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## CHEMICAL ANALYSIS, DATABASING, AND STATISTICAL ANALYSIS OF SMOKELESS POWDERS FOR FORENSIC APPLICATION

by

# DANA-MARIE KARINE DENNIS B.S. University of Central Florida, 2009

A dissertation submitted in partial fulfillment of the requirements for the degree of Doctor of Philosophy in the Department of Chemistry in the College of Sciences at the University of Central Florida Orlando, Florida

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Major Professor: Michael E. Sigman

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## ABSTRACT

Smokeless powders are a set of energetic materials, known as low explosives, which are typically utilized for reloading ammunition. There are three types which differ in their primary energetic materials; where single base powders contain nitrocellulose as their primary energetic material, double and triple base powders contain nitroglycerin in addition to nitrocellulose, and triple base powders also contain nitroguanidine. Additional organic compounds, while not proprietary to specific manufacturers, are added to the powders in varied ratios during the manufacturing process to optimize the ballistic performance of the powders. The additional compounds function as stabilizers, plasticizers, flash suppressants, deterrents, and opacifiers. Of the three smokeless powder types, single and double base powders are commercially available, and have been heavily utilized in the manufacture of improvised explosive devices.

Forensic smokeless powder samples are currently analyzed using multiple analytical techniques. Combined microscopic, macroscopic, and instrumental techniques are used to evaluate the sample, and the information obtained is used to generate a list of potential distributors. Gas chromatography – mass spectrometry (GC-MS) is arguably the most useful of the instrumental techniques since it distinguishes single and double base powders, and provides additional information about the relative ratios of all the analytes present in the sample. However, forensic smokeless powder samples are still limited to being classified as either single or double base powders, based on the absence or presence of nitroglycerin, respectively. In this work, the goal was to develop statistically valid classes, beyond the single and double base designations, based on multiple organic compounds which are commonly encountered in commercial smokeless powders. Several chemometric techniques were applied to smokeless powder GC-MS data for determination of the classes, and for assignment of test samples to these novel classes. The total ion spectrum (TIS), which is calculated from the GC-MS data for each sample, is obtained by summing the intensities for each mass-to-charge (m/z) ratio across the entire chromatographic profile. A TIS matrix comprising data for 726 smokeless powder samples was subject to agglomerative hierarchical cluster (AHC) analysis, and six distinct classes were identified. Within each class, a single m/z ratio had the highest intensity for the majority of samples, though the m/z ratio was not always unique to the specific class. Based on these observations, a new classification method known as the *Intense Ion Rule (IIR)* was developed and used for the assignment of test samples to the AHC designated classes.

Discriminant models were developed for assignment of test samples to the AHC designated classes using *k*-Nearest Neighbors (*k*NN) and linear and quadratic discriminant analyses (LDA and QDA, respectively). Each of the models were optimized using leave-one-out (LOO) and leave-group-out (LGO) cross-validation, and the performance of the models was evaluated by calculating correct classification rates for assignment of the cross-validation (CV) samples to the AHC designated classes. The optimized models were utilized to assign test samples to the AHC designated classes. Overall, the QDA LGO model achieved the highest correct classification rates for assignment of the test samples to the AHC designated classes.

In forensic application, the goal of an explosives analyst is to ascertain the manufacturer of a smokeless powder sample. In addition, knowledge about the probability of a forensic sample being produced by a specific manufacturer could potentially decrease the time invested by an analyst during investigation by providing a shorter list of potential manufacturers. In this work, Bayes' Theorem and Bayesian Networks were investigated as an additional tool to be utilized in forensic casework. Bayesian Networks were generated and used to calculate posterior probabilities of a test sample belonging to specific manufacturers. The networks were designed to include manufacturer controlled powder characteristics such as shape, color, and dimension; as well as, the relative intensities of the class associated ions determined from cluster analysis. Samples were predicted to belong to a manufacturer based on the highest posterior probability. Overall percent correct rates were determined by calculating the percentage of correct predictions; that is, where the known and predicted manufacturer were the same. The initial overall percent correct rate was 66%. The dimensions of the smokeless powders were added to the network as average diameter and average length nodes. Addition of average diameter and length resulted in an overall prediction rate of 70%.

This work is dedicated to my mother – my confidante, my moral compass, my biggest supporter, my most outspoken critic, my friend; Georgette Marie Howell.

I love and miss you beyond words.

*Until we meet again, rest in peace. May 6, 1958 – February 17, 2014.* 

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# LIST OF ACRONYMS

2,4-DNT	2,4-Dinitrotoluene
2-nDIPH	2-Nitrodiphenylamine
2-nsoDIPH	2-Nitrosodiphenylamine
4-nDIPH	4-Nitrodiphenylamine
4-nsoDIPH	4-Nitrosodiphenylamine
AEDPA	Antiterrorism and Effective Death Penalty Act
AHC	Agglomerative Hierarchical Cluster
amap	Another Multidimensional Analysis Package
ATR	Attenuated Total Reflectance
BATFE	Bureau of Alcohol Tobacco Firearms and Explosives
BN	Bayesian Network
caret	Classification and Regression Training
cba	Clustering for Business Analytics
$CH_2Cl_2$	Methylene Chloride
CRAN	Comprehensive R Archive Network
CV	Cross - Validation
DAG	Directed Acyclic Graph
DAG DbPHTH	Directed Acyclic Graph Dibutyl Phthalate
DbPHTH	Dibutyl Phthalate

DNT	Dinitrotoluene
DoPHTH	Dioctyl Phthalate
dRI	Difference in Refractive Indices
EC	Ethyl Centralite
EI	Electron Ionization
FBI	Federal Bureau of Investigation
FID	Flame Ionization Detection
FPR	False Positive Rate
FTIR	Fourier Transform Infrared Spectroscopy
GC	Gas Chromatograph
GC-MS	Gas Chromatography – Mass Spectrometry
gRain	Graphical Independence Networks with the gRain Package
for R	
gRbase	A Common Platform for Graphical Models in R: The
gRbase Package	
GRIM	Glass Refractive Index Measurements
gRim	Graphical Interaction Models
HPD	Heavy Petroleum Distillate
HS-SPME	Headspace Solid Phase Microextraction
IED	Improvised Explosive Device
IIR	Intense Ion Rule

IMS	Ion Mobility Spectrometry
IMS	Ion Mobility Spectrometry
IQR	Interquartile Range
IR	Infrared
kNN	k-Nearest Neighbors
LDA	Linear Discriminant Analysis
LEMS	Laser Electrospray Mass Spectrometry
LGO	Leave-Group-Out
LGOCV	Leave-Group-Out - Cross-Validation
LOO	Leave-One-Out
LOOCV	Leave-One-Out - Cross-Validation
LR	Likelihood Ratio
m/z	Mass-to-Charge
MASS	Modern Applied Statistics with S
MC	Methyl Centralite
MEIS	Most intense Extracted Ion Spectrum
MS	Mass Spectrometer
NAS	National Academy of Sciences
NC	Nitrocellulose
NCFS	National Center for Forensic Science
nESI-MS	Nanoelectrospray Ionization Mass Spectrometry
NFI	Netherlands Forensic Institute

NG	Nitroglycerin
NGG	Nitroguanidine
NIR-HSI	Near Infrared Hyperspectral Imaging
NRC	National Research Council
PA	Polyacrylate
PC	Principal Component
PCA	Principal Components Analysis
pcaPP	Robust PCA by Projection Pursuit
PDMS	Polydimethylsiloxane
PLS-DA	Partial Least Squares – Discriminant Analysis
PSPME	Planar Solid Phase Microextraction
QDA	Quadratic Discriminant Analysis
ROC	Receiver Operating Characteristic
SWGFEX	Scientific Working Group for Fire and Explosions
SEM-EDX	Scanning Electron Microscopy – Energy Dispersive X-Ray
SPME	Solid Phase Microextraction
SRN	Sample Reference Number
TIC	Total Ion Chromatogram
TIS	Total Ion Spectrum
TOF-SIMS	Time-of-Flight – Secondary Ion Mass Spectrometry
TPR	True Positive Rate

UPLC-MS-MS

Ultra Performance Liquid Chromatography – Tandem Mass

Spectrometry

## **CHAPTER 1: INTRODUCTION**

In 2006, the National Academy of Sciences (NAS) assembled a committee comprised of members of the scientific and legal communities. The committee was charged with the task of identifying the disparities and needs of the various disciplines within the forensic science community. The NAS report, "Strengthening Forensic Science in the United States: A Path Forward"[1], was published in 2009, and addressed the need for the development of error rates, associated with the interpretation of evidence, which are founded in scientific methodology. Since forensic analysts play a significant role in criminal proceedings, there is great concern regarding whether the analytical protocols utilized for the evaluation of evidence are in fact rooted in rigorous scientific practice. The advent of nuclear DNA analysis has resulted in a number of exonerations where convictions were previously secured based on expert testimony of forensic scientists. In a number of these cases, testimony was based on the expert's interpretation of observed characteristic patterns in the evidence. The interpretation of the evidence within a number of forensic disciplines is perceived as subjective, and as such are considered to be founded on "less rigorous" practices when compared to DNA analysis.

### 1.1. History of Smokeless Powders

Low explosives are a subset of a larger group known as energetic materials. Low explosives undergo decomposition by deflagration or rapid burning [2], and the material decomposes at rates up to 1000 m/s [3-6]. Confinement of low explosives results in the buildup of heat, and

significant increase in pressure due to the release of gases within the containment. The increase in pressure can lead to explosion. The use of low explosives began with the discovery of black powder, also known as gunpowder. The material is comprised of charcoal, sulfur, and potassium nitrate in the ratio 15:10:75 [5, 7]. The date of invention and the inventor of black powder remains unknown [2, 5, 7], but the material was utilized in a number of applications including rock blasting, demolition, and as propellant charges in civilian and military firearms and artillery [7]. The utility of black powder, however, demonstrated inherent drawbacks as upon discharge, it produced a dense cloud of smoke which betrayed the shooter's position while decreasing visibility [5, 7]. To address the issues associated with using black powder, a number of countries invested resources toward the development of a more stable material which produced significantly less smoke than black powders.

The first smokeless powder was developed by Austrian Chemist, Frederick Volkmann, in 1871 [8]. The powder was manufactured by dissolving wood fiber in nitric acid, followed by a water wash to remove the acid. The by-product was then gelatinized using an ether-alcohol mixture which resulted in the formation of a plastic colloid. The product, known as nitrocellulose (NC), was marketed in Austria, until the Government stopped paying the licensing fees, which caused the facilities to close down. To move away from using black powders, the French Government began using cartridges which were filled with smokeless powders developed by French Chemist, Paul Vielle, in 1886 [5, 7, 8]. Smokeless powders, like their predecessor, are low explosive propellants which are utilized in civilian and military ammunition. There are three smokeless

powder types which differ in their primary energetic materials. A single base powder, the first type developed, has NC as its primary energetic material. Double and triple base powders contain nitroglycerin (NG) in addition to NC, and triple base powders also contain nitroguanidine (NGG). The energetic materials facilitate the explosion, where NC is the base charge, NG increases the powder's energy, and NGG reduces the flame temperature. In addition, NGG regulates the relationship between the powder's energy and flame temperature [4]. Other organic compounds and some inorganics are also blended into the chemical formulation of smokeless propellants, or are otherwise incorporated as separate grains. These compounds function as stabilizers, plasticizers, flash suppressants, deterrents, dyes and opacifiers [4]. Diphenylamine (DIPH) and methyl and ethyl centralite (MC and EC, respectively) are commonly encountered stabilizers in smokeless propellants. Stabilizers increase the shelf life of the propellants by slowing the rate at which NC and NG decompose. Plasticizers such as NG, ethyl centralite (EC) and dibutyl phthalate (DbPHTH) are incorporated to soften the propellant, and to suppress hygroscopicity. Deterrents reduce the initial surface burn rate, as well as, the ignitability and the initial flame temperature. Common deterrents are DbPHTH, dinitrotoluene (DNT), EC and MC, and dioctyl phthalate (DoPHTH). Flash suppressants are usually alkaline earth salts which function to repress secondary flash. The most common opacifier is carbon, and its function is to enhance the burning rate of the material. Dyes are used as markers to aid in the identification of specific brands.

The constituents found in smokeless powders are not proprietary to specific manufacturers; however, the ratio of the additives are controlled by each manufacturer to improve the safety and ballistic capabilities of their propellants [4, 7, 9, 10]. In addition to chemical composition, manufacturer's produce powders of different size and morphology (shape) to optimize performance. The chemical composition, shape, and size affect the propellant's ballistic characteristics such as its stability, pressure, and burn rate. Common smokeless powder shapes, shown in Figure 1, include ball, cylinder, disk (with and without perforation), flattened ball and lamel.

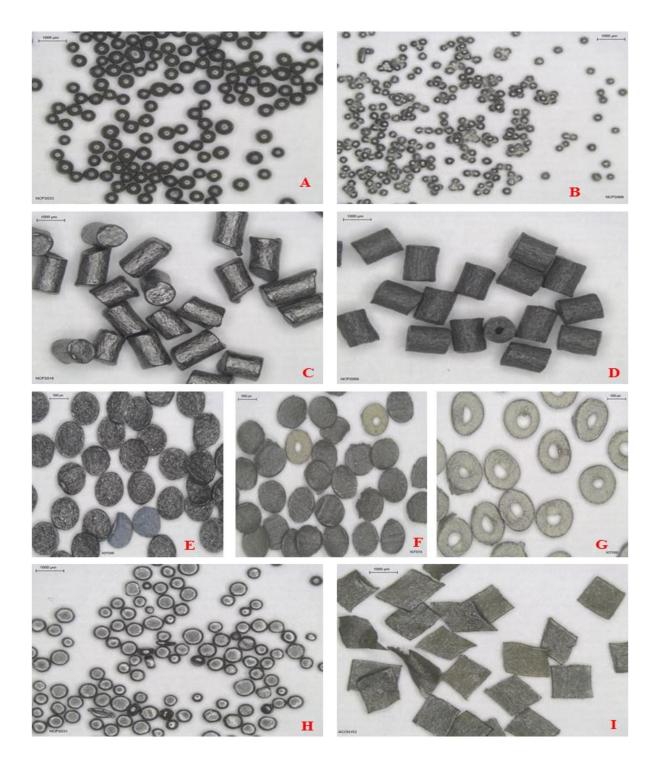


Figure 1: Common smokeless powder shapes Ball (A and B), cylinder (without perforation (C) and with perforation (D)), disk (including marker (E and F) and with perforation (F and G), flattened ball (H) and lamel (I)

As previously discussed, there are three types of smokeless powders. Of the three types, single and double base propellants are commercially available and are easily procured from a number of sporting goods retailers. Accessibility of smokeless powders contributes to their use in the production of improvised explosive devices (IEDs), and the majority of bombing incidents worldwide involve the use of smokeless powders [11-18].

### 1.2. Current Practices and Limitations in Smokeless Powders Analysis

The Scientific Working Group for Fire and Explosions (SWGFEX) has published guidelines for the analysis of intact explosives, and post-blast explosive residues [19, 20]. The guidelines list a variety of analytical techniques which can be utilized for the analysis of explosives, categorized by the information that the technique can potentially provide. There are four categories: "(1) those that provide significant structural and/or elemental information, (2) those that provide limited structural or elemental information, (3) those that provide a high degree of selectivity, and (4) those that are useful but do not fall in either of the other categories" [19]. The guidelines recommend the use of multiple analytical techniques for the identification of smokeless powders and the instrumental technique(s) employed are determined by the categories in which they are listed. Techniques listed in category one are sufficient for identification of the propellant while those listed in categories two to four require one, two, or three supporting techniques, respectively. Gas chromatography-mass spectrometry (GC-MS) and Fourier transform infrared spectroscopy (FTIR) are listed in category one of the guidelines, while stereomicroscopy is listed in category three. In the United States, the accepted laboratory protocol for the analysis and identification of intact smokeless powders involve the macroscopic and microscopic examination of the sample prior to instrumental analysis [4, 5, 10, 19]. Macroscopic and microscopic analyses are performed for the determination of the particle's shape, color and size. Analysis by FTIR is employed primarily for the identification of nitrocellulose, and positive identification is indicative of a smokeless powder. GC-MS is utilized for the identification of organic analytes which are present in the smokeless powder. From a forensic standpoint, NG is currently the most important of the organic analytes as its presence distinguishes single and double base powders. Analysis of a forensic sample using a combination of techniques results in the generation of a short list of potential distributors (Alliant, Hercules, IMR), and in some cases, the identification of a specific brand (Blue Dot, Bullseye, 3031).

#### 1.3. Research Goals

Multiple analytical techniques are employed for the identification of smokeless powders. In forensic casework, the information obtained from combined analyses of smokeless powders is used to generate a short list of potential distributors; however, the potential distributors identified in this list can fall only into one of two categories: single or double base. Currently, there are no established methods for the determination of smokeless powders beyond the single and double base types. Further characterization of smokeless powders could improve their evidentiary value provided that distinct chemical patterns, which are characteristic of these novel groups, can be

identified. Additional class designations could aid an investigation if the novel groups contain fewer distributors than the broader single and double base categories. Such a development could facilitate faster identification of a powder's source. The goal of this work was to investigate whether smokeless powders of the single and double base types can be further classified into statistically valid, chemically distinct groups, based on multiple organic compounds which are commonly encountered in commercial smokeless powders. In addition, discriminant analyses methods were employed to determine classification rates of independent samples into these novel groups. The ultimate goal of an explosives analyst is to ascertain the brand of a forensic smokeless powder sample. In this research, Bayesian Networks were also investigated as an additional tool to be utilized in forensic casework.

## **CHAPTER 2: BACKGROUND**

2.1. Previous Studies in Smokeless Powders Analysis

Smokeless powders identification remains an active area of research due to their high availability, and use in the manufacture of improvised explosive and other incendiary devices. Research is primarily focused on improving current techniques and developing novel techniques for the rapid detection, identification, and classification of smokeless powders products. A brief review of the research is given here.

### 2.1.1 Instrumental Analyses

Scherperel *et al.* developed a nanoelectrospray ionization mass spectrometry (nESI-MS) method for the characterization of smokeless powders [21]. In this study, smokeless powder particles were extracted from seven commercially available cartridges produced by Federal, Smith and Wesson, Winchester, and Remington-Peters. The intact smokeless powder particles were evaluated using stereomicroscopy, as well as, a tandem mass spectrometric method post extraction of the powders with methanol. Using stereomicroscopy, the authors made determinations about the particle size and morphology, color, and surface characteristics, such as texture, for each smokeless powder. The smokeless powders were divided into two groups based solely on their physical characteristics. Another parameter subject to evaluation was the extraction yield. The powders were grouped based on low and high extraction yields, and the authors reported the identical group membership as observed in the groups based on physical appearance. Overall, the authors argue the successful differentiation of seven smokeless powders after considering their physical characteristics, extraction yields, and mass spectral identification of the target analytes. While characterization and differentiation of forensic smokeless powder samples is desirable, it is known that manufacturer's habitually produce smokeless powders with varied physical characteristics and chemical compositions in order to optimize product performance; therefore, these differences are expected, and in fact are typically relied upon for source determination in forensic settings.

In an article published in 2009 [22], Joshi and her group reported the first extraction of smokeless powder additives from the headspace of commercial smokeless powders using a polydimethylsiloxane (PDMS) solid phase microextraction (SPME) fiber. Extraction profiles for each of the smokeless powder target analytes were obtained using SPME-GC-MS, and the powder extracts were evaluated using SPME Ion Mobility Spectrometry (IMS). Successful detection of the target analytes: DIPH, EC, and 2,4-Dinitrotoluene (2,4-DNT) was achieved using the SPME-IMS technique. The same research group designed a dynamic planar solid phase microextraction (PSPME) to target and extract volatile chemicals from the headspace of commercial smokeless powders [23]. Dynamic sampling, an alternative approach to traditional SPME sampling, was achieved by exposing the fiber to a stream of gas to facilitate adsorption of volatile compounds unto the fiber's surface. The planar design of the fiber provided a larger surface area for extraction of the organic compounds. The extraction and detection of DIPH, EC,

and 2,4-DNT using the PSPME fiber was compared to the extraction and detection of the same compounds using the manufacturer's Teflon filters which were provided by the manufacturer with the IMS. The PSPME fiber demonstrated better extraction and detection for DIPH and 2,4-DNT when compared to the Teflon filters; however, their performances were equivalent for EC. In real world application, methodology for the rapid detection and identification of smokeless powder target analytes is in demand. The utility of IMS is widely demonstrated in a number of applications, most notably at screening checkpoints in the airport. The rapid screening, and high sensitivity of the method allows for detection and identification of a number of volatile organic compounds; however, the technique is employed strictly for the purposes of screening, therefore, additional analytical techniques are necessary for determination of source.

Chang *et al.* developed a headspace SPME (HS-SPME) method for the extraction of volatile organics in smokeless powders [24]. The SPME fibers were subjected to an optimization process in an attempt to maximize the amount of each compound extracted from the samples. The group employed a multivariate design to investigate parameters including sample weight, incubation time, extraction time, and sample temperature. The first step of the multivariate optimization process involved the study of the aforementioned parameters to evaluate their interaction, and to determine which of them were influential. The second step of the multivariate process was focused on optimizing the parameters which were determined to have the most influence. Three types of fibers; two PDMS fibers of different dimensions, and a polyacrylate (PA) fiber were used in the study. Smokeless powder particles extracted from commercial cartridges were also

utilized, and separation of the constituents in each sample was achieved using gas chromatography. Flame ionization detection (FID) was used for determination of the retention times for each constituent, and mass spectrometry was employed for further confirmation of their identities. Observations made from this work demonstrated that increasing the sample's extraction time and temperature resulted in higher extractions of the target analytes, as evidenced by an increase in their peak areas.

Ultra performance liquid chromatography with tandem mass spectrometry (UPLC-MS-MS) has also been used for the separation and detection of additives in smokeless powders [25]. Using this technique, Thomas *et al.* was able to identify 18 target analytes attributable to smokeless powders. Smokeless powder brands were characterized and differentiated based on the presence or absence of specific additives. In addition, the authors report the ability to differentiate lots of specific brands based on the proportions of the organic compounds between the lots.

The development of new methodology for the detection, and identification of smokeless powder target analytes is highly desirable in forensic investigations. Characterization of smokeless powders is achieved by a suite of analytical methods including those employed for the determination of the powder's physical characteristics. While chemical analysis allows for identification of the organic volatiles, which may potentially lead to identification of the powder brand, there is still a need for probabilistic inference for characterization of forensic smokeless powder samples.

### 2.1.2 Chemometric Studies

The term "chemometrics" which originated in 1972 [26] is defined as "a chemical discipline that uses mathematics, statistics and formal logic (a) to design or select optimal experimental procedures; (b) to provide maximum relevant chemical information by analyzing chemical data; and (c) to obtain knowledge about chemical systems" [27]. The application of chemometric methodology to the analysis of smokeless powders provides an avenue for the statistical analysis, and probabilistic characterization of smokeless powders. Research has been conducted previously for the characterization of smokeless powders using chemometric methods, and a review is given here.

Mahoney *et al.* [28] applied principal components analysis (PCA) to data obtained from analysis of three smokeless powders, four black powders, and two black powder substitutes using timeof-flight secondary ion mass spectrometry (TOF-SIMS). The scores associated with the first and second principal components (PC), which reproduced 87% of the variance within the data, were used to generate a plot depicting separation of the smokeless powders. Based on the scores and loadings plots, the authors argue the ability to differentiate between the smokeless powders; however, this is not surprising since two of the three powders were of the double base designation and a distinction can always be made between single and double base powders based on nitroglycerin's absence or presence, respectively. Furthermore, it is common knowledge that manufacturer's vary the ratios of smokeless powder additives during the manufacturing process; thus, smokeless powders can be distinguished based on the different ratios of the additives. No chemical distinction was made between the black powders and black powder substitutes using PCA; however, a distinction was made based on the differences in their grain sizes.

PCA was also employed in a smokeless powders study conducted at Temple University [29]. In this study, five commercially available smokeless powders were analyzed using laser electrospray mass spectrometry (LEMS), and ten mass spectra from each smokeless powder were retained for PCA analysis. For each of the smokeless powders, three randomly selected mass spectra were designated as the training set, and the remaining spectra were designated as the test set. PCA was performed on the training set, and the scores associated with the first, second, and third PCs were used to construct PCA space. The product of the mean-centered test data, and the training set eigenvectors were projected into the PC space for classification of the smokeless powder samples. PCA is an unsupervised multivariate technique which is used to reduce data dimensionality. Reduction of the data is achieved by projecting higher dimensions onto lower dimensional space. The goal of PCA is to find a set of variables which reproduce maximum variance within the data. Though PCA seeks these variables which are representative of the original data, which can provide significant information about inherent groups, it is not sufficient for classification. Additionally, the authors utilized mass spectral data for the five smokeless powders for both construction of the PCA space, and for projection into the PCA space; therefore, it is not surprising that the training and test sets grouped within the same PCA space since both the test and training data were collected from the same sample set.

Young *et al.* has used receiver operating characteristic (ROC) curves as a tool for comparing the performance of PSPME fibers to traditional SPME using different instrumental techniques [30]. Smokeless powders and some high explosives were utilized in this study. True positive rates (TPR) and false positive rates (FPR) were calculated and used to construct ROC curves for each experimental scenario. The authors were able to demonstrate the equivalent performance of PSPME-IMS for explosives detection, compared to traditional SPME methods, through the evaluation of the ROC curves.

A collaborative study conducted in Spain and Denmark used near infrared hyperspectral imaging (NIR-HSI) and partial-least squares discriminant analysis (PLS-DA) for detection and classification of explosive residue in handprints [31]. Explosives considered in the study included ammonium nitrate, black powder, dynamite, and single and double base smokeless powders. Hyperspectral images of explosive contaminated handprints were collected and preprocessed to eliminate features in the spectra, such as noise, dead pixels, spikes, and scattering effects which are produced during operation of the system; PLS-DA was applied to the pretreated data for classification of the explosive residues. The method demonstrated the ability to distinguish smokeless powders from the other explosive types; however, little to no distinction was observed for the different smokeless powder designations. The authors attributed this observation to the high percentage composition of nitrocellulose in the smokeless powder samples.

### 2.2. Instrumentation

As previously mentioned, GC-MS is a category one analytical method prescribed in the SWGFEX guidelines for the separation and identification of target analytes in forensic smokeless powder samples [19]. Separation of the components in a sample is achieved by the gas chromatograph (GC), and each component is identified by the mass spectrometer (MS) based on its fragmentation pattern. During analysis, a liquid sample is introduced to the GC via the injection port where it is vaporized prior to entering a capillary column which contains a stationary phase. The capillary column is housed in a temperature programmable oven. The vaporized sample is transported through the capillary column by means of a carrier gas which functions as the mobile phase. Components within the sample are retained in the column based on their affinities for either the stationary or mobile phase [32, 33]. The components in the sample elute, or exit the column, at different times based on mass, where lighter (low boiling point) compounds elute prior to heavier (high boiling point) compounds. The total time a compound is retained in the column is known as its retention time. Separation of the components in a sample can be optimized by adjusting the oven temperature, the column type, and the carrier gas flow. The chromatographic data is recorded as a total ion chromatogram (TIC), which displays the retention time of each compound within the sample [32]. Once the compounds exit the GC, they are passed into the MS via a transfer line. The MS is comprised of (1) the ion source, (2) the mass analyzer, and (3) the detector [32]. Using electron ionization (EI), each component is bombarded with a 70eV electron beam in the ion source, which causes weaker bonds to break resulting in the formation of ions [34]. Mass-to-charge (m/z) ratios are typically

used to characterize formed ions. The ions travel to the mass analyzer where specific m/z ratios are selected and transferred to the detector [35]. The number of ions corresponding to each m/zratio is recorded by the detector. For each of the components which are introduced to the MS, a mass spectrum is generated. A mass spectrum represents the abundance of the ions which are detected for its corresponding m/z ratio. The TIC for a single base smokeless powder is shown in Figure 2, where the retention times are displayed on the *x*-axis, and abundance is shown on the *y*axis. Figure 3 represents the mass spectrum corresponding to the 2,4-DNT peak between retention times 7.730 and 7.754 minutes. The m/z ratios are shown on the *x*-axis, and their abundance is displayed on the *y*-axis.

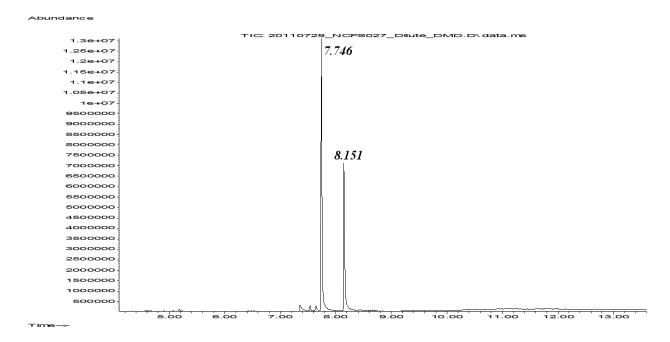
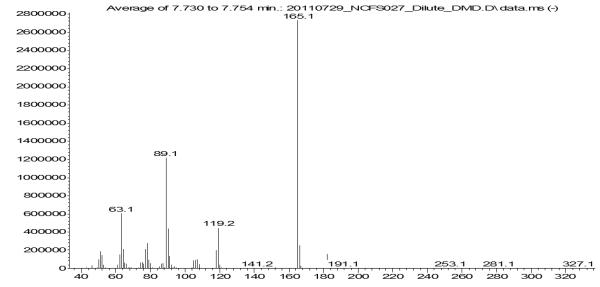


Figure 2: TIC for a commercial single base smokeless powder The 2,4-DNT was identified at retention time 7.746 minutes, and DIPH was identified at retention time 8.151 minutes

Abundance



m⁄z–>

Figure 3: Mass spectrum corresponding to the 2, 4-Dinitrotoluene peak The 2,4-DNT peak was recorded between retention times 7.730 and 7.754 minutes. Three major ions associated with 2,4-DNT (m/z 165, m/z 89 and m/z 63) are shown.

### 2.3. Total Ion Spectrum

Current laboratory protocol for the identification of smokeless powder target analytes involves the extraction and analysis of smokeless powder, and subsequent interpretation of the TIC. Although the TIC provides significant structural information for the components which are present in a sample, the retention times can shift between intra- and inter-laboratory analyses. The total ion spectrum (TIS) has been utilized in this work, and its use eliminates the issue associated with shifting retention times. The utility of the TIS for the evaluation of data has been demonstrated [36-38]. Figure 4 illustrates the partial reconstruction of an original GC-MS dataset (shown in blue) for a commercial smokeless powder, as well as, the TIC (shown in red) and TIS (shown in black), which correspond to the specified region of data. The TIC is calculated by summing the intensities at each mass scan across all m/z ratios, while the TIS is calculated by summing the intensities for each m/z ratio across the entire chromatographic profile. Data preprocessing methods may be utilized for treatment of the TIS data prior to statistical analyses.

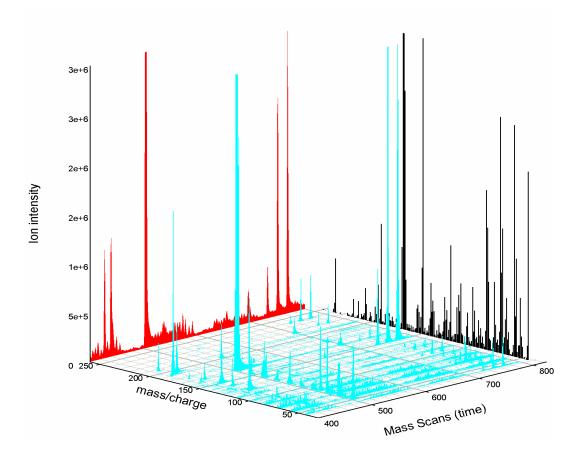


Figure 4: Three-Dimensional reconstruction of a partial GC-MS dataset for a commercial smokeless powder The GC-MS data is shown in blue, the TIC and TIS corresponding to the region of GC-MS data are shown in red and black, respectively.

### 2.4. Cluster Analysis

Cluster analysis is an unsupervised learning method which is employed for the determination of inherent patterns or groupings within data. The method is unsupervised because there is no prior knowledge about groupings or clusters in the data. Cluster analysis considers the distance of objects relative to each other in multidimensional space, and shorter distances are indicative of highly similar objects. The goal of cluster analysis is to identify inherent groups, or clusters, where the similarities are maximized within the clusters, but minimized between the clusters [26, 39, 40].

Several metrics are available to be used to calculate the distances between objects [26, 39-42]; however, correlation distance was used in this work and will be discussed here. The correlation distance, also known as the "Centered Pearson", is described by Equation 2.1, where r is the Pearson correlation coefficient, and  $d_{corr}$  is the distance. The coefficient which describes the linear relationship between two variables can range from -1 to 1 [26, 27]; therefore,  $d_{corr}$  can range from 0 to 2. If a variable, x, is perfectly linearly related to another variable, y, then r is equal to 1 [26]. Equation 2.2 is used to calculate r, where n is the total number of samples. The correlation distance between x and y is measured for each sample, i, where  $\bar{x}$  and  $\bar{y}$  represent the means of the variables for all samples considered.

$$d_{corr} = 1 - r \tag{2.1}$$

$$r = \frac{\Sigma_{i=1}^{n} (x_{i} - \bar{x})(y_{i} - \bar{y})}{\sqrt{\Sigma_{i=1}^{n} (x_{i} - \bar{x})^{2} \Sigma_{i=1}^{n} (y_{i} - \bar{y})^{2}}}$$
(2.2)

A number of clustering methods exist which may be applied for analysis of data [39]; however, agglomerative hierarchical cluster (AHC) analysis was employed in this research and will be further discussed. In AHC analysis, the clustering process is initiated by assigning each object as

an individual cluster. The distances between the clusters are then calculated, and similar objects, represented by shorter distances, are merged to form a new cluster. The clustering process ends when a single cluster remains [39, 43-46]. At each step of the clustering process, the distances between newly formed clusters are recalculated as specified by a linkage metric [44]. Several linkage metrics are available to facilitate clustering of the objects; however, average and complete linkage will be discussed. Average linkage is determined by calculating the average distance between objects within the clusters. There are two alternatives for calculation of the distances based on average linkage [40]. In this research, the un-weighted average was calculated. Un-weighted average means that the number of objects within each of the clusters was considered in the calculation [46, 47]. The weighted average divides the summed distances by two, and does not account for the number of objects within the clusters [40]. Complete linkage is also referred to as furthest neighbor method. The method considers the largest distance between objects in two independent clusters during the clustering process [39, 46].

The most appropriate distance and linkage combination may be determined by calculating the cophenetic correlation coefficient. The coefficient, which ranges from 0 to 1, describes the relationship between the distances in the original data matrix and the clustered distance matrix. The distances in the clustered matrix most accurately reflect the distances in the original matrix when the coefficient is equal to 1. The cophenetic correlation coefficient is calculated using the Pearson correlation coefficient [27, 48, 49], Equation 2.2.

The results obtained from cluster analysis of data can be shown graphically in a binary hierarchical tree, or dendrogram. Objects are displayed as "leaves" in the dendrogram, and "branches" represent the linkage of the objects [39, 44]. Optimal leaf ordering can be used to "maximize the sum of similarity of adjacent elements" [43]. Figure 5 represents the dendrogram achieved from cluster analysis of six objects using correlation distance and average linkage. Optimally ordered objects are shown along the *x*-axis, while the *y*-axis is the clustering height, or distance, at which the objects were merged [47]. Low clustering heights are indicative of objects which were merged initially during the clustering process. An example is shown Figure 5, where objects 2 and 5 initially merged to form a cluster, while objects 1 and 3 merged to form a separate cluster. The cluster containing objects 2 and 5 was merged with object 4 to form a new cluster, which was subsequently merged with object 6 to create a new cluster. The merging process was terminated upon the formation of a single cluster comprised of the six objects.

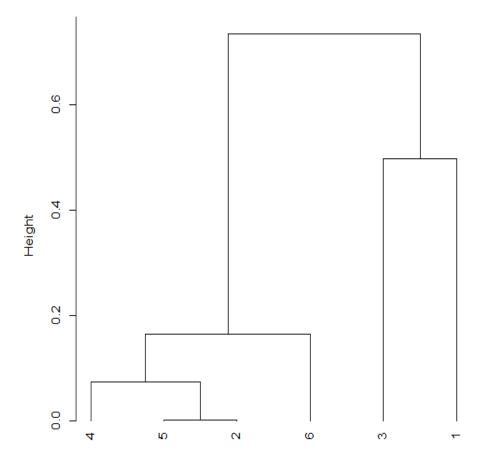


Figure 5: Example dendrogram of six objects clustered using correlation distance and average linkage

Similarities can be calculated for the objects using Equation 2.3, where s is the similarity and d is the distance previously calculated in the clustering step. Correlation distance, Equation 2.2, which can range from 0 to 2, was used in this research; therefore, similarity values can range from 0 to 1. Pairwise comparison of identical objects will yield a similarity equal to 1.

$$s = 1 - \frac{d}{2} \tag{2.3}$$

To visualize the relative similarities of objects within and between clusters, heat maps can be generated [50, 51]. Figure 6 is an exemplar heat map for the six objects which were clustered using correlation distance and average linkage.

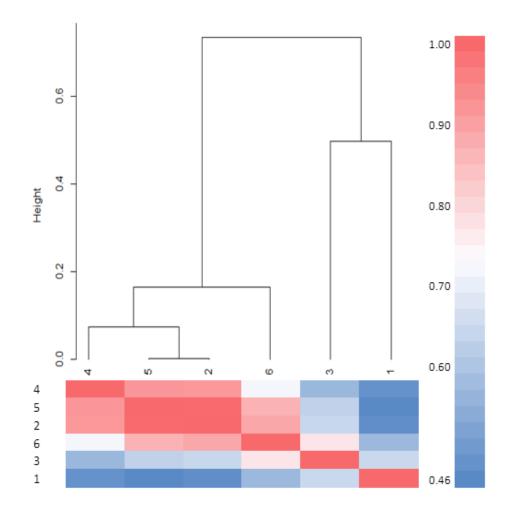


Figure 6: Heat map of the six objects clustered using correlation distance and average linkage

The diagonal of the heat map represents the similarities for pairwise comparisons of identical objects; while off diagonal values indicate different object comparisons. Two clusters result when the dendrogram is cut at a link height of 0.6. Objects in cluster 1 (that is, objects 2, 4, 5 and 6) exhibit high similarity in comparison to other objects within the cluster, but low similarity to objects in cluster 2 (i.e., objects 1 and 3). Additionally, object 3 is more similar to object 6 than to object 1, even though objects 1 and 3 are merged together in cluster 2. The arrangement of the objects makes sense as optimal leaf ordering was applied during cluster analysis of the data.

### 2.5. Discriminant Analysis

Discriminant analysis methods are known as supervised techniques because prior knowledge of group (class) membership is required for sample assignment [26, 40, 52]. The discriminant analysis methods which were utilized in this work are: the intense ion rule, *k*-Nearest neighbors, linear discriminant analysis, and quadratic discriminant analysis.

### 2.5.1. The Intense Ion Rule

The intense ion rule (IIR) has been developed for use in this work for sample assignment to known classes. The IIR considers the relative intensities of select ions, and sample assignment is achieved based on visual inspection of these ion intensities. The criterion for assignment of a sample to a given class using the IIR was developed based on the results obtained from cluster analysis. A detailed description of the methodology will be given in section 4.2.3.

### 2.5.2. k-Nearest Neighbors

*k*-Nearest Neighbors (*k*NN) is a mathematically simple classification method for assignment of an unknown sample, *x*, to a known class. The method works by calculating the distance between *x* and objects of known class membership, in multidimensional space, as specified by a distance metric. A number of metrics may be used for the calculation, but Euclidean distance is most frequently employed [26, 39, 40, 49, 53]. The distance between *x* and all objects in the data set are calculated, and *x* is assigned to the corresponding class that contains the majority of the *k* nearest neighbors [26, 39, 49, 53]. Figure 7 illustrates class assignment of object *x* when k = 3. In this case, *x* is classified as a square.

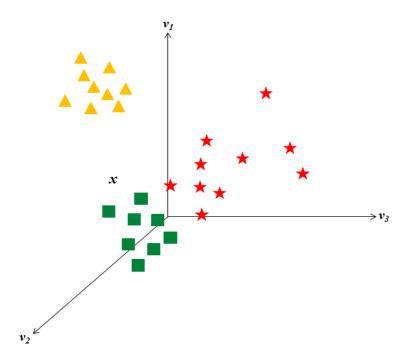


Figure 7: Classification of object *x* using kNN, k = 3

Optimization of k is achieved by performing cross-validation (CV) on the data set of known class membership using different values for k [39, 53]. The value for k should not exceed the number of samples in the smallest class; and k is optimized when the number of misclassifications is minimized [53].

The *k*NN method is advantageous due to its computational simplicity, easy application to multiclass problems, and its lack of statistical assumptions, such as, normal distribution in the data; however, some limitations are associated with its use. One limitation arises if there is a significant difference in the number of objects within each class; that is, the volume occupied by the objects in the class with more members may be larger than the volume occupied by objects in the remaining classes, so *x* can incorrectly assign to the class with the greatest number of members based solely on spatial distribution [40, 49]. Another limitation is the assumption of equal significance for each variable considered in the calculation. This is problematic because not all the variables may be diagnostic of class membership. To overcome this issue, diagnostic variables may be selected prior to classification. Finally, *k*NN does not account for variance within the data. Despite these limitations, *k*NN is favorable as a classification method based on its simplicity. Additional classification methods can be utilized for comparison of the results to those obtained using *k*NN.

### 2.5.3. Bayesian Discriminant Analysis

Bayesian linear and quadratic discriminant analysis (LDA and QDA, respectively) consider prior and posterior probabilities in the classification of an unknown object. Prior probabilities are the natural or theoretical probabilities of an object belonging to a group, and it is reasonable to assume equal prior probabilities before performing the calculation [39]. For classification, decision boundaries are constructed between the classes being considered. The decision boundary is constructed at the point where the posterior probabilities for the classes are equal [39]. For LDA, the decision boundary is represented by linear discriminant functions, while quadratic discriminant functions are generated for QDA. During classification, posterior probabilities are assigned to the object for each class considered, and the object is assigned to the class with the largest posterior probability. In addition to probabilities, LDA and QDA take into account the covariance for the classes. LDA requires the covariance matrices to be pooled for all classes considered. In order to pool the matrices, the covariance for the classes must be equivalent. Covariance matrices are considered equivalent when the 95% confidence ellipsoids have equal volume and orientation in space, corresponding to equal variance and covariance, respectively. If the covariance matrices are not equal, QDA is more suitable for classification [49].

Bayesian LDA and QDA are hard classification techniques that assign class membership based on a discriminant function, g(x) [39]. Hard classification methods require the assignment of an object to one class; thus, neither multiple class assignment nor failure to assign to a class are options. An object is assigned to a class  $\omega_i$  given  $g_i(x) > g_j(x)$  for all classes, where each class is unique. The variable, x, describes a vector of parameters for each case being considered [54]. Equation 2.4 yields the minimum-error-rate classification function, where  $p(x \mid \omega_i)$  is the classconditional probability density, and  $p(\omega_i)$  is the prior probability of encountering class  $\omega_i$ .

$$g_i(x) = \ln[p(x|\omega_i)] + \ln[P(\omega_i)]$$
(2.4)

For multivariate normal class-conditional probability densities, the discriminant function is given by Equation 2.5.

$$g_i(x) = -\frac{1}{2} \ln[|\Sigma_i|] - \frac{1}{2} (x - \mu_i)^t \Sigma_i^{-1} (x - \mu_i) + \ln[P(\omega_i)]$$
(2.5)

In Equation 2.5,  $\mu_i$  represents the mean vector, while  $\Sigma_i$  and  $|\Sigma_i|$  are the covariance matrix, and the determinant of the covariance matrix, respectively, for class  $\omega_i$ . The squared Mahalanobis distance from x to the center of class  $\omega_i$  is given by the term  $(x - \mu_i)^t \Sigma_i^{-1} (x - \mu_i)$ . Equation 2.6 represents the discriminant function which is quadratic in x, and is utilized for the multivariate normal case where the covariance matrices are not equivalent.

$$g_i(x) = -\frac{1}{2} \ln[|\Sigma_i|] - \frac{1}{2} x^t \Sigma_i^{-1} x + x^t \Sigma_i^{-1} \mu_i - \frac{1}{2} \mu_i^t \Sigma_i^{-1} \mu_i + \ln[P(\omega_i)]$$
(2.6)

For equivalent covariance matrices, the term  $x^t \Sigma_i^{-1} x$  simplifies to  $x^t \Sigma^{-1} x$  to represent a covariance matrix which is the same across all the classes considered. The resulting discriminant

function, shown in Equation 2.7, is linear in x. As stated previously, the object will be assigned to the class with the largest posterior probability, which is equivalent to the largest discriminant function [54].

$$g_i(x) = -\frac{1}{2} \ln[|\Sigma_i|] + x^t \Sigma_i^{-1} \mu_i - \frac{1}{2} \mu_i^t \Sigma_i^{-1} \mu_i + \ln[P(\omega_i)]$$
(2.7)

## 2.5.4. The Likelihood Ratio Test

The equivalence of class covariance matrices determines which classification method, LDA or QDA, is suitable for class assignment of objects. The likelihood ratio test is employed to determine whether the covariance matrices between two classes are equivalent. The likelihood ratio test statistic is calculated using Equation 2.8, where  $n_1$  and  $n_2$  represent the sample populations for classes 1 and 2, respectively.

$$-2\log_e \lambda = (n_1 + n_2)\log_e \left| \hat{\Sigma} \right| - n_1 \log_e \left| \hat{\Sigma}_1 \right| - n_2 \log_e \left| \hat{\Sigma}_2 \right|$$
(2.8)

The maximum likelihood estimates which are calculated jointly  $(\hat{\Sigma})$  and individually  $(\hat{\Sigma}_1 \text{ and } \hat{\Sigma}_2)$ , for the two classes under consideration, are given in Equations 2.9, 2.10, and 2.11, respectively.

$$\hat{\Sigma} = \frac{1}{n_1 + n_2} (C_1 + C_2) \tag{2.9}$$

$$\hat{\Sigma}_1 = \frac{1}{n_1} C_1 \tag{2.10}$$

$$\hat{\Sigma}_2 = \frac{1}{n_2} C_2 \tag{2.11}$$

Variables  $C_1$  and  $C_2$ , shown in Equations 2.12 and 2.13, represent the product matrices for classes 1 and 2, respectively. The product matrix is calculated by multiplication of the mean centered data and its transpose for each class being considered.

$$C_1 = \sum_{i=1}^{n_1} (x_i - \bar{x})(x_i - \bar{x})'$$
(2.12)

$$C_2 = \sum_{i=1}^{n_2} (y_i - \bar{y})(y_i - \bar{y})'$$
(2.13)

In Equation 2.8, the likelihood ratio test statistic,  $-2log_e\lambda$ , follows a chi-squared distribution with  $\frac{1}{2}p(p+1)$  degrees of freedom; p represents the number of variables. In testing the null hypothesis, which states that the covariance matrices are equivalent, the calculated test statistic is compared to a chi-squared table statistic. The null hypothesis is accepted if the table statistic is less than the test statistic [55].

#### 2.6. The Probability of the Manufacturer

In criminal proceedings, the role of the forensic scientist is limited to the evaluation and interpretation of evidence which is presented to them; that is, the forensic scientist is solely concerned with the match probability between a questioned and known sample. In nuclear DNA analysis, it is standard practice to associate probabilities with one's findings. In other disciplines, forensic testimony is most often based on the characteristic patterns observed in the evidence, as well as, the credentials and expertise of the analyst. Probabilistic interpretation of evidence is increasingly sought after in forensic testimony, and Bayes' theorem provides an avenue to express the value of the evidence based on probabilities.

#### 2.6.1. Bayes' Theorem and the Likelihood Ratio

Bayes' theorem, derived from the third law of probability, relates conditional and unconditional probabilities. The general form of Bayes' theorem is given in Equation 2.14.

$$P(X|Y) = \frac{P(Y|X)P(X)}{P(Y)}$$
(2.14)

Here, the | symbol means "given", and the expression reads "the probability that event X occurred given event Y, is equal to the product of the probability that event Y occurred given X and the probability that event X occurred, divided by the probability that event Y occurred." In a criminal case, the role of prosecution is to prove a suspect's guilt through the presentation of evidence, while the defense presents alternative arguments to prove the suspect is not guilty. The presumption of guilt, G, can be made based on the evidence, E, and the competing hypotheses of the prosecution and defense may be expressed as an odds ratio, Equation 2.15. The numerator represents the prosecution hypothesis, the probability of the suspect's guilt given the evidence;

while the denominator represents the defense hypothesis, the probability that the suspect is not guilty given the evidence [56].

$$Odds(G|E) = \frac{P(G|E)}{P(\bar{G}|E)}$$
(2.15)

The unconditional and conditional probabilities mentioned previously are equivalent to prior and class-conditional probabilities, respectively [54, 57]. Equation 2.16 describes the posterior probability of a suspect's guilt given the evidence, P(G|E), as the product of the class-conditional probability, P(E|G), and the prior probability, P(G), divided by the sum of P(E|G)P(G) and  $P(E|\bar{G})P(\bar{G})$ . The same expansion of the argument applies for the defense hypothesis, Equation 2.17. The ratio of the prosecution and defense hypothesis Equation 2.18 is simplified to Equation 2.19.

$$P(G|E) = \frac{P(E|G)P(G)}{[P(E|G)P(G)] + [P(E|\bar{G})P(\bar{G})]}$$
(2.16)

$$P(\bar{G}|E) = \frac{P(E|\bar{G})P(\bar{G})}{[P(E|G)P(G)] + [P(E|\bar{G})P(\bar{G})]}$$
(2.17)

$$\frac{P(G|E)}{P(\bar{G}|E)} = \frac{\frac{P(E|G)P(G)}{[P(E|G)P(G)] + [P(E|\bar{G})P(\bar{G})]}}{\frac{P(E|\bar{G})P(\bar{G})}{[P(E|G)P(G)] + [P(E|\bar{G})P(\bar{G})]}}$$
(2.18)

$$\frac{P(G|E)}{P(\bar{G}|E)} = \frac{P(E|G)}{P(E|\bar{G})} \frac{P(G)}{P(\bar{G})}$$
(2.19)

$$\frac{P(G|E)}{P(\bar{G}|E)} = \frac{P(E|G)}{P(E|\bar{G})}, \text{ where } P(G) = P(\bar{G}) = 0.5$$
(2.20)

$$\frac{P(G|E)}{P(\bar{G}|E)} \frac{P(\bar{G})}{P(G)} = \frac{P(E|G)}{P(E|\bar{G})}, \text{ where } P(G) \neq P(\bar{G})$$
(2.21)

The left side of Equation 2.19 represents the ratio of the posterior probabilities,  $\frac{P(G|E)}{P(G|E)}$ , which is equal to the product of the likelihood ratio (LR),  $\frac{P(E|G)}{P(E|G)}$ , and the prior odds,  $\frac{P(G)}{P(G)}$ . If the prior probabilities for the prosecution and defense hypotheses are equal; that is,  $P(G) = P(\overline{G}) = 0.5$ , the prior odds are equal to 1 and Equation 2.19 is simplified to Equation 2.20. In this equation, the ratio of the posterior probabilities, shown on the left, is equal to the LR, shown on the right. Likewise, when the prior probabilities are not equal; that is,  $P(G) \neq P(\overline{G})$ , Equation 2.19 is rearranged to yield Equation 2.21. In this case, the LR is equal to the product of the posterior odds, and the inverse of the prior odds. The LR, which is directly dependent on the evidence and the propositions to which that evidence lends support, can be used to express the value of the evidence [56]. An LR greater than 1 lends support to the prosecution hypothesis; an LR less than 1 lends support to the defense hypothesis, and an LR equal to 1 does not discriminate between the prosecution and defense hypotheses [58].

### 2.6.2. Bayesian Networks

Bayes Nets (BNs) are also referred to as causal networks, or belief networks [54]. BNs are graphical representations which encode probabilistic relationships between component variables, or events of interest. In constructing a BN, one must "(1) correctly identify the goals of modeling, (2) identify many possible observations that may be relevant to the problem, (3) determine what subset of these observations is worthwhile to model, and (4) organize the observations into variables having mutually exclusive and collectively exhaustive states" [59]. The structure of the BN, known as a directed acyclic graph (DAG), is comprised of nodes and arcs which collectively describe the probabilistic relationships between the component variables. Figure 8 illustrates a BN representing the relationships between variables A, B, C, and D.

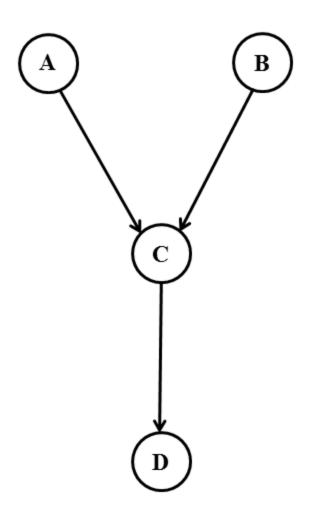


Figure 8: Illustration of a BN for variables A, B, C, and D

In figure 8, the variables are represented as nodes, and the causal dependencies between the variables are represented by arcs, which are illustrated as arrows in the graphical model. Here, the nodes that do not have arcs directed into them are referred to as parent nodes, while nodes with directed arcs are known as child nodes. Parent nodes are conditionally independent of other nodes in the model; child nodes are conditionally dependent on their parent nodes, and

conditionally independent of other child nodes given their parents. Probability tables are associated with each node within the graphical model; where tables associated with parent nodes encode prior probabilities, and tables associated with child nodes encode class-conditional probabilities [60]. Figure 9 depicts variables A, B, C, and D and their associated probability tables. Within the model, uppercase letters represent discrete variables, or events. The number of states, or possible outcomes for each event, is depicted in the associated probability table as lowercase letters.

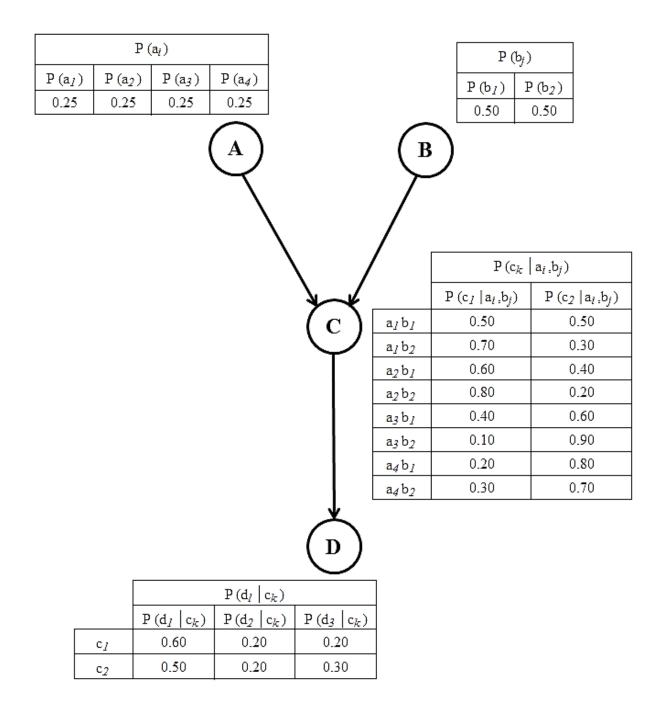


Figure 9: Illustration of a BN for variables A, B, C, and D with their associated probability tables Tables associated with parent nodes A and B encode prior probabilities for nodes A and B, respectively. Tables associated with child nodes C and D encode class-conditional probabilities for nodes C and D, respectively.

Using a BN, and through the application of Bayes theorem, determinations can be made about the probability of any configuration of variables in the joint distribution. Bayes' Theorem serves as a simple tool for updating the posterior probability of a given event when new evidence is observed. The calculations are easy to perform for a simple problem; however, the calculations become tedious for problems where inference needs to be made for a collection or sequence of events. In addition, the calculation becomes more difficult as the number of states for a given event increases. Bayesian networks can be used to perform the calculations. Here, the design of the network is important to ensure that the correct prior, and class-conditional probabilities, are utilized for the inference problem under consideration. Once evidence is observed, the network is instantiated in order to update the posterior probability. That is, the prior probabilities are updated to posterior probabilities through observation of the evidence.

#### 2.6.2.1. Bayes Nets and the Likelihood Ratio in Forensic Science

As previously discussed, the value of evidence may be expressed by the LR [56, 58]; that is, the LR is indicative of the level of discrimination between alternative hypotheses. BNs and the LR have been utilized in forensic application, and a review is given here.

In a two part publication, Beidermann and colleagues used BNs in the forensic investigation of fire incidents. In the first installment [61], Beidermann *et al.* made the assumption that a flammable liquid was detected in a fire debris sample. The proposed BN provided a means for reconsidering the degree of belief in propositions that were not directly observed, in light of the

detection of the flammable liquid. The results of this work demonstrated the utility of BNs for the representation of the relationship between a set of variables, each representing relevant propositions for the forensic fire debris problem. Additionally, this work demonstrated that the strength of a causal relationship can be expressed from examination of the BN. In the second installment [62], Beidermann et al. used BNs to evaluate forensic evidence collected from two separate fire incidents. The first incident involved the detection of terpenes at the fire scene. The authors constructed a BN to evaluate the weight of the evidence, detected terpenes, by considering a number of additional propositions. The propositions taken into consideration included, but were not limited to, fire cause, the presence of terpenes at the sampling point, background presence of terpenes at the sampling point, and detected terpenes. Each proposition was represented as a node in the BN. Probability tables were generated for each of the nodes, and instantiation of the "detected terpenes" node demonstrated strong support for the proposition that terpenes were present at the sampling point. The second BN was constructed to evaluate the cause of a fire after gasoline and heavy petroleum distillate (HPD) were detected in a fire debris sample. Instantiation of the "detected HPD and gasoline" node resulted in high posterior probabilities supporting the hypothesis that the fire resulted from human action. Overall, the authors argue the utility of BNs for introducing scientific rigor where forensic questions were previously answered solely by expert opinions.

Zadora has applied BNs and the LR in the evaluation of evidentiary value of forensic glass fragments [63]. Data collected from glass refractive index measurements (GRIM), and scanning

electron microscopy–energy dispersive x-ray (SEM-EDX) spectrometry were utilized in this study, and Zadora demonstrated the utility of BNs for comparison of alternate hypotheses, and for classification of the glass samples. For analysis of the glass fragments using the GRIM method, Zadora calculated the difference in refractive indices (dRI) before and after a simulated annealing process. The result of this calculation, dRI, was used for comparison and classification of the glass fragments, and Zadora noted that if dRI could not be determined, classification would not be possible. Regarding spectral data obtained from the SEM-EDX, Zadora argued that evaluations should be based solely on the LR; that is, attempts at classification increased the complexity of the network, causing a loss in simplicity compared to the LR.

Zadora has also applied BNs to classification of diesel fuel and kerosene samples; for the comparison of car paint, and for the comparison of fiber samples [64]. The results in this work demonstrated that BNs can be used for performing LR calculations for the evaluation of data when there is limited information about the analyzed objects.

BNs will be utilized in this research to calculate posterior probabilities of smokeless powders belonging to specific manufacturers using powder properties which are controlled by the manufacturer during production.

# **CHAPTER 3: EXPERIMENTAL**

### 3.1. Smokeless Powders Database

Increased concerns about incidents of terror, such as the bombing of the World Trade Center in 1993, and the 1995 bombing of the Murrah Federal Building in Oklahoma City, led to the passing of the Antiterrorism and Effective Death Penalty Act (AEDPA) by the United States Congress. The AEDPA, which passed in 1996, mandated reexamination of the advantages and disadvantages of adding markers and taggants to explosives for purposes of detection and identification, as well as, the determination of whether such an addition was feasible. The National Research Council (NRC) appointed the Committee on Smokeless and Black Powders in response to this mandate. The committee's task was to determine whether addition of taggants would (1) pose risks to human safety, (2) significantly assist law enforcement agencies in their investigations, (3) impair the powder's quality and performance, (4) lead to adverse environmental effects, (5) have a limited cost to benefit tradeoff, and (6) be simple to evade using terrorism counter-measures. The NRC report, "Black and Smokeless Powders: Technologies for finding Bombs and the Bomb Makers" [14], was published in 1998, and the committee's findings discouraged the addition of taggants to black and smokeless powders. In addition, the committee cited heavy use of internal powder databases at the Federal Bureau of Investigations (FBI), and the Bureau of Alcohol Tobacco Firearms and Explosives (BATFE) in forensic casework; however, these databases were incomplete, and were not available for use by smaller law enforcement agencies. Recommendations were made for the development of a

publicly accessible national powder database to be used as an investigative tool to assist law enforcement agencies in their casework.

Development of the smokeless powders database began in 2009 as a collaborative project between the Explosives Database Committee of SWGFEX and NCFS. The database [65] is an internet accessible reference collection of commercial smokeless powders which is frequently updated with analytical data for powders representing various manufacturers. The database was designed to assist in the characterization, classification, and comparison of smokeless powder samples based on their physicochemical characteristics. The database contains analytical data contributed by the FBI, NCFS, and the Netherlands Forensic Institute (NFI). There are 779 smokeless powder records in the database at the time of this writing. The methods prescribed by the SWGFEX Explosives Database Committee for analysis of the smokeless powder samples are Stereomicroscopy, Attenuated Total Reflectance Fourier Transform Infrared Spectroscopy (ATR-FTIR), and GC-MS. The analytical protocol for each contributing agency can be accessed from the database; however, a description of the NCFS methodology is given here.

### 3.1.1. Stereomicroscopy and Micrometry

A Leica S8APO stereomicroscope equipped with a Leica DFC290 camera was used to record micrographs of the smokeless powder samples, and to facilitate micrometry or physical measurements of the smokeless powder particles. A 50 mm micrometer scale with 0.1 mm divisions (Graticles, Ltd.) was used to calibrate the micron bar within the camera's software. For

each smokeless powder sample, fifty particles were placed against a white background and photographed at X10.1 magnification. The smokeless powder micrograph was recorded with the calibrated micron bar superimposed in the image. Figure 10 depicts the micrometer scale and a smokeless powder micrograph with the calibrated micron bar.

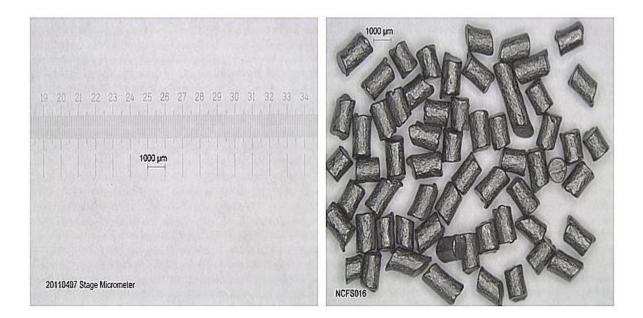


Figure 10: Stage micrometer and smokeless powder micrograph The micron bar is first calibrated in the Leica camera software using the stage micrometer. The calibrated micron bar is superimposed in the smokeless powder micrograph.

ImageTool software was used to measure the diameter and length of the smokeless powder particles [66]. The measuring apparatus in ImageTool was calibrated using the micron bar in the smokeless powder micrograph. Calibration of the measuring tool was achieved at a 1:1 image zoom, and physical measurements were performed at a 1:2 image zoom. The physical measurements were recorded in a Microsoft Excel (2010) spreadsheet, and the averages and standard deviations were calculated. Figure 11 illustrates the method used for measuring the smokeless powder particles, and addition of the powder's dimensions to the Excel spreadsheet.

1000 µm	Smo keless Powd er Measurements		
ATAA. BA.P	SRN	134	
A AMARIAN	Distributor	Alliant Powder	
TOMINAL A	Product Name	Reloder 22 NCFS	
AVER24 MAN	Data Source		
Les El mail 4	Source SRN	NCFS016	
UNICERALIONAA		length	diameter
AT STREET ()		( <b>mm</b> )	(mm)
OP INC PALINCA	1	1.8	1.1
	2	1.6	1.0
DUI MAYVAX V	5	1.8	1.2
Vakala alk	49	1.2	1.1
AMACAN	50	1.5	1.1
	Average	1.5	1.1
ELESA LA ALES	Stand ard D eviation	0.2	0.0
M CO. All	Maximum	1.9	1.2
NCFS016	M inim um	0.8	1.0

Figure 11: Measurement of smokeless powder particles Length and diameter measurements are performed as illustrated, and the powder's dimensions are recorded in a Microsoft Excel spreadsheet.

3.1.2. Sample Preparation and Instrumental Parameters

# 3.1.2.1. ATR-FTIR

As previously discussed, NC is the only primary energetic material present in both single and double base powders. NC is the most abundant compound, and ATR-FTIR is employed for its

detection so as to confirm that the material is a smokeless powder. Sample preparation involved the extraction of 2.5 mg of uncut smokeless powder particles with 80  $\mu$ L of acetone for 30 minutes. Approximately one half of the supernatant was spotted onto a clean microscope slide, and the acetone was allowed to evaporate to form a film. The remaining supernatant was overlaid on the preexisting film, with evaporation of the solvent to form a double layered film.

Analyses of the films were conducted using an ATI Mattson Infinity Series FTIR equipped with a Spectra Tech IR Plan Advantage microscope. A silicon internal reflectance element was utilized to contact the film so as to perform attenuated total reflectance measurements on the smokeless powder sample. The smokeless powder absorbance spectra were collected in the mid-IR region with the number of scans equal to 32 at a spectral resolution of 4 cm<sup>-1</sup>. OMNIC software was used to apply an ATR correction for variance in the penetration depth. The absorbance spectra were converted to percent transmittance prior to database upload, Figure 12.

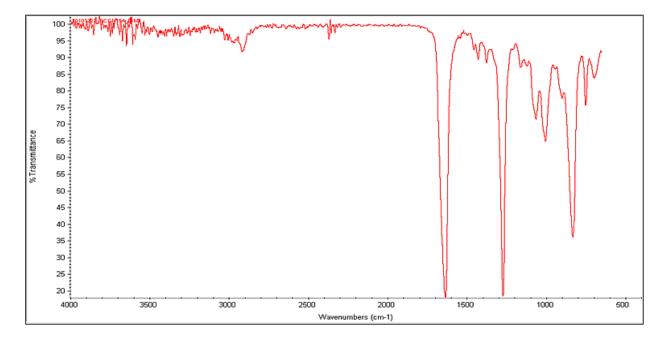


Figure 12: IR spectrum of a smokeless powder sample

#### 3.1.2.2. GC-MS

Sample preparation for GC-MS analysis involved cutting approximately 10 mg of the smokeless powder particles. Extraction of the analytes was achieved by placing the cut particles into 300  $\mu$ L of methylene chloride (CH<sub>2</sub>Cl<sub>2</sub>) with 10 ppm undecane as internal standard. The extraction was allowed to proceed for three hours to ensure optimal extraction of the analytes. For quality assurance, two analysts performed individual extractions for each smokeless powder sample. The supernatant and a 1:10 dilution were analyzed for each smokeless powder extract. A smokeless powder standard was also analyzed, and a list of the target analytes contained in the standard can be found in Appendix A.

A Hewlett-Packard 6890 GC, operating in EI mode and interfaced to a Hewlett-Packard 5973 MS, was utilized for sample analysis. An Agilent G2614A auto sampler injector was used to introduce 1 µL aliquots of the smokeless powder extract into the GC. The injection port temperature was set to 170 °C. Separation of the analytes was achieved using a 30 mm 5% phenyl methyl siloxane capillary column with a nominal diameter of 250 µm, and a film thickness of 0.25 µm. Helium carrier gas was maintained on the column at a flow rate of 1.2 mL/minute, with an average velocity of 40 cm/second. The initial oven temperature was set to 40 °C and held for one minute, followed by a 25 °C/minute ramp to a final temperature of 280 °C. The final temperature was held for three minutes. The MS transfer line was maintained at 250 °C, the ionization source was set to 230 °C, and the quadrupole temperature was set to 150 °C. The mass analyzer began scanning after a four minute solvent delay within a 43 - 400 mass range, at a rate of three to four scans per second. The smokeless powder target analytes were identified based on retention time, a 3:1 signal-to-noise ratio, and the presence of at least three major ions. Figure 13 shows a TIC of a smokeless powder sample with the target analytes identified.

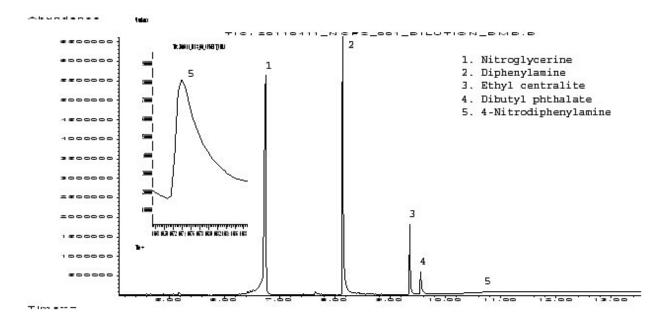


Figure 13: Labelled GC-MS TIC for a smokeless powder database sample

# 3.1.3. Database Structure

The smokeless powders database contains information pertaining to each contributing agency, as well as, contact information for the members of the SWGFEX Explosives Database Committee. The search area of the database is divided into three sections; product information, chemical composition, and physical characteristics. The database can be searched by selecting a single criterion; otherwise, an "AND" search can be initiated by selecting multiple criteria from any or all of three sections. Once a search is conducted, the user can specify how to display the results. For each record, the sample details can be accessed, and the corresponding analytical data can be downloaded. The results layout for a smokeless powder database record is shown in Figure 14.

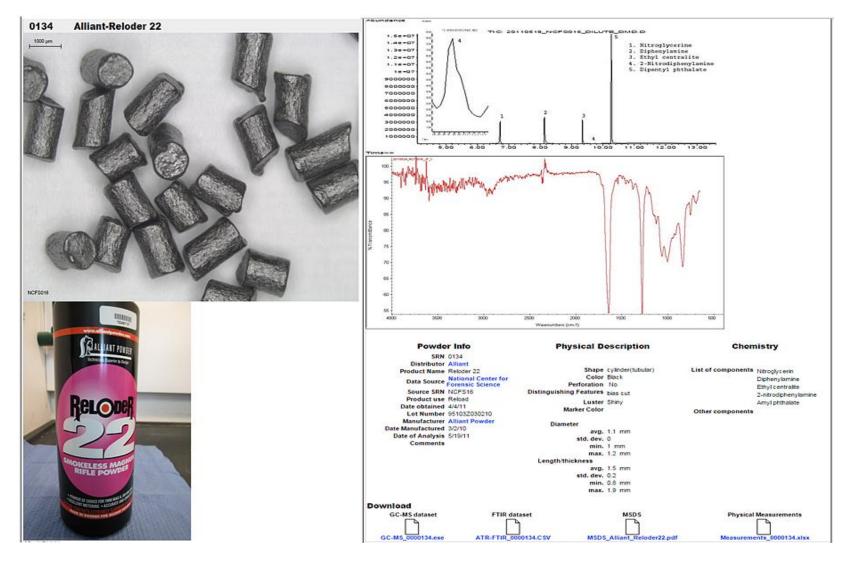


Figure 14: Result layout for a smokeless powder database sample record

Another useful feature of the database includes a "Help" option which provides guidance about selection of user-specified search criteria. For example, the user can select the "Help" option associated with powder shape to receive guidance if there is uncertainty about morphology of the sample. An illustration is provided in Figure 15. Additionally, within "Powder Information", users can access information about the data source for a given sample, as well as, information pertaining to the powder's distributor and manufacturer.

Home Search Databa		Powders D			
Search Powders	Physical Descrip	tion Chemistry	Result La	rout	
Shape	Select Value		,	Help	
Perforation	Select Value			Shape	
Distinguishing Features	lamel		ened ball	Diameter Disk: An extruded form of smokeless powder cut into thin circular disks which may have a central	Ball: A generally spherical type of smokeless powder without flattening or other alteration. The flattened
Color	other			perforation according to the manufacturer's choice. The thickness is normally less than its diameter.	ball is a ball powder further modified by a flattening
Luster	Agglomerate	d image day		+	process and is found in its own category in the
Marker Color	flatten ball and ball with irregu flatten ball and	ular flatten ball		Diameter	database.  Thickness
Diameter	min.	mm	max.	Length	Diameter
	Average	mm	+/-	Cylinder (Tubular): An extruded form of smokeless	<b>.</b>
Length/thickness	min.	mm	max.	powder cut into think rods whose length normally	Flattened Ball: The flattened ball is a ball powder further modified by a flattening process and may be
	Average	mm	+1-	either equals or exceeds their diameter. Most, but not all examples will have a central perforation and	elongated, have cracked margins, or other similar morphology.
Clear Parameters				will possess fairly uniform dimensions of length and diameter. Length Lamel: A type of smokeless propellant in which the individual particles are in the shape of thin square, diamond, or parallelogram – shapes. In some examples, the shape and dimensions of the particles are closely controlled while others may show considerable variation.	Irregular: A type of smokeless powder whose final form has been so highly modified by the manufacturer to achieve the desired performance characteristics that none of the morphology of the original particles has survived. The resultant particles have no consistently measurable dimensions such as length and diameter. Based on the Association of Firearm and Toolmark Examiners (AFTE) glossary of gunshot residue terms. Accessed on December 11, 2012. http://www.firearmsid.com/glossary/index.asp

Figure 15: Illustration of the "Help" option associated with powder shape.

#### 3.2. Cluster Analysis

## 3.2.1. Data Set

A matrix comprised of TIS data for 639 FBI and 87 NCFS smokeless powder samples was evaluated using AHC analysis. The samples are representative of various manufacturers, and lists of the FBI and NCFS samples are provided in Appendices B and C, respectively. Cluster analysis was employed for the determination of inherent groupings within the smokeless powders data. For each sample, a TIS was calculated within the 43 - 400 mass range as previously described in Section 2.3. The sample TIS was normalized using the "base peak" method. Base peak normalization was performed by dividing the intensity for each m/z ratio by the intensity of the base peak; therefore, the intensity for each m/z ratio is expressed as a percentage of the base peak. The TIS data matrix was subject to cluster analysis in its original form; where the matrix was oriented with the samples in the rows, and the m/z ratios in the matrix was oriented with the m/z ratios along the rows, and the samples in the columns. The code utilized for cluster analysis is provided in Appendix F.

# 3.2.2. Distances and Linkages

Several distance and linkage metrics are available for use in AHC analysis. Multiple distance and linkage combinations were investigated to determine which combination resulted in a dendrogram with distinct, chemically meaningful groups, and a large cophenetic correlation value. Calculations were performed in R [67] using the *stats* and *amap* packages. Within the *amap* package [41], accessed from the Comprehensive R Archive Network (CRAN), nine distances are available: Binary, Canberra, Correlation, Euclidean, Kendall, Manhattan, Maximum, Pearson, and Spearman. The *stats* package [67], available in the basic R software, lists seven linkage metrics: Average, Centroid, Complete, McQuitty, Median, Single, and Ward. Sixty-three distance and linkage combinations were utilized to test the TIS data matrices described in Section 3.2.1.

Dendrograms of the clustered samples were generated using the R *stats* package. The *cba* package [68], which is accessed through the CRAN, was used to optimally order the samples in the dendrogram. Optimal ordering of the samples was performed so that highly similar samples were arranged in the center of the cluster.

# 3.2.3. Heat Maps

## 3.2.3.1. Pairwise Sample Comparisons

A distance matrix of pairwise sample comparisons was generated during cluster analysis. A matrix of similarity values was calculated from the distance matrix using Equation 2.3; thus, samples with no distance between them have similarity values equal to 1. A heat map of the pairwise sample comparisons was generated using the conditional formatting option in Microsoft Excel (2010); where the formatting was applied to the matrix of similarity values. Figure 16 illustrates conversion of the distance matrix to a similarity matrix, and generation of a heat map from the similarity matrix.

SRN	400	494	239	521	24	22
400	0	0.003	0.004	0.475	0.764	0.911
494	0.003	0	0.001	0.425	0.737	0.913
239	0.004	0.001	0	0.407	0.727	0.914
521	0.475	0.425	0.407	0	0.747	0.985
24	0.764	0.737	0.727	0.747	0	0.966
22	0.911	0.913	0.914	0.985	0.966	0

			↓			
SRN	400	494	239	521	24	22
400	1	0.999	0.998	0.763	0.618	0.545
494	0.999	1	0.999	0.788	0.631	0.544
239	0.998	0.999	1	0.796	0.637	0.543
521	0.763	0.788	0.796	1	0.627	0.508
24	0.618	0.631	0.637	0.627	1	0.517
22	0.545	0.544	0.543	0.508	0.517	1

Equation 2.3

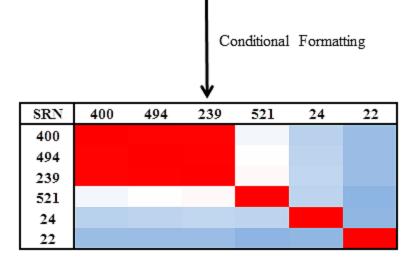


Figure 16: Illustration of a heat map generated from a similarity matrix

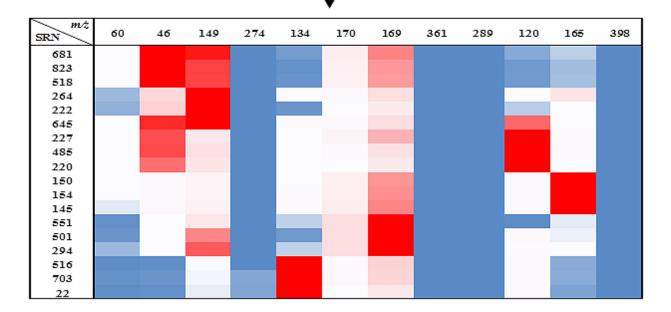
The similarity matrix is calculated from the distance matrix using Equation 2.3, and the heat map is generated from the similarity matrix through the application of conditional formatting using Microsoft Excel (2010).

In Figure 16, SRN represents the sample reference number assigned to the smokeless powder record in the database. The areas shaded red indicate high similarities between the samples being evaluated in the comparison; while regions shaded blue indicate low similarity values. The white portions of the map indicate samples with mid-point similarities. Similarity values for same sample comparisons lie along the diagonal of the heat map and are equal to one.

# 3.2.3.2. Ordered TIS

The TIS data was ordered using the results obtained from cluster analysis of the matrix in its original and transposed orientations. A heat map of the ordered TIS matrix was generated using the conditional formatting option in Microsoft Excel. The heat map was generated to visualize the degree of contribution of each of the m/z ratios to sample groupings within the similarity heat map. An excerpt of the heat map is shown in Figure 17.

m/z SRN	60	46	149	274	134	170	169	361	289	120	165	398
681	0.007	1	0.913	0	0.001	0.063	0.486	0	0	0.001	0.002	0
823	0.006	1	0.740	0	0	0.052	0.405	0	0	0.001	0.002	0
518	0.006	1	0.733	0	0	0.050	0.391	0	0	0.001	0.002	0
264	0.002	0.150	1	0	0.006	0.015	0.121	0	0	0.005	0.100	0
222	0.001	0.177	1	0	0	0.010	0.076	0	0	0.002	0.011	0
645	0.007	0.836	1	0	0.004	0.016	0.128	0	0	0.589	0.010	0
227	0.005	0.693	0.089	0	0.007	0.038	0.300	0	0	1	0.012	0
485	0.005	0.707	0.111	0	0.006	0.014	0.112	0	0	1	0.012	0
220	0.004	0.564	0.099	0	0.006	0.010	0.082	0	0	1	0.011	0
150	0.004	0.018	0.041	0	0.011	0.055	0.417	0	0	0.018	1	0
154	0.005	0.016	0.040	0	0.012	0.058	0.438	0	0	0.018	1	0
145	0.003	0.020	0.049	0	0.013	0.064	0.485	0	0	0.019	1	0
551	0	0.005	0.094	0	0.002	0.127	1	0	0	0	0.003	0
501	0	0.004	0.474	0	0.001	0.127	1	0	0	0.018	0.003	0
294	0.002	0.008	0.650	0	0.002	0.128	1	0	0	0.015	0.006	0
516	0	0	0.004	0	1	0.022	0.169	0	0	0.019	0.001	0
703	0	0	0.004	0.001	1	0.020	0.161	0	0	0.018	0.001	0
22	0	0	0.003	0.001	1	0.011	0.086	0	0	0.019	0.001	0



Conditional Formatting

Figure 17: Illustration of a heat map generated from the ordered TIS data matrix

In Figure 17, SRN represents the sample reference number assigned to the smokeless powder record in the database. The shading in the heat map represents the relative intensities contributed by the m/z ratios within the 43 - 400 mass range. The regions shaded white and blue represent low intensities; areas shaded pink represent mid to high intensities, and red regions are indicative of the most intense contributions of the m/z ratio.

#### 3.3. Discriminant Analysis

# 3.3.1. Data Sets

## 3.3.1.1. Samples used for Model Development

The TIS data matrix described in Section 3.2.1 was processed based on the results obtained from cluster analysis. The processed data matrix, which will be described in Section 4.1.2, was used to develop discriminant models for the IIR, LDA, QDA, and *k*NN. The data was normalized, using the "base peak" method, prior to processing.

## 3.3.1.2. Samples used for Classification

As previously discussed, NCFS smokeless powder samples were extracted in duplicate by two analysts. The 87 NCFS samples extracted by the second analyst were classified using the discriminant methods. The TIS for each sample in this dataset was calculated and base peak normalized as described in Section 3.2.1. The resulting data matrix was processed based on the results obtained from cluster analysis. Correct classification rates for the samples were determined by comparing the known classes for the NCFS samples in the model to the class assignments of the NCFS duplicate samples.

#### 3.3.2. The IIR

The IIR was developed at NCFS based on the results obtained from cluster analysis. As mentioned previously, the IIR considers the relative intensities of ions which were selected based on deductions which were made from cluster analysis. Class assignment of the smokeless powder samples using the IIR was achieved based on visual inspection of the ion intensities. A detailed description of the IIR method will be given in Section 4.2.3.

# 3.3.3. Cross-Validation

Cross-validation (CV) is used to optimize and estimate the performance of discriminant models. The method involves random selection of samples from the dataset; where randomly selected samples are withheld as the validation test set, and remaining samples are used for development of the model. Several cross-validation techniques exist; however, leave-one-out and leave-group-out cross-validation were utilized in this work. Leave-one-out cross-validation (LOOCV) involves random selection of a lone sample, which is withheld as the validation sample; the remaining samples are used for model development. Leave-group-out cross-validation (LGOCV) involves random selection of a percentage of the samples from the dataset, to be used as the

validation set, prior to development of the model. In both cases, class assignment of the withheld samples is achieved based on the model.

# 3.3.4. kNN

The NCFS test samples described in Section 3.3.1.2 were classified using *k*NN. The *k*NN model was developed using the dataset described in Section 3.3.1.1, and the model's performance was evaluated using LOOCV and LGOCV. Calculations were performed in R using the *caret* and *class* packages, which were accessed from the CRAN. The *caret* package [69] was used to select the portion of the data to be used as the validation set in LGOCV. The *class* package [70] was used to perform the calculations for model development, as well as for class assignment of the test samples.

# 3.3.5. The Likelihood Ratio Test

The likelihood ratio test was used to determine whether the covariance matrices between the classes were equivalent. The test evaluates two classes for each comparison; therefore, in comparing multiple classes, each class is tested against all other classes. For example, in evaluating three classes, Class 1 would be compared to Class 2, Class 1 to Class 3, and Class 2 to Class 3. The TIS for each sample within the original data matrix was normalized using the "summed to one" method. Summed to one normalization was performed by dividing the intensity for each m/z ratio by the sample's summed intensity value. The "summed to one" data

matrix was processed based on the results obtained from cluster analysis. The likelihood ratio test was applied to the processed data.

#### 3.3.6. *LDA/QDA*

Models were developed for LDA and QDA using the dataset mentioned in Section 3.3.1.1. The samples described in Section 3.3.1.2 were classified using LDA and QDA. Calculations were performed using the *MASS* package [70], which was accessed from the CRAN, and the LDA and QDA models were evaluated using LOOCV and LGOCV. Discriminant functions for quadratic and linear combinations of the data for each class were calculated using Equations 2.6 and 2.7, respectively. For classification, a sample was assigned to the class with the largest discriminant value; that is, the largest posterior probability. The code which was utilized in LDA and QDA is provided in Appendix H.

## 3.4. Bayesian Networks

Bayesian Networks were developed using the 119 NCFS smokeless powder samples listed in Appendices B and C. The networks were developed to calculate posterior probabilities for a smokeless powder belonging to specific manufacturers given that evidence is observed. The networks were generated using the *gRain* [71], *gRbase* [72], and *gRim* [73] packages which were accessed from the CRAN repository in R software. For each network, the DAG design, which is based on the joint probability distribution, was specified using the "dag" function in the

*gRbase* package. The probability tables associated with each node in the DAG were extracted from the smokeless powder dataset using the *gRim* package, and the "extractCPT" function in the *gRain* package. The probability tables were compiled using the "compileCPT" function which was also available in the *gRain* package. The "grain" function within the *gRain* package, and the "compile" function in the *gRbase* package were used to build and compile functional networks comprising the nodes, and their corresponding probability tables. The compiled networks were instantiated, and queried, using the "querygrain" function in the *gRain* package. Instantiation of the network was achieved through the entering of evidence into specific nodes by invoking the "setEvidence" function. The prior probabilities were updated to posterior probabilities after instantiation of the networks.

# **CHAPTER 4: RESULTS AND DISCUSSION**

## 4.1. Cluster Analysis

The TIS data matrix described in Section 3.2.1 was subject to cluster analysis in both its original and transposed form. In the original matrix, the samples within the dataset were oriented in the rows, while the m/z ratios were oriented in the columns. Within the transposed matrix, m/z ratios were oriented in the rows, and samples were oriented in the columns. Cluster analysis of the matrix in its original and transposed orientations resulted in clustering of the samples and the m/z ratios, respectively.

# 4.1.1. Heat Maps

# 4.1.1.1. Pairwise Sample Comparisons

A high cophenetic correlation value of 0.935 was achieved for cluster analysis of the samples using correlation distance and average linkage. The combination of correlation distance and complete linkage resulted in a correlation value of 0.642 for clustering the m/z ratios. The correlation distance was calculated using Equation 2.1, where r is the Pearson correlation coefficient, which is defined in Equation 2.2. The linear relationship between two variables is described by the Pearson correlation coefficient which ranges from -1 to 1; thus, correlation distances range from 0 to 2. The distance matrix of pairwise sample comparisons was converted to a similarity matrix using Equation 2.3. Using this equation and the correlation distance, the

similarity values can potentially range from 0 to 1; therefore, a pair of samples with a short distance between them would yield a large similarity value for the comparison.

Correlation distances were calculated for samples in the TIS data matrix. The samples were clustered using average linkage, and a dendrogram reflecting the arrangement of the samples was generated. Optimal leaf ordering was employed for orientation of highly similar samples in the center of the cluster. The distance matrix of pairwise sample comparisons was converted first to a similarity matrix, and then to a heat map as described in Section 3.2.3.1. Figure 18 depicts the heat map which was generated from the similarity matrix. Samples within the heat map were arranged using the optimal leaf order in the dendrogram. The color gradient in the heat map represents the range of similarity values observed for samples within the dataset, where red is indicative of high similarities, blue represents low similarities, and white represents mid-point similarity values. The scale illustrating the range of similarity values in the heat map is shown to the right of Figure 18. As mentioned previously, correlation distance was used in this research; therefore, similarity values can range from 0 to 1. However, the data used in this research had a minimum similarity value of 0.49; therefore, the similarity values ranged from 0.49 to 1.

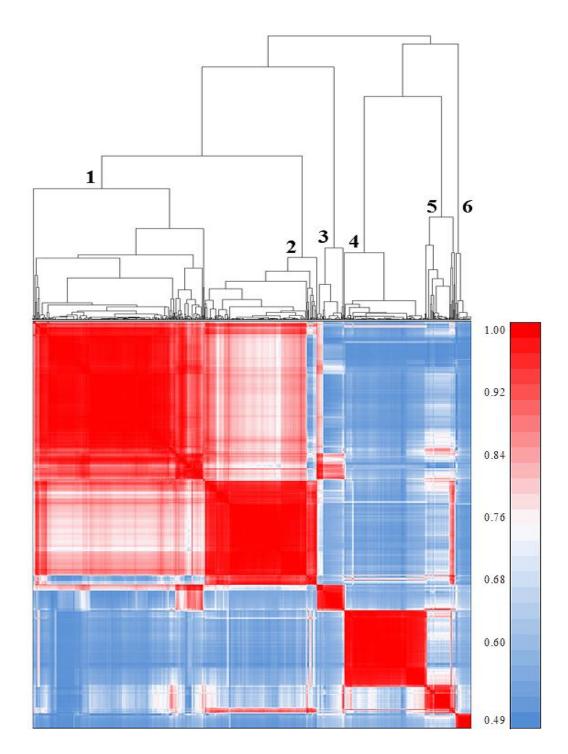
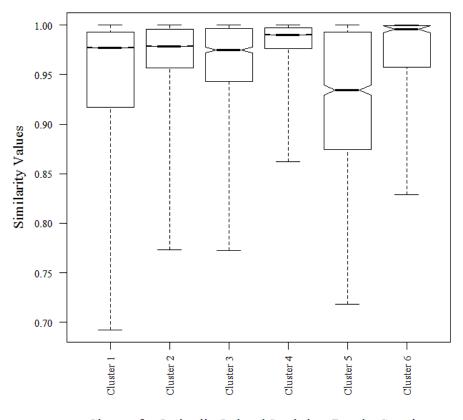


Figure 18: Dendrogram and heat map for 639 FBI and 87 NCFS smokeless powder database samples The samples were clustered using correlation distance and average linkage, and are arranged using the optimal leaf order in the dendrogram

Six distinct clusters were identified in the smokeless powders dataset from observation of the combined dendrogram and heat map. The clusters are labeled 1 through 6 in Figure 18. The range of similarity values demonstrated that there was some similarity between all the samples in the data set; however, there were still enough differences which contributed to formation of distinct clusters. The samples within the clusters are highly similar to each other; however, there is some variation in the similarities between a few samples within each of the clusters. In addition, the majority of samples in Cluster 2 are very similar to samples in Cluster 1; all samples in Cluster 3 exhibit relatively high similarities to a few samples in Cluster 1, and some Cluster 5 samples are very similar to all samples in Cluster 2, and a few samples in Clusters 1, 2, and 4. Samples in Clusters 4 and 6 exhibit minimal similarity to samples in the other clusters. The chemical composition of the samples within the clusters was examined to identify target analytes which were present, and to determine whether these analytes were unique within each cluster. Diphenylamine (DIPH), Ethyl centralite (EC), 2-nitrodiphenylamine (2-nDIPH), 4nitrodiphenylamine (4-nDIPH), and a variety of phthalates were present in samples across the six clusters. Nitroglycerin (NG), 2,4-Dinitrotoluene (2,4-DNT), Methyl centralite (MC), 2nitrosodiphenylamine (2-nsoDIPH), and 4-nitrosodiphenylamine (4-nsoDIPH) were identified in Cluster 1 samples. With the exception of 2-nsoDIPH, the compounds mentioned previously were also present in samples from Clusters 2 and 5. Finally, in addition to chemical constituents which were present in samples across all clusters, NG and 4-nsoDIPH were also identified in Cluster 3 samples; while, 2-4-DNT and MC were identified in samples from Clusters 4 and 6, respectively.

Inspecting the chemical composition of the clustered samples did not provide insight about chemical variation in the samples; thus, to illustrate variation of the similarity values between and within the smokeless powder clusters, the boxplots shown in Figure 19, were generated using R software [67].



Clusters for Optimally Ordered Smokeless Powder Samples

Figure 19: Boxplots illustrating variation in the smokeless powder clusters

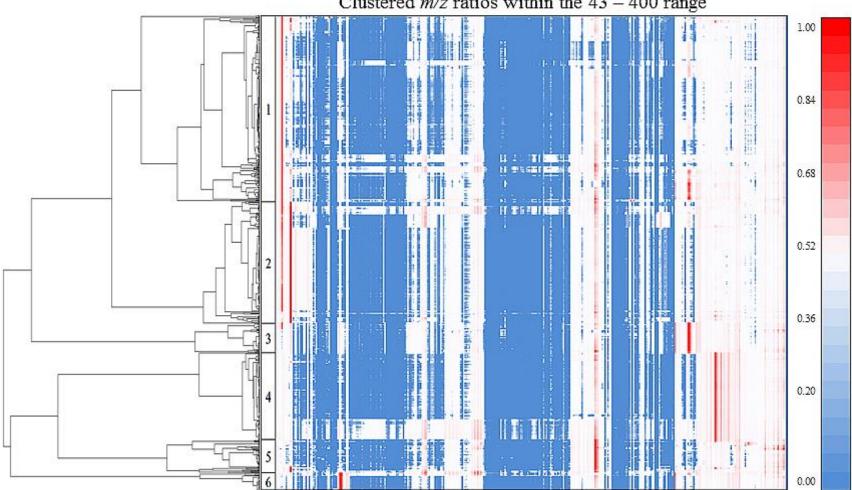
The range of similarity values observed in the clusters is shown on the y-axis of Figure 19, while cluster identifiers are shown on the x-axis. The boxes, which represent 50% of the data

associated with each cluster, were constructed around the first and third quartiles. The thick, dark horizontal lines are indicative of the median similarity values within each cluster. The dashed lines drawn parallel to the *y*-axis represent the range of similarity values, and the horizontal lines at the outermost regions of the range indicate minimum and maximum similarities for each cluster. The notches observed on the boxes represent a 95% confidence interval around the median,  $\pm \frac{1.57 \times IQR}{\sqrt{n}}$ , where IQR is the interquartile range, and n is the number of samples. A significant overlap in the range of similarity values is observed between five of the six clusters. This observation was expected as a number of target analytes were common across all the clusters. Within the clusters, the most amount of variation was observed in Cluster 5; while the least variation was observed in Cluster 4. In addition, the notches for each of the clusters did not overlap, which indicated that there were significant differences between the clusters. Despite differences in the similarities, additional determinations could not be made about specific characteristics which contributed to formation of the clusters.

# 4.1.1.2. Ordered TIS

The TIS data matrix described in Section 3.2.1 was ordered using the results obtained from clustering the samples, and the m/z ratios. The result obtained from clustering the samples was used to sort the rows of the TIS matrix so that the ordering of the samples reflected the optimal leaf order observed in the dendrogram. The result obtained from cluster analysis of the m/z ratios was used to sort the columns of the TIS matrix; therefore, m/z ratios were arranged in non-sequential order. Conversion of the ordered TIS matrix to a heat map was achieved as described

in Section 3.2.3.2. The ordered TIS heat map, Figure 20, was examined to determine the relationship between the clusters identified, and the m/z ratios within the 43 – 400 range.



Clustered m/z ratios within the 43 - 400 range

Figure 20: Heat map generated from the ordered TIS data matrix.

Samples along the rows are ordered to reflect optimal leaf order in the dendrogram; m/z ratios are ordered based on results obtained from cluster analysis of m/z ratios, and are therefore not in sequence.

The scale illustrating intensity values, which ranged from 0 to 1, is shown to the right of Figure 20. The color gradient in the heat map represents the range of intensities associated with each of the m/z ratios within the 43 – 400 range; where blue represents little or no intensity, white represents mid-point intensities, and shades of red indicate the highest intensities including the base peak. Examination of the heat map indicated that only a few m/z ratios contributed significantly to formation of the clusters as observed in specific regions of the map, where the associated intensities were the highest; therefore, the distinction between the clusters was based on the relative intensities of these contributing ions.

## 4.1.1.3. Most Intense Extracted Ion Spectrum

As previously discussed, examination of the TIS heat map shown in Figure 20 demonstrated that a small number of m/z ratios contributed significantly to the formation of six distinct clusters. The m/z ratios which were identified as minor contributing ions were removed from the ordered TIS matrix; and the reduced matrix demonstrated that the relative intensities of six major ions were responsible for formation of the six clusters. That is, within each of the six clusters, a single m/z ratio was responsible for clustering the samples, and that specific ion was most intense for the majority of samples within the cluster. The reduced TIS heat map, henceforth referred to as the most intense extracted ion spectrum (MEIS), is shown in Figure 21.

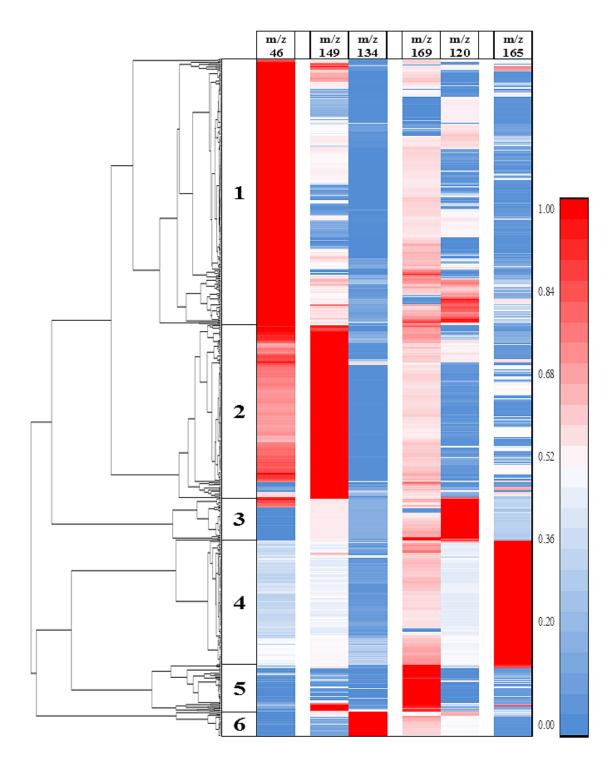


Figure 21: Heat map generated from the MEIS

Samples along the rows are ordered to reflect the optimal leaf order in the dendrogram; m/z ratios represent the six ions responsible for clustering samples into the six clusters.

In this figure, the arrangement of the samples within their respective clusters, shown on the yaxis, reflect the optimal leaf order in the dendrogram. The m/z ratios which were identified as major contributing ions are shown on the x-axis. The color gradient represents the range of intensities associated with these ions; where blue represents little or no intensity, white represents mid-point intensities, and shades of red represent the range of highest intensities. The scale illustrating the range of intensity values, synonymous with the relative contributions of the ions within each of the clusters, is shown to the right of Figure 21.

As previously mentioned, some analytes were observed in samples across the six clusters; however, close inspection of the MEIS demonstrated that a single m/z ratio was the base peak for the majority of the samples within a given cluster. Table 1 provides an illustration for the six clusters.

Cluster	SRN	Cluster 1 <i>m/z</i> , 46	Cluster 2 <i>m/z</i> 149	Cluster 3 <i>m/z</i> 120	Cluster 4 <i>m/z</i> , 165	Cluster 5 <i>m/z</i> 169	Cluster 6 <i>m/z</i> 134
	7	1	0.081	0.897	0.012	0.643	0.005
1	80	1	0.161	0.960	0.011	0.521	0.006
	455	1	0.240	0.769	0.047	0.435	0.005
	179	0.860	1	0.012	0.005	0.442	0.005
2	180	0.917	1	0.003	0.006	0.409	0.005
	186	0.931	1	0.003	0.005	0.363	0.005
	49	0	0.087	1	0.012	0.995	0.006
3	51	0	0.091	1	0.011	0.806	0.006
	706	0	0.086	1	0.011	0.351	0.006
	63	0.013	0.280	0.017	1	0.250	0.001
4	213	0.012	0.026	0.016	1	0.529	0.003
	417	0.013	0.019	0.017	1	0.571	0.004
	31	0.013	0.019	0.015	0.833	1	0.003
5	506	0.010	0.019	0.014	0.875	1	0.001
	787	0.010	0.137	0.011	0.617	1	0.001
	167	0	0.080	0.360	0.014	0.034	1
6	181	0	0.082	0.322	0.012	0.037	1
	183	0	0.113	0.298	0.016	0.063	1

 Table 1: Illustration of the sample clusters within the MEIS

 Samples along the rows are ordered to reflect the optimal leaf order in the dendrogram; m/z ratios represent the six ions responsible for clustering the samples into six distinct classes

As can be seen, samples grouped in Cluster 1 based on m/z 46 which is the major ion indicative of NG. Cluster 2 samples grouped based on m/z 149, one of the major ions for PHTH, even though the majority of these samples also contained NG. Samples grouped in Cluster 3 based on m/z 120, which is indicative of the presence of EC. Mass-to-charge ratio 165, indicative of 2,4-DNT, was the base peak for all samples within Cluster 4. The major ion indicative of DIPH, m/z 169, was most intense for the majority of samples in Cluster 5; while m/z 134, indicative of MC, was the base peak for all Cluster 6 samples. The clusters, their corresponding ions, and the associated compounds are summarized in Table 2.

Cluster	Number of samples	Mass-to-charge ( $m/z$ )	Associated compound(s)
1	285	46	Nitroglycerin (NG)
2	186	149	Phthalates (PHTH)
3	45	120	Ethyl centralite (EC)
4	133	165	2,4-Dinitrotoluene (2,4-DNT)
5	51	169	Diphenylamines (DIPH)
6	26	134	Methyl centralite (MC)

Table 2: Smokeless powder clusters, their ions, and associated compound(s)

Some anomalies, shown in Table 3, were observed for samples grouped in Clusters 1 and 5. Four samples in Cluster 1, and one sample in Cluster 5 were not grouped within their respective clusters due to the base peak. That is, the intensities associated with the m/z ratios identified in the MEIS were the second most intense ion, within the 43 – 400 mass range, for each of these samples. The ions associated with the base peak for the samples in Clusters 1 and 5 were m/z 225 and m/z 207, respectively. The compound associated with m/z 225 was identified as diphenyl phthalate, and this compound was not one of the target analytes utilized in this work; m/z 207

was attributed to column bleed. Considering only the MEIS, these samples still grouped within the clusters associated with the ions of highest intensity, despite the absence of the base peak.

 Table 3: Samples identified within clusters where most intense ion was not the base peak

 The sample labeled "SRN NA" represents an FBI sample which was not included in the NCFS smokeless powders database. There are only two samples within the dataset which were not included in the database

Cluster	SRN	Cluster 1 <i>m/z</i> 46	Cluster 2 <i>m/</i> z 149	Cluster 3 <i>m/z</i> 120	Cluster 4 <i>m/z</i> , 165	Cluster 5 <i>m/z</i> 169	Cluster 6 <i>m/z</i> , 134	<i>m/z</i> 207	m/z 225
	239	0.764	0.121	0.042	0.033	0.177	0.001	0.053	1
4	400	0.634	0.085	0.048	0.009	0.173	0.001	0.060	1
I	494	0.734	0.101	0.039	0.033	0.211	0.001	0.052	1
	NA	0.946	0.139	0.002	0.051	0.205	0.000	0.058	1
5	580	0.000	0.003	0.001	0.004	0.787	0.000	1	0.001

Another significant observation was made for a few samples grouped within Clusters 2, 3, and 5. In each of these cases, the base peak was observed for its associated cluster; however, the samples did not group according to the base peak. Instead, the majority of the samples grouped within the cluster associated with the second most intense ion. The MEIS for these samples is shown in Table 4.

Cluster	SRN	Cluster 1 m/z 46	Cluster 2 <i>m/z</i> 149	Cluster 3 <i>m/z</i> 120	Cluster 4 <i>m/z</i> , 165	Cluster 5 m/z 169	Cluster 6 <i>m/z</i> 134
	16	1	0.798	0.001	0.001	0.373	0.000
	136	1	0.700	0.002	0.006	0.548	0.005
	187	1	0.927	0.011	0.006	0.372	0.004
2	518	1	0.733	0.001	0.002	0.391	0.000
	681	1	0.913	0.001	0.002	0.486	0.001
	822	1	0.716	0.001	0.002	0.381	0.000
	823	1	0.740	0.001	0.002	0.405	0.000
2	47	0.000	0.048	0.555	0.007	1	0.003
3	701	0.001	0.070	0.782	0.010	1	0.005
	105	0.002	1	0.008	0.016	0.893	0.021
	176	0.000	1	0.004	0.008	0.824	0.013
	190	0.006	1	0.010	0.475	0.978	0.002
5	258	0.003	1	0.219	0.005	0.520	0.005
	299	0.006	1	0.006	0.005	0.798	0.002
	416	0.011	1	0.016	0.931	0.917	0.005
	500	0.002	1	0.004	0.005	0.887	0.001

Table 4: Samples grouped to clusters based on ions other than the base peak The samples shown in this figure represent every sample within the entire dataset which grouped within the cluster associated with the ion of second highest intensity

As can be seen, the samples in Cluster 2 were grouped based on m/z 149, the second most intense ion, even though the base peak was observed for m/z 46, which is the ion synonymous with Cluster 1. Similar observations were made for some samples in Clusters 3 and 5; that is, the samples were grouped based on their second most intense ions, m/z 120 and m/z 169, respectively. A single sample in Cluster 5, SRN 416, clustered based on the ion of third highest intensity. Though the majority of the samples within the dataset were grouped in clusters due to their most intense ion (or the base peak), the clustering calculation did not group a few samples into clusters where the most intense ion within the sample TIS corresponded to the most intense ion associated with that cluster. The set of most intense ions corresponding to the six clusters  $(m/z \ 46, \ 120, \ 134, \ 149, \ 165, \ and \ 169)$  were identified using visual feature selection. The feature ions, as defined in the MEIS, were used for smokeless powder classification as described in the remainder of this chapter.

#### 4.2. Discriminant Analysis

#### 4.2.1. Samples used for Model Development

The TIS data matrix, comprised of 726 smokeless powder database samples, was subject to AHC analysis. Six clusters, henceforth referred to as classes, were identified from cluster analysis. Each of the six classes was associated with a single m/z ratio, where the base peak (or the most intense ion) was observed for the majority of the samples within that class. The TIS matrix was amended, using visual feature selection, to exclude the ions which did not contribute significantly to formation of the classes; thus, only data associated with the feature selected ions in the MEIS was utilized for model development. Within the models, the 87 NCFS samples were used as ground truth samples, and correct classification rates were calculated after assignment of the NCFS test samples to the six classes.

## 4.2.2. Samples used for Classification

As previously mentioned in Section 3.1.2.2., each NCFS smokeless powder sample was extracted and analyzed by two analysts. For each sample from the second analyst, the TIS were calculated, base peak normalized, and processed to generate the MEIS. Class assignment of the test samples was achieved using the IIR, kNN, LDA, and QDA.

# 4.2.3. The IIR

A new classification rule, the IIR, was developed in this work based on the results obtained from AHC analysis. The results from cluster analysis demonstrated that six ions were primarily responsible for the formation of six distinct classes. In addition, for the majority of the samples within a given class, the most significant contributions (i.e., the highest intensities) were observed for a single ion. The IIR considers the six ions that distinguish the classes, or the MEIS. Cross-validation was not utilized to evaluate the IIR since the rule is implemented strictly based on visual inspection of the sample MEIS; where the sample is always assigned to the class associated with the ion of highest intensity. The results obtained for assignment of the smokeless powder test samples are summarized in a confusion matrix, Table 5.

			Predictions based on the IIR								
		Class 1	Class 2	Class 3	Class 4	Class 5	Class 6	Sum	% Correct		
	Class 1	33						33	100		
	Class 2	4	11					15	73		
AHC designated	Class 3	1	NCFS smoke	less powder s	amples neithe	r clustered in 1	nor were assig	ned to Clas	s 3		
class	Class 4				31			31	100		
	Class 5		2			1		3	33		
	Class 6						5	5	100		
	Sum	37	13	0	31	1	5	87	<del>9</del> 3		

Table 5: Confusion matrix summarizing assignment of the NCFS test samples based on the IIR

In Table 5, the rows represent the AHC designated classes for the NCFS ground truth samples; columns represent the predictions which were made using the IIR for assignment of the test samples to the classes. Values along the diagonal of the matrix represent correct class assignment of the test samples, where samples both clustered in, and were assigned to the respective class. Off-diagonal values represent sample misclassifications by the model. Samples were assigned to Classes 1, 4, and 6 with high correct classification rates of 100%. Less than perfect classification rates of 73% and 33% were observed for assignment of Class 2, and Class 5 samples, respectively. Four Class 2 samples were incorrectly assigned to Class 1, while two Class 5 samples were misclassified to Class 2. Finally, NCFS samples neither clustered in Class 3, nor were they assigned to that class using the IIR. The low correct classification rates for sample

assignment to Classes 2 and 5 reduced the overall correct classification rate to 93%. Table 6 provides a summary of the samples which were misclassified using the IIR.

Table 6: Misclassifications of the NCFS test samples using the IIR The column titled "AHC designated class" represents the class of the NCFS ground truth samples determined from cluster analysis. The column titled "Predicted" represents class assignment of the test samples based on the IIR

			MEIS for the NCFS test samples							
SRN	Predicted	AHC designated class	Class 1 m/z 46	Class 2 m/z 149	Class 3 m/z 120	Class 4 m/z 165	Class 5 m/z 169	Class 6 m/z 134		
105	Class 2	Class 5	0.003	1	0.008	0.014	0.751	0.018		
136	Class 1	Class 2	1	0.797	0.003	0.007	0.611	0.006		
160	Class 1	Class 2	1	0.904	0.008	0.008	0.475	0.006		
176	Class 2	Class 5	0.000	1	0.003	0.008	0.830	0.015		
180	Class 1	Class 2	1	0.982	0.003	0.006	0.392	0.005		
187	Class 1	Class 2	1	0.920	0.011	0.006	0.368	0.004		

In this table, the column titled "AHC designated class" represents the class of the NCFS ground truth sample determined from cluster analysis; the column titled "Predicted" represents the class assignment of the NCFS test sample based on the IIR. Four of the six misclassified samples, namely SRN 105, 136, 176, and 187, were previously identified as anomalies from cluster analysis. Recall from Table 4, these samples clustered based on their second most intense ion, but were assigned to the class associated with their most intense ion. The two remaining

misclassified samples, SRN 160 and 180, were designated Class 2 samples based on cluster analysis, but were assigned to Class 1 based on the IIR. The MEIS for the ground truth samples for SRN 160 and 180 is shown in Table 7. As can be seen, the samples were clustered in Class 2; where m/z 149 was the base peak for both samples. However, the SRN 160 and 180 test samples were not assigned to Class 2, using the IIR, because m/z 149 was the second most intense ion in the MEIS for each of the test samples. Using the IIR, each test sample was assigned to the class which corresponded with the most intense ion in the sample' MEIS, Class 1. Despite these misclassifications, a high overall correct classification rate was observed using the IIR.

Table 7: AHC designated classes of the NCFS ground truth samples misclassified by the IIRThe ground truth samples had m/z 149 (Class 2) as the most intense ion; while the test samples had m/z 46 (Class 1)as the most intense ion (Table 5)

		MEIS for the NCFS ground truth samples									
SRN	AHC designated class	Class 1 m/z 46	Class 2 m/z 149	Class 3 m/z 120	Class 4 m/z 165	Class 5 m/z 169	Class 6 m/z 134				
105	Class 5	0.002	1	0.008	0.016	0.893	0.021				
136	Class 2	1	0.700	0.002	0.006	0.548	0.005				
160	Class 2	0.841	1	0.009	0.007	0.425	0.005				
176	Class 5	0.000	1	0.004	0.008	0.824	0.013				
180	Class 2	0.917	1	0.003	0.006	0.409	0.005				
187	Class 2	1	0.927	0.011	0.006	0.372	0.004				

### 4.2.4. kNN

As previously discussed, the kNN method predicts the class of an unknown object based on its distance to objects of known class membership in multidimensional space. In this research, Euclidean distance was utilized for assignment of the NCFS test samples to the AHC designated classes. Cross-validation methods were employed to optimize the number of nearest neighbors, k, to be considered for sample classification. Leave-one-out cross-validation (LOOCV) was achieved by withholding one sample, which was used as a validation test sample, prior to development of the model. Leave-group-out cross-validation (LGOCV) was achieved by withholding 10% of the data, which was used as the validation test set, prior to model development. For each model, the lowest number of sample misclassifications was achieved when k was equal to five.

### 4.2.4.1. LOOCV

The results for assignment of the validation test samples using the *k*NN LOO model are summarized in a confusion matrix, Table 8. The row headings represent the classes which were determined from cluster analysis, and column headings represent class predictions by the model. Values along the diagonal represent correct classifications; where the samples both clustered in, and were assigned to the same AHC designated class. Sample misclassifications by the model are represented as off-diagonal values.

			Predictions based on the kNN LOO model										
		Class 1	Class 1 Class 2 Class 3 Class 4 Class 5 Class 6 Sum % Correct										
	Class 1	284	1					285	99				
	Class 2		184			2		186	99				
AHC designated	Class 3			45				45	100				
class	Class 4				133			133	100				
	Class 5		1			50		51	98				
	Class 6						26	26	100				
	Sum	284	186	45	133	52	26	726	99				

Table 8: Confusion matrix summarizing assignment of the CV samples using the kNN LOO model

High correct classification rates of 99%, 99%, and 98% were observed for assignment of the validation samples to Classes 1, 2, and 5, respectively. In addition, no misclassifications were observed for assignment of the validation samples to Classes 3, 4, and 6, which resulted in a 100% correct classification rate for sample assignment to these classes. For the misclassified samples, one Class 1 sample was incorrectly assigned to Class 2; two Class 2 samples were misclassified to Class 5, and one Class 5 sample incorrectly assigned to Class 2. The misclassified Class 1 and Class 2 samples were grouped within their respective classes according to the base peak, and assigned to the classes associated with the second most intense ion.

Conversely, the misclassified Class 5 was clustered due to its second most intense ion, and assigned to the class associated with its base peak.

#### 4.2.4.2. LGOCV

The confusion matrix, shown in Table 9, summarizes the results obtained for assignment of the percent withheld validation samples using the kNN LGO model. As previously described, the classes determined from cluster analysis are represented by the row headings; while column headings represent class predictions by the model. Correct classifications, where samples both clustered in, and were assigned to the same class, are shown on the diagonal of the matrix. Off-diagonal values indicate misclassifications by the model.

		Predictions based on the kNN LGO model										
		Class 1	Class 2	Class 3	Class 4	Class 5	Class 6	Sum	% Correct			
	Class 1	27	1					28	96			
	Class 2		18					18	100			
AHC designated	Class 3			4				4	100			
class	Class 4				13			13	100			
	Class 5					5		5	100			
	Class 6						2	2	100			
	Sum	27	19	4	13	5	2	70	99			

Table 9: Confusion matrix summarizing assignment of the CV samples using the kNN LGO model

A single Class 1 sample incorrectly assigned to Class 2, resulting in a high correct classification rate of 96%; while no misclassifications occurred for sample assignment to Classes 2, 3, 4, 5, and 6. The misclassified sample was placed in the class associated with its base peak ion, and assigned to the class associated with the ion of second highest intensity.

### 4.2.4.3. Class Assignment of the NCFS Test Samples

The optimized *k*NN LOO and LGO models were used for assignment of the NCFS test samples. Euclidean distance was utilized in each model, and *k* was set equal to five. The results obtained for assignment of the test samples to the AHC designated classes using the *k*NN LOO and LGO models are reported together since the results were identical using both models.

#### 4.2.4.3.1. Classification based on the kNN LOO and LGO models

The results obtained for assignment of the NCFS test samples are summarized in the confusion matrix, Table 10. The row headings represent the AHC designated classes for the NCFS ground truth samples in the model; column headings represent class assignment of the NCFS test samples based on the model. High correct classification rates were achieved for sample assignment to Classes 1, 2, 4, 5, and 6. In addition, NCFS samples neither clustered in, nor were assigned to Class 3.

 Table 10: Confusion matrix summarizing assignment of the NCFS test samples using the kNN LOO and LGO models

 The set of the

			Predictions based on the <i>k</i> NN LOO model										
		Class 1	Class 2	Class 3	Class 4	Class 5	Class 6	Sum	% Correct				
	Class 1	33						33	100				
	Class 2		15					15	100				
AHC designated	Class 3	N	NCFS smokeless powder samples neither clustered in nor were assigned to Class 3										
class	Class 4				31			31	100				
	Class 5					3		3	100				
	Class 6						5	5	100				
	Sum	33	15	0	31	3	5	87	100				

The results obtained using the LOO and LGO models are reported as the same confusion matrix since the results using both models were identical

High correct classification rates were achieved for sample assignment to Classes 1, 2, 4, 5, and 6. In addition, NCFS samples neither clustered in, nor were assigned to Class 3. The overall correct classification rate was 100% for assignment of the test samples to the AHC designated classes.

## 4.2.5. The Likelihood Ratio Test

The likelihood ratio test is employed to determine whether the covariance matrices between classes can be considered equal. If the test, which is a pairwise comparison between the classes, reveals that the classes are equivalent, then LDA is better suited for classification. Conversely, if the classes are not equivalent, QDA is the most appropriate method for sample classification. As

previously mentioned in Section 3.3.5., the TIS for each of the samples in the model were normalized using the "summed to one" method. The "summed to one" data was processed to include only the data associated with the MEIS for the AHC designated classes. The covariance matrices for the six classes were calculated using the "summed to one" MEIS data. The likelihood ratio test was used to determine equivalence between the class covariance matrices, which were found to be statistically different. Based on this result, QDA was the most appropriate classification method for sample assignment to the classes. To visualize the differences between the covariance matrices for each pairwise comparison, the "covplot" function was employed to generate the plots using the *pcaPP* package [74], accessed from the R software. The plots for each two class comparison are illustrated in Figures 22 to 36.

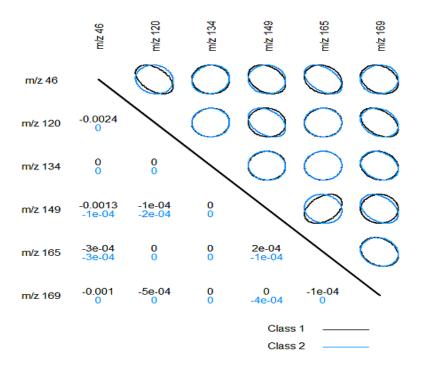


Figure 22: Comparison of the Class 1 and Class 2 covariance matrices

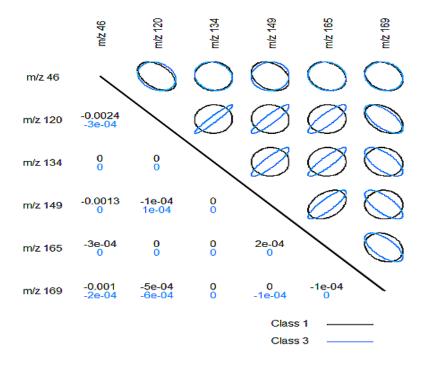


Figure 23: Comparison of Class 1 and Class 3 covariance matrices

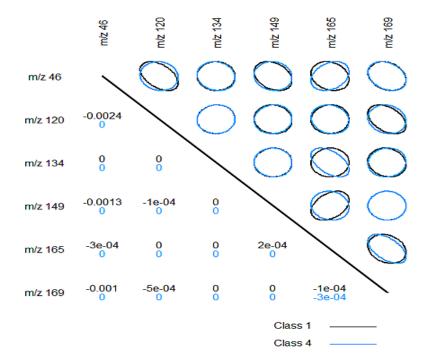


Figure 24: Comparison of Class 1 and Class 4 covariance matrices

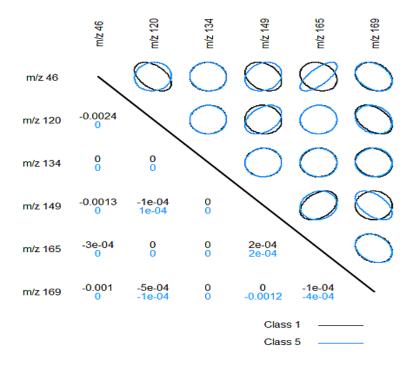


Figure 25: Comparison of Class 1 and Class 5 covariance matrices

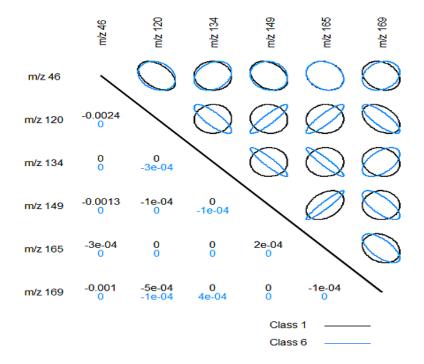


Figure 26: Comparison of Class 1 and Class 6 covariance matrices

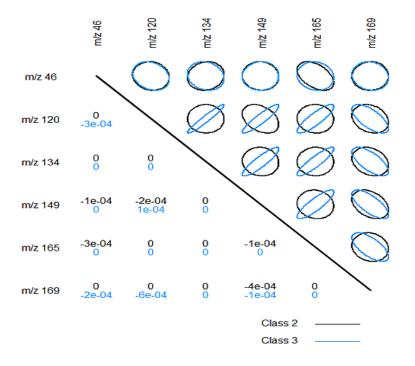


Figure 27: Comparison of Class 2 and Class 3 covariance matrices

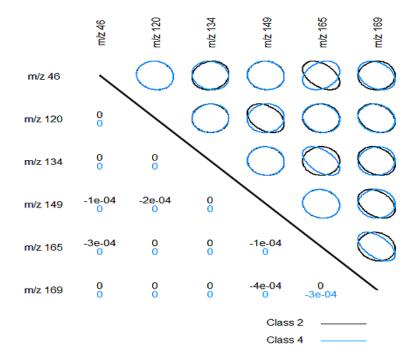


Figure 28: Comparison of Class 2 and Class 4 covariance matrices

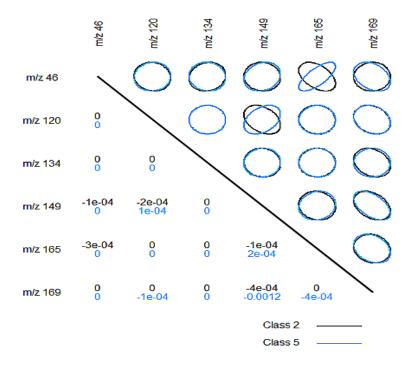


Figure 29: Comparison of Class 2 and Class 5 covariance matrices

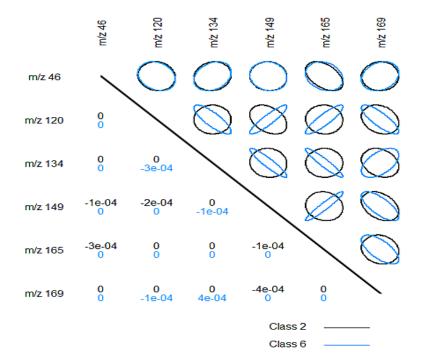


Figure 30: Comparison of Class 2 and Class 6 covariance matrices

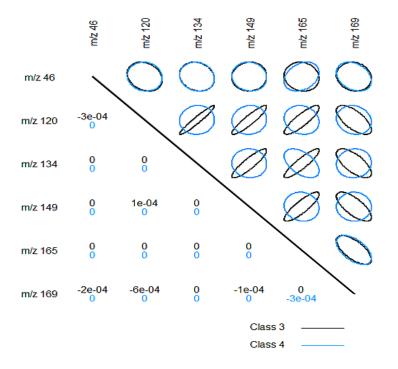


Figure 31: Comparison of Class 3 and Class 4 covariance matrices

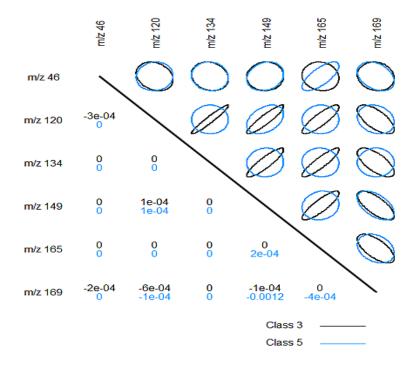


Figure 32: Comparison of Class 3 and Class 5 covariance matrices

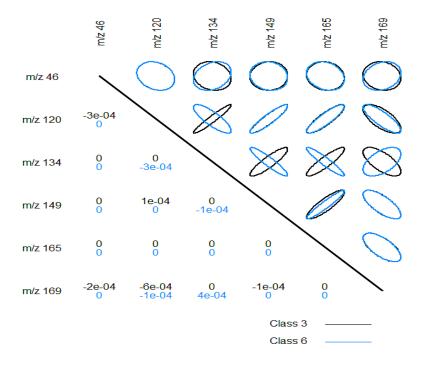


Figure 33: Comparison of Class 3 and Class 6 covariance matrices

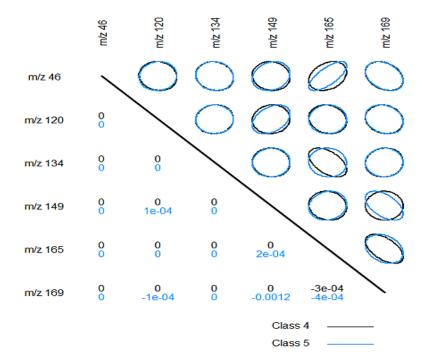


Figure 34: Comparison of Class 4 and Class 5 covariance matrices

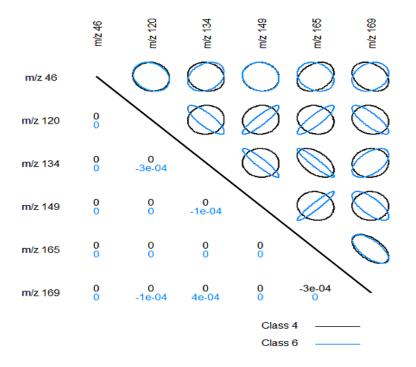


Figure 35: Comparison of Class 4 and Class 6 covariance matrices

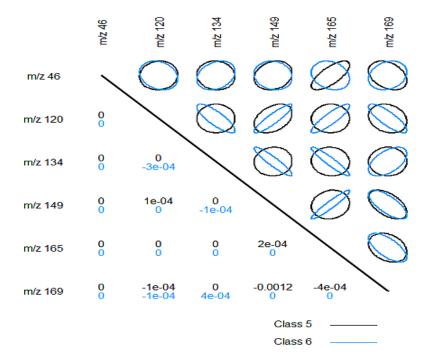


Figure 36: Comparison of Class 5 and Class 6 covariance matrices

In each plot, the covariance ellipses are shown above the diagonal; while the covariance values for each of the class associated ions are shown below the diagonal. In addition, for each comparison, the covariance values and ellipses for each class is shown as one color. For example, in Figure 22, the values and ellipses for Class 1 are shown in black, while the values and ellipses for Class 2 are shown in blue. For each of the two class comparisons, the covariance ellipses were observed to have different volumes and orientations in space, which demonstrated that the covariance matrices were not equivalent. Though QDA was determined to be the more appropriate classification method, LDA is more commonly used; therefore, the method was also utilized for classification in this work.

#### 4.2.6. *LDA/QDA*

#### 4.2.6.1. Development of the Discriminant Models

Classification models were developed for sample assignment to known classes using LDA and QDA. The dataset utilized for model development was comprised of the AHC designated class associated MEIS data for the 639 FBI and 87 NCFS ground truth samples. Leave-one-out and leave-group-out cross-validation was employed to optimize the models, and for evaluation of model performance. Leave-one-out cross-validation was achieved by withholding a lone sample, which was used as a validation test sample, prior to development of the model. For LGOCV, data representing 10% of each class was withheld to be used as a validation test set, prior to model development. For each model type, the prior probabilities for each class were set equal,

and a sample was assigned to the class with the highest posterior probability. The results for assignment of the cross-validation samples to the six AHC designated classes are summarized in confusion matrices. In each matrix, row headings represent the AHC designated classes for the CV samples, while column headings represent class predictions by the model. Values on the diagonal represent correct classifications; where samples both clustered in, and were assigned to the same class. Sample misclassifications are represented by the off-diagonal values. Correct classification rates for assignment of the CV samples to the AHC designated classes were calculated, and are listed under the column titled "% Correct" in the matrix.

### 4.2.6.1.1 Assignment of the CV samples using the LDA LOO model

The results for assignment of the CV samples using the LDA LOO model are summarized in Table 11.

			Predictions based on the LDA LOO model										
		Class 1	Class 1 Class 2 Class 3 Class 4 Class 5 Class 6 Sum % Correct										
	Class 1	281	2	2				285	99				
	Class 2		186					186	100				
AHC designated	Class 3			43		2		45	96				
class	Class 4				133			133	100				
	Class 5		5		4	42		51	82				
	Class 6						26	26	100				
	Sum	281 193 45 137 44 26 726 9											

Table 11: Confusion matrix summarizing assignment of the CV samples using the LDA LOO model

A few misclassifications were observed for sample assignment to Classes 1, 3, and 5, resulting in correct classification rates of 99%, 96%, and 82%, respectively. No misclassifications were observed when assigning the CV samples to Classes 2, 4, and 6. For the misclassified samples, four Class 1 samples were incorrectly assigned; where two samples misclassified to Class 2, and two samples misclassified to Class 3. Additional misclassifications were observed when two Class 3 samples incorrectly assigned to Class 5, and nine Class 5 samples misclassified; where five samples incorrectly assigned to Class 2, and four samples misclassified to Class 4. Despite these misclassifications, an overall correct classification rate of 98% was achieved. Three of the four misclassified Class 1 samples were each assigned to the class associated with the ion of

second highest intensity. That is, the AHC designated class was the class associated with the base peak ion; while the samples were assigned to classes associated with the ion of second highest intensity. The fourth sample was clustered in the class associated with the second most intense ion, and assigned to the class associated with the third most intense ion. Conversely, two Class 3 samples which clustered according to the second most intense ion, were assigned to the class synonymous with the base peak ion (Class 5). For the nine remaining misclassifications, five samples were designated Class 5, which was the class associated with the second most intense ion, but were assigned to the classes corresponding to the base peak ion. In addition, three samples were designated Class 5 due to the base peak, but were assigned to Class 4 according to the second most intense ion. The remaining Class 5 sample was clustered according to its most intense ion, and assigned to Class 4 based on the ion of second highest intensity.

### 4.2.6.1.2. Assignment of the CV samples using the LDA LGO model

The results for assignment of the CV samples using the LDA LGO model are given in Table 12. Correct classification rates of 100% were achieved for assignment of the samples to Classes 2, 3, 4, 5, and 6. Misclassification of one Class 1 sample to Class 3 resulted in a high correct classification rate of 96%. The misclassified sample was designated Class 1 due to the base peak, and assigned to Class 3, which was the class associated with the second most intense ion.

			Predictions based on the LDA LGO model									
		Class 1	Class 2	Class 3	Class 4	Class 5	Class 6	Sum	% Correct			
	Class 1	27		1				28	96			
	Class 2		18					18	100			
AHC designated	Class 3			4				4	100			
class	Class 4				13			13	100			
	Class 5					5		5	100			
	Class 6						2	2	100			
	Sum	27	18	5	13	5	2	70	99			

Table 12: Confusion matrix summarizing assignment of the CV samples using the LDA LGO model

#### 4.2.6.1.3. Assignment of the CV samples using the QDA LOO model

Table 13 provides a summary for assignment of the CV samples to the AHC designated classes using the QDA LOO model. Four Class 1 samples, two Class 3 samples, and nine Class 5 samples were misclassified to other classes, resulting in correct classification rates of 99%, 96%, and 82%, respectively. Samples were assigned to Classes 2, 4, and 6 with correct classification rates of 100%. An overall correct classification rate of 98% was achieved for assignment of the CV samples to the AHC designated classes using this model.

			Predictions based on the QDA LOO model									
		Class 1	Class 2	Class 3	Class 4	Class 5	Class 6	Sum	% Correct			
	Class 1	281	2	2				285	99			
	Class 2		186					186	100			
AHC designated	Class 3			43		2		45	96			
class	Class 4				133			133	100			
	Class 5		5		4	42		51	82			
	Class 6						26	26	100			
	Sum	281	193	45	137	44	26	726	98			

Table 13: Confusion matrix summarizing assignment of the CV samples using the QDA LOO model

The same observations which were made for assignment of the CV samples to the AHC designated classes using the LDA LOO model were also made using this model. That is, the majority of the misclassified samples were either clustered in the class associated with the base peak ion, and assigned to the class associated with the second most intense ion, or the opposite was true. One exception was observed where one Class 5 sample clustered due to the third most intense ion, and assigned to the class associated with the ion of second highest intensity.

#### 4.2.6.1.4. Assignment of the CV samples using the QDA LGO model

The results obtained for assignment of the CV samples using the QDA LGO model are summarized in Table 14. An overall correct classification rate of 100% was observed for sample assignment to the AHC designated classes.

			Predictions based on the QDA LGO model										
		Class 1	Class 2	Class 3	Class 4	Class 5	Class 6	Sum	% Correct				
	Class 1	28						28	100				
	Class 2		18					18	100				
AHC designated	Class 3			4				4	100				
class	Class 4				13			13	100				
	Class 5					5		5	100				
	Class 6						2	2	100				
	Sum	28	18	4	13	5	2	70	100				

Table 14: Confusion matrix summarizing assignment of the CV samples using the QDA LGO model

### 4.2.6.2. Class Assignment of the NCFS test samples

As mentioned previously, 87 NCFS smokeless powder samples were extracted and analyzed by two analysts. The models developed for LDA and QDA comprised 639 FBI and 87 NCFS ground truth samples from one analyst. The optimized models were used to classify the NCFS test samples from the second analyst. The NCFS test samples were described previously in Section 3.2.2. Correct classification rates for assignment of the test samples were calculated by comparing the AHC designated classes for the ground truth samples, to predictions made by the model for class assignment of the test samples. The results for class assignment of the test samples are given in confusion matrices; where row headings represent the AHC designated classes for the NCFS ground truth samples, and column headings represent class predictions by the model.

### 4.2.6.2.1. Classification based on the LDA LOO and LGO models

The results obtained for assignment of the NCFS test samples to the AHC designated classes using the LDA LOO and LGO models are reported together since the results were identical using both models. Table 15 provides a summary of the results. The test samples assigned to Classes 1, 2, 4, and 6 with 100% correct classification rates; however, a low correct classification rate of 33% was observed for sample assignment to Class 5. Of the three samples belonging to Class 5, two were incorrectly assigned to Class 2. In addition, NCFS samples neither clustered in, nor were assigned to Class 3.

			Predictions based on the LDA LOO/LGO models										
		Class 1	Class 1 Class 2 Class 3 Class 4 Class 5 Class 6 Sum % Correct										
	Class 1	33						33	100				
	Class 2		15					15	100				
AHC designated	Class 3	N	NCFS smokeless powder samples neither clustered in nor were assigned to Class 3										
class	Class 4				31			31	100				
	Class 5		2			1		3	33				
	Class 6						5	5	100				
	Sum	33	17	0	31	1	5	87	98				

Table 15: Confusion matrix summarizing assignment of the NCFS test samples using the LDA models The results obtained using the LOO and LGO models are reported as the same confusion matrix since the results using both models were identical

The misclassified Class 5 samples clustered within the class corresponding to their second most intense ion, and were assigned to the class corresponding to their base peak ion.

# 4.2.6.2.2. Classification based on the QDA LOO and LGO models

The results obtained for assignment of the NCFS test samples to the AHC designated classes using the QDA LOO and LGO models are reported together since the results were identical using both models. The results are summarized in Table 16.

			Bradictions have done the ODA LOOT COmpatible										
			Predictions based on the QDA LOO/LGO models										
		Class 1	Class 1 Class 2 Class 3 Class 4 Class 5 Class 6 Sum % Correct										
	Class 1	33						33	100				
	Class 2		15					15	100				
AHC designated	Class 3	NCFS smokeless powder samples neither clustered in nor were assigned to Class 3											
class	Class 4				31			31	100				
	Class 5					3		3	100				
	Class 6						5	5	100				
	Sum	33	15	0	31	3	5	87	100				

Table 16: Confusion matrix summarizing assignment of the NCFS test samples using the QDA models The results obtained using the LOO and LGO models are reported as the same matrix since the results using both models were identical

As can be seen, no misclassifications were observed for assignment of the test samples to the AHC designated classes; thus, a 100% overall correct classification rate was achieved. Additionally, NCFS samples neither clustered in, no were assigned to Class 3.

### 4.2.7. Comparison of the Classification Methods

A new classification rule, the IIR, was developed in this work for sample assignment to AHC designated classes. In addition, discriminant models were developed for sample assignment to the AHC designated classes using kNN, LDA, and QDA. The models were optimized using LOO

and LGOCV. The performance of the discriminant models was evaluated by calculating correct classification rates for assignment of the CV samples to the AHC designated classes. Cross-validation was not used to evaluate the performance of the IIR since the rule is implemented simply by visual inspection of the sample MEIS; where the sample is assigned to the class associated with the most intense ion. The IIR and the optimized *k*NN, LDA, and QDA models were utilized for class assignment of the NCFS smokeless powder test samples. Within the models, NCFS smokeless powder samples were taken as ground truth samples, and correct classification rates were calculated by comparing the AHC designated classes of the ground truth samples, to predictions made by the model for class assignment of the test samples. Table 17 summarizes the overall correct classification rates for class assignment of the RFS end QDA.

Samples assigned by the	Discriminant Model										
Discriminant Model	IID	k I	NN	LI	DA	QDA					
	IIR	LOO	LGO	LOO	LGO	LOO	LGO				
CV samples	_	<del>9</del> 9	99	98	99	<mark>9</mark> 8	100				
NCFS test samples	93	100	100	98	98	100	100				

Table 17: Overall correct classification rates for sample assignment to AHC designated classes

High overall correct classification rates were achieved for assignment of the CV samples to the AHC designated classes using *k*NN, LDA, and QDA. High overall correct classification rates

were also observed for assignment of the NCFS test samples to the AHC designated classes using the IIR, *k*NN, LDA, and QDA. The lowest correct classification rate was observed for class assignment of the test samples using the IIR. The misclassified CV and NCFS test samples are summarized in Tables 18 and 19, respectively.

AHC designated	SRN	<b>k</b> ]	NN	LI	DA	QDA		
class		L00	LGO	LOO	LGO	LOO	LGO	
Class 5	31			Class 4		Class 4		
Class 3	47			Class 5		Class 5		
Class 1	80			Class 3	Class 3	Class 3		
Class 5	105			Class 2		Class 2		
Class 1	129			Class 3		Class 3		
Class 5	176			Class 2		Class 2		
Class 1	189		Class2	Class 2		Class 2		
Class 1	196	Class 2		Class 2		Class 2		
Class 5	206			Class 4		Class 4		
Class 5	258	Class 2		Class 2		Class 2		
Class 5	299			Class 2		Class 2		
Class 5	416			Class 4		Class 4		
Class 5	500			Class 2		Class 2		
Class 5	506			Class 4		Class 4		
Class 3	701			Class 5		Class 5		
Class 2	785	Class 5						
Class 2	788	Class 5						

Table 18: Comparison of the misclassified CV samples using the kNN, LDA, and QDA models

AHC designated class	SRN	IIR	k NN		LDA		QDA	
			L00	LGO	L00	LGO	L00	LGO
Class 5	105	Class 2			Class 2	Class 2		
Class 2	136	Class 1						
Class 2	160	Class 1						
Class 5	176	Class 2			Class 2	Class 2		
Class 2	180	Class 1						
Class 2	187	Class 1						

Table 19: Comparison of the misclassified NCFS test samples using the IIR, *k*NN, LDA, and QDA models

In Tables 18 and 19, the column titled "SRN" represents the sample reference number assigned to the smokeless powder sample record in the database; while the column titled "AHC designated class" represents the class of the sample determined from cluster analysis. Within the "SRN" column, the samples shown in green, black, and red represent samples which clustered in their respective class according to the base peak, the ion of second highest intensity, and the third most intense ion, respectively. The cell entries represent the class to which the sample was assigned using the respective model. For all samples shown in green, the AHC designated class was associated with the base peak ion, while the predicted class was associated with the ion of second highest intensity. The samples shown in black grouped within their AHC designated classes based on the ion of second highest intensity, but were assigned to the class associated with the base peak ion. For example, SRN 31 clustered in Class 5 according to the base peak, but was incorrectly assigned to Class 4, the class associated with the ion of second highest intensity, using the LDA and QDA LOO models. In addition, the sample did not misclassify using any other model. The only exceptions to this trend were observed for SRN 160, 180, and 416. For each of these samples, the predicted class associated with the most intense ion in each test sample MEIS was not the same as the AHC designated class for the ground truth samples. That is, the ground truth samples for SRN 160 and 180 both clustered in Class 2, where m/z 149 was the base peak ion for both ground truth samples; however, the test samples were assigned to Class 1 (m/z 46) which was the base peak ion for both test samples using the IIR. In addition, the models did not misclassify these samples despite the presence of the base peak. For SRN 416, the sample clustered to the class associated with the third most intense ion, and was assigned to

the class associated with the ion of second highest intensity. As is evident within each table, the misclassified samples were all incorrectly assigned to the same classes using the IIR and the discriminant models.

A few samples in the model dataset were clustered within classes associated with the ion of second highest intensity. One exception was observed for SRN 416, which clustered within the class associated with the third most intense ion. These samples were also assigned to their respective AHC designated classes using kNN, LDA, and QDA. Tables 20 and 21 provide lists of the CV and NCFS test samples which were assigned using the each of the models. The outline of each of the tables is the same as described for Tables 18 and 19. As can be seen, the models assigned the samples to their AHC designated classes instead of the class associated with the base peak ion.

AHC designated class	SRN	k NN		LDA		QDA	
		L00	LGO	L00	LGO	L00	LGO
Class 2	16	Class 2		Class 2		Class 2	
Class 3	47	Class 3					
Class 5	105	Class 5					
Class 2	136	Class 2		Class 2	Class 2	Class 2	
Class 5	176	Class 5					
Class 2	187	Class 2		Class 2		Class 2	
Class 5	190	Class 5				Class 5	
Class 5	299	Class 5					Class 5
Class 5	416	Class 5					
Class 5	500	Class 5					
Class 2	518	Class 2		Class 2	Class 2	Class 2	
Class 2	681	Class 2		Class 2		Class 2	
Class 3	701	Class 3					
Class 2	822	Class 2		Class 2		Class 2	
Class 2	823	Class 2		Class 2		Class 2	

Table 20: Comparison of the CV sample anomalies within the kNN, LDA, and QDA models

AHC designated class	SRN	k NN		LDA		QDA	
		L00	LGO	L00	LGO	L00	LGO
Class 5	105	Class 5	Class 5			Class 5	Class 5
Class 2	136	Class 2					
Class 5	176	Class 5	Class 5			Class 5	Class 5
Class 2	187	Class 2					

Table 21: Comparison of the NCFS test sample anomalies within the *k*NN, LDA, and QDA models

#### 4.3. Smokeless Powders Bayes Nets

As previously discussed, Bayesian Networks (BN) are graphical representations which encode probabilistic relationships between events of interest in a joint probability distribution. The structure of the BN or the directed acyclic graph (DAG) is comprised of nodes, each of which represents a random variable, or an event of interest; and arcs or arrows, which describe the causal relationships between the nodes. Each node can take a number of states, or possible outcomes, for the event defined by that node. Within the network, nodes without directed arcs are referred to as parent nodes; while nodes with arcs directed into them are referred to as child nodes. Parent nodes are conditionally independent of other nodes in the DAG; while child nodes are conditionally dependent on their parents, and conditionally independent of other child nodes given their parents. Conditional independence between the child nodes can be determined from the structure of the DAG using a visual method, which states that nodes are conditionally independent if they are *d*-separated (directionally separated), given their parents [58]. Two child nodes are *d*-separated when evidence is observed in their common parent; that is, the nodes are d-separated and conditionally independent if they have a parent in common, and that parent is instantiated. Each node in the DAG has an associated probability table, where tables associated with parent nodes encode prior probabilities, and tables associated with child nodes encode class-conditional probabilities. That is, the table associated with the parent node encodes the probabilities of possible outcomes for the event within that node; while the table associated with the child node encodes probabilities for possible outcomes for the event within that node, conditioned on its parent. Bayesian Networks are used to calculate the probabilities for events through the observation of evidence. Once evidence is observed, the network is instantiated, and the prior probabilities are updated to posterior probabilities.

An R code was written in-house to develop BNs to calculate posterior probabilities of a smokeless powder belonging to a specific manufacturer through the observation of evidence. Within the code, 100 iterations were performed for development of the BN. For each repetition, 5% of the data was withheld as the test set, and the remaining 95% was used to develop the functional network comprising the nodes and their associated probability tables. The networks, which were developed using the 119 NCFS smokeless powder database samples, are shown in Figures 37 and 38.

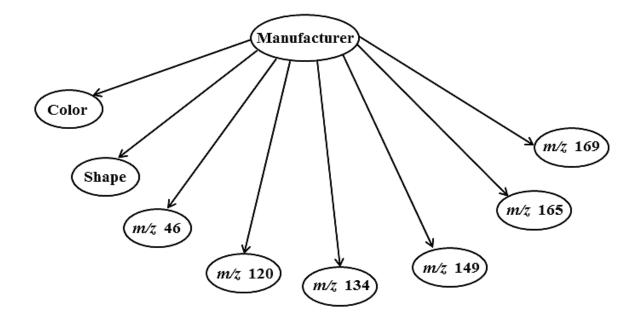


Figure 37: Bayesian Network excluding the average diameter (D) and average length (L) child nodes

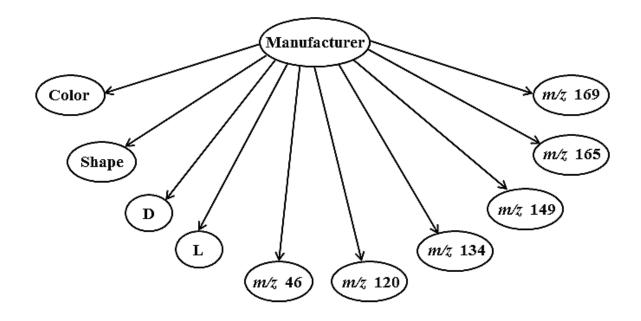


Figure 38: Bayesian Network including the average diameter (D) and average length (L) child nodes

The structures of the networks shown in Figures 37 and 38 were determined by looking at the causal dependencies between the events under study, as well as the inference problem under consideration. That is, each of the powder characteristics such as shape, color, dimension, and chemical composition is controlled by the manufacturer, while none of the aforementioned properties determine the manufacturer. Therefore, causal dependencies exist between the manufacturer and each of the states (color, shape, etc.), but there are no causal dependencies between the states and the manufacturer. In addition, the posterior probability of a smokeless powder belonging to a certain manufacturer represents the inference problem in this work. In each network, the parent node is the Manufacturer, and the child nodes are Color, Shape, m/z 46 (Class 1), *m/z* 149 (Class 2), *m/z* 120 (Class 3), *m/z* 165 (Class 4), *m/z* 169 (Class 5), and *m/z* 134 (Class 6). Two additional child nodes, representing average diameter (D) and average length (L), were included in the network shown in Figure 38. The states within the Manufacturer node were Alliant Powder Company, Hodgdon Powder Company, Norma Precision AB, Vihta Vuori, and Western Powders. The states in the Shape node were ball, cylinder (tubular), disk, and flattened ball. Within each node for the class associated ions, the states represented the intensity of the ion as zero, weak, medium, or strong; where zero indicated the absence of a peak for the ion, a range greater than 0 and less than or equal to 0.33 was assigned as weak, ranges greater than 0.33 and less than or equal to 0.66 were medium, and intensities indicated as strong were in the range greater than 0.66, and less than or equal to 1. Six states were assigned within the average diameter (D) and average length (L) nodes; where the states took values d1 (11) greater than 0 mm and less than or equal to 0.4 mm, d2 (12) greater than 0.4 mm and less than or equal to 0.8

mm, d3 (13) greater than 0.8 mm and less than or equal to 1.2 mm, d4 (14) greater than 1.2 mm and less than or equal to 1.6 mm, d5 (15) greater than 1.6 mm and less than or equal to 2.0 mm, and d6 (16) greater than 2.0 mm and less than or equal to 2.4 mm. The child nodes within each network were assumed to be conditionally independent, given the Manufacturer, since evidence was never observed (i.e., no instantiation) in the Manufacturer node; in addition, there were no causal dependencies between any of the manufacturer controlled powder properties. The prior and class-conditional probabilities for each state within the nodes were calculated based on their frequencies within the dataset. The prior probability table associated with the Manufacturer node for both networks is shown in Table 22.

Manufacturer	Prior Probabilities
Alliant Powder Company	0.17
Hodgdon Powder Company	0.55
Norma Precision AB	0.07
Vihta Vuori	0.06
Western Powders	0.15
SUM	1

Table 22: Prior probability table associated with the Manufacturer node shown in Figures 37 and 38

Smokeless powders manufactured by the Hodgdon Powder Company comprise more than 50% of the data; while powders manufactured by Norma Precision AB, and Vihta Vuori occur with the lowest probabilities. The child nodes within each network were instantiated using the states observed for each sample in the test set, and the prior probabilities in the Manufacturer node were updated to posterior probabilities after observation of the evidence. The posterior probabilities which were calculated for the manufacturers for each test sample, using the DAG design shown in Figure 37, are summarized in Tables 23 through 27. In each table, the column titled "SRN" represents the sample reference number for the smokeless powder sample record in the database; while the column titled "Known Manufacturer" represents the known manufacturer for the test samples. As mentioned previously, 100 iterations were performed during development of the network. For each repetition, 5% of the data was randomly withheld from the entire dataset to be used as a test set; therefore, a number of repetitions for each sample were included in the test data set. The replicate samples which were assigned to different manufacturers based on the highest posterior probabilities are shown in red. The manufacturer posterior probabilities which were calculated for each test sample are listed in the columns titled "Alliant Powder Company", "Hodgdon Powder Company", "Norma Precision AB", "Vihta Vuori", and "Western Powders". For example, the known manufacturer of SRN 121 (shown in Table 23) was Alliant Powder Company, and the posterior probability of the sample belonging to Alliant Powder Company was 0.98. With the exception of test samples manufactured by Norma Precision AB, the majority of the samples were identified as belonging to their respective manufacturer with fairly high to high posterior probabilities.

# Table 23: Posterior probabilities calculated for smokeless powders manufactured by Alliant Powder Company (data excludes average diameter and average length)

			Pos	terior Probabilities			
SRN	Known Manufacturer	Alliant Powder Company	Hodgdon Powder Company	Norma Precision AB	Vihta Vuori	Western Powders	SUM
SRN 119	Alliant Powder Company	0.79	0.21	0	0	0	1
SRN 120	Alliant Powder Company	0.84	0.16	0	0	0	1
SRN 121	Alliant Powder Company	0.98	0.02	0	0	0	1
SRN 122	Alliant Powder Company	0.98	0.02	0	0	0	1
SRN 123	Alliant Powder Company	0.98	0.02	0	0	0	1
SRN 124	Alliant Powder Company	0.98	0.02	0	0	0	1
SRN 125	Alliant Powder Company	0.94	0.06	0	0	0	1
SRN 126	Alliant Powder Company	0.98	0.02	0	0	0	1
SRN 127	Alliant Powder Company	0.42	0.06	0.45	0	0.07	1
SRN 127	Alliant Powder Company	0.45	0.06	0.42	0	0.07	1
SRN 128	Alliant Powder Company	0.51	0.06	0.36	0	0.08	1
SRN 130	Alliant Powder Company	0.33	0.09	0.48	0	0.10	1
SRN 130	Alliant Powder Company	0.41	0.10	0.36	0	0.12	1
SRN 131	Alliant Powder Company	1	0	0	0	0	1
SRN 132	Alliant Powder Company	0.29	0.09	0.52	0	0.09	1
SRN 132	Alliant Powder Company	0.42	0.11	0.36	0	0.11	1
SRN 133	Alliant Powder Company	0.46	0.05	0.43	0	0.06	1
SRN 134	Alliant Powder Company	0.41	0.06	0.46	0	0.08	1
SRN 134	Alliant Powder Company	0.47	0.05	0.40	0	0.07	1
SRN 135	Alliant Powder Company	1	0	0	0	0	1
SRN 303	Alliant Powder Company	0.36	0.07	0.47	0	0.10	1
SRN 303	Alliant Powder Company	0.42	0.12	0.37	0	0.10	1
SRN 349	Alliant Powder Company	0.36	0.09	0.47	0	0.08	1

 Table 24: Posterior probabilities calculated for smokeless powders manufactured by the Hodgdon Powder Company (data excludes average diameter and average length)

			Pos	terior Probabilities			
SRN	Known Manufacturer	Alliant Powder Company	Hodgdon Powder Company	Norma Precision AB	Vihta Vuori	Western Powders	SUM
SRN 136	Hodgdon Powder Company	0.87	0.13	0	0	0	1
SRN 137	Hodgdon Powder Company	0	1	0	0	0	1
SRN 138	Hodgdon Powder Company	0	1	0	0	0	1
SRN 139	Hodgdon Powder Company	0	0.39	0	0	0.61	1
SRN 140	Hodgdon Powder Company	0	0.24	0	0	0.76	1
SRN 141	Hodgdon Powder Company	0	0.48	0	0	0.52	1
SRN 141	Hodgdon Powder Company	0	0.78	0	0	0.22	1
SRN 142	Hodgdon Powder Company	0	0.37	0	0	0.63	1
SRN 143	Hodgdon Powder Company	0	0.32	0	0	0.68	1
SRN 144	Hodgdon Powder Company	0	0.59	0	0	0.41	1
SRN 145	Hodgdon Powder Company	0	1	0	0	0	1
SRN 146	Hodgdon Powder Company	0	1	0	0	0	1
SRN 147	Hodgdon Powder Company	0	1	0	0	0	1
SRN 148	Hodgdon Powder Company	0	0.57	0	0	0.43	1
SRN 149	Hodgdon Powder Company	0	0.41	0	0	0.59	1
SRN 150	Hodgdon Powder Company	0	1	0	0	0	1
SRN 151	Hodgdon Powder Company	0	0.03	0	0	0.97	1
SRN 152	Hodgdon Powder Company	0	0.46	0	0	0.54	1
SRN 152	Hodgdon Powder Company	0	0.55	0	0	0.45	1
SRN 153	Hodgdon Powder Company	0	1	0	0	0	1
SRN 154	Hodgdon Powder Company	0	1	0	0	0	1
SRN 155	Hodgdon Powder Company	0	1	0	0	0	1

			Pos	terior Probabilities			
SRN	Known Manufacturer	Alliant Powder Company	Hodgdon Powder Company	Norma Precision AB	Vihta Vuori	Western Powders	SUM
SRN 156	Hodgdon Powder Company	0	1	0	0	0	1
SRN 157	Hodgdon Powder Company	0	1	0	0	0	1
SRN 158	Hodgdon Powder Company	0	1	0	0	0	1
SRN 159	Hodgdon Powder Company	0	1	0	0	0	1
SRN 160	Hodgdon Powder Company	0.36	0.07	0.47	0	0.10	1
SRN 160	Hodgdon Powder Company	0.43	0.06	0.41	0	0.10	1
SRN 161	Hodgdon Powder Company	0	0.27	0	0	0.73	1
SRN 162	Hodgdon Powder Company	0	0.25	0	0	0.75	1
SRN 163	Hodgdon Powder Company	0	1	0	0	0	1
SRN 164	Hodgdon Powder Company	0	1	0	0	0	1
SRN 165	Hodgdon Powder Company	0	1	0	0	0	1
SRN 166	Hodgdon Powder Company	0	1	0	0	0	1
SRN 167	Hodgdon Powder Company	0	0	0	0	1	1
SRN 168	Hodgdon Powder Company	0	1	0	0	0	1
SRN 169	Hodgdon Powder Company	0	1	0	0	0	1
SRN 170	Hodgdon Powder Company	0	1	0	0	0	1
SRN 171	Hodgdon Powder Company	0	1	0	0	0	1
SRN 172	Hodgdon Powder Company	0	1	0	0	0	1
SRN 173	Hodgdon Powder Company	0	1	0	0	0	1
SRN 174	Hodgdon Powder Company	0.92	0.08	0	0	0	1
SRN 175	Hodgdon Powder Company	0	1	0	0	0	1
SRN 176	Hodgdon Powder Company	0	0	0	1	0	1

			Pos	terior Probabilities			
SRN	Known Manufacturer	Alliant Powder Company	Hodgdon Powder Company	Norma Precision AB	Vihta Vuori	Western Powders	SUM
SRN 177	Hodgdon Powder Company	0.92	0.08	0	0	0	1
SRN 178	Hodgdon Powder Company	0	1	0	0	0	1
SRN 305	Hodgdon Powder Company	0	1	0	0	0	1
SRN 306	Hodgdon Powder Company	0	0.35	0	0	0.65	1
SRN 306	Hodgdon Powder Company	0	0.76	0	0	0.24	1
SRN 307	Hodgdon Powder Company	0	0.42	0	0	0.58	1
SRN 307	Hodgdon Powder Company	0	0.53	0	0	0.47	1
SRN 308	Hodgdon Powder Company	0	1	0	0	0	1
SRN 309	Hodgdon Powder Company	0	1	0	0	0	1
SRN 311	Hodgdon Powder Company	0	1	0	0	0	1
SRN 314	Hodgdon Powder Company	0	1	0	0	0	1
SRN 321	Hodgdon Powder Company	0	1	0	0	0	1
SRN 322	Hodgdon Powder Company	0	1	0	0	0	1
SRN 323	Hodgdon Powder Company	0	1	0	0	0	1
SRN 324	Hodgdon Powder Company	0	1	0	0	0	1
SRN 325	Hodgdon Powder Company	0	1	0	0	0	1
SRN 326	Hodgdon Powder Company	0	1	0	0	0	1
SRN 329	Hodgdon Powder Company	0	1	0	0	0	1
SRN 330	Hodgdon Powder Company	0	0.35	0	0	0.65	1
SRN 331	Hodgdon Powder Company	0	1	0	0	0	1
SRN 332	Hodgdon Powder Company	0	1	0	0	0	1
SRN 335	Hodgdon Powder Company	0	0.30	0	0	0.70	1

SRN	Known Manufacturer	Alliant Powder Company	Hodgdon Powder Company	Norma Precision AB	Vihta Vuori	Western Powders	SUM		
SRN 336	Hodgdon Powder Company	0	0.32	0	0	0.68	1		
SRN 336	Hodgdon Powder Company	0	0.53	0	0	0.47	1		
SRN 337	Hodgdon Powder Company	0	1	0	0	0	1		
SRN 338	Hodgdon Powder Company	0	1	0	0	0	1		
SRN 345	Hodgdon Powder Company	0	0.03	0	0	0.97	1		
SRN 348	Hodgdon Powder Company	0	1	0	0	0	1		

#### **Posterior Probabilities**

 Table 25: Posterior probabilities calculated for smokeless powders manufactured by Norma Precision AB (data excludes average diameter and average length)

			Posterior Probabilities							
SRN	Known Manufacturer	Alliant Powder Company	Hodgdon Powder Company	Norma Precision AB	Vihta Vuori	Western Powders	SUM			
SRN 300	Norma Precision AB	0.49	0.09	0.31	0	0.11	1			
SRN 301	Norma Precision AB	0.50	0.10	0.32	0	0.08	1			
SRN 302	Norma Precision AB	1	0	0	0	0	1			
SRN 339	Norma Precision AB	0.49	0.10	0.32	0	0.09	1			
SRN 341	Norma Precision AB	0.55	0.05	0.33	0	0.06	1			
SRN 342	Norma Precision AB	0.59	0.06	0.27	0	0.07	1			
SRN 343	Norma Precision AB	0.59	0.06	0.27	0	0.07	1			
SRN 344	Norma Precision AB	0.59	0.06	0.27	0	0.08	1			

Table 26: Posterior probabilities calculated for smokeless powders manufactured by Vihta Vuori (data excludes average diameter and average length)

SRN	Known Manufacturer	Alliant Powder Company	Hodgdon Powder Company	Norma Precision AB	Vihta Vuori	Western Powders	SUM	
SRN 312	Vihta Vuori	0	0	0	1	0	1	
SRN 313	Vihta Vuori	0	0	0	1	0	1	
SRN 327	Vihta Vuori	0	0	0	1	0	1	
SRN 328	Vihta Vuori	0	0	0	1	0	1	
SRN 333	Vihta Vuori	0	0	0	1	0	1	
SRN 346	Vihta Vuori	0	0	0	1	0	1	
SRN 347	Vihta Vuori	0	0.33	0	0.67	0	1	

**Posterior Probabilities** 

# Table 27: Posterior probabilities calculated for smokeless powders manufactured by Western Powders (data excludes average diameter and average length)

		Posterior Probabilities					
SRN	Known Manufacturer	Alliant Powder Company	Hodgdon Powder Company	Norma Precision AB	Vihta Vuori	Western Powders	SUM
SRN 179	Western Powders	0	0.90	0	0	0.10	1
SRN 180	Western Powders	0	0.11	0	0	0.89	1
SRN 181	Western Powders	0	0.11	0	0	0.89	1
SRN 182	Western Powders	0	0	0	0	1	1
SRN 183	Western Powders	0	0	0	0	1	1
SRN 184	Western Powders	0	0.10	0	0	0.90	1
SRN 185	Western Powders	0	0.90	0	0	0.10	1
SRN 186	Western Powders	0	0.12	0	0	0.88	1
SRN 187	Western Powders	0	0.08	0	0	0.92	1
SRN 310	Western Powders	0	1	0	0	0	1
SRN 310	Western Powders	0	0	0	0	1	1
SRN 315	Western Powders	0	1	0	0	0	1
SRN 315	Western Powders	0	0.13	0	0	0.87	1
SRN 316	Western Powders	0.60	0.28	0	0	0.12	1
SRN 317	Western Powders	0	0.45	0	0	0.55	1
SRN 317	Western Powders	0	0.60	0	0	0.40	1
SRN 318	Western Powders	0	0.45	0	0	0.55	1
SRN 318	Western Powders	0	0.59	0	0	0.41	1
SRN 319	Western Powders	0	0.09	0	0	0.91	1
SRN 320	Western Powders	0	0	0	0	1	1
SRN 334	Western Powders	0	0.67	0	0.28	0.05	1
SRN 340	Western Powders	0	0.88	0	0	0.12	1

The percent correct rates obtained for calculating the posterior probabilities for each manufacturer are summarized in Table 28.

Manufacturer	Percent Correct
Alliant Powder Company	73
Hodgdon Powder Company	71
Norma Precision AB	0
Vihta Vuori	100
Western Powders	62
OVERALL	66

 Table 28: Percent correct for manufacturer predictions based on posterior probabilities (data excludes average diameter and average length)

The Vihta Vuori powders were all predicted to have been manufactured by Vihta Vuori; while none of the Norma Precision AB powders were predicted to have been manufactured by Norma Precision AB. An overall percent correct of 66% was obtained for predicting the manufacturer of the test samples based on the highest posterior probabilities.

The posterior probabilities which were calculated for the manufacturers for each test sample, using the DAG design shown in Figure 38, are summarized in Tables 29 through 33. The outline for each table is the same as previously described on Tables 23 through 27. As mentioned before,

the posterior probabilities which were calculated for each test sample are listed in the columns titled "Alliant Powder Company", "Hodgdon Powder Company", "Norma Precision AB", "Vihta Vuori", and "Western Powders".

Table 29: Posterior probabilities for smokeless powders manufactured by Alliant Powder Company (data includes average diameter and average length)

		Posterior Probabilities								
SRN	Known Manufacturer	Alliant Powder Company	Hodgdon Powder Company	Norma Precision AB	Vihta Vuori	Western Powders	SUM			
SRN 119	Alliant Powder Company	0.98	0.02	0	0	0	1			
SRN 120	Alliant Powder Company	0.98	0.02	0	0	0	1			
SRN 121	Alliant Powder Company	1	0	0	0	0	1			
SRN 122	Alliant Powder Company	1	0	0	0	0	1			
SRN 123	Alliant Powder Company	0.96	0.04	0	0	0	1			
SRN 124	Alliant Powder Company	1	0	0	0	0	1			
SRN 125	Alliant Powder Company	0.99	0.01	0	0	0	1			
SRN 126	Alliant Powder Company	0	1	0	0	0	1			
SRN 127	Alliant Powder Company	0.36	0.03	0	0	0.61	1			
SRN 127	Alliant Powder Company	0.52	0.04	0	0	0.44	1			
SRN 128	Alliant Powder Company	0.69	0.10	0	0	0.22	1			
SRN 130	Alliant Powder Company	0.10	0.06	0.84	0	0	1			
SRN 131	Alliant Powder Company	1	0	0	0	0	1			
SRN 132	Alliant Powder Company	0.05	0.03	0.86	0	0.06	1			
SRN 133	Alliant Powder Company	0.11	0.02	0.84	0	0.03	1			
SRN 134	Alliant Powder Company	0.06	0.02	0.87	0	0.04	1			
SRN 135	Alliant Powder Company	1	0	0	0	0	1			
SRN 303	Alliant Powder Company	0.68	0.32	0	0	0	1			
SRN 349	Alliant Powder Company	0.11	0.05	0.60	0	0.24	1			

#### **Posterior Probabilities**

Table 30: Posterior probabilities calculated for smokeless powders manufactured by Hodgdon Powder Company (data includes average diameter and length)

			Pos	terior Probabilities			
SRN	Known Manufacturer	Alliant Powder Company	Hodgdon Powder Company	Norma Precision AB	Vihta Vuori	Western Powders	SUM
SRN 136	Hodgdon Powder Company	0.99	0.01	0	0	0	1
SRN 137	Hodgdon Powder Company	0	1	0	0	0	1
SRN 138	Hodgdon Powder Company	0	1	0	0	0	1
SRN 139	Hodgdon Powder Company	0	0.36	0	0	0.64	1
SRN 140	Hodgdon Powder Company	0	0.07	0	0	0.93	1
SRN 141	Hodgdon Powder Company	0	0.65	0	0	0.35	1
SRN 141	Hodgdon Powder Company	0	0.46	0	0	0.54	1
SRN 142	Hodgdon Powder Company	0	1	0	0	0	1
SRN 143	Hodgdon Powder Company	0	0.30	0	0	0.70	1
SRN 144	Hodgdon Powder Company	0	0.51	0	0	0.49	1
SRN 144	Hodgdon Powder Company	0	0.48	0	0	0.52	1
SRN 145	Hodgdon Powder Company	0	1	0	0	0	1
SRN 146	Hodgdon Powder Company	0	1	0	0	0	1
SRN 147	Hodgdon Powder Company	0	1	0	0	0	1
SRN 148	Hodgdon Powder Company	0	0.23	0	0	0.77	1
SRN 149	Hodgdon Powder Company	0	0.18	0	0	0.82	1
SRN 150	Hodgdon Powder Company	0	1	0	0	0	1
SRN 151	Hodgdon Powder Company	0	0.01	0	0	0.99	1
SRN 152	Hodgdon Powder Company	0	0.43	0	0	0.57	1
SRN 152	Hodgdon Powder Company	0	0.55	0	0	0.45	1
SRN 153	Hodgdon Powder Company	0	1	0	0	0	1
SRN 154	Hodgdon Powder Company	0	1	0	0	0	1

	Posterior Probabilities						
SRN	Known Manufacturer	Alliant Powder Company	Hodgdon Powder Company	Norma Precision AB	Vihta Vuori	Western Powders	SUM
SRN 156	Hodgdon Powder Company	0	1	0	0	0	1
SRN 157	Hodgdon Powder Company	0	1	0	0	0	1
SRN 158	Hodgdon Powder Company	0	1	0	0	0	1
SRN 159	Hodgdon Powder Company	0	1	0	0	0	1
SRN 160	Hodgdon Powder Company	0.10	0.06	0.84	0	0	1
SRN 161	Hodgdon Powder Company	0	0.25	0	0	0.75	1
SRN 162	Hodgdon Powder Company	0	0.07	0	0	0.93	1
SRN 163	Hodgdon Powder Company	0	1	0	0	0	1
SRN 164	Hodgdon Powder Company	0	1	0	0	0	1
SRN 165	Hodgdon Powder Company	0	1	0	0	0	1
SRN 166	Hodgdon Powder Company	0	1	0	0	0	1
SRN 167	Hodgdon Powder Company	0	0	0	0	1	1
SRN 168	Hodgdon Powder Company	0	1	0	0	0	1
SRN 169	Hodgdon Powder Company	0	1	0	0	0	1
SRN 170	Hodgdon Powder Company	0	1	0	0	0	1
SRN 171	Hodgdon Powder Company	0	1	0	0	0	1
SRN 172	Hodgdon Powder Company	0	1	0	0	0	1
SRN 173	Hodgdon Powder Company	0	1	0	0	0	1
SRN 174	Hodgdon Powder Company	1	0	0	0	0	1
SRN 175	Hodgdon Powder Company	0	1	0	0	0	1
SRN 177	Hodgdon Powder Company	0.94	0.06	0	0	0	1

		Posterior Probabilities						
SRN	Known Manufacturer	Alliant Powder Company	Hodgdon Powder Company	Norma Precision AB	Vihta Vuori	Western Powders	SUM	
SRN 305	Hodgdon Powder Company	0	1	0	0	0	1	
SRN 306	Hodgdon Powder Company	0	0.11	0	0	0.89	1	
SRN 306	Hodgdon Powder Company	0	0.53	0	0	0.47	1	
SRN 307	Hodgdon Powder Company	0	0.40	0	0	0.60	1	
SRN 307	Hodgdon Powder Company	0	0.50	0	0	0.50	1	
SRN 308	Hodgdon Powder Company	0	1	0	0	0	1	
SRN 309	Hodgdon Powder Company	0	1	0	0	0	1	
SRN 311	Hodgdon Powder Company	0	1	0	0	0	1	
SRN 314	Hodgdon Powder Company	0	1	0	0	0	1	
SRN 321	Hodgdon Powder Company	0	1	0	0	0	1	
SRN 322	Hodgdon Powder Company	0	1	0	0	0	1	
SRN 323	Hodgdon Powder Company	0	1	0	0	0	1	
SRN 324	Hodgdon Powder Company	0	1	0	0	0	1	
SRN 325	Hodgdon Powder Company	0	1	0	0	0	1	
SRN 326	Hodgdon Powder Company	0	1	0	0	0	1	
SRN 329	Hodgdon Powder Company	0	1	0	0	0	1	
SRN 330	Hodgdon Powder Company	0	0.33	0	0	0.67	1	
SRN 331	Hodgdon Powder Company	0	1	0	0	0	1	
SRN 332	Hodgdon Powder Company	0	1	0	0	0	1	
SRN 335	Hodgdon Powder Company	0	0.09	0	0	0.91	1	
SRN 336	Hodgdon Powder Company	0	0.35	0	0	0.65	1	
SRN 336	Hodgdon Powder Company	0	0.51	0	0	0.49	1	

SRN	Known Manufacturer	Alliant Powder Company	Hodgdon Powder Company	Norma Precision AB	Vihta Vuori	Western Powders	SUM
SRN 337	Hodgdon Powder Company	0	1	0	0	0	1
SRN 338	Hodgdon Powder Company	0	1	0	0	0	1
SRN 345	Hodgdon Powder Company	0	0.01	0	0	0.99	1
SRN 348	Hodgdon Powder Company	0	1	0	0	0	1

**Posterior Probabilities** 

Table 31: Posterior probabilities for smokeless powders manufactured by Norma Precision AB (data includes average diameter and average length)

		Posterior Probabilities						
SRN	Known Manufacturer	Alliant Powder Company	Hodgdon Powder Company	Norma Precision AB	Vihta Vuori	Western Powders	SUM	
SRN 300	Norma Precision AB	0.15	0.04	0.75	0	0.06	1	
SRN 301	Norma Precision AB	0.79	0.21	0	0	0	1	
SRN 302	Norma Precision AB	1	0	0	0	0	1	
SRN 339	Norma Precision AB	0.11	0.05	0.75	0	0.09	1	
SRN 341	Norma Precision AB	0.82	0.18	0	0	0	1	
SRN 342	Norma Precision AB	0.49	0.08	0.43	0	0	1	
SRN 343	Norma Precision AB	0.19	0.02	0.72	0	0.06	1	
SRN 344	Norma Precision AB	0.20	0.03	0.73	0	0.05	1	

Table 32: Posterior probabilities for smokeless powders manufactured by Vihta Vuori (data includes average diameter and average length)

SRN	Known Manufacturer	Alliant Powder Company	Hodgdon Powder Company	Norma Precision AB	Vihta Vuori	Western Powders	SUM
SRN 312	Vihta Vuori	0	0	0	1	0	1
SRN 313	Vihta Vuori	0	0	0	1	0	1
SRN 327	Vihta Vuori	0	0	0	1	0	1
SRN 328	Vihta Vuori	0	0	0	1	0	1
SRN 333	Vihta Vuori	0	0	0	1	0	1
SRN 346	Vihta Vuori	0	1	0	0	0	1
SRN 347	Vihta Vuori	0	0.18	0	0.82	0	1

**Posterior Probabilities** 

Table 33: Posterior probabilities for smokeless powders manufactured by Western Powders (data includes average diameter and average length)

	Posterior Probabilities							
SRN	Known Manufacturer	Alliant Powder Company	Hodgdon Powder Company	Norma Precision AB	Vihta Vuori	Western Powders	SUM	
SRN 179	Western Powders	0	0.77	0	0	0.23	1	
SRN 180	Western Powders	0	0.03	0	0	0.97	1	
SRN 181	Western Powders	0	0.08	0	0	0.92	1	
SRN 182	Western Powders	0	0	0	0	1	1	
SRN 183	Western Powders	0	0	0	0	1	1	
SRN 184	Western Powders	0	0.03	0	0	0.97	1	
SRN 185	Western Powders	0	0.54	0	0	0.46	1	
SRN 185	Western Powders	0	0.49	0	0	0.51	1	
SRN 186	Western Powders	0	0.05	0	0	0.95	1	
SRN 187	Western Powders	0	0.02	0	0	0.98	1	
SRN 310	Western Powders	0	0	0	0	1	1	
SRN 315	Western Powders	0	1	0	0	0	1	
SRN 315	Western Powders	0	0.05	0	0	0.95	1	
SRN 316	Western Powders	0.50	0.39	0	0	0.11	1	
SRN 317	Western Powders	0	0.21	0	0	0.79	1	
SRN 318	Western Powders	0	0.48	0	0	0.52	1	
SRN 318	Western Powders	0	0.55	0	0	0.45	1	
SRN 319	Western Powders	0	0.02	0	0	0.98	1	
SRN 320	Western Powders	0	0	0	0	1	1	
SRN 334	Western Powders	0	0.16	0	0.79	0.05	1	
SRN 340	Western Powders	0	0.90	0	0	0.10	1	

The majority of the test samples were predicted as belonging to their respective manufacturers with fairly high to high posterior probabilities. The percent correct obtained for calculating the posterior probabilities for each manufacturer are summarized in Table 34.

Manufacturer	Percent Correct
Alliant Powder Company	65
Hodgdon Powder Company	71
Norma Precision AB	57
Vihta Vuori	89
Western Powders	70
OVERALL	70

 Table 34: Percent correct for manufacturer predictions based on posterior probabilities (data includes average diameter and average length)

The correct prediction rates were improved for assigning the test samples, based on high posterior probabilities, to Norma Precision AB and Western Powders. Though the correct prediction rates for Alliant Powder Company, Hodgdon Powder Company, and Vihta Vuori were 65%, 71%, and 89% respectively, they were slightly lower than previously observed. The overall percent correct obtained when predicting the manufacturer for the test samples, based on the highest posterior probabilities, improved from 66% to 70% when the average diameter and average length nodes were added to the network and instantiated.

### **CHAPTER 5: CONCLUSIONS**

#### 5.1. Significance

Commercial smokeless powders are currently designated as either single or double base due to the absence or presence, respectively, of one organic compound, nitroglycerin. The goal of this research was to identify novel, chemically distinct classes, based on multiple organic compounds which are typically incorporated into smokeless powders during the manufacturing process. In addition, the research focused on classification of smokeless powder test samples into novel classes. A suite of chemometric techniques was employed for identification of the novel classes, and for classification of the smokeless powder test samples.

The TIS, which was calculated by summing the intensities for each m/z ratio across the full chromatographic profile, was used in this work. The TIS data matrix, comprising 726 commercial smokeless powders, was subject to AHC analysis. Cluster analysis was utilized to investigate whether inherent clusters could be identified in the data. Six distinct clusters were identified through examination of a combined dendrogram and similarity heat map of the clustered samples. Examination of the samples within the six clusters (classes) demonstrated that multiple compounds were prevalent across the classes; however, ordering of the TIS matrix demonstrated that only six m/z ratios which were contributing significantly to formation of the six classes. Furthermore, though some of the m/z ratios were evidently contributing to multiple classes, the most significant contribution from a single m/z ratio was limited to a single class;

where the m/z ratio was the base peak for the majority of samples within the class. Based on observations made from cluster analysis, the TIS data matrix was processed by removing the non-contributing m/z ratios, using visual feature selection, to generate the most intense extracted ion spectrum (MEIS). The MEIS was used during the rest of this work for smokeless powder classification. In addition, a new classification method, the intense ion rule (IIR), was developed. The IIR is implemented by looking at the feature selected m/z ratios in the MEIS. Using the IIR, a test sample is assigned to its respective class through visual inspection of the intensities of the feature ions in the MEIS; the sample is assigned to the class associated with the most intense ion. The overall correct classification rate for assignment of the test samples to AHC designated classes was 93%.

Though the IIR achieved the lowest overall correct classification rate for assignment of the test samples to the AHC designated classes, the performance of the method was still comparable to the performance of kNN, LDA, and QDA. Additionally, the IIR is easy to implement in practice, since it requires a simple calculation of the sample TIS, followed by isolation of the MEIS, and assignment to an AHC designated class through visual inspection of the MEIS.

Another area of the research focused on the use of Bayes' Theorem and Bayesian Networks to calculate posterior probabilities of a smokeless powder belonging to specific manufacturers, Smokeless powder samples representing five manufacturers were used for development of the networks, and for calculating posterior probabilities of the test samples belonging to each manufacturer. The networks were designed to include powder characteristics determined by the manufacturer such as shape, color, and dimension; as well as, relative intensities of the six class associated m/z ratios. Predictions of the manufacturer were based on the highest posterior probability calculated for the test sample. Using the DAG design shown in Figure 37, the highest percent correct for the manufacturer predictions was achieved for Vihta Vuori samples; while the lowest percent correct was observed for Norma Precision AB powders. The overall percent correct was 66% which is significantly better than the random 20% chance of correct prediction, using current methods, when considering the five manufacturers. Addition of the average diameter and average length to the network resulted in an overall correct prediction rate of 70%. The most significant improvement for manufacturer rate was achieved for the Norma Precision AB powders, which increased from 0% to 57%.

The results obtained using Bayes' Theorem and Bayesian Networks provides a promising investigative approach in the analysis of forensic smokeless powder samples. The ability to ascertain the manufacturer of a forensic smokeless powder sample, along with the probability of the sample belonging to the manufacturer would provide the analyst with fewer, yet viable investigative leads.

#### 5.2. Future Work

The research utilized data obtained from the analysis of intact pre-blast smokeless powder particles. Additional research is required to investigate post-blast samples, and explosive residues, to determine whether the AHC designated classes are still viable or if additional classes can be identified. Furthermore, work will need to be conducted to include investigation of potential degradation products which can form in smokeless powders as a consequence of storage conditions and environment.

In the future, the Bayesian Networks can be improved by expanding the datasets to include samples which are represented of smokeless powder manufacturers. A larger population dataset will be more representative of the true product availability in the smokeless powders market. In addition, likelihood ratios (LR) could be investigated as another tool to aid explosives analysts in interpreting and communicating the value of the evidence in a manner which is easy to understand by a jury.

Finally, the NCFS smokeless powders database could be restructured to include a Bayesian Network application which would allow an explosives analyst to submit evidence to calculate manufacturer posterior probabilities and LRs for a forensic sample. Such an application would significantly decrease the time invested by an analyst during an investigation.

## APPENDIX A: SMOKELESS POWDER TARGET ANALYTES

STRUCTURE	SPECIFICATIONS			
$O_2N$	Name: CAS* Number: Molecular Formula: Molecular Weight (g mol <sup>-1</sup> ): Major Ions (% Abundance):	2,4-Dinitrotoluene 121-14-2 C <sub>7</sub> H <sub>6</sub> N <sub>2</sub> O <sub>4</sub> 182.1335 165 (100) 89 (50) 63 (27)		
H NO2 H N	Name: CAS* Number: Molecular Formula: Molecular Weight (g mol <sup>-1</sup> ): Major Ions (% Abundance):	2-Nitrodiphenylamine 119-75-5 C <sub>12</sub> H <sub>10</sub> N <sub>2</sub> O <sub>2</sub> 214.2200 167 (100) 214 (82) 169 (37)		
H N NO <sub>2</sub>	Name: CAS* Number: Molecular Formula: Molecular Weight (g mol <sup>-1</sup> ): Major Ions (% Abundance):	4-Nitrodiphenylamine 836-30-6 C <sub>12</sub> H <sub>10</sub> N <sub>2</sub> O <sub>2</sub> 214.2200 214 (100) 167 (83) 168 (40)		

STRUCTURE	SPECIFICATIONS			
ON H	Name: CAS* Number: Molecular Formula: Molecular Weight (g mol <sup>-1</sup> ): Major Ions (% Abundance):	4-Nitrosodiphenylamine 156-10-5 C <sub>12</sub> H <sub>10</sub> N <sub>2</sub> O 198.2206 167 (100) 198 (92) 168 (67)		
	Name: CAS* Number: Molecular Formula: Molecular Weight (g mol <sup>-1</sup> ): Major Ions (% Abundance):	Camphor 76-22-2 C <sub>10</sub> H <sub>16</sub> O 152.2334 95 (100) 41 (64) 81 (72)		
	Name: CAS* Number: Molecular Formula: Molecular Weight (g mol <sup>-1</sup> ): Major Ions (% Abundance):	Dibutyl Phthalate 84-74-2 C <sub>16</sub> H <sub>22</sub> O <sub>4</sub> 278.3435 149 (100) 223 (6) 205 (5)		

STRUCTURE	SPECIFICATIONS		
	Name: CAS* Number: Molecular Formula: Molecular Weight (g mol <sup>-1</sup> ): Major Ions (% Abundance): Name: CAS* Number: Molecular Formula: Molecular Weight (g mol <sup>-1</sup> ): Major Ions (% Abundance):	Diethyl Phthalate 84-66-2 $C_{12}H_{14}O_4$ 222.2372 149 (100) 177 (26) 105 (7) Dioctyl Phthalate 117-81-7 $C_{24}H_{38}O_4$ 390.5561 149 (100) 167 (50) 57 (37)	
	Name: CAS* Number: Molecular Formula: Molecular Weight (g mol <sup>-1</sup> ): Major Ions (% Abundance):	Dipentyl (Amyl) Phthalate 131-18-0 C <sub>18</sub> H <sub>26</sub> O <sub>4</sub> 306.3966 149 (100) 43 (19) 237 (8)	

STRUCTURE	SPECIFICATIONS		
	Name: CAS* Number: Molecular Formula: Molecular Weight (g mol <sup>-1</sup> ): Major Ions (% Abundance): Name: CAS* Number: Molecular Formula: Molecular Weight (g mol <sup>-1</sup> ): Major Ions (% Abundance):	Diphenylamine 122-39-4 $C_{12}H_{11}N$ 169.2224 169 (100) 51 (21) 84 (18) Ethyl Centralite 85-98-3 $C_{17}H_{20}N_{2}O$ 268.3535 120 (100) 148 (79) 77 (39)	
	Name: CAS* Number: Molecular Formula: Molecular Weight (g mol <sup>-1</sup> ): Major Ions (% Abundance):	Methyl Centralite 611-92-7 C <sub>15</sub> H <sub>16</sub> N <sub>2</sub> O 240.3003 134 (100) 240 (62) 106 (35)	

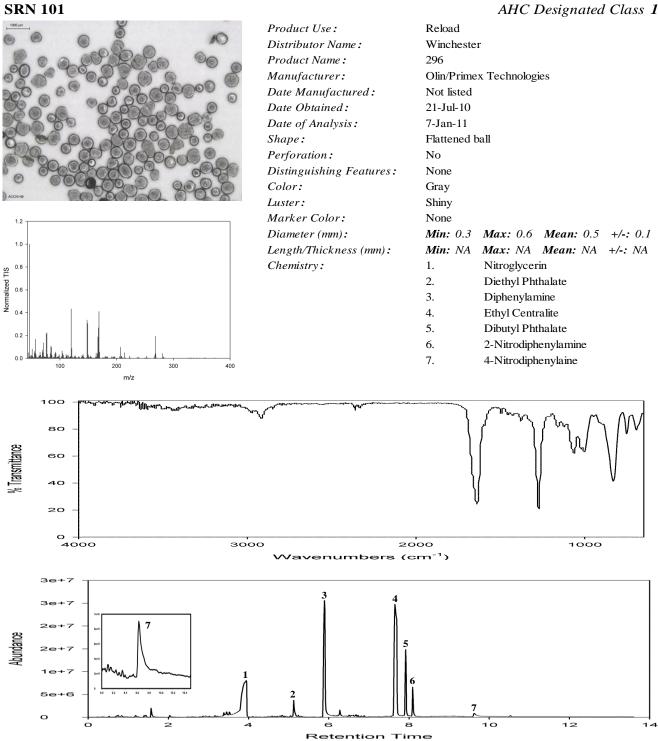
STRUCTURE	SPECIFICATIONS		
$ \begin{array}{c}                                     $	Name: CAS* Number: Molecular Formula: Molecular Weight (g mol <sup>-1</sup> ): Major Ions (% Abundance):	Nitroglycerin† 55-63-0 C <sub>3</sub> H <sub>5</sub> N <sub>3</sub> O <sub>9</sub> 227.0865 46 (100) 76 (57)	
	Name: CAS* Number: Molecular Formula: Molecular Weight (g mol <sup>-1</sup> ): Major Ions (% Abundance):	Undecane ‡ 1120-21-4 C <sub>11</sub> H <sub>24</sub> 156.3083 57 (100) 43 (90) 71 (55)	

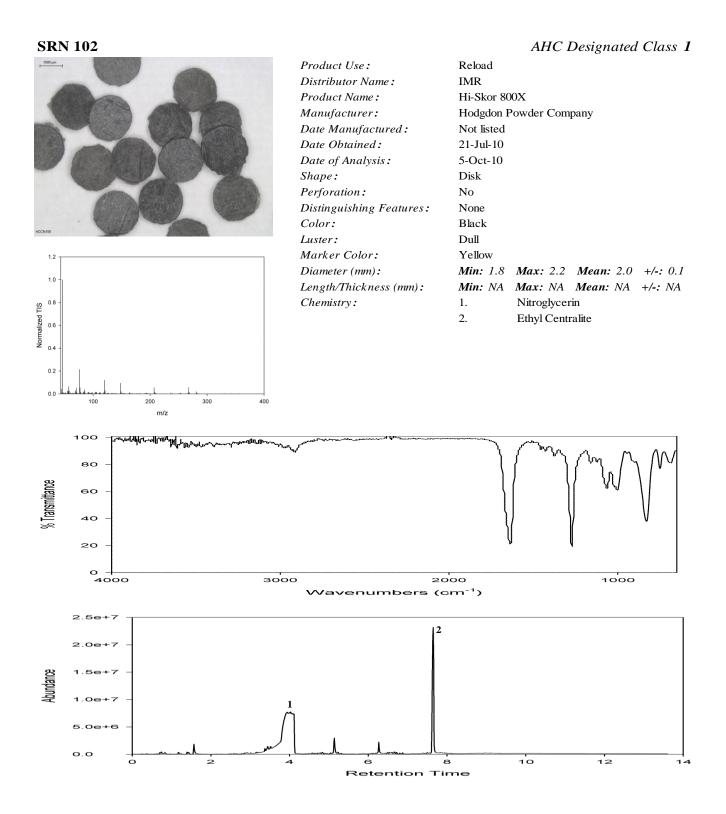
 $\dagger$  Primary energetic material; a component of double base smokeless powders

‡ Denotes Internal Standard

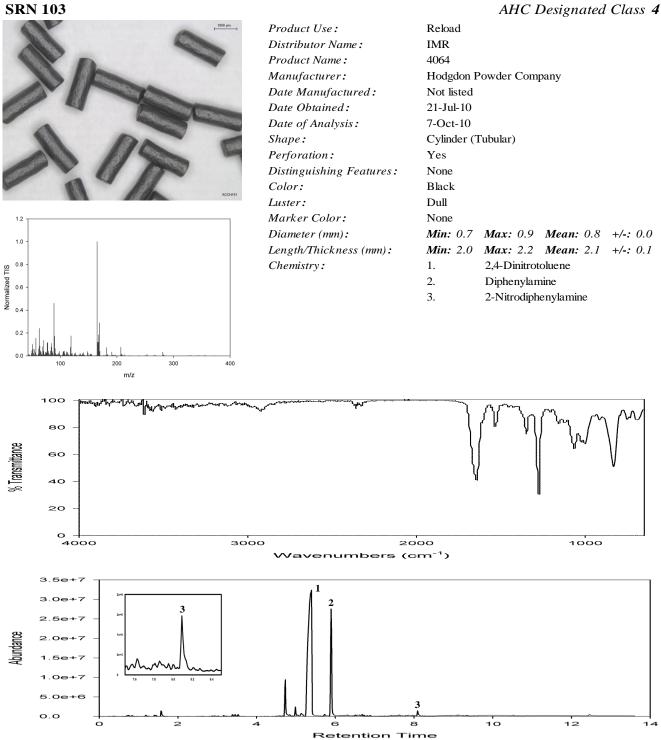
## APPENDIX B: NCFS DATABASE SAMPLES USED FOR DEVELOPMENT OF THE DISCRIMINANT ANALYSIS MODELS

### AHC Designated Class 1

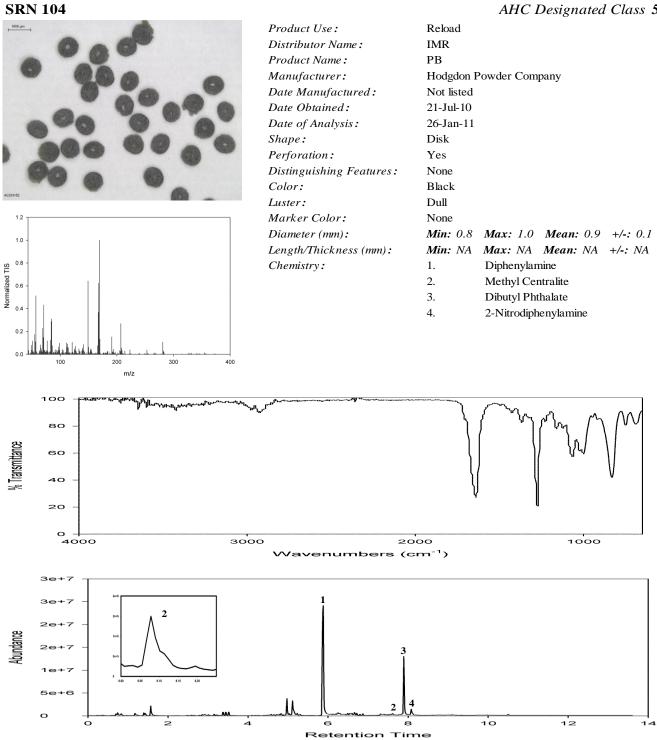


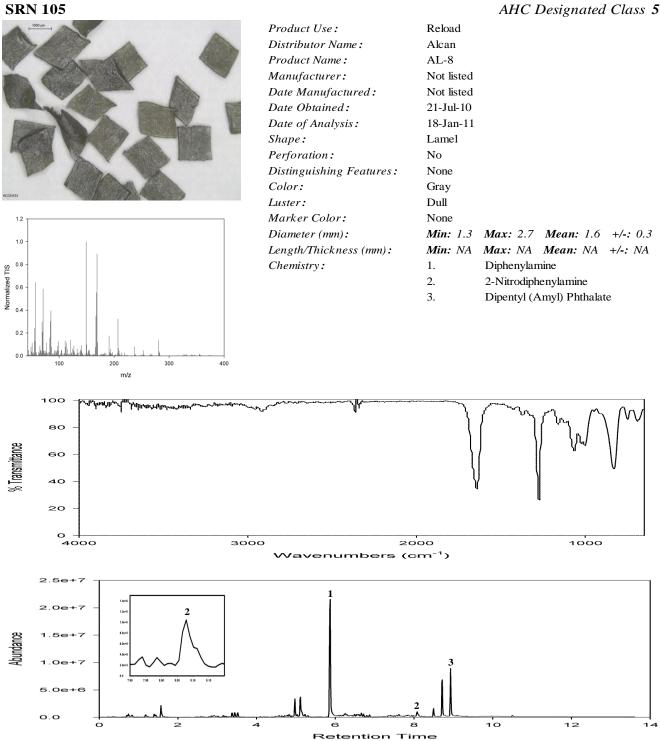


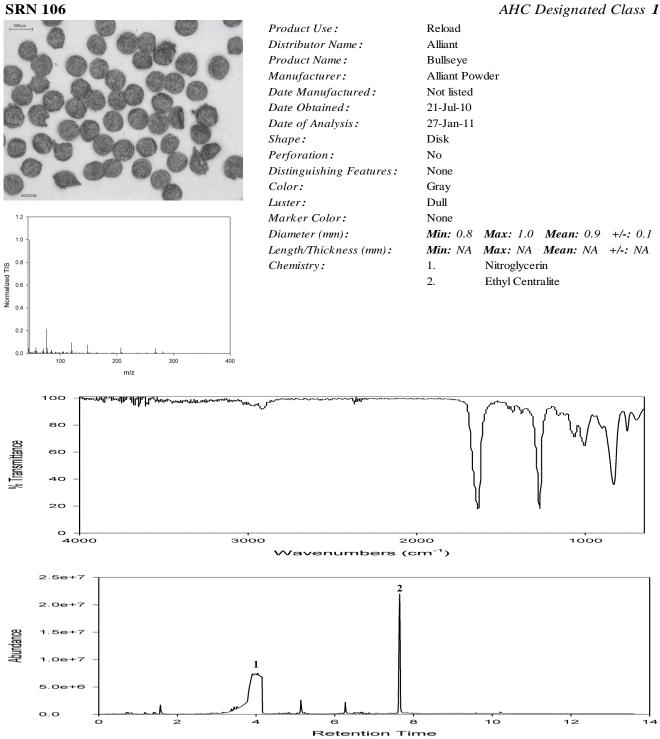
### AHC Designated Class 4

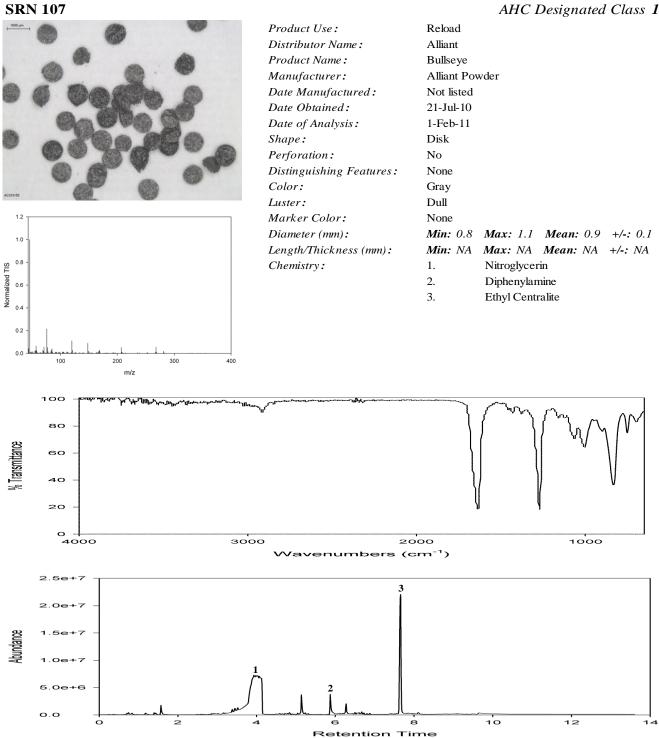


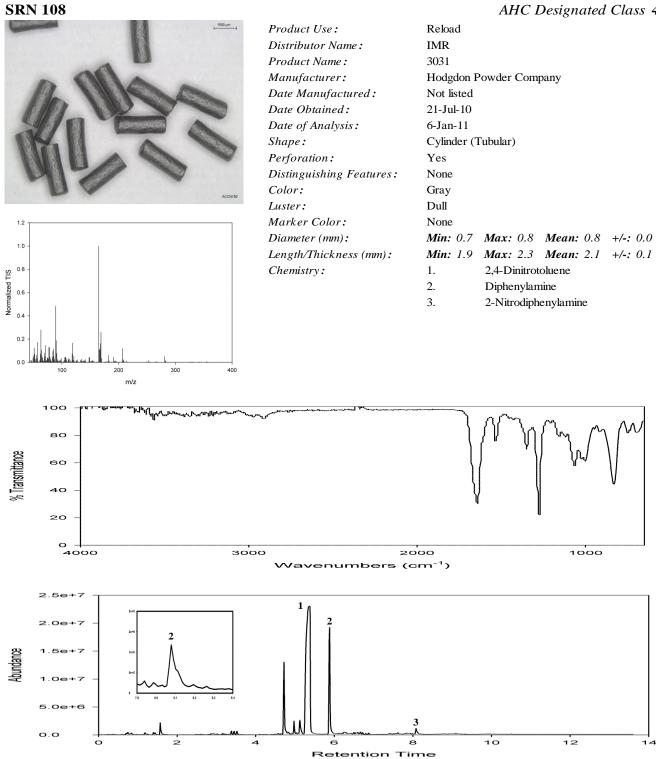
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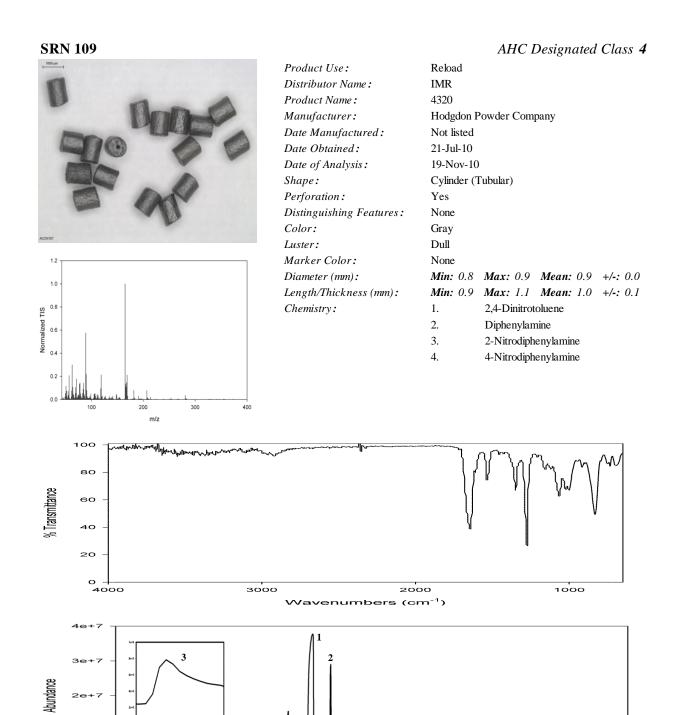








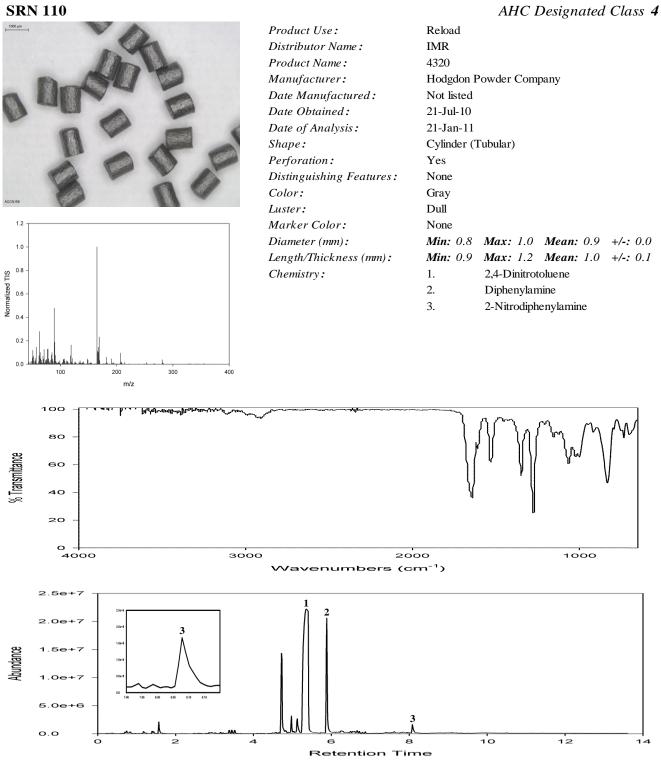


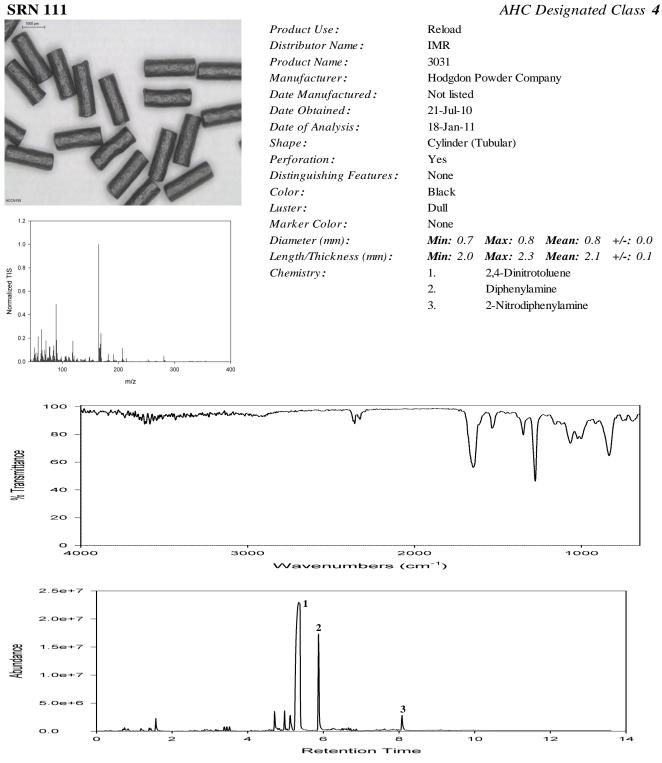


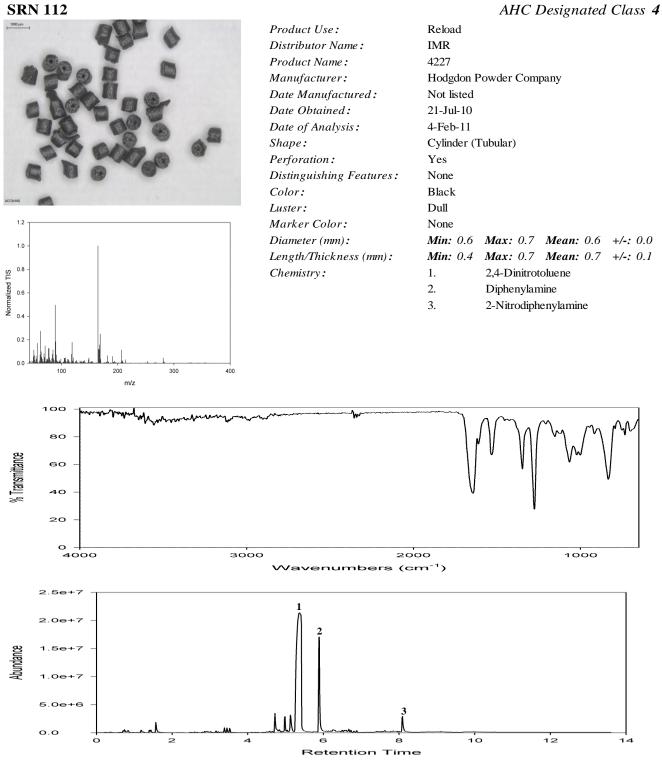
**Retention** Time

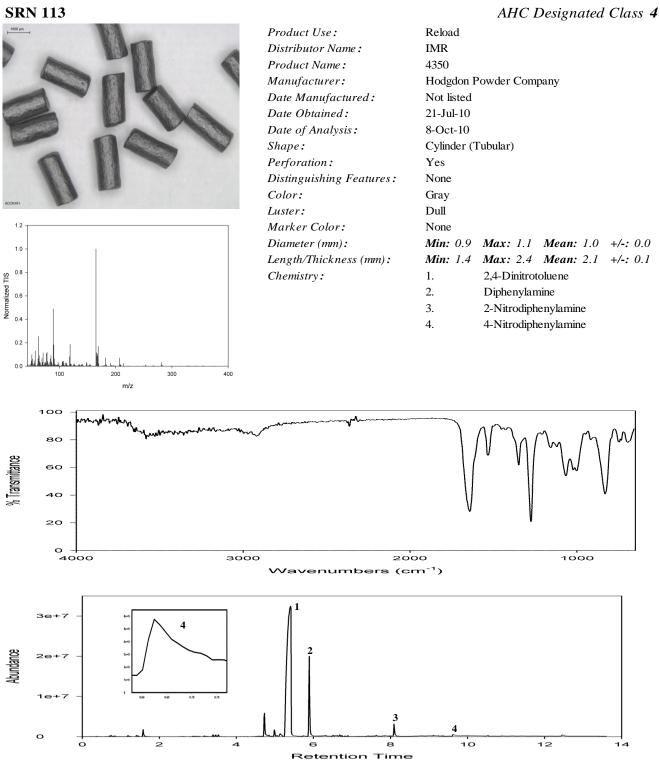
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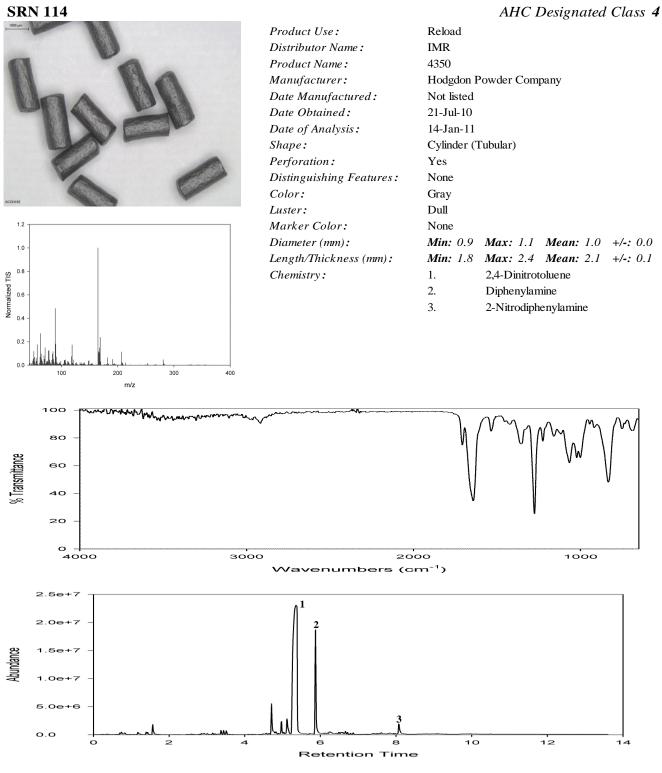
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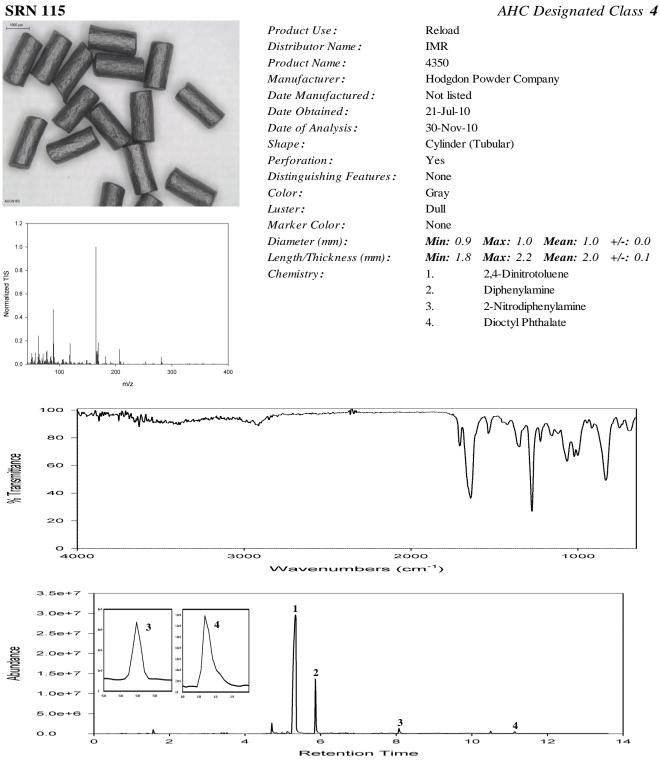


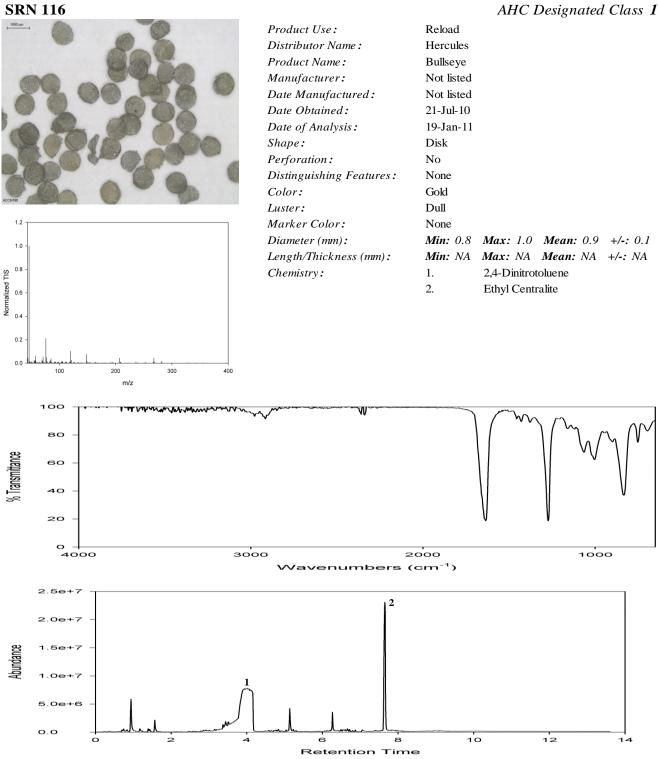


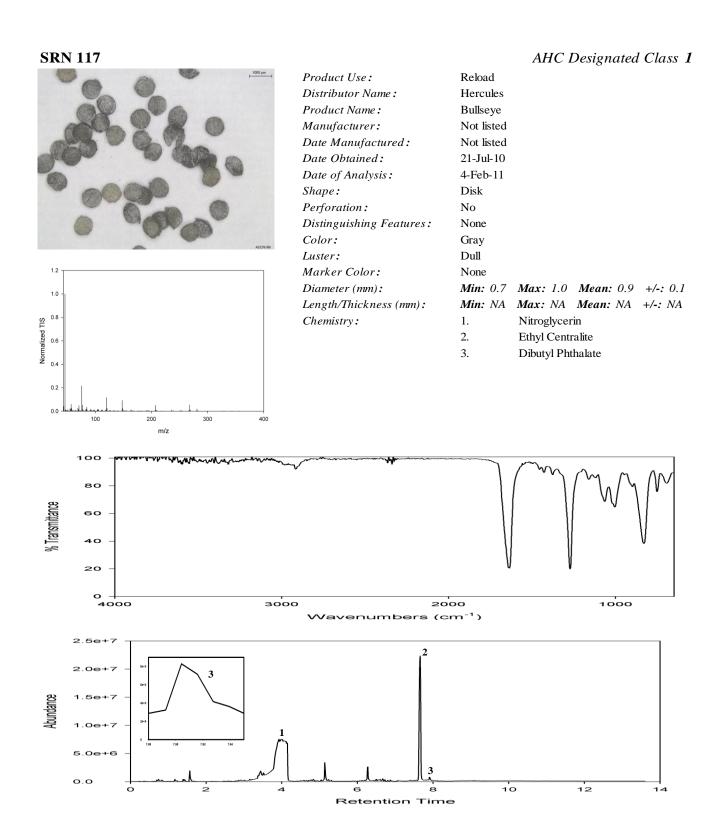




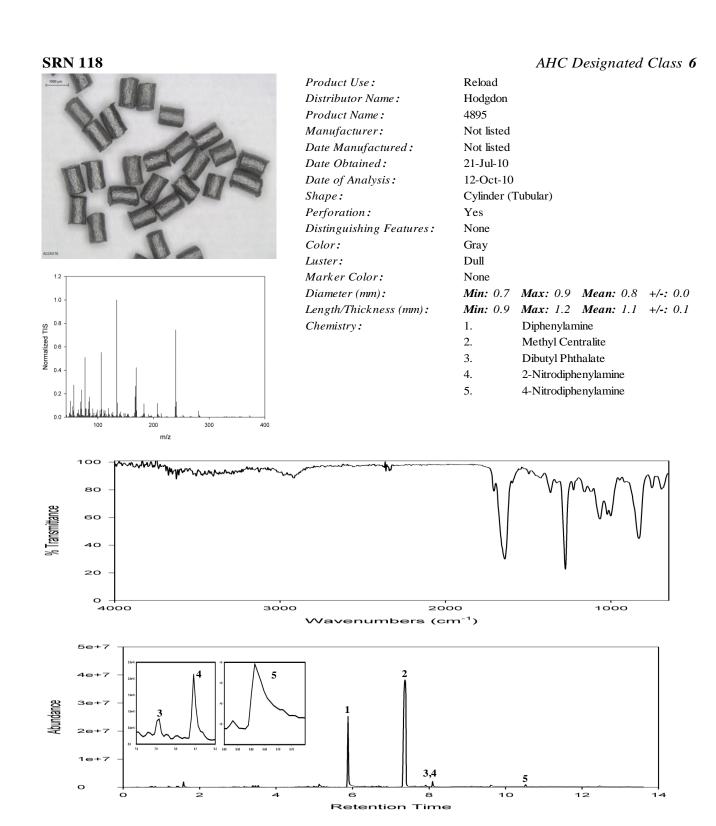


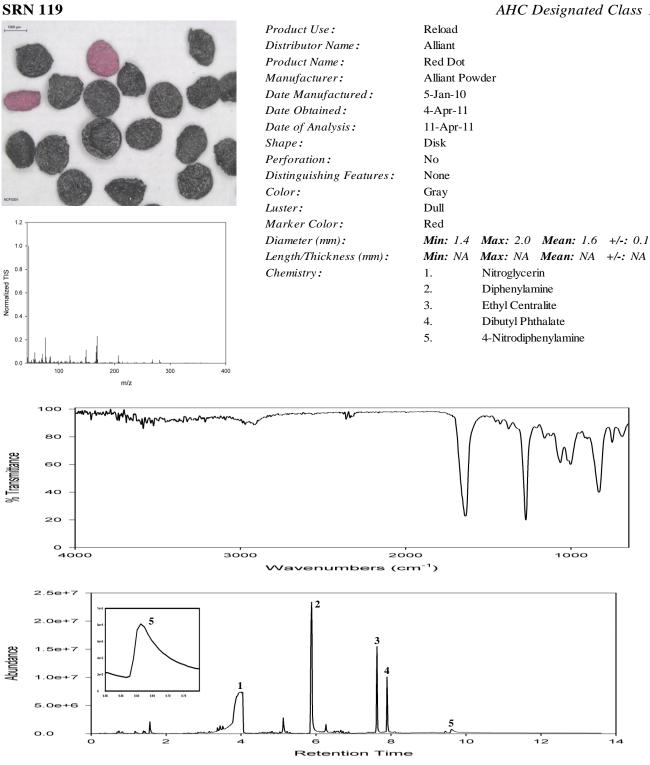


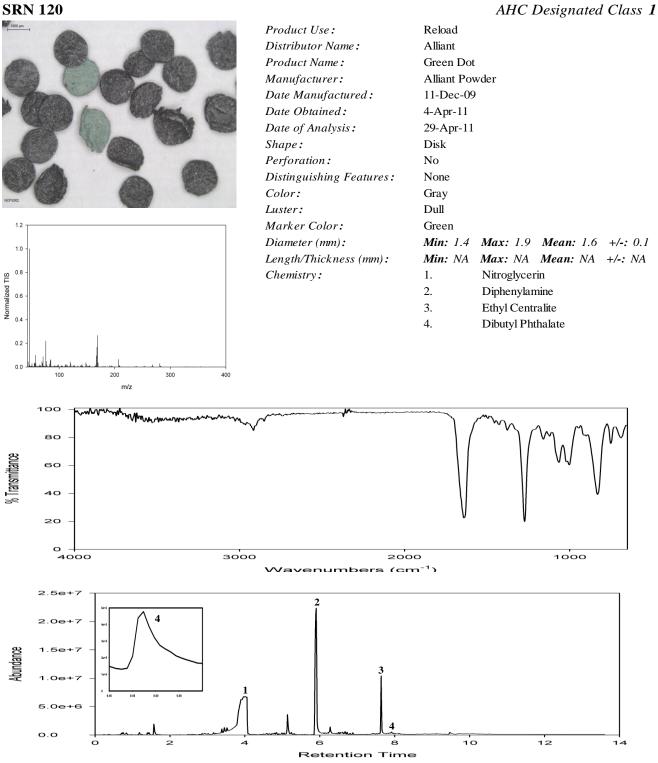


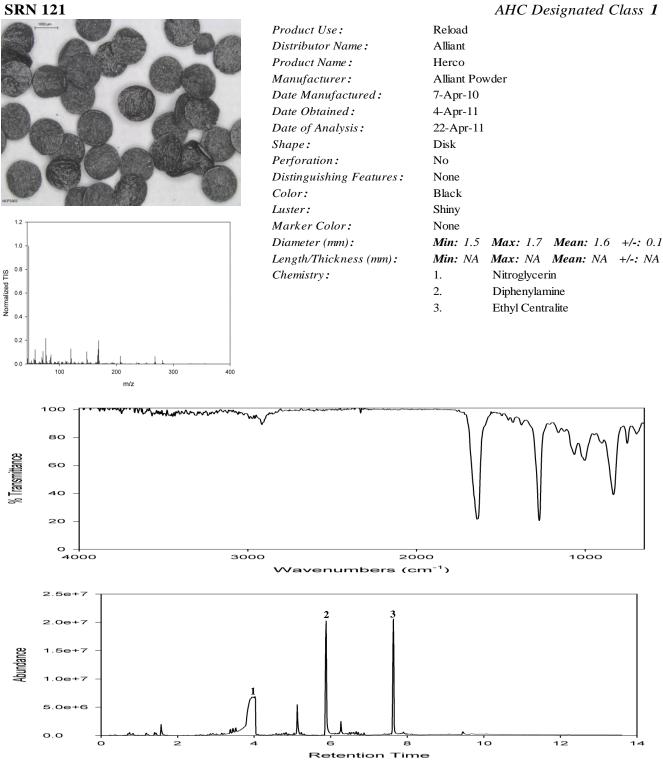


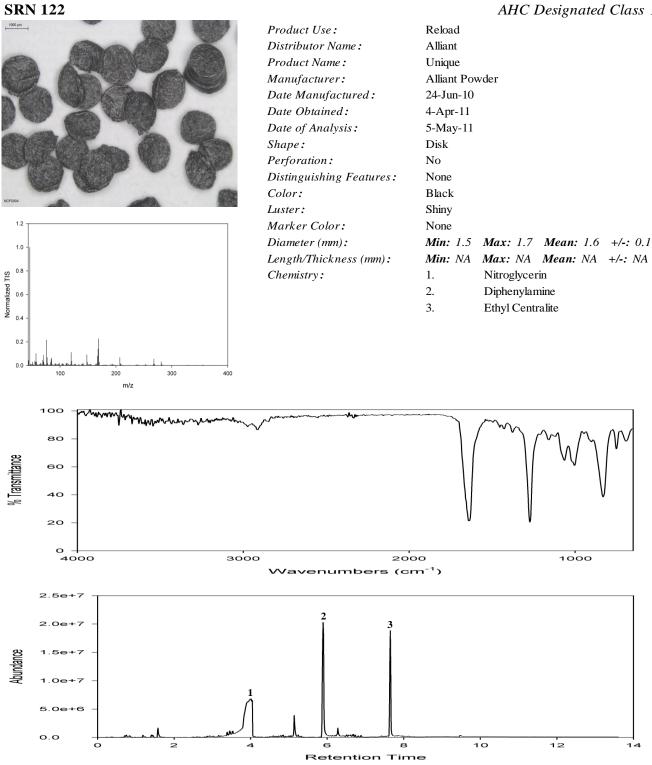
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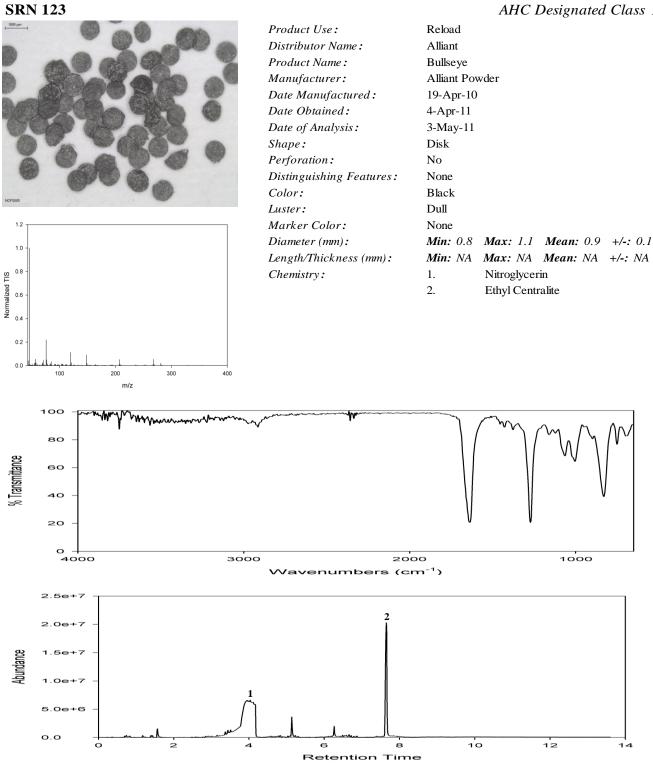


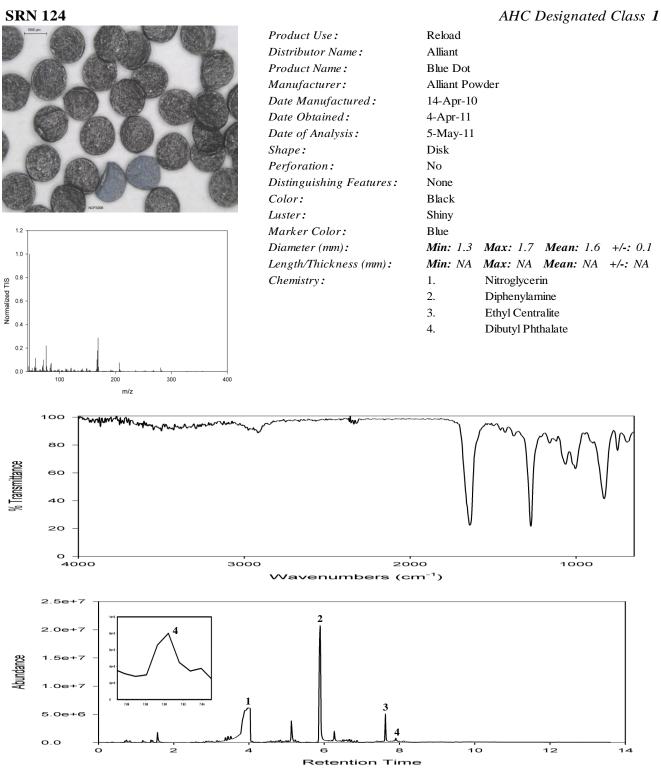


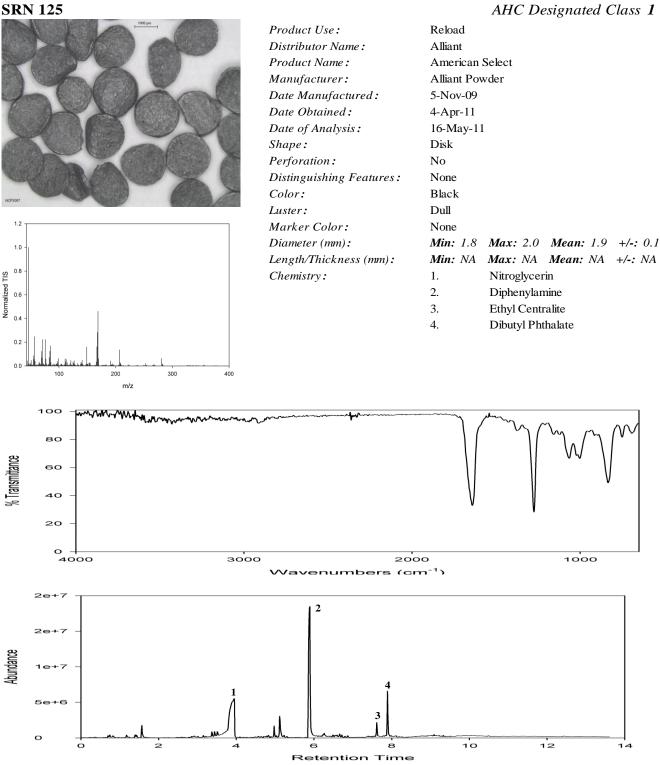


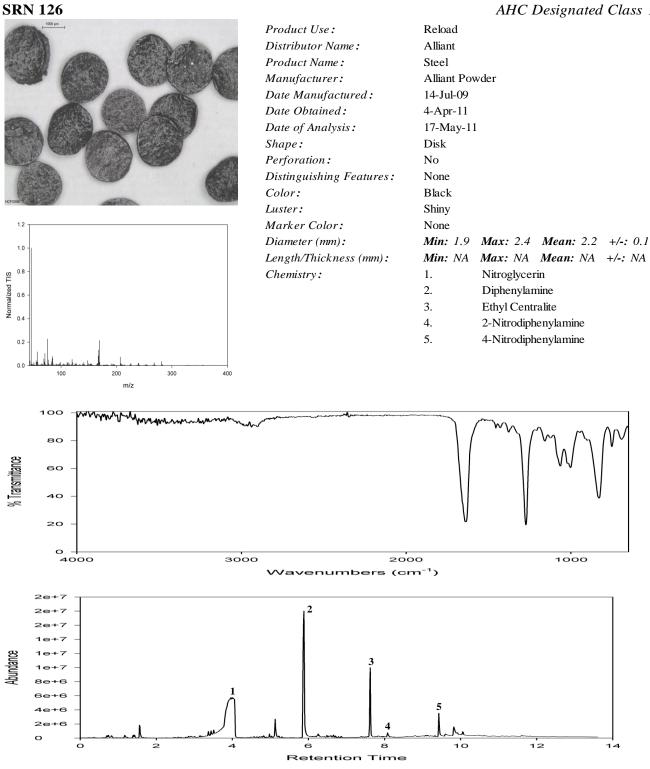




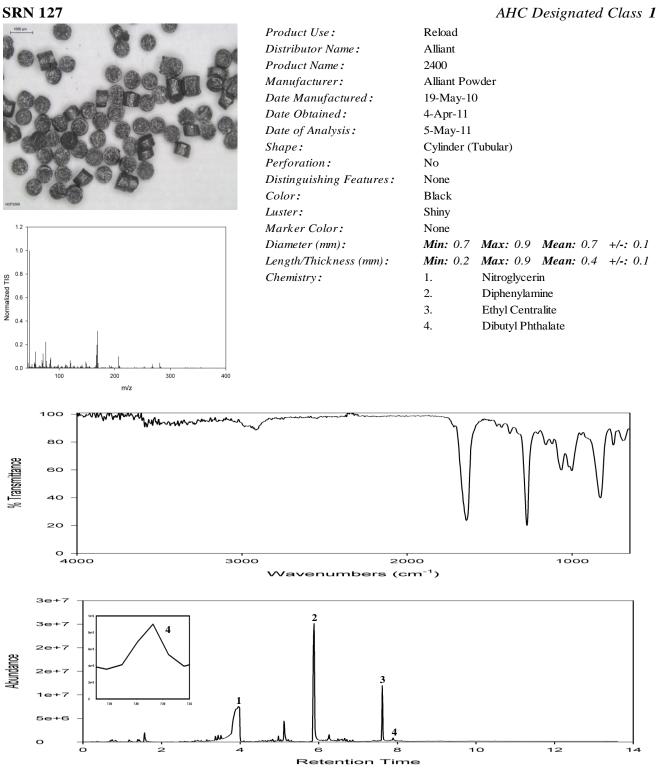


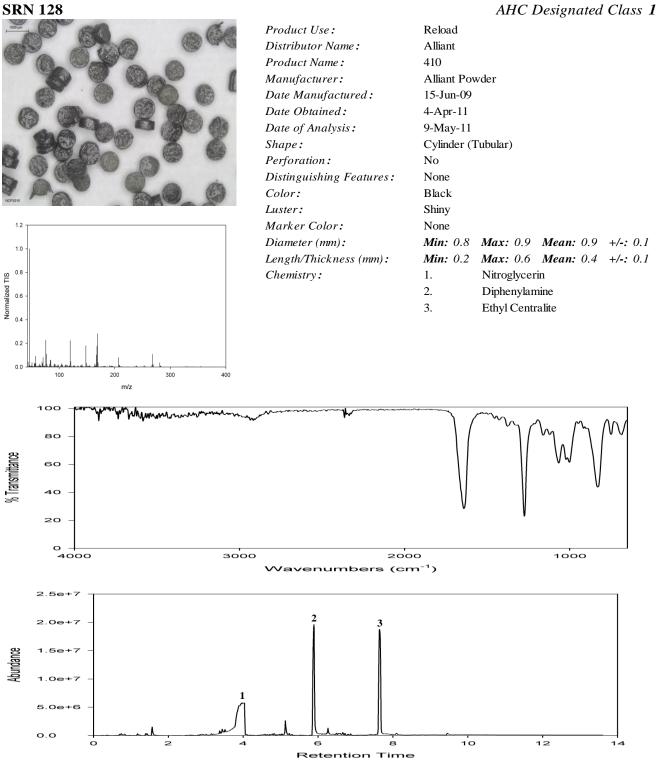


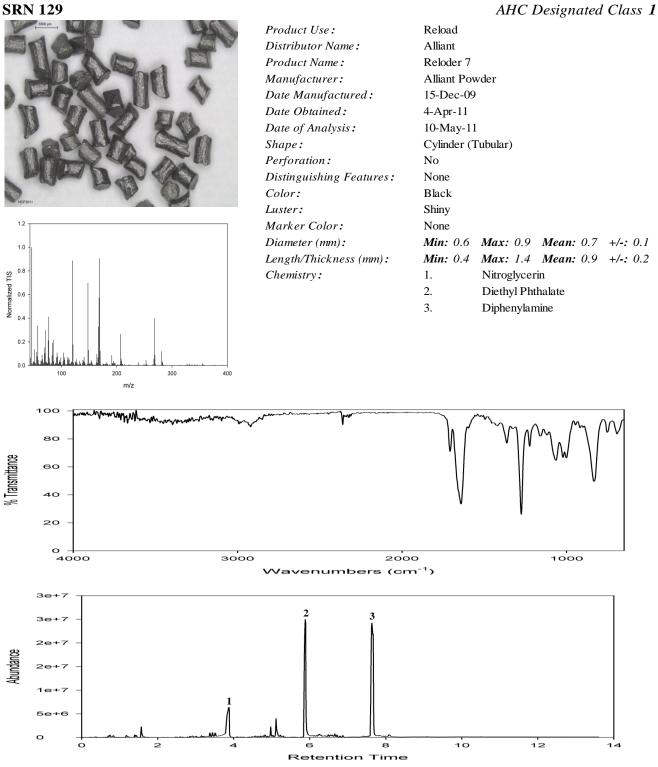


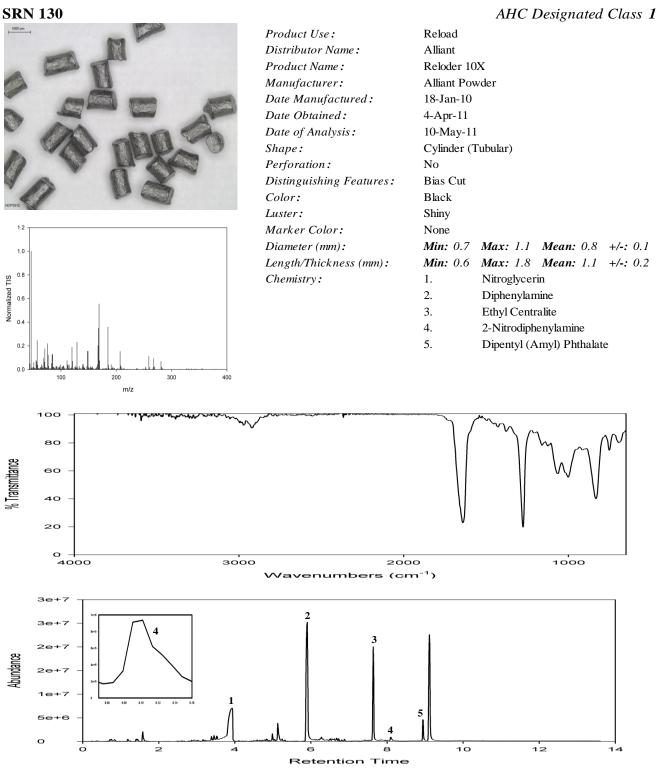


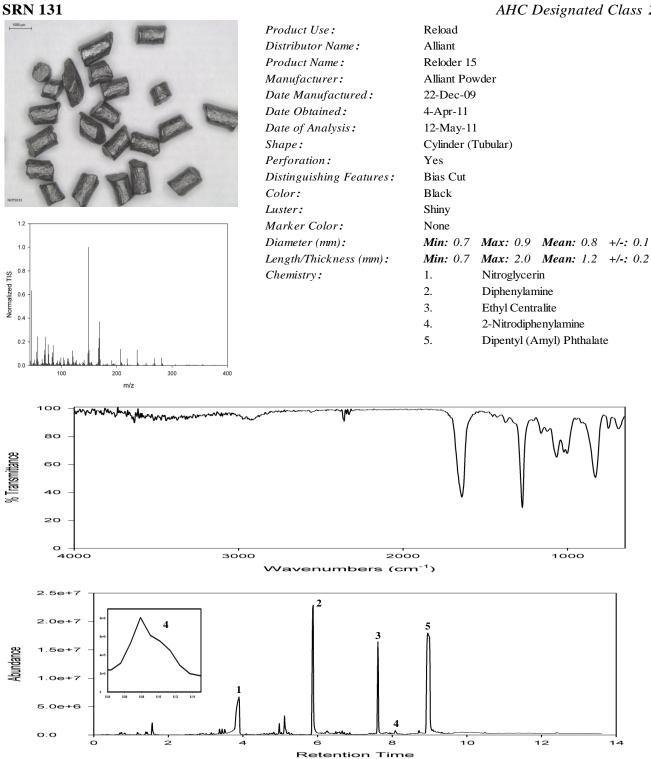
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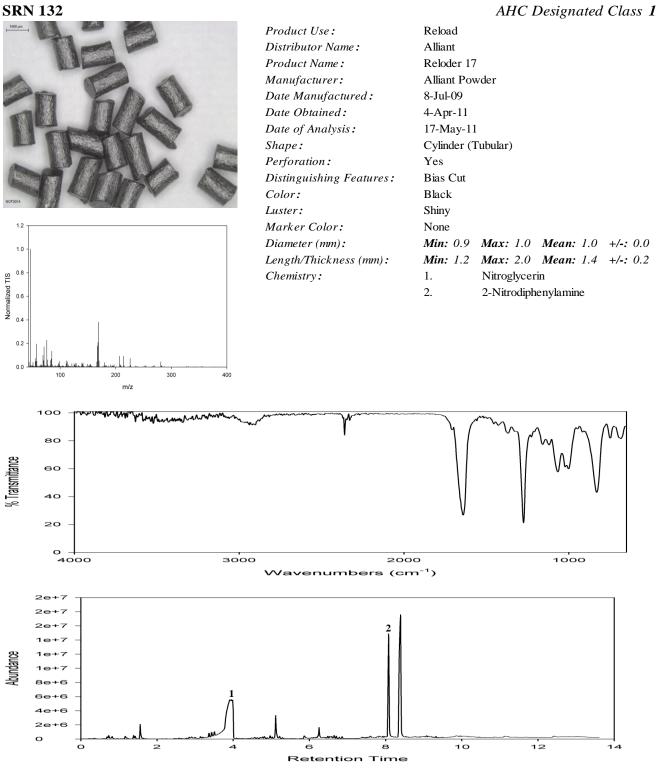


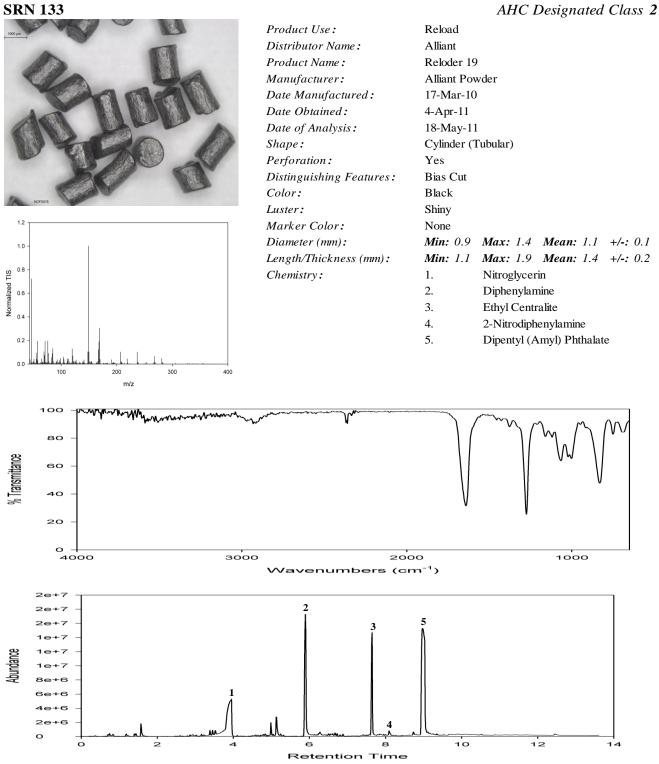


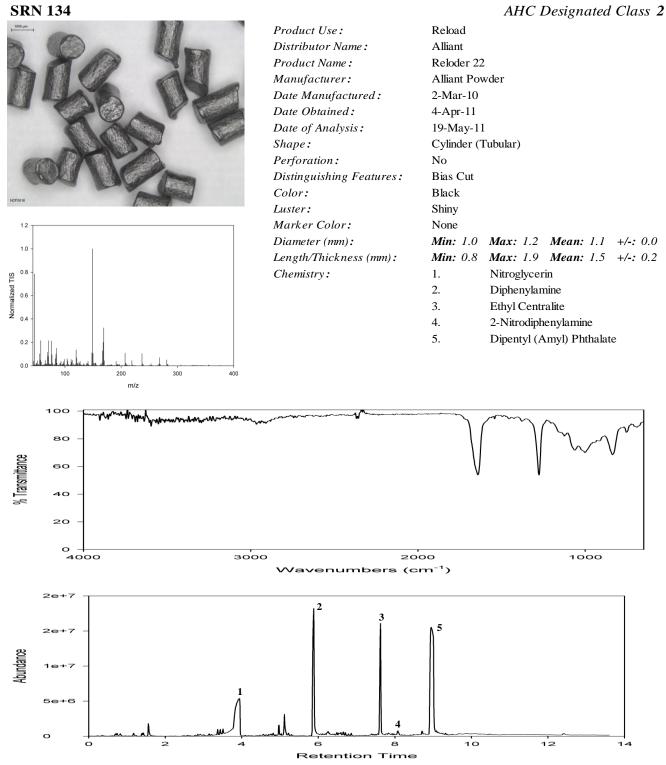


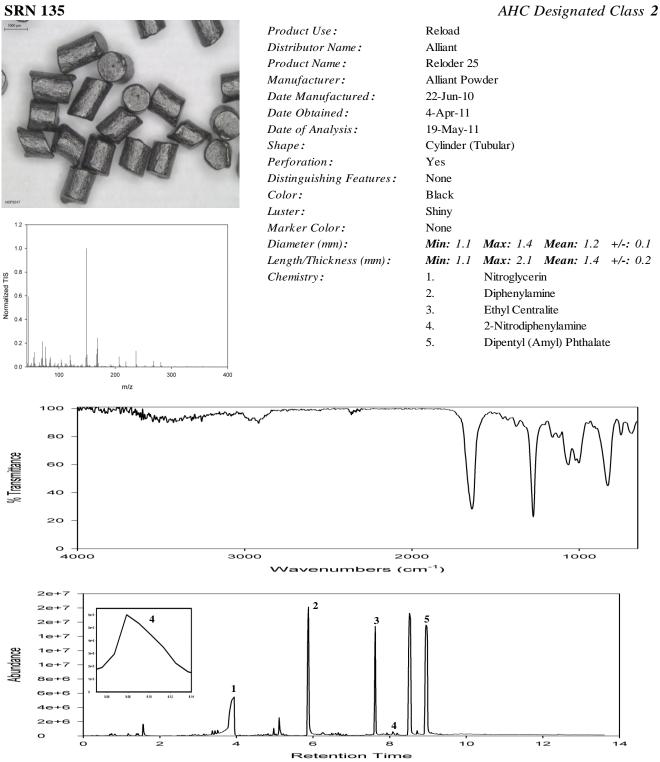


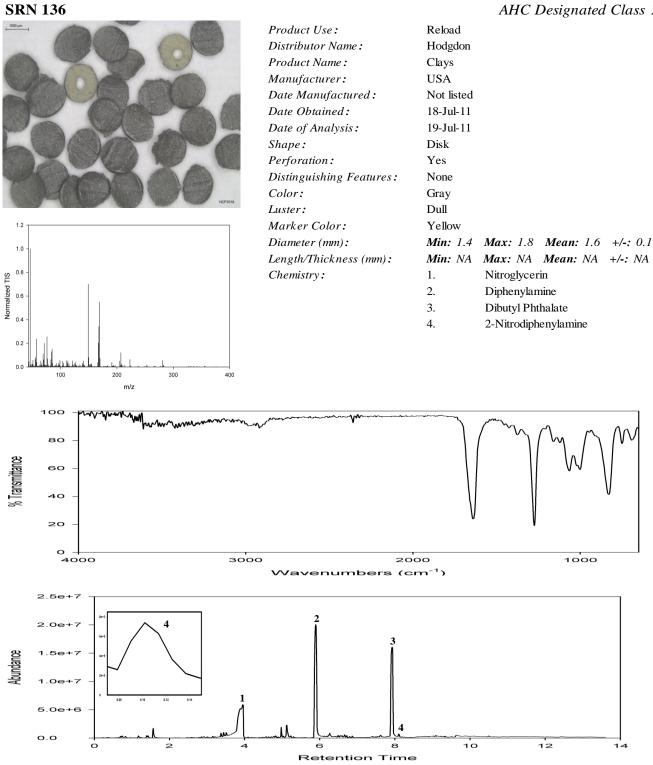


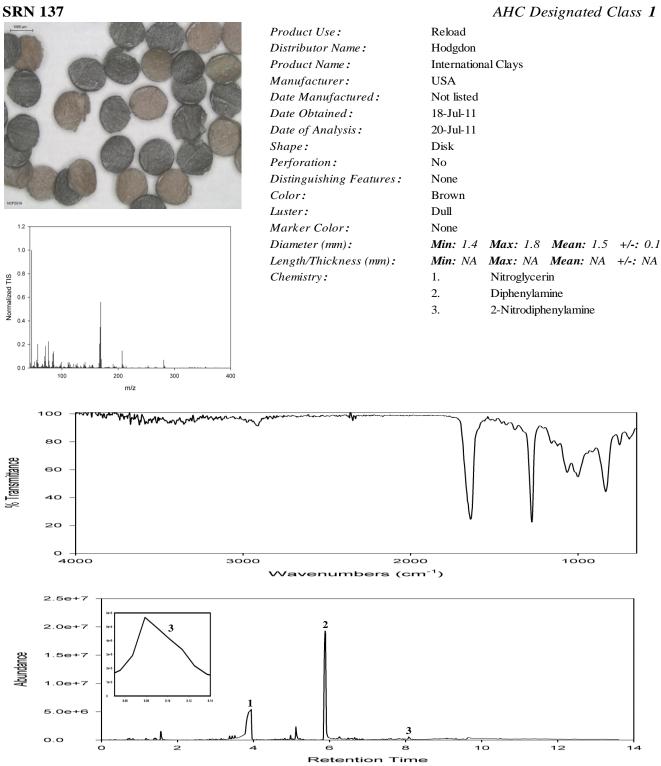


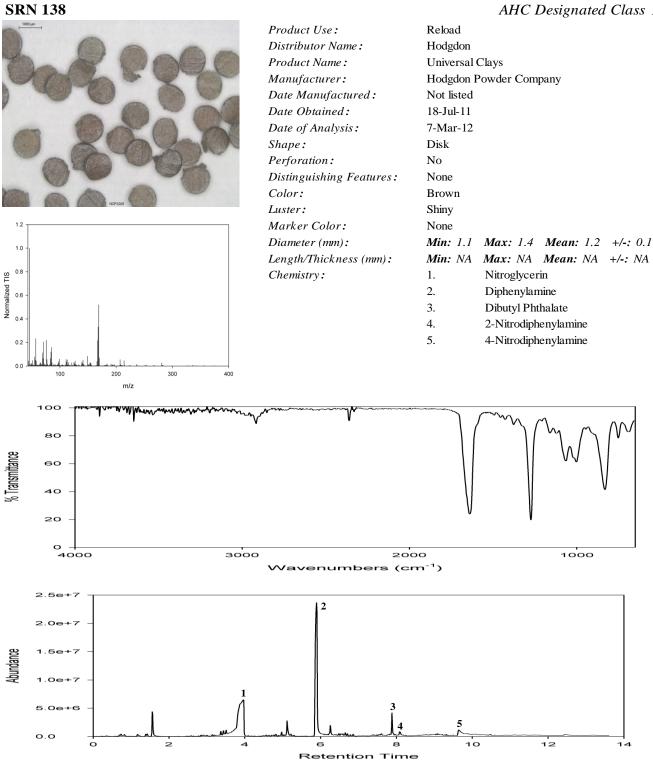


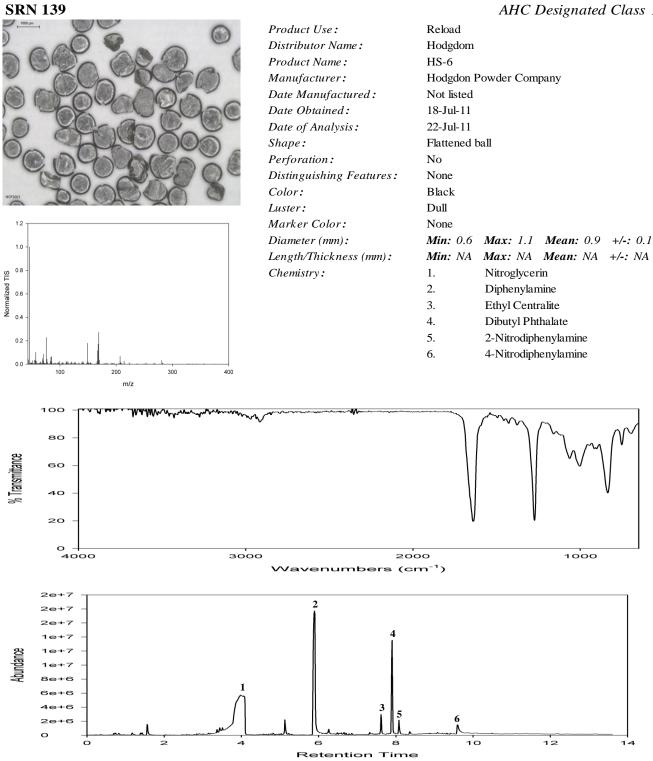


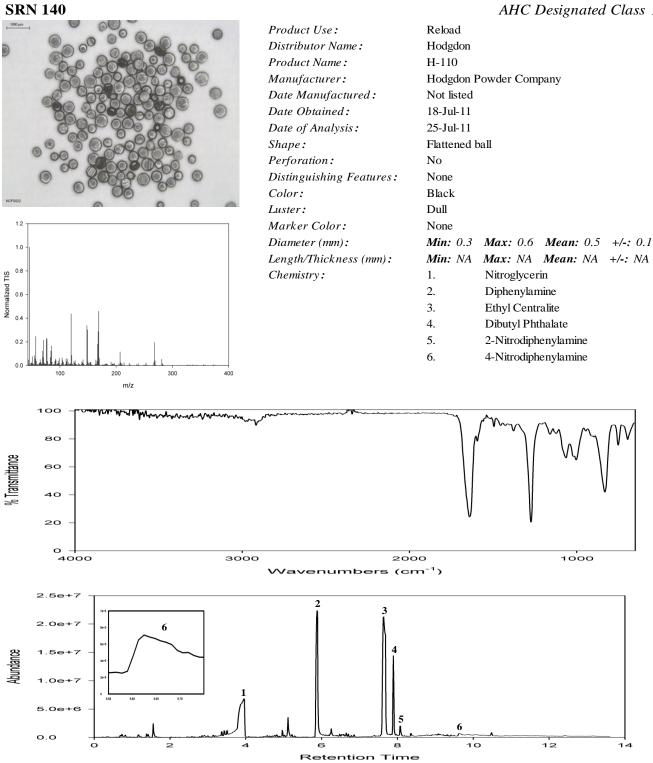


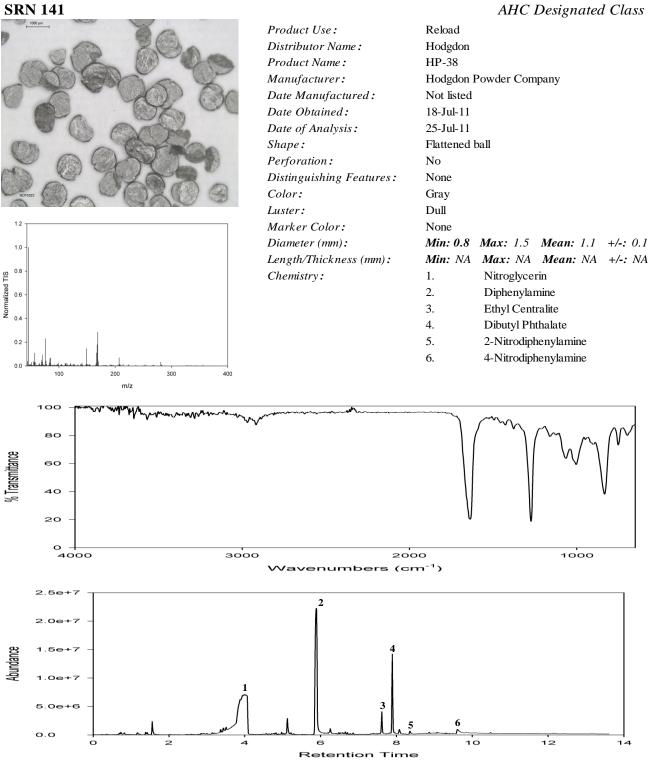


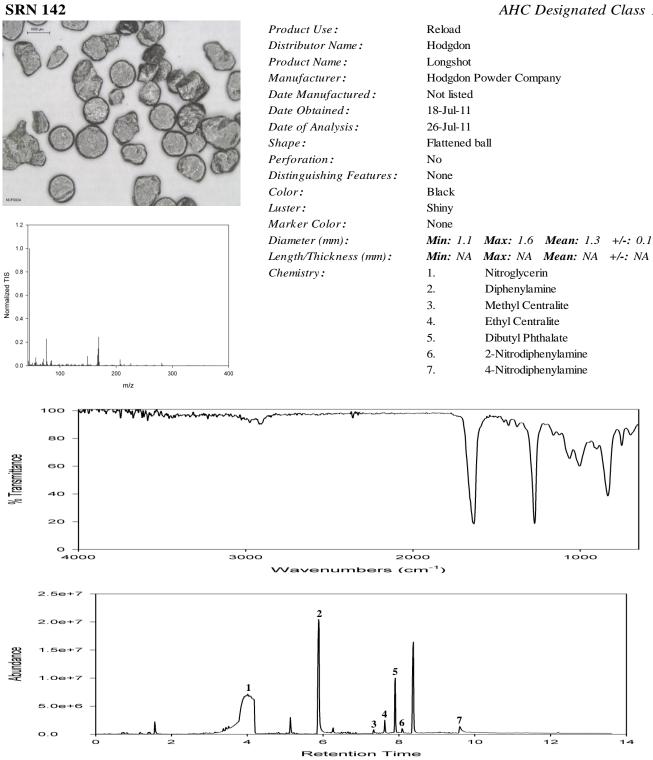


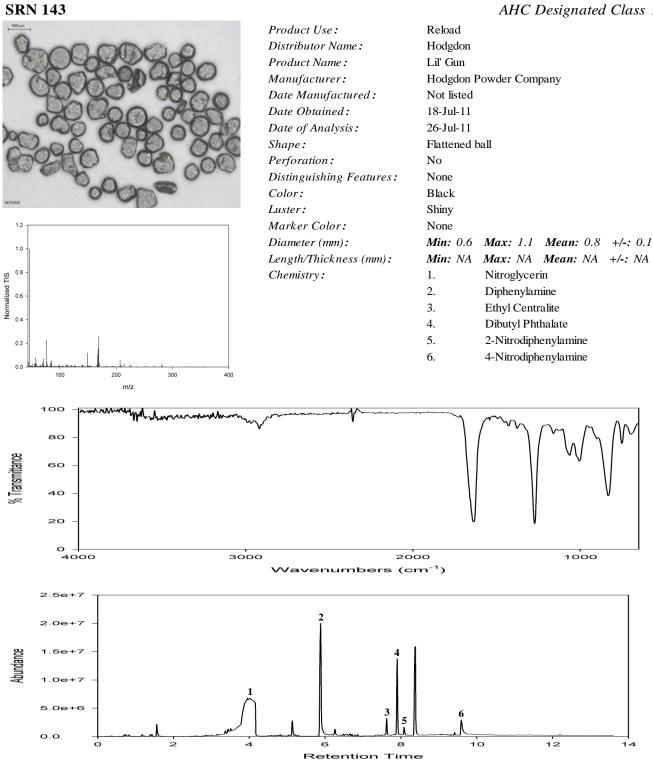


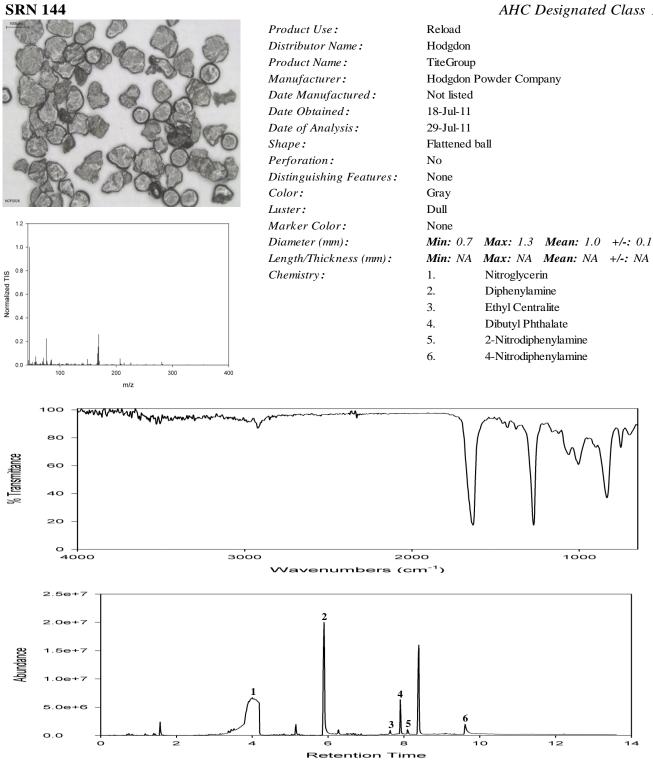


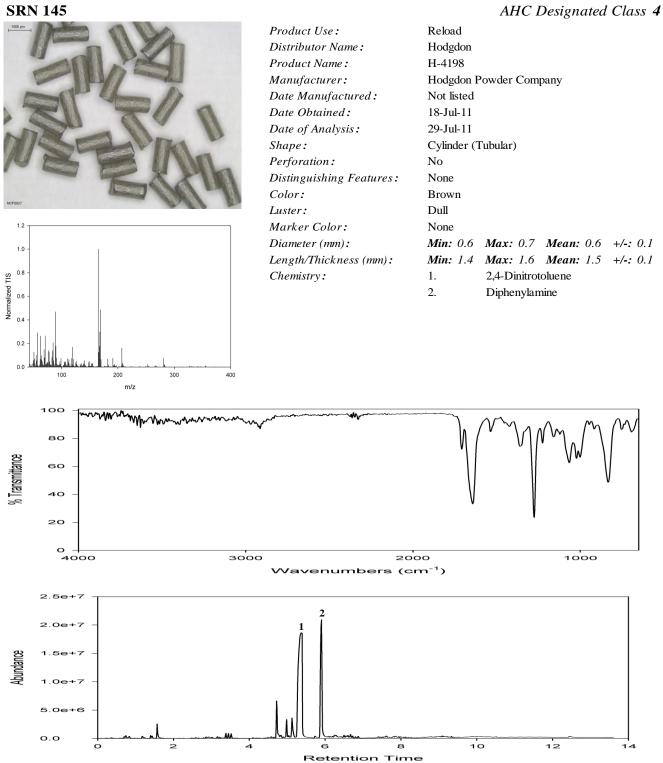


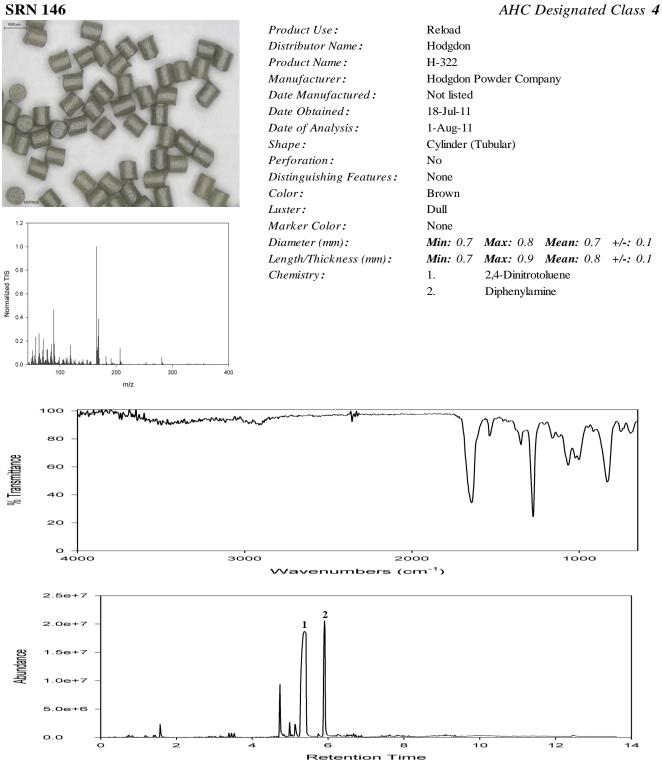


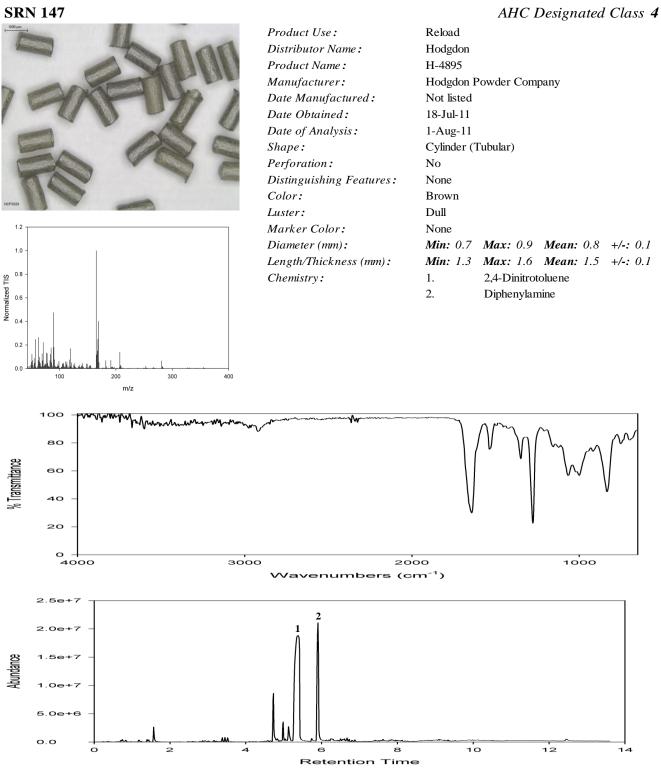


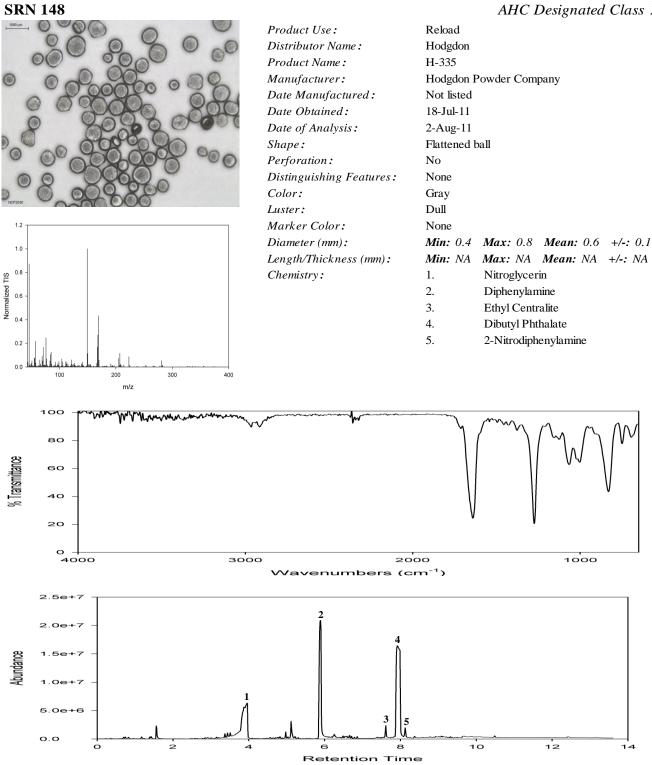


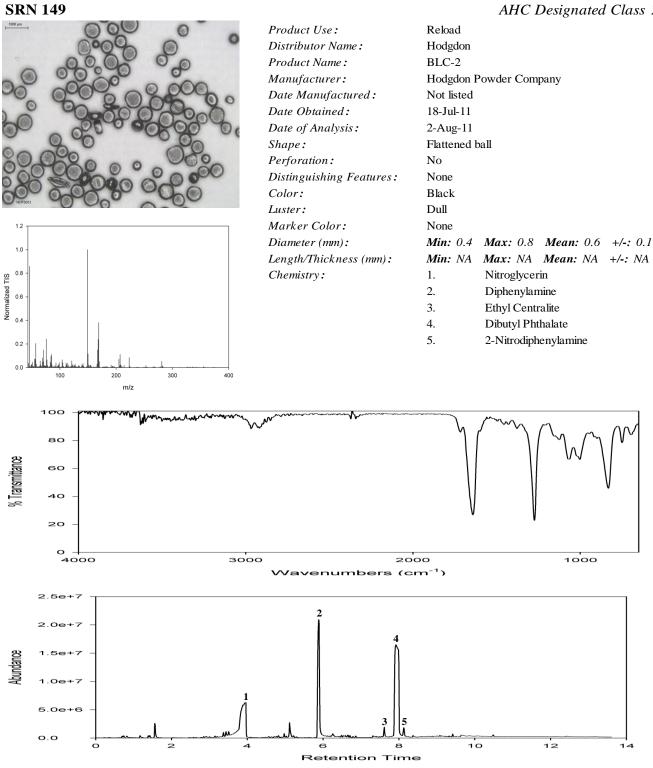


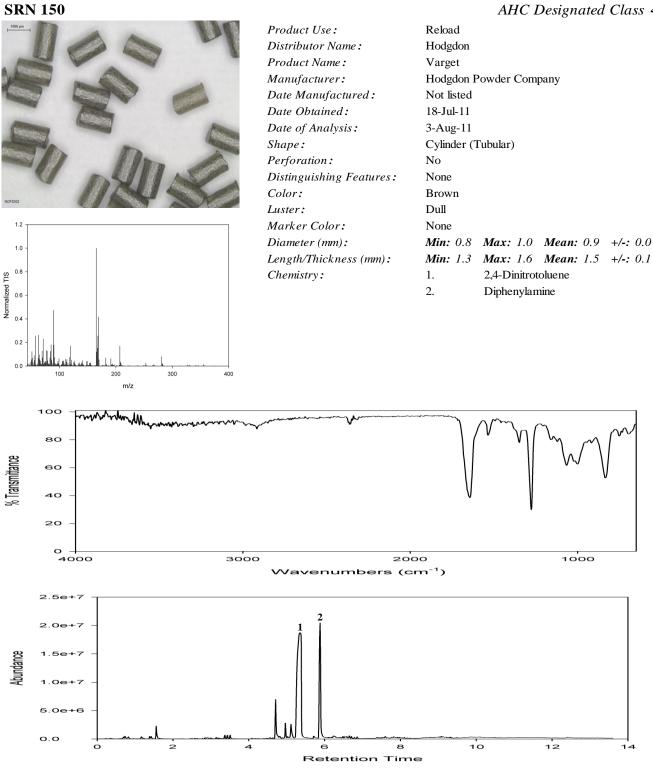


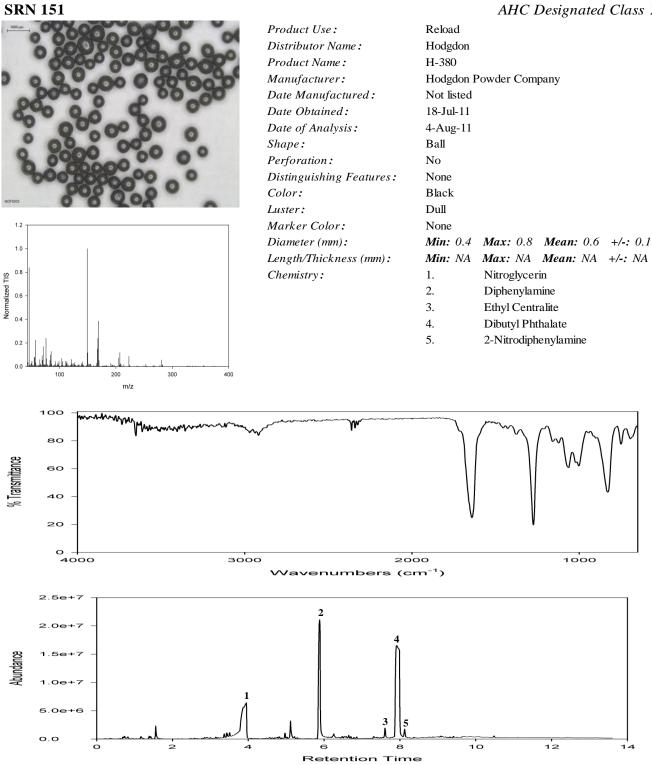


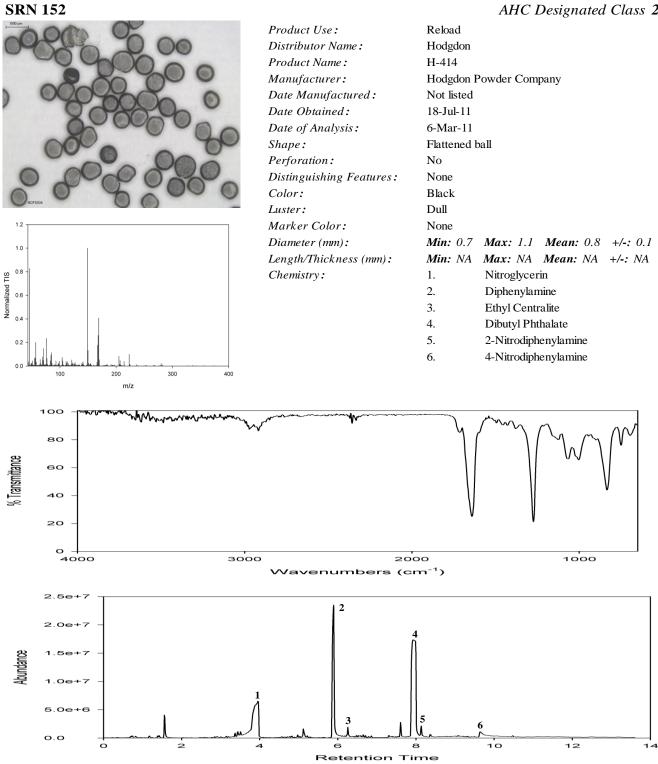




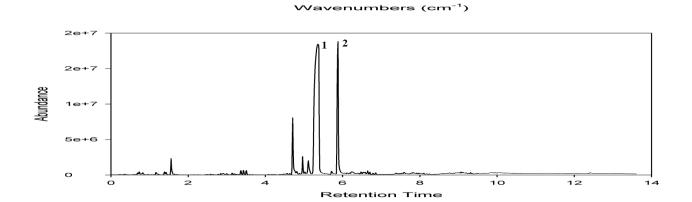








#### **SRN 153** AHC Designated Class 4 1000 µm Product Use: Reload Distributor Name: Hodgdon H-4350 Product Name: Manufacturer: Hodgdon Powder Company Date Manufactured: Not listed Date Obtained: 18-Jul-11 Date of Analysis: 10-Aug-11 Cylinder (Tubular) Shape: Perforation: No Distinguishing Features: None Brown Color: Luster: Dull Marker Color: None 1.2 Diameter (mm): Min: 0.9 Max: 1.1 Mean: 1.0 +/-: 0.0 1.0 Length/Thickness (mm): Min: 1.3 Max: 1.6 Mean: 1.5 +/-: 0.1 Normalized TIS 0.0 0.4 Chemistry: 1. 2,4-Dinitrotoluene 2. Diphenylamine 0.4 0.2 0.0 300 100 200 400 m/z 100 80 % Transmittance 60 40 20

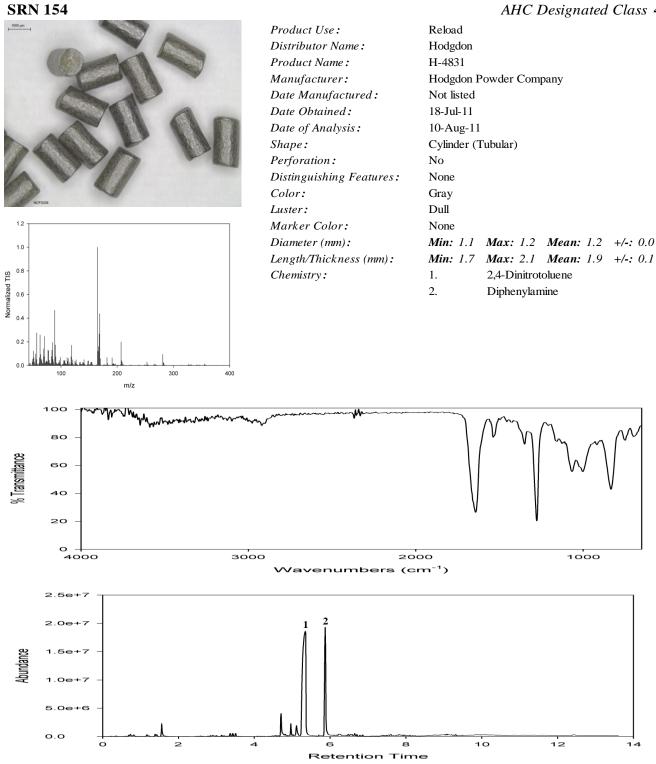


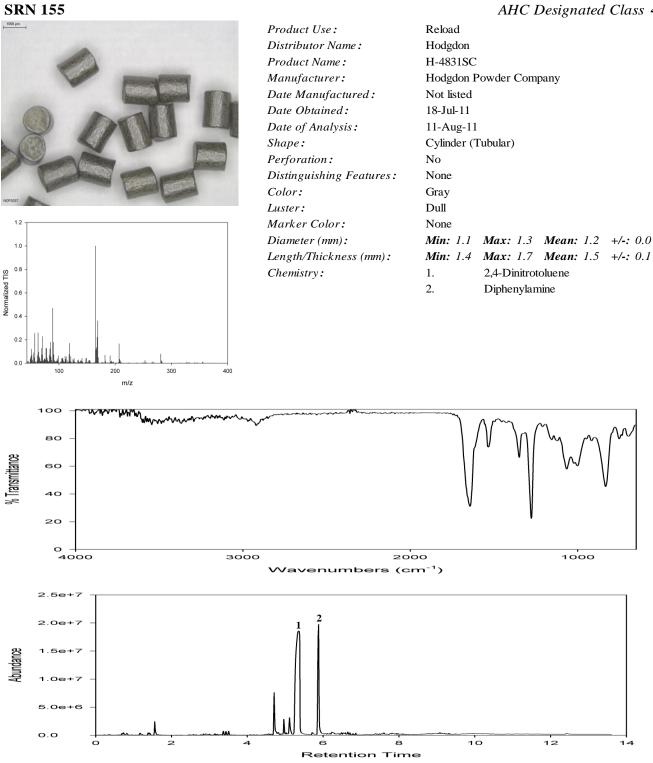
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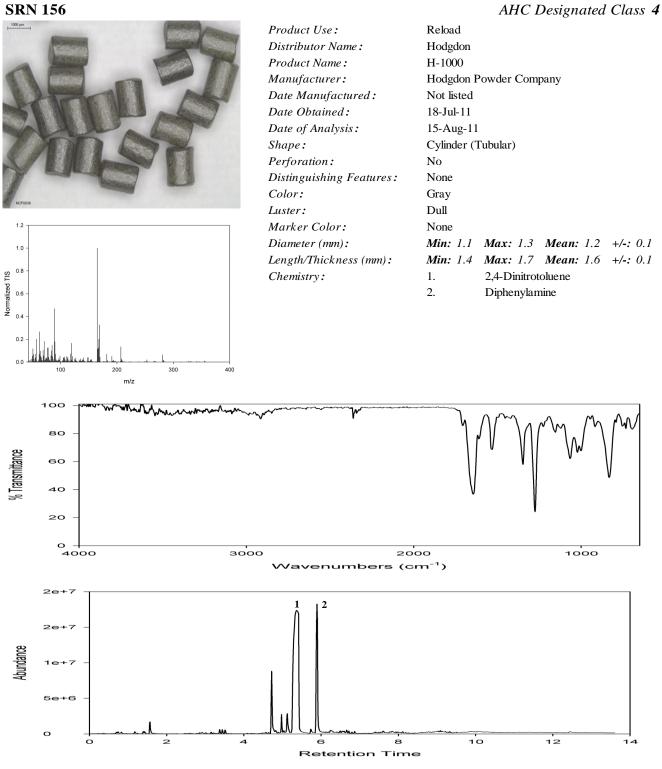
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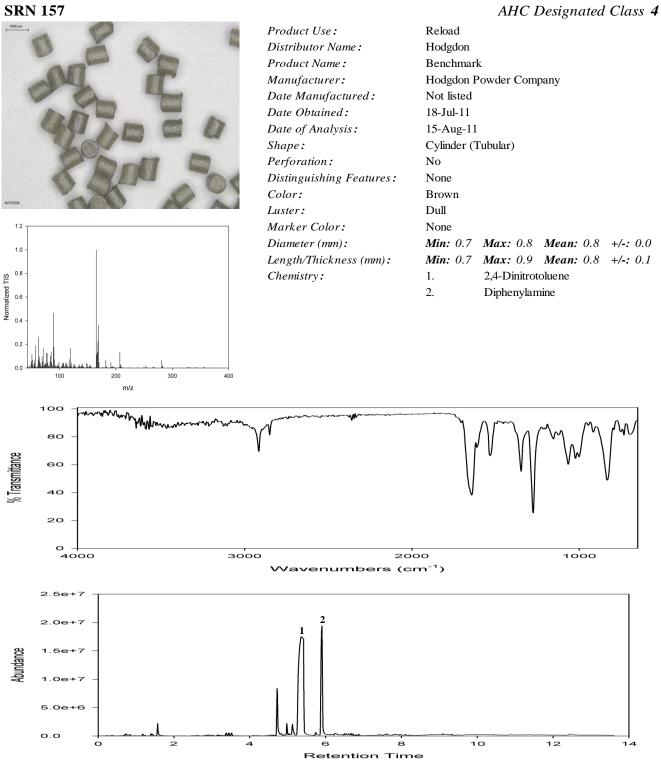
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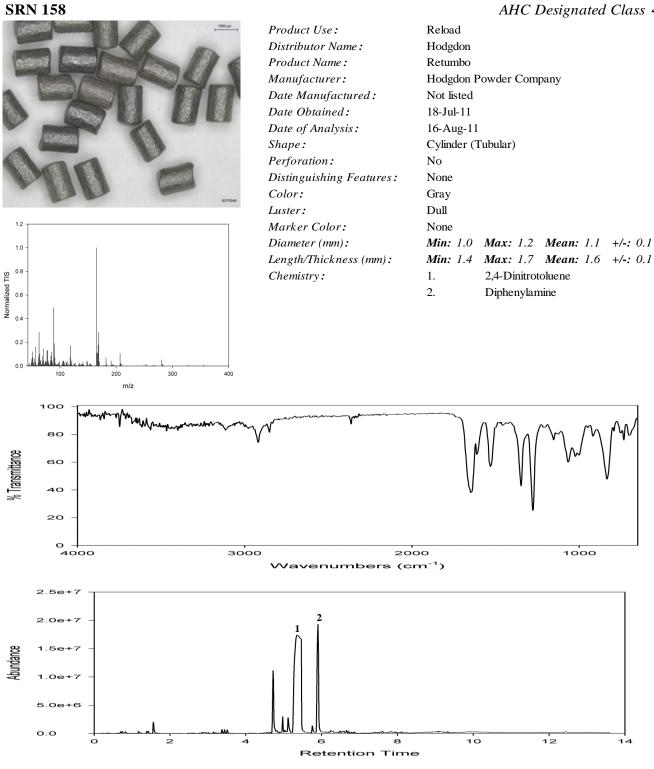
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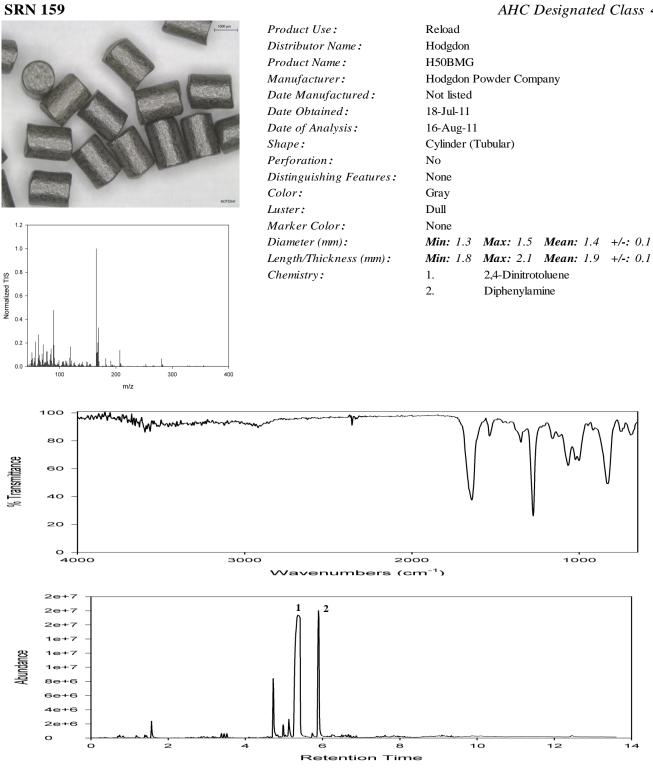


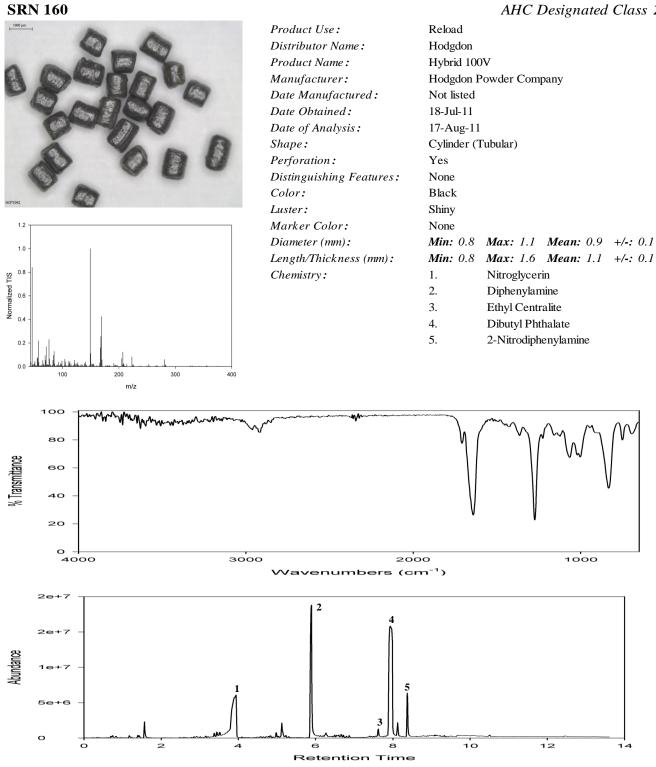


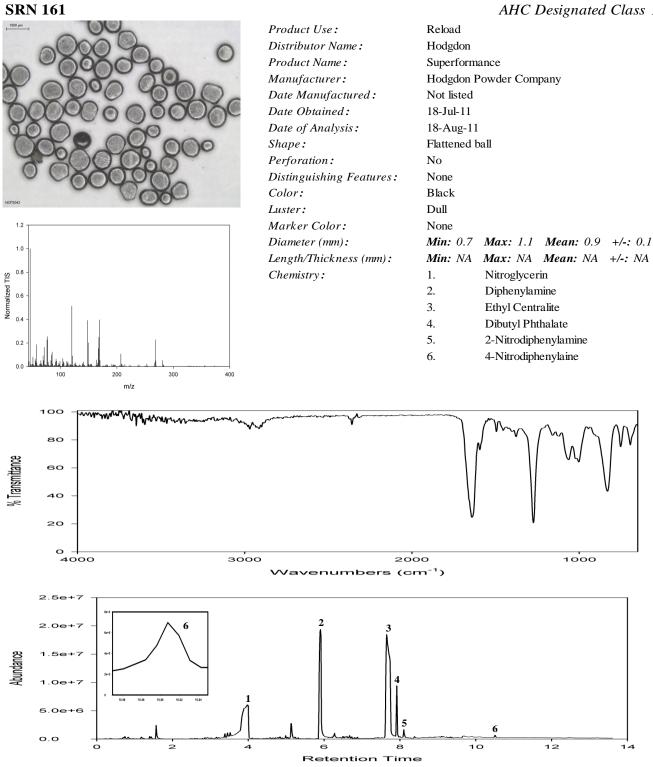


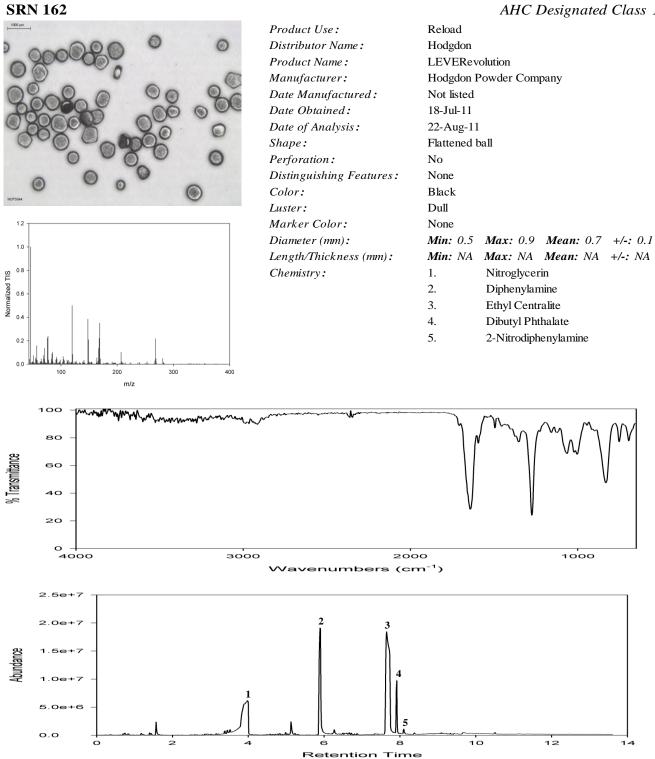


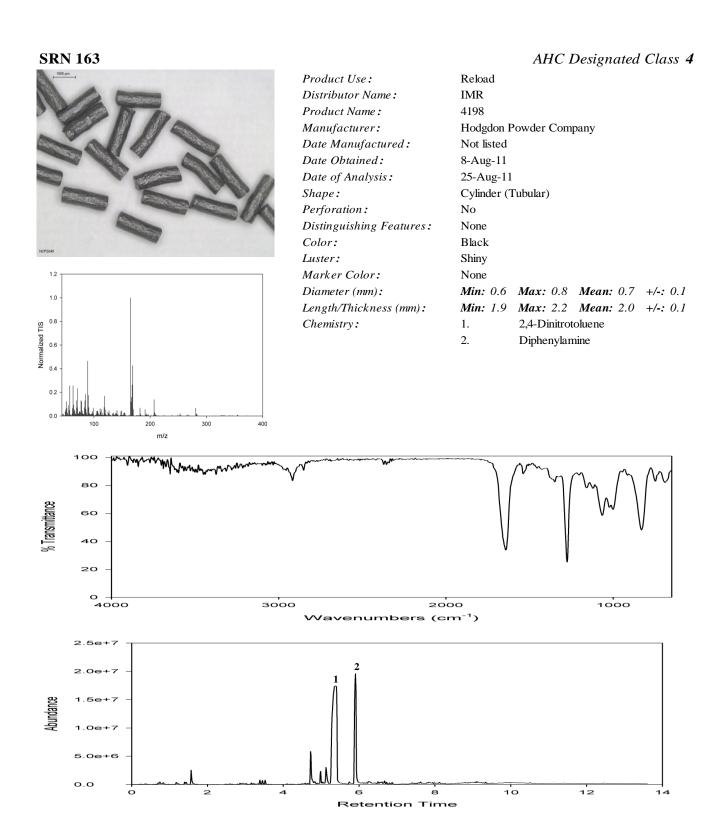




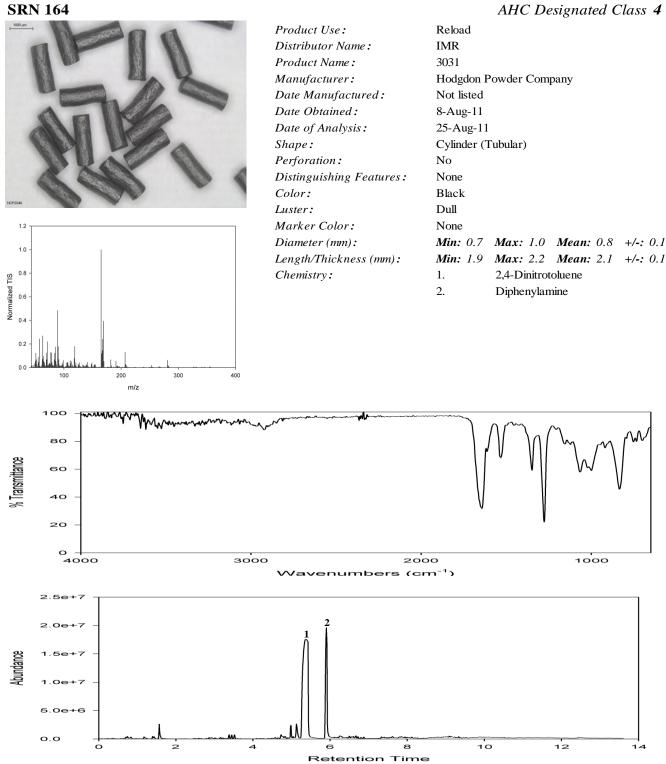


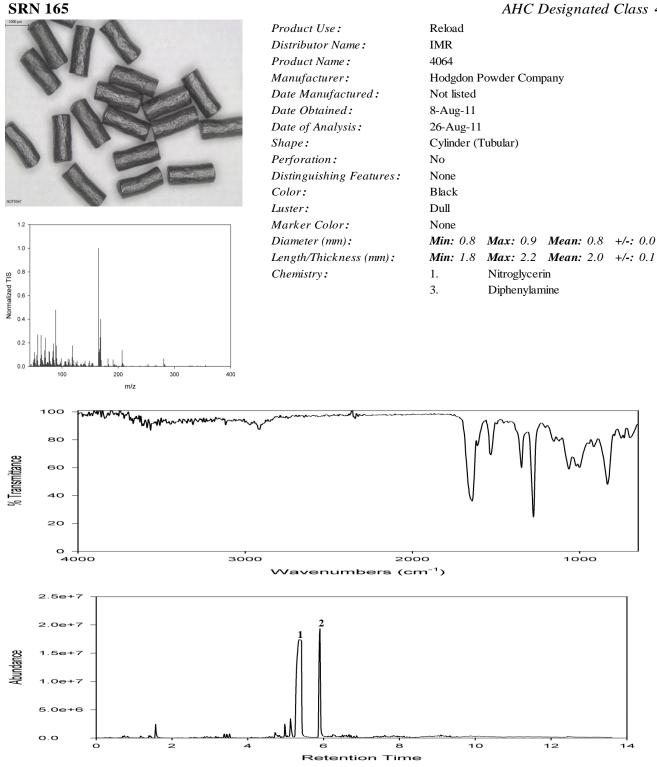


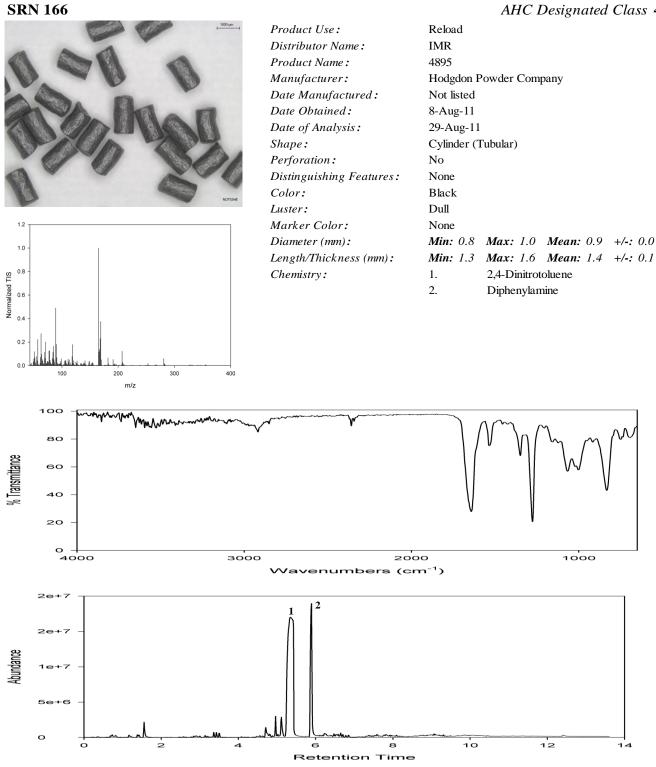


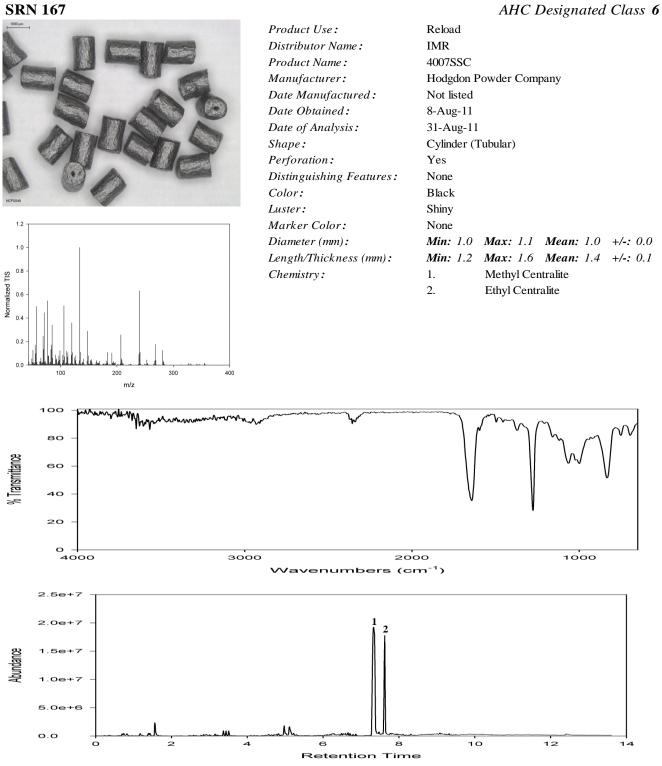


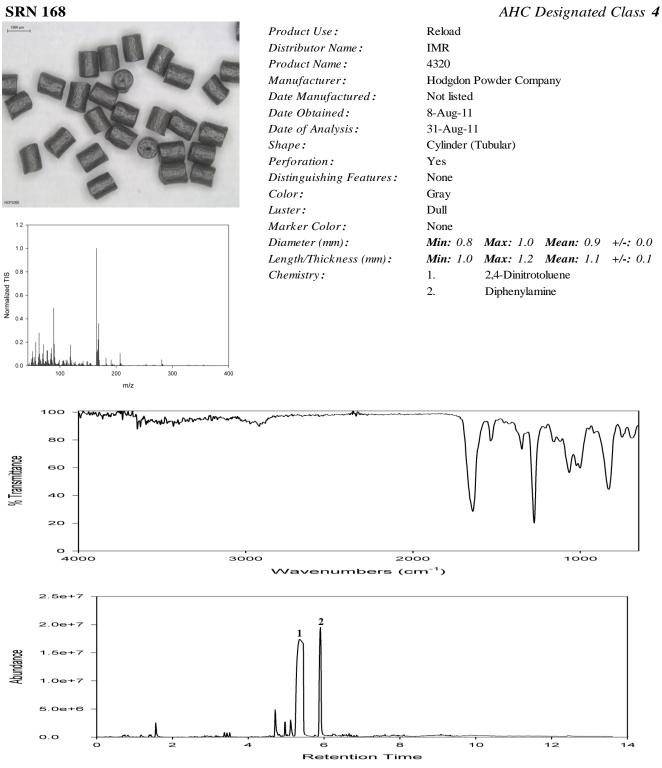
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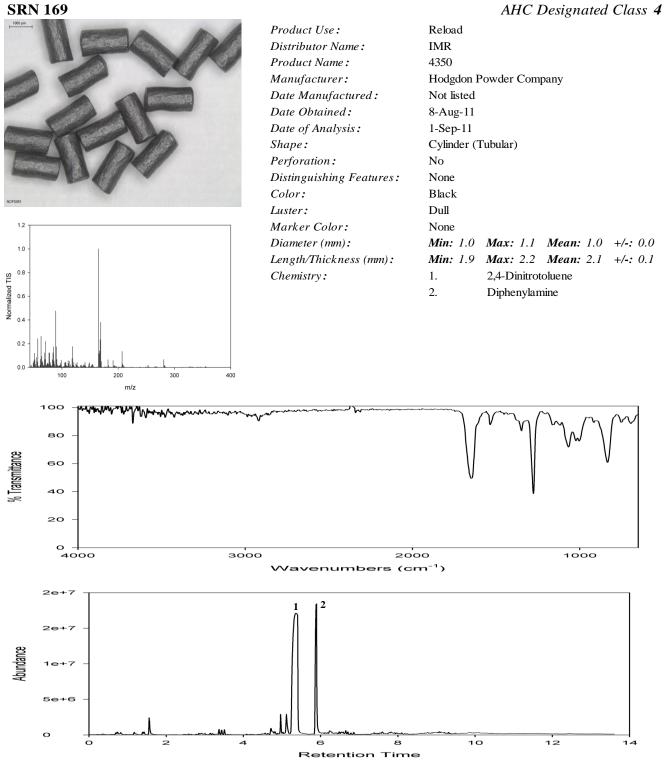


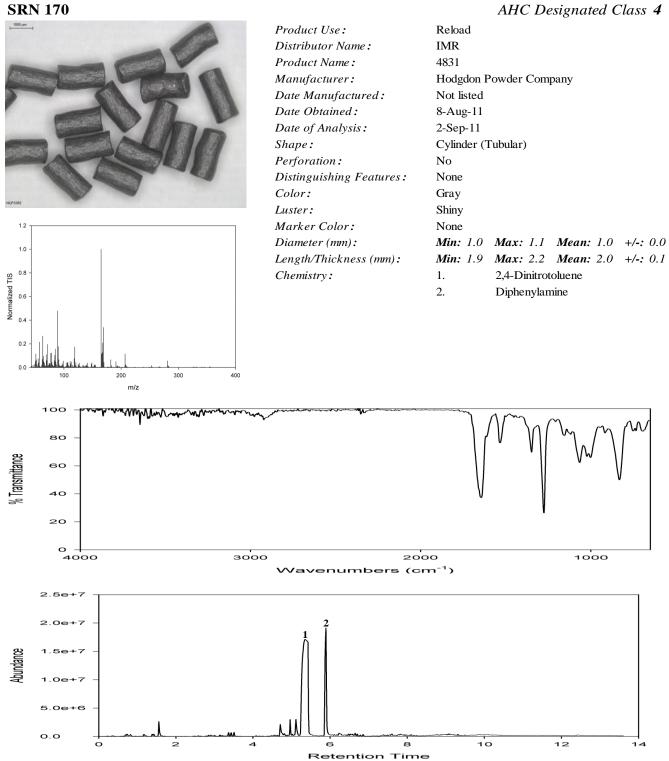


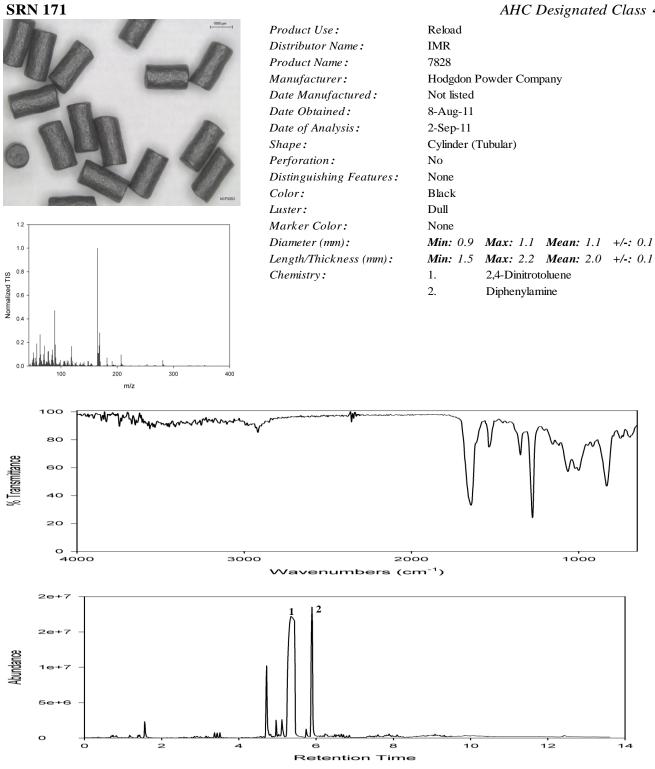


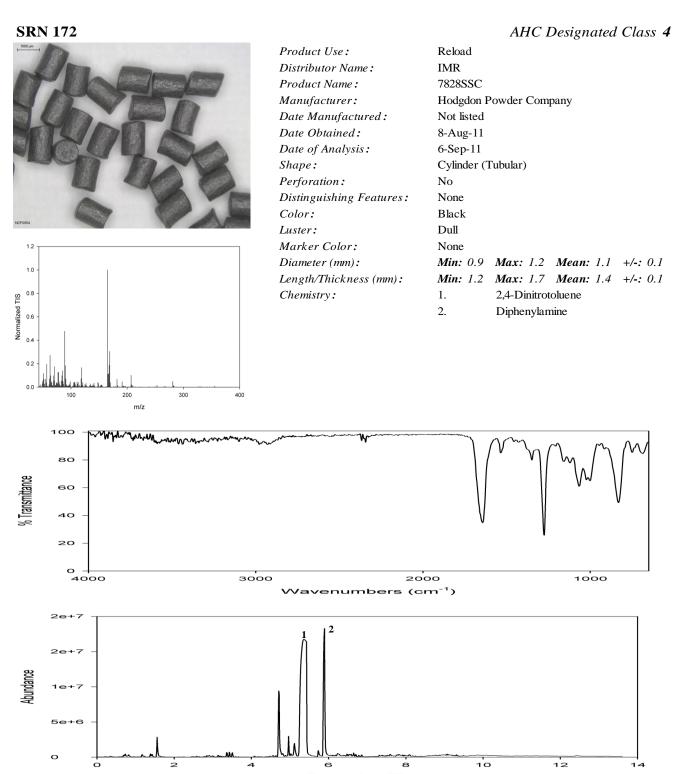


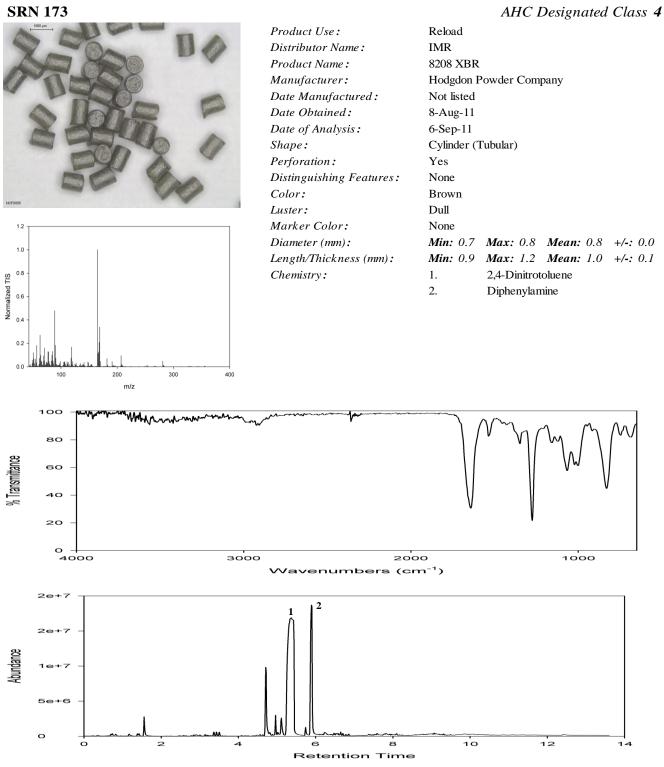


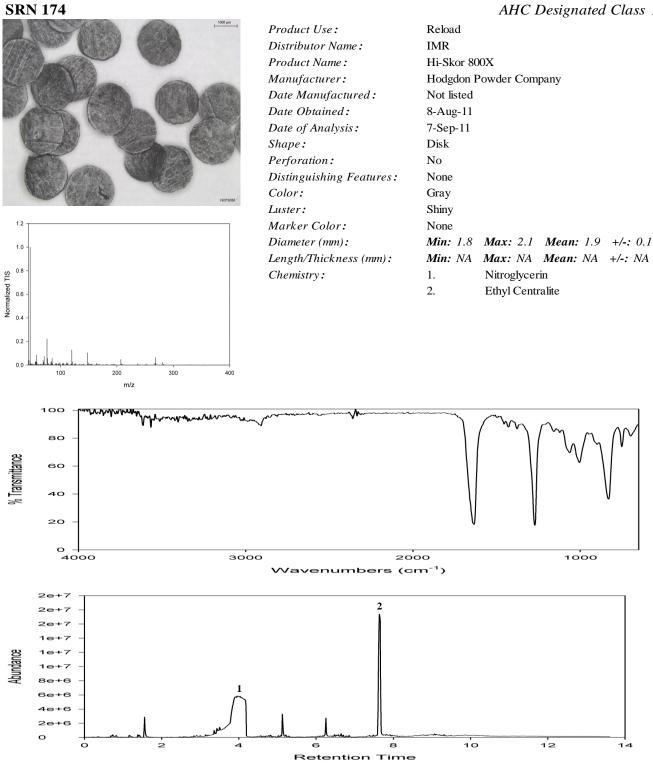


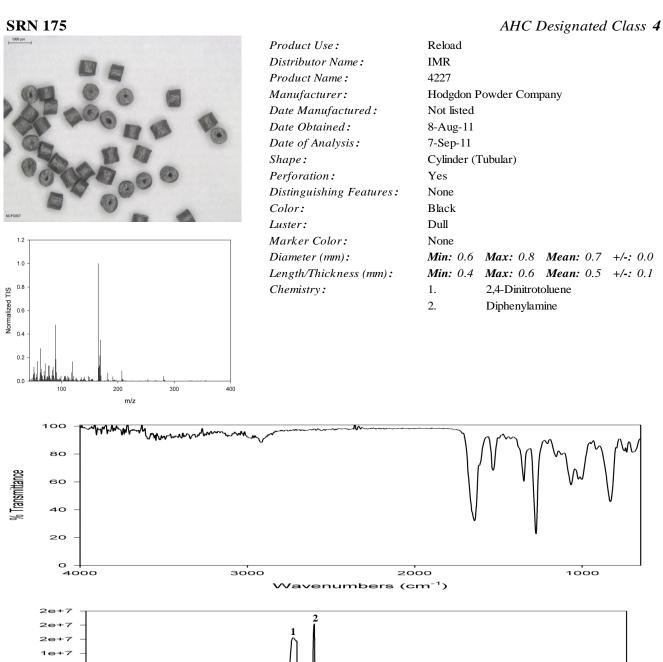












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**Retention Time** 

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8

12

14

Abundance

1e+7 1e+7 8e+6 6e+6 4e+6 2e+6 0

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2

#### **SRN 176** AHC Designated Class 5 1000 µm Product Use: Reload Distributor Name: IMR SR4759 Product Name: Manufacturer: Hodgdon Powder Company Date Manufactured: Not listed Date Obtained: 8-Aug-11 Date of Analysis: 8-Sep-11 Cylinder (Tubular) Shape: Perforation: Yes Distinguishing Features: None Black Color: Luster: Dull 1.2 Marker Color: None Diameter (mm): Min: 1.1 Max: 1.3 Mean: 1.2 +/-: 0.1 1.0 Length/Thickness (mm): Min: 1.3 Max: 1.7 Mean: 1.5 +/-: 0.1 Normalized TIS 0.0 0.4 Chemistry: 1. Diphenylamine 2. Dibutyl Phthalate 0.4 0.2 0.0 100 200 300 400 m/z 100 M 80 % Transmittance 60 40 20 o ↓ 4000 3000 2000 1000 nbers (cm<sup>-1</sup>) 2e+7 1 2 2e+7 Abundance

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Retention Time

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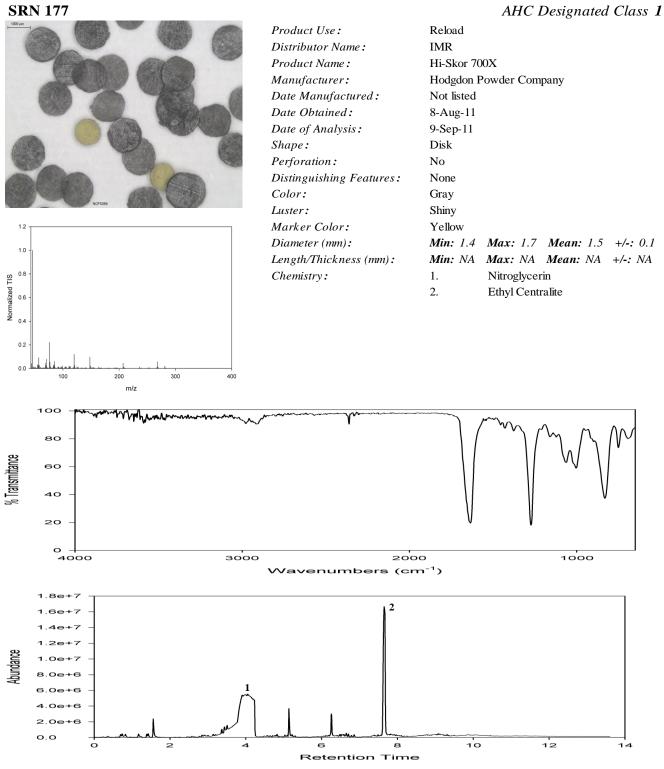
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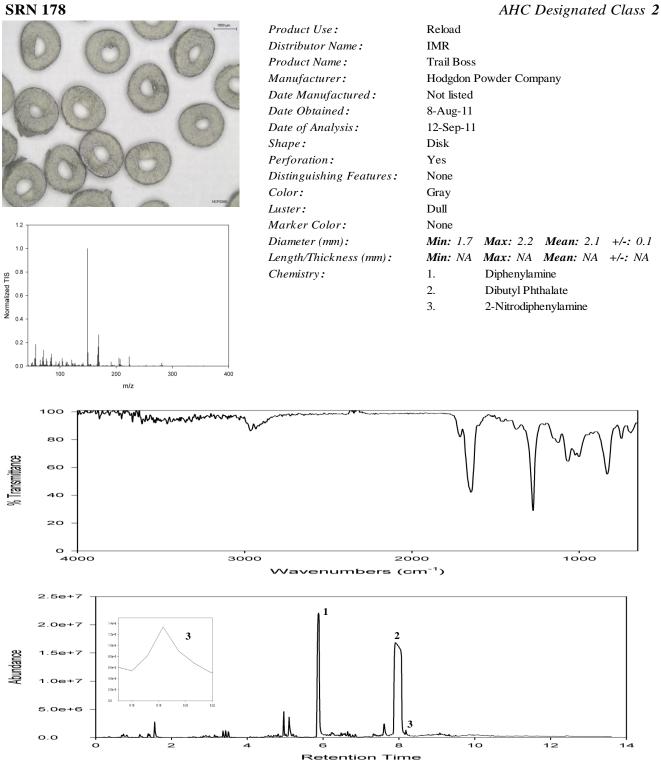
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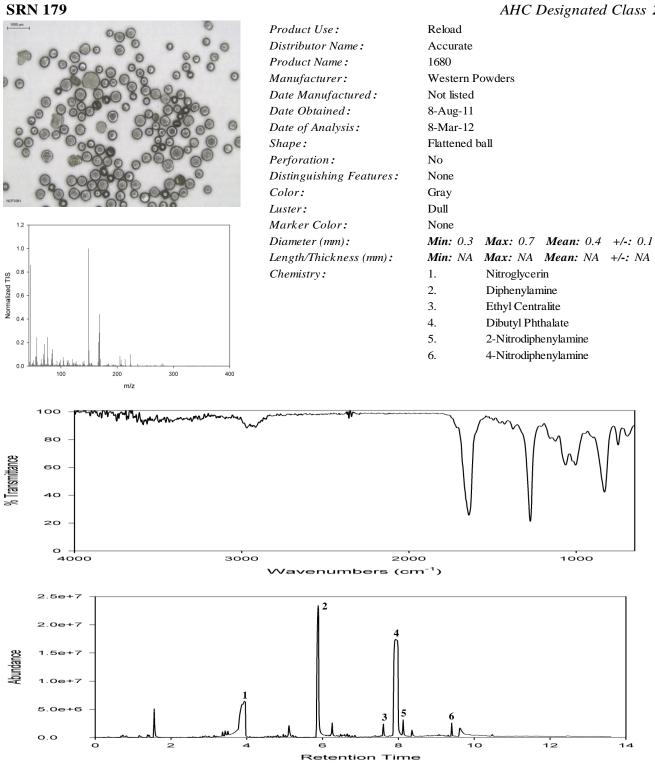
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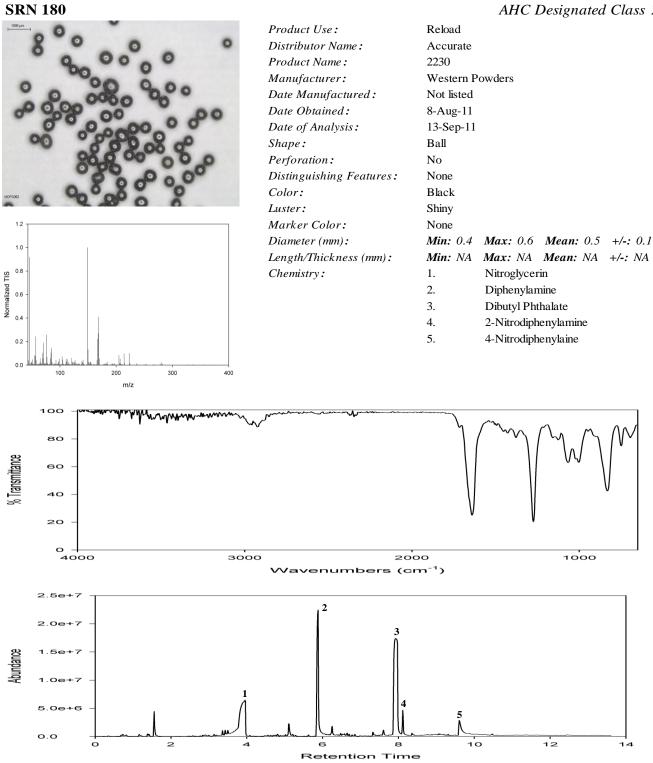
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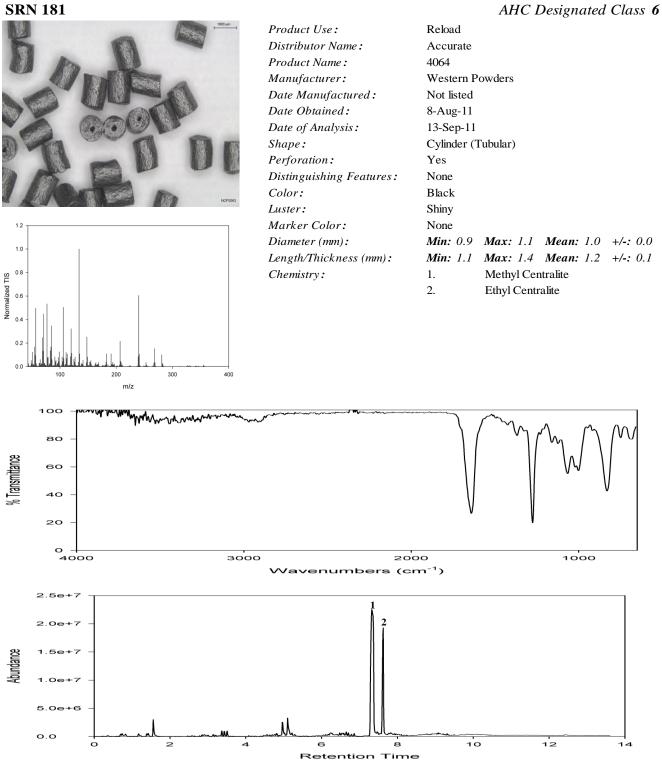
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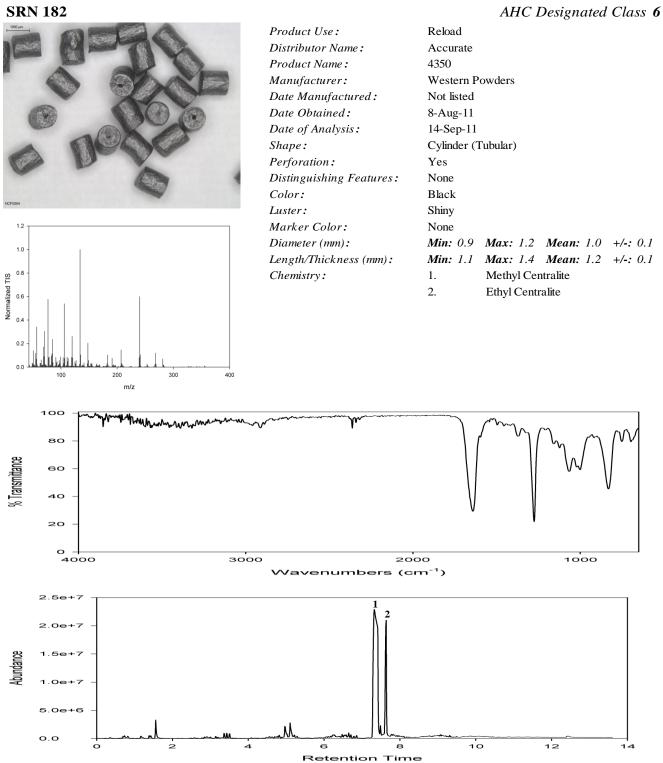


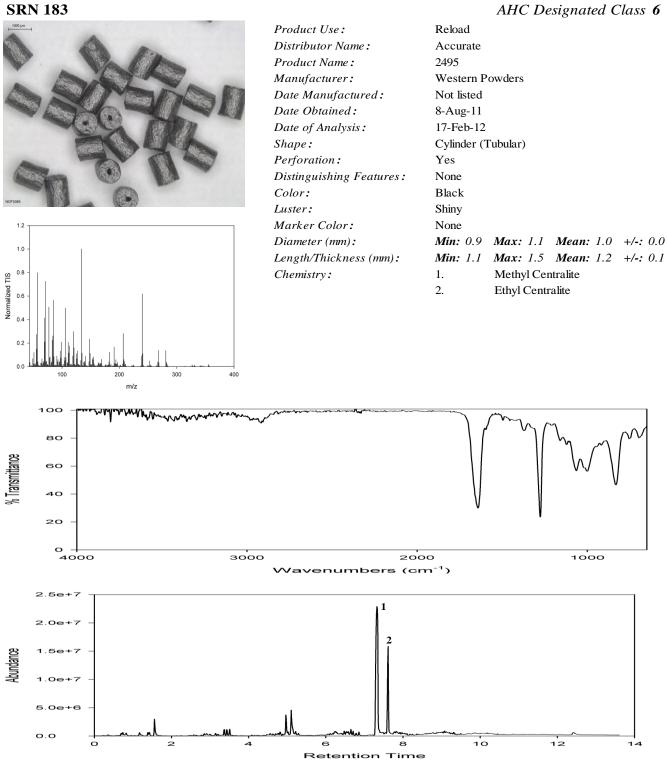


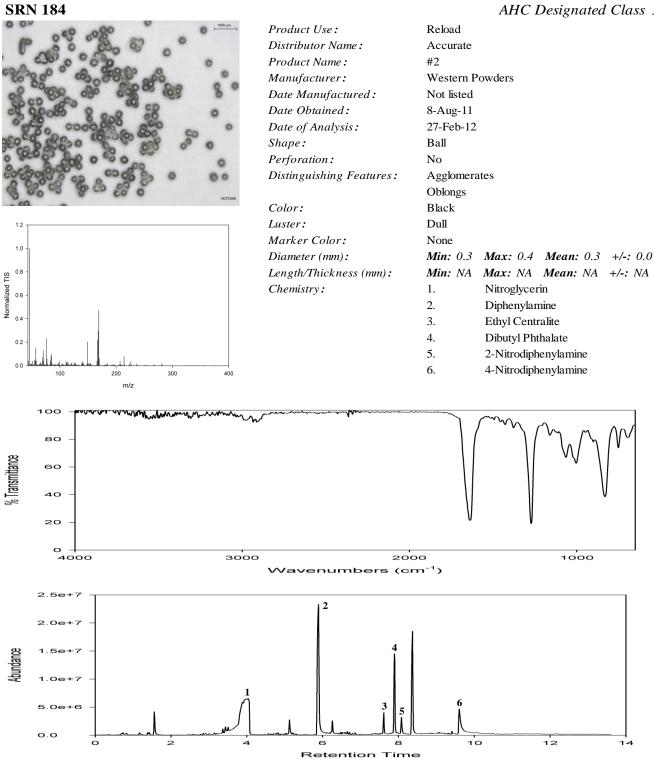


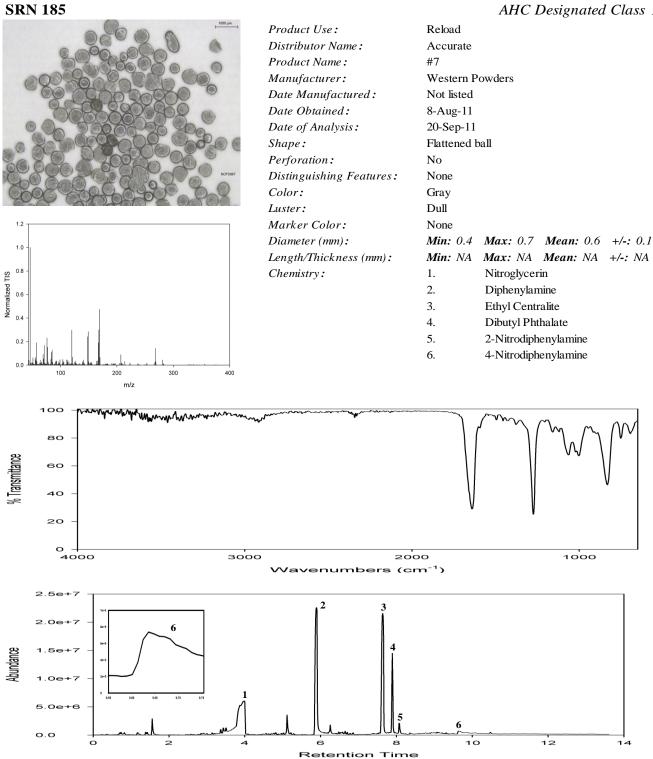


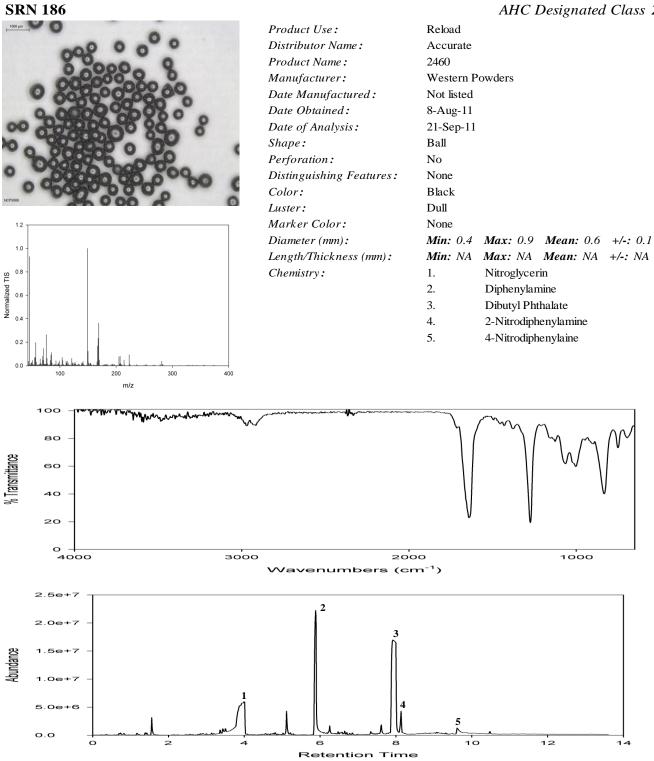


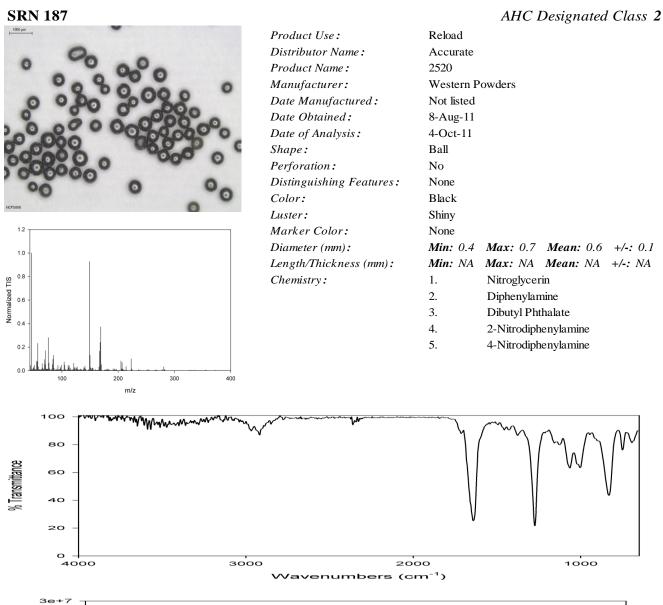


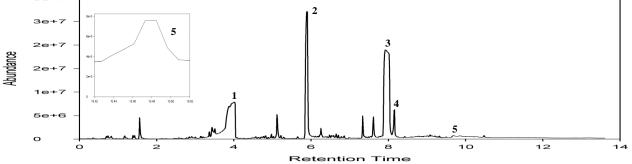












# APPENDIX C: NCFS SMOKELESS POWDER REFERENCE COLLECTION SAMPLES

SRN	Source SRN	Product Name	Class assignment based on the IIR
300	NCFS 070	Norma URP	Class 1
301	NCFS 071	Norma 217	Class 1
302	NCFS 072	Norma 204	Class 1
303	NCFS 073	Alliant Power Pro 4000MR	Class 1
304	NCFS 074	Alliant Reloder 50	Class 1
305	NCFS 075	Hodgdon H4198	Class 4
306	NCFS 076	Hodgdon LEVERevolution	Class 1
307	NCFS 077	Hodgdon US869	Class 1
308	NCFS 078	Hodgdon H50BMG	Class 4
309	NCFS 079	IMR 7828	Class 4
310	NCFS 080	Accurate 4064	Class 6
311	NCFS 081	IMR 4064	Class 4
312	NCFS 082	VihtaVuori N150	Class 3
313	NCFS 083	VihtaVuori N160	Class 3
314	NCFS 084	Hodgdon H4831	Class 4
315	NCFS 085	Accurate 2460	Class 1
316	NCFS 086	Accurate 5744	Class 1
317	NCFS 087	Accurate 2200	Class 1
318	NCFS 088	Accurate MagPro	Class 1
319	NCFS 089	Accurate 2015	Class 6
320	NCFS 090	Accurate 2495	Class 6
321	NCFS 091	Hodgdon Benchmark	Class 4
322	NCFS 092	IMR 7828SSC	Class 4
323	NCFS 093	IMR 4831	Class 4
324	NCFS 094	IMR 4320	Class 4

SRN	Source SRN	Product Name	Class assignment based on the IIR
325	NCFS 095	IMR 4895	Class 4
326	NCFS 096	IMR 8208 XBR	Class 4
327	NCFS 097	VihtaVuori N135	Class 3
328	NCFS 098	VihtaVuori N165	Class 3
329	NCFS 099	Hodgdon H322	Class 4
330	NCFS 100	Hodgdon H414Class 1Hodgdon H4350Class 4	
331	NCFS 101	Hodgdon H4350 Class 4	
332	NCFS 102	IMR 4227	Class 4
333	NCFS 103	VihtaVuori N133	Class 3
334	NCFS 104	Accurate LT-32	Class 5
335	NCFS 105	Hodgdon H335	Class 1
336	NCFS 106	Hodgdon Superformance	Class 1
337	NCFS 107	IMR 3031	Class 4
338	NCFS 108	Hodgdon Retumbo	Class 4
339	NCFS 109	Norma 203B	Class 1
340	NCFS 110	Accurate No. 4350	Class 2
341	NCFS 111	Norma 200	Class 1
342	NCFS 112	Norma 201	Class 1
343	NCFS 113	Norma 202	Class 1
344	NCFS 114	Norma MRP	Class 1
345	NCFS 115	Hodgdon H380	Class 1
346	NCFS 116	VihtaVuori 3N37	Class 5
347	NCFS 117	VihtaVuori N140	Class 5
348	NCFS 118	Hodgdon Hybrid 100V	Class 1
349	NCFS 119	Alliant Reloder 10X	Class 1

## APPENDIX D: FBI DATABASE SAMPLES USED FOR DEVELOPMENT OF THE DISCRIMINANT ANALYSIS MODELS

SRN	Powder Type	AHC Designated	Distributor	Product Name	Shape	Color
1	Double Base	Class 1	Alliant	2400	Disk	Gray
2	Double Base	Class 1	Alliant	Promo	Disk	Gray
3	Double Base	Class 1	Alliant	American Select	Disk	Gray
4	Double Base	Class 1	Alliant	Power Pistol	Disk	Gray
5	Double Base	Class 1	Alliant	Steel	Disk	Black
6	Double Base	Class 1	Alliant	Blue Dot	Disk	Black
7	Double Base	Class 1	Alliant	Reloder 7	Cylinder (Tubular)	Gold
8	Double Base	Class 2	Alliant	Reloder 10x	Cylinder (Tubular)	Gray
9	Double Base	Class 2	Alliant	Reloder 15	Cylinder (Tubular)	Gray
10	Double Base	Class 2	Alliant	Reloder 22	Cylinder (Tubular)	Gray
11	Double Base	Class 2	Alliant	Reloder 25	Cylinder (Tubular)	Gray
12	Double Base	Class 1	Alliant	410	Disk	Gray
13	Double Base	Class 1	Alliant	e3	Disk	Black
14	Double Base	Class 1	Accurate	#2	Ball	Gray
15	Double Base	Class 1	Accurate	#5	Flattened Ball	Gray
16	Double Base	Class 2	Accurate	#7	Flattened Ball	Gray
17	Double Base	Class 1	Accurate	#9	Ball	Gray
18	Double Base	Class 2	Accurate	1680	Flattened Ball	Black
19	Single Base	Class 3	Accurate	2015	Cylinder (Tubular)	Gray
20	Double Base	Class 2	Accurate	2230	Flattened Ball	Gray
21	Double Base	Class 2	Accurate	2460	Flattened Ball	Gray
22	Single Base	Class 6	Accurate	2495	Cylinder (Tubular)	Gray

SRN	Powder Type	AHC Designated	Distributor	Product Name	Shape	Color
23	Double Base	Class 2	Accurate	2520	Ball	Gray
24	Double Base	Class 2	Accurate	2700	Flattened Ball	Gray
25	Single Base	Class 4	Accurate	3100	Cylinder (Tubular)	Gray
26	Single Base	Class 3	Accurate	4064	Cylinder (Tubular)	Gray
27	Single Base	Class 4	Accurate	4350	Cylinder (Tubular)	Gray
28	Double Base	Class 1	Accurate	5744	Cylinder (Tubular)	Gray
29	Double Base	Class 2	Accurate	8700	Flattened Ball	Gray
30	Double Base	Class 2	Accurate	MagPro	Flattened Ball	Gray
31	Single Base	Class 5	Accurate	Solo 1000	Disk	Gray
32	Double Base	Class 1	Accurate	Nitro 100	Disk	Gray
33	Single Base	Class 5	Accurate	Solo 1250	Disk	Gray
34	Double Base	Class 1	Winchester	231	Irregular Flattened Ball	Gray
35	Double Base	Class 1	Winchester	296	Flattened Ball	Gray
36	Double Base	Class 1	Winchester	WST	Flattened Ball & Irregular Flattened Ball	Gray
37	Double Base	Class 1	Winchester	WSF	Irregular Flattened Ball	Gray
38	Double Base	Class 2	Winchester	748	Flattened Ball	Gray
39	Double Base	Class 2	Winchester	760	Flattened Ball	Gray
40	Double Base	Class 2	Winchester	WXR	Cylinder (Tubular)	Black
41	Single Base	Class 3	VihtaVuori	N120	Cylinder (Tubular)	Gray
42	Single Base	Class 3	VihtaVuori	N130	Cylinder (Tubular)	Gray
43	Single Base	Class 3	VihtaVuori	N133	Cylinder (Tubular)	Gray
44	Single Base	Class 3	VihtaVuori	N135	Cylinder (Tubular)	Gray

SRN	Powder Type	AHC Designated	Distributor	Product Name	Shape	Color
45	Single Base	Class 3	VihtaVuori	N165	Cylinder (Tubular)	Gray
46	Single Base	Class 3	VihtaVuori	N170	Cylinder (Tubular)	Gray
47	Single Base	Class 3	VihtaVuori	N105	Cylinder (Tubular)	Gray
48	Single Base	Class 5	VihtaVuori	3N37	Cylinder (Tubular)	Gold
49	Single Base	Class 3	VihtaVuori	3N38	Cylinder (Tubular)	Gray
50	Single Base	Class 5	VihtaVuori	N310	Cylinder (Tubular)	Gold
51	Single Base	Class 3	VihtaVuori	N110	Cylinder (Tubular)	Gray
52	Single Base	Class 5	VihtaVuori	N320	Cylinder (Tubular)	Gold
53	Single Base	Class 5	VihtaVuori	Oy N330	Cylinder (Tubular)	Gray
54	Single Base	Class 5	VihtaVuori	N340	Cylinder (Tubular)	Gold
55	Single Base	Class 5	VihtaVuori	N350	Cylinder (Tubular)	Gold
56	Double Base	Class 1	VihtaVuori	N540	Cylinder (Tubular)	Gray
57	Double Base	Class 1	VihtaVuori	N550	Cylinder (Tubular)	Gray
58	Double Base	Class 1	VihtaVuori	N560	Cylinder (Tubular)	Gray
59	Single Base	Class 3	VihtaVuori	Oy N3SH	Lamel	Gray
60	Single Base	Class 3	VihtaVuori	N3SL	Lamel	Gray
61	Single Base	Class 3	VihtaVuori	20N29	Cylinder (Tubular)	Gray
62	Single Base	Class 3	VihtaVuori	24N41	Cylinder (Tubular)	Gray
63	Single Base	Class 4	Hodgdon	H1000	Cylinder (Tubular)	Gold
64	Single Base	Class 4	Hodgdon	Varget	Cylinder (Tubular)	Gold
65	Single Base	Class 4	Hodgdon	H322	Cylinder (Tubular)	Gold
66	Double Base	Class 2	Hodgdon	H335	Flattened Ball	Gray

SRN	Powder Type	AHC Designated	Distributor	Product Name	Shape	Color
67	Double Base	Class 2	Hodgdon	H380	Ball	Gray
68	Double Base	Class 2	Hodgdon	H414	Flattened Ball	Gray
69	Single Base	Class 4	Hodgdon	H4227	Cylinder (Tubular)	Gold
70	Single Base	Class 4	Hodgdon	H4350	Cylinder (Tubular)	Gold
71	Single Base	Class 4	Hodgdon	H4831	Cylinder (Tubular)	Gold
72	Single Base	Class 4	Hodgdon	H4831 SC	Cylinder (Tubular)	Gold
73	Single Base	Class 4	Hodgdon	H4895	Cylinder (Tubular)	Gold
74	Single Base	Class 4	Hodgdon	H50BMG	Cylinder (Tubular)	Gray
75	Double Base	Class 2	Hodgdon	BL-C(2)	Flattened Ball	Gray
76	Single Base	Class 4	Hodgdon	Benchmark	Cylinder (Tubular)	Gold
77	Single Base	Class 4	Hodgdon	Retumbo	Cylinder (Tubular)	Gold
78	Double Base	Class 1	Hodgdon	HS-6	Flattened Ball	Black
79	Double Base	Class 1	Hodgdon	HS-7	Flattened Ball	Gray
80	Double Base	Class 1	Hodgdon	H110	Flattened Ball	Black
81	Double Base	Class 1	Hodgdon	HP-38	Flattened Ball	Gray
82	Double Base	Class 1	Hodgdon	Titegroup	Irregular Flattened Ball	Gray
83	Double Base	Class 1	Hodgdon	Titewad	Irregular Flattened Ball	Gray
84	Double Base	Class 2	Hodgdon	Clays	Disk	Gray
85	Double Base	Class 1	Hodgdon	International Clays	Disk	Gray
86	Double Base	Class 1	Hodgdon	Universal Clays	Disk	Gray
87	Double Base	Class 1	Hodgdon	Longshot	Irregular Flattened Ball	Gray
88	Double Base	Class 1	Hodgdon	Lil'Gun	Flattened Ball	Gray

SRN	Powder Type	AHC Designated	Distributor	Product Name	Shape	Color
89	Double Base	Class 1	Ramshot	Competition	Irregular Flattened Ball	Gray
90	Double Base	Class 1	Ramshot	Zip	Flattened Ball	Gray
91	Double Base	Class 1	Ramshot	Silhouette	Flattened Ball	Gray
92	Double Base	Class 1	Ramshot	True Blue	Ball	Black
93	Double Base	Class 2	Ramshot	Enforcer	Ball	Black
94	Double Base	Class 2	Ramshot	X-Terminator	Ball	Black
95	Double Base	Class 2	Ramshot	TAC	Flattened Ball	Gray
96	Double Base	Class 2	Ramshot	Big Game	Ball	Black
97	Double Base	Class 2	Ramshot	Hunter	Ball	Black
98	Double Base	Class 2	Ramshot	Magnum	Flattened Ball	Black
99	Single Base	Class 4	Hodgdon	H4198	Cylinder (Tubular)	Gold
100	Single Base	Class 3	VihtaVuori	N160	Cylinder (Tubular)	Black
188	Double Base	Class 1	Hercules	2400	Disk	Gray
189	Double Base	Class 1	Hodgdon	240	Disk	Gray
190	Single Base	Class 5	Dupont	Hi-Skor	Disk	Gray
191	Single Base	Class 5	Dupont	#5 Pistol	Disk	Gray
192	Double Base	Class 1	Hercules	Bullseye	Disk	Gray
193	Double Base	Class 1	Hercules	Blue Dot	Disk	Gray
194	Double Base	Class 1	Hercules	Green Dot	Disk	Gray
195	Double Base	Class 1	Dupont	700X	Disk	Black
196	Double Base	Class 1	Herters	164	Disk	Black
197	Double Base	Class 1	Herters	162	Disk	Gray

SRN	Powder Type	AHC Designated	Distributor	Product Name	Shape	Color
198	Double Base	Class 1	Hercules	Red Dot	Disk	Gray
199	Double Base	Class 1	Norma	2020	Disk	Gray
200	Double Base	Class 1	Herters	160	Disk	Gray
201	Double Base	Class 1	Norma	1010	Disk	Gray
202	Double Base	Class 1	Hercules	Unique	Disk	Black
203	Double Base	Class 1	Hercules	SS #1	Disk	Gray
204	Double Base	Class 1	Hercules	Herco	Disk	Gray
205	Single Base	Class 5	Dupont	PB	Disk	Gray
206	Double Base	Class 5	Dupont	SR-7625	Disk	Black
207	Double Base	Class 1	Hodgdon	HP-38	Flattened Ball	Gray
212	Double Base	Class 1	Dupont	Hi-Skor 800-X	Disk	Black
213	Single Base	Class 4	Dupont	SR-4756	Disk	Gray
214	Double Base	Class 1	Hercules	Red Dot	Disk	Gray
215	Double Base	Class 1	Hercules	Herco	Disk	Gray
216	Double Base	Class 1	Hercules	Blue Dot	Disk	Gray
217	Double Base	Class 1	Hercules	Unique	Disk	Gray
218	Double Base	Class 1	Hercules	Bullseye	Disk	Gray
219	Double Base	Class 1	Hercules	2400	Disk	Gray
220	Double Base	Class 3	Hercules	RL-7	Disk	Gray
221	Double Base	Class 3	Hercules	RL-12	Cylinder (Tubular)	Black
222	Double Base	Class 2	Dupont	Ball C	Ball	Black
223	Double Base	Class 1	Hodgdon	H-110	Flattened Ball	Black

SRN	Powder Type	AHC Designated	Distributor	Product Name	Shape	Color
224	Double Base	Class 2	Hodgdon	BLC-2	Flattened Ball	Black
225	Single Base	Class 4	Hodgdon	H-4831	Cylinder (Tubular)	Gray
226	Double Base	Class 1	Winchester	AA20S	Agglomerate	Gray
227	Double Base	Class 3	Hercules	RL-21	Cylinder (Tubular)	Gray
228	Double Base	Class 1	Hercules	Hi-Vel-2	Cylinder (Tubular)	Gray
229	Double Base	Class 2	Hodgdon	H-375	Flattened Ball	Gray
230	Double Base	Class 2	Hodgdon	H-380	Ball	Black
231	Single Base	Class 4	Dupont	IMR-4759	Cylinder (Tubular)	Gray
232	Double Base	Class 2	Hodgdon	H-414	Flattened Ball	Gray
233	Double Base	Class 2	Hodgdon	H-870	Ball	Black
234	Single Base	Class 5	Dupont	Bulk	Other	Orange
235	Single Base	Class 4	C Dupont	IMR-4831	Cylinder (Tubular)	Gray
236	Double Base	Class 1	Winchester	571	Flattened Ball	Gray
237	Double Base	Class 2	Winchester	785	Flattened Ball	Gray
238	Double Base	Class 1	Winchester	231	Flattened Ball & Irregular Flattened Ball	Gray
239	Double Base	Class 1	Winchester	452AA	Flattened Ball & Irregular Flattened Ball	Gray
240	Double Base	Class 2	Winchester	680	Flattened Ball	Black
241	Double Base	Class 2	Winchester	296	Flattened Ball	Black
242	Double Base	Class 1	Winchester	540	Flattened Ball	Gray
243	Double Base	Class 2	Winchester	748	Flattened Ball	Gray
244	Double Base	Class 2	Winchester	760	Flattened Ball	Gray
245	Double Base	Class 2	Hodgdon	H-335	Flattened Ball	Gray

SRN	Powder Type	AHC Designated	Distributor	Product Name	Shape	Color
246	Double Base	Class 1	Hodgdon	Trap 100	Flattened Ball & Irregular Flattened Ball	Gray
247	Double Base	Class 1	Hodgdon	HS-6	Flattened Ball	Gray
248	Double Base	Class 2	Hodgdon	H-760	Ball	Black
249	Double Base	Class 1	Hercules	RL-15	Cylinder (Tubular)	Gray
250	Double Base	Class 2	Hercules	RL-19	Cylinder (Tubular)	Gray
251	Double Base	Class 2	Hercules	RL-22	Cylinder (Tubular)	Gray
252	Double Base	Class 1	WPR	280	Flattened Ball & Irregular Flattened Ball	Gray
253	Double Base	Class 2	Winchester	749	Flattened Ball & Irregular Flattened Ball	Gray
254	Double Base	Class 2	Winchester	760	Flattened Ball	Gray
255	Double Base	Class 1	Winchester	473AA	Flattened Ball & Irregular Flattened Ball	Gray
256	Single Base	Class 4	Hodgdon	H-4227	Cylinder (Tubular)	Gray
257	Single Base	Class 4	Hodgdon	H-4198	Cylinder (Tubular)	Gray
258	Single Base	Class 5	Norma	R-1	Cylinder (Tubular)	Gray
259	Single Base	Class 4	Dupont	IMR-4227	Cylinder (Tubular)	Black
261	Single Base	Class 6	Hodgdon	H-4198	Cylinder (Tubular)	Gray
262	Single Base	Class 2	Norma	R-123	Cylinder (Tubular)	Gray
263	Double Base	Class 3	Hercules	RL-7	Cylinder (Tubular)	Gray
264	Double Base	Class 2	Norma	N-203	Cylinder (Tubular)	Gray
265	Single Base	Class 4	Dupont	IMR-4320	Cylinder (Tubular)	Gray
266	Single Base	Class 6	Herters	102	Cylinder (Tubular)	Gray
267	Single Base	Class 6	Hodgdon	Н-322	Cylinder (Tubular)	Gray
268	Single Base	Class 6	Herters	103	Cylinder (Tubular)	Gray

SRN	Powder Type	AHC Designated	Distributor	Product Name	Shape	Color
269	Double Base	Class 2	Norma	N-201	Cylinder (Tubular)	Gray
270	Double Base	Class 2	Norma	N-200	Cylinder (Tubular)	Gray
271	Single Base	Class 4	Hodgdon	H-4895	Cylinder (Tubular)	Gray
272	Double Base	Class 2	Norma	Magnum Rifle	Cylinder (Tubular)	Gray
273	Double Base	Class 2	Norma	205	Cylinder (Tubular)	Gray
274	Double Base	Class 2	Norma	204	Cylinder (Tubular)	Gray
275	Single Base	Class 4	C Dupont	IMR-4198	Cylinder (Tubular)	Gray
276	Single Base	Class 4	C Dupont	IMR-3031	Cylinder (Tubular)	Gray
277	Single Base	Class 4	C Dupont	IMR-4350	Cylinder (Tubular)	Gray
278	Single Base	Class 6	Herters	101	Cylinder (Tubular)	Gray
279	Single Base	Class 4	C Dupont	IMR-4064	Cylinder (Tubular)	Gray
280	Double Base	Class 2	Hodgdon	BLC-2	Flattened Ball	Black
281	Single Base	Class 4	Hodgdon	H-322	Cylinder (Tubular)	Gray
282	Double Base	Class 2	Hodgdon	Н-335	Flattened Ball	Gray
283	Single Base	Class 6	Hodgdon	H-4895	Cylinder (Tubular)	Gray
284	Double Base	Class 2	Hodgdon	H-414	Flattened Ball	Gray
285	Double Base	Class 2	Hodgdon	H-380	Ball	Black
286	Double Base	Class 2	Hodgdon	H-450	Ball	Black
287	Single Base	Class 6	Hodgdon	H-4831	Cylinder (Tubular)	Gray
288	Double Base	Class 2	Hodgdon	H-870	Ball	Black
289	Double Base	Class 1	Hodgdon	H-110	Flattened Ball	Gray
290	Double Base	Class 1	Hodgdon	HP-38	Flattened Ball & Irregular Flattened Ball	Gray

SRN	Powder Type	AHC Designated	Distributor	Product Name	Shape	Color
291	Double Base	Class 1	Hodgdon	HS-6	Flattened Ball	Gray
292	Double Base	Class 1	Hodgdon	HS-7	Flattened Ball	Gray
294	Single Base	Class 5	Alcan	AL-5	Lamel	Black
295	Double Base	Class 1	Dupont	MX	Irregular	Black
296	Double Base	Class 1	Dupont	#6 Pistol	Irregular	Black
297	Single Base	Class 5	Alcan	AL-8	Lamel	Gray
298	Double Base	Class 1	Nike	Unknown	Lamel	Red
299	Single Base	Class 5	Alcan	AL-7	Lamel	Black
400	Double Base	Class 1	Hodgdon	Trap 100	Flattened Ball & Irregular Flattened Ball	Gray
401	Double Base	Class 1	Winchester	571	Flattened Ball	Gray
402	Double Base	Class 1	WMG	535	Flattened Ball & Irregular	Gray
403	Double Base	Class 1	Winchester	814	Flattened Ball	Gray
404	Double Base	Class 1	Winchester	818	Flattened Ball	Gray
405	Double Base	Class 1	Dupont	700X	Disk	Gray
406	Double Base	Class 1	Dupont	800-X	Disk	Gray
407	Single Base	Class 5	Dupont	PB	Disk	Gray
408	Single Base	Class 4	Dupont	IMR-3031	Cylinder (Tubular)	Gray
409	Single Base	Class 4	Dupont	IMR-4064	Cylinder (Tubular)	Gray
410	Single Base	Class 4	Dupont	IMR-4198	Cylinder (Tubular)	Gray
411	Single Base	Class 4	Dupont	IMR-4227	Cylinder (Tubular)	Gray
412	Single Base	Class 4	Dupont	IMR-4320	Cylinder (Tubular)	Gray
413	Single Base	Class 4	Dupont	IMR-4350	Cylinder (Tubular)	Gray

SRN	Powder Type	AHC Designated	Distributor	Product Name	Shape	Color
414	Single Base	Class 4	Dupont	IMR-4895	Cylinder (Tubular)	Gray
415	Single Base	Class 4	Dupont	SR-4759	Cylinder (Tubular)	Gray
416	Single Base	Class 5	IMR	SR-7625	Disk	Gray
417	Single Base	Class 4	Dupont	SR-4756	Disk	Gray
418	Single Base	Class 4	Dupont	IMR-7828	Cylinder (Tubular)	Gray
419	Double Base	Class 1	Winchester	452AA	Irregular Flattened Ball	Gray
420	Double Base	Class 1	Winchester	230	Irregular Flattened Ball	Gray
421	Double Base	Class 2	Winchester	748	Flattened Ball	Gray
422	Double Base	Class 1	Winchester	540	Flattened Ball	Black
423	Double Base	Class 1	Winchester	571	Flattened Ball	Black
424	Double Base	Class 1	Winchester	231	Flattened Ball & Irregular	Gray
425	Double Base	Class 2	Winchester	680	Flattened Ball	Gray
426	Double Base	Class 2	Winchester	748	Flattened Ball	Gray
427	Double Base	Class 2	Winchester	760	Flattened Ball	Gray
428	Double Base	Class 1	WSX	150	Flattened Ball	Gray
429	Double Base	Class 1	WMG	575	Flattened Ball & Irregular	Gray
430	Double Base	Class 1	Winchester	232	Flattened Ball & Irregular	Gray
431	Double Base	Class 2	Winchester	755	Flattened Ball	Black
432	Double Base	Class 1	Winchester	AA80	Flattened Ball & Irregular Flattened Ball	Gray
433	Double Base	Class 2	Winchester	662	Flattened Ball	Black
434	Single Base	Class 4	Accurate	MR-3100	Cylinder (Tubular)	Gray
435	Double Base	Class 1	Accurate	5744	Cylinder (Tubular)	Black

SRN	Powder Type	AHC Designated	Distributor	Product Name	Shape	Color
436	Double Base	Class 2	Accurate	8700	Flattened Ball	Black
437	Double Base	Class 2	Accurate	MR-223	Flattened Ball	Black
438	Double Base	Class 2	Accurate	MR-2460	Flattened Ball	Black
439	Double Base	Class 2	Accurate	2520	Ball	Black
440	Double Base	Class 1	Accurate	No. 2	Ball & Irregular Flattened Ball	Gray
441	Double Base	Class 1	Accurate	No. 5	Flattened Ball	Gray
442	Double Base	Class 1	WSX	120	Flattened Ball & Irregular Flattened Ball	Gray
443	Double Base	Class 1	Winchester	231	Flattened Ball	Gray
444	Double Base	Class 1	Winchester	296	Flattened Ball & Irregular Flattened Ball	Gray
445	Double Base	Class 1	WMG	525	Flattened Ball & Irregular Flattened Ball	Gray
446	Double Base	Class 1	Winchester	669	Ball	Black
447	Double Base	Class 2	Winchester	728	Flattened Ball	Gray
448	Double Base	Class 2	Winchester	680	Flattened Ball	Gray
449	Double Base	Class 2	Winchester	844	Flattened Ball	Black
450	Double Base	Class 1	WSX	170	Flattened Ball & Irregular Flattened Ball	Black
451	Double Base	Class 1	Winchester	AA20	Flattened Ball & Irregular Flattened Ball	Gray
452	Double Base	Class 1	Winchester	615	Flattened Ball	Gray
453	Double Base	Class 2	Winchester	732	Flattened Ball	Black
454	Double Base	Class 2	Winchester	785	Flattened Ball	Gray
455	Double Base	Class 1	Winchester	295 S	Flattened Ball	Black
456	Double Base	Class 2	Winchester	860	Flattened Ball	Black
457	Double Base	Class 1	Winchester	237	Irregular Flattened Ball	Gray

SRN	Powder Type	AHC Designated	Distributor	Product Name	Shape	Color
458	Double Base	Class 1	WMG	555	Flattened Ball & Irregular Flattened Ball	Gray
459	Double Base	Class 1	Winchester	235	Flattened Ball	Gray
460	Double Base	Class 2	Winchester	846	Flattened Ball	Gray
461	Double Base	Class 1	WSX	130	Flattened Ball & Irregular Flattened Ball	Gray
462	Double Base	Class 2	Winchester	759	Flattened Ball	Black
463	Double Base	Class 1	Winchester	AA60	Flattened Ball & Irregular Flattened Ball	Gray
464	Double Base	Class 1	WSX	110	Flattened Ball & Irregular Flattened Ball	Gray
465	Double Base	Class 1	WMG	585	Flattened Ball	Black
466	Double Base	Class 1	Winchester	540	Flattened Ball	Gray
467	Double Base	Class 2	Winchester	852H	Ball	Black
468	Double Base	Class 1	WSX	140	Irregular Flattened Ball	Gray
469	Double Base	Class 2	Winchester	730	Flattened Ball	Gray
470	Single Base	Class 4	Dupont	IMR-4198	Cylinder (Tubular)	Gray
471	Single Base	Class 6	Hodgdon	H-4198	Cylinder (Tubular)	Gray
472	Double Base	Class 2	Hodgdon	H-870	Ball	Black
473	Double Base	Class 2	Hodgdon	H-414	Flattened Ball	Gray
474	Double Base	Class 2	Hodgdon	H-380	Ball	Black
475	Double Base	Class 2	Hodgdon	Н-335	Flattened Ball	Gray
476	Single Base	Class 6	Hodgdon	H-322	Cylinder (Tubular)	Gray
477	Double Base	Class 2	Hodgdon	BLC-2	Flattened Ball	Gray
478	Double Base	Class 1	Hercules	Herco	Disk	Black
479	Double Base	Class 1	Hercules	Blue Dot	Disk	Gray

SRN	Powder Type	AHC Designated	Distributor	Product Name	Shape	Color
480	Double Base	Class 1	Hercules	Red Dot	Disk	Gray
481	Double Base	Class 1	Hercules	Unique	Disk	Gray
482	Double Base	Class 1	Hercules	2400	Disk	Gray
483	Double Base	Class 1	Hercules	Green Dot	Disk	Gray
484	Double Base	Class 1	Hercules	Bullseye	Disk	Gray
485	Double Base	Class 3	Hercules	RL-7	Disk	Gray
486	Double Base	Class 2	Winchester	785	Flattened Ball	Gray
487	Double Base	Class 2	Winchester	760	Flattened Ball	Gray
488	Double Base	Class 2	Winchester	748	Flattened Ball	Gray
489	Double Base	Class 2	Winchester	680	Flattened Ball & Irregular Flattened Ball	Gray
490	Double Base	Class 1	Winchester	571	Flattened Ball	Gray
491	Double Base	Class 1	Winchester	630	Flattened Ball	Gray
492	Double Base	Class 1	Winchester	540	Flattened Ball	Gray
493	Double Base	Class 1	Winchester	473AA	Flattened Ball	Gray
494	Double Base	Class 1	Winchester	452AA	Flattened Ball	Gray
495	Double Base	Class 2	Winchester	296	Flattened Ball	Gray
496	Double Base	Class 1	Winchester	231	Flattened Ball & Irregular Flattened Ball	Gray
497	Double Base	Class 1	Winchester	230 P	Irregular Flattened Ball	Gray
498	Single Base	Class 6	Hodgdon	H-4895	Cylinder (Tubular)	Gray
499	Single Base	Class 5	Alcan	AL-8	Lamel	Gray
500	Single Base	Class 5	Alcan	AL-7	Lamel	Gray
501	Single Base	Class 5	Alcan	AL-5	Lamel	Black

SRN	Powder Type	AHC Designated	Distributor	Product Name	Shape	Color
502	Single Base	Class 5	Dupont	PB	Disk	Gray
503	Double Base	Class 1	Dupont	Hi-Skor 800-X	Disk	Gray
504	Double Base	Class 1	Dupont	Hi-Skor 700-X	Disk	Gray
505	Single Base	Class 5	Dupont	SR-7625	Disk	Gray
506	Single Base	Class 5	Dupont	SR-4756	Disk	Gray
507	Single Base	Class 4	Dupont	IMR-4895	Cylinder (Tubular)	Gray
508	Single Base	Class 4	Dupont	IMR-4831	Cylinder (Tubular)	Gray
509	Single Base	Class 4	Dupont	IMR-4350	Cylinder (Tubular)	Gray
510	Single Base	Class 4	Dupont	IMR-4320	Cylinder (Tubular)	Gray
511	Single Base	Class 4	Dupont	IMR-4227	Disk	Gray
512	Single Base	Class 4	Dupont	IMR-4198	Cylinder (Tubular)	Gray
513	Single Base	Class 6	Dupont	IMR-4064	Cylinder (Tubular)	Gray
514	Single Base	Class 4	Dupont	IMR-3031	Cylinder (Tubular)	Gray
515	Single Base	Class 6	Hodgdon	H-4227	Disk	Gray
516	Single Base	Class 6	Hodgdon	H-4831	Cylinder (Tubular)	Gray
517	Double Base	Class 2	Accurate	No. 9	Flattened Ball	Black
518	Double Base	Class 2	Accurate	No. 7	Flattened Ball	Gray
519	Double Base	Class 1	Scot	Royal Scot	Disk	Black
520	Single Base	Class 5	Scot	Solo 1000	Disk	Black
521	Double Base	Class 1	Dupont	Hi-Skor 800-X	Disk	Gray
522	Double Base	Class 1	IMR	Hi-Skor 800-X	Disk	Gray
523	Double Base	Class 1	Winchester	Magnum Rifle	Flattened Ball	Gray

SRN	Powder Type	AHC Designated	Distributor	Product Name	Shape	Color
524	Double Base	Class 1	Winchester	Superfield AA	Flattened Ball & Irregular Flattened Ball	Gray
525	Double Base	Class 1	Winchester	Super-Lite WSL1	Flattened Ball & Irregular Flattened Ball	Gray
526	Double Base	Class 1	Winchester	Action Pistol WAP1	Flattened Ball & Irregular Flattened Ball	Gray
527	Double Base	Class 1	Dupont	Hi-Skor 700-X	Disk	Gray
528	Double Base	Class 1	IMR	Hi-Skor 700-X	Disk	Gray
529	Single Base	Class 5	Dupont	PB	Disk	Gray
530	Single Base	Class 4	IMR	IMR-4227	Cylinder (Tubular)	Gray
531	Single Base	Class 4	IMR	IMR-4064	Cylinder (Tubular)	Gray
532	Single Base	Class 4	IMR	IMR-7828	Cylinder (Tubular)	Gray
533	Single Base	Class 4	IMR	IMR-4198	Cylinder (Tubular)	Gray
534	Single Base	Class 4	IMR	IMR-4831	Cylinder (Tubular)	Gray
535	Single Base	Class 4	IMR	IMR-4895	Cylinder (Tubular)	Gray
536	Single Base	Class 4	IMR	IMR-4350	Cylinder (Tubular)	Gray
537	Single Base	Class 4	IMR	IMR-4320	Cylinder (Tubular)	Gray
538	Single Base	Class 4	IMR	IMR-3031	Cylinder (Tubular)	Gray
539	Single Base	Class 4	Accurate	4350	Cylinder (Tubular)	Gray
540	Double Base	Class 2	Accurate	2700	Flattened Ball & Ball	Gray
541	Single Base	Class 5	Accurate	2495BR	Cylinder (Tubular)	Gray
542	Double Base	Class 2	Accurate	2230	Flattened Ball & Irregular Flattened Ball	Gray
543	Single Base	Class 2	Accurate	2015BR	Cylinder (Tubular)	Gray
544	Double Base	Class 2	Accurate	1680	Flattened Ball	Gray
545	Single Base	Class 4	Accurate	Magnum Rifle	Cylinder (Tubular)	Gray

SRN	Powder Type	AHC Designated	Distributor	Product Name	Shape	Color
546	Double Base	Class 1	Accurate	Nitro 100	Disk	Gray
547	Double Base	Class 1	Scot	Nitro 100	Disk	Gray
548	Double Base	Class 1	Hodgdon	Clays	Disk	Gray
549	Double Base	Class 1	Hodgdon	Universal Clays	Disk	Brown
550	Double Base	Class 1	Hodgdon	International Clays	Disk	Gray
551	Single Base	Class 5	IMR	PB	Disk	Black
552	Single Base	Class 6	Scot	Brigadier 4065	Cylinder (Tubular)	Gray
553	Double Base	Class 1	Hercules	Blue Dot	Disk	Gray
554	Double Base	Class 1	Hercules	Red Dot	Disk	Gray
555	Double Base	Class 1	Hercules	Green Dot	Disk	Gray
556	Double Base	Class 1	Winchester	Superfield AA (dup)	Flattened Ball & Irregular	Gray
557	Double Base	Class 2	Norma	202	Cylinder (Tubular)	Gray
558	Double Base	Class 1	Winchester	Supertarget AA	Flattened Ball & Irregular	Gray
559	Single Base	Class 4	Hodgdon	H-4831 SC	Cylinder (Tubular)	Gray
560	Single Base	Class 6	Hodgdon	H-1000	Cylinder (Tubular)	Gray
561	Single Base	Class 5	Scot	Royal Scot D	Disk	Gray
562	Double Base	Class 1	Scot	Scot 453	Flattened Ball	Gray
563	Single Base	Class 6	Scot	Brigadier 4351	Cylinder (Tubular)	Gray
564	Single Base	Class 6	Scot	Brigadier 3032	Cylinder (Tubular)	Gray
565	Single Base	Class 6	Scot	Brigadier 4065	Cylinder (Tubular)	Gray
566	Single Base	Class 6	Scot	Brigadier 4197	Cylinder (Tubular)	Gray
567	Double Base	Class 1	Scot	Pearl Scot	Disk	Black

SRN	Powder Type	AHC Designated	Distributor	Product Name	Shape	Color
568	Single Base	Class 5	Scot	Solo 1500	Disk	Black
569	Double Base	Class 2	Hercules	RL-22	Cylinder (Tubular)	Gray
570	Single Base	Class 4	Accurate	5010	Cylinder (Tubular)	Gray
571	Double Base	Class 1	Accurate	No. 2	Flattened Ball	Gray
572	Double Base	Class 2	Accurate	MR 2520	Ball	Black
573	Single Base	Class 3	VihtaVuori	Oy V-N110	Cylinder (Tubular)	Gray
574	Single Base	Class 3	VihtaVuori	Oy V-N120	Cylinder (Tubular)	Gray
575	Single Base	Class 3	VihtaVuori	Oy V-N135	Cylinder (Tubular)	Gray
576	Single Base	Class 3	VihtaVuori	Oy V-N140	Cylinder (Tubular)	Gray
577	Single Base	Class 5	VihtaVuori	Oy V-N310	Cylinder (Tubular)	Gray
578	Single Base	Class 5	VihtaVuori	Oy V-N330	Cylinder (Tubular)	Gray
579	Single Base	Class 5	VihtaVuori	Oy V-N340	Cylinder (Tubular)	Gray
580	Single Base	Class 5	VihtaVuori	Oy V-N350	Cylinder (Tubular)	Gray
581	Single Base	Class 3	VihtaVuori	Oy N318-N3SL	Lamel	Gray
582	Single Base	Class 3	VihtaVuori	Oy N130	Cylinder (Tubular)	Gray
583	Single Base	Class 3	VihtaVuori	Oy N165	Cylinder (Tubular)	Gray
584	Single Base	Class 3	VihtaVuori	Oy N133	Cylinder (Tubular)	Gray
585	Single Base	Class 3	VihtaVuori	Oy N160	Cylinder (Tubular)	Gray
586	Single Base	Class 5	VihtaVuori	Oy 3N37	Cylinder (Tubular)	Gray
587	Single Base	Class 3	VihtaVuori	Oy 24N64	Cylinder (Tubular)	Gray
588	Single Base	Class 3	VihtaVuori	Oy 20N29	Cylinder (Tubular)	Gray
589	Single Base	Class 3	VihtaVuori	Oy N150	Cylinder (Tubular)	Gray

SRN	Powder Type	AHC Designated	Distributor	Product Name	Shape	Color
590	Single Base	Class 5	VihtaVuori	Oy N320	Cylinder (Tubular)	Gray
591	Single Base	Class 3	VihtaVuori	Oy N170	Cylinder (Tubular)	Gray
592	Single Base	Class 3	VihtaVuori	Oy N35-N3SM	Lamel	Gray
593	Double Base	Class 1	VihtaVuori	Oy High Energy NC-Powder N560	Cylinder (Tubular)	Gray
594	Double Base	Class 1	VihtaVuori	Oy High Energy NC-Powder N550	Cylinder (Tubular)	Gray
595	Double Base	Class 1	VihtaVuori	Oy High Energy NC-Powder N540	Cylinder (Tubular)	Gray
596	Double Base	Class 1	VihtaVuori	Oy High Energy NC-Powder N530	Cylinder (Tubular)	Gray
597	Double Base	Class 1	Hercules	Red Dot	Disk	Gray
598	Double Base	Class 2	Accurate	No. 9	Flattened Ball & Irregular	Black
599	Double Base	Class 1	Accurate	No. 2 Improved	Flattened Ball	Gray
600	Double Base	Class 2	Accurate	1680	Flattened Ball	Gray
601	Double Base	Class 1	Accurate	2460	Ball	Gray
602	Double Base	Class 1	Accurate	2520	Flattened Ball	Gray
603	Double Base	Class 1	Accurate	2230	Flattened Ball	Gray
604	Double Base	Class 1	Accurate	No. 7	Flattened Ball	Gray
604	Single Base	Class 4	Accurate	4350	Flattened Ball	Gray
605	Single Base	Class 2	Accurate	2015BR	Cylinder (Tubular)	Gray
606	Single Base	Class 5	Accurate	2495BR	Cylinder (Tubular)	Black
607	Double Base	Class 2	Accurate	2700	Ball	Black
608	Double Base	Class 2	Accurate	8700	Flattened Ball	Black
609	Single Base	Class 4	Accurate	3100	Cylinder (Tubular)	Gray
610	Single Base	Class 4	Accurate	Magnum Rifle	Cylinder (Tubular)	Gray

SRN	Powder Type	AHC Designated	Distributor	Product Name	Shape	Color
611	Double Base	Class 1	Accurate	Nitro 100	Disk	Gray
612	Double Base	Class 1	Accurate	No. 5	Flattened Ball	Gray
613	Single Base	Class 4	Hodgdon	H-1000	Cylinder (Tubular)	Gray
614	Double Base	Class 1	Hodgdon	HP-38	Irregular Flattened Ball	Gray
615	Double Base	Class 1	Hodgdon	HP-38	Flattened Ball	Gray
616	Double Base	Class 1	Winchester	231	Flattened Ball & Irregular	Gray
617	Double Base	Class 1	Hodgdon	HS-7	Flattened Ball	Black
618	Double Base	Class 1	Hodgdon	HS-6	Flattened Ball	Black
619	Single Base	Class 4	Hodgdon	H-4831 SC	Cylinder (Tubular)	Gray
620	Double Base	Class 3	Alliant	Reloder 7	Disk	Gray
621	Double Base	Class 2	Alliant	Reloder 15	Cylinder (Tubular)	Gray
622	Double Base	Class 2	Alliant	Reloder 19	Cylinder (Tubular)	Gray
623	Double Base	Class 2	Alliant	Reloder 22	Cylinder (Tubular)	Gray
624	Double Base	Class 1	Alliant	Red Dot	Disk	Gray
625	Double Base	Class 2	Accurate	No. 9	Ball & Flattened Ball	Black
626	Double Base	Class 2	Accurate	No. 9	Ball & Flattened Ball	Black
627	Double Base	Class 2	Accurate	2230	Flattened Ball	Gray
628	Double Base	Class 1	Alliant	Bullseye	Disk	Gray
629	Double Base	Class 1	Alliant	Blue Dot	Disk	Gray
630	Double Base	Class 1	Alliant	Unique	Disk	Gray
631	Double Base	Class 1	Alliant	2400	Disk	Gray
632	Double Base	Class 1	Alliant	Herco	Disk	Gray

SRN	Powder Type	AHC Designated	Distributor	Product Name	Shape	Color
633	Double Base	Class 1	Alliant	Green Dot	Disk	Gray
634	Double Base	Class 2	Hodgdon	H-380	Ball	Gray
635	Double Base	Class 2	Hodgdon	H-450	Ball	Black
636	Double Base	Class 2	Winchester	748	Flattened Ball	Gray
637	Double Base	Class 2	Accurate	2230	Flattened Ball	Gray
638	Double Base	Class 2	Accurate	8700	Ball	Black
639	Double Base	Class 2	Accurate	8700	Flattened Ball	Black
640	Double Base	Class 2	Accurate	2700	Ball	Black
641	Double Base	Class 2	Accurate	2700	Ball	Black
642	Double Base	Class 2	Accurate	2700	Ball	Black
643	Double Base	Class 1	Remington	Peters 16 ga.	Disk	Gray
644	Double Base	Class 1	Alliant	Power Pistol	Disk	Gray
645	Double Base	Class 2	Accurate	2520	Flattened Ball	Gray
646	Double Base	Class 1	Accurate	2460	Flattened Ball	Gray
647	Double Base	Class 2	Accurate	1680	Flattened Ball	Gray
648	Single Base	Class 4	IMR	IMR-4198	Cylinder (Tubular)	Gray
649	Single Base	Class 5	Dupont	SR-4759	Cylinder (Tubular)	Gray
650	Single Base	Class 4	IMR	IMR-4831	Cylinder (Tubular)	Gray
651	Double Base	Class 1	Alliant	American Select	Disk	Gray
652	Double Base	Class 1	Hodgdon	Lil'Gun	Flattened Ball	Gray
653	Single Base	Class 4	IMR	SR-4759	Cylinder (Tubular)	Gray
654	Single Base	Class 4	IMR	IMR-3031	Cylinder (Tubular)	Gray

SRN	Powder Type	AHC Designated	Distributor	Product Name	Shape	Color
655	Single Base	Class 4	Hodgdon	Benchmark	Cylinder (Tubular)	Gold
656	Single Base	Class 4	Dupont	4320 Rifle Powder	Cylinder (Tubular)	Gray
657	Double Base	Class 1	Accurate	MP-5744	Cylinder (Tubular)	Gray
658	Double Base	Class 1	Winchester	Magnum Rifle	Flattened Ball	Black
659	Double Base	Class 1	Winchester	Superlite WSL1	Flattened Ball & Irregular Flattened Ball	Gray
660	Double Base	Class 1	Winchester	WST Super-Target	Irregular Flattened Ball	Gray
661	Double Base	Class 1	IMR	Hi-Skor 800-X	Disk	Gray
662	Double Base	Class 2	Winchester	WXR	Cylinder (Tubular)	Gray
663	Single Base	Class 4	IMR	IMR-4064	Cylinder (Tubular)	Gray
664	Single Base	Class 4	IMR	IMR-4227	Cylinder (Tubular)	Gray
665	Single Base	Class 5	IMR	SR-4756	Disk	Gray
666	Double Base	Class 1	Winchester	540	Flattened Ball & Irregular Flattened Ball	Gray
667	Single Base	Class 5	Dupont	SR-4759	Cylinder (Tubular)	Gray
668	Double Base	Class 2	Accurate	MR-8700	Ball	Black
669	Double Base	Class 1	Hercules	Herco	Disk	Gray
670	Double Base	Class 1	Hodgdon	Trap 100	Flattened Ball & Irregular Flattened Ball	Gray
671	Single Base	Class 4	Hodgdon	H-4350	Cylinder (Tubular)	Gray
672	Single Base	Class 4	Hodgdon	H-5010	Cylinder (Tubular)	Gray
673	Single Base	Class 4	Hodgdon	Varget	Cylinder (Tubular)	Gray
674	Double Base	Class 2	Hodgdon	BLC-2	Flattened Ball	Gray
675	Single Base	Class 4	Hodgdon	H-1000	Cylinder (Tubular)	Gray
676	Double Base	Class 3	Hercules	RL-12	Cylinder (Tubular)	Gray

SRN	Powder Type	AHC Designated	Distributor	Product Name	Shape	Color
677	Double Base	Class 1	Hercules	2400	Disk	Gray
678	Double Base	Class 1	Winchester	WSF Super-Field	Irregular Flattened Ball	Gray
679	Double Base	Class 2	Hercules	RL-19	Cylinder (Tubular)	Gray
680	Double Base	Class 1	Hercules	2400	Disk	Gray
681	Double Base	Class 2	Accurate	No. 7	Ball & Flattened Ball	Gray
682	Double Base	Class 1	Accurate	No. 5	Flattened Ball	Gray
683	Double Base	Class 2	Alliant	Reloder 25	Cylinder (Tubular)	Gray
684	Double Base	Class 2	Norma	Magnum Rifle	Cylinder (Tubular)	Gray
684	Single Base	Class 4	Dupont	SR-4759	Cylinder (Tubular)	Gray
685	Double Base	Class 1	Hercules	Red Dot	Disk	Black
686	Double Base	Class 1	Hercules	Red Dot	Disk	Gray
687	Double Base	Class 1	Hercules	RL-15	Cylinder (Tubular)	Gray
688	Double Base	Class 1	Hercules	Green Dot	Disk	Gray
689	Double Base	Class 1	Hercules	Blue Dot	Disk	Gray
690	Double Base	Class 2	Scot	4100	Ball	Black
691	Single Base	Class 4	Accurate	3100	Cylinder (Tubular)	Gray
692	Double Base	Class 2	Accurate	2460	Ball & Flattened Ball	Gray
693	Double Base	Class 2	Accurate	MR-223	Ball & Flattened Ball	Gray
694	Double Base	Class 3	Hercules	RL-7	Disk	Gray
695	Double Base	Class 2	Hercules	RL-19	Cylinder (Tubular)	Gray
696	Double Base	Class 2	Hercules	RL-15	Cylinder (Tubular)	Gray
697	Double Base	Class 1	Alliant	Bullseye	Disk	Gray

SRN	Powder Type	AHC Designated	Distributor	Product Name	Shape	Color
698	Double Base	Class 1	Hercules	Red Dot	Disk	Gray
699	Double Base	Class 1	Hercules	Bullseye	Disk	Gray
700	Double Base	Class 2	Hodgdon	H-414	Flattened Ball	Gray
701	Single Base	Class 3	Scot	Solo 1250	Disk	Gray
702	Double Base	Class 1	X-truded	XMP 5744	Cylinder (Tubular)	Gray
703	Single Base	Class 6	X-truded	XMR 2495	Cylinder (Tubular)	Gray
704	Double Base	Class 2	Norma	204	Cylinder (Tubular)	Gray
705	Double Base	Class 2	Accurate	8700	Flattened Ball	Gray
706	Single Base	Class 3	X-truded	XMR 2015	Cylinder (Tubular)	Gray
707	Single Base	Class 4	IMR	IMR-4064	Cylinder (Tubular)	Gray
708	Single Base	Class 3	X-truded	XMR 4064	Cylinder (Tubular)	Gray
709	Single Base	Class 4	X-truded	XMR 3100	Cylinder (Tubular)	Gray
710	Double Base	Class 1	IMR	Hi-Skor 700-X	Disk	Black
711	Single Base	Class 4	X-truded	XMR 4350	Cylinder (Tubular)	Gray
712	Double Base	Class 2	Accurate	2700	Flattened Ball	Gray
713	Single Base	Class 4	IMR	IMR-7828	Cylinder (Tubular)	Unknown
714	Single Base	Class 4	IMR	IMR-4895	Cylinder (Tubular)	Gray
715	Single Base	Class 5	Scot	Solo 1500	Disk	Gray
716	Double Base	Class 2	Norma	Magnum Rifle	Cylinder (Tubular)	Gray
717	Double Base	Class 2	Hodgdon	BLC-2	Flattened Ball	Gray
718	Single Base	Class 5	IMR	SR-7625	Disk	Gray
719	Double Base	Class 1	Hodgdon	H-322	Flattened Ball & Irregular Flattened Ball	Black

SRN	Powder Type	AHC Designated	Distributor	Product Name	Shape	Color
720	Double Base	Class 2	Accurate	8700	Ball	Gray
721	Single Base	Class 4	Accurate	3100	Cylinder (Tubular)	Gray
722	Double Base	Class 2	Hodgdon	BLC-2	Ball & Flattened Ball	Gray
723	Single Base	Class 4	Accurate	3100	Cylinder (Tubular)	Gray
724	Double Base	Class 2	Accurate	8700	Ball & Flattened Ball	Gray
725	Single Base	Class 4	Accurate	4350	Cylinder (Tubular)	Gray
726	Double Base	Class 2	Accurate	2460	Ball & Flattened Ball	Gray
727	Double Base	Class 2	Accurate	2460	Ball & Flattened Ball	Gray
728	Double Base	Class 2	Norma	Magnum Rifle	Cylinder (Tubular)	Gray
729	Single Base	Class 2	Norma	R-123	Cylinder (Tubular)	Gray
730	Double Base	Class 1	Accurate	No. 5	Ball & Irregular Flattened Ball	Gray
731	Double Base	Class 1	Accurate	No. 2	Ball & Irregular Flattened Ball	Gray
732	Double Base	Class 1	Accurate	No. 2	Ball & Irregular Flattened Ball	Gray
733	Double Base	Class 1	Accurate	No. 5	Ball & Irregular Flattened Ball	Gray
734	Double Base	Class 2	Accurate	1680	Flattened Ball	Black
735	Double Base	Class 2	Accurate	2520	Ball	Gray
736	Double Base	Class 2	Accurate	MR-2520	Ball	Gray
737	Double Base	Class 2	Accurate	MR-223	Flattened Ball	Gray
738	Single Base	Class 3	Accurate	2015BR	Cylinder (Tubular)	Gray
739	Single Base	Class 2	Accurate	2015BR	Cylinder (Tubular)	Gray
740	Single Base	Class 5	Accurate	2495BR	Cylinder (Tubular)	Gray
741	Single Base	Class 5	Accurate	2495BR	Cylinder (Tubular)	Gray

SRN	Powder Type	AHC Designated	Distributor	Product Name	Shape	Color
742	Single Base	Class 5	Accurate	2495BR	Cylinder (Tubular)	Gray
743	Single Base	Class 4	Accurate	3100	Cylinder (Tubular)	Gray
744	Single Base	Class 4	Accurate	3100	Cylinder (Tubular)	Gray
745	Single Base	Class 4	Accurate	4350	Cylinder (Tubular)	Gray
746	Single Base	Class 4	Accurate	4350	Cylinder (Tubular)	Gray
747	Single Base	Class 4	Accurate	4350	Cylinder (Tubular)	Gray
748	Double Base	Class 1	Accurate	XMP-5744	Cylinder (Tubular)	Gray
749	Double Base	Class 1	Accurate	5744	Cylinder (Tubular)	Gray
750	Double Base	Class 1	Accurate	Nitro 100	Disk	Gray
751	Double Base	Class 1	Accurate	Nitro 100	Disk	Gray
752	Single Base	Class 5	Accurate/Scot	Solo 1000	Disk	Gray
753	Double Base	Class 1	Accurate/Scot	Nitro 100	Disk	Black
754	Double Base	Class 1	Accurate	No. 2 Improved	Flattened Ball	Gray
755	Double Base	Class 1	Alliant	Power Pistol	Disk	Gray
756	Single Base	Class 4	Accurate	5010	Cylinder (Tubular)	Gray
757	Single Base	Class 2	Accurate	2015BR	Cylinder (Tubular)	Gold
758	Double Base	Class 1	Alliant	Red Dot	Disk	Gray
759	Double Base	Class 1	Alliant	Blue Dot	Disk	Black
760	Double Base	Class 1	Alliant	Unique	Disk	Gray
761	Double Base	Class 1	Winchester	571	Flattened Ball & Irregular Flattened Ball	Gray
762	Double Base	Class 1	Winchester	296	Flattened Ball	Gray
763	Double Base	Class 1	Winchester	231	Flattened Ball & Irregular	Gray

SRN	Powder Type	AHC Designated	Distributor	Product Name	Shape	Color
764	Double Base	Class 2	Winchester	760	Flattened Ball	Gray
765	Double Base	Class 2	Winchester	748	Flattened Ball	Black
766	Double Base	Class 1	Hodgdon	Tite Wad	Irregular Flattened Ball	Gray
767	Double Base	Class 1	Alliant	Green Dot	Disk	Gray
768	Double Base	Class 1	Ramshot	Silhouette	Flattened Ball & Irregular Flattened Ball	Gray
769	Double Base	Class 1	Ramshot	Silhouette	Flattened Ball & Irregular Flattened Ball	Gray
770	Double Base	Class 1	Ramshot	Competition	Irregular Flattened Ball	Gray
771	Double Base	Class 1	Ramshot	Zip Pistol	Irregular Flattened Ball	Gray
772	Double Base	Class 2	Ramshot	Big Boy Rifle Powder	Flattened Ball	Black
773	Double Base	Class 2	Ramshot	Big Game Rifle Powder	Ball	Black
774	Double Base	Class 1	Ramshot	TAC Rifle Powder	Flattened Ball	Black
775	Double Base	Class 2	Ramshot	X-Terminator	Ball	Black
776	Double Base	Class 2	Ramshot	Enforcer Pistol Powder	Ball	Black
777	Double Base	Class 1	Ramshot	True Blue Pistol Powder	Ball	Black
778	Double Base	Class 1	VihtaVuori	High Energy NC Powder N550	Cylinder (Tubular)	Gray
779	Double Base	Class 1	VihtaVuori	High Energy NC Powder N540	Cylinder (Tubular)	Gray
780	Single Base	Class 3	VihtaVuori	Oy N135	Cylinder (Tubular)	Gray
781	Double Base	Class 1	Unknown	Unknown Chinese Powder	Disk	Gray
782	Double Base	Class 1	Hodgdon	International Clays	Disk	Gray
783	Double Base	Class 1	IMR	Hi-Skor 700-X	Disk	Gray
784	Double Base	Class 1	IMR	Hi-Skor 800-X	Disk	Black
785	Single Base	Class 2	IMR	PB	Disk	Gray

SRN	Powder Type	AHC Designated	Distributor	Product Name	Shape	Color
787	Single Base	Class 5	IMR	SR-4759	Cylinder (Tubular)	Gray
788	Single Base	Class 2	IMR	SR-7625	Disk	Gray
789	Single Base	Class 4	IMR	IMR 3031	Cylinder (Tubular)	Gray
791	Single Base	Class 4	IMR	IMR 4198	Cylinder (Tubular)	Gray
792	Single Base	Class 4	IMR	IMR 4227	Cylinder (Tubular)	Gray
792	Single Base	Class 4	IMR	IMR 4320	Cylinder (Tubular)	Gray
793	Single Base	Class 4	IMR	IMR 4350	Cylinder (Tubular)	Gray
794	Single Base	Class 4	IMR	IMR 4831	Cylinder (Tubular)	Gray
795	Single Base	Class 4	IMR	IMR 4895	Cylinder (Tubular)	Gray
796	Single Base	Class 4	IMR	IMR 7828	Cylinder (Tubular)	Gray
797	Single Base	Class 4	IMR	IMR 7828 SSC	Cylinder (Tubular)	Gray
798	Double Base	Class 1	Alliant	Red Dot	Disk	Gray
799	Double Base	Class 1	Alliant	Green Dot	Disk	Gray
800	Double Base	Class 1	Alliant	Bullseye	Disk	Gray
801	Double Base	Class 1	Alliant	Herco	Disk	Gray
802	Double Base	Class 1	Alliant	Unique	Disk	Gray
821	Single Base	Class 2	IMR	Trail Boss	Disk	Gray
822	Double Base	Class 2	Accurate	No. 7	Ball & Irregular Flattened Ball	Black
823	Double Base	Class 2	Accurate	No. 7	Ball & Irregular Flattened Ball	Black
824	Double Base	Class 2	Accurate	No. 9	Ball & Flattened Ball	Black
825	Double Base	Class 2	Accurate	No. 9	Ball & Flattened Ball	Black
826	Double Base	Class 2	Accurate	2230	Ball & Flattened Ball	Black

SRN	Powder Type	AHC Designated	Distributor	Product Name	Shape	Color
827	Double Base	Class 2	Accurate	2460	Flattened Ball	Black
828	Double Base	Class 1	Hercules	Herco	Disk	Black
829	Double Base	Class 3	Hercules	RL-7	Cylinder (Tubular)	Black
830	Double Base	Class 2	Accurate	No. 9	Ball & Flattened Ball	Black
831	Double Base	Class 3	Hercules	RL-7	Cylinder (Tubular)	Black
832	Double Base	Class 1	Hercules	Red Dot	Disk	Black
833	Double Base	Class 1	Hercules	Green Dot	Disk	Black
834	Double Base	Class 1	Accurate	No. 7	Flattened Ball	Black
835	Double Base	Class 1	Accurate	No. 7	Ball & Irregular Flattened Ball	Gray
836	Double Base	Class 2	Accurate	No. 9	Ball & Flattened Ball	Black
837	Double Base	Class 1	Accurate	No. 5	Flattened Ball & Irregular Flattened Ball	Gray
838	Double Base	Class 1	Accurate	No. 5	Ball & Flattened Ball	Black
839	Double Base	Class 2	Accurate	2230	Flattened Ball	Gray
840	Double Base	Class 1	Accurate	2230	Flattened Ball	Unknown
841	Double Base	Class 2	Accurate	1680	Ball & Flattened Ball	Black
842	Double Base	Class 2	Accurate	1680	Flattened Ball	Black
843	Double Base	Class 1	Accurate	2460	Flattened Ball	Black
844	Double Base	Class 1	Accurate	No. 2 Improved	Ball & Flattened Ball	Gray
845	Double Base	Class 1	Accurate	2520	Ball & Flattened Ball	Black
846	Double Base	Class 2	Accurate	Scot 4100	Ball	Black
847	Double Base	Class 2	Accurate	MR-2520	Ball	Black
NA	Double Base	Class 1	Winchester	473AA	Flattened Ball & Irregular Flattened Ball	Gray
NA	Double Base	Class 2	Accurate	1680	Ball & Flattened Ball	Gray

## APPENDIX E: CLASS IDENTIFICATION OF SMOKELESS POWDERS DATABASE SAMPLES

Powder Type	Class	Shape	Color	Distributor	Product Name	SRN
			Gold	Accurate	2015BR	757
						605
		Calindary (Trabalar)		Accurate	2015BR	543
		Cylinder (Tubular)	Gray			739
	2			Norma	R-123	262
	2			TOTIK	K-125	729
					РВ	785
		Disk	Gray	IMR	SR-7625	788
		Disk	Giay	IIVIIX	Trail Boss	178
					Than Doss	821
			Black	VihtaVuori	N160	100
					2015	19
				Accurate	4064	26
					2015BR	738
Single Base					20N29	61
Single Dase					24N41	62
					3N38	49
					N105	47
					N110	51
	3	Cylinder (Tubular)			N120	41
	Ŭ	- ) ()	Gray		N130	42
				VihtaVuori	N133	43
					N135	44
					N165	45
					N170	46
					Oy 20N29	588
					Oy 24N64	587
					Oy N130	582
					Oy N133	584
					Oy N135	780

Powder Type	Class	Shape	Color	Distributor	Product Name	SRN
					Oy N150	589
					Oy N160	585
					Oy N165	583
				VihtaVuori	Oy N170	591
		Culindan (Turburbar)	Crew	vinta vuori	Oy V-N110	573
		Cylinder (Tubular)	Gray		Oy V-N120	574
					Oy V-N135	575
	3				Oy V-N140	576
				<b>V</b> ( 1 1	XMR 2015	706
				X-truded	XMR 4064	708
		Disk	Gray	Scot	Solo 1250	701
					N3SL	60
		Lamel	Crew	VihtaVuori	Oy N318-N3SL	581
		Lamer	Gray	vinta vuori	Oy N35-N3SM	592
Single Dece					Oy N3SH	59
Single Base				Dupont	4227	259
					3031	111
					5051	164
					4064	103
						165
			Black		4198	163
			Ыаск	IMR	4227	112
	4	Cylinder (Tubular)			4227	175
					4350	169
					4895	166
					7828	171
					7828 SSC	172
					Benchmark	157
			Brown	Hodgdon	H322	146
					H4198	145

Powder Type	Class	Shape	Color	Distributor	Product Name	SRN
					H4350	153
			Brown	Hodgdon	H4895	147
					Varget	150
				IMR	8208XBR	173
						655
					Benchmark	76
					H1000	63
					H322	65
					H4198	99
			<b>C</b> 11		H4227	69
			Gold	Hodgdon	H4350	70
					H4831	71
					H4831 SC	72
					H4895	73
Single Dege	4	Cylinder (Tubular)			Retumbo	77
Single Base	4				Varget	64
					3100	25
						691
						744
						723
						743
						609
			Gray	Accurate		721
			Ciay	Acculate		747
						539
					4350	746
						27
						745
						725
					5010	570

Powder Type	Class	Shape	Color	Distributor	Product Name	SRN
					5010	756
						545
				Accurate	Magnum Rifle	610
					MR-3100	434
					3031	276
					4064	279
				C Dupont	4198	275
					4350	277
					4831	235
					2021	514
					3031	408
					4064	409
		4 Cylinder (Tubular)	Gray		4198	410
						512
Charle Dave						470
Single Base	4				4227	411
					4320	412
						510
				Dunant		265
				Dupont		656
					4350	413
					4550	509
					4759	231
					4831	508
					1005	507
					4895	414
					7828	418
					CD 4750	415
					SR-4759	684
				Hodgdon	H1000	613

Powder Type	Class	Shape	Color	Distributor	Product Name	SRN
					111000	675
					H1000	156
					H322	281
					H4198	257
					H4227	256
					H4350	671
					114021	225
					H4831	154
				Hodgdon		619
					H4831 SC	559
						155
			Gray		H4895	271
					H5010	672
					H50BMG	74
Single Dece	4	Cylinder (Tubular)			HJUBINO	159
Single Base	4	Cymider (Tubular)			Retumbo	158
					Varget	673
					3031	108
						654
						538
						789
						707
					4064	531
				IMR		663
						533
				4198	648	
					791	
				4227	664	
					530	
						792

Powder Type	Class	Shape	Color	Distributor	Product Name	SRN
						109
						110
					4320	168
						537
						792
						115
						113
					4350	114
						536
						793
				IMR	4831	170
		Cylinder (Tubular)	Gray			650
		Cymider (Tubular)				534
	4					794
Single Dece	4					714
Single Base					4895	535
						795
					7828	532
					7828	796
					7828 SSC	797
					SR-4759	653
				X-truded	XMR 3100	709
				A-titudeu	XMR 4350	711
			Unknown	IMR	7828	713
					4227	511
		Disk	Gray	Dupont	SR-4756	213
					51-4/30	417
		Flattened Ball (FB)	Gray	Accurate	4350	604
	5	Cylinder (Tubular)	Black	Accurate	2495BR	606
	3		DIACK	IMR	SR-4759	176

Powder Type	Class	Shape	Color	Distributor	Product Name	SRN
					3N37	48
					N310	50
			Gold	VihtaVuori	N320	52
					N340	54
					N350	55
						541
					240500	740
				Accurate	2495BR	741
						742
					CD 4750	667
		Cylinder (Tubular)		Dupont	SR-4759	649
				IMR	SR-4759	787
			Gray	Norma	R-1	258
					Oy 3N37	586
Single Dece	5	5			Oy N320	590
Single Base	5				Oy N330	53
				VihtaVuori	Oy V-N310	577
					Oy V-N330	578
					Oy V-N340	579
					Oy V-N350	580
				Accurate	Solo 1000	31
			Gray	Accurate	Solo 1250	33
				Accurate/Scot	Solo 1000	752
		Disk		IMR	PB	551
			Dlaalr	IWIK	PD	104
			Black	Scot	Solo 1000	520
				Scot	Solo 1500	568
					AL-5	294
		Lamel	Black	Alcan	AL-J	501
					AL-7	299

Powder Type	Class	Shape	Color	Distributor	Product Name	SRN
					AL-7	500
		Lamel	Cross	Alcan		499
		Lamer	Gray	Alcali	AL-8	297
						105
					#5 Pistol	191
					Hi-Skor	190
						407
				Dunant	РВ	205
	5			Dupont	FD	502
	5					529
		Disk	Gray		SR-4756	506
				SR-7625	505	
				IMR	SR-4756	665
					SR-7625	718
Single Base					SIC-702.5	416
Single Dase				Scot	Royal Scot D	561
				Beet	Solo 1500	715
		Other	Orange	Dupont	Bulk	234
					2495	183
			Black	Accurate	4064	181
			DIACK		4350	182
				IMR	4007SSC	167
				Accurate	2495	22
	6	Cylinder (Tubular)		Dupont	4064	513
	U				101	278
			Gray	Herters	102	266
		Gray		103	268	
				Hodgdon	4895	118
				Scot	Brigadier 3032	564
				5001	Brigadier 4065	552

Powder Type	Class	Shape	Color	Distributor	Product Name	SRN
					H1000	560
					11222	476
					H322	267
					114100	471
				Hodgdon	H4198	261
					114021	287
		Cylinder (Tubular)	Gray		H4831	516
Single Base	6				114905	283
					H4895	498
					Brigadier 4065	565
				Scot	Brigadier 4197	566
					Brigadier 4351	563
				X-truded	XMR 2495	703
		Disk	Gray	Hodgdon	H4227	515
		Agglomerate	Gray	Winchester	AA20S	226
			Black	Accurate	#2	184
				Ramshot	True Blue	92
					The Due	777
		Ball		Winchester	669	446
				Accurate	2460	601
			Gray		#2	14
Deally Dear	1				#9	17
Double Base	1		Dlasta	A	2520	845
		Ball & Flattened Ball (FB)	Black	Accurate	No. 5	838
			Gray	Accurate	No. 2 Improved	844
						440
					No. 2	732
		Ball & Irregular FB	Gray	Accurate		731
						733
					No. 5	730

Powder Type	Class	Shape	Color	Distributor	Product Name	SRN
		Ball & Irregular FB	Gray	Accurate	No. 7	835
				Accurate	5744	435
					410	128
			Black		2400	127
			DIACK	Alliant	Reloder 10X	130
					Reloder 17	132
					Reloder 7	129
			Gold	Alliant	Reloder 7	7
					5744	749
				Accurate	5744	28
				Acculate	MP-5744	657
		Cylinder (Tubular)			XMP 5744	748
			Gray	Hercules	Hi-Vel-2	228
					RL-15	249 687
Double Base	1			VihtaVuori	High Energy NC Powder N540	779
					High Energy NC Powder N550	778
					N540	56
					N550	57
					N560	58
					Oy High Energy NC-Powder N530	596
					Oy High Energy NC-Powder N540	595
					Oy High Energy NC-Powder N550	594
					Oy High Energy NC-Powder N560	593
				X-truded	XMP 5744	702
				Accurate/Scot	Nitro 100	753
					American Select	125
		Disk	Black	A 11: 4		759
				Alliant	Blue Dot	6
						124

Powder Type	Class	Shape	Color	Distributor	Product Name	SRN
					Bullseye	123
					e3	13
				4.11	Herco	121
				Alliant	a 1	5
					Steel	126
					Unique	122
				D	700X	195
				Dupont	Hi-Skor 800X	212
					Green Dot	833
			DI I			478
			Black		Herco	828
				Hercules		685
				Red Dot	832	
					Unique	202
	1	Disk		Herters	164	196
Double Base	1	DISK		IMR	Hi-Skor 700X	710
					U: Ch., , 900V	784
					Hi-Skor 800X	102
				Scot	Pearl Scot	567
					Royal Scot	519
					International Clays	137
			Brown	Hodgdon	Universal Clays	549
					Universar Clays	138
			Gold	Hercules	Bullseye	116
						751
						750
			Grow	Accurate	Nitro 100	546
		Gray			611	
					32	
				Alliant	410	12

Powder Type	Class	Shape	Color	Distributor	Product Name	SRN	
					2400	631	
					2400	1	
					American Select	3	
					American Select	651	
					Blue Dot	629	
						800	
						628	
					Bullseye	697	
						106	
						107	
						799	
				Alliant	Green Dot	633	
						767	
						120	
Double Base	1	Disk	Gray		ay Herco	Herco	801
						632	
						755	
					Power Pistol	644	
						4	
					Promo	2	
						798	
					Red Dot	624	
						758	
						119	
					<b>T</b> T '	802	
				Unique	630		
			├		760		
				Dupont	Hi-Skor 700X	405	
				Dupont	HI-SKOT /UUX	406	
						504	

Powder Type	Class	Shape	Color	Distributor	Product Name	SRN
						527
				Dupont	Hi-Skor 800X	503
						521
						482
						677
					2400	680
						188
						219
						479
						193
					Blue Dot	689
				Bullseye Hercules		216
						553
						218
Double Base	1	Disk	Gray			484
Double Dase	-				Bullseye	192
						699
						117
					Green Dot	194
						483
						688
				_		555
						669
					Herco	215
					204	
					198	
					480	
				Red Dot	214	
						597
						554

Powder Type	Class	Shape	Color	Distributor	Product Name	SRN
					Red Dot	698
					Ked Dot	686
				Hercules	SS #1	203
					Unique	217
					Unique	481
				Herters	160	200
				nenters	162	197
					240	189
					Clays	548
				Hadadan		550
				Hodgdon	International Clays	85
		Diek	Gray			782
	Disk	Glay		Universal Clays	86	
						177
Double Base	1				Hi-Skor 700X	783
Double Dase	1			IMR		528
				IIVIK	Hi-Skor 800X	174
						661
						522
				Norma	1010	201
				Noma	2020	199
				Remington	Peters 16 ga.	643
				Scot	Nitro 100	547
				Unknown	Unknown Chinese Powder	781
			Black	WSX	170	450
			DIACK	Hodgdon	H322	719
		Flattened Ball & Irregular FB		Accurate	No. 5	837
		Fatteneu Dan & meguiai FD	Gray		HP-38	290
			Ulay	Hodgdon	Trap 100	400
					11ap 100	670

Powder Type	Class	Shape	Color	Distributor	Product Name	SRN
				Hodgdon	Trap 100	246
				Ramshot	Silhouette	769
				Kamsnot	Sinouette	768
					231	238
					251	496
					296	444
					540	666
					571	761
					452AA	239
					172 & A	NA
				Winchester	473AA	255
				winchester	AA20	451
	Flattened Ball & Irregular FB	Gray		AA60	463	
					AA80	432
Double Base	1				Action Pistol WAP1	526
Double Dase	1				Superfield AA	524
					Superlite WSL1	659
					Superine w SEI	525
					WST	36
				WMG	525	445
				W MO	555	458
				WPR	280	252
					110	464
				WSX	120	442
					130	461
		Flattened Ball (FB)		Accurate	2460	843
				Accurate	No. 7	834
			Black		H110	80
				Hodgdon		140
						223

Powder Type	Class	Shape	Color	Distributor	Product Name	SRN
						618
					HS-6	78
						139
				Hadadan	HS-7	617
				Hodgdon	Leverevolution	162
					LIL' GUN	143
			Black		Longshot	142
			ыаск		Superformance	161
				Ramshot	TAC	774
					540	422
				Winchester	571	423
				Winchester	295 S	455
				Magnum Rifle	658	
			WMG	585	465	
Double Base	1	Elattanad Dall (ED)			2230	603
Double Dase	1	1 Flattened Ball (FB)		2460	646	
					2520	602
					#5	15
					#7	185
				Accurate	No. 2	571
				Accurate	No. 2 Improved	754
			Gray		No. 2 improved	599
			Giay			441
					No. 5	682
						612
				No. 7	604	
				H110	289	
			Hodgdon		207	
			nougdon	HP-38	615	
						81

Powder Type	Class	Shape	Color	Distributor	Product Name	SRN
					HP-38	141
						291
					HS-6	247
				II-d-d-n	110 7	79
				Hodgdon	HS-7	292
					LilCur	652
					Lil'Gun	88
					Titegroup	144
				Ramshot	Silhouette	91
				Kamsnot	Zip	90
				Scot	Scot 453	562
					231	443
					235 296	459
						101
Double Base	1	1 Flattened Ball (FB)	Gray			762
Double Dase	1	Flattened Dali (FD)	Glay			35
						242
					540	492
						466
				Winchester		490
				w inchester	571	236
						401
					615	452
					630	491
					814	403
					818	404
					452AA	494
					473AA	493
					Magnum Rifle	523
				WSX	150	428

Powder Type	Class	Shape	Color	Distributor	Product Name	SRN
		Flattened Ball (FB)	Unknown	Accurate	2230	840
						424
					231	763
				Winchester		616
		Flattened Ball (FB) & Irregular Gray	Graz	winchester	232	430
		Flattened Ball (FB) & megular	Glay		Superfield AA	556
					Supertarget AA	558
				WMG	535	402
				W MG	575	429
		Irregular	Black	Duncat	#6 Pistol	296
		Inegular	DIACK	Dupont	МХ	295
					HP-38	614
					Longshot	87
				Hodgdon	Titegroup	82
	1				TiteWad	766
Double Base					The w ad	83
					Competition	770
				Ramshot		89
					Zip Pistol	771
		Irregular Flattened Ball (FB)	Gray		230	420
					231	34
					237	457
				Winchester	230 P	497
				winchester	452AA	419
					WSF	37
					WSF Super-Field	678
					WST Super-Target	660
				WSX	140	468
		Lamel	Red	Nike	Unknown	298
	2	Ball	Black	Accurate	2230	180

Powder Type	Class	Shape	Color	Distributor	Product Name	SRN
					2460	186
					2520	187
					2520	439
						607
					2700	641
				Accurate	2700	642
				Acculate		640
					8700	638
					MD 2520	572
					MR-2520	847
					MR-8700	668
					Scot 4100	846
				Dupont		222
						151
Double Base	2	2 Ball	Black		11290	285
Double Dase	2				П380	474
						230
				Hadadan	H450	635
				Hodgdon	H450	286
					H760	248
						472
					H870	288
						233
					Big Game	96
					Big Game	773
					Enforcer	93
				Ramshot	Enforcer	776
					Hunter	97
					X-Terminator	94
						775

Powder Type	Class	Shape	Color	Distributor	Product Name	SRN
				Scot	4100	690
			Black	Winchester	852H	467
					2520	735
		Ball		Accurate	2520	23
		Ball	Gray	Accurate	8700	720
			Giay		MR-2520	736
				Hodgdon	H380	67
				Houguon	H380	634
					1680	841
					2230	826
					No. 9	836
			Black	Accurate		625
						825
						830
Double Base	2					626
Double Dase	2	Ball & Flattened Ball (FB)				824
		Dali & Flattened Dali (FD)	Gray		1680	NA
					2460	727
						726
				Accurate		692
			Giay		8700	724
					MR-223	693
					No. 7	681
				Hodgdon	BLC-2	722
		Ball & Irregular FB	Black	Accurate	No. 7	823
		Dan & megular i D	DIACK	neculate	110. /	822
					Reloder 15	131
		Cylinder (Tubular)	Black	Alliant	Reloder 19	133
		Cymider (Tubulai)			Reloder 22	134
			Black	Alliant	Reloder 25	135

Powder Type	Class	Shape	Color	Distributor	Product Name	SRN
			Dlash	Hodgdon	Hybrid 100V	160
			Black	Winchester	WXR	40
					Reloder 10X	8
					Reloder 15	621
					Reloder 15	9
				Alliant	Reloder 19	622
				Amant	Reloder 22	623
					Reloael 22	10
					Reloder 25	683
					Reloael 25	11
					RL-15	696
						679
				Hercules	RL-19	250
		Cylinder (Tubular)		Thereares		695
Double Base	2		Gray		RL-22	251
Double Dase	2		Glay		NL-22	569
					202	557
					204	704
					204	274
					205	273
					Magnum Rifle	272
				Norma		716
						684
						728
					N-200	270
					N-201	269
					N-203	264
				Winchester	WXR	662
		Disk	Gray	Hodgdon	Clays	136
		2101	uy	nouguon	<i>Cia j</i> 0	84

Powder Type	Class	Shape	Color	Distributor	Product Name	SRN
				Accurate	2230	542
		Flattened Ball & Irregular FB	Gray	Winchester	680	489
				Winchester	749	253
						842
					1680	734
						18
					2460	827
				Accurate		608
				Accurate	8700	639
				436		
				MR-223	437	
					MR-2460	438
					No. 9	517
						149
Double Base	2			Hodgdon	MR-2460	224
Double Dase	2		Black	Hougdon		280
		Flattened Ball (FB)			H414	152
				Ramshot	Big Boy	772
				Kalibilot	Magnum	98
					296	241
					662	433
					680	240
					732	453
				Winchester	748	765
					755	431
					759	462
					844	449
					860	456
			Gray	Accurate	1680	179
			Ciay	Accurate	1000	600

Powder Type	Class	Shape	Color	Distributor	Product Name	SRN
					1/200	647
					1080	544
						637
					2230	839
					2230	627
						20
					2460	21
				Accurate	2520	645
				Accurate	1680       2230       2460       2520       2700       8700       #7       MagPro       MR-223       No. 7       BLC-2       H335	24
					2700	712
					8700	705
					8700	29
		Flattened Ball (FB)	Gray		#7	16
					MagPro	30
Double Base	2				MR-223	737
Double Dase	2	Thattened Dan (TD)	Giuy		No. 7	518
						75
					BLC-2	477
						674
						717
						66
						148
				Hodgdon	H335	475
				nouguon		245
						282
					H375	229
						68
					H414	473
						232
					H414	700

Powder Type	Class	Shape	Color	Distributor	Product Name	SRN		
				Hodgdon	H414	284		
				Ramshot	TAC	95		
					296	495		
					680	425		
					080	448		
					728	447		
					730	469		
						243		
						426		
					748	38		
					/48	636		
		Flattened Ball (FB)	Gray	Winchester		488		
	2					421		
						487		
Double Base						244		
Double Dase					760	254		
					700	39		
						427		
						284 95 495 425 448 447 469 243 426 38 636 488 421 487 244 254 39		
						486		
					785	454		
						237		
					846	460		
		Flattened Ball (FB) & Ball	Gray	Accurate	2700	540		
		Flattened Ball (FB) & Irregular	Black	Accurate	No. 9	598		
					RL-12	221		
			Black	Hercules		831		
	3	Cylinder (Tubular)			RL-7	829		
			Grou	Hercules	RL-12	676		
			Gray	nercules	RL-21	227		

Powder Type	Class	Shape	Color	Distributor	Product Name	SRN
		Cylinder (Tubular)	Gray	Hercules	RL-7	263
Double Base				Alliant	Reloder 7	620
	3	D' 1	G			485
		Disk	Gray	Hercules	RL-7	220
						694
	5	Disk	Black	Dupont	SR-7625	206

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