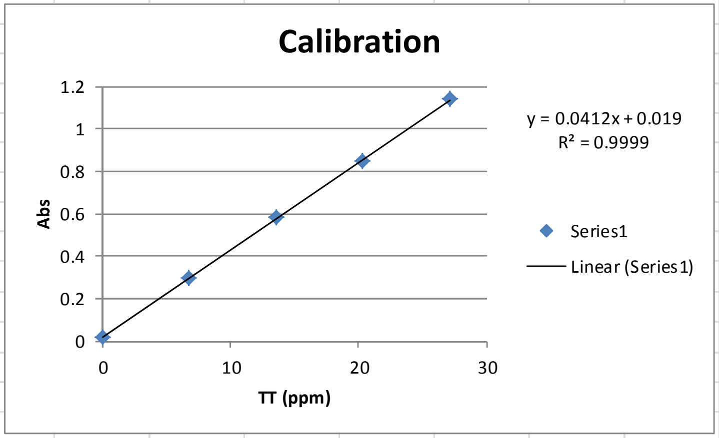
7Aug15_0.710%pH6						
			flow rate=	0.7		
			volume=	350		
			resid time	482		
			rate const	0.000139229		
wavelength=	430					
time (min)	abs		C/Co	model	sum squares	
0	1.135949	57.61835	1	1	0	
5	1.136509	57.64783	1.000512	0.999307695	1.45E-06	
10	1.136356	57.63977	1.000372	0.998623011	3.06E-06	
15	1.133659	57.49787	0.997909	0.997945864	1.36E-09	
20	1.135735	57.6071	0.999805	0.997276172	6.39E-06	
25	1.132789	57.45207	0.997114	0.996613852	2.5E-07	
30	1.131438	57.38095	0.99588	0.995958824	6.25E-09	
35	1.130947	57.35512	0.995432	0.995311006	1.45E-08	
40	1.12988	57.29894	0.994457	0.99467032	4.57E-08	
45	1.130819	57.34839	0.995315	0.994036686	1.63E-06	
50	1.127042	57.14959	0.991864	0.993410029	2.39E-06	
55	1.12904	57.25472	0.993689	0.992790269	8.08E-07	
60	1.128965	57.2508	0.993621	0.992177333	2.08E-06	
65	1.126539	57.12312	0.991405	0.991571144	2.76E-08	
70	1.125101	57.0474	0.990091	0.990971628	7.76E-07	
75	1.124281	57.00426	0.989342	0.990378712	1.07E-06	
80	1.127293	57.16278	0.992093	0.989792323	5.29E-06	
85	1.124302	57.00538	0.989362	0.98921239	2.23E-08	
90	1.125315	57.05871	0.990287	0.98863884	2.72E-06	
95	1.121895	56.87869	0.987163	0.988071605	8.26E-07	
100	1.124196	56.99979	0.989264	0.987510614	3.08E-06	
105	1.122017	56.88512	0.987274	0.986955799	1.01E-07	
110	1.122243	56.897	0.987481	0.986407091	1.15E-06	
115	1.120697	56.81563	0.986068	0.985864424	4.15E-08	
120	1.119913	56.77435	0.985352	0.985327731	5.87E-10	
125	1.118212	56.68482	0.983798	0.984796946	9.98E-07	
130	1.118621	56.70635	0.984172	0.984272005	1.01E-08	
135	1.12048	56.80421	0.98587	0.983752842	4.48E-06	
140	1.117733	56.65965	0.983361	0.983239394	1.48E-08	
145	1.116923	56.617	0.982621	0.982731599	1.22E-08	
150	1.11489	56.50997	0.980763	0.982229394	2.15E-06	
155	1.115063	56.51909	0.980922	0.981732717	6.58E-07	
160	1.113545	56.43923	0.979536	0.981241508	2.91E-06	
165	1.116035	56.57025	0.98181	0.980755706	1.11E-06	
170	1.114957	56.51355	0.980826	0.980275253	3.03E-07	
175	1.114368	56.48255	0.980288	0.979800088	2.38E-07	
180	1.116046	56.57085	0.98182	0.979330155	6.2E-06	
185	1.11055	56.2816	0.9768	0.978865395	4.27E-06	
190	1.11261	56.39002	0.978682	0.978405751	7.61E-08	
195	1.113291	56.42585	0.979303	0.977951167	1.83E-06	
200	1.111294	56.32073	0.977479	0.977501587	5.07E-10	
205	1.111622	56.33799	0.977779	0.977056957	5.21E-07	
210	1.109736	56.23875	0.976056	0.976617221	3.15E-07	
215	1.109013	56.20066	0.975395	0.976182326	6.2E-07	
220	1.109881	56.24635	0.976188	0.975752219	1.9E-07	
225	1.108029	56.14892	0.974497	0.975326846	6.88E-07	
230	1.106954	56.09233	0.973515	0.974906157	1.94E-06	
235	1.106275	56.0566	0.972895	0.974490098	2.54E-06	
240	1.107944	56.14444	0.974419	0.97407862	1.16E-07	
245	1.109468	56.22461	0.975811	0.973671671	4.58E-06	
250	1.106345	56.06025	0.972958	0.973269203	9.67E-08	
255	1.105801	56.03163	0.972462	0.972871165	1.68E-07	
260	1.104737	55.97565	0.97149	0.972477509	9.75E-07	
265	1.105033	55.99123	0.97176	0.972088186	1.07E-07	
270	1.106849	56.0868	0.973419	0.971703149	2.94E-06	
275	1.105606	56.02135	0.972283	0.971322351	9.23E-07	
280	1.102301	55.84745	0.969265	0.970945745	2.83E-06	
285	1.103265	55.89817	0.970145	0.970573285	1.83E-07	
290	1.104669	55.97205	0.971427	0.970204925	1.49E-06	
295	1.101388	55.79934	0.96843	0.96984062	1.99E-06	
300	1.101436	55.80188	0.968474	0.969480326	1.01E-06	
				sum=	8.27E-05	

Calibratio Curve

a=	0.0412
b=	0.019

%	TT (ppm)	abs
0	0	0.0191
0.25	6.7775	0.2962
0.5	13.555	0.5849
0.75	20.3325	0.8502
1	27.11	1.1395

pH Before	6.418
pH After	6.103



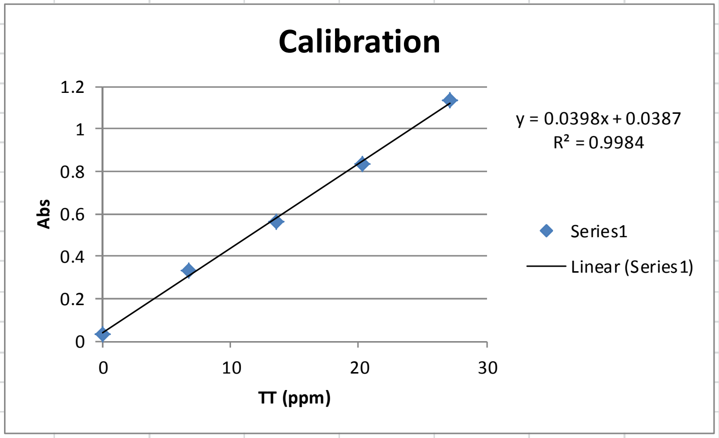
11Aug15_0.7@50%pH7						
			flow rate=	0.7		
			volume=	350		
			resid time	482		
			rate const	0.000589571		
wavelength=	430					
time (min)	abs		C/Co	model	sum squares	
0	1.085213	27.01325	1	1	0	
5	1.082503	26.94323	0.997408	0.997071692	1.13E-07	
10	1.078604	26.84247	0.993678	0.994182134	2.54E-07	
15	1.076399	26.78551	0.991569	0.991330814	5.68E-08	
20	1.073431	26.70882	0.98873	0.988517225	4.54E-08	
25	1.071326	26.65442	0.986716	0.985740868	9.52E-07	
30	1.067713	26.56105	0.98326	0.983001251	6.7E-08	
35	1.065177	26.49553	0.980835	0.980297886	2.88E-07	
40	1.061877	26.41025	0.977677	0.977630296	2.22E-09	
45	1.058661	26.32717	0.974602	0.974998005	1.57E-07	
50	1.054651	26.22354	0.970766	0.972400548	2.67E-06	
55	1.05318	26.18554	0.969359	0.969837462	2.29E-07	
60	1.051256	26.13582	0.967518	0.967308294	4.42E-08	
65	1.047453	26.03754	0.96388	0.964812594	8.69E-07	
70	1.046785	26.02029	0.963242	0.96234992	7.95E-07	
75	1.042467	25.90871	0.959111	0.959919834	6.54E-07	
80	1.039421	25.83001	0.956198	0.957521905	1.75E-06	
85	1.038562	25.8078	0.955376	0.955155709	4.84E-08	
90	1.035735	25.73475	0.952671	0.952820823	2.24E-08	
95	1.033502	25.67707	0.950536	0.950516836	3.65E-10	
100	1.030085	25.58877	0.947267	0.948243337	9.53E-07	
105	1.027503	25.52203	0.944797	0.945999923	1.45E-06	
110	1.027251	25.51552	0.944556	0.943786196	5.92E-07	
115	1.023493	25.41843	0.940961	0.941601763	4.1E-07	
120	1.02168	25.37158	0.939227	0.939446237	4.8E-08	
125	1.018552	25.29074	0.936235	0.937319235	1.18E-06	
130	1.01756	25.26512	0.935286	0.935220379	4.34E-09	
135	1.01487	25.1956	0.932712	0.933149297	1.91E-07	
140	1.013318	25.1555	0.931228	0.931105622	1.5E-08	
145	1.012193	25.12644	0.930152	0.929088991	1.13E-06	
150	1.009536	25.05778	0.92761	0.927099046	2.62E-07	
155	1.008079	25.02012	0.926217	0.925135434	1.17E-06	
160	1.004908	24.93818	0.923183	0.923197806	2.12E-10	
165	1.004433	24.92592	0.922729	0.921285818	2.08E-06	
170	1.00059	24.82663	0.919054	0.919399132	1.19E-07	
175	0.999627	24.80172	0.918132	0.917537413	3.53E-07	
180	0.996477	24.72034	0.915119	0.915700329	3.38E-07	
185	0.99549	24.69483	0.914175	0.913887556	8.24E-08	
190	0.993267	24.63738	0.912048	0.912098771	2.57E-09	
195	0.991893	24.60188	0.910734	0.910333656	1.6E-07	
200	0.990628	24.56921	0.909524	0.9085919	8.69E-07	
205	0.988232	24.50728	0.907232	0.906873192	1.29E-07	
210	0.986259	24.4563	0.905344	0.905177228	2.8E-08	
215	0.983828	24.39348	0.903019	0.903503706	2.35E-07	
220	0.982707	24.36451	0.901947	0.90185233	8.91E-09	
225	0.981167	24.32473	0.900474	0.900222806	6.31E-08	
230	0.978725	24.26162	0.898138	0.898614846	2.28E-07	
235	0.976968	24.21622	0.896457	0.897028165	3.26E-07	
240	0.976627	24.20741	0.896131	0.895462479	4.47E-07	
245	0.974318	24.14775	0.893923	0.893917512	2.53E-11	
250	0.972218	24.09349	0.891914	0.89239299	2.3E-07	
255	0.970516	24.04951	0.890286	0.890888642	3.64E-07	
260	0.969312	24.01839	0.889134	0.8894042	7.32E-08	
265	0.967896	23.98182	0.88778	0.887939403	2.55E-08	
270	0.967058	23.96015	0.886978	0.886493989	2.34E-07	
275	0.965288	23.91442	0.885285	0.885067701	4.71E-08	
280	0.963418	23.86609	0.883496	0.883660288	2.71E-08	
285	0.96187	23.82609	0.882015	0.8822715	6.59E-08	
290	0.961069	23.8054	0.881249	0.880901089	1.21E-07	
295	0.959384	23.76187	0.879637	0.879548812	7.85E-09	
300	0.957799	23.7209	0.878121	0.87821443	8.73E-09	
				sum=	2.31E-05	

Calibratio Curve

a=	0.0398
b=	0.0387

%	TT (ppm)	abs
0	0	0.0346
0.25	6.7775	0.3301
0.5	13.555	0.561
0.75	20.3325	0.8332
1	27.11	1.1313

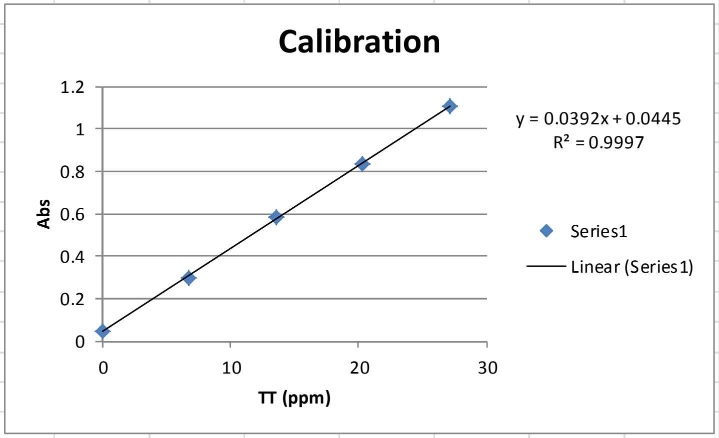
pH Before	6.998
pH After	7.809



12Aug15 0.7@70%pH6Redo						
			flow rate=	0.7		
			volume=	350		
			resid time	482		
			rate const	0.000827011		
wavelength=	430					
time (min)	abs		C/Co	model	sum squares	
0	1.102453	23.89334	1	1	0	
5	1.100628	23.85231	0.998283	0.995894796	5.7E-06	
10	1.095645	23.74033	0.993596	0.991848723	3.05E-06	
15	1.090592	23.62678	0.988844	0.987860928	9.66E-07	
20	1.08634	23.53125	0.984846	0.983930573	8.37E-07	
25	1.083332	23.46364	0.982016	0.980056829	3.84E-06	
30	1.079538	23.37838	0.978448	0.976238882	4.88E-06	
35	1.074848	23.27298	0.974036	0.972475928	2.44E-06	
40	1.070246	23.16957	0.969708	0.968767174	8.86E-07	
45	1.066439	23.08403	0.966128	0.965111841	1.03E-06	
50	1.064003	23.02929	0.963837	0.961509158	5.42E-06	
55	1.058832	22.91307	0.958973	0.957958367	1.03E-06	
60	1.054184	22.80863	0.954602	0.954458721	2.06E-08	
65	1.051183	22.74119	0.951779	0.951009483	5.93E-07	
70	1.047515	22.65876	0.94833	0.947609927	5.18E-07	
75	1.044743	22.59646	0.945722	0.944259337	2.14E-06	
80	1.041429	22.52201	0.942606	0.940957008	2.72E-06	
85	1.03848	22.45573	0.939832	0.937702246	4.54E-06	
90	1.036399	22.40896	0.937875	0.934494364	1.14E-05	
95	1.031456	22.29789	0.933226	0.931332687	3.59E-06	
100	1.029141	22.24586	0.931049	0.928216551	8.02E-06	
105	1.025234	22.15807	0.927375	0.925145299	4.97E-06	
110	1.022443	22.09536	0.92475	0.922118284	6.92E-06	
115	1.018155	21.99898	0.920716	0.91913487	2.5E-06	
120	1.01675	21.96742	0.919395	0.916194428	1.02E-05	
125	1.012429	21.87032	0.915331	0.91329634	4.14E-06	
130	1.010344	21.82346	0.91337	0.910439995	8.59E-06	
135	1.007299	21.75504	0.910506	0.907624792	8.3E-06	
140	1.004207	21.68556	0.907598	0.904850138	7.55E-06	
145	1.000716	21.6071	0.904315	0.90211545	4.84E-06	
150	0.998714	21.56212	0.902432	0.899420152	9.07E-06	
155	0.995652	21.49331	0.899553	0.896763676	7.78E-06	
160	0.992335	21.41876	0.896432	0.894145464	5.23E-06	
165	0.9885	21.33258	0.892826	0.891564963	1.59E-06	
170	0.984617	21.24532	0.889173	0.889021632	2.3E-08	
175	0.982647	21.20107	0.887321	0.886514934	6.5E-07	
180	0.981081	21.16587	0.885848	0.884044341	3.25E-06	
185	0.978202	21.10117	0.88314	0.881609335	2.34E-06	
190	0.974944	21.02795	0.880076	0.879209402	7.51E-07	
195	0.971807	20.95746	0.877126	0.876844037	7.93E-08	
200	0.970357	20.92489	0.875762	0.874512742	1.56E-06	
205	0.966934	20.84796	0.872543	0.872215026	1.08E-07	
210	0.964964	20.80369	0.87069	0.869950407	5.47E-07	
215	0.963171	20.7634	0.869004	0.867718406	1.65E-06	
220	0.958723	20.66344	0.86482	0.865518554	4.88E-07	
225	0.957354	20.63269	0.863533	0.863350389	3.34E-08	
230	0.955742	20.59646	0.862017	0.861213453	6.45E-07	
235	0.951058	20.49119	0.857611	0.859107298	2.24E-06	
240	0.949965	20.46663	0.856583	0.857031478	2.01E-07	
245	0.947483	20.41085	0.854248	0.854985559	5.43E-07	
250	0.944219	20.33751	0.851179	0.852969108	3.2E-06	
255	0.941684	20.28054	0.848795	0.850981702	4.78E-06	
260	0.939484	20.23111	0.846726	0.849022922	5.28E-06	
265	0.936888	20.17275	0.844284	0.847092356	7.89E-06	
270	0.93481	20.12606	0.842329	0.845189597	8.18E-06	
275	0.933935	20.10641	0.841507	0.843314245	3.27E-06	
280	0.930198	20.02243	0.837992	0.841465905	1.21E-05	
285	0.927795	19.96843	0.835732	0.839644188	1.53E-05	
290	0.925263	19.91154	0.833351	0.837848711	2.02E-05	
295	0.923193	19.86501	0.831404	0.836079095	2.19E-05	
300	0.922865	19.85764	0.831095	0.834334969	1.05E-05	
				sum=	0.000273	

Calibratio Curve					
a=	0.0392		%	TT (ppm)	abs
b=	0.0445		0	0	0.0506
			0.25	6.7775	0.2991
			0.5	13.555	0.5817
			0.75	20.3325	0.8358
			1	27.11	1.109

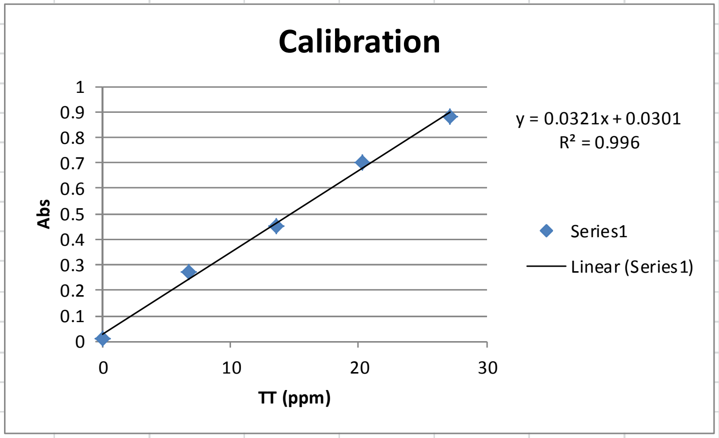
pH Before	6.287
pH After	5.825



13Aug15_0.7@100%pH8					
			flow rate=	0.7	
			volume=	350	
			resid time	482	
			rate const	0.000481987	
wavelength=	430				
time (min)	abs		C/Co	model	sum squares
0	0.886178	28.37468	1	1	0
5	0.884311	28.31265	0.997814	0.997605403	4.35E-08
10	0.882251	28.24421	0.995402	0.995241222	2.59E-08
15	0.880215	28.17659	0.993019	0.992907072	1.25E-08
20	0.87921	28.1432	0.991842	0.990602569	1.54E-06
25	0.875454	28.01842	0.987444	0.988327339	7.8E-07
30	0.874237	27.97797	0.986019	0.986081008	3.84E-09
35	0.873425	27.95099	0.985068	0.983863211	1.45E-06
40	0.871652	27.89209	0.982992	0.981673584	1.74E-06
45	0.868176	27.77661	0.978923	0.979511769	3.47E-07
50	0.867583	27.75692	0.978228	0.977377414	7.24E-07
55	0.865969	27.70327	0.976338	0.97527017	1.14E-06
60	0.864342	27.64925	0.974434	0.973189692	1.55E-06
65	0.863009	27.60495	0.972873	0.97113564	3.02E-06
70	0.861036	27.53941	0.970563	0.969107679	2.12E-06
75	0.859778	27.49762	0.96909	0.967105477	3.94E-06
80	0.85854	27.45646	0.96764	0.965128707	6.31E-06
85	0.857226	27.41283	0.966102	0.963177046	8.55E-06
90	0.855329	27.3498	0.963881	0.961250175	6.92E-06
95	0.853385	27.28521	0.961604	0.959347779	5.09E-06
100	0.850805	27.19951	0.958584	0.957469547	1.24E-06
105	0.849569	27.15845	0.957137	0.955615173	2.32E-06
110	0.846902	27.06982	0.954013	0.953784353	5.24E-08
115	0.846894	27.06958	0.954005	0.951976788	4.11E-06
120	0.845816	27.03376	0.952742	0.950192183	6.5E-06
125	0.843396	26.95334	0.949908	0.948430246	2.18E-06
130	0.843031	26.94124	0.949482	0.946690689	7.79E-06
135	0.840505	26.85732	0.946524	0.944973228	2.41E-06
140	0.839405	26.82076	0.945236	0.943277582	3.83E-06
145	0.838957	26.80589	0.944712	0.941603474	9.66E-06
150	0.836054	26.70945	0.941313	0.939950631	1.86E-06
155	0.833192	26.61434	0.937961	0.938318783	1.28E-07
160	0.834859	26.66974	0.939914	0.936707662	1.03E-05
165	0.832813	26.60176	0.937518	0.935117005	5.76E-06
170	0.829926	26.50584	0.934137	0.933546553	3.49E-07
175	0.828333	26.45293	0.932272	0.93199605	7.64E-08
180	0.828459	26.4571	0.932419	0.93046524	3.82E-06
185	0.82706	26.41063	0.930782	0.928953875	3.34E-06
190	0.825253	26.3506	0.928666	0.927461707	1.45E-06
195	0.823357	26.28761	0.926446	0.925988493	2.1E-07
200	0.822253	26.25094	0.925154	0.924533992	3.84E-07
205	0.821189	26.21557	0.923907	0.923097966	6.55E-07
210	0.820607	26.19623	0.923226	0.92168018	2.39E-06
215	0.818388	26.12253	0.920628	0.920280403	1.21E-07
220	0.816922	26.07383	0.918912	0.918898406	1.81E-10
225	0.814557	25.99524	0.916142	0.917533963	1.94E-06
230	0.81367	25.96579	0.915104	0.916186851	1.17E-06
235	0.813168	25.94909	0.914516	0.91485685	1.16E-07
240	0.811962	25.90903	0.913104	0.913543743	1.93E-07
245	0.809648	25.83215	0.910395	0.912247316	3.43E-06
250	0.807932	25.77514	0.908385	0.910967355	6.67E-06
255	0.808161	25.78275	0.908654	0.909703652	1.1E-06
260	0.80775	25.7691	0.908172	0.908456001	8.05E-08
265	0.804625	25.66529	0.904514	0.907224198	7.35E-06
270	0.80379	25.63753	0.903536	0.906008041	6.11E-06
275	0.802029	25.57903	0.901474	0.904807332	1.11E-05
280	0.802023	25.57885	0.901467	0.903621874	4.64E-06
285	0.801314	25.5553	0.900637	0.902451474	3.29E-06
290	0.79999	25.51128	0.899086	0.90129594	4.88E-06
295	0.798743	25.46988	0.897627	0.900155084	6.39E-06
300	0.796776	25.4045	0.895323	0.899028719	1.37E-05
				sum=	0.000188

Calibratio Curve				
a=	0.0321	%	TT (ppm)	abs
b=	0.0301	0	0	0.0122
		0.25	6.7775	0.2738
		0.5	13.555	0.4505
		0.75	20.3325	0.7028
		1	27.11	0.8842

pH Before	8.229
pH After	8.712



Appendix R: LED Degradation over Time of Use

Bulb No.	Time (Hrs)	Output	Slope
1	0	3.89E-04	-8.82E-07
1	102	2.99E-04	
2	0	4.05E-04	-2.94E-06
2	102	1.05E-04	
3	0	na	--
3	110.75	3.32E-04	
4	0	4.17E-04	-2.65E-07
4	111	3.88E-04	
5	0	na	--
5	110.75	4.71E-05	
6	0	4.55E-04	-1.12E-06
6	111	3.31E-04	
7	0	na	--
7	110.75	3.47E-04	
Average	0	4.16E-04	-1.43E-06
Average	106.5	2.64E-04	

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14. ABSTRACT

Water treatment capability is required for military operations, production of drinking water, and industrial wastewater treatment. The Advanced Oxidation Process (AOP) is one of many viable steps for treating water; however, it is important to understand the byproducts of the treatment process to avoid creating other constituents more severe than the first. Tartrazine (TAR) was oxidized with pulsed Ultra-Violet (UV) Light Emitting Diodes (LEDs) in combination with hydrogen peroxide (H2O2) in an AOP at the laboratory scale. The relative concentration of TAR was reduced from 1 to between 1 – 0.75 over pH values between 6 and 9, and at Duty Cycles (DCs) ranging from 0% to100%. The first order rate constant for TAR removal was statistically and positively correlated with DC, was statistically and negatively correlated with pH, and was typically greatest at pH6. DC and pH were variables in a regression model of the first order rate constant with adjusted R2 of 0.85. Chromatographic contrast angle determinations revealed that the byproduct profile was most significantly influenced by pH 7 under both positive and negative ionization, by the 70% DC for the positive ionization, and 50% DC for the negative ionization. DC and pH were variables in regression models…

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