

Supplementary material for the article:

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Synthesis, Characterization and in Vitro Cytotoxic Activities of New Steroidal
Thiosemicarbazones and Thiadiazolines. *RSC Advances* **2016**, *6* (41), 34312–34333.
<https://doi.org/10.1039/c6ra01516f>

Supplementary data

Synthesis, characterization and *in vitro* cytotoxic activities of new steroidal thiosemicarbazones and thiadiazolines

Marijana B. Živković^a, Ivana Z. Matic^b, Marko V. Rodić^c, Irena T. Novaković^a, Dušan M. Sladić^d, Natalija M. Krstić^a

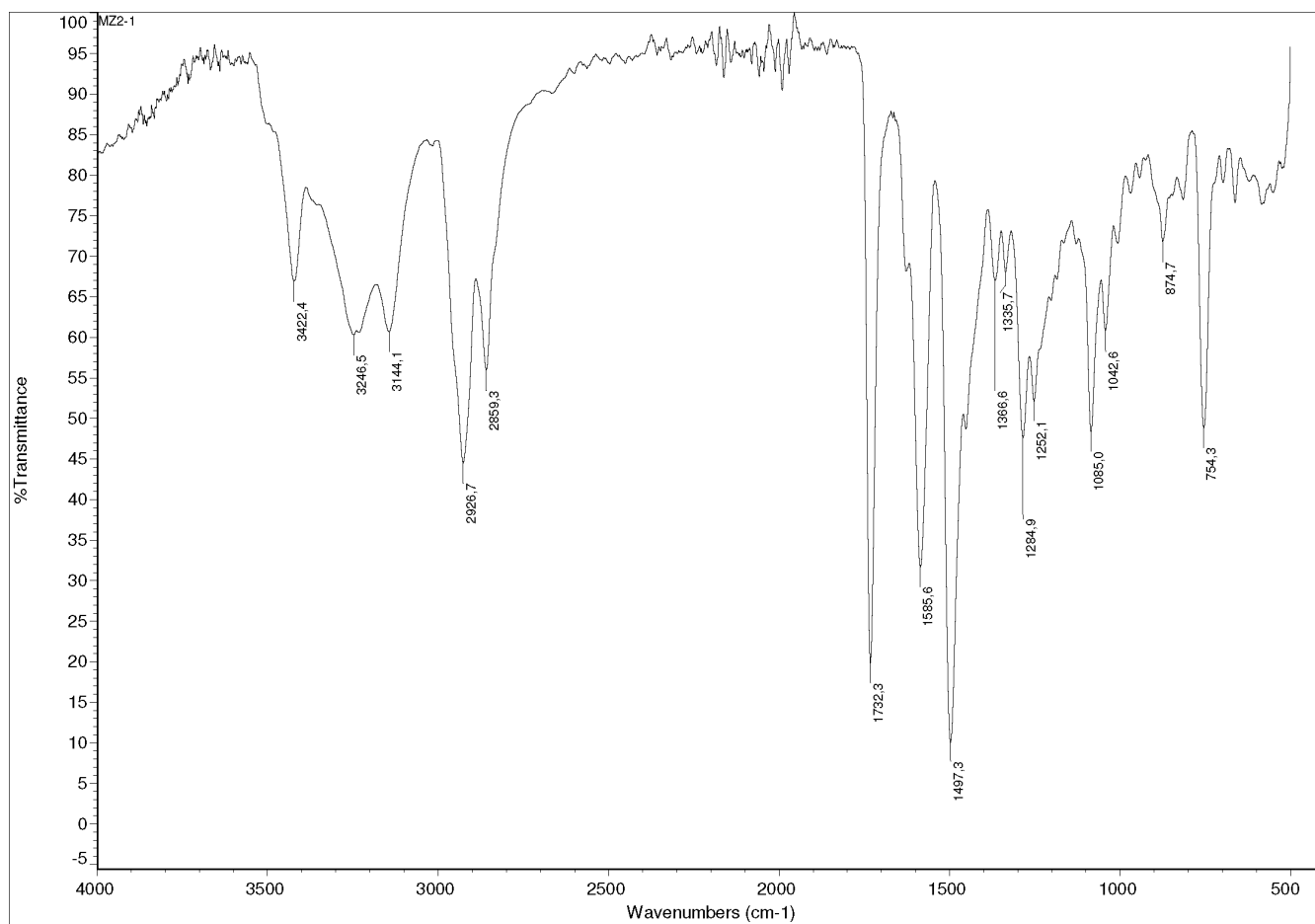
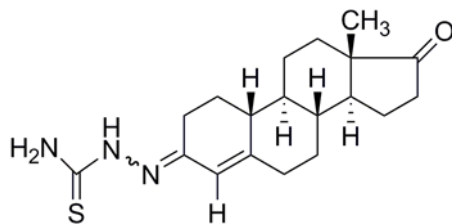
^aCenter for Chemistry, Institute of Chemistry, Technology and Metallurgy, University of Belgrade, Studentski trg 12-16, P. O. Box 473, 11001 Belgrade, Republic of Serbia

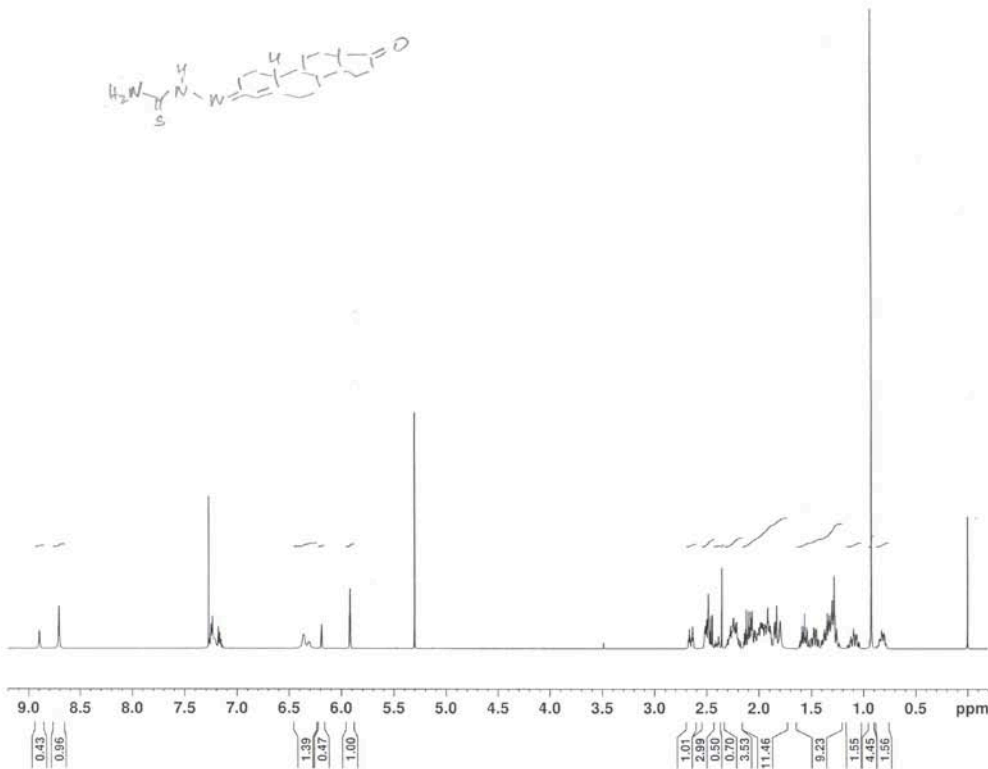
^bInstitute for Oncology and Radiology of Serbia, Pasterova 14, 11000 Belgrade, Republic of Serbia

^cFaculty of Sciences, University of Novi Sad, Trg D. Obradovića 3, 21000 Novi Sad, Republic of Serbia

^dFaculty of Chemistry, University of Belgrade, Studentski trg 12-16, P. O. Box 158, 11001 Belgrade, Republic of Serbia

Compound 2a



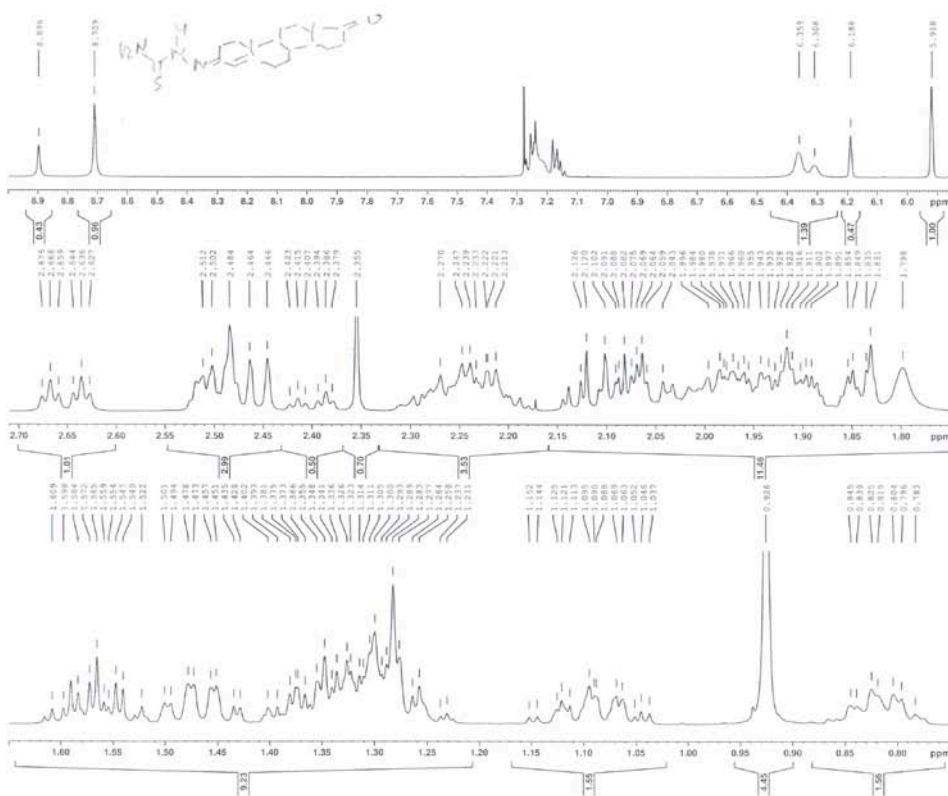


Current Data Parameters
 NAME M22
 EXPNO 1
 PROCNO 1

F2 - Acquisition Parameters
 Date_ 20100602
 Time 11:29
 INSTRUM spect
 PROBHD 5 mm BBO BB-1H
 PULPROG zg30
 TD 32768
 SOLVENT CDCl3
 NS 16
 DS 0
 SWH 5376.344 Hz
 FIDRES 0.164073 Hz
 AQ 3.0474241 sec
 RG 128
 DW 93.000 usec
 DE 6.50 usec
 TE 298.0 K
 D1 2.00000000 sec
 TDO 1

----- CHANNEL f1 -----
 SFO1 500.2623242 MHz
 NUC1 1H
 P1 9.35 usec
 PLW1 27.37999916 W

F2 - Processing parameters
 SI 32768
 SF 500.2600048 MHz
 WDW EM
 SSB 0
 LB 0.20 Hz
 GB 0
 PC 1.00

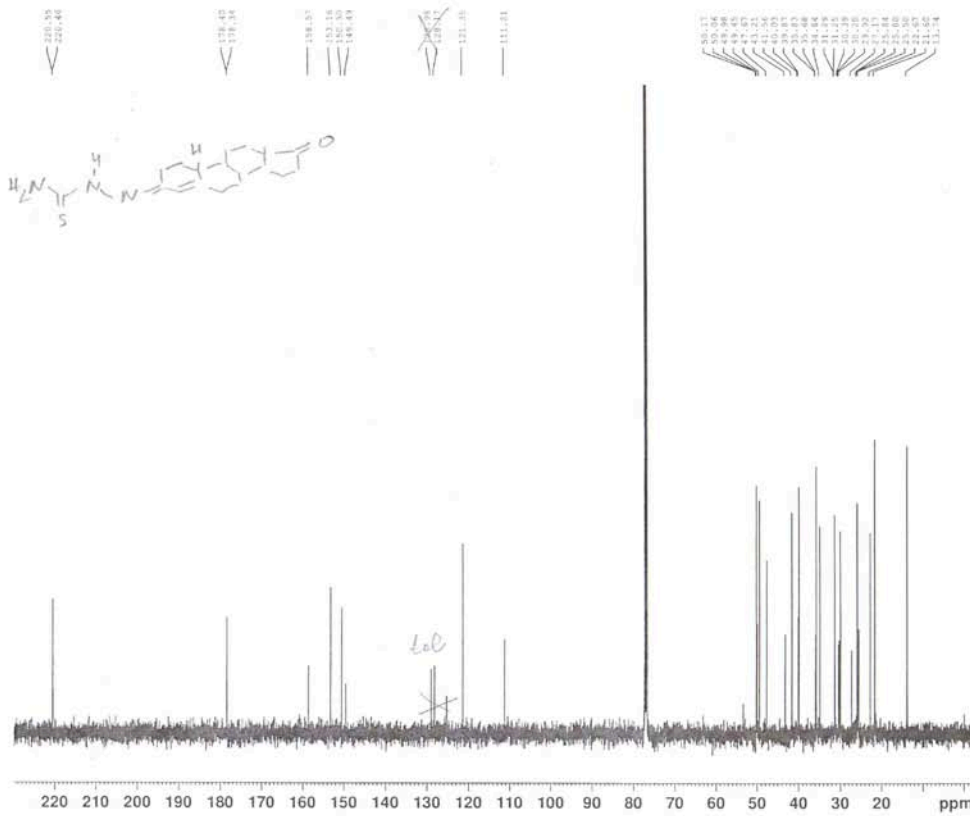


Current Data Parameters
 NAME M22
 EXPNO 1
 PROCNO 1

F2 - Acquisition Parameters
 Date_ 20100602
 Time 11:29
 INSTRUM spect
 PROBHD 5 mm BBO BB-1H
 PULPROG zg30
 TD 32768
 SOLVENT CDCl3
 NS 16
 DS 0
 SWH 5376.344 Hz
 FIDRES 0.164073 Hz
 AQ 3.0474241 sec
 RG 128
 DW 93.000 usec
 DE 6.50 usec
 TE 298.0 K
 D1 2.00000000 sec
 TDO 1

----- CHANNEL f1 -----
 SFO1 500.2623242 MHz
 NUC1 1H
 P1 9.35 usec
 PLW1 27.37999916 W

F2 - Processing parameters
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 WDW EM
 SSB 0
 LB 0.20 Hz
 GB 0
 PC 1.00



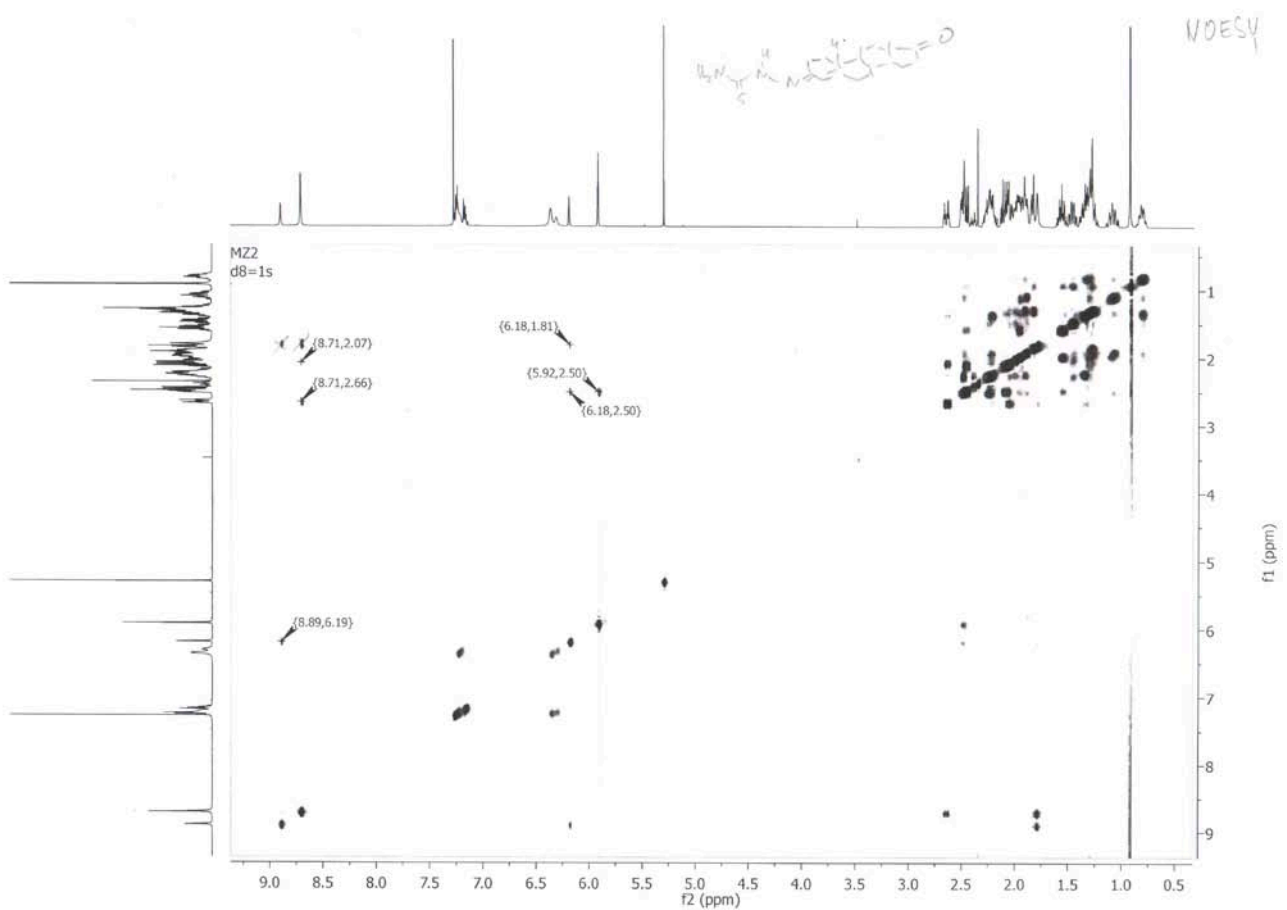
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 EXPNO 2
 PROCNO 1

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 Date_ 20140602
 Time 11.52
 INSTRUM spect
 PROBHD 5 mm BBO BB-1H
 PULPROG zgpg30
 TD 32768
 SOLVENT CDCl3
 NS 257
 DS 4
 SWH 32894.738 Hz
 FIDRES 1.003868 Hz
 AQ 0.4980736 sec
 RG 1030
 DW 15.200 usec
 DE 6.50 usec
 TE 298.0 K
 D1 2.0000000 sec
 D11 0.0300000 sec
 TDO 1

----- CHANNEL f1 -----
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 NUC1 13C
 P1 11.50 usec
 PL1 32.22800064 W

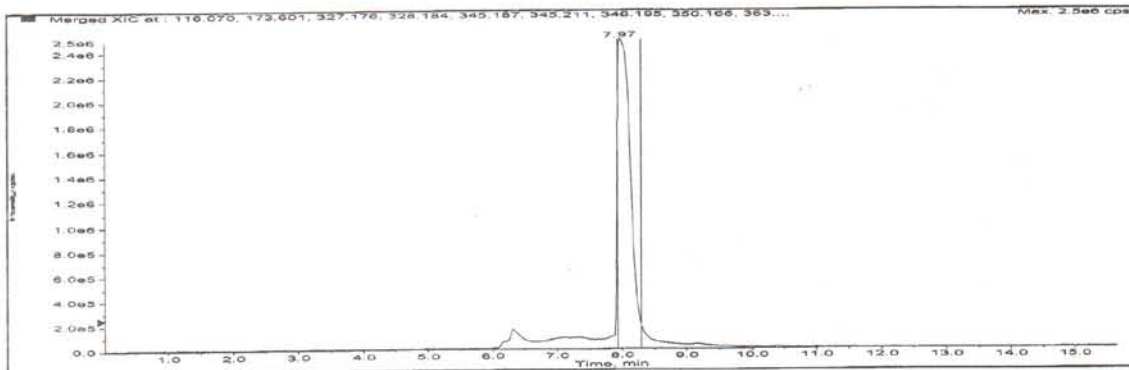
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 SFO2 500.2623242 MHz
 NUC2 1H
 CTDPRG2 waltz16
 PCPD2 80.00 usec
 PLM2 20.77000045 W
 PLM3 0.39267001 W
 PLM3 0.25130999 W

F2 - Processing parameters
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 SF 125.7904843 MHz
 WDN EM
 SSB 0
 LS 1.50 Hz
 GB 0
 FC 1.40

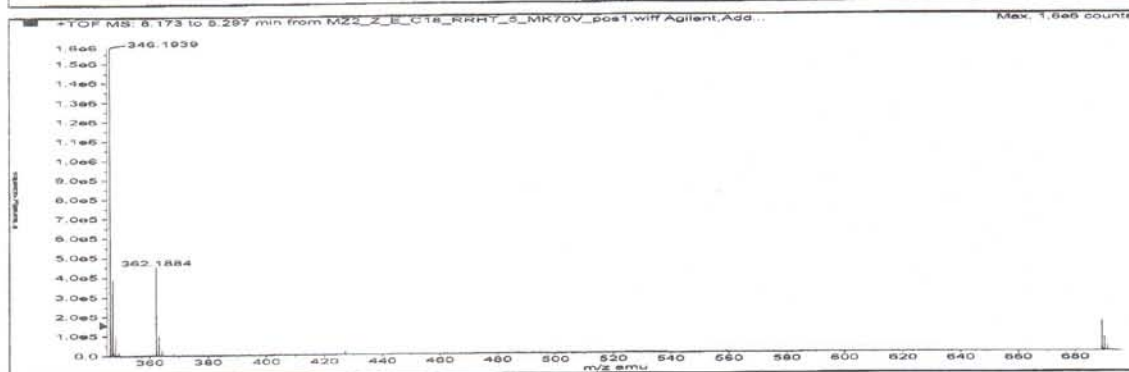
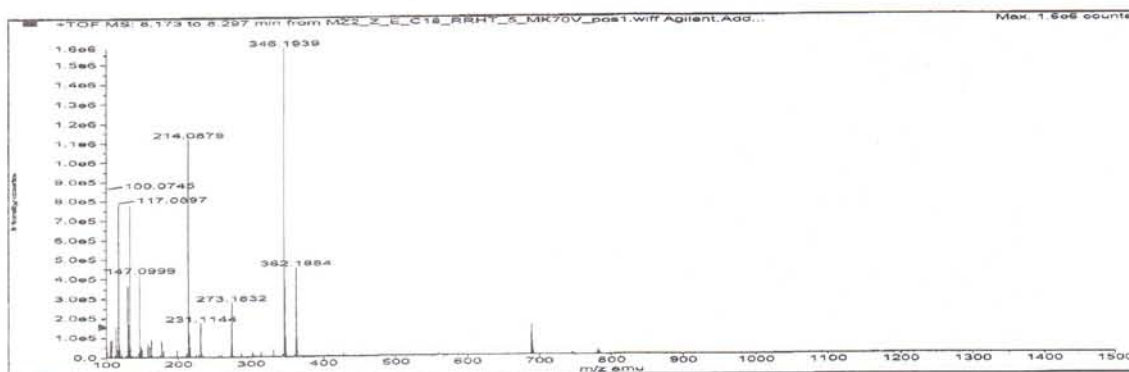


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 PM
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One or more scans have failed IRM. Review the data file for details.

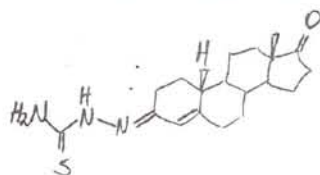


Merged XIC, Period#: 1 Experiment#: 1

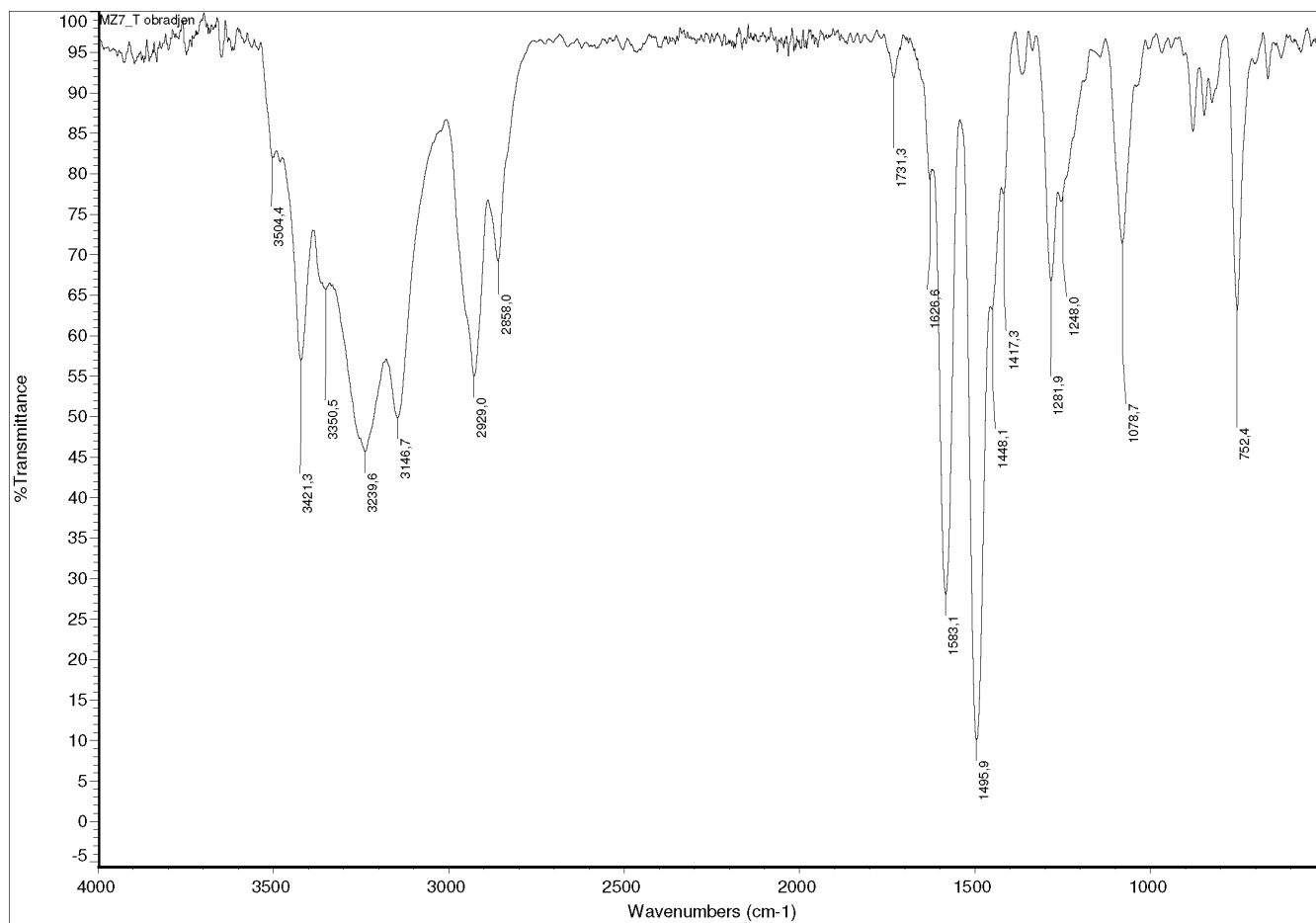
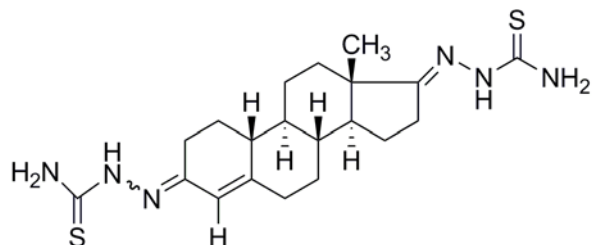


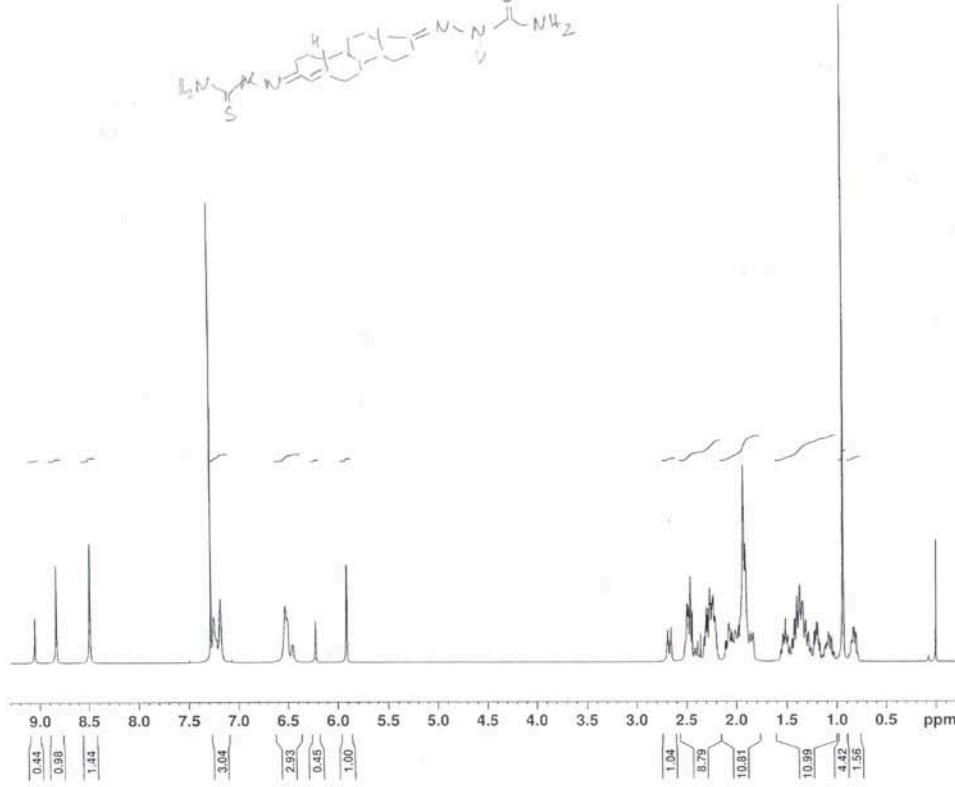
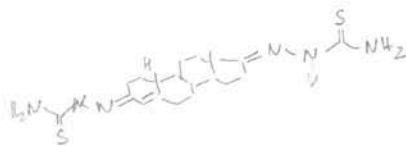
Formula	Compound name	Mass	Peak RT. (min)	Peak area	Description
C ₁₉ H ₂₇ N ₃ O ₅	-	345.18748	7.97	3.42837 E7	-

Species	Abundance (counts)	Ion Mass	Measured Mass	Error (mDa)	Error (ppm)	Ret. Time Error (min)
[M+H] ⁺	1592200.42	346.19476	346.19388	-0.88163	-2.55	--
[M+NH ₄] ⁺	98766.01	363.22131	363.19179	-29.52256	81.29	--
[2M+H] ⁺	29112.46	691.38224	691.36763	-14.60880	21.13	--



Compound 3a



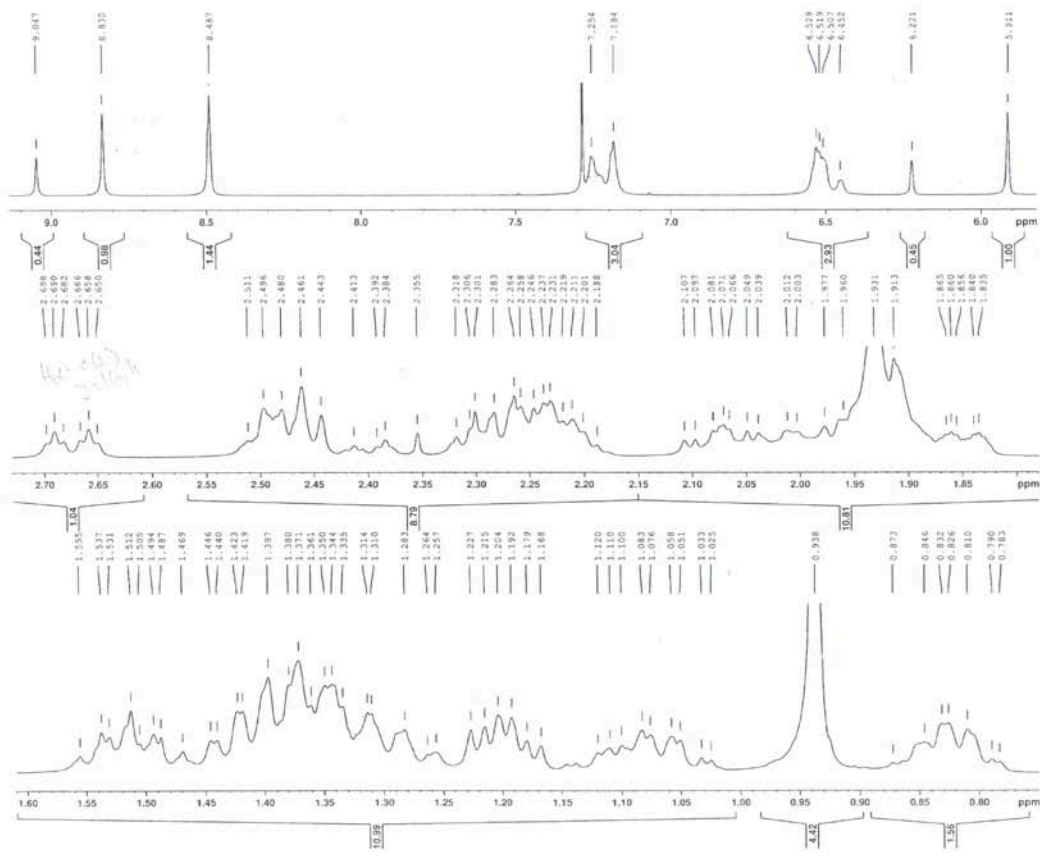


Current Data Parameters
 NAME MD7
 EXPNO 1
 PROCNO 1

F2 - Acquisition Parameters
 Date_ 20140602
 Time 13.55
 INSTRUM spect
 PROBHD 5 mm BBO BB-1H
 PULPROG zg30
 TD 32768
 SOLVENT CDCl3
 NS 16
 DS 0
 SWH 5357.143 Hz
 FIDRES 0.163487 Hz
 AQ 3.0583467 sec
 RG 128
 DW 93.333 usec
 DE 6.50 usec
 TE 298.0 K
 D1 2.0000000 sec
 TDO 1

----- CHANNEL f1 -----
 SFO1 500.2623246 MHz
 NUCL1 1H
 P1 9.35 usec
 PLW1 27.37999916 W

F2 - Processing parameters
 SI 32768
 SF 500.2600014 MHz
 WDW EM
 SSB 0
 LB 0.20 Hz
 GB 0
 PC 1.00

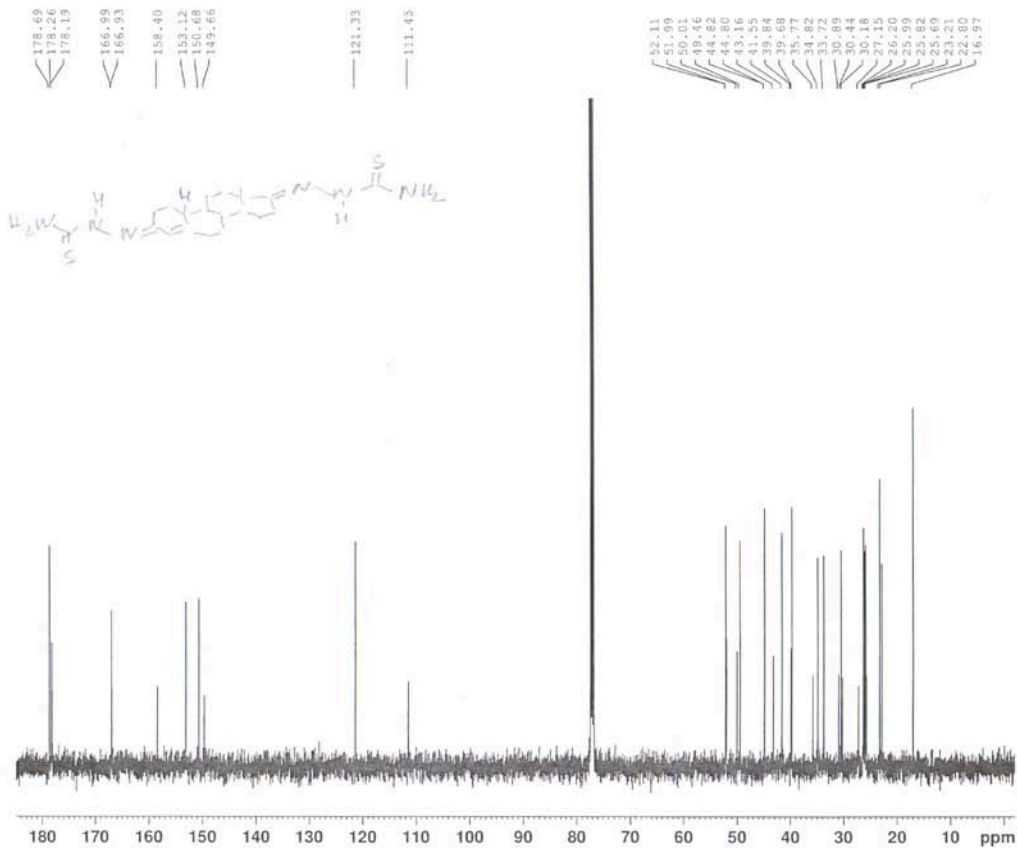


Current Data Parameters
 NAME MD7
 EXPNO 1
 PROCNO 1

F2 - Acquisition Parameters
 Date_ 20140602
 Time 13.59
 INSTRUM spect
 PROBHD 5 mm BBO BB-1H
 PULPROG zg30
 TD 32768
 SOLVENT CDCl3
 NS 16
 DS 0
 SWH 5357.143 Hz
 FIDRES 0.163487 Hz
 AQ 3.0583467 sec
 RG 128
 DW 93.333 usec
 DE 6.50 usec
 TE 298.0 K
 D1 2.0000000 sec
 TDO 1

----- CHANNEL f1 -----
 SFO1 500.2623246 MHz
 NUCL1 1H
 P1 9.35 usec
 PLW1 27.37999916 W

F2 - Processing parameters
 SI 32768
 SF 500.2600014 MHz
 WDW EM
 SSB 0
 LB 0.20 Hz
 GB 0
 PC 1.00



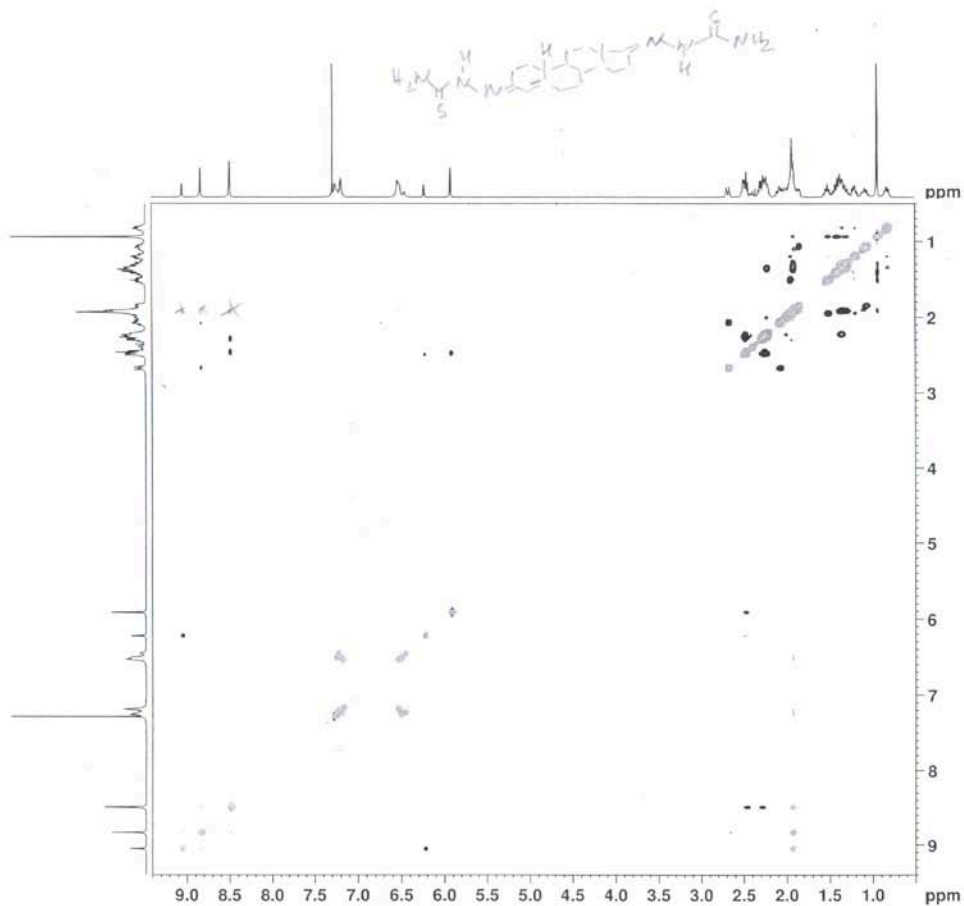
Current Data Parameters
NAME M27
EXPNO 2
PROCNO 1

F2 - Acquisition Parameters
Date_ 20140602
Time 14.06
INSTRUM spect
PROBHD 5 mm BBO BB-1H
PULPROG zgpg30
TD 32768
SOLVENT CDCl3
NS 320
DS 4
SWH 32894.738 Hz
FIDRES 1.003868 Hz
AQ 0.4980736 sec
RG 1030
DW 15.200 usec
DE 6.50 usec
TE 298.0 K
D1 2.0000000 sec
D11 0.0300000 sec
TD0 1

----- CHANNEL f1 -----
SFO1 125.8055719 MHz
NUC1 13C
P1 11.50 usec
PLW1 32.22800064 W

----- CHANNEL f2 -----
SFO2 500.2623247 MHz
NUC2 1H
CDEPRG2 waltz16
PCPD2 80.00 usec
PLW2 20.77000046 W
PLW12 0.39267001 W
PLW13 0.25130999 W

F2 - Processing parameters
SI 32768
SF 125.7904867 MHz
WDW EM
SSB 0
LB 1.50 Hz
GB 0
PC 1.40



Current Data Parameters
NAME M27
EXPNO 5
PROCNO 1

F2 - Acquisition Parameters
Date_ 20140602
Time 15.02
INSTRUM spect
PROBHD 5 mm BBO BB-1H
PULPROG noesypph
TD 1024
SOLVENT CDCl3
NS 4
DS 16
SWH 4618.227 Hz
FIDRES 4.509987 Hz
AQ 0.1108651 sec
RG 287
DW 108.267 usec
DE 6.50 usec
TE 298.0 K
D0 0.0000940 sec
D1 2.0000000 sec
D8 1.0000000 sec
D16 0.0000000 sec
IN0 0.00021660 sec

----- CHANNEL f1 -----
SFO1 500.2624918 MHz
NUC1 1H
P1 9.25 usec
P2 18.70 usec
PLW1 27.37999916 W

----- GRADIENT CHANNEL -----
GPNAM[1] SINE100
GR1 40.00 Hz
P16 1000.00 usec

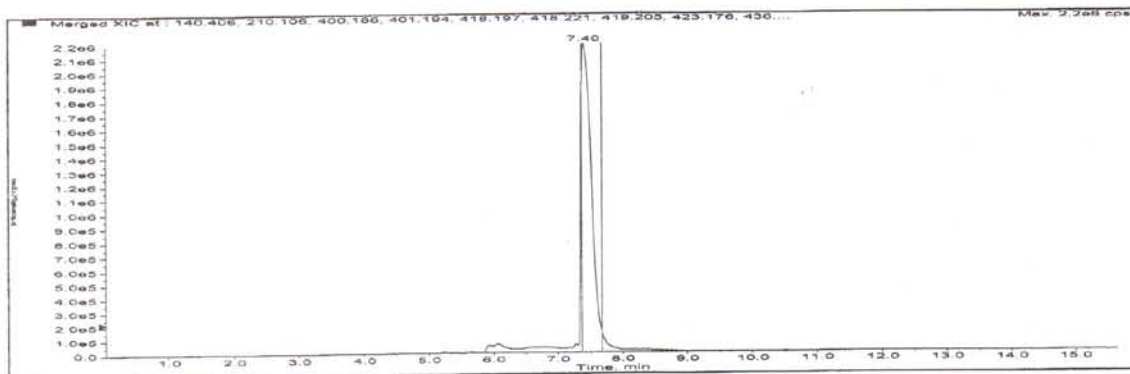
F1 - Acquisition parameters
SI 1024
TD 256
SFO1 500.2625 MHz
FIDRES 18.034395 Hz
SW 5.229 ppm
PnMODE States-TPP1

F2 - Processing parameters
SI 1024
SF 500.2599993 MHz
WDW COSTUME
SSB 2
LB 0 Hz
GB 0
PC 1.00

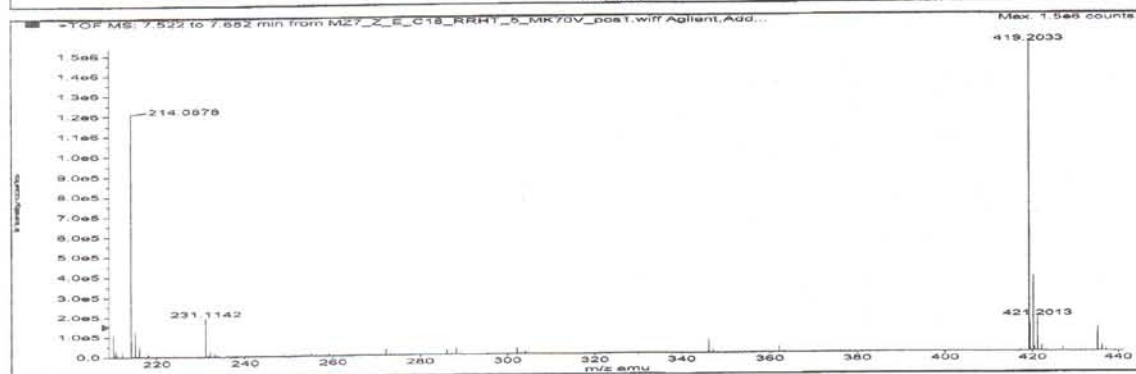
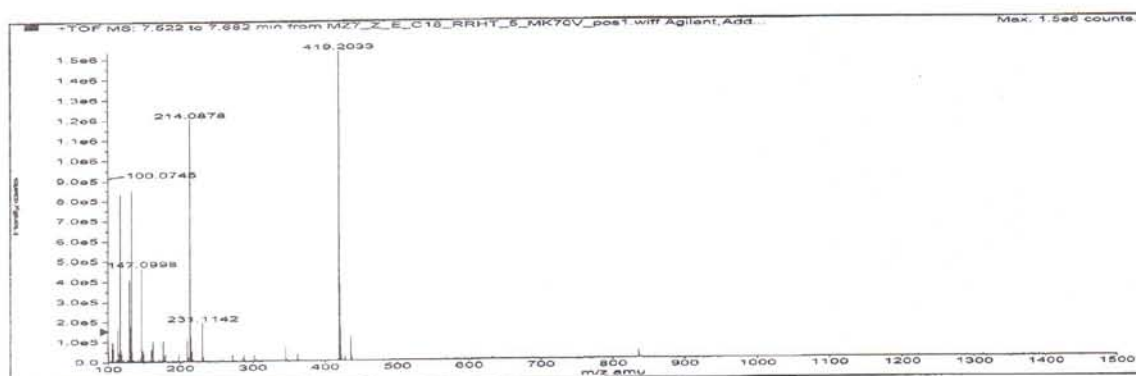
F1 - Processing parameters
SI 1024
MC2 States-TPP1
SF 500.2599992 MHz
WDW COSTUME
SSB 2
LB 0 Hz
GB 0

Sample Name: MZ7 Sample Location: P1-C8 Sample Id: Operator: Milka
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 PM
 Method: d:\TOF_Data\damethods\Night_Seq_Comp_ident1.anml\etc.xml

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



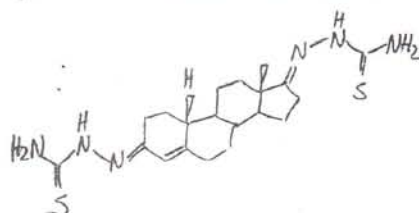
Merged XIC, Period#: 1 Experiment#: 1



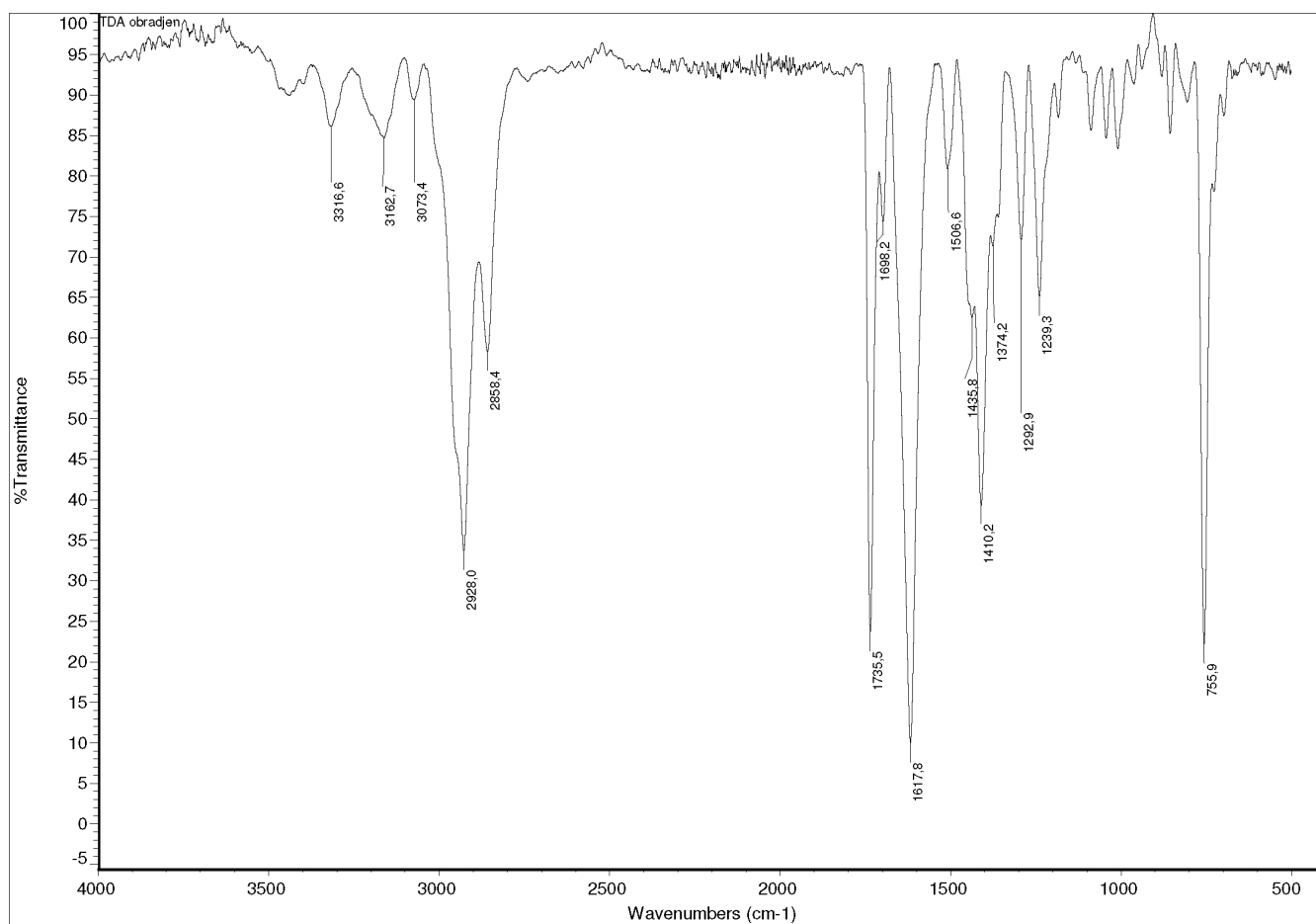
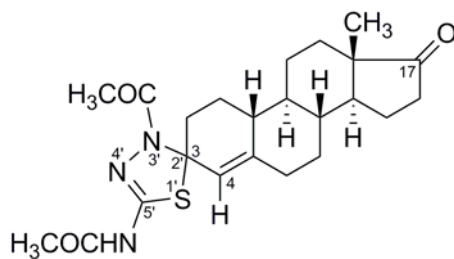
Formula	Compound name	Mass	Peak RT (min)	Peak area	Description
C20H30N6S2	-	418.19734	7.40	2.50483 E7	-

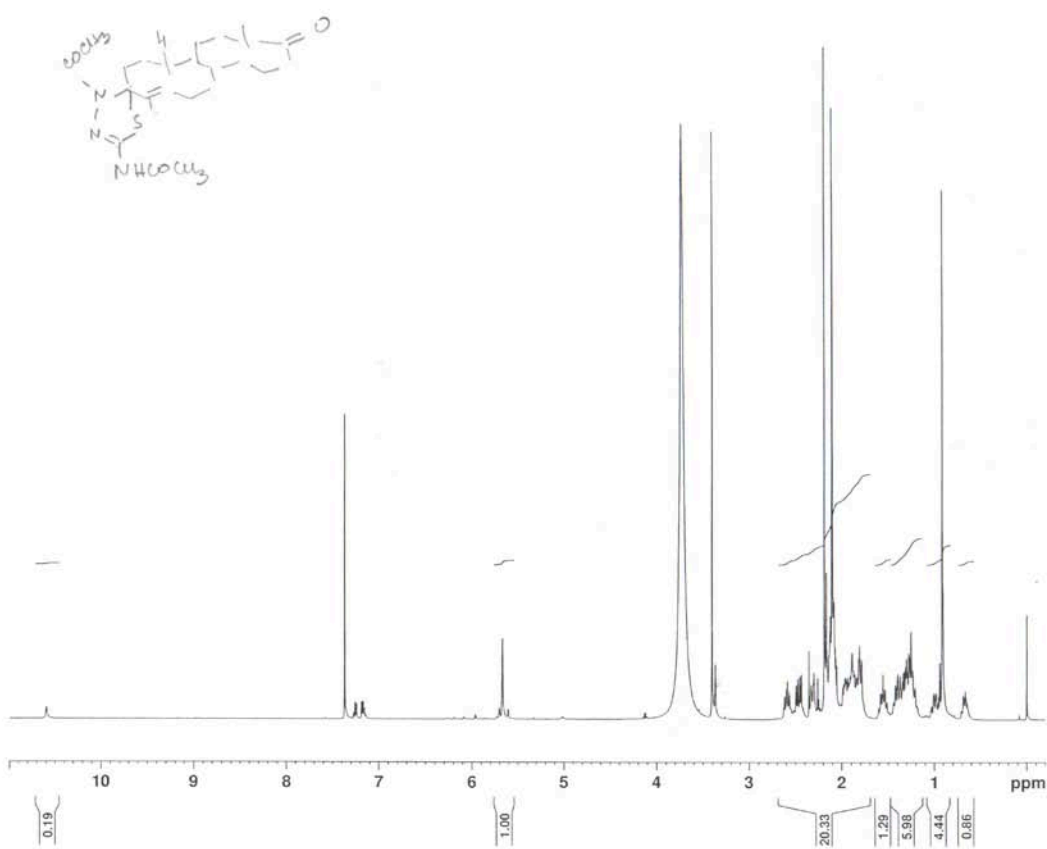
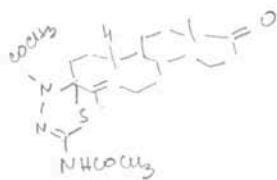
Species	Abundance (counts)	Ion Mass	Measured Mass	Error (mDa)	Error (ppm)	Ret. Time Error (min)
[M+2H] ²⁺	110876.65	210.10594	210.10428	-1.66827	-7.94	
[M+H] ⁺	1536715.77	419.20461	419.20335	-1.26756	-3.02	
[M+NH4] ⁺	29241.75	436.23116	436.20049	-30.67147	-70.32	

OK, MS



Compound 4a



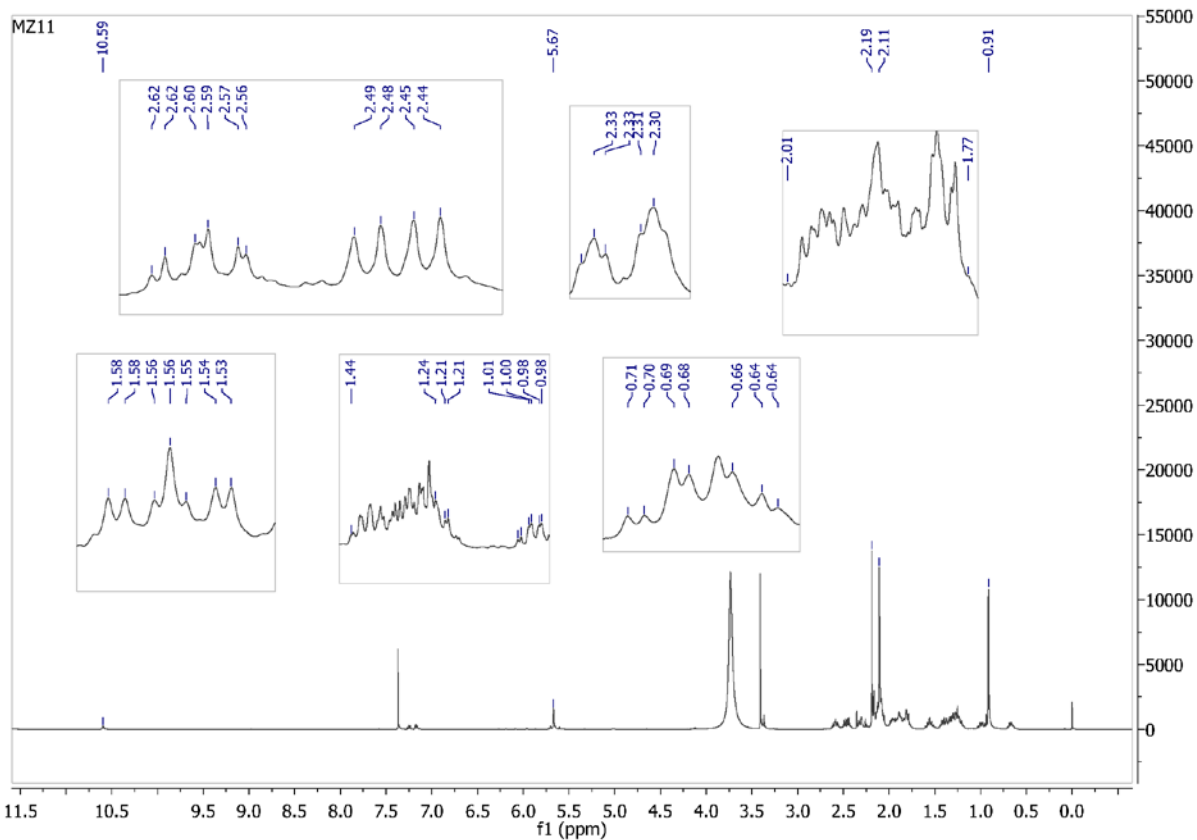


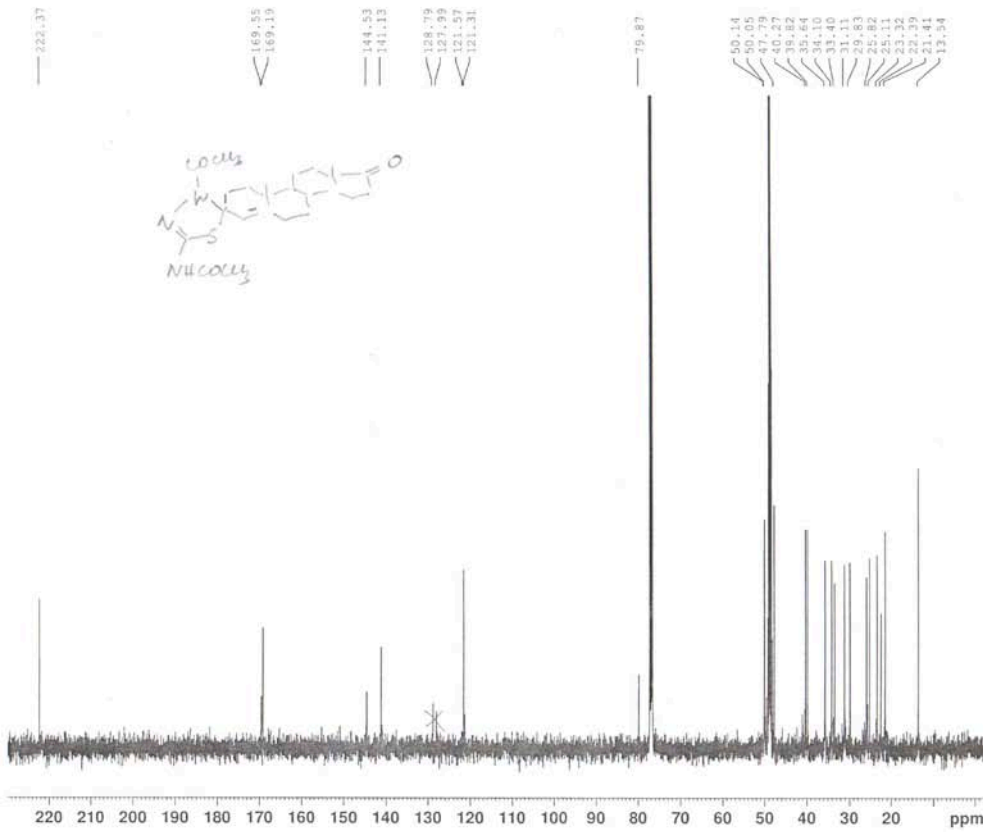
Current Data Parameters
 NAME MZ11
 EXPNO 1
 PROCNO 1

F2 - Acquisition Parameters
 Date_ 20140604
 Time 14.30
 INSTRUM spect
 PROBNM 5 mm BBO BB-1H
 PULPROG zg30
 TD 32768
 SFO1 500.2599573 MHz
 SOLVENT CDCl3
 NS 32
 DS 0
 SWH 6127.451 Hz
 FIDRES 0.186995 Hz
 AQ 2.6738689 sec
 RG 128
 DW 81.600 usec
 DE 8.50 usec
 TE 298.0 K
 D1 2.00000000 sec
 TDO 1

===== CHANNEL f1 =====
 SFO1 500.2599573 MHz
 NUC1 1H
 P1 9.15 usec
 PLW1 27.37999916 W

F2 - Processing parameters
 SI 32768
 SF 500.2599573 MHz
 WDW EM
 SSB 0
 LB 0.20 Hz
 CB 0
 PC 1.00





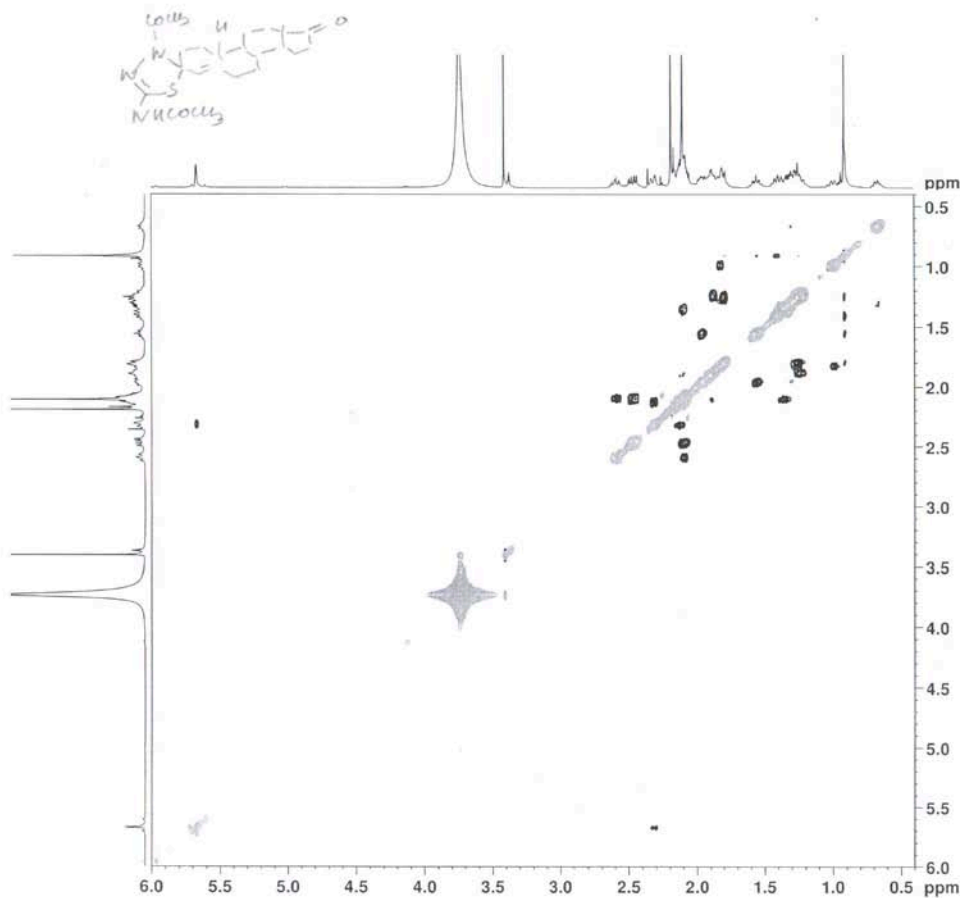
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NAME MZ11
EXPNO 2
PROCNO 1

F2 - Acquisition Parameters
Date_ 20140504
Time 14.40
INSTRUM spect
PROBHD 5 mm BBO BB-1H
PULPROG zgpg30
TD 32768
SOLVENT CDCl₃
NS 4
DS 4
SWH 32894.738 Hz
FIDRES 1.003868 Hz
AQ 0.4980736 sec
RG 1030
DM 15.200 usec
DE 6.50 usec
TE 298.0 K
D1 2.0000000 sec
D11 0.0300000 sec
TD0 1

----- CHANNEL f1 -----
SFO1 125.8055719 MHz
NUC1 13C
P1 11.50 usec
PLW1 32.22800064 W

----- CHANNEL f2 -----
SFO2 500.2626919 MHz
NUC2 1H
CPDPRG2 waltz16
PCPD2 80.00 usec
PLK2 20.77000046 W
PLW2 0.39267001 W
PLW3 0.25130999 W

F2 - Processing parameters
SI 32768
SF 125.7904907 MHz
WDW EM
SSB 0
LB 1.50 Hz
GB 0
PC 1.40



NOESY

Current Data Parameters
NAME MZ11
EXPNO 5
PROCNO 1

F2 - Acquisition Parameters
Date_ 20140504
Time 15.56
INSTRUM spect
PROBHD 5 mm BBO BB-1H
PULPROG noesypph
TD 1024
SOLVENT CDCl₃
NS 4
DS 4
SWH 3059.976 Hz
FIDRES 2.988257 Hz
AQ 0.1673216 sec
RG 287
DM 163.400 usec
DE 6.50 usec
TE 298.0 K
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D1 2.00000000 sec
D6 1.00000000 sec
D16 0.00020000 sec
IND 0.00032680 sec

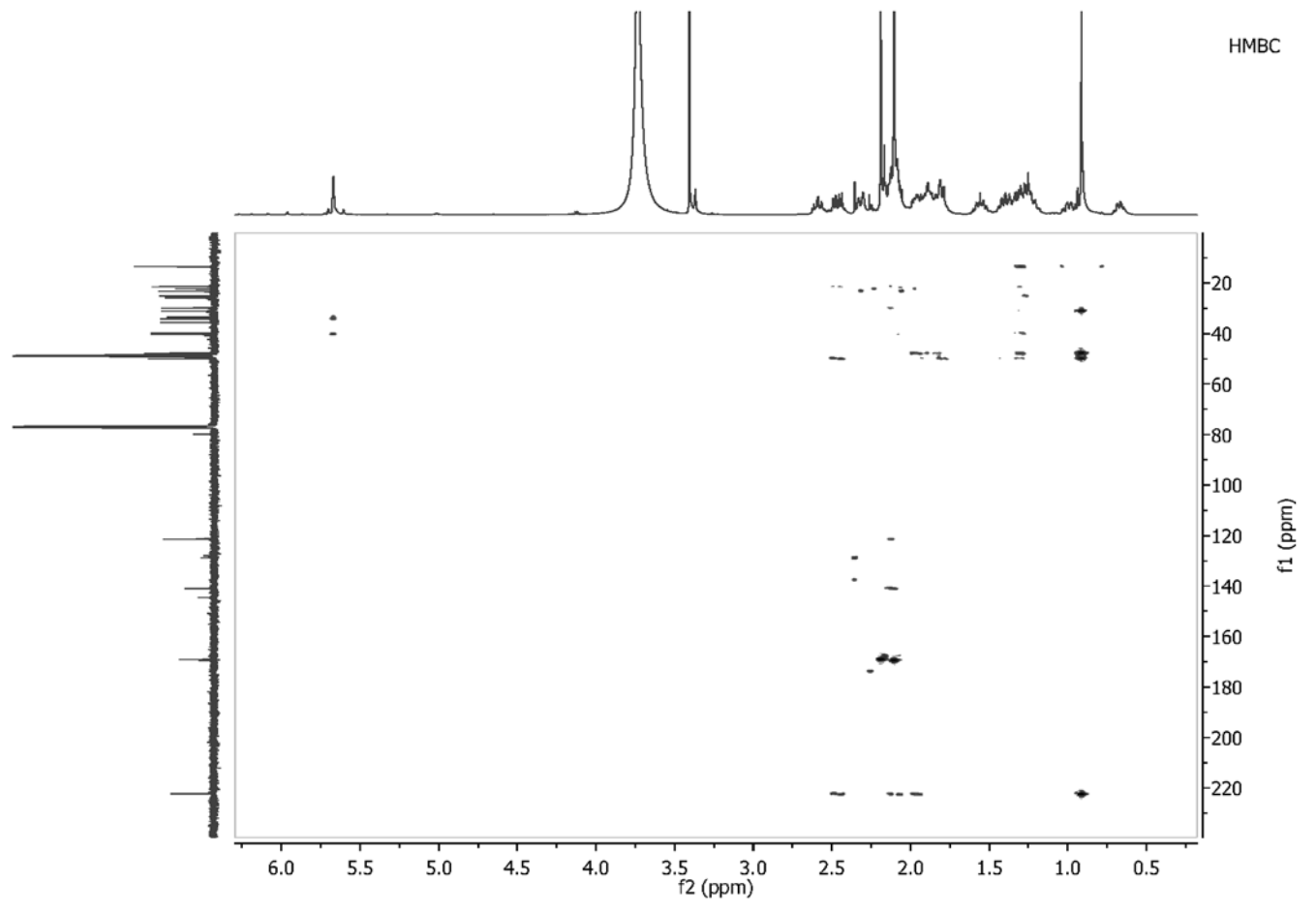
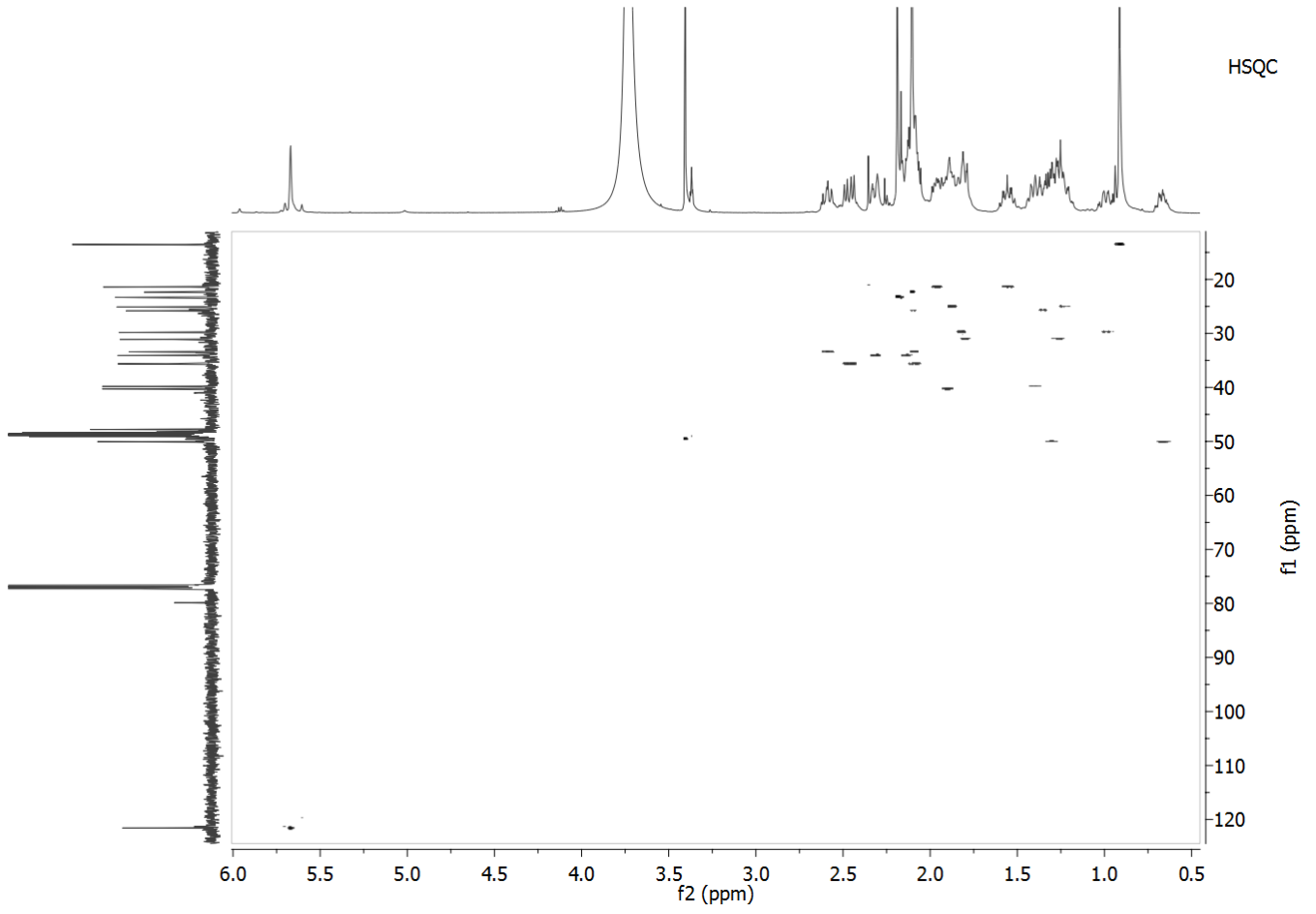
----- CHANNEL f1 -----
SFO1 500.2615733 MHz
NUC1 1H
P1 9.35 usec
P2 18.70 usec
PLW1 27.37999916 W

----- GRADIENT CHANNEL -----
GPRM[1] SINE 100
GPE1 40.00 V
P16 1000.00 usec

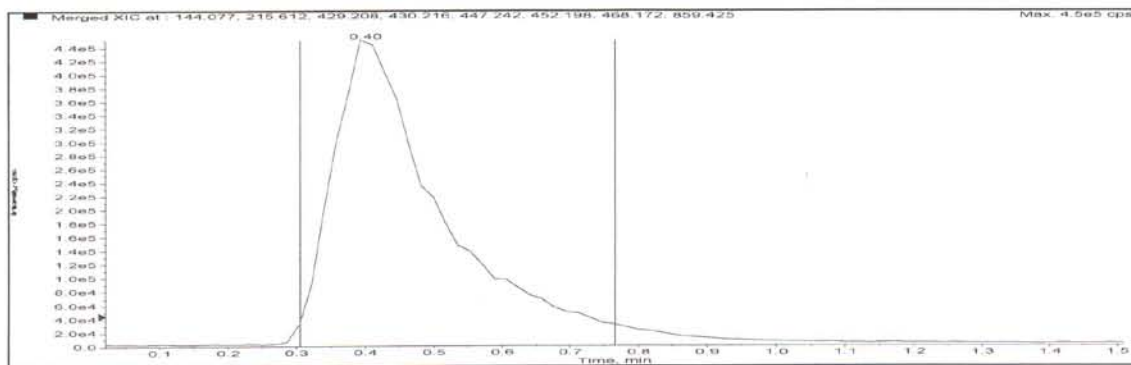
F1 - Acquisition parameters
TD 160
SFO1 500.2616 MHz
FIDRES 19.124847 Hz
SW 6.117 ppm
F0MODE States-TPP1

F2 - Processing parameters
SI 1024
SF 500.259560 MHz
WDW GSIIME
SSB 2
LB 0 Hz
GB 0
PC 1.00

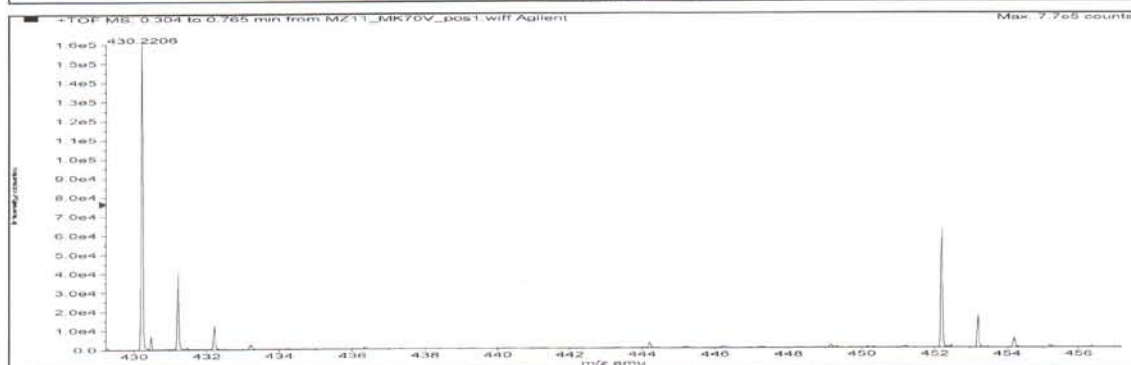
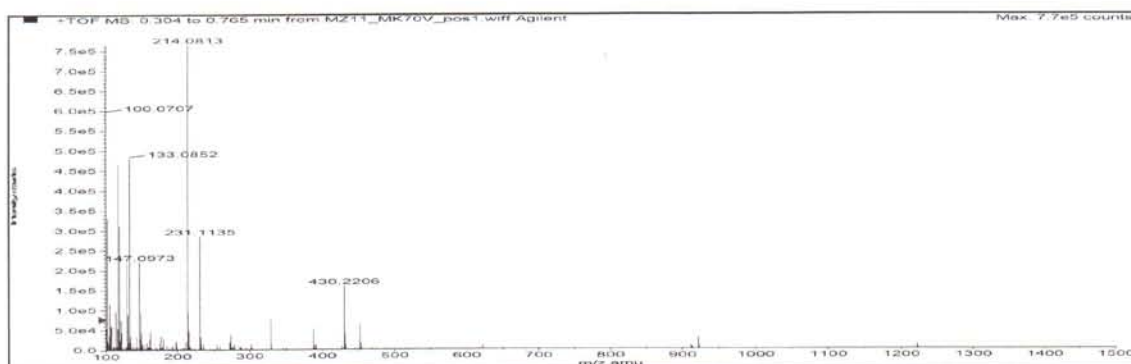
F1 - Processing parameters
SI 1024
MC2 States-TPP1
SF 500.259564 MHz
WDW GSIIME
SSB 2
LB 0 Hz
GB 0



Sample Name: MZ11 Sample Location: P1-C1 Sample Id: Operator: Milka
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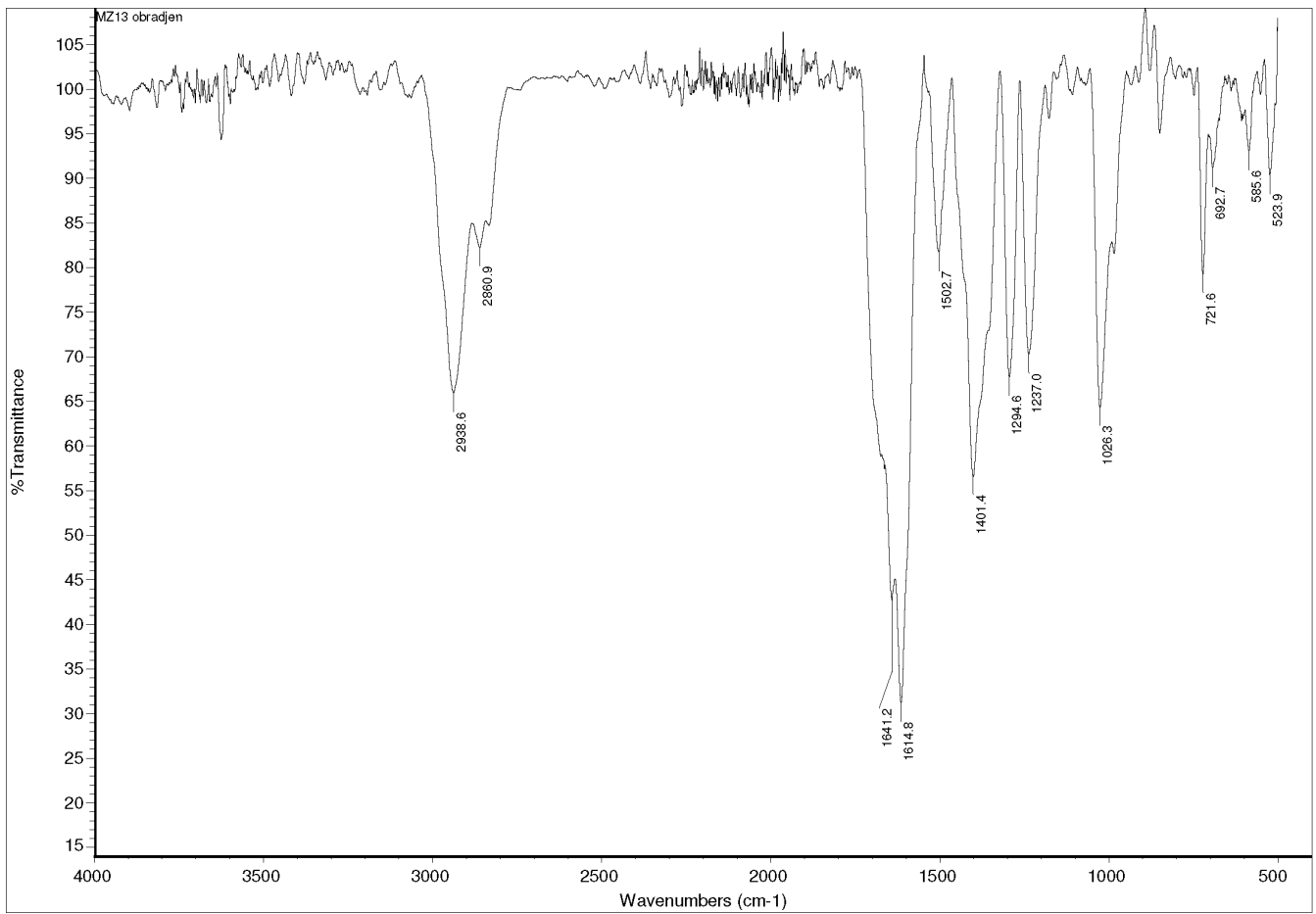
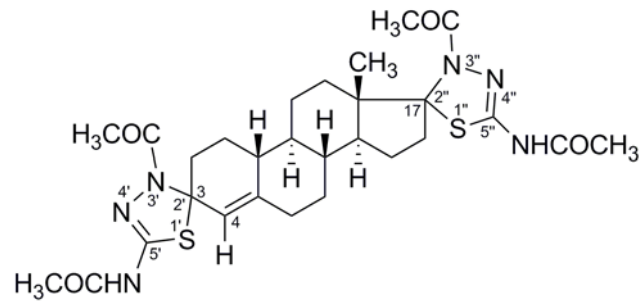
Merged XIC, Period# : 1 Experiment# : 1

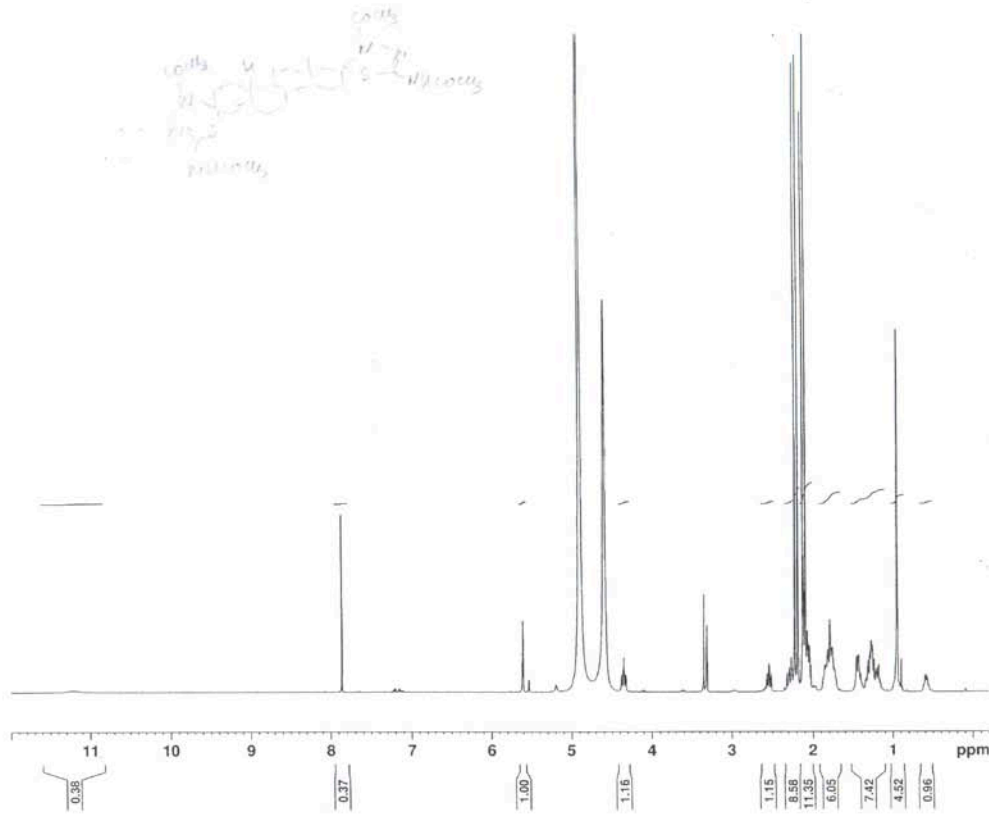


Formula	Compound name	Mass	Peak RT (min)	Peak area	Description
C23H31N3O3S	--	429.20861	0.40	4.98363 E6	--

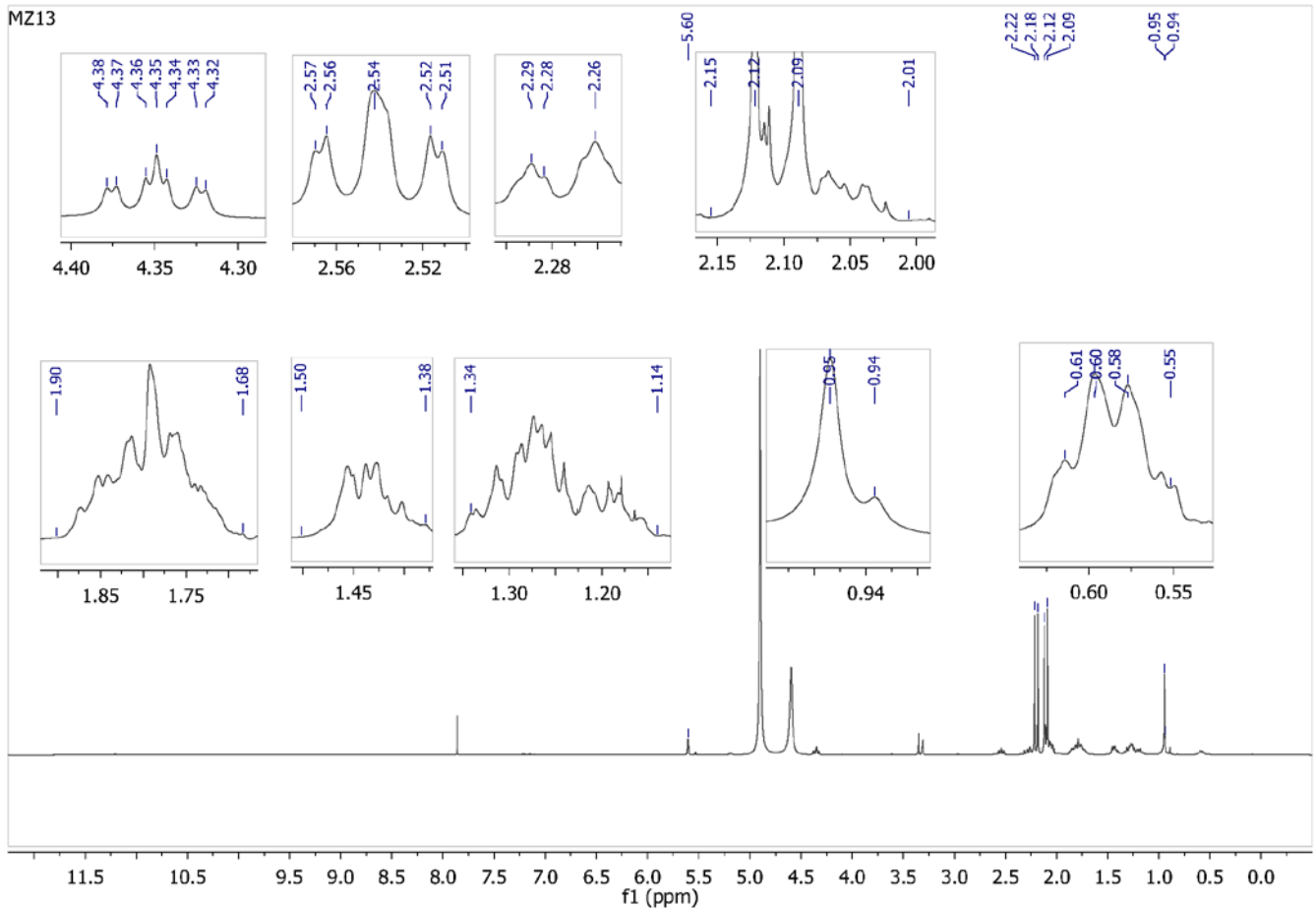
Species	Abundance (counts)	Ion Mass	Measured Mass	Error (mDa)	Error (ppm)	Ret. Time Error (min)
[M+H] ⁺	162128.32	430.21589	430.21581	-0.08124	-0.19	--
[M+Na] ⁺	63766.11	452.19783	452.19790	0.06355	0.14	--

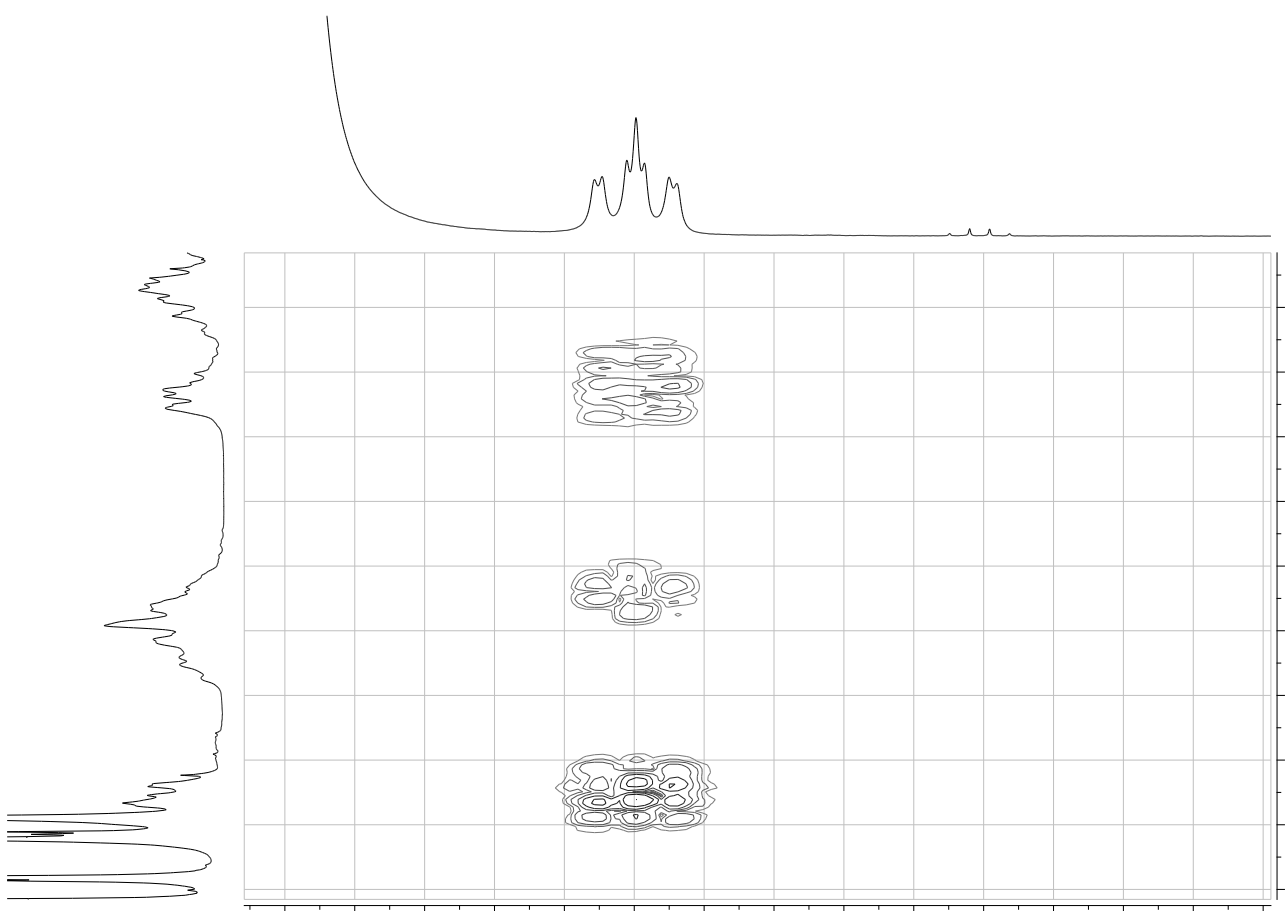
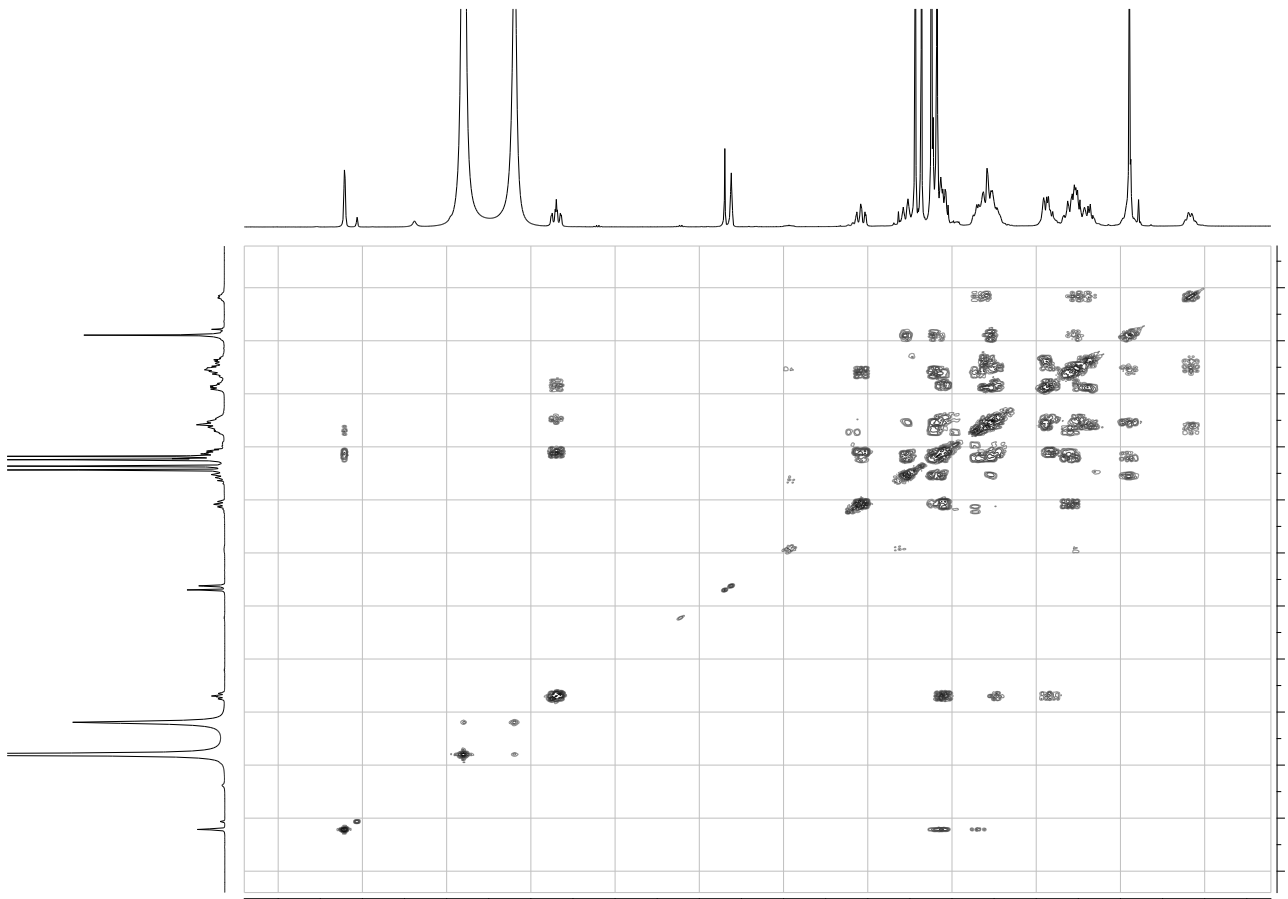
Compound 5a

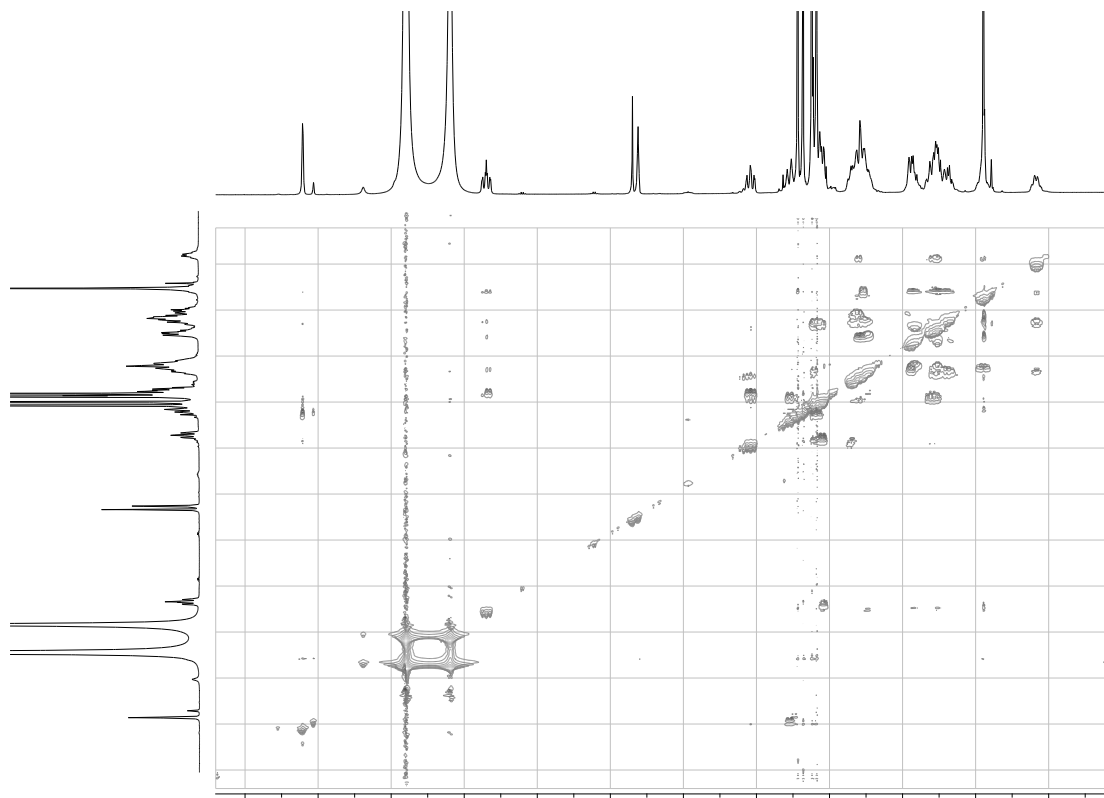




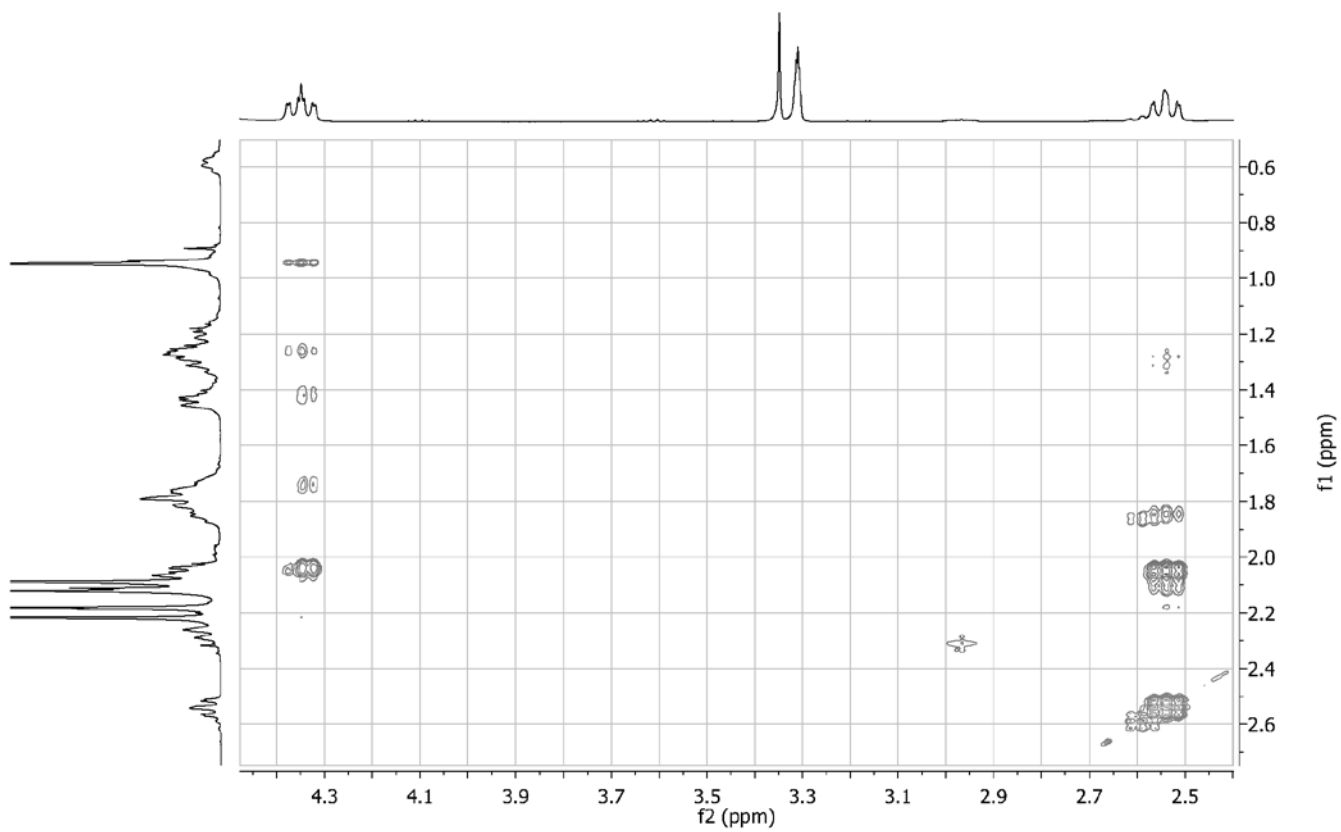
MZ13



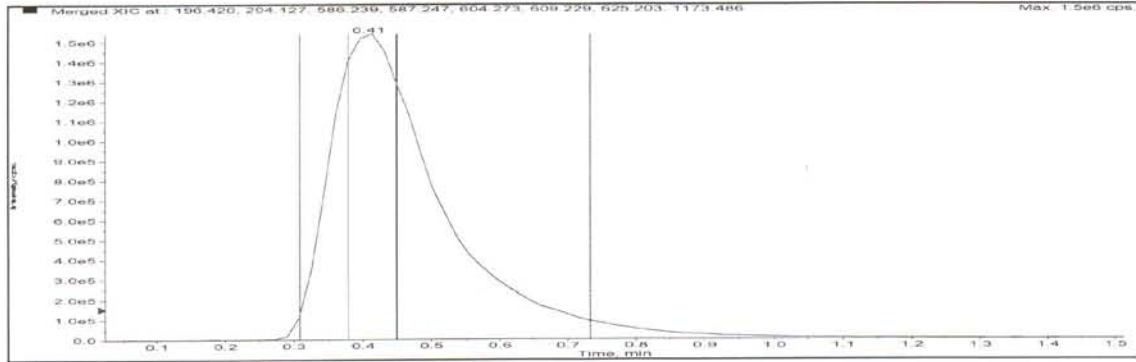




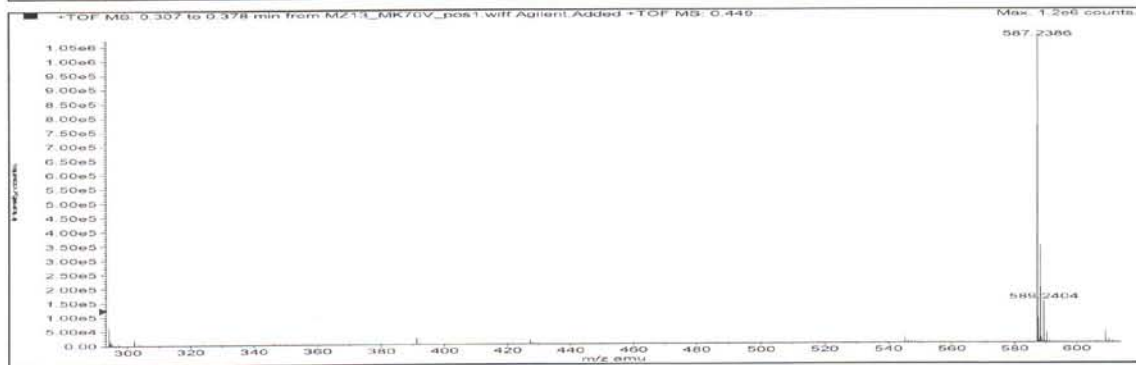
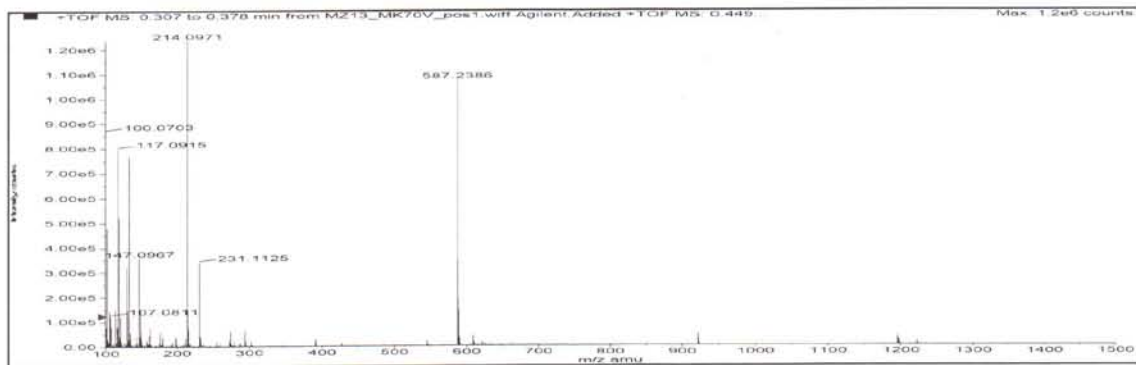
ROESY



Sample Name: MZ13 Sample Location: P1-C3 Sample Id: Operator: Milka
 Data File Name: D:\PE Sciex Data\Projects\Sladic\Data\MZ13_MK70V_pos1.wiff Acq Time: August 05 2014, 11:20:27 AM
 Method: d:\TOF_Data\damethods\Night_Seq_Comp_ident1.anml\efc.xml



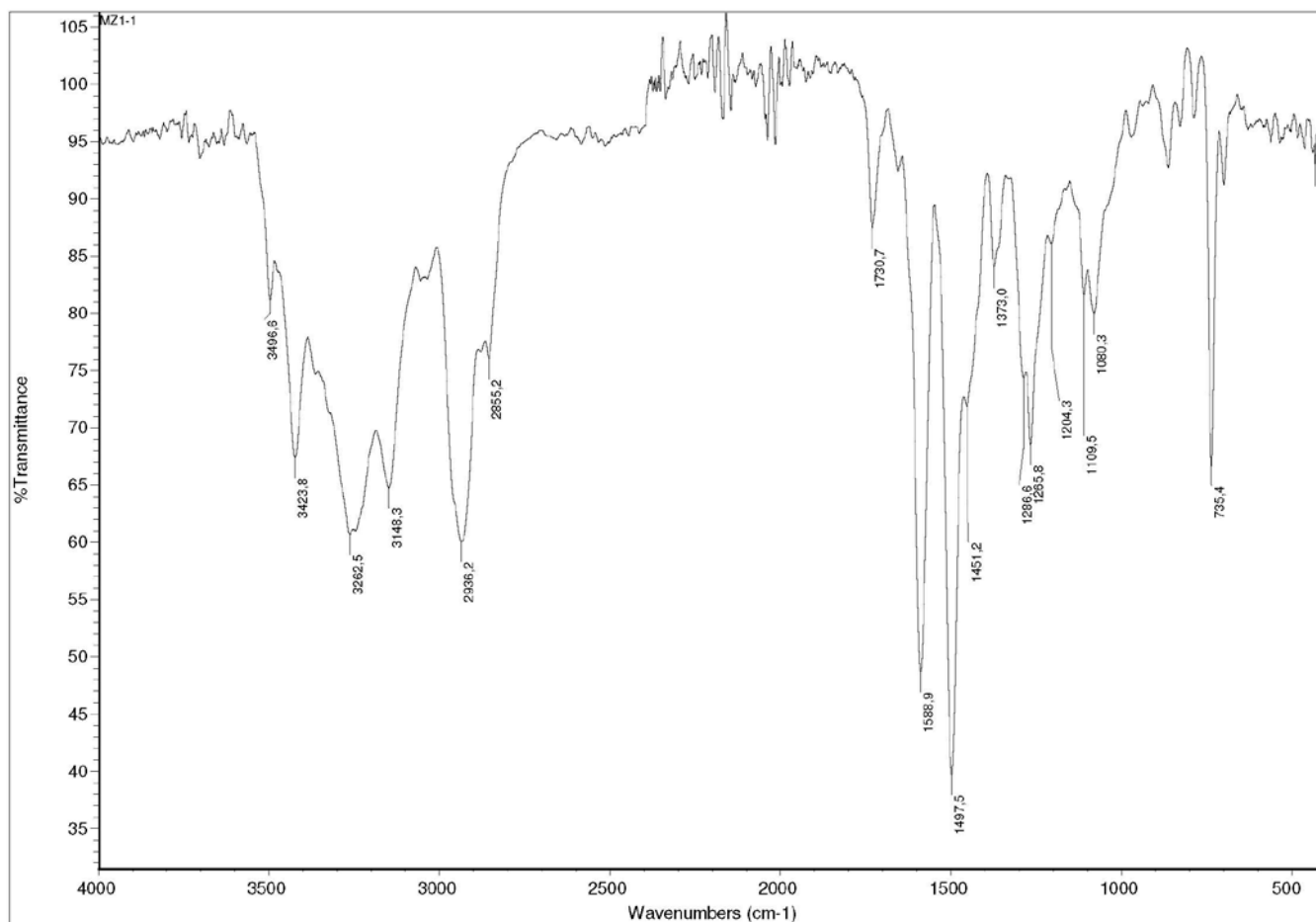
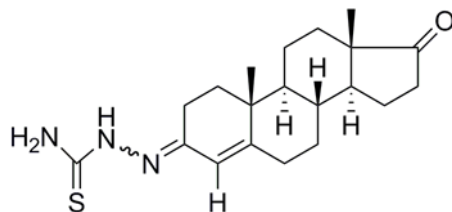
Merged XIC, Period# : 1 Experiment# : 1

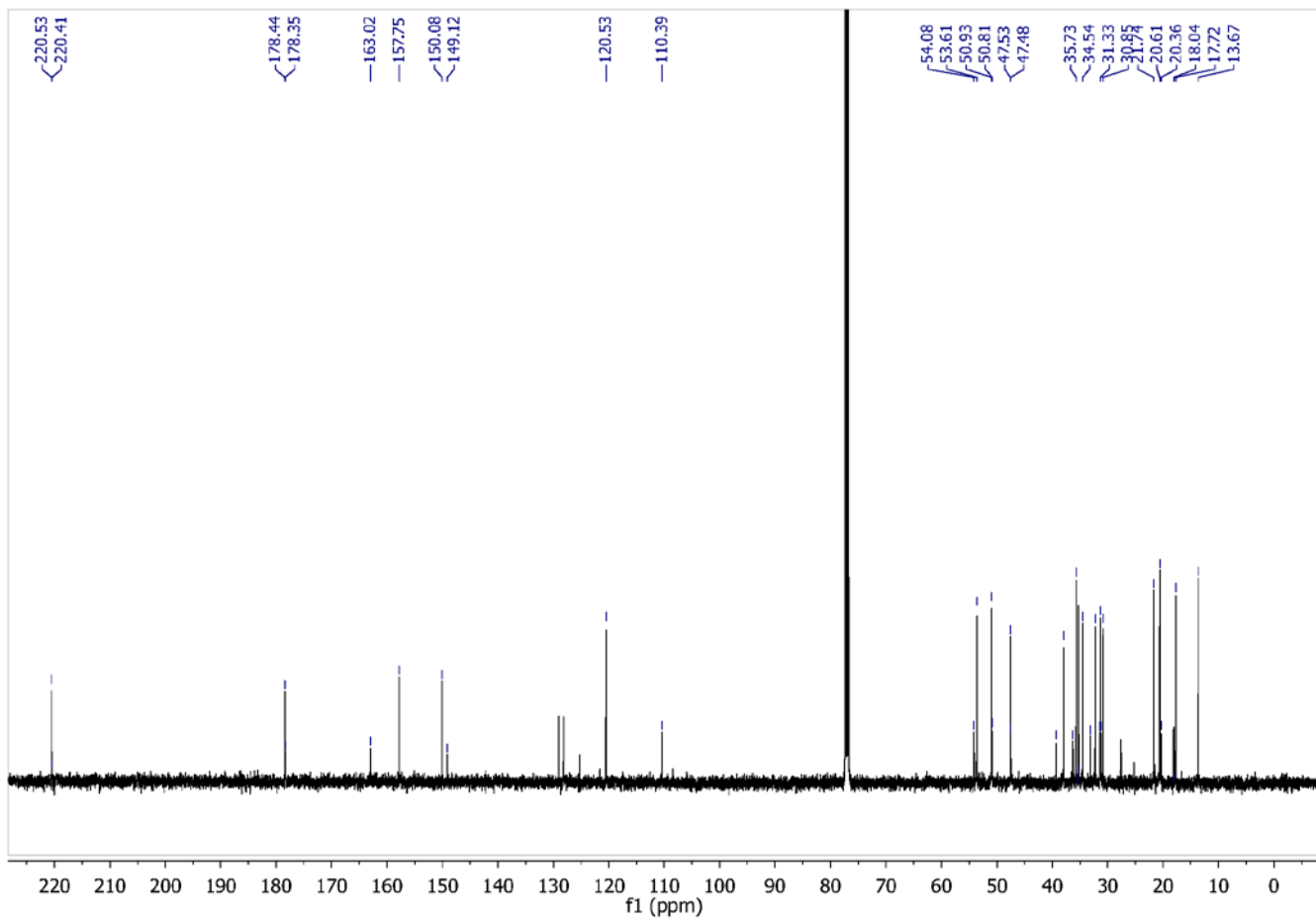
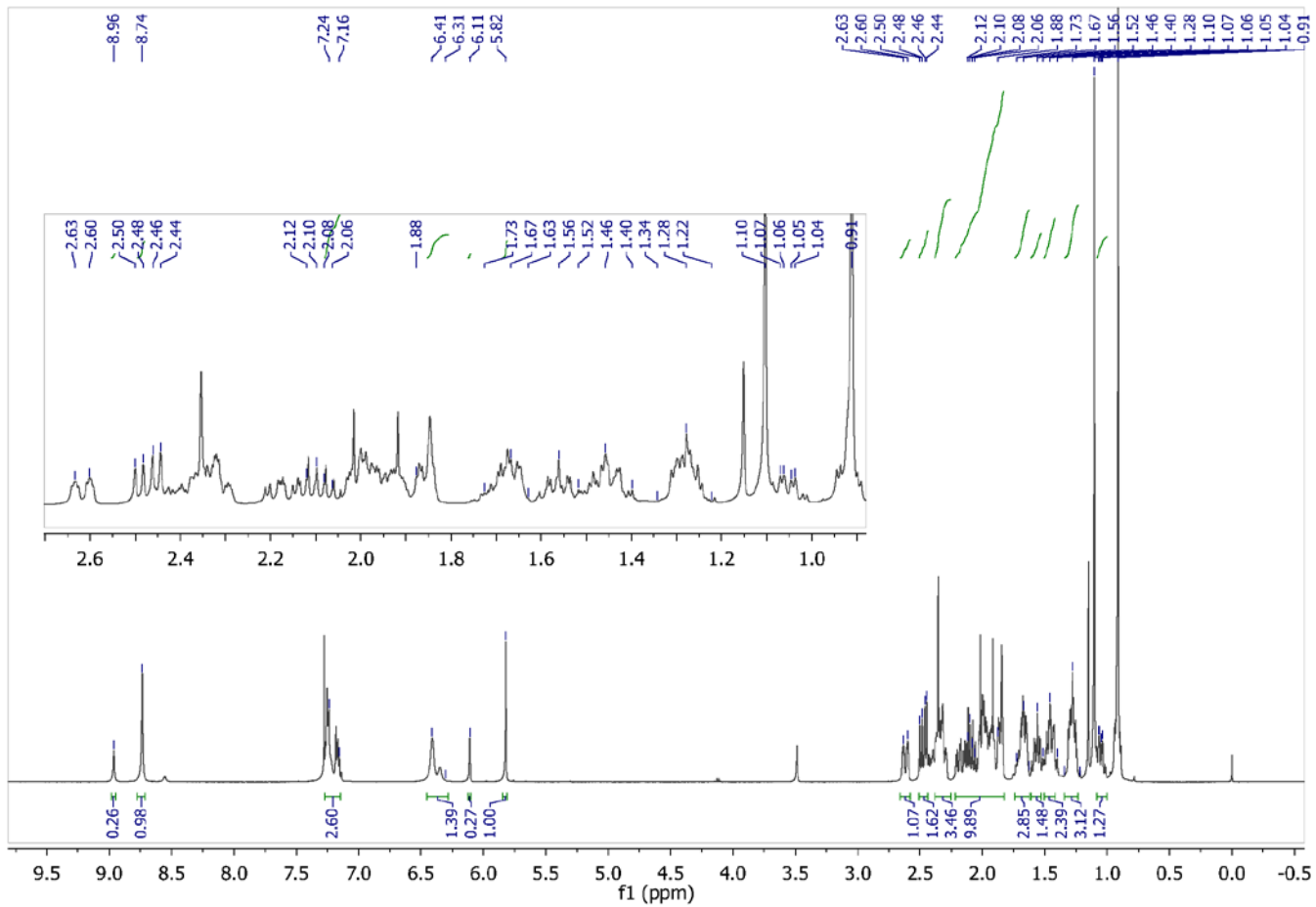


Formula	Compound name	Mass	Peak RT (min)	Peak area	Description
C28H38N6O4S2	--	586.23960	0.41	1.72010 E7	--

Species	Abundance (counts)	Ion Mass	Measured Mass	Error (mDa)	Error (ppm)	Ret. Time Error (min)
[M+2H] ²⁺	63313.91	294.12707	294.12704	-0.03354	-0.11	--
[M+H] ⁺	1100522.81	587.24687	587.24700	0.12510	0.21	--
[M+Na] ⁺	43472.35	609.22882	609.22878	-0.03344	-0.05	--

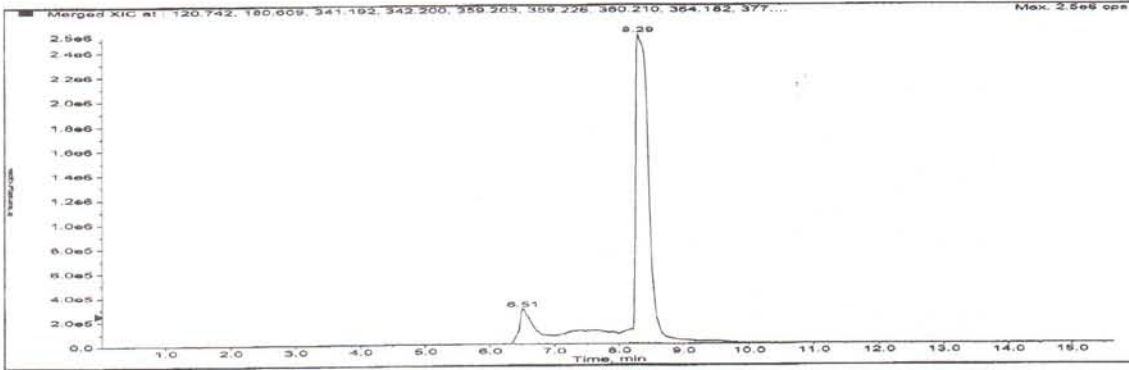
Compound 2b



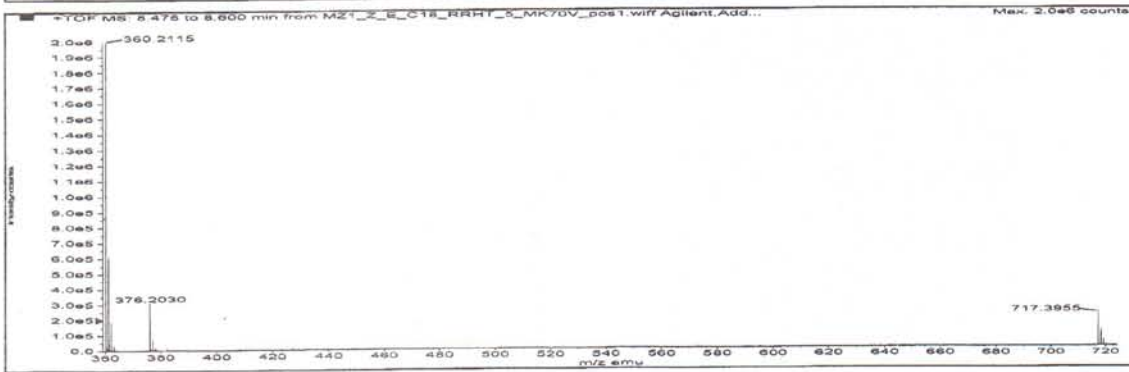
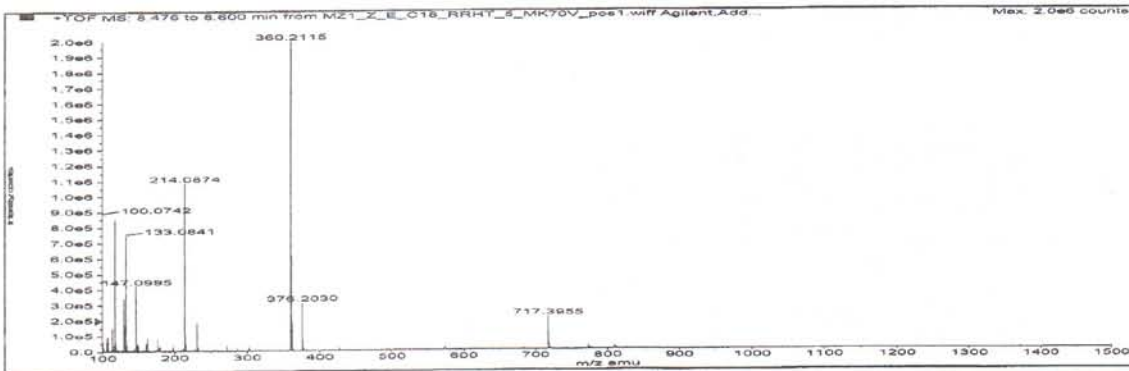


Sample Name: MZ1 Sample Location: P1-C4 Sample Id: Operator: Milka
 Data File Name: D:\PE Sciex Data\Projects\Stadic\Data\MZ1_Z_E_C18_RRHT_5_MK70V_pos1.wiff Acq Time: March 24 2014 01:14:01
 PM
 Method: g:\TOF_Data\damethods\Night_Seq_Comp_ident1\anmlcfc.xml

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



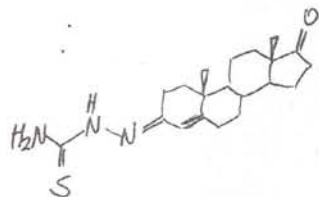
Merged XIC, Period#: 1 Experiment#: 1



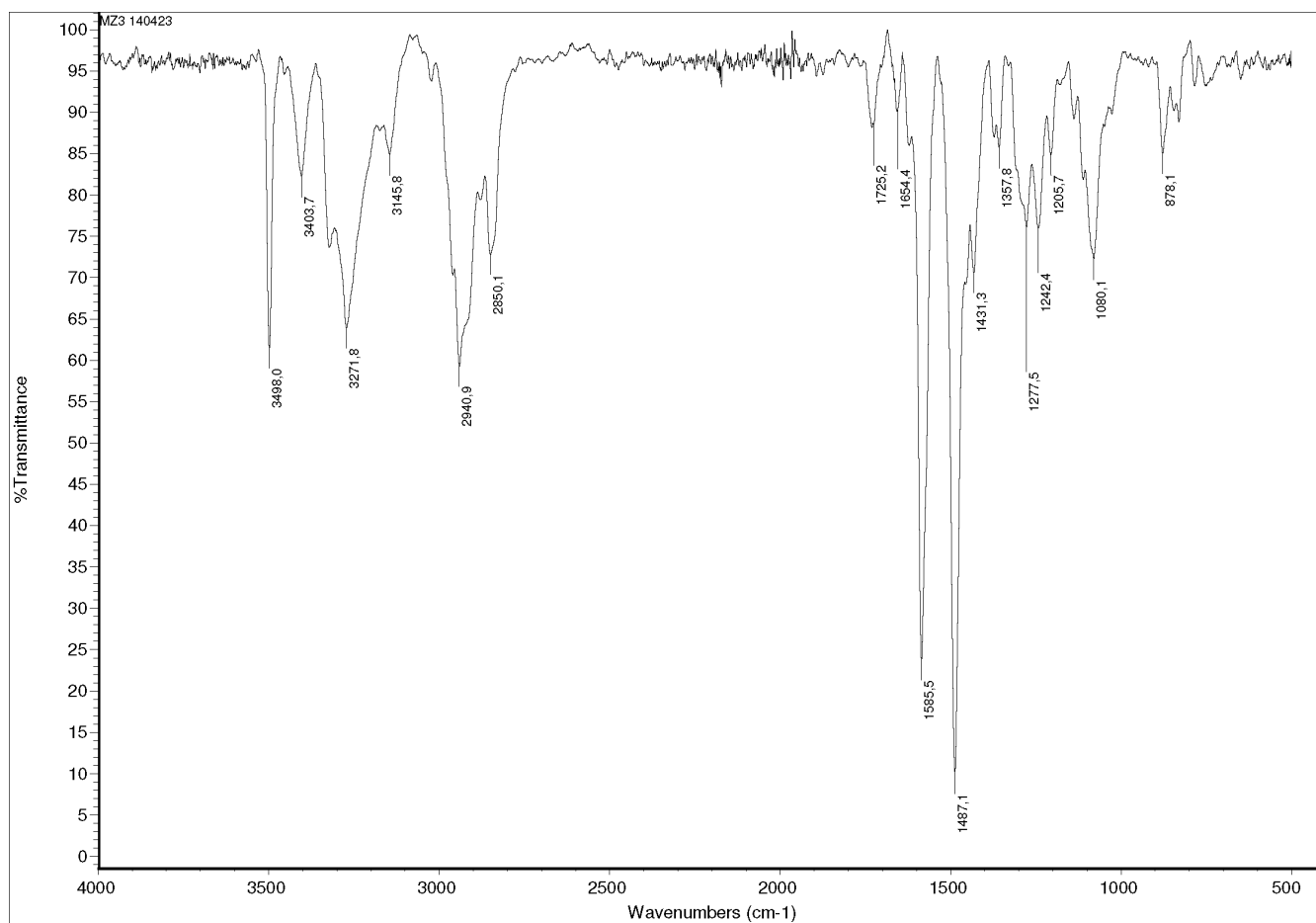
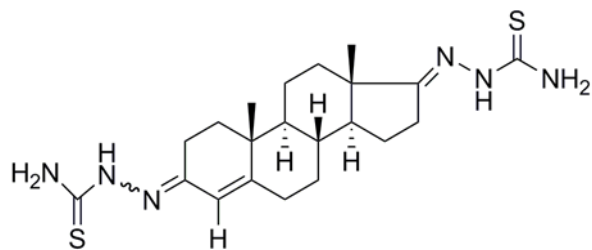
Formula	Compound name	Mass	Peak RT (min)	Peak area	Description
C20H29N3OS	--	359.20313	8.29	3.29119 E7	--

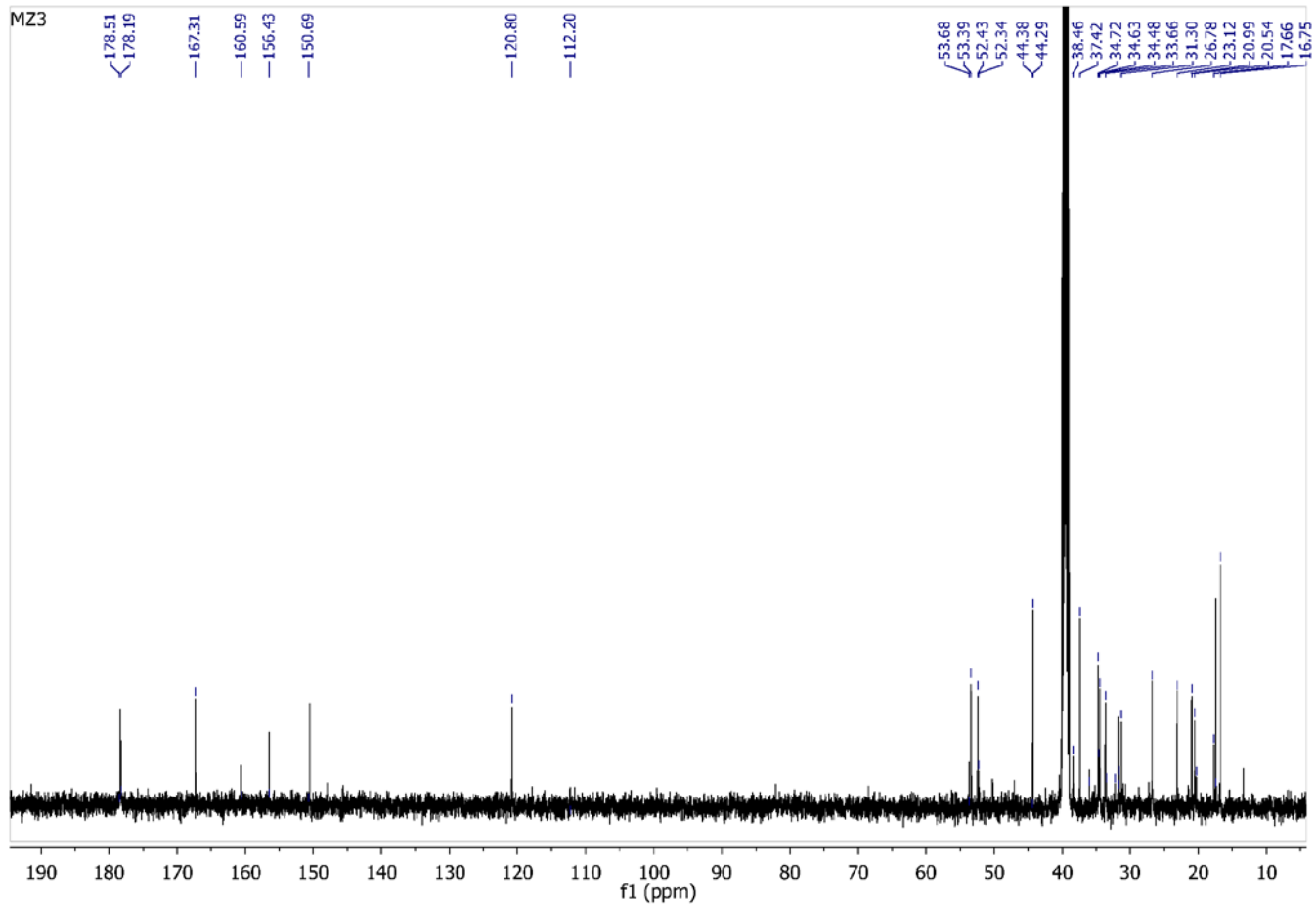
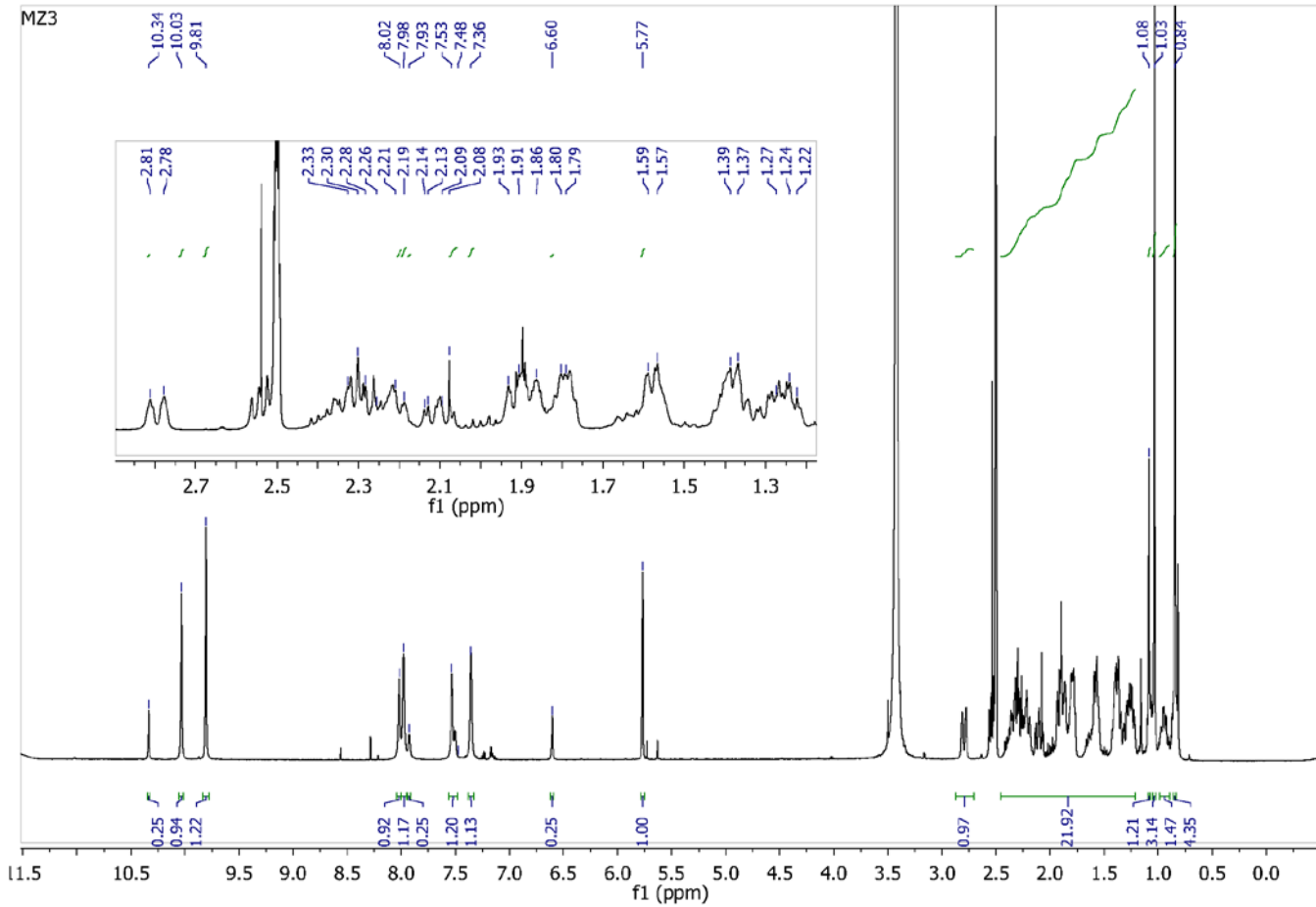
Species	Abundance (counts)	Ion Mass	Measured Mass	Error (mDa)	Error (ppm)	Ret. Time Error (min)
[M+H] ⁺	2118045.71	360.21041	360.21148	1.07232	2.98	--
[M+NH4] ⁺	71633.36	377.23696	377.20593	-31.02970	-82.26	--
[2M+H] ⁺	41919.78	719.41354	719.39735	-16.19003	-22.50	--

OK, MZ



Compound 3b

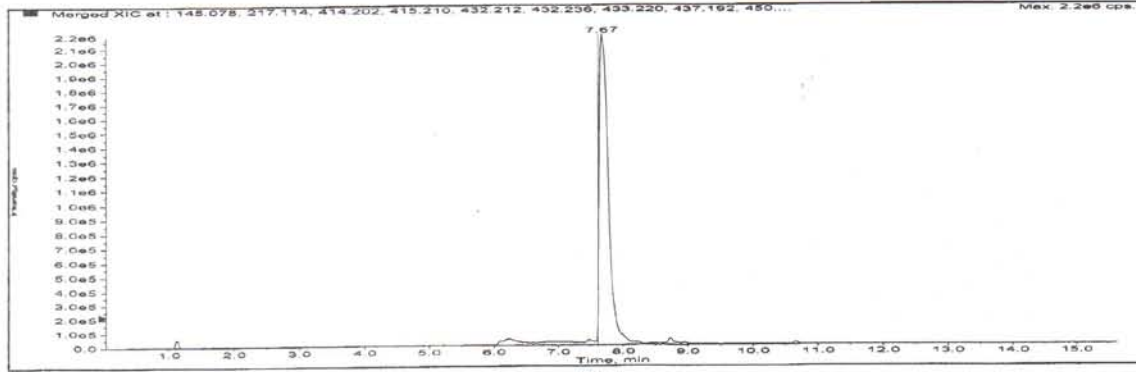




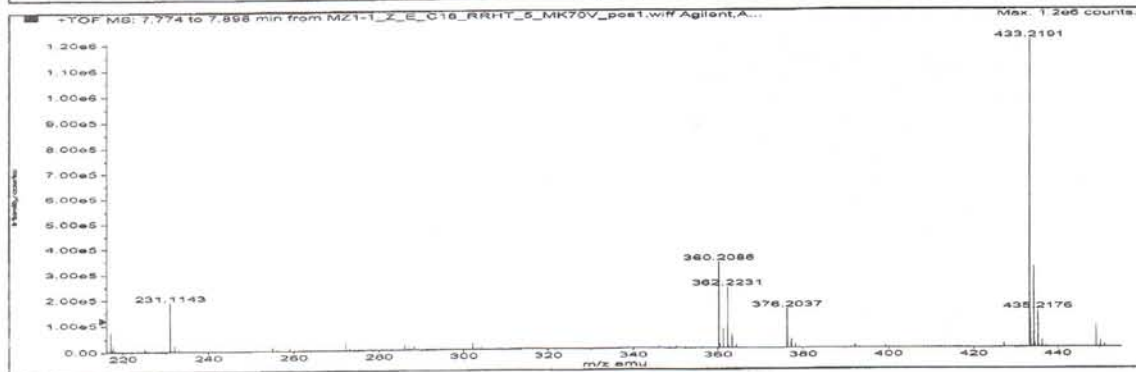
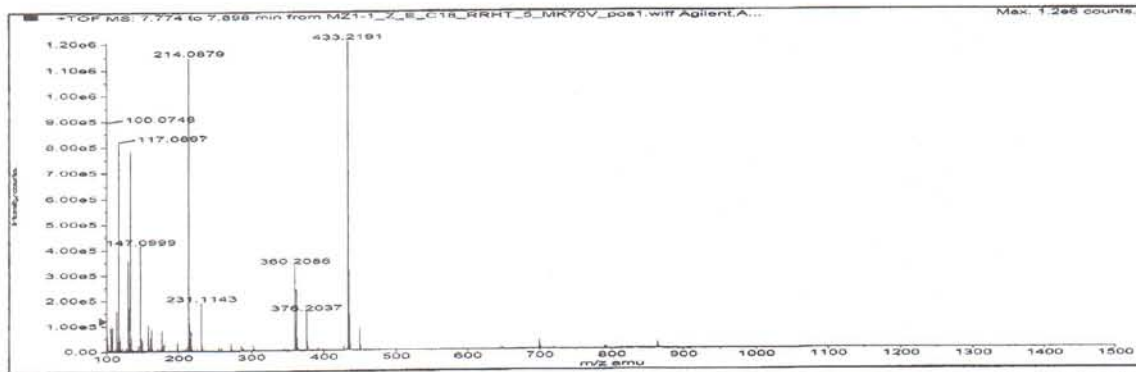
MZ3

Sample Name: MZ1-1 Sample Location: P1-C5 Sample Id: Operator: Milka
 Data File Name: D:\PE ScieX Data\Projects\SIadic\Data\MZ1-1_Z_E_C18_RRHT_5_MK70V_pos1.wiff Acq Time: March 24 2014,
 01:33:50 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.



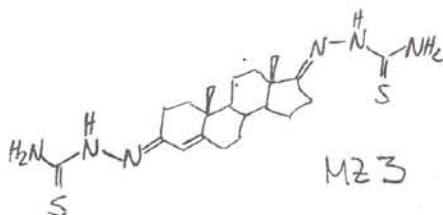
Merged XIC, Period# : 1 Experiment# : 1



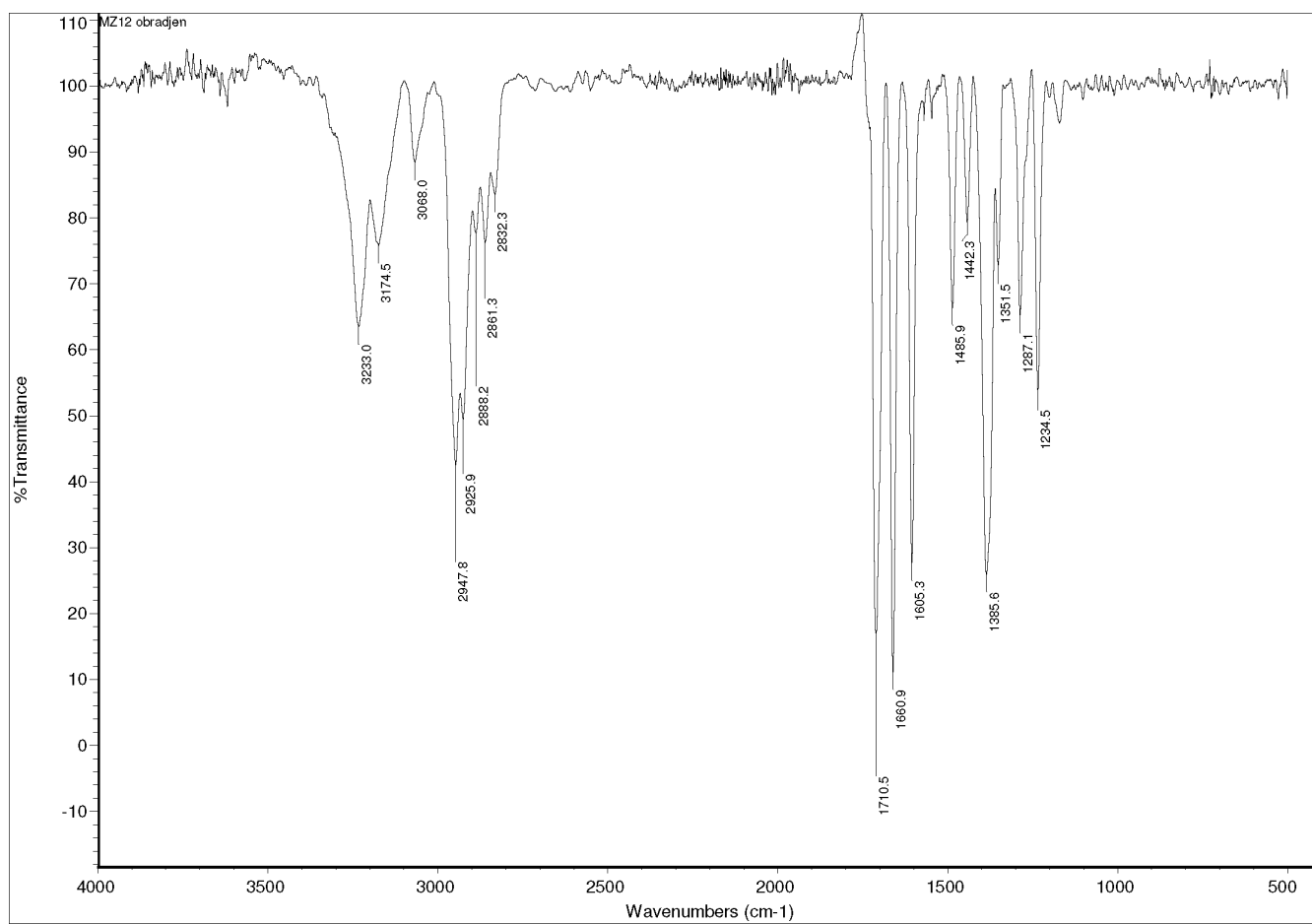
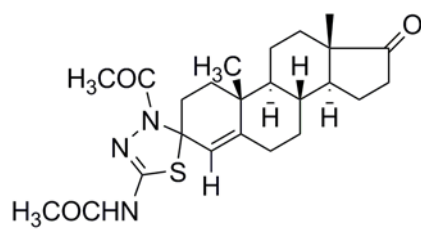
Formula	Compound name	Mass	Peak RT (min)	Peak area	Description
C21H32N6S2	--	432.21299	7.67	2.05709 E7	--

Species	Abundance (counts)	Ion Mass	Measured Mass	Error (mDa)	Error (ppm)	Ret. Time Error (min)
[M+2H] ²⁺	80952.69	217.11377	217.11160	-2.16649	-9.98	
[M+H] ⁺	1259507.50	433.22026	433.21908	-1.17879	-2.72	
[M+NH4] ⁺	24836.46	460.24681	460.21780	-29.01626	-64.46	

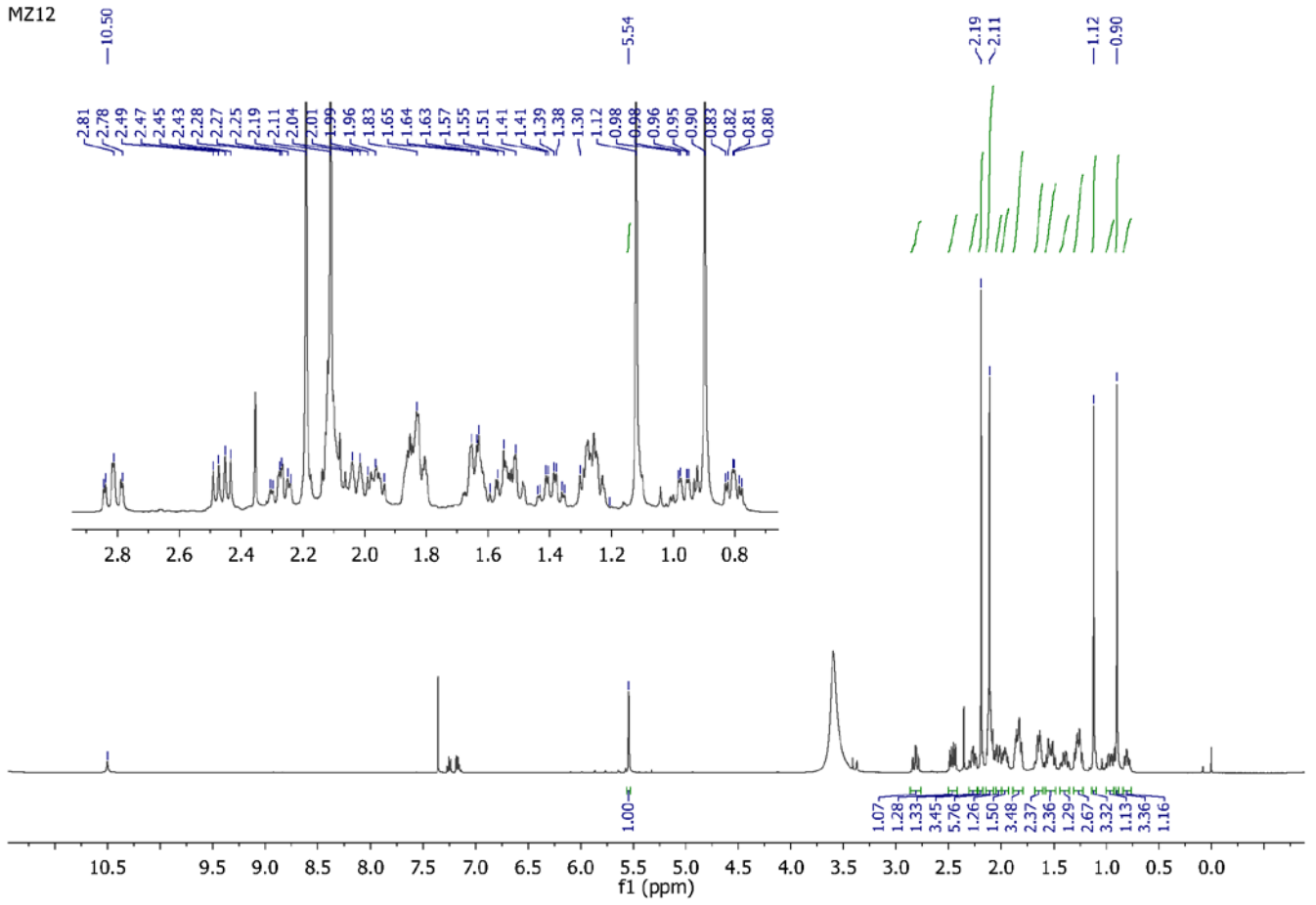
OK, MJ



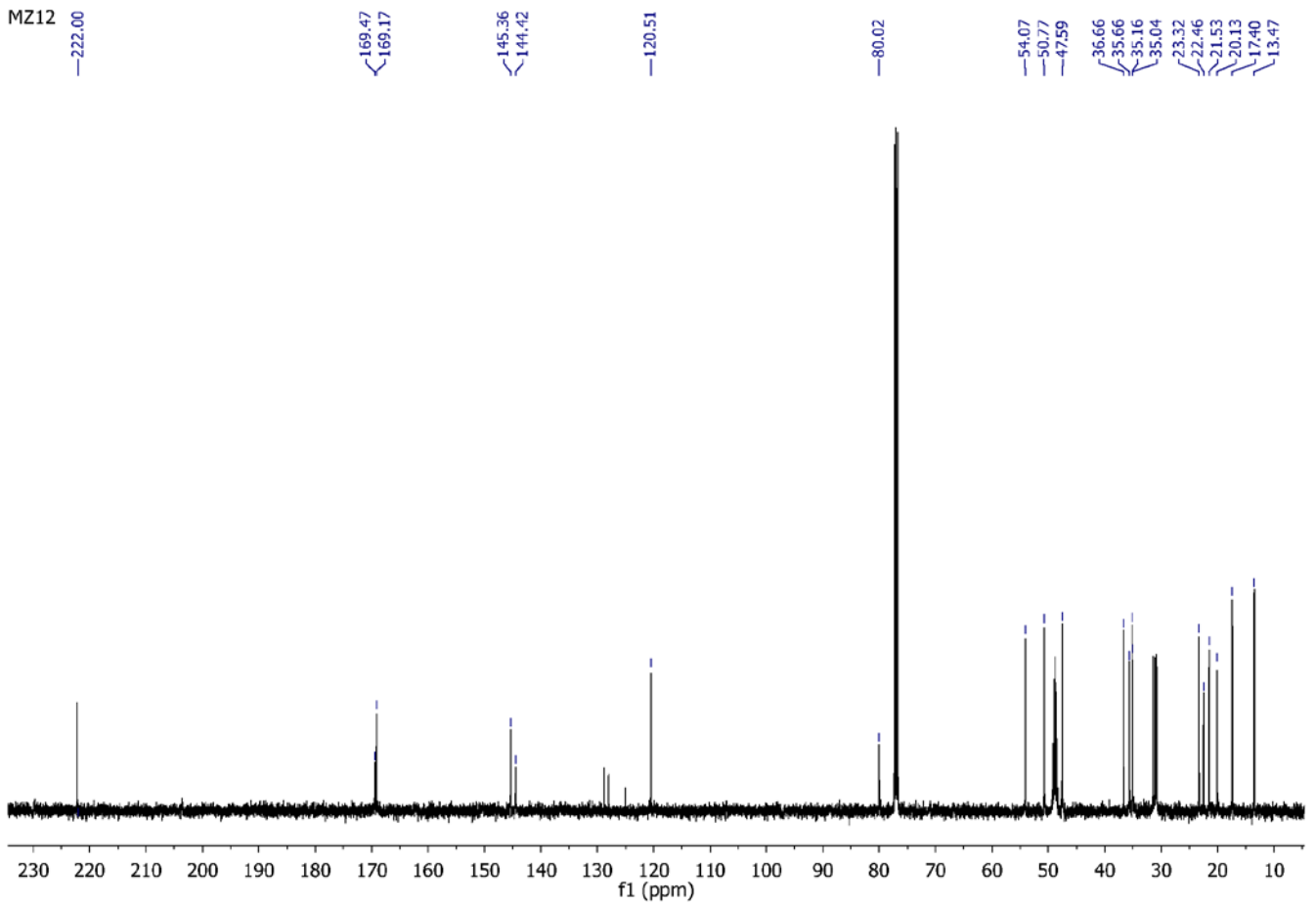
Compound 4b



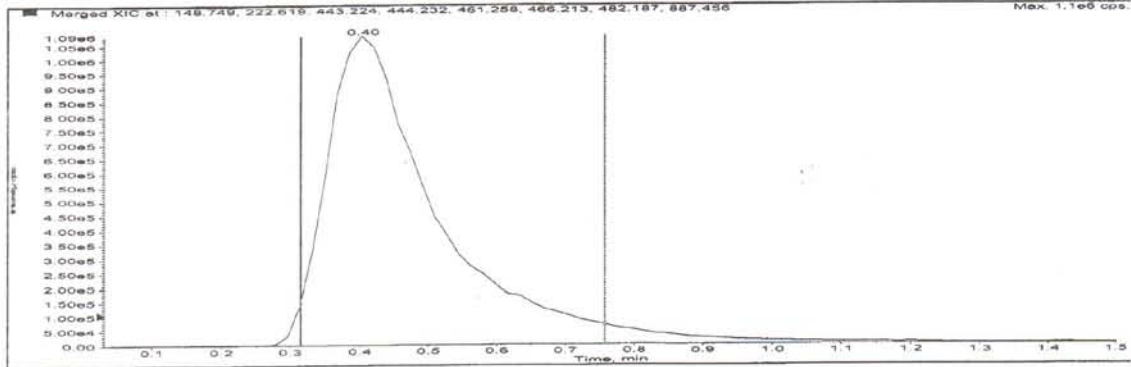
MZ12



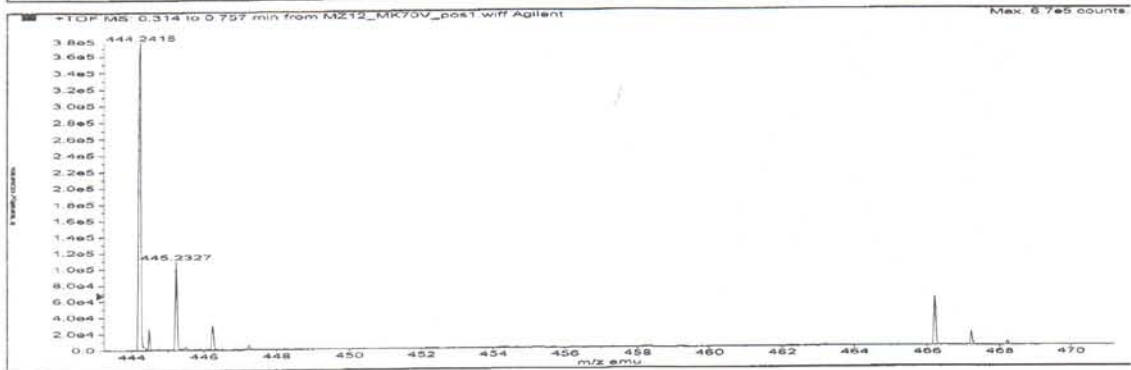
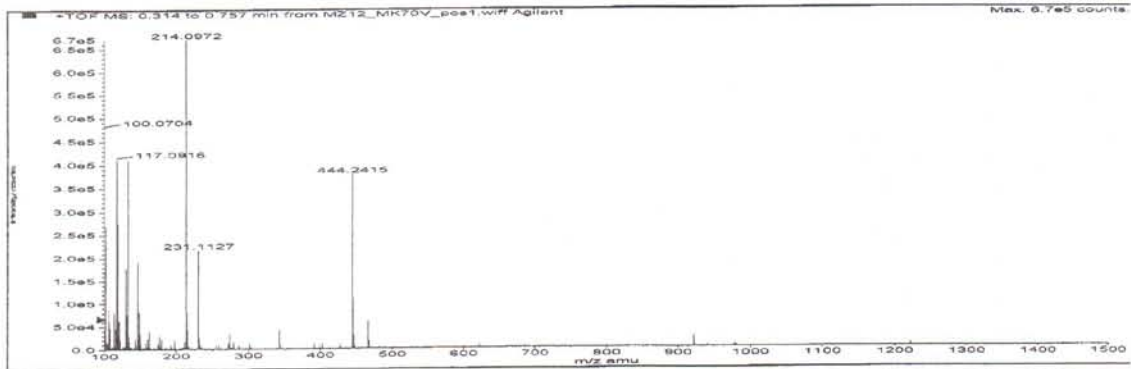
MZ12



Sample Name: MZ12 Sample Location: P1-C2 Sample Id: Operator: Milka
 Data File Name: D:\PE Sciex Data\Projects\Sladic\Data\MZ12_MK70V_pos1.wiff Acq Time: August 05 2014, 11:17:46 AM
 Method: d:\TOF_Data\damethods\Night_Seq_Comp_ident1.an\mefc.xml



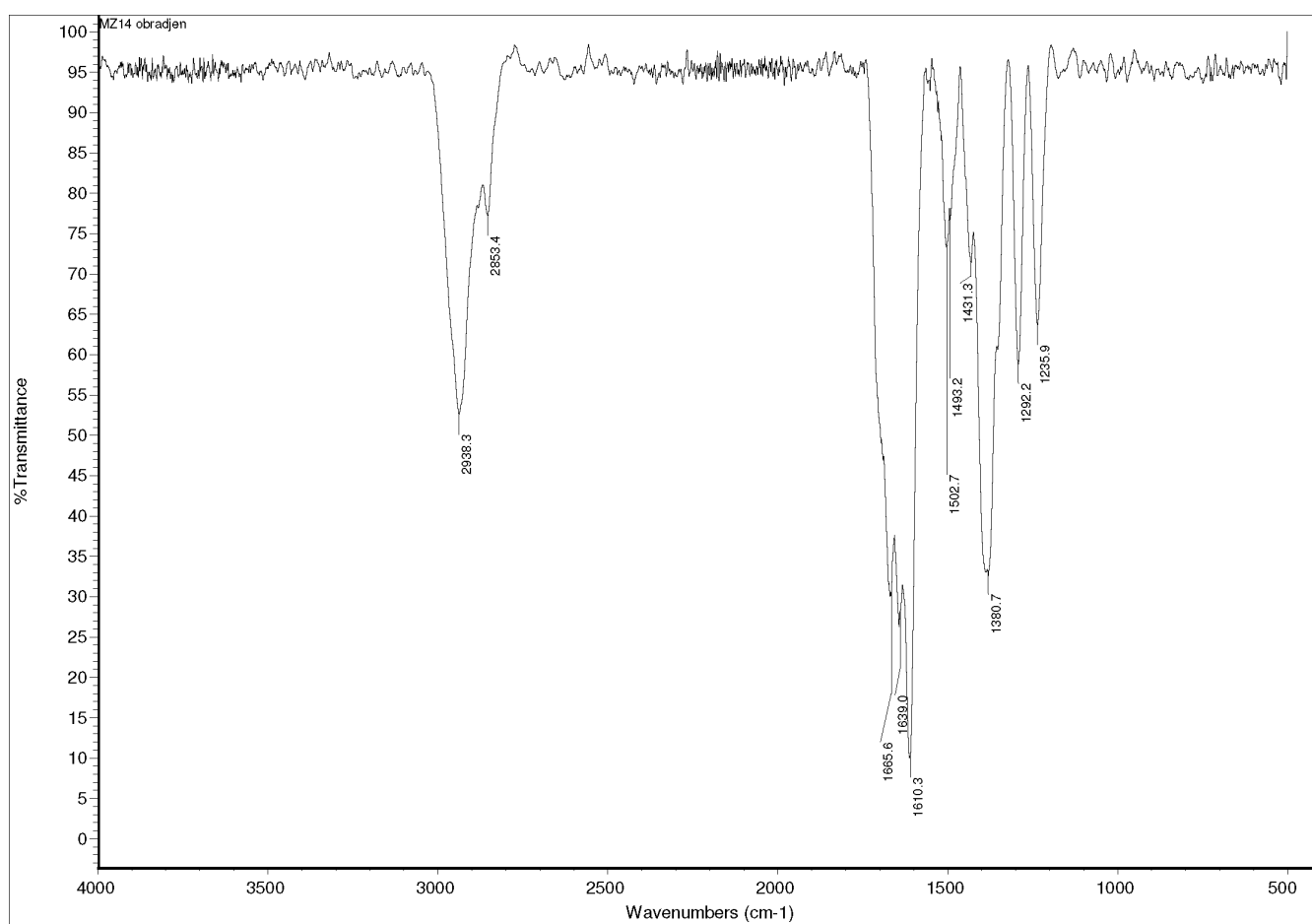
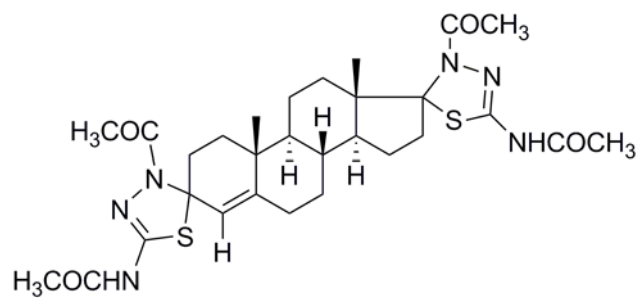
Merged XIC, Period# : 1 Experiment# : 1



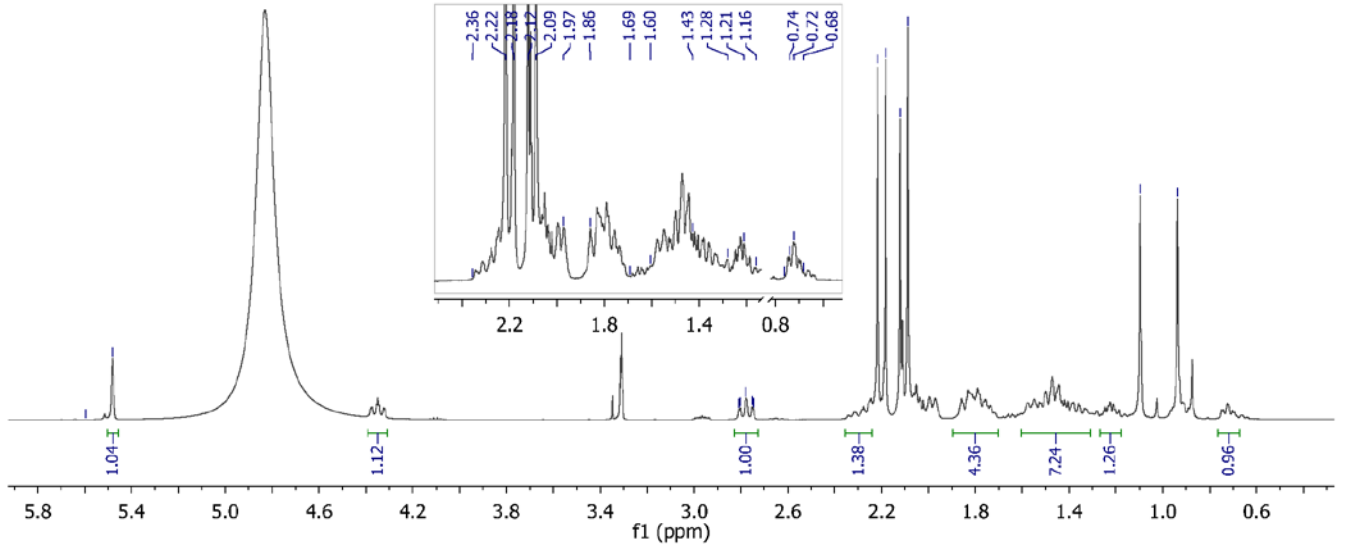
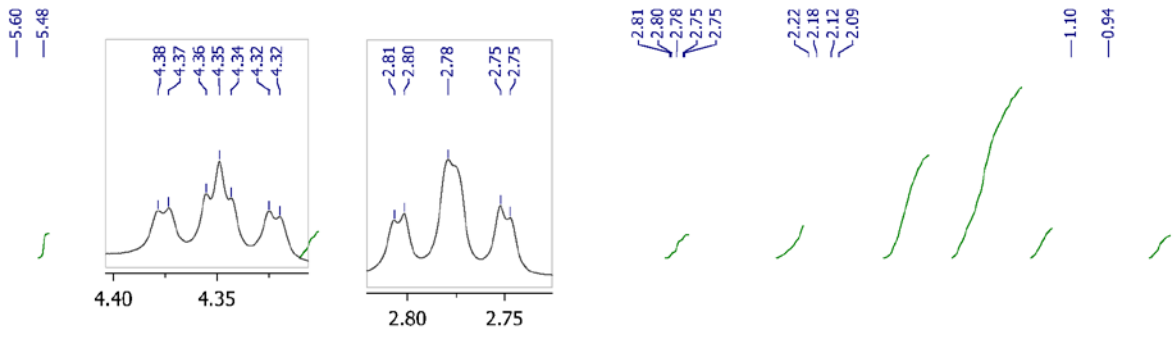
Formula	Compound name	Mass	Peak RT (min)	Peak area	Description
C24H33N3O3S	--	443.22426	0.40	1.19248 E7	--

Species	Abundance (counts)	Ion Mass	Measured Mass	Error (mDa)	Error (ppm)	Ret. Time Error (min)
[M+H] ⁺	399940.43	444.23154	444.23112	-0.41601	-0.94	--
[M+Na] ⁺	62367.77	466.21348	466.21310	-0.38718	-0.83	--

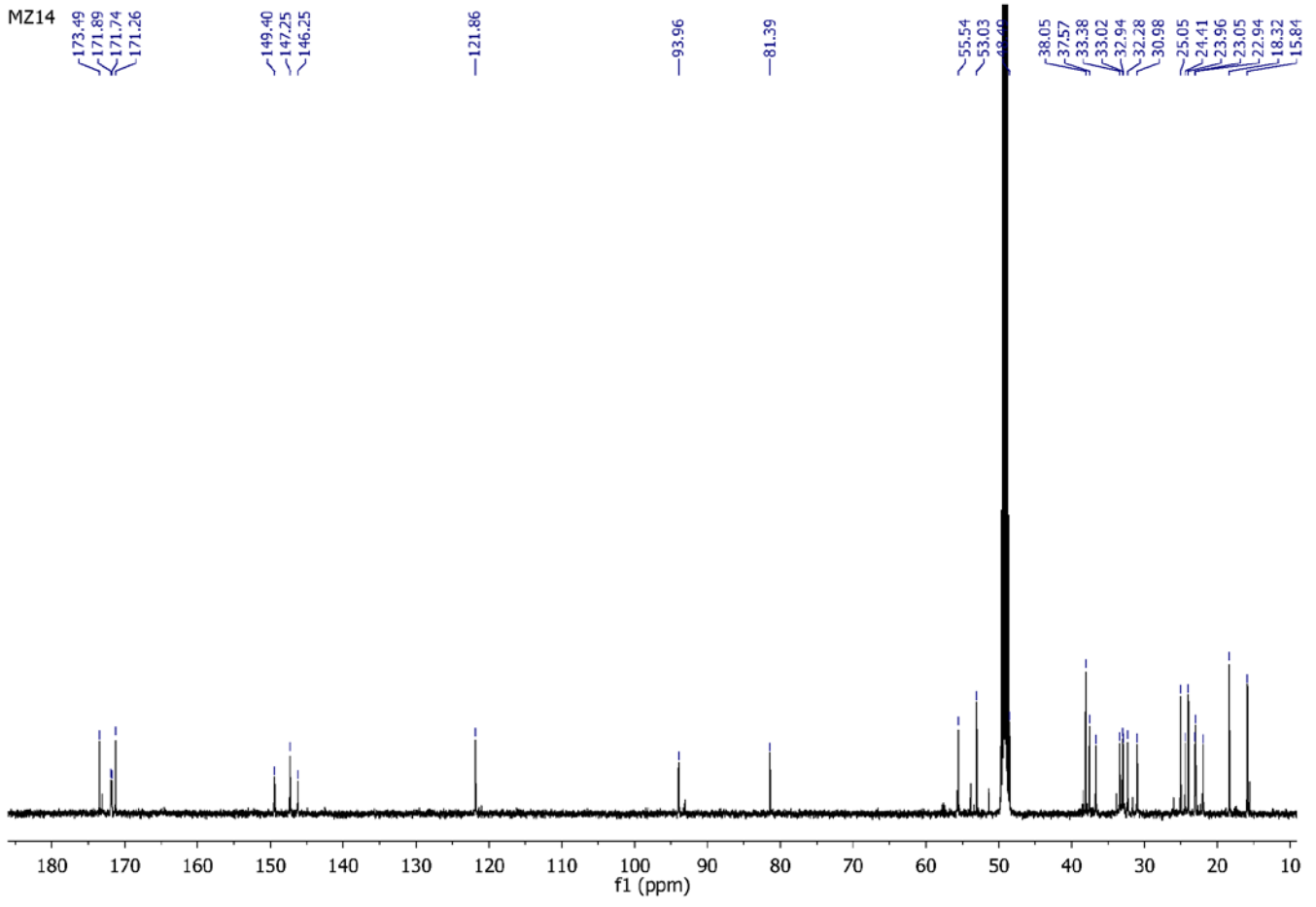
Compound 5b



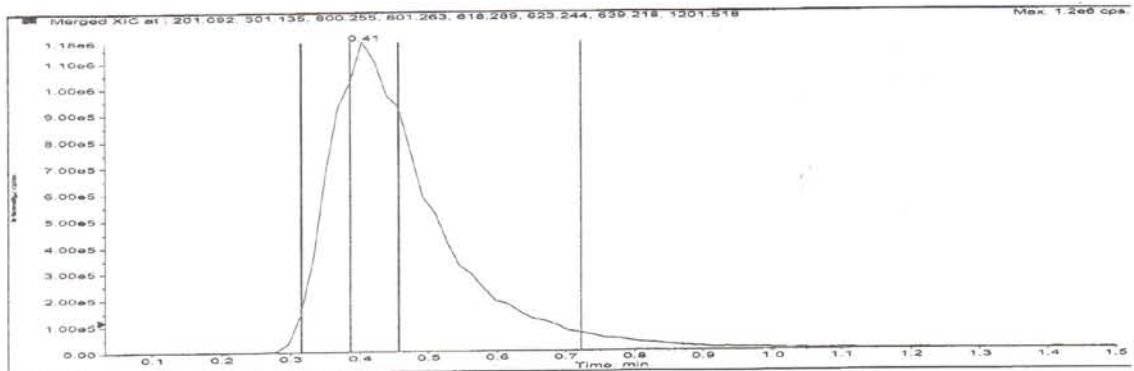
MZ14



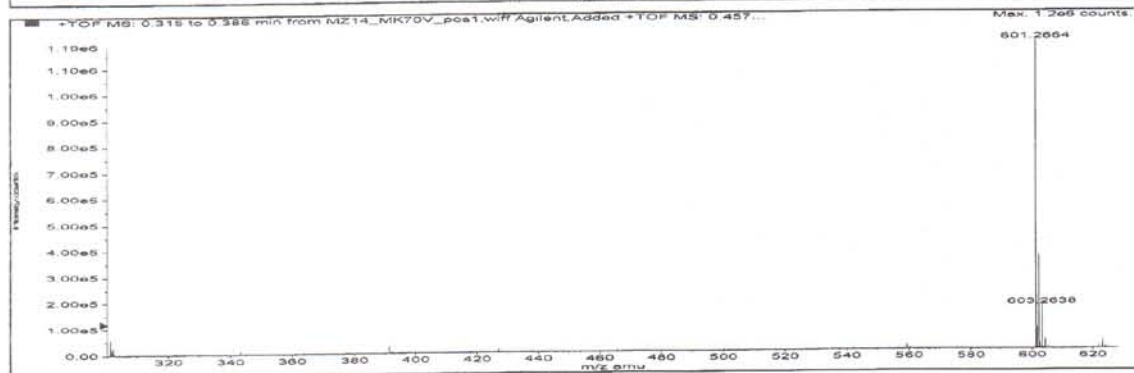
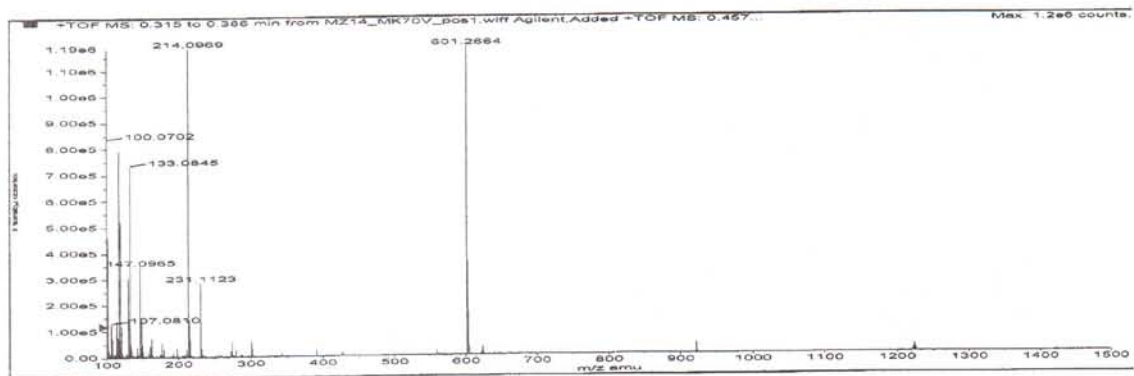
MZ14



Sample Name: MZ14 Sample Location: P1-C4 Sample Id: Operator: Milka
 Data File Name: D:\PE ScieX Data\Projects\Sladic\Data\MZ14_MK70V_pos1.wiff Acq Time: August 05 2014, 11:22:57 AM
 Method: d:\TOF_Data\damethods\Night_Seq_Comp_ident1_anmlefc.xml



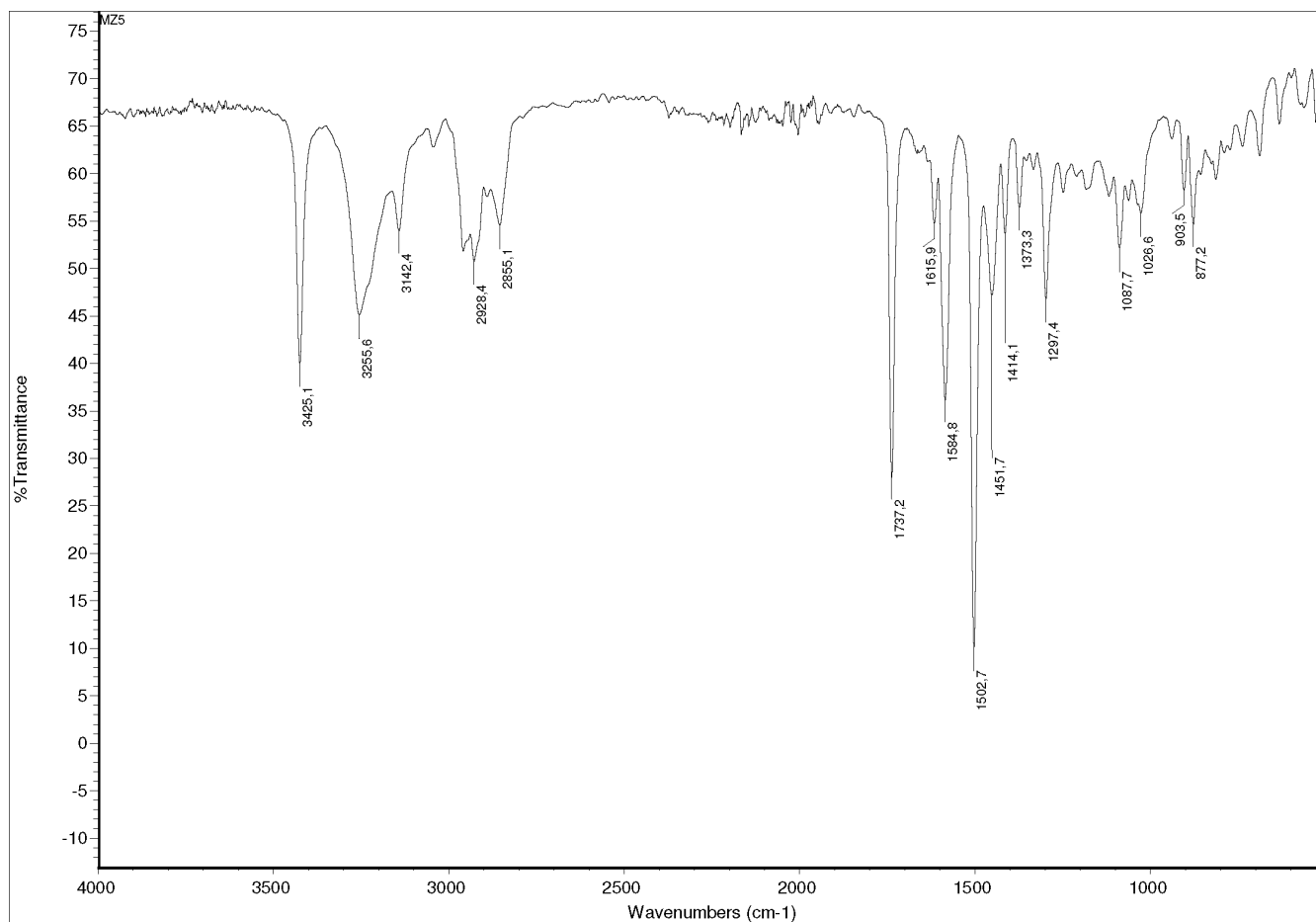
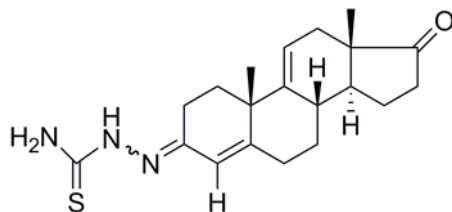
Merged XIC, Period#: 1 Experiment#: 1

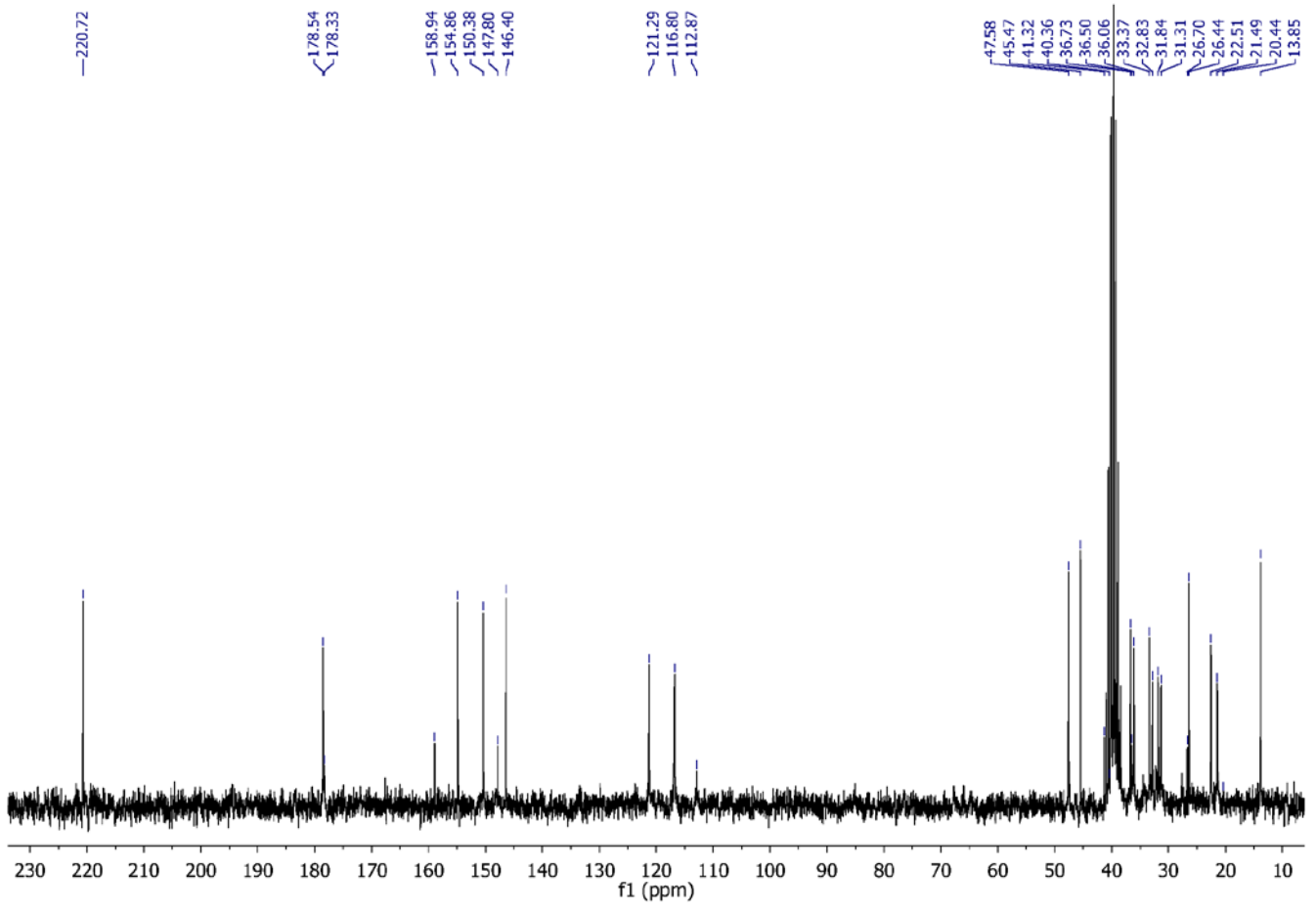
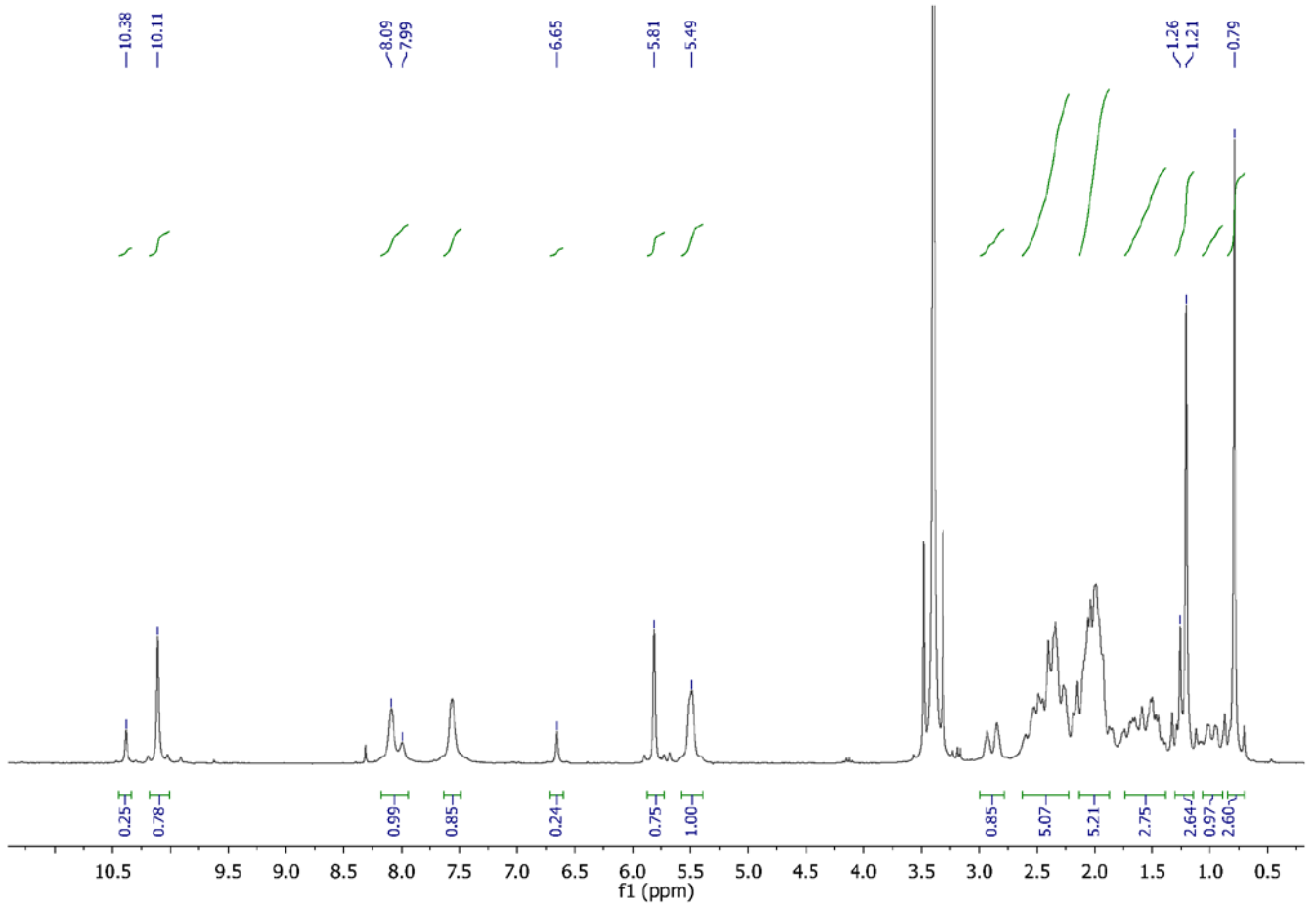


Formula	Compound name	Mass	Peak RT (min)	Peak area	Description
C29H40N6O4S2	--	600.25525	0.41	1.23775 E7	--

Species	Abundance (counts)	Ion Mass	Measured Mass	Error (mDa)	Error (ppm)	Ret. Time Error (min)
[M+2H] ²⁺	62126.89	301.13490	301.13535	0.45015	1.49	--
[M+H] ⁺	1190849.86	601.26252	601.26266	0.14036	0.23	--
[M+Na] ⁺	33383.24	623.24447	623.24458	0.11073	0.18	--

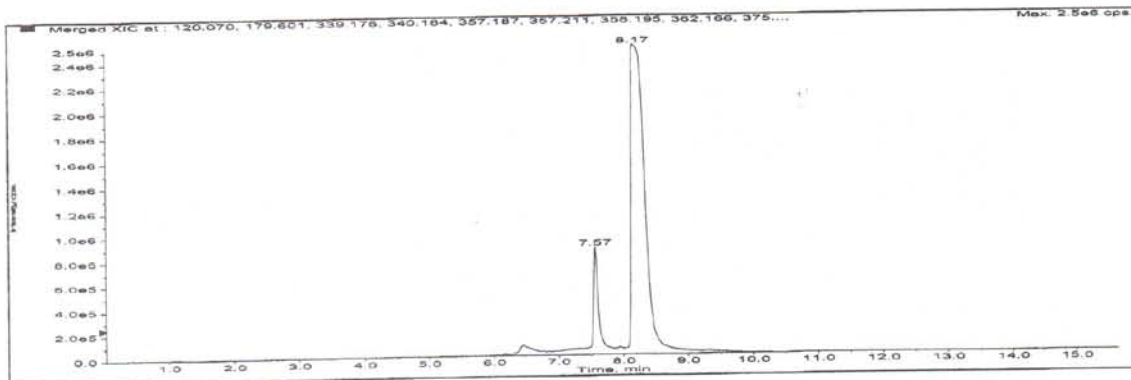
Compound 2c



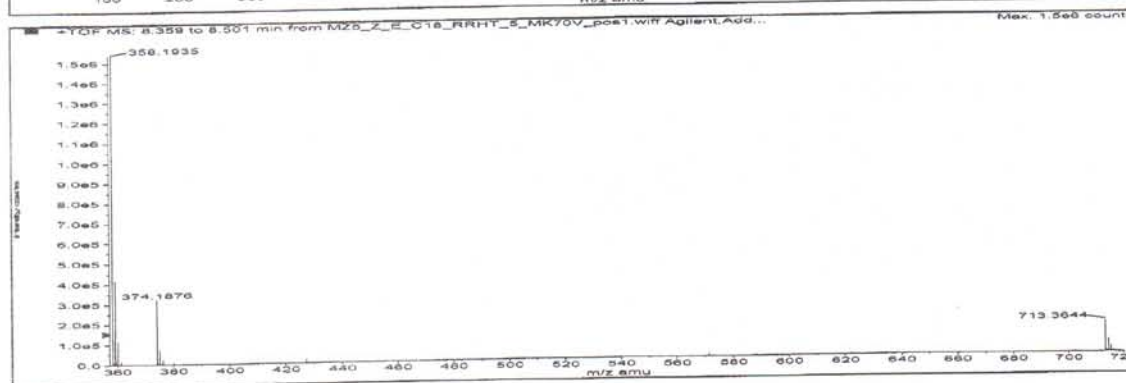
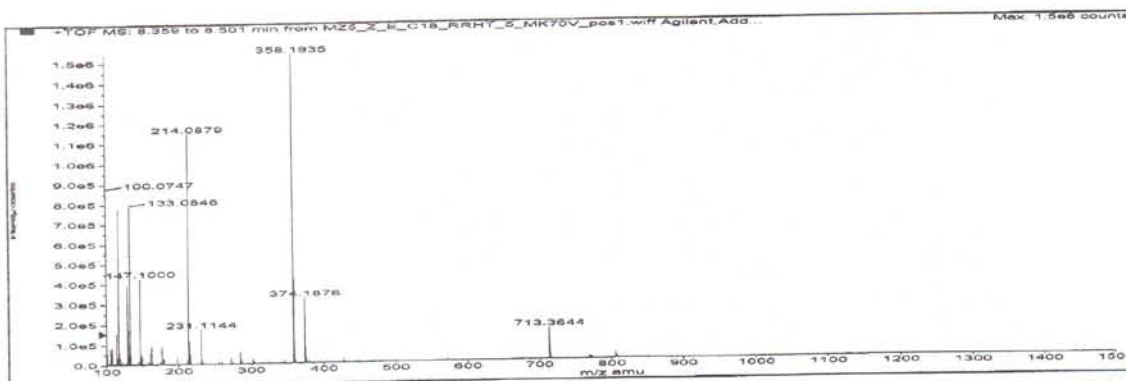


Sample Name: MZ5 Sample Location: P1-C7 Sample Id: Operator: Milka
 Data File Name: D:\PE Sciex Data\Projects\Sladic\Data\MZ5_Z_E_C18_RRHT_5_MK70V_pos1.wiff Acq Time: March 24 2014, 02:13:28
 PM
 Method: d:\TOF_Data\damethods\Night_Seq_Comp_Ident1.anml\etc.xml

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

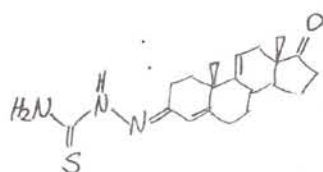


Merged XIC, Period# : 1 Experiment# : 1

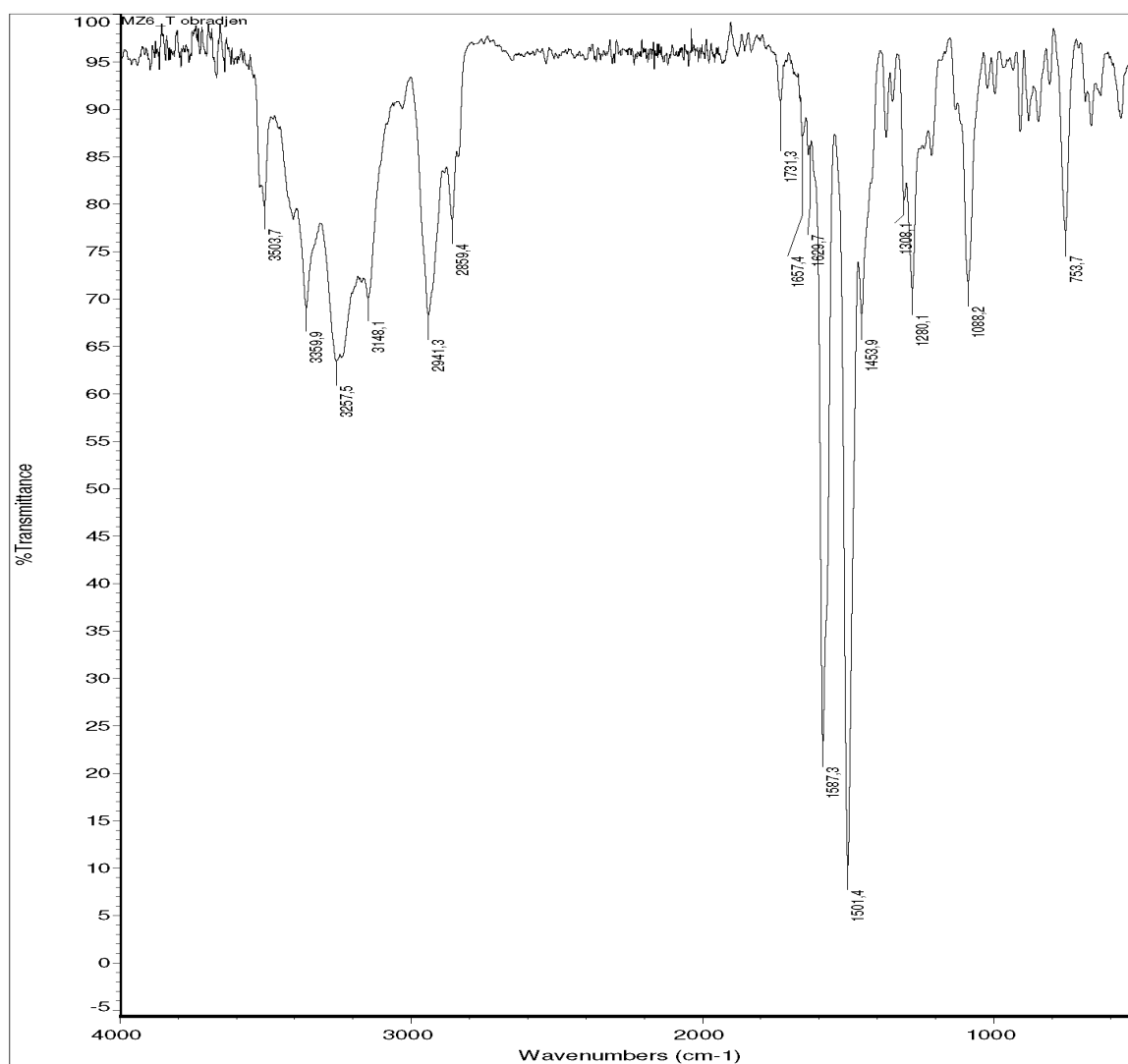
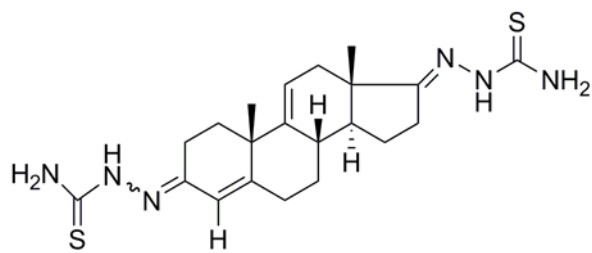


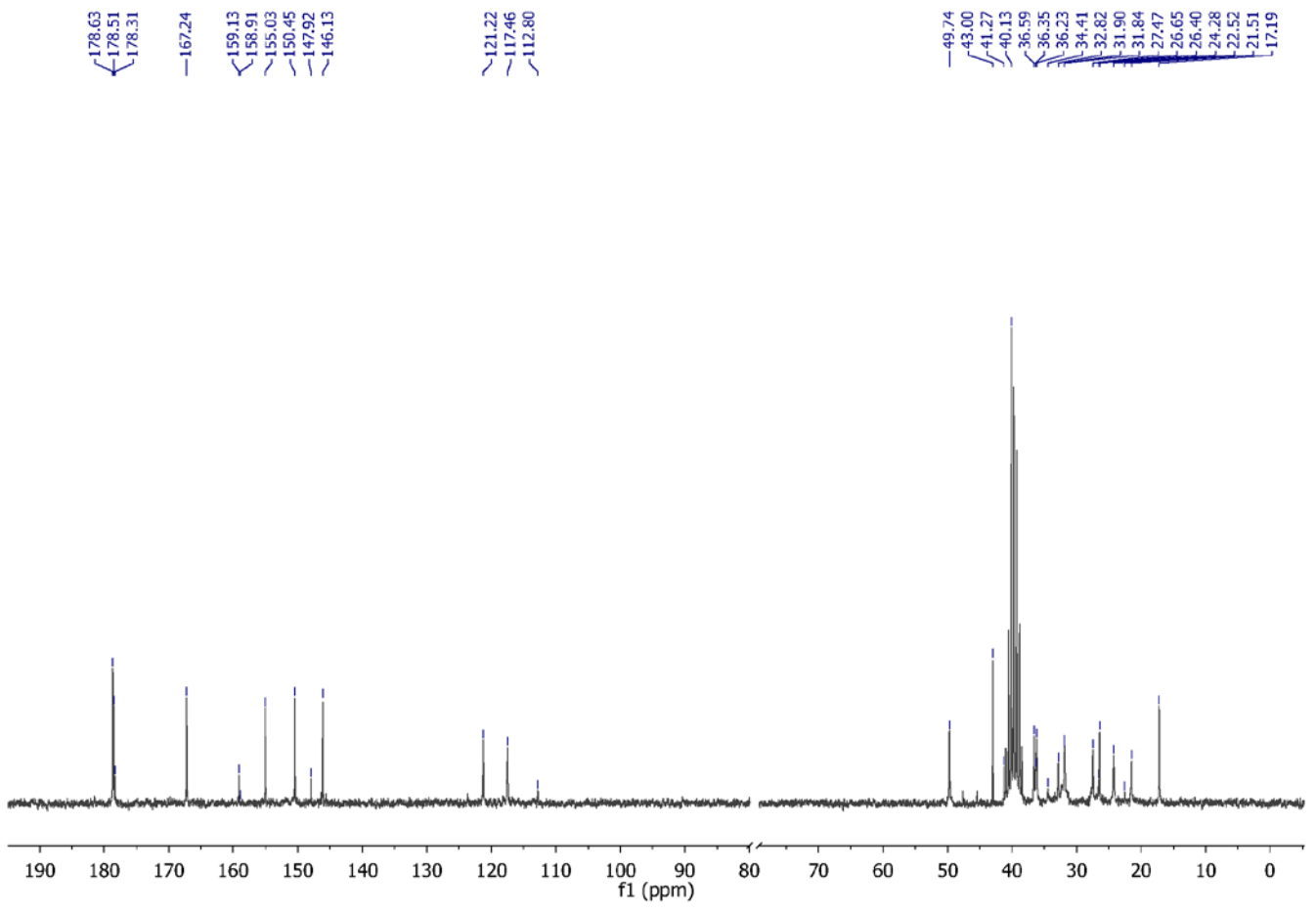
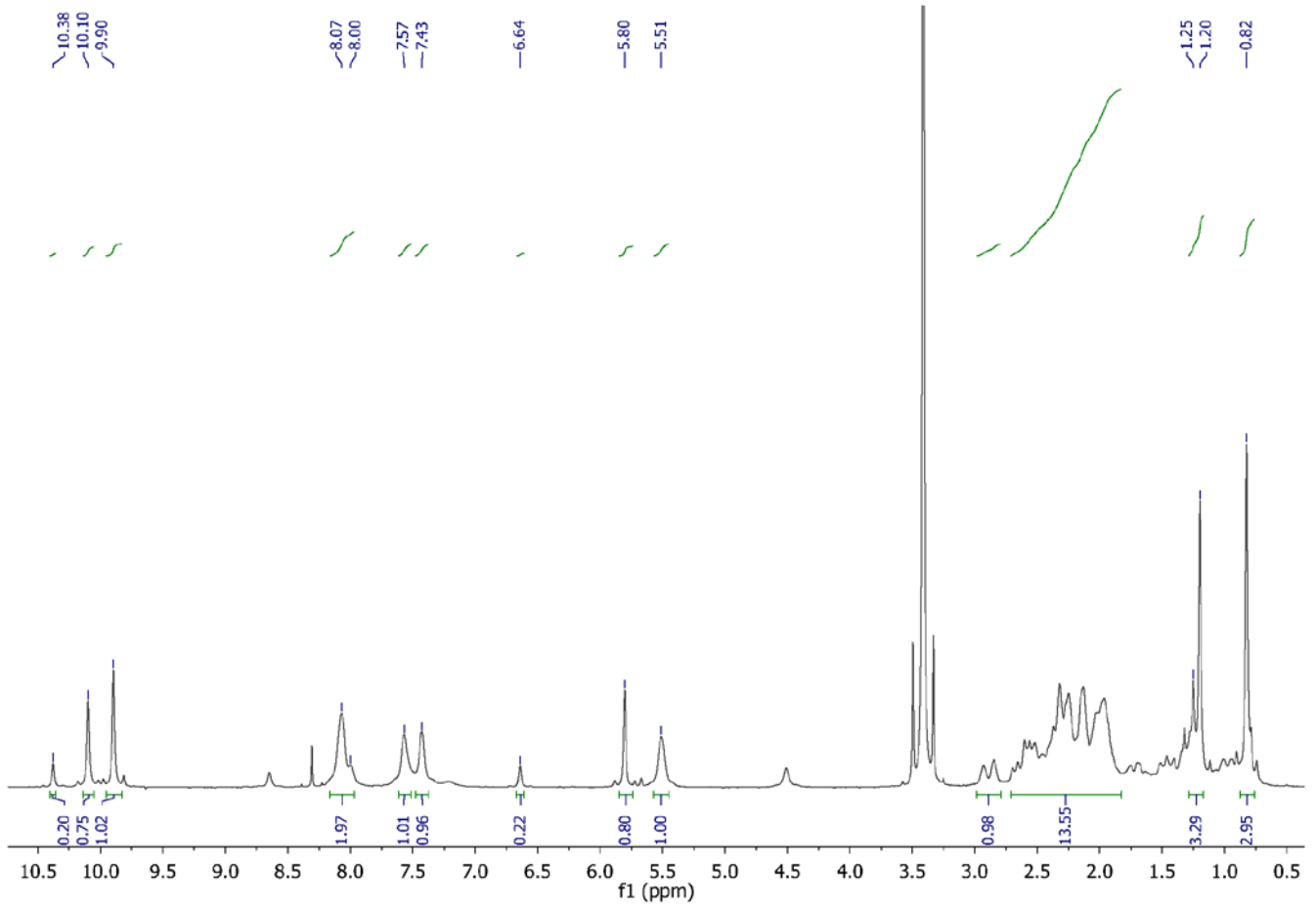
Formula	Compound name	Mass	Peak RT (min)	Peak area	Description
C20H27N3OS	--	357.18748	8.17	3.48884 E7	--

Species	Abundance (counts)	Ion Mass	Measured Mass	Error (mDa)	Error (ppm)	Ret. Time Error (min)
[M+H] ⁺	1606346.42	358.19476	358.19350	-1.25947	-3.52	--
[M+NH4] ⁺	75377.06	375.22131	375.19111	-30.19601	-80.48	--
[2M+H] ⁺	29439.09	715.38224	715.36655	-15.69705	-21.94	--



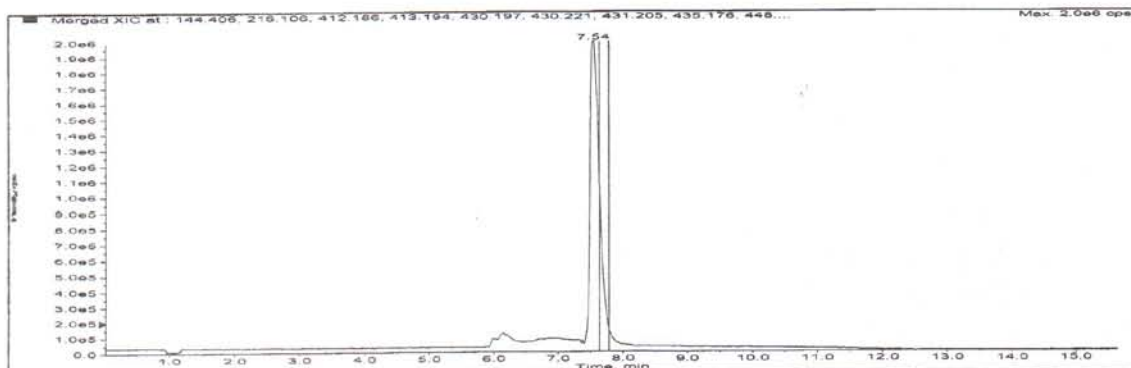
Compound 3c



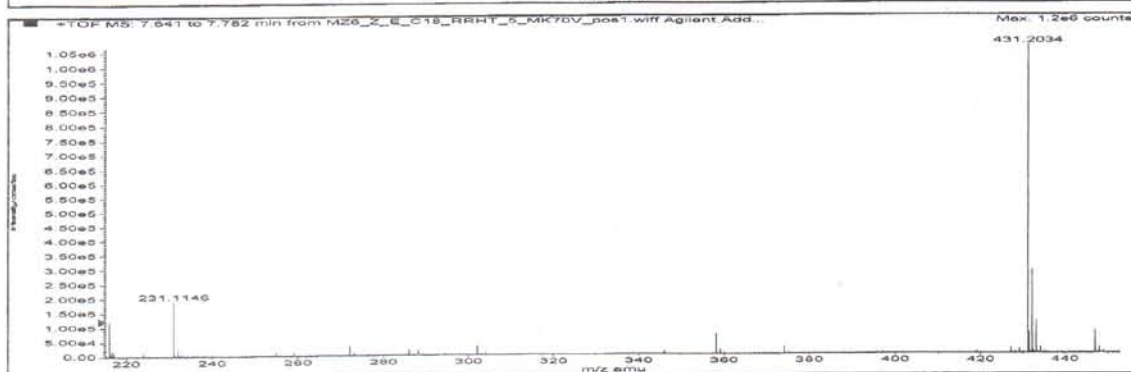
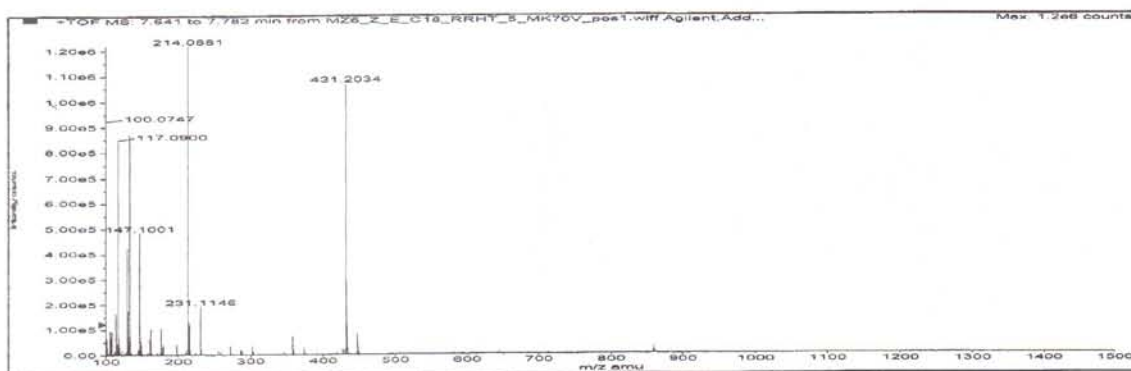


Sample Name: MZ6 Sample Location: P1-C9 Sample Id: Operator: Milka
 Data File Name: D:\PE_Sciex_Data\Projects\Stadici\Data\MZ6_Z-E_C18_RRHT_5_MK70V_pos1.wiff Acq Time: March 24 2014 02:55:59
 PM
 Method: d:\TOF_Data\damethods\Night_Seq_Comp_ident1.an\lfc.xml

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

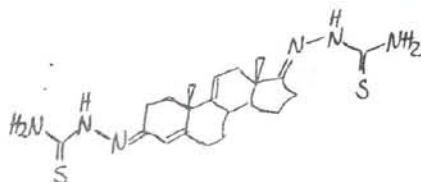


Merged XIC, Period# : 1 Experiment# : 1



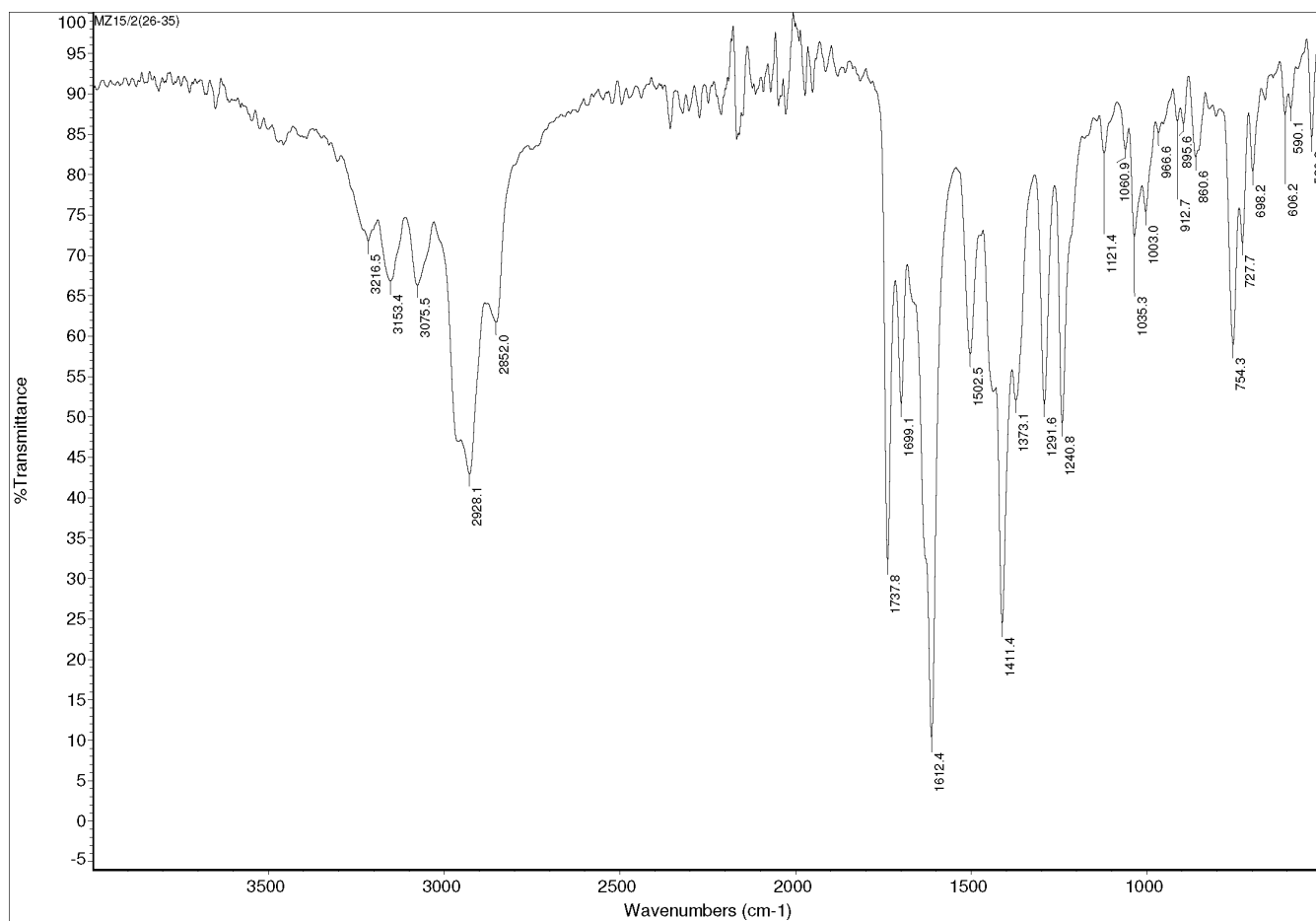
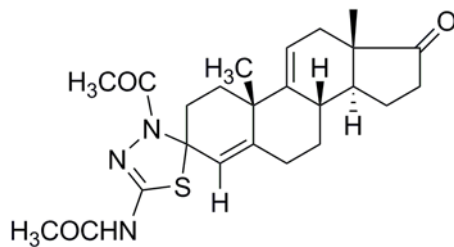
Formula	Compound name	Mass	Peak RT (min)	Peak area	Description
C21H30N6S2	-	430.19734	7.54	1.96986 E7	-

Species	Abundance (counts)	Ion Mass	Measured Mass	Error (mDa)	Error (ppm)	Ret. Time Error (min)
[M+2H] ²⁺	120512.45	216.10594	216.09697	-8.97379	-41.53	
[M+H] ⁺	1105903.79	431.20461	431.20339	-1.22762	-2.85	
[M+NH4] ⁺	22141.87	448.23116	448.20094	-30.22452	-67.44	

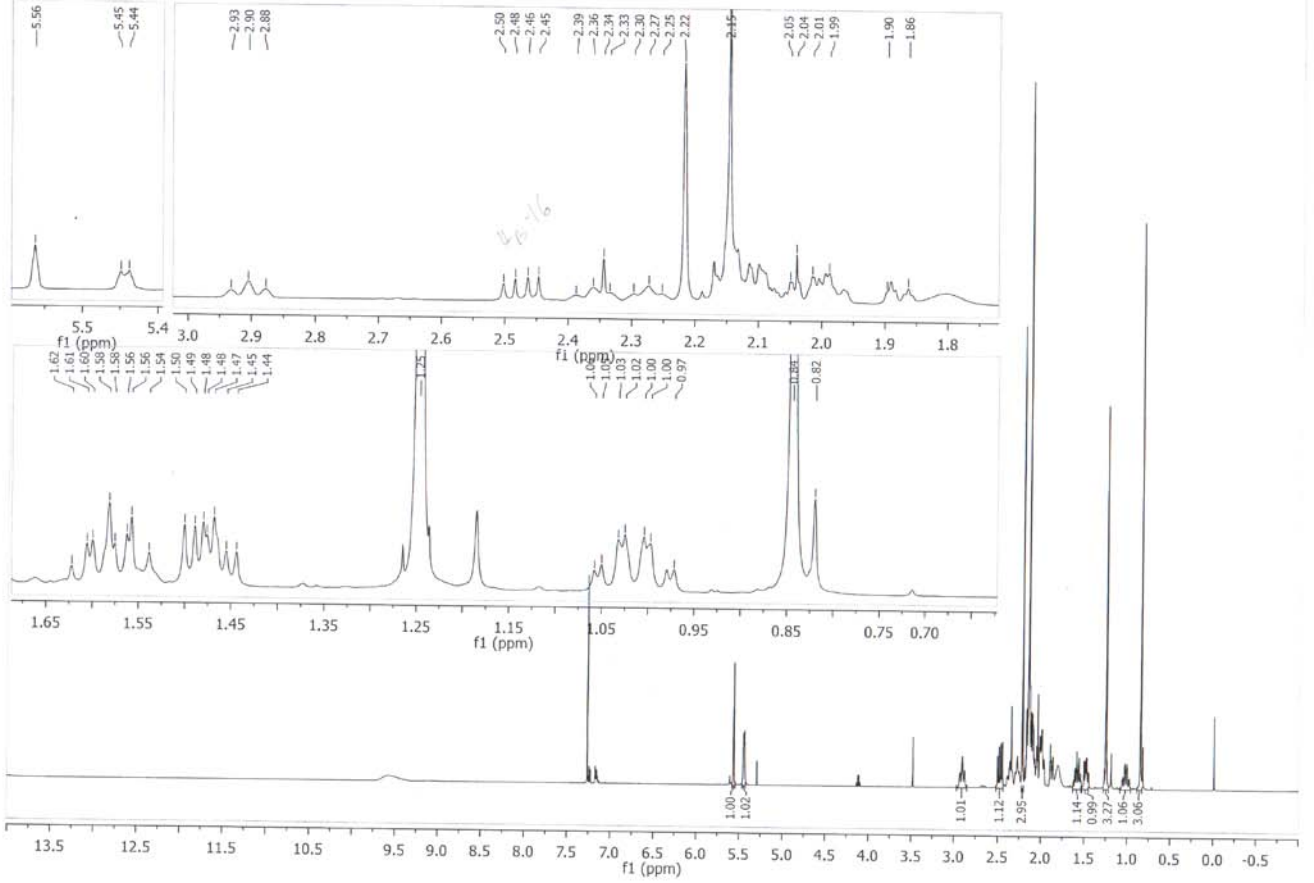


OK, jg

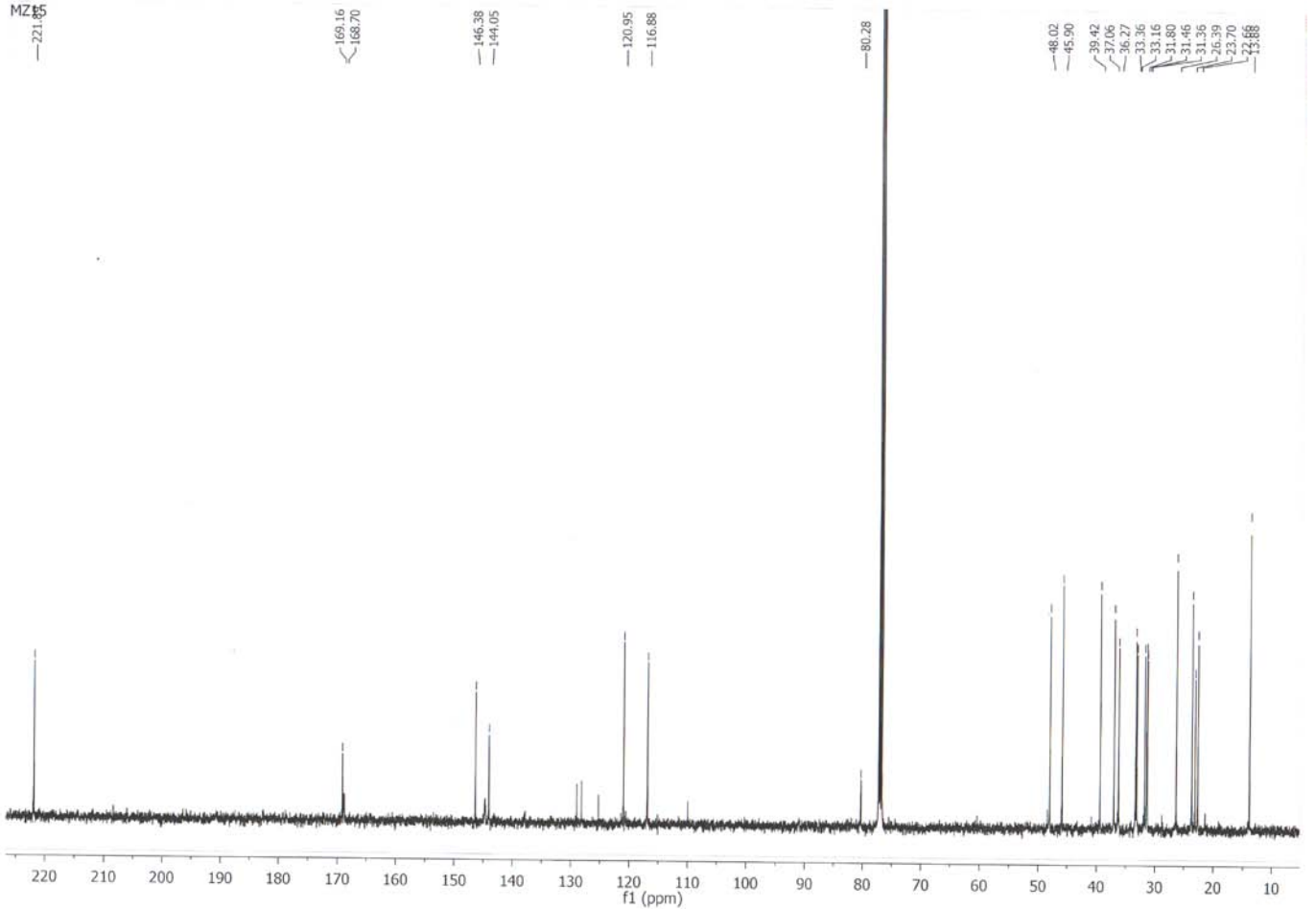
Compound 4c



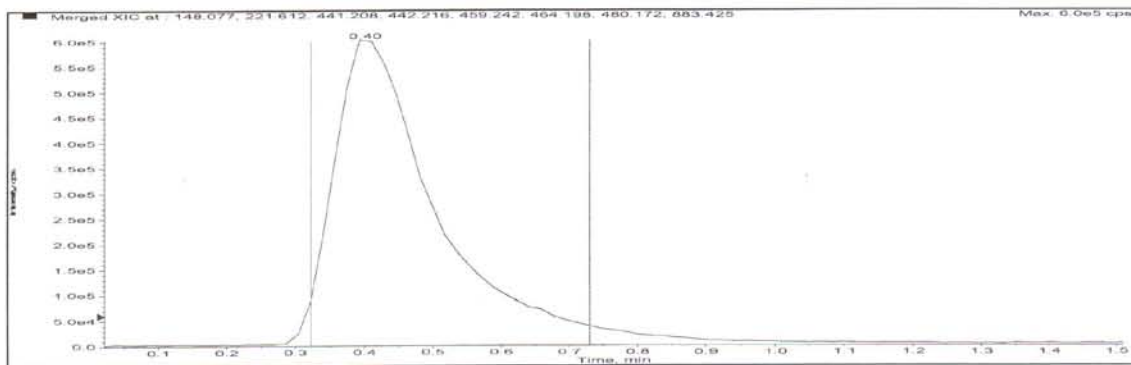
Desktop 11/2/15



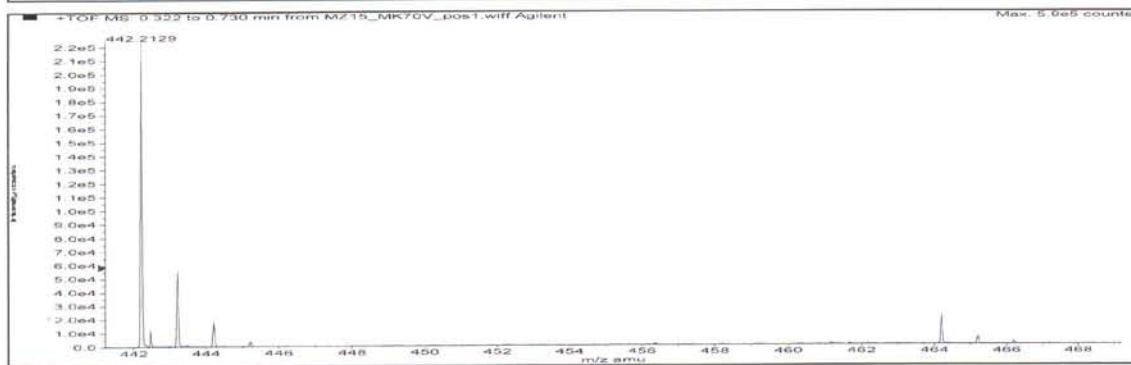
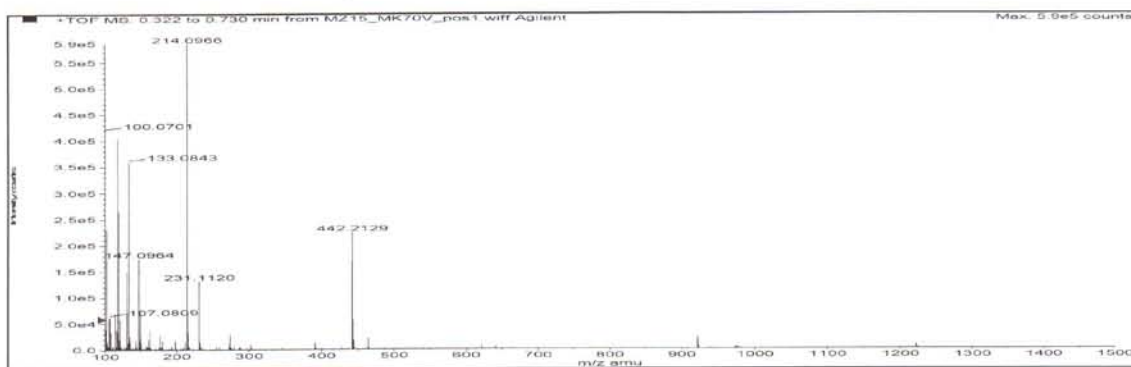
MZ15



Sample Name: MZ15 Sample Location: P1-C5 Sample Id: Operator: Milka
 Data File Name: D:\PE Sclex Data\Projects\Sladic\Data\MZ15_MK70V_pos1.wiff Acq Time: August 05 2014, 11:25:25 AM
 Method: d:\TOF_Data\damethods\Night_Seq_Comp_Ident1.anmlfc.xml



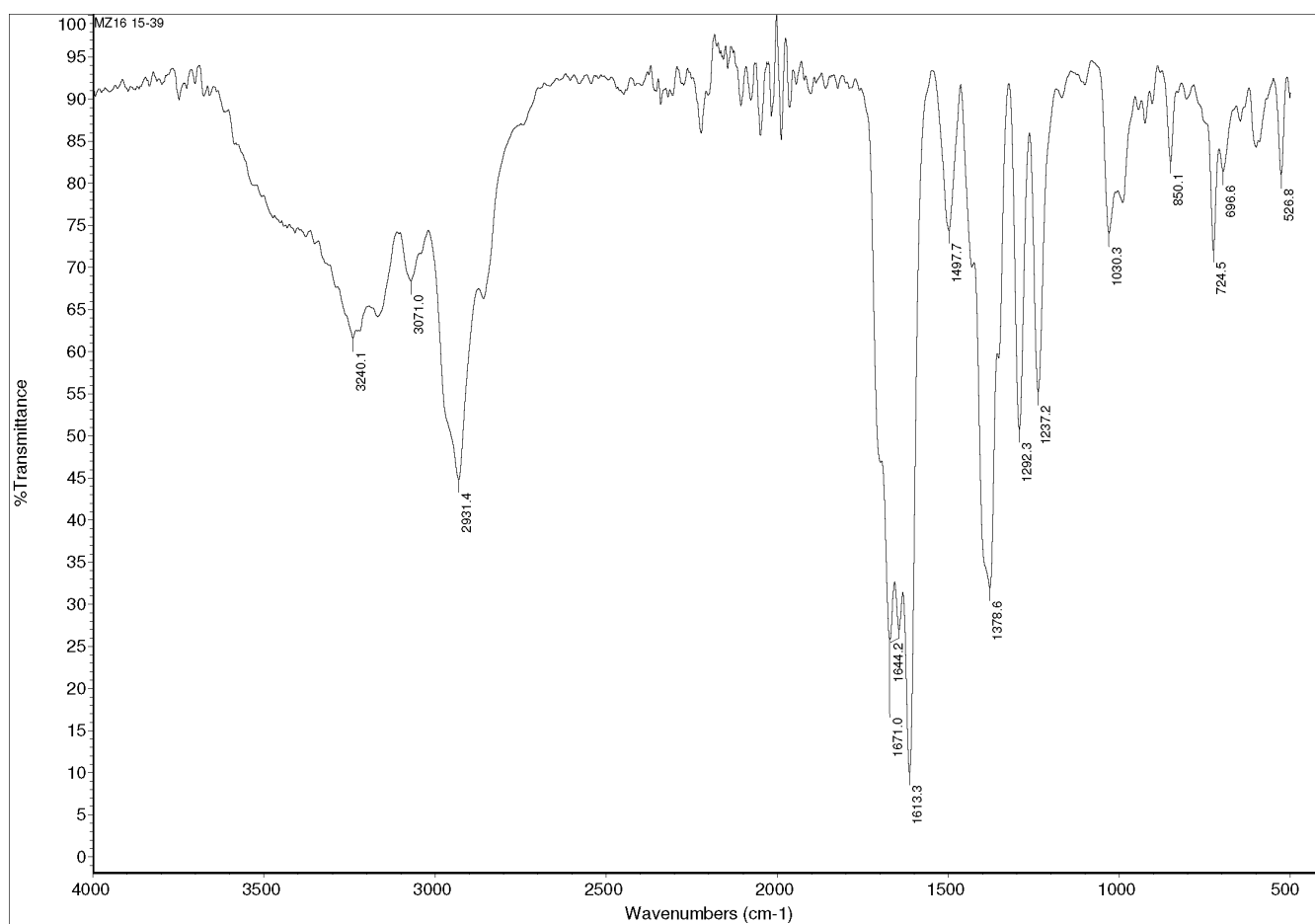
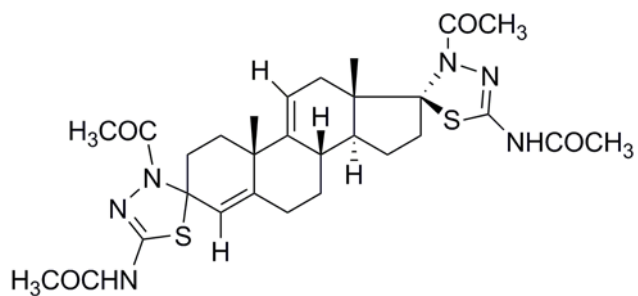
Merged XIC, Period# : 1 Experiment# : 1

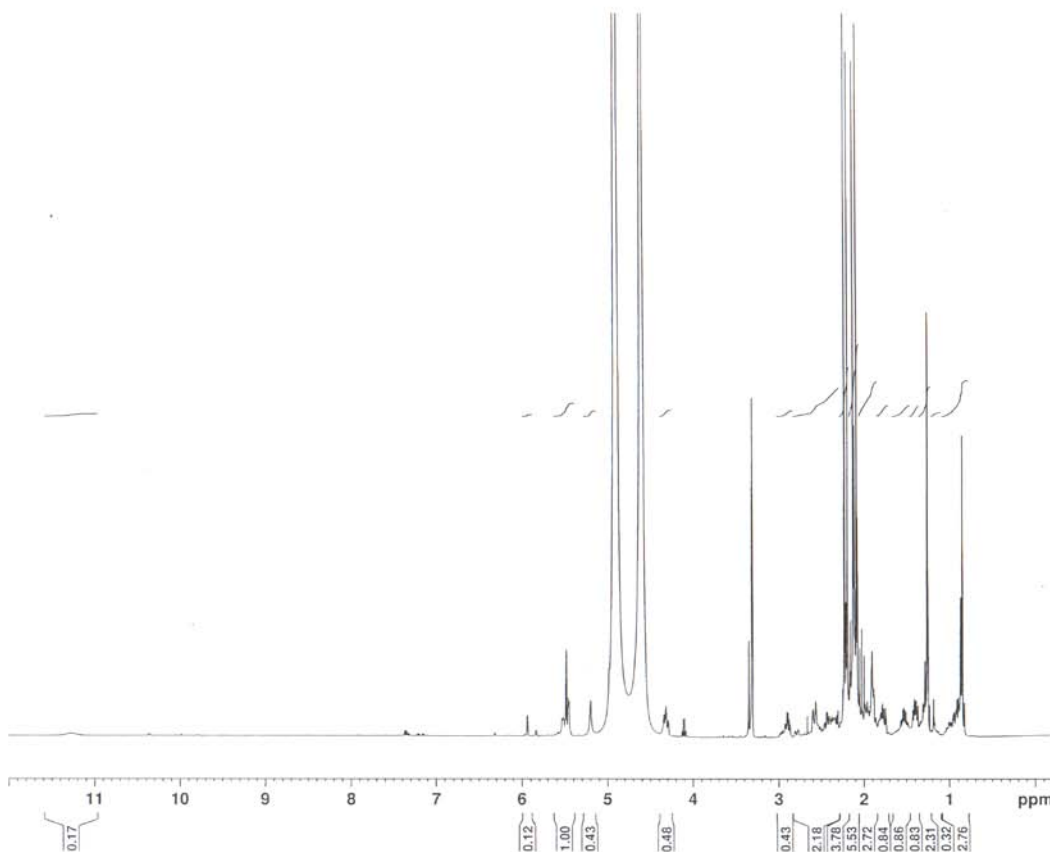


Formula	Compound name	Mass	Peak RT (min)	Peak area	Description
C24H31N3O3S	--	441.20861	0.40	6.26847 E6	--

Species	Abundance (counts)	Ion Mass	Measured Mass	Error (mDa)	Error (ppm)	Ret. Time Error (min)
[M+H] ⁺	224776.54	442.21589	442.21584	-0.04842	-0.11	--
[M+Na] ⁺	21273.69	464.19783	464.19803	0.19545	0.42	--

Compound 5c





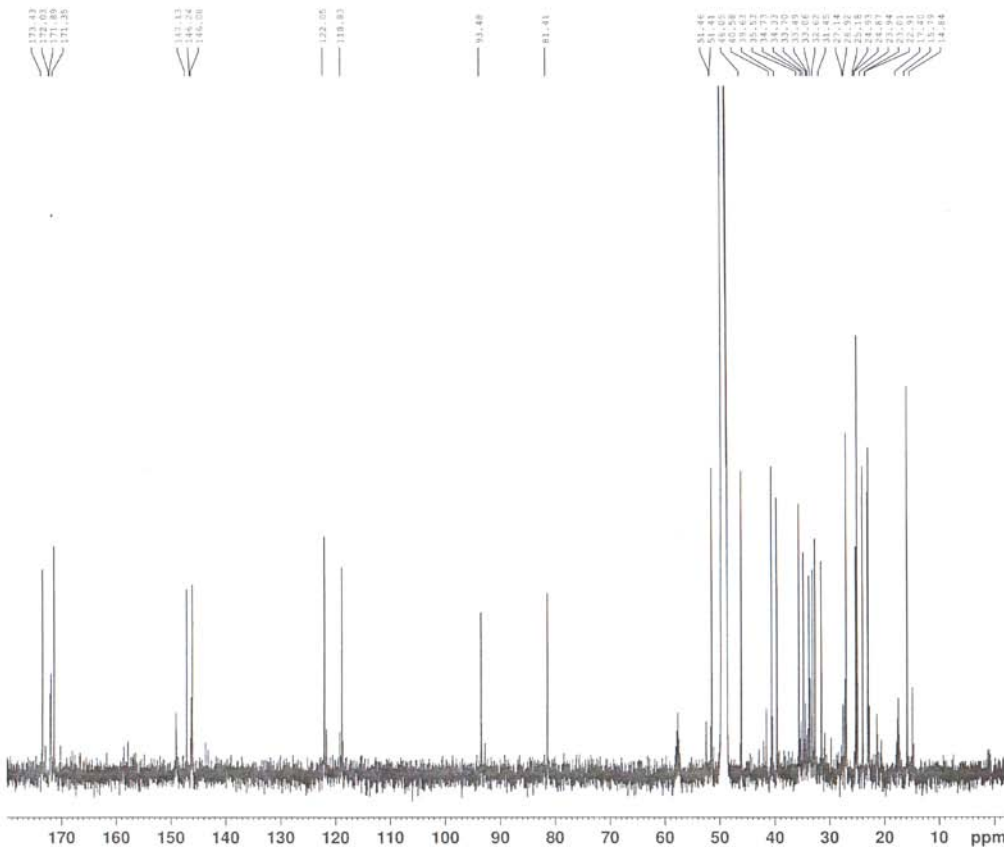
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Current Data Parameters
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EXPNO    1
PROCNO   1

F2 - Acquisition Parameters
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Time     15.19
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PULPROG  zg30
TD        32768
SOLVENT  MeOD
NS        32
DS         0
SWH       6510.417 Hz
FIDRES    0.198462 Hz
AQ        2.5165825 sec
RG         49.3
DW        76.800 usec
DE         6.50 usec
TE        298.0 K
D1        2.0000000 sec
TD0       1

----- CHANNEL f1 -----
SF01     500.2630115 MHz
NUC1      1H
P1        9.35 usec
PLW1     27.379999516 W

F2 - Processing parameters
SI        32768
SF        500.2600000 MHz
WDW       EM
SSB       0
LB        0.20 Hz
GB        0
FC        1.00
  
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```

Current Data Parameters
NAME      MZ16
EXPNO    6
PROCNO   1

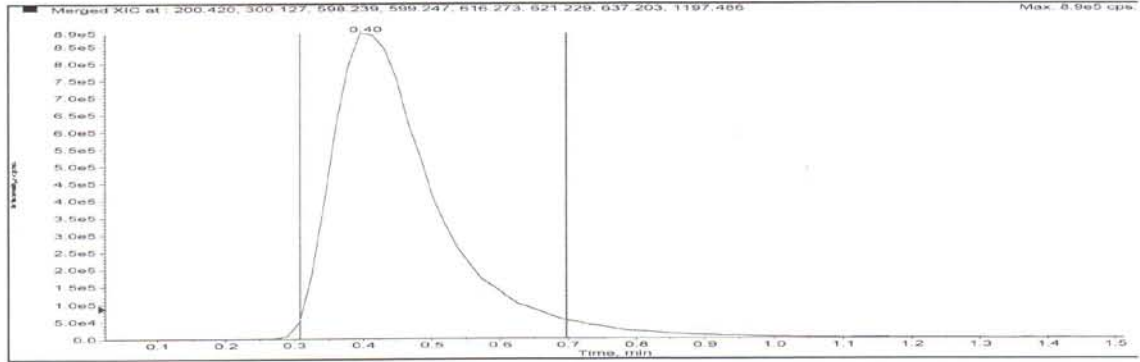
F2 - Acquisition Parameters
Date_    20140625
Time     7.59
INSTRUM  spect
PROBHD   5 mm BBO BB-1H
PULPROG  zgpg30
TD        32768
SOLVENT  MeOD
NS        3267
DS         4
SWH       32894.738 Hz
FIDRES    1.003868 Hz
AQ        0.4980736 sec
RG         1030
DW        15.200 usec
DE         6.50 usec
TE        298.0 K
D1        2.0000000 sec
D11       0.0300000 sec
TD0       1

----- CHANNEL f1 -----
SF01     125.8055719 MHz
NUC1      13C
P1        11.50 usec
PLW1     32.22800064 W

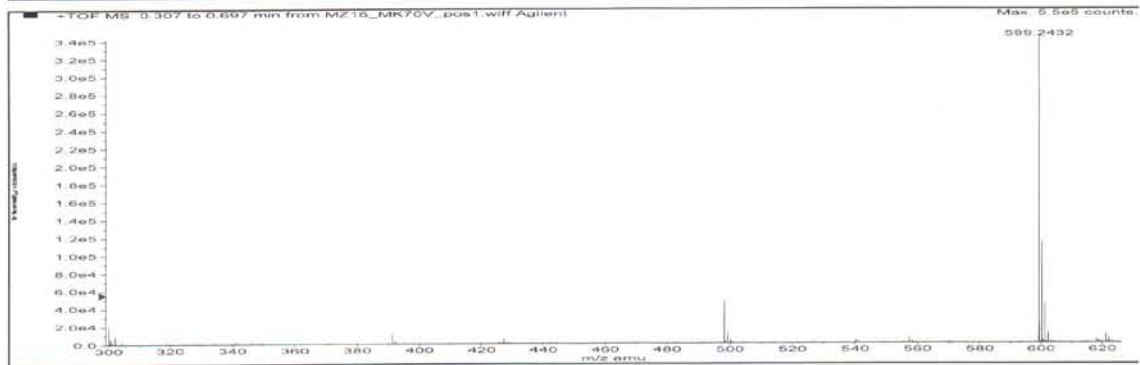
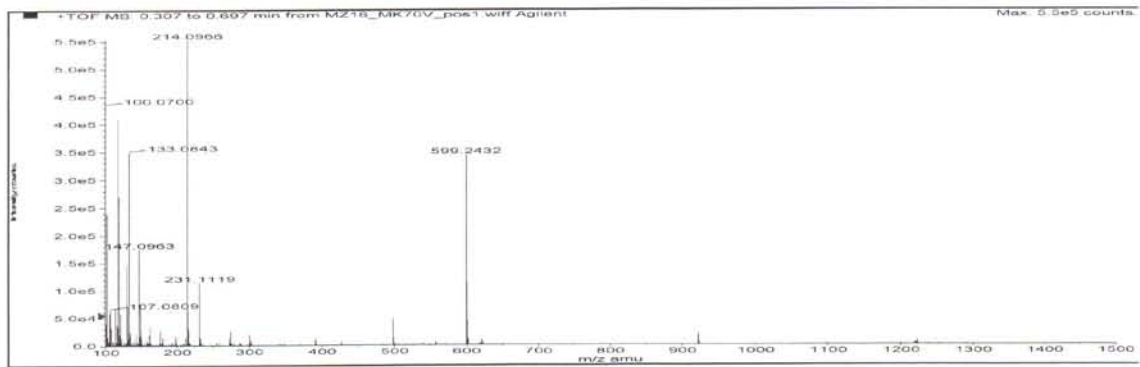
----- CHANNEL f2 -----
SF02     500.2630116 MHz
NUC2      1H
CPDPRG12 waltz16
PCPD2    80.00 usec
PLW2     20.77000046 W
PLW12    0.39267001 W
PLW13    0.25130999 W

F2 - Processing parameters
SI        32768
SF        125.7902882 MHz
WDW       EM
SSB       0
LB        1.50 Hz
GB        0
FC        1.40
  
```

Sample Name: MZ16 Sample Location: P1-C6 Sample Id: Operator: Milka
 Data File Name: D:\PE_Sciex_Data\Projects\Sladic\Data\MZ16_MK70V_pos1.wiff Acq Time: August 05 2014, 11:27:55 AM
 Method: d:\TOF_Data\damethods\Night_Seq_Comp_ident1.anmlfc.xml



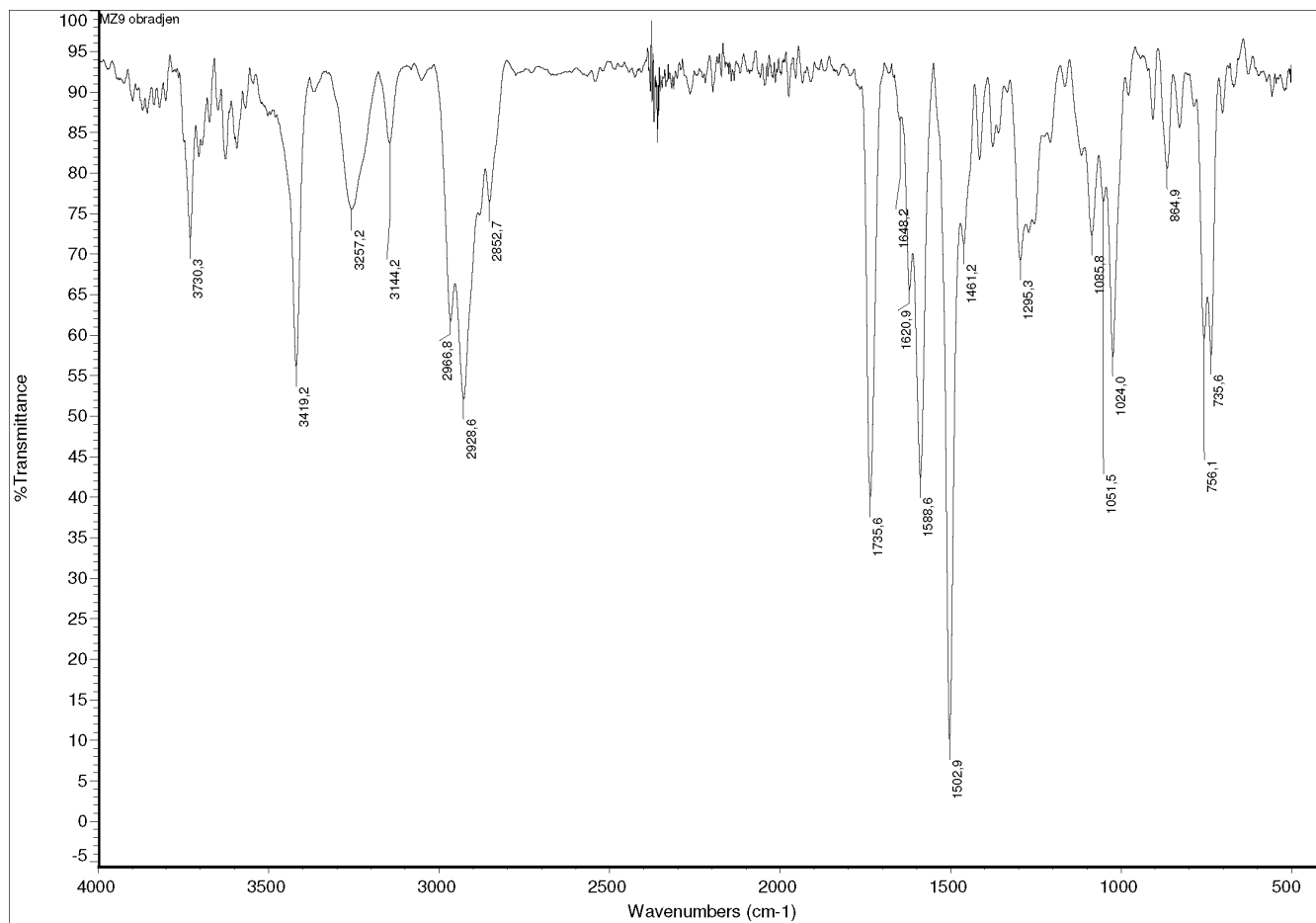
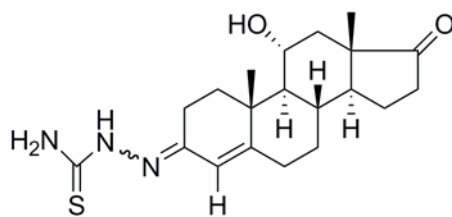
Merged XIC, Period# : 1 Experiment# : 1

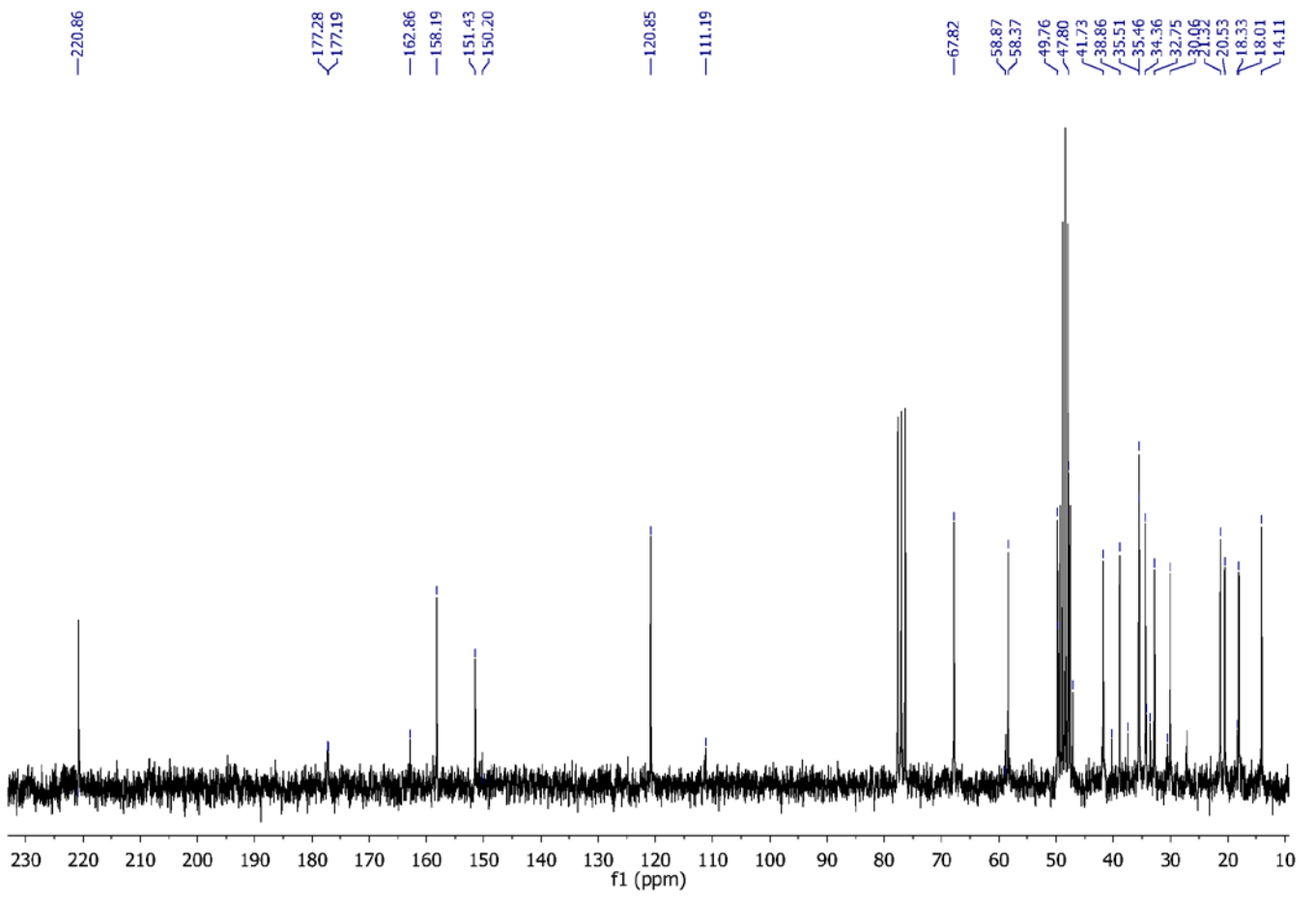
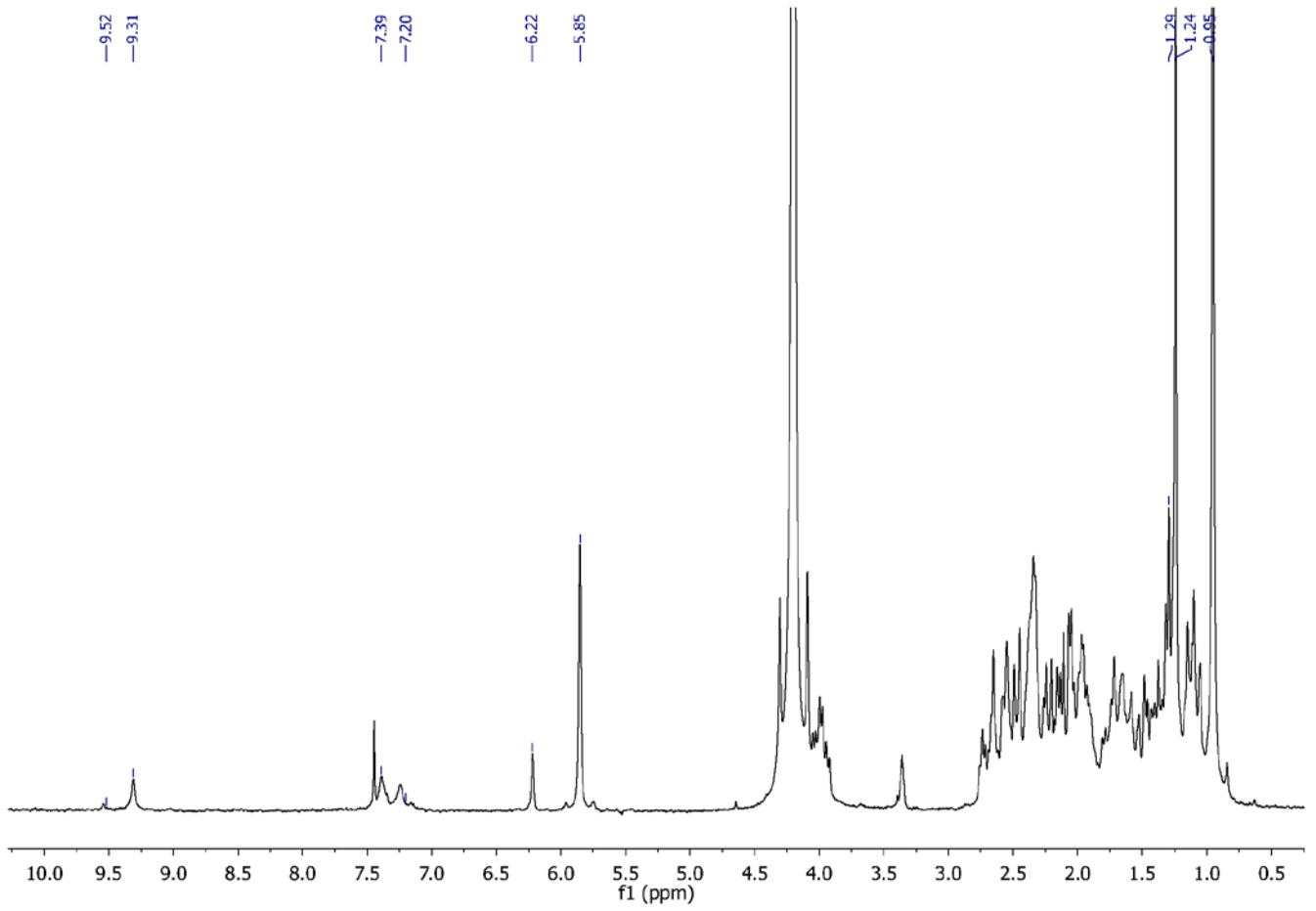


Formula	Compound name	Mass	Peak RT (min)	Peak area	Description
C29H38N6O4S2	--	598.23960	0.40	9.30051 E6	--

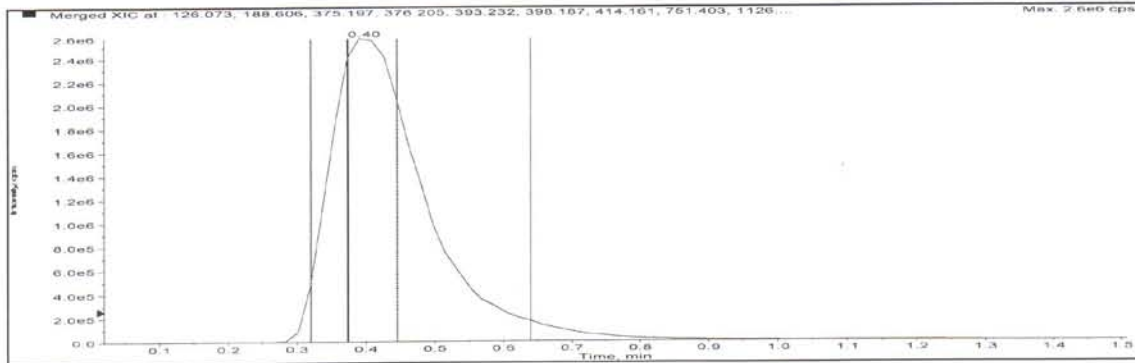
Species	Abundance (counts)	Ion Mass	Measured Mass	Error (mDa)	Error (ppm)	Ret. Time Error (min)
[M+2H] ²⁺	20361.33	300.12707	300.12731	0.23612	0.79	--
[M+H] ⁺	344152.86	599.24687	599.24660	-0.27645	-0.46	--
[M+Na] ⁺	11180.87	621.22882	621.22859	-0.22286	-0.36	--

Compound 2d

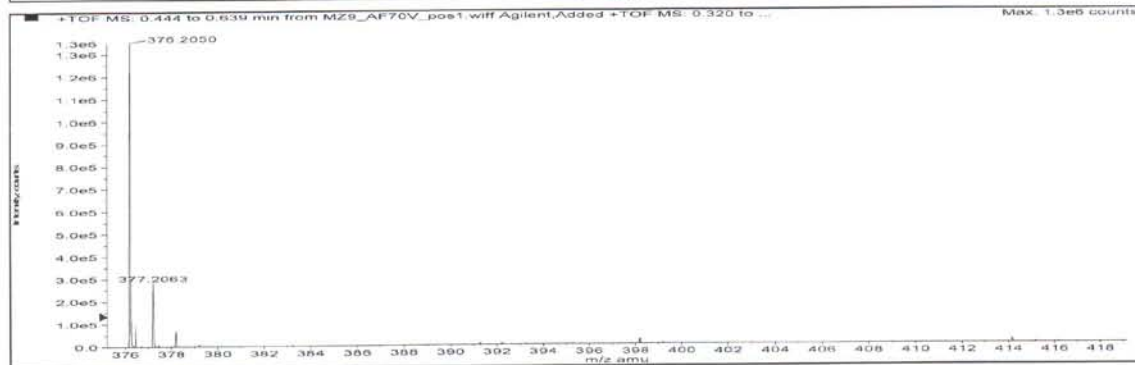
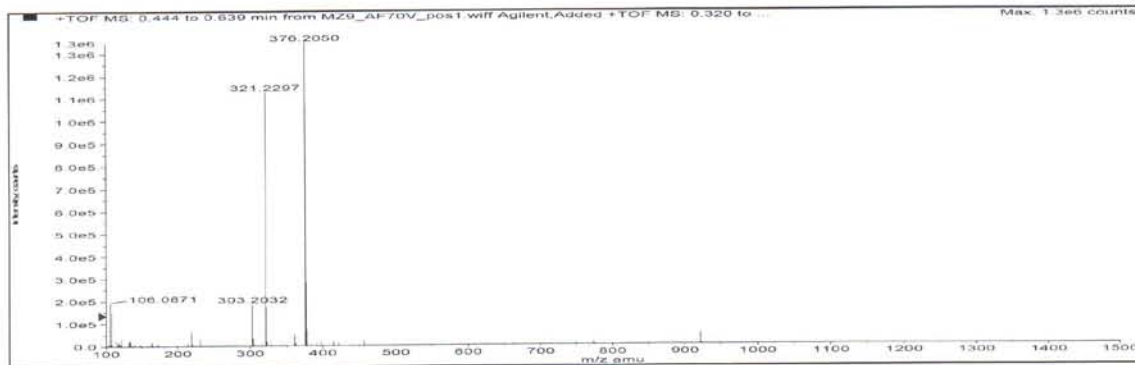




Sample Name: MZ9 Sample Location: P1-D1 Sample Id: Operator: Milka
 Data File Name: D:\PE_Sciex_Data\Projects\SladiciData\MZ9_AF70V_pos1.wiff Acq Time: May 07 2015, 11:21:01 AM
 Method: d:\TOF_Data\methods\Night_Seq_Comp_ident1.an\lefc.xml



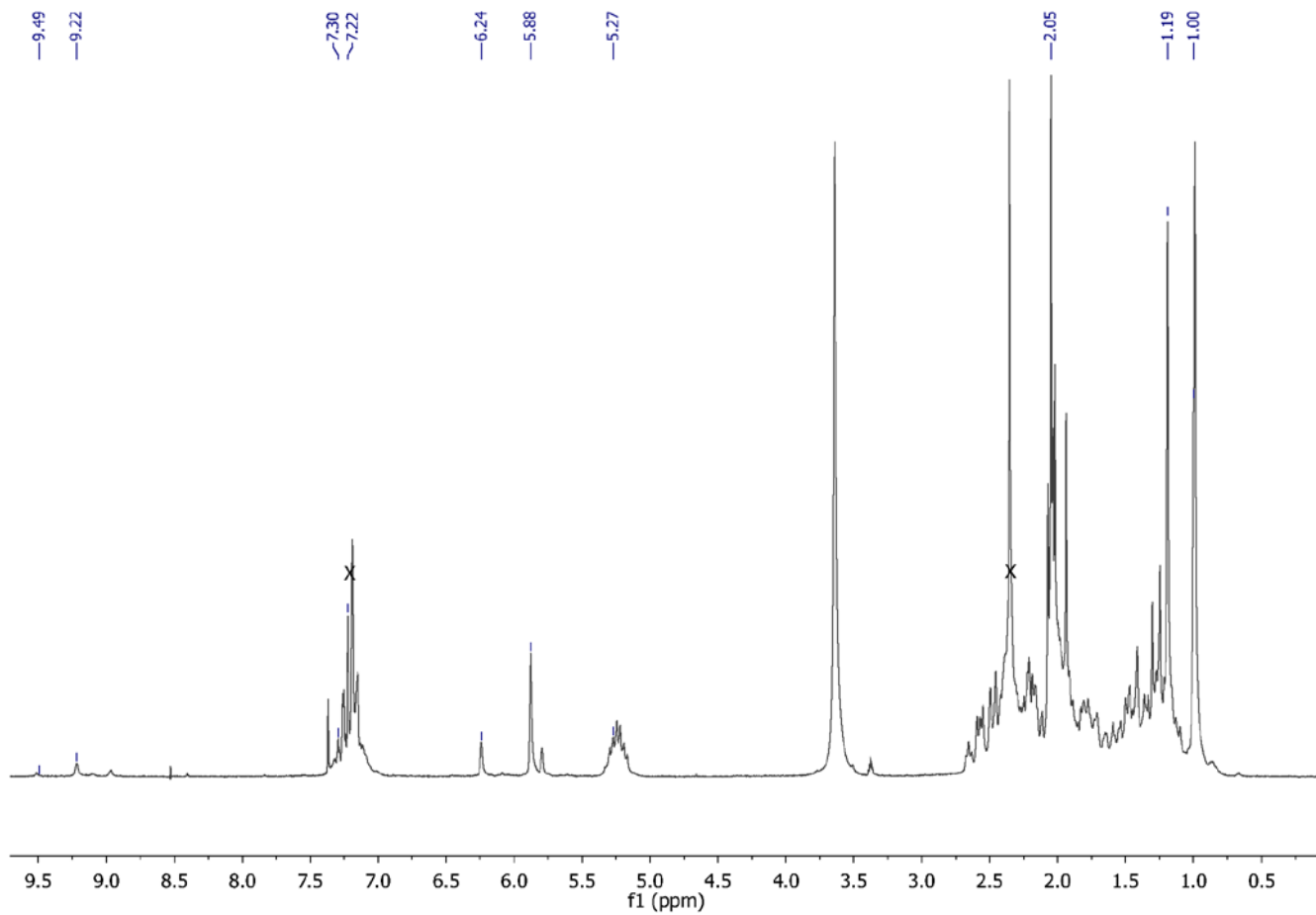
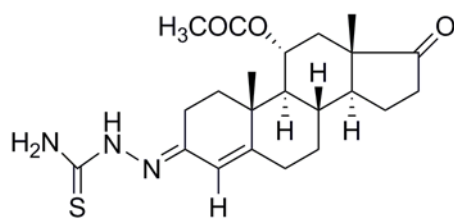
Merged XIC, Period# : 1 Experiment# : 1



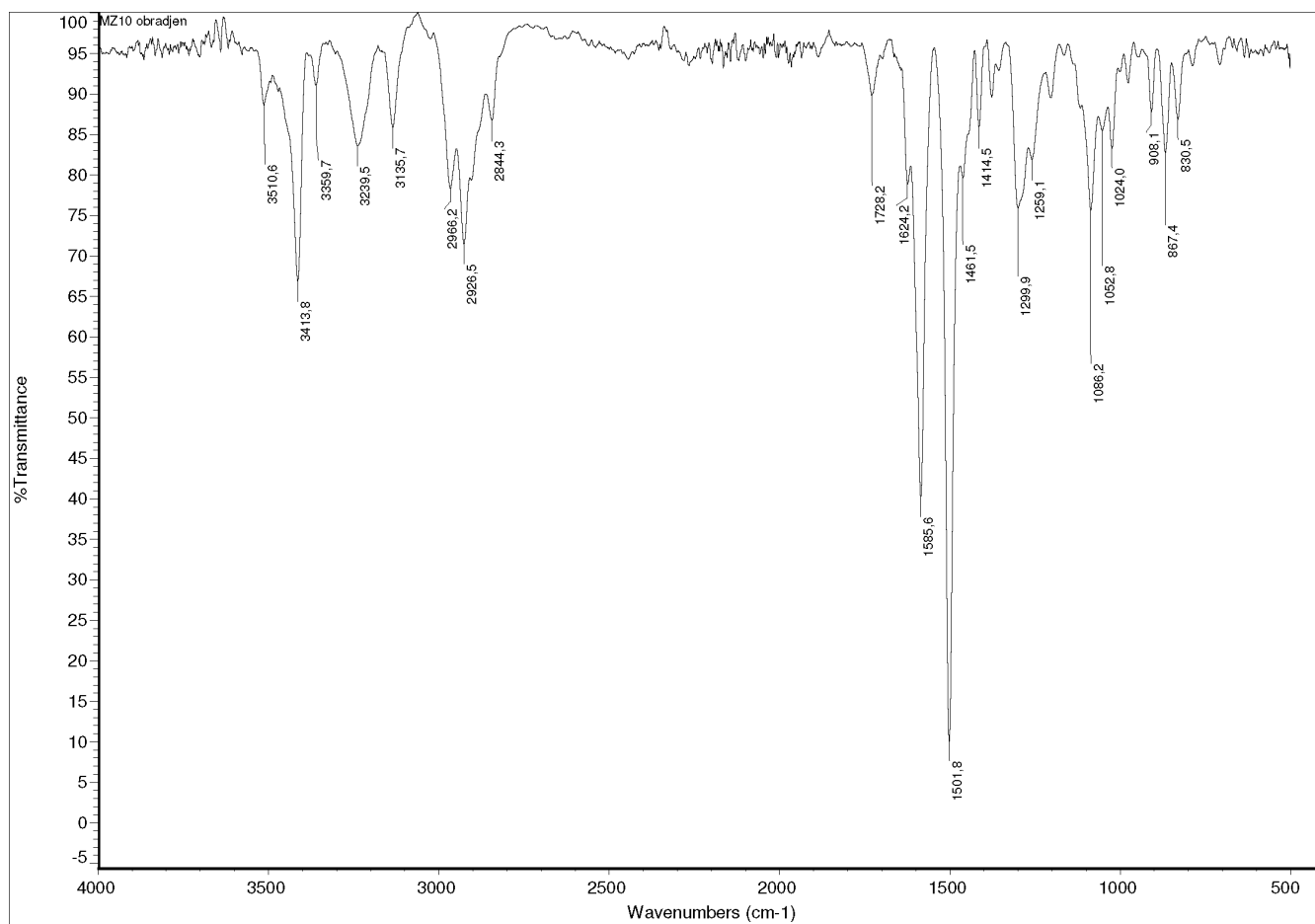
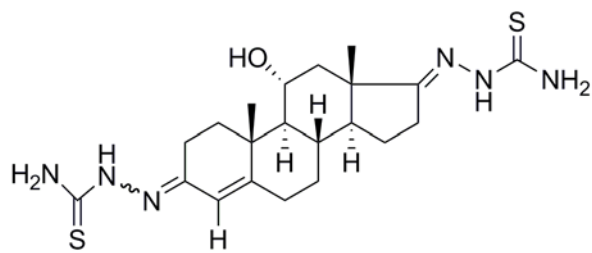
Formula	Compound name	Mass	Peak RT (min)	Peak area	Description
C ₂₀ H ₂₉ N ₃ O ₂ S	--	375.19805	0.40	2.45542 E7	--

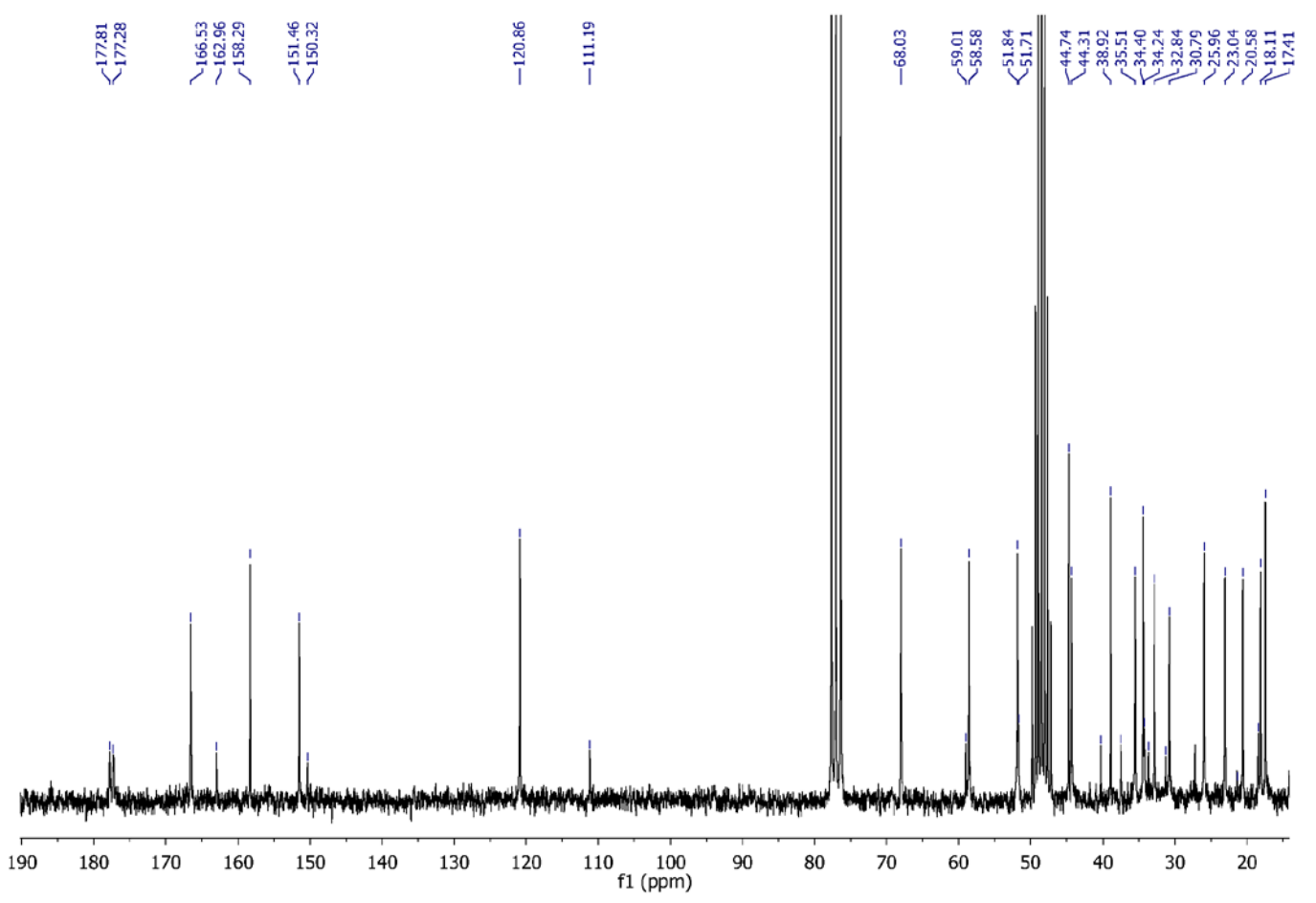
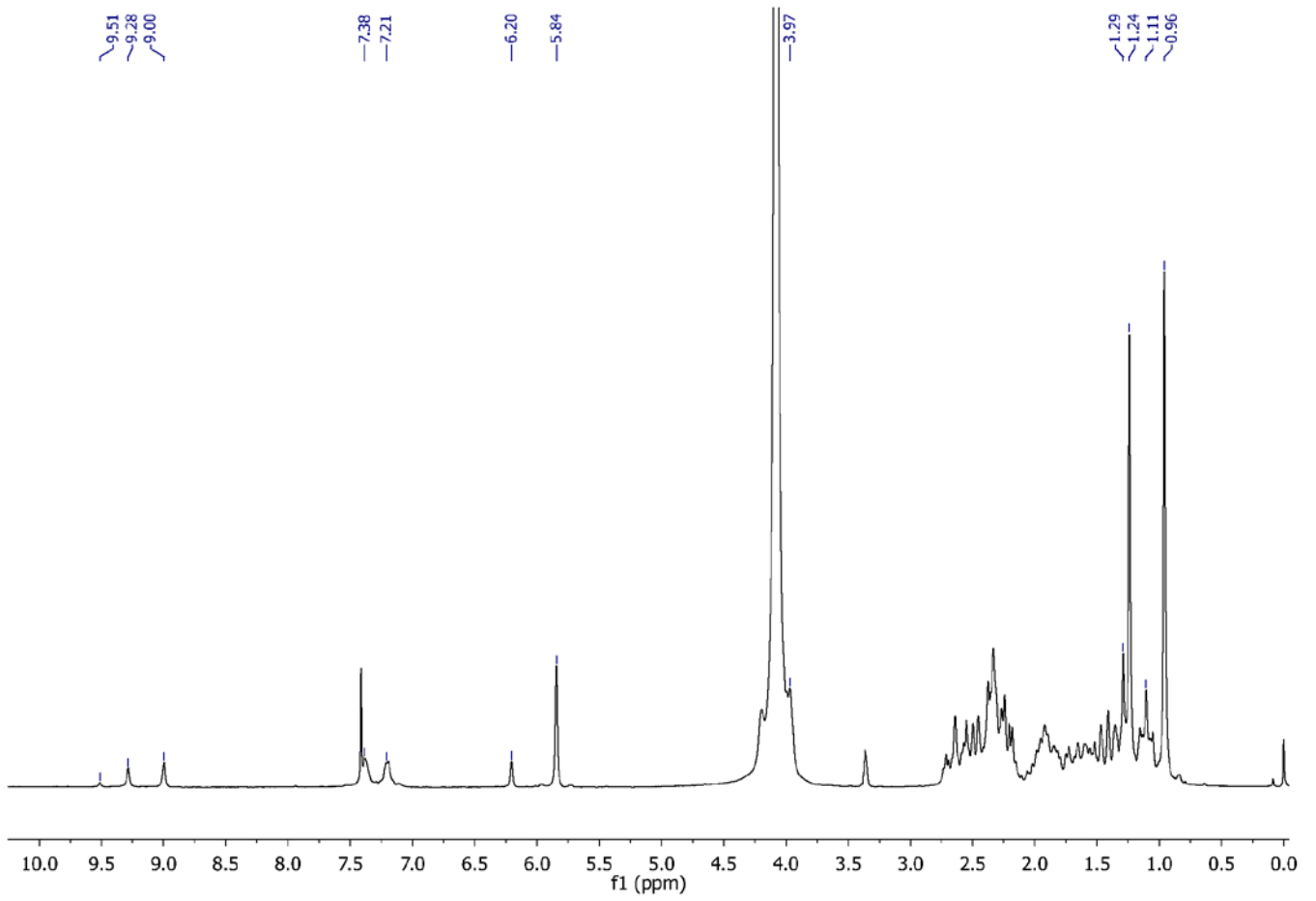
Species	Abundance (counts)	Ion Mass	Measured Mass	Error (mDa)	Error (ppm)	Ret. Time Error (min)
[M+H] ⁺	1349547.36	376.20532	376.20446	-0.86587	-2.30	--
[M+Na] ⁺	22984.79	398.18727	398.18694	-0.33013	-0.83	--
[M+K] ⁺	14207.43	414.16121	414.16159	0.37987	0.92	--

Compound 2d-OAc

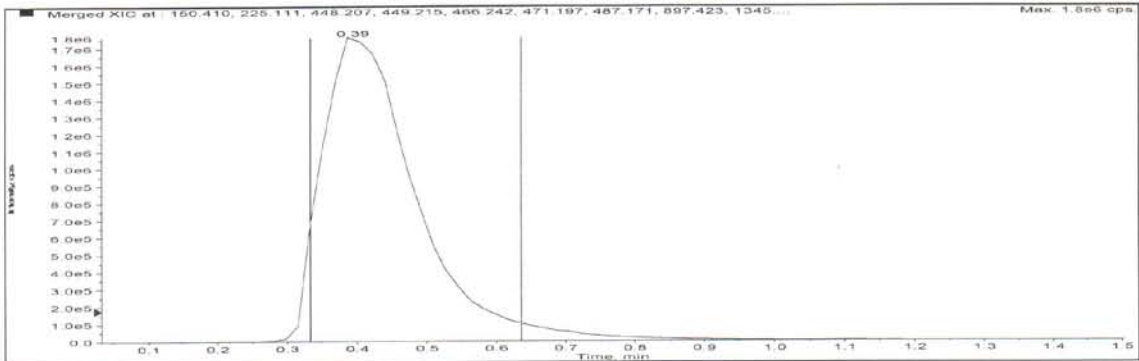


Compound 3d

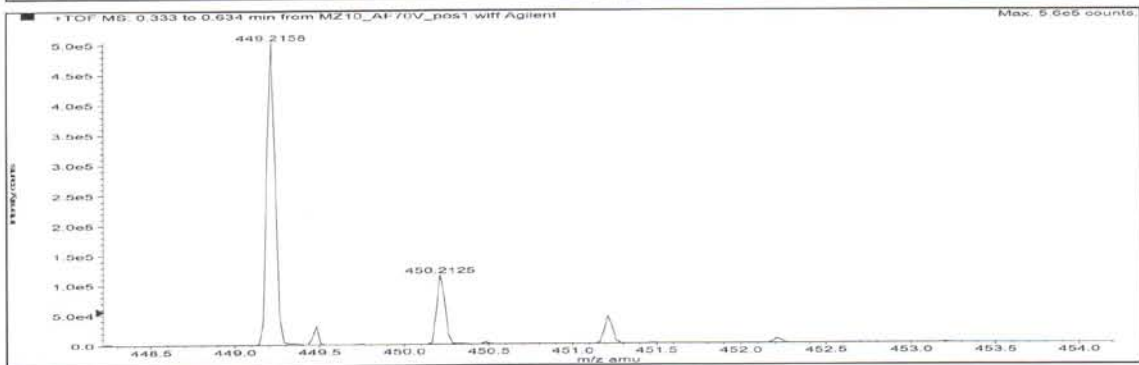
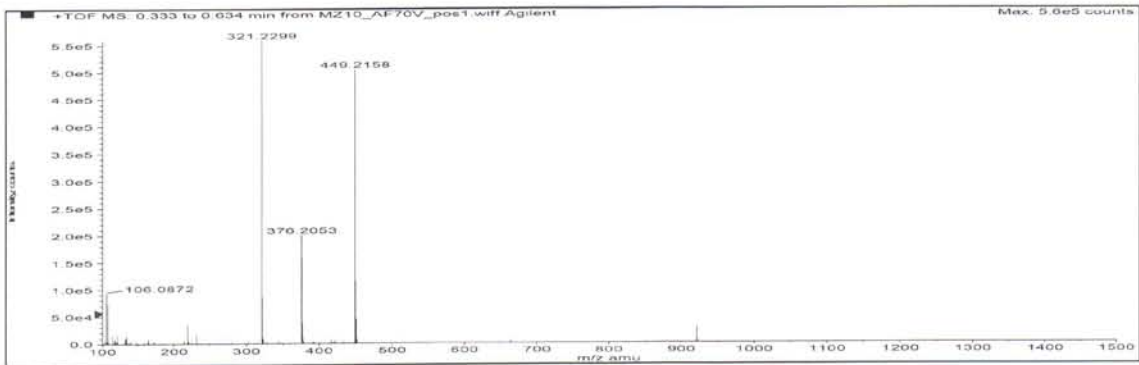




Sample Name: MZ10 Sample Location: P1-D2 Sample Id: Operator: Milka
 Data File Name: D:\PE Sciex Data\Projects\Sladic\Data\MZ10_AF70V_pos1.wiff Acq Time: May 07 2015, 11:23:36 AM
 Method: d:\TOF_Data\damethods\Night_Seq_Comp_ident1.anm\efc.xml

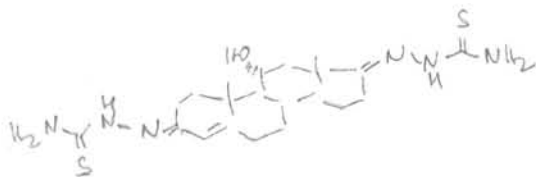


Merged XIC, Period# : 1 Experiment# : 1

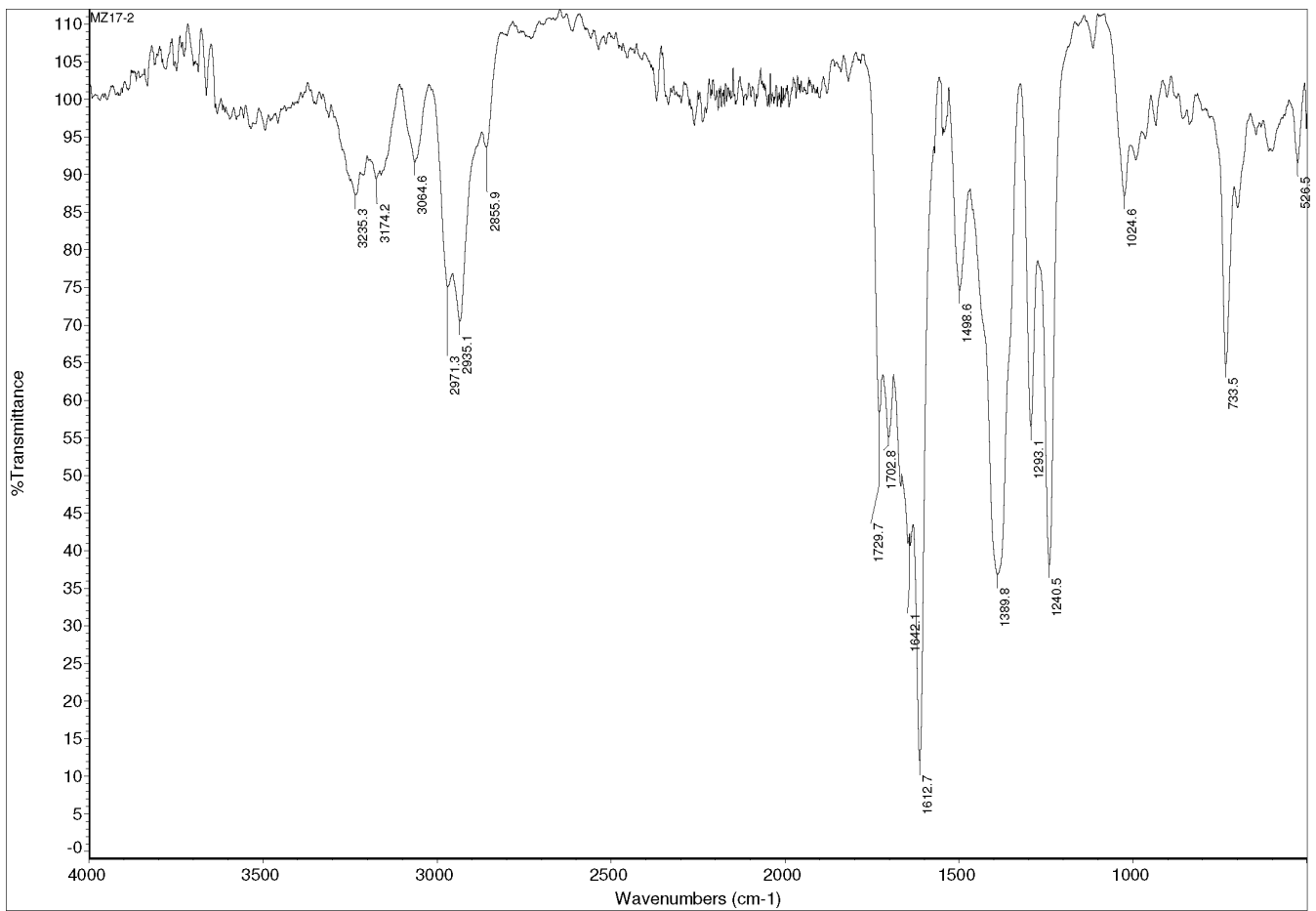
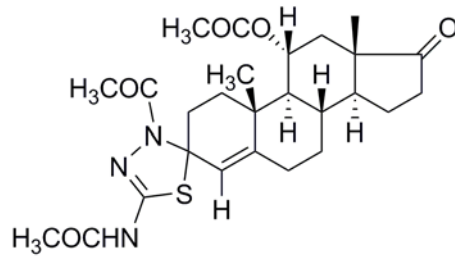


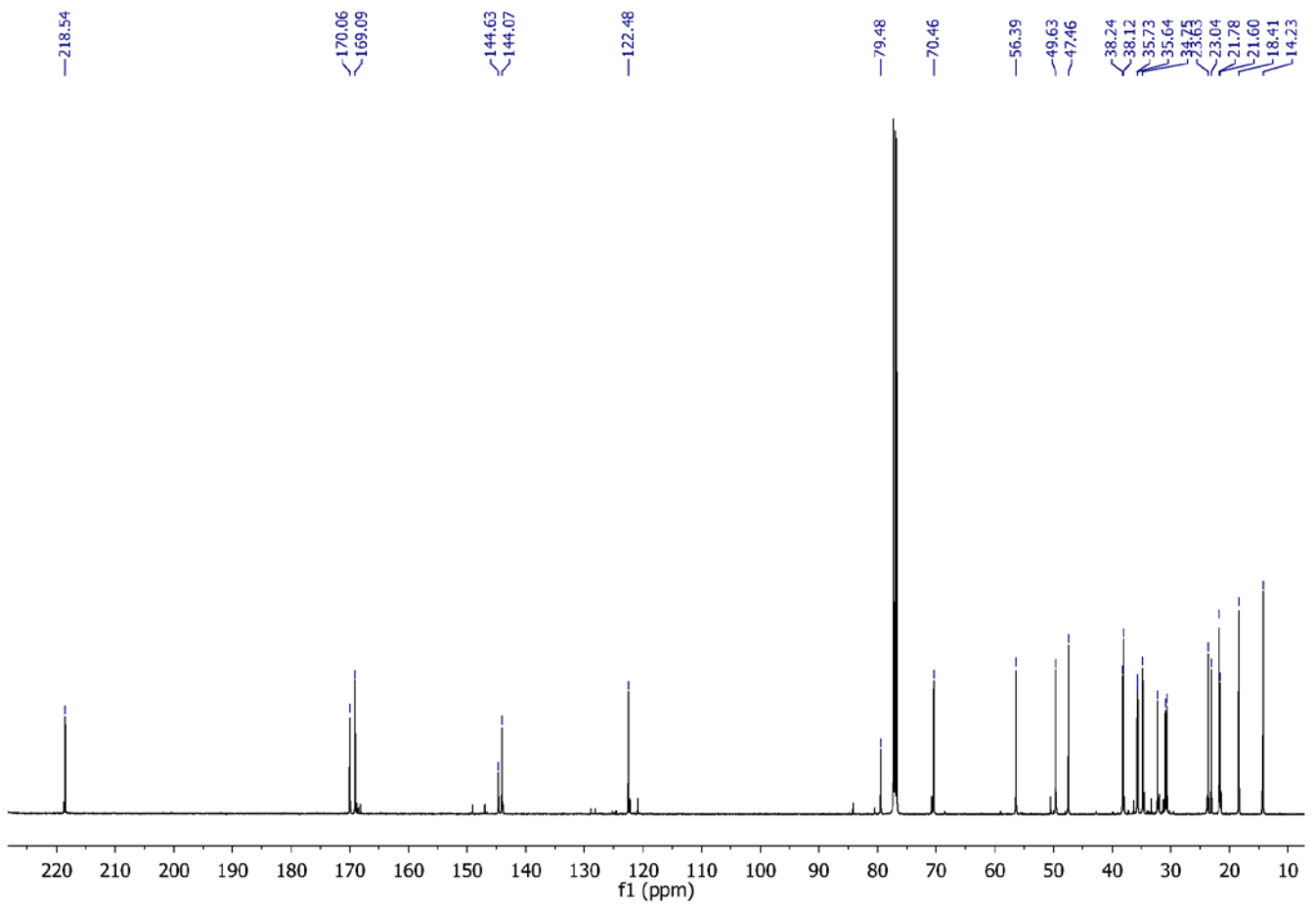
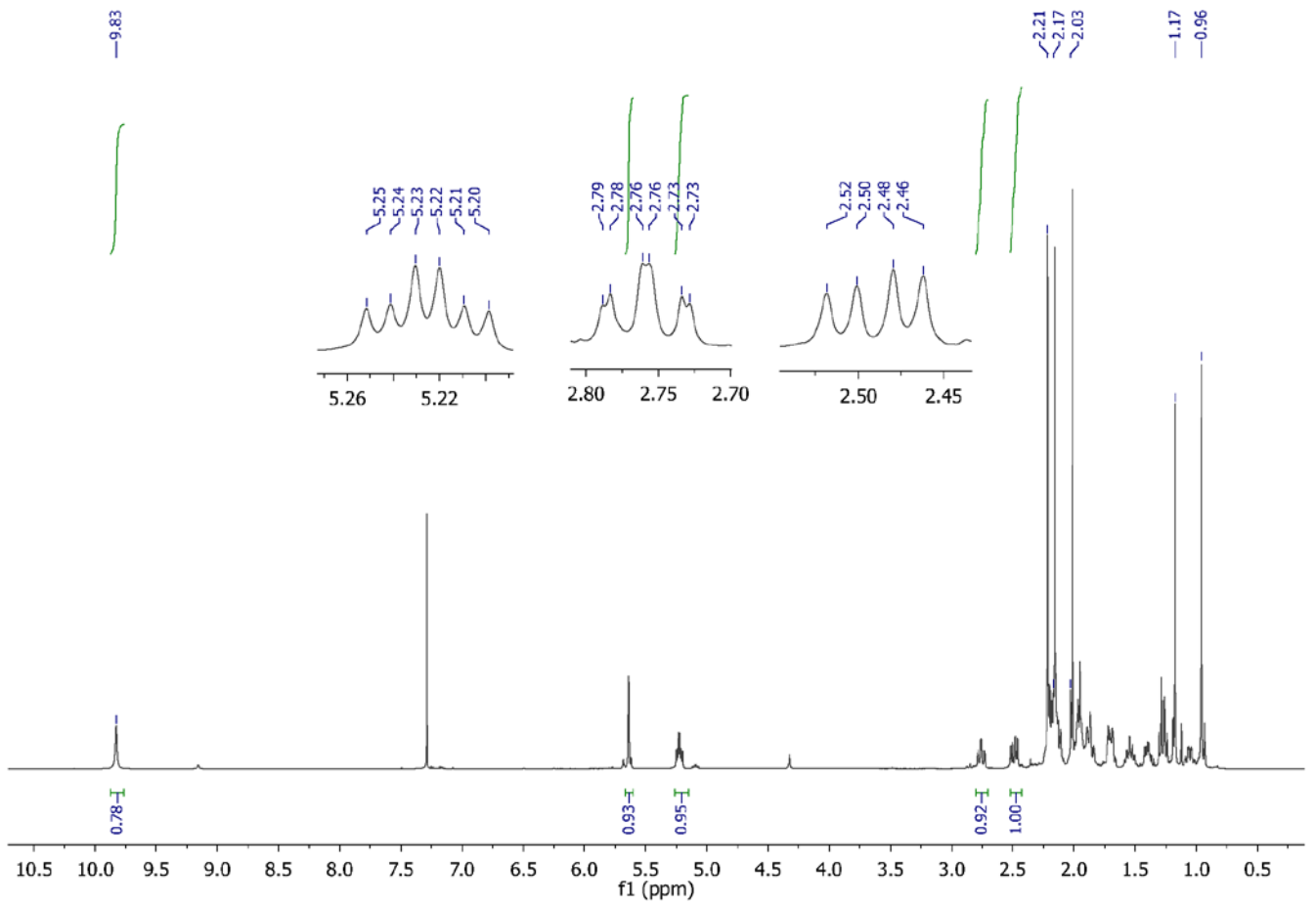
Formula	Compound name	Mass	Peak RT (min)	Peak area	Description
C21H32N6OS2	-	448.20790	0.39	1.63724 E7	--

Species	Abundance (counts)	Ion Mass	Measured Mass	Error (mDa)	Error (ppm)	Ret. Time Error (min)
[M+H] ⁺	505028.62	449.21518	449.21447	-0.70987	-1.58	--

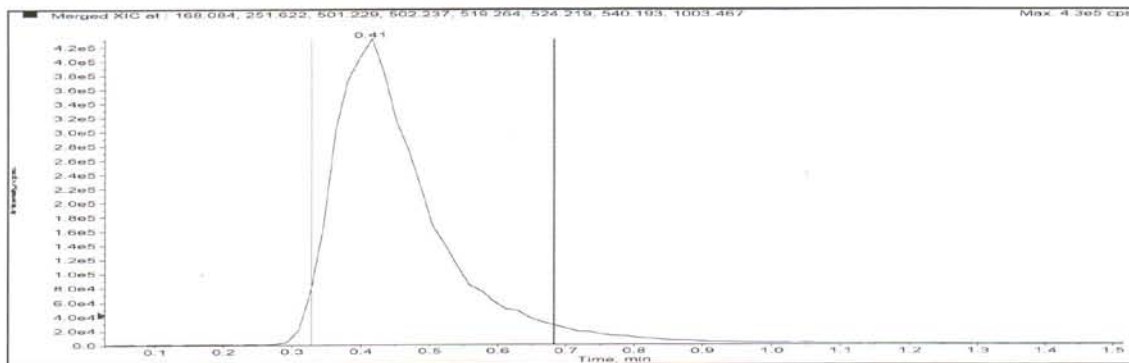


Compound 4d-OAc

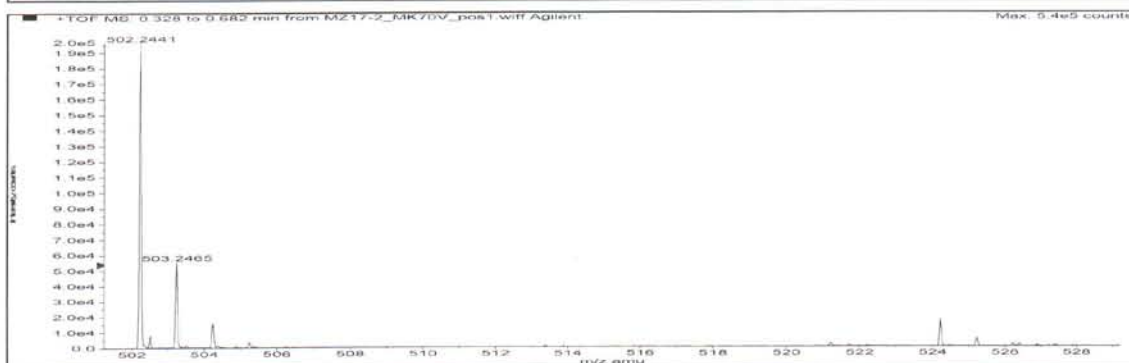
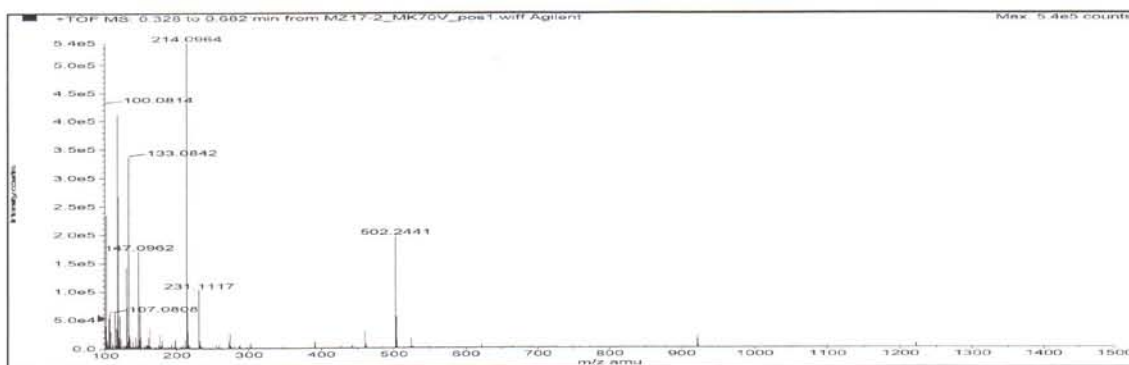




Sample Name: MZ17-2 Sample Location: P1-C7 Sample Id: Operator: Milka
 Data File Name: D:\PE Sciex Data\Projects\Sladic\Data\MZ17-2_MK70V_pos1.wiff Acq Time: August 05 2014, 11:30:24 AM
 Method: d:\TOF_Data\damethods\Night_Seq_Comp_ident1.an\lfe.c.xml

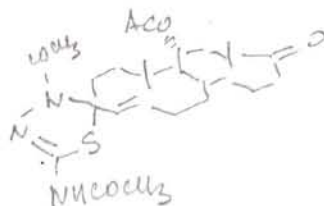


Merged XIC, Period# : 1 Experiment# : 1

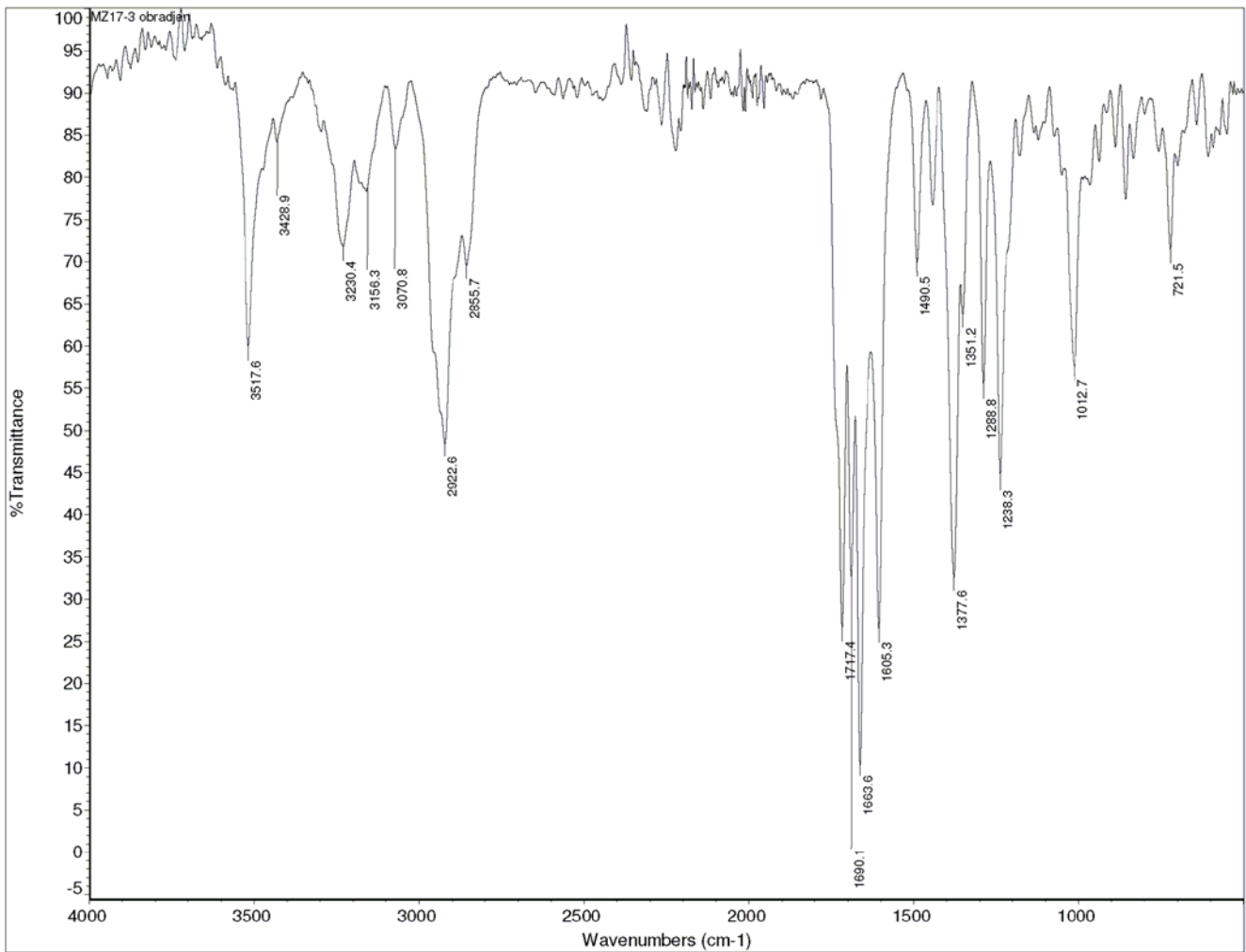
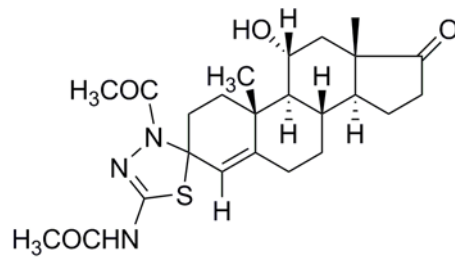


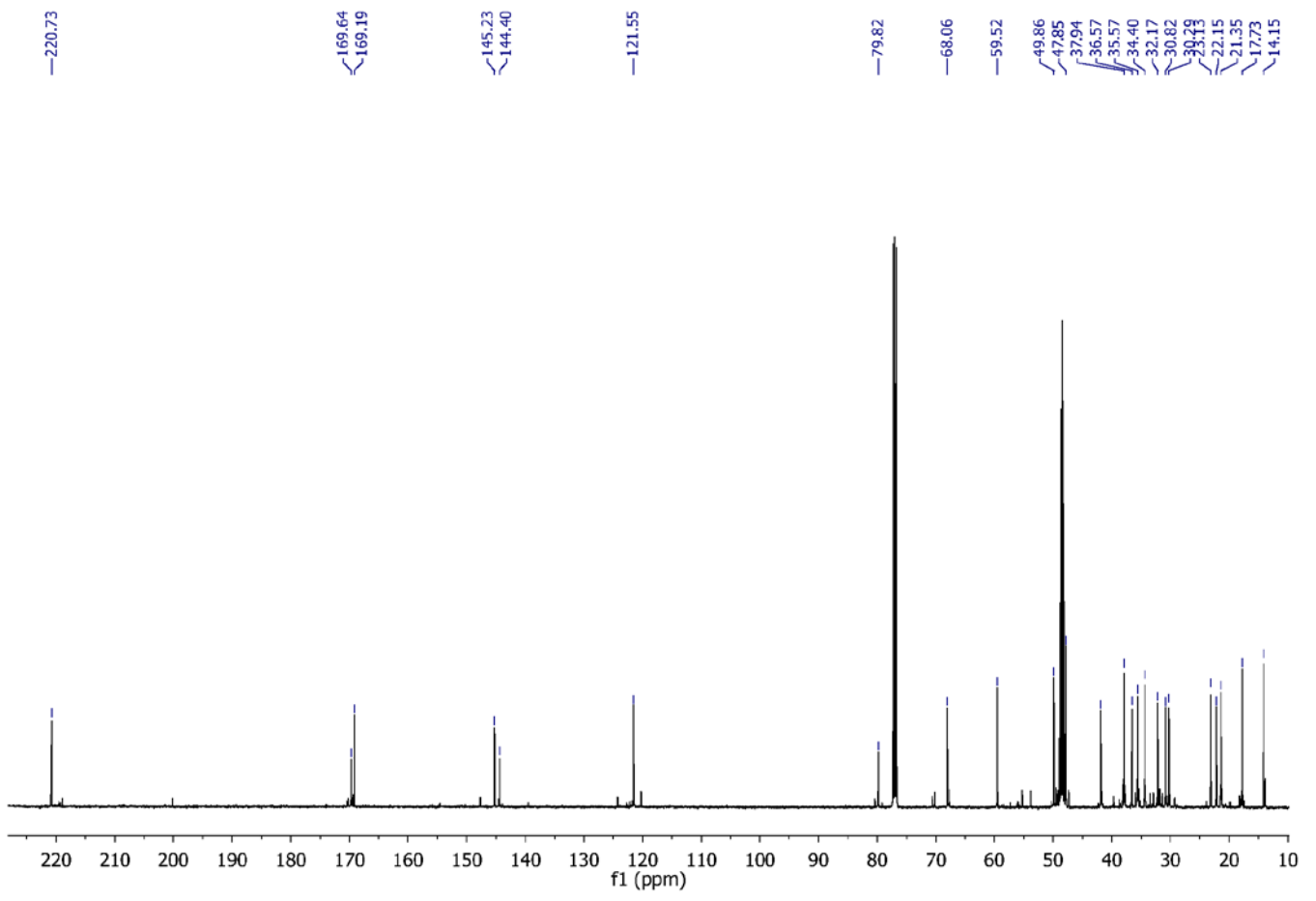
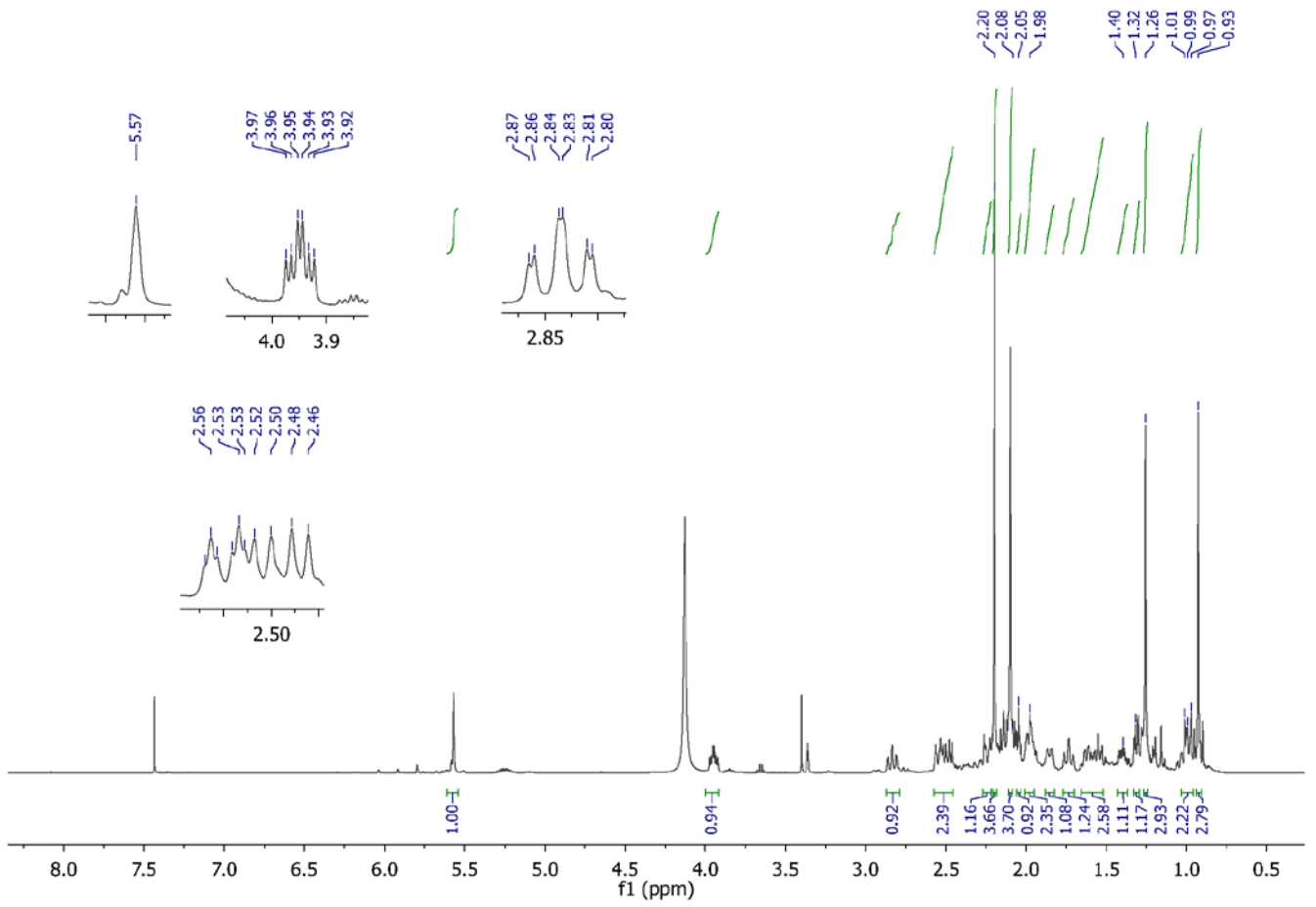
Formula	Compound name	Mass	Peak RT (min)	Peak area	Description
C26H35N3O5S	--	501.22974	0.41	4.14084 E6	--

Species	Abundance (counts)	Ion Mass	Measured Mass	Error (mDa)	Error (ppm)	Ret. Time Error (min)
[M+H] ⁺	201169.49	502.23702	502.23678	-0.23730	-0.47	--
[M+Na] ⁺	17471.65	524.21896	524.21936	0.39577	0.75	--

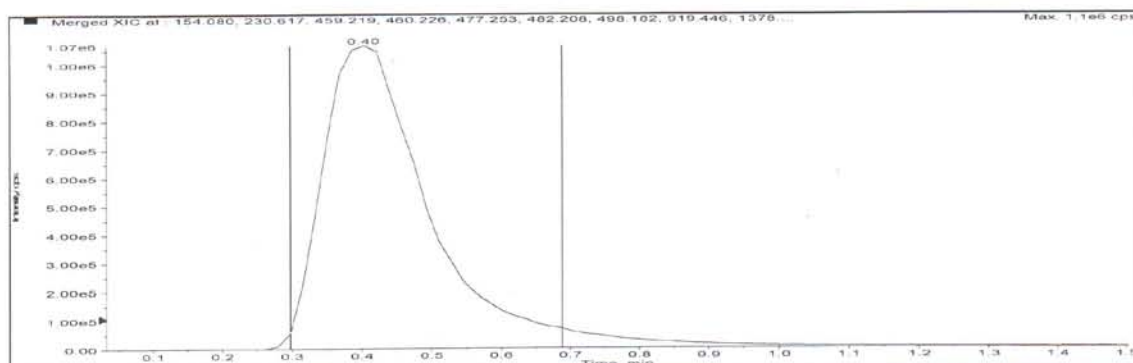


Compound 4d-OH

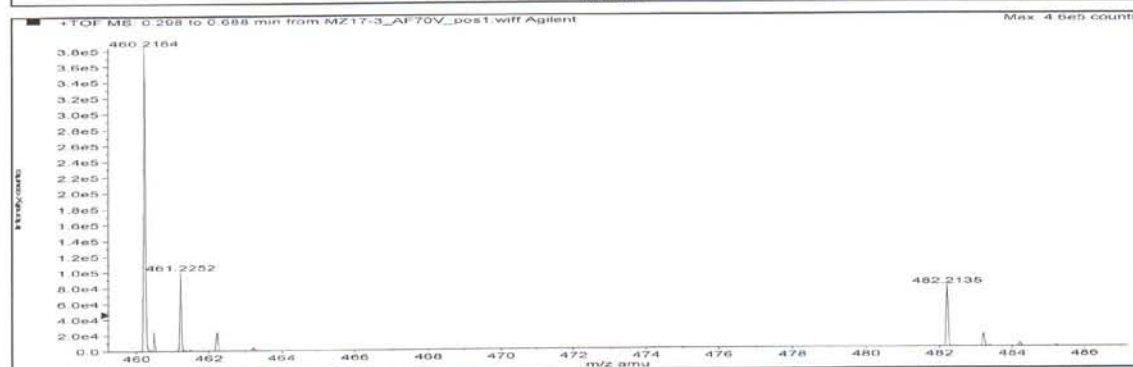
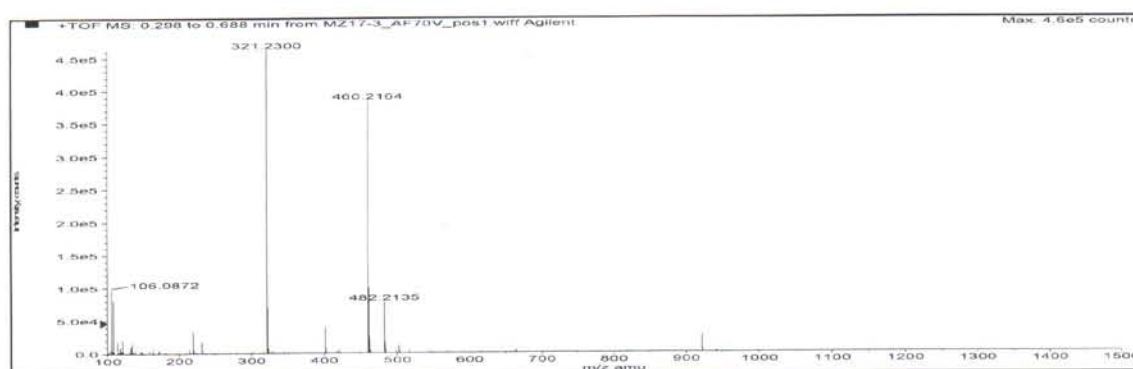




Sample Name: MZ17-3 Sample Location: P1-D3 Sample Id: Operator: Milka
 Data File Name: D:\PE Sciex Data\Projects\Sladlc\Data\MZ17-3_AF70V_pos1.wiff Acq Time: May 07 2015, 11:26:09 AM
 Method: d:\TOF_Data\damethods\Night_Seq_Comp_ident1.anmlefc.xml

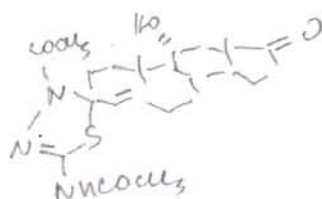


Merged XIC, Period#: 1 Experiment#: 1

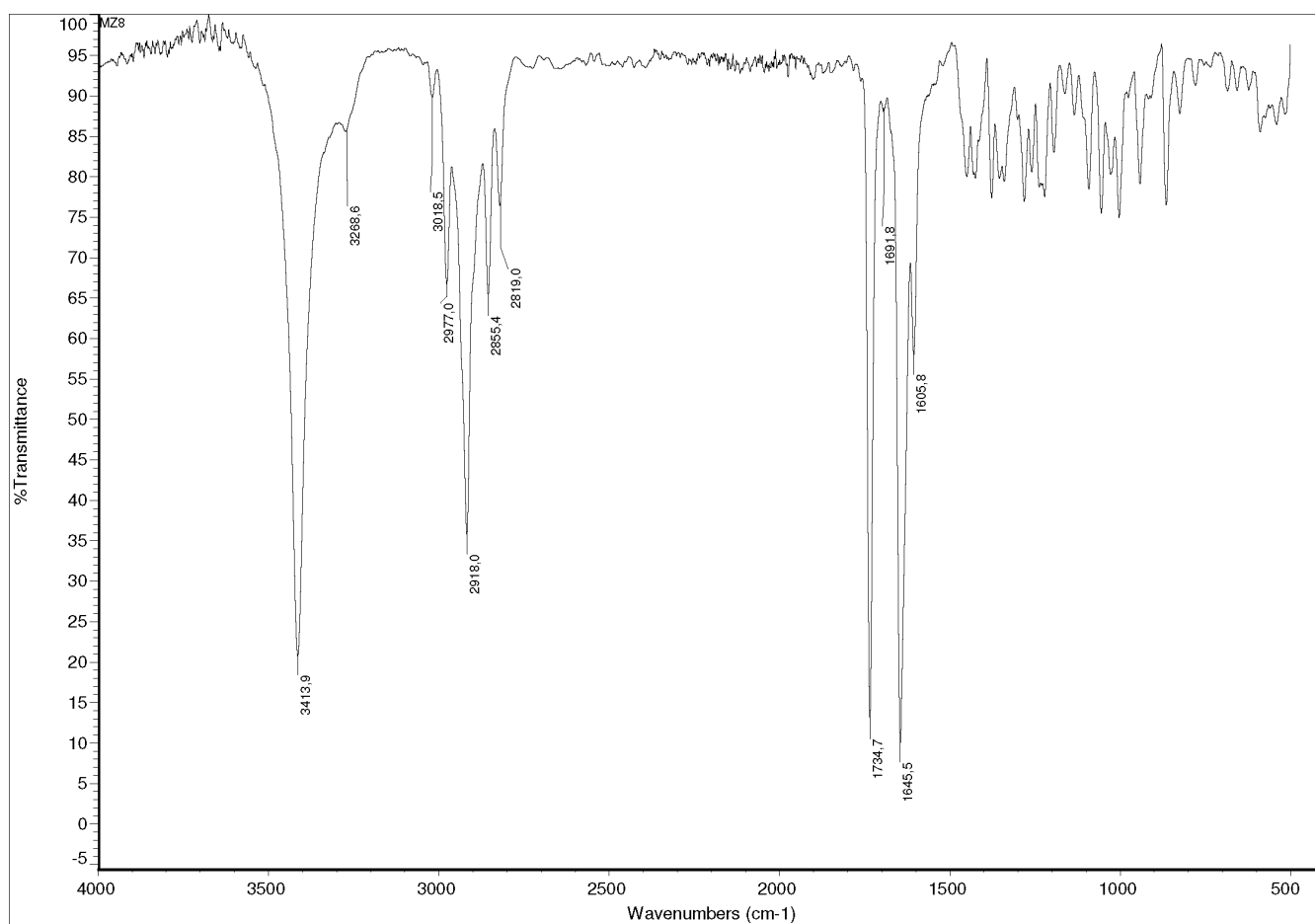
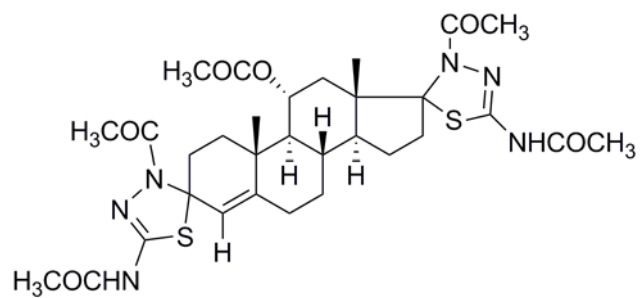


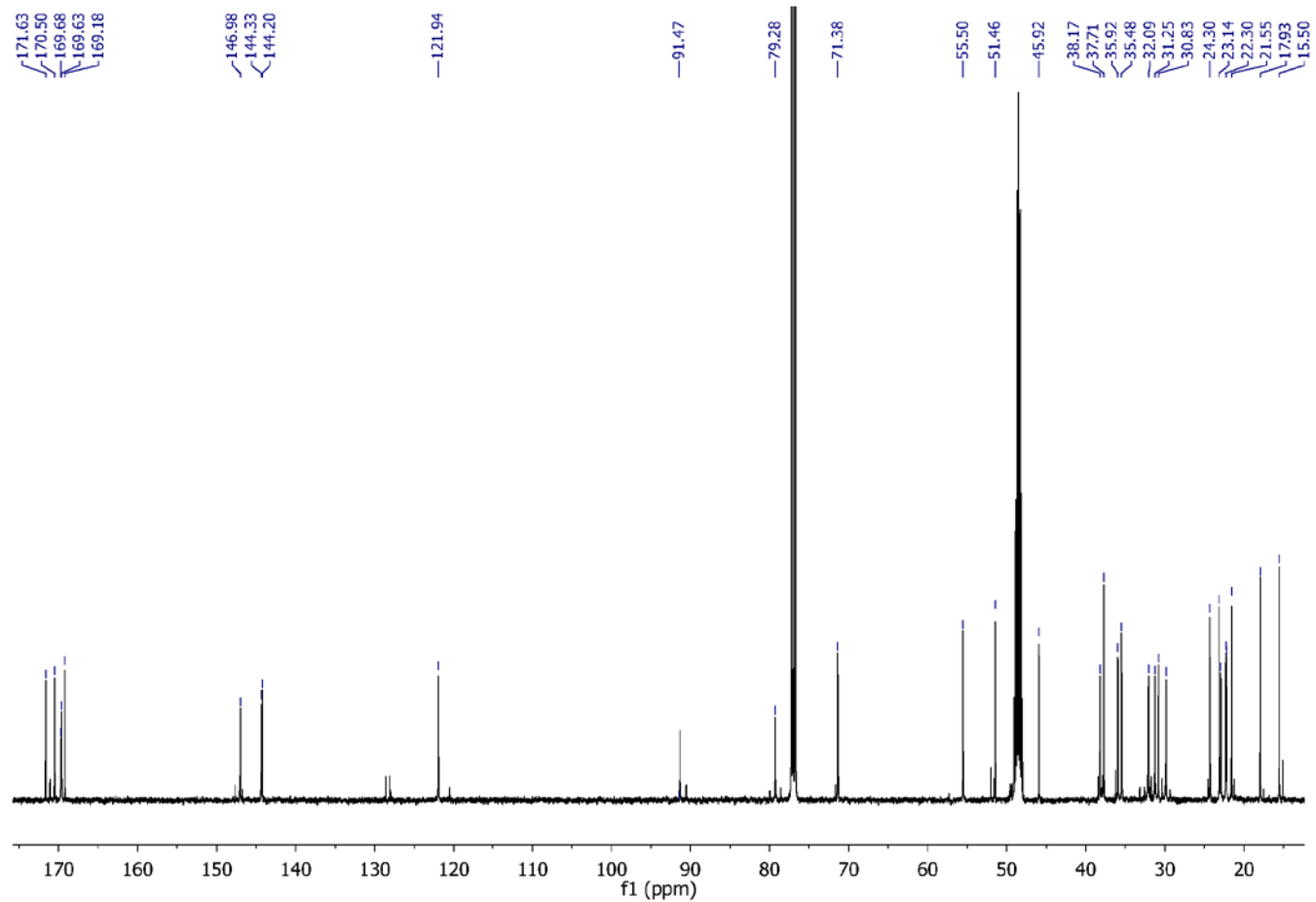
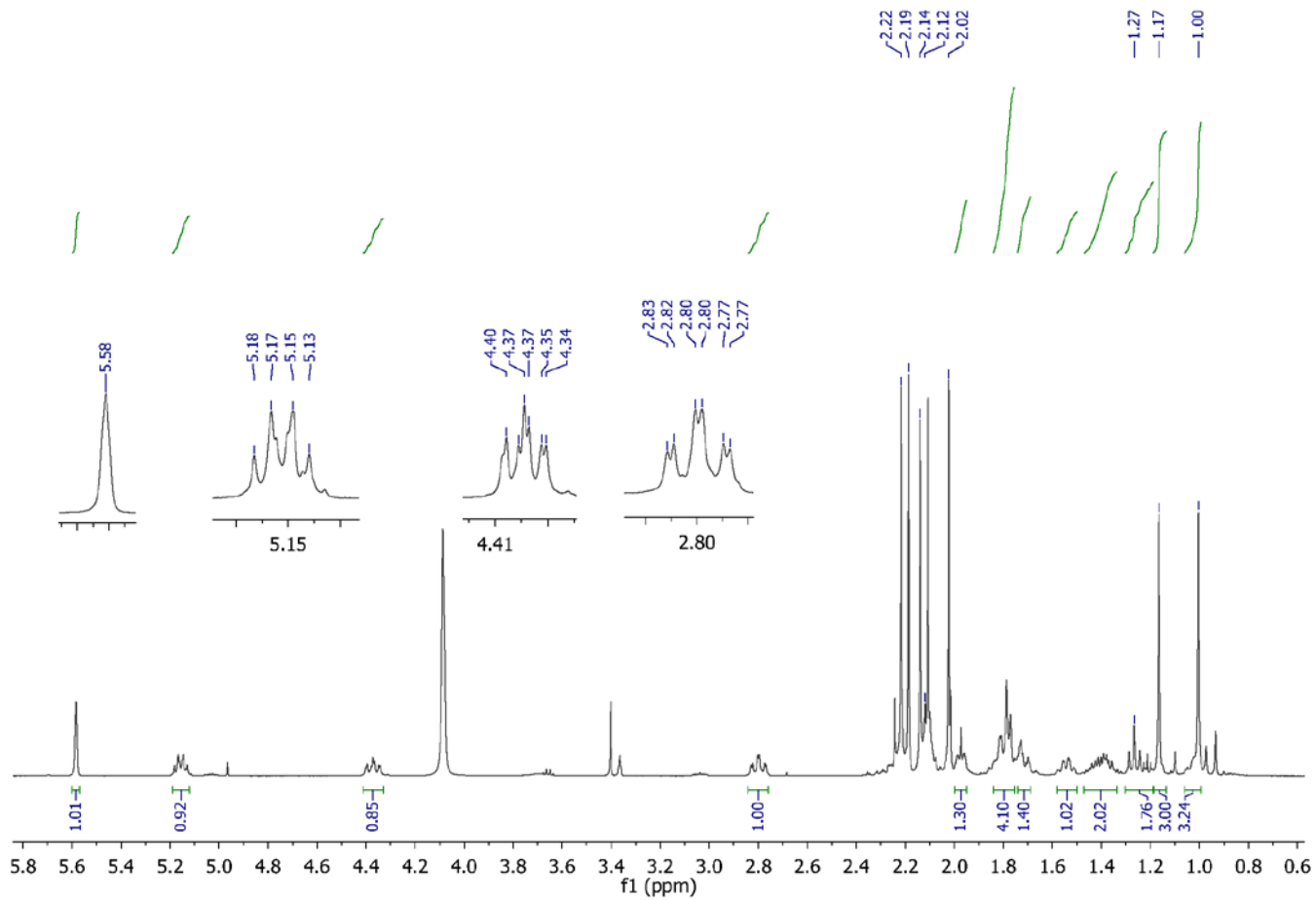
Formula	Compound name	Mass	Peak RT (min)	Peak area	Description
C24H33N3O4S	--	459.21918	0.40	1.11991 E7	--

Species	Abundance (counts)	Ion Mass	Measured Mass	Error (mDa)	Error (ppm)	Ret. Time Error (min)
[M+H] ⁺	401111.19	460.22645	460.22563	-0.82686	-1.80	--
[M+Na] ⁺	78642.74	482.20840	482.20780	-0.59397	-1.23	--

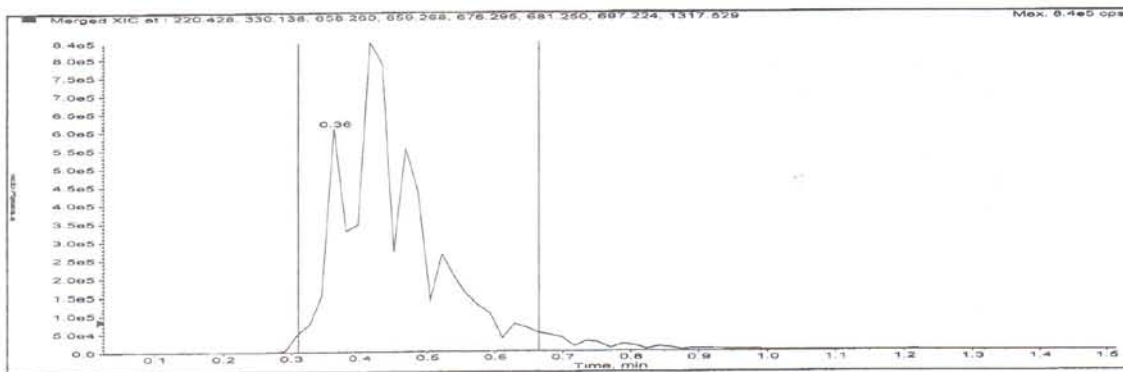


Compound 5d

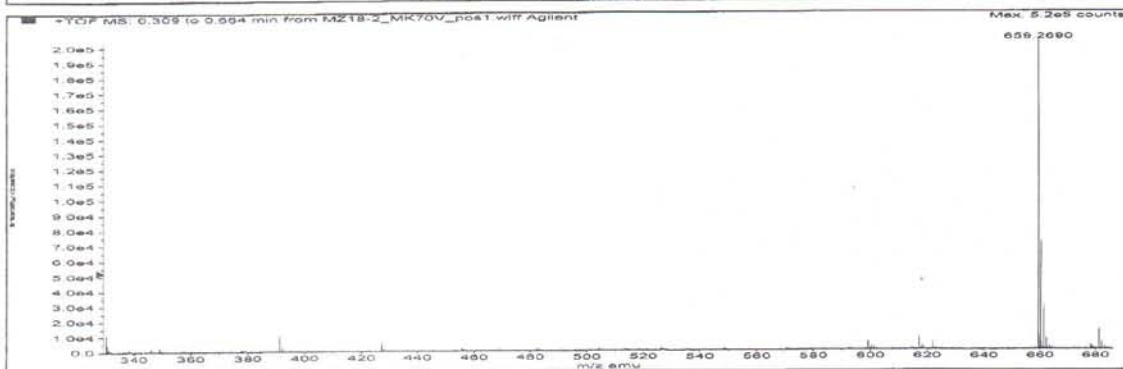
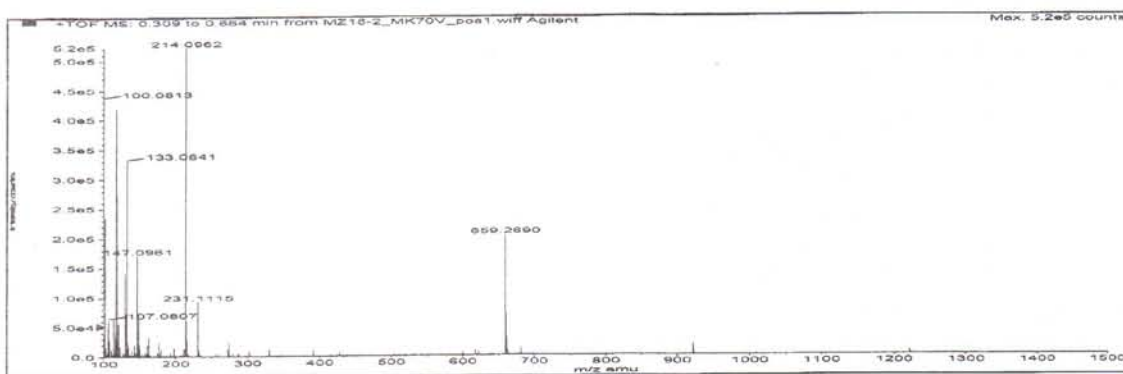




Sample Name: MZ18-2 Sample Location: P1-C8 Sample Id: Operator: Milka
 Data File Name: D:\PE Sciex Data\Projects\Sladic\Data\MZ18-2_MK70V_pos1.wiff Acq Time: August 05 2014, 11:32:53 AM
 Method: d:\TOF_Data\damethods\Night_Seq_Comp_ident1.anmlefc.xml

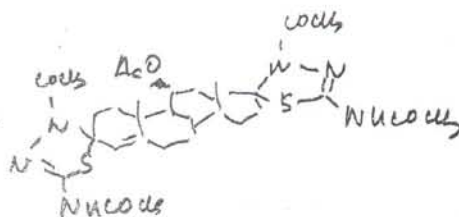


Merged XIC, Period# : 1 Experiment# : 1

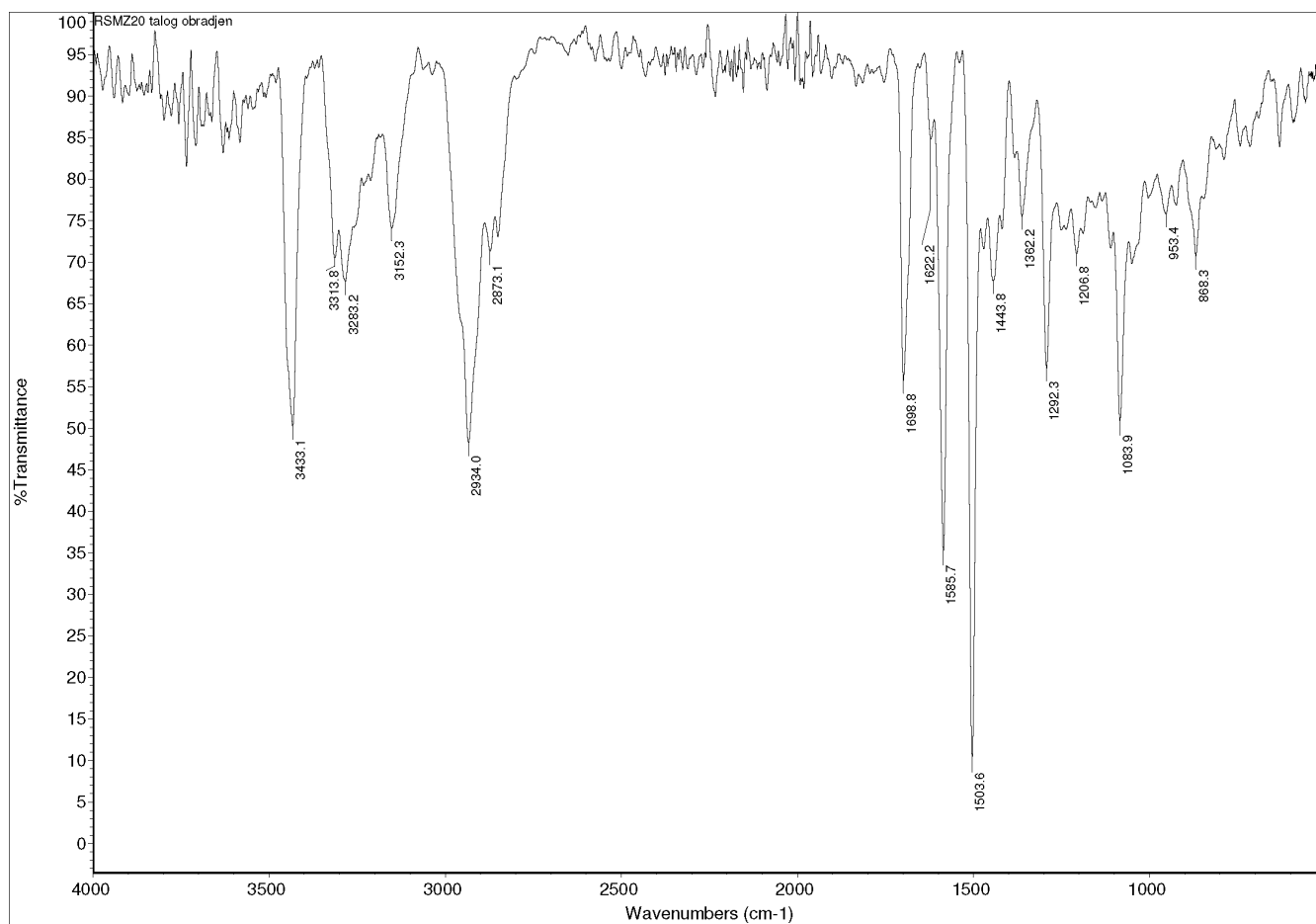
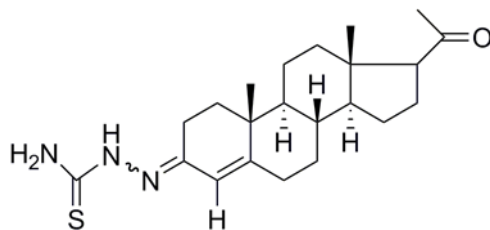


Formula	Compound name	Mass	Peak RT (min)	Peak area	Description
C31H42N6O6S2	--	658.26072	0.42	6.22477 E6	--

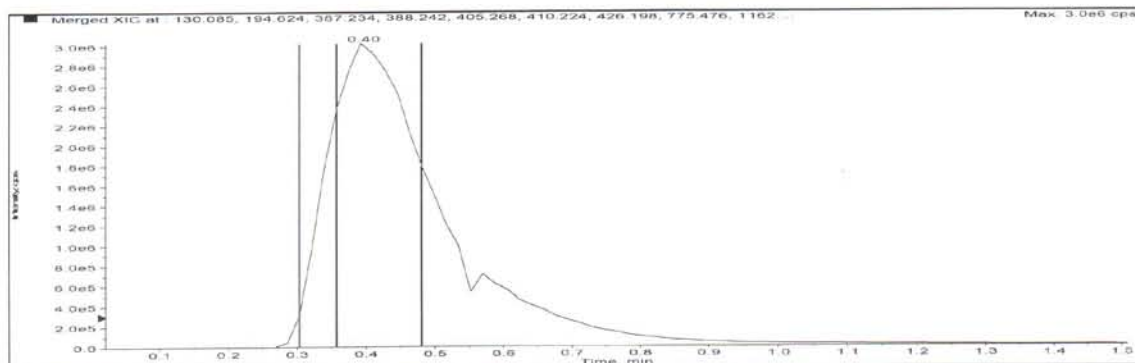
Species	Abundance (counts)	Ion Mass	Measured Mass	Error (mDa)	Error (ppm)	Ret. Time Error (min)
[M+2H] ²⁺	11227.02	330.13764	330.13822	0.57808	1.75	--
[M+H] ⁺	203144.82	659.26800	659.26750	-0.50395	-0.76	--
[M+Na] ⁺	13686.55	681.24995	681.24989	-0.05726	-0.08	--



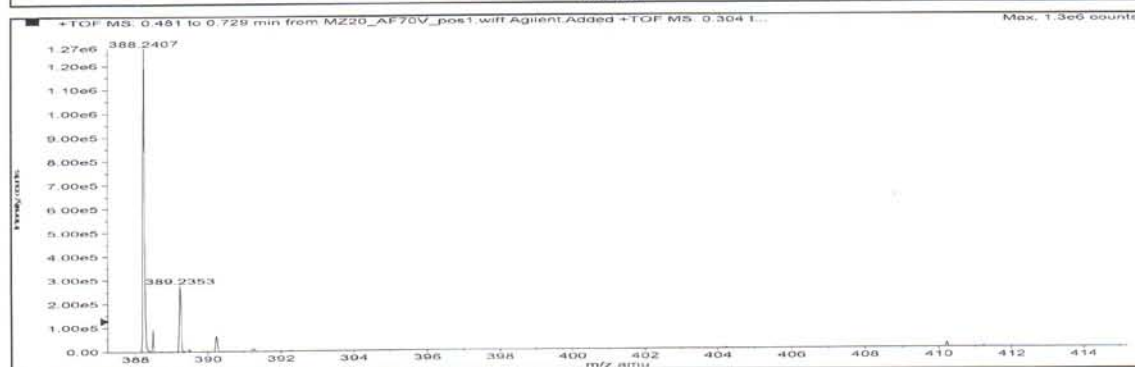
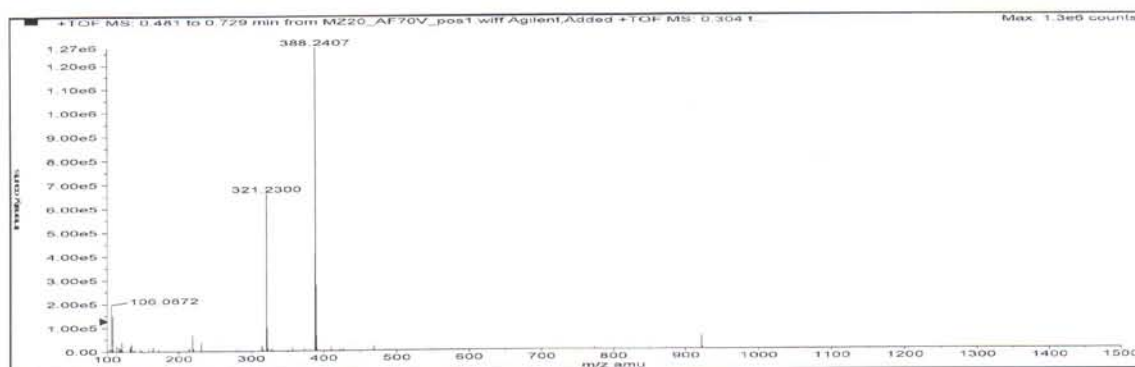
Compound 2e



Sample Name: MZ20 Sample Location: P1-D4 Sample Id: Operator: Milka
 Data File Name: D:\PE Sciex Data\Projects\SIadici\Data\MZ20_AF70V_pos1.wiff Acq Time: May 07 2015, 11:28:41 AM
 Method: d:\TOF_Data\damethods\Night_Seq_Comp_ident1.anm\efc.xml

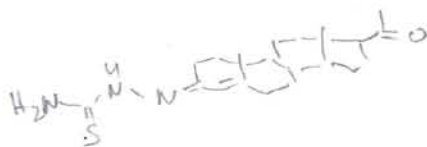


Merged XIC, Period# : 1 Experiment# : 1

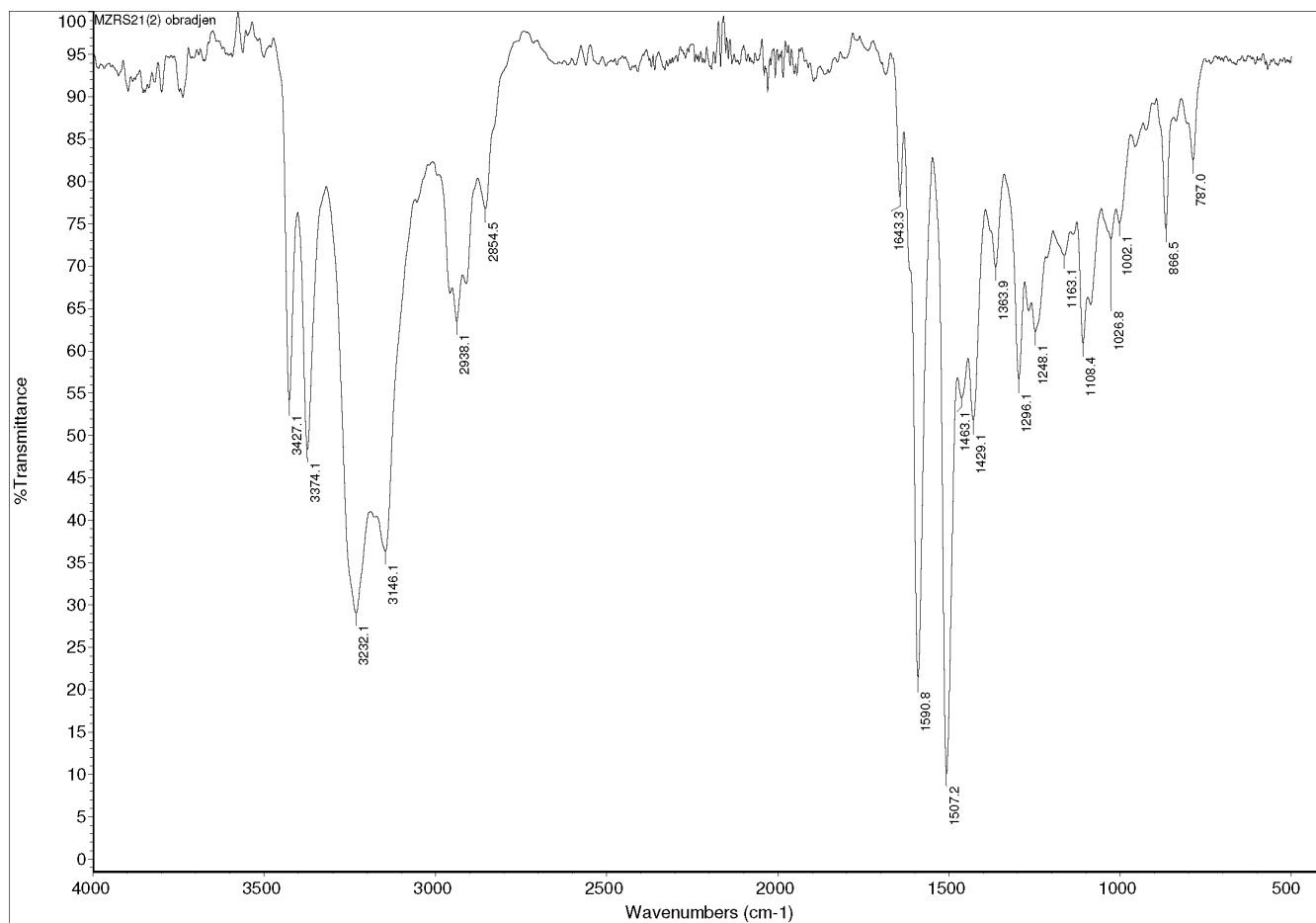
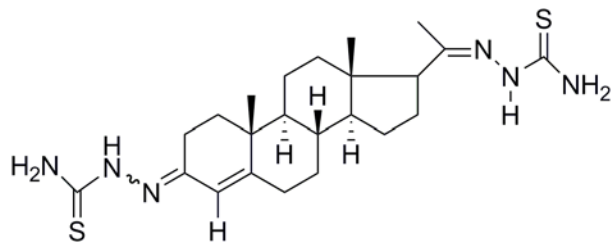


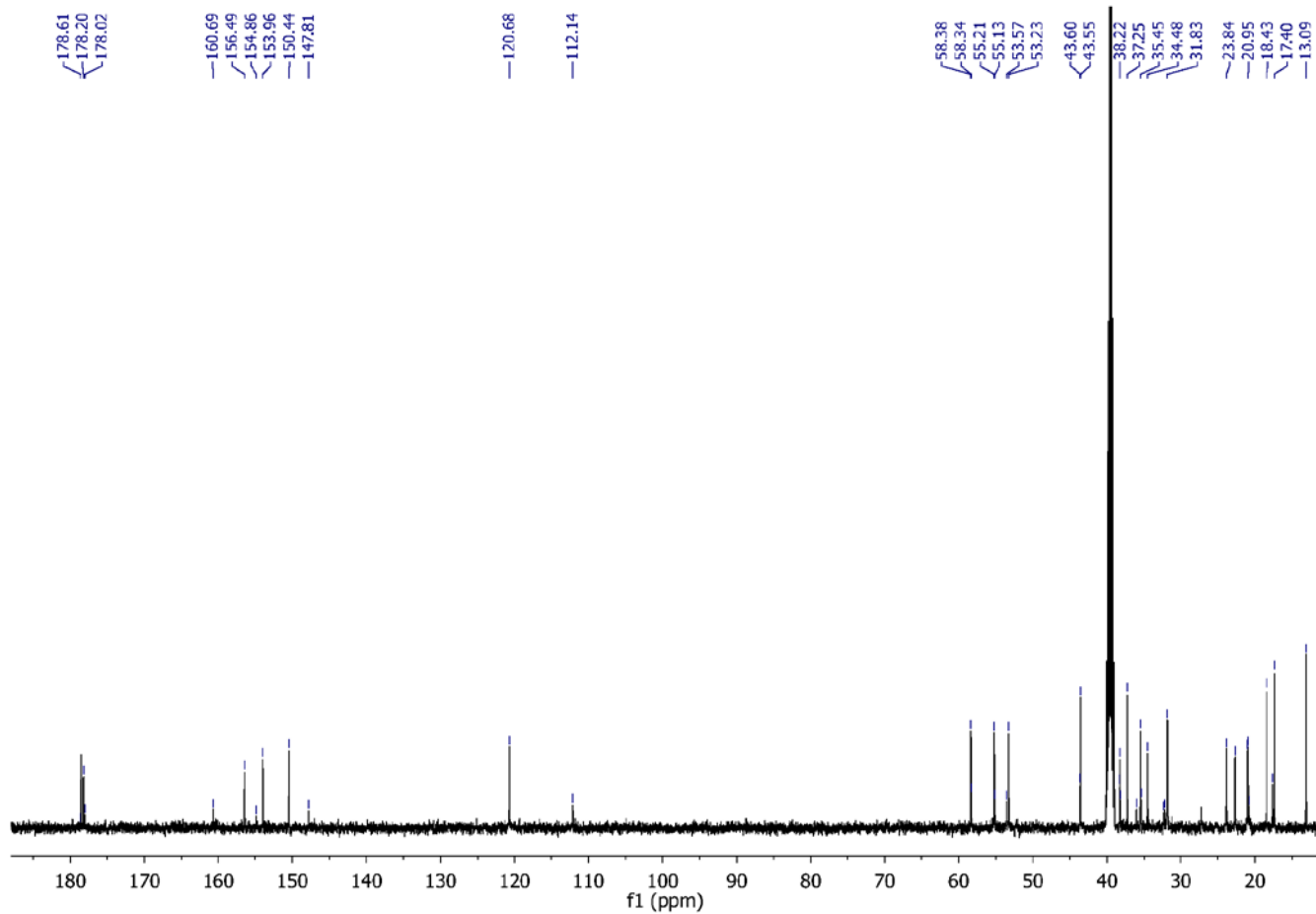
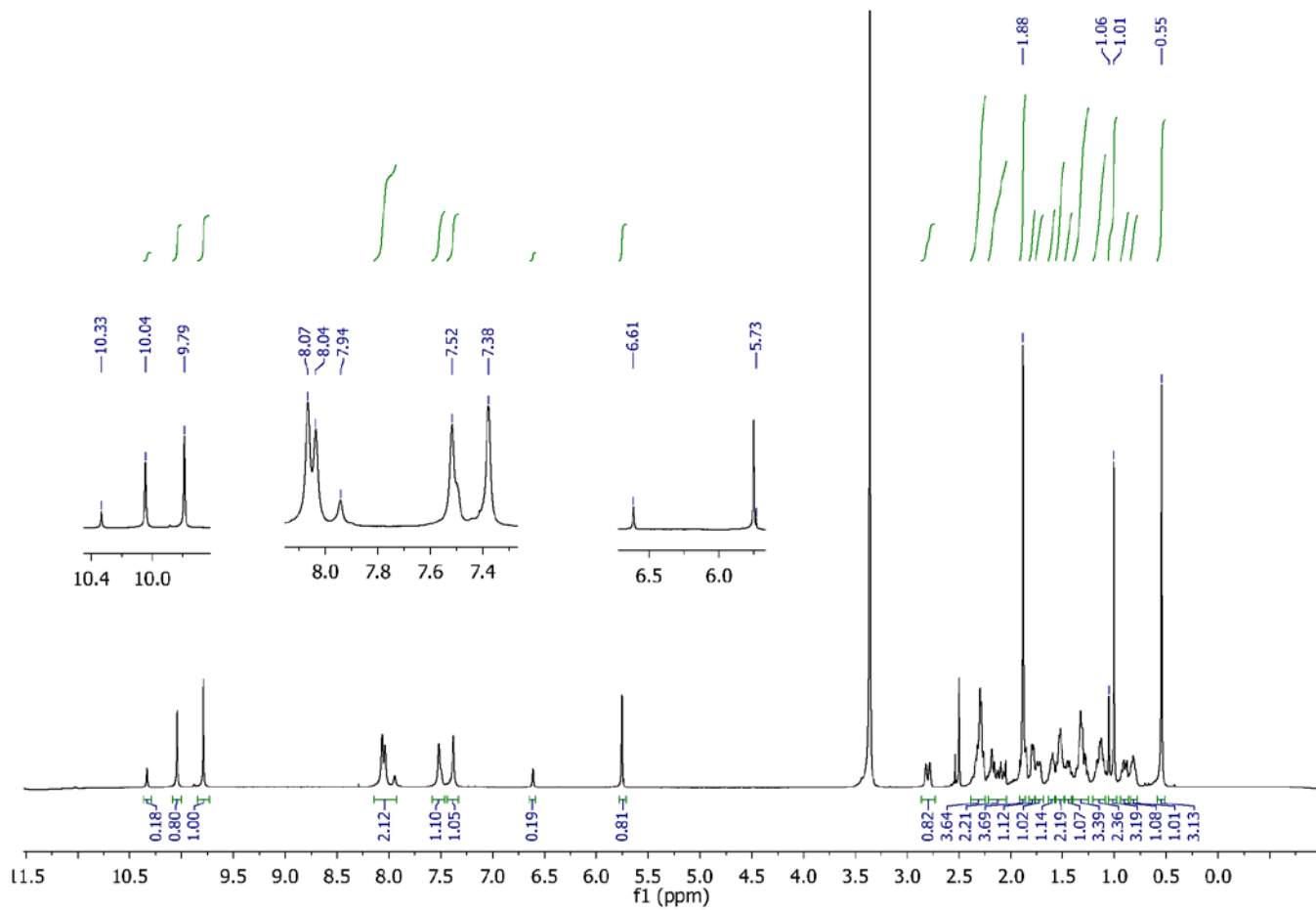
Formula	Compound name	Mass	Peak RT (min)	Peak area	Description
C22H33N3OS	--	387.23443	0.40	3.43590 E7	--

Species	Abundance (counts)	Ion Mass	Measured Mass	Error (mDa)	Error (ppm)	Ret. Time Error (min)
[M+H] ⁺	1274663.73	388.24171	388.24102	-0.68812	-1.77	--
[M+Na] ⁺	18648.17	410.22365	410.22379	0.13069	0.32	--

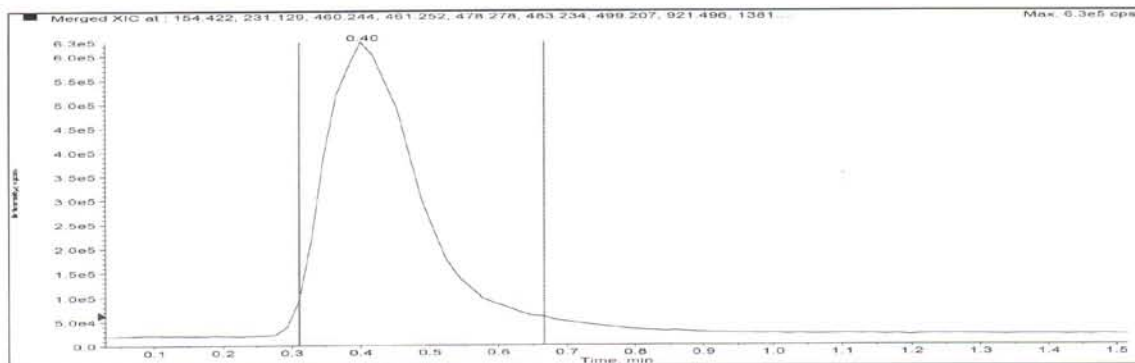


Compound 3e

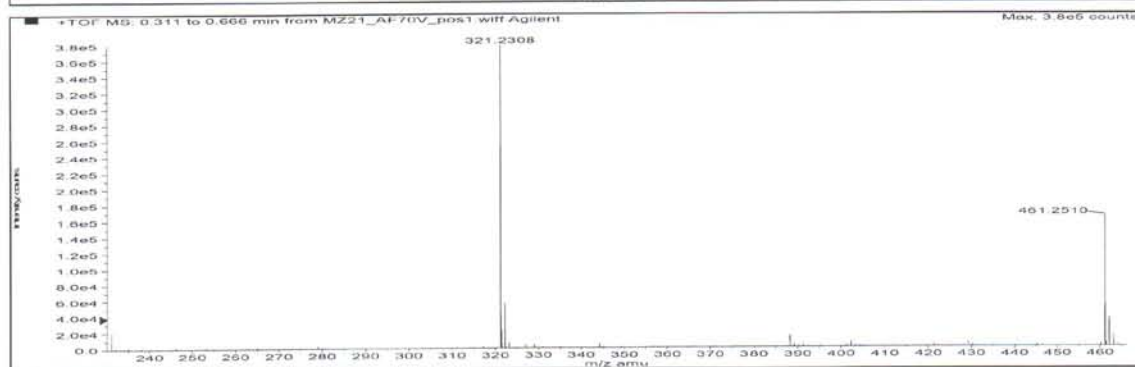
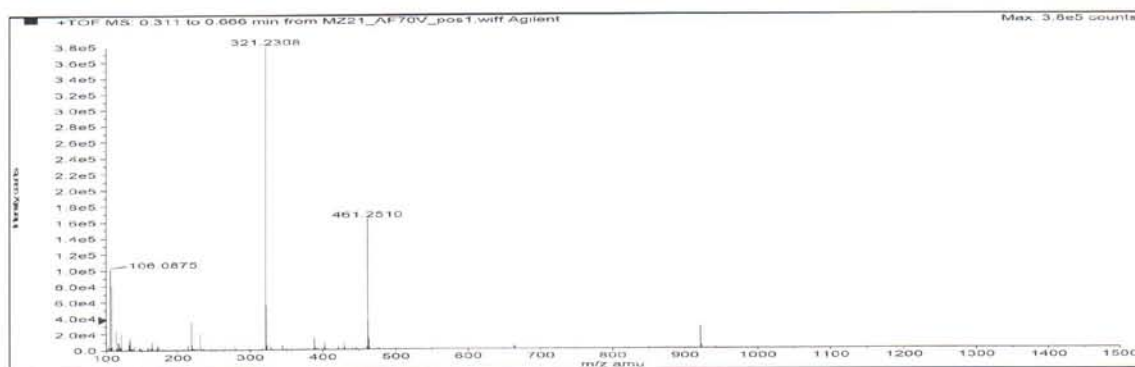




Sample Name: MZ21 Sample Location: P1-D5 Sample Id: Operator: Milka
 Data File Name: D:\PE Sciex Data\Projects\Sladic\Data\MZ21_AF70V_pos1.wiff Acq Time: May 07 2015, 11:42:07 AM
 Method: d:\TOF_Data\damethods\Night_Seq_Comp_ident1.anm\efc.xml



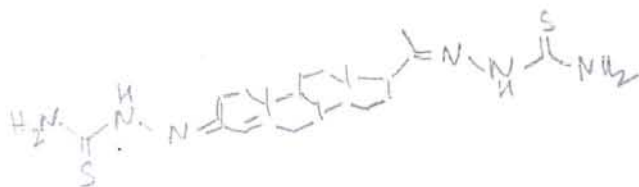
Merged XIC, Period# : 1 Experiment# : 1



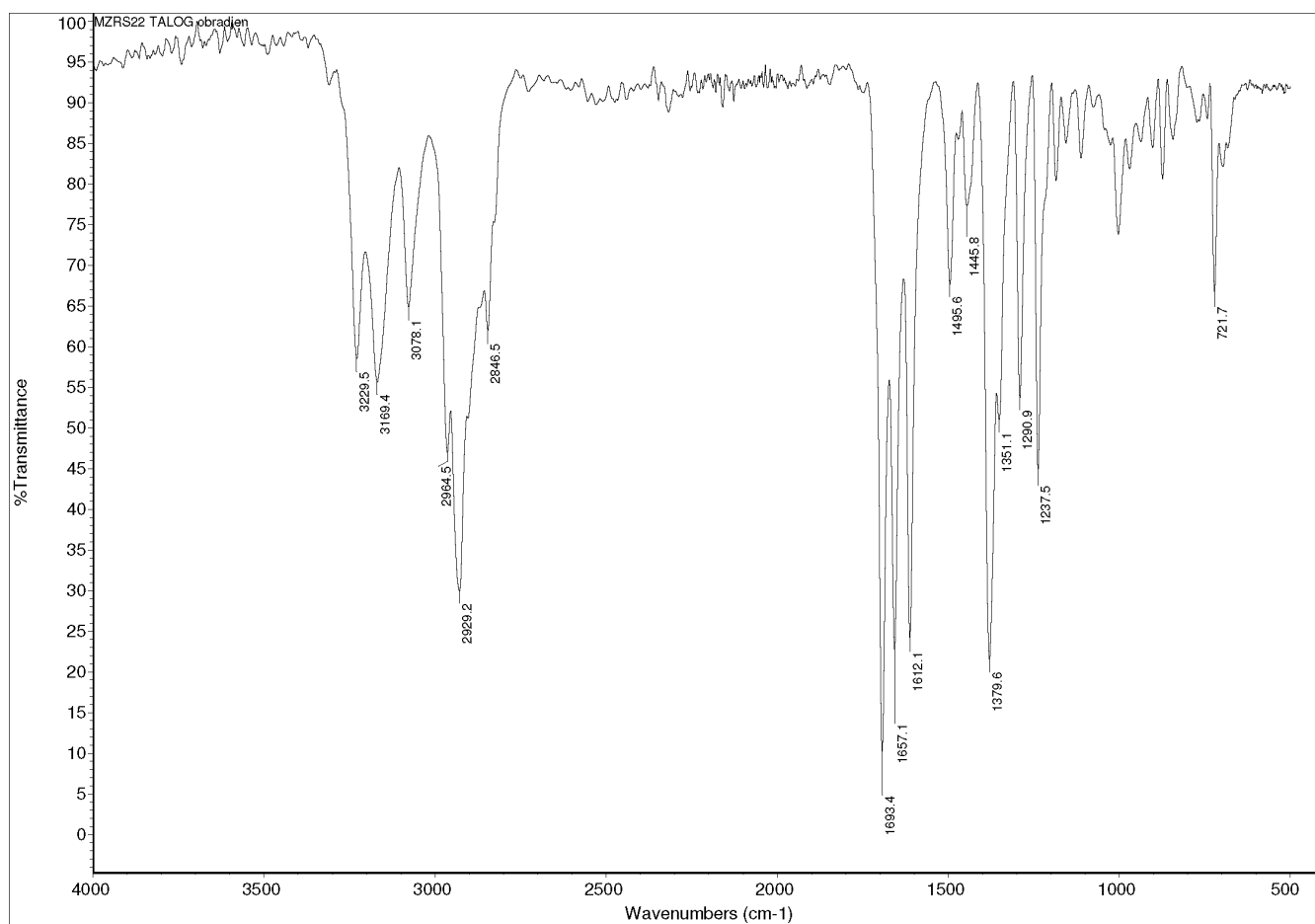
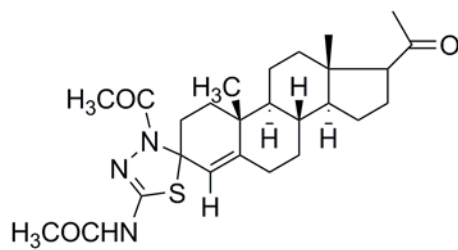
Formula	Compound name	Mass	Peak RT (min)	Peak area	Description
C23H36N6S2	--	460.24429	0.40	6.00059 E6	--

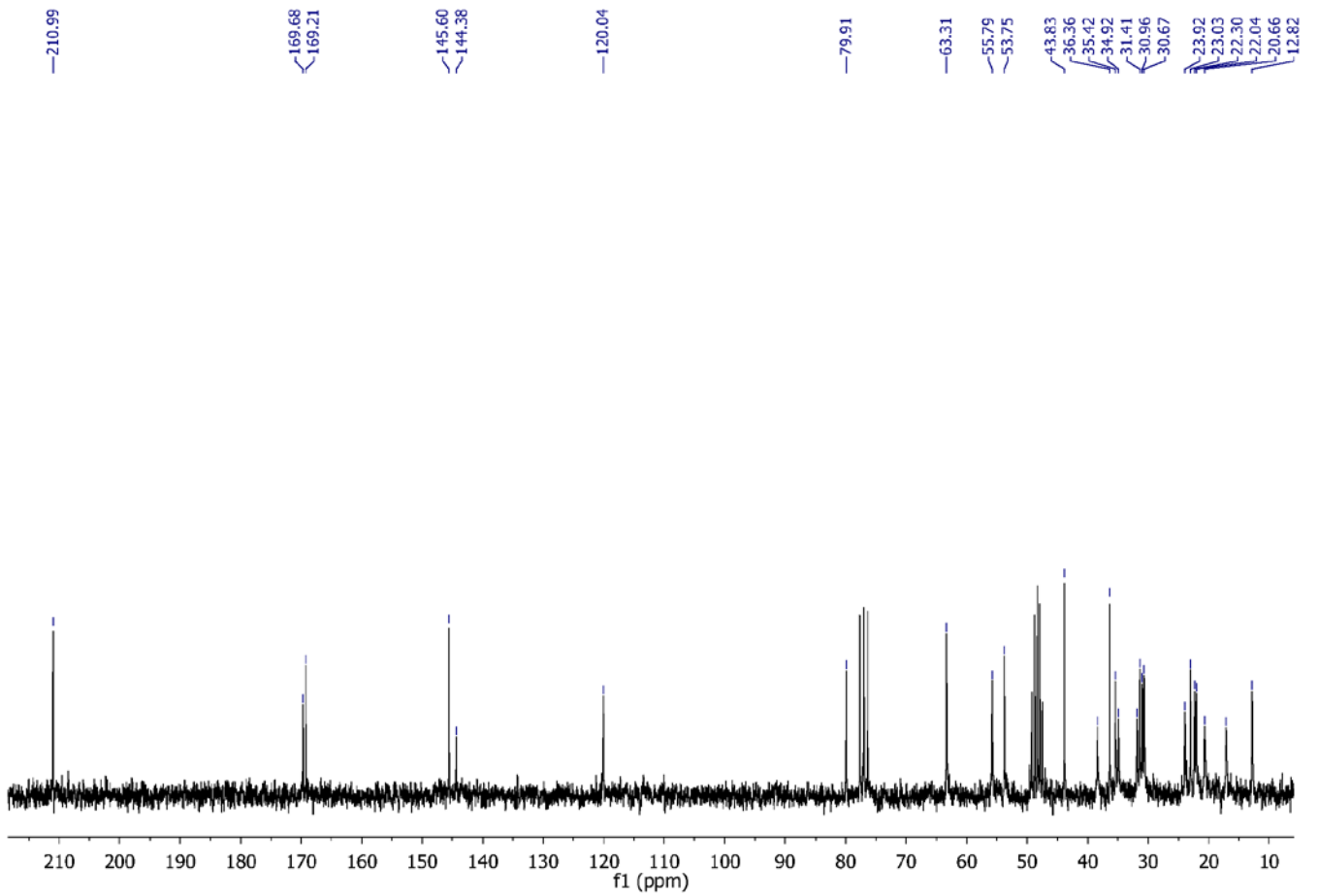
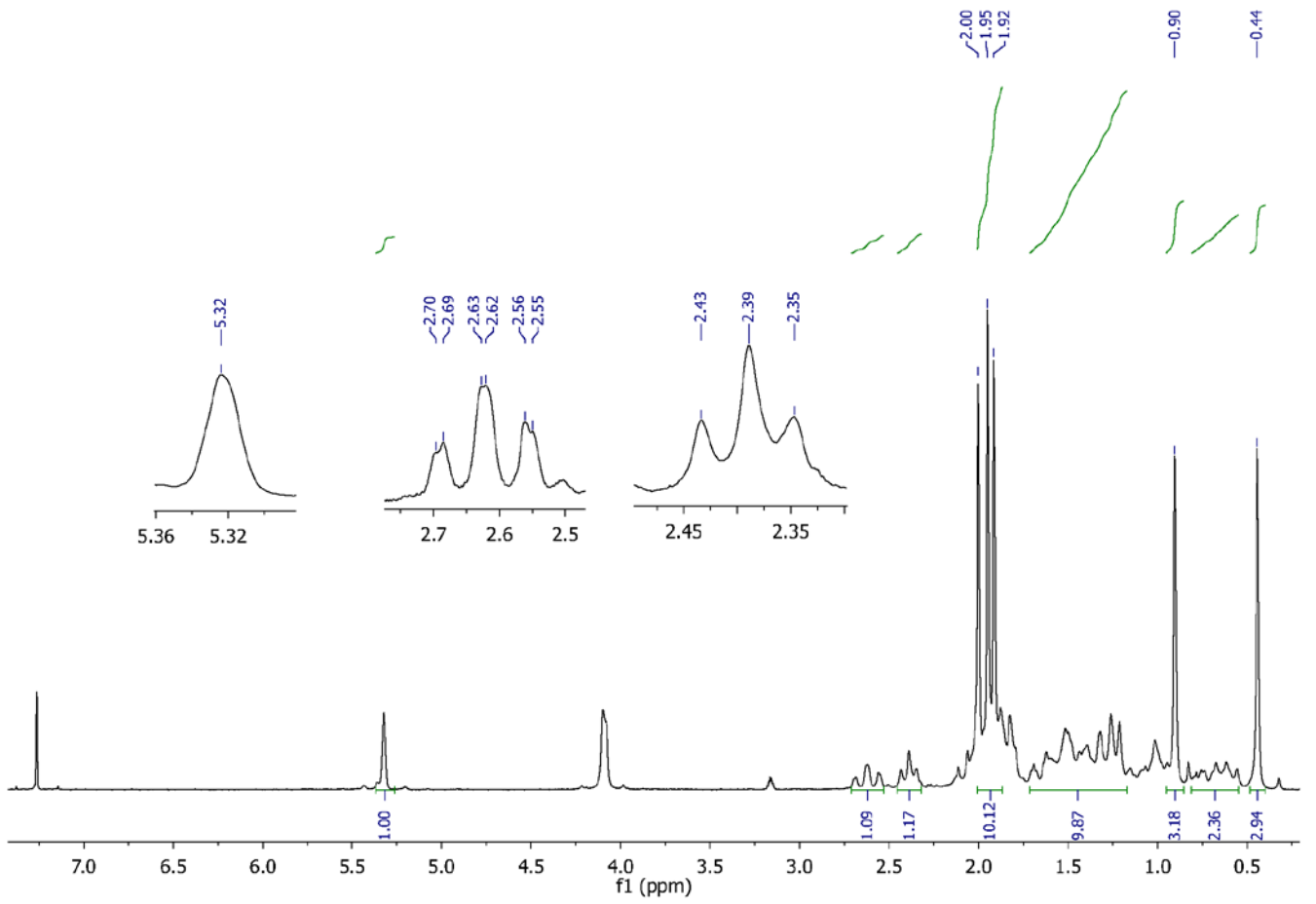
Species	Abundance (counts)	Ion Mass	Measured Mass	Error (mDa)	Error (ppm)	Ret. Time Error (min)
[M+2H] ²⁺	21283.91	231.12942	231.11850	-10.92236	-47.26	--
[M+H] ⁺	183573.95	461.25156	461.25130	-0.25807	-0.56	--

OK! JG

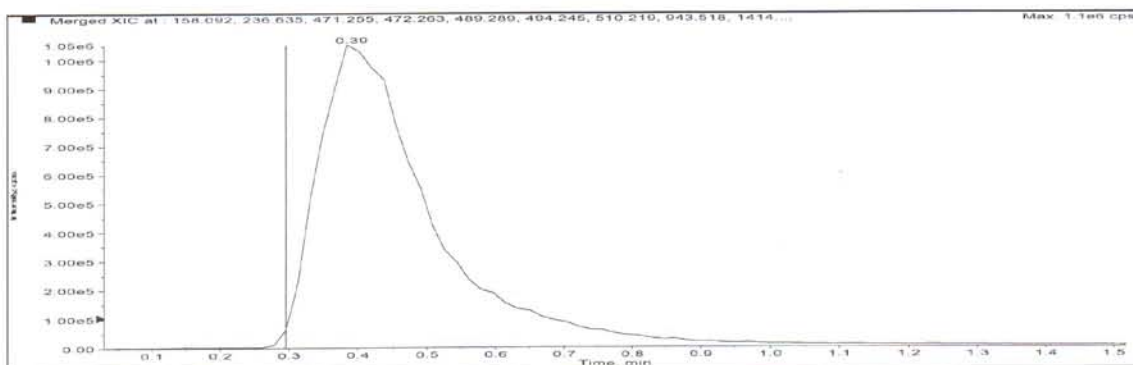


Compound 4e

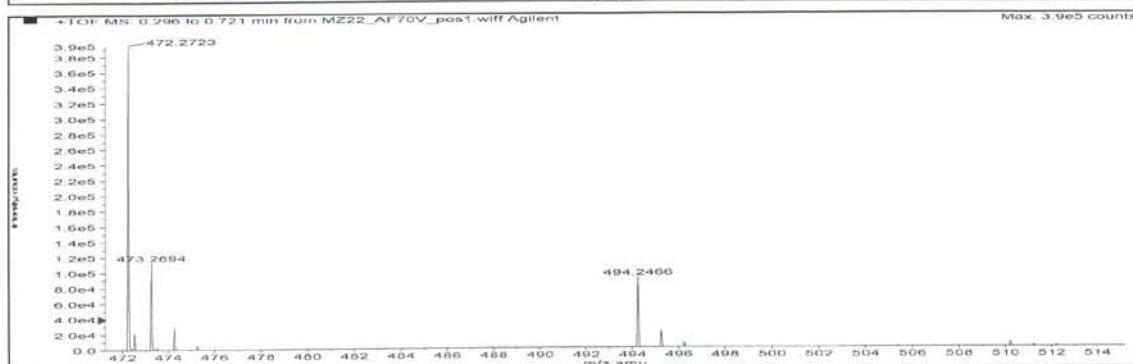
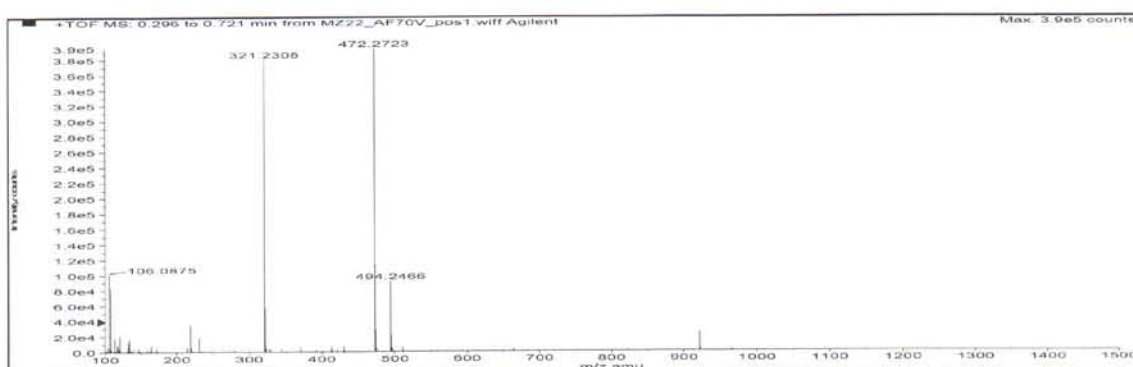




Sample Name: MZ22 Sample Location: P1-D6 Sample Id: Operator: Milka
 Data File Name: D:\PE Sclex Data\Projects\Sladici\Data\MZ22_AF70V_pos1.wiff Acq Time: May 07 2015, 11:44:39 AM
 Method: d:\TOF_Data\damethods\Night_Seq_Comp_ident1.anml\efc.xml

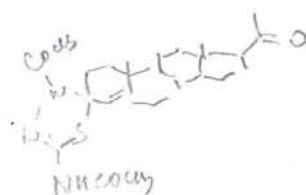


Merged XIC, Period# : 1 Experiment# : 1

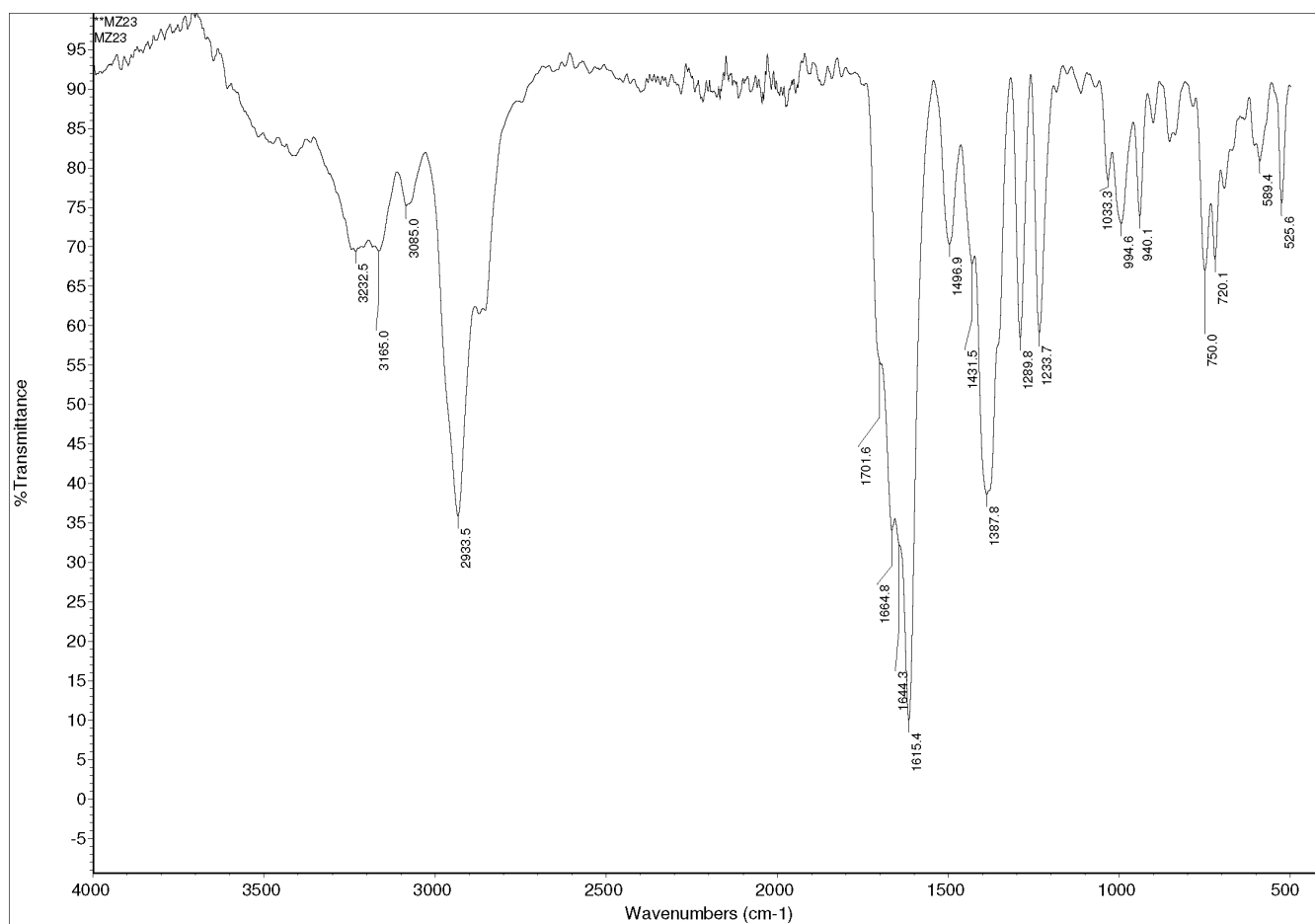
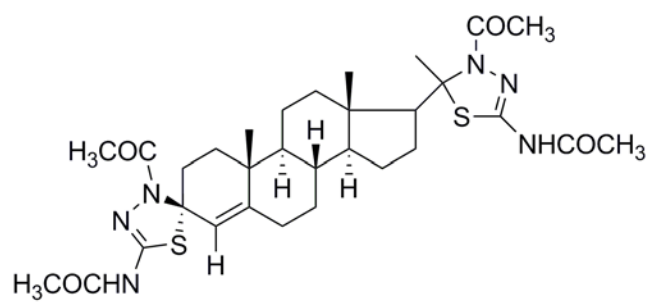


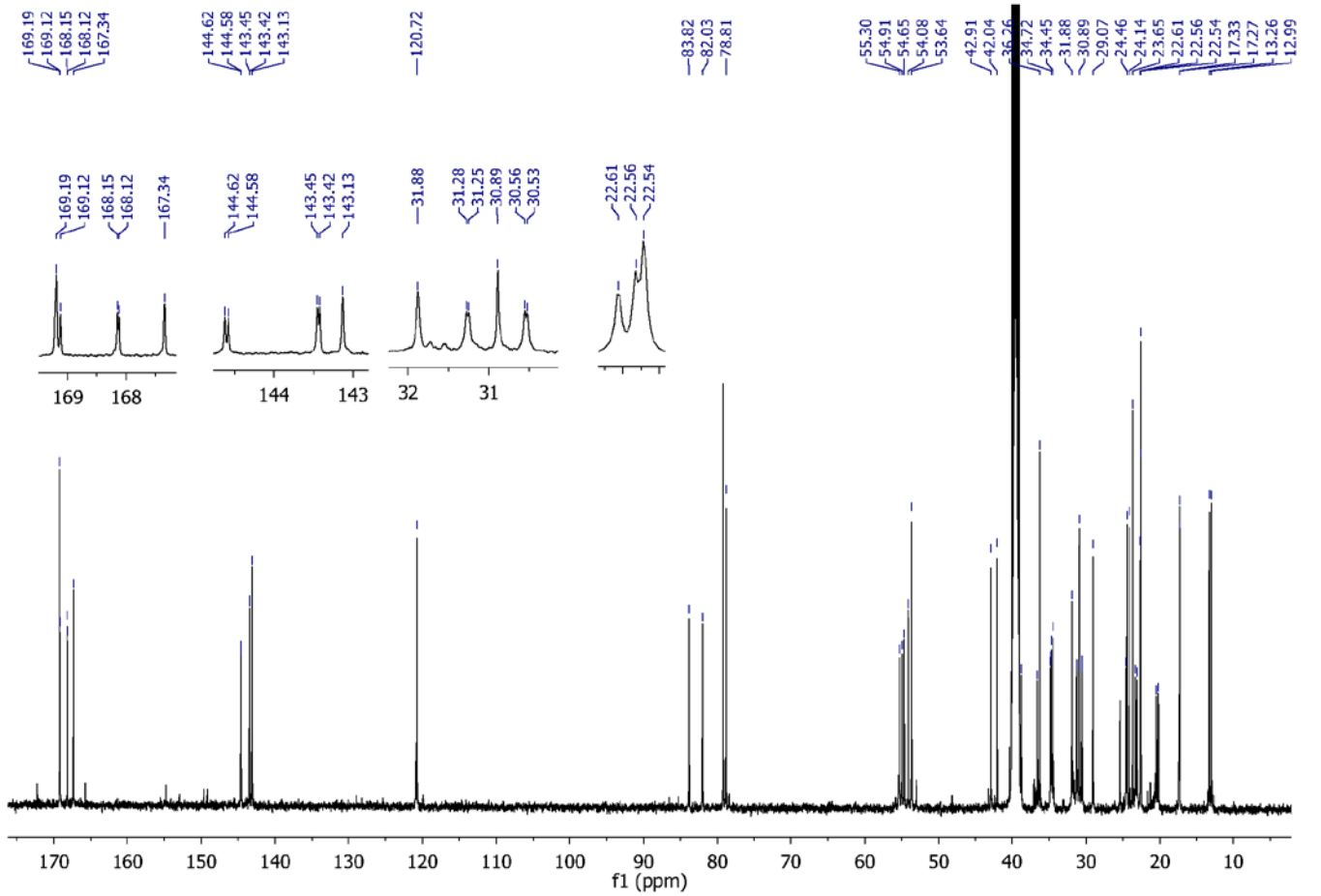
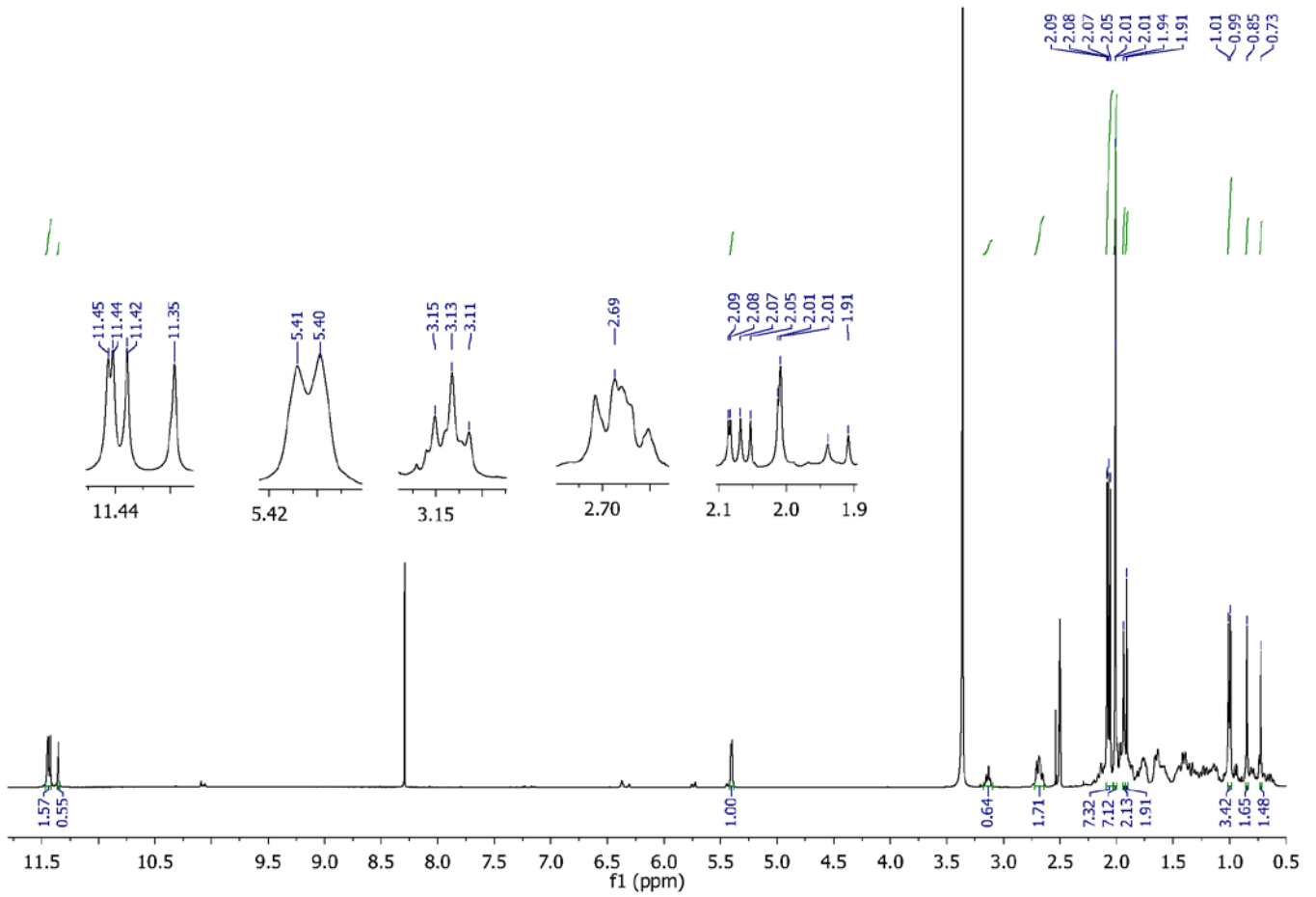
Formula	Compound name	Mass	Peak RT (min)	Peak area	Description
C26H37N3O3S	--	471.25556	0.39	1.16231 E7	--

Species	Abundance (counts)	Ion Mass	Measured Mass	Error (mDa)	Error (ppm)	Ret. Time Error (min)
[M+H] ⁺	417053.04	472.26284	472.26186	-0.97699	-2.07	--
[M+Na] ⁺	92126.24	494.24478	494.24438	-0.40077	-0.81	--
[M+K] ⁺	6330.56	510.21872	510.21919	0.47390	0.93	--

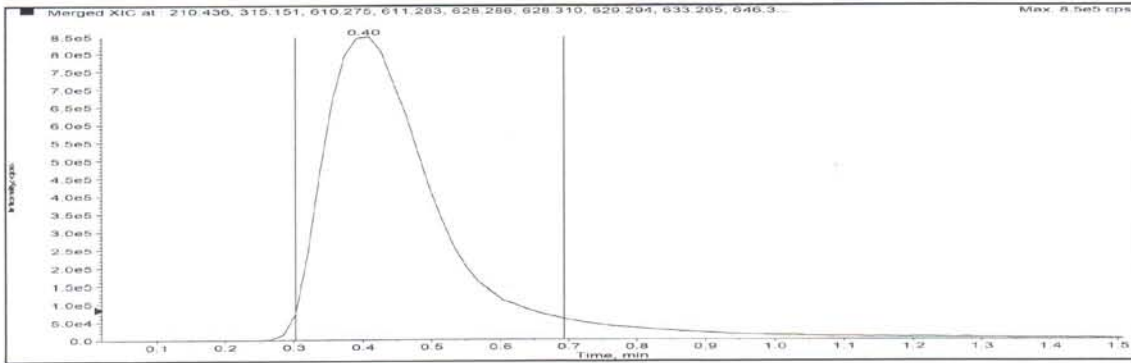


Compound 5e

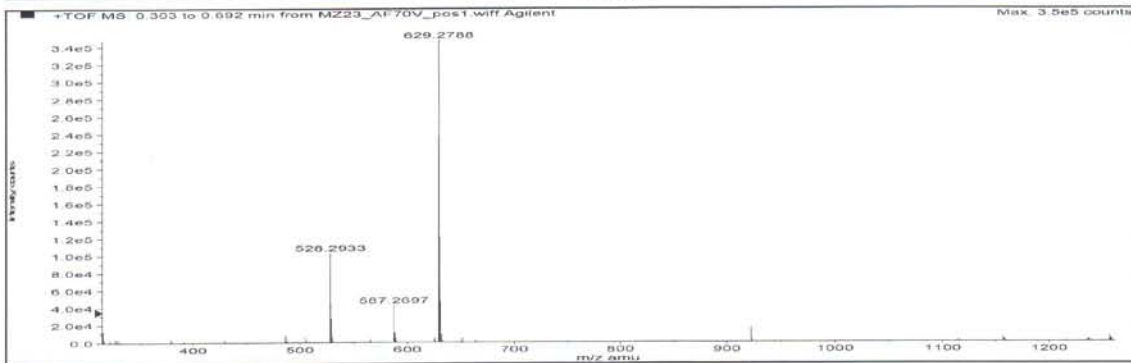
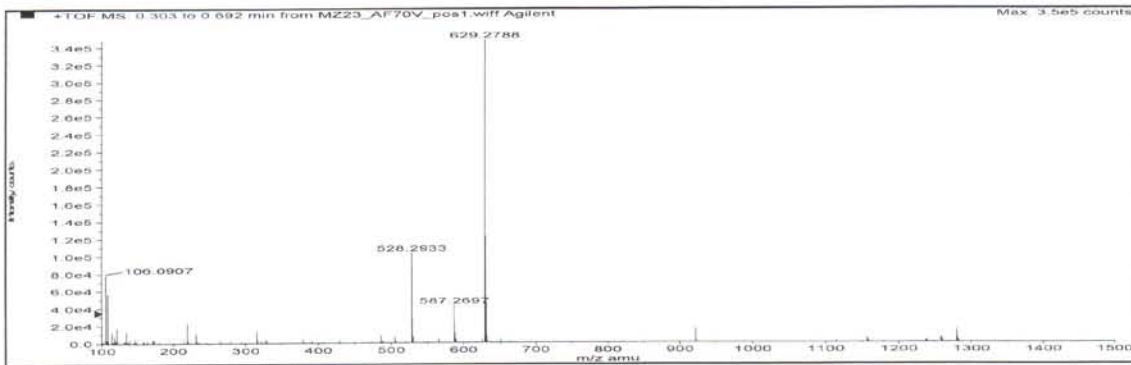




Sample Name: MZ23 Sample Location: P1-F6 Sample Id: Operator: Milka
 Data File Name: D:\PE Sciex Data\Projects\Sladici\Data\MZ23_AF70V_pos1.wiff Acq Time: May 08 2015, 01:31:35 PM
 Method: d:\TOF_Data\damethods\Night_Seq_Comp_ident1.an\lfc.xml



Merged XIC, Period# : 1 Experiment# : 1



Formula	Compound name	Mass	Peak RT (min)	Peak area	Description
C31H44N6O4S2	--	628.28655	0.40	9.40326 E6	--

Species	Abundance (counts)	Ion Mass	Measured Mass	Error (mDa)	Error (ppm)	Ret. Time Error (min)
[M+2H] ²⁺	12959.73	315.15055	315.15006	-0.48824	-1.55	--
[M+H] ⁺	369767.78	629.29382	629.29187	-1.94983	-3.10	--
[M+Na] ⁺	4818.21	651.27577	651.27484	-0.93039	-1.43	--
[2M+H] ⁺	6238.23	1257.58037	1257.57804	-2.32970	-1.85	--

