

Supplementary data for article:

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Indirect *N*-vinylation of indoles via isomerisation of *N*-allyl derivatives. Synthesis of (±)-debromoarborescidine B

Gordana Tasic^a, Milena Simic^a, Stanimir Popovic^a, Suren Husinec^b, Veselin Maslak^c, Vladimir Savic^a

^a University of Belgrade, Faculty of Pharmacy, Vojvode Stepe 450, 11221 Belgrade, Serbia

^b Institute for Chemistry, Technology and Metallurgy, Centre for Chemistry, PO Box 815, Njegoseva 12, 11000 Belgrade, Serbia

^c University of Belgrade, Faculty of Chemistry, Studentski Trg 12-16, 11000 Belgrade, Serbia

SUPPLEMENTARY INFORMATION

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1. General

The NMR spectra were recorded on a Bruker Avance III (500 MHz) spectrometer. Chemical shifts are given in parts per million (δ) downfield from tetramethylsilane as the internal standard. Deuteriochloroform was used as a solvent, unless otherwise stated. Mass spectral data were recorded using Agilent MSD TOF spectrometer coupled with Agilent 1200 HPLC or Agilent Technologies 5975C MS coupled with Agilent Technologies 6890N GC. IR spectra were recorded on a IR Termo Scientific NICOLET iS10 (4950) spectrometer. Flash chromatography employed silica gel 60 (230-400 mesh) while thin layer chromatography was carried out using alumina plates with 0.25 mm silica layer (Kieselgel 60 F₂₅₄, Merck). Compounds were visualized by staining with potassium permanganate solution. The solvents were purified by distillation before use. Melting points were not corrected.

2. Synthetic procedures

2.1. General procedure for the *t*-BuOK promoted *N*-allyl to *N*-vinyl double bond migration

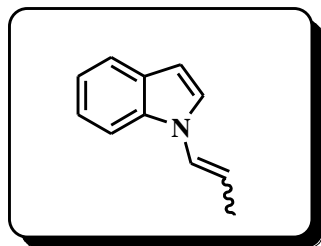
A mixture of allyl indoles (0.1 mmol), and *t*-BuOK (0.45 mmol, 4.5 eq) in DMSO (3.0 mL) was stirred at r.t. The reaction was monitored by t.l.c. and when completed (1-3 h) Et₂O (30 mL) was added and the mixture washed with H₂O (3 x 5 mL). The combined ethereal layers were then dried (Na₂SO₄) and the solid separated by filtration. The filtrate was evaporated under reduced pressure and the oily residue was purified by column chromatography (SiO₂, petroleum ether/ether) to afford the product.

2.2. General procedure for the NaH promoted *N*-allyl to *N*-vinyl double bond migration

A mixture of allyl indoles (0.38 mmol), and NaH (1.72 mmol, 4.5 eq) in DMSO (11.5 mL) was stirred at r.t. The reaction was monitored by t.l.c. and when completed (3-24 h) Et₂O (50 mL) was added and the mixture washed with H₂O (3 x 10 mL). The combined ethereal layers were then dried (Na₂SO₄) and the solid separated by filtration. The filtrate was evaporated under reduced pressure and the oily residue was purified by column chromatography (SiO₂, petroleum ether/ether) to afford the product.

2.3. Spectral data for synthesised compounds

1-(Prop-1-enyl)-1*H*-indole (6)



Isolated after column chromatography (SiO₂ petroleum ether) as colourless oil in 85 % yield as *E* isomer. The other isomer is present in trace amount.

IR ν_{max} : 1671, 1460, 1325, 1228, 737 cm⁻¹.

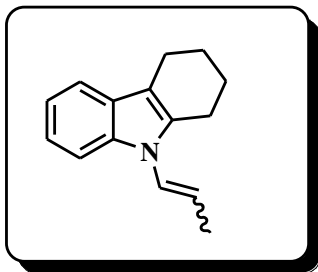
¹H NMR (500 MHz, CDCl₃) δ 1.88 (dd, 3H, CH₃, *J*=6.5 and 1.5 Hz), 5.71-5.79 (m, 1H, CH₃CHCHN), 6.56 (d, 1H, ArH, *J*=3.0 Hz), 6.97 (dd, 1H, CH₃CHCHN, *J*=14.0 and 1.5 Hz), 7.10-7.14 (m, 1H, ArH), 7.21-7.24 (m, 1H, ArH), 7.32 (d, 1H, ArH, *J*=3.0 Hz), 7.44 (dd, 1H, ArH, *J*=8.0 and 0.5 Hz), 7.60 (dt, 1H, ArH, *J*=8.0 and 1.0 Hz);

¹³C NMR (125 MHz, CDCl₃) δ 15.3, 103.7, 109.5, 110.8, 120.2, 121.0, 122.2, 124.3, 124.8, 128.7, 135.3;

m/z (EI): 157.1 (M⁺), 142, 130.1, 117, 102, 89.1.

HRMS (ESI): calculated for C₁₁H₁₁N (M+H)⁺ 158.09643, found 158.09503.

6,7,8,9-(Tetrahydro-9-prop-1-enyl)-5H-carbazole (8)



Isolated after column chromatography (SiO₂ 98:2 v/v petroleum ether-ether) as a colourless oil in 99 % yield as 1:5 mixture of *Z/E* isomers.

IR ν_{max} : 2923, 1668, 1460, 1373, 734 cm⁻¹

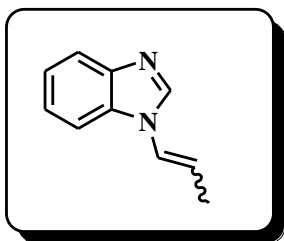
¹H NMR (500 MHz, CDCl₃) δ 1.59 (dd, 3H, CH₃, *Z* isomer, *J*=7.0 and 2.0 Hz), 1.84-1.91 (dd+m, 8H, CH₃, *E* isomer+5H *Z/E* CH₂ groups, *J*=7.0 and 2.0 Hz), 2.60-2.62 (m, 2H, *Z* isomer, CH₂ groups), 2.69-2.73 (m, 9H, *Z/E* CH₂ groups), 5.77-5.84 (m, 2H, CH₃CHCHN, *E* and *Z* isomers), 6.52 (dq, 1H, CH₃CHCHN *Z* isomer, *J*=8.0 and 2.0 Hz), 6.71 (dq, 1H, CH₃CHCHN, *E* isomer, *J*=14.3 and 2.0 Hz), 7.07-7.16 (m, 5H, ArH, *Z* and *E* isomers), 7.43-7.46 (m, 3H, ArH, *Z* and *E* isomers);

¹³C NMR (125 MHz, CDCl₃) δ 13.3, 15.8, 21.0, 22.6, 22.9, 23.2, 23.3, 23.4, 110.1, 110.2, 111.0, 116.3, 117.6, 117.7, 119.1, 119.6, 120.8, 121.2, 123.9, 124.3, 125.5, 127.9, 135.1, 135.7;

m/z (EI): 211.1 (M⁺), 196.1, 183.1, 168.1, 154.1, 143.0.

HRMS (ESI): calculated for C₁₅H₁₇N (M+H)⁺ 212.14338, found 212.14269.

1-(Prop-1-enyl)-1H-benzo[d]imidazole (10)



Isolated after column chromatography (SiO₂ ether) as colourless oil in 68 % yield as 5:1 mixture of *Z/E* isomers.

IR ν_{max} : 1489, 1458, 1229, 934, 739 cm⁻¹

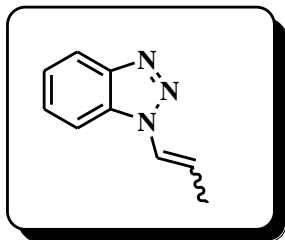
¹H NMR (500 MHz, CDCl₃) δ 1.80 (dd, 3H, CH₃, *Z* isomer, *J*=7.0 and 2.0 Hz), 1.93 (dd, 3H, CH₃, *E* isomer, *J*=7.0 and 1.5 Hz), 5.81-5.87 (m, 1H, CH₃CHCHN, *Z* isomer), 6.03-6.10 (m, 1H, CH₃CHCHN, *E* isomer), 6.75 (dq, 1H, CH₃CHCHN, *Z* isomer, *J*=8.3 and 2.0 Hz), 6.87 (dq, 1H, CH₃CHCHN, *E* isomer, *J*=14.0 and 1.5 Hz), 7.30-7.36 (m, 5H, ArH, *Z/E* isomer), 7.48-7.51 (m, 1H, ArH, *E* isomer), 7.82-7.84 (m, 2H, ArH, *Z/E* isomer), 7.99, (s, 1H, ArH, *Z* isomer), 8.06 (s, 1H, ArH, *E* isomer);

¹³C NMR (125 MHz, CDCl₃) δ 12.8, 15.3, 110.2, 117.8, 120.2, 120.4, 121.7, 122.6, 122.6, 123.4, 123.5, 123.6, 133.7, 140.9, 142.3, 142.9;

m/z (EI): 158.1 (M⁺), 141.9, 130.0, 118.1, 104.0, 91.0;

HRMS (ESI): calculated for C₁₀H₁₀N₂ (M+H)⁺ 159.09167 found 159.09170.

1-(Prop-1-enyl)-1H-benzo[*d*][1,2,3]triazole (12)



Isolated after column chromatography (SiO₂ 4:1 v/v petroleum ether-ethyl-acetate) as colourless oil in 51 % yield as 1:8 mixture of *Z/E* isomers.

IR ν_{max} : 1677, 1453, 1175, 1053, 934 cm⁻¹

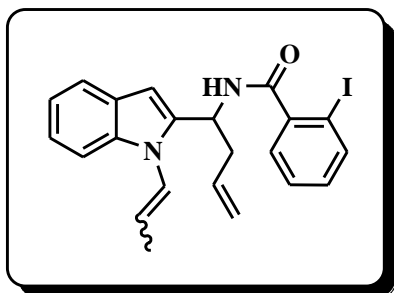
¹H NMR (500 MHz, CDCl₃) δ 1.98 (dd, 3H, CH₃, *Z* isomer, *J*=7.0 and 2.0 Hz), 2.01 (dd, 3H, CH₃, *E* isomer, *J*=7.0 and 1.5 Hz), 5.96-5.99 (m, 1H, CH₃CH₂CHN, *Z* isomer), 6.50-6.57 (m, 1H, CH₃CH₂CHN, *E* isomer), 7.06 (dd, 1H, CH₃CHCHN, *Z* isomer, *J*=9.0 and 2.0 Hz), 7.32 (dq, 1H, CH₃CHCHN, *E* isomer, *J*=14.3 and 1.5 Hz), 7.34-7.42 (m, 2H, ArH, *Z/E*), 7.47-7.64 (m, 3H, ArH, *Z/E*), 7.64-7.66 (m, 1H, ArH, *E* isomer), 8.06-8.09 (m, 2H, ArH, *Z/E*);

¹³C NMR (125 MHz, CDCl₃) δ 15.5, 110.0, 118.7, 120.2, 123.8, 124.3, 127.9, 146.1;

m/z (EI): 159.0 (M⁺), 130.0, 116.0, 103.0, 91.0, 77.1;

HRMS (ESI): calculated for C₉H₉N₃ (M+H)⁺ 160.08692 found 160.08708.

2-Iodo-N-(1-(1-(prop-1-enyl)-1H-indol-2-yl)but-3-enyl)benzamide (14)



Isolated after column chromatography (SiO₂ 3:2 v/v petroleum ether-ether) as colourless solid (mp 127-129 °C) in 95 % yield as 2:1 mixture of *Z/E* isomers.

IR ν_{max} : 3272, 1661, 1521, 1458, 739 cm⁻¹

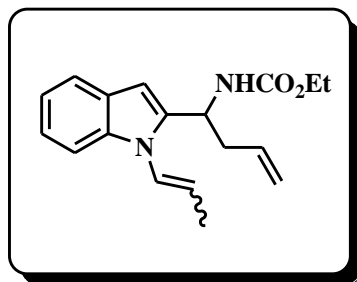
¹H NMR (500 MHz, CDCl₃) δ 1.57 (d, 3H, CH₃, *Z* isomer, *J*=5.0 Hz), 1.97 (d, 3H, CH₃, *E* isomer, *J*=6.5 Hz), 2.81-2.87 (m, 2H, =CHCH₂CH), 5.12-5.26 (m, 2H, CH₂=CHCH₂CH), 5.48 (q, 1H, CH₂CHNH, *Z* isomer, *J*=7.0 Hz), 5.60 (q, 1H, CH₂CHNH, *E* isomer, *J*=7.0 Hz), 5.89-5.96 (m, 2H, =CHCH₂CHNH), 6.03-6.06 (m, 1H, CH₃CH=CHN, *Z* and *E* isomers), 6.55 (d, 1H, ArH, *J*=15.0 Hz), 6.74 (d, 1H, CH₃CH=CHN, *Z* isomer, *J*=8.0 Hz), 6.86 (d, 1H, CH₃CH=CHN, *E* isomer, *J*=14.0 Hz), 7.08-7.21 (m, 4H, ArH), 7.33-7.34 (m, 2H, ArH), 7.50-7.59 (m, 1H, ArH), 7.85 (d, 1H, ArH, *J*=8.0 Hz);

¹³C NMR (125 MHz, CDCl₃) δ 13.1 (CH₃, *Z* isomer), 15.7 (CH₃, *E* isomer), 38.8 (=CHCH₂CH), 38.9 (=CHCH₂CH), 45.8, 46.2, 92.4, 100.5, 100.9, 110.9, 111.0, 118.7 (CH₂=CHCH₂CH), 120.1, 120.4, 120.5 (2C), 122.2, 122.4, 123.6 (CH₃CH=CHN *Z* isomer), 124.3 (CH₃CH=CHN *E* isomer), 127.4, 127.7, 128.1, 128.2, 129.0, 131.2, 133.6, 133.7, 136.7, 136.8, 138.8, 139.4, 140.1, 141.7, 167.9;

m/z (EI): 456.1 (M⁺), 415.1, 281.0, 253.1, 230.9, 207.0, 168.0;

HRMS (ESI): calculated for $C_{22}H_{21}IN_2O$ ($M+H$)⁺ 457.07713 found 457.07780.

Ethyl 1-(1-(prop-1-enyl)-1*H*-indol-2-yl)but-3-enylcarbamate (16)



Isolated after column chromatography (SiO_2 4:1 v/v petroleum ether-ether) as a white solid (mp 104-106 °C) in 56 % yield as 4:1 mixture of *Z/E* isomers.

IR ν_{max} : 3294, 1688, 1541, 1460, 1265, 742 cm^{-1}

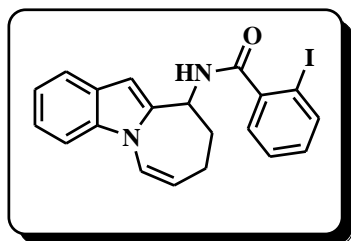
1H NMR (500 MHz, $CDCl_3$) δ 1.23 (t, 3H, $NHCO_2CH_2CH_3$, $J=7.0$ Hz), 1.53-1.55 (m, 3H, CH_3CHCHN), 2.62-2.67 (m, 2H, $CH_2=CHCH_2CH$), 4.11 (q, 2H, $NHCO_2CH_2CH_3$, $J=7.0$ Hz), 4.83-4.86 (m, 1H, NH), 4.96-4.98 (m, 1H, $CH_2=CHCH_2CH$), 5.09-5.17 (m, 2H, $CH_2=CHCH_2CH$), 5.73-5.81 (m, 1H, $CH_2=CHCH_2CH$), 5.97-6.03 (m, 1H, $CH_3=CHCH_2N$), 6.50 (s, 1H, ArH), 6.62-6.63 (m, 1H, $CH_3CH=CHN$), 7.09-7.14 (m, 2H, ArH), 7.17-7.20 (m, 1H, ArH), 7.56-7.58 (m, 1H, ArH);

^{13}C NMR (125 MHz, $CDCl_3$) δ 12.9 (CH_3CHCHN), 14.6 ($NHCO_2CH_2CH_3$), 39.4 (CH_2CHCH_2CH), 47.6 ($CH_2=CHCH_2CH$), 60.9 ($NHCO_2CH_2CH_3$), 99.9, 110.7, 118.4, 120.00 ($CH_2=CHCH_2CH$), 120.4, 122.0, 123.7, 127.5, 129.0, 133.6, 136.7 ($CH_2=CHCH_2N$), 140.4 ($CH_2=CHCH_2CH$), 155.7;

m/z (EI): 298.1 (M^+), 257.1, 211.1, 196.1, 183.1, 168.1;

HRMS (ESI): calculated for $C_{18}H_{22}N_2O_2$ ($M+H$)⁺ 299.17540 found 299.17567.

***N*-((*Z*)-9,10-Dihydro-8*H*-azepino[1,2-*a*]indol-10-yl)-2-iodobenzamide (18)**



Flash chromatography (SiO_2 , 4:1 v/v ether-petroleum ether) afforded the product **18** (79 %) as a white solid (mp 182-185 °C).

IR ν_{max} : 3289, 2923, 2853, 1636, 1518, 1463, 732 cm^{-1}

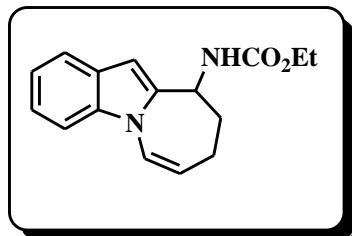
1H NMR (500 MHz, $CDCl_3$) δ 2.26-2.32 (m, 1H, CH_2CH_2CH ring), 2.43-2.49 (m, 1H, CH_2CH_2CH ring), 2.61-2.64 (m, 2H, CH_2CH_2CH ring), 5.24 (dt, 1H, $=CHCH_2CH_2$ ring, $J=10.0$ and 4.5 Hz), 5.69 (t, 1H, CH_2CH_2CH ring, $J=8.5$ Hz), 6.23 (d, 1H, NH , $J=8.0$ Hz), 6.57 (s, 1H, ArH), 7.00-7.02 (m, 1H, $CH=CHCH_2$ ring), 7.09-7.16 (m, 2H, ArH), 7.22-7.25 (m, 1H, ArH), 7.35-7.44 (m, 3H, ArH), 7.56 (d, 1H, ArH, $J=7.5$ Hz), 7.87 (d, 1H, ArH, $J=8.0$ Hz)

^{13}C NMR (125 MHz, $CDCl_3$) δ 25.6, 30.6, 48.1, 92.3, 102.6, 109.4, 112.0, 120.7, 120.9, 122.5, 122.5, 127.5, 128.2, 128.4, 131.3, 137.1, 139.9, 140.3, 141.9, 168.3;

m/z (EI): 429.0, 354.9, 331.1, 281.0, 252.9, 207.0.

HRMS (ESI): calculated for $C_{20}H_{17}IN_2O$ (M+H)⁺ 429.04583, found 429.04578.

Ethyl (Z)-9,10-dihydro-8H-azepino[1,2-a]indol-10-ylcarbamate (20)



Isolated after column chromatography (SiO₂ 7:3 v/v petroleum ether-ethyl acetate) as a white solid (mp 118-120 °C) in 97 % yield.

IR ν_{max} : 3320, 1683, 1525, 1245, 1041, 742 cm⁻¹

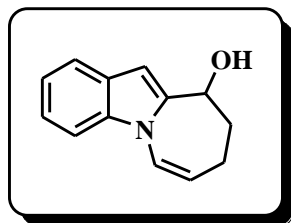
¹H NMR (500 MHz, CDCl₃) δ 1.26 (t, 3H, NHCO₂CH₂CH₃, *J*=7.0 Hz), 2.12-2.18 (m, 2H, =CHCH₂CH₂ ring), 2.21-2.26 (m, 2H, =CHCH₂CH₂ ring), 4.15 (q, 2H, NHCO₂CH₂CH₃, *J*=7.0 Hz), 5.16-5.23 (m, 3H, (NH + =CHCH₂CH₂CH ring)), 6.45 (s, 1H, ArH), 6.98 (dt, 1H, CH=CHCH₂ ring, *J*=9.5 and 2.0 Hz), 7.13 (dd, 1H, ArH, *J*=7.5 and 1.0 Hz), 7.21 (dd, 1H, ArH, *J*=7.0 and 1.0 Hz), 7.34 (d, 1H, ArH, *J*=8.5 Hz), 7.54 (d, 1H, ArH, *J*=8.0 Hz);

¹³C NMR (125 MHz, CDCl₃) δ 14.6, 25.4, 31.4, 49.0, 61.1, 101.8, 109.3, 111.9, 120.63, 120.8, 122.3, 122.5, 127.6, 137.0, 141.4, 155.7;

m/z (EI): 270.1 (M⁺), 224.1, 197.1, 181.1, 168.1, 154.1.

HRMS (ESI): calculated for $C_{16}H_{18}N_2O_2$ (M+H)⁺ 271.14410 found 271.14323.

(Z)-9,10-Dihydro-8H-azepino[1,2-a]indol-10-ol (22)



Isolated after column chromatography (SiO₂ 4:1 v/v petroleum ether-ether) as a yellow solid (mp 98-99 °C) in 98 % yield.

IR ν_{max} : 3274, 15670, 1458, 1343, 1292, 1040, 733 cm⁻¹

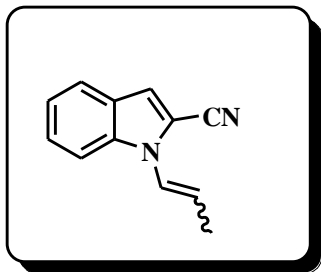
¹H NMR (500 MHz, CDCl₃) δ 1.98 (d, 1H, OH, *J*=5.0 Hz), 2.13-2.19 (m, 1H, CH₂CHHCH ring), 2.26-2.32 (m, 1H, CH₂CHHCH ring), 2.41-2.48 (m, 1H, =CHCHHCH₂ ring), 2.63-2.71 (m, 1H, =CHCHHCH₂ ring), 5.12 (ddd, 1H, CH₂CHOH ring, *J*=8.0, 5.0 and 1.0 Hz), 5.21 (dt, 1H, CH=CHN ring, *J*=10.0 and 4.5 Hz), 6.53 (s, 1H, ArH), 6.99 (dt, 1H, CH=CHN ring, *J*=10.0 and 1.5 Hz), 7.14 (td, 1H, ArH, *J*=8.0 and 1.0 Hz), 7.21-7.25 (m, 1H, ArH), 7.37 (d, 1H, ArH, *J*=8.0 Hz), 7.55-7.57 (m, 1H, ArH);

¹³C NMR (125 MHz, CDCl₃) δ 24.2, 32.1, 67.8, 102.30, 109.4, 111.9, 120.7, 122.0, 122.4, 127.5, 137.1, 143.3;

m/z (EI): 199.1, 181.1, 167.0, 152.0;

HRMS (ESI): calculated for $C_{13}H_{13}NO$ (M+H)⁺ 200.10699, found 200.10651.

1-(Prop-1-enyl)-1*H*-indole-2-carbonitrile (24)



Isolated after column chromatography (SiO₂ 99:1 v/v petroleum ether-ether) as a colourless oil in 73 % yield as 3.2:1 mixture of *Z/E* isomers.

IR ν_{max} : 2223, 1449, 1345, 936, 735 cm⁻¹

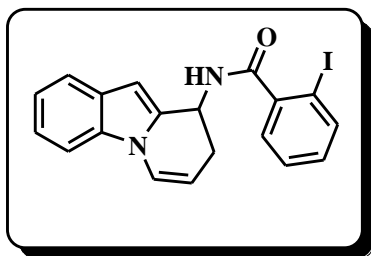
¹H NMR (500 MHz, CDCl₃) δ 1.67 (dd, 3H, *J*=7.0 and 2.0 Hz, CH₃, *Z* isomer), 1.96 (dd, 3H, *J*=7.0 and 1.5 Hz, CH₃, *E* isomer), 6.05-6.11 (m, 1H, CH₃CHCHN, *Z* isomer), 6.17-6.24 (m, 1H, CH₃CHCHN, *E* isomer), 6.71 (dq, 1H, *J*=8.0 and 2.0 Hz, CH₃CHCHN, *Z* isomer), 6.87 (dq, 1H, *J*=13.5 and 1.5 Hz, CH₃CHCHN, *E* isomer), 7.21-7.25 (m, 4H, ArH), 7.38-7.41 (m, 4H, ArH), 7.48 (dd, 1H, ArH, *J*=8.5 and 0.5 Hz), 7.63-7.68 (m, 1H, ArH);

¹³C NMR (125 MHz, CDCl₃) δ 13.2, 15.5, 108.9, 110.1, 111.1, 111.3, 113.6, 113.7, 113.9, 114.8, 121.8, 122.0, 122.2, 122.3, 122.4, 122.5, 123.1, 126.0, 126.1, 126.2 (2C), 129.7, 136.9, 137.4;

***m/z* (EI)**: 182.1 (M⁺), 167.0, 154.0, 142.1, 128.0, 115.0.

HRMS (ESI): calculated for C₁₂H₁₀N₂ (M+H)⁺ 183.09167, found 183.09084.

N-(8,9-Dihydropyrido[1,2-*a*]indol-9-yl)-2-iodobenzamide (25)



Isolated after column chromatography (SiO₂ 3:2 v/v petroleum ether-ether) as a white needles (mp 178-181 °C) in 92 % yield.

IR ν_{max} : 3436, 2921, 1647, 1462, 740 cm⁻¹

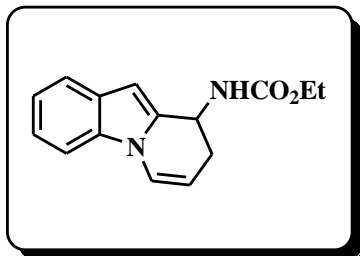
¹H NMR (500 MHz, CDCl₃) δ 2.58-2.63 (m, 1H, =CH₂CHNH ring), 2.83-2.87 (m, 1H, =CH₂CHNH ring), 5.40-5.43 (dt, 1H, CH₂CHNH ring, *J*=7.5 and 4.4 Hz), 5.66-5.70 (m, 1H, CH=CHCH₂ ring), 6.17 (d, 1H, CH=CHCH₂ ring, *J*=8.0 Hz), 6.62 (s, 1H, ArH), 7.08-7.15 (m, 2H, ArH), 7.18-7.25 (m, 2H, ArH), 7.36-7.43 (m, 3H, ArH), 7.58 (d, 1H, ArH, *J*=7.7 Hz), 7.85 (d, 1H, ArH, *J*=8.0 Hz);

¹³C NMR (125 MHz, CDCl₃) δ 27.9 (=CH₂CHNH ring), 43.7 (CH=CHCH₂ ring), 92.3, 101.1, 105.7 (=CHCH₂CH ring), 108.6, 120.9, 121.1, 122.6, 122.8, 128.0, 128.2, 128.4, 131.3, 133.9, 134.4, 139.9, 141.8, 168.5;

***m/z* (EI)**: 413.1 (M⁺¹), 281.1, 230.9, 207.0, 167.0, 139.0

HRMS (ESI): calculated for C₁₉H₁₅IN₂O (M+H)⁺ 415.03018 found 415.02942.

Ethyl 8,9-dihidropyrido [1,2-a]indole-9-ylcarbamate (26)



Isolated after column chromatography (SiO₂ 4:1 v/v petroleum ether-ether) as a pale yellow solid (mp 125-128 °C) in 88 % yield.

IR ν_{max} : 3290, 1683, 1543, 1461, 1313, 716 cm⁻¹

¹H NMR (500 MHz, CDCl₃) δ 1.26 (t, 3H, NHCO₂CH₂CH₃, *J*=7.0 Hz), 2.34-2.38 (m, 1H, CH₂ ring), 2.68-2.71 (m, 1H, CH₂ ring), 4.15 (q, 2H, NHCO₂CH₂CH₃, *J*=7.0 Hz), 5.10-5.19 (m, 2H, CH=CH-N), 5.32-5.36 (m, 1H, CHNHCO₂CH₂CH₃), 6.49 (s, 1H, ArH), 7.10-7.14 (m, 2H, 1 ArH + NH), 7.20-7.25 (m, 1H, ArH), 7.34 (d, 1H, ArH, *J*=4.0 Hz), 7.55 (d, 1H, ArH, *J*=4.0 Hz);

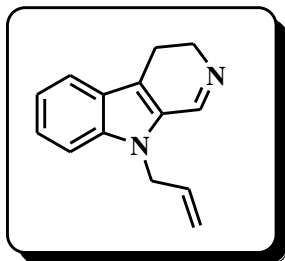
¹³C NMR (125 MHz, CDCl₃) δ 14.6 (NHCO₂CH₂CH₃), 28.4 (CH₂ ring), 44.9 (CH=CH-N), 61.1 (NHCO₂CH₂CH₃), 100.3, 105.6 (CHNHCO₂CH₂CH₃), 108.5, 120.7, 120.9, 122.4, 122.7, 128.0, 134.4, 135.0, 155.8;

m/z (EI): 281.1 (M⁺), 256.1 209.1 183.1, 167.1, 154.1;

HRMS (ESI): calculated for C₁₅H₁₆N₂O₂ (M+H)⁺ 257.12845 found 257.12879.

4. Synthesis of (±)-debromoarborescidine B

9-Allyl-4,9-dihydro-3H-β-carboline (28)¹



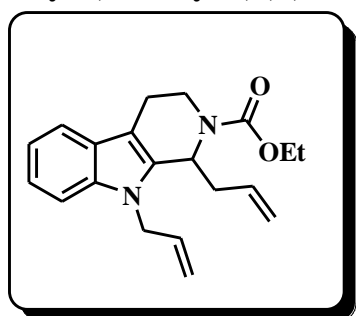
To a suspension of sodium hydride (44 mg, 1.0 mmol of a 60 % dispersion in mineral oil) in anhydrous DMF (1.0 mL) a solution of 3,4-dihydro-β-carboline **27** (100 mg, 0.59 mmol) in DMF (0.5 mL) was added dropwise with stirring at -10 °C under nitrogen. The mixture was stirred for 1 h at -10 °C and then cooled to -60 °C followed by dropwise addition of a solution of allyl bromide (78 mg, 0.64 mmol) in DMF (0.5 mL). Stirring was maintained for 2 h at -60 °C and methanol (0.1 mL), water (0.1 mL) and brine (6 mL) were added successively. The solution was extracted with dichloromethane (3 x 15 mL), the organic extracts were combined, washed with water (10 mL) and dried over sodium sulphate. The solvent was removed under reduced pressure and the residue was purified by flash chromatography (SiO₂, ether saturated with aqueous ammonia) to afford **28** as a colourless crystals (49 mg, 40 %), mp 125-127°C.

¹H NMR (500 MHz, CDCl₃) δ 2.89 (t, 2H, CH₂CH₂N, *J*=8.5 Hz), 3.91 (dd, 2H, CH₂CH₂N, *J*=8.5 and 2.5 Hz), 4.83 (dt, 2H, CH₂CH=CH₂, *J*=5.0 and 1.5 Hz), 4.99 (dq, 1H, CH₂CH=CH₂, *J*=17.0 and 1.0 Hz), 5.18 (dq, 1H, CH₂CH=CH₂, *J*=10.5 and 1.0 Hz), 6.01-5.94 (m, 1H, CH₂CH=CH₂), 7.14 (ddd, 1H, ArH,

$J = 8.2, 8.0$ and 2.0 Hz), 7.29-7.30 (m, 2H, ArH), 7.59 (d, 1H, ArH, $J = 8.0$ Hz), 8.44 (t, 1H, $\text{CH}=\text{N}$, $J = 2.5$ Hz);

^{13}C NMR (125 MHz, CDCl_3) δ 19.1, 45.5, 48.5, 110.2, 115.9, 117.0, 120.1, 120.2, 124.3, 124.9, 129.0, 133.1, 137.3, 150.2;

Ethyl 1,9-diallyl-1,2,3,4-tetrahydro- β -carboline carboxylate (**29**)



Compound **29** was synthesised following the modified literature procedure²: To a solution of **28** (75 mg, 0.36 mmol) in THF (2 mL) ethyl chloroformate (43 mg, 0.40 mmol) was added dropwise with stirring under nitrogen at room temperature. The mixture was stirred at room temperature for additional 40 minutes. Indium powder (83 mg, 0.72 mmol) and allyl bromide (124 mg, 1.0 mmol) were added to the solution and the resulting mixture was stirred at room temperature for 2 hours. The reaction was monitored by t.l.c. Upon completion of the reaction, the solvent was removed under reduced pressure and the residue was purified by flash chromatography (SiO_2 , 4:1 v/v petroleum ether-ether) to afford the product **29** (93 mg, 81 %) as a colourless oil.

IR ν_{max} : 3054, 2979, 2914, 1697, 1465, 1423, 1232, 1190, 1107, 1027, 920, 743 cm^{-1} .

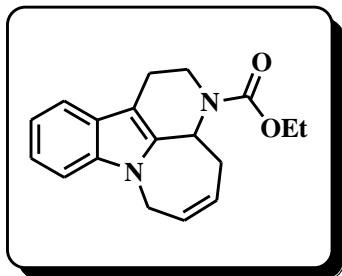
^1H NMR (500 MHz, CDCl_3) δ (rotamers): 1.26 (t, 3H, $J = 7.0$ Hz, CH_3), 1.29 (t, 3H, CH_3 , $J = 7.0$ Hz), 2.49-2.56 (m, 2H), 2.64-2.68 (m, 2H), 2.72-2.77 (m, 2H), 2.82-2.95 (m, 2H), 3.24-3.52 (m, 2H), 4.14-4.26 (m, 4H), 4.34 (dd, 1H, $J = 13.5$ and 5.5 Hz), 4.56 (dd, 1H, $J = 13.5$ and 5.5 Hz), 4.63-4.74 (m, 4H), 4.94 (t, 2H, $J = 16.0$ Hz), 5.06-5.19 (m, 6H), 5.31 (dd, 1H, $J = 9.0$ and 4.5 Hz), 5.54 (dd, 1H, $J = 10.0$ and 3.0 Hz), 5.80-5.98 (m, 4H), 7.08-7.11 (m, 2H), 7.16-7.19 (m, 2H), 7.23-7.25 (m, 2H), 7.46-7.50 (m, 2H);

^{13}C NMR (125 MHz, CDCl_3) δ (rotamers): 14.6 (2 C), 20.9, 21.3, 37.4, 37.9, 38.8, 38.9, 45.9, 46.0, 50.0, 50.3, 62.0, 62.2, 107.6, 108.3, 109.6, 109.8, 116.8, 116.9, 117.4, 117.7, 118.1, 118.3, 119.3, 119.5, 121.5, 121.7, 126.7, 133.0, 133.1, 133.9, 134.2, 134.5, 134.9, 136.9, 155.9, 156.3;

m/z (EI): 324.2 (M^+), 283.1, 255.1, 211.1, 169.1;

HRMS (ESI): calculated for $\text{C}_{20}\text{H}_{24}\text{N}_2\text{O}_2$ ($\text{M}+\text{H}$)⁺ 325.19105, found 325.19007.

2-Carboethoxy-1,9-(2-butenediyl)-1,2,3,4-tetrahydro- β -carboline (30)



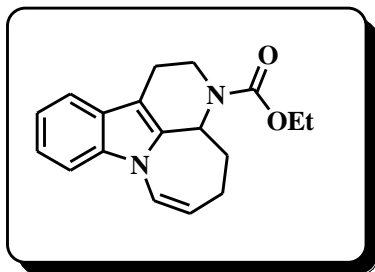
To a solution of **29** (39 mg, 0.1 mmol) in dry dichloromethane (2.0 mL) Grubbs catalyst 2nd generation (4.1 mg, 4 mol %) was added under nitrogen atmosphere. The resulting mixture was stirred under reflux for 30 minutes. Upon completion of the reaction, the solvent was removed under reduced pressure and the residue was purified by flash chromatography (SiO₂, 7:3 v/v petroleum ether-ether) to afford the product **30** (35 mg, 98 %) as a colourless oil. Compound **30** was used in following reaction of isomerisation without further purification.

IR ν_{max} : 3351, 2979, 2917, 1696, 1466, 1423, 1238, 1109, 909, 738 cm⁻¹.

¹H NMR (500 MHz, CDCl₃) δ (rotamers) 1.31 (t, 3H, CH₃, $J=7.0$ Hz), 2.59-2.77 (m, 2H), 2.77-2.83 (m, 2H), 3.13-3.18 (m, 1H), 4.21-4.22 (m, 2H), 4.39-4.64 (m, 2H), 4.77-4.80 (m, 1H), 5.47-5.63 (m, 1H), 5.82-5.84 (m, 2H), 7.09 (t, 1H, ArH, $J=7.5$ Hz), 7.19 (t, 1H, ArH, $J=7.5$ Hz), 7.27 (d, 1H, ArH, $J=8.0$ Hz), 7.50 (d, 1H, ArH, $J=6.0$ Hz);

HRMS (ESI): calculated for C₁₈H₂₀N₂O₂ (M+H)⁺ 297.15975, found 297.15828.

2-Carboethoxy-1,9-(1-butenediyl)-1,2,3,4-tetrahydro- β -carboline (31)



Compound **31** was synthesised from carbamate **30** following the general isomerisation procedure 2.1 and 2.2. The product was isolated after column chromatography (SiO₂, 7:3 v/v petroleum ether-ether) as a colourless oil in 75 % yield.

IR ν_{max} : 3051, 2924, 1697, 1445, 1442, 1306, 1231, 1109, 739 cm⁻¹.

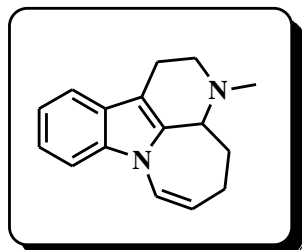
¹H NMR (500 MHz, CDCl₃) δ 1.31 (t, 3H, CH₃, $J=7.0$ Hz), 2.11-2.18 (m, 2H, CH₂CHN), 2.48-2.49 (m, 2H, CH₂CH=CHN), 2.74-2.83 (m, 2H, CH₂CH₂N), 3.04-3.09 (m, 1H, CH₂CH₂N), 4.22 (q, 2H, $J=5.0$ Hz), 4.47-4.55 (m, 1H, CH₂CH₂N), 5.07-5.17 (m, 1H, CH₂CHN), 5.19 (dt, 1H, NCH=CH, $J=9.5$ and 5.0 Hz), 6.96 (dt, 1H, NCH=CH, $J=10.0$ and 1.5 Hz), 7.13-7.16 (m, 1H, ArH), 7.22 (td, 1H, ArH, $J=7.0$ and 1.0 Hz), 7.35 (d, 1H, ArH, $J=8.0$ Hz), 7.49 (d, 1H, ArH, $J=8.0$ Hz)

¹³C NMR (125 MHz, CDCl₃) δ 14.7 (CH₃), 21.7 (CH₂CH₂N), 26.7 (CH₂CH=CHN), 31.9 (CH₂CHN), 39.1 (CH₂CHN), 52.3 (CH₂CH₂N), 61.5 (CH₂O), 109.2 (ArC), 111.6 (NCH=CH), 118.2 (ArC), 120.3 (ArC), 121.7 (ArC), 122.0 (NCH=CH), 126.8 (ArC), 135.9 (ArC), 155.5 (C=O);

m/z (EI): 296.1 (M⁺), 267.1, 223.1, 194.1, 167.1;

HRMS (ESI): calculated for C₁₈H₂₀N₂O₂ (M+H)⁺ 297.15975, found 297.15863.

(±)-Debromoarborescidine B (1b)



To a suspension of LiAlH₄ (14 mg, 0.37 mmol, 60 % dispersion in mineral oil) in dry THF (2.0 mL) solution of **31** (21 mg, 0.07 mmol) in THF (1.0 mL) was added dropwise with stirring under nitrogen atmosphere at room temperature. The resulting mixture was stirred under reflux for 3 hours. The reaction mixture was then cooled to room temperature, and the excess of LiAlH₄ decomposed with H₂O (0.1 mL) and 15 % NaOH (0.02 mL). After the filtration the residue was extracted with Et₂O (3 x 15 mL). The combined organic extracts were dried over sodium sulphate. The solvent was removed under reduced pressure and the residue was purified by flash chromatography (SiO₂, ether saturated with aqueous ammonia) to afford the product **1b** (13.5 mg, 80 %) as a colourless amorphous solid (mp 97-102 °C).

IR ν_{\max} : 3047, 2924, 2845, 2785, 1673, 1464, 1438, 1384, 1309, 740 cm⁻¹.

¹H NMR (500 MHz, CDCl₃) δ 1.85-1.92 (m, 1H, CH₂CHN), 2.33-2.38 (m, 1H, CH₂CHN), 2.40-2.45 (m, 1H, CH₂CH=CHN), 2.51-2.57 (m, 4H, CH₃, CH₂CH=CHN), 2.69-2.75 (m, 2H, CH₂CH₂N, CH₂CH₂N), 2.90-2.97 (m, 1H, CH₂CH₂N), 3.14 (ddd, 1H, CH₂CH₂N, *J*=11.0, 5.5 and 2.0 Hz), 3.41 (brd, 1H, CH₂CHN, *J*=10.5 Hz), 5.04-5.08 (m, 1H, NCH=CH), 6.93 (dt, 1H, NCH=CH, *J*=10.0 and 2.0 Hz), 7.11-7.15 (m, 1H, ArH), 7.18-7.21 (m, 1H, ArH), 7.33 (d, 1H, ArH, *J*=8.0 Hz), 7.47 (d, 1H, ArH, *J*=7.5 Hz);

¹³C NMR (125 MHz, CDCl₃) δ 20.7 (CH₂CH₂N), 28.0 (CH₂CH₂CH=), 30.0 (CH₂CH₂CH=), 42.5 (NCH₃), 52.9 (CH₂CH₂N), 62.6 (CH₂CHN), 109.1, 109.3, 110.0 (NCH=CH), 118.2 (ArC), 120.1 (ArC), 121.8 (ArC), 122.0 (NCH=CH), 127.0 (ArC), 136.2 (ArC), 137.3 (ArC);

m/z (EI): 238.2 (M⁺), 223.1, 209.1, 195.1, 180.1, 167.1;

HRMS (ESI): calculated for C₁₆H₁₈N₂ (M+H)⁺ 239.15428, found 239.15319.

References

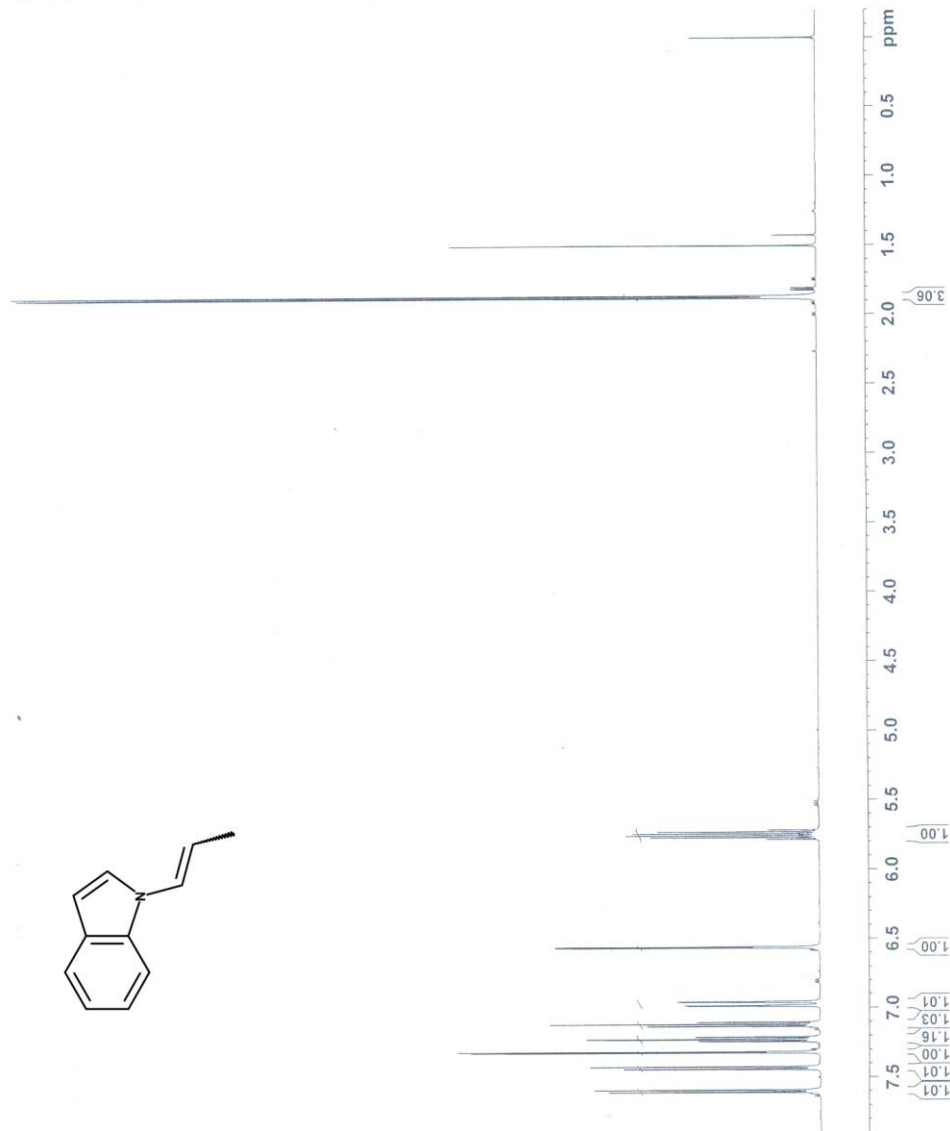
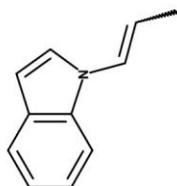
1. González-Gómez, Á.; Domínguez, G.; Pérez-Castells, J. *Tetrahedron*, **2009**, *65*, 3378–3391.
2. Lee, S.H.; Park, Y.S.; Nam, M.H.; Yoon, C.M. *Org. Biomol. Chem*, **2004**, *2*, 2170-2172.

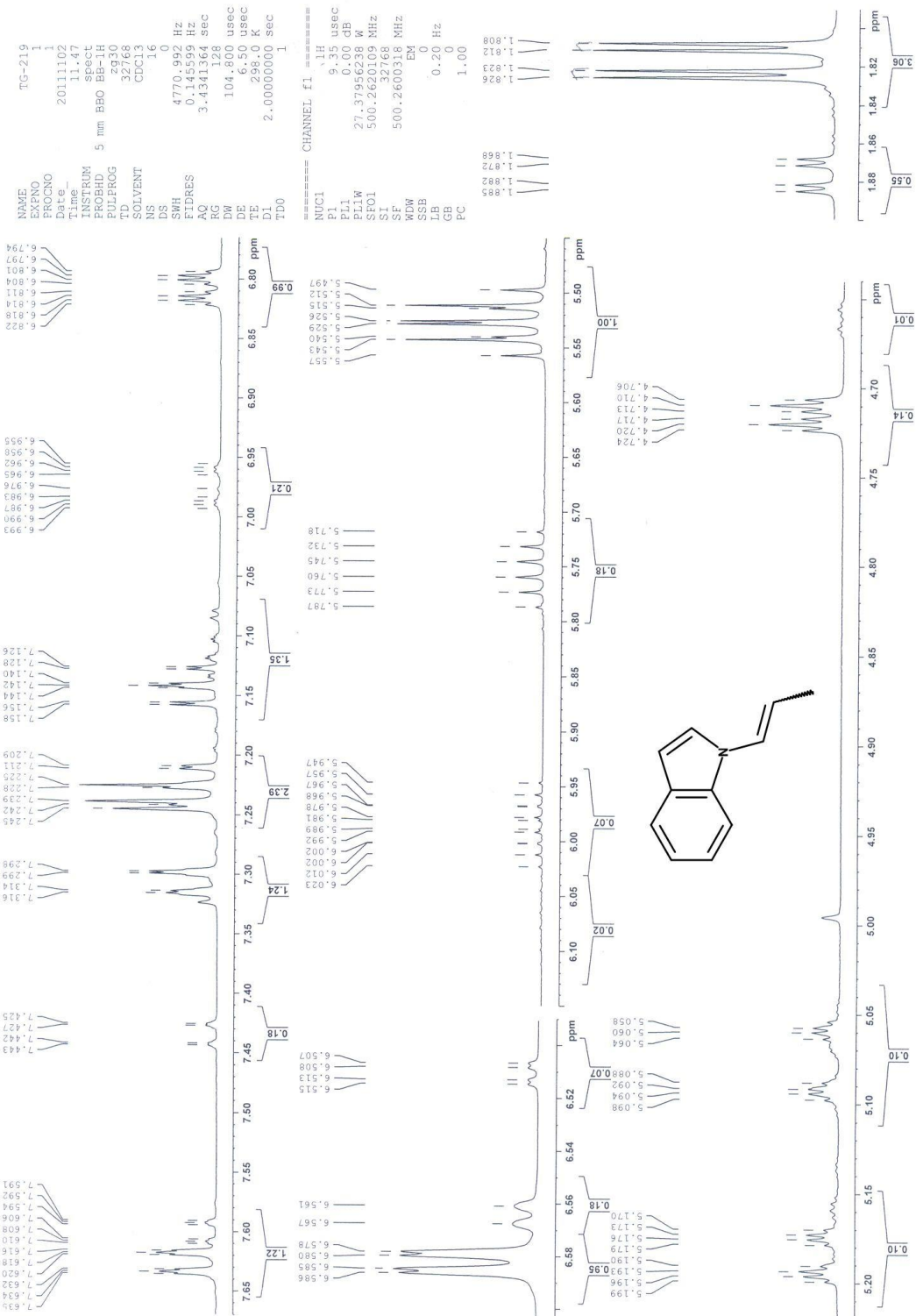
5. Copies of spectra

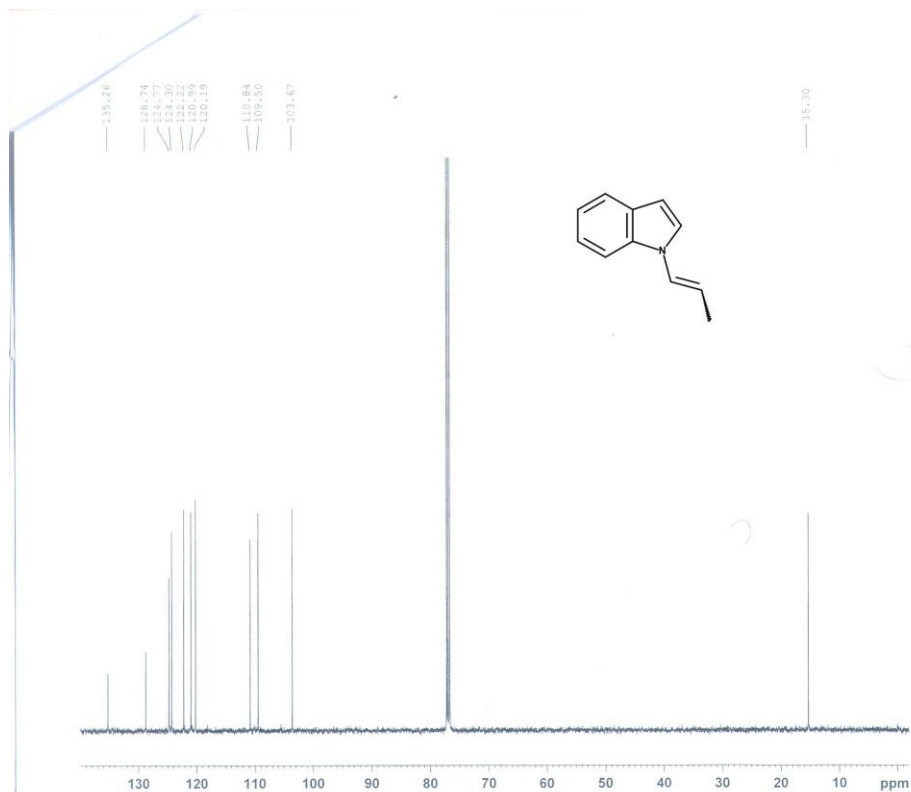
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PROCNO 1
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DS 16
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SMH 4587.156 Hz
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TDI 298.0 K
TDO 2.0000000 sec

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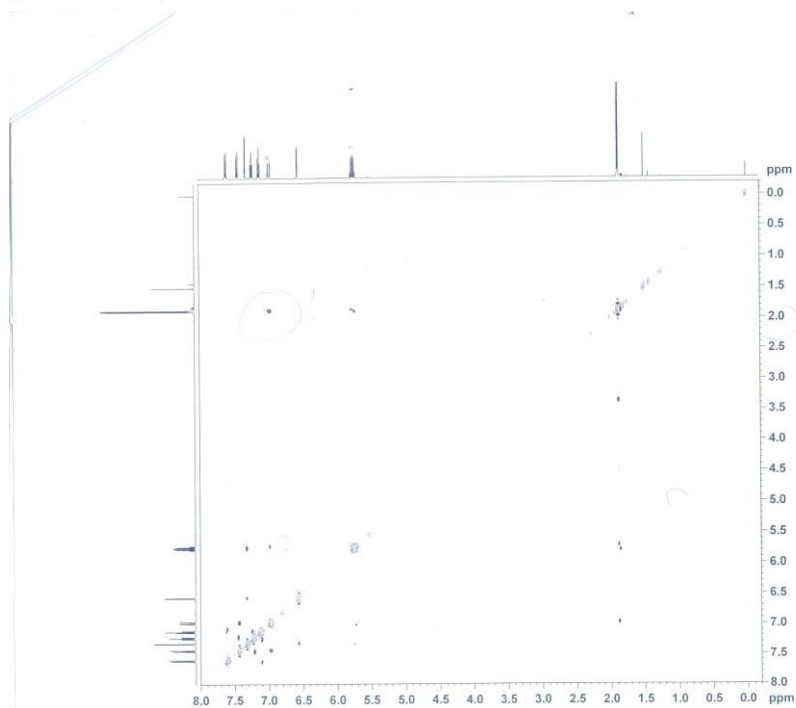
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TE            298.0 K
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D11           0.0300000 sec
TDO           1
  
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SFO1         125.8043140 MHz
  
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NUC2          1H
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PL12          18.40 dB
PL13          18.40 dB
PL2W         20.76952171 W
PL12W        0.39575511 W
PL13W        0.39575511 W
SFO2         500.2619725 MHz
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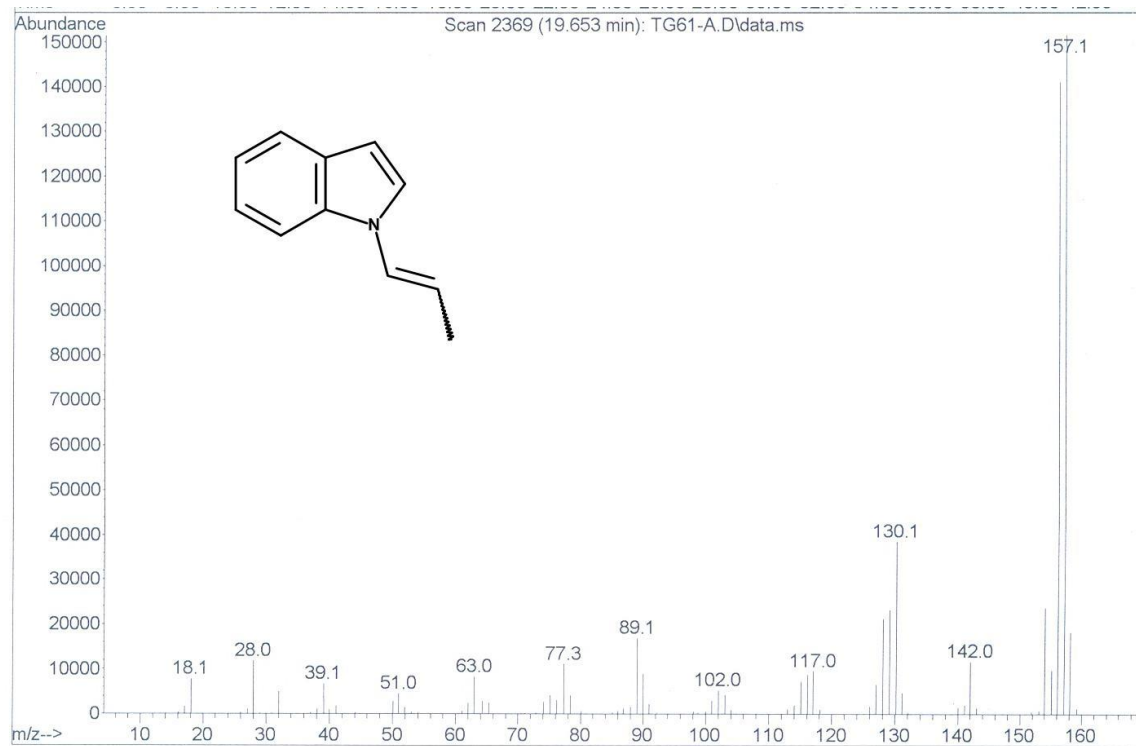
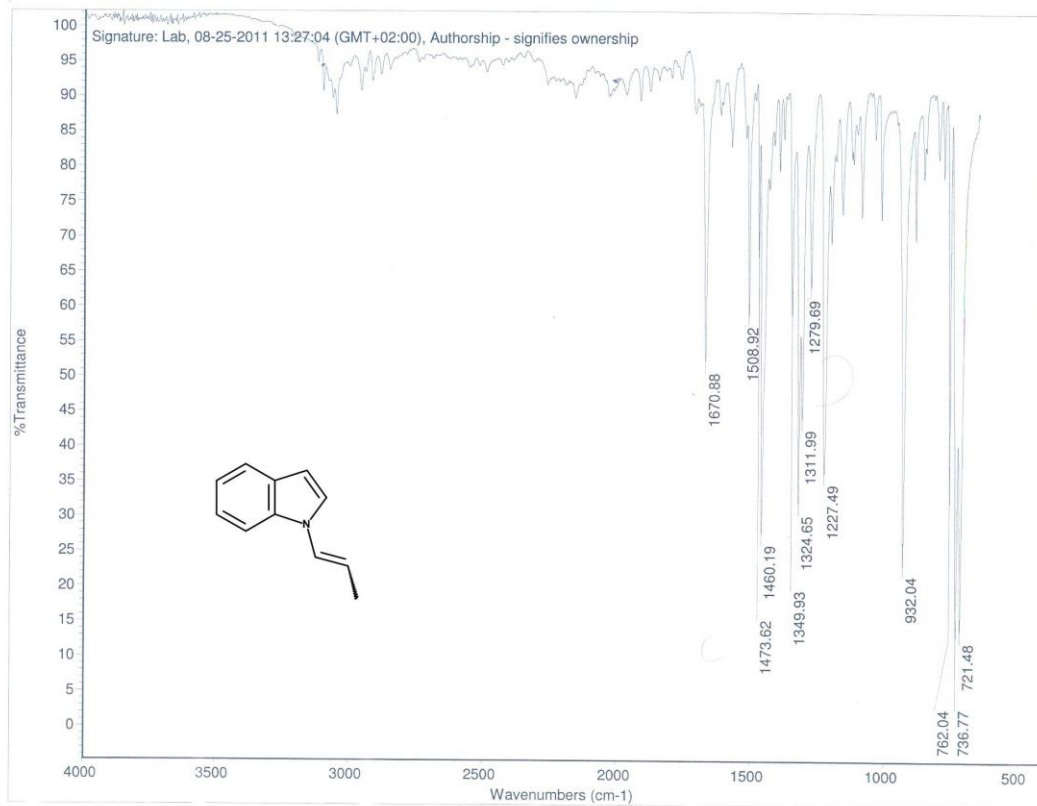


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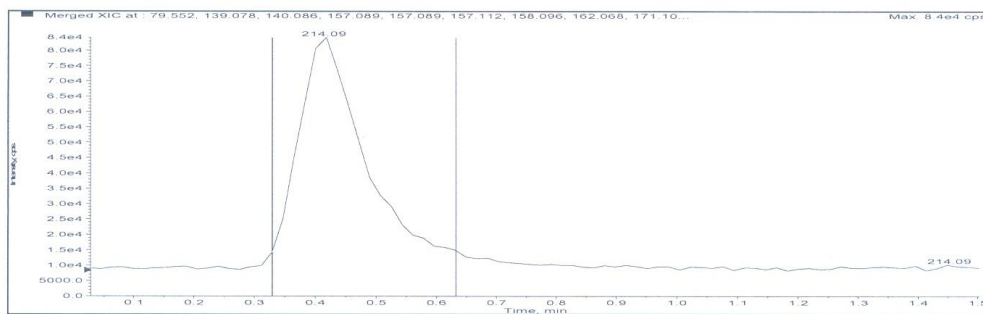
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DS            4
SWH           4387.156 Hz
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RG            181
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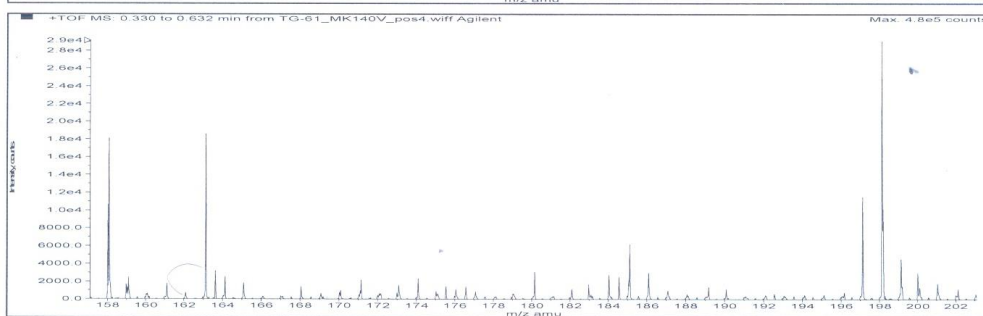
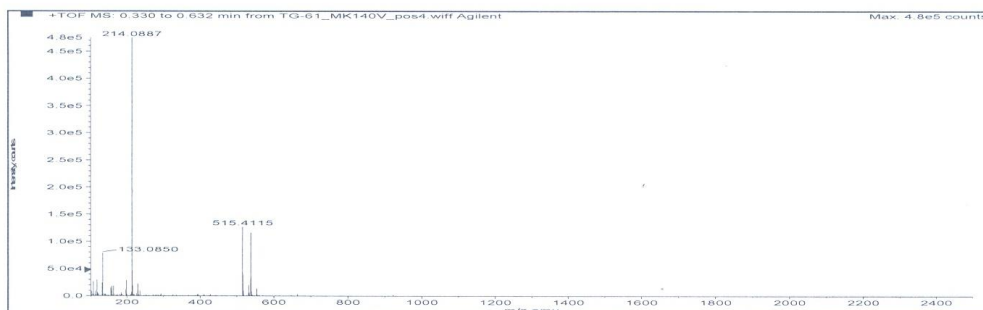
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SWH           26.89179 Hz
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SBB           0
LB            0.00 Hz
GB            0
  
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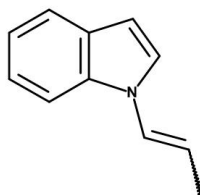


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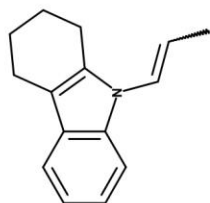


Formula	Compound name	Mass	Peak RT (min)	Peak area	Description
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Species	Abundance (counts)	Ion Mass	Measured Mass	Error (mDa)	Error (ppm)	Ret. Time Error (min)
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[M+CH3CN] ⁺	29347.39	198.11515	198.12624	11.09070	55.98	--

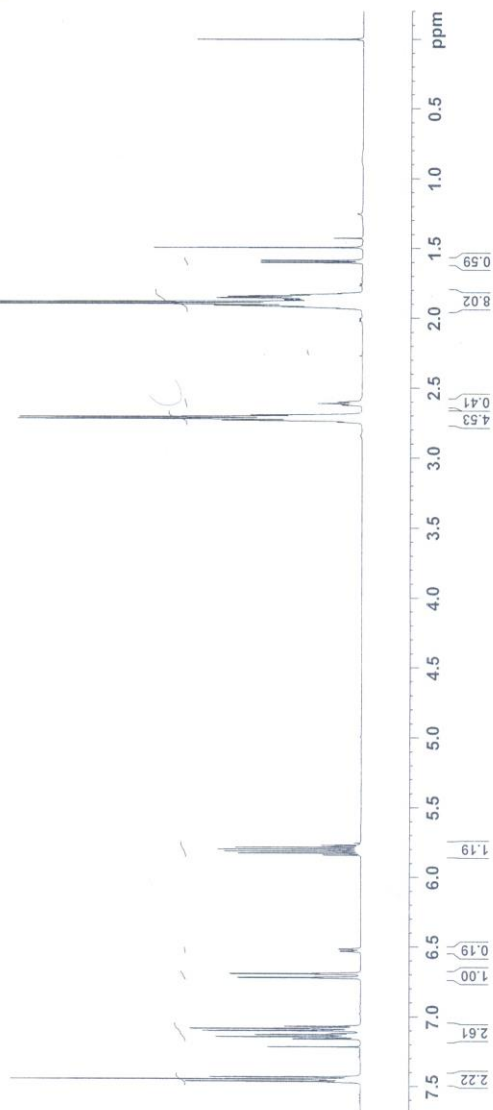


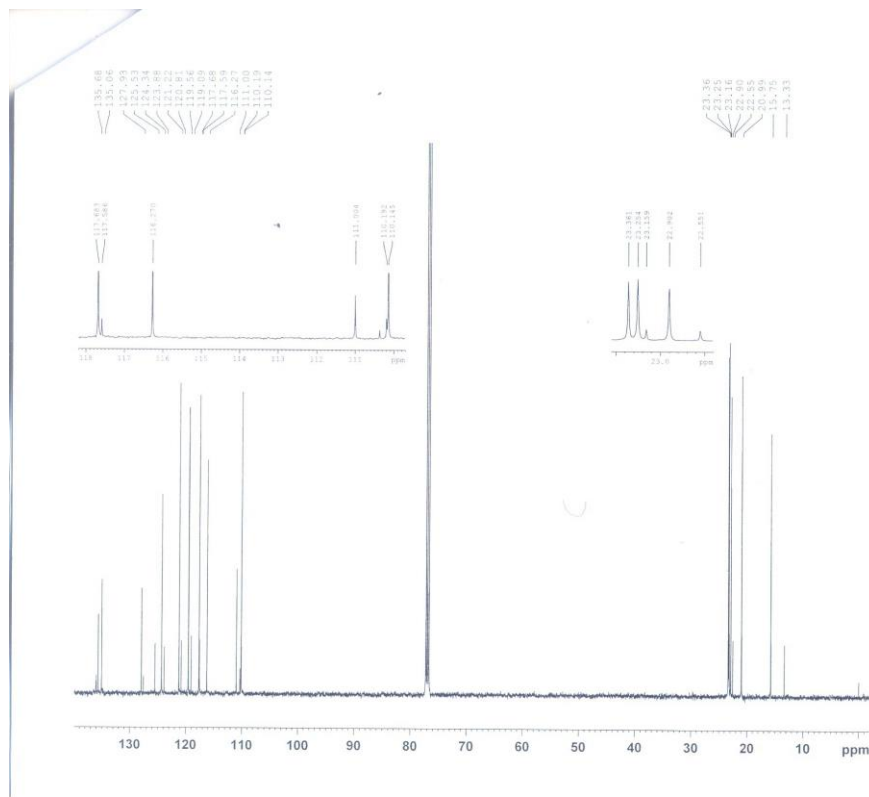
Compound 8



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TD0           1
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PL12          0.00 dB
PL13          0.00 dB
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WDW           EM
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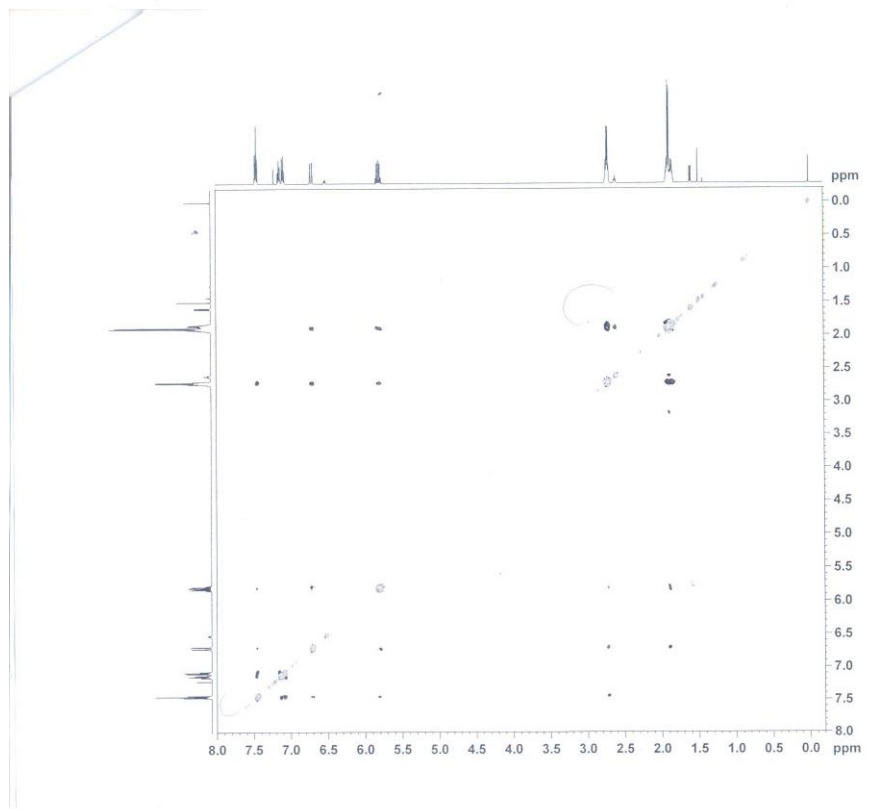
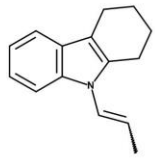


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INSTRUM       spect
PROBHD        5 mm BBO BB-1H
PULPROG       zgpg30
TD            32768
SOLVENT       CDCl3
NS            524
DS            4
SWH           29761.904 Hz
FIDRES        0.908261 Hz
AQ            0.5505524 sec
RG            724
DW            16.400 usec
DE            6.50 usec
TE            298.0 K
D1            2.0000000 sec
D11           0.0300000 sec
TD0           1

===== CHANNEL f1 =====
NUC1          13C
P1            11.50 usec
PL1           3.00 dB
PL1W          32.2284892 W
SFO1          125.8043340 MHz

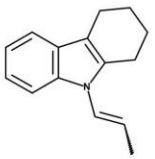
===== CHANNEL f2 =====
CPDPRG2       waltz16
NUC2          1H
PCPD2         80.00 usec
PL2           1.20 dB
PL12          18.40 dB
PL13          18.40 dB
PL2W          20.76952171 W
PL1W          0.39575511 W
SFO2          500.2619610 MHz
SI            32768
SF            125.7904857 MHz
WDW           EM
SSB           0
LB            1.50 Hz
GB            0
PC            1.40
  
```

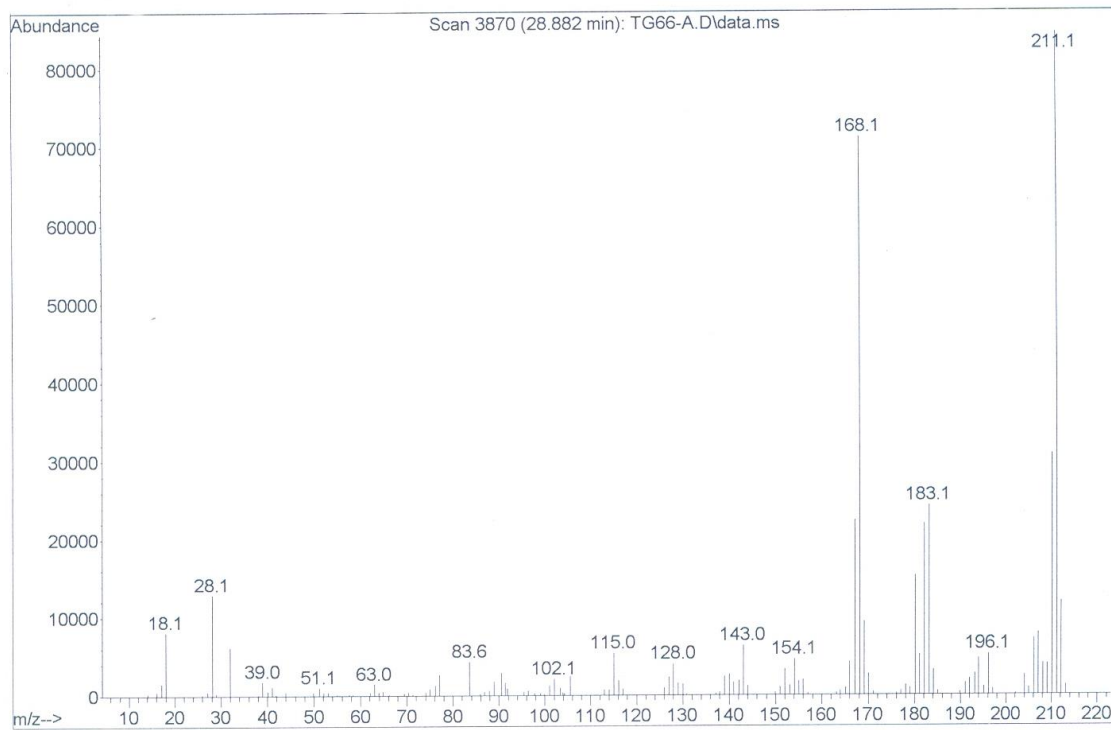
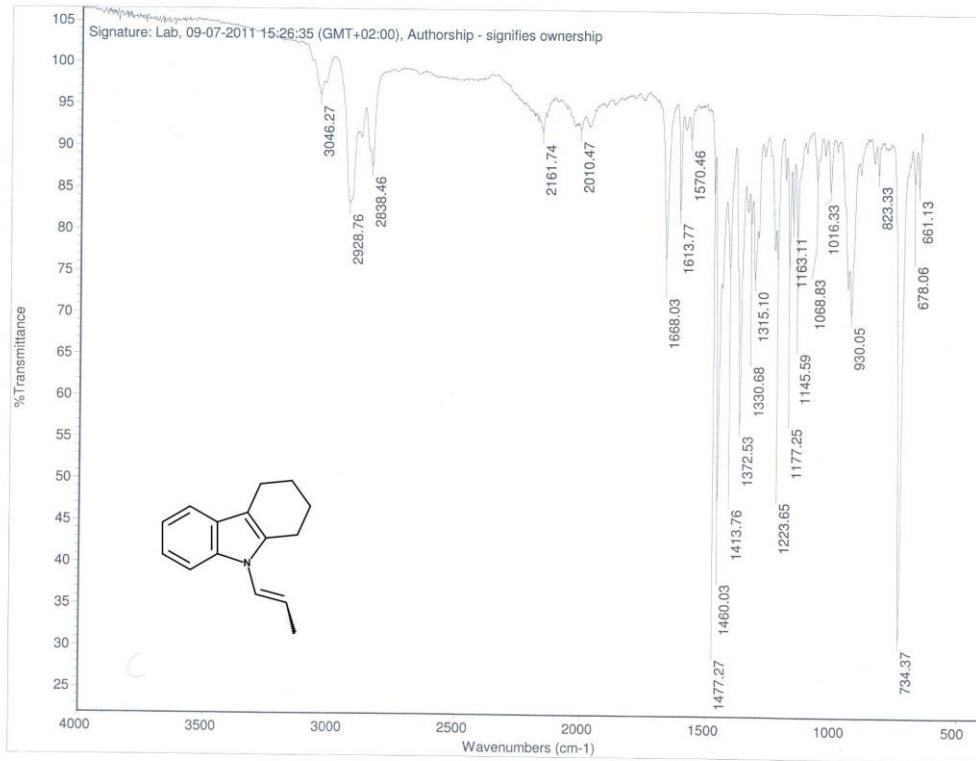


```

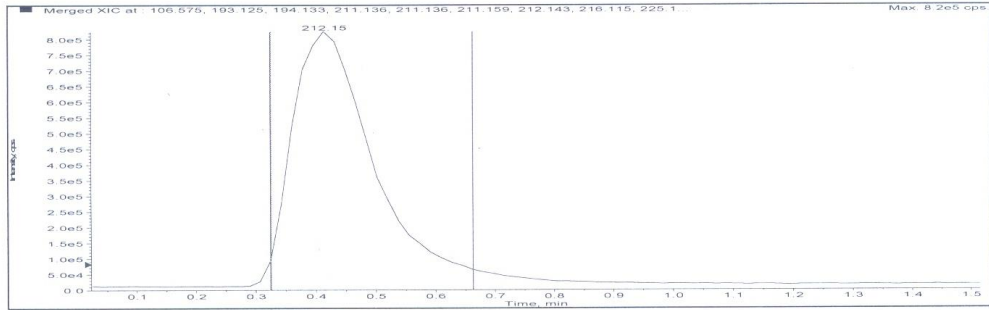
NAME          TG-66
EXPNO         4
PROCNO        1
Date_         20101007
Time          11.16
INSTRUM       spect
PROBHD        5 mm BBO BB-1H
PULPROG       zgpg30
TD            1124
SOLVENT       CDCl3
NS            4
DS            16
SWH           4619.227 Hz
FIDRES        4.50987 Hz
AQ            0.1109151 sec
RG            114
DW            108.267 usec
DE            4.50 usec
TE            298.0 K
D0            0.00009636 sec
D2            2.0000000 sec
D8            1.0000000 sec
WDW           0.0021659 sec

===== CHANNEL f1 =====
NUC1          1H
P1            9.35 usec
PL1           0.00 dB
PL1W          27.37954238 W
SFO1          500.2619610 MHz
NUC2          13C
P2            25.00 usec
SFO2          300.362 MHz
FIDRES        18.039915 Hz
SW            9.353 FPM
F2MODE        States-TPPI
SI            1124
SF            500.2600144 MHz
WDW           Q01MG
SSB           0
LB            0.00 Hz
GB            0
PC            1.00
D1            10.00 sec
MC2           States-TPPI
SF            500.7600343 MHz
WDW           Q01MG
SSB           0
LB            0.00 Hz
GB            0
  
```

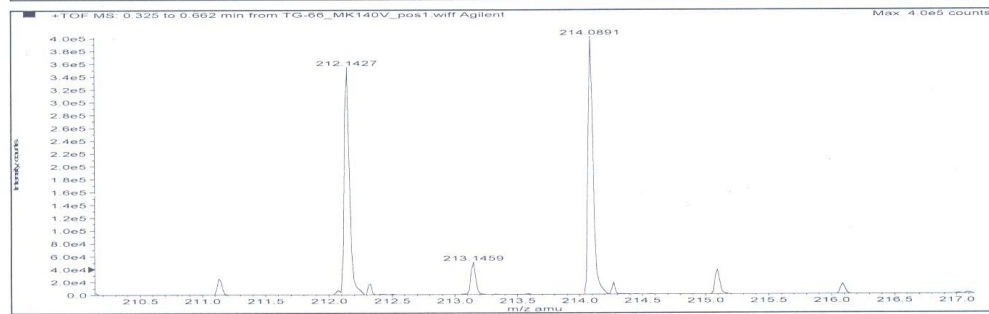
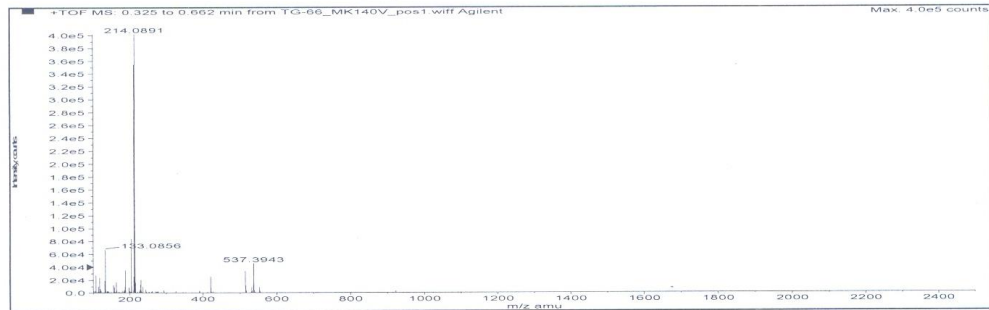




Sample Name: TG-66 Sample Location: P1-D5 Sample Id: Operator: Milka
 Data File Name: D:\PE ScieX Data\Projects\Farmaceutski fakultet\Data\TG-66_MK140V_pos1.wiff Acq Time: November 12 2010,
 02:11:12 PM
 Method: D:\TOF_Data\damethods\Night_Seq_Comp_ident1.anmlefc.xml

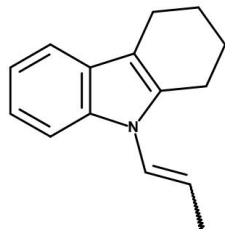


Merged XIC, Period# : 1 Experiment# : 1

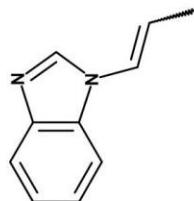


Formula	Compound name	Mass	Peak RT (min)	Peak area	Description
C15H17N	--	211.13610	0.41	7.83379 E6	--

Species	Abundance (counts)	Ion Mass	Measured Mass	Error (mDa)	Error (ppm)	Ret. Time Error (min)
[M+H2O-H2O]+	26310.05	211.13555	211.13496	-0.59335	-2.81	--
[M+H]+	357859.60	212.14338	212.14269	-0.69049	-3.25	--

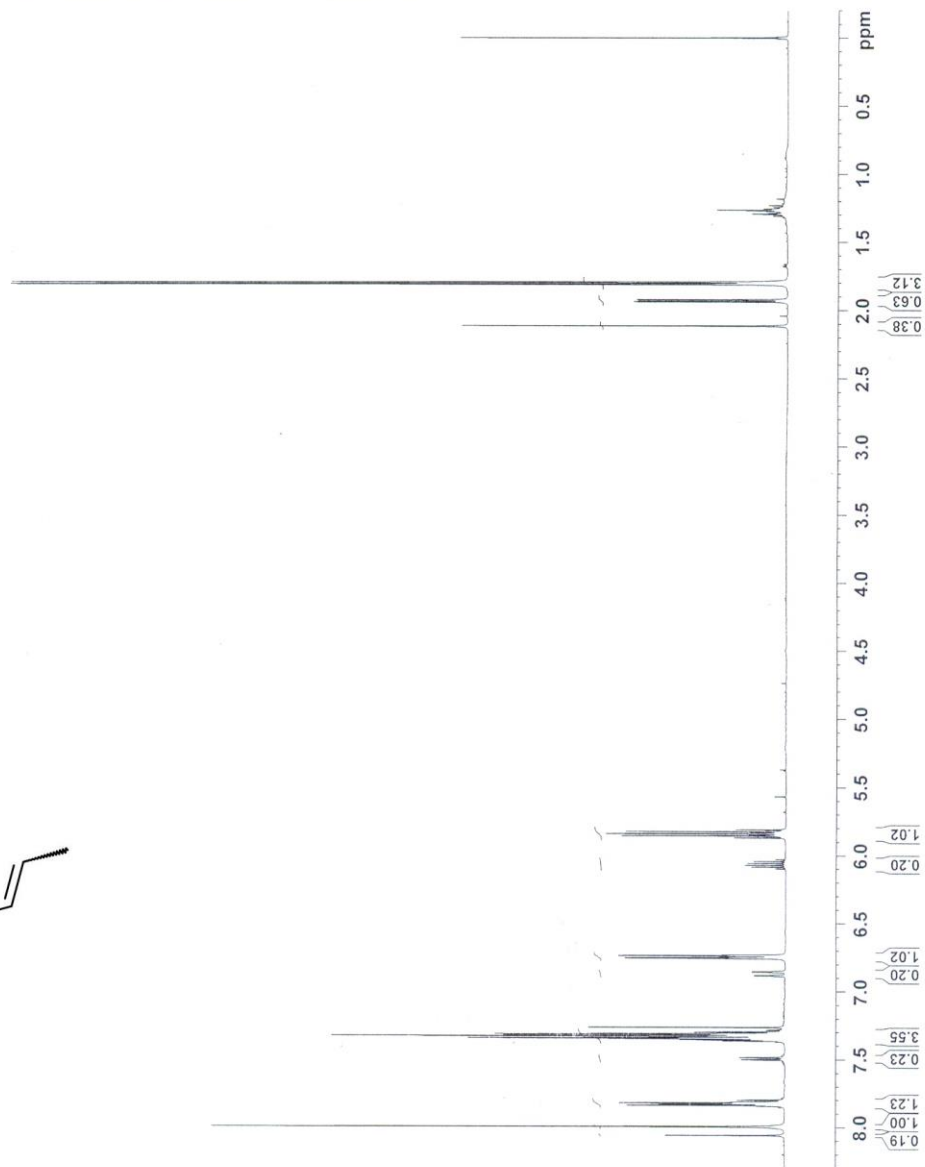


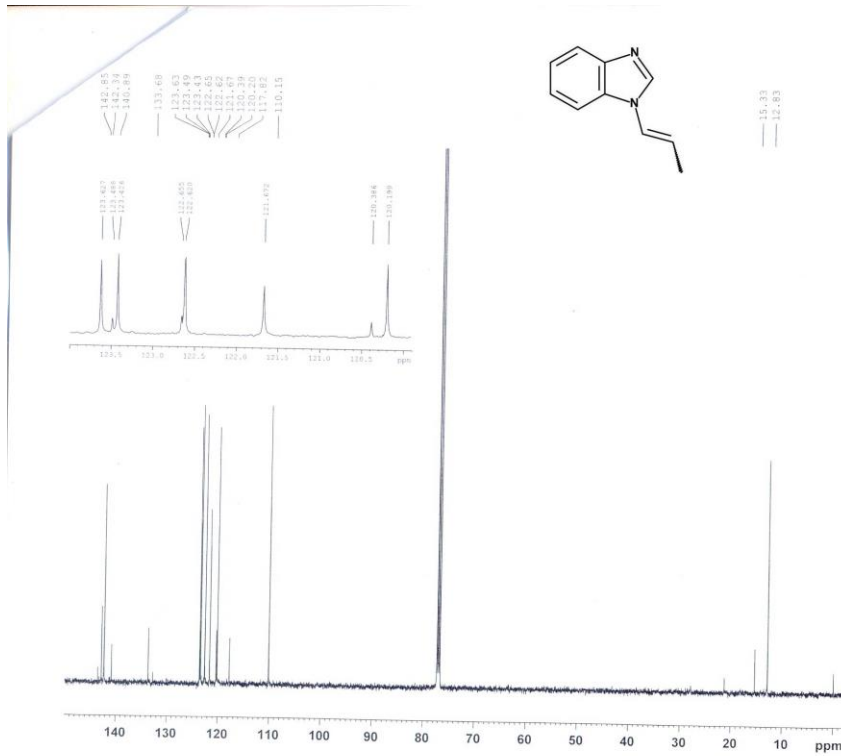
Compound 10



```

NAME          MV5
EXPNO         1
PROCNO        1
Date_         20101006
Time          11:00:00
INSTRUM       spect
PROBHD        5 mm BBO BE-1H
PULPROG       zg30
TD            32768
SOLVENT       CDCl3
NS            16
DS            4
SWH           4873.284 Hz
FIDRES        0.148721 Hz
AQ            3.3620467 sec
RG            181
DW            102.600 usec
DE            6.50 usec
TE            298.0 K
TD0           1
===== CHANNEL f1 =====
NUC1          1H
P1            9.35 usec
PL1           0.00 dB
SFO1          27.375623 W
SI            32768
SF            500.260130 MHz
WDW           EM
SSB           0
LB            0.20 Hz
GB            0
PC            1.00
  
```





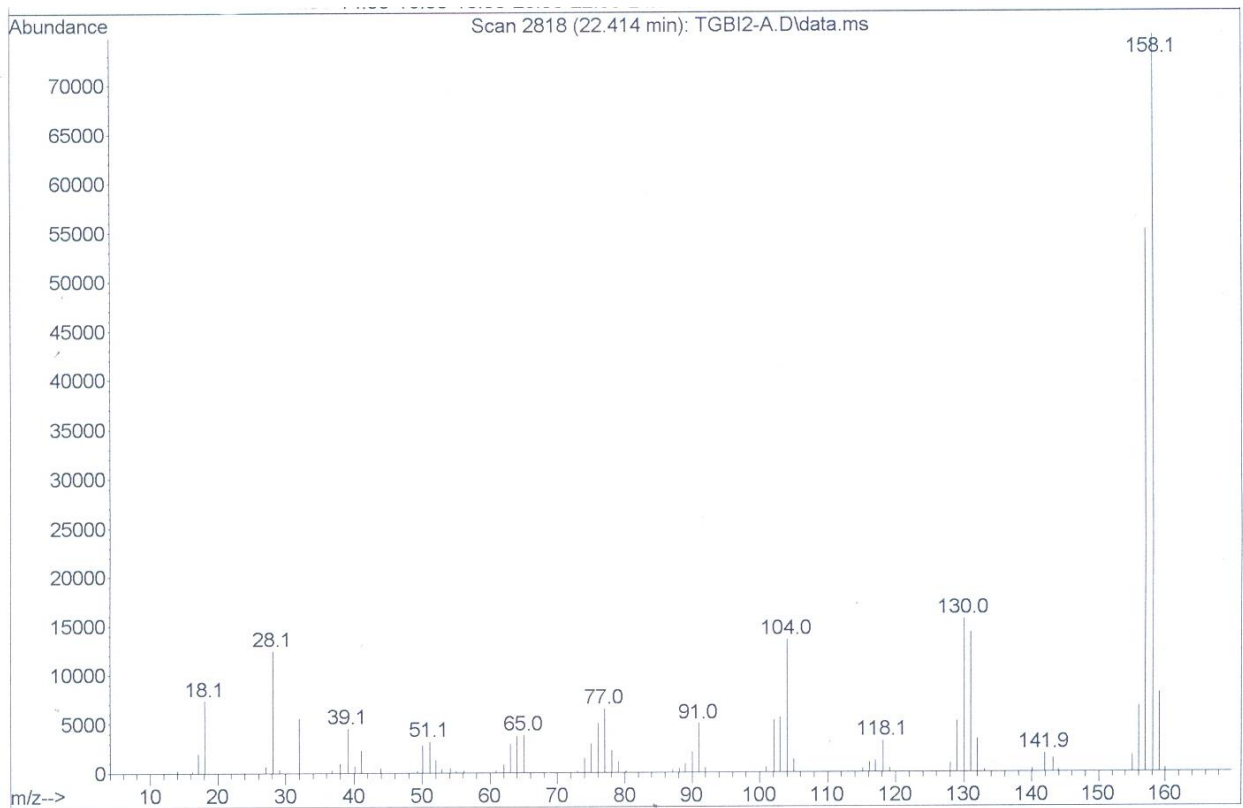
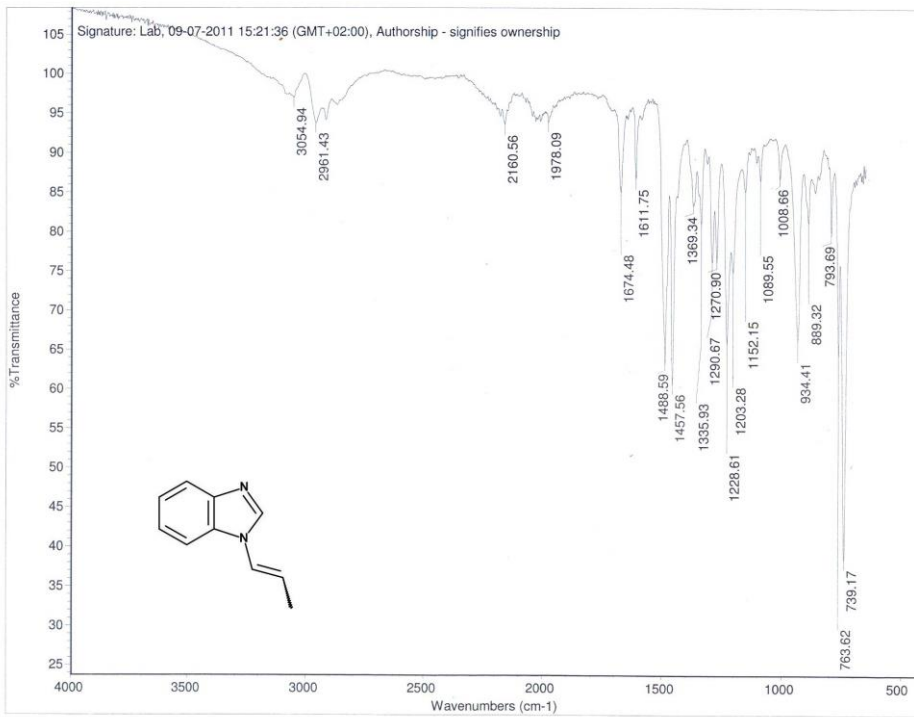
```

NAME          NV5
EXNO          2
PROCHO       1
Date_        20101006
Time         13.06
INSTRUM      spect
PFORMO       5 mm BBO BB-1H
PULPROG      zgpg30
TD           32768
SOLVENT      CDCl3
NS           805
DS           4
SWH          25761.904 Hz
FIDRES       0.908261 Hz
AQ           0.550524 sec
RG           812
DW           16.800 usec
DE           6.50 usec
TE           298.0 K
D1           2.00000000 sec
D11          0.03000000 sec
TDO          1

----- CHANNEL f1 -----
NUC1         13C
P1           11.50 usec
PL1          3.00 dB
PLLW        32.22848892 W
SFO1        125.8941140 MHz

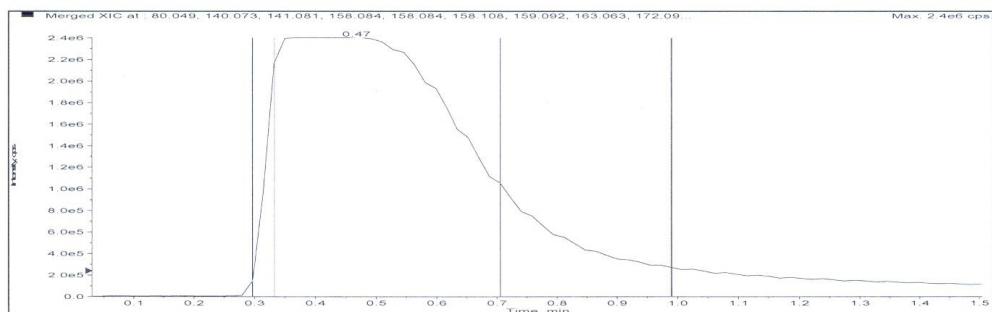
----- CHANNEL f2 -----
CPDPRG2      waltz16
NUC2         1H
P2           80.00 usec
PL2          1.20 dB
PL12        18.40 dB
PL13        18.40 dB
PL2W        20.76952171 W
PL1W        0.19575511 W
PL13W       0.39575511 W
SFO2        500.2620786 MHz
SI           32768
SF          125.7904835 MHz
WDW          EM
SSB          0
LB           1.50 Hz
GB           0
PC           1.40

```

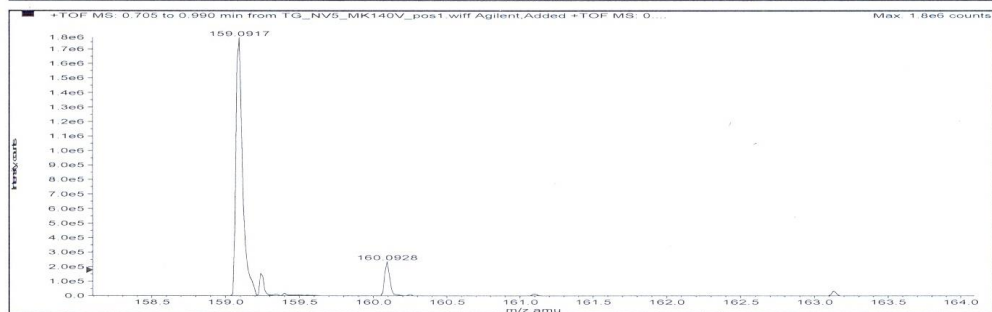
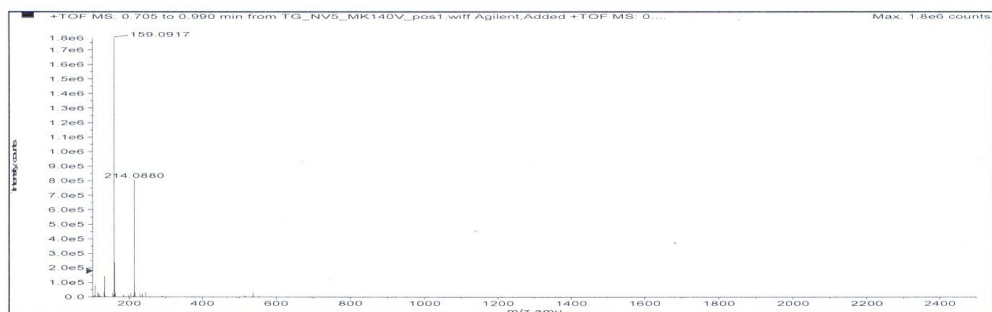


Sample Name: NV5 Sample Location: P1-D4 Sample Id: Operator: Milka
 Data File Name: D:\PE Sciex Data\Projects\Farmaceutski fakultet\Data\TG_NV5_MK140V_pos1.wiff Acq Time: December 10 2010,
 01:25:13 PM
 Method: D:\TOF_Data\damethods\Night_Seq_Comp_ident1.anmlefc.xml

One or more scans have failed IRM. Review the data file for details.

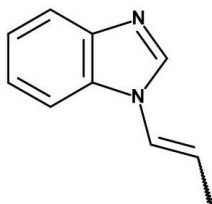


Merged XIC, Period# : 1 Experiment# : 1



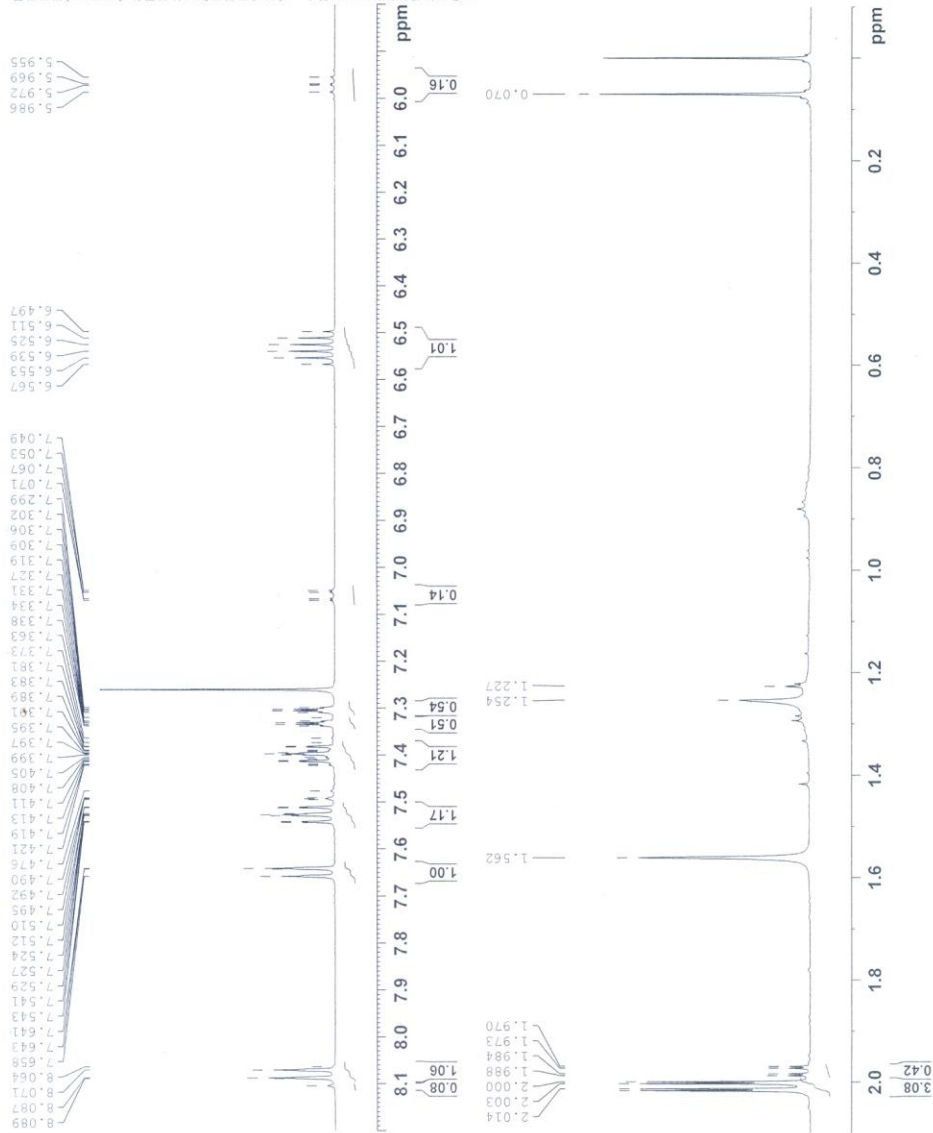
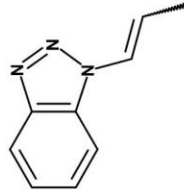
Formula	Compound name	Mass	Peak RT (min)	Peak area	Description
C10H10N2	--	158.08440	0.47	5.57397 E7	--

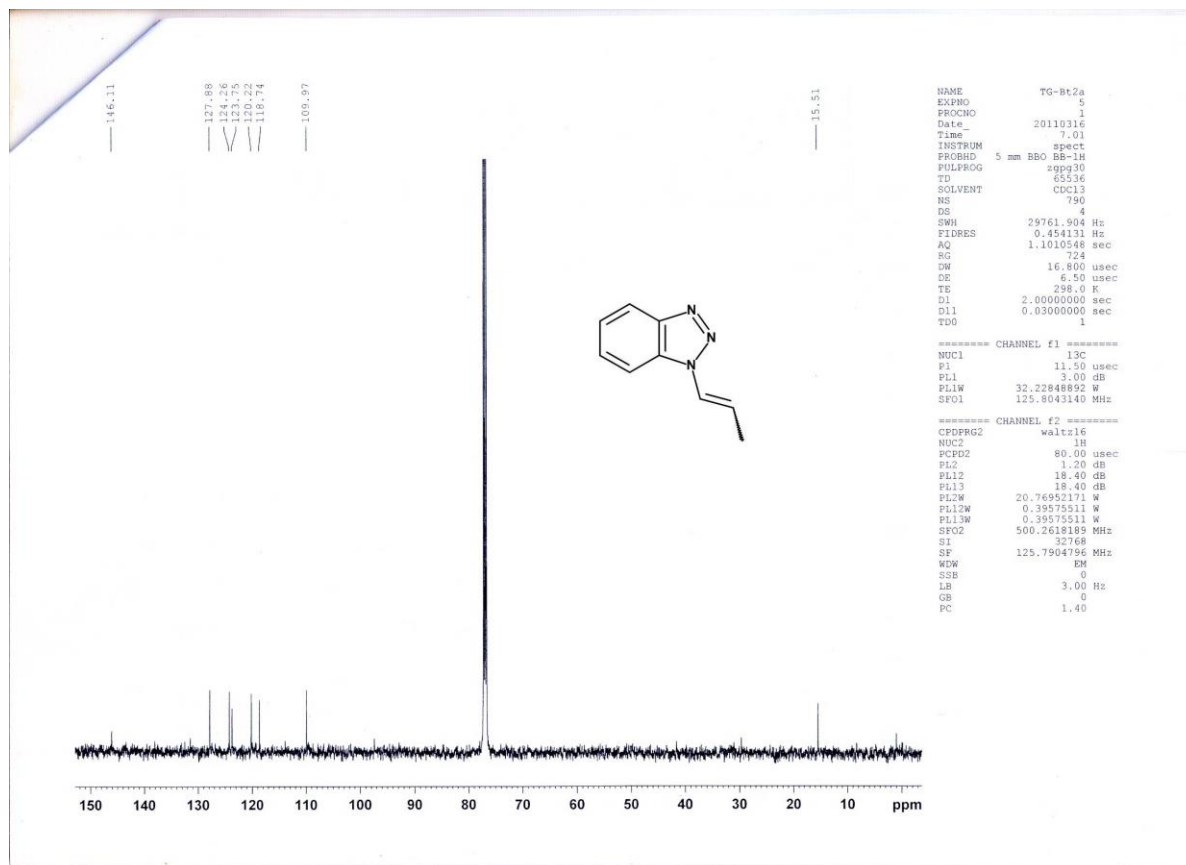
Species	Abundance (counts)	Ion Mass	Measured Mass	Error (mDa)	Error (ppm)	Ret. Time Error (min)
[M+H] ⁺	1808648.31	159.09167	159.09170	0.02656	0.17	--

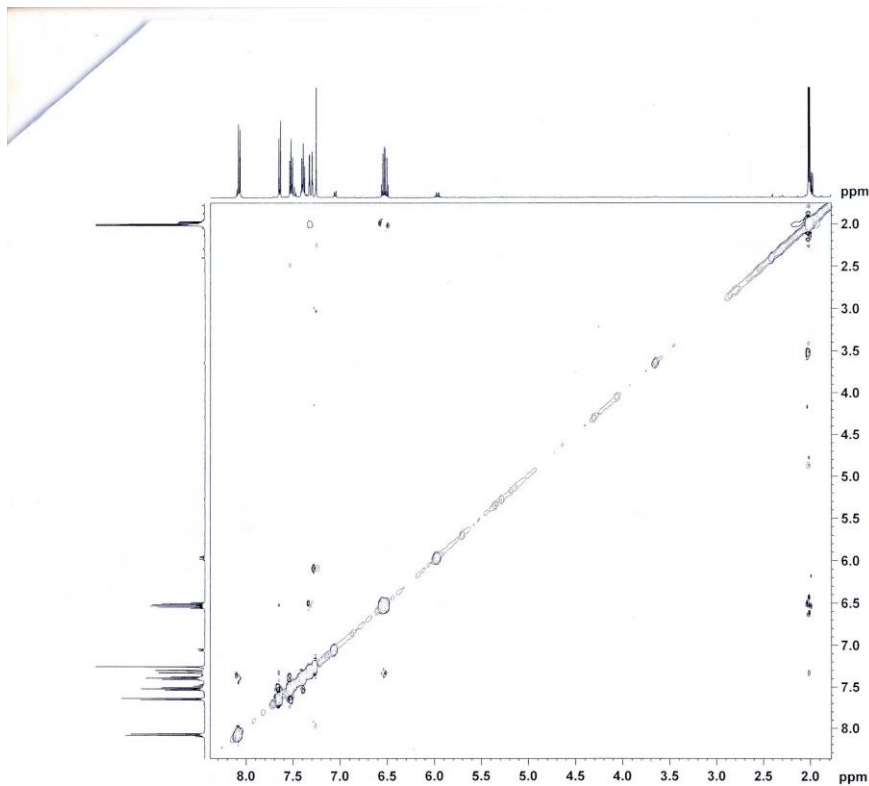


Compounds 12

NAME TC-B12a
 F11
 Date 20110316
 Time 6.53
 INSTRUM spect
 PROBEID 5 mm BB-1H
 TD 32768
 TD0 1
 SOLVENT CDCl3
 NS 32
 DS 0
 SWH 5000.000 Hz
 F1 9.35 usec
 F2 0.00 usec
 AQ 3.276800 sec
 RG 406
 TDW 100.000 usec
 DE 6.50 usec
 TE 298.0 K
 DT 0.00 sec
 TDO 2.0000000 sec







```

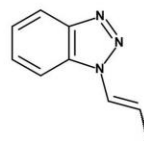
NAME          TG-BL2a
EXPNO         1
PROCNO        1
Date_         20110316
Time          7.36
INSTRUM       spect
PROBHD        5 mm BBO BB-H
PULPROG       zgpg30
TD            1024
SOLVENT       CDCl3
NS            8
DS            16
SWH           5000.000 Hz
FIDRES       4.882813 Hz
AQ           0.1024500 sec
RG            406
SW           160.000 usec
DE           6.50 usec
TE           298.0 K
DC           0.0000000 sec
D1           2.0000000 sec
DS           1.0000000 sec
INO           0.0001990 sec

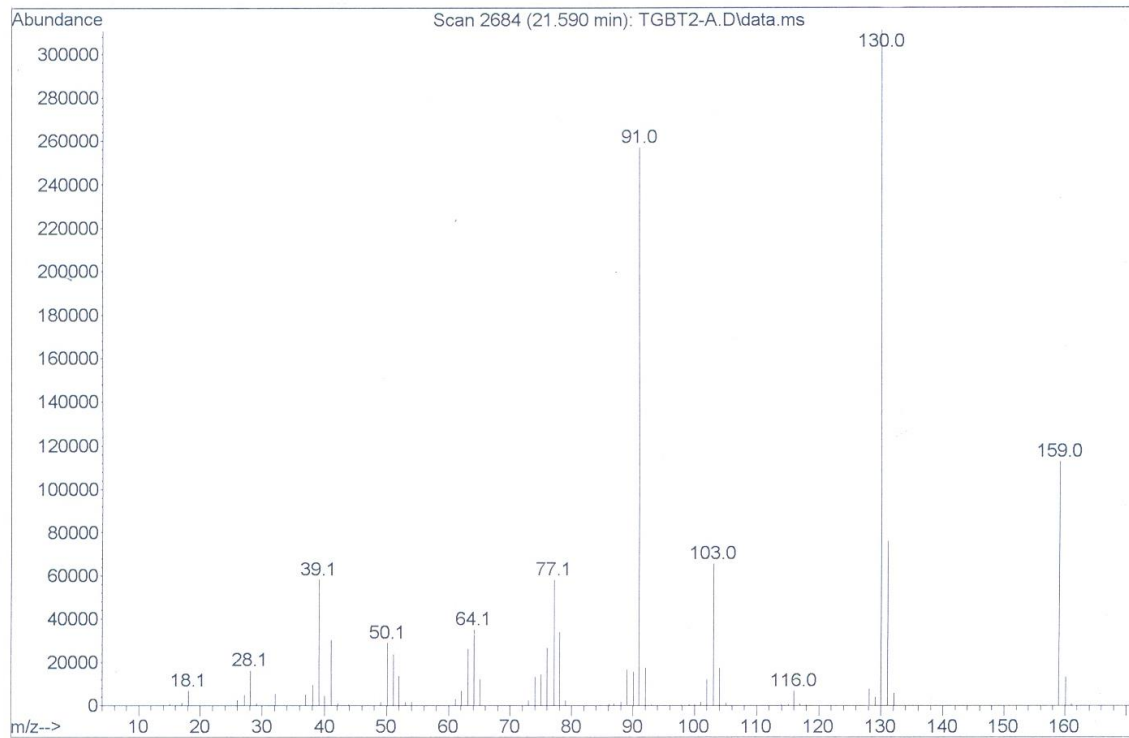
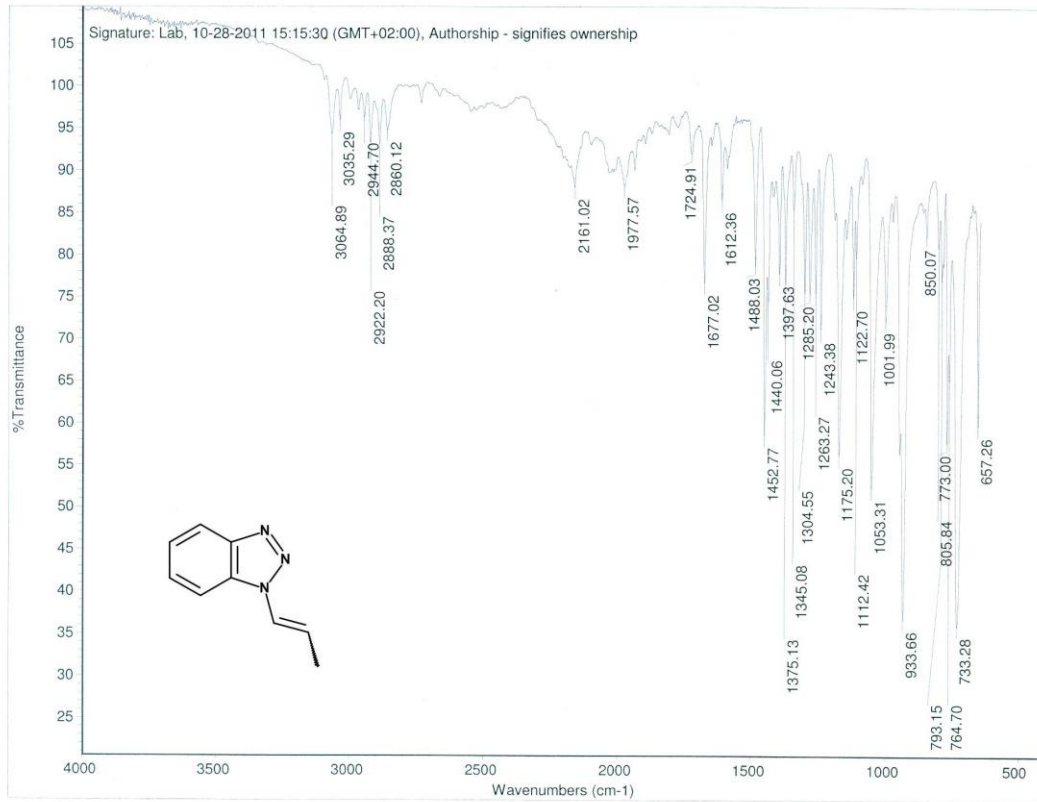
```

```

----- CHANNEL f1 -----
NUC1          1H
P1            9.25 usec
PL1           0.00 dB
PL1W         27.37296238 W
SFO1         500.2621011 MHz
RG            1
TD            128
SFO1         500.26211 MHz
FIDRES       39.082977 Hz
SW           10.000 ppm
PRMODE       States-TPPI
SI            512
SF           500.2600064 MHz
WDW          Q3LINE
SSB           2
LB            0.00 Hz
GB            0
PC            1.00
CI            512
MC2          States-TPPI
SF           500.2600103 MHz
WDW          Q3LINE
SSB           2
LB            0.00 Hz
GB            0

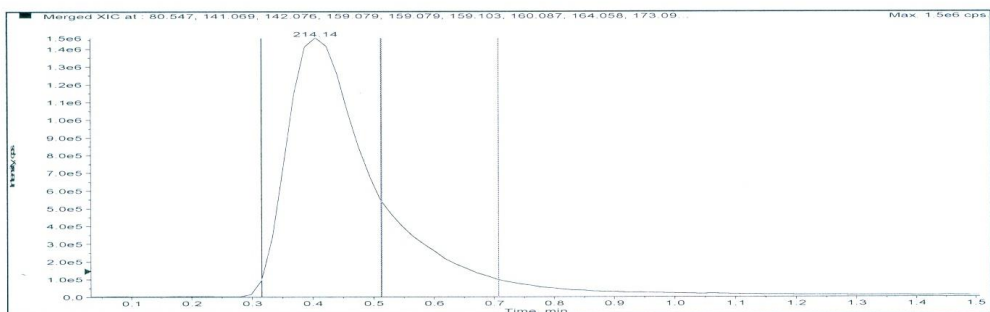
```



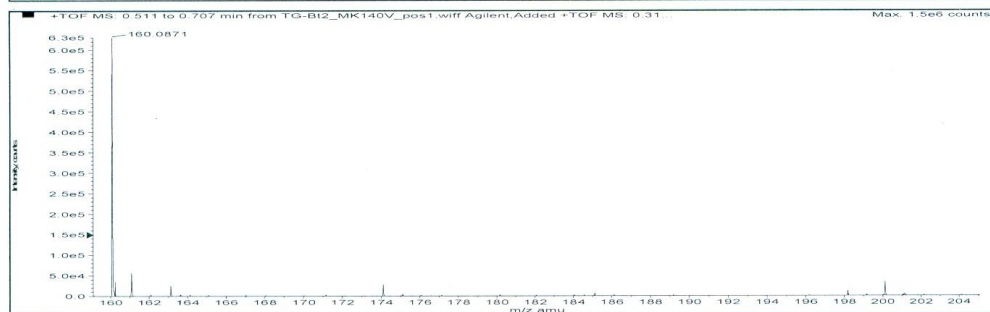
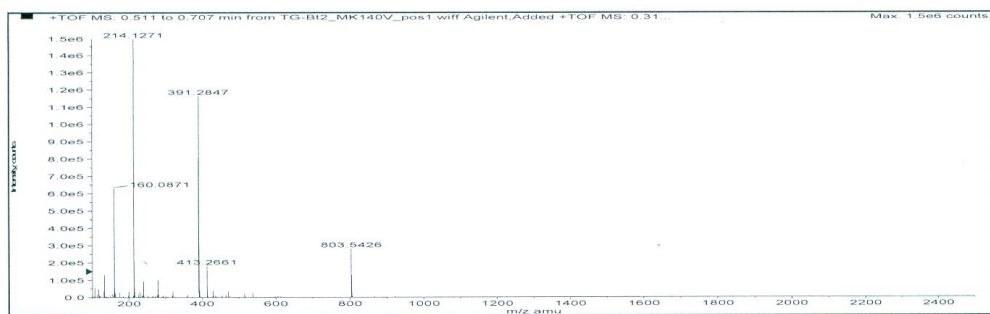


Sample Name: TG-Bt2 Sample Location: P1-D3 Sample Id: Operator: Milka
 Data File Name: D:\PE_Sciex_Data\Projects\Farmaceutski fakulteti\Data\TG-Bt2_MK140V_pos1.wiff Acq Time: November 12 2010,
 02:05:46 PM
 Method: D:\TOF_Data\damethods\Night_Seq_Comp_ident1.anmlefc.xml

One or more scans have failed IRM. Review the data file for details.

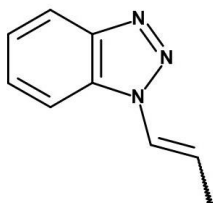


Merged XIC, Period# : 1 Experiment# : 1

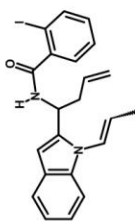


Formula	Compound name	Mass	Peak RT (min)	Peak area	Description
C9H9N3	--	159.07965	0.40	1.46881 E7	--

Species	Abundance (counts)	Ion Mass	Measured Mass	Error (mDa)	Error (ppm)	Ret. Time Error (min)
[M+H] ⁺	648951.48	160.08692	160.08708	0.15564	0.97	--
[M+CH3CN] ⁺	33814.14	200.10565	200.11844	12.79212	63.92	--



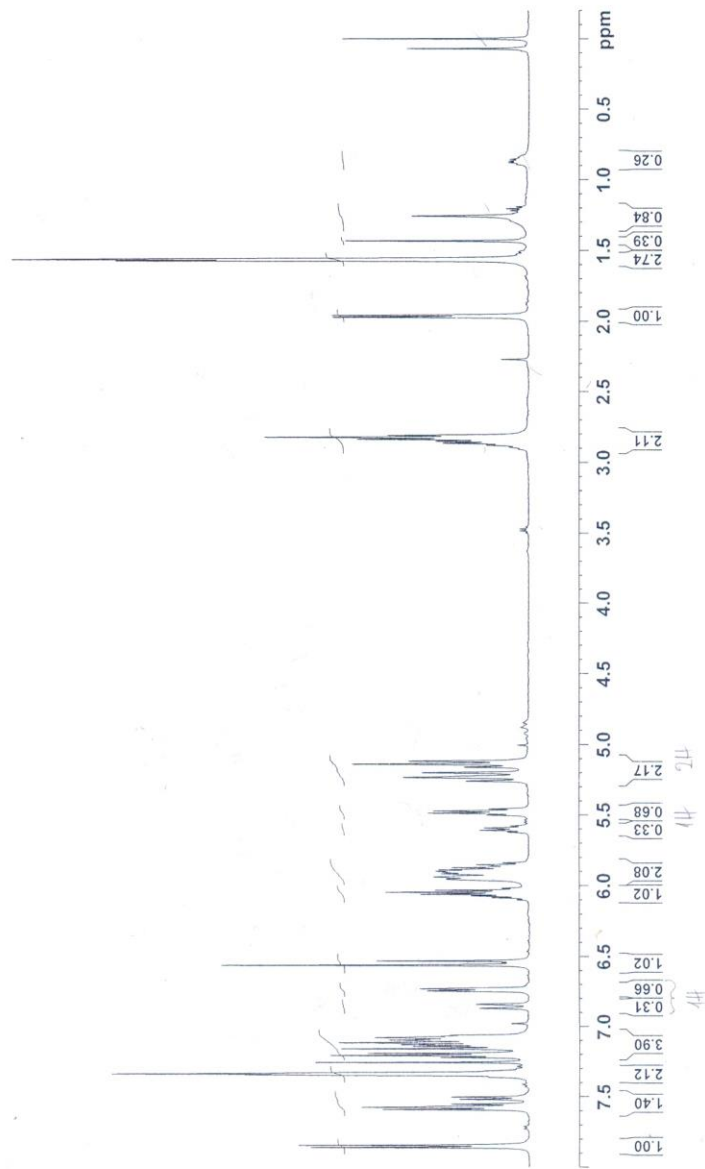
Compound 14

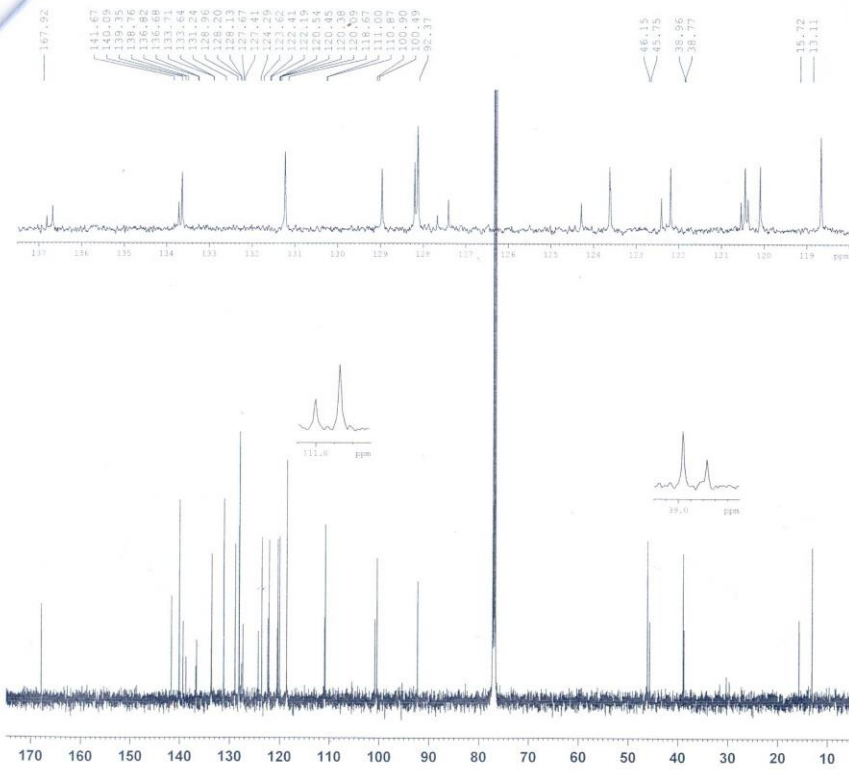


```

NAME          TG-9
EXPNO         1
PROCNO        1
F2ACQ0        20100315
Time_         15.31
INSTRUM       spect
PROBHD        5 mm BBO BB-1H
PULPROG       zgpg30
TD            32768
SOLVENT       CDCl3
NS            10
DS            1
SWH           4716.981 Hz
FIDRES        0.143951 Hz
AQ            3.4734581 sec
RG            256
DM            106.000 usec
DE            6.00 usec
TE            300.2 K
D1            2.00000000 sec
TD0           1

===== CHANNEL f1 =====
NUC1          1H
P1            9.35 usec
PL1           0.00 dB
PT1M         27.37965550 sec
SFO1          500.2619936 MHz
SI            32768
SF            500.2600172 MHz
WDW           EM
SSB           0
LB            0.20 Hz
GB            0
PC            1.00
    
```



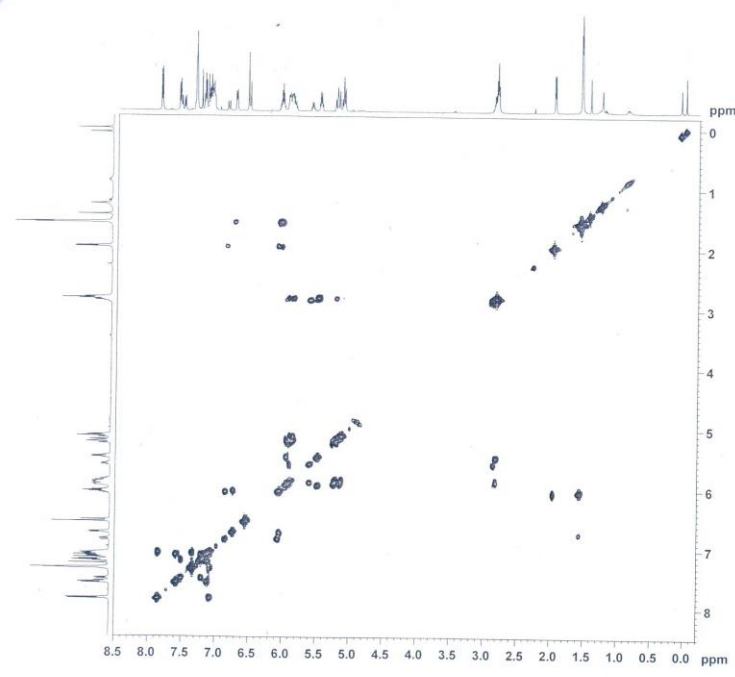
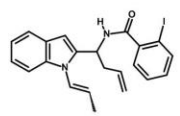


```

NAME          TG-91
EXPNO         5
PROCNO        1
Date_         20100315
Time          16.32
INSTRUM       spect
PROBHD        5 mm BBO BB-1H
PULPROG       zgpg30
TD            32768
SOLVENT       CDCl3
NS            643
DS            4
SWH           25761.904 Hz
FIDRES        0.908261 Hz
AQ            0.5505524 sec
RG            3440
DM            16.800 usec
DE            6.50 usec
TE            298.0 K
D1            2.0000000 sec
d11           0.0300000 sec
TDO           1

----- CHANNEL F1 -----
NUC1          13C
P1            11.50 usec
PL1           3.00 dB
PL1W          32.22848862 W
SFO1          125.8043140 MHz

----- CHANNEL F2 -----
CPDPRG2       waitz16
NUC2          1H
PCPD2         80.00 usec
PL2           1.20 dB
PL12          18.40 dB
PL13          18.40 dB
PL1W          20.76952171 W
PL2W          0.39575511 W
PL13W         0.39575511 W
SFO2          500.2619935 MHz
SI            32768
SF            125.7904814 MHz
WDW           EM
SSB           0
LB            1.50 Hz
GB            0
PC            1.40
  
```

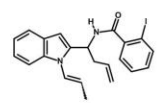


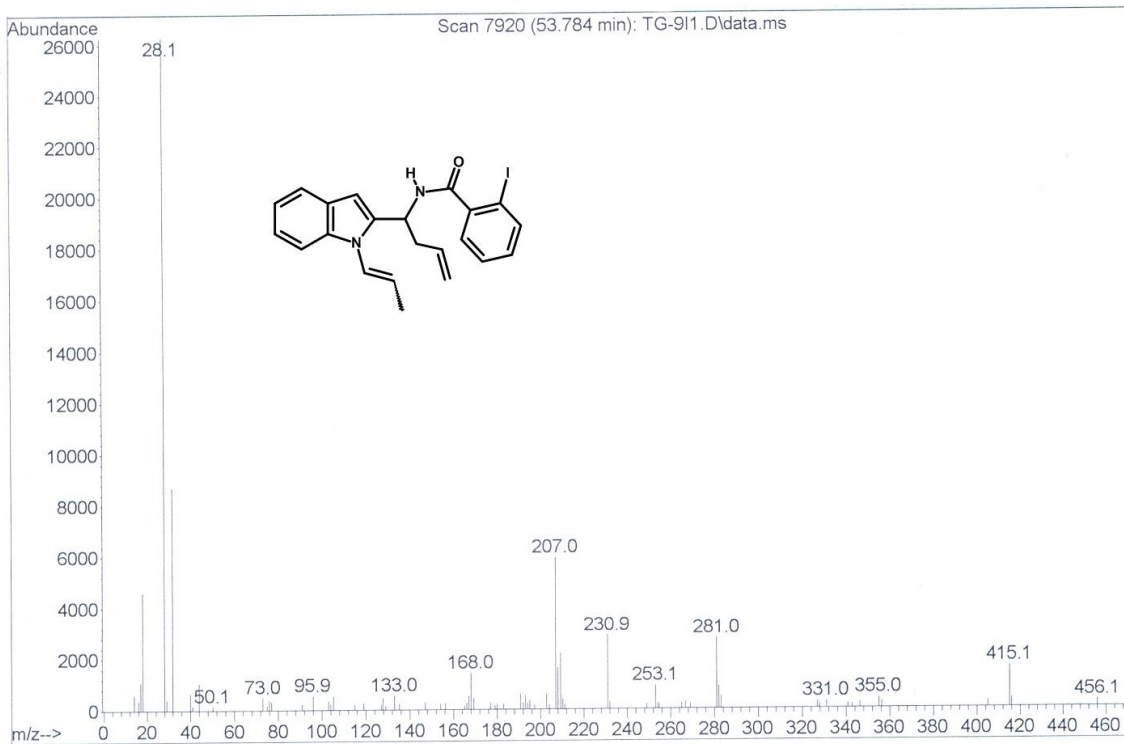
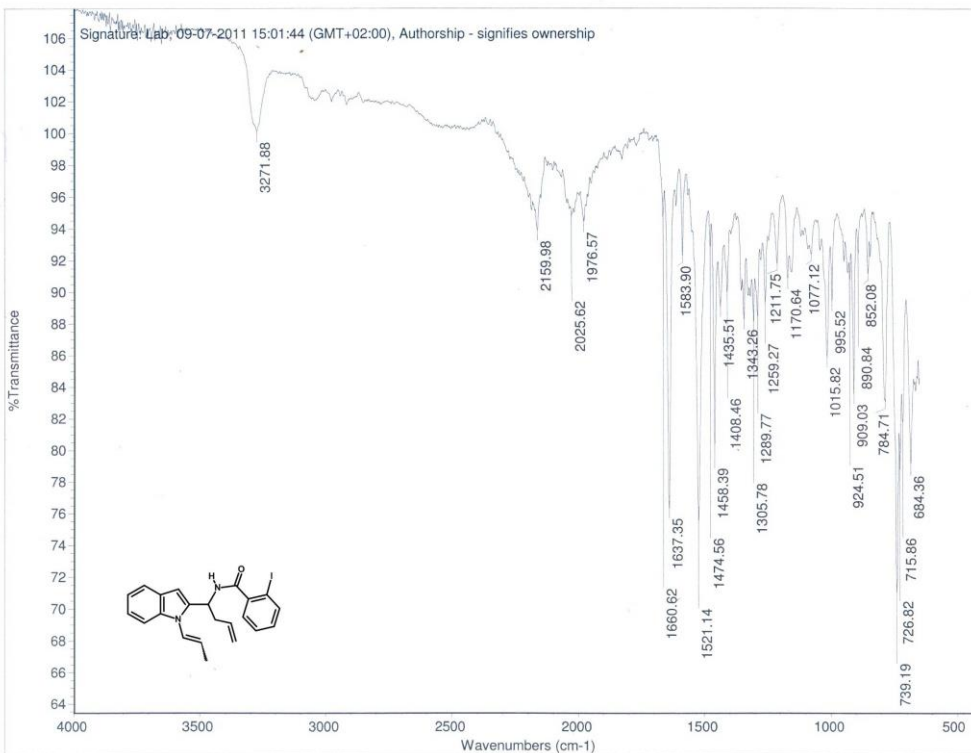
```

NAME          TG-91
EXPNO         1
PROCNO        1
Date_         20100315
Time          15.47
INSTRUM       spect
PROBHD        5 mm BBO BB-1H
PULPROG       zgpg30
TD            1024
SOLVENT       CDCl3
NS            64
DS            4
SWH           4716.901 Hz
FIDRES        8.404417 Hz
AQ            0.1982940 sec
RG            296
DM            104.000 usec
DE            6.50 usec
TE            291.0 K
D1            0.0000000 sec
d11           1.0000000 sec
d12           0.0000400 sec
T1R          0.0002000 sec
T1G          0.0002100 sec

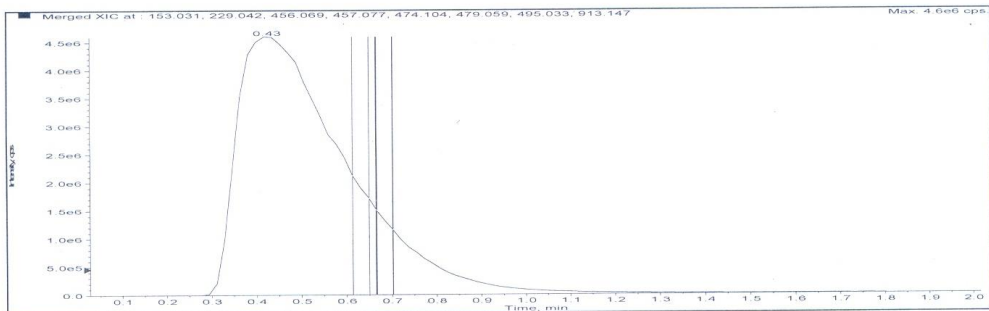
----- CHANNEL F1 -----
NUC1          1H
P1            9.15 usec
PL1           0.00 dB
PL1W          27.37956238 W
SFO1          500.2619935 MHz

----- GRADIENT CHANNEL -----
GPMAG1        SINE 100
GZ1           10.00 V
P1G           1000.00 usec
MAG1          1
TD            128
SFO2          500.2602 MHz
FIDRES        36.891330 Hz
SF            9.429 ppm
PULSEPRG      CP
SF            500.260128 MHz
WDW           SINE
SSB           0
LB            0.00 Hz
GB            0
PC            1.40
SI            512
MAG2          CP
SF            300.2600114 MHz
WDW           SINE
SSB           0
LB            0.00 Hz
GB            0
  
```

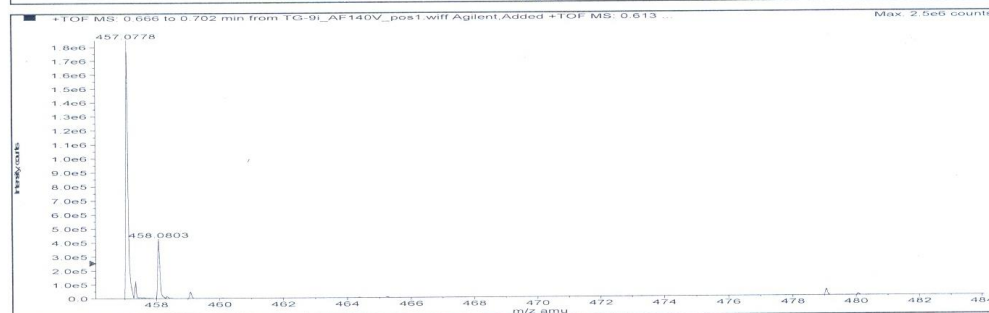
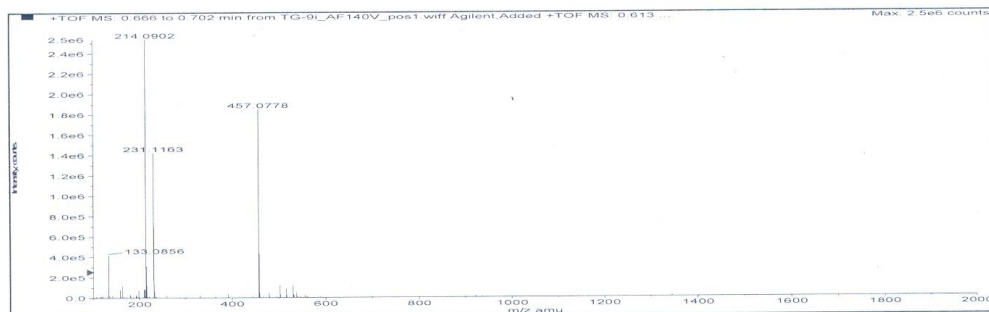




Sample Name: TG-9I Sample Location: P1-C6 Sample Id: Operator: Milka
 Data File Name: D:\PE Sciex Data\Projects\Farmaceutski fakultet\Data\TG-9I_AF140V_pos1.wiff Acq Time: November 02 2011,
 01:28:01 PM
 Method: D:\TOF_Data\damethods\Night_Seq_Comp_ident1.anml\efc.xml

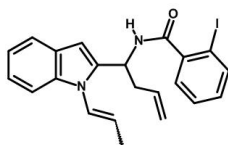


Merged XIC, Period# : 1 Experiment# : 1

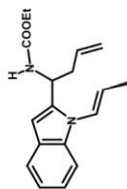


Formula	Compound name	Mass	Peak RT (min)	Peak area	Description
C22H21N2O	--	456.06986	0.43	7.67715 E7	--

Species	Abundance (counts)	Ion Mass	Measured Mass	Error (mDa)	Error (ppm)	Ret. Time Error (min)
[M+H] ⁺	1849025.23	457.07713	457.07780	0.66274	1.45	--
[M+Na] ⁺	45633.57	479.05908	479.05918	0.09931	0.21	--

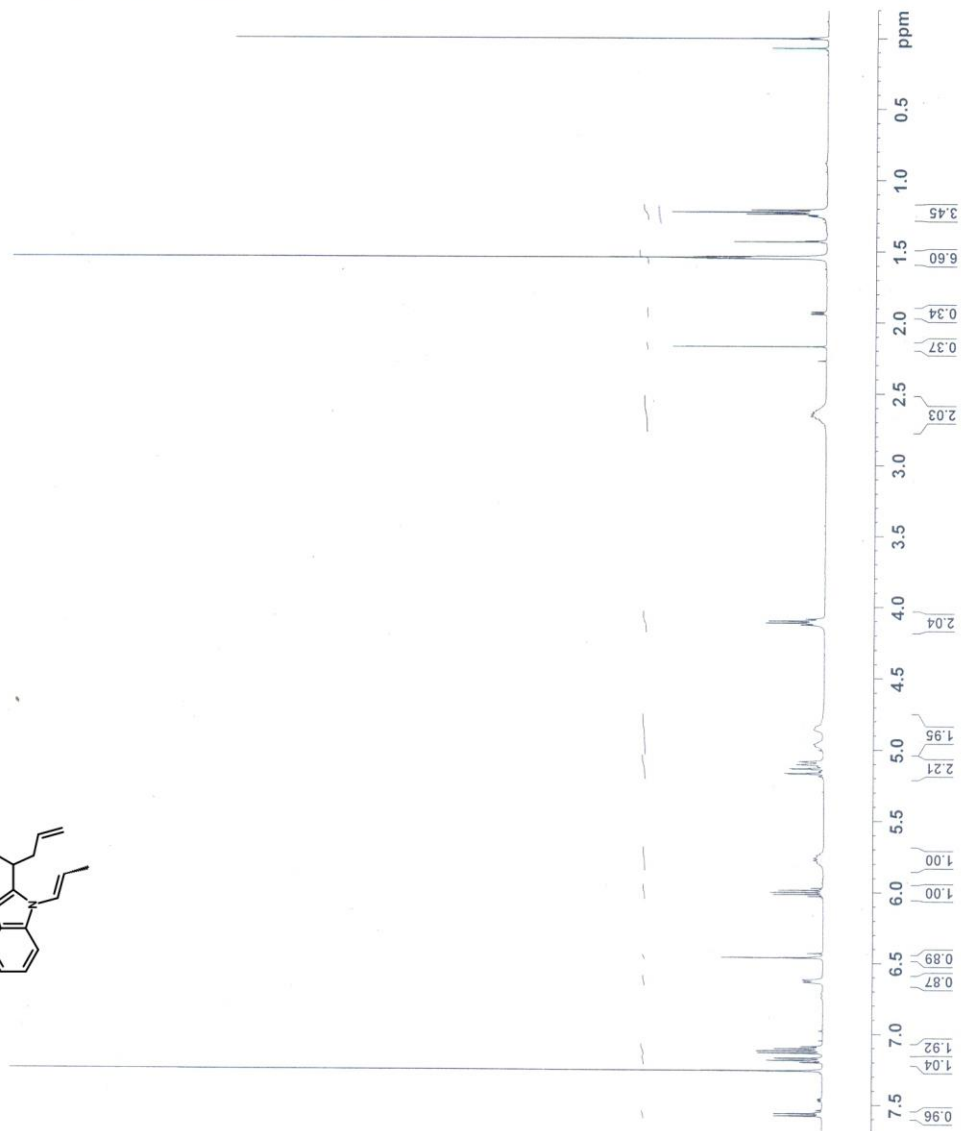


Compound 16



```

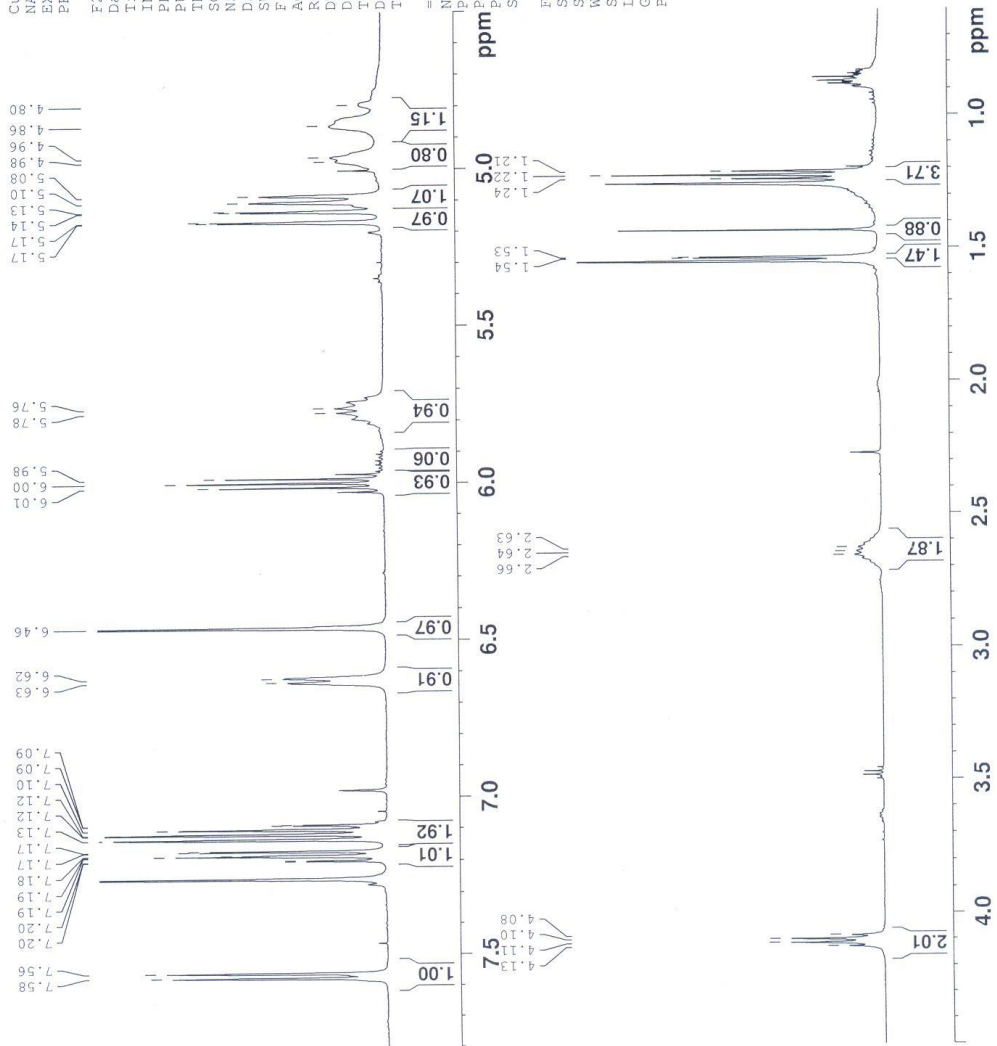
NAME          TG-160
EXPNO         1
PROCNO        1
PROC        20110513
PULPROG       zgpg30
INSTRUM       spect
PROBHD        5 mm BBO BB-1H
PULPROG       zgpg30
TD            32768
SOLVENT       CDCl3
NS            70
DS            4
SWH           4746.835 Hz
FIDRES        0.144862 Hz
AQ           3.4516127 sec
RG           105.256
DE           1.05330 usec
TE           298.0 K usec
D1           2.00000000 sec
TD0          1
===== CHANNEL f1 =====
NUC1          1H
P1           9.35 usec
PL1          0.00 dB
PL1W         27.37956238 W
SFO1         500.2618954 MHz
SI           32768
WDW          EM
SSB          0
LB           0.20 Hz
GB           0
PC           1.00
  
```

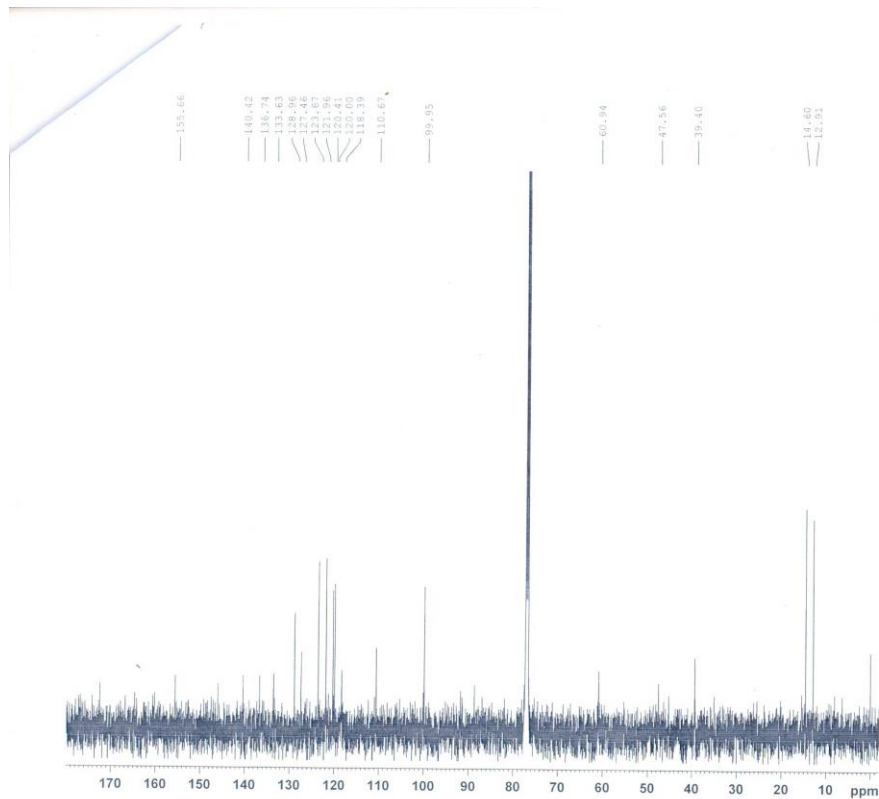


Current Data Parameters
 NAME TC-246
 EXPNO 1
 PROCNO 1

F2 - Acquisition Parameters
 Date_ 20111212
 Time_ 8:18
 INSTRUM spect
 PROBHD 5 mm BBO BB-H
 PULPROG zg30
 ID 32768
 SOLVENT CDCl3
 NS 64
 DS 0
 SWH 5000.000 Hz
 FIDRES 0.152588 Hz
 AQ 3.2768500 sec
 RG 287
 DW 100.000 usec
 DE 6.50 usec
 TE 298.0 K
 TD0 2.00000000 sec
 D1 1

===== CHANNEL f1 =====
 NUC1 1H
 P1 9.35 usec
 PL1 0.00 dB
 PL1W 27.37956238 W
 SF01 500.2620208 MHz
 F2 - Processing parameters
 SI 32768
 SF 500.2600156 MHz
 WDW EM
 SSB 0
 LB 0.20 Hz
 GB 0
 PC 1.00





```

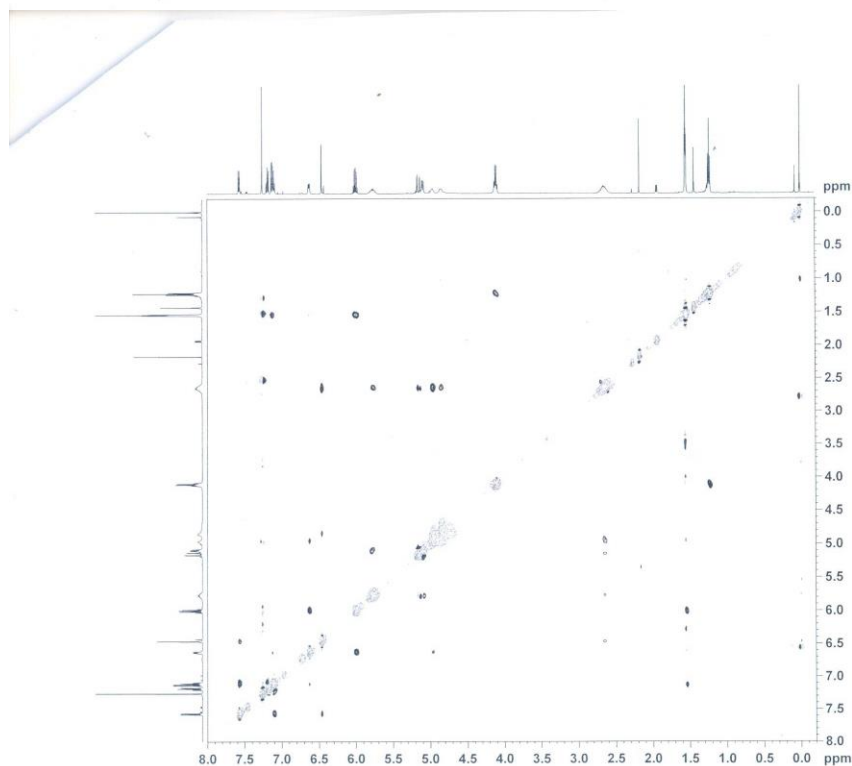
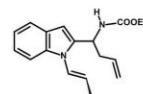
NAME      TG-160
EXPNO    2
PROCNO   1
Date_    20110513
Time     14.22
INSTRUM  spect
PROBHD   5 mm BBO BB-1H
PULPROG  zgpg30
TD        32768
SOLVENT  CDCl3
NS        2000
DS        4
SWH       25761.504 Hz
FIDRES   0.908261 Hz
AQ        0.5505524 sec
RG        724
AQ        16.800 usec
DE        6.50 usec
TE        298.0 K
D1        2.0000000 sec
D11       0.0300000 sec
TD0       1
  
```

```

----- CHANNEL f1 -----
NUC1      13C
P1        11.50 usec
PL1       3.00 dB
PL1W     32.22848892 W
SF01     125.8043140 MHz
  
```

```

----- CHANNEL f2 -----
CDDPRG2  waltz16
NUC2      1H
PCPDZ    80.00 usec
PL2       1.20 dB
PL12     18.40 dB
PL13     18.40 dB
PL1W     20.76952171 W
EL12W   0.39575511 W
EL13W   0.39575511 W
SF02     500.2618955 MHz
SI        32768
SF        125.7904793 MHz
WDW      EM
SSB       0
GB         1.50 Hz
GB         0
PC         1.40
  
```

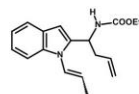


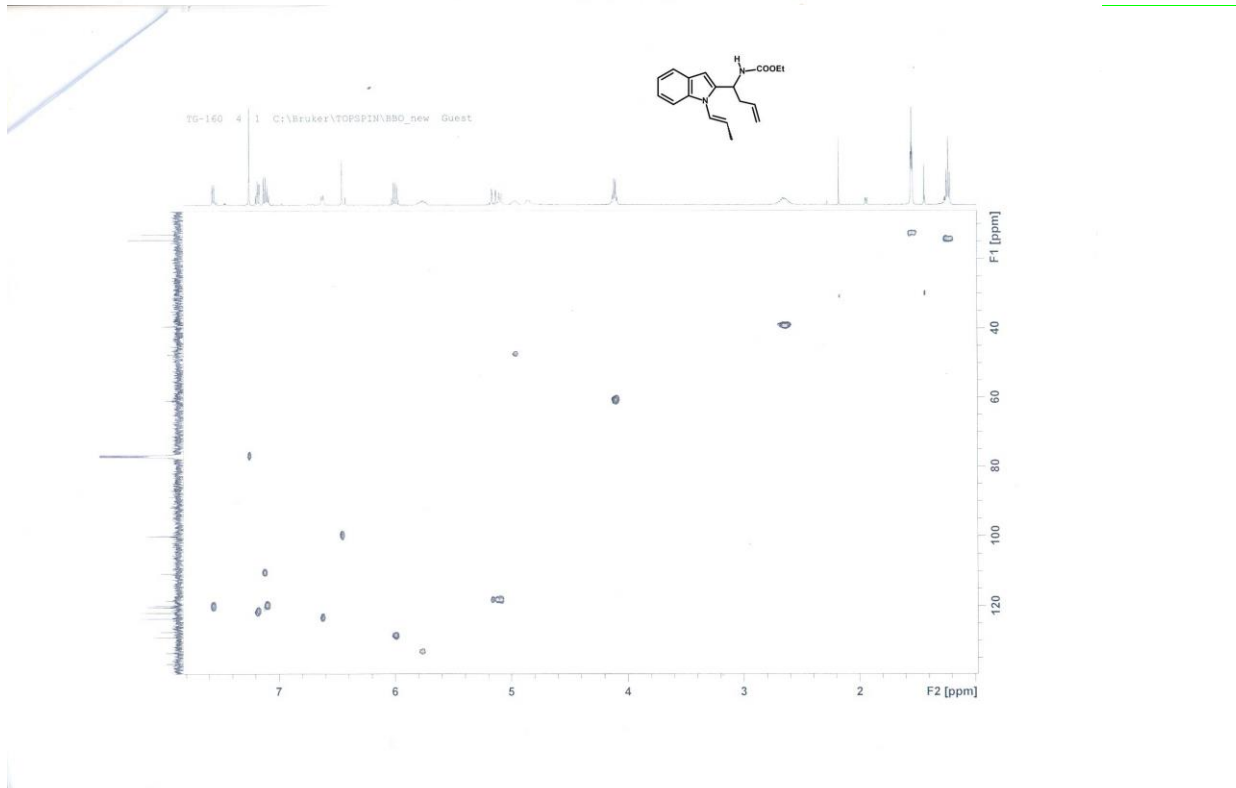
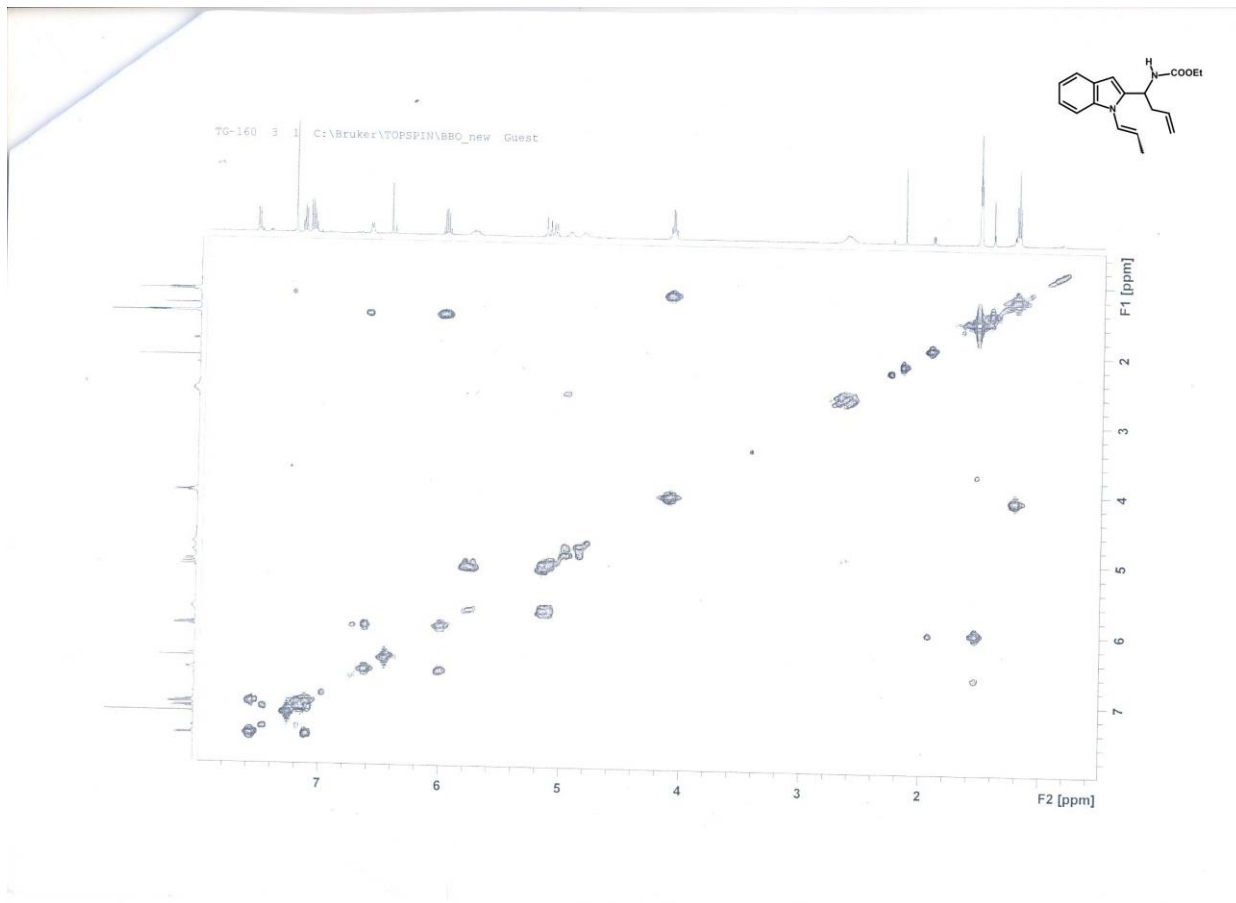
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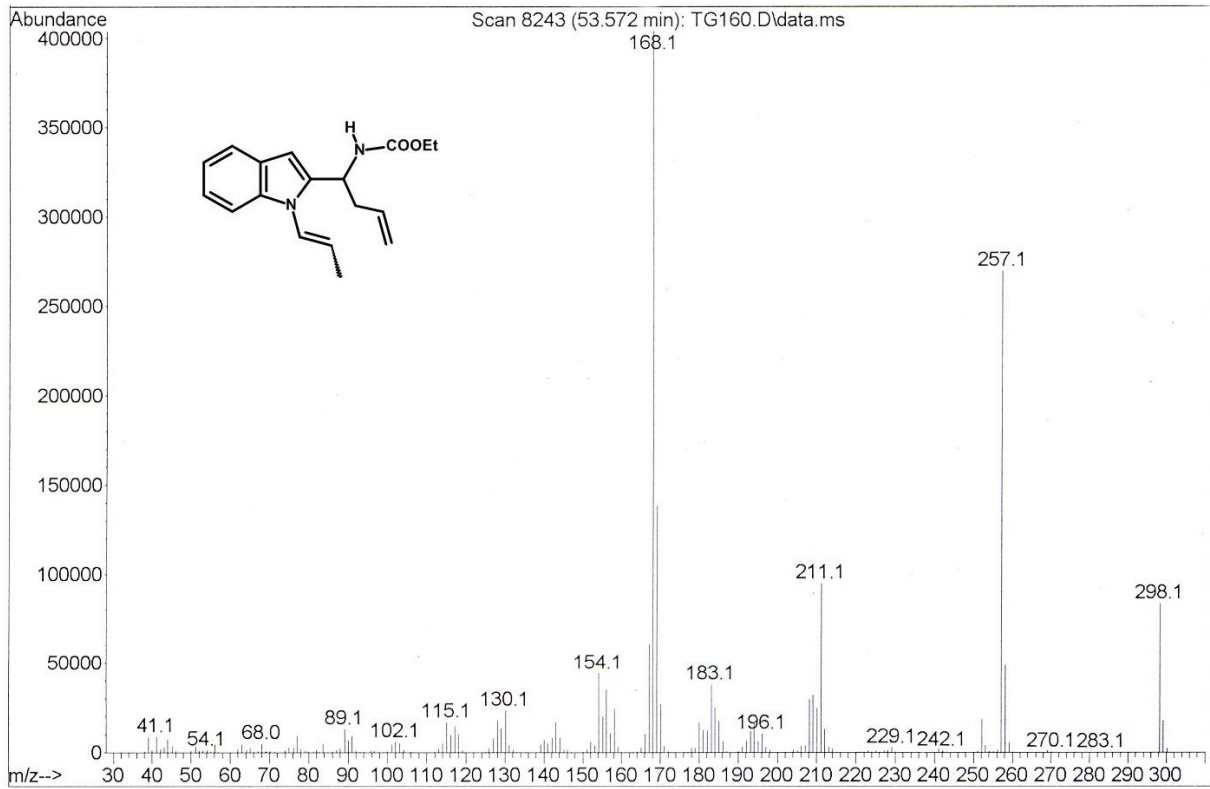
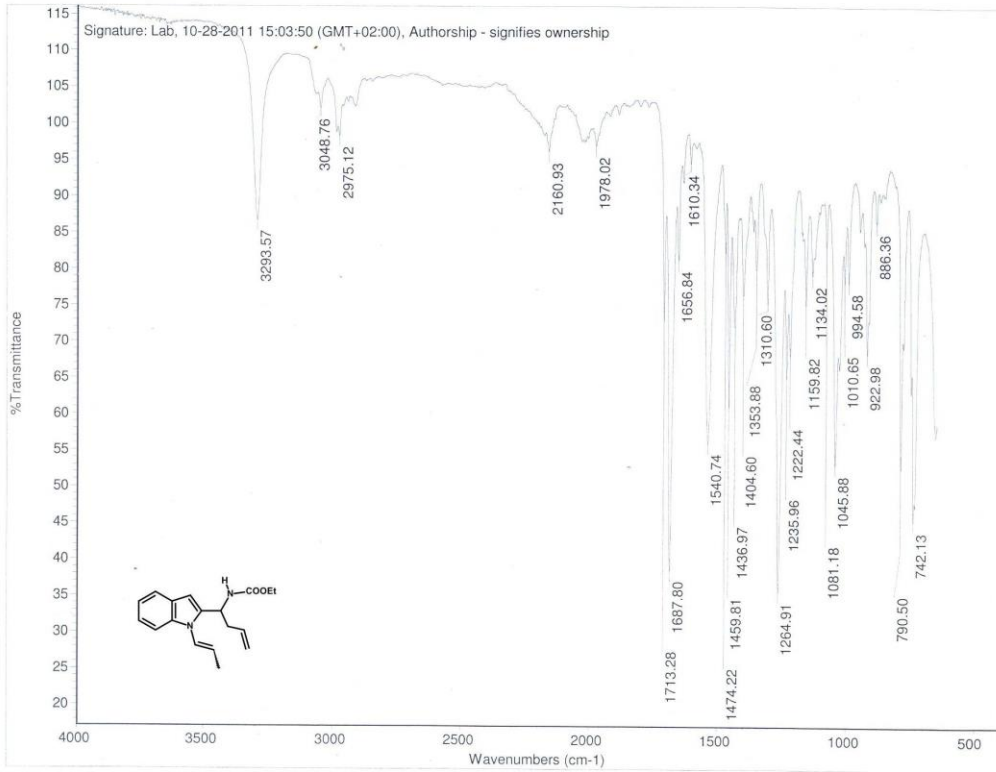
NAME      TG-160
EXPNO    1
PROCNO   1
Date_    20110513
Time     16.35
INSTRUM  spect
PROBHD   5 mm BBO BB-1H
PULPROG  nonezg
TD        1324
SOLVENT  CDCl3
NS        8
DS        16
SWH       4746.835 Hz
FIDRES   4.635581 Hz
AQ        0.1079113 sec
RG        258
AQ        109.333 usec
DE        6.50 usec
TE        298.0 K
D1        0.0000000 sec
D11       2.0000000 sec
D12       1.0000000 sec
D13       0.0001063 sec
  
```

```

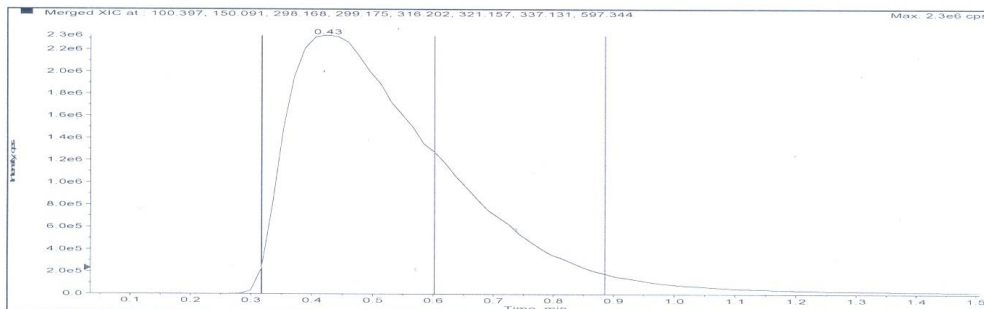
----- CHANNEL f1 -----
NUC1      1H
P1        9.35 usec
PL1       0.00 dB
PL1W     27.91946238 W
SF01     500.2618955 MHz
NUC2      13C
P2        138
SF02     500.2619 MHz
FIDRES   37.064668 Hz
SM        5.489 ppm
FMRDCX   States-TPT1
SI        512
SF        500.2601022 MHz
WDW      gq130
SSB       2
GB         0.00 Hz
PC         1.00
SI        512
MCX      States-TPT1
SF        500.2601024 MHz
WDW      gq130
SSB       2
GB         0.00 Hz
PC         0
  
```



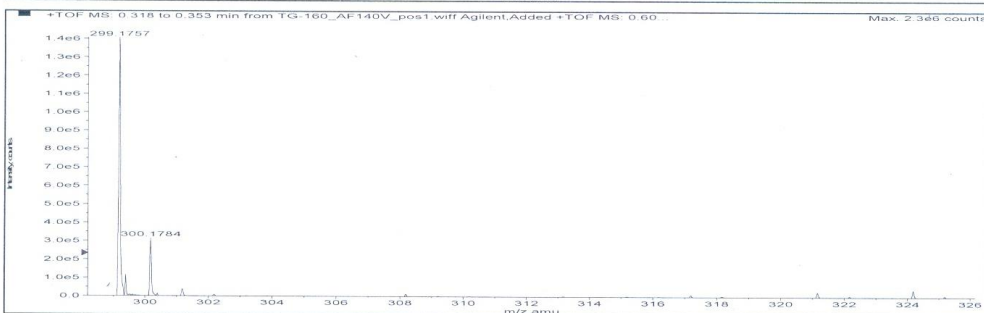
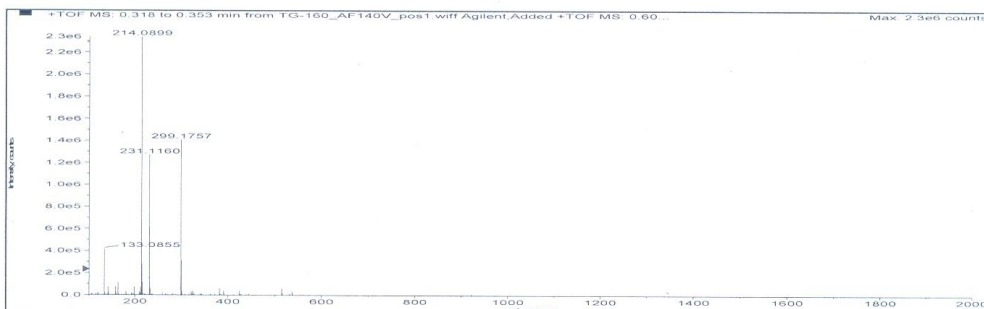




Sample Name: TG-160 Sample Location: P1-D1 Sample Id: Operator: Milka
 Data File Name: D:\PE Sciex Data\Projects\Farmaceutski fakultet\Data\TG-160_AF140V_pos1.wiff Acq Time: November 02 2011,
 01:39:26 PM
 Method: D:\TOF_Data\damethods\Night_Seq_Comp_ident1.anm\efc.xml

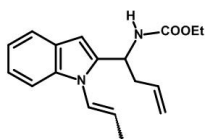


Merged XIC, Period# : 1 Experiment# : 1

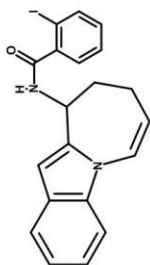


Formula	Compound name	Mass	Peak RT (min)	Peak area	Description
C18H22N2O2	--	298.16813	0.43	4.11011 E7	--

Species	Abundance (counts)	Ion Mass	Measured Mass	Error (mDa)	Error (ppm)	Ret. Time Error (min)
[M+H] ⁺	1485863.86	299.17540	299.17567	0.26518	0.89	--
[M+Na] ⁺	29108.30	321.15735	321.15755	0.20025	0.62	--



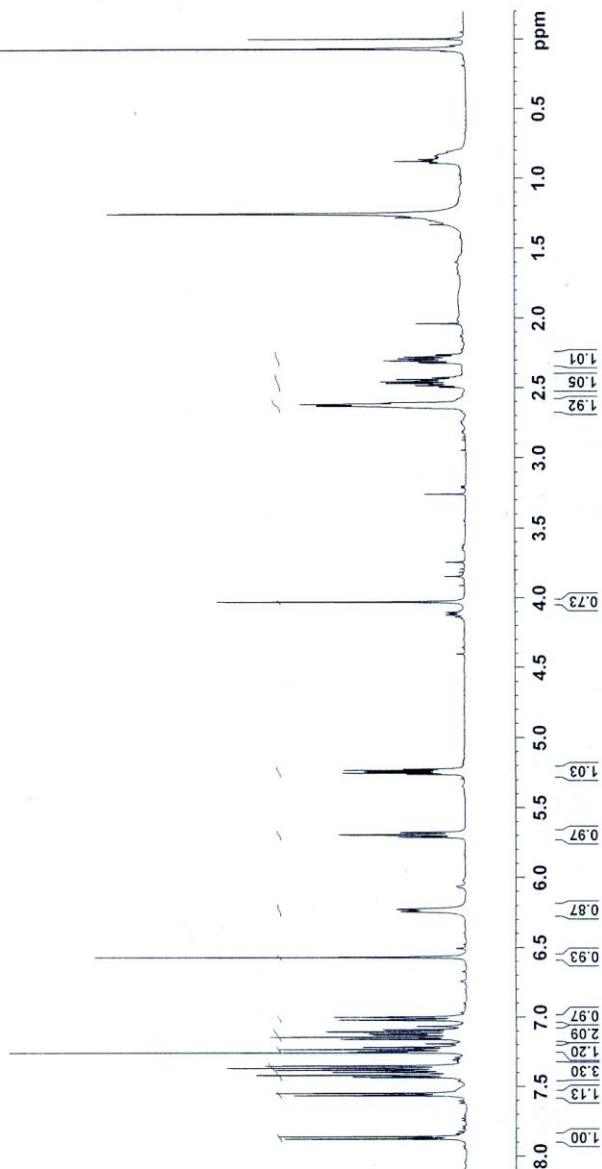
Compound 18

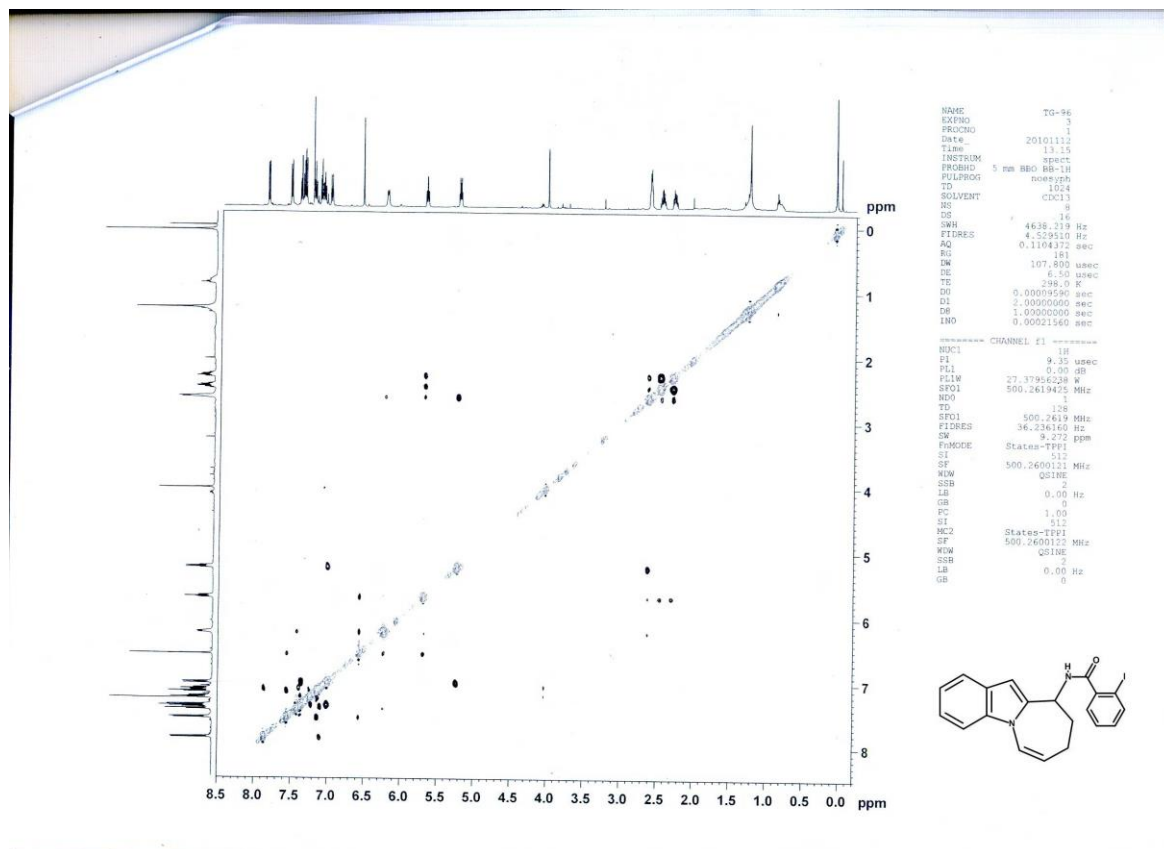
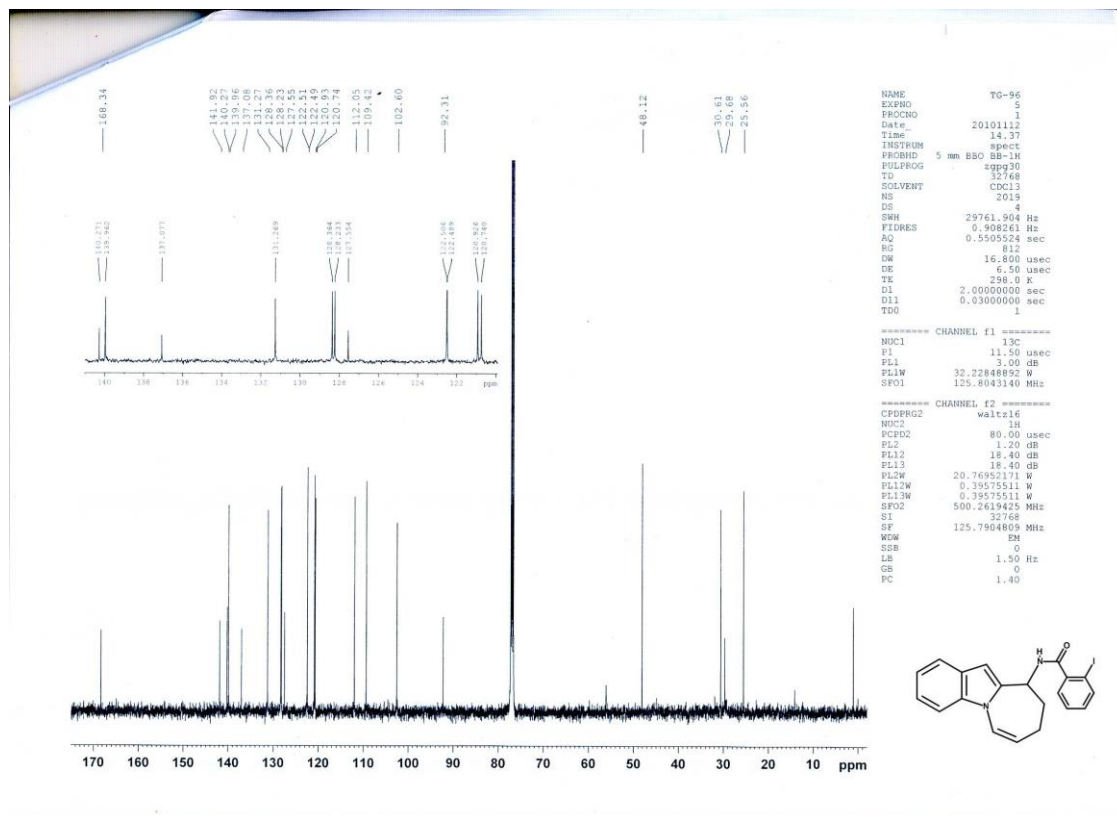


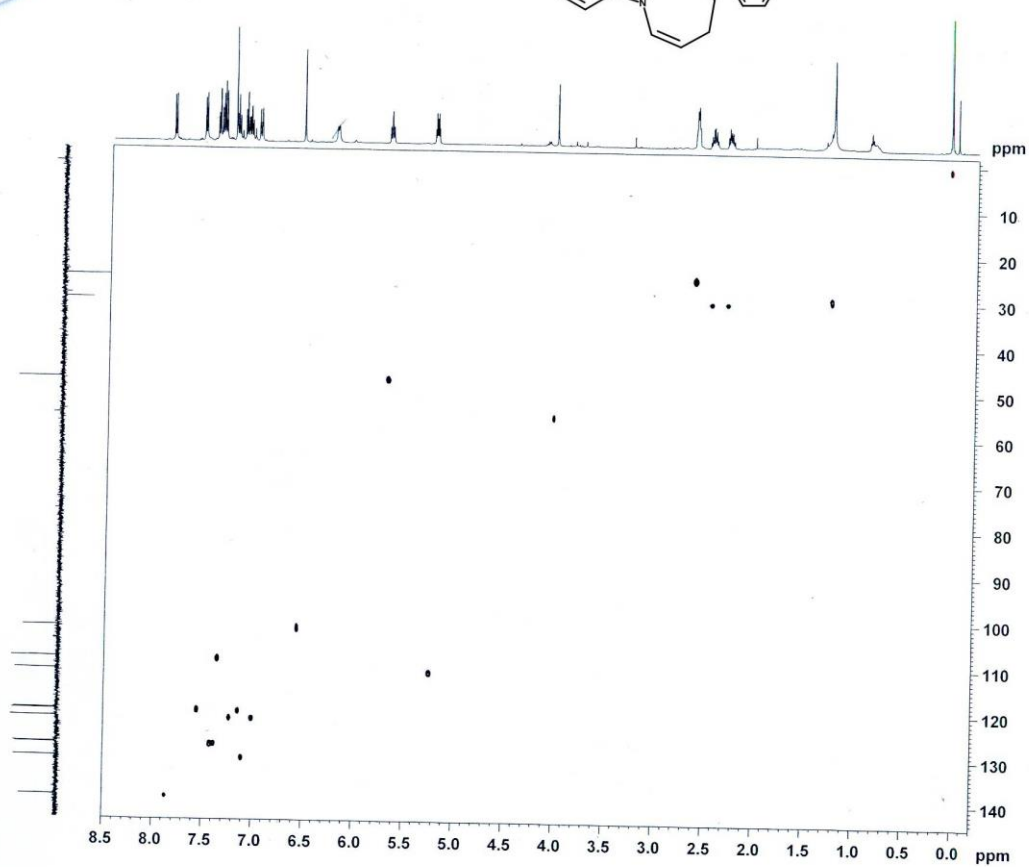
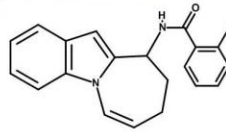
```

NAME          TG-96
EXPNO         1
PROCNO        1
Date_         20101111
Time          12:56
INSTRUM       spect
PROBHD        5 mm BBO BB-1H
PULPROG       zg30
TD            32768
SOLVENT       CDCl3
NS            10
DS            10
SWH           4638.219 Hz
FIDRES        0.141547 Hz
AQ            3.5324404 sec
RG            107.800 usec
DE            38.61466 usec
TE            300.2 K
D1            2.00000000 sec
TDO           1

===== CHANNEL f1 =====
NUC1          1H
P1            9.35 usec
PL1           0.00 dB
PL12          27.37945500 dB
SFO1          500.2619425 MHz
SI            32768
SF            500.2600160 MHz
WDW           EM
SSB           0
LB            0.20 Hz
GB            0
PC            1.00
    
```







```

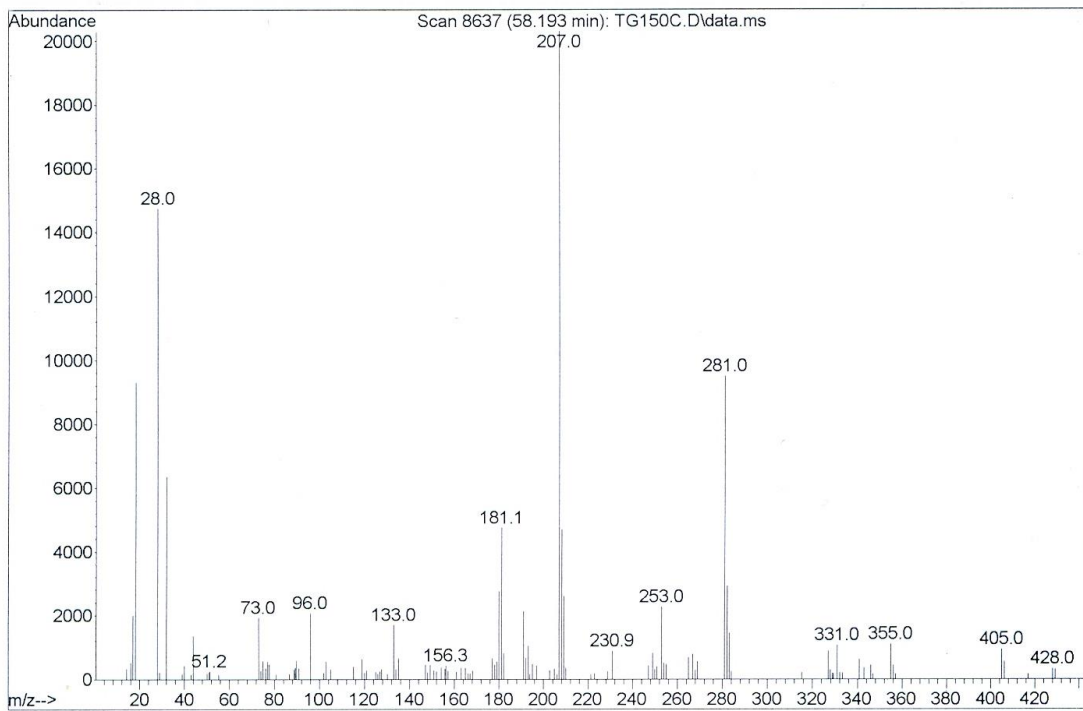
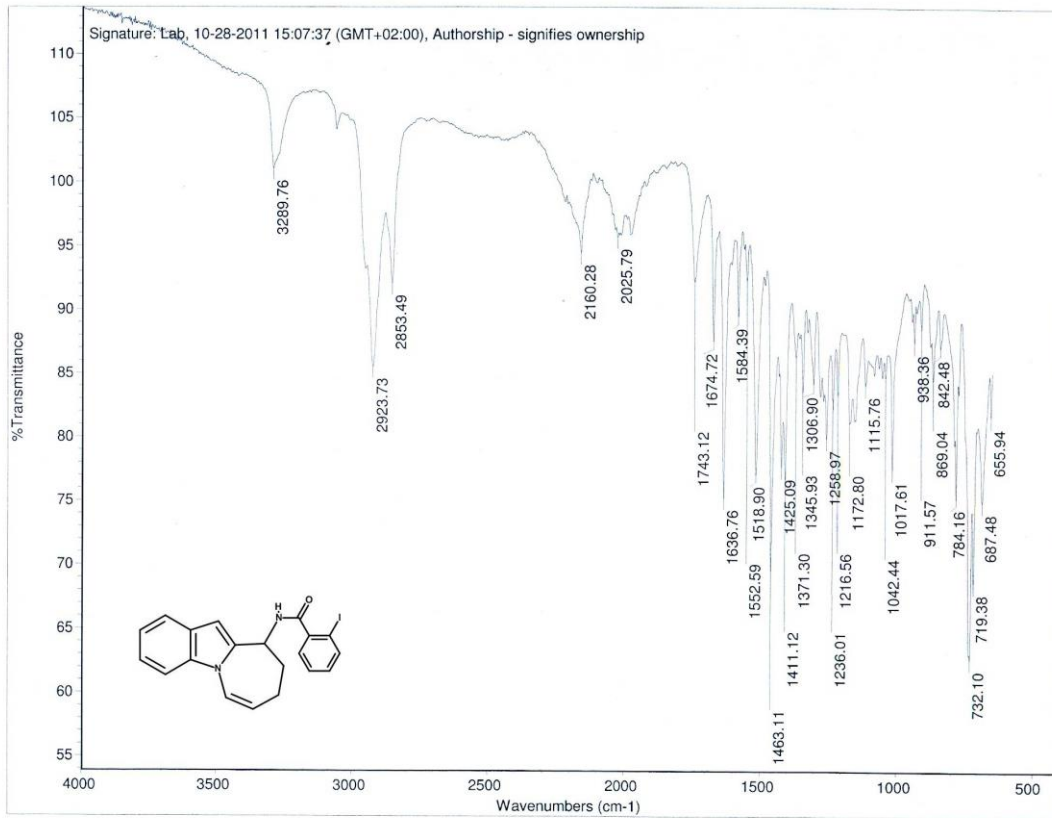
NAME          TC-96
EXPNO         4
PROCNO        4
Date_         20101112
Time          14.08
INSTRUM       spect
PROBHD        5 mm BBO BB-1H
PULPROG       hsqcqtpr1
TD            3274
SOLVENT       CDCl3
NS            4
DS            16
SWH           4638.219 Hz
FIDRES       4.529510 Hz
AQ           0.1104232 sec
RG            2500
IN          107.800 usec
DE           6.30 usec
TE           298.1 K
CQF2         145.000000 sec
D0           0.00000000 sec
D1           2.00000000 sec
D4           0.0017214 sec
D11          0.03000000 sec
D13          0.00000000 sec
D14          0.00920000 sec
D24          0.00086207 sec
IN0          0.00002485 sec
ZGPTMS

----- CHANNEL f1 -----
NUC1          13C
P1            9.25 usec
P2            18.70 usec
P28           1000.00 usec
PL1           0.00 dB
PL12          27.3798238 W
SFO1          500.2619425 MHz

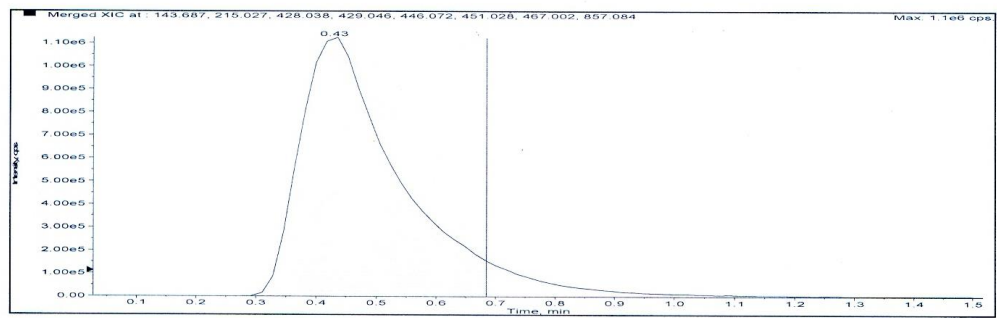
----- CHANNEL f2 -----
CFOFREQ2     9atp
NUC2          13C
P3            11.50 usec
P4            23.00 usec
PCPD2        70.00 usec
PL2           3.00 dB
PL12         18.00 dB
PL28         32.22848892 W
PL12W        1.01919201 W
SFO2         125.7992823 MHz

----- GRADIENT CHANNEL -----
GPRAM1       SINE_100
GPRAM2       SINE_100
GPRAM3       SINE_100
GPRAM4       SINE_100
GF21         80.00 %
GF22         20.10 %
GF23         11.00 %
GF24         -5.00 %
F16          1000.00 usec
F19          600.00 usec
MOD          2
TD           128
SFO1         125.7993 MHz
F1RES        157.24930 Hz
SW           160.000 ppm
FMODE        Echo-Antiecho
SI           1024
SF           500.260138 MHz
SFB          0.00 Hz
LS           2
GB           0
PC           1.40
ST           256
MC2          echo-antlecho
TE           125.790443 MHz
SFB          0.00 Hz
LS           0
GB           0

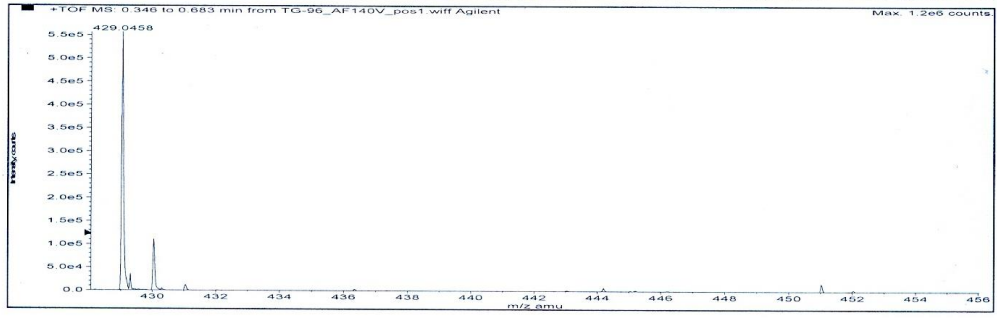
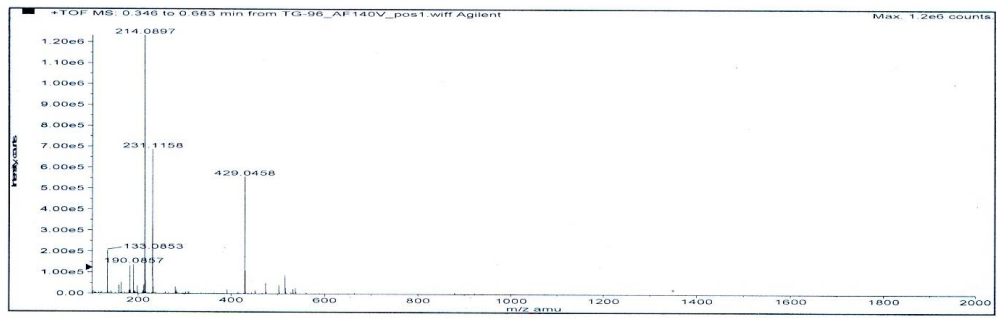
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Sample Name: TG-96 Sample Location: P1-C7 Sample Id: Operator: Milka
 Data File Name: D:\PE Sclex Data\Projects\Farmaceutski fakultet\Data\TG-96_AF140V_pos1.wiff Acq Time: November 02 2011, 01:31:19 PM
 Method: D:\TOF_Data\damethods\Night_Seq_Comp_ident1.anmlefc.xml

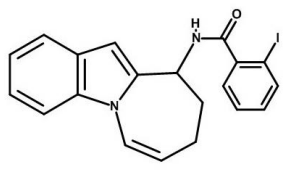


Merged XIC, Period# : 1 Experiment# : 1

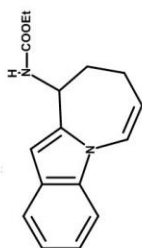


Formula	Compound name	Mass	Peak RT (min)	Peak area	Description
C20H17IN2O	--	428.03856	0.43	1.31293 E7	--

Species	Abundance (counts)	Ion Mass	Measured Mass	Error (mDa)	Error (ppm)	Ret. Time Error (min)
[M+H] ⁺	560676.24	429.04583	429.04578	-0.05360	-0.12	--
[M+Na] ⁺	16460.08	451.02778	451.02741	-0.36566	-0.81	--



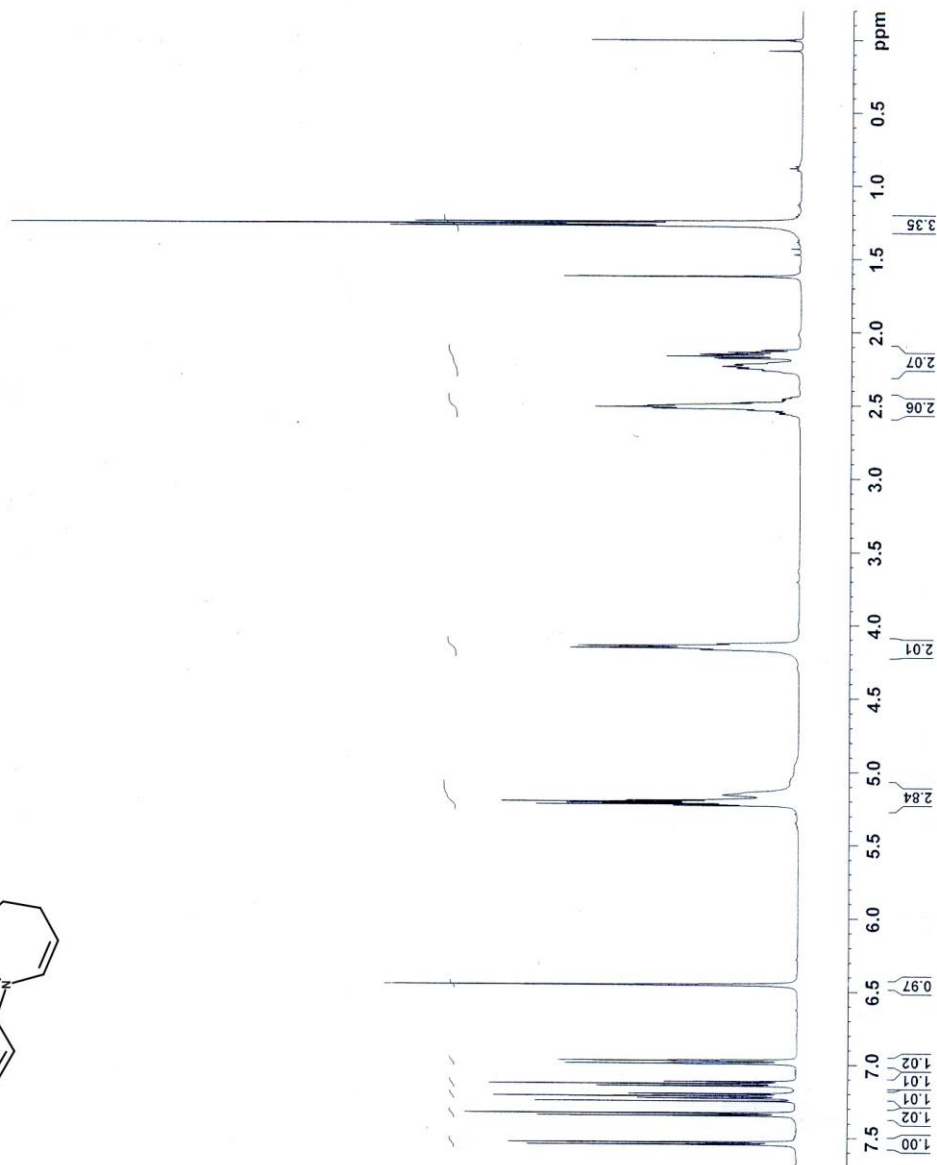
Compound 20



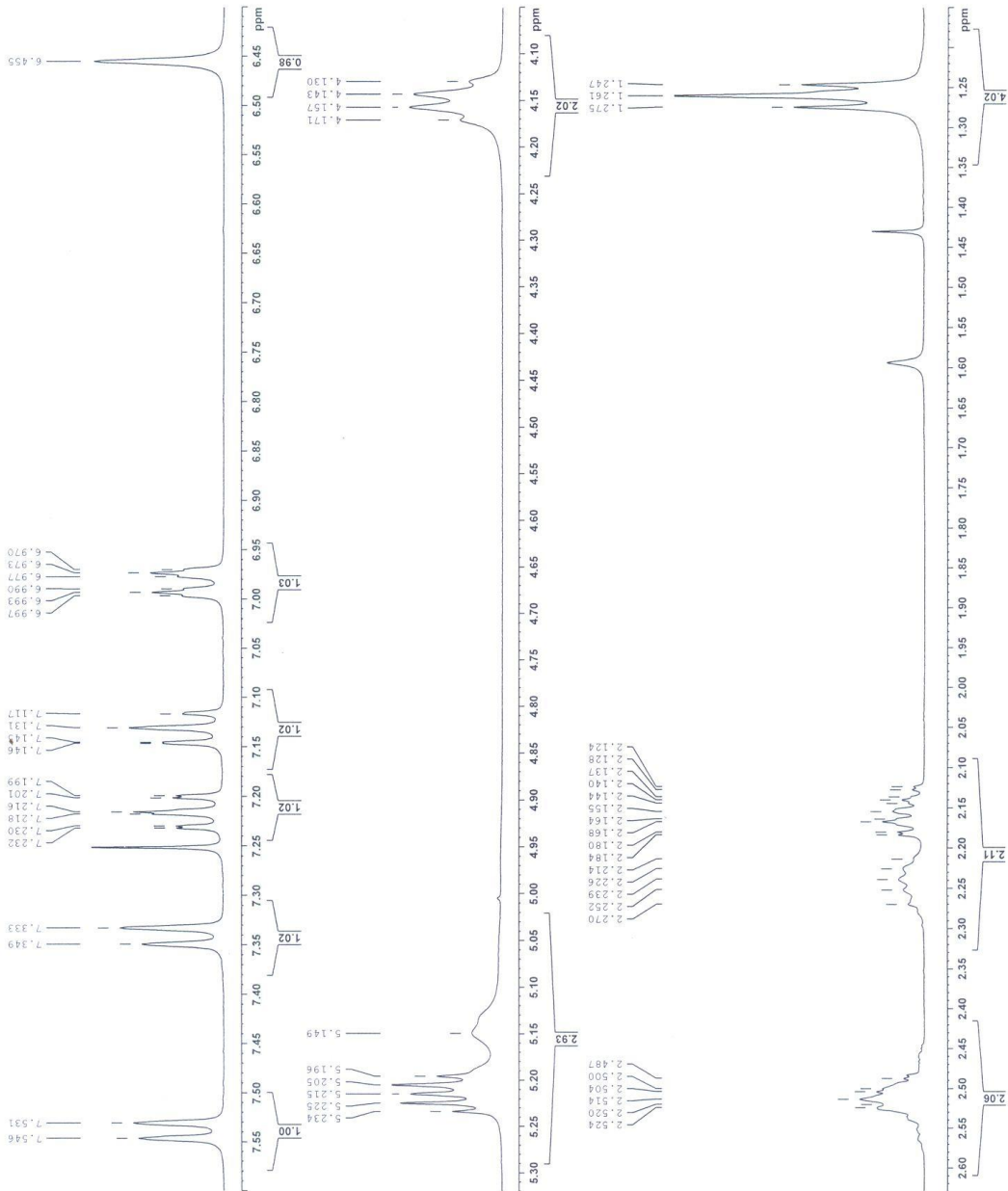
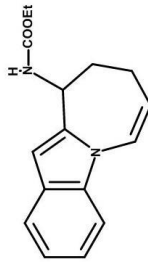
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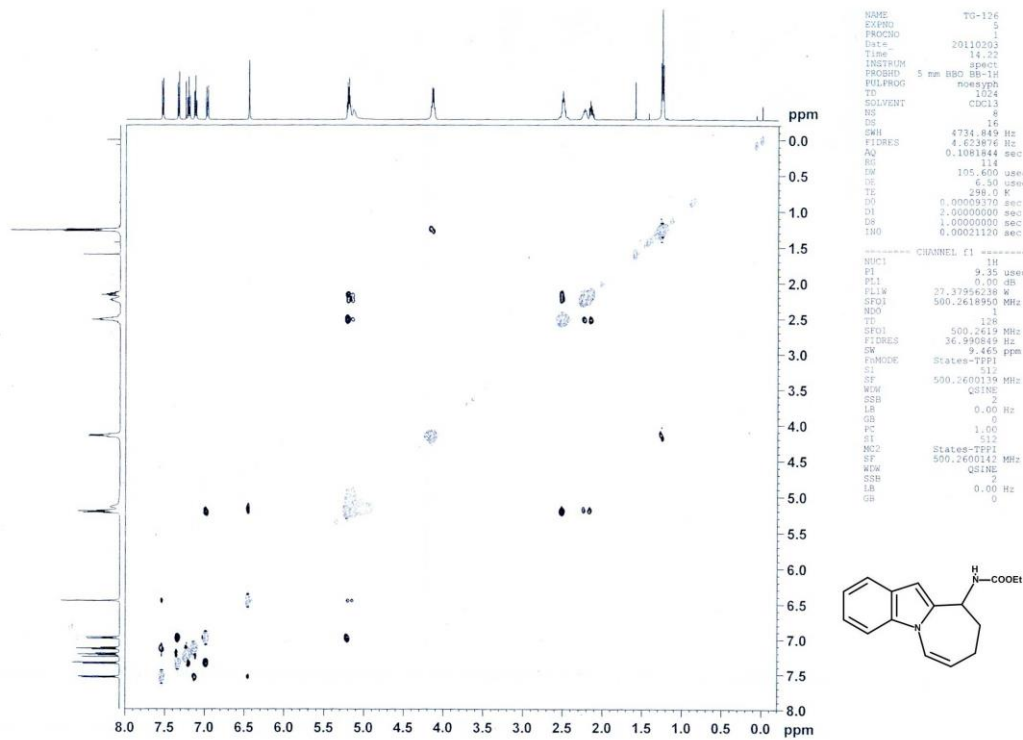
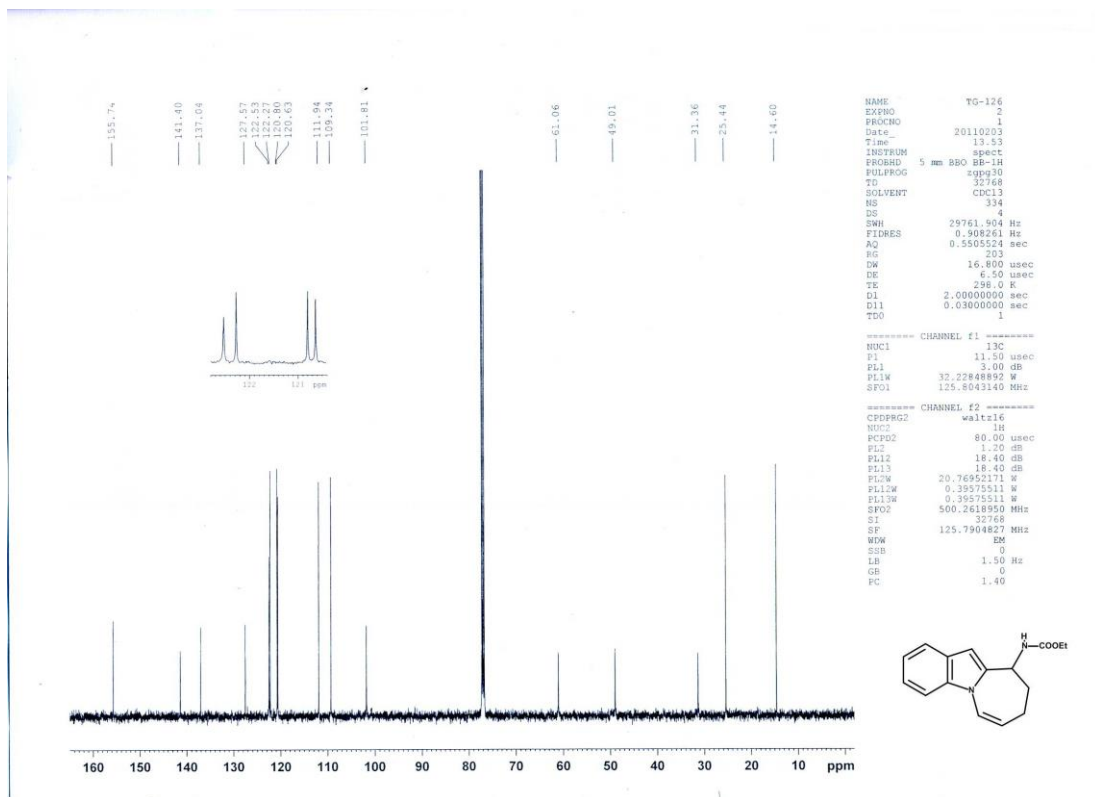
NAME          TC-126a
EXPNO         1
PROCNO        1
Date_         20110721
Time          11.16
INSTRUM       spect
PROBHD        5 mm BBO BB-1H
PULPROG       zgpg30
TD            32768
SOLVENT       CDCl3
NS            10
DS            10
SWH           4835.590 Hz
FIDRES        0.147570 Hz
AQ            3.3882613 sec
RG            114
DW           103.400 usec
TE            6.50 usec
DE            2.00 usec
DI            2.00000000 sec
TD0           1

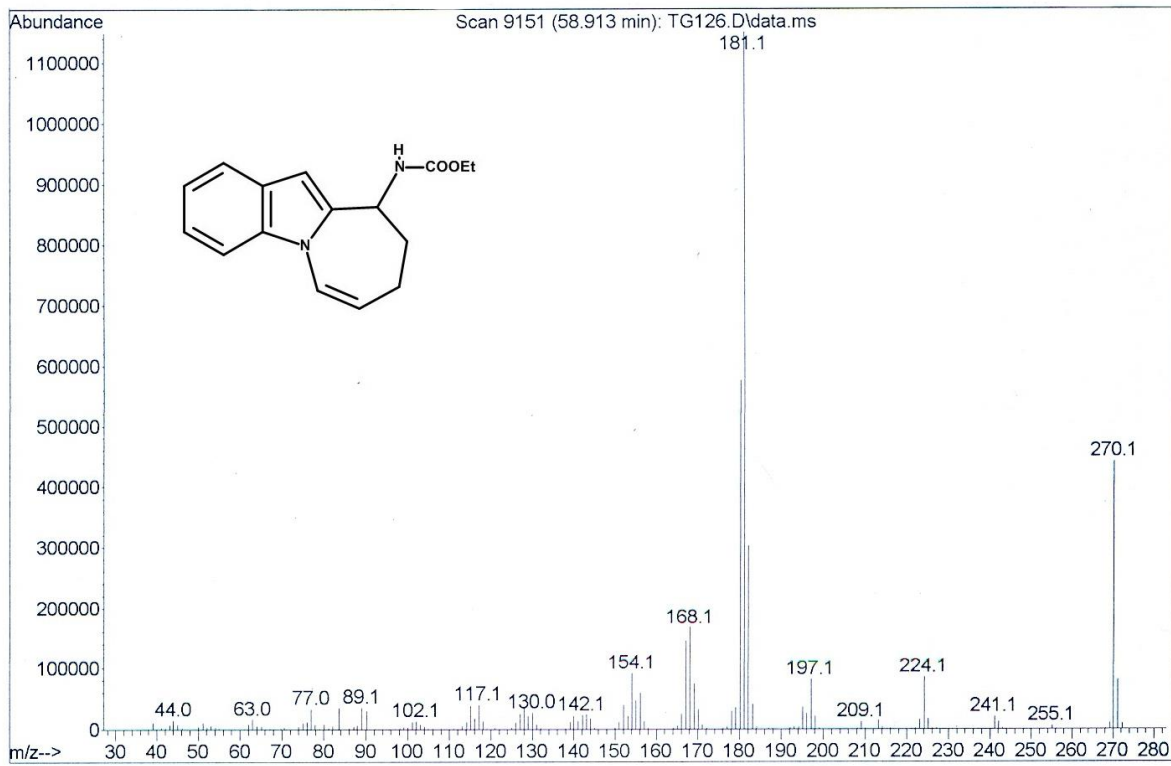
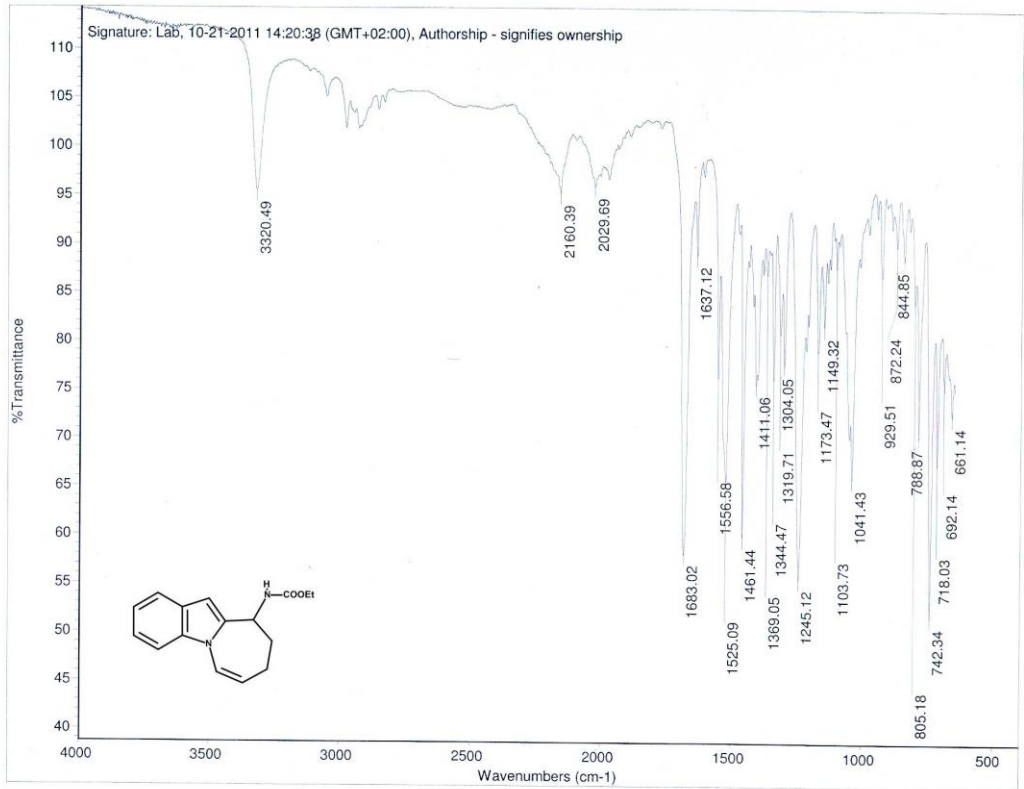
===== CHANNEL f1 =====
NUC1          1H
P1            9.35 usec
PL1           0.00 dB
PL2           0.00 dB
PL3           0.00 dB
PL4           0.00 dB
PL5           0.00 dB
SFO1          500.2613475 MHz
SI            32768
SF            500.2600202 MHz
WDW           EM
SSB           0
GB            0
PC            1.00
  
```



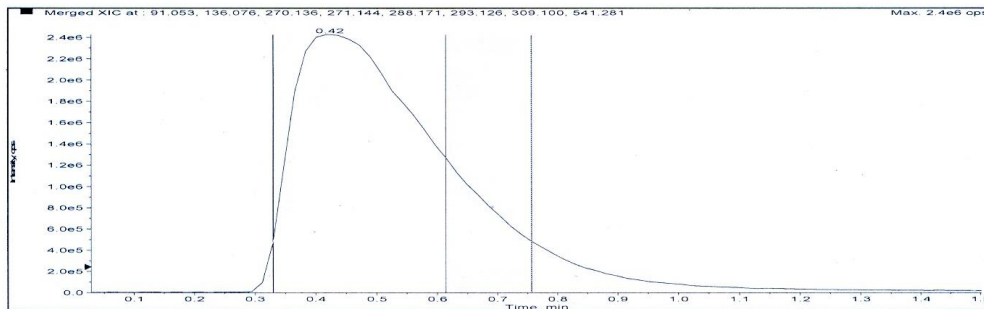
TG-236
 NAME 1
 EXENO 1
 PROCNO 2011129
 Date 11/13/29
 Time 3:37
 INSTRUM spect
 PROBDH 5 mm BBO BB-1H
 PULPROG zg30
 TD 32768
 SOLVENT CDC13
 NS 16
 DS 0
 SWH 4528.985 Hz
 FIDRES 0.138214 Hz
 AQ 3.6176372 sec
 SFO 203
 RG 110.40 usec
 DE 298.0 usec
 TE 298.0 K
 DI 2.0000000 sec
 TDO 1
 =====
 CHANNEL f1
 NUC1 1H
 P1 9.35 usec
 PL1 0.00 dB
 PL1W 27.37956238 W
 SFOL 500.2619418 MHz
 SI 32768
 SFO 500.2600188 MHz
 KW 160
 SSB 0
 LB 0.20 Hz
 GB 0
 PC 1.00



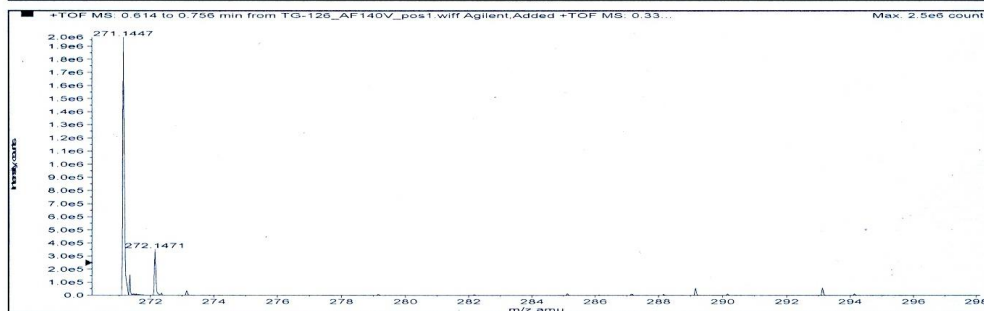
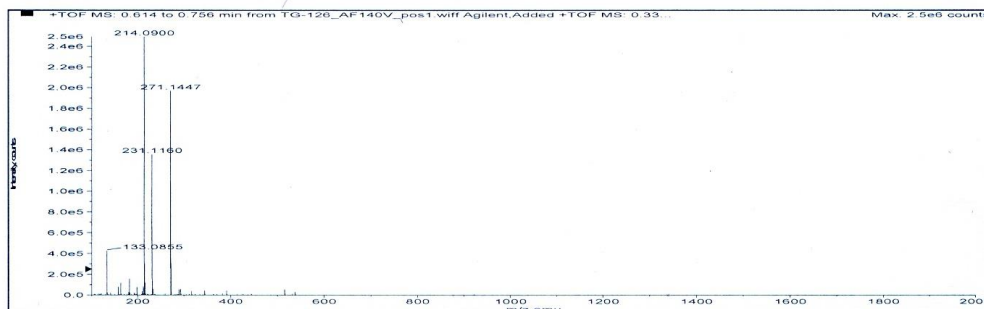




Sample Name: TG-126 Sample Location: P1-C8 Sample Id: Operator: Milka
 Data File Name: D:\PE Sciex Data\Projects\Farmaceutski fakultet\Data\TG-126_AF140V_pos1.wiff Acq Time: November 02 2011,
 01:34:02 PM
 Method: D:\TOF_Data\damethods\Night_Seq_Comp_ident1.anmlefc.xml

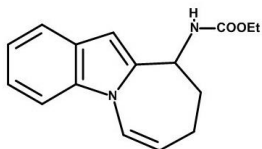


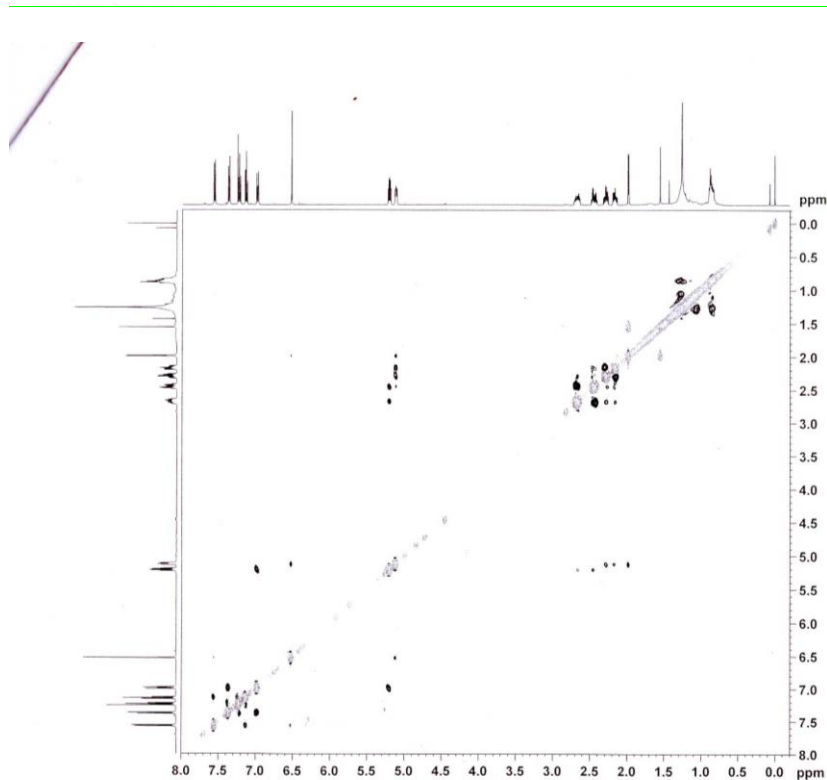
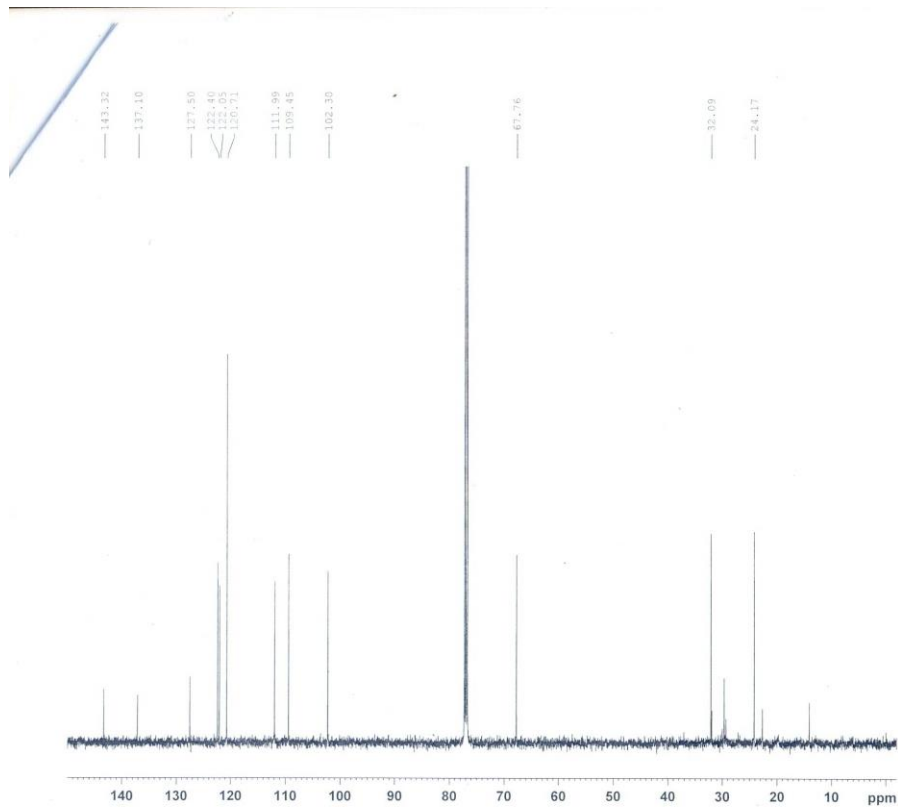
Merged XIC, Period# : 1 Experiment# : 1

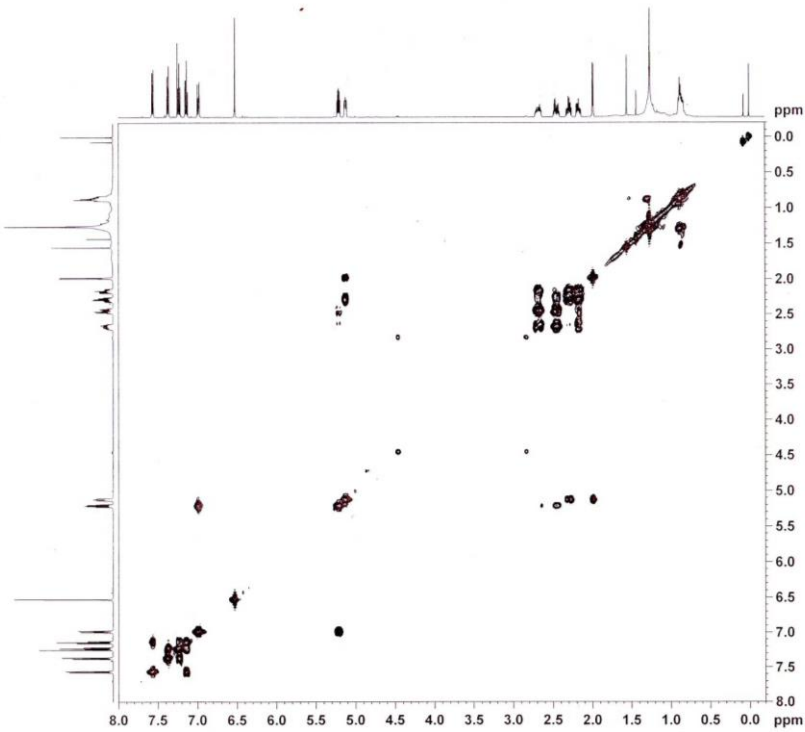


Formula	Compound name	Mass	Peak RT (min)	Peak area	Description
C16H18N2O2	--	270.13683	0.42	4.27005 E7	--

Species	Abundance (counts)	Ion Mass	Measured Mass	Error (mDa)	Error (ppm)	Ret. Time Error (min)
[M+H] ⁺	1972670.34	271.14410	271.14471	0.60693	2.24	--
[M+Na] ⁺	60289.49	293.12605	293.12618	0.13354	0.46	--





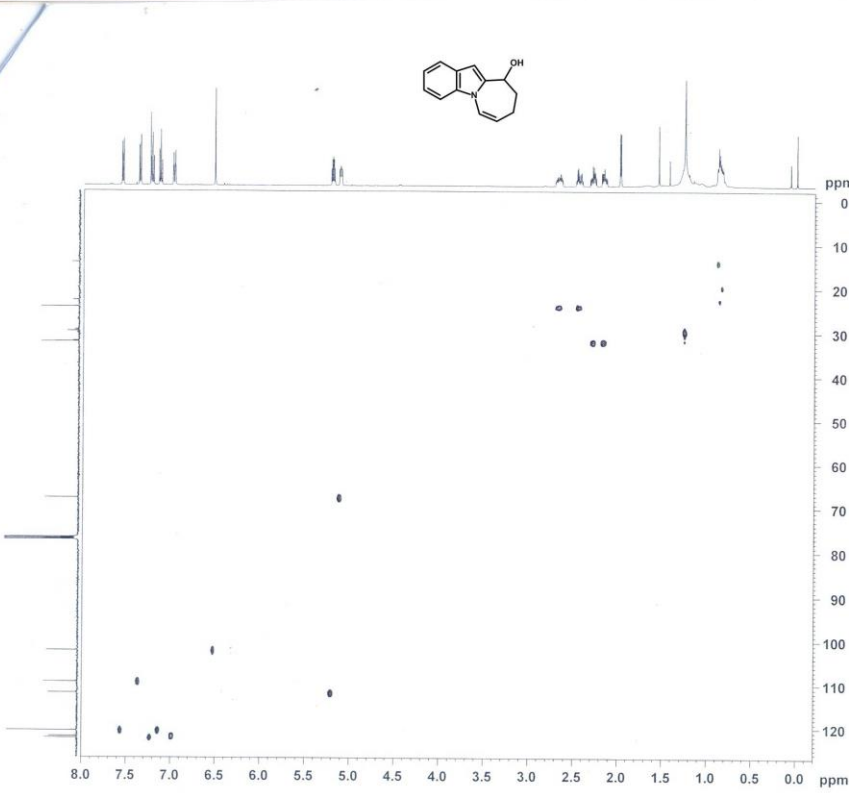
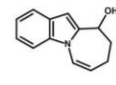


```

NAME          TU-133
EXPNO         3
PROCNO        1
Date_         20110314
Time          11.21
INSTRUM       spect
PROBHD        5 mm BBO BB-1H
PULPROG       zgpg30
TD            65536
SOLVENT       CDCl3
NS            4
DS            16
SFR          4838.219 Hz
F2RES        4.329310 Hz
AQ           0.1104372 sec
RG           203
SW           107.800 usec
DE           6.50 usec
TE           297.9 K
DQ           0.0000000 sec
DI           1.0000000 sec
D13          0.0000000 sec
D16          0.0002000 sec
RG           0.0001560 sec

----- CHANNEL f1 -----
NUC1          1H
P1           9.35 usec
PT           2.35 usec
PL1          0.00 dB
PL12         27.3796428 W
SFO1          500.2618455 MHz

----- GRADIENT CHANNEL -----
GPRAM1       SINE.100
GPRM1        SINE.100
P16          1000.00 usec
TD           2
SFO1         500.2618455 MHz
F2RES        38.236160 Hz
SW           9.272 ppm
FAMODE       CF
F1           512
SF           500.2600139 MHz
MVM          SINE
SVM          0
LB           0.00 Hz
GB           1.40
PC           517
MC2          0
SF           500.2600139 MHz
MVM          SINE
SVM          0
LB           0.00 Hz
GB           0
  
```



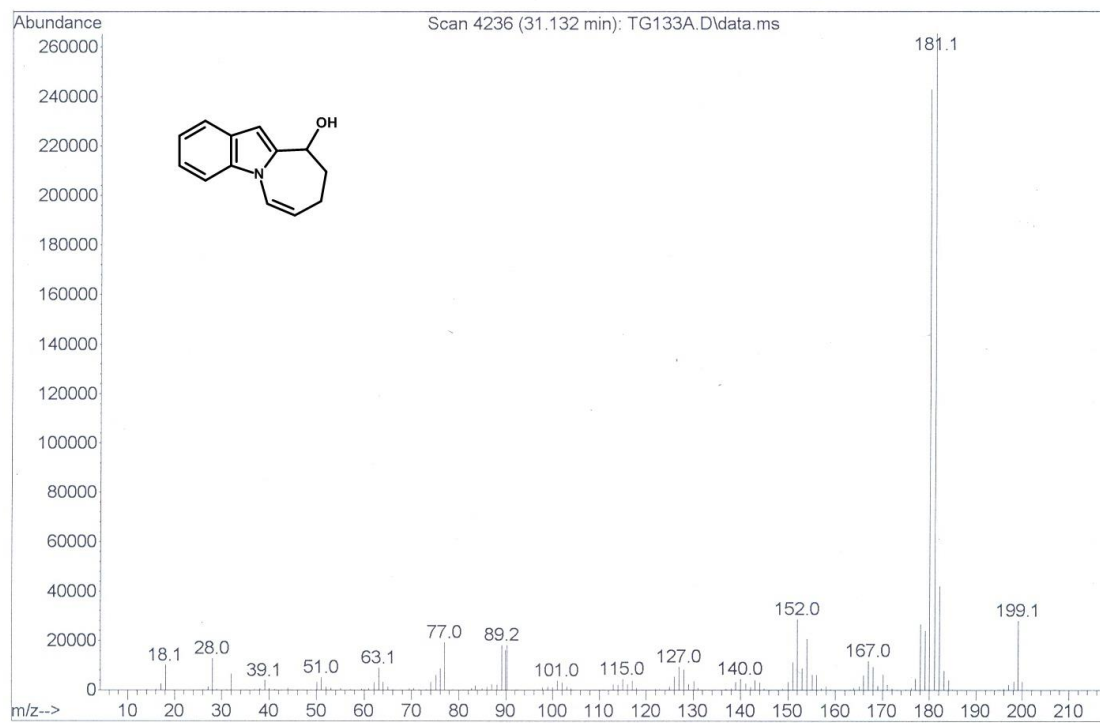
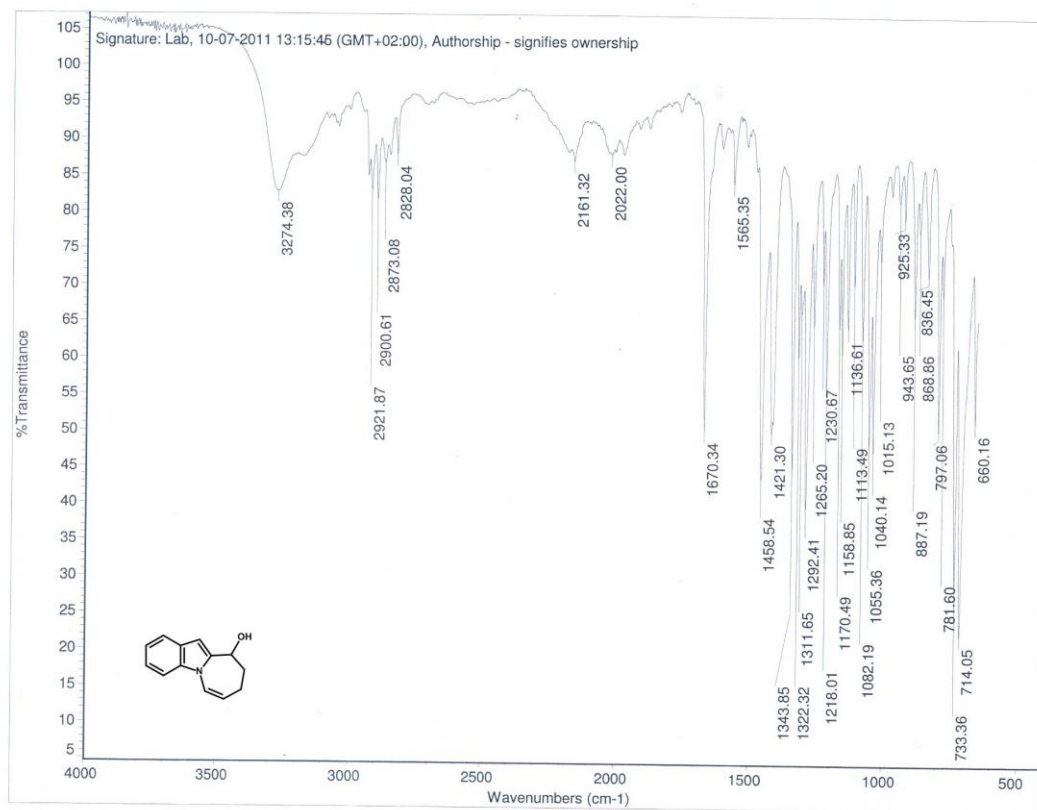
```

NAME          TU-133
EXPNO         4
PROCNO        1
Date_         20110314
Time          11.03
INSTRUM       spect
PROBHD        5 mm BBO BB-1H
PULPROG       zgpg30
TD            65536
SOLVENT       CDCl3
NS            4
DS            16
SFR          4838.219 Hz
F2RES        4.329310 Hz
AQ           0.1104372 sec
RG           203
SW           107.800 usec
DE           6.50 usec
TE           297.9 K
DQ           0.0000000 sec
DI           2.0000000 sec
D13          0.0017844 sec
D16          0.0000000 sec
D18          0.0000000 sec
D19          0.0000000 sec
D20          0.0000000 sec
D21          0.0000000 sec
D22          0.0000000 sec
D23          0.0000000 sec
D24          0.0000000 sec
D25          0.0000000 sec
D26          0.0000000 sec
D27          0.0000000 sec
D28          0.0000000 sec
D29          0.0000000 sec
D30          0.0000000 sec
D31          0.0000000 sec
D32          0.0000000 sec
D33          0.0000000 sec
D34          0.0000000 sec
D35          0.0000000 sec
D36          0.0000000 sec
D37          0.0000000 sec
D38          0.0000000 sec
D39          0.0000000 sec
D40          0.0000000 sec
D41          0.0000000 sec
D42          0.0000000 sec
D43          0.0000000 sec
D44          0.0000000 sec
D45          0.0000000 sec
D46          0.0000000 sec
D47          0.0000000 sec
D48          0.0000000 sec
D49          0.0000000 sec
D50          0.0000000 sec
D51          0.0000000 sec
D52          0.0000000 sec
D53          0.0000000 sec
D54          0.0000000 sec
D55          0.0000000 sec
D56          0.0000000 sec
D57          0.0000000 sec
D58          0.0000000 sec
D59          0.0000000 sec
D60          0.0000000 sec
D61          0.0000000 sec
D62          0.0000000 sec
D63          0.0000000 sec
D64          0.0000000 sec
D65          0.0000000 sec
D66          0.0000000 sec
D67          0.0000000 sec
D68          0.0000000 sec
D69          0.0000000 sec
D70          0.0000000 sec
D71          0.0000000 sec
D72          0.0000000 sec
D73          0.0000000 sec
D74          0.0000000 sec
D75          0.0000000 sec
D76          0.0000000 sec
D77          0.0000000 sec
D78          0.0000000 sec
D79          0.0000000 sec
D80          0.0000000 sec
D81          0.0000000 sec
D82          0.0000000 sec
D83          0.0000000 sec
D84          0.0000000 sec
D85          0.0000000 sec
D86          0.0000000 sec
D87          0.0000000 sec
D88          0.0000000 sec
D89          0.0000000 sec
D90          0.0000000 sec
D91          0.0000000 sec
D92          0.0000000 sec
D93          0.0000000 sec
D94          0.0000000 sec
D95          0.0000000 sec
D96          0.0000000 sec
D97          0.0000000 sec
D98          0.0000000 sec
D99          0.0000000 sec
D100         0.0000000 sec

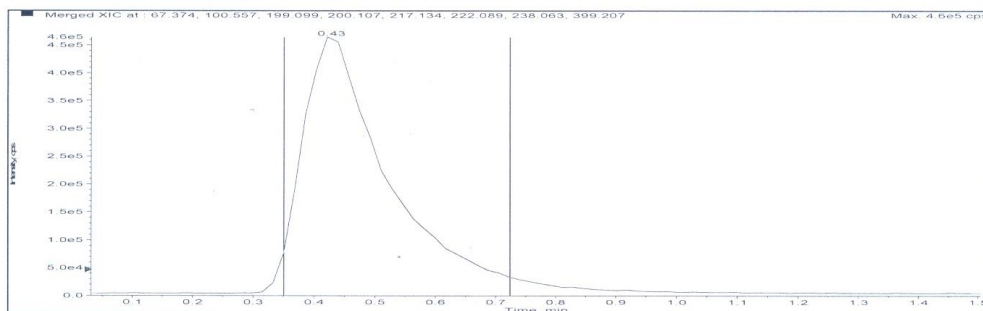
----- CHANNEL f1 -----
NUC1          1H
P1           9.35 usec
PT           2.35 usec
PL1          0.00 dB
PL12         27.3796428 W
SFO1          500.2618455 MHz

----- CHANNEL f2 -----
NUC2          13C
P2           11.50 usec
PT           7.00 usec
PL2          0.00 dB
PL22         18.00 dB
PL24         18.00 dB
PL26         18.00 dB
PL28         18.00 dB
PL30         18.00 dB
PL32         18.00 dB
PL34         18.00 dB
PL36         18.00 dB
PL38         18.00 dB
PL40         18.00 dB
PL42         18.00 dB
PL44         18.00 dB
PL46         18.00 dB
PL48         18.00 dB
PL50         18.00 dB
PL52         18.00 dB
PL54         18.00 dB
PL56         18.00 dB
PL58         18.00 dB
PL60         18.00 dB
PL62         18.00 dB
PL64         18.00 dB
PL66         18.00 dB
PL68         18.00 dB
PL70         18.00 dB
PL72         18.00 dB
PL74         18.00 dB
PL76         18.00 dB
PL78         18.00 dB
PL80         18.00 dB
PL82         18.00 dB
PL84         18.00 dB
PL86         18.00 dB
PL88         18.00 dB
PL90         18.00 dB
PL92         18.00 dB
PL94         18.00 dB
PL96         18.00 dB
PL98         18.00 dB
D100         18.00 dB

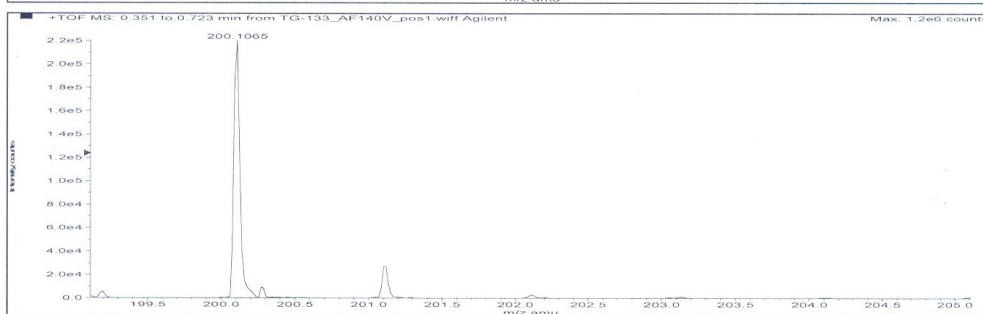
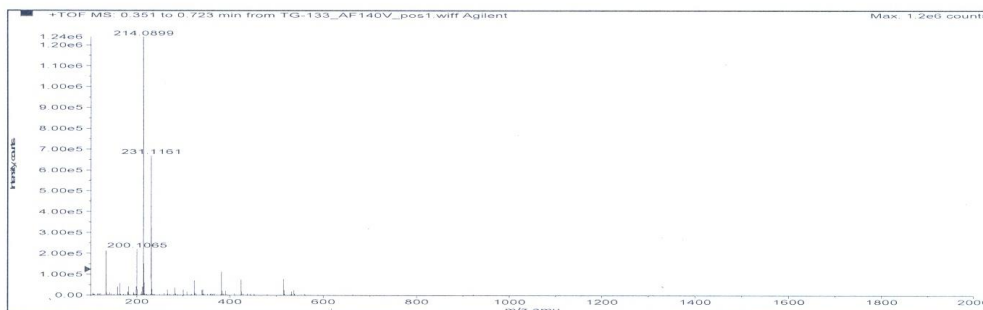
----- GRADIENT CHANNEL -----
GPRAM1       SINE.100
GPRM1        SINE.100
P16          1000.00 usec
TD           2
SFO1         125.7683 MHz
F2RES        137.34000 Hz
SW           140.000 ppm
FAMODE       Echo-antiEcho
F1           124
SF           125.7660139 MHz
MVM          SINE
SVM          0
LB           0.00 Hz
GB           1.40
PC           517
MC2          0
SF           125.7660139 MHz
MVM          SINE
SVM          0
LB           0.00 Hz
GB           0
  
```



Sample Name: TG-133 Sample Location: P1-C9 Sample Id: Operator: Milka
 Data File Name: D:\PE Sciex Data\Projects\Farmaceutski fakultet\Data\TG-133_AF140V_pos1.wiff Acq Time: November 02 2011,
 01:36:47 PM
 Method: D:\TOF_Data\damethods\Night_Seq_Comp_ident1.anmlefc.xml

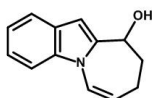


Merged XIC, Period#: 1 Experiment#: 1

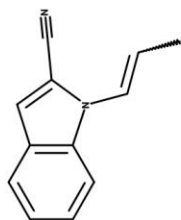


Formula	Compound name	Mass	Peak RT (min)	Peak area	Description
C13H13NO	--	199.09971	0.43	4.58983 E6	--

Species	Abundance (counts)	Ion Mass	Measured Mass	Error (mDa)	Error (ppm)	Ret. Time Error (min)
[M+H] ⁺	224658.69	200.10699	200.10651	-0.48393	-2.42	--



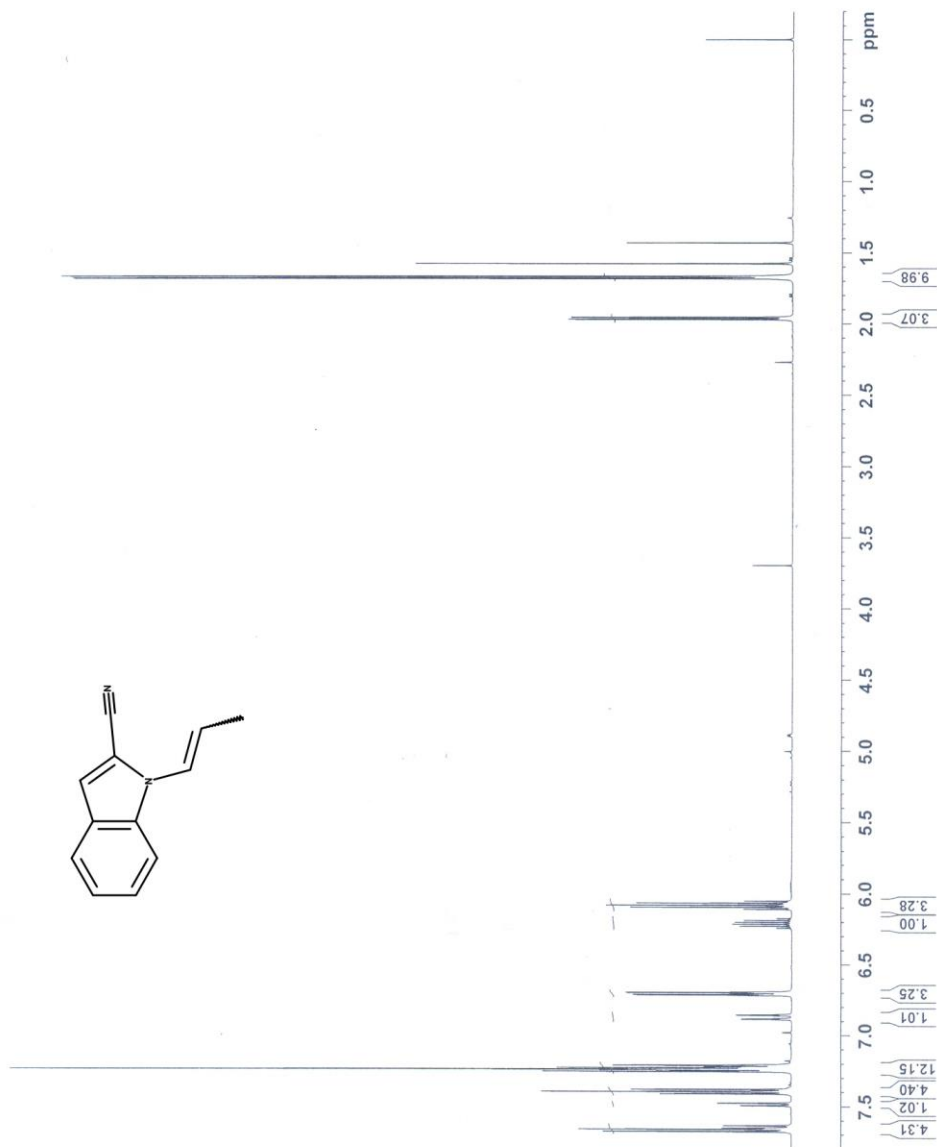
Compound 24

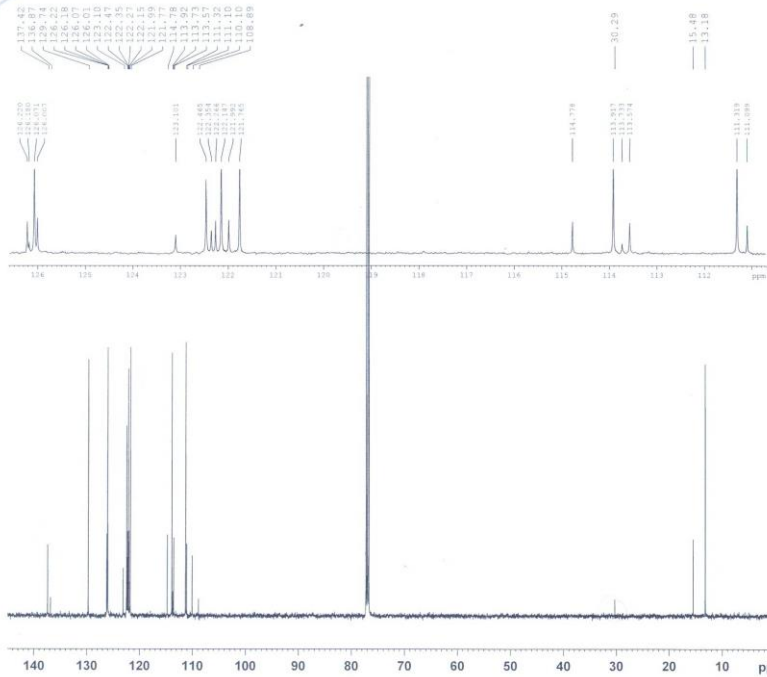


```

NAME          TG-50
EXPNO         1
PROCNO        1
Date_         20100629
Time          11.38
INSTRUM       spect
PROBHD        5 mm BBO BB-1H
PULPROG       zgpg30
TD            32768
SOLVENT       CDCl3
NS            16
DS            0
SWH           4618.227 Hz
AQ            0.140931 Hz
RG            3.547761 sec
WDW           EM
SSB           0
GB            0
PC            1.00
DE           108.267 usec
TE            298.0 K
D1            2.00000000 sec
TD0           1

===== CHANNEL f1 =====
NUC1          1H
P1            9.35 usec
PL1           0.00 dB
PL12          27.37956238 W
SFO1          500.261524 MHz
SF            500.260207 MHz
MOM           EM
SBB           0
LB            0
GB            0
PC            1.00
  
```





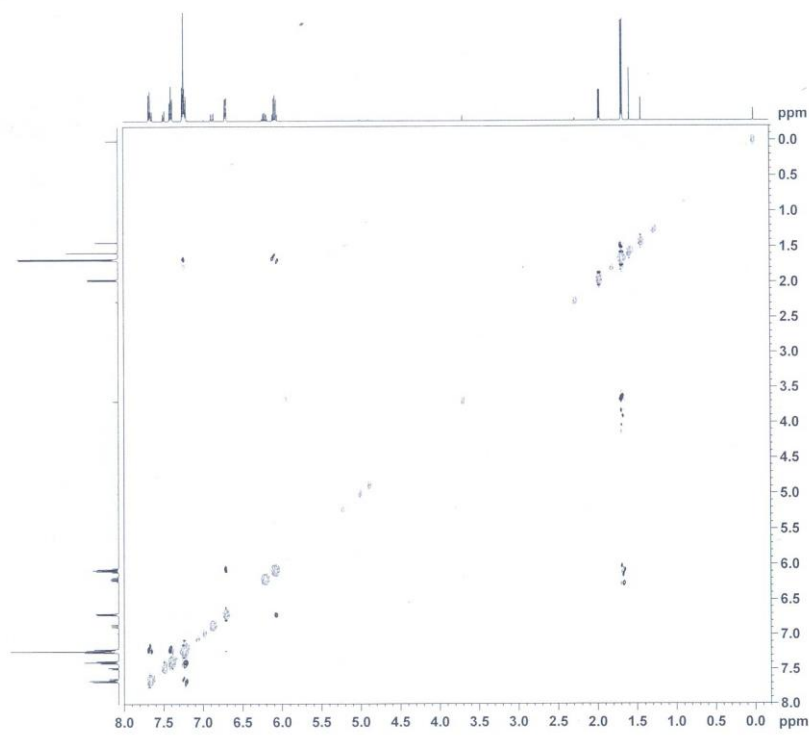
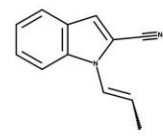
```

NAME          TG-50
EXPNO         2
PROCNO        1
Date_         20100629
Time          11.51
INSTRUM       spect
PROBHD        5 mm BBO BB-1H
PULPROG       zgpg30
TD            32768
SOLVENT       CDCl3
NS            816
DS            4
SWH           29761.984 Hz
FIDRES        0.908261 Hz
AQ            0.5505524 sec
RG            912
DW            16.800 usec
DE            6.50 usec
TE            298.0 K
D1            2.0000000 sec
d11           0.0300000 sec
TD0           1
  
```

```

----- CHANNEL f1 -----
NUC1          13C
P1            11.50 usec
PL1           3.00 dB
PL1W          32.2284892 W
SFO1          125.8043140 MHz

----- CHANNEL f2 -----
CPDPRG2       waltz16
NUC2          1H
PCPD2         80.00 usec
PL2           1.20 dB
PL12          18.40 dB
PL13          18.40 dB
PL2W          20.76952171 W
PL12W         0.39575511 W
PL13W         0.39575511 W
SFO2          500.2619545 MHz
SI            32768
SF            125.7904851 MHz
WDW           EM
SSB           0
LB            1.50 Hz
GB            0
PC            1.40
  
```

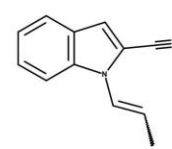


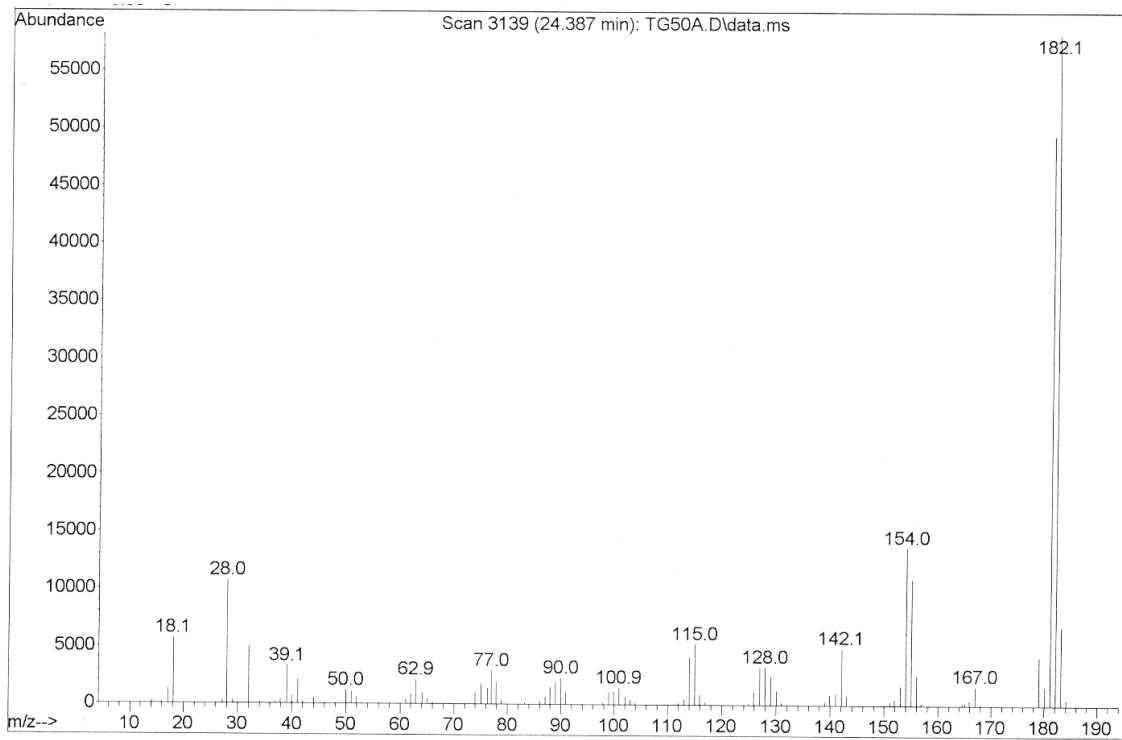
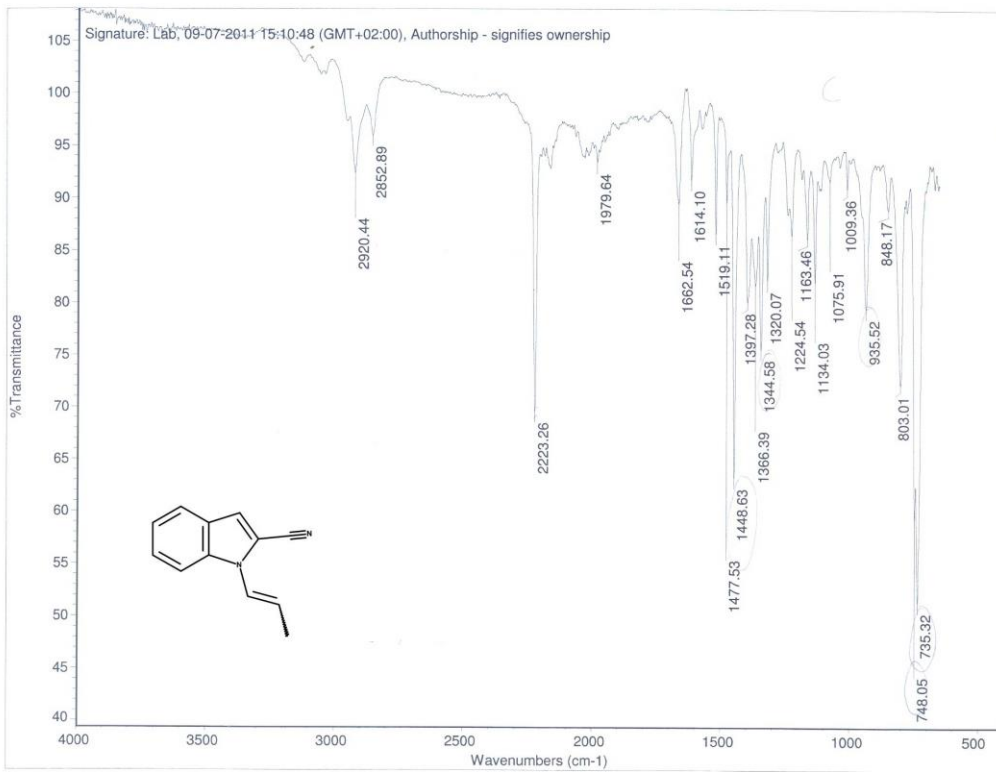
```

NAME          TG-50
EXPNO         3
PROCNO        1
Date_         20100629
Time          12.04
INSTRUM       spect
PROBHD        5 mm BBO BB-1H
PULPROG       noesypr
TD            1024
SOLVENT       CDCl3
NS            816
DS            4
SWH           4618.277 Hz
FIDRES        4.509967 Hz
AQ            0.1109151 sec
RG            281
DW            108.267 usec
DE            6.50 usec
TE            298.0 K
D0            0.00059636 sec
D1            2.0000000 sec
D8            1.0000000 sec
IBO           0.00021655 sec
  
```

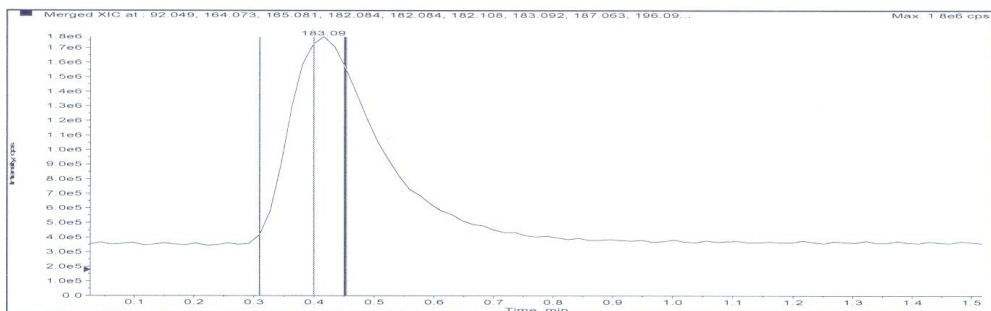
```

----- CHANNEL f1 -----
NUC1          1H
P1            9.35 usec
PL1           0.00 dB
PL1W          27.3756238 W
SFO1          500.2619545 MHz
NUC2          13C
TD            128
SFO2          500.262 MHz
FIDRES        36.079830 Hz
SW            States-TPPI
SI            512
SF            500.2600160 MHz
WDW           QO1MC
SSB           2
LB            0.00 Hz
GB            0
PC            1.00
MC2           States-TPPI
SF            500.2600177 MHz
WDW           QO1MC
SSB           2
LB            0.00 Hz
GB            0
  
```

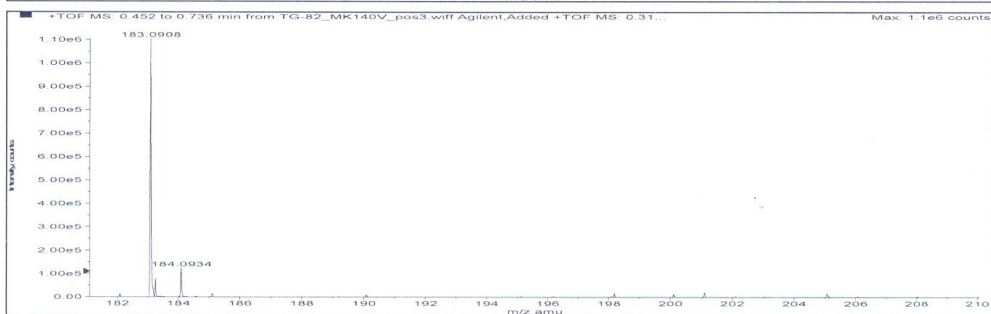
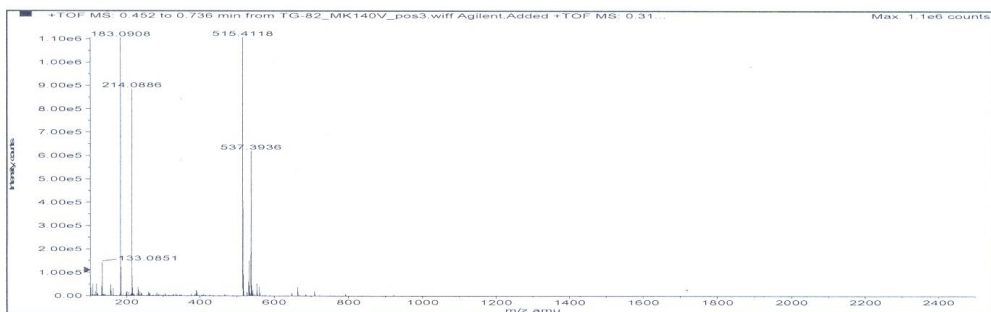




Sample Name: TG-82 Sample Location: P1-D6 Sample Id: Operator: Milka
 Data File Name: D:\PE_Sciex_Data\Projects\Farmaceutski fakultet\Data\TG-82_MK140V_pos3.wiff Acq Time: November 12 2010,
 02:40:16 PM
 Method: D:\TOF_Data\damethods\Night_Seq_Comp_ident1.anm\efc.xml

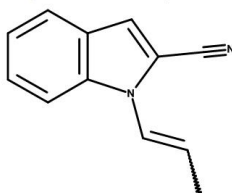


Merged XIC, Period# : 1 Experiment# : 1

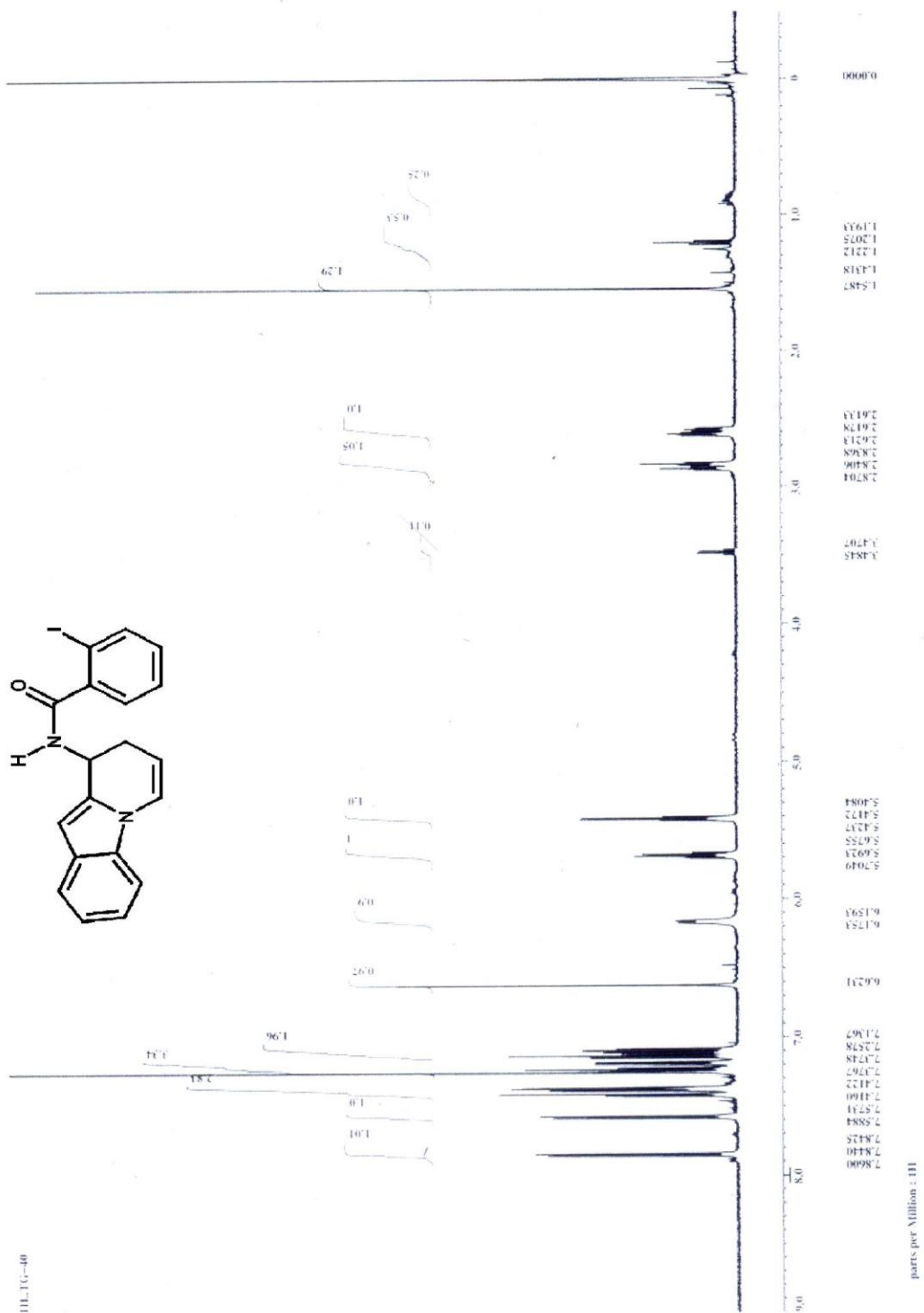


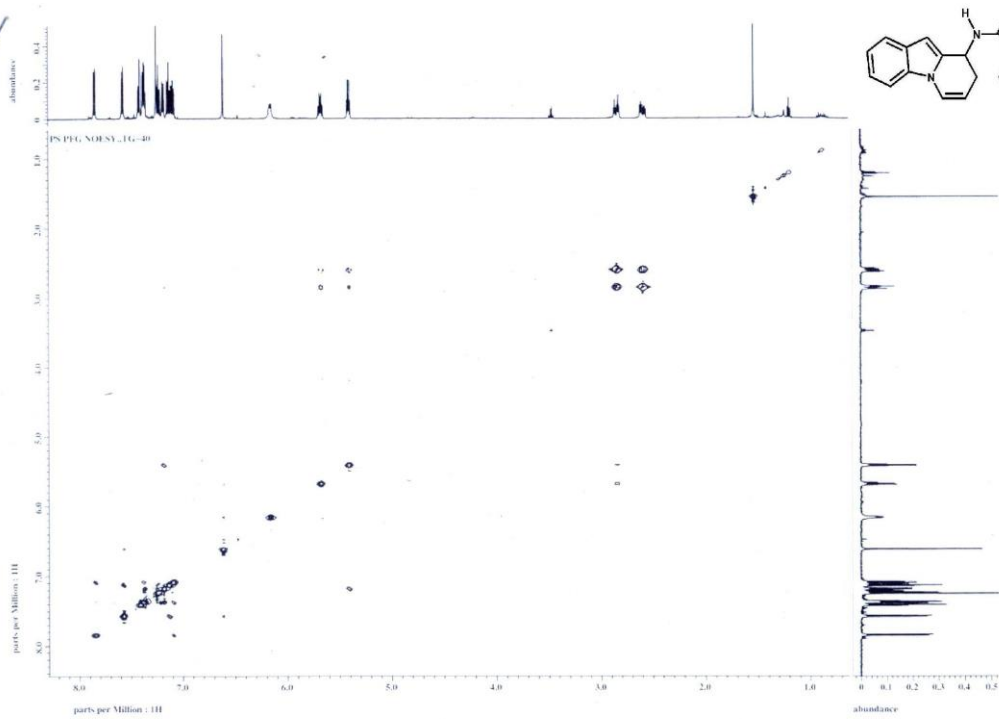
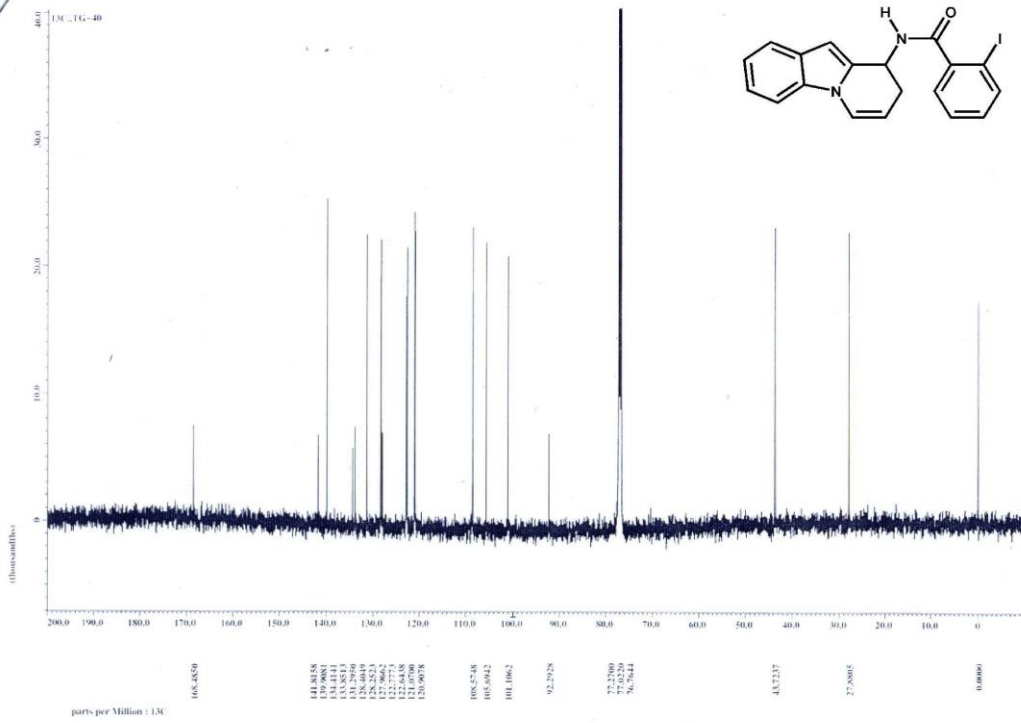
Formula	Compound name	Mass	Peak RT (min)	Peak area	Description
C12H10N2	--	182.08440	0.41	1.49963 E7	--

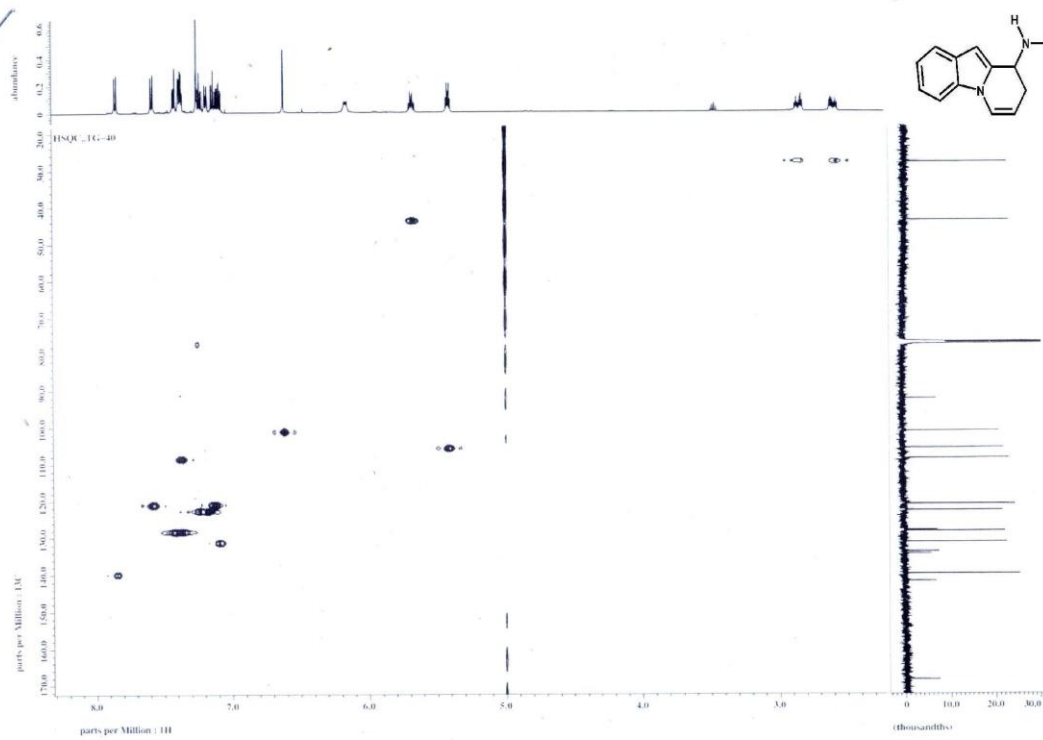
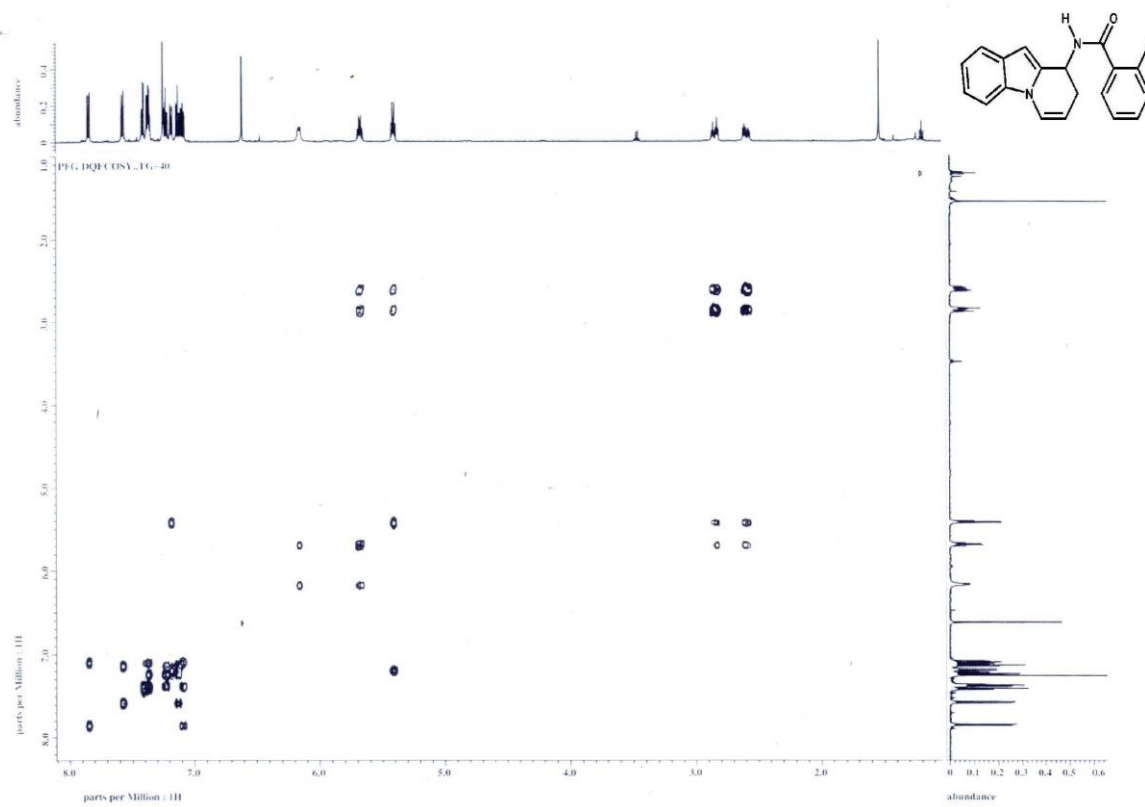
Species	Abundance (counts)	Ion Mass	Measured Mass	Error (mDa)	Error (ppm)	Ret. Time Error (min)
[M+H2O-H2O]+	13128.65	182.08385	182.09119	7.34506	40.34	--
M+	13128.65	182.08385	182.09119	7.34506	40.34	--
[M+NH4-H2O]+	13128.65	182.10766	182.09119	-16.46439	-90.42	--
[M+H]+	1106251.11	183.09167	183.09084	-0.83694	-4.57	--
[M+H2O]+	13490.30	200.09441	200.11130	16.88498	84.38	--
[M+NH4]+	13490.30	200.11822	200.11130	-6.92447	-34.60	--

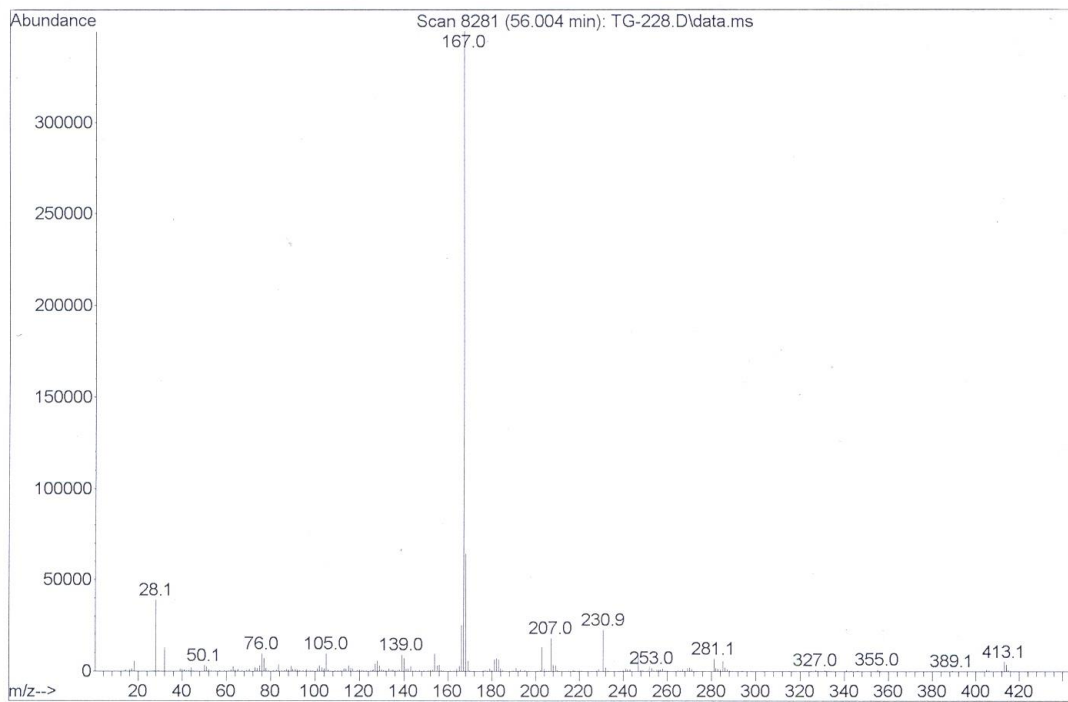
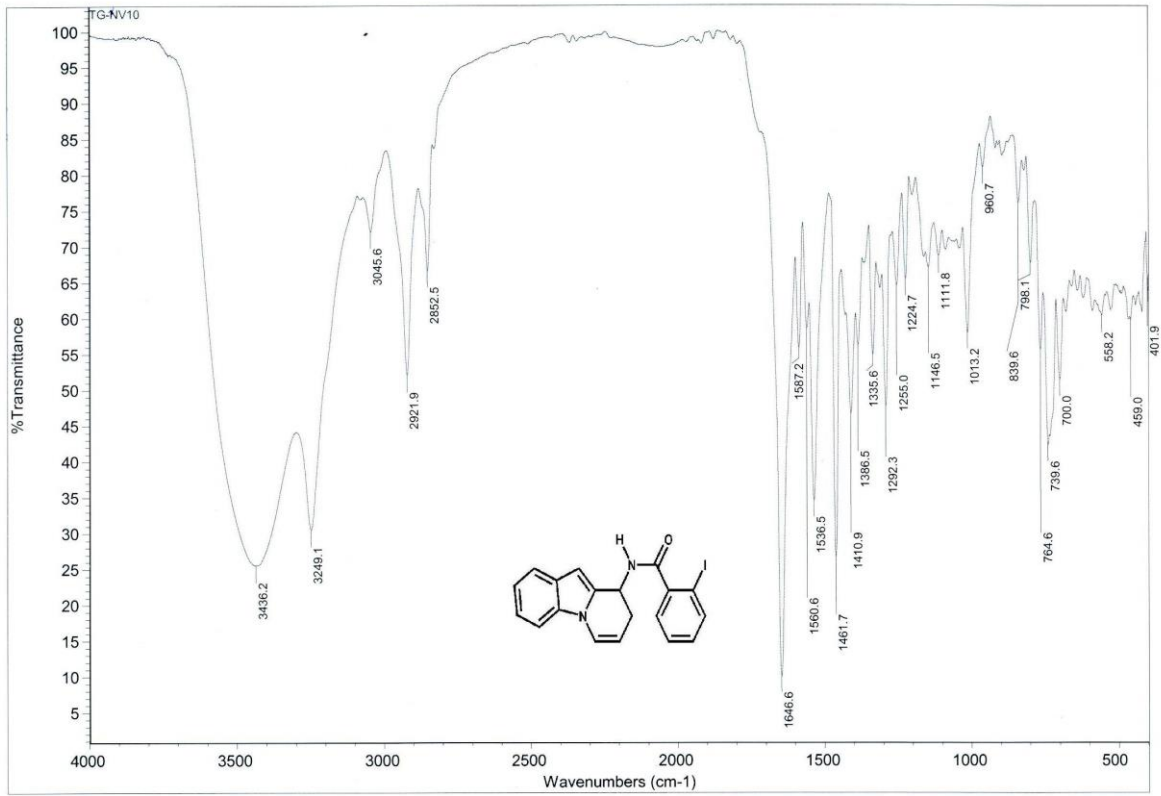


Compound 25

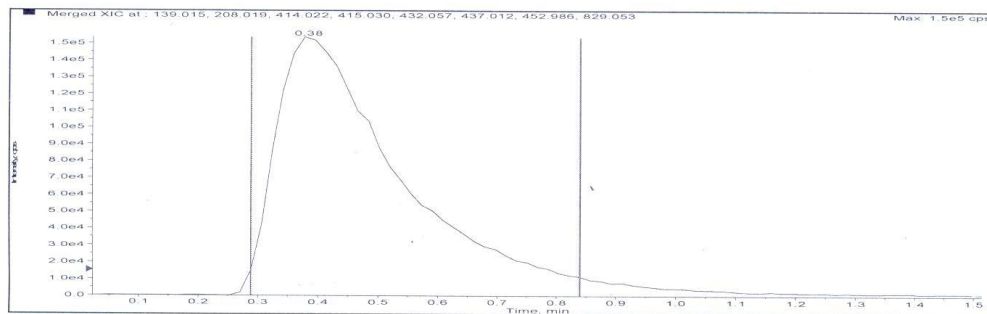




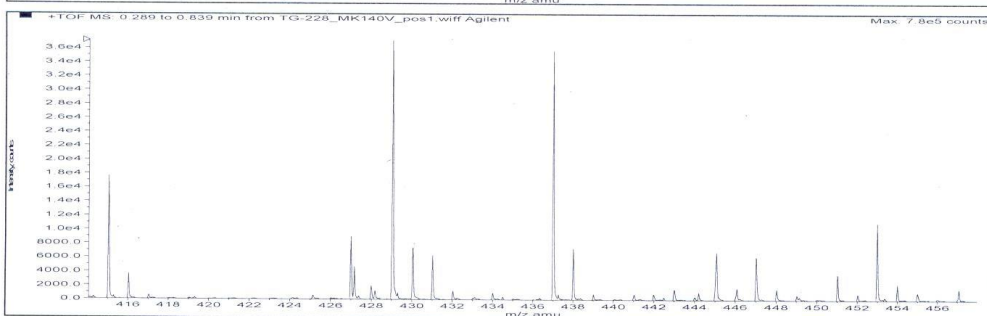
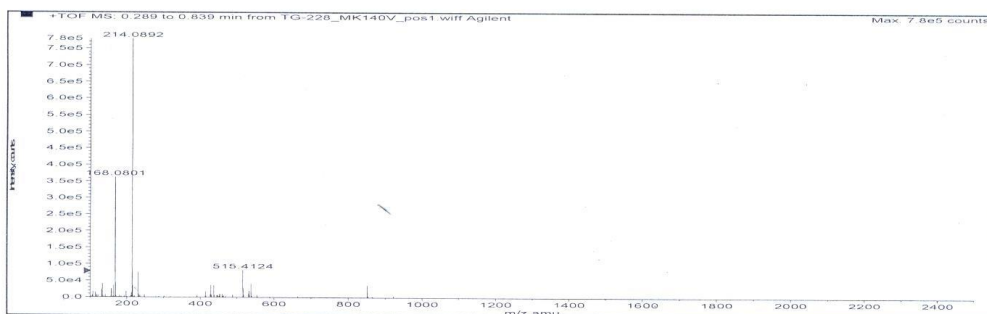




Sample Name: TG-228 Sample Location: P1-E9 Sample Id: Operator: Milka
 Data File Name: D:\PE_Sciex_Data\Projects\Farmaceutski fakultet\Data\TG-228_MK140V_pos1.wiff Acq Time: December 02 2011, 02:36:53 PM
 Method: D:\TOF_Data\damethods\Night_Seq_Comp_ident1.anm\efc.xml

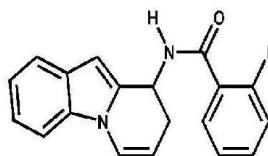


Merged XIC, Period# : 1 Experiment# : 1

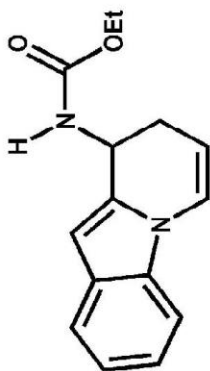
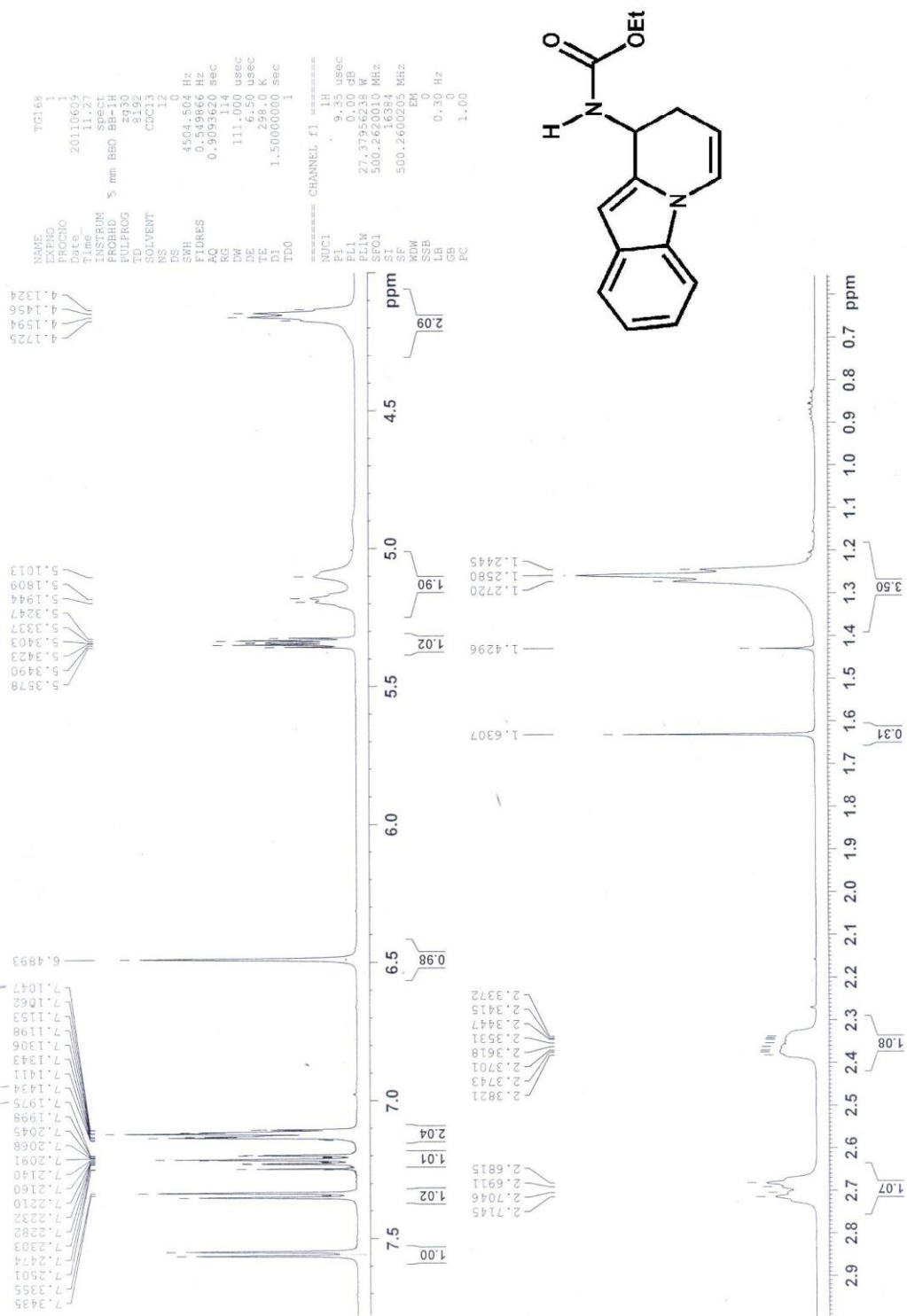


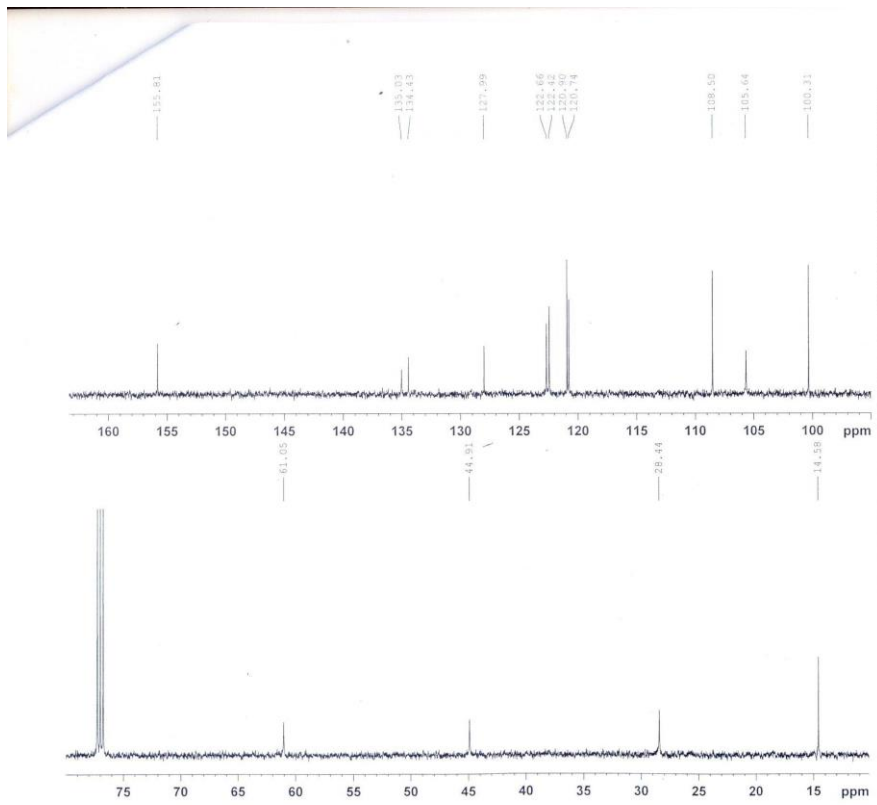
Formula	Compound name	Mass	Peak RT (min)	Peak area	Description
C19H15N2O	--	414.02291	0.38	2.21091 E6	--

Species	Abundance (counts)	Ion Mass	Measured Mass	Error (mDa)	Error (ppm)	Ret. Time Error (min)
[M+H] ⁺	17904.01	415.03018	415.02942	-0.76738	-1.85	--
[M+Na] ⁺	36478.79	437.01213	437.01181	-0.32054	-0.73	--
[M+K] ⁺	11040.89	452.98606	452.98711	1.04793	2.31	--



Compound 26



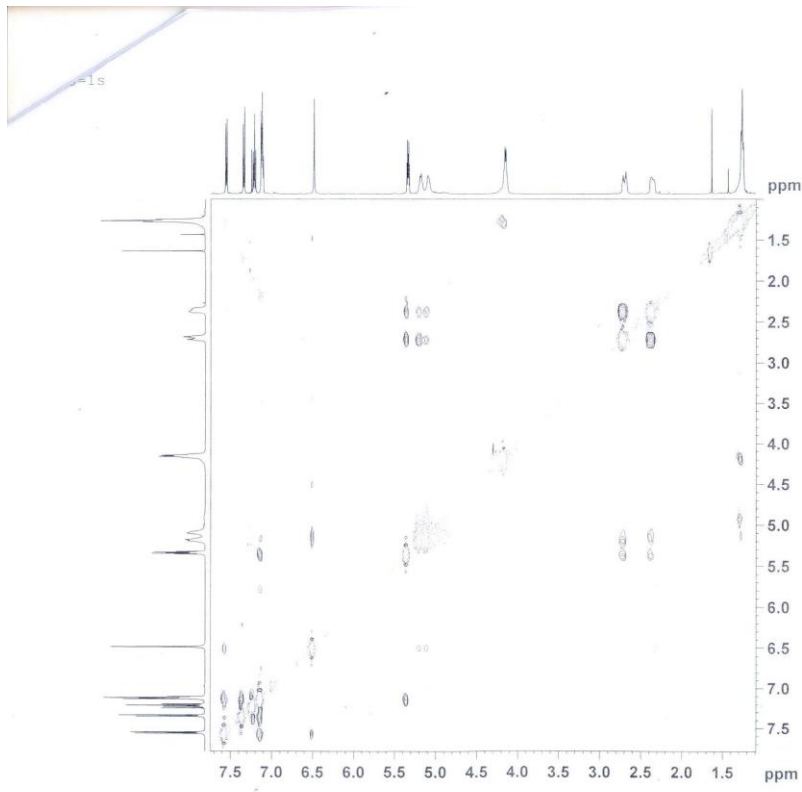
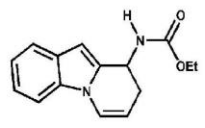


```

NAME          TG168
EXPNO         2
PROCNO        1
Date_         20110609
Time          11.36
INSTRUM       spect
PROBHD        5 mm BBO BB-1H
PULPROG       zgpg30
TD            32768
SOLVENT       CDCl3
NS            90
DS            4
SWH           29761.904 Hz
FIDRES        0.908261 Hz
AQ            0.5505524 sec
RG            812
DW            16.800 usec
DE            6.50 usec
TE            298.1 K
D1            2.0000000 sec
D11           0.0300000 sec
TD0           1

----- CHANNEL f1 -----
NUC1          13C
P1            11.90 usec
PL1           3.00 dB
PL1W         32.2288892 W
SFO1         125.8043140 MHz

----- CHANNEL f2 -----
CPDPRG2      waltz16
NUC2          1H
PCPD2        80.00 usec
PL2           1.20 dB
PL12         18.40 dB
PL13         18.40 dB
PL1W         20.76552171 W
PL12W        0.39575511 W
PL13W        0.39575511 W
SFO2         500.2622612 MHz
SI            32768
SF           125.7904834 MHz
WDW           EM
SSB           0
LB            1.50 Hz
GB            0
PC            1.40
  
```

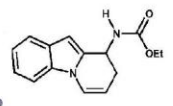


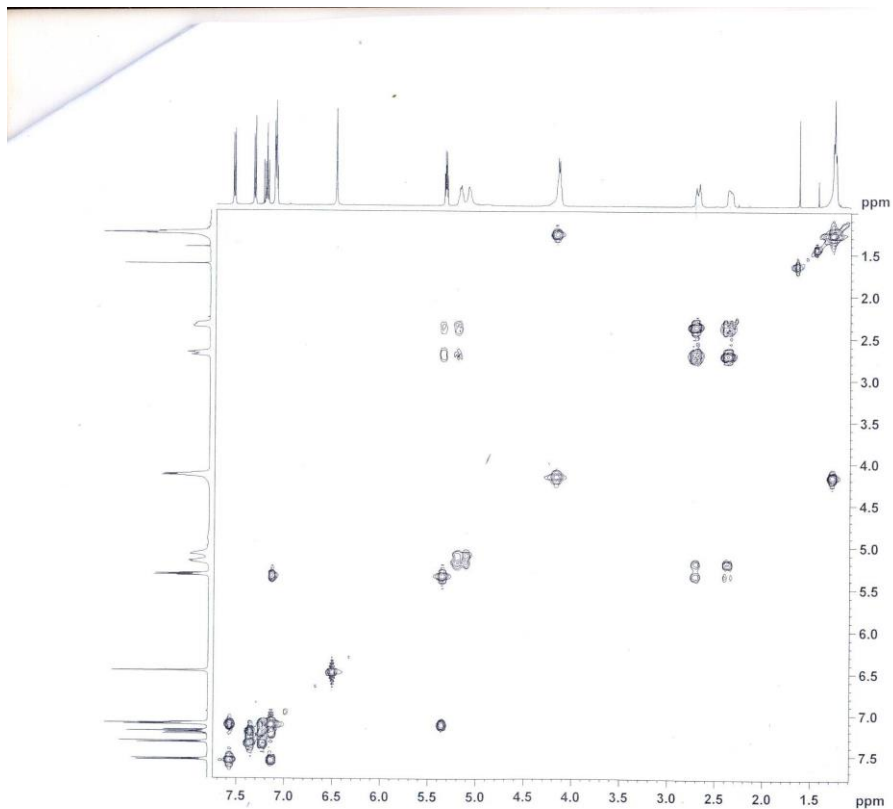
BRUKER

```

NAME          TG168
EXPNO         20
PROCNO        1
Date_         20110609
Time          11.58
INSTRUM       spect
PROBHD        5 mm BBO BB-1H
PULPROG       noesyph
TD            1024
SOLVENT       CDCl3
NS            4
DS            16
SWH           4504.504 Hz
FIDRES        4.398930 Hz
AQ            0.1137140 sec
RG            114
DW            111.000 usec
DE            6.50 usec
TE            298.0 K
D0            0.00009915 sec
D1            2.0000000 sec
D8            1.0000000 sec
IN0           0.00022210 sec

----- CHANNEL f1 -----
NUC1          1H
P1            9.35 usec
PL1           0.00 dB
PL1W         27.37956238 W
SFO1         500.2620010 MHz
NUC2          1
TD            100
SFO2         500.262 MHz
FIDRES        45.023579 Hz
SW            9.000 ppm
EXMODE        States-TFPI
SI            512
SF           500.2600062 MHz
WDW           QSIINE
SSB           2
LB            0.00 Hz
GB            0
PC            1.00
SI            512
MC2           States-TFPI
SF           500.2600064 MHz
WDW           QSIINE
SSB           2
LB            0.00 Hz
GB            0
  
```





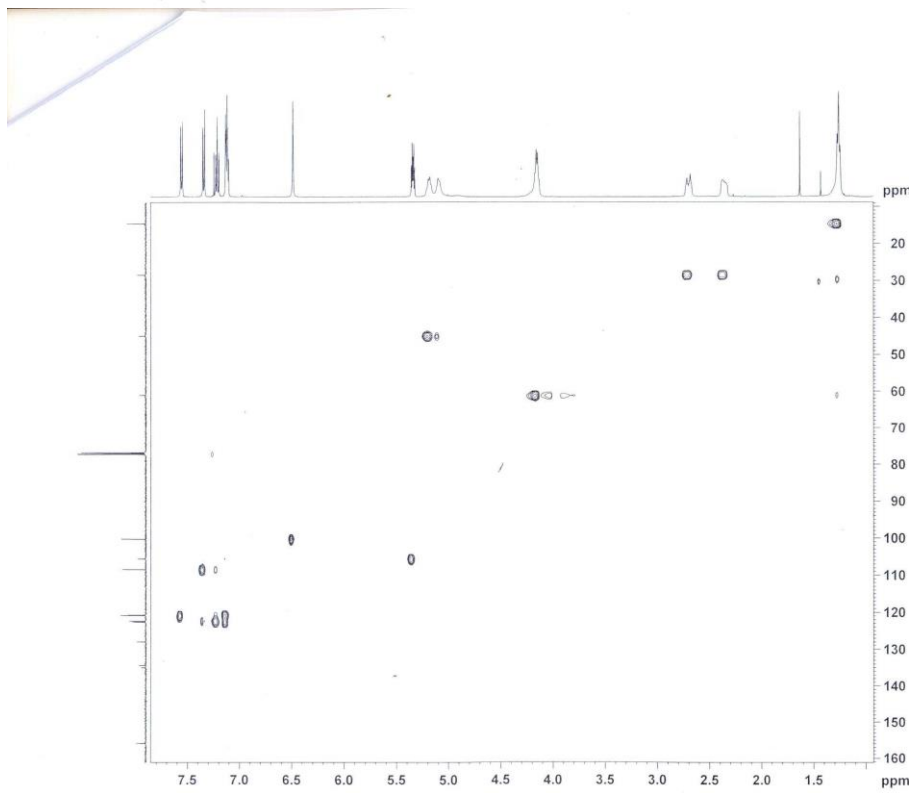
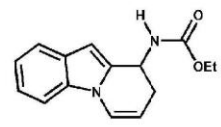
```

NAME          T0148
EXPNO         12
PROCNO        1
Date_         20110813
Time          21.33
INSTRUM       spect
PROBHD        5 mm BBO 5mm-1H
PULPROG       zgpg30
TD            65536
SOLVENT       CDCl3
AQ            4
RG            14
DS            4504.504 Hz
FIDRES        4.338930 Hz
AQ            0.1137140 sec
RG            114
DS            111.000 usec
TE            300.2 K
FIDRES        4.55 usec
AQ            0.0000000 sec
RG            237.25 F
DS            0.0000000 sec
TE            0.0000000 sec
RG            0.0000000 sec
TE            0.0000000 sec
RG            0.0002210 sec
RG            0.0002210 sec

===== CHANNEL f1 =====
NUC1          1H
P1            9.35 usec
PL1           0.00 dB
PL12          0.00 dB
PL1W          23.3794238 W
SFO1          500.2620010 MHz

===== GRADIENT CHANNEL =====
GPRG1        SINE 120
GFL1         10.00 %
P13          1000.00 usec
TD           4
TE           128
SFO1         500.142 MHz
FIDRES       35.174671 Hz
DS           9.500 ppm
FAMODE       QF
SI           512
SF           500.2600000 MHz
WCH          SINE
SFR          0
LB           0.00 Hz
GB           0
PC           1.40
ST           312
MC2          QF
SF           500.2600000 MHz
WCH          SINE
SFR          0
LB           0.00 Hz
GB           0

```



```

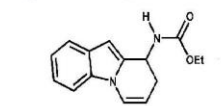
NAME          T0148
EXPNO         12
PROCNO        1
Date_         20110813
Time          21.33
INSTRUM       spect
PROBHD        5 mm BBO 5mm-1H
PULPROG       zgpg30
TD            65536
SOLVENT       CDCl3
AQ            4
RG            14
DS            4504.504 Hz
FIDRES        4.338930 Hz
AQ            0.1137140 sec
RG            114
DS            111.000 usec
TE            300.2 K
FIDRES        4.55 usec
AQ            0.0000000 sec
RG            237.25 F
DS            0.0000000 sec
TE            0.0000000 sec
RG            0.0000000 sec
TE            0.0002210 sec
RG            0.0002210 sec

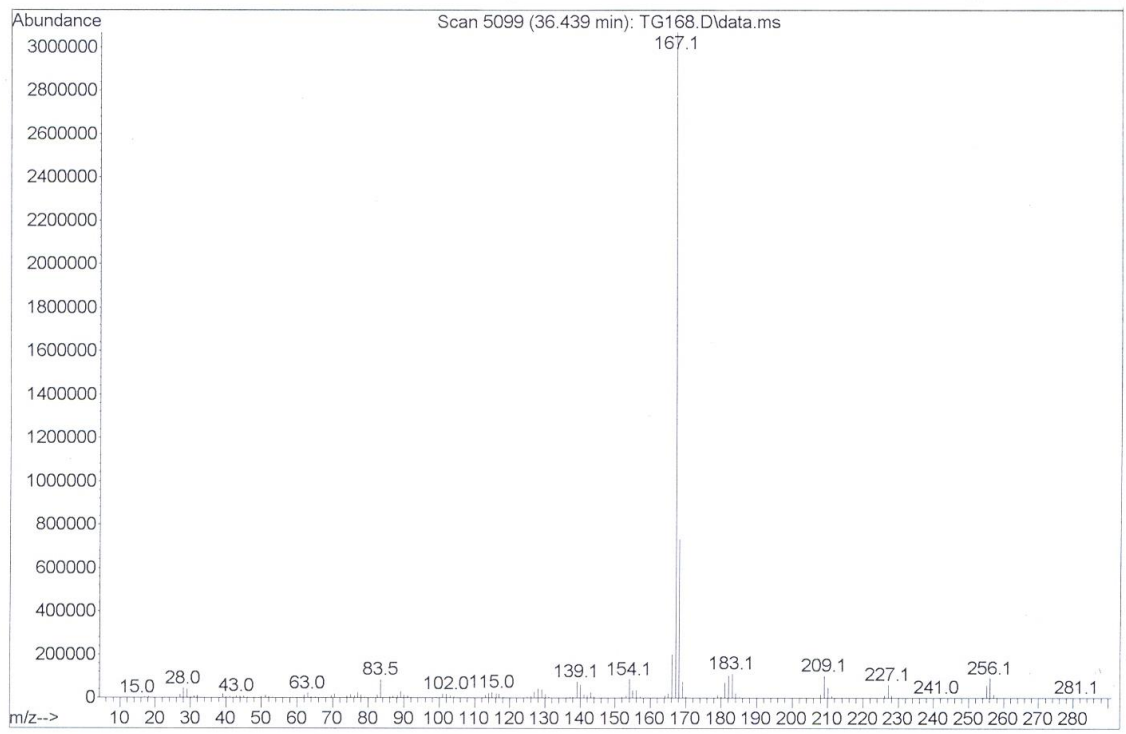
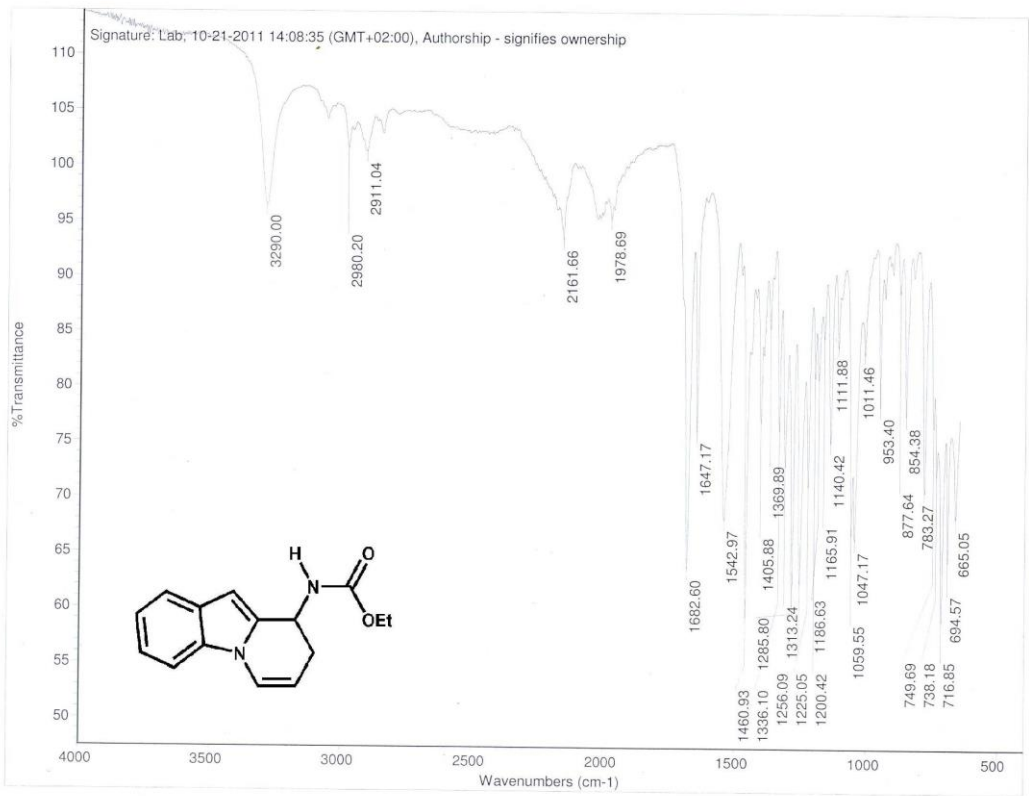
===== CHANNEL f1 =====
NUC1          1H
P1            9.35 usec
PL1           0.00 dB
PL12          0.00 dB
PL1W          23.3794238 W
SFO1          500.2620010 MHz

===== CHANNEL f2 =====
NUC2          13C
P2            11.50 usec
PL2           0.00 dB
PL22          0.00 dB
PL2W          70.00 usec
SFO2          125.7611492 MHz

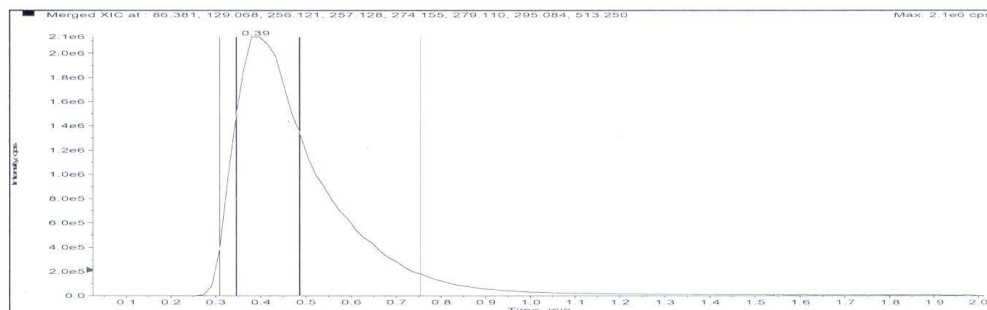
===== GRADIENT CHANNEL =====
GPRG1        SINE 120
GFL1         10.00 %
P13          1000.00 usec
TD           4
TE           128
SFO1         500.142 MHz
FIDRES       35.174671 Hz
DS           9.500 ppm
FAMODE       QF
SI           512
SF           500.2600000 MHz
WCH          SINE
SFR          0
LB           0.00 Hz
GB           0
PC           1.40
ST           312
MC2          QF
SF           500.2600000 MHz
WCH          SINE
SFR          0
LB           0.00 Hz
GB           0

```

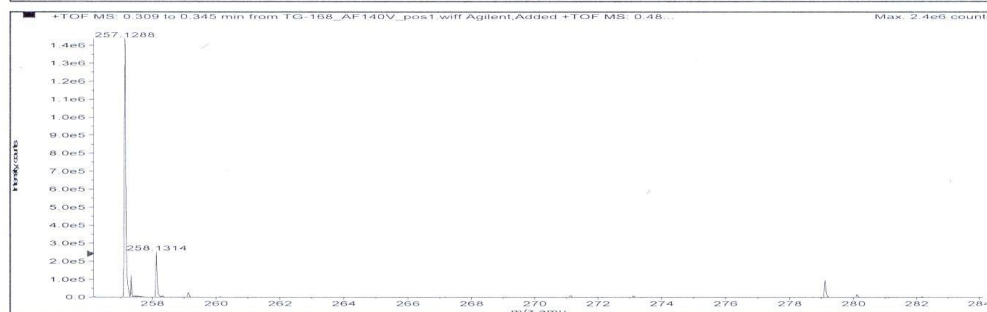
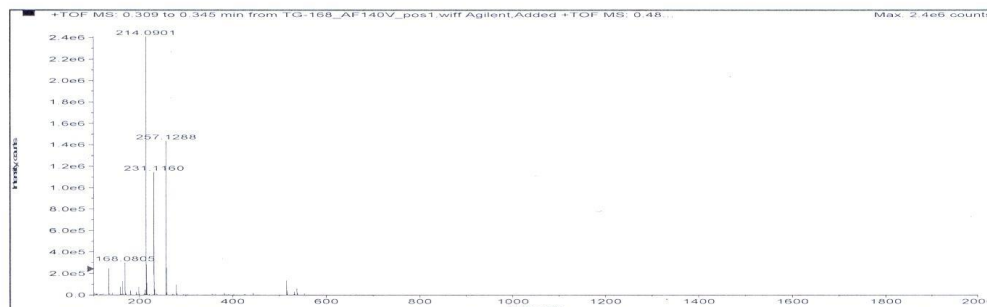




Sample Name: TG-168 Sample Location: P1-D5 Sample Id: Operator: mLKA
 Data File Name: D:\PE Sciex Data\Projects\Farmaceutski fakultet\Data\TG-168_AF140V_pos1.wiff Acq Time: November 14 2011, 04:30:02 PM
 Method: D:\TOF_Data\damethods\Night_Seq_Comp_ident1.anmlefc.xml

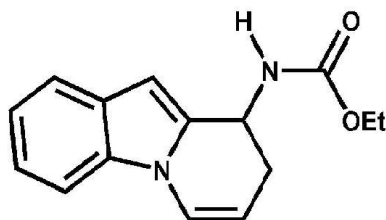


Merged XIC, Period#: 1 Experiment#: 1

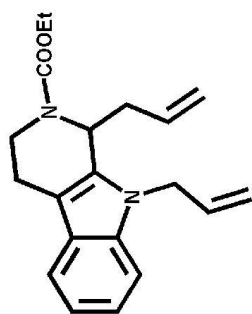


Formula	Compound name	Mass	Peak RT (min)	Peak area	Description
C15H16N2O2	--	256.12118	0.39	2.81253 E7	--

Species	Abundance (counts)	Ion Mass	Measured Mass	Error (mDa)	Error (ppm)	Ret. Time Error (min)
[M+H] ⁺	1533601.20	257.12845	257.12879	0.33703	1.31	--
[M+Na] ⁺	99123.98	279.11040	279.11146	1.06470	3.81	--



Compound 29



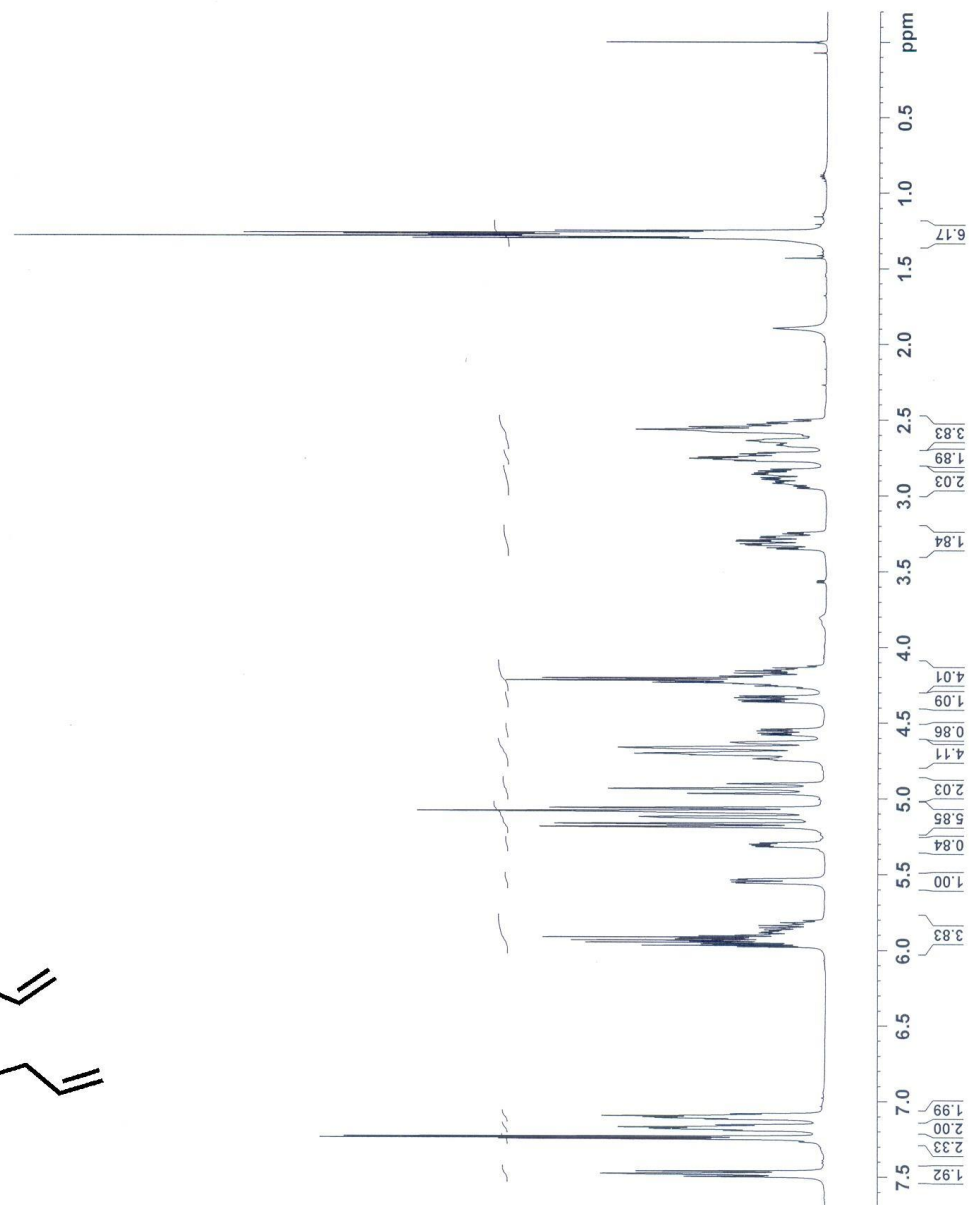
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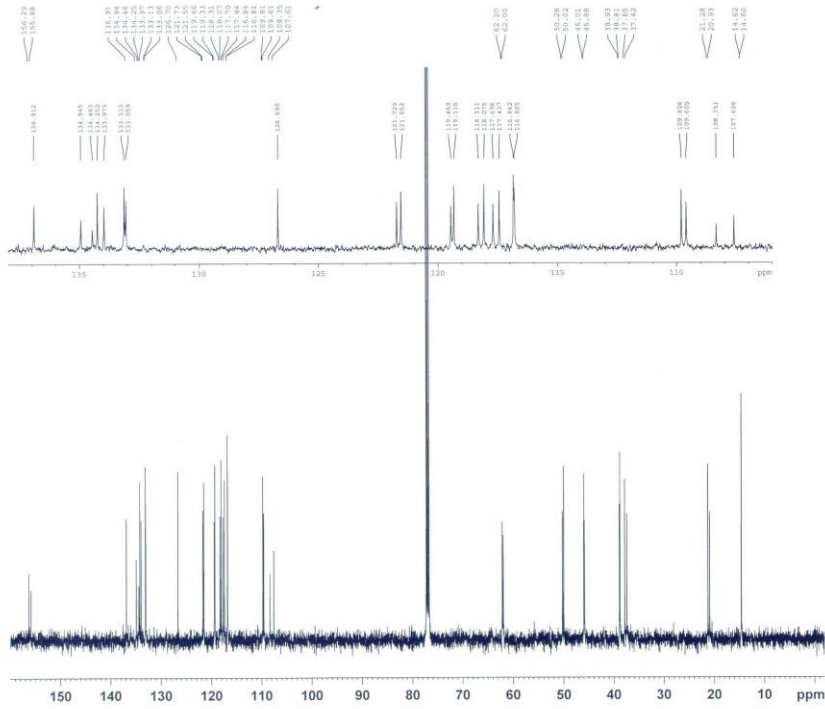
Current Data Parameters
NAME      MS-313
EXPNO     1
PROCNO    1

F2 - Acquisition Parameters
Date_     20130326
Time      15.45
INSTRUM   spect
PROBHD    5 mm BBO BB-1H
PULPROG   zg30
TD         32768
SOLVENT   CDCl3
NS         16
DS         4
SWH        4562.044 Hz
FIDRES     0.139223 Hz
AQ         3.5913727 sec
RG         128
DW         109.600 usec
DE         6.50 usec
TE         298.0 K
D1         2.00000000 sec
TD0        1

===== CHANNEL f1 =====
SF01      500.2618743 MHz
NUC1      1H
P1         9.35 usec
PL1        27.37999916 W

F2 - Processing parameters
SI         32768
SF         500.2600250 MHz
WDW        EM
SSB        0
LB         0.20 Hz
GB         0
PC         1.00
  
```





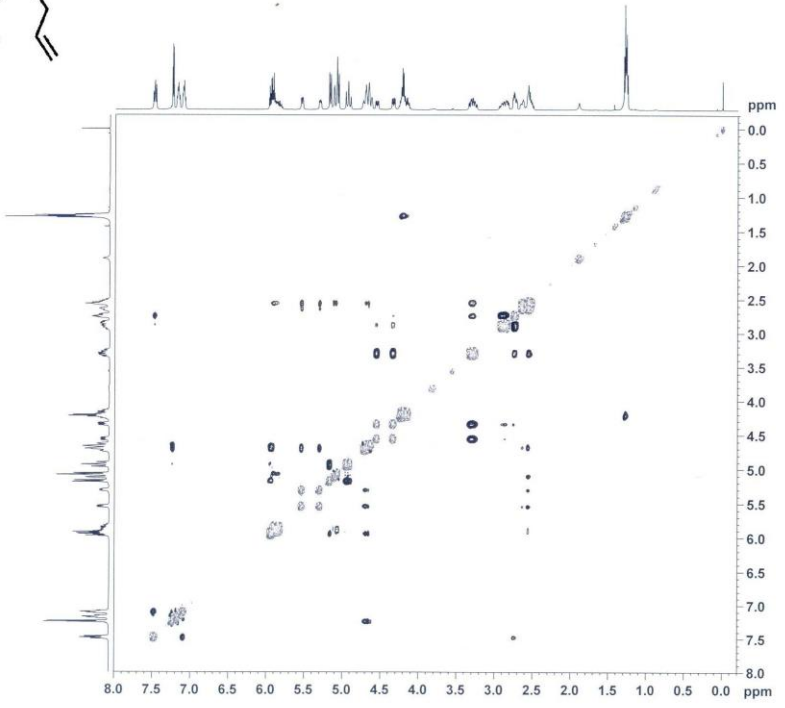
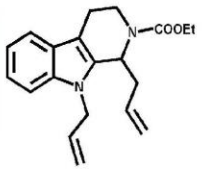
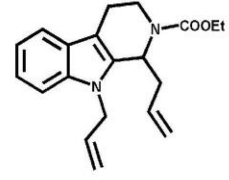
Current Data Parameters
 NAME MS-113
 EXPNO 2
 PROCNO 1

F2 - Acquisition Parameters
 Date_ 20130326
 Time 15.53
 INSTRUM spect
 PROBHD 5 mm BBO BB-1H
 PULPROG zgpg30
 TD 32768
 SOLVENT CDCl3
 NS 320
 DS 4
 SWE 29761.994 Hz
 FIDRES 0.908261 Hz
 AQ 0.5505024 sec
 RG 912
 DW 16.800 usec
 DE 6.50 usec
 TE 298.0 K
 D1 2.0000000 sec
 D11 0.0300000 sec
 TDO 1

----- CHANNEL f1 -----
 SFO1 125.8043340 MHz
 NUC1 13C
 P1 11.50 usec
 PLW1 32.22800664 W

----- CHANNEL f2 -----
 SFO2 500.2618745 MHz
 NUC2 1H
 CPDPRG2 waltz16
 PCPD2 60.00 usec
 PLW2 20.77000046 W
 PLW12 0.39257051 W
 PLW13 0.25130999 W

F2 - Processing parameters
 SI 12768
 SF 125.7904843 MHz
 WDW EM
 SSB 0
 LB 1.50 Hz
 GB 0
 PC 1.40



Current Data Parameters
 NAME MS-113
 EXPNO 5
 PROCNO 1

F2 - Acquisition Parameters
 Date_ 20130326
 Time 16.39
 INSTRUM spect
 PROBHD 5 mm BBO BB-1H
 PULPROG hmcyspph
 TD 1024
 SOLVENT CDCl3
 NS 4
 DS 16
 SWE 4562.044 Hz
 FIDRES 4.455121 Hz
 AQ 0.1122104 sec
 RG 128
 DW 109.600 usec
 DE 6.50 usec
 TE 298.0 K
 D0 0.0000970 sec
 D1 2.0000000 sec
 D8 1.0000000 sec
 D16 0.0002000 sec
 INO 0.00021930 sec

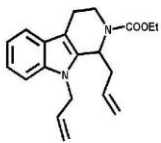
----- CHANNEL f1 -----
 SFO1 500.2618745 MHz
 NUC1 1H
 P1 9.35 usec
 P2 16.70 usec
 PLW1 27.37999916 W

----- GRADIENT CHANNEL -----
 GRAM1 2188.100
 GP21 40.00 %
 P16 1000.00 usec

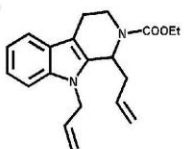
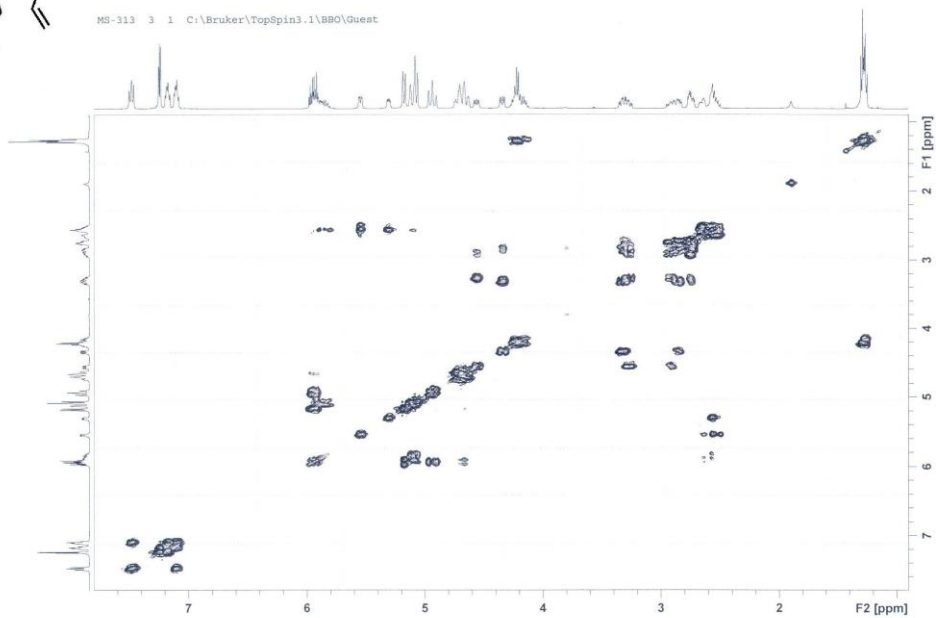
F1 - Acquisition parameters
 TD 140
 SFO1 500.2619 MHz
 FIDRES 28.622774 Hz
 SW 9.119 ppm
 FREQCZ States-TPP1

F2 - Processing parameters
 SI 812
 SF 500.2602025 MHz
 WDW Q918E
 SSB 2
 LB 0 Hz
 GB 0
 PC 1.00

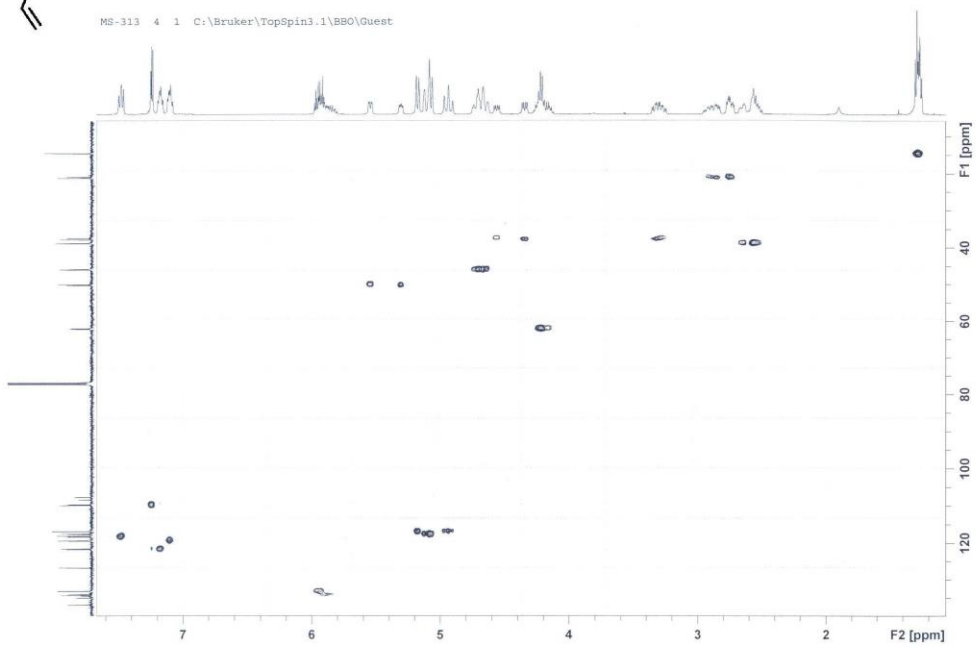
F1 - Processing parameters
 SI 812
 MC2 States-TPP1
 SF 500.2603196 MHz
 WDW Q918E
 SSB 2
 LB 0 Hz
 GB 0

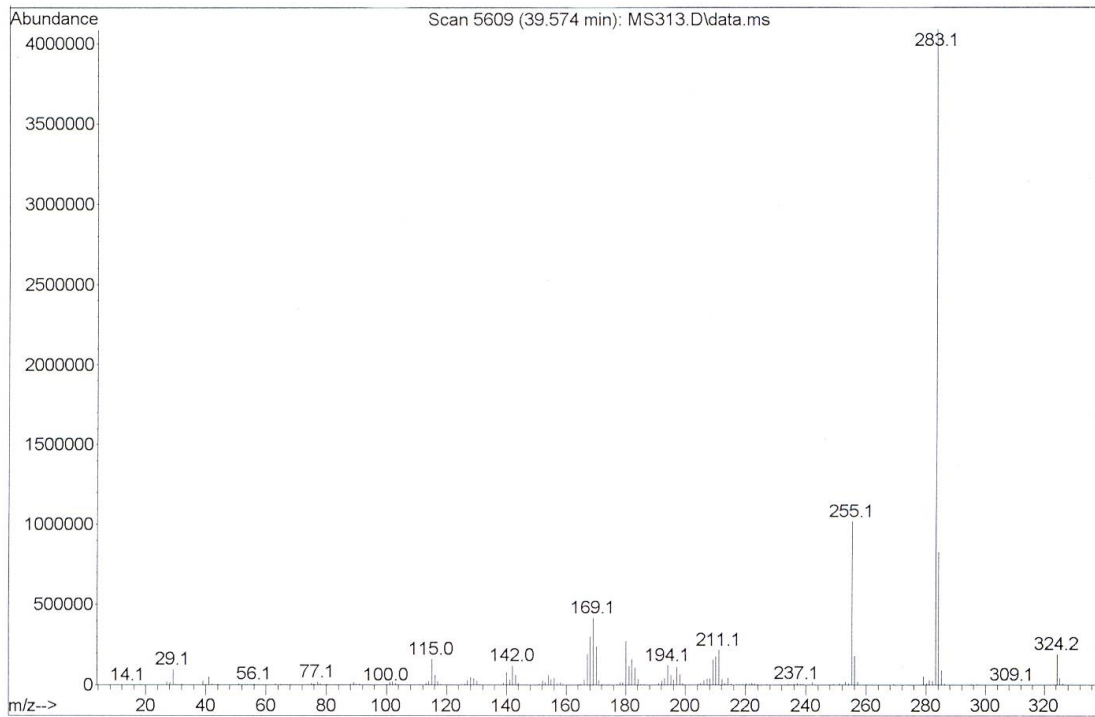
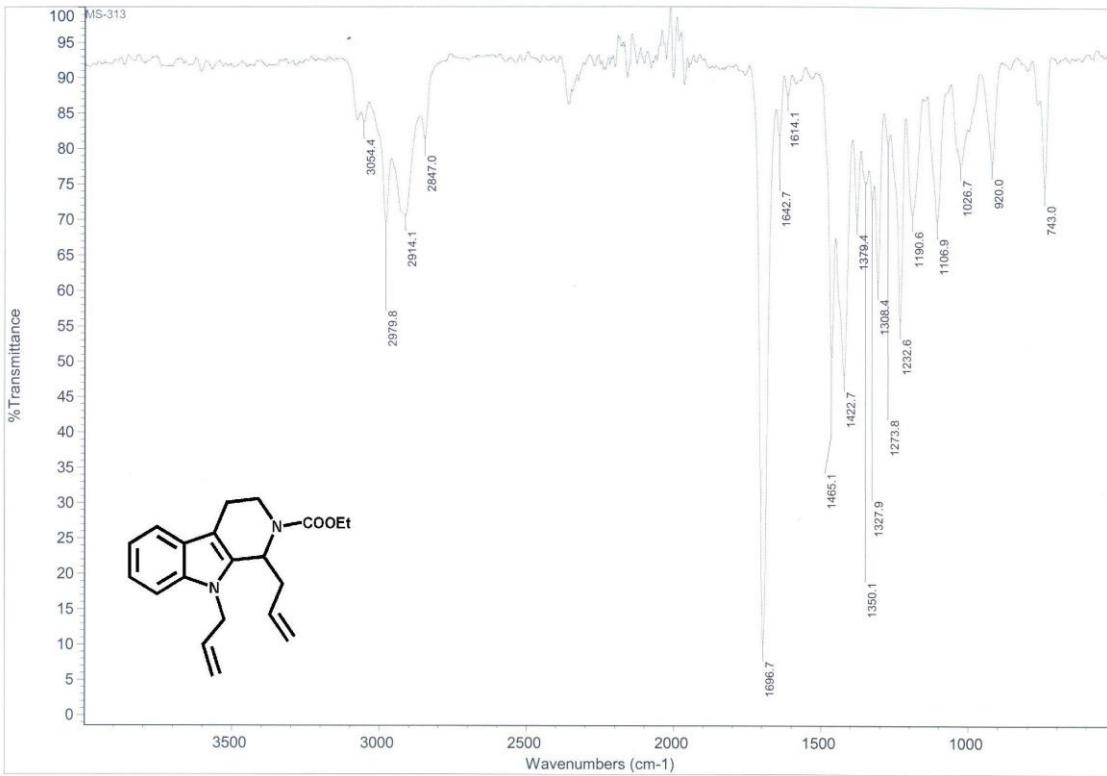


MS-313 3 1 C:\Bruker\TopSpin3.1\BBO\Guest

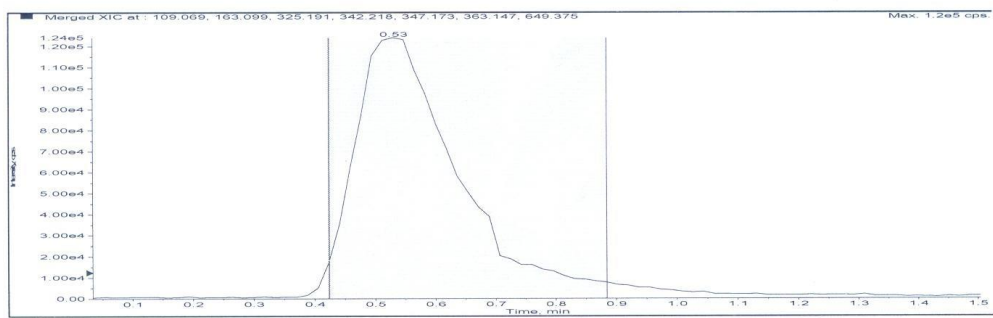


MS-313 4 1 C:\Bruker\TopSpin3.1\BBO\Guest

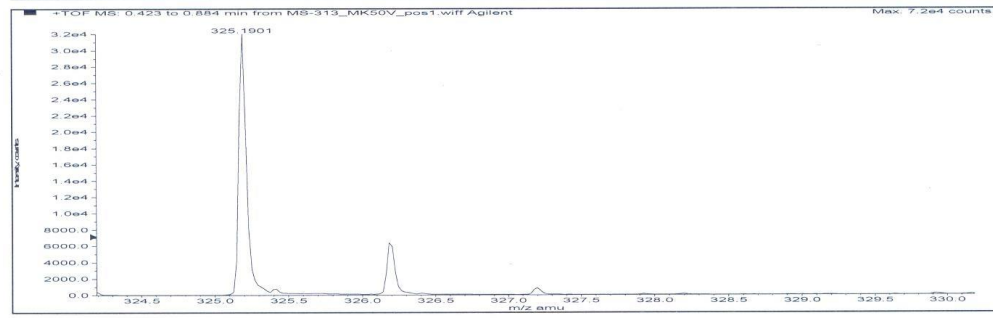
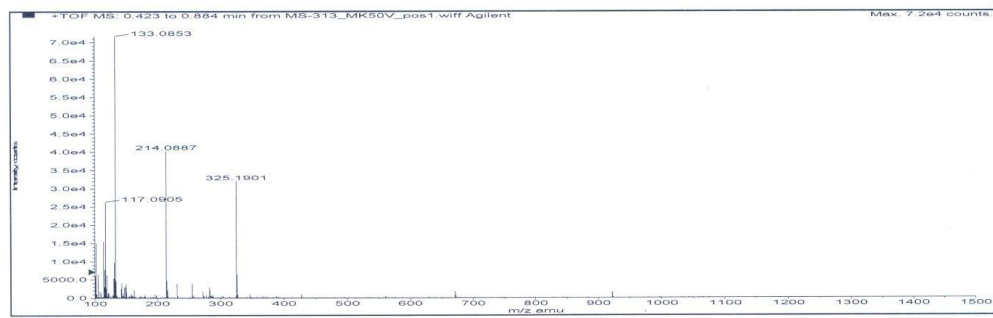




Sample Name: MS-313 Sample Location: P1-D6 Sample Id: Operator: Gordana
 Data File Name: D:\PE Sciex Data\Projects\Novi Sad\Data\MS-313_MK50V_pos1.wiff Acq Time: April 11 2013, 12:48:29 PM
 Method: d:\TOF_Data\damethods\Night_Seq_Comp_Ident1.anml\efc.xml

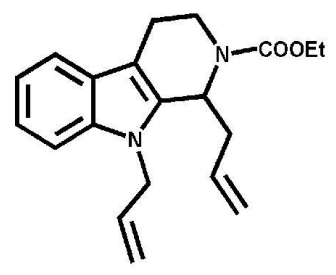


Merged XIC, Period# : 1 Experiment# : 1

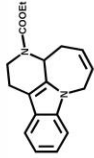


Formula	Compound name	Mass	Peak RT (min)	Peak area	Description
C20H24N2O2	--	324.18378	0.53	1.48519 E6	--

Species	Abundance (counts)	Ion Mass	Measured Mass	Error (mDa)	Error (ppm)	Ret. Time Error (min)
[M+H] ⁺	32035.80	325.19105	325.19007	-0.98183	-3.02	--



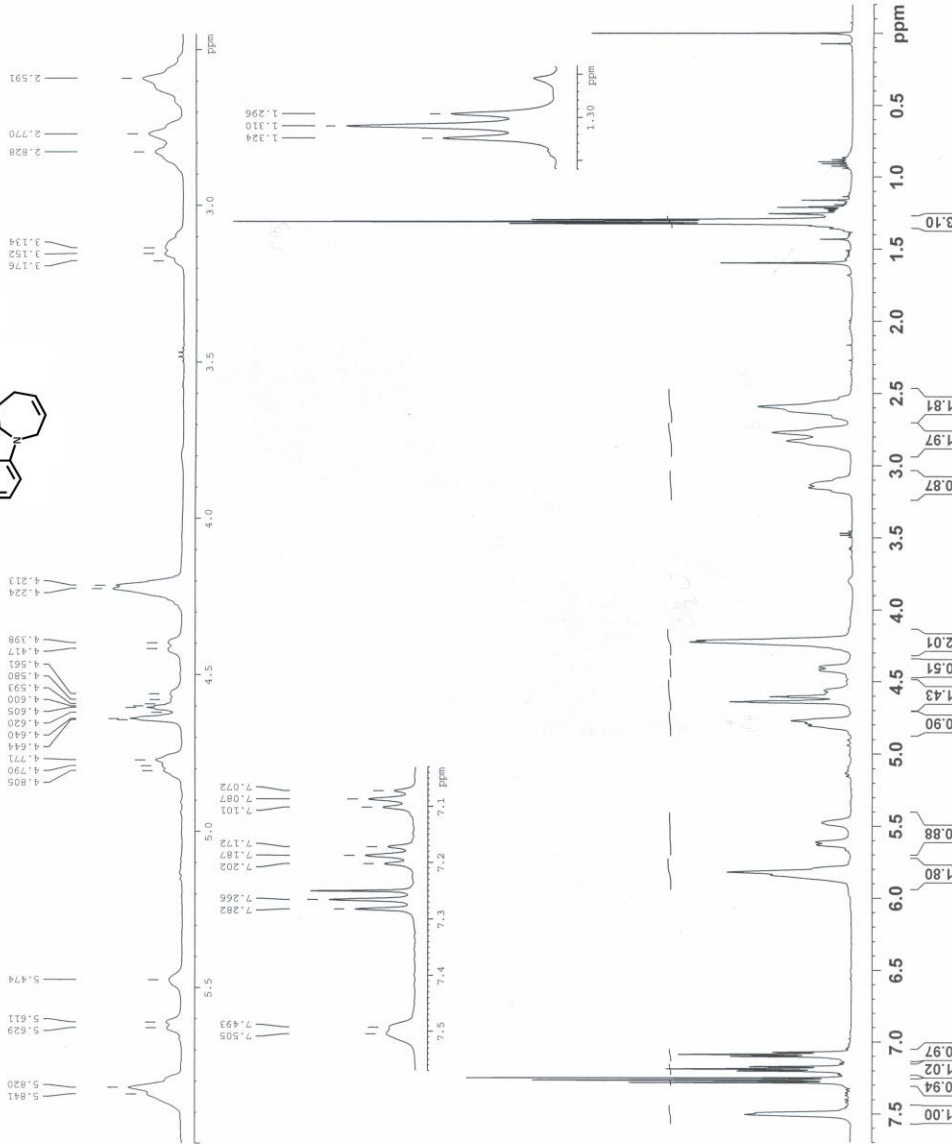
Compound 30

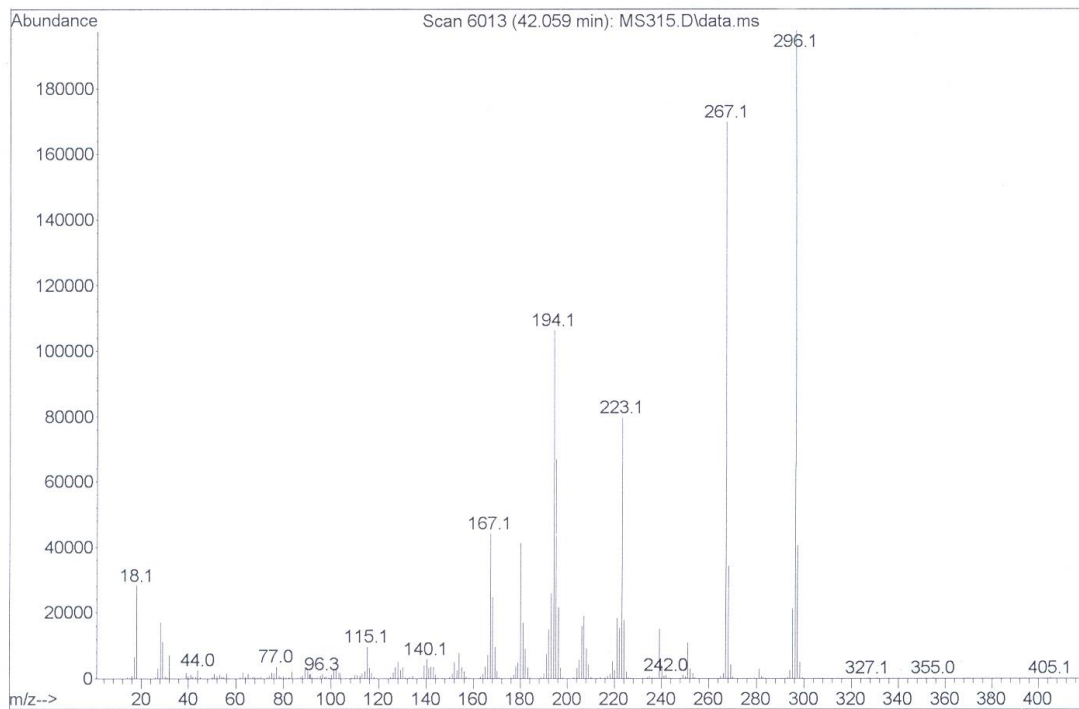
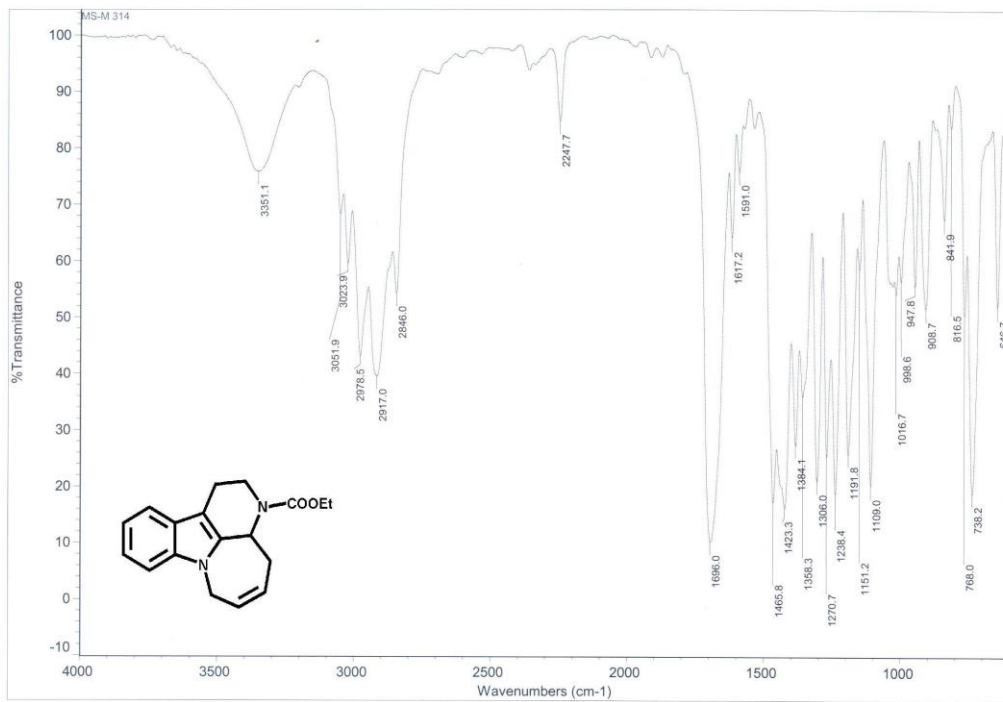


Current Data Parameters
 NAME MS-314
 EXPNO 1
 PROCNO 1

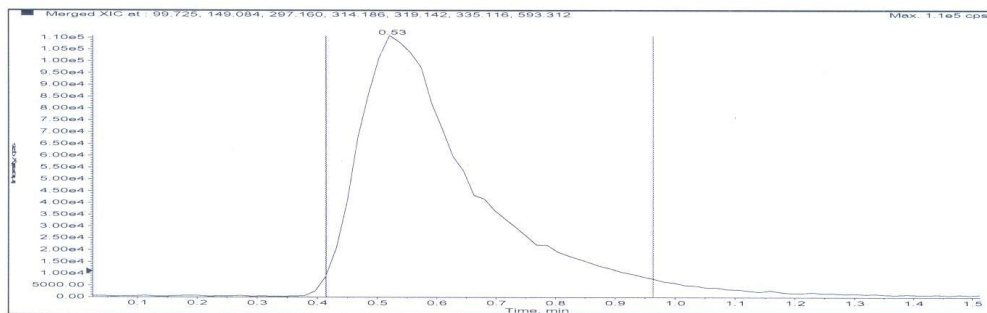
F2 - Acquisition Parameters
 Date_ 20130211
 Time_ 14.28
 INSTRUM spect
 PULPROG zgpg30
 TD 32768
 SOLVENT CDCl3
 NS 16
 DS 0
 SWH 4761.905 Hz
 FWHZ 14520.0
 AQ 3.44166400 sec
 RG 203
 DW 105.000 usec
 DE 6.50 usec
 TE 298.0 K
 TD 2.00000000 sec
 TDO 1

===== CHANNEL f1 =====
 SF01 500.2620149 MHz
 NUC1 1H
 P1 8.35 usec
 PL1 27.37999916 W
 F2 - Processing parameters
 SF 500.2600194 MHz
 EM
 LB 0
 GB 0
 PC 1.00

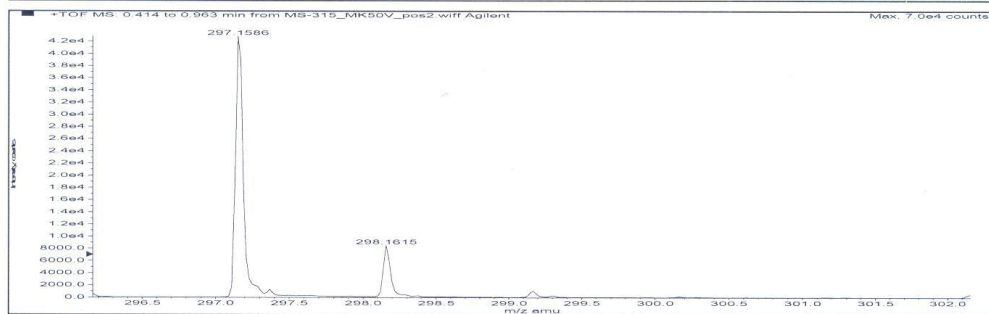
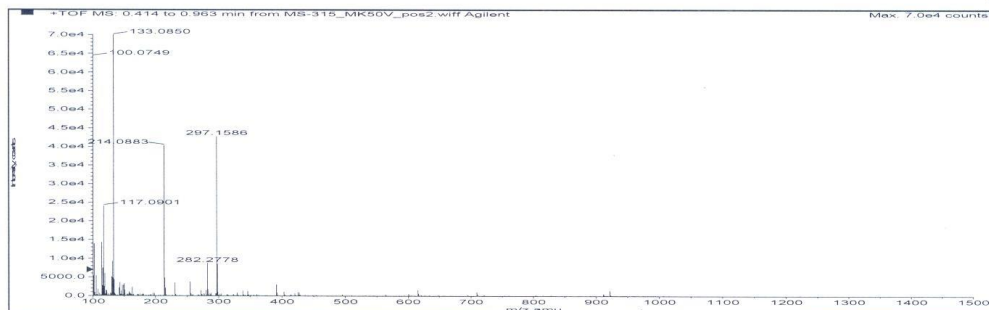




Sample Name: MS-315 Sample Location: P1-D8 Sample Id: Operator: Gordana
 Data File Name: D:\PE Sciex Data\Projects\Novi Sad\Data\MS-315_MK50V_pos2.wiff Acq Time: April 11 2013, 01:12:31 PM
 Method: d:\TOF_Data\damethods\Night_Seq_Comp_ident1.anmefc.xml

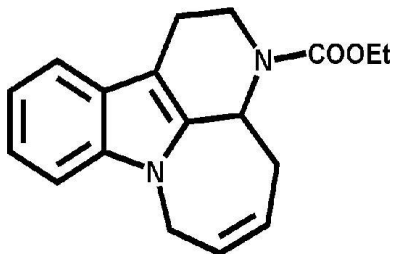


Merged XIC, Period# : 1 Experiment# : 1

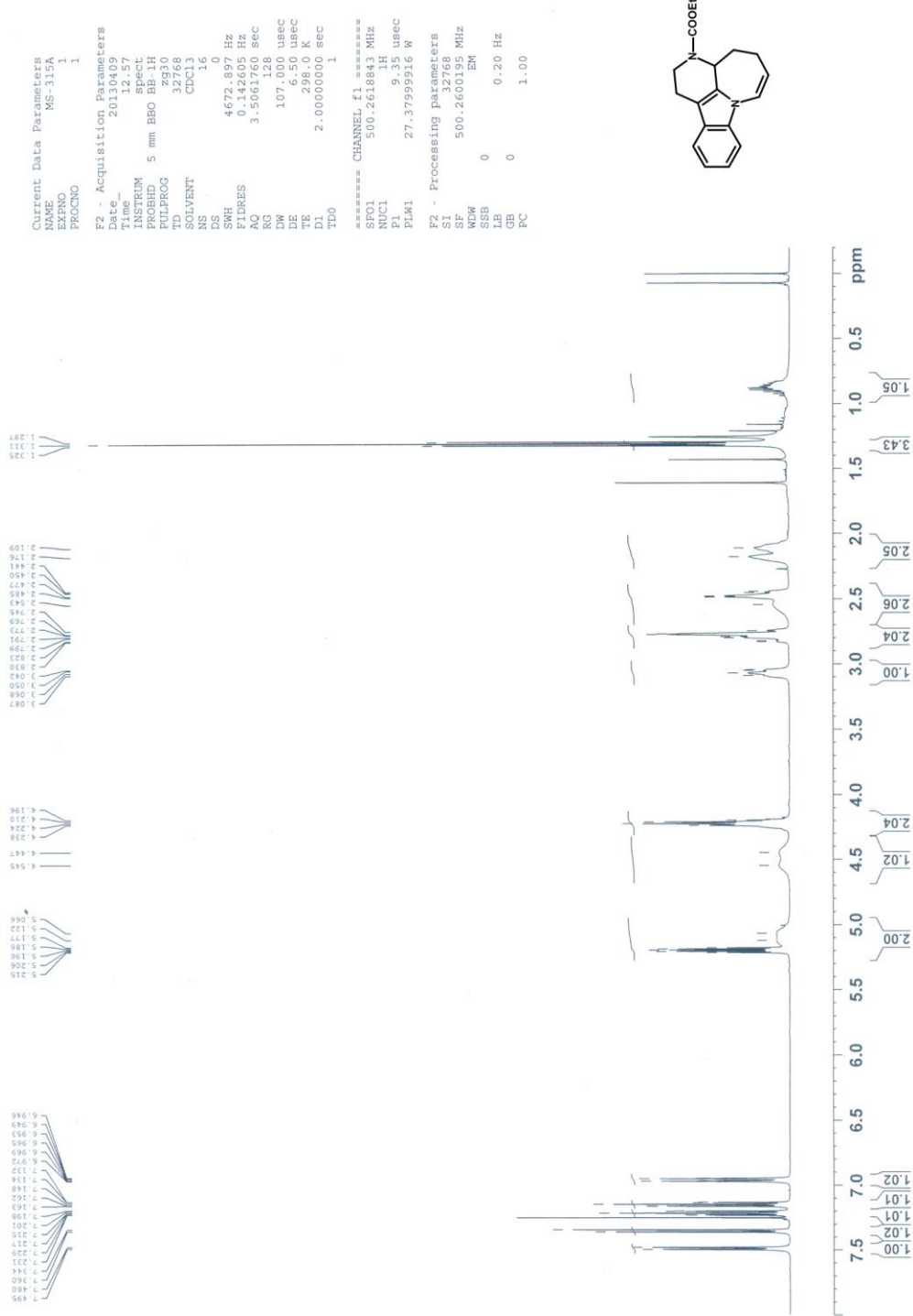


Formula	Compound name	Mass	Peak RT (min)	Peak area	Description
C18H20N2O2	--	296.15248	0.53	1.50638 E6	--

Species	Abundance (counts)	Ion Mass	Measured Mass	Error (mDa)	Error (ppm)	Ret. Time Error (min)
[M+H] ⁺	44700.62	297.15975	297.15863	-1.12193	-3.78	--



Compound 31

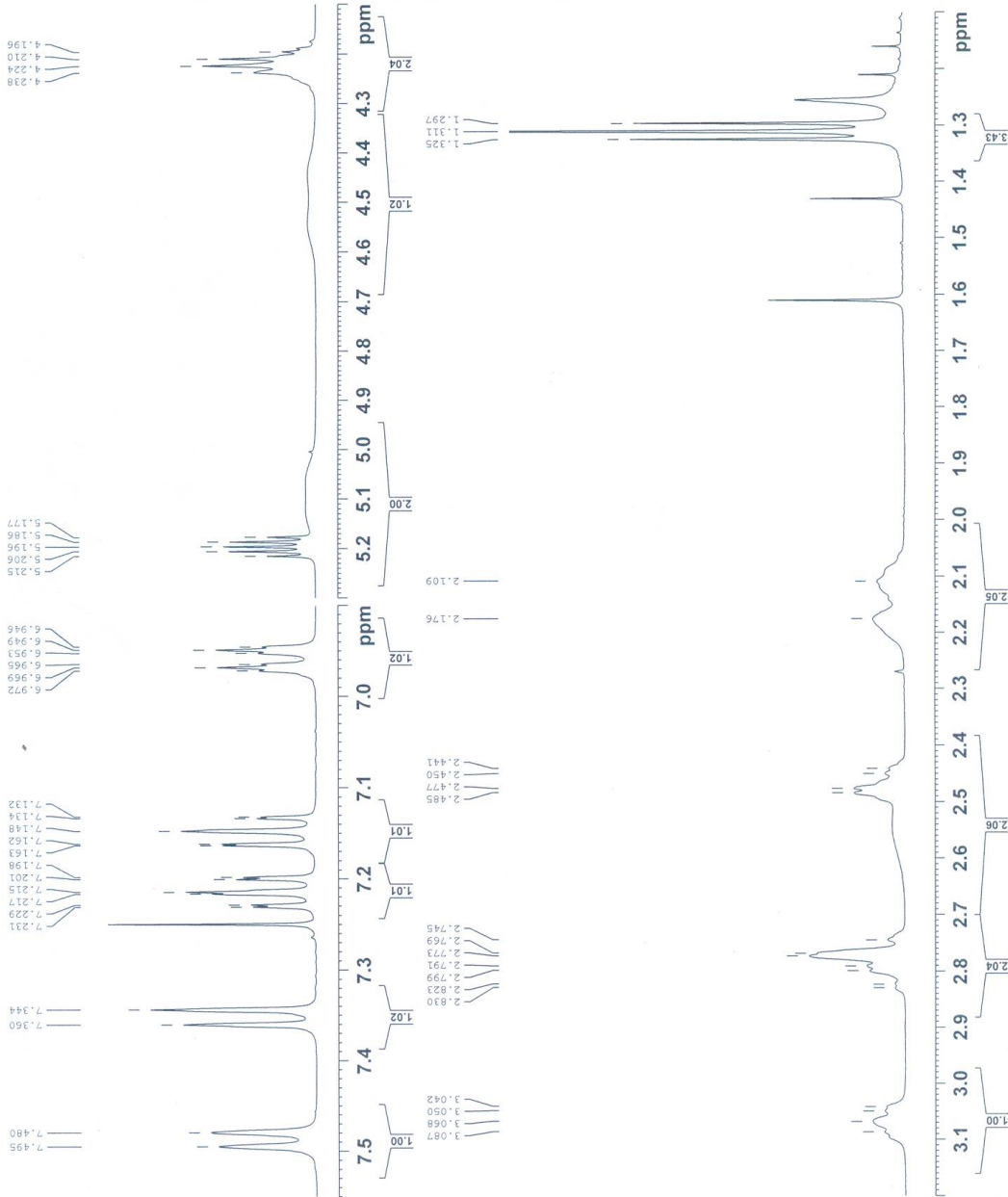
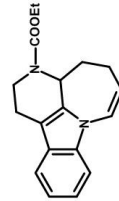


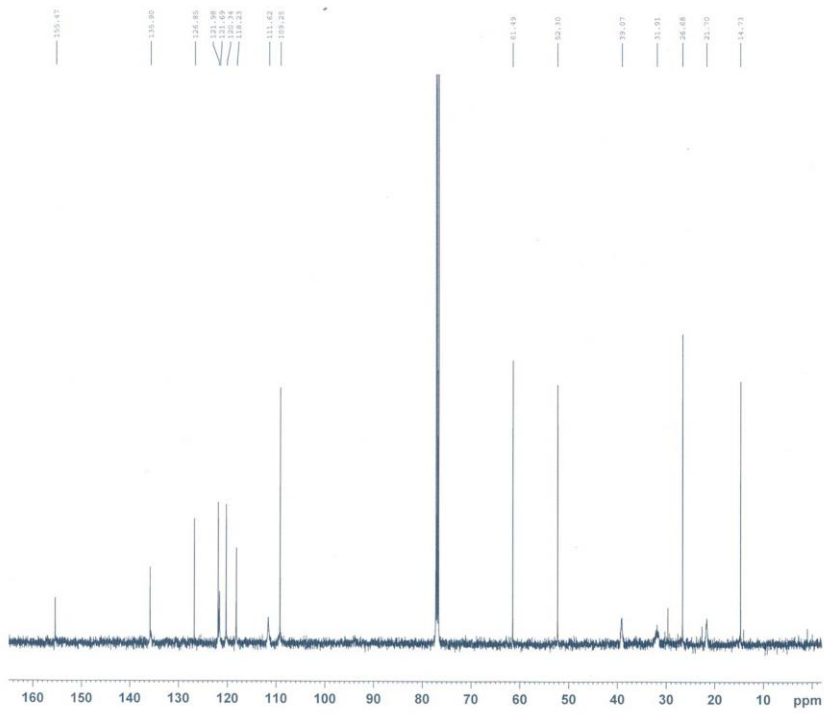
Current Data Parameters
 NAME MS-315A
 EXPNO 1
 PROCNO 1

F2 - Acquisition Parameters
 Date_ 20130409
 Time_ 12:57
 INSTRUM spect
 PROBHD 5 mm BBO BB-1H
 PULPROG zg30
 TD 32768
 SOLVENT CDCl3
 NS 16
 DS 0
 SWH 4672.897 Hz
 FIDRES 0.142605 Hz
 AQ 3.5061760 sec
 RG 106
 DW 107.006 usec
 DE 6.50 usec
 TE 298.0 K
 D1 2.00000000 sec
 TD0 1

===== CHANNEL f1 =====
 SF01 500.2618843 MHz
 NUC1 1H
 P1 9.35 usec
 PL1 27.37999916 W

F2 - Processing Parameters
 SF 500.2600195 MHz
 WDW EM
 SSB 0
 LB 0.20 Hz
 GB 0
 PC 1.00





```

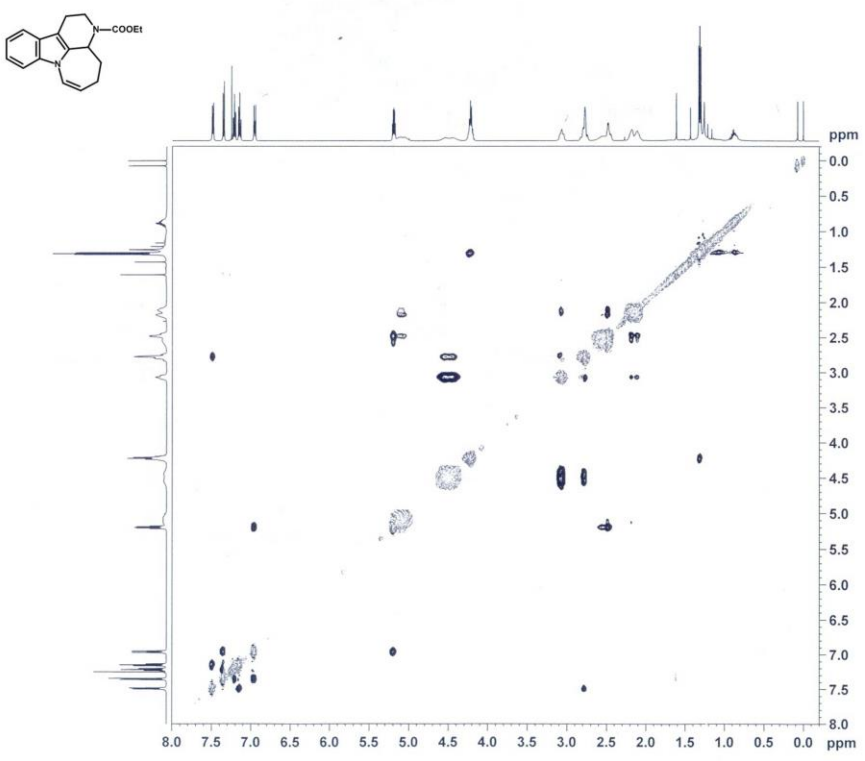
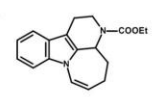
Current Data Parameters
NAME      MS-315A
EXPNO    2
PROCNO   1

F2 - Acquisition Parameters
Date_    20130409
Time     13.10
INSTRUM  spect
PROBHD   5 mm BBO BB-1H
PULPROG  zgpg30
TD       32768
SOLVENT  CDCl3
NS       644
DS       4
SWH      29761.904 Hz
FIDRES   0.598261 Hz
AQ       0.550524 sec
RG       812
DM       16.600 usec
DE       6.50 usec
TE       298.0 K
D1       2.0000000 sec
D11      0.0300000 sec
TD0      1

===== CHANNEL f1 =====
SFO1     125.8043140 MHz
NUC1     13C
P1       11.50 usec
PLW1     32.22800064 W

===== CHANNEL f2 =====
SFO2     500.2618845 MHz
NUC2     1H
CPDPRG2  waltz16
PCPD2    80.00 usec
PLW2     20.77000146 W
PLW12    0.39267001 W
PLW13    0.25130999 W

F2 - Processing parameters
SI       32768
SF       125.7904826 MHz
WDW      EM
SSB      0
LB       1.50 Hz
GB       0
PC       1.40
  
```



```

Current Data Parameters
NAME      MS-315A
EXPNO    5
PROCNO   1

F2 - Acquisition Parameters
Date_    20130409
Time     14.01
INSTRUM  spect
PROBHD   5 mm BBO BB-1H
PULPROG  noesygpg3
TD       1024
SOLVENT  CDCl3
NS       8
DS       16
SWH      4672.897 Hz
FIDRES   4.563376 Hz
AQ       0.1099680 sec
RG       128
DM       107.000 usec
DE       6.50 usec
TE       298.0 K
D0       0.0000510 sec
D1       2.0000000 sec
D8       1.0000000 sec
D16      0.0020000 sec
IN0      0.00021400 sec

===== CHANNEL f1 =====
SFO1     500.2618845 MHz
NUC1     1H
P1       9.35 usec
PLW1     18.70 usec
PLM1     27.37999916 W

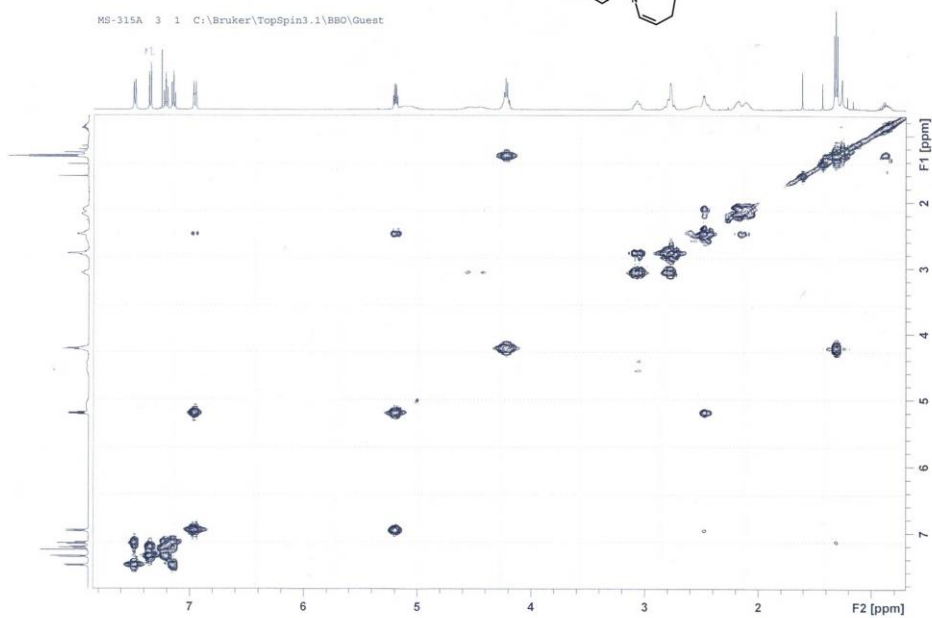
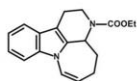
===== GRADIENT CHANNEL =====
GPRAM(1) SINE.100
OP1      40.00 Hz
P16      1000.00 usec

F1 - Acquisition parameters
TD       139
SFO1     500.2619 MHz
FIDRES   33.617966 Hz
SW       9.241 ppm
F0MODE   States-TPPI

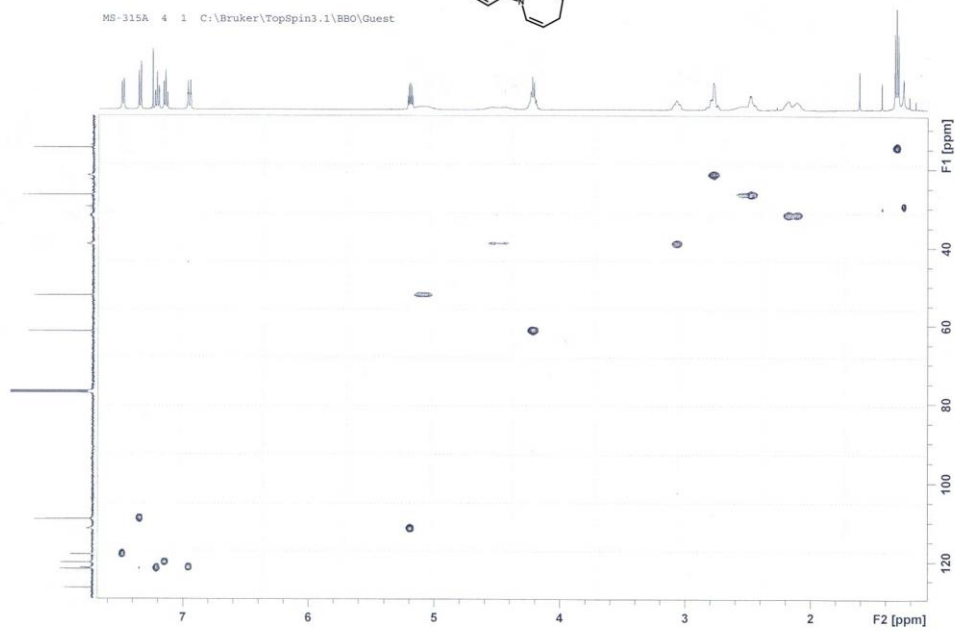
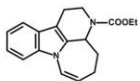
F2 - Processing parameters
SI       512
SF       500.2600128 MHz
WDW      OSINE
SSB      2
LB       0 Hz
GB       0
PC       1.00

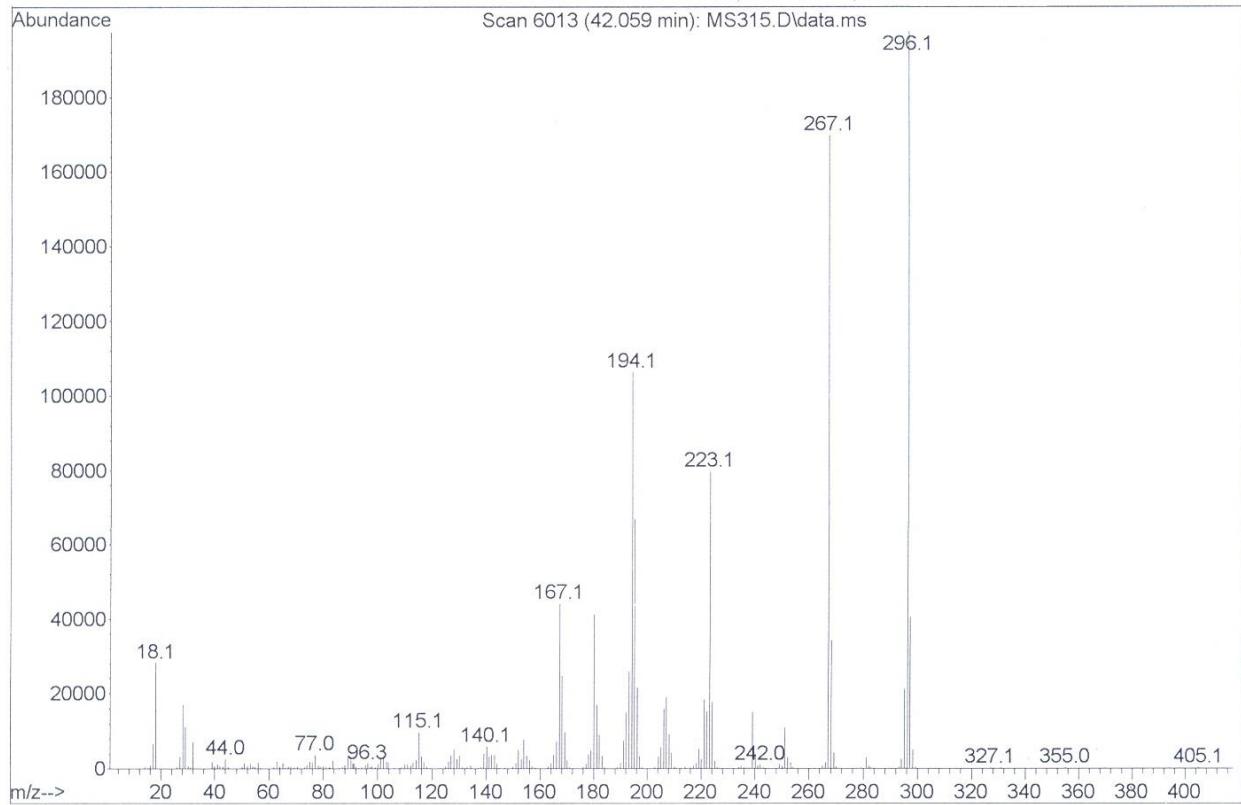
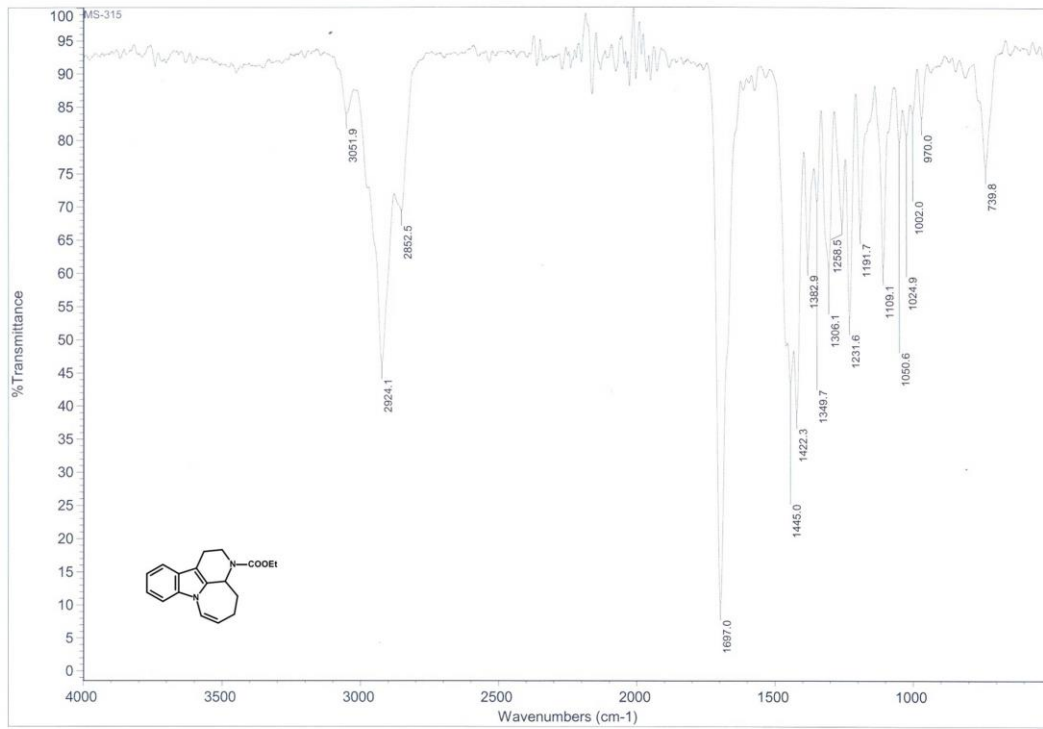
F1 - Processing parameters
SI       512
MC2      States-TPPI
SF       500.2600164 MHz
WDW      OSINE
SSB      2
LB       0 Hz
GB       0
  
```

MS-315A 3 1 C:\Bruker\TopSpin3.1\BBO\Guest

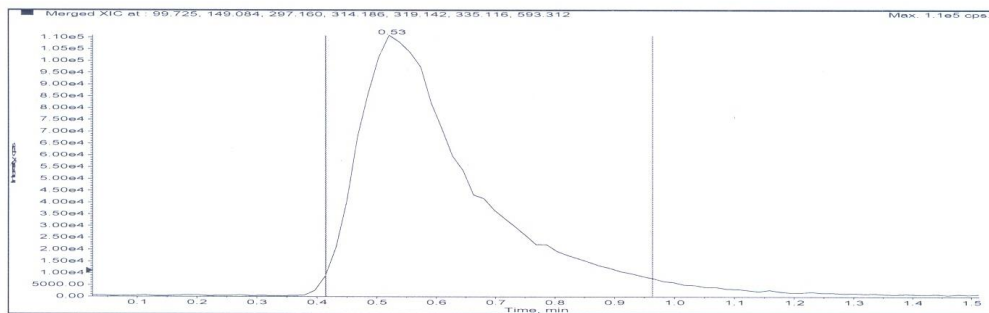


MS-315A 4 1 C:\Bruker\TopSpin3.1\BBO\Guest

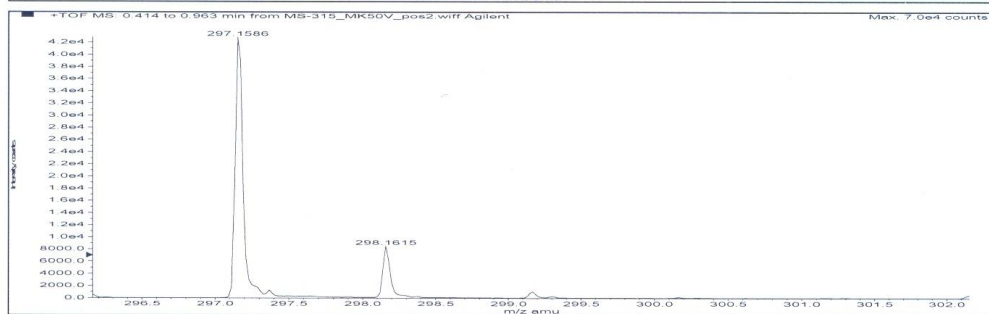
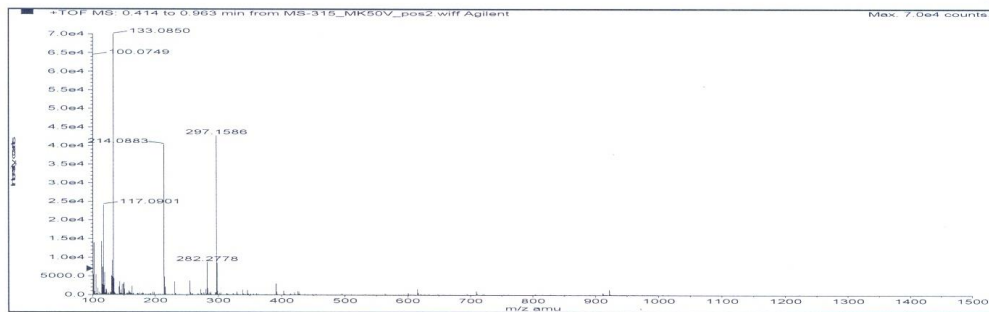




Sample Name: MS-315 Sample Location: P1-D8 Sample Id: Operator: Gordana
 Data File Name: D:\PE Sciex Data\Projects\Novi Sad\Data\MS-315_MK50V_pos2.wiff Acq Time: April 11 2013, 01:12:31 PM
 Method: d:\TOF_Data\damethods\Night_Seq_Comp_ident1.anm\efc.xml

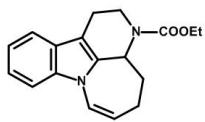


Merged XIC, Period# : 1 Experiment# : 1

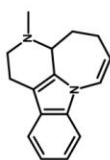


Formula	Compound name	Mass	Peak RT (min)	Peak area	Description
C18H20N2O2	--	296.15248	0.53	1.50638 E6	--

Species	Abundance (counts)	Ion Mass	Measured Mass	Error (mDa)	Error (ppm)	Ret. Time Error (min)
[M+H] ⁺	44700.62	297.15975	297.15863	-1.12193	-3.78	--



Compound 1b

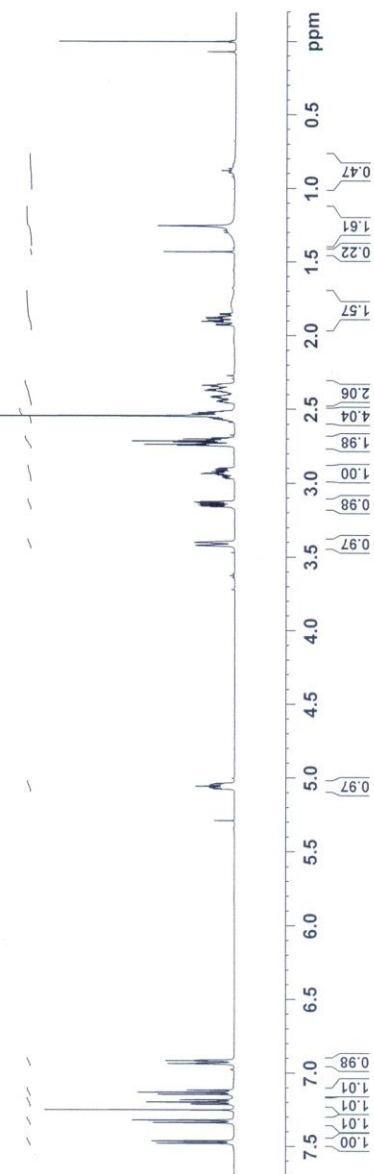


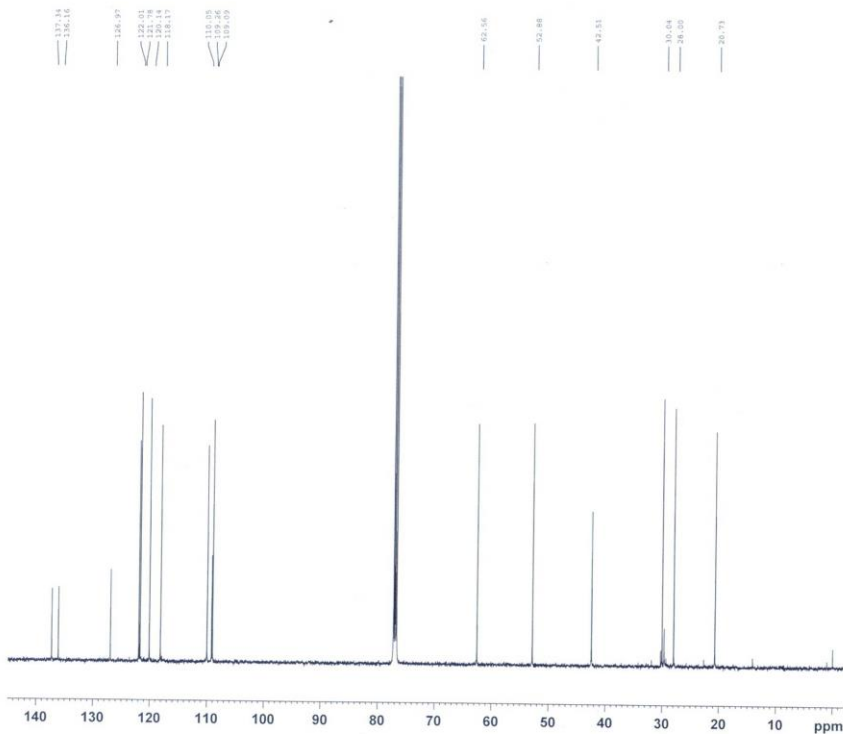
Current Data Parameters
 NAME VM-MS327A
 EXPNO 1
 PROCNO 1

F2 - Acquisition Parameters
 Date_ 2010042
 Time 1743
 INSTRUM spect
 PROBHD 5 mm BBO BB-1H
 PULPROG zg30
 TD 32768
 SOLVENT CDCl3
 NS 16
 DS 4
 SWH 4553.734 Hz
 FIDRES 0.138969 Hz
 AQ 3.5979264 sec
 RG 144
 DW 109.800 usec
 DE 6.50 usec
 DI 298.0 K
 D1 2.0000000 sec
 TDO 1

===== CHANNEL f1 =====
 SFO1 500.2619841 MHz
 NUC1 1H
 PL1 9.35 usec
 PLM1 27.37999916 W

F2 - Processing parameters
 SI 32768
 SF 500.2600185 MHz
 MDW 0 EM
 SSB 0
 LB 0
 GB 0
 PC 1.00





```

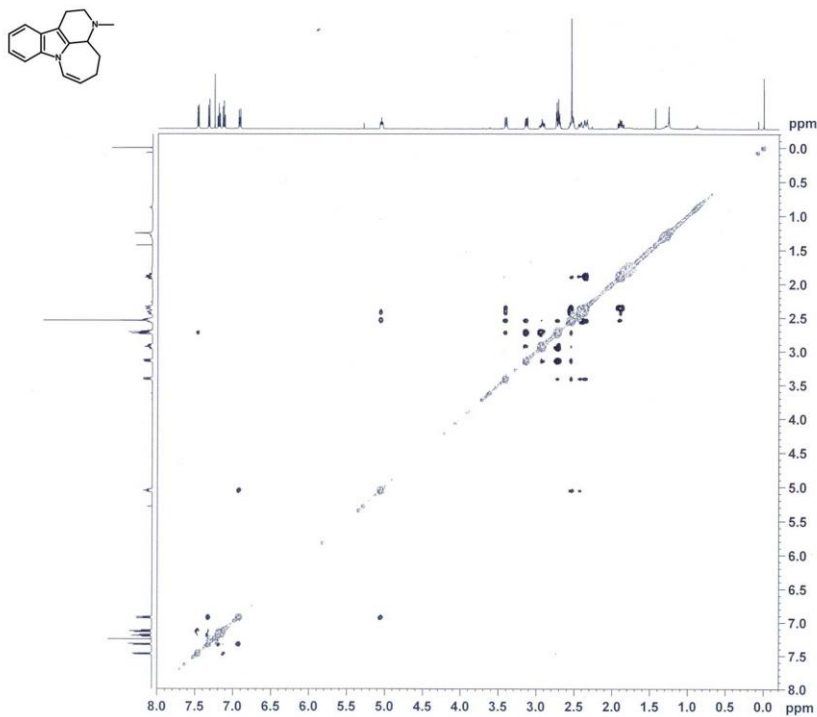
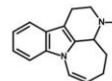
Current Data Parameters
NAME      VM-M327A
EXPNO    6
PROCNO   1

F2 - Acquisition Parameters
Date_    20130403
Time     7.13
INSTRUM  spect
PROBHD   5 mm BBO BB-1H
PULPROG  zgpg30
TD       32768
SOLVENT  CDCl3
NS       5200
DS       4
SWH      29761.904 Hz
FIDRES   0.908261 Hz
AQ       0.5505024 sec
RG       812
DM       16.800 usec
DE       6.50 usec
TE       298.0 K
D1       2.0000000 sec
D11      0.0300000 sec
TD0      1

===== CHANNEL f1 =====
SFO1     125.8043140 MHz
NUC1     13C
P1       11.50 usec
PLW1     32.22800064 W

===== CHANNEL f2 =====
SFO2     500.2619840 MHz
NUC2     1H
CPDPRG2  waltz16
PCPD2    80.00 usec
PLW2     20.77000046 W
PLW12    0.39267001 W
PLW13    0.25130999 W

F2 - Processing parameters
SI       32768
SF       125.7904811 MHz
WDW      EM
SSB      0
LB       1.50 Hz
GB       0
PC       1.40
  
```



```

Current Data Parameters
NAME      VM-M327A
EXPNO    1
PROCNO   1

F2 - Acquisition Parameters
Date_    20130403
Time     19.14
INSTRUM  spect
PROBHD   5 mm BBO BB-1H
PULPROG  noesypph
TD       1024
SOLVENT  CDCl3
NS       16
DS       16
SWH      4553.734 Hz
FIDRES   4.447058 Hz
AQ       0.1124352 sec
RG       144
DM       109.800 usec
DE       6.50 usec
TE       298.0 K
D1       0.0000790 sec
D11      2.0000000 sec
D8       1.0000000 sec
D16      0.0002000 sec
IND      0.00021960 sec

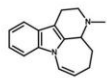
===== CHANNEL f1 =====
SFO1     500.2619840 MHz
NUC1     1H
P1       9.35 usec
P2       18.70 usec
PLW1     27.37999916 W

===== GRADIENT CHANNEL =====
GPRAM[1] SINE:150
GPE1    40.00 %
P16     1000.00 usec

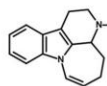
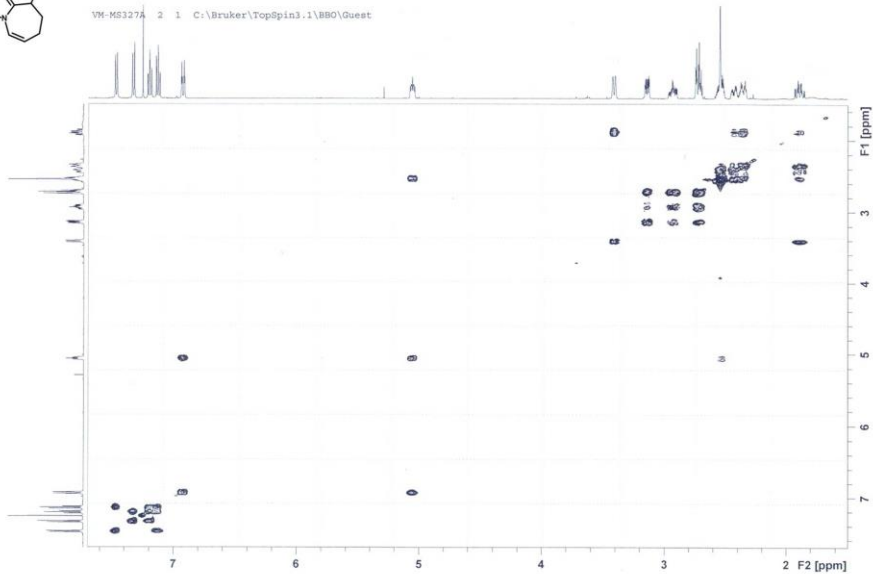
F1 - Acquisition parameters
TD       256
SFO1     500.262 MHz
FIDRES   17.788023 Hz
SW       9.103 ppm
FHM00DE States-TPPI

F2 - Processing parameters
SI       512
SF       500.2600140 MHz
WDM      Q3192
SSB      2
LB       0 Hz
GB       0
PC       1.00

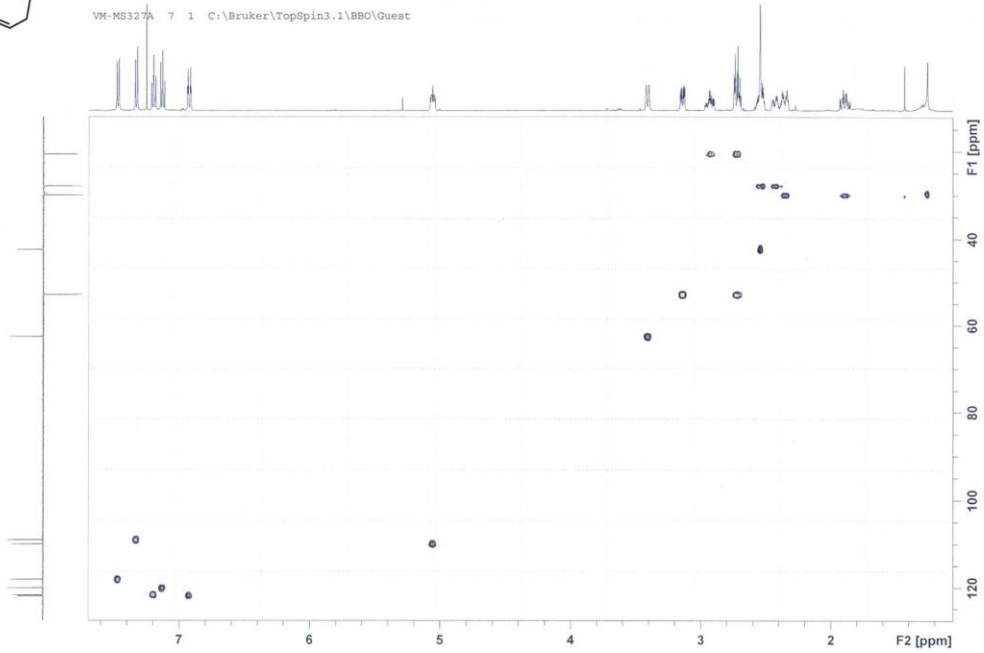
F1 - Processing parameters
SI       512
MC2     States-TPPI
SF       500.2600139 MHz
WDM      Q3192
SSB      2
LB       0 Hz
GB       0
  
```

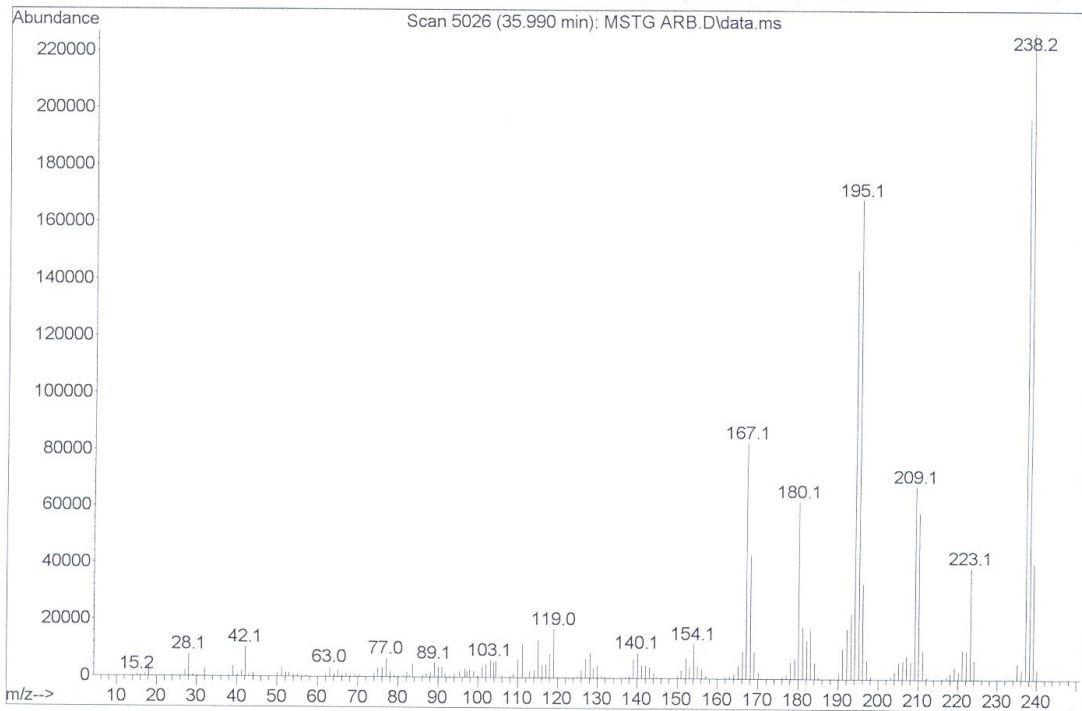
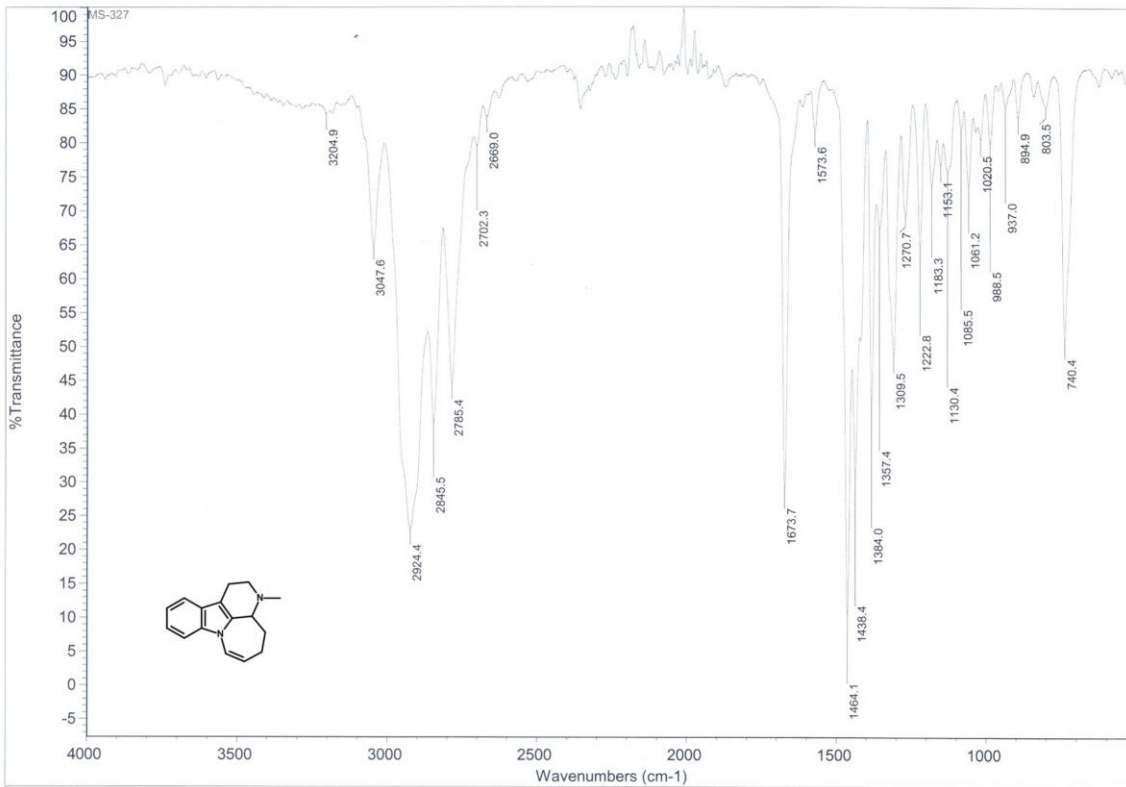


VM-MS327A 2 1 C:\Bruker\TopSpin3.1\BBO\Guest

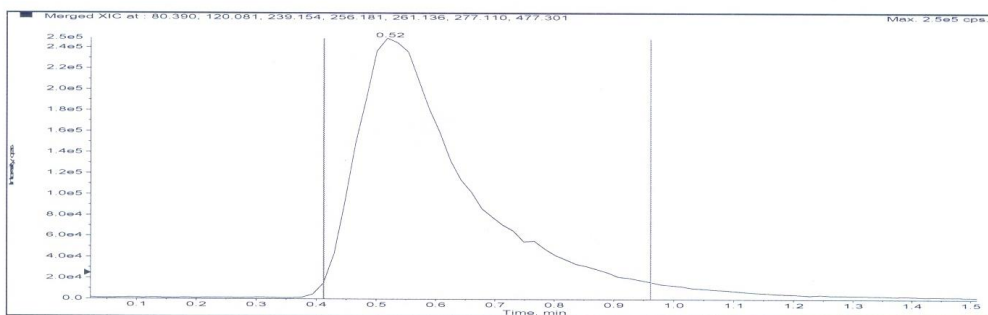


VM-MS327A 7 1 C:\Bruker\TopSpin3.1\BBO\Guest

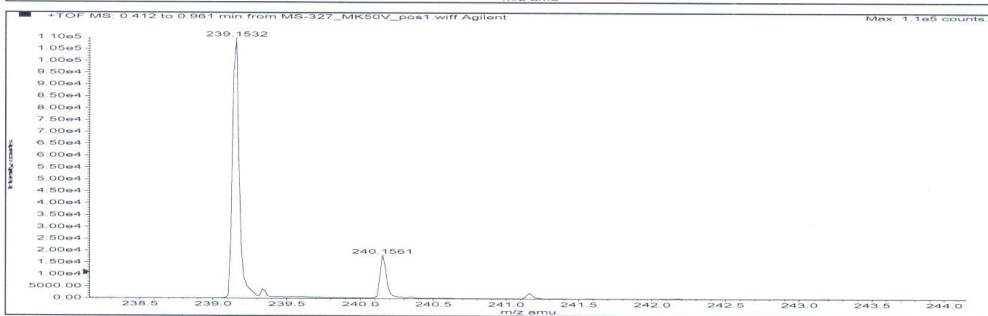
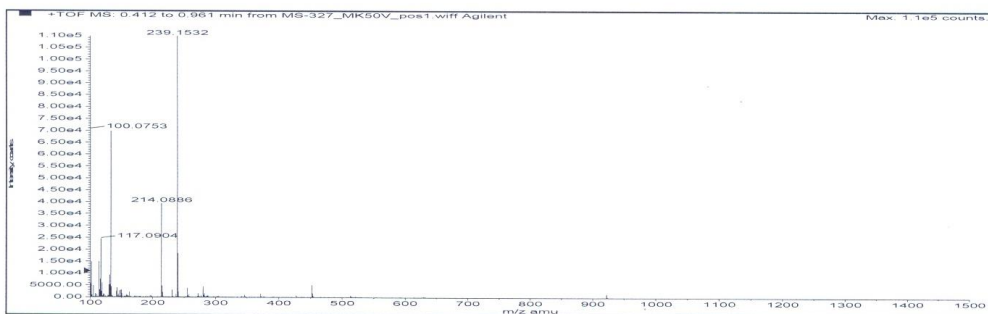




Sample Name: MS-327 Sample Location: P1-D9 Sample Id: Operator: Gordana
 Data File Name: D:\PE_Sciex_Data\Projects\Novi Sad\Data\MS-327_MK50V_pos1.wiff Acq Time: April 11 2013, 12:56:00 PM
 Method: d:\TOF_Data\damethods\Night_Seq_Comp_Ident1.an\mlefc.xml



Merged XIC, Period# : 1 Experiment# : 1



Formula	Compound name	Mass	Peak RT (min)	Peak area	Description
C16H18N2	--	238.14700	0.52	3.30369 E6	--

Species	Abundance (counts)	Ion Mass	Measured Mass	Error (mDa)	Error (ppm)	Ret. Time Error (min)
[M+H] ⁺	112304.21	239.15428	239.15319	-1.08311	-4.53	--

