

Supplementary data

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

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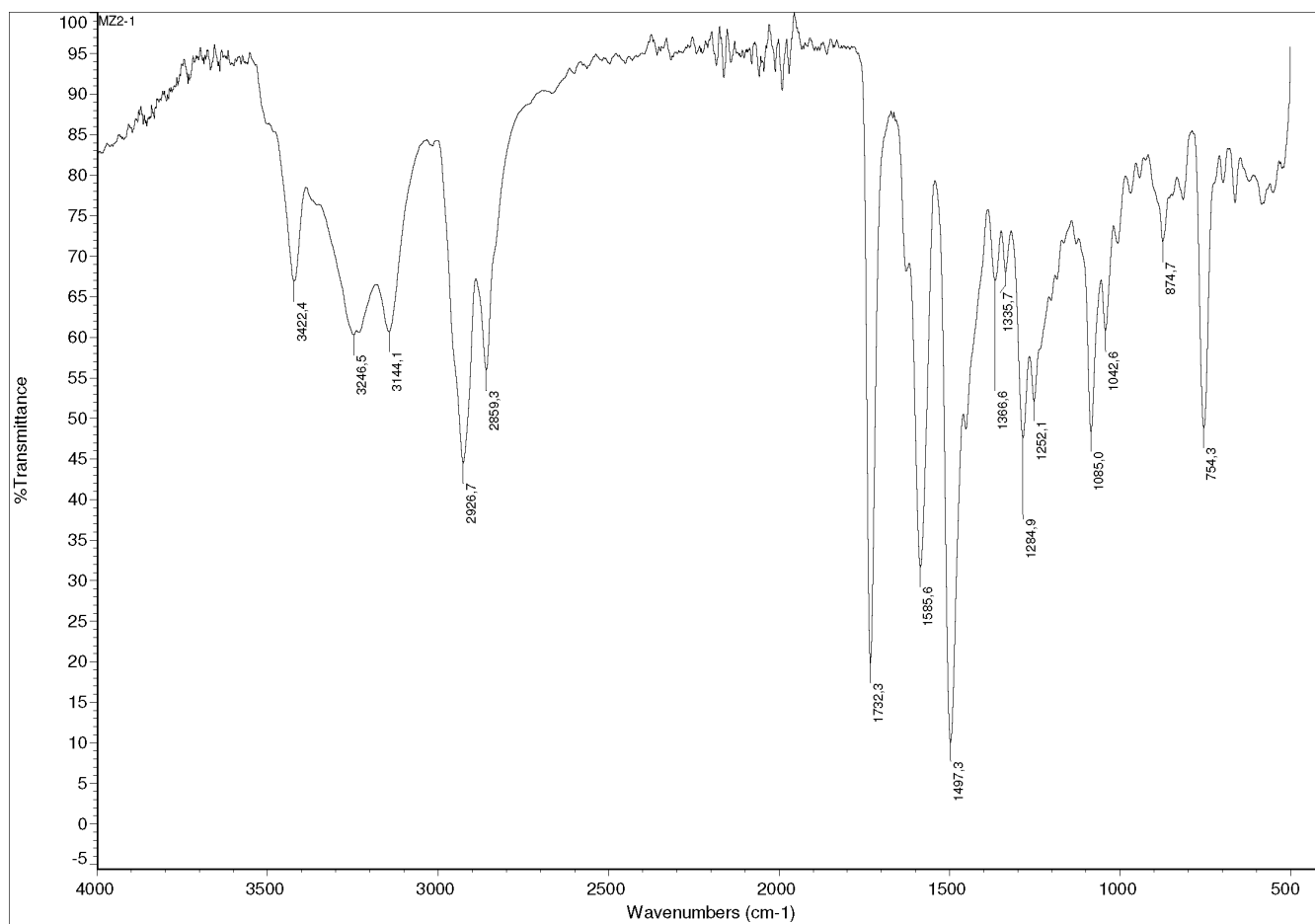
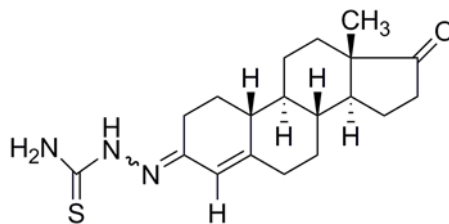
^aCenter for Chemistry, Institute of Chemistry, Technology and Metallurgy, University of Belgrade, Studentski trg 12-16, P. O. Box 473, 11001 Belgrade, Republic of Serbia

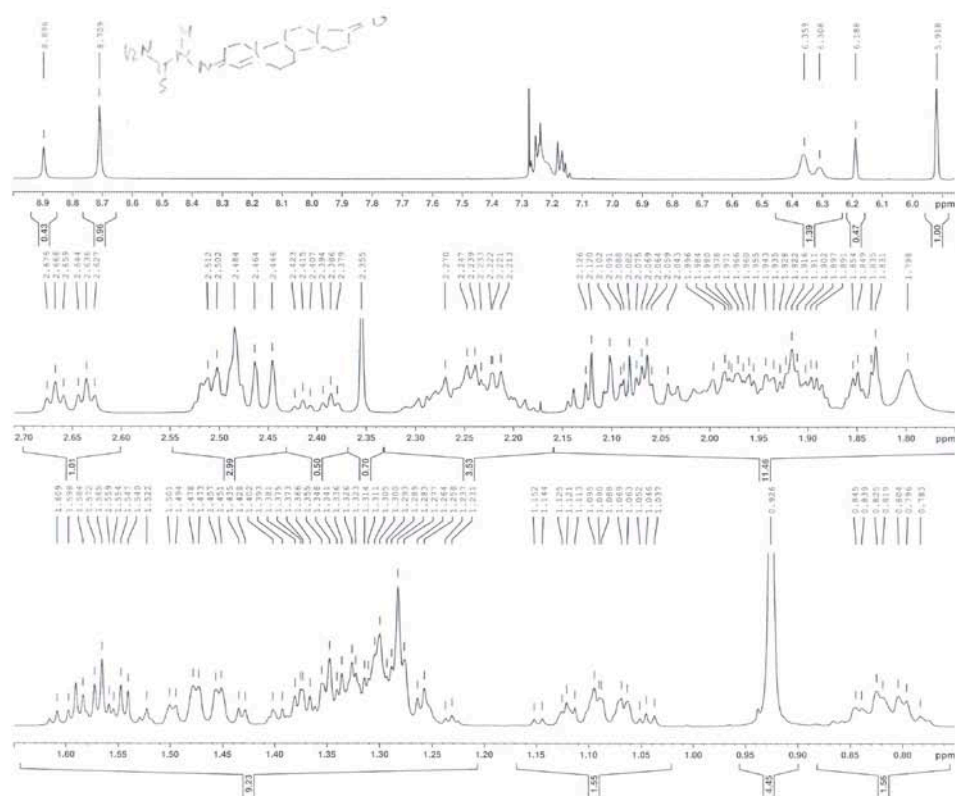
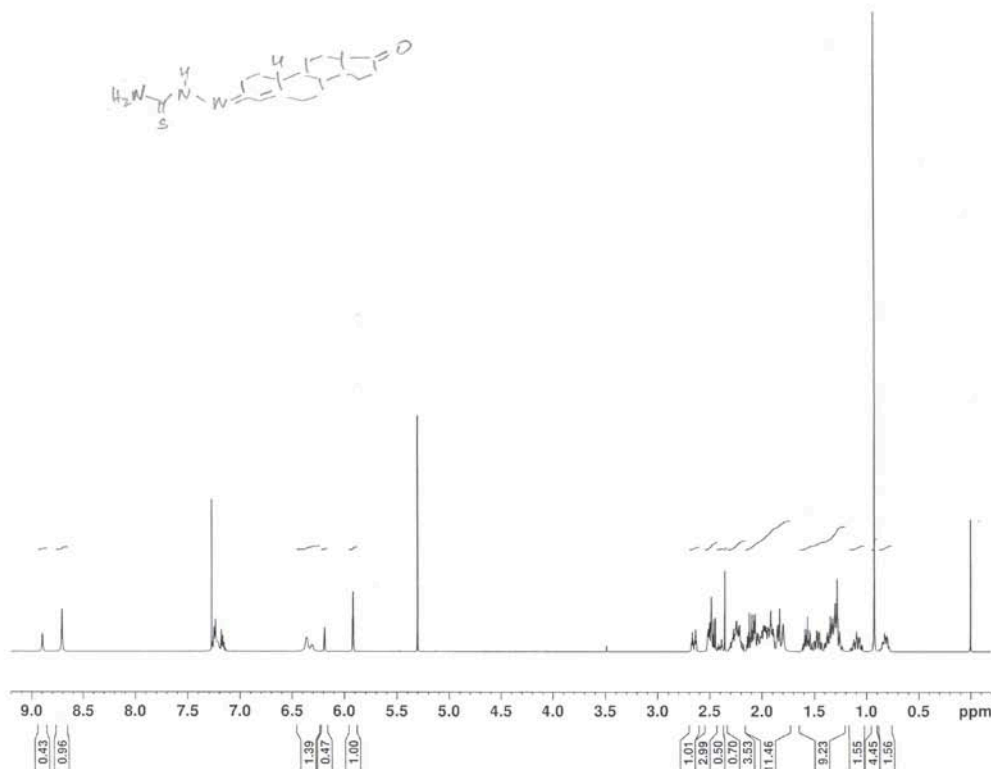
^bInstitute for Oncology and Radiology of Serbia, Pasterova 14, 11000 Belgrade, Republic of Serbia

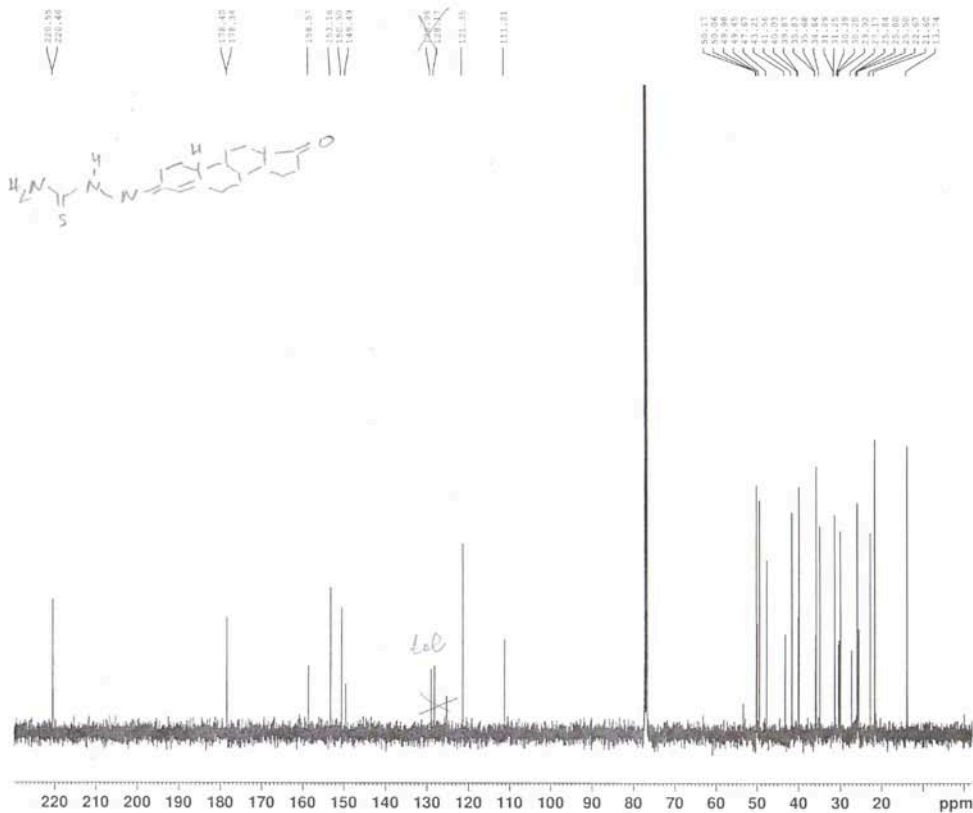
^cFaculty of Sciences, University of Novi Sad, Trg D. Obradovića 3, 21000 Novi Sad, Republic of Serbia

^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 2
PROCNO 1

F2 - Acquisition Parameters

Date_ 20140602
Time 11.52
INSTRUM spect
PROBHD 5 mm BBO BB-1H
PULPROG zgpg30
TD 32768
SOLVENT CDCl3
NS 257
DS 4
SWH 32694.738 Hz
FIDRES 1.003868 Hz
AQ 0.4980736 sec
RG 1030
DW 15.200 usec
DE 6.50 usec
TE 298.0 K
D1 2.00000000 sec
D11 0.03000000 sec
TD0 1

===== CHANNEL f1 =====

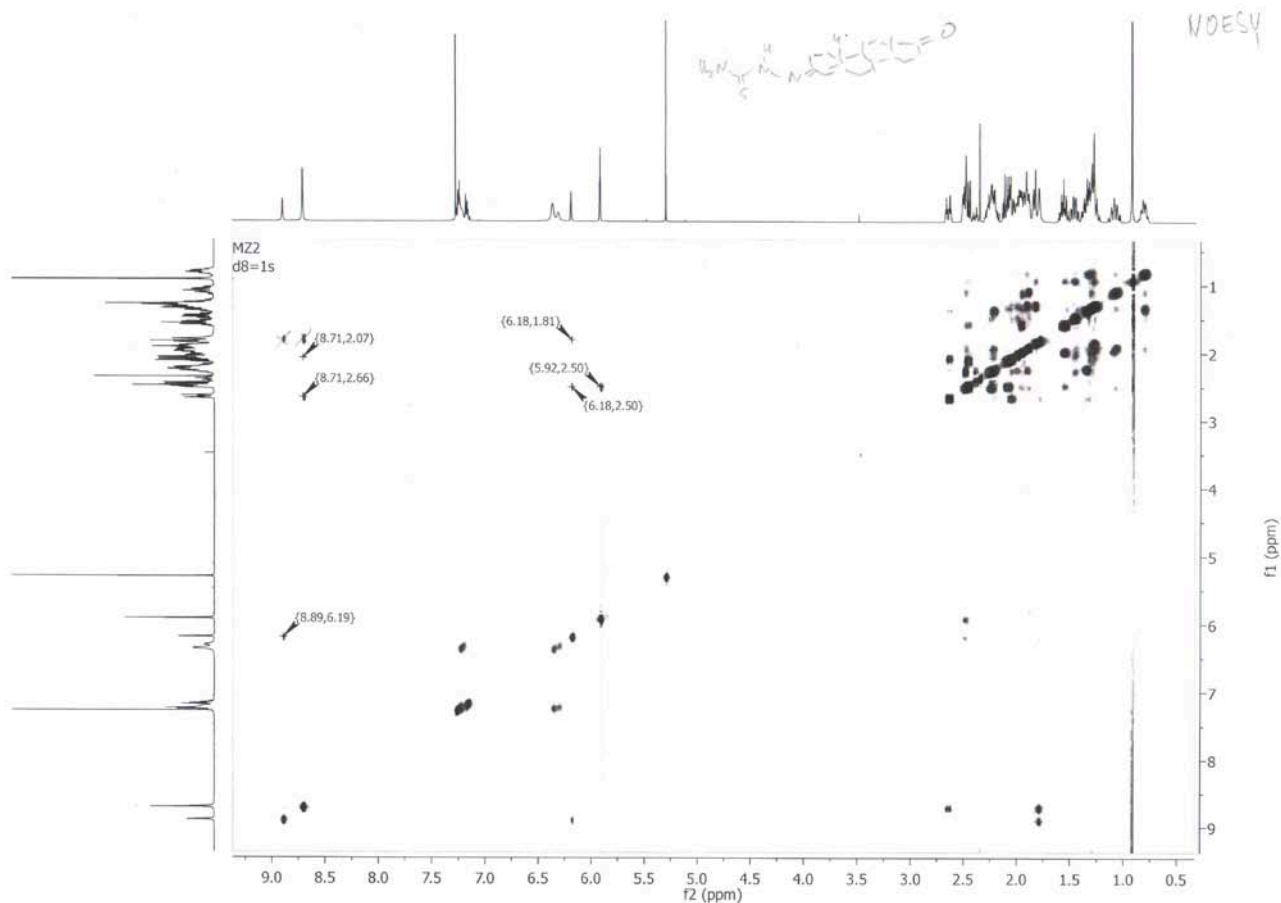
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NUC1 13C
P1 11.50 usec
PLM1 32.22800064 W

===== CHANNEL f2 =====

SFO2 500.2623242 MHz
NUC2 1H
CTDPRG12 waltz16
PCPD2 80.00 usec
PLM2 20.77000046 W
PLM12 0.38267001 W
PLM13 0.25130999 W

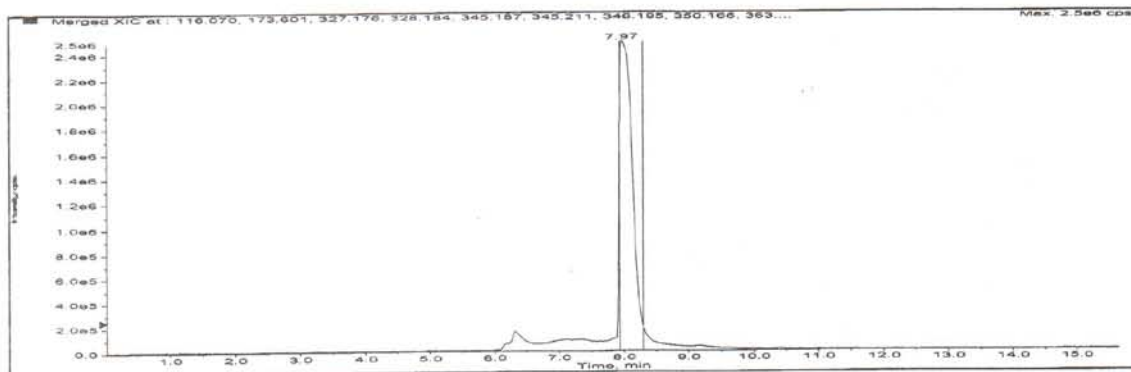
F2 - Processing parameters

SF 125.7904843 MHz
WDW EM
SSB 0
LS 1.50 Hz
GB 0
PC 1.40

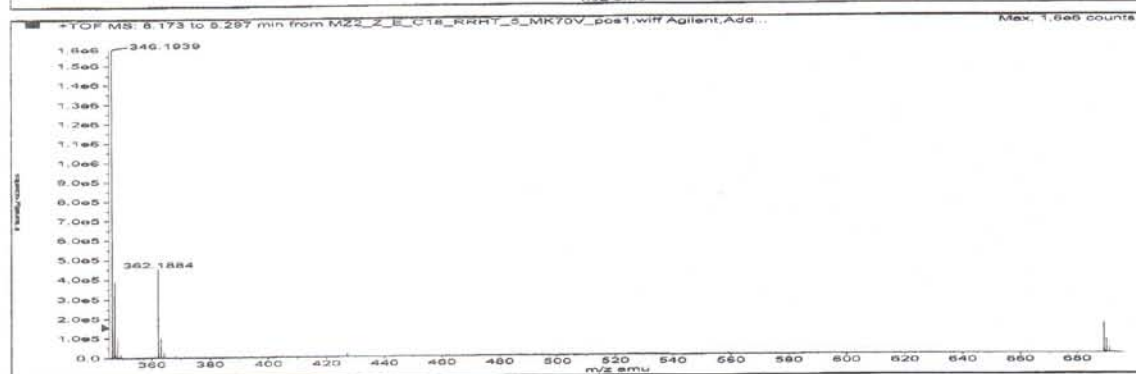
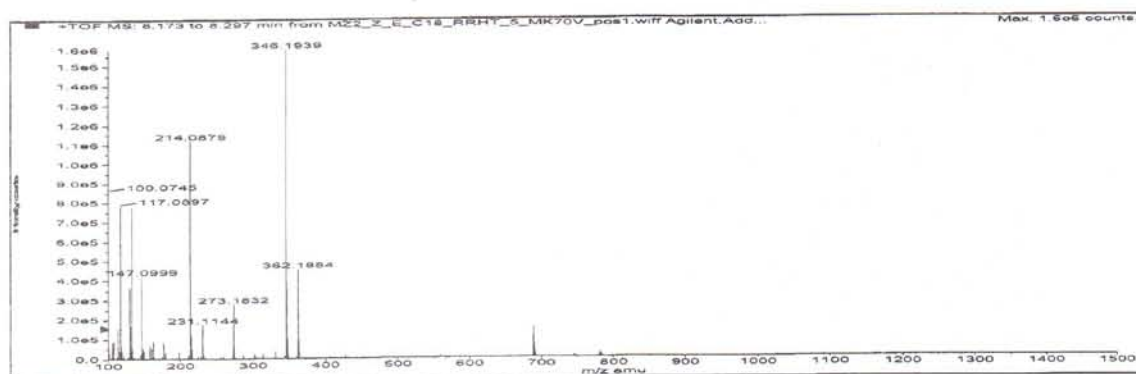


Sample Name: MZ2 Sample Location: P1-C6 Sample Id: Operator: Milka
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One or more scans have failed IRM. Review the data file for details.

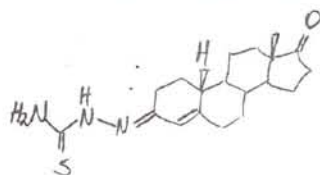


Merged XIC, Period# : 1 Experiment# : 1

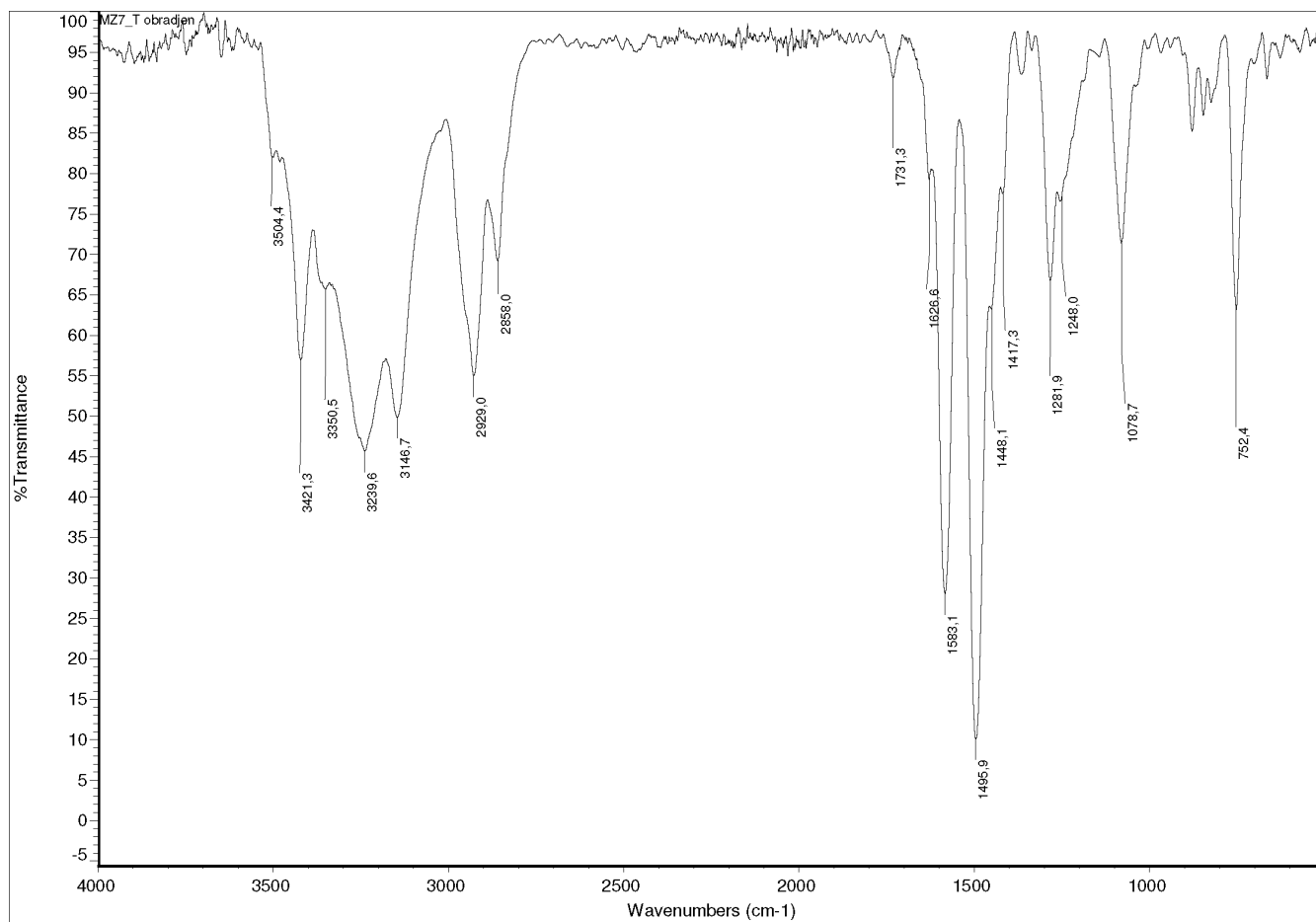
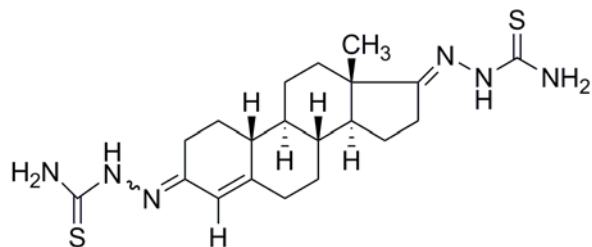


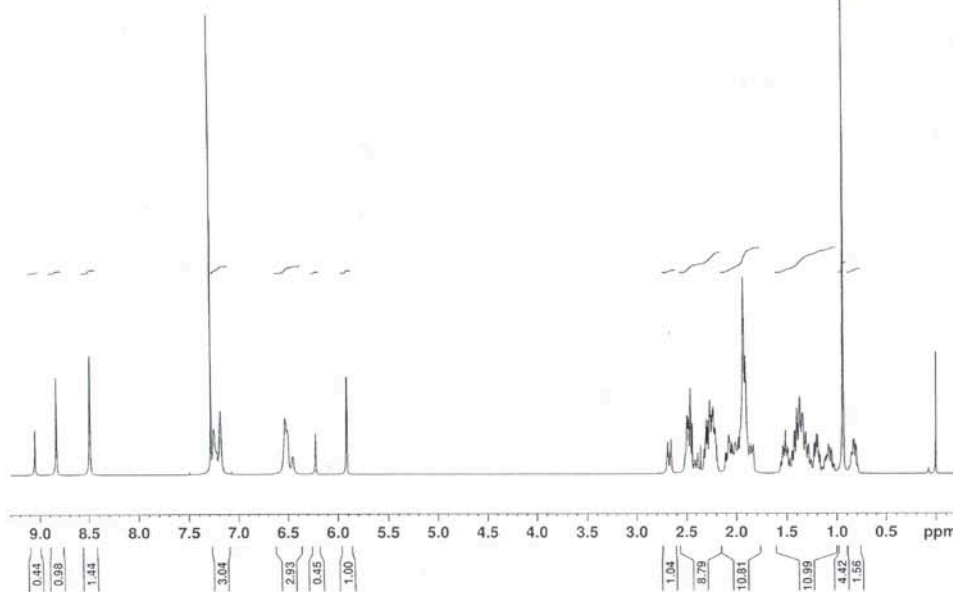
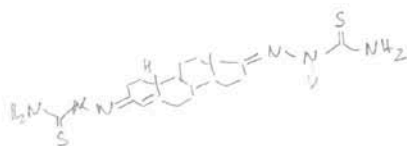
Formula	Compound name	Mass	Peak RT. (min)	Peak area	Description
C ₁₉ H ₂₇ N ₃ O ₅	—	345.18748	7.97	3.42837 E7	—

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] ⁺	98766.91	363.22131	363.19179	-29.52256	-81.20	—
[2M+H] ⁺	29112.46	691.38224	691.36763	-14.60880	-21.13	—



Compound 3a



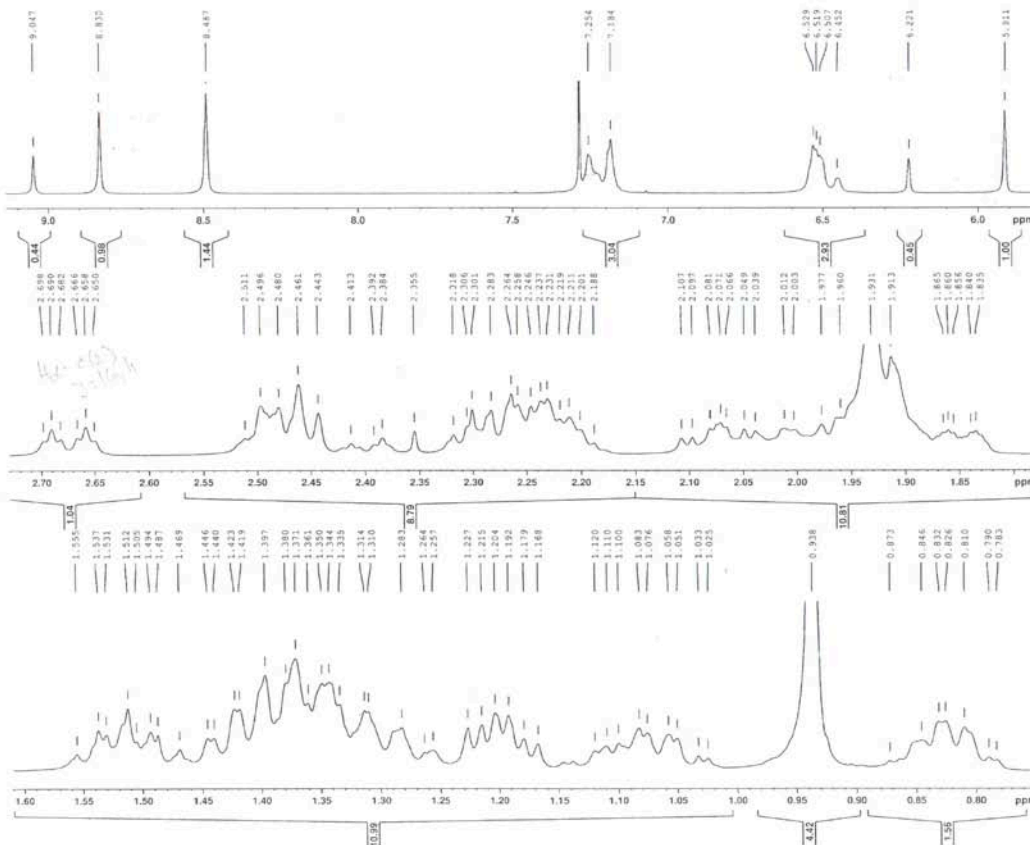


Current Data Parameters
NAME MD7
EXPNO 1
PROCNO 1

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Date_ 20140602
Time 13.55
INSTRUM spect
PROBHD 5 mm BBO BB-1H
PULPROG zg30
TD 32768
SOLVENT CDCl3
NS 16
DS 6
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
NUC1 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

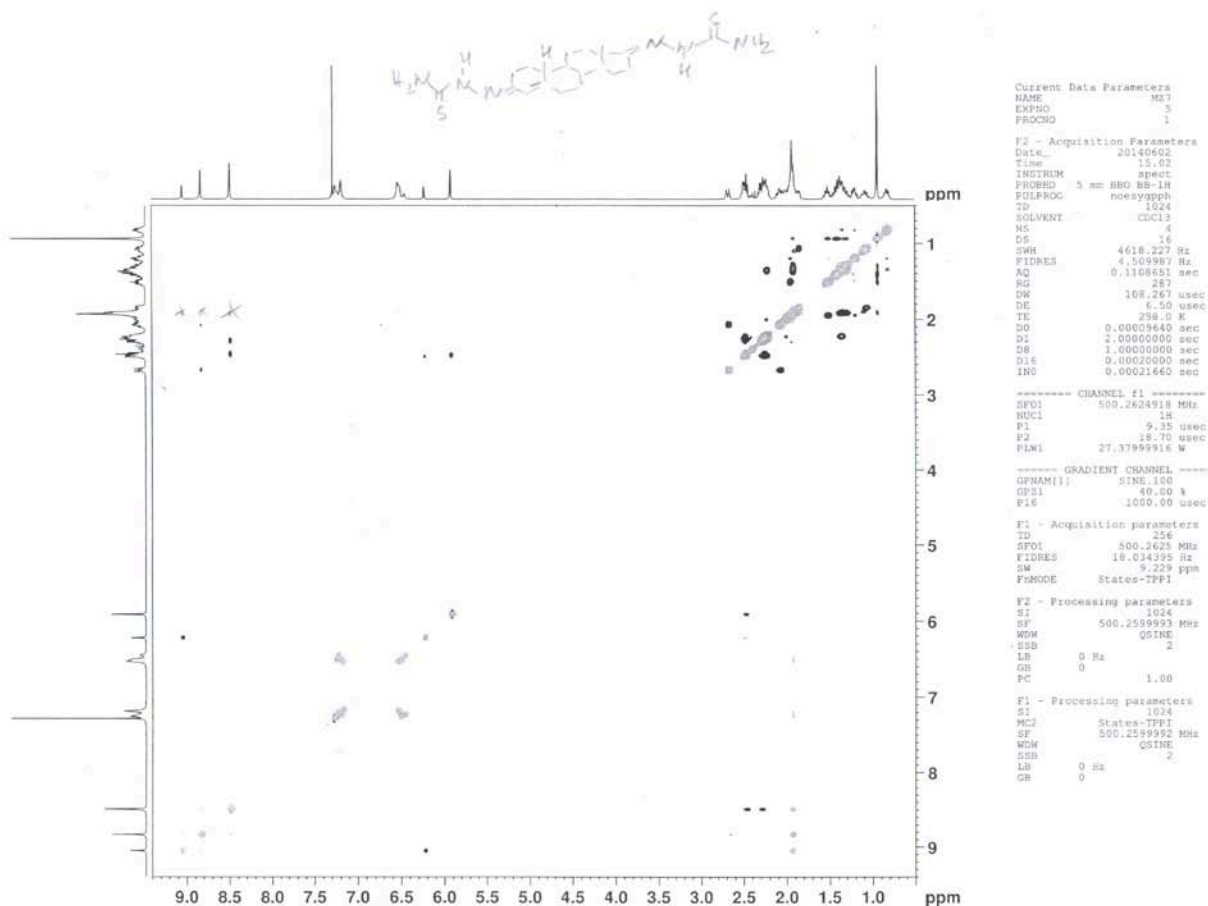
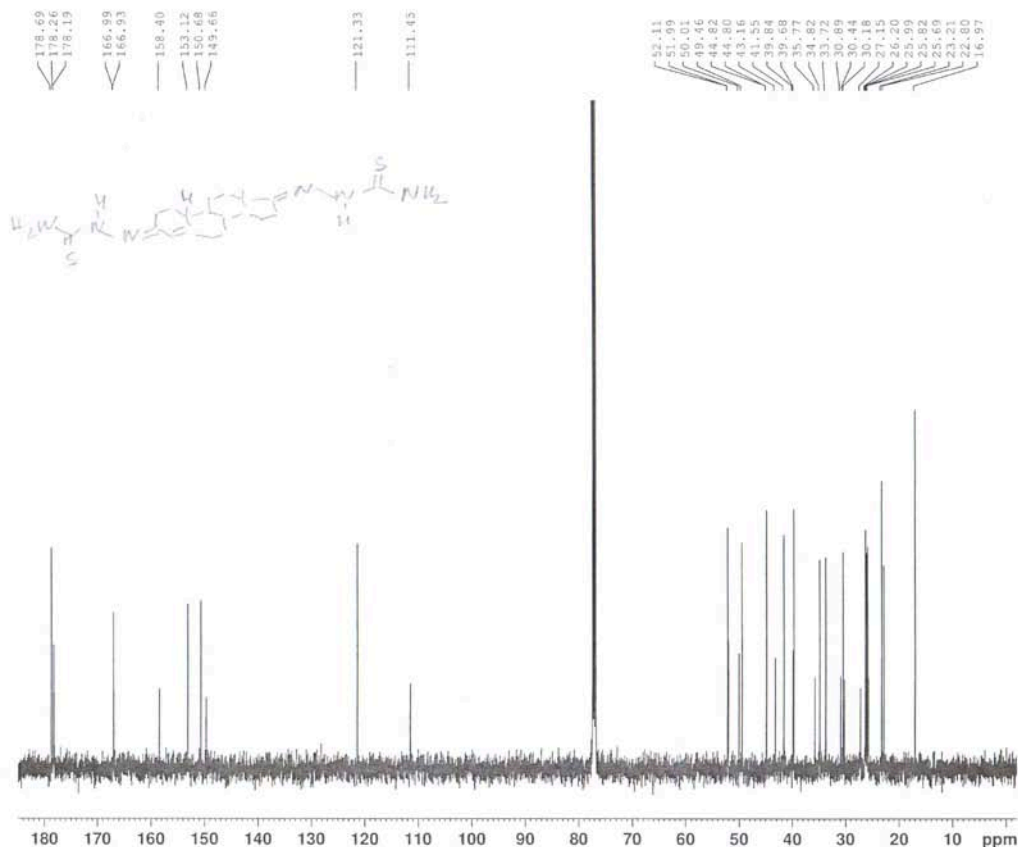


Current Data Parameters
NAME MD7
EXPNO 1
PROCNO 1

F2 - Acquisition Parameters
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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

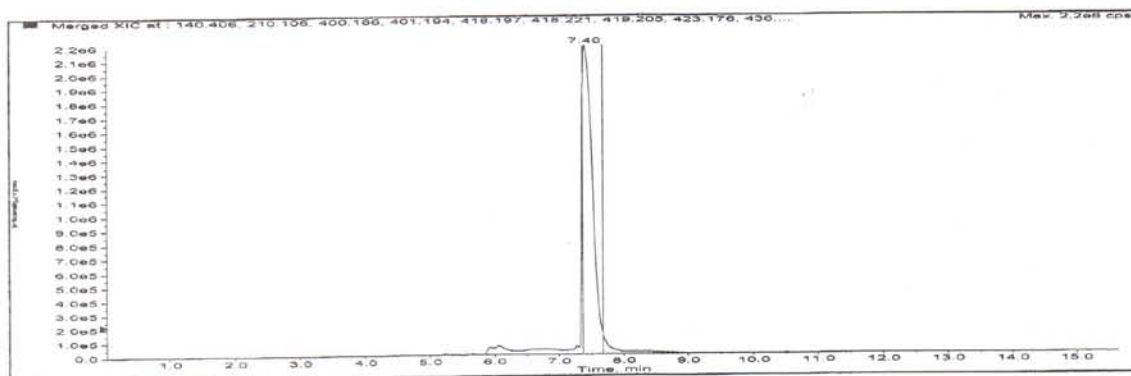
----- CHANNEL f1 -----
SFO1 500.2623246 MHz
NUC1 1H
P1 9.35 usec
PLW1 27.37999916 W

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

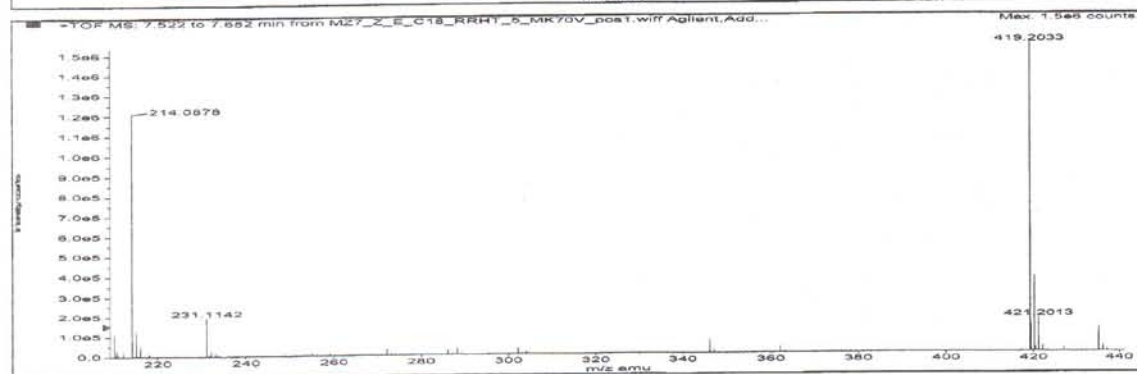
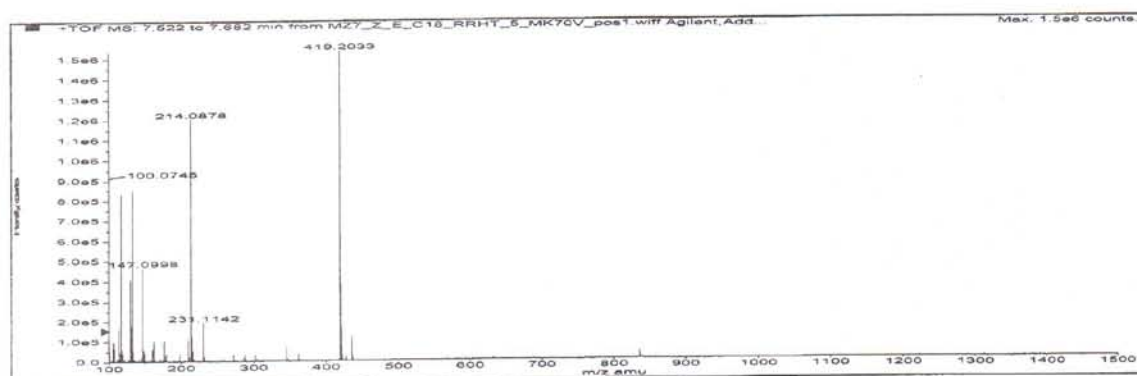


Sample Name: MZ7 Sample Location: P1-C8 Sample Id: Operator: Milka
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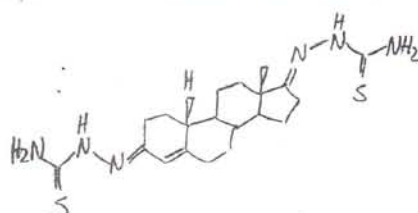
Merged XIC, Period#: 1 Experiment#: 1



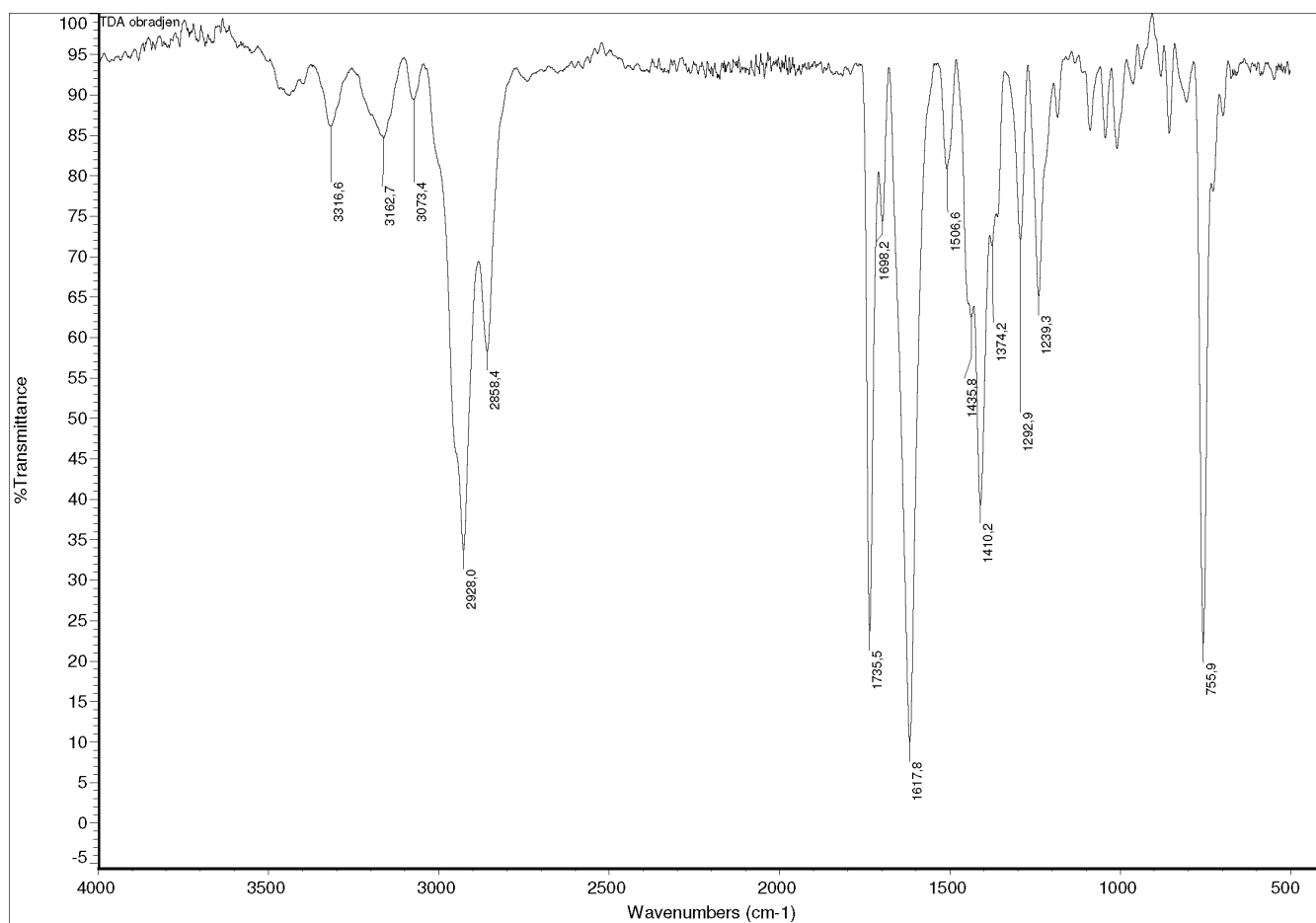
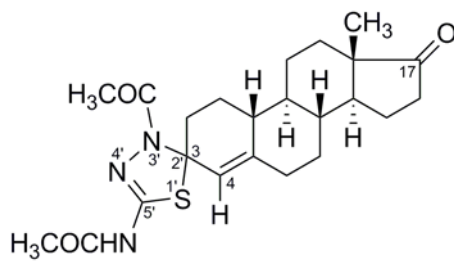
Formula	Compound name	Mass	Peak RT (min)	Peak area	Description
C20H30N6S2	-	418.19734	7.40	2.50483 E7	-

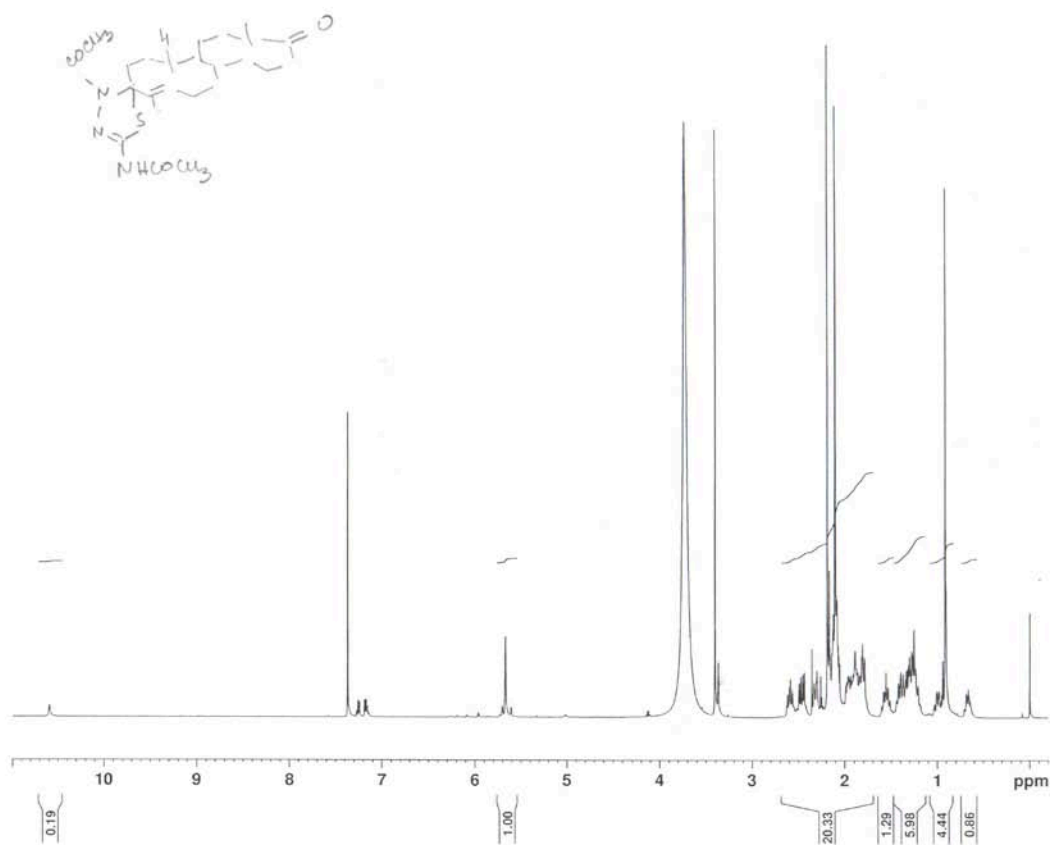
Species	Abundance (counts)	Ion Mass	Measured Mass	Error (mDa)	Error (ppm)	Ret. Time Error (min)
[M+2H] ²⁺	110876.65	210.10594	210.10428	-1.66827	-7.94	
[M+H] ⁺	1536715.77	419.20461	419.20335	-1.26756	-3.02	
[M+NH4] ⁺	29241.75	436.23116	436.20049	-30.67147	-70.32	

OK, MZ



Compound 4a





Current Data Parameters

NAME	MZ11
EXPNO	1
PROCNO	1

F2 - Acquisition Parameters

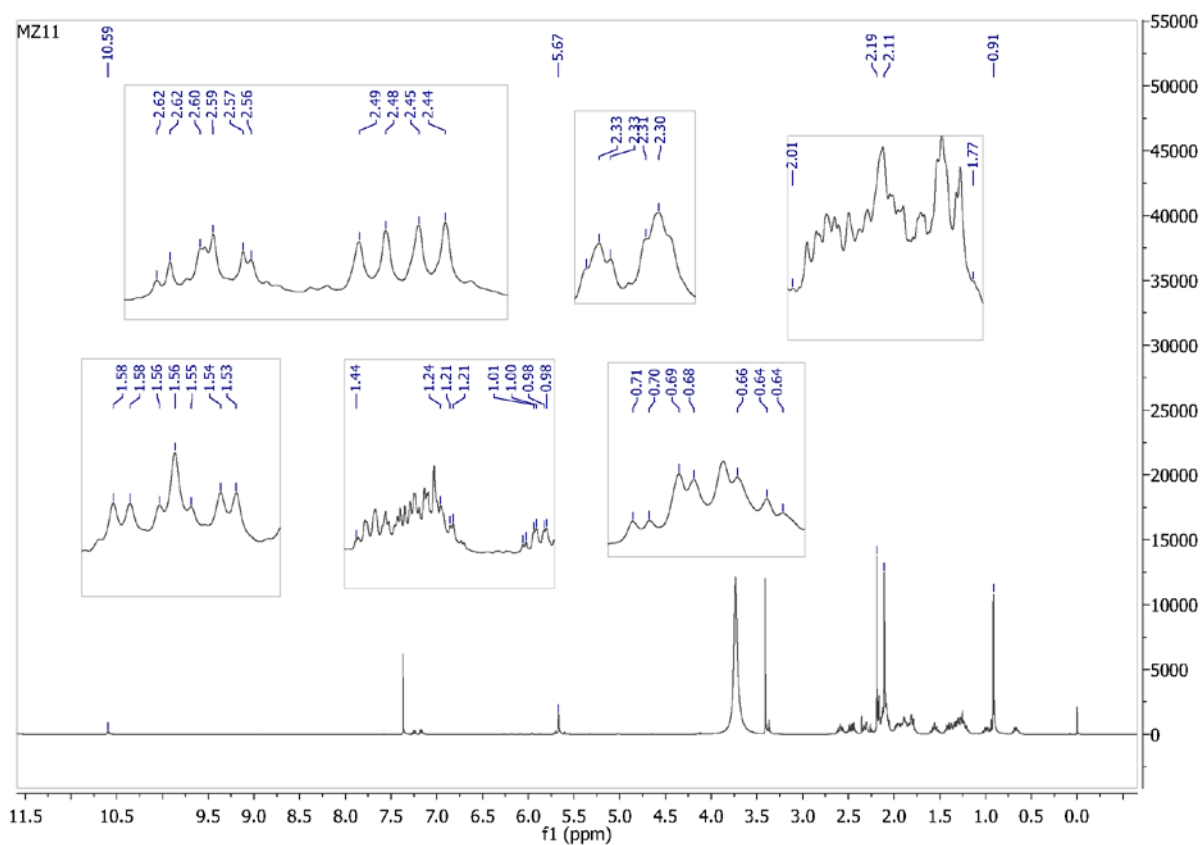
Date_	20140604
Time	14.30
INSTRUM	spnc
PROBHD	5 mm BBO BB-1H
PULPROG	zg30
TD	32768
SOLVENT	CDCl3
NS	32
DS	0
SWH	6127.451 Hz
FIDRES	0.186995 Hz
AQ	2.6738689 sec
RG	128
DW	81.600 usec
DE	8.50 usec
TE	298.0 K
D1	2.00000000 sec
TDC	1

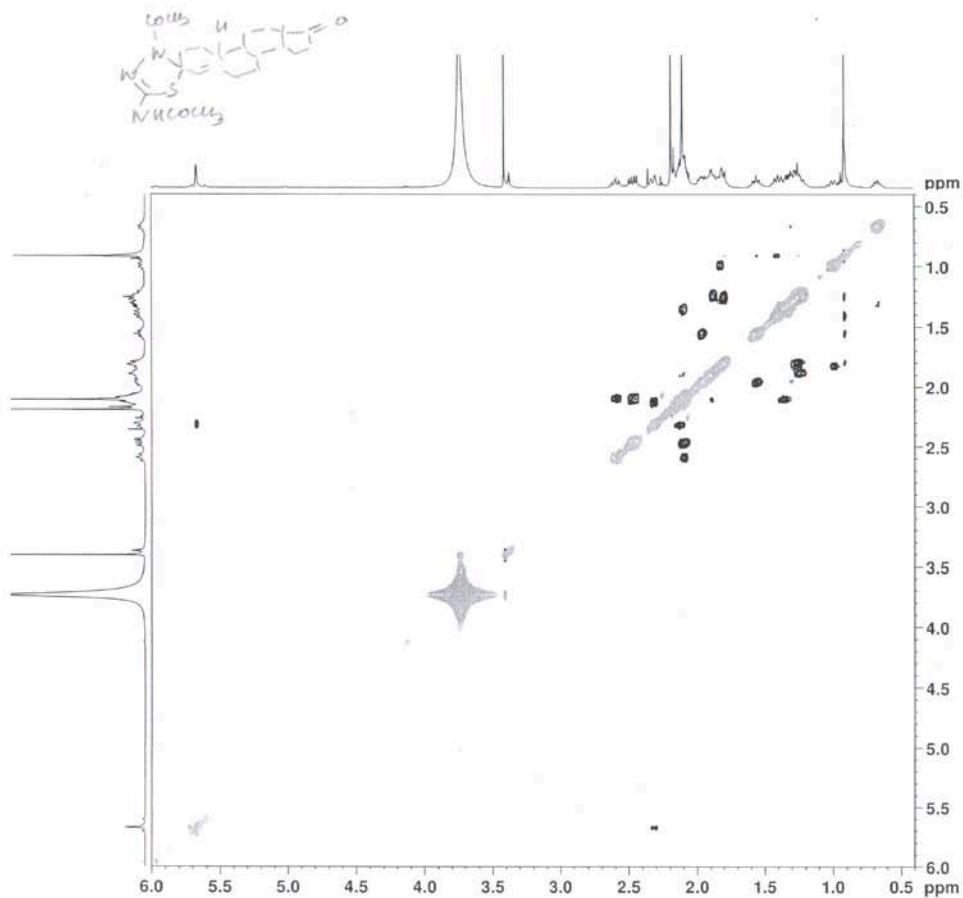
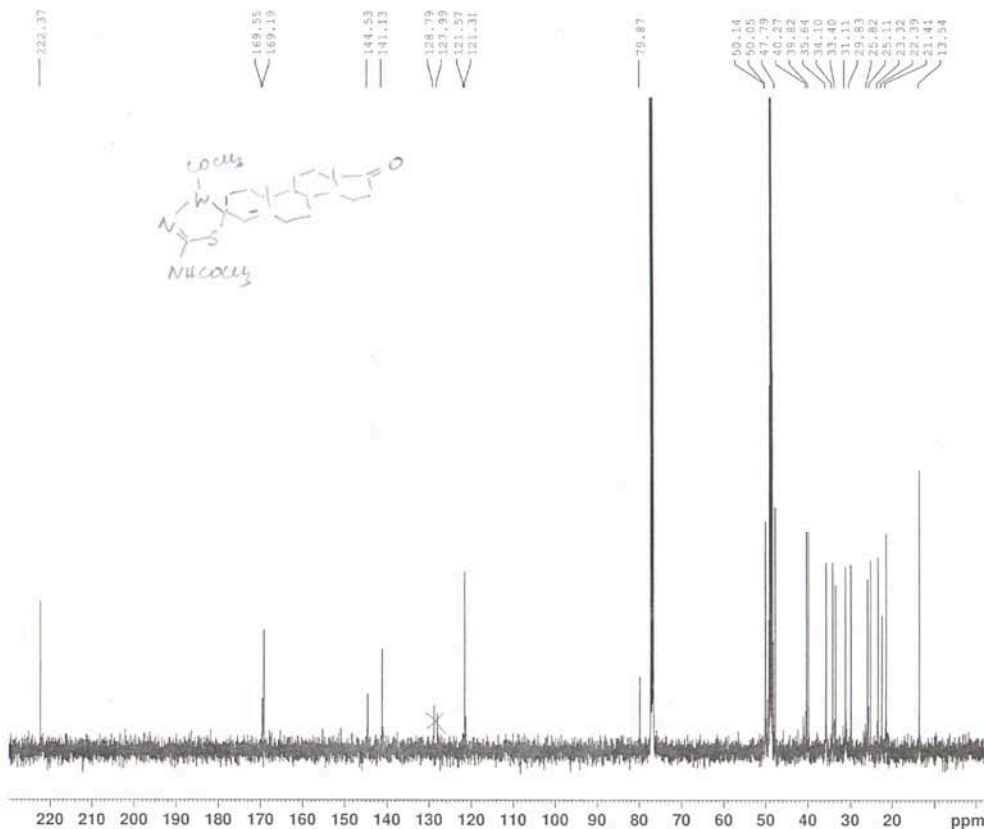
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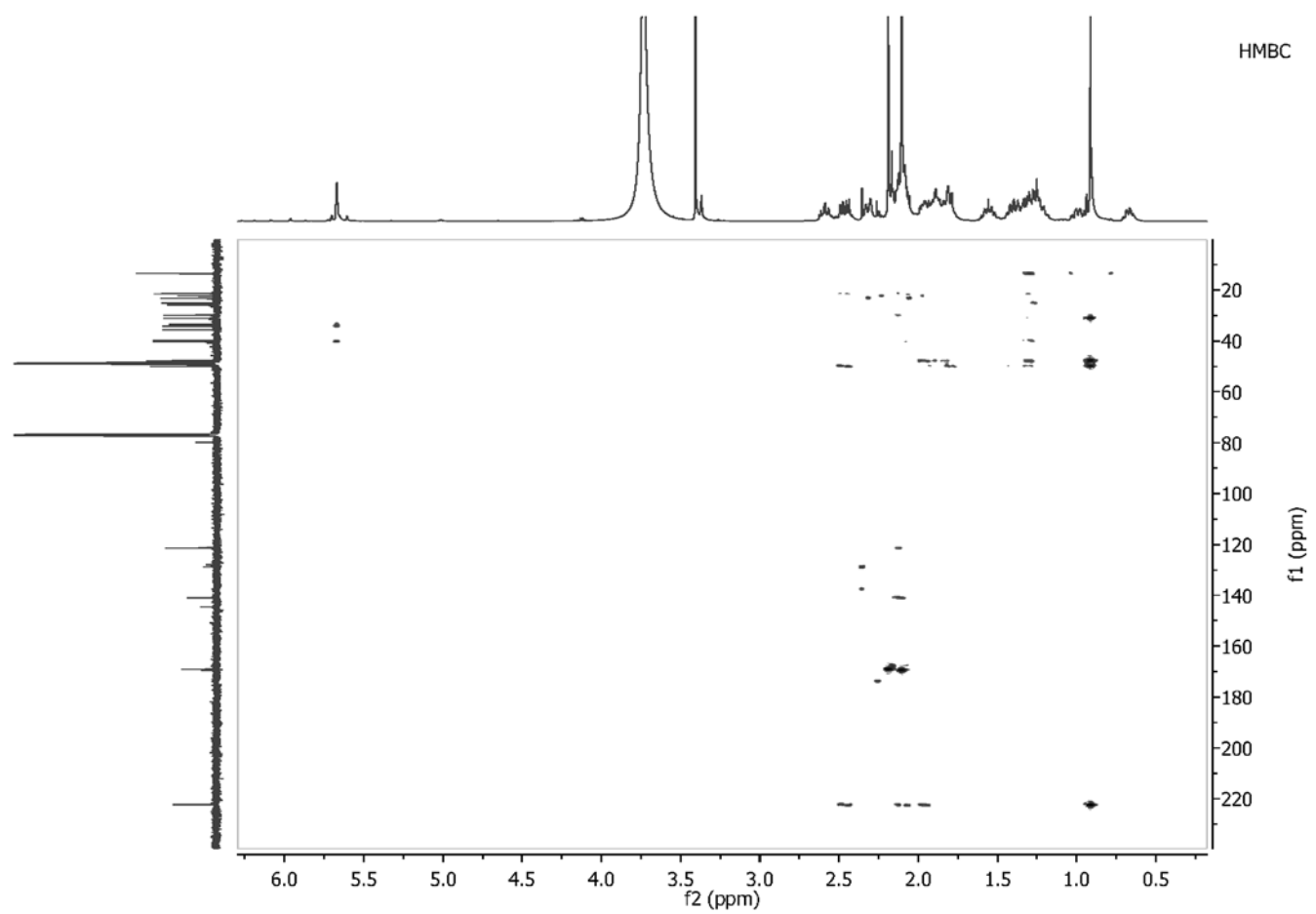
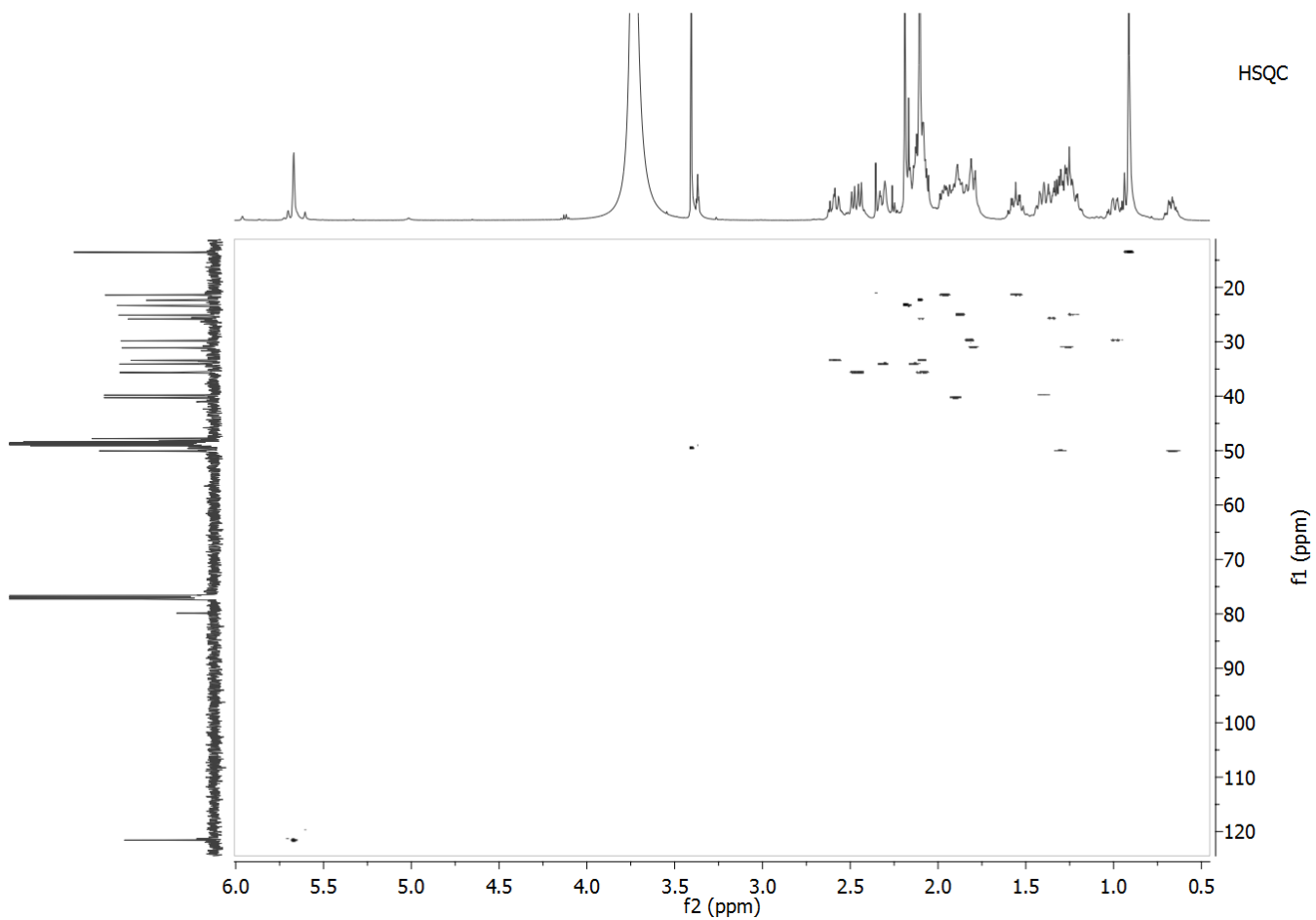
SFO1	500.2626919 MHz
NUC1	1H
P1	9.15 usec
PLW1	27.37999916 W

F2 - Processing parameters

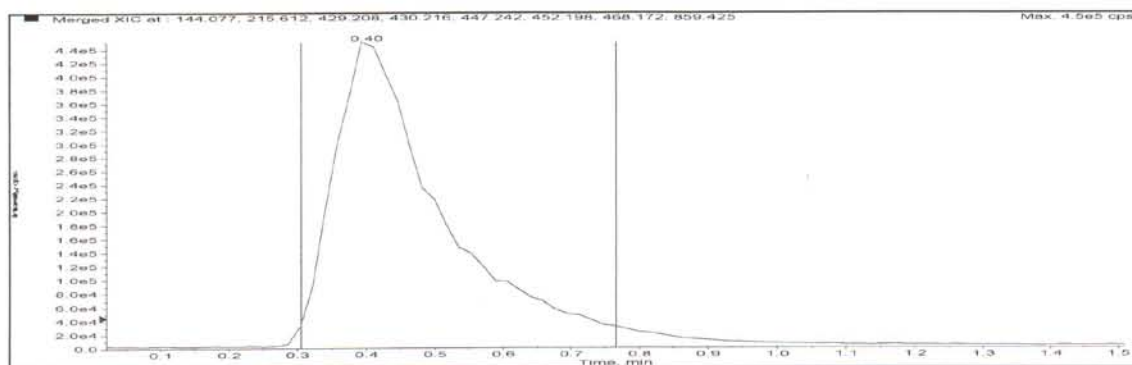
SI	32768
SF	500.2599573 MHz
WDW	EM
SSB	0
LB	0.20 Hz
CB	0
PC	1.00



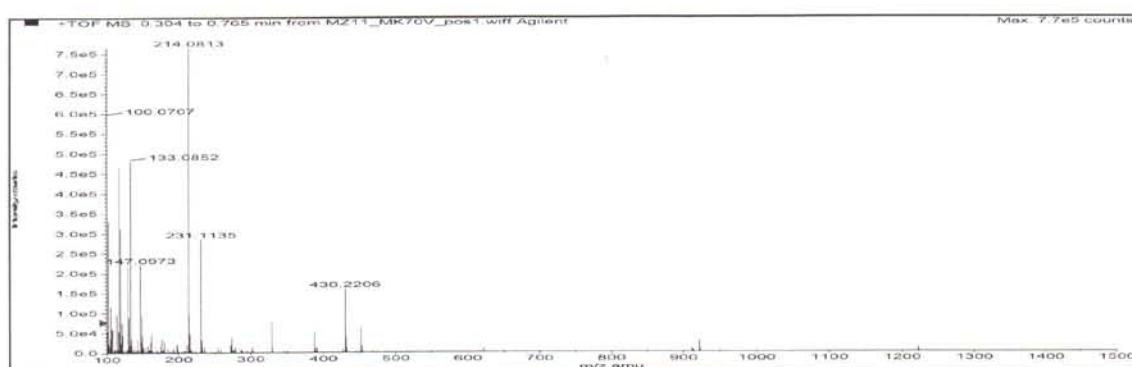




Sample Name: MZ11 Sample Location: P1-C1 Sample Id: Operator: Milka
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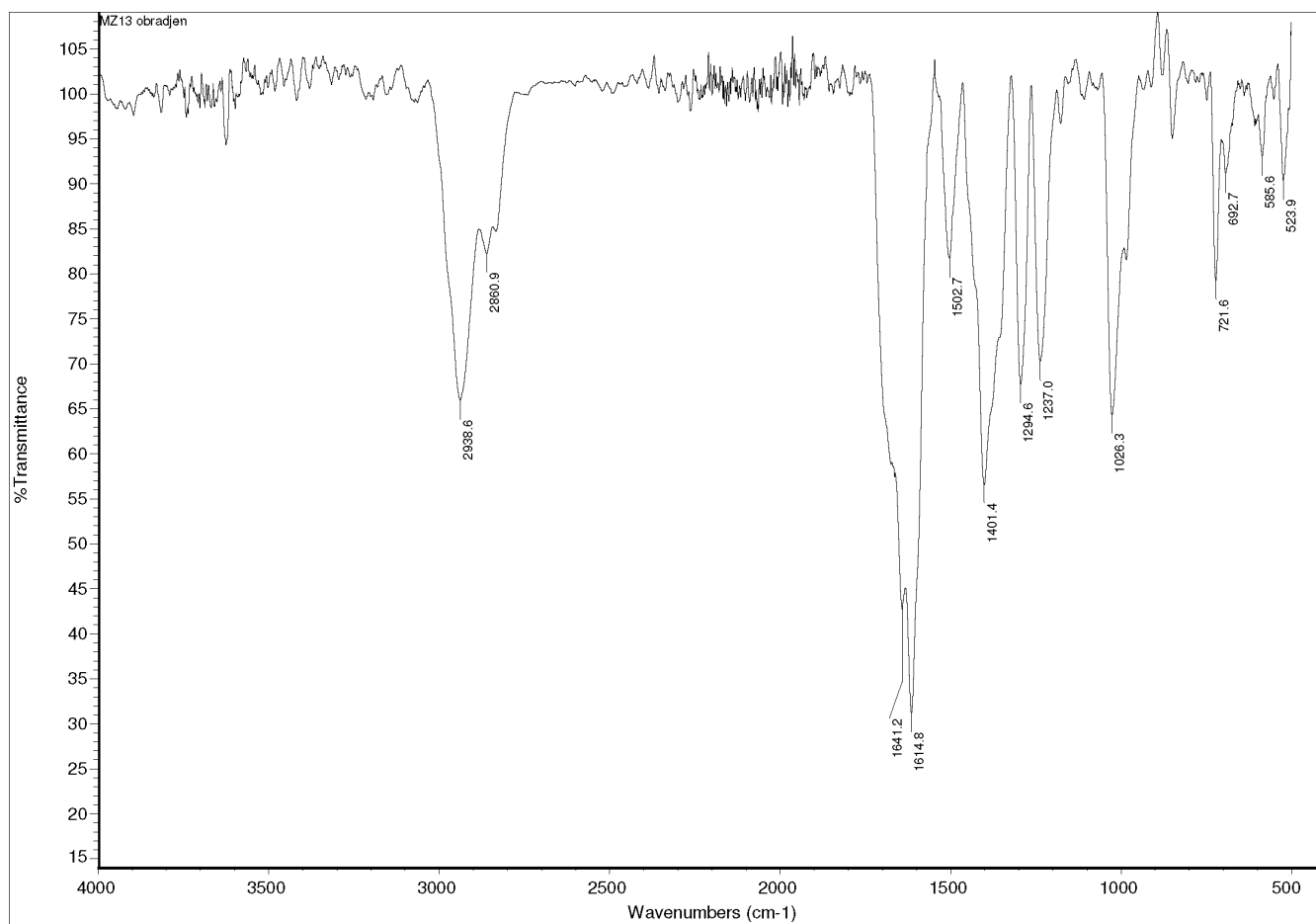
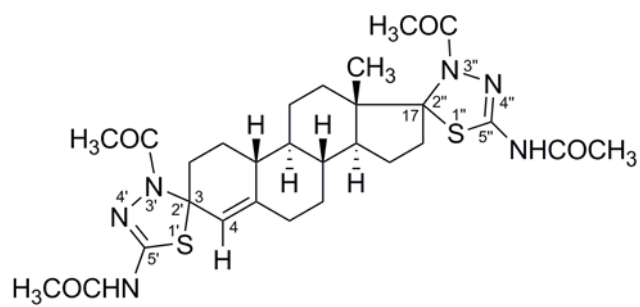
Merged XIC, Period# : 1 Experiment# : 1

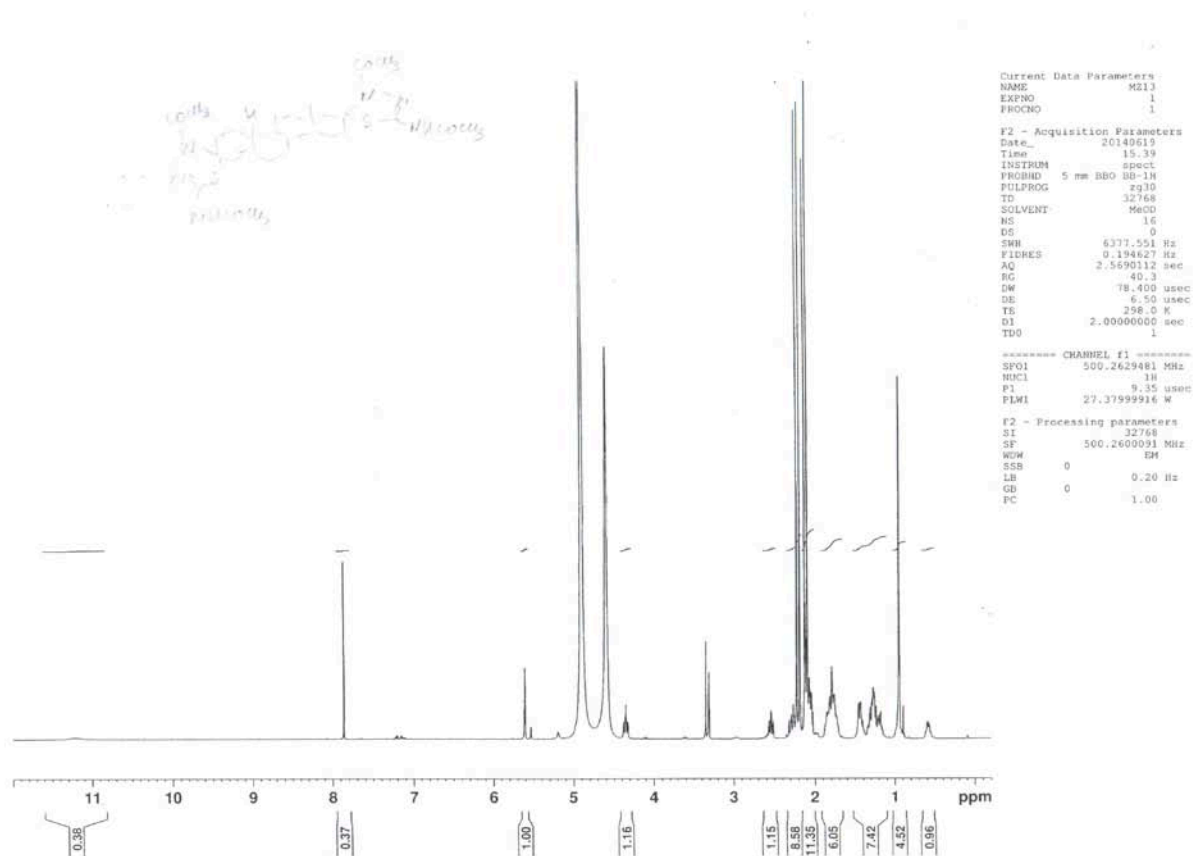


Formula	Compound name	Mass	Peak RT (min)	Peak area	Description
C23H31N3O3S	—	429.20861	0.40	4.98363 E6	—

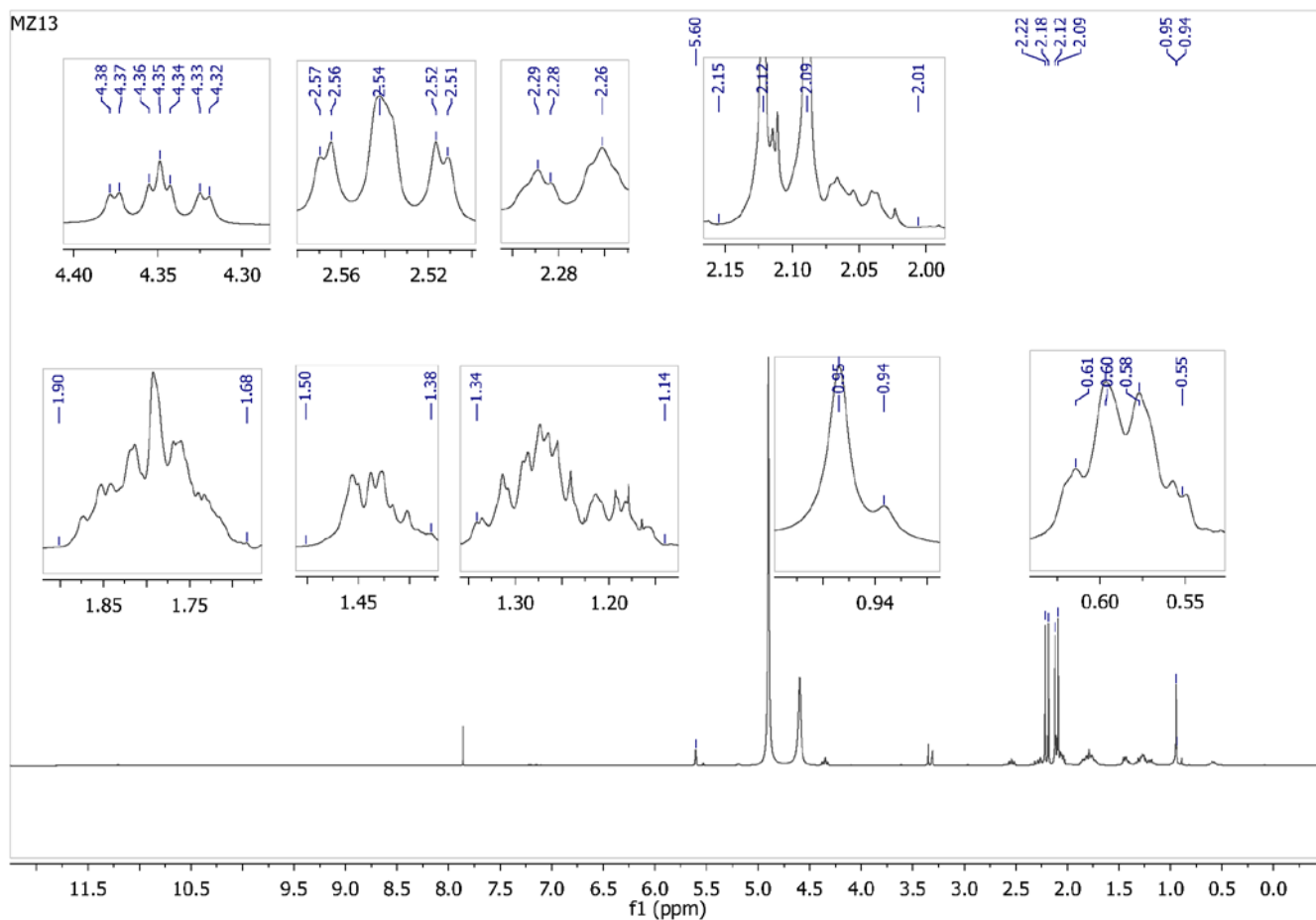
Species	Abundance (counts)	Ion Mass	Measured Mass	Error (mDa)	Error (ppm)	Ret. Time Error (min)
[M+H] ⁺	162128.32	430.21589	430.21581	-0.08124	-0.19	—
[M+Na] ⁺	63766.11	452.19783	452.19790	0.06355	0.14	—

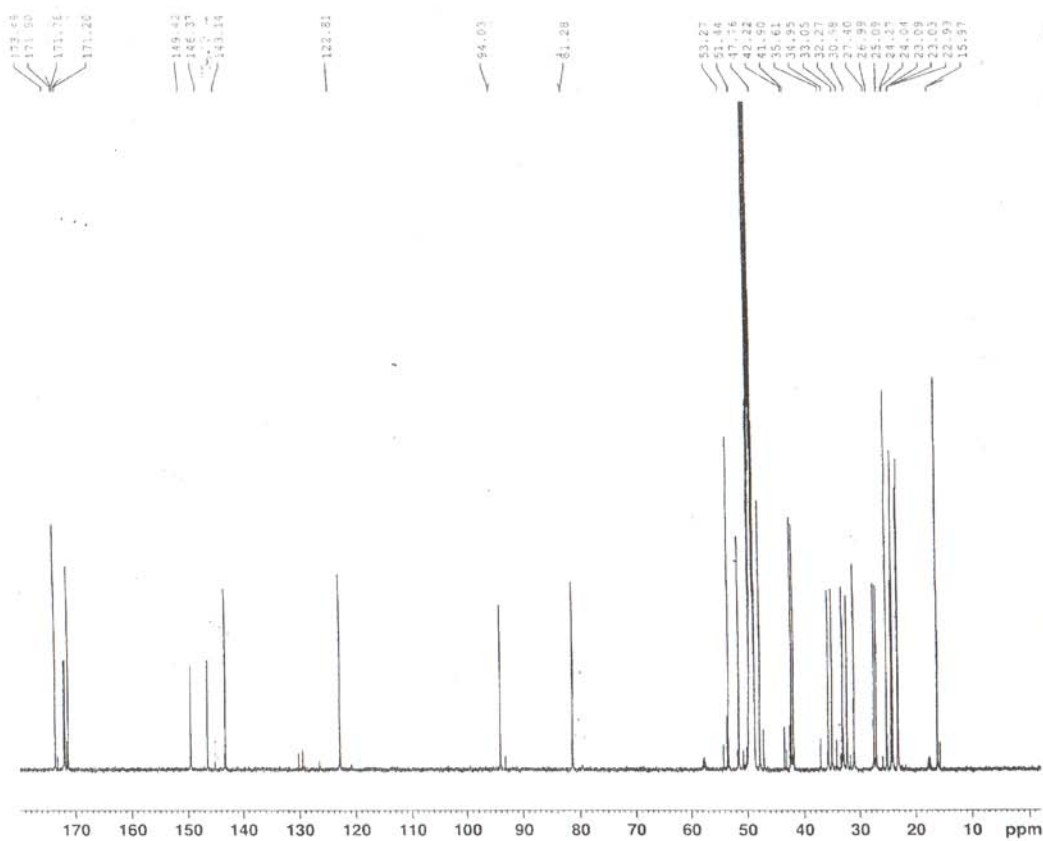
Compound 5a





MZ13





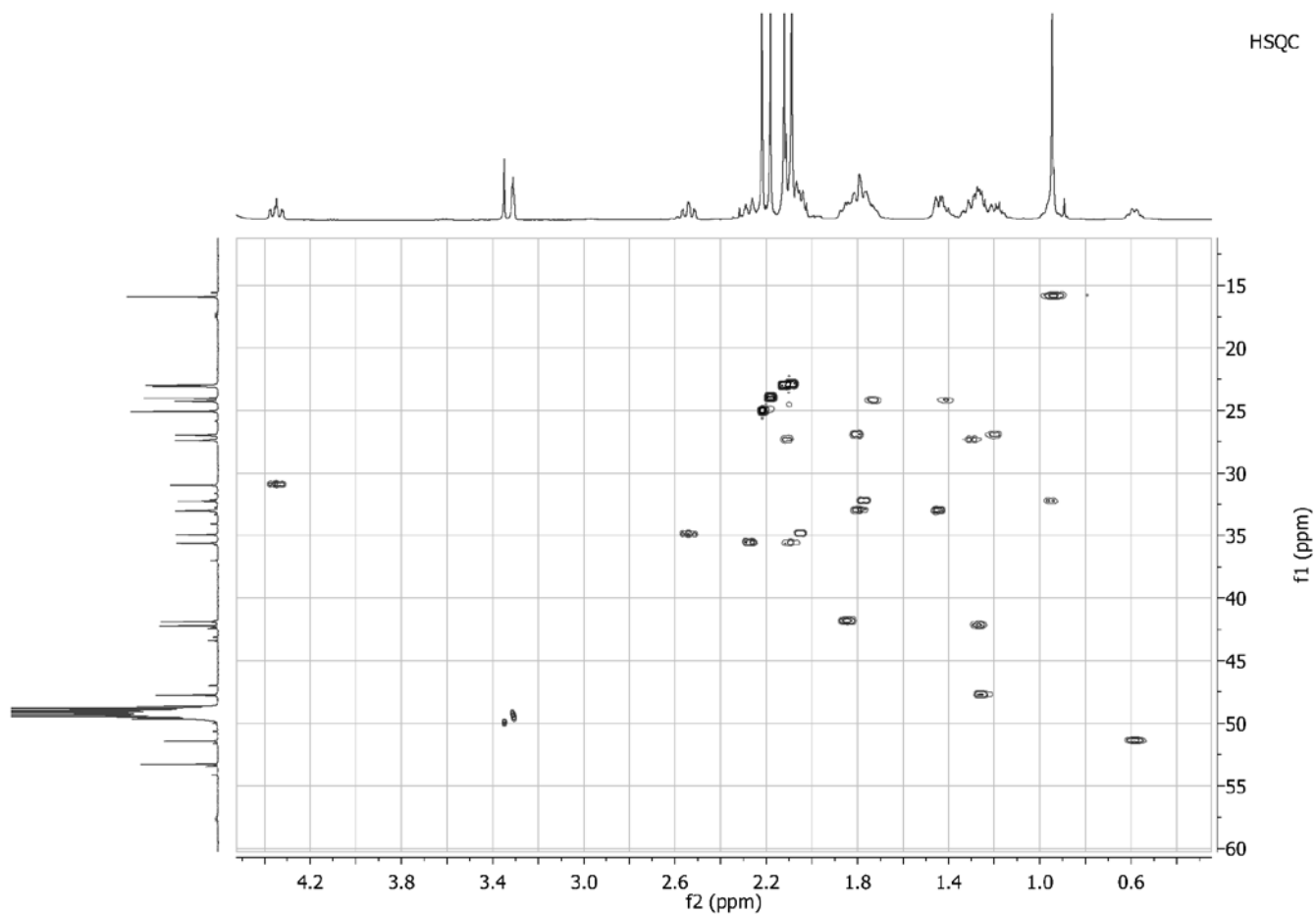
Current Data Parameters
NAME M213
EXPNO 6
PROCNO 1

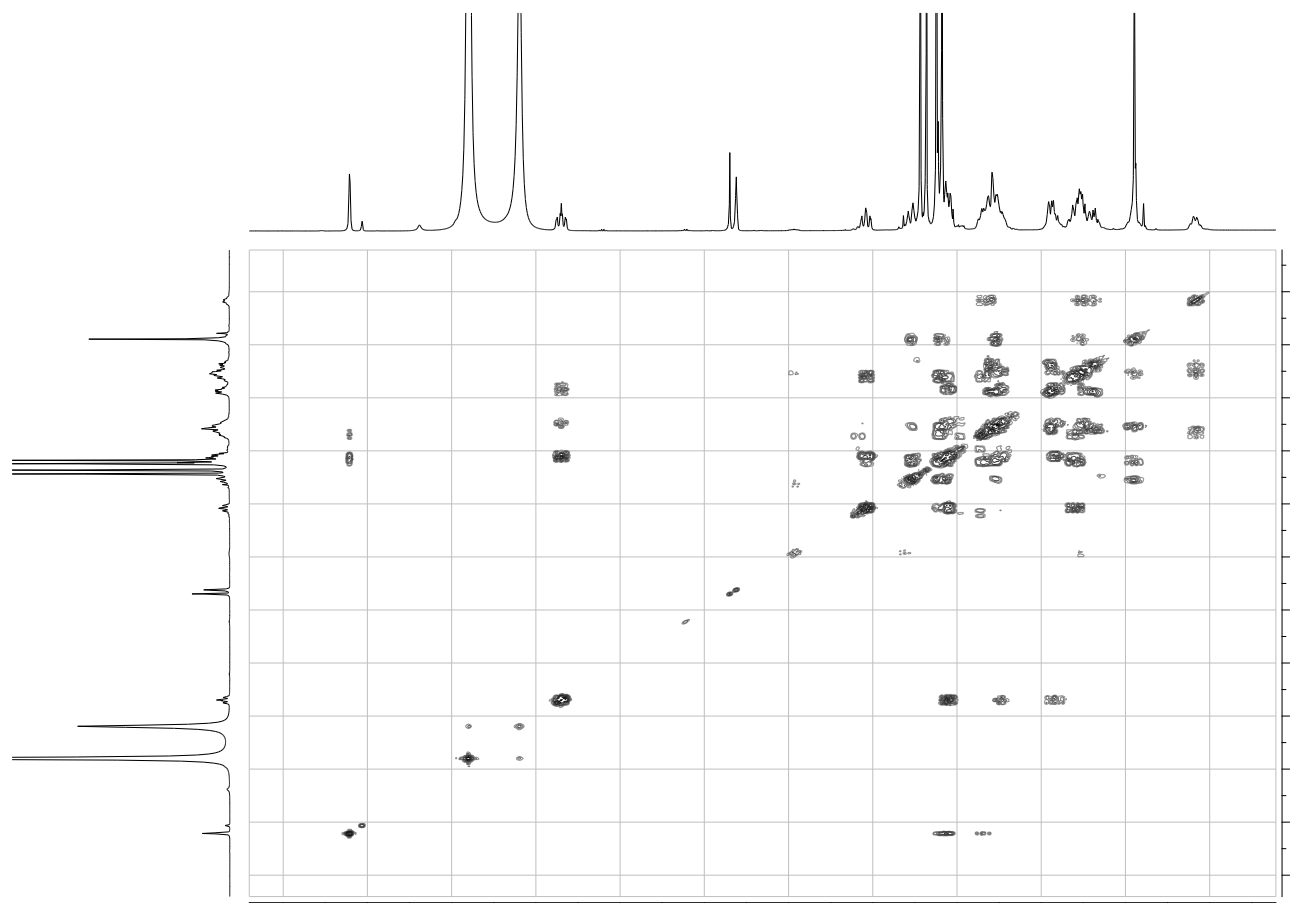
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Date_ 20140620
Time 8.53
INSTRUM spect
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PULPROG zgpg30
TD 32768
SOLVENT MeOD
NS 6197
DS 4
SWH 32894.738 Hz
FIDRES 1.003868 Hz
AQ 0.4980736 sec
RG 2050
DW 15.200 usec
DE 6.50 usec
TE 298.0 K
D1 2.00000000 sec
D11 0.03000000 sec
TD0 1

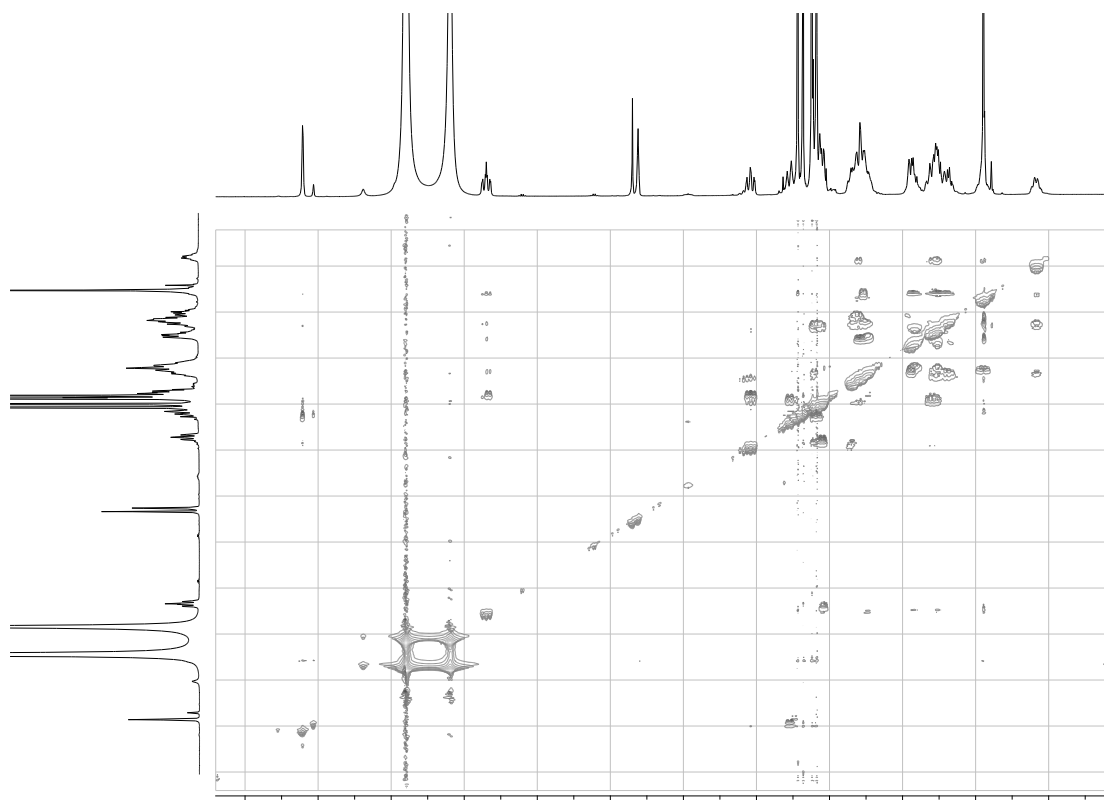
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NUC1 13C
P1 11.50 usec
PLW1 32.22800064 W

===== CHANNEL f2 =====
SFO2 500.2629480 MHz
NUC2 1H
CPDPRG12 waltz16
PCPD2 80.00 usec
PLW2 20.77000046 W
PLW12 0.39267001 W
PLW13 0.25130999 W

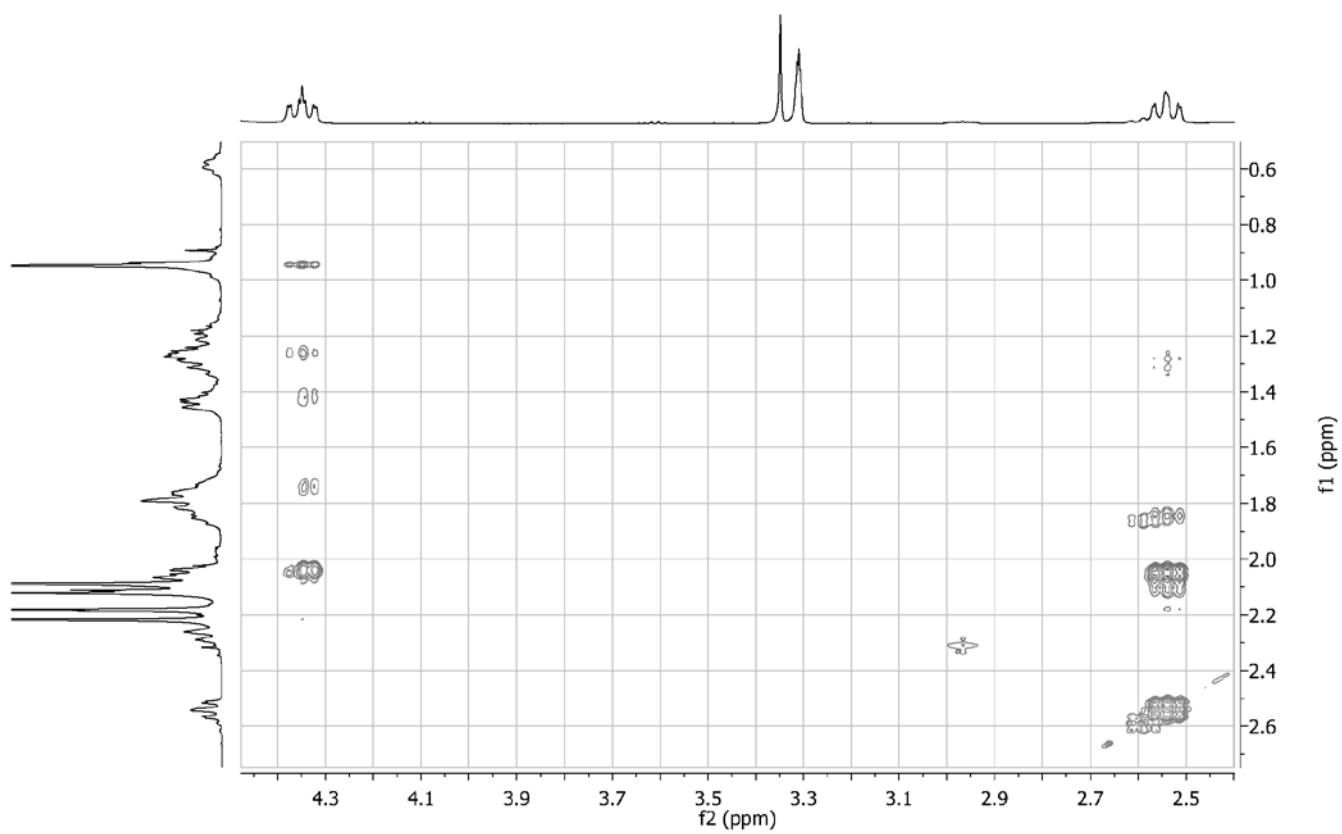
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SI 32768
SF 125.7902920 MHz
WDW EM
SSB 0
LB 1.50 Hz
GB 0
PC 1.40



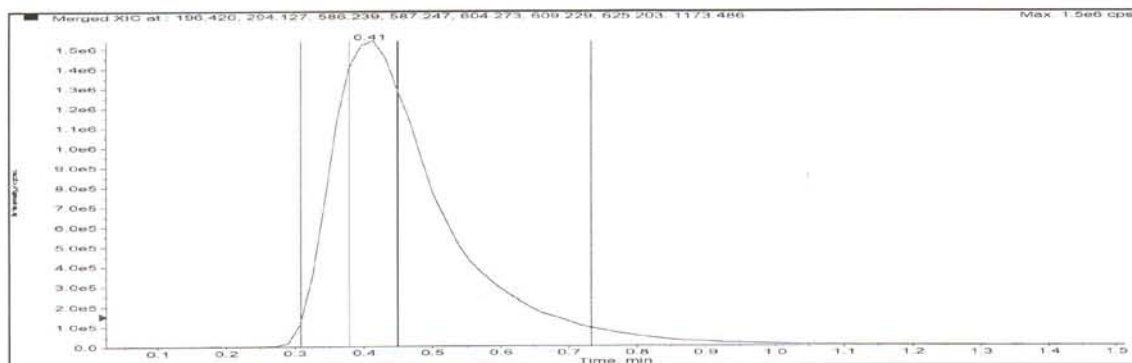




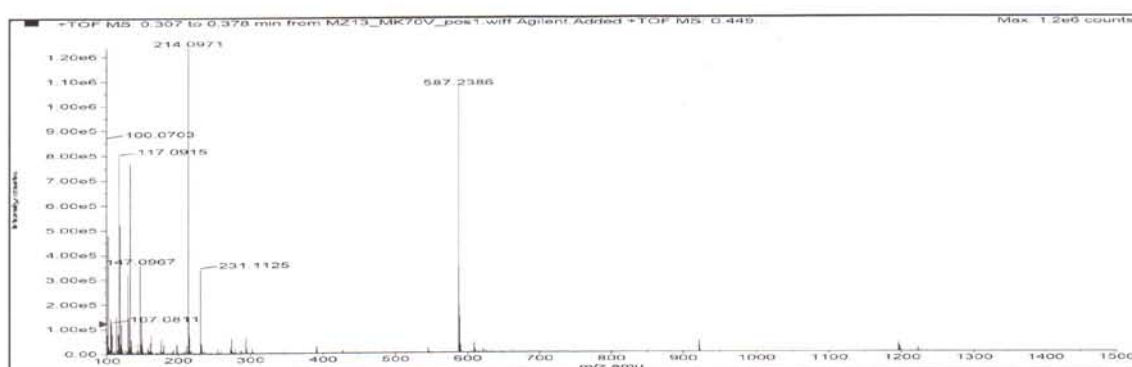
ROESY



Sample Name: MZ13 Sample Location: P1-C3 Sample Id: Operator: Milka
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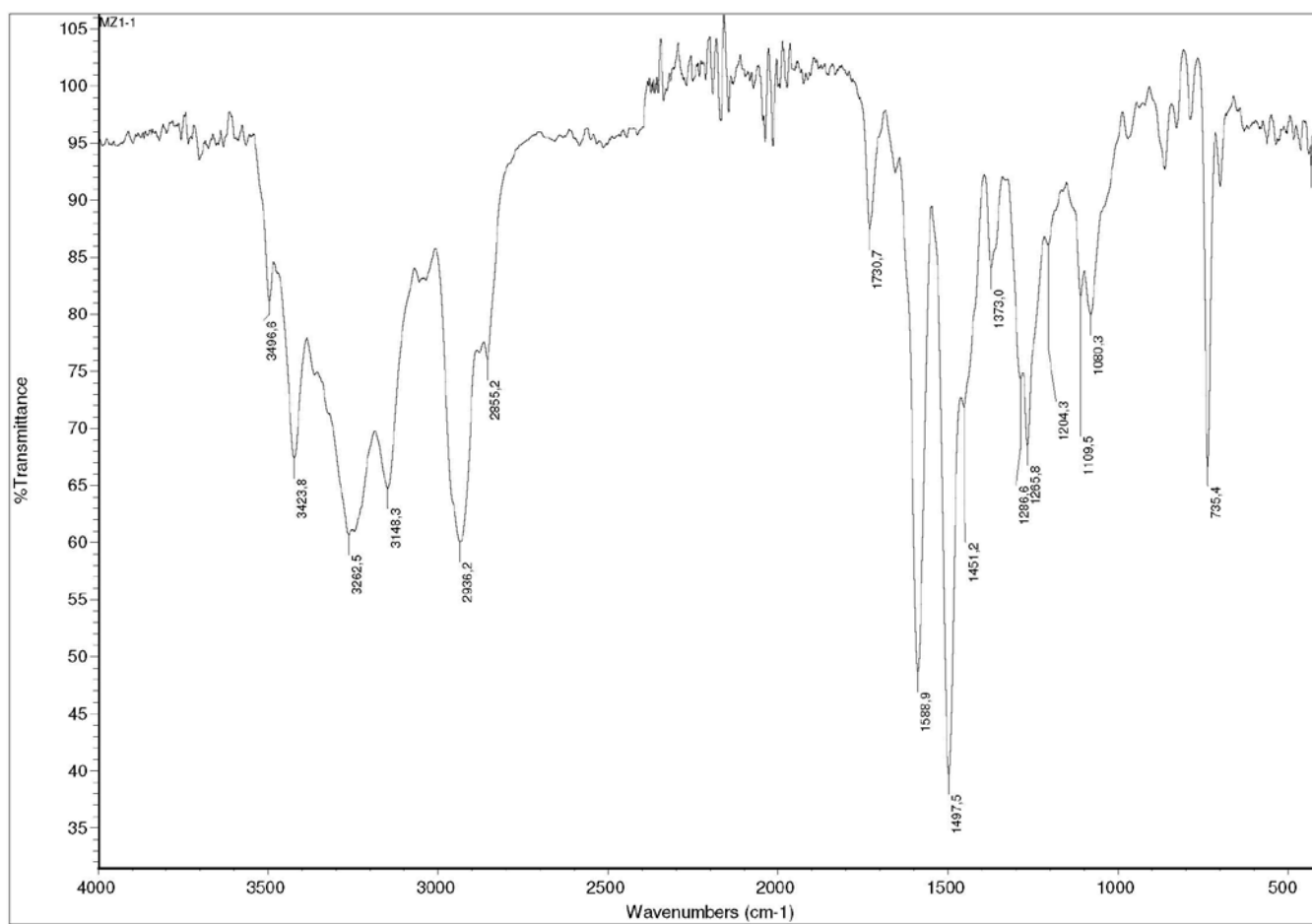
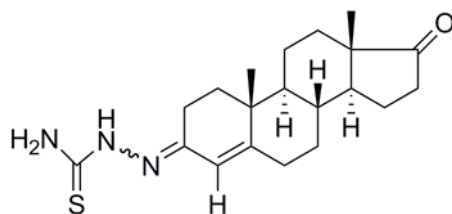
Merged XIC, Period# : 1 Experiment# : 1



Formula	Compound name	Mass	Peak RT (min)	Peak area	Description
C ₂₈ H ₃₈ N ₆ O ₄ S ₂	--	586.23960	0.41	1.72010 E7	--

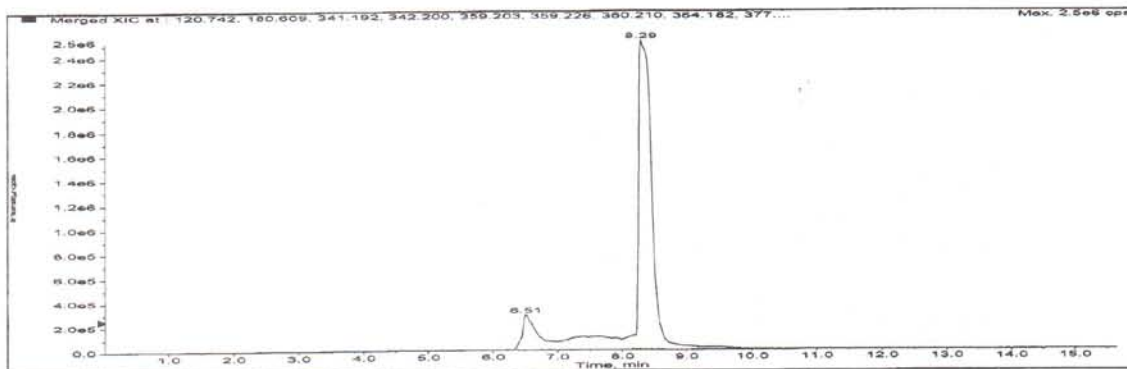
Species	Abundance (counts)	Ion Mass	Measured Mass	Error (mDa)	Error (ppm)	Ret. Time Error (min)
[M+2H] ²⁺	63313.91	294.12707	294.12704	-0.03354	-0.11	--
[M+H] ⁺	1100522.81	587.24687	587.24700	0.12510	0.21	--
[M+Na] ⁺	43472.35	609.22882	609.22878	-0.03344	-0.05	--

Compound 2b

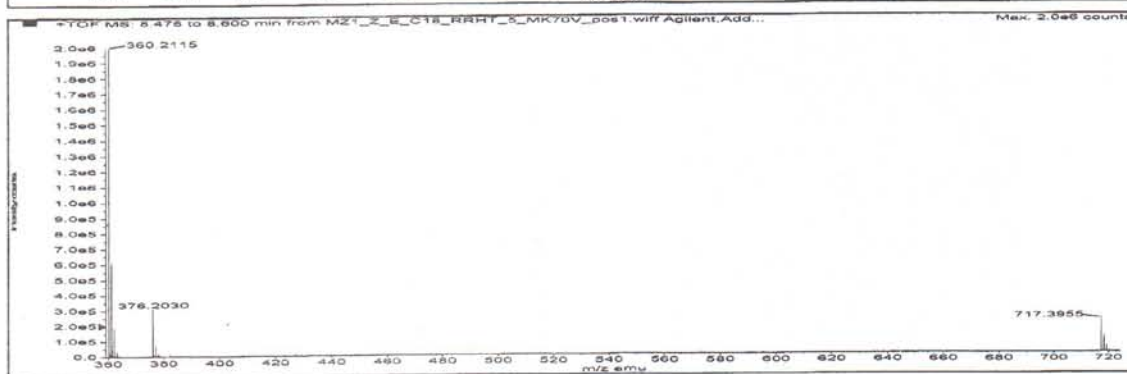
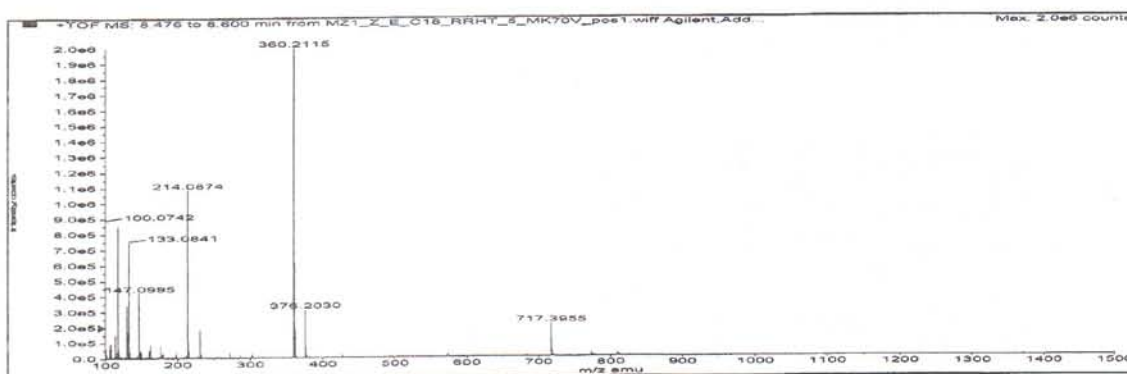


Sample Name: MZ1 Sample Location: P1-C4 Sample Id: Operator: Milka
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 Method: d:\TOF_Data\damethods\Night_Seq_Comp_ident1.anm\efc.xml

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



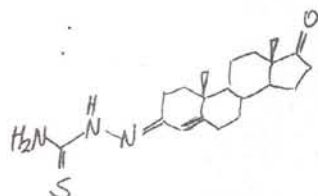
Merged XIC, Period# : 1 Experiment# : 1



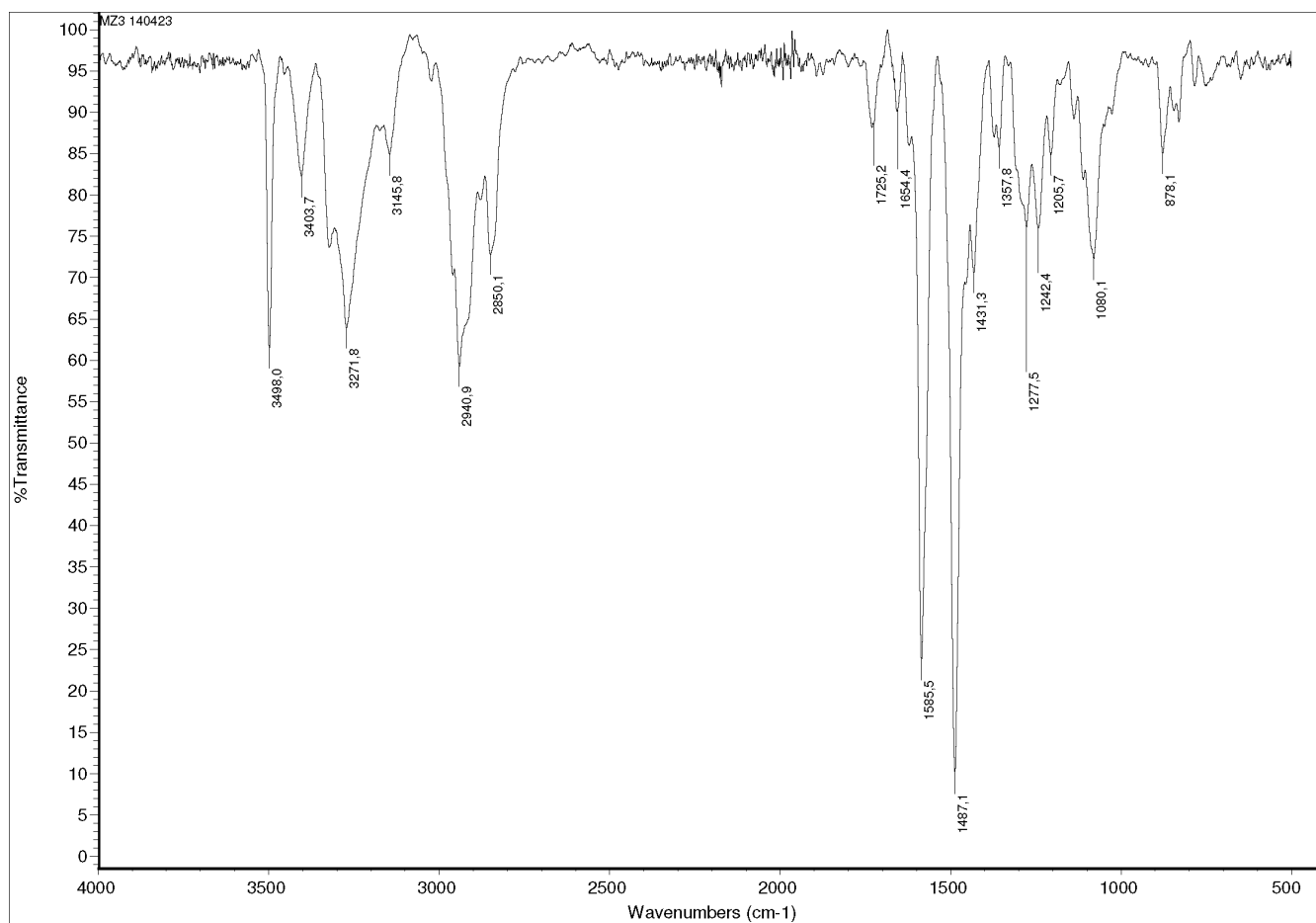
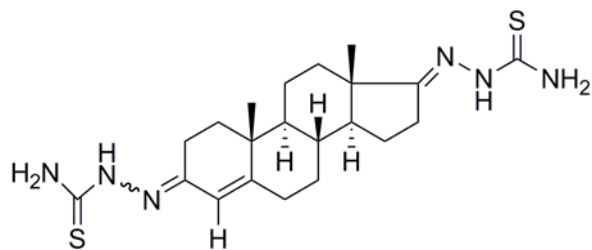
Formula	Compound name	Mass	Peak RT (min)	Peak area	Description
C ₂₀ H ₂₉ N ₃ O ₃	--	359.20313	8.29	3.29119 E7	--

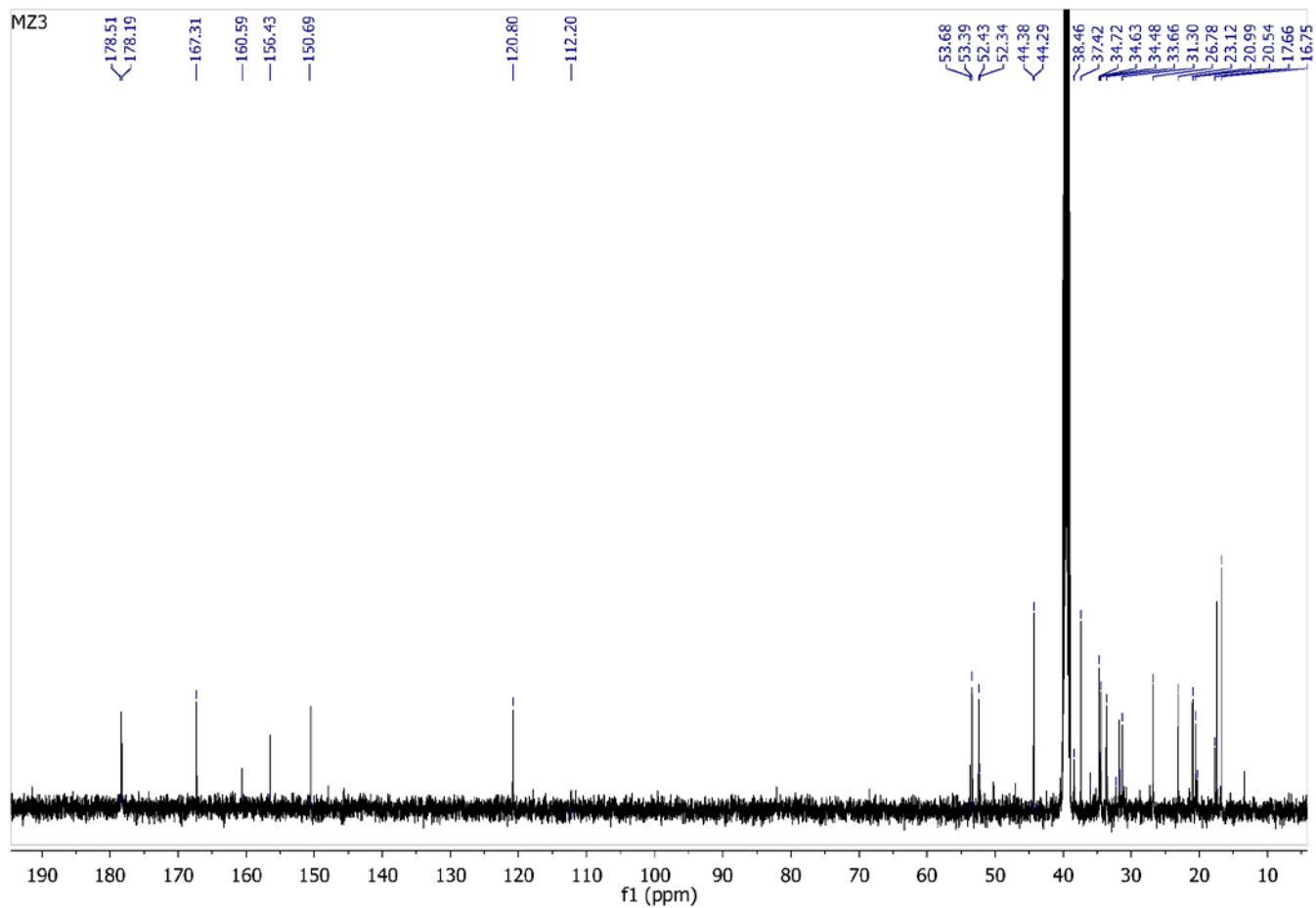
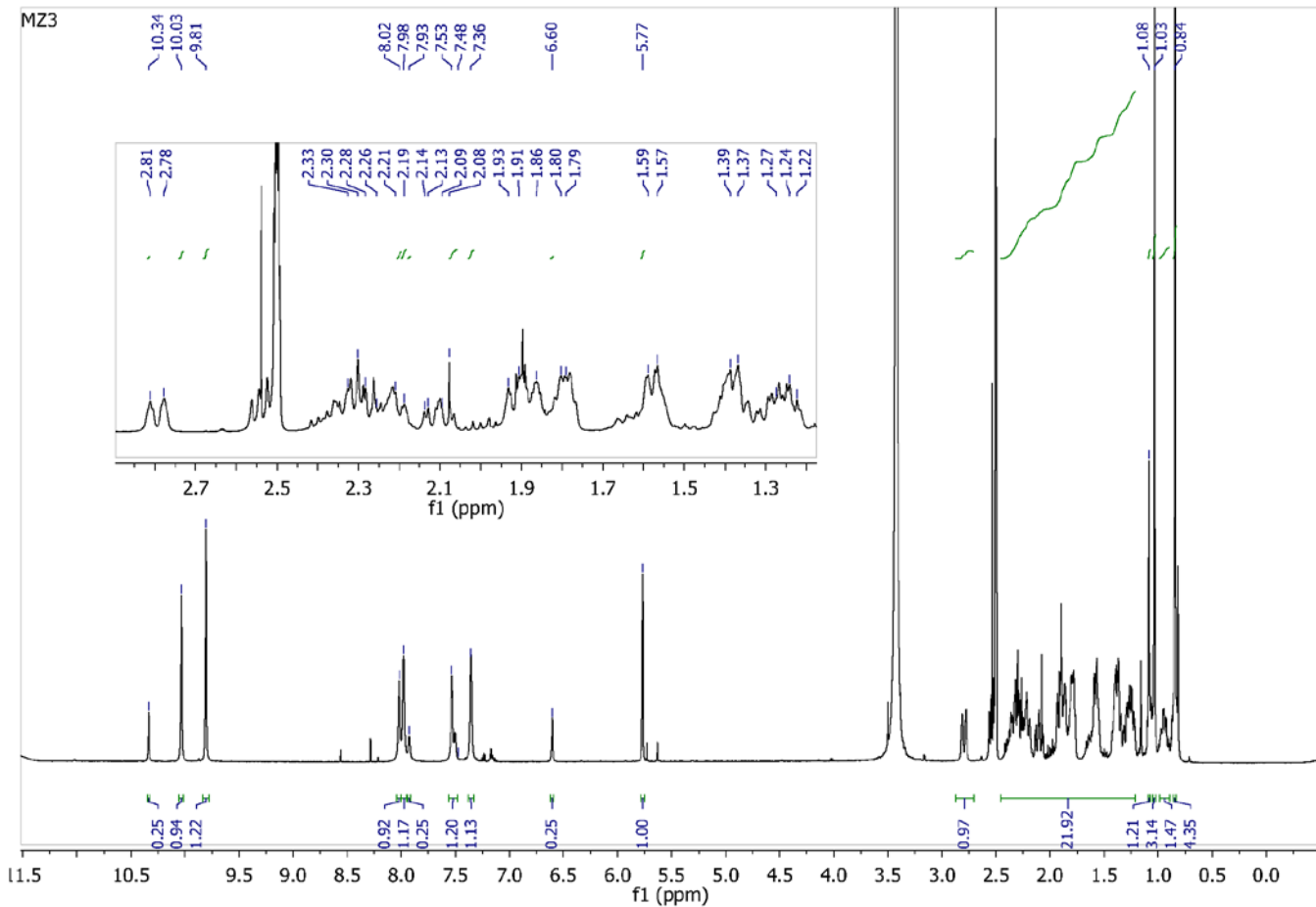
Species	Abundance (counts)	Ion Mass	Measured Mass	Error (mDa)	Error (ppm)	Ret. Time Error (min)
[M+H] ⁺	2118045.71	360.21041	360.21148	1.07232	2.98	--
[M+NH ₄] ⁺	71633.36	377.23696	377.20593	-31.02970	-82.26	--
[2M+H] ⁺	41919.78	719.41354	719.39735	-16.19003	-22.50	--

OK, MZ



Compound 3b

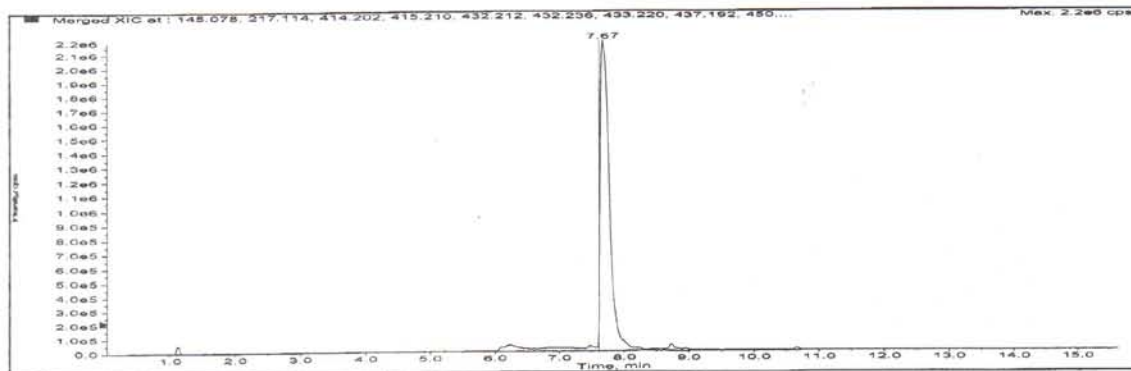




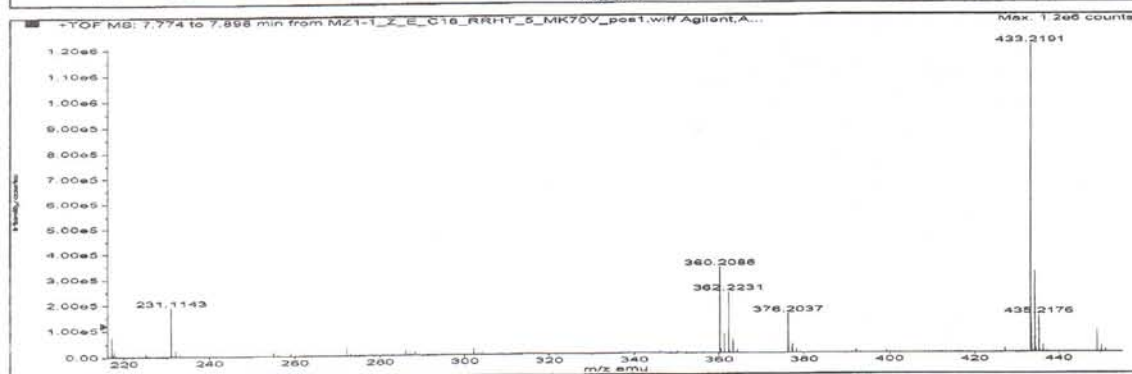
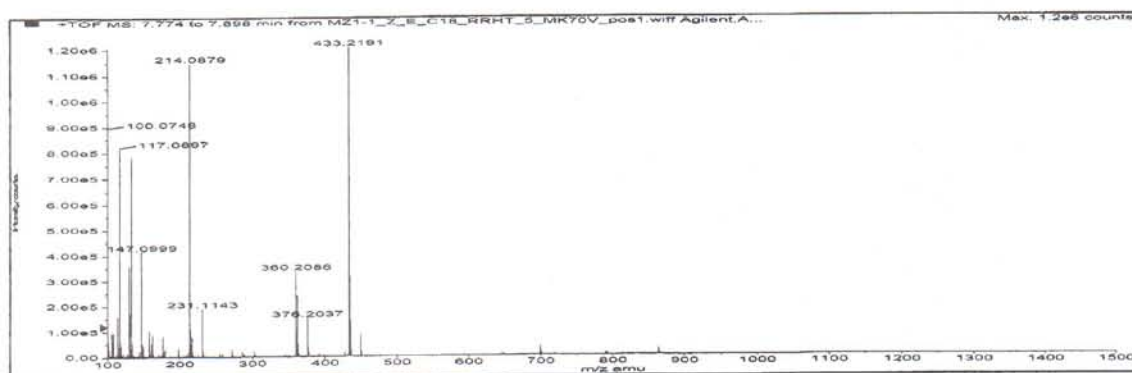
MZ3

Sample Name: MZ1-1 Sample Location: P1-C5 Sample Id: Operator: Milka
 Data File Name: D:\PE Sciex Data\Projects\Sladic\Data\MZ1-1_Z_E_C18_RRHT_5_MK70V_pos1.wiff Acq Time: March 24 2014,
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 Method: d:\TOF_Data\damethods\Night_Seq_Comp_ident1.anmlefc.xml

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



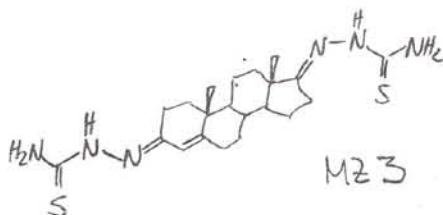
Merged XIC, Period# : 1 Experiment# : 1



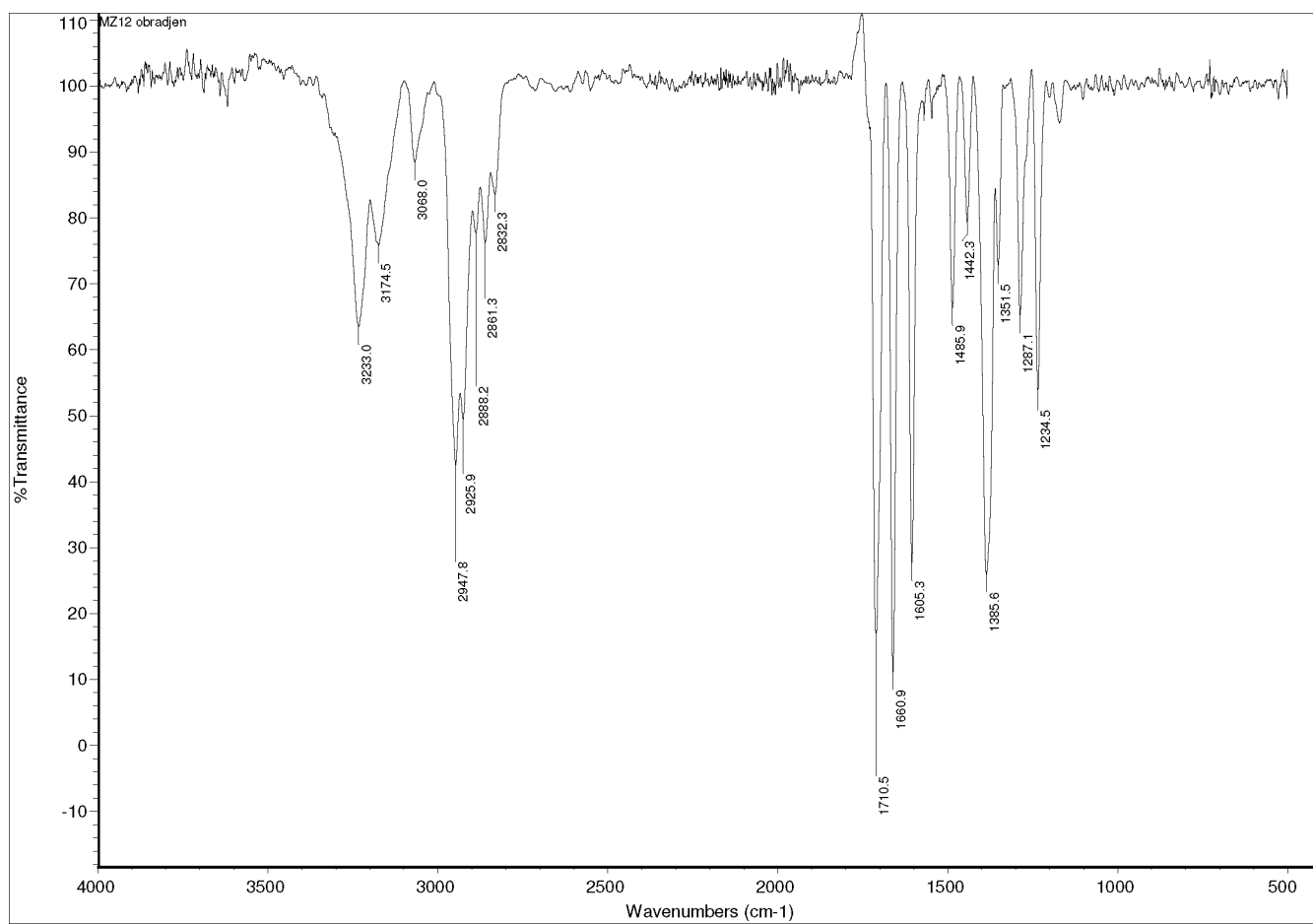
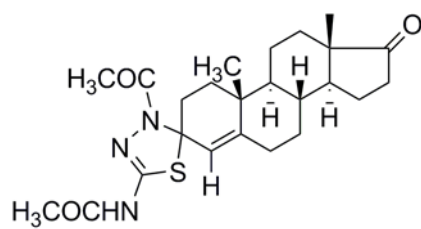
Formula	Compound name	Mass	Peak RT (min)	Peak area	Description
C21H32N6S2	--	432.21298	7.67	2.05709 E7	--

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	450.24681	450.21780	-29.01626	-64.45	

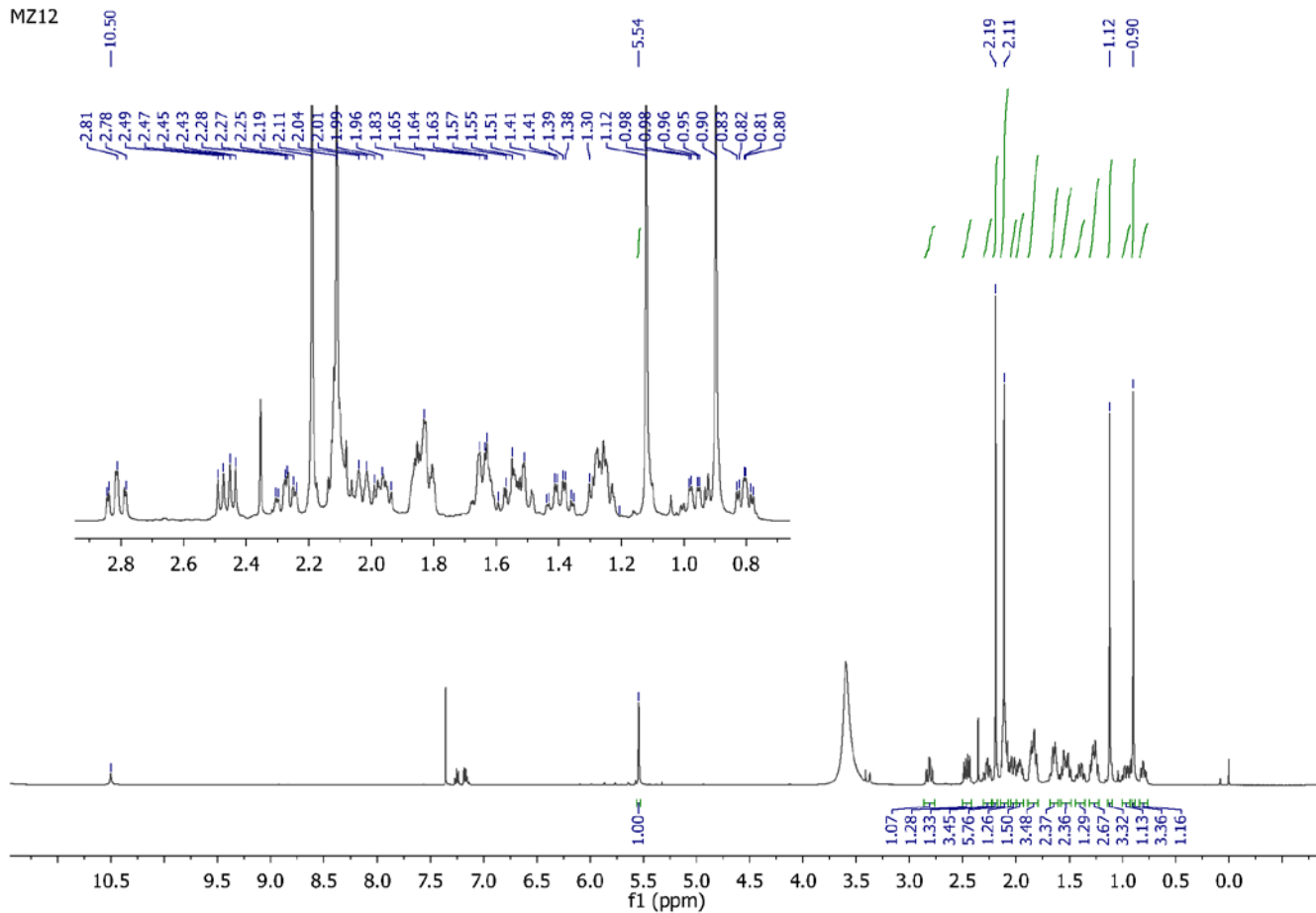
OK, MZ



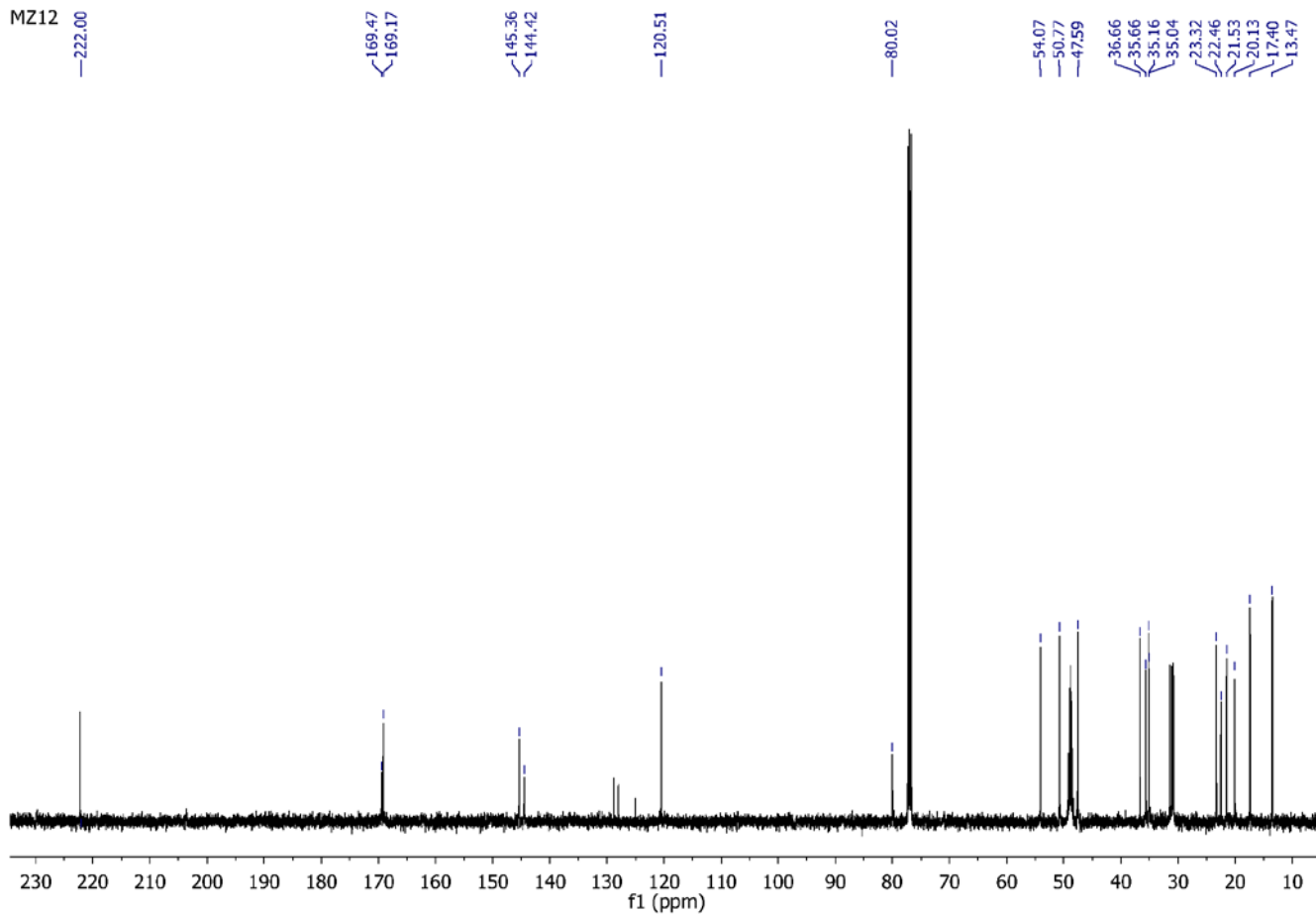
Compound 4b



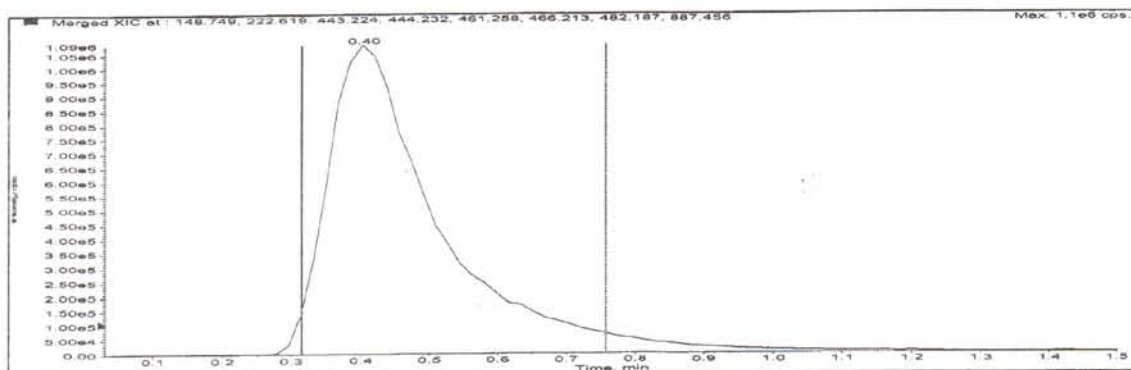
MZ12



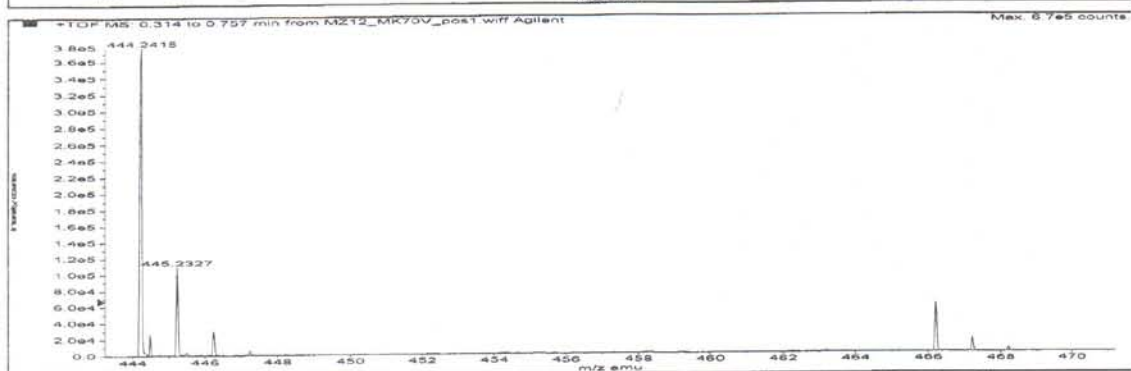
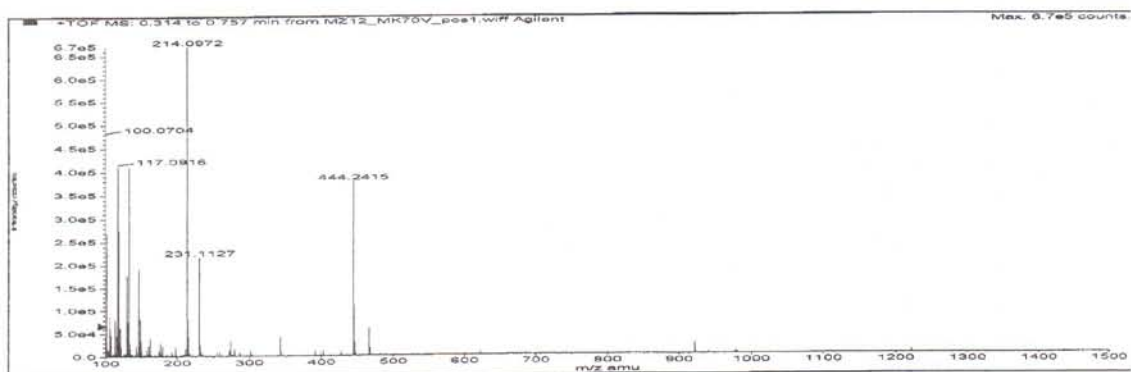
MZ12



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



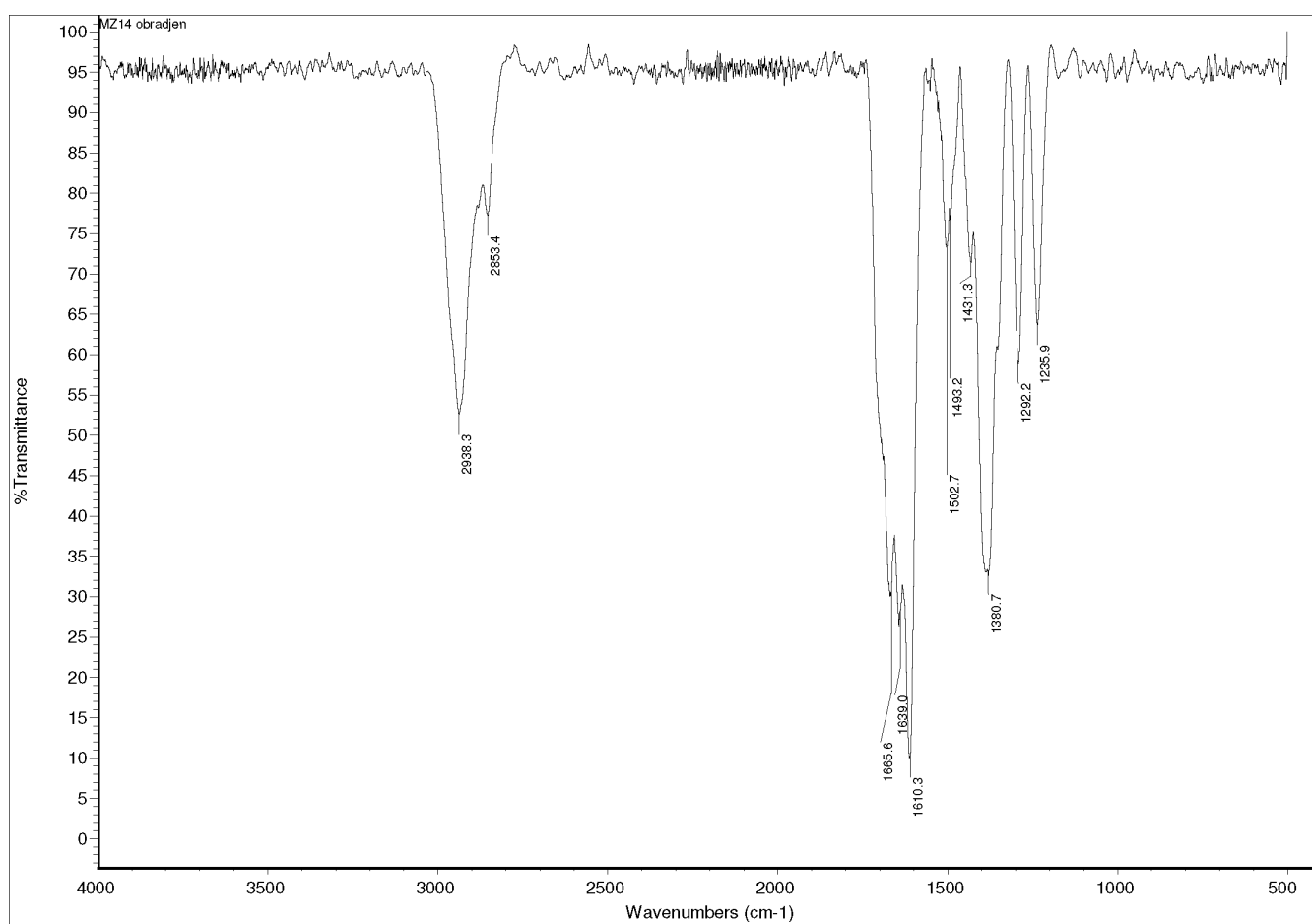
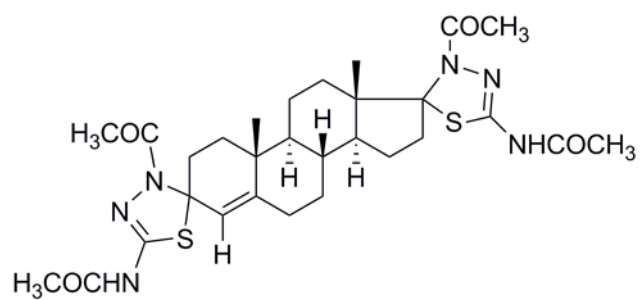
Merged XIC, Period# : 1 Experiment# : 1



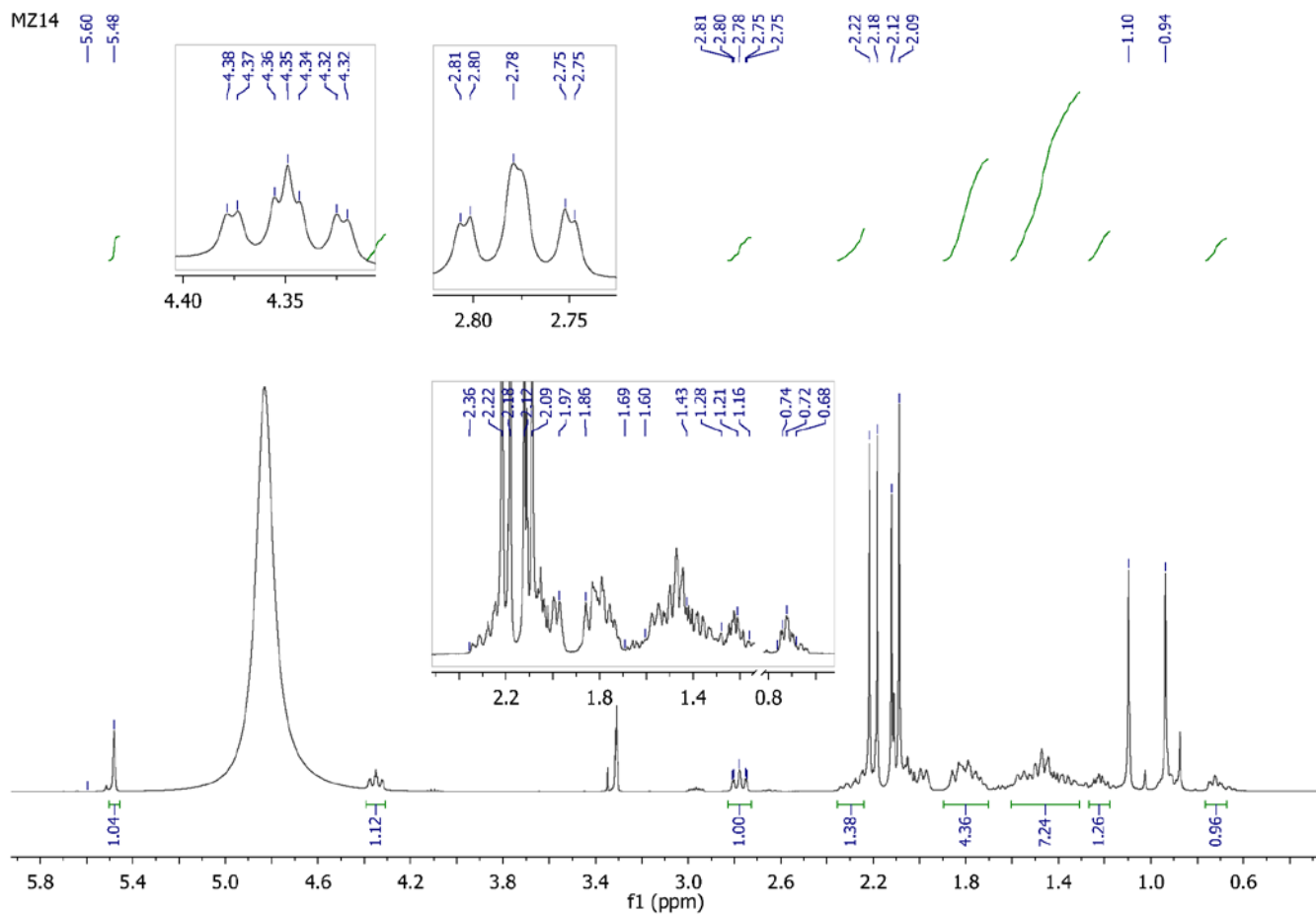
Formula	Compound name	Mass	Peak RT (min)	Peak area	Description
C24H33N3O3S	--	443.22426	0.40	1.19248 E7	--

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	--

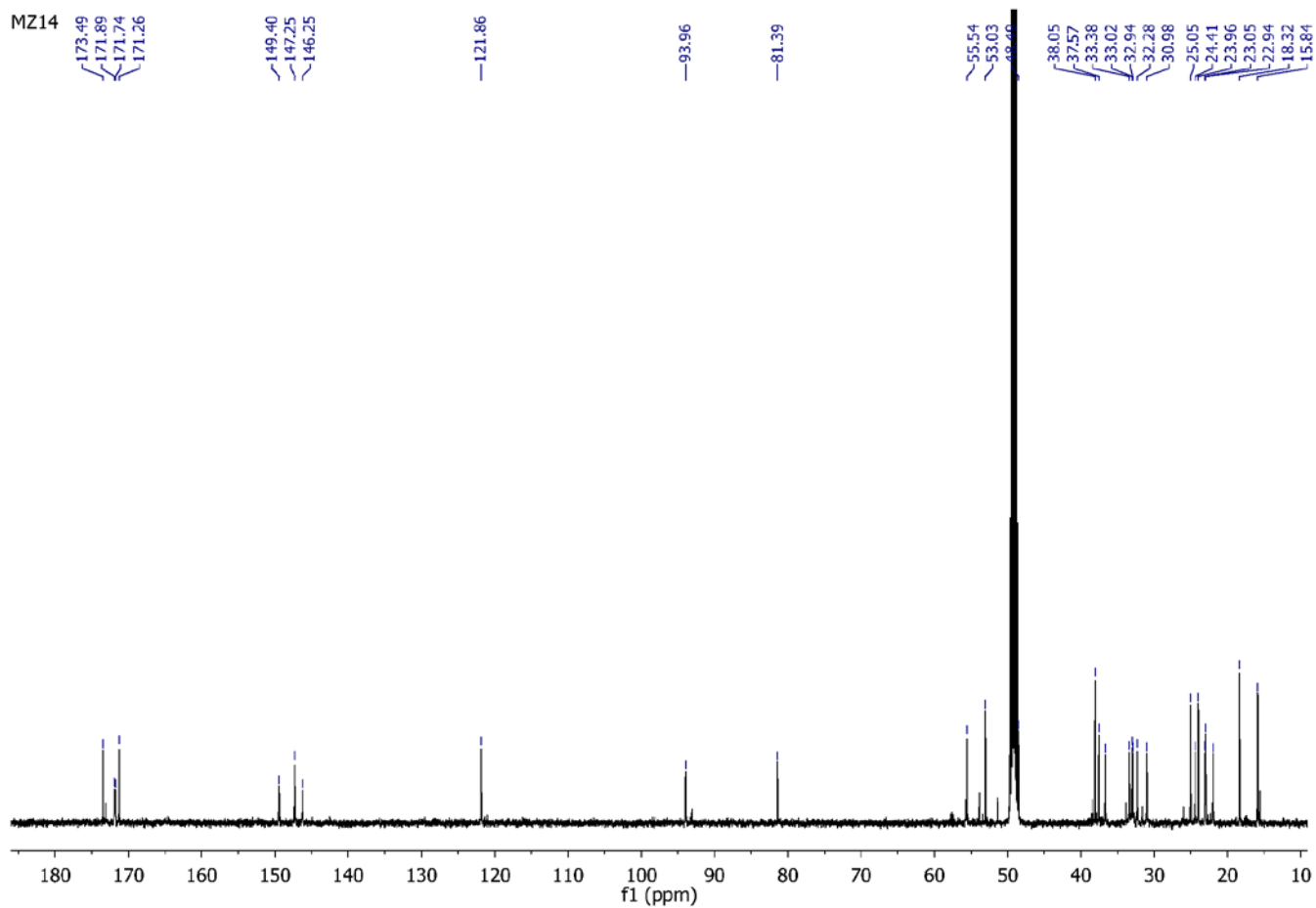
Compound **5b**



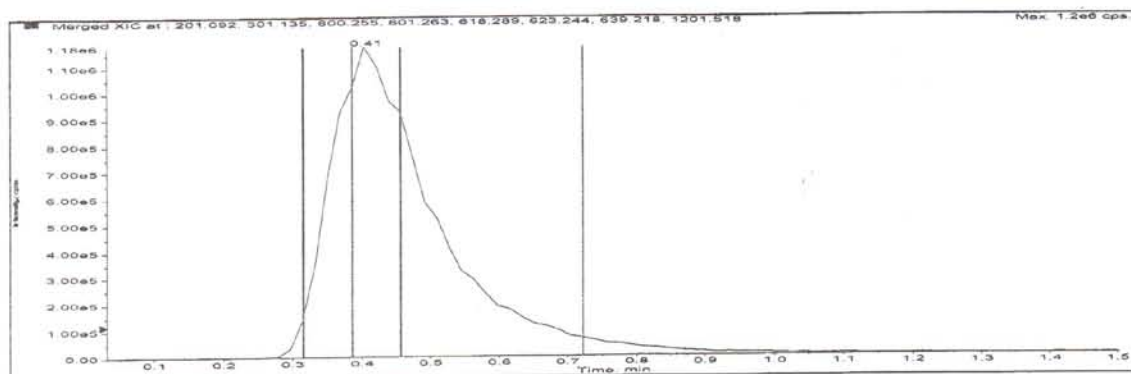
MZ14



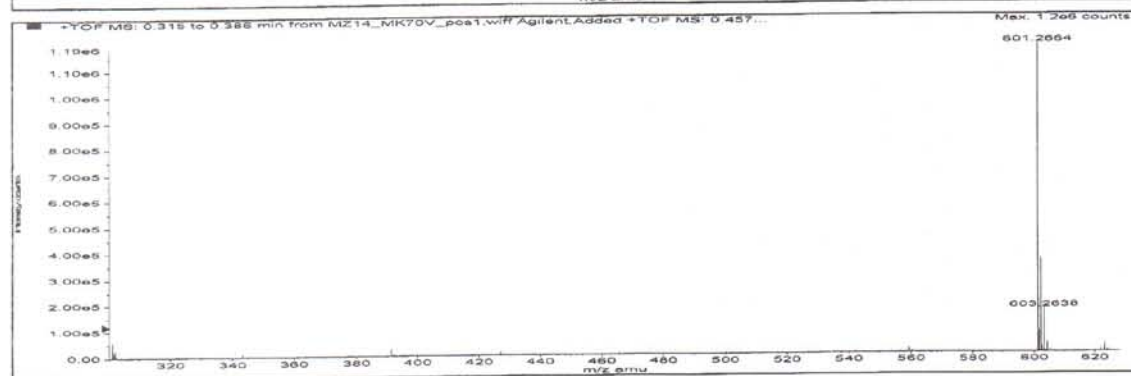
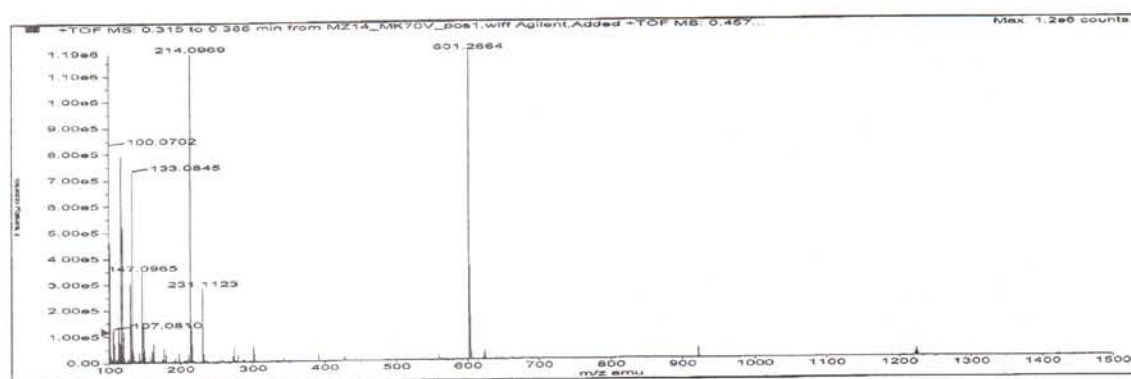
MZ14



Sample Name: MZ14 Sample Location: P1-C4 Sample Id: Operator: Milka
 Data File Name: D:\PE Sciex Data\Projects\Sladice\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



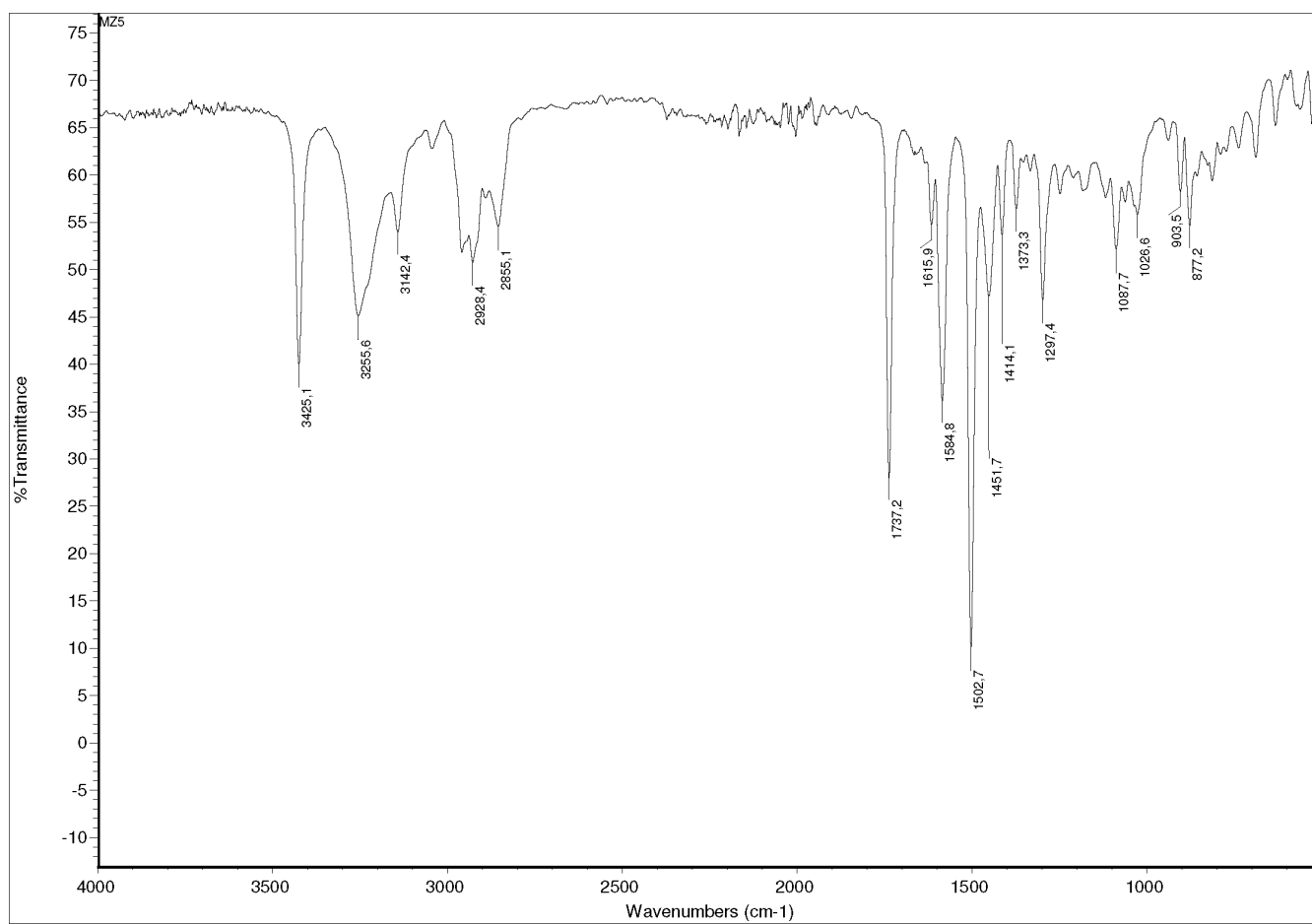
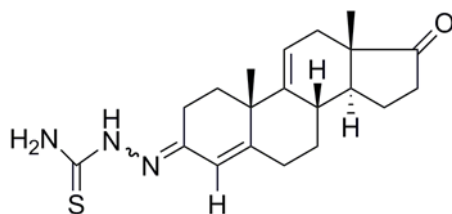
Merged XIC, Period# : 1 Experiment# : 1

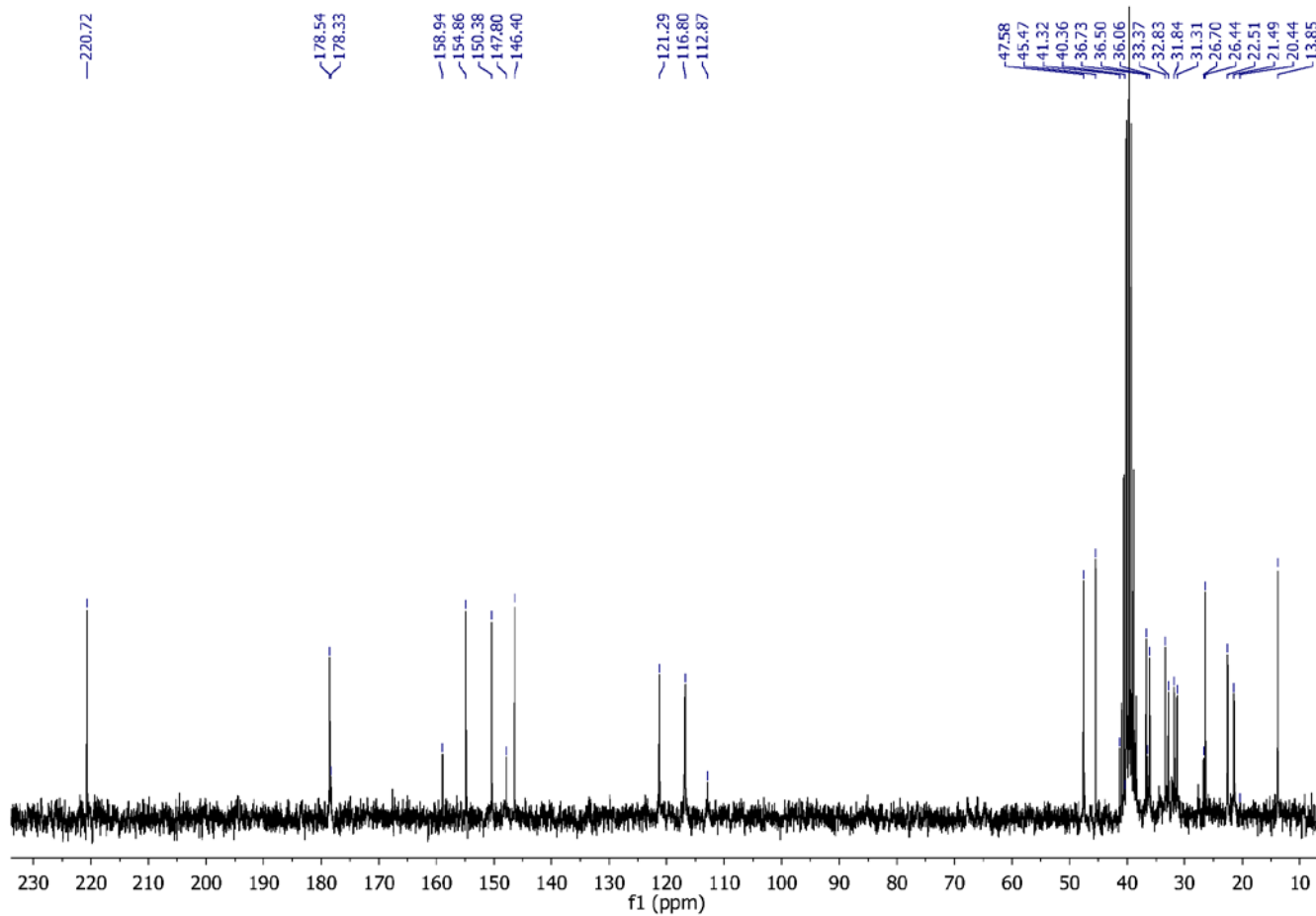
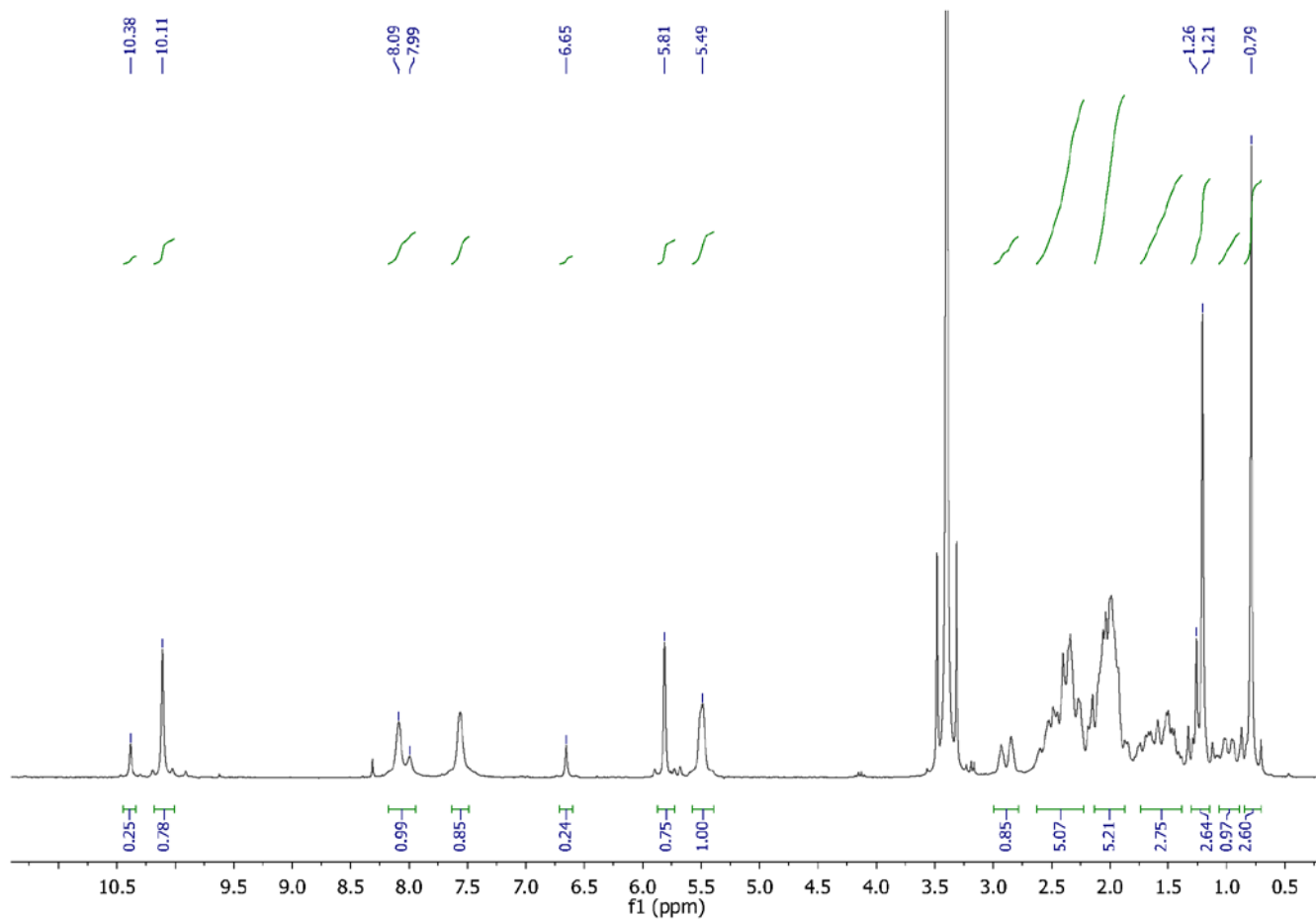


Formula	Compound name	Mass	Peak RT (min)	Peak area	Description
C29H40N6O4S2	—	600.25525	0.41	1.23775 E7	—

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	—

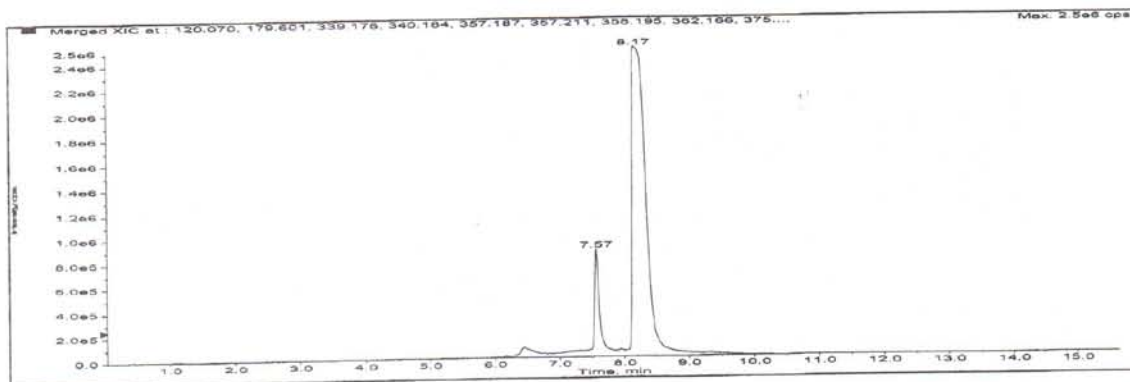
Compound 2c



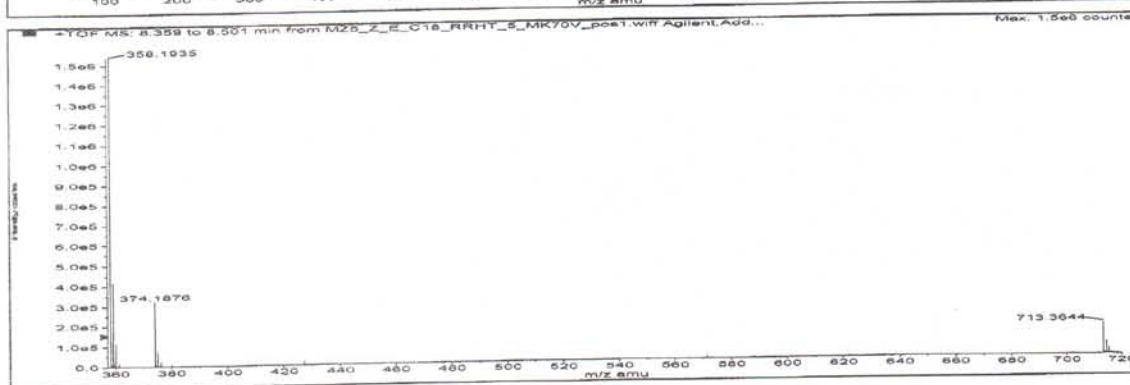
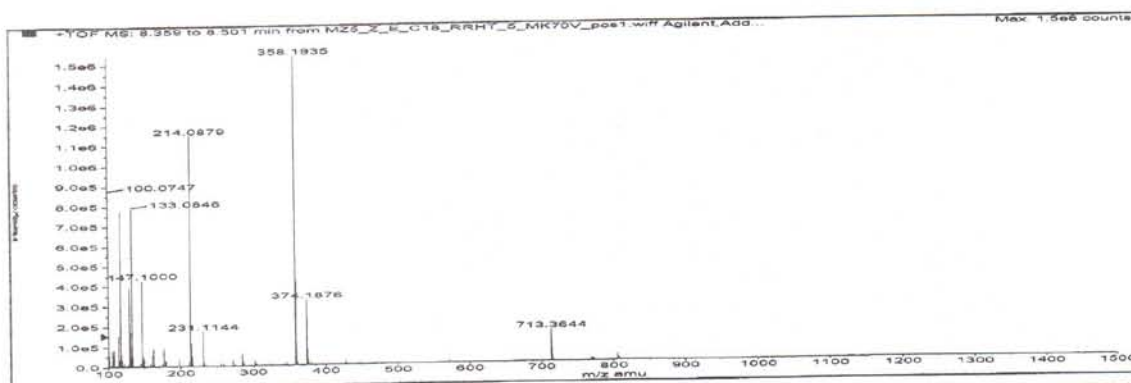


Sample Name: MZ5 Sample Location: P1-C7 Sample Id: Operator: Milka
 Data File Name: D:\PE Sciex Data\Projects\Sladic\Data\MZ5_Z_E_C18_RRHT_5_MK70V_pos1.wiff Acq Time: March 24 2014, 02:13:28
 PM
 Method: d:\TOF_Data\amethods\Night_Seq_Comp_Ident1.anml\etc.xml

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

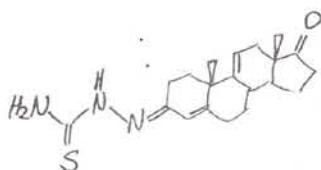


Merged XIC, Period# : 1 Experiment# : 1

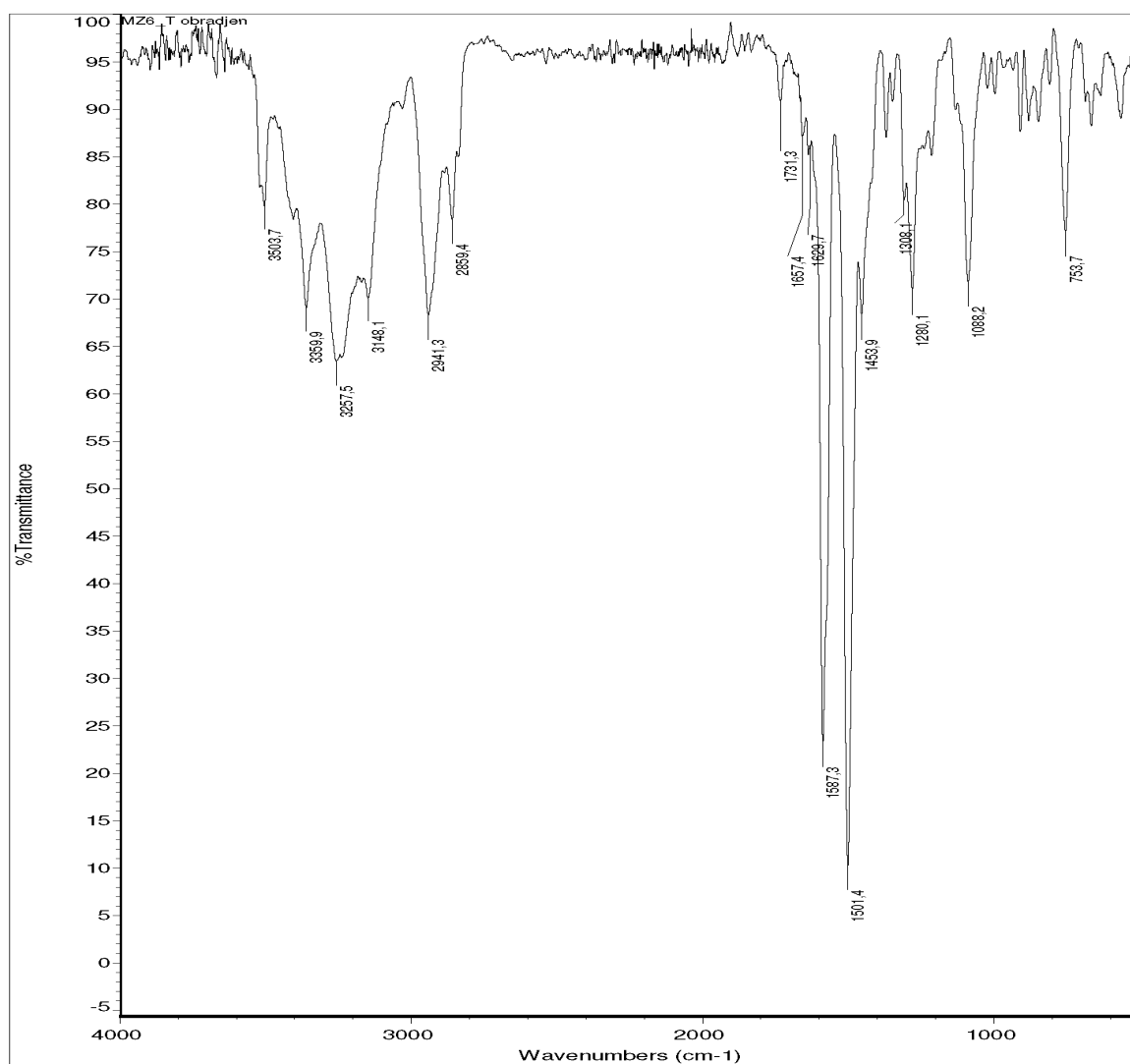
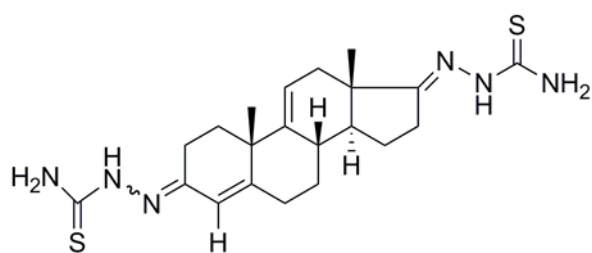


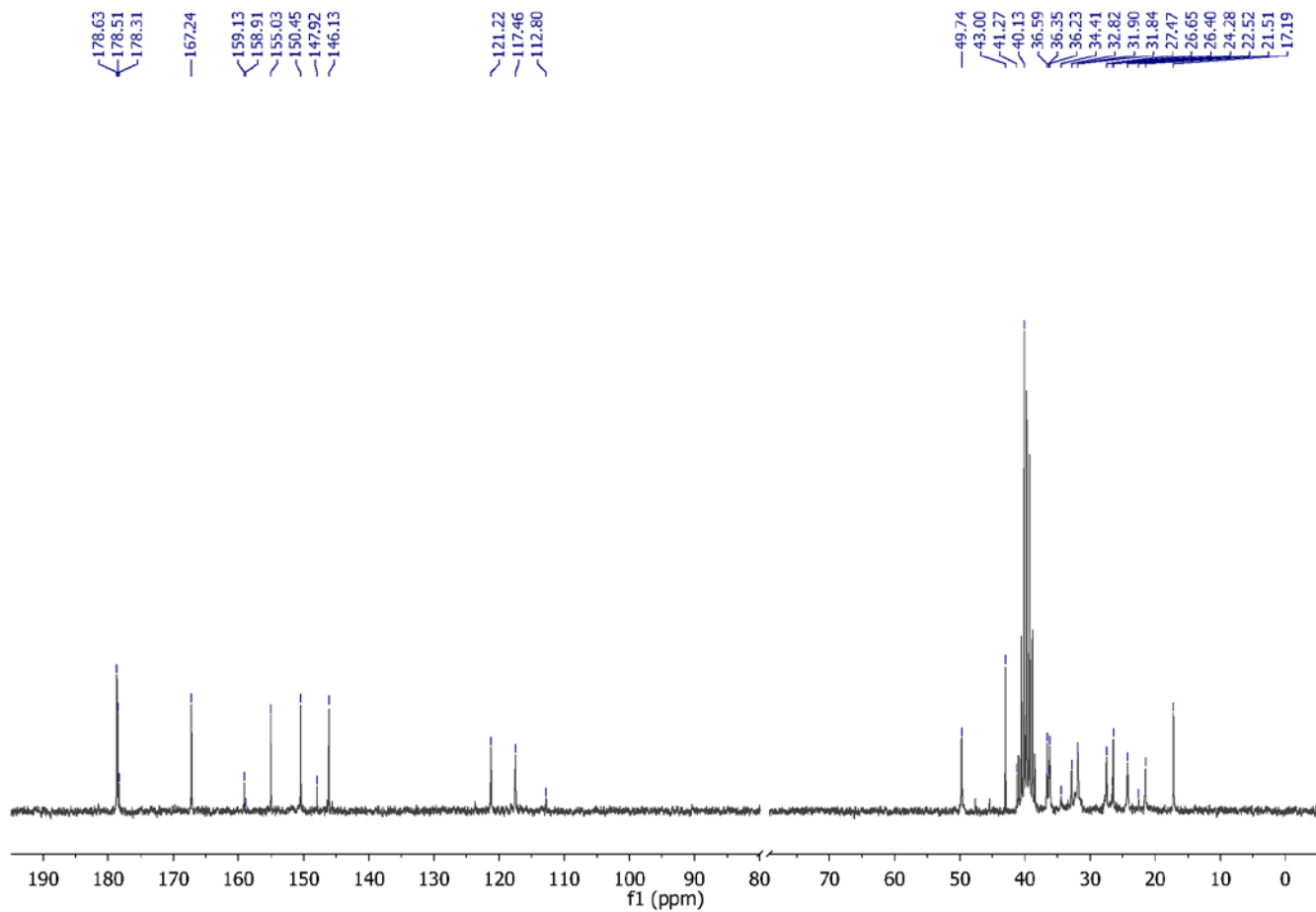
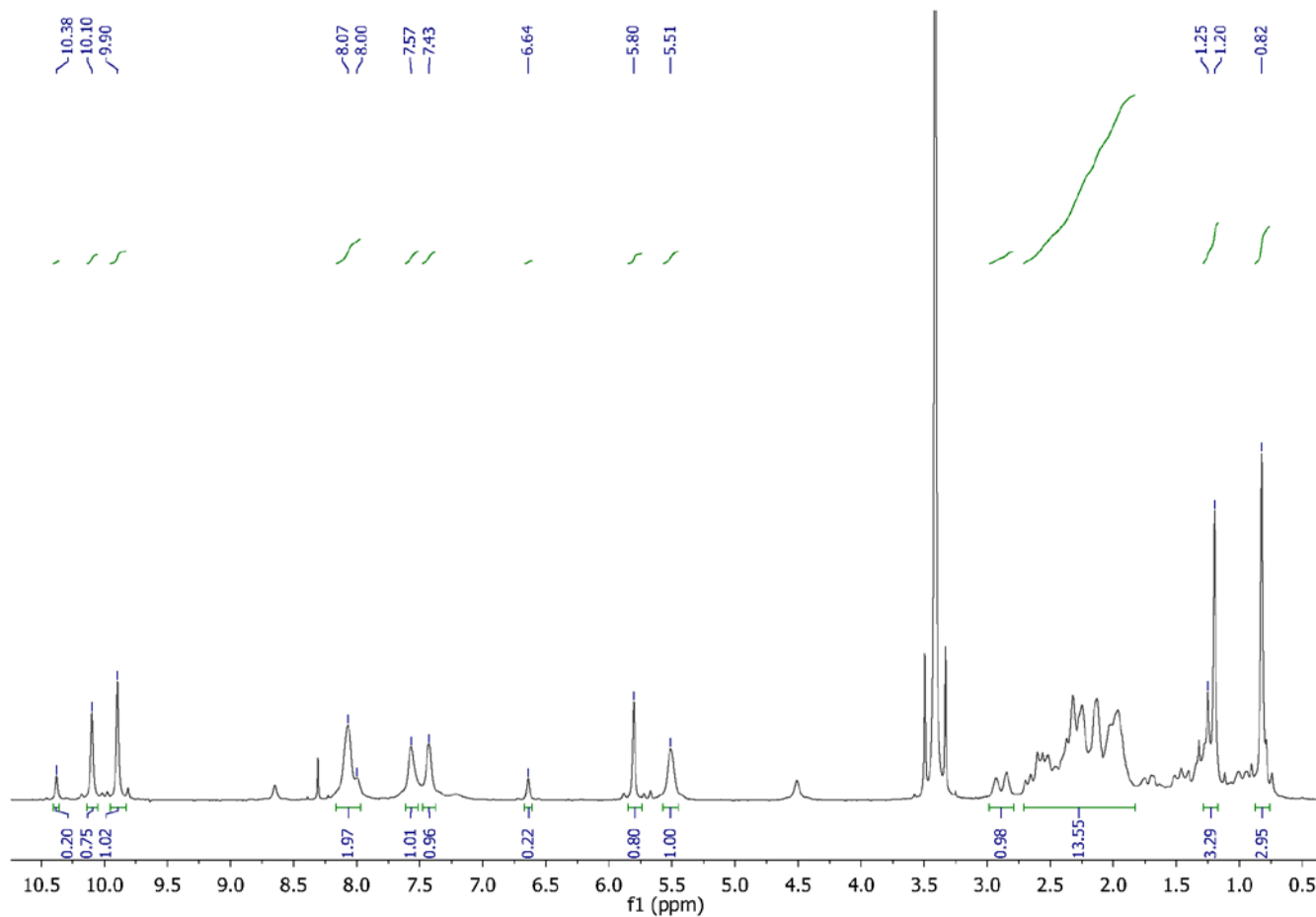
Formula	Compound name	Mass	Peak RT (min)	Peak area	Description
C20H27N3OS	--	357.18748	8.17	3.48884 E7	--

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	--



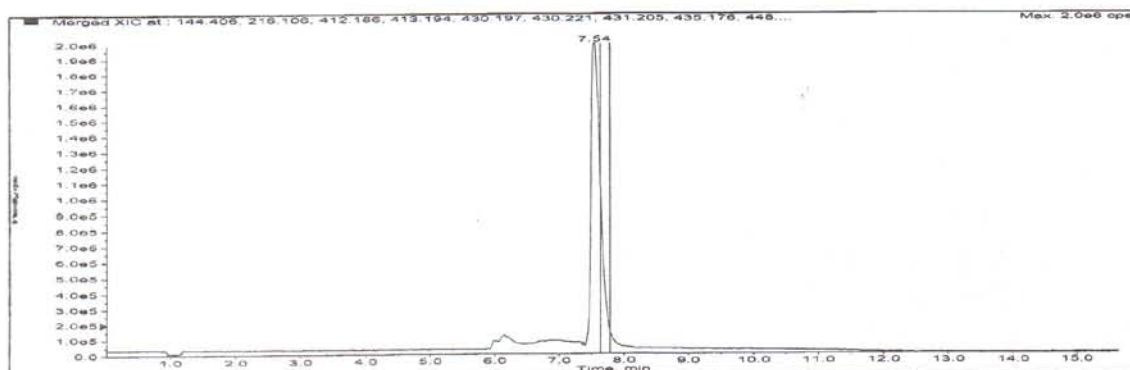
Compound 3c



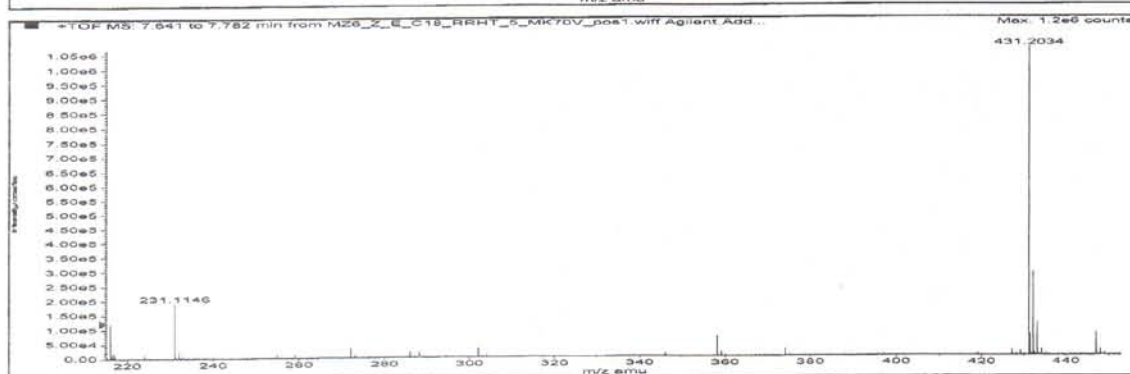
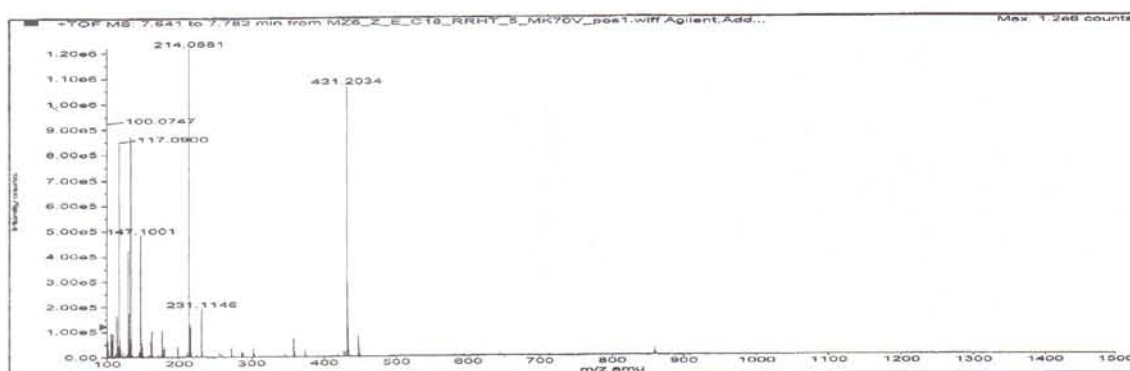


Sample Name: MZ6 Sample Location: P1-C9 Sample Id: Operator: Milka
 Data File Name: D:\PE Sciex Data\Projects\StadiciData\MZ6_Z-E_C18-RRHT_5_MK70V_pos1.wiff Acq Time: March 24, 2014, 02:55:59 PM
 Method: d:\TOF_Data\damethods\Night_Seq_Comp_ident1.anmlc.xml

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

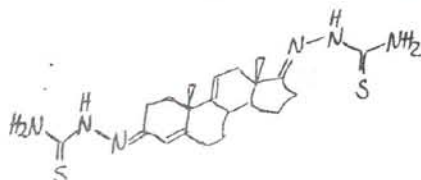


Merged XIC, Period# : 1 Experiment# : 1

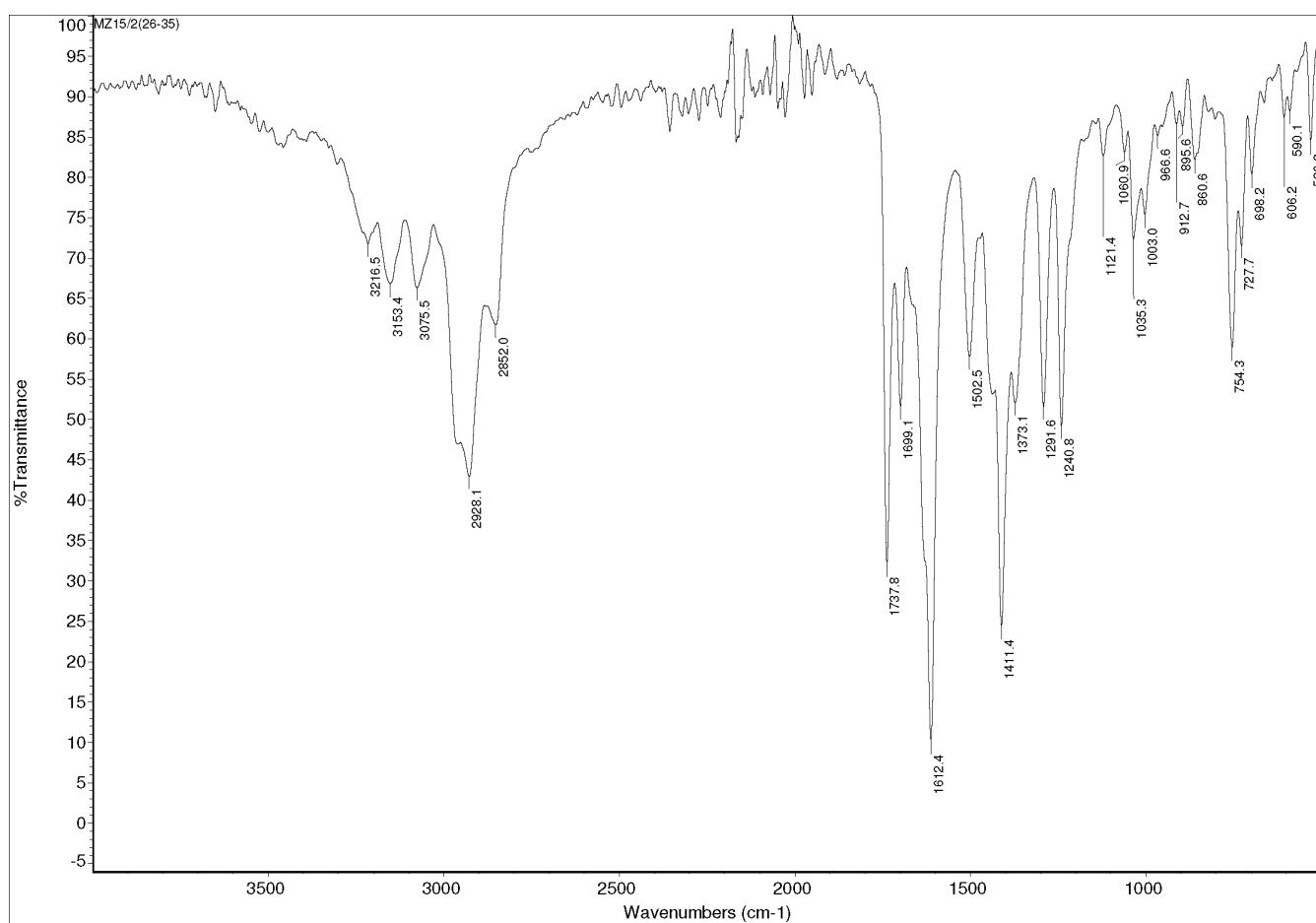
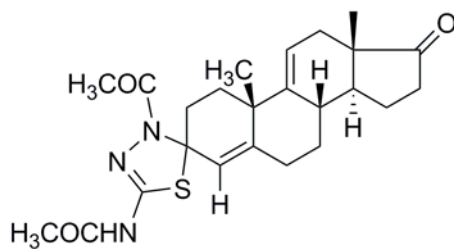


Formula	Compound name	Mass	Peak RT (min)	Peak area	Description
C21H30N6S2	—	430.19734	7.54	1.96986 E7	—

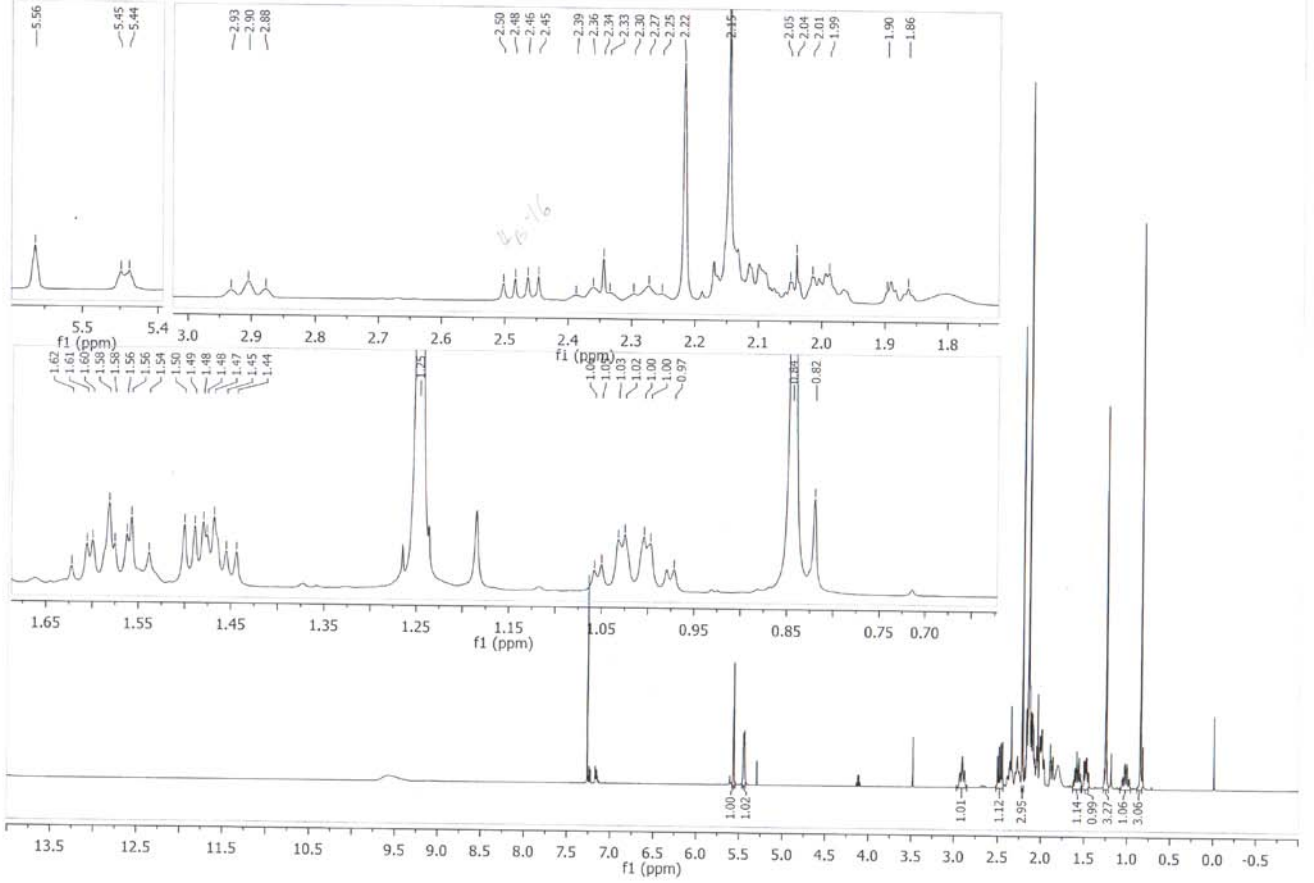
Species	Abundance (counts)	Ion Mass	Measured Mass	Error (mDa)	Error (ppm)	Ret. Time Error (min)
[M+2H] ²⁺	120512.45	216.10594	216.09697	-8.97379	-41.53	
[M+H] ⁺	1105903.79	431.20461	431.20339	-1.22762	-2.85	
[M+NH4] ⁺	22141.87	448.23116	448.20094	-30.22452	-67.44	



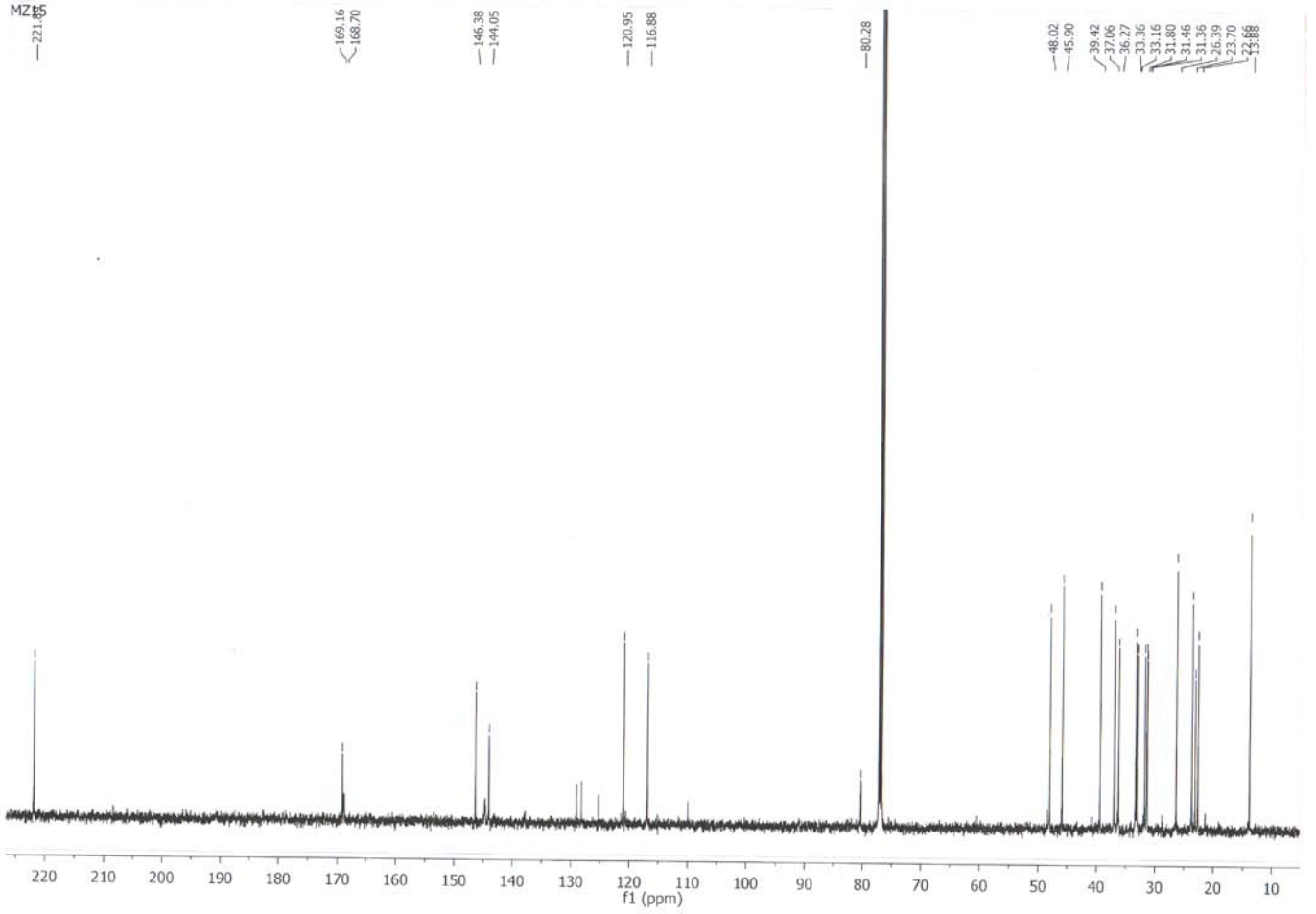
Compound 4c



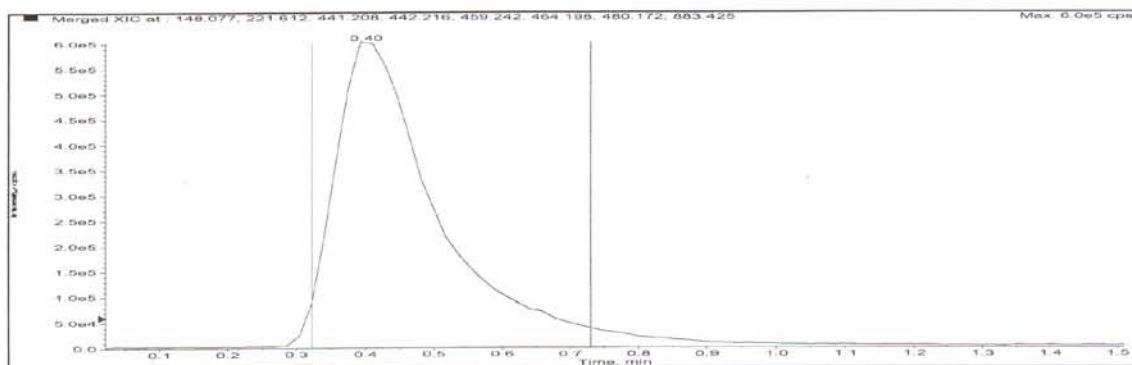
Desktop 11.7.15



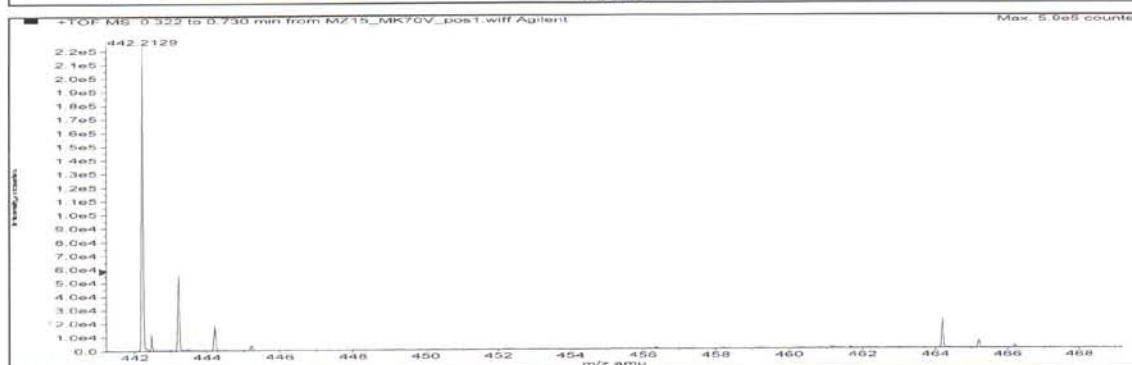
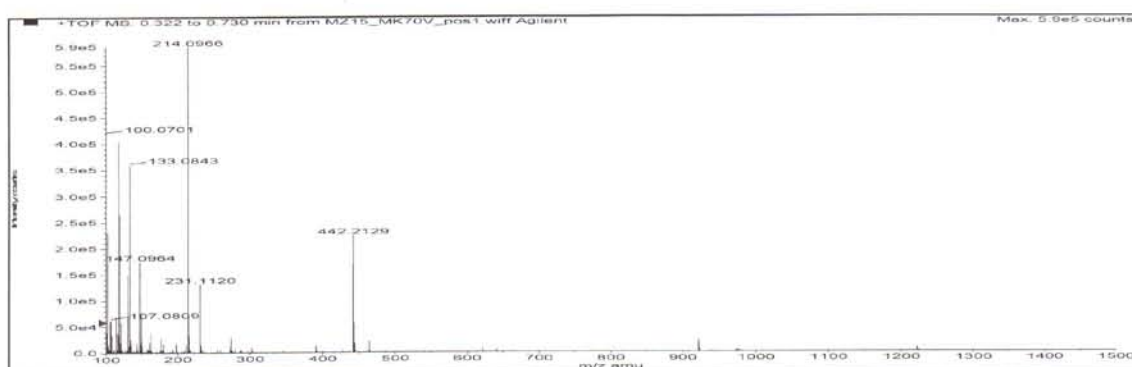
MZ 15



Sample Name: MZ15 Sample Location: P1-C5 Sample Id: Operator: Milka
 Data File Name: D:\PE Sciex 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.anml\efc.xml



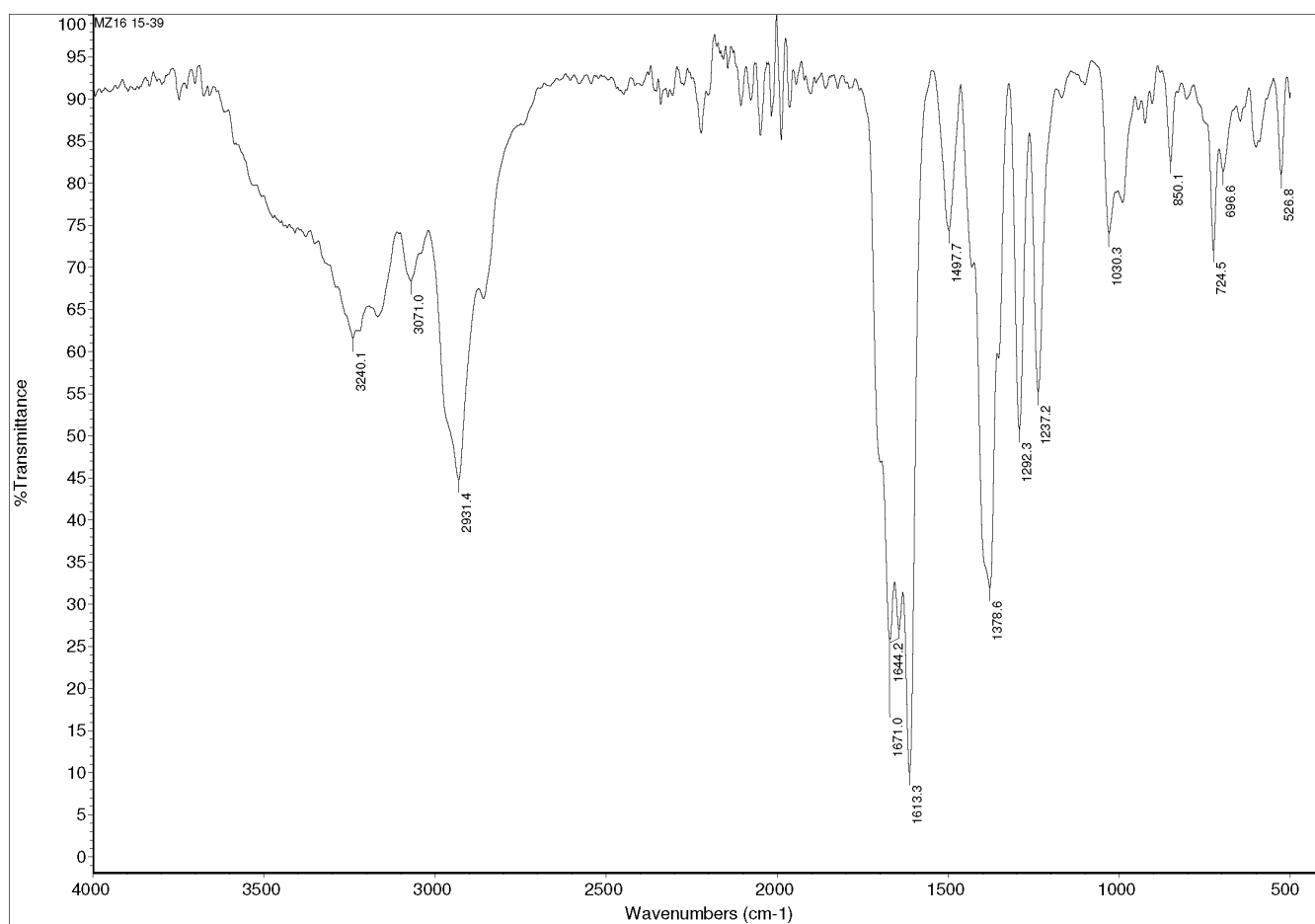
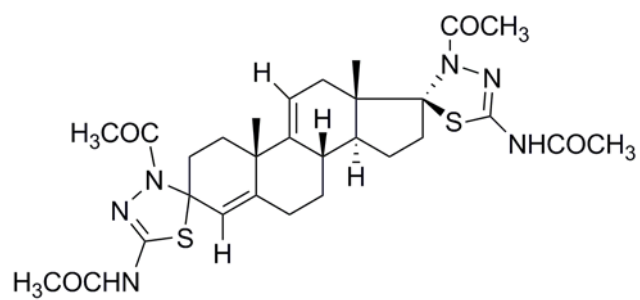
Merged XIC, Period# : 1 Experiment# : 1

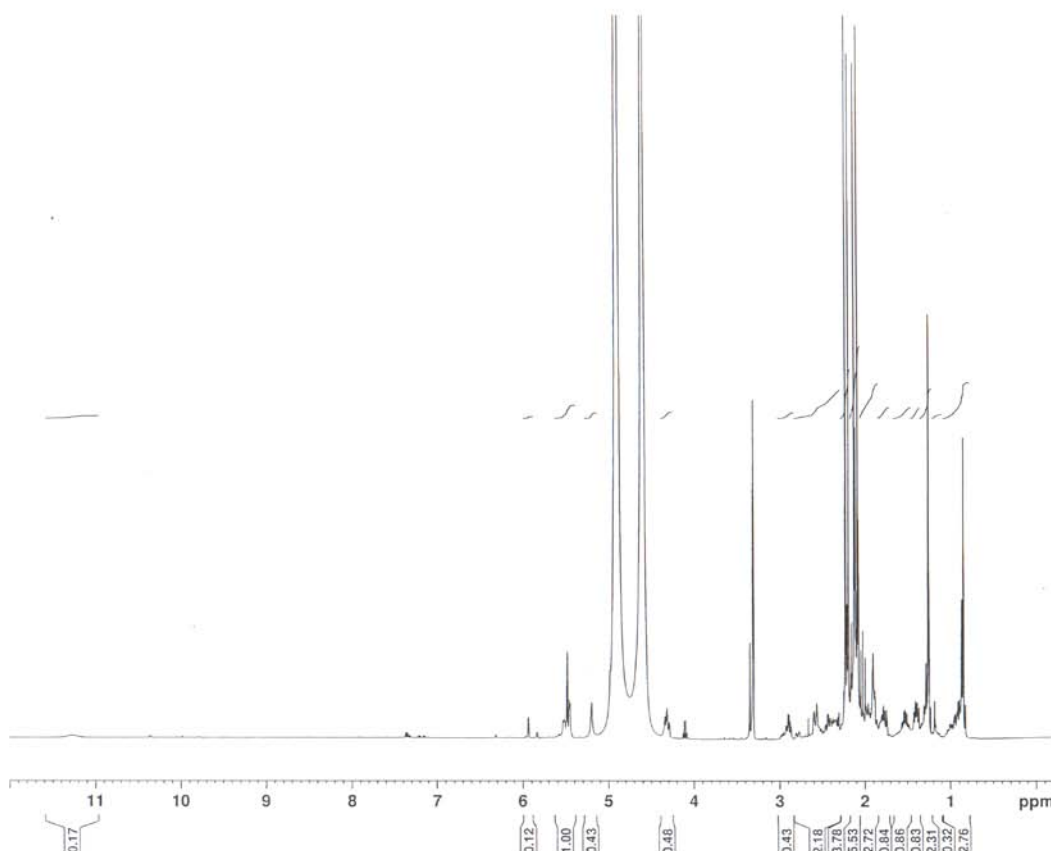


Formula	Compound name	Mass	Peak RT (min)	Peak area	Description
C24H31N3O3S	--	441.20861	0.40	6.26847 E6	--

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



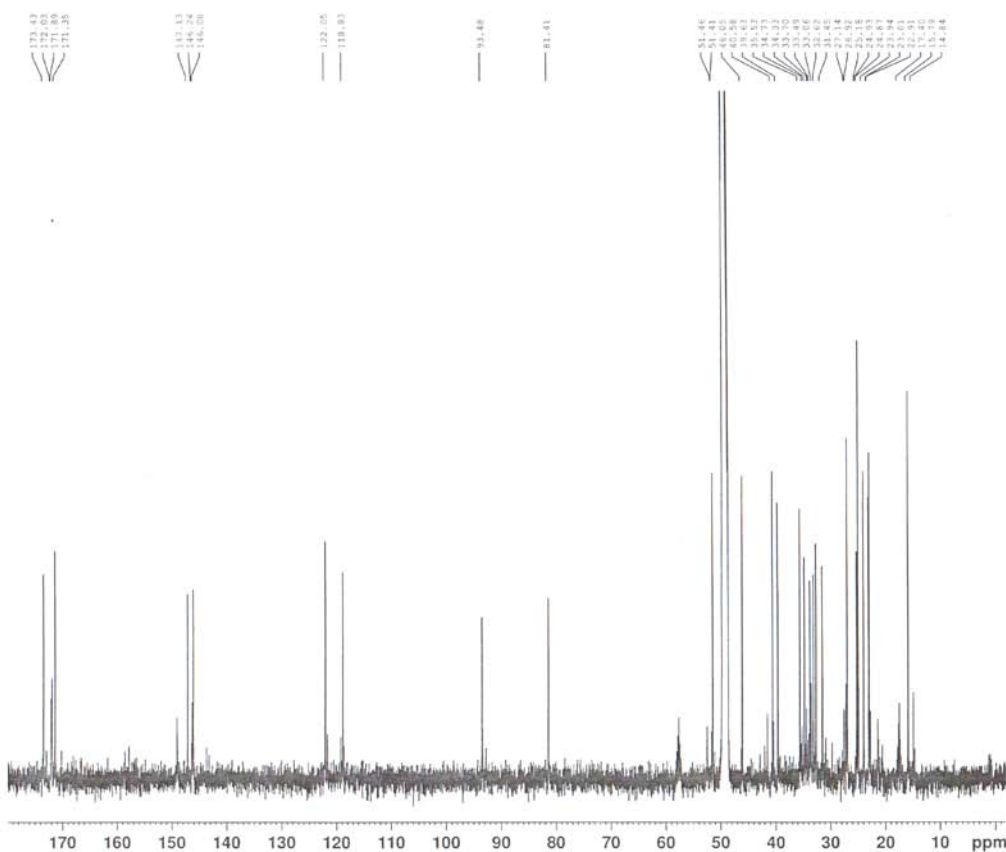


Current Data Parameters
NAME MZ16
EXPNO 1
PROCNO 1

F2 - Acquisition Parameters
Date_ 20140624
Time 15.19
INSTRUM spect
PROBHD 5 mm BBO BB-1H
PULPROG zg30
TD 32768
SOLVENT MeOD
NS 32
DS 0
SWH 6510.417 Hz
FIDRES 0.198682 Hz
AQ 2.5165825 sec
RG 40.3
DW 76.800 usec
DE 6.50 usec
TE 298.0 K
D1 2.00000000 sec
TD0 1

***** CHANNEL f1 *****
SFO1 500.2630115 MHz
NUC1 1H
P1 9.35 usec
PLW1 27.37999916 W

F2 - Processing parameters
SI 32768
SF 500.2600090 MHz
WDW EM
SSB 0
LB 0.20 Hz
GB 0
FC 1.00



Current Data Parameters
NAME MZ16
EXPNO 6
PROCNO 1

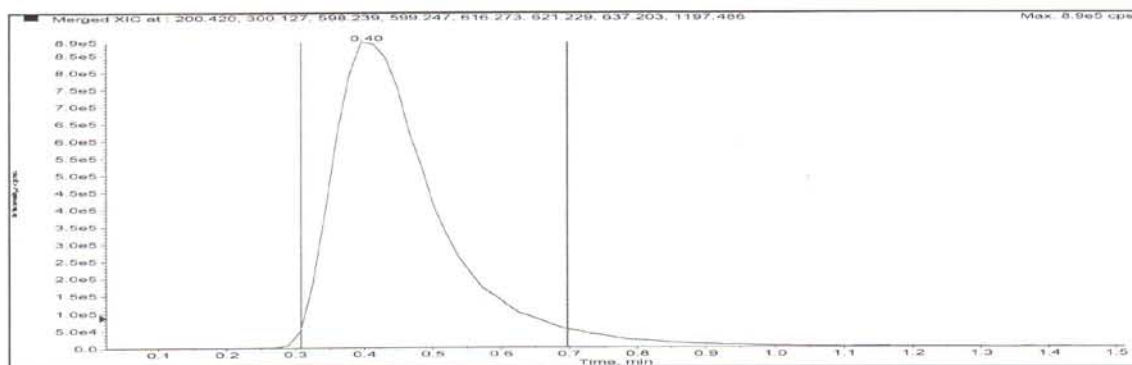
F2 - Acquisition Parameters
Date_ 20140625
Time 7.59
INSTRUM spect
PROBHD 5 mm BBO BB-1H
PULPROG zgpg30
TD 32768
SOLVENT MeOD
NS 3267
DS 4
SWH 32894.738 Hz
FIDRES 1.003868 Hz
AQ 0.4980736 sec
RG 1030
DW 15.200 usec
DE 6.50 usec
TE 298.0 K
D1 2.00000000 sec
D11 0.03000000 sec
TD0 1

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

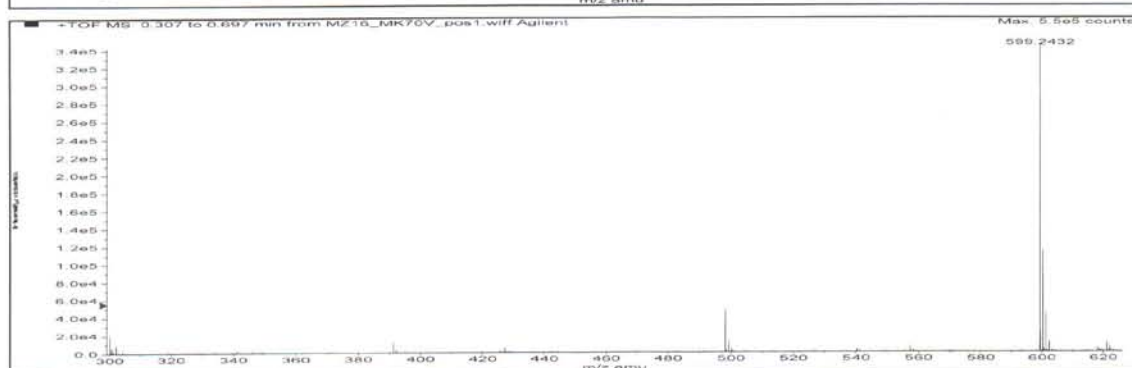
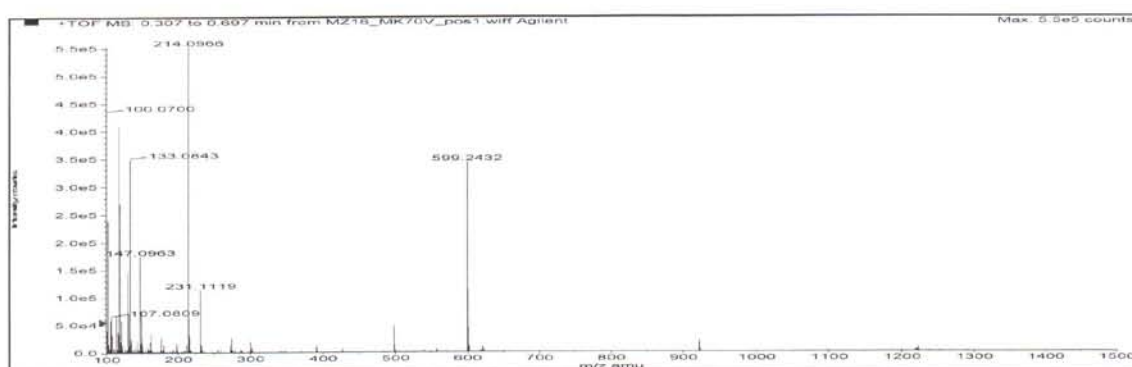
***** CHANNEL f2 *****
SFO2 500.2630116 MHz
NUC2 1H
PCPDPRG12 waitz16
PCPD2 80.00 usec
PLW2 20.77000004 W
PLW12 0.19267001 W
PLW13 0.25130999 W

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.anml\efc.xml



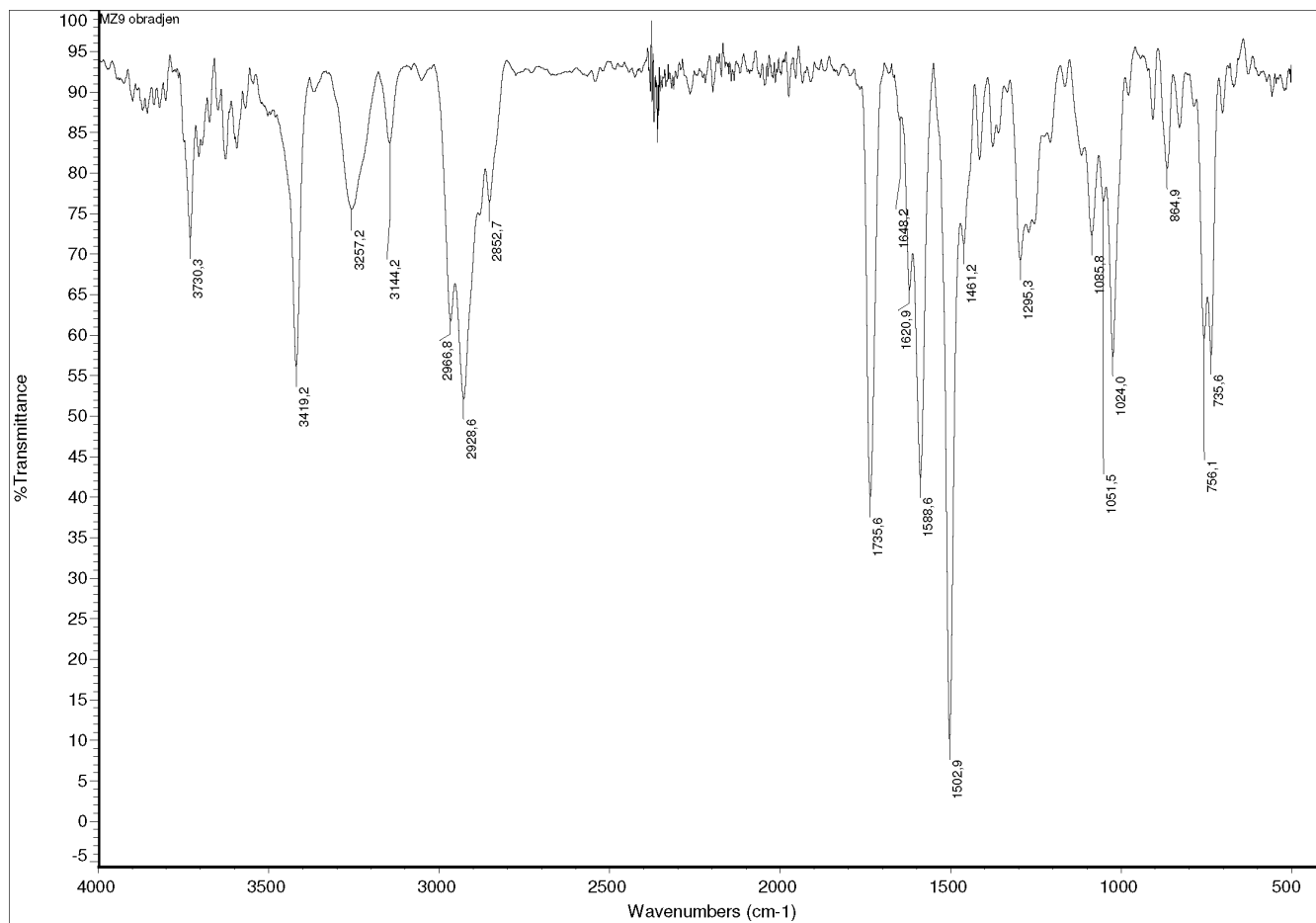
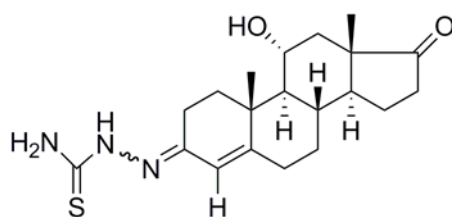
Merged XIC, Period# : 1 Experiment# : 1

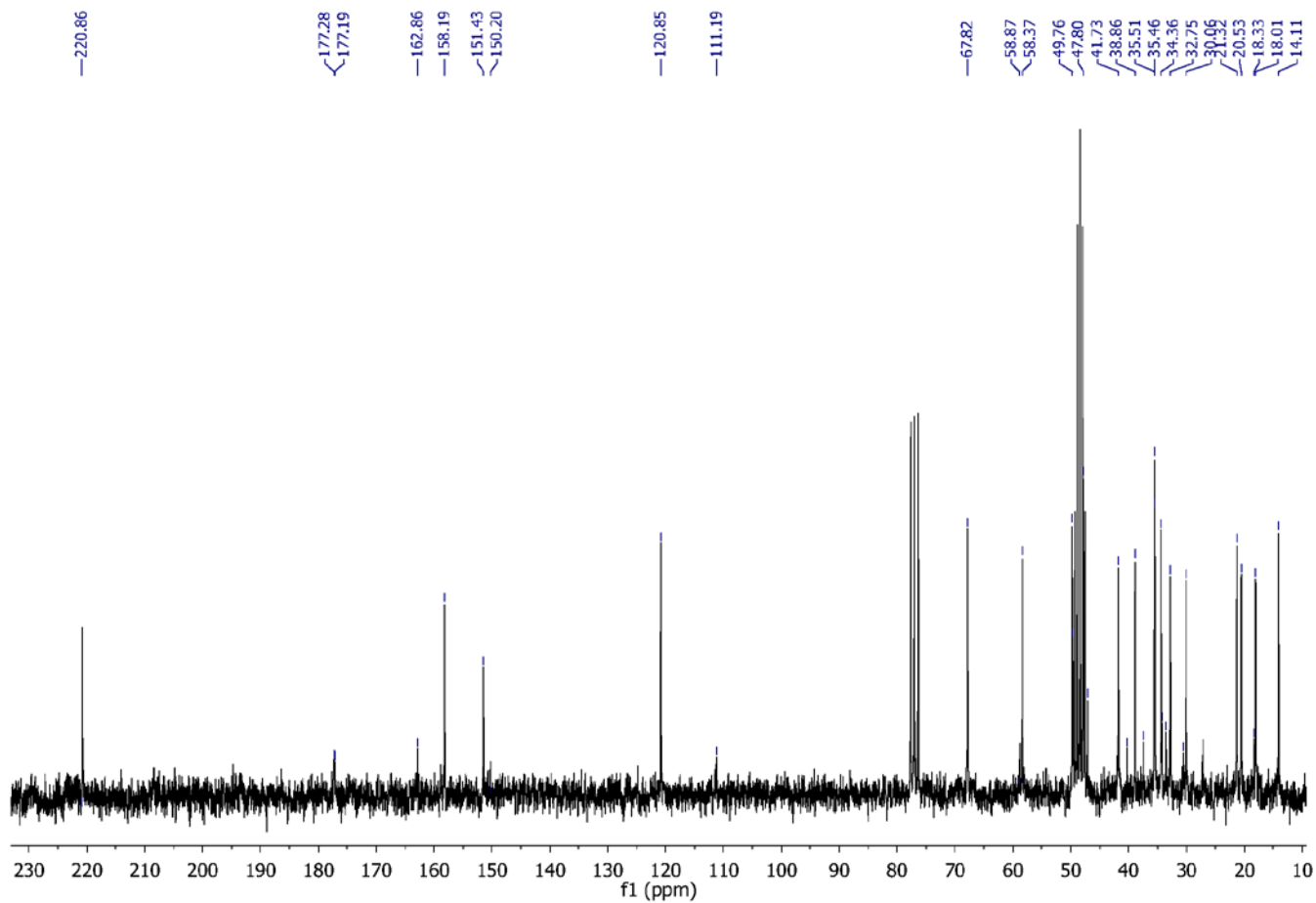
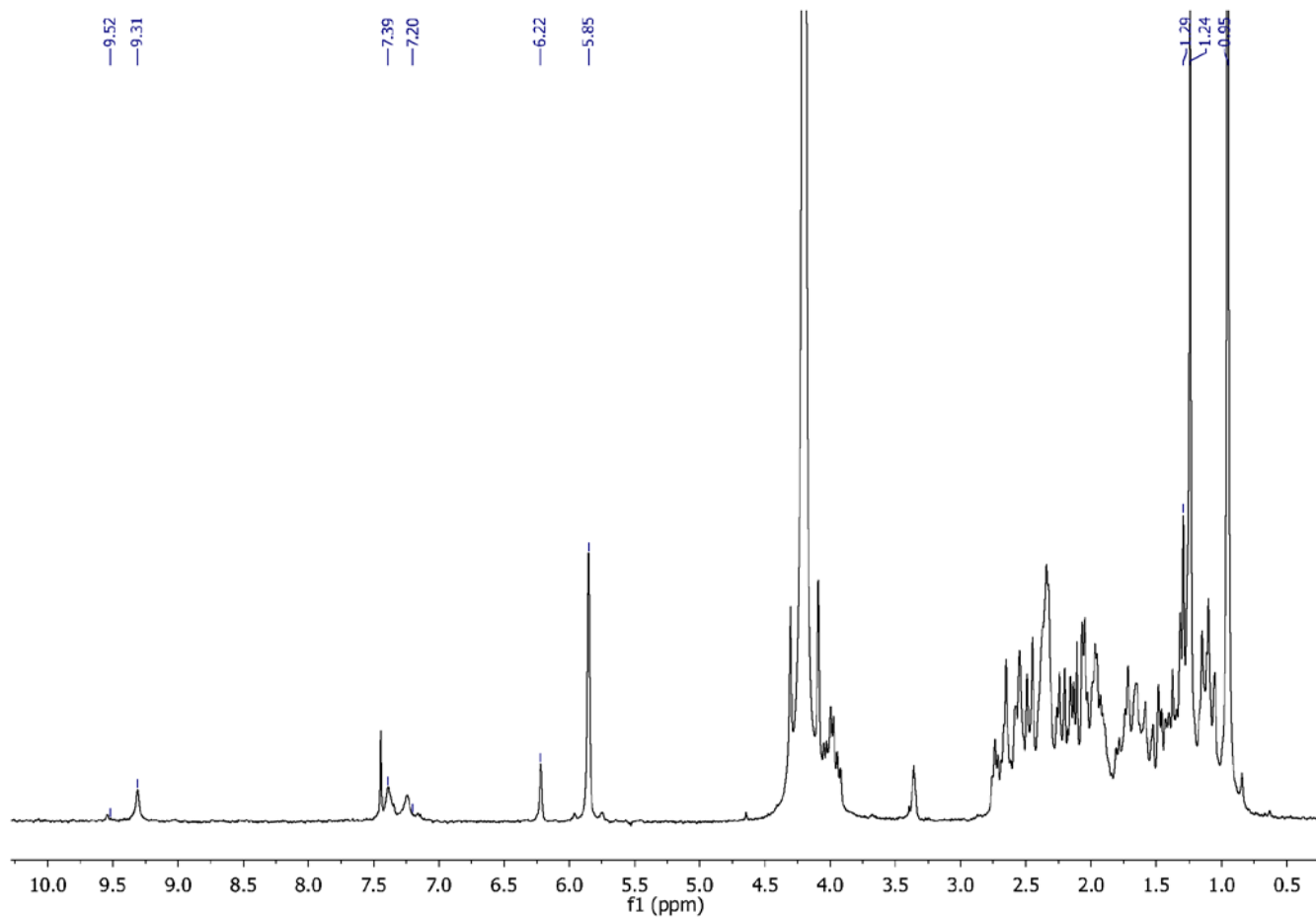


Formula	Compound name	Mass	Peak RT (min)	Peak area	Description
C29H38N6O4S2	—	598.23960	0.40	9.30051 E6	—

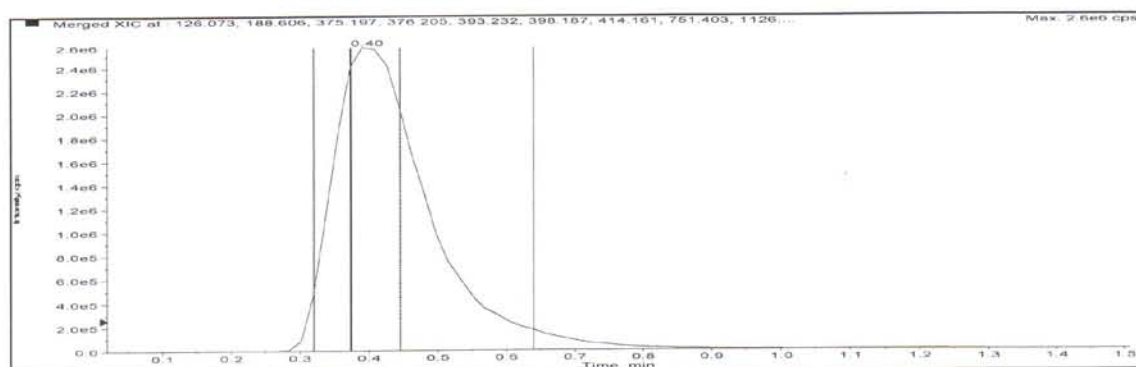
Species	Abundance (counts)	Ion Mass	Measured Mass	Error (mDa)	Error (ppm)	Ret. Time Error (min)
[M+2H] ²⁺	20361.33	300.12707	300.12731	0.23612	0.79	--
[M+H] ⁺	344152.86	599.24687	599.24660	-0.27645	-0.46	--
[M+Na] ⁺	11180.87	621.22882	621.22859	-0.22286	-0.36	--

Compound **2d**

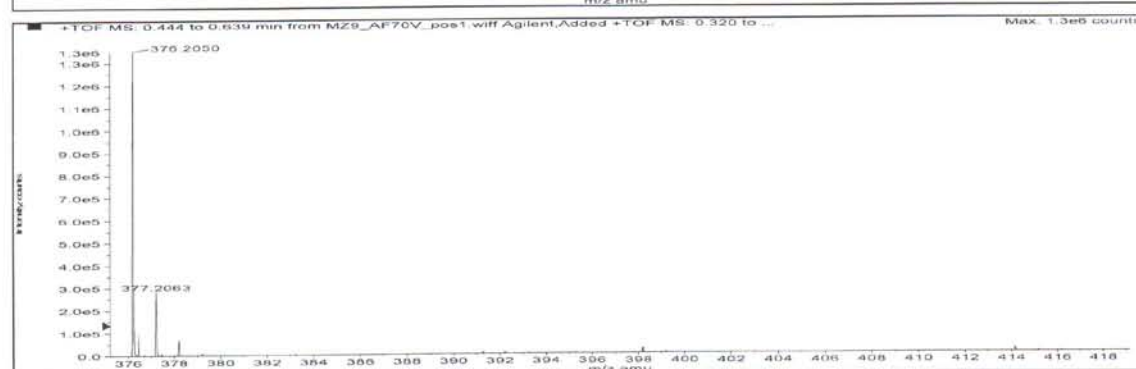
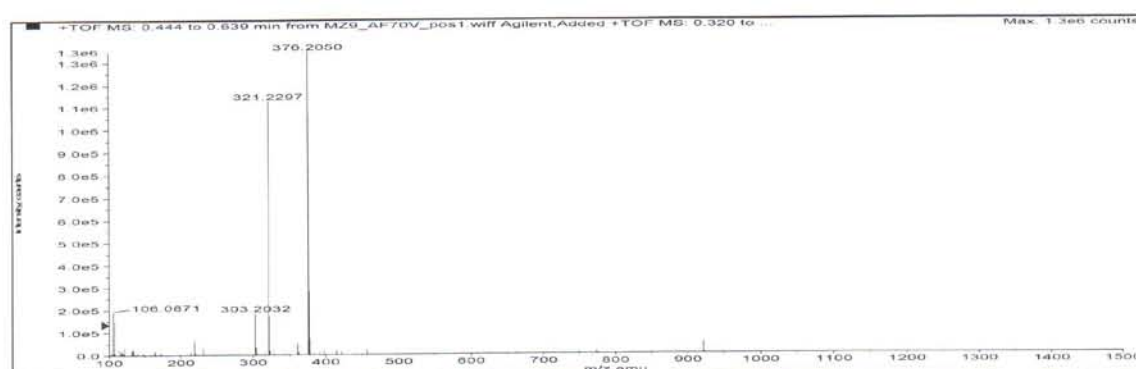




Sample Name: **MZ9** Sample Location: **P1-D1** Sample Id: Operator: **Milka**
 Data File Name: **D:\PE Sciex Data\Projects\SladiciData\MZ9_AF70V_pos1.wiff** Acq Time: **May 07 2015, 11:21:01 AM**
 Method: **d:\TOF_Data\damethods\Night_Seq_Comp_ident1.anmlefc.xml**



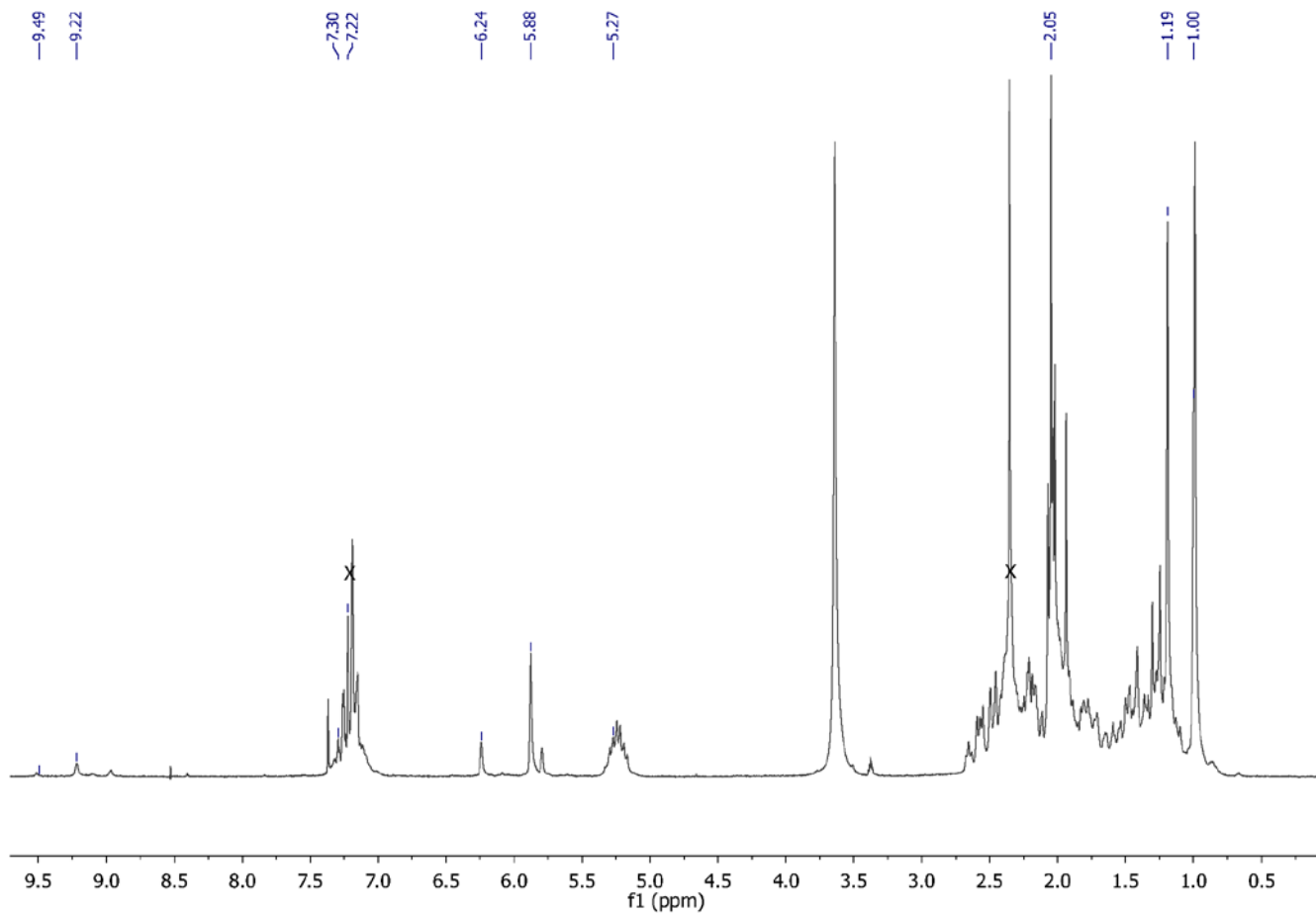
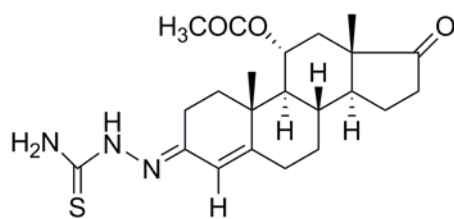
Merged XIC, Period# : 1 Experiment# : 1



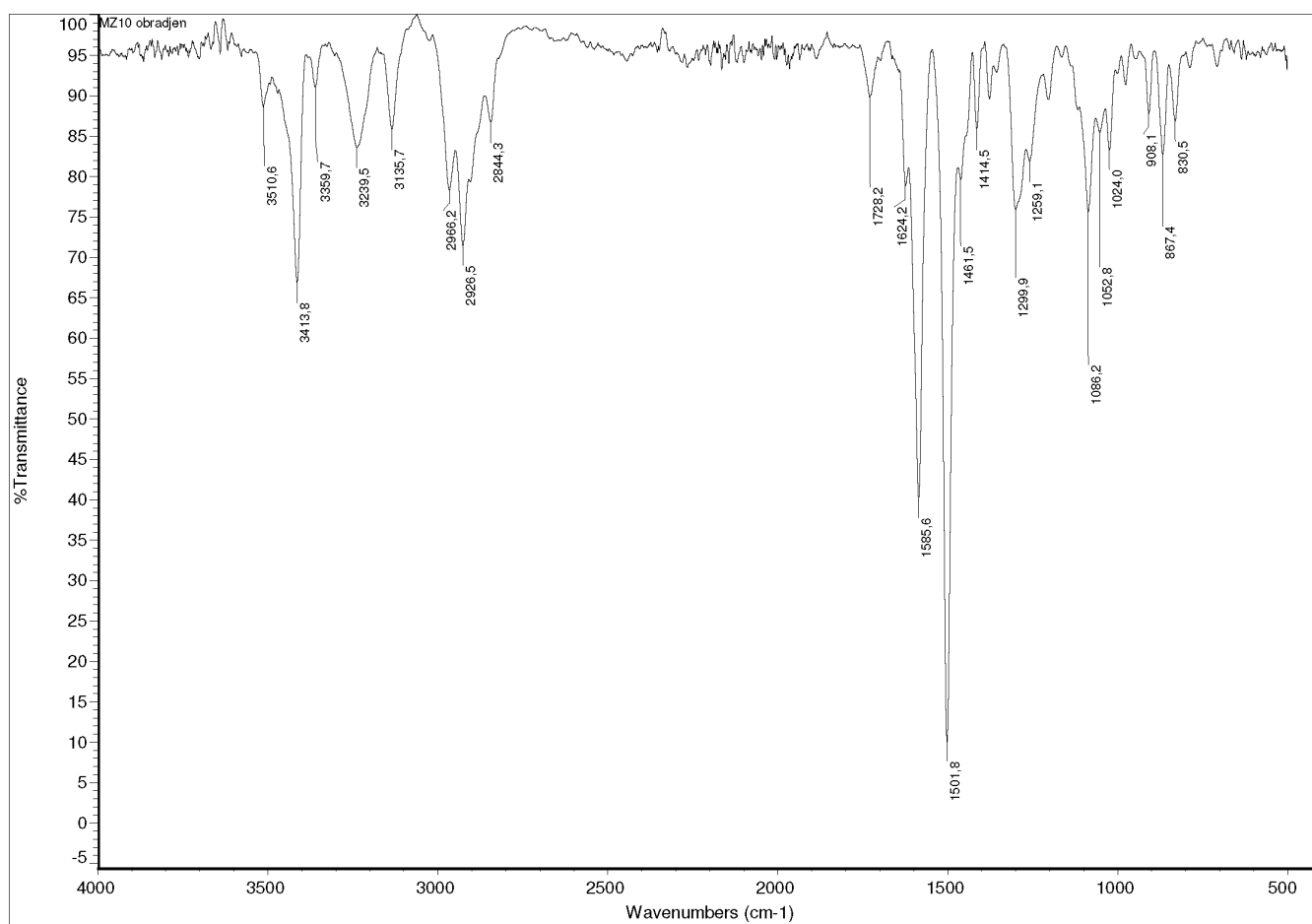
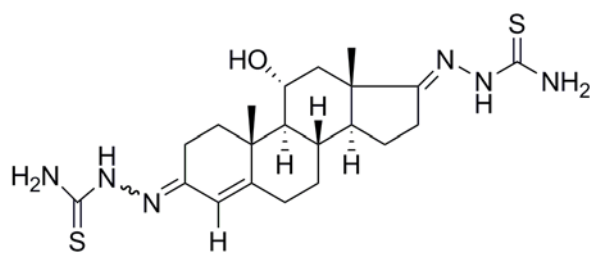
Formula	Compound name	Mass	Peak RT (min)	Peak area	Description
C ₂₀ H ₂₉ N ₃ O ₂ S	--	375.19805	0.40	2.45542 E7	--

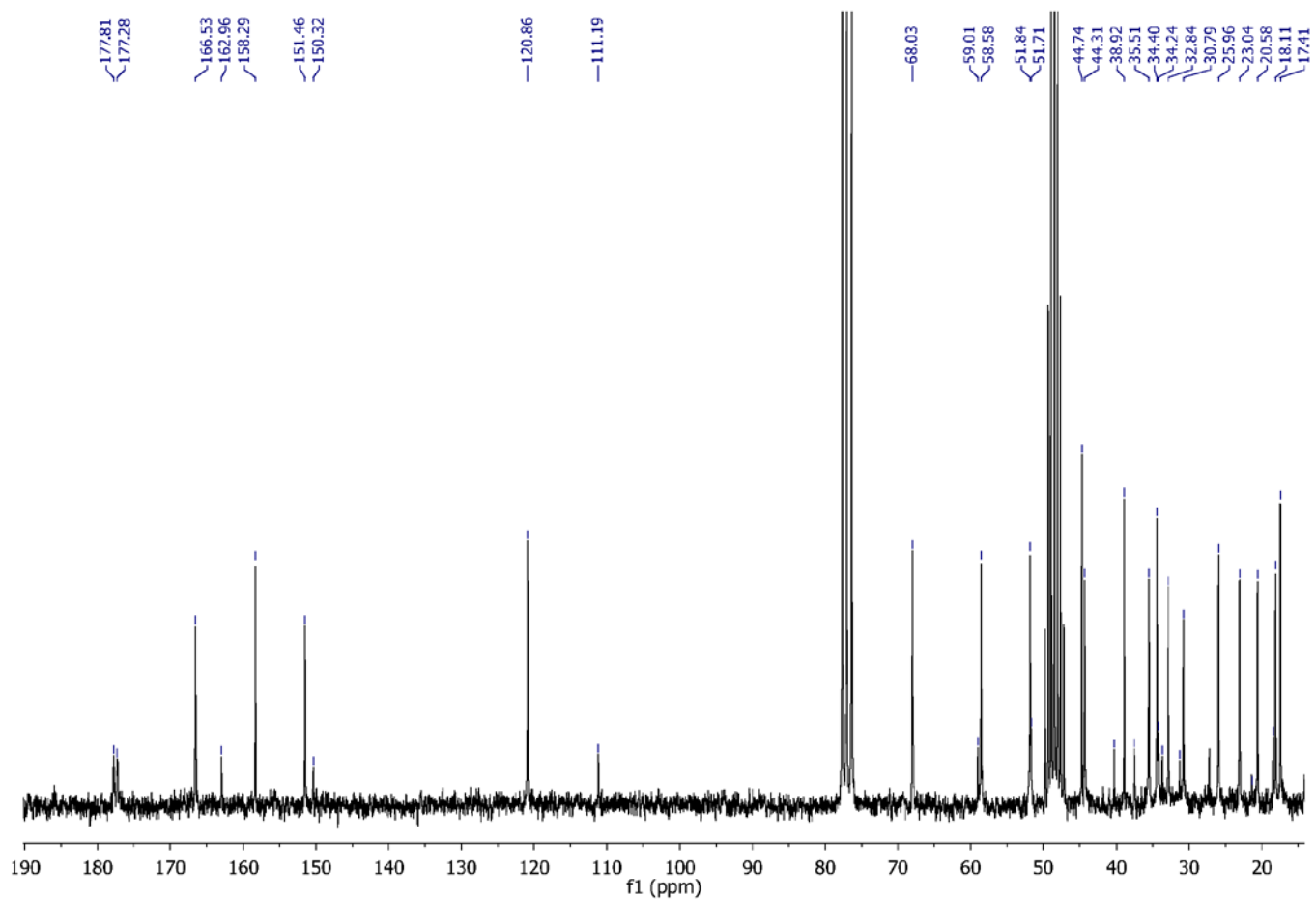
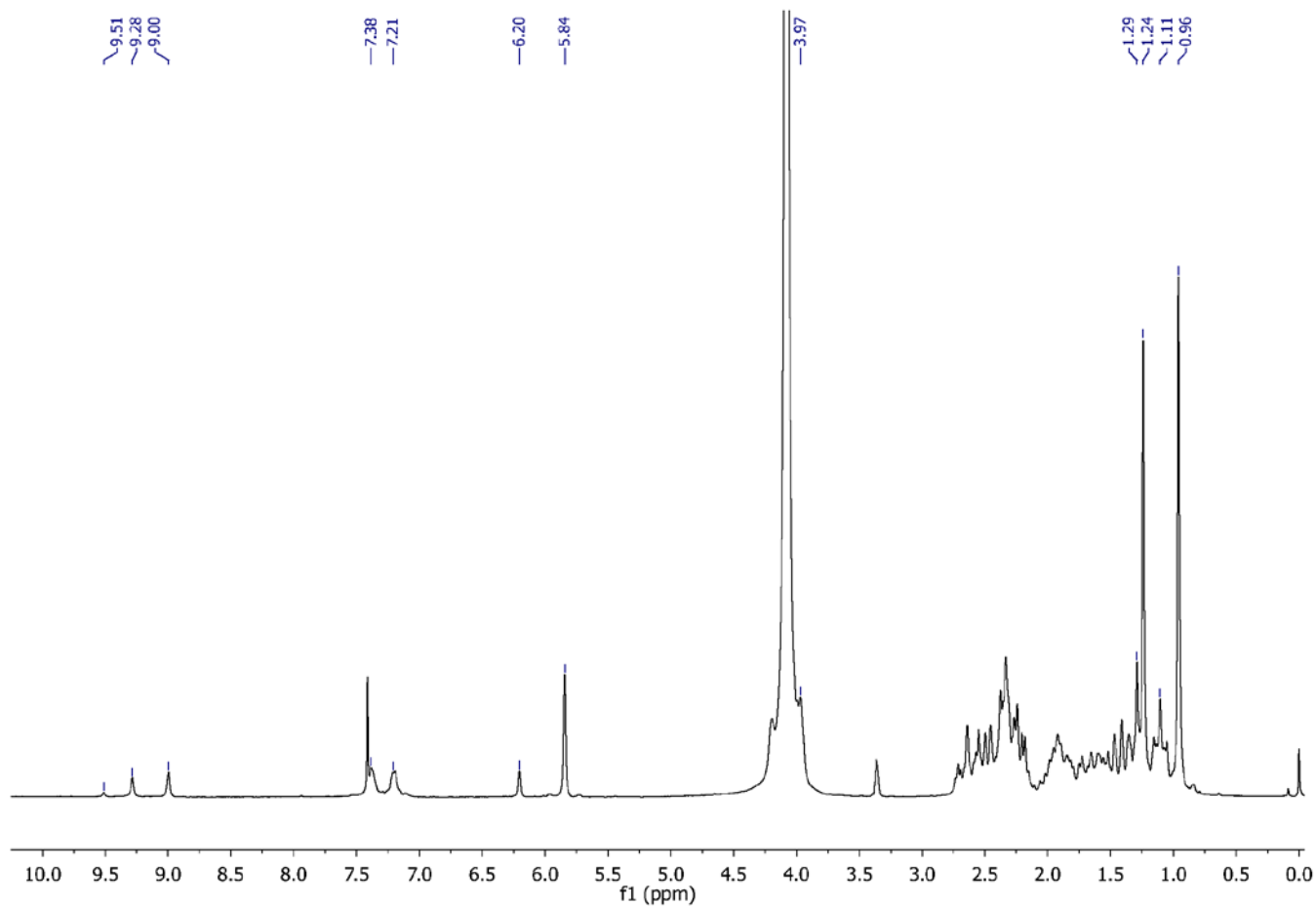
Species	Abundance (counts)	Ion Mass	Measured Mass	Error (mDa)	Error (ppm)	Ret. Time Error (min)
[M+H] ⁺	1349547.36	376.20532	376.20446	-0.86587	-2.30	--
[M+Na] ⁺	22984.79	398.18727	398.18694	-0.33013	-0.83	--
[M+K] ⁺	14207.43	414.16121	414.16159	0.37987	0.92	--

Compound **2d-OAc**

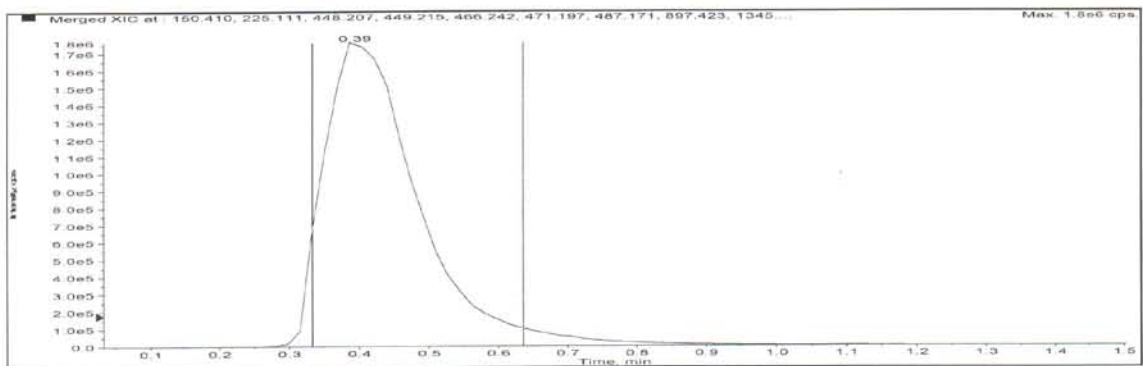


Compound 3d

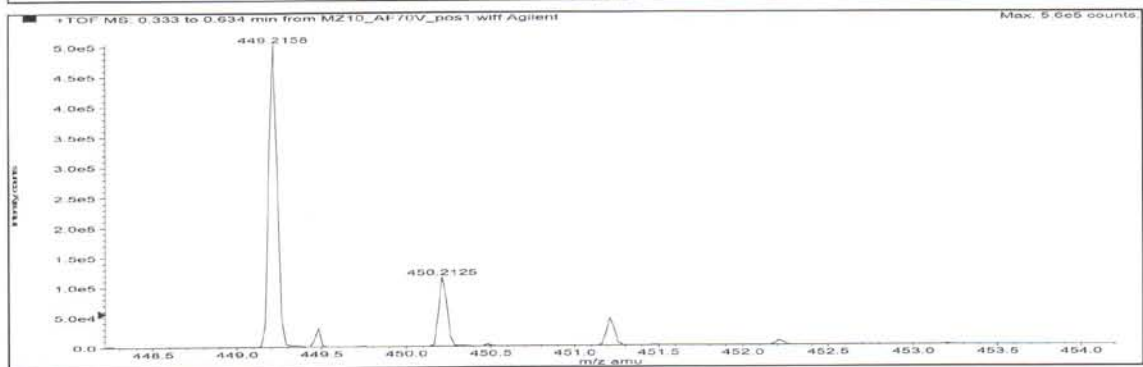
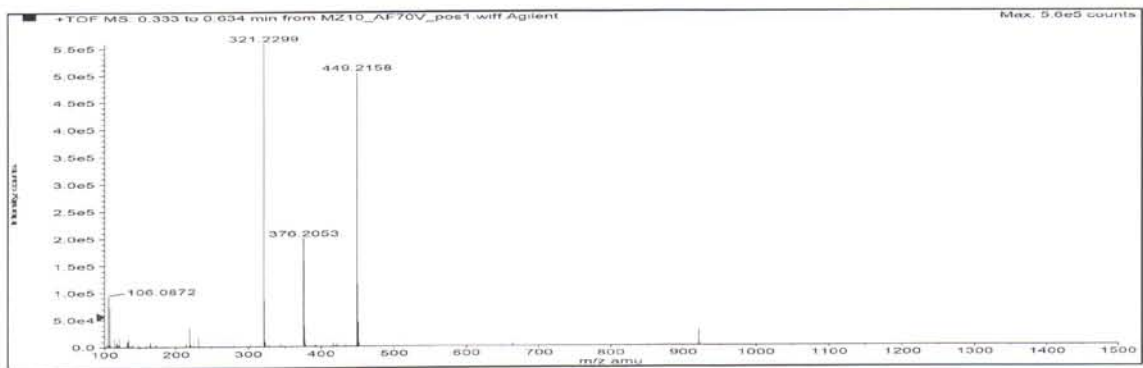




Sample Name: MZ10 Sample Location: P1-D2 Sample Id: Operator: Milka
 Data File Name: D:\PE Sciex Data\Projects\Sladic\Data\MZ10_AF70V_pos1.wiff Acq Time: May 07 2015, 11:23:36 AM
 Method: d:\TOF_Data\damethods\Night_Seq_Comp_ident1.anm\efc.xml

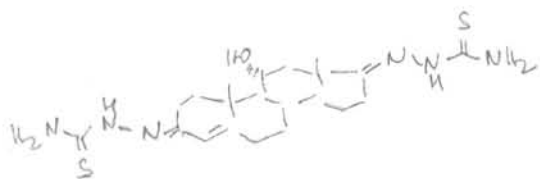


Merged XIC, Period# : 1 Experiment# : 1

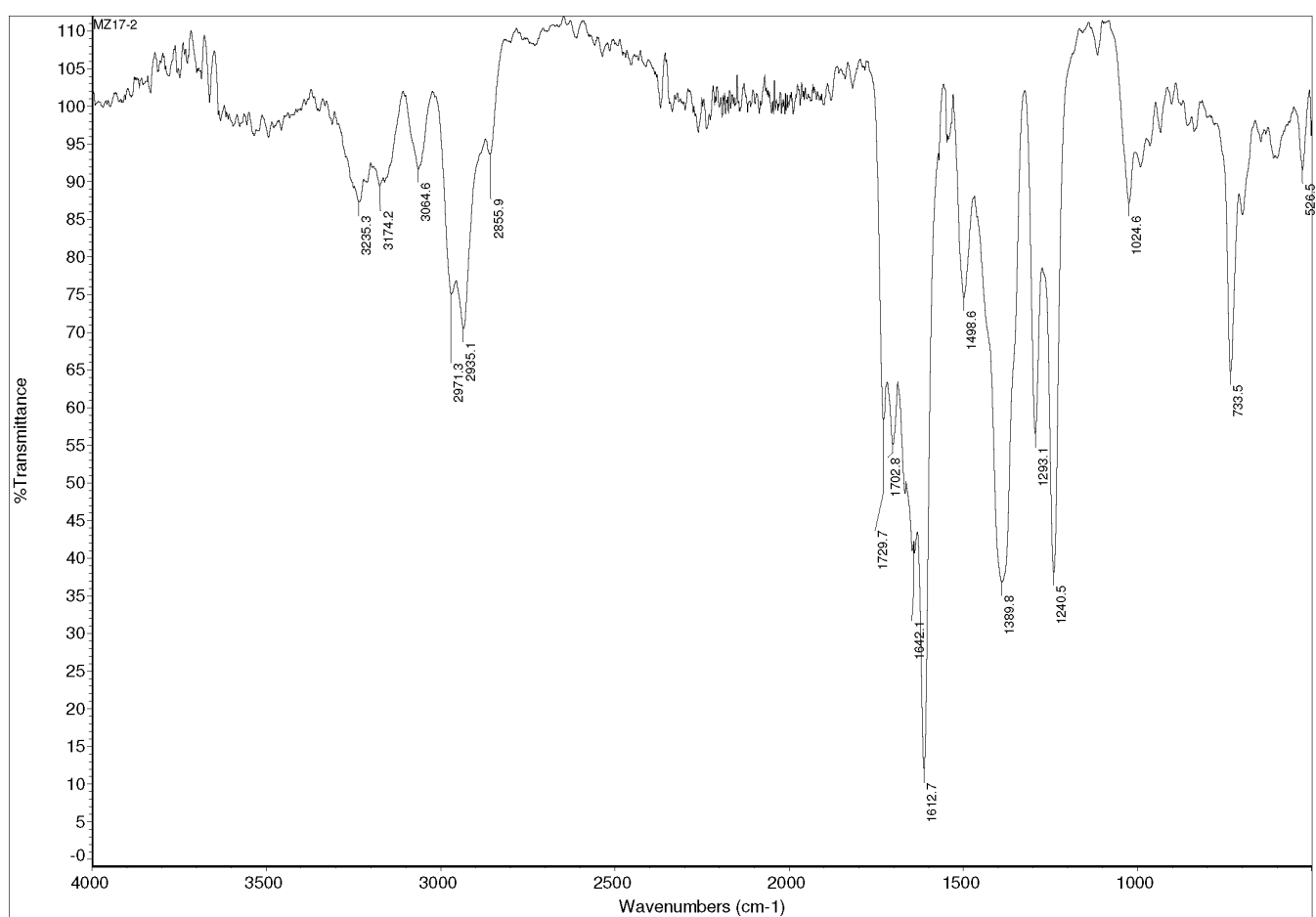
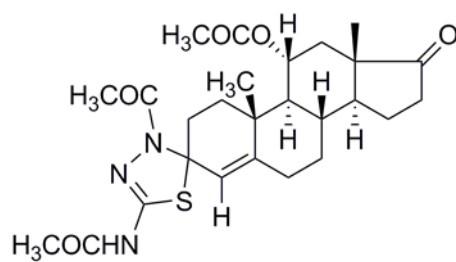


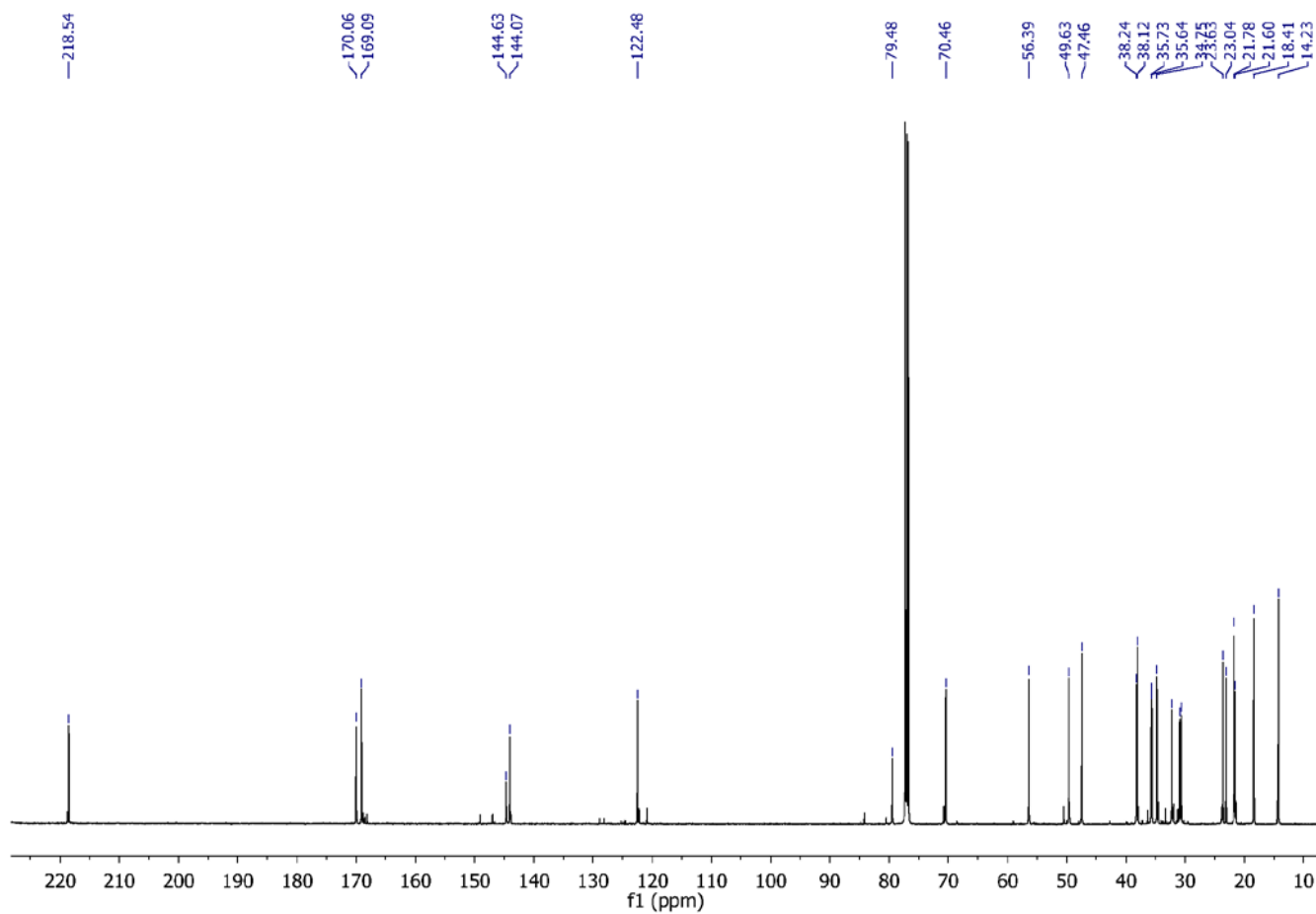
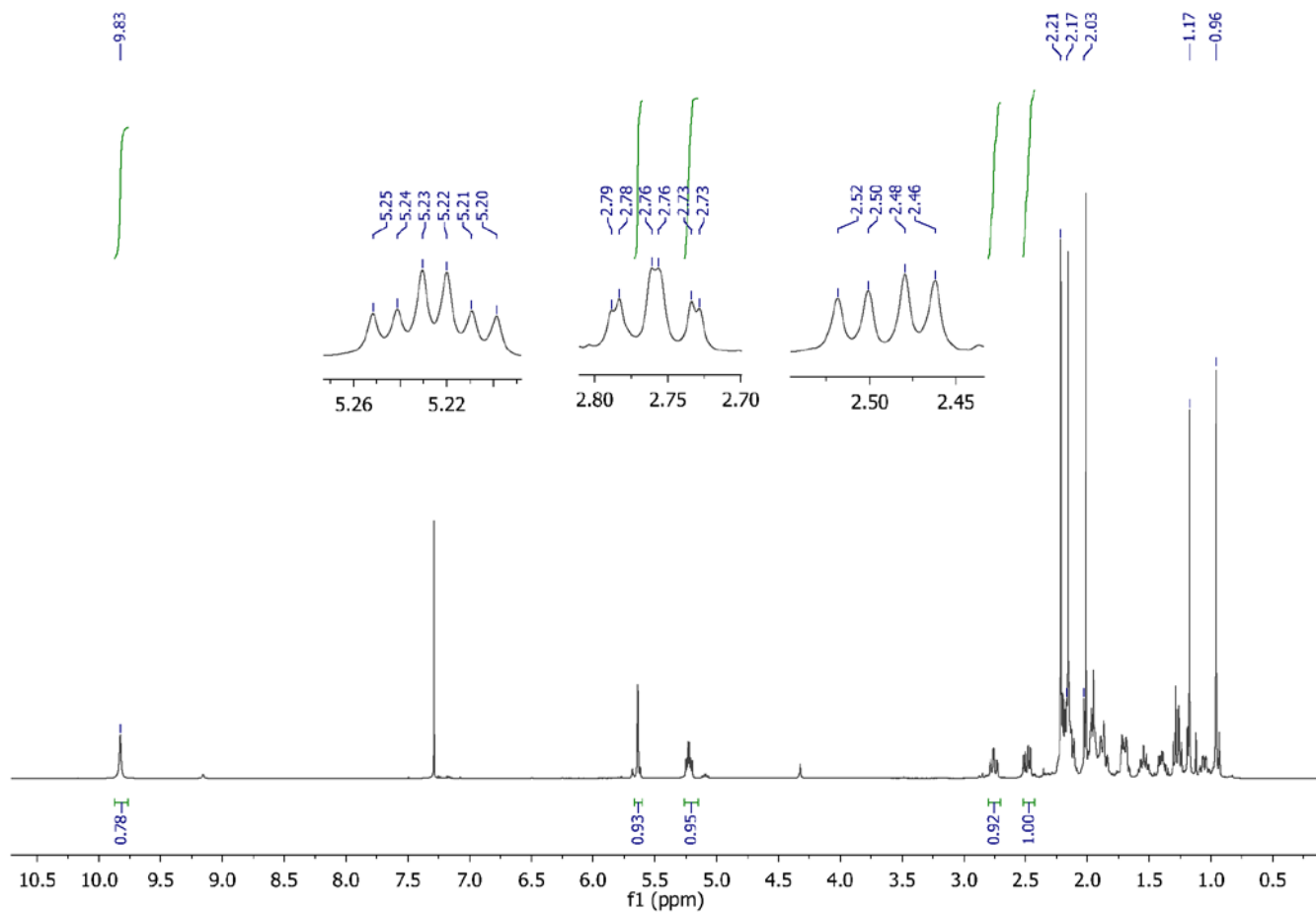
Formula	Compound name	Mass	Peak RT (min)	Peak area	Description
C21H32N6OS2	—	448.20790	0.39	1.63724 E7	—

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	—

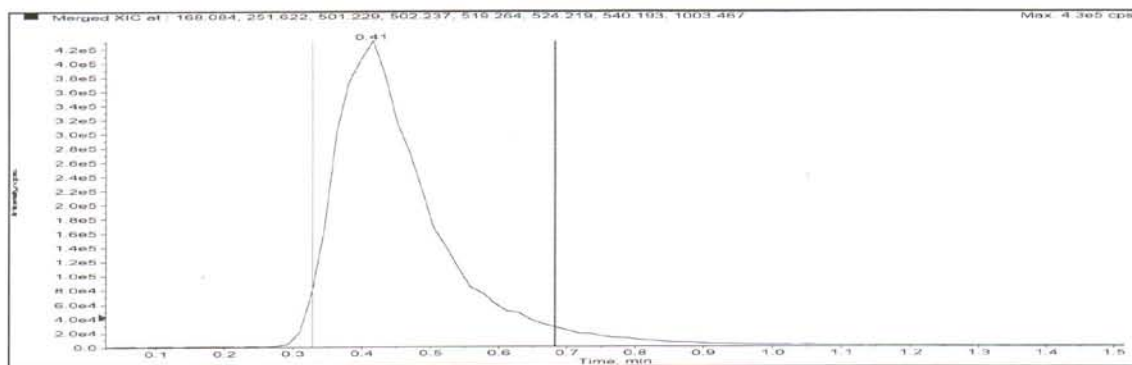


Compound **4d-OAc**

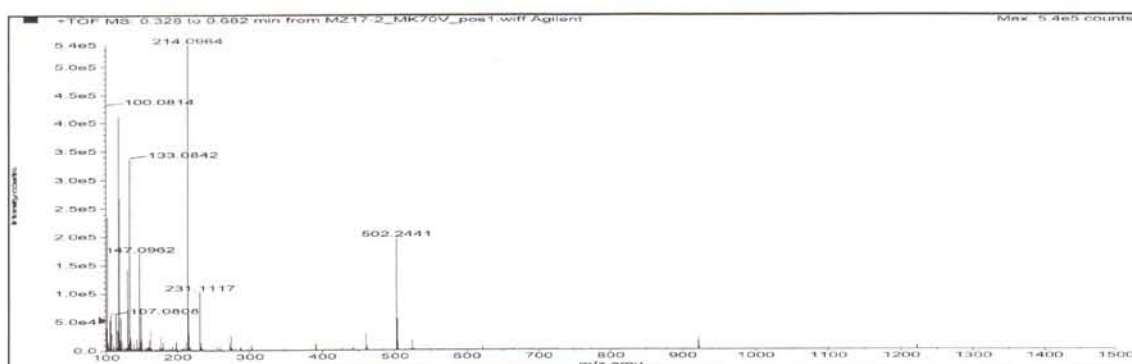




Sample Name: MZ17-2 Sample Location: P1-C7 Sample Id: Operator: Milka
 Data File Name: D:\PE Sciex Data\Projects\Sladic\Data\MZ17-2_MK70V_pos1.wiff Acq Time: August 05 2014, 11:30:24 AM
 Method: d:\TOF_Data\damethods\Night_Seq_Comp_ident1.an\lfe.c.xml

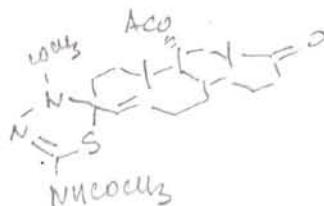


Merged XIC, Period# : 1 Experiment# : 1

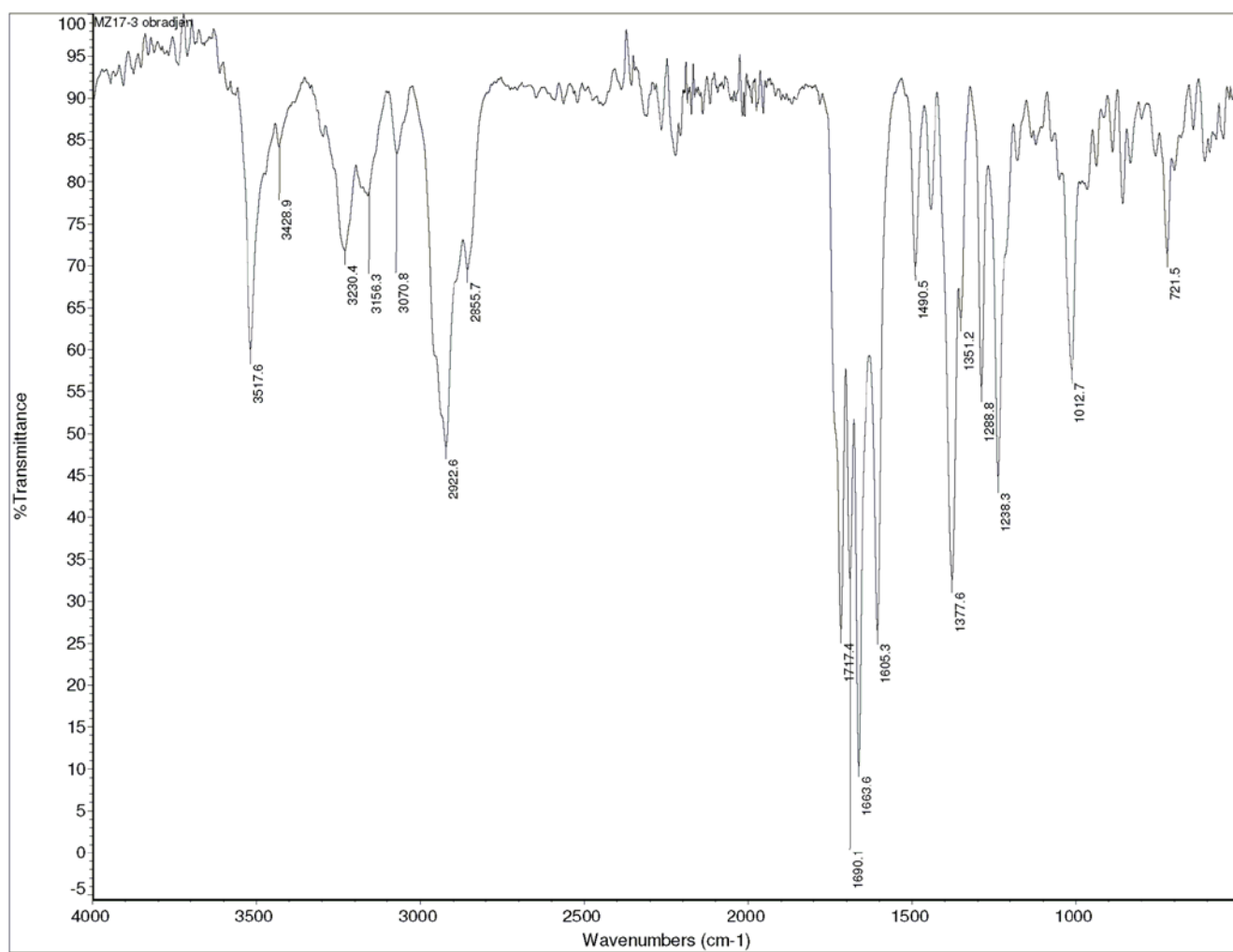
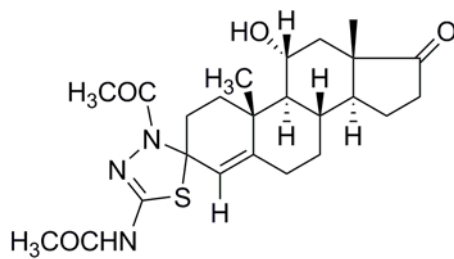


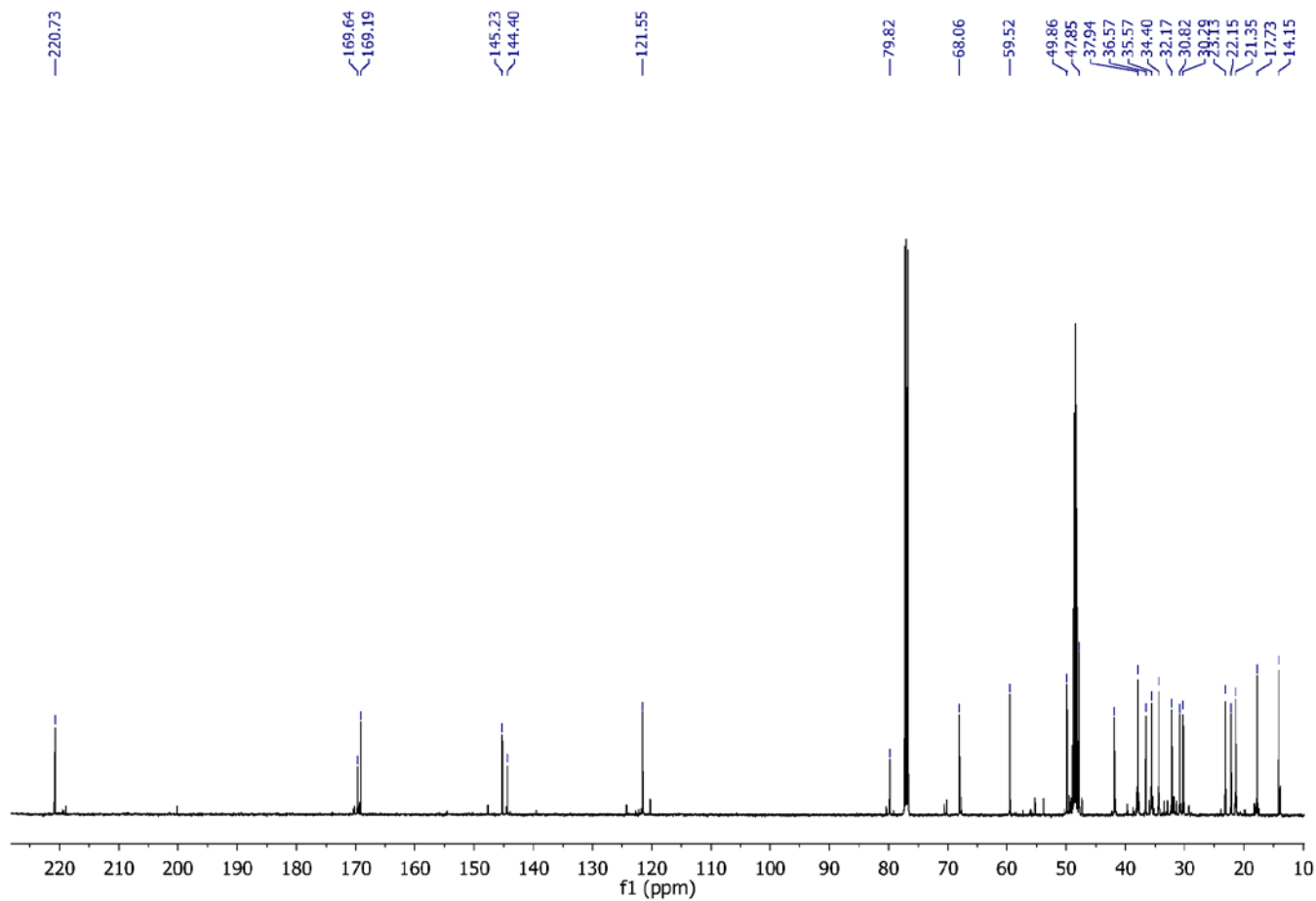
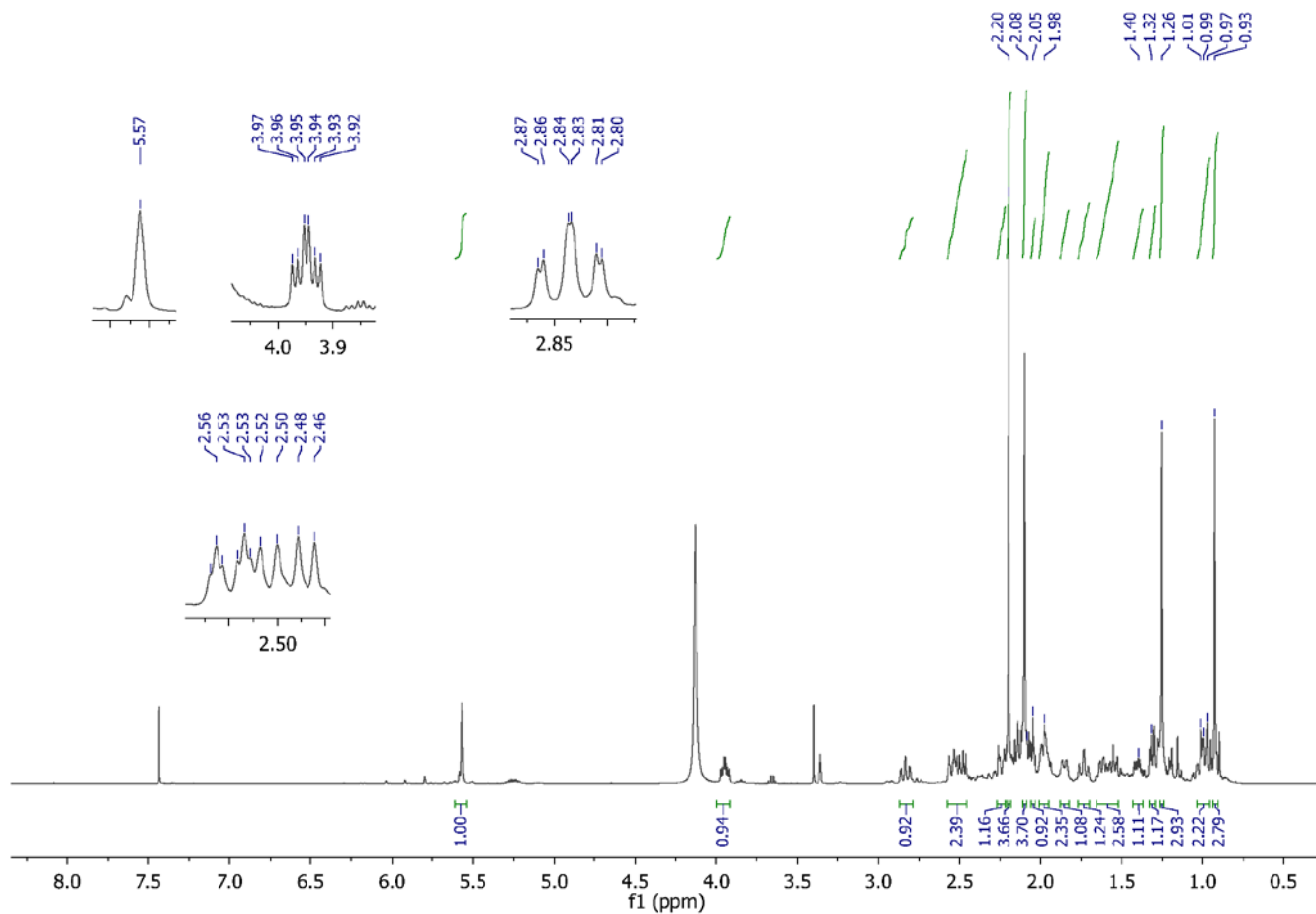
Formula	Compound name	Mass	Peak RT (min)	Peak area	Description
C26H35N3O5S	—	501.22974	0.41	4.14084 E6	—

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	—

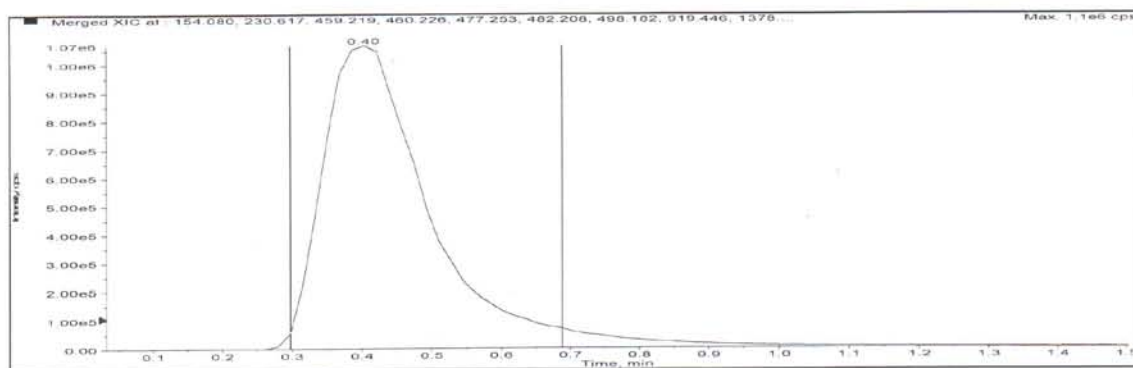


Compound **4d-OH**

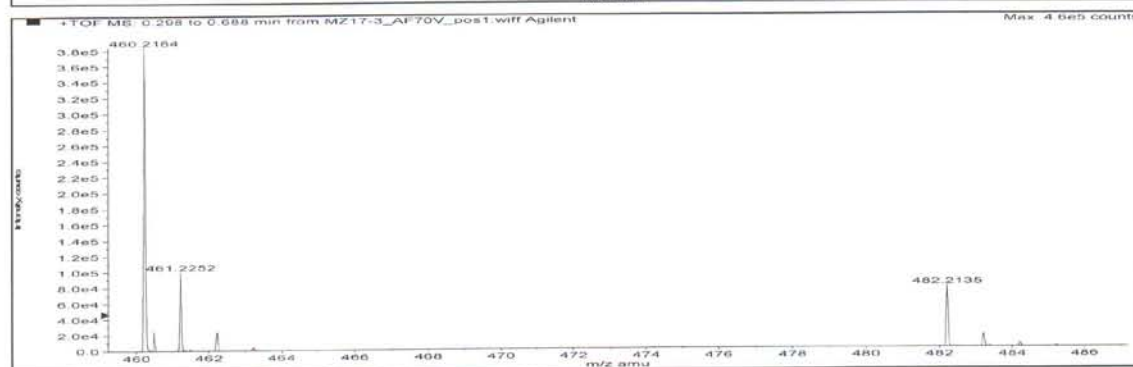
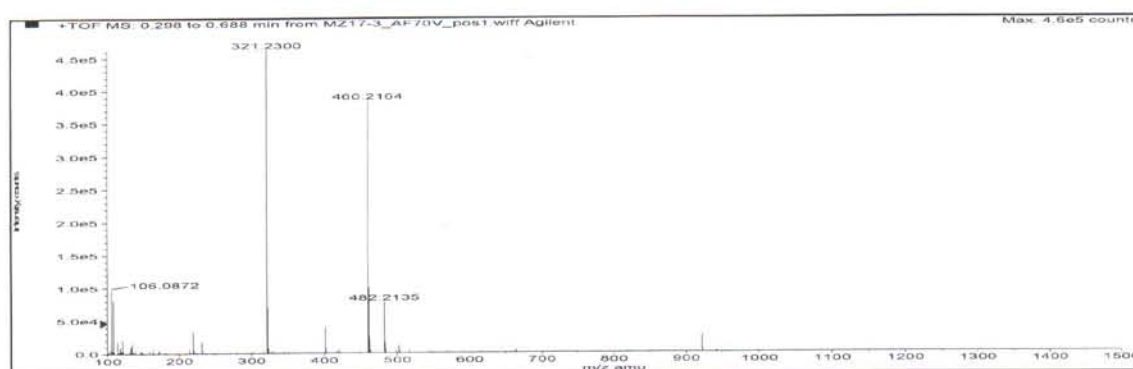




Sample Name: MZ17-3 Sample Location: P1-D3 Sample Id: Operator: Milka
 Data File Name: D:\PE Sclex Data\Projects\SladlcData\MZ17-3_AF70V_pos1.wiff Acq Time: May 07 2015, 11:26:09 AM
 Method: d:\TOF_Data\damethods\Night_Seq_Comp_ident1.anmlefc.xml

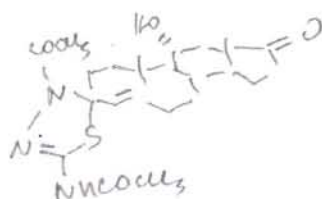


Merged XIC, Period# : 1 Experiment# : 1

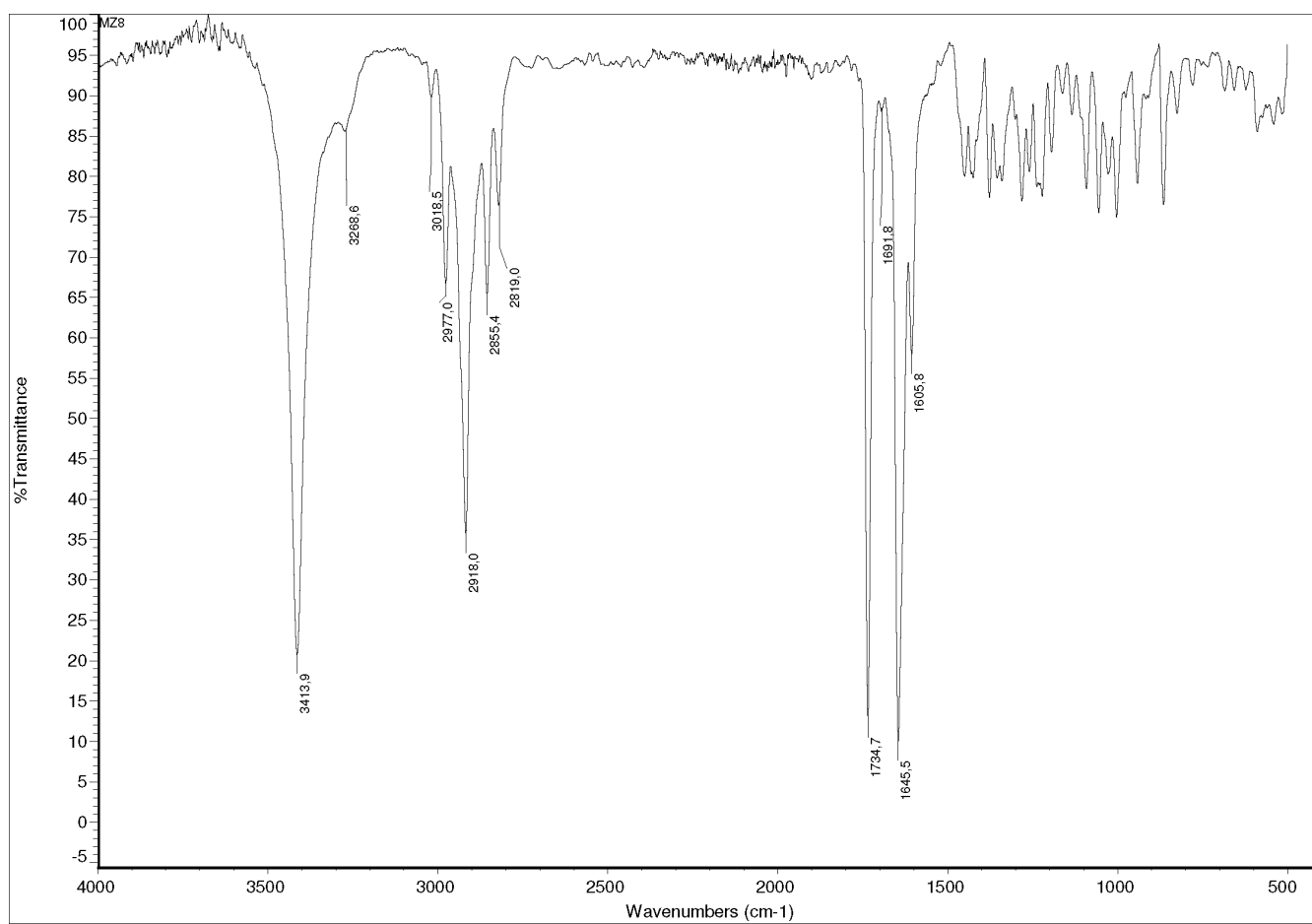
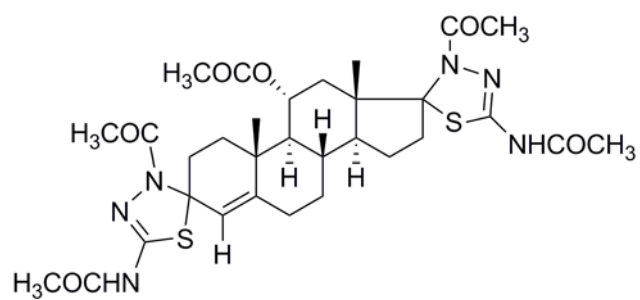


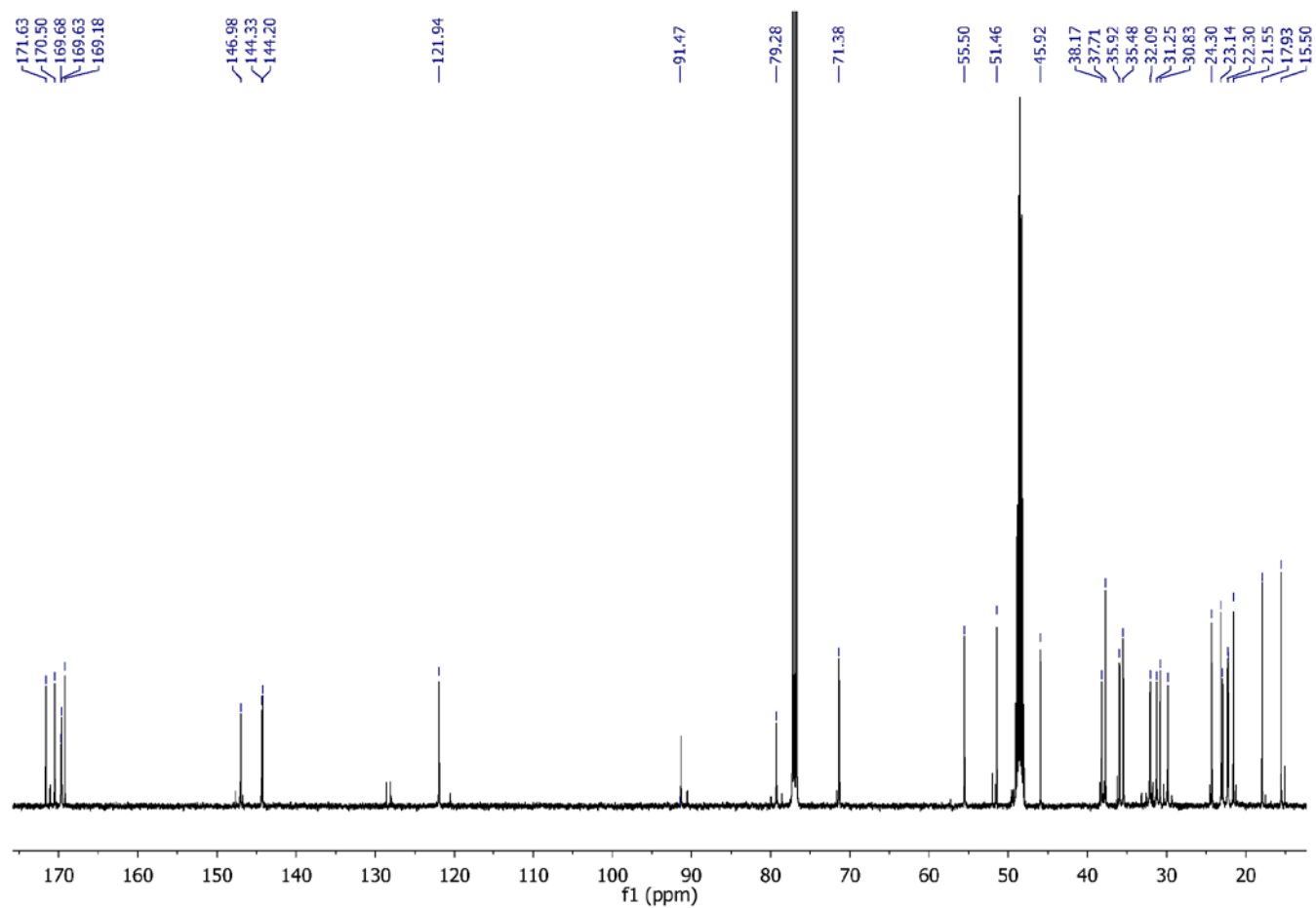
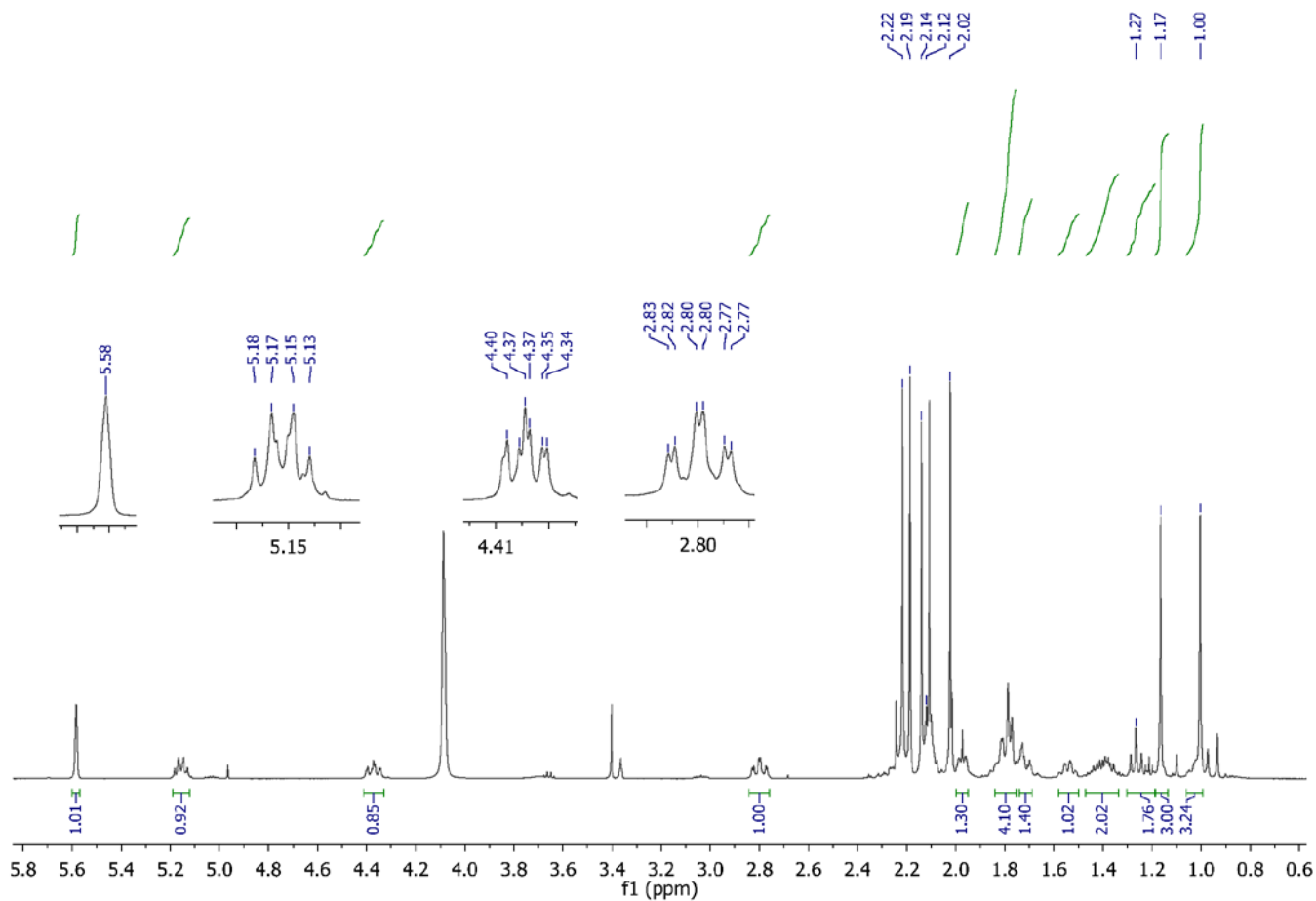
Formula	Compound name	Mass	Peak RT (min)	Peak area	Description
C24H33N3O4S	--	459.21918	0.40	1.11991 E7	--

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	--

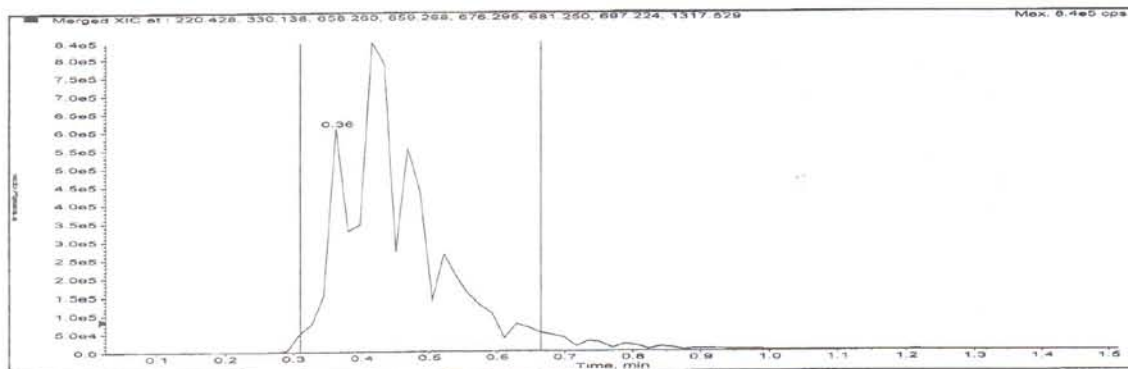


Compound 5d

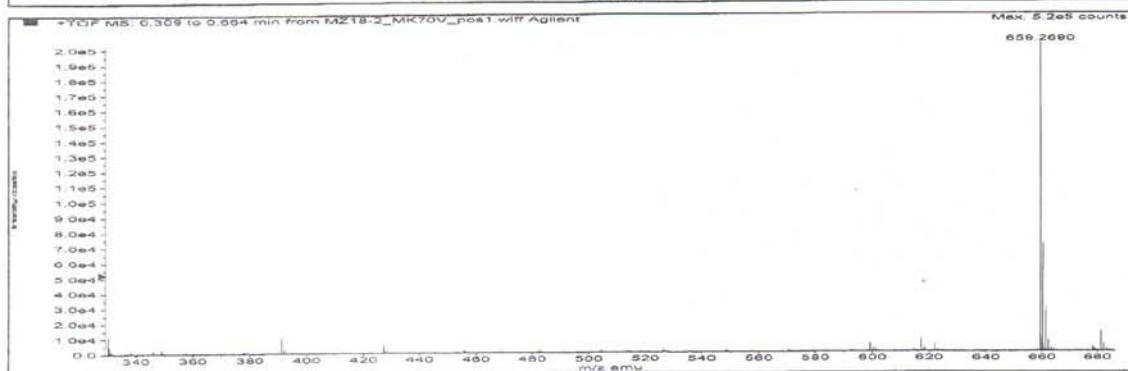
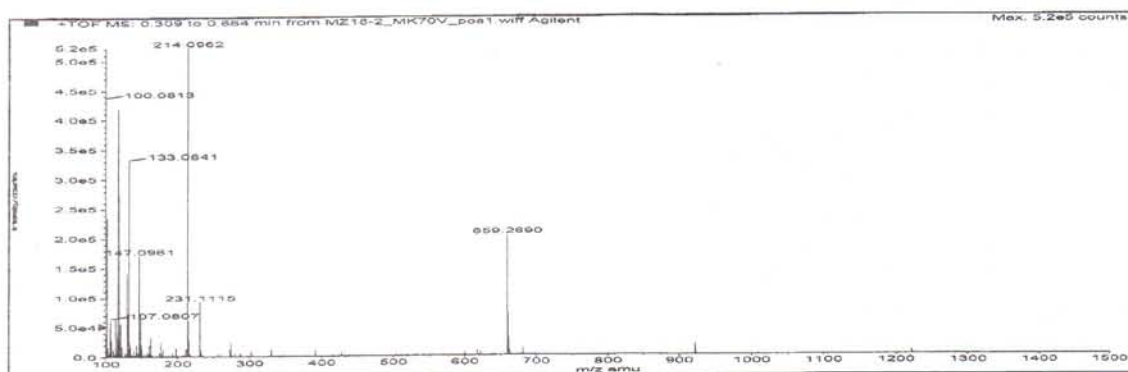




Sample Name: MZ18-2 Sample Location: P1-C8 Sample Id: Operator: Milka
 Data File Name: D:\PE Sciex Data\Projects\Sladic\Data\MZ18-2_MK70V_pos1.wiff Acq Time: August 05 2014, 11:32:53 AM
 Method: d:\TOF_Data\damethods\Night Seq Comp_ident1.anmlefc.xml

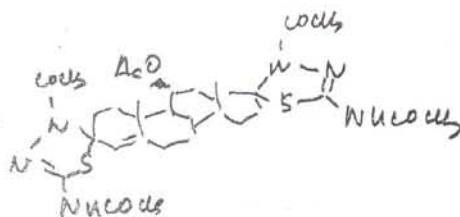


Merged XIC, Period# : 1 Experiment# : 1

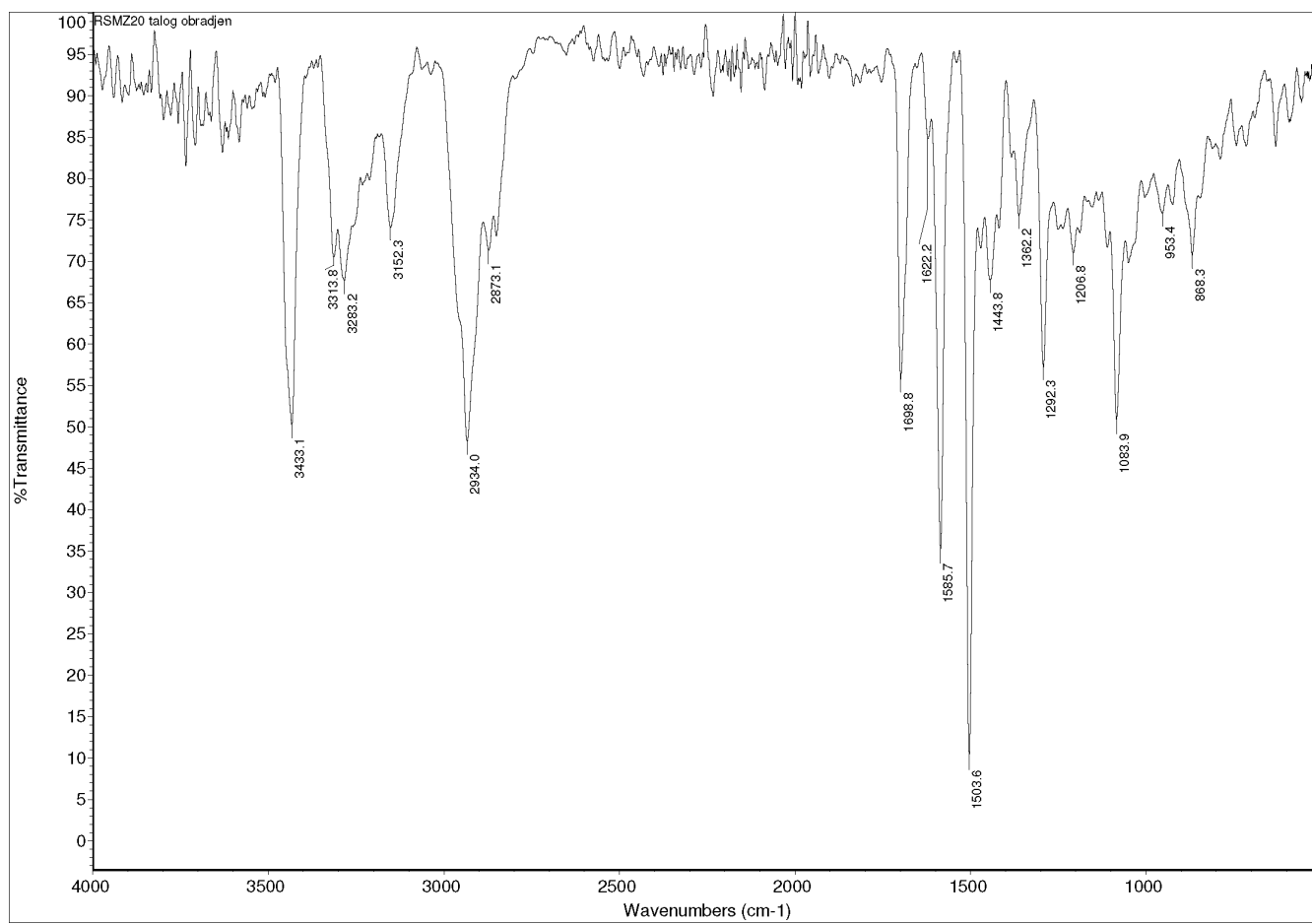
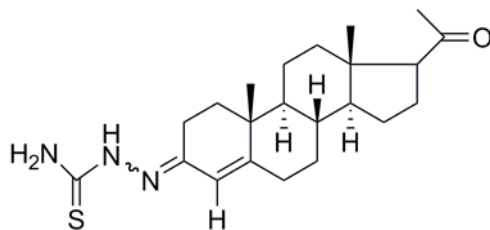


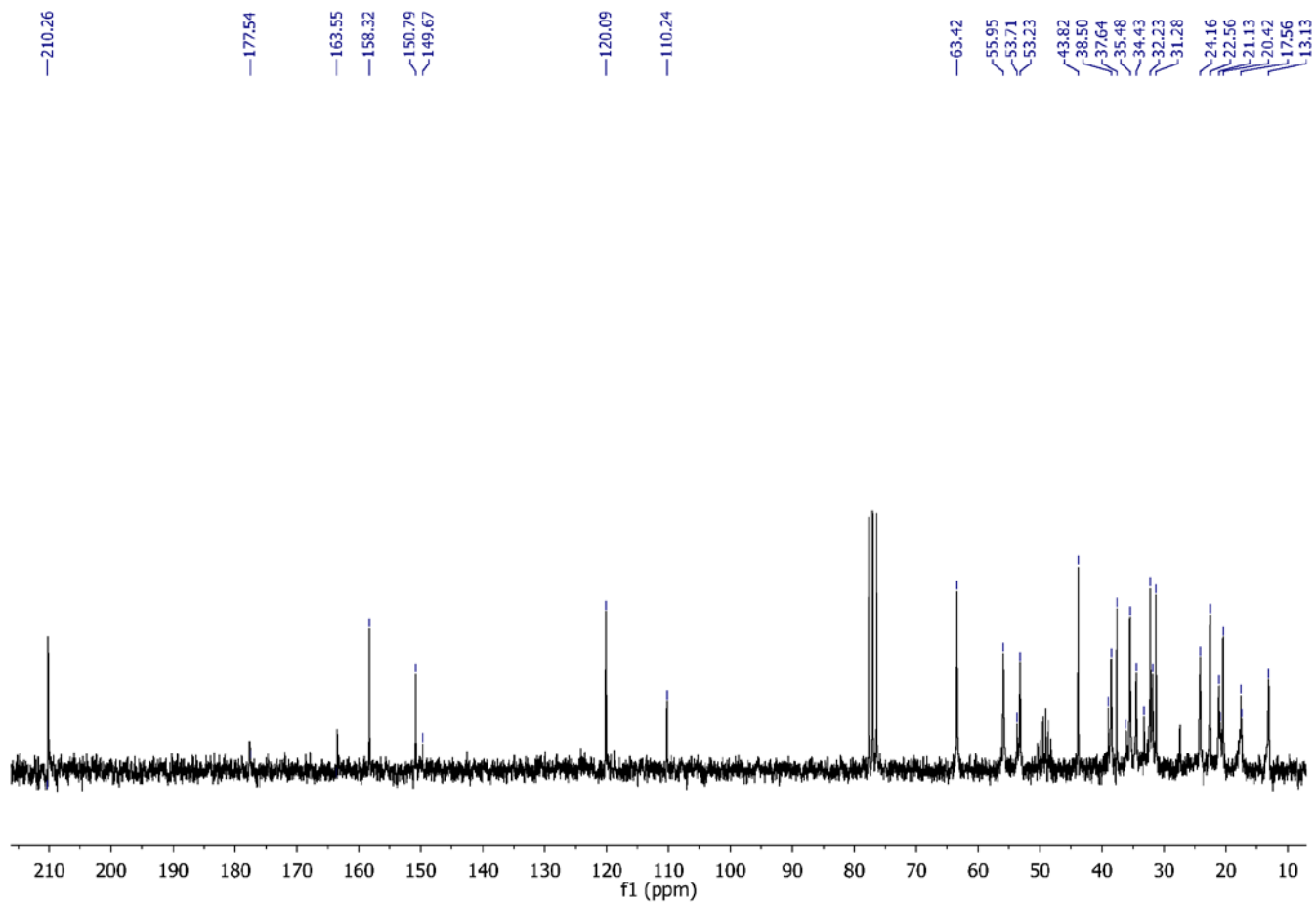
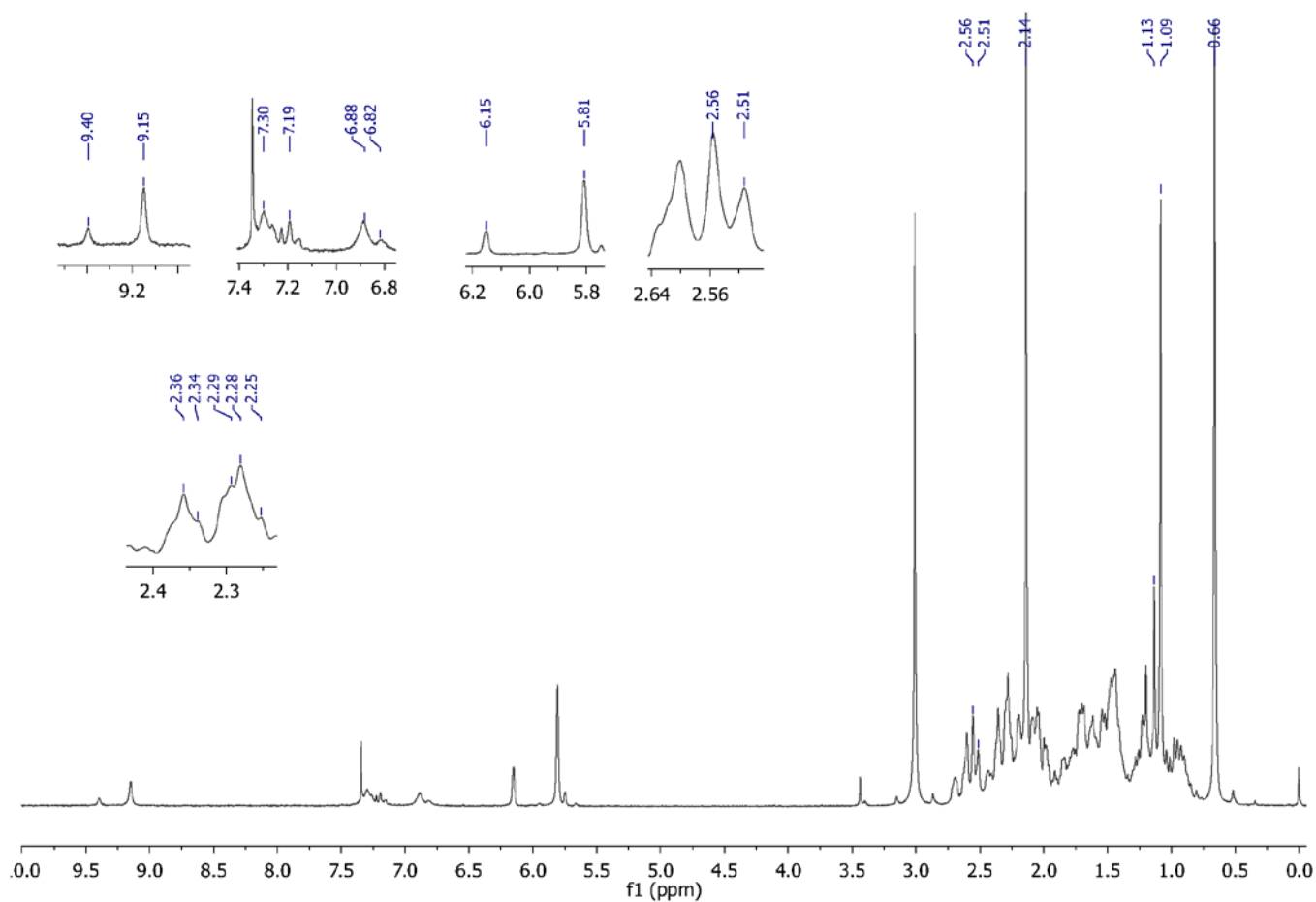
Formula	Compound name	Mass	Peak RT (min)	Peak area	Description
C ₃₁ H ₄₂ N ₆ O ₆ S ₂	--	658.26072	0.42	6.22477 E6	--

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	--

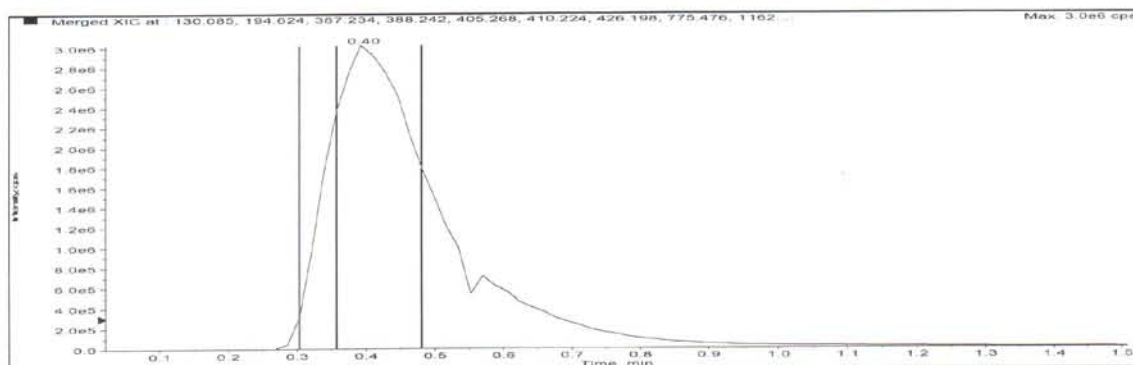


Compound 2e

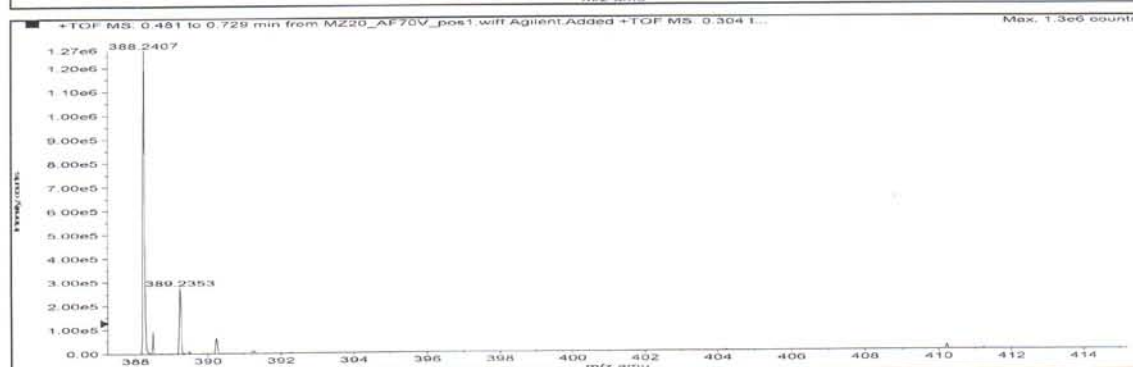
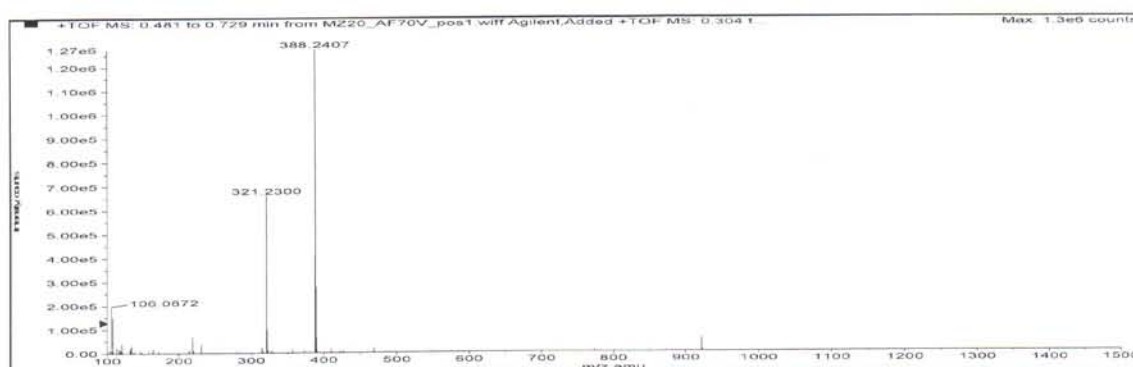




Sample Name: MZ20 Sample Location: P1-D4 Sample Id: Operator: Milka
 Data File Name: D:\PE Sclex Data\Projects\Sladic\Data\MZ20_AF70V_pos1.wiff Acq Time: May 07 2015, 11:28:41 AM
 Method: d:\TOF_Data\damethods\Night_Seq_Comp_ident1.anm\efc.xml

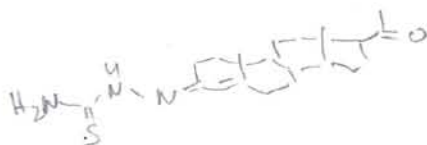


Merged XIC, Period# : 1 Experiment# : 1

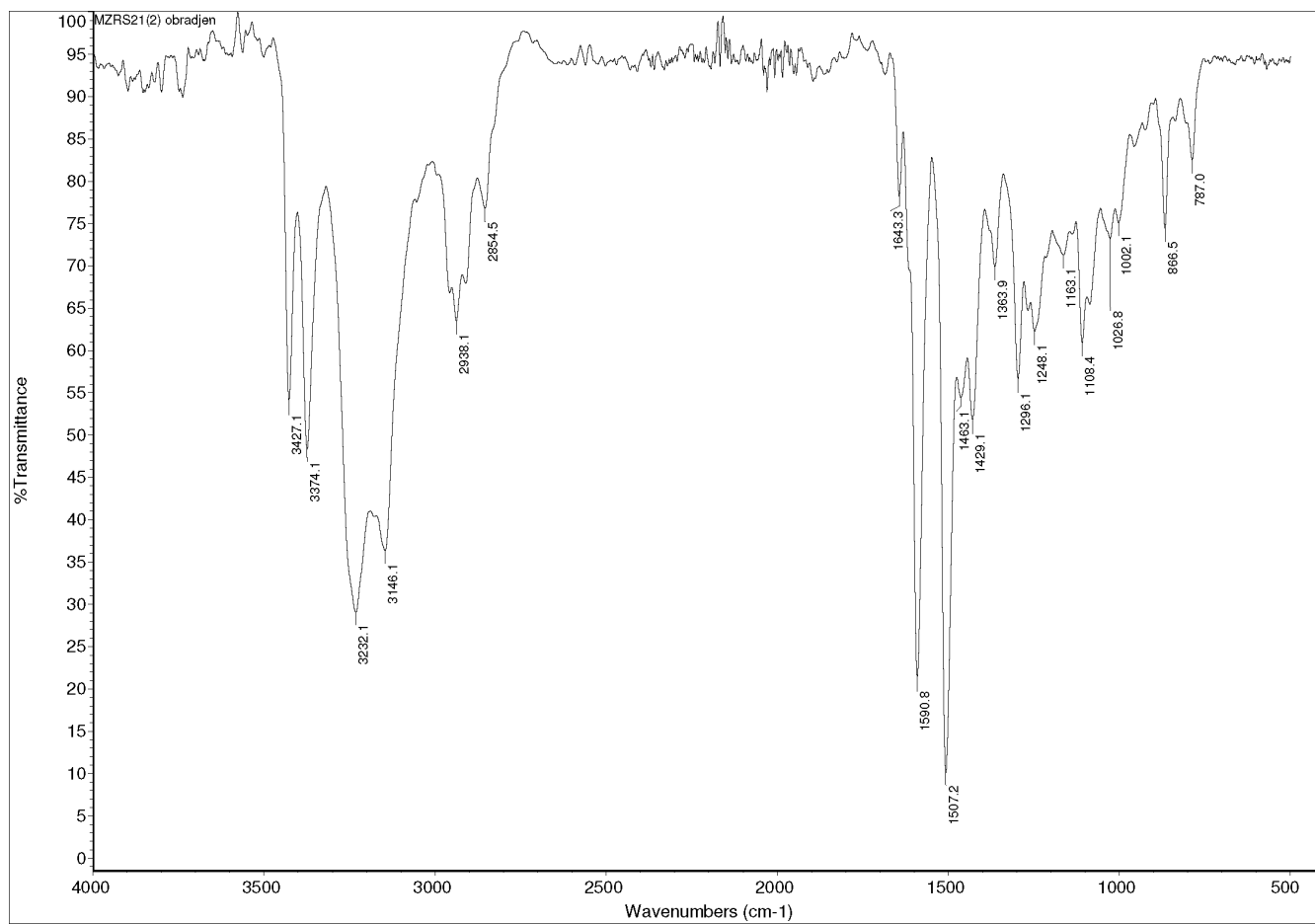
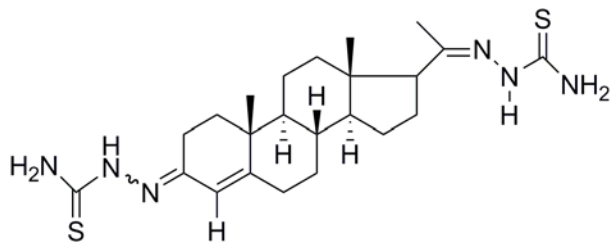


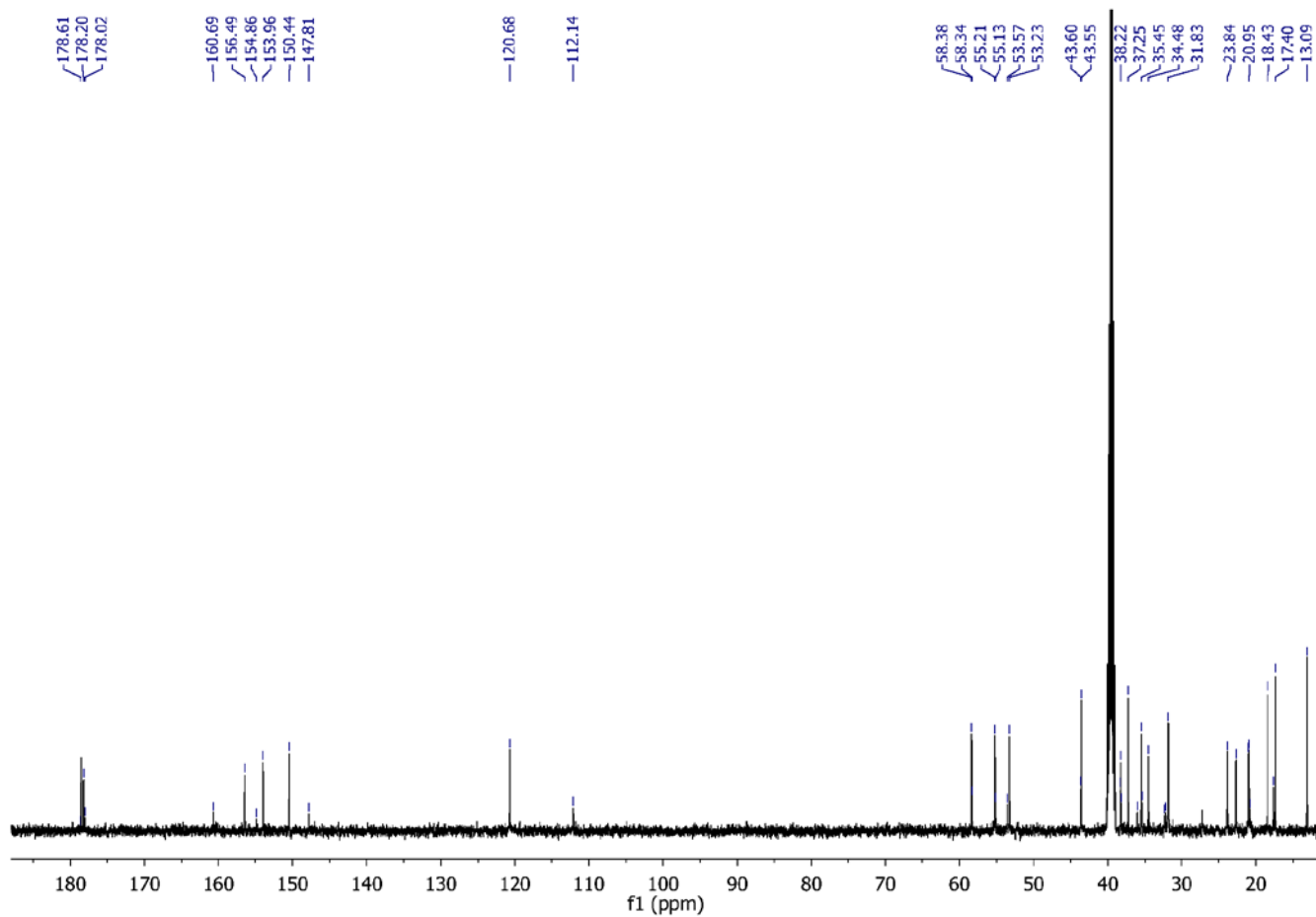
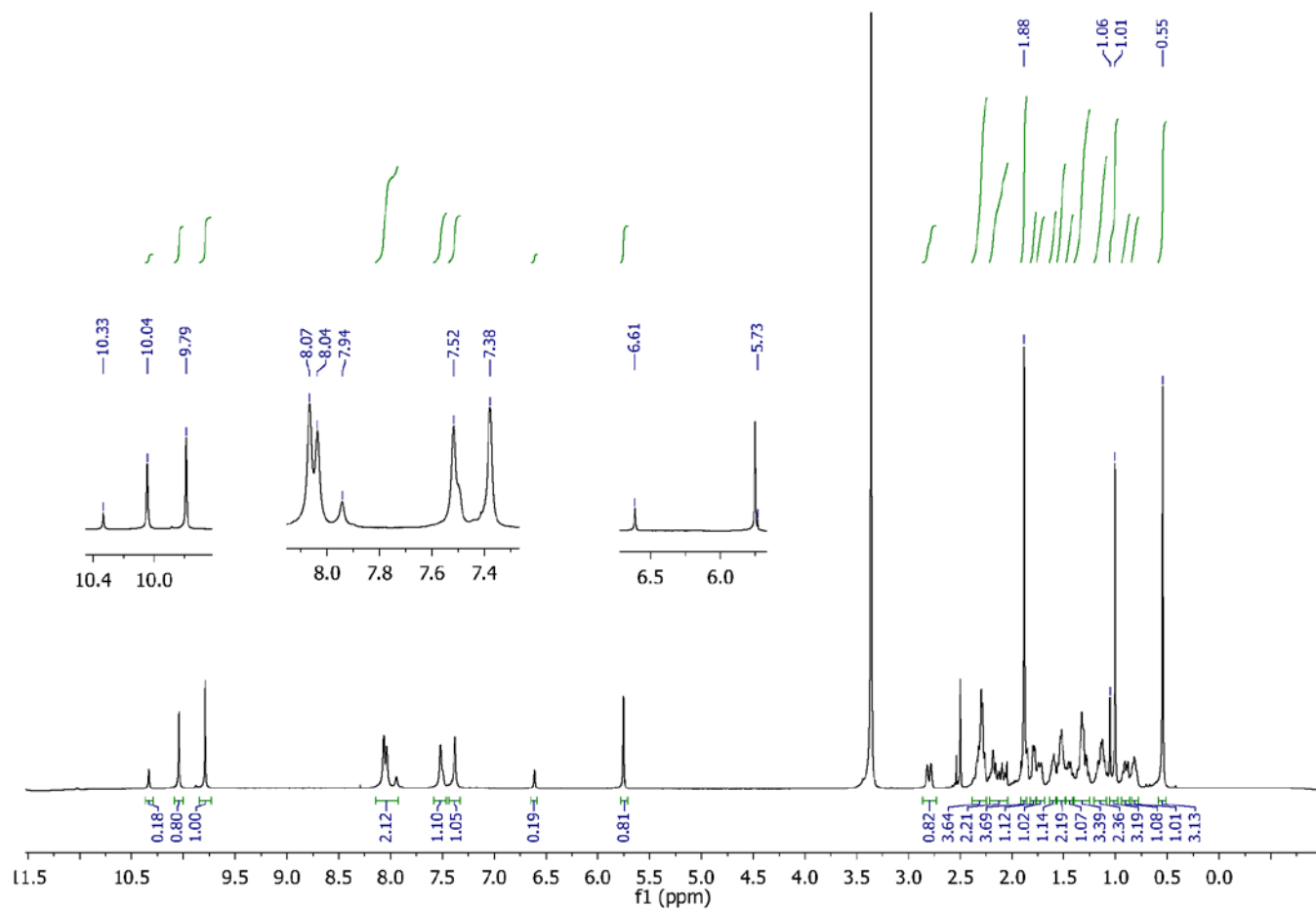
Formula	Compound name	Mass	Peak RT (min)	Peak area	Description
C22H33N3OS	--	387.23443	0.40	3.43590 E7	--

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	--

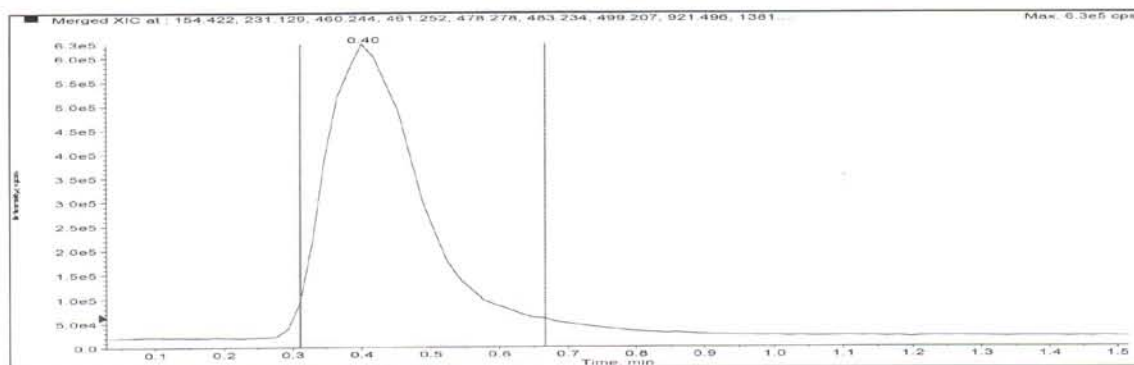


Compound 3e

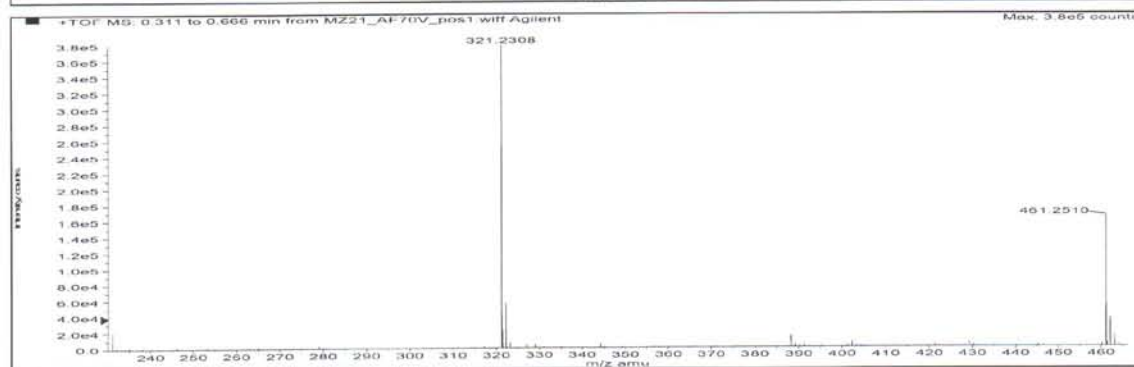
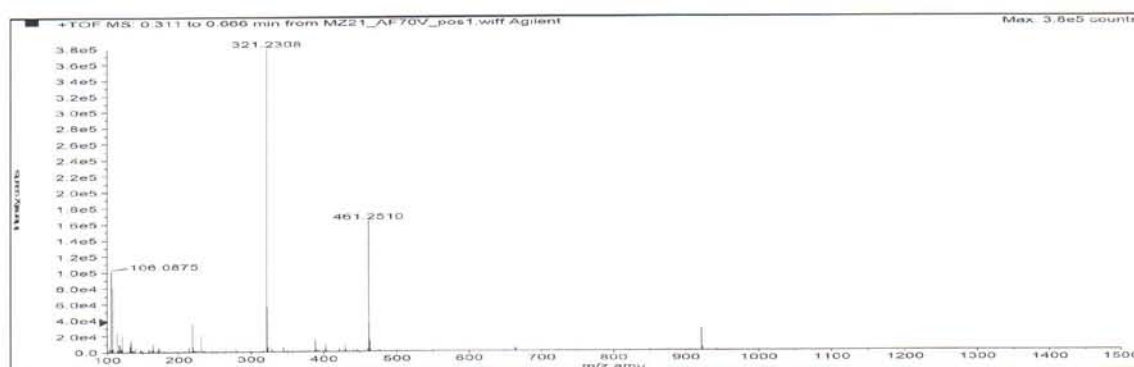




Sample Name: MZ21 Sample Location: P1-D5 Sample Id: Operator: Milka
 Data File Name: D:\PE Sciex Data\Projects\Sladic\Data\MZ21_AF70V_pos1.wiff Acq Time: May 07 2015, 11:42:07 AM
 Method: d:\TOF_Data\damethods\Night_Seq_Comp_ident1.anm\efc.xml



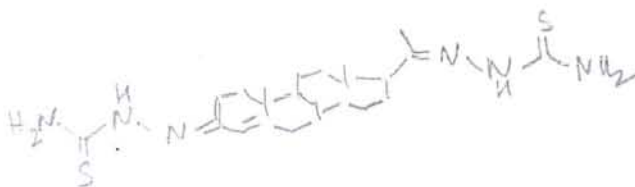
Merged XIC, Period# : 1 Experiment# : 1



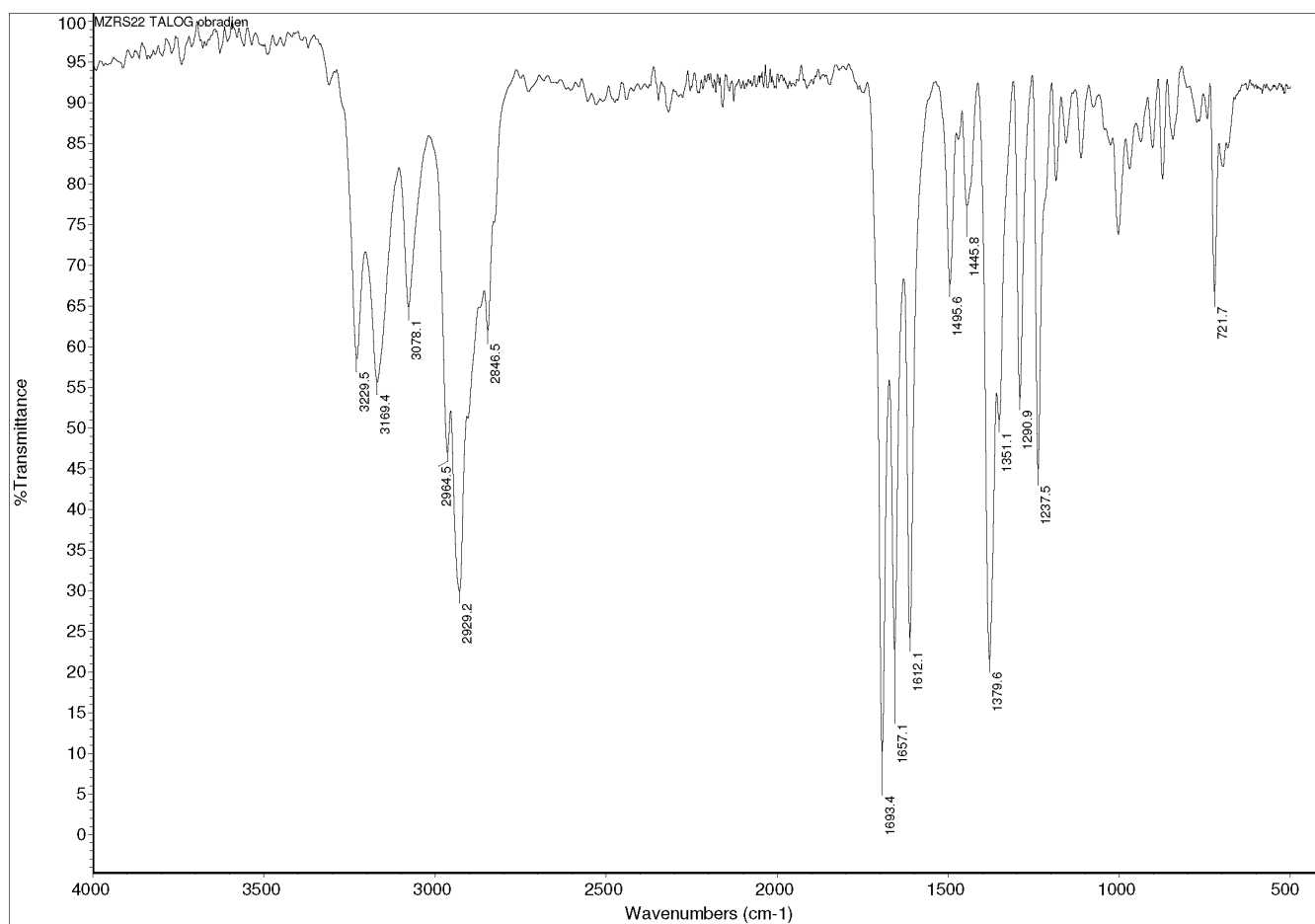
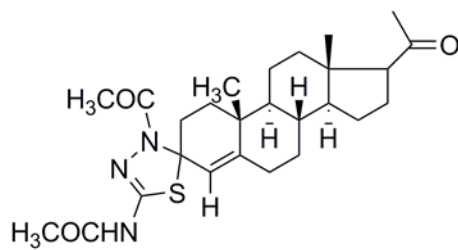
Formula	Compound name	Mass	Peak RT (min)	Peak area	Description
C23H36N6S2	--	460.24429	0.40	6.00059 E6	--

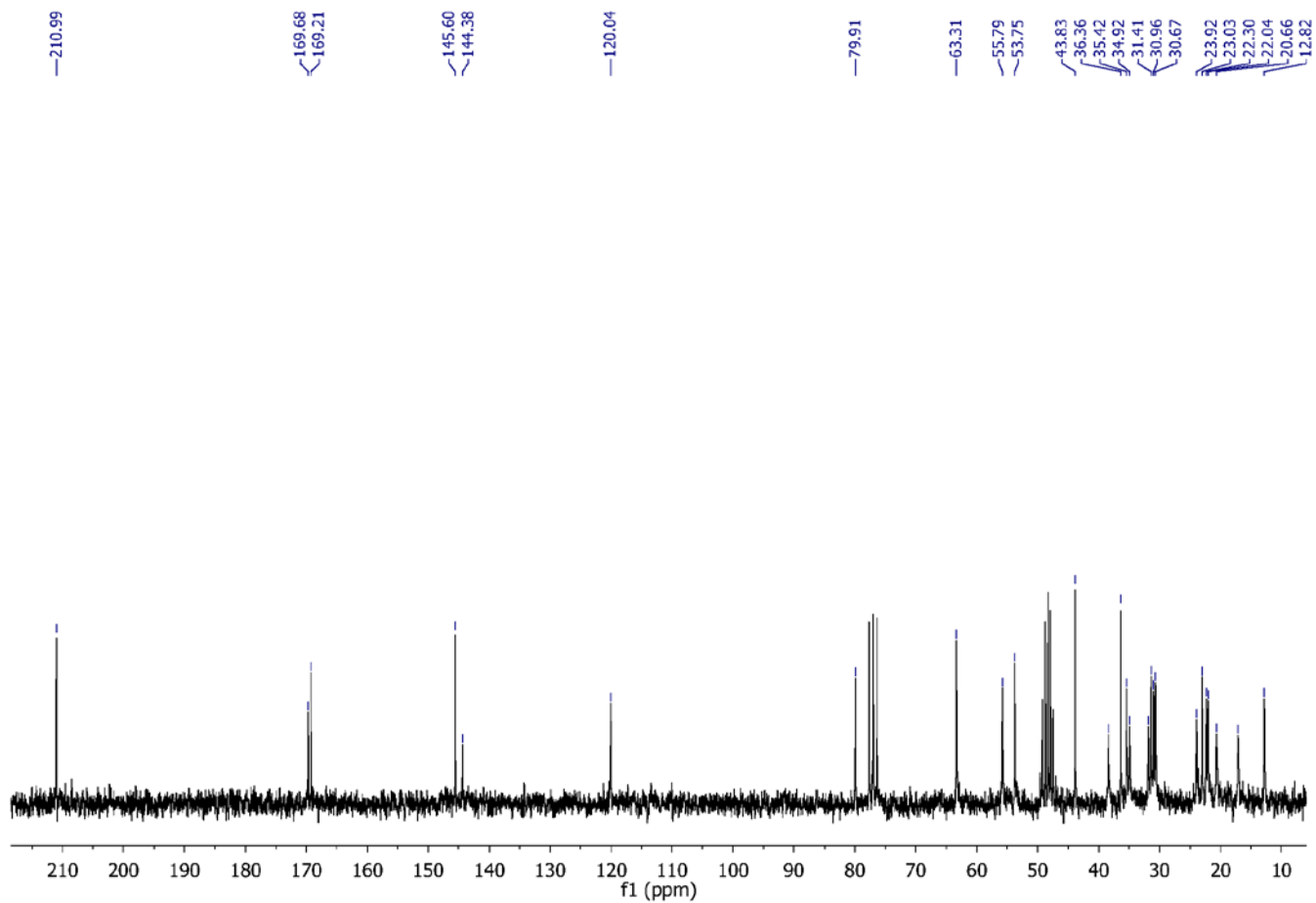
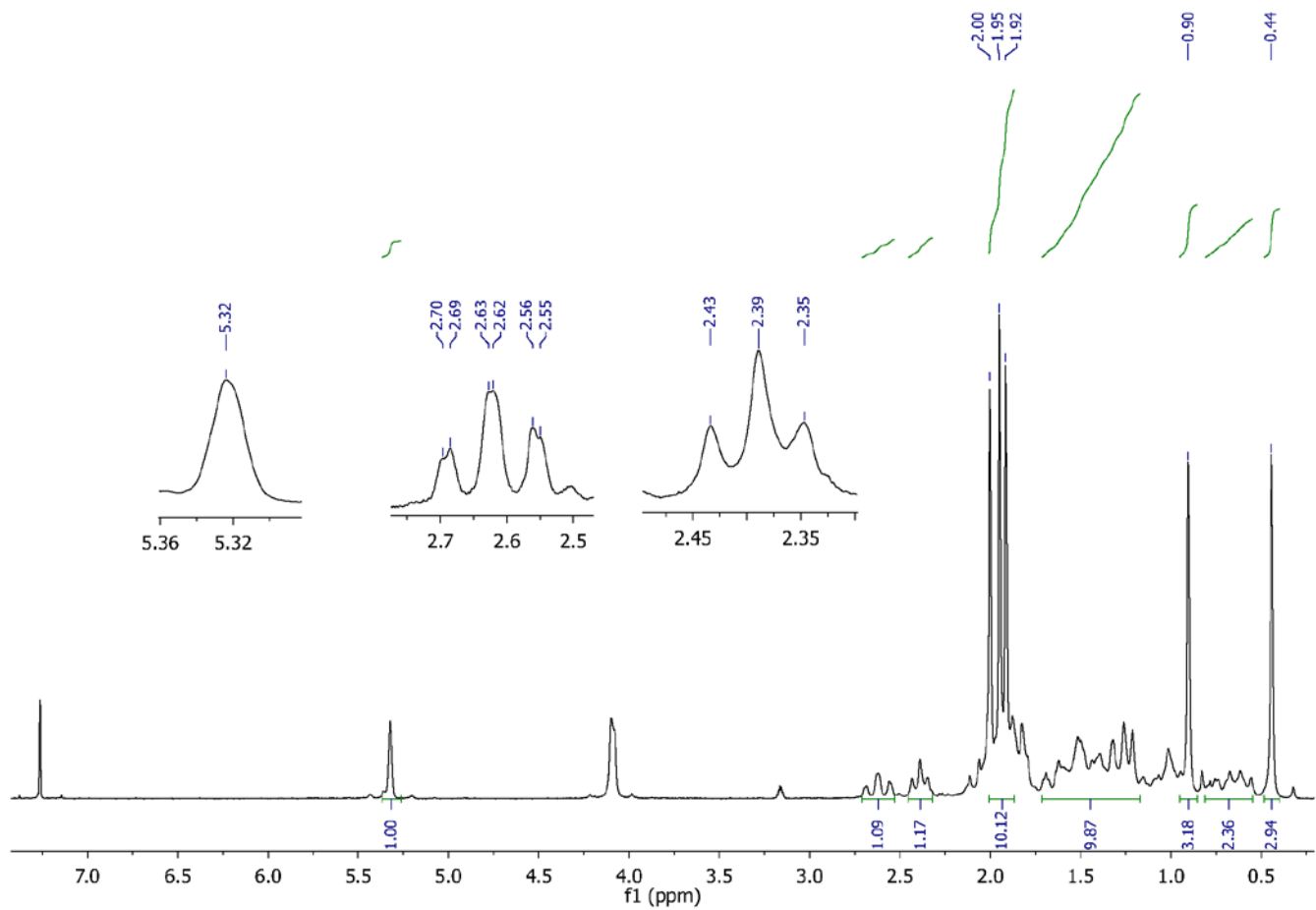
Species	Abundance (counts)	Ion Mass	Measured Mass	Error (mDa)	Error (ppm)	Ret. Time Error (min)
[M+2H] ²⁺	21283.91	231.12942	231.11850	-10.92236	-47.26	--
[M+H] ⁺	163573.95	461.25156	461.25130	-0.25807	-0.56	--

OK! JG

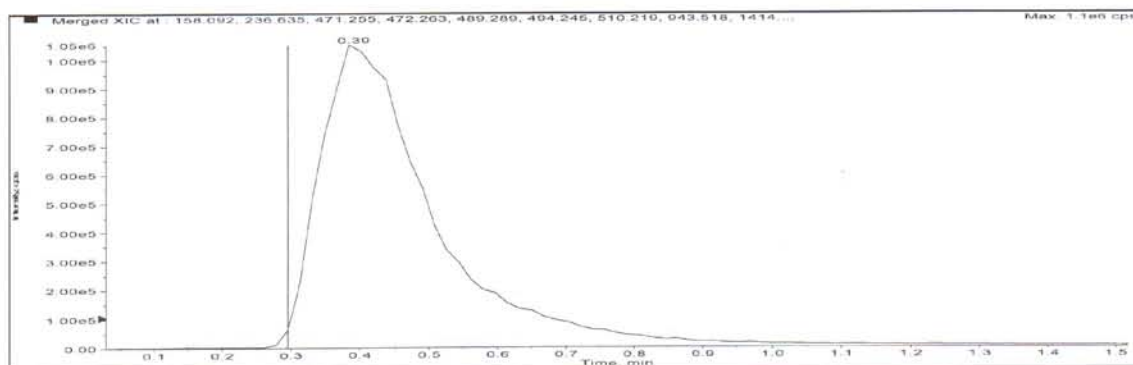


Compound 4e

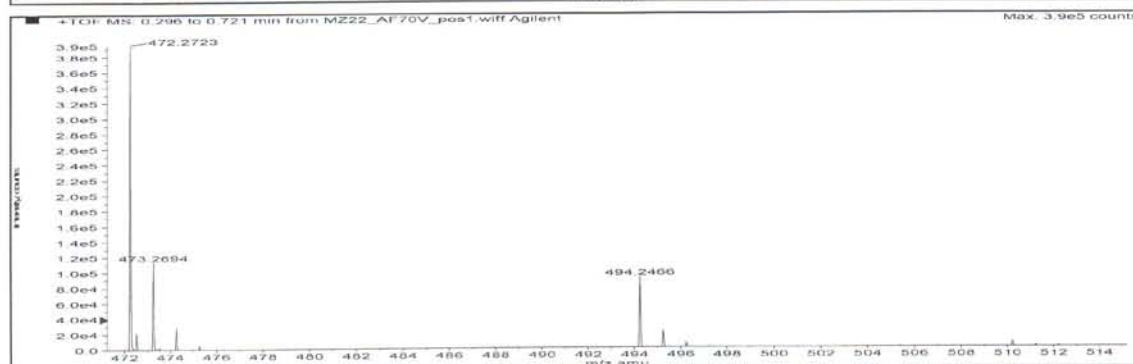
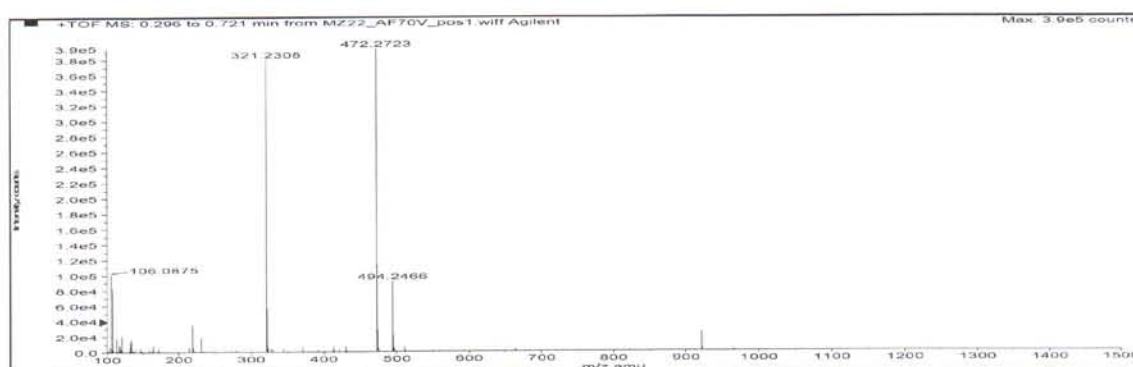




Sample Name: **MZ22** Sample Location: **P1-D6** Sample Id: Operator: **Milka**
 Data File Name: **D:\PE Sclex Data\Projects\SladiciData\MZ22_AF70V_pos1.wiff** Acq Time: **May 07 2015, 11:44:39 AM**
 Method: **d:\TOF_Data\damethods\Night_Seq_Comp_Ident1.anm\lefc.xml**

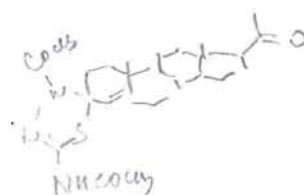


Merged XIC, Period# : 1 Experiment# : 1

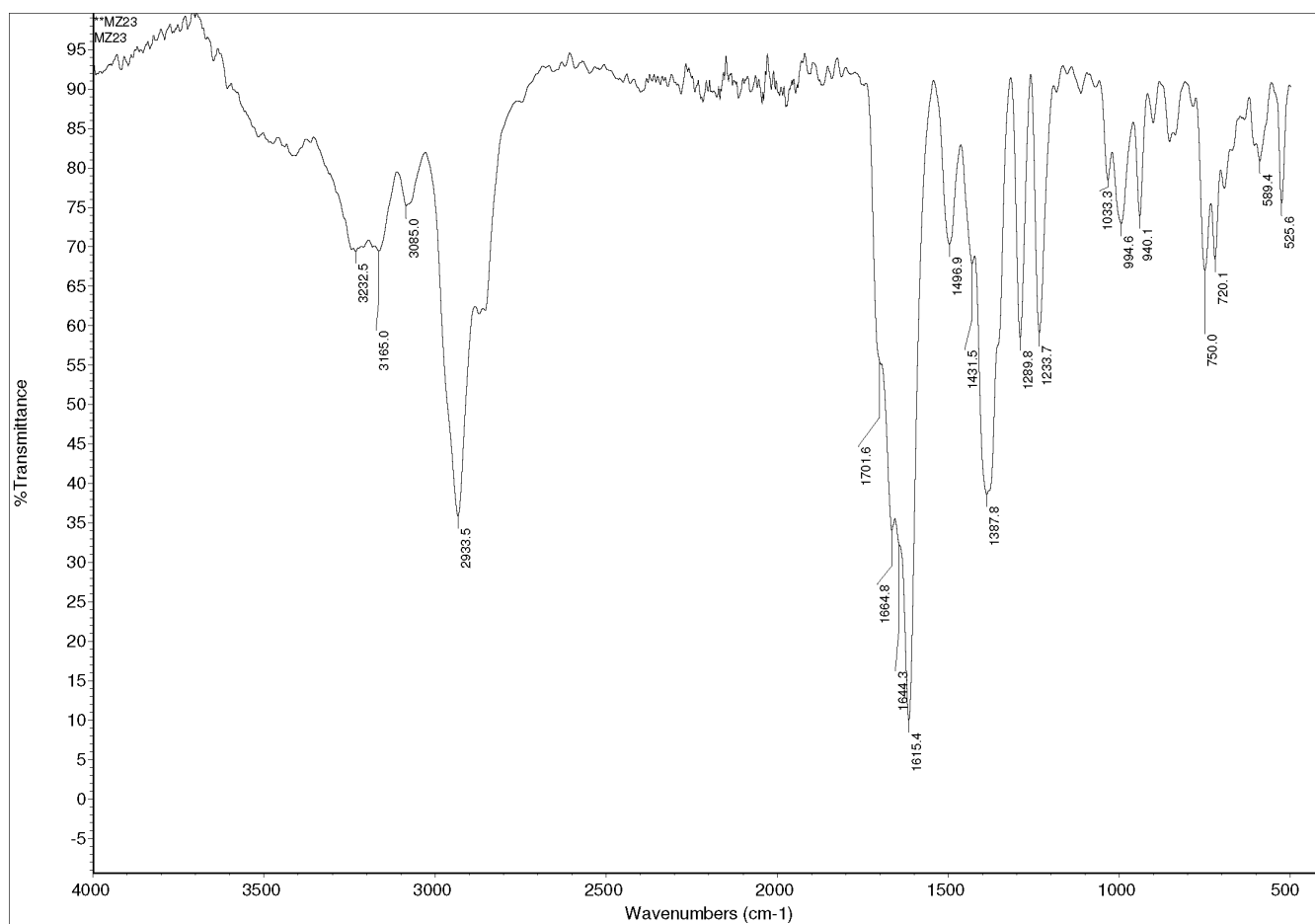
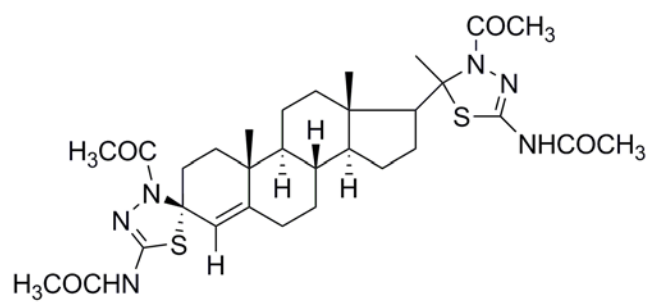


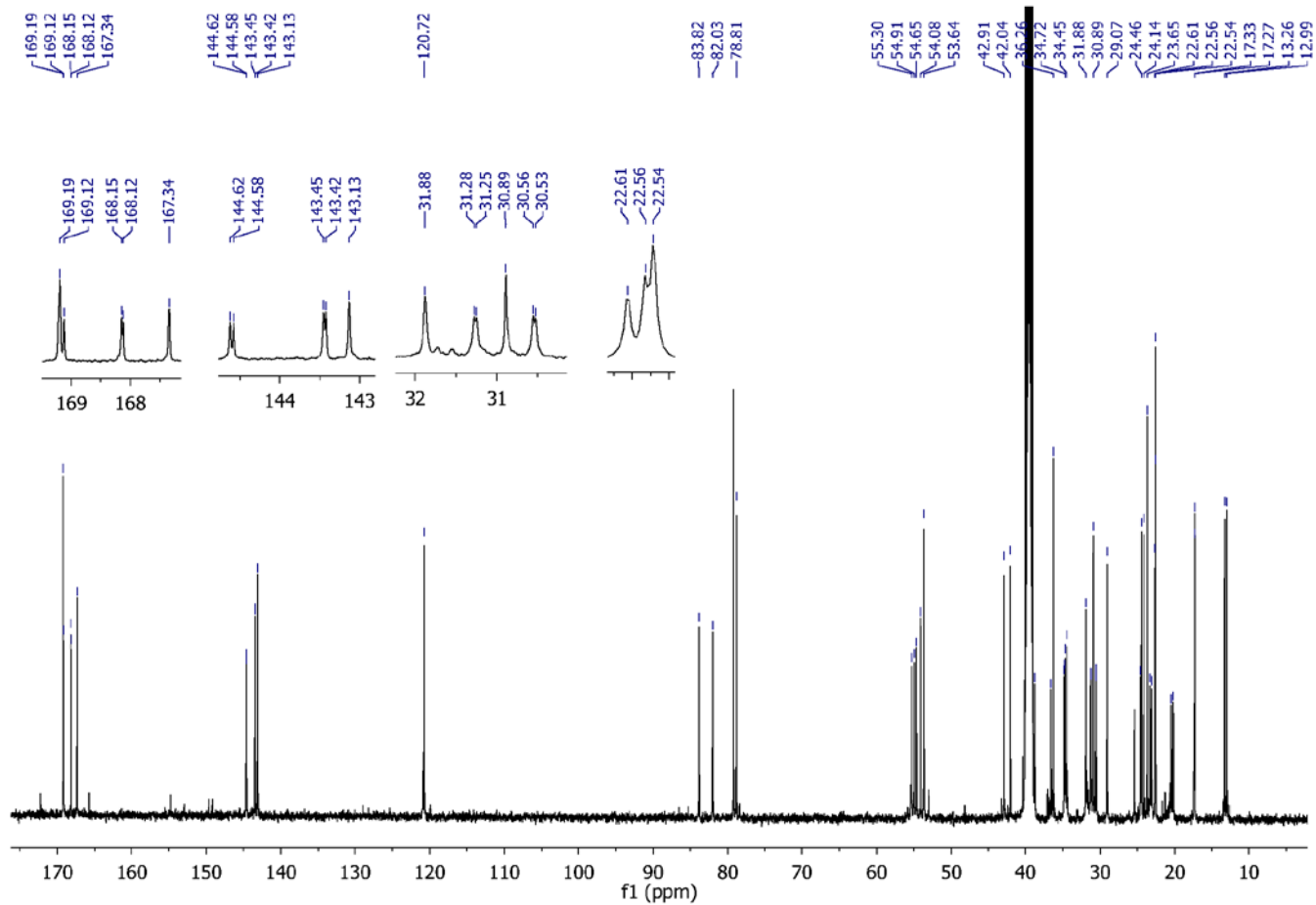
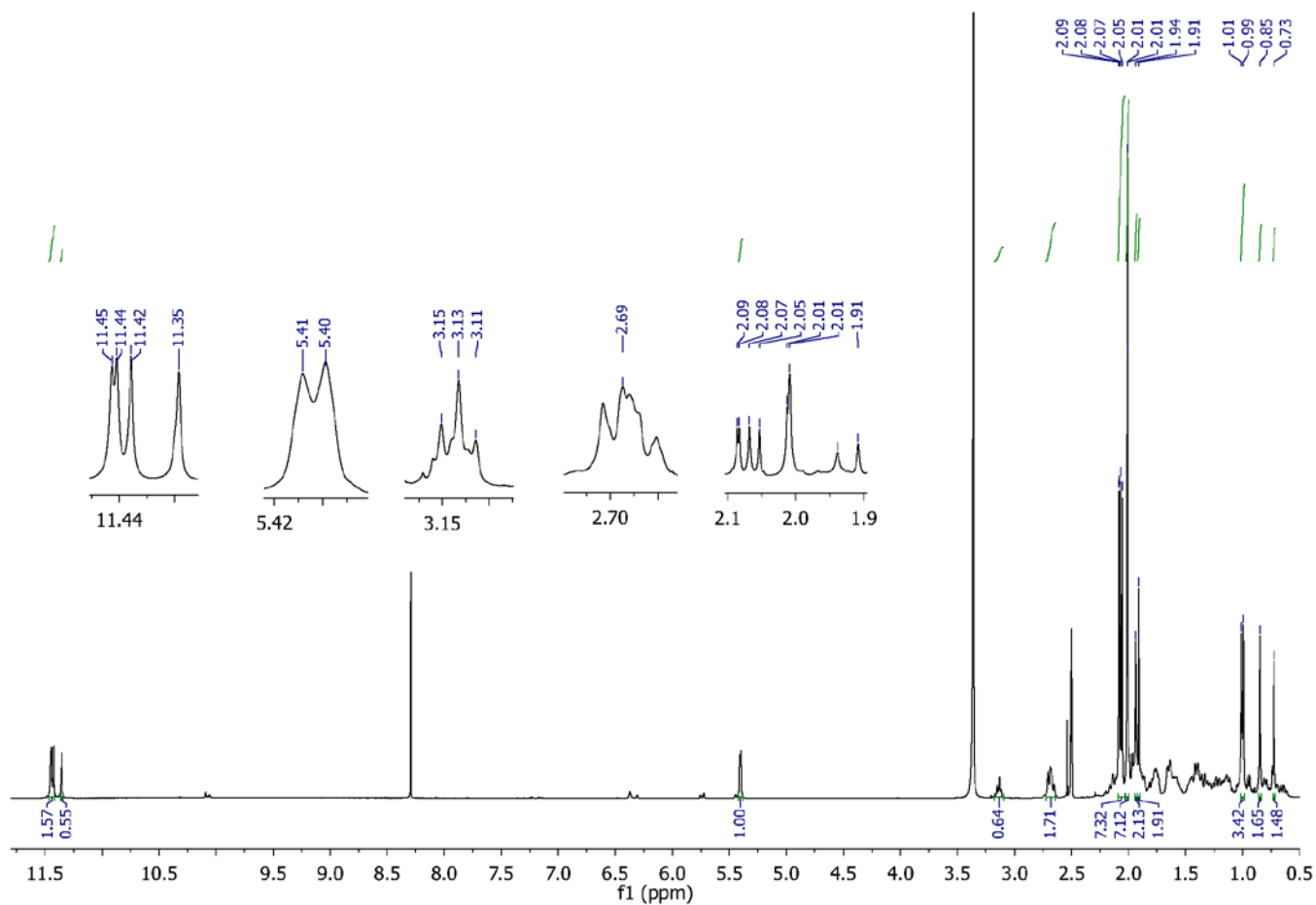
Formula	Compound name	Mass	Peak RT (min)	Peak area	Description
C ₂₆ H ₃₇ N ₃ O ₃ S	--	471.25556	0.39	1.16231 E7	--

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	--

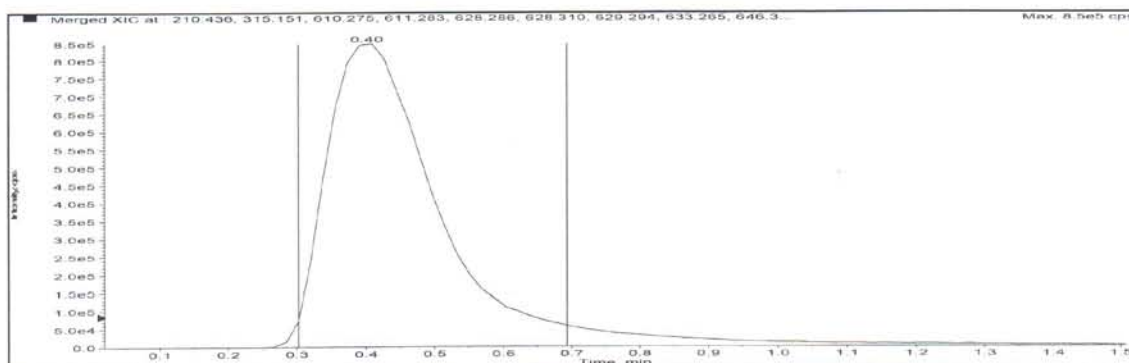


Compound 5e

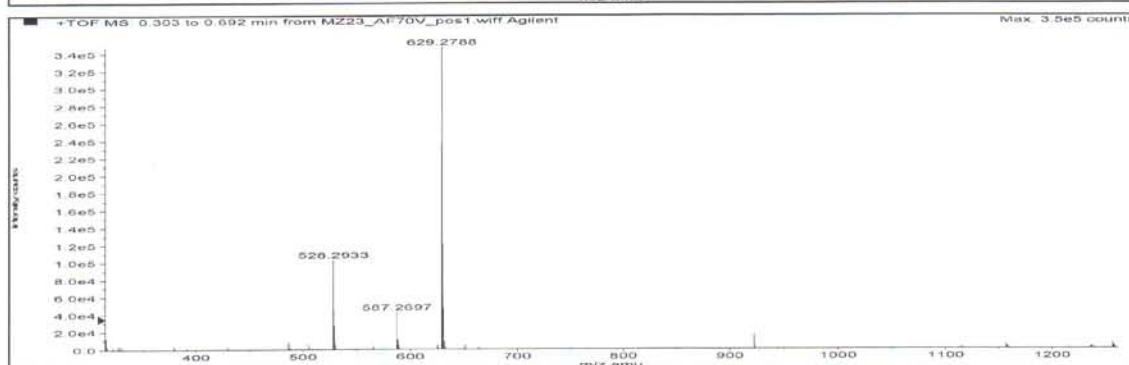
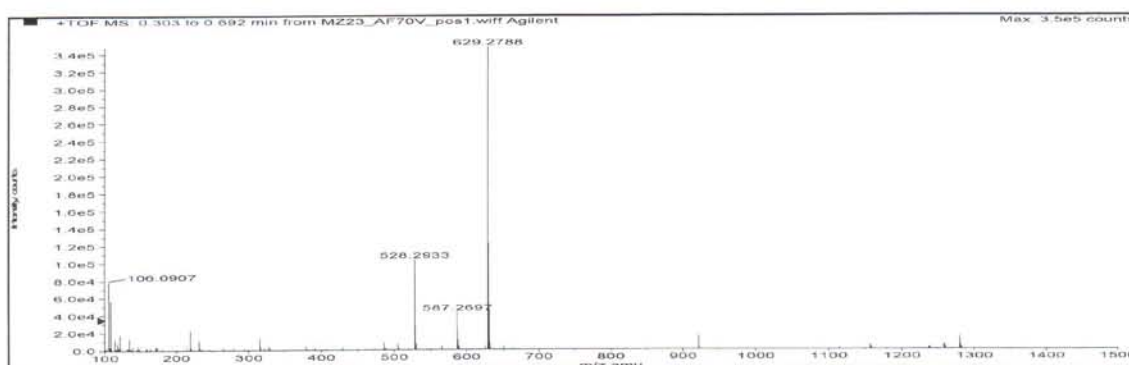




Sample Name: MZ23 Sample Location: P1-F6 Sample Id: Operator: Milka
 Data File Name: D:\PE Sciex Data\Projects\Sladici\Data\MZ23_AF70V_pos1.wiff Acq Time: May 08 2015, 01:31:35 PM
 Method: d:\TOF_Data\damethods\Night_Seq_Comp_Ident1.an\lefc.xml



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	--

