

Supplementary data for article:

Živković, M. B.; Novaković, I. T.; Matić, I. Z.; Sladić, D. M.; Krstić, N. M. Synthesis and Preliminary Screening for the Biological Activity of Some Steroidal Δ^4 -Unsaturated Semicarbazone Derivatives. *Steroids* **2019**, *148*, 36–46.

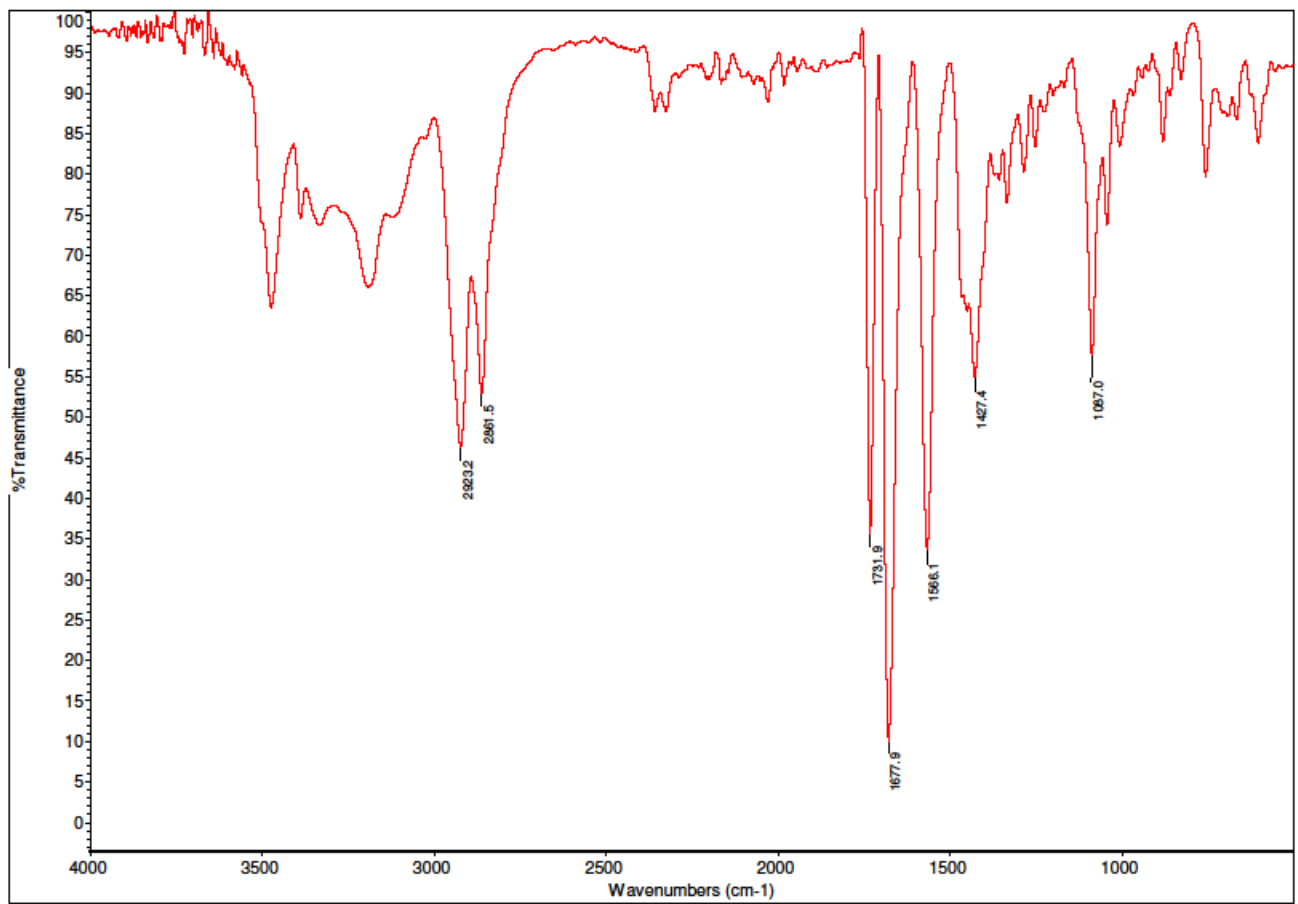
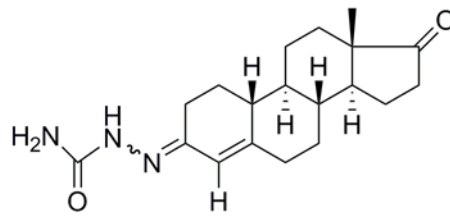
<https://doi.org/10.1016/j.steroids.2019.04.010>

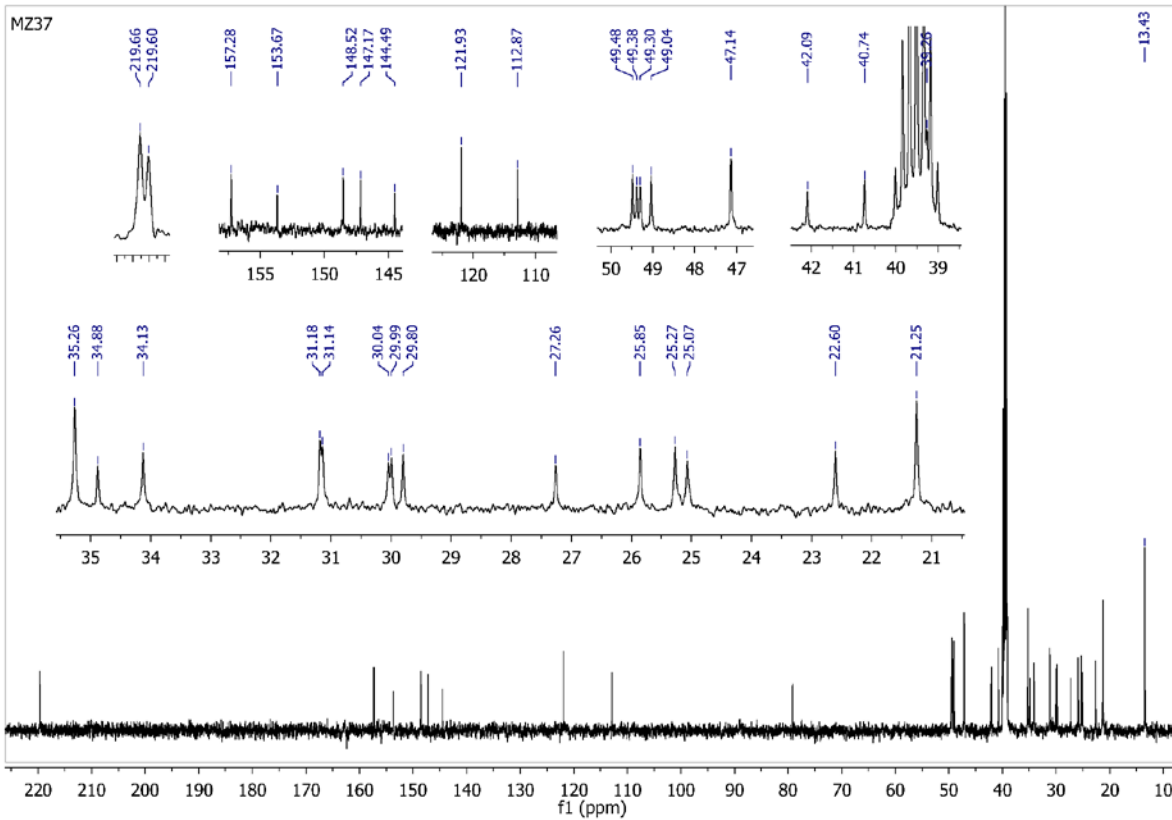
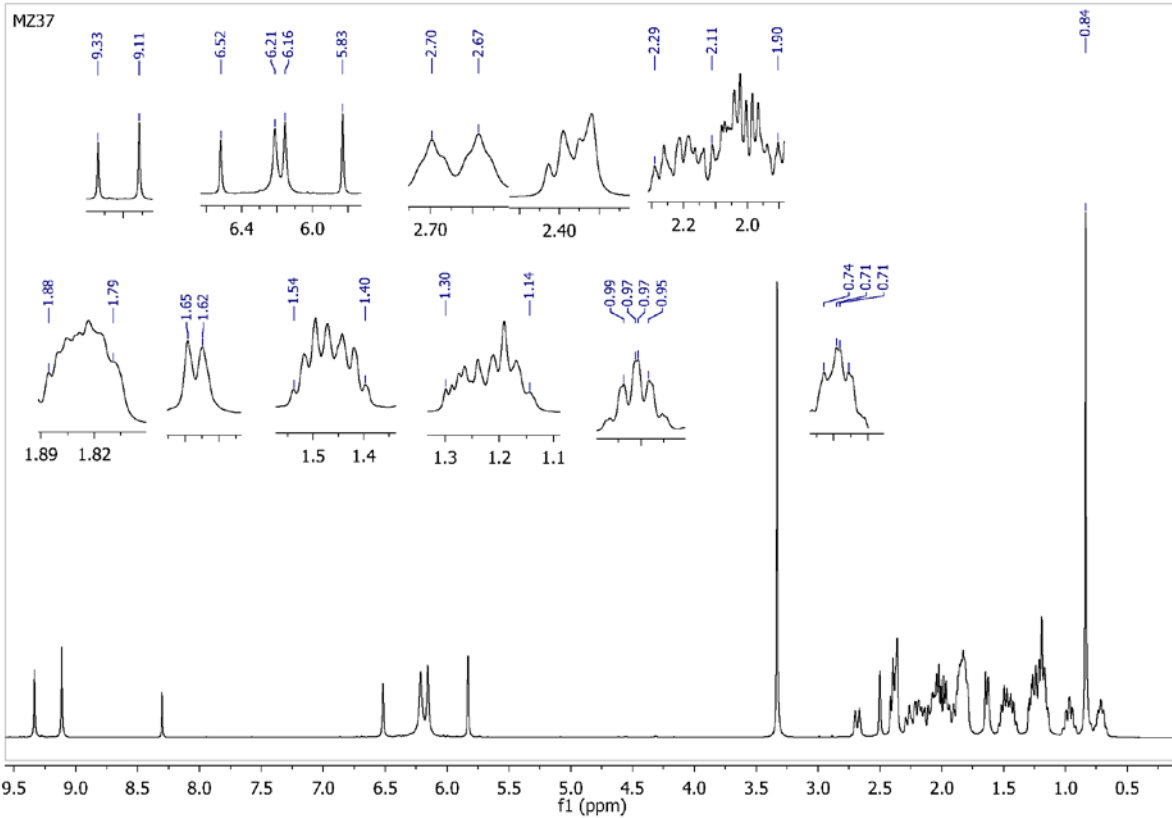
Supplementary data

Synthesis and preliminary screening for the biological activity of some steroidal Δ^4 -unsaturated semicarbazone derivatives

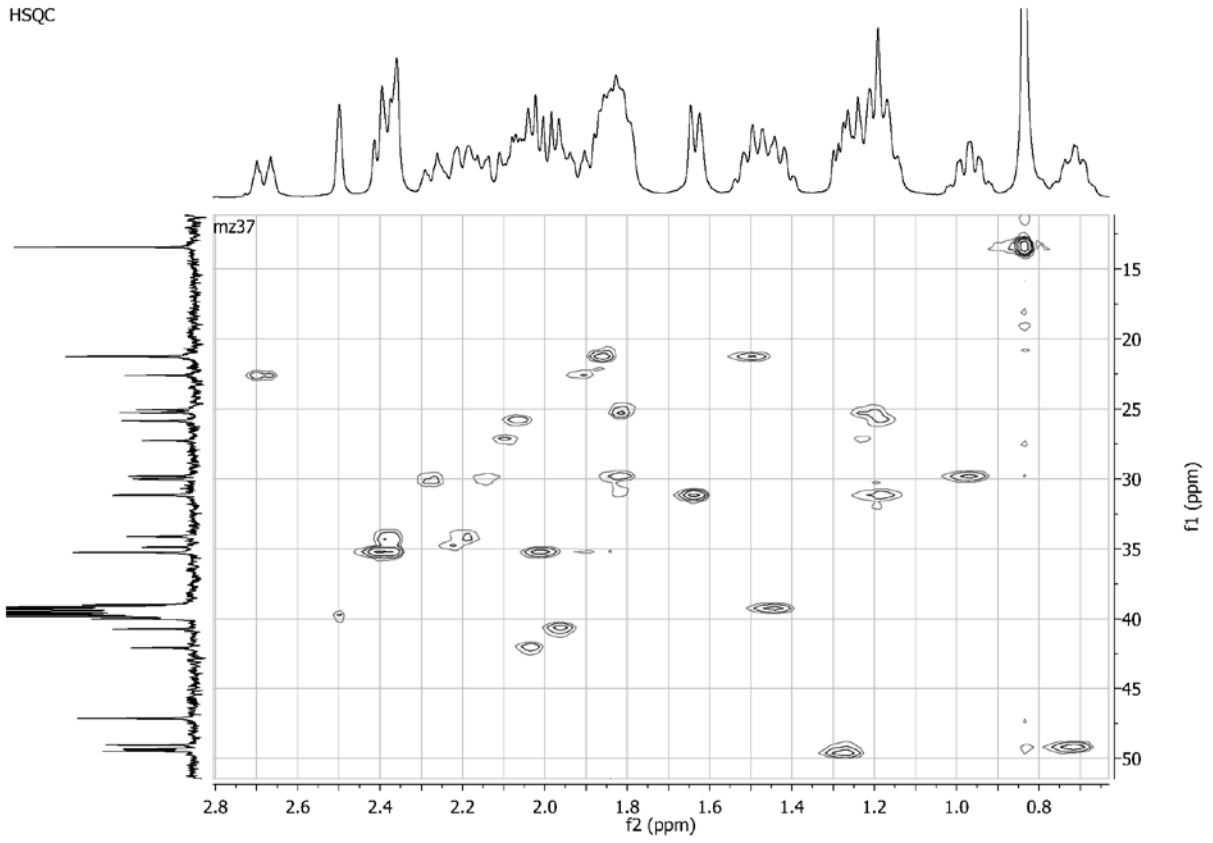
Marijana B. Živković, Irena T. Novaković, Ivana Z. Matić, Dušan M. Sladić,
Natalija M. Krstić

Compound 2a

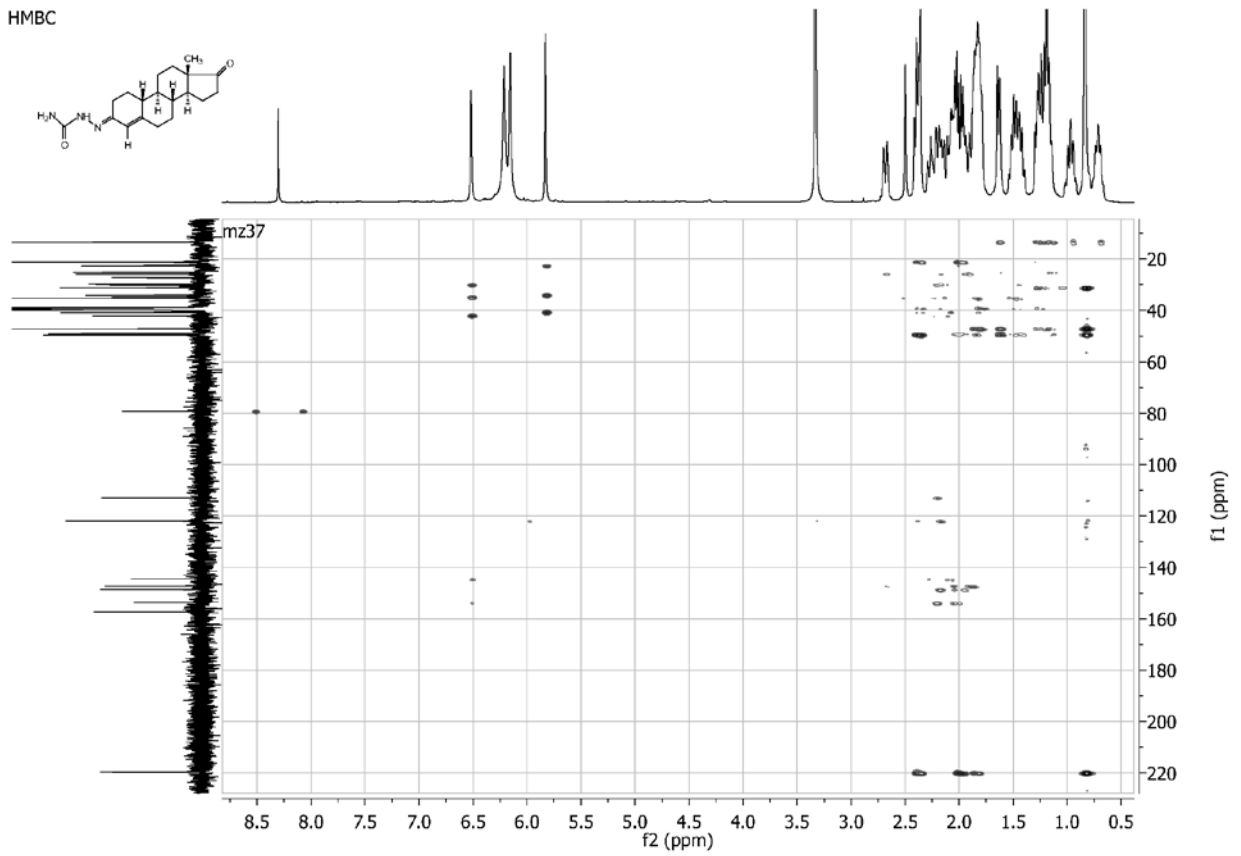




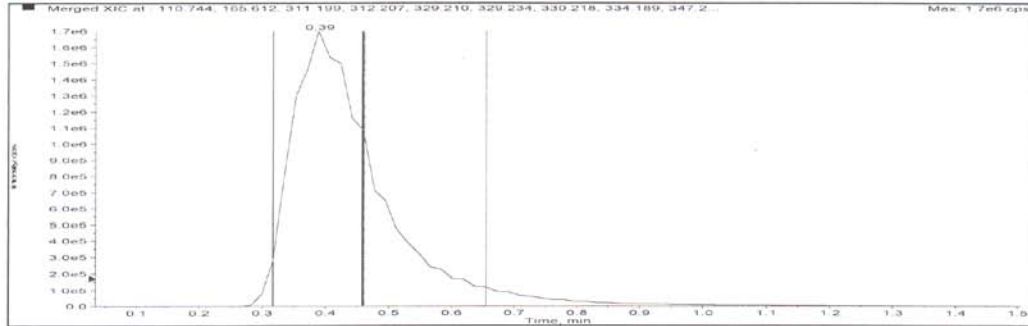
HSQC



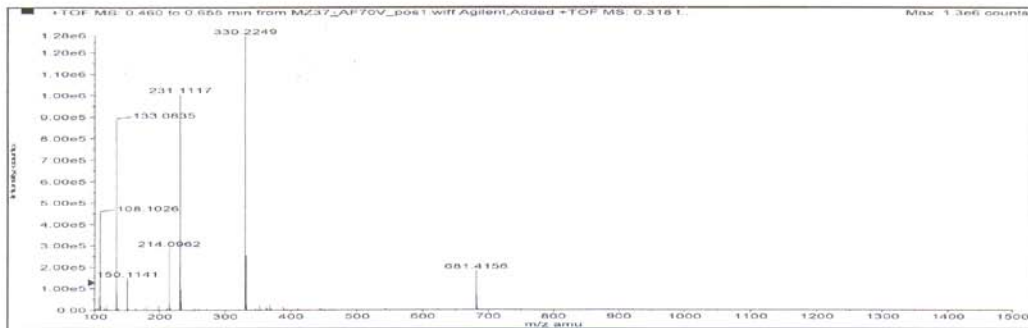
HMBC



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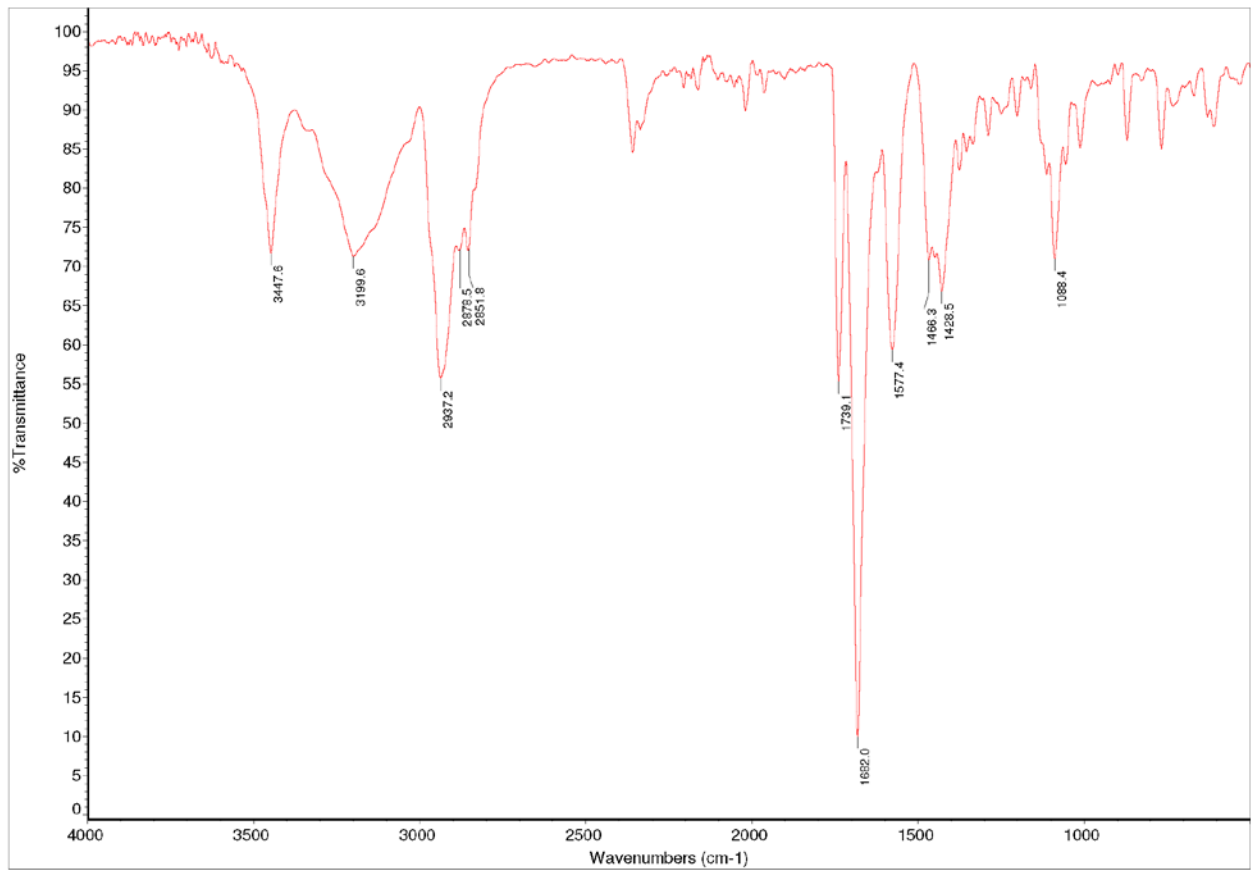
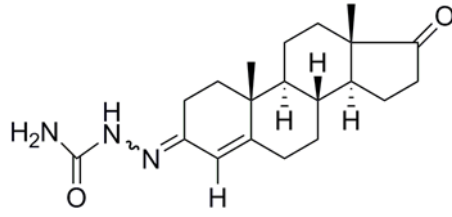
Merged XIC, Period#: 1 Experiment#: 1



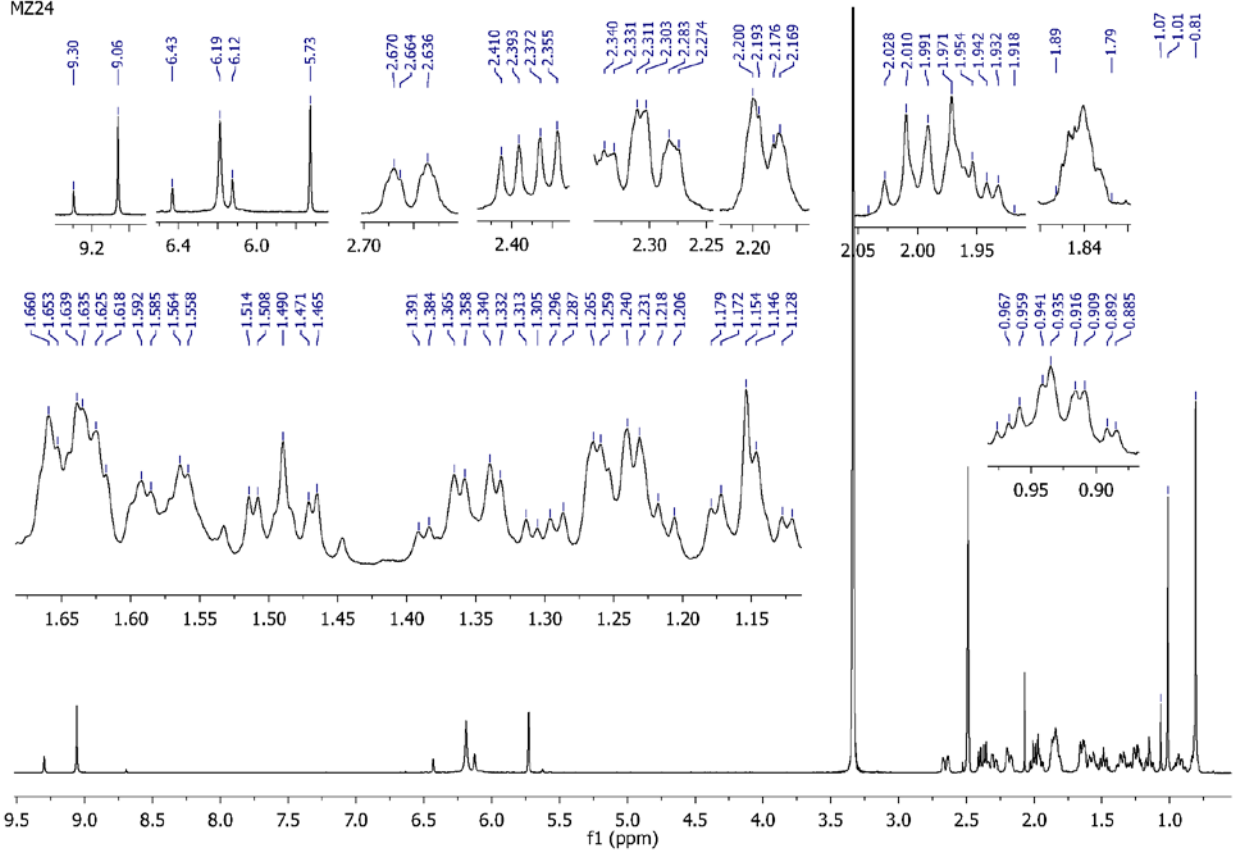
Formula	Compound name	Mass	Peak RT (min)	Peak area	Description
C19H27N3O2	--	329.21033	0.39	1.57992 E7	--

Species	Abundance (counts)	Ion Mass	Measured Mass	Error (mDa)	Error (ppm)	Ret. Time Error (min)
[M+H] ⁺	1336551.29	330.21760	330.21713	-0.47805	-1.45	--
[M+Na] ⁺	19101.79	352.19955	352.20030	0.74953	2.13	--
[M+K] ⁺	20570.61	368.17349	368.17497	1.48547	4.03	--

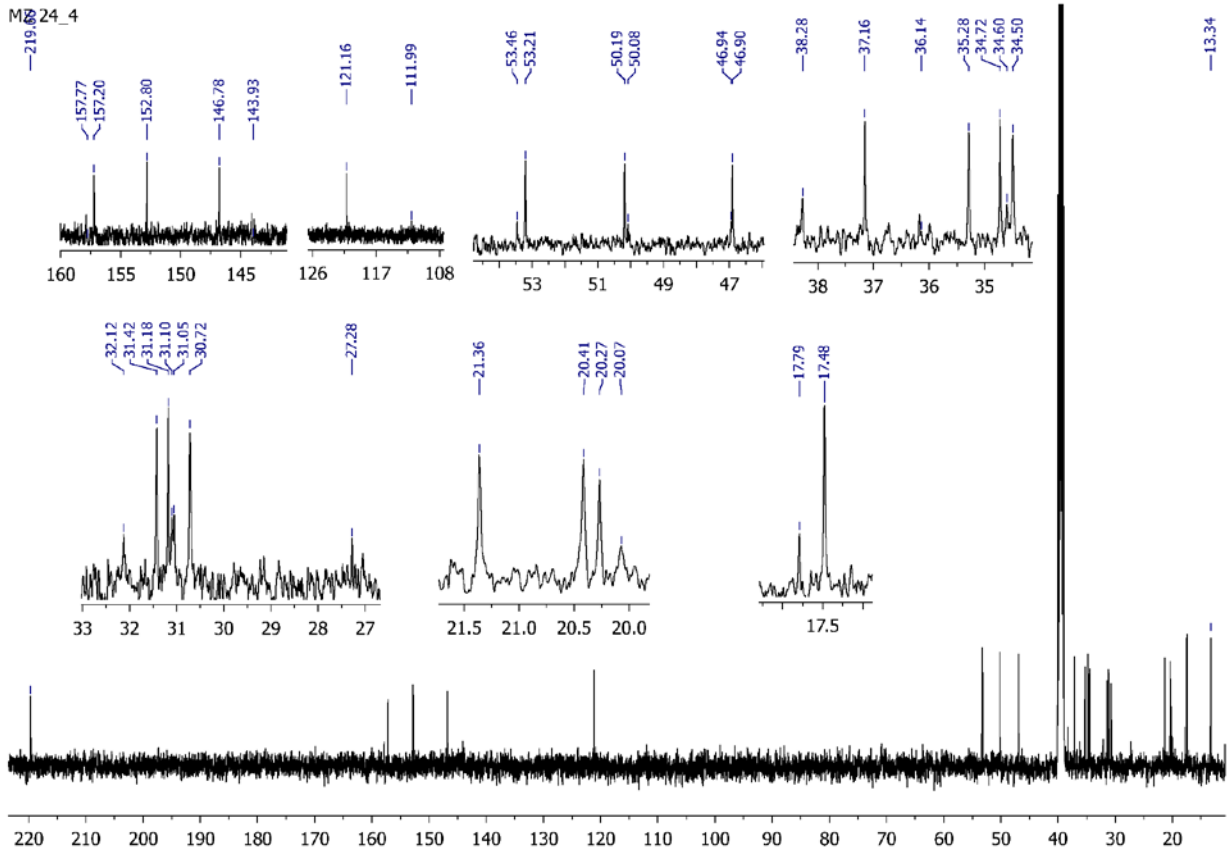
Compound 2b



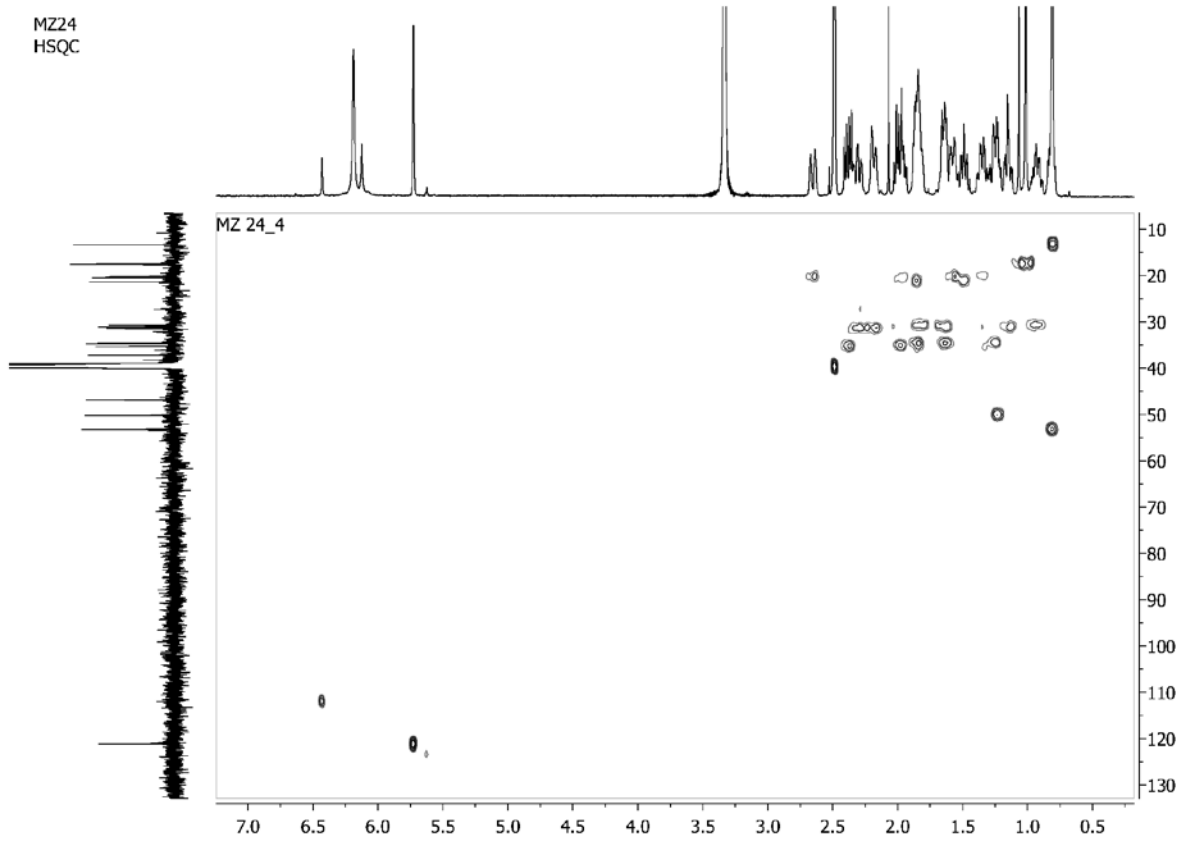
MZ24



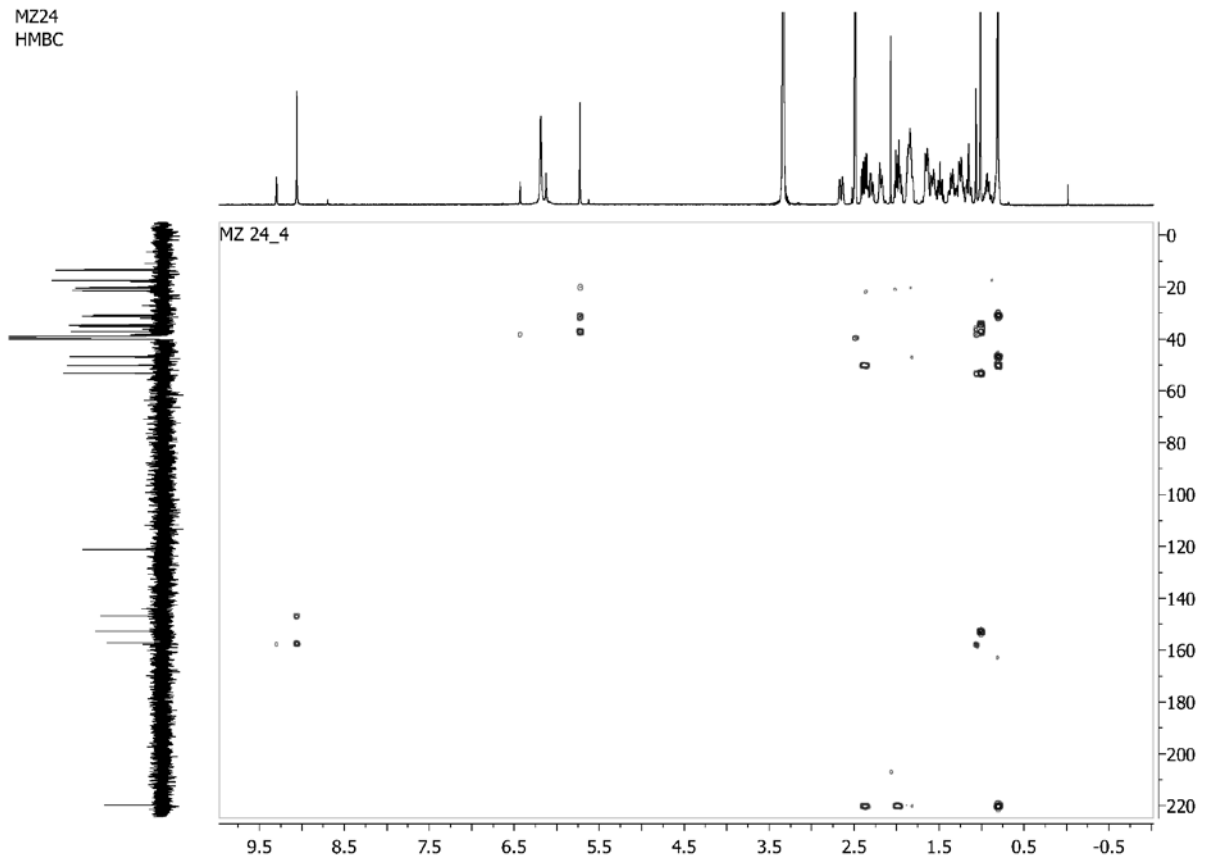
MZ24.4



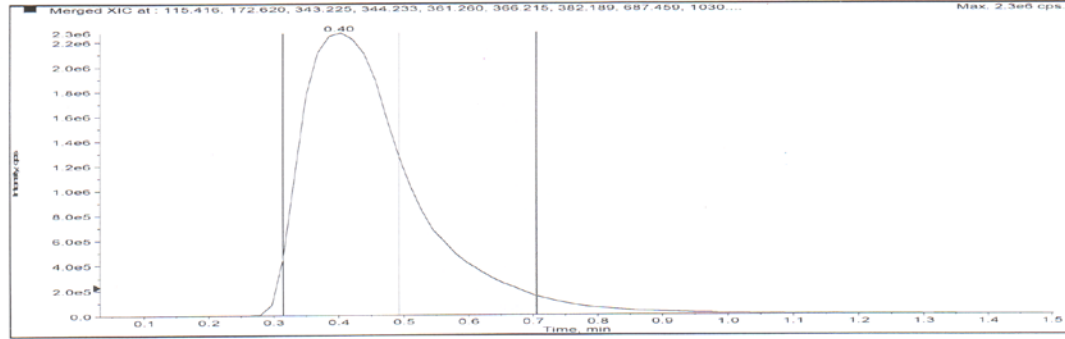
MZ24
HSQC



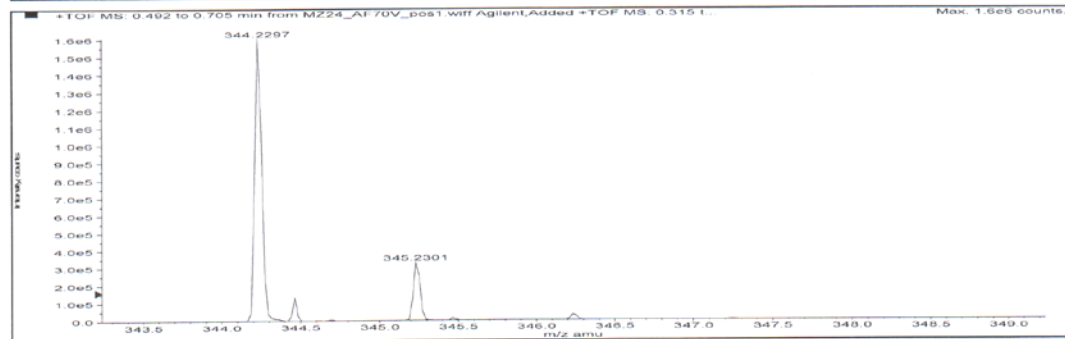
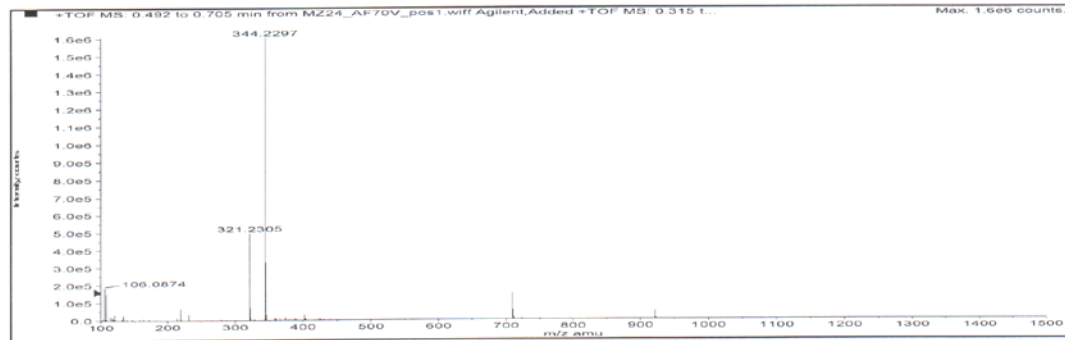
MZ24
HMBC



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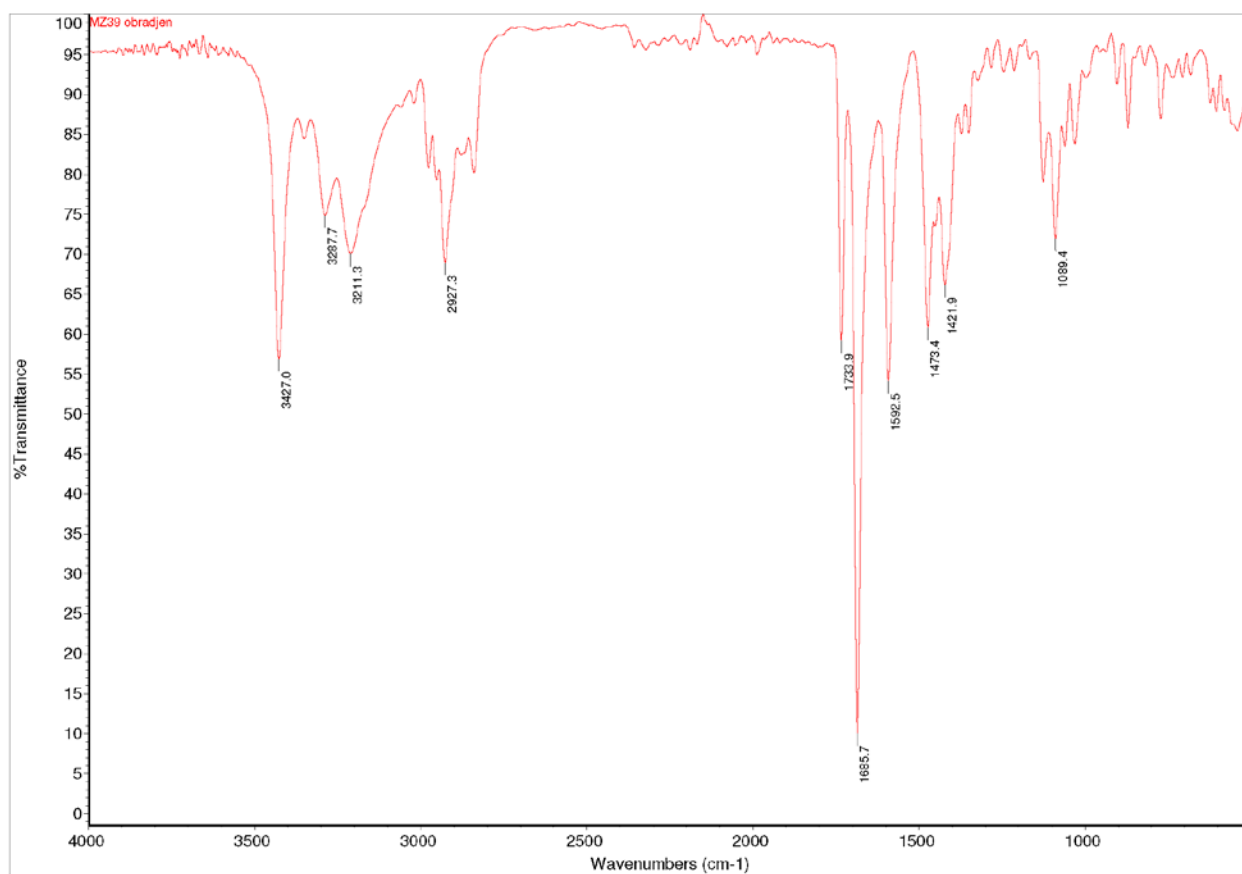
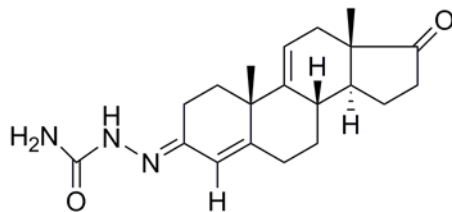
Merged XIC, Period#: 1 Experiment#: 1

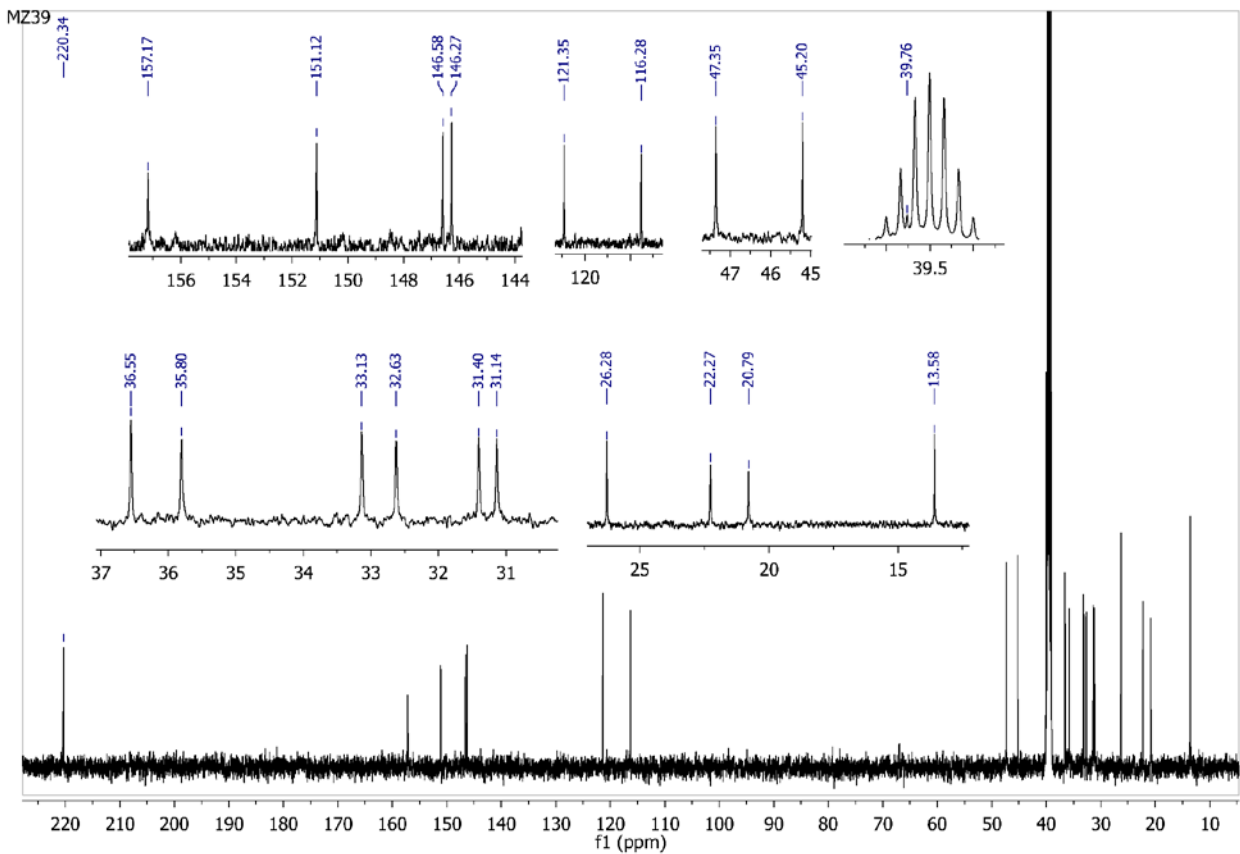
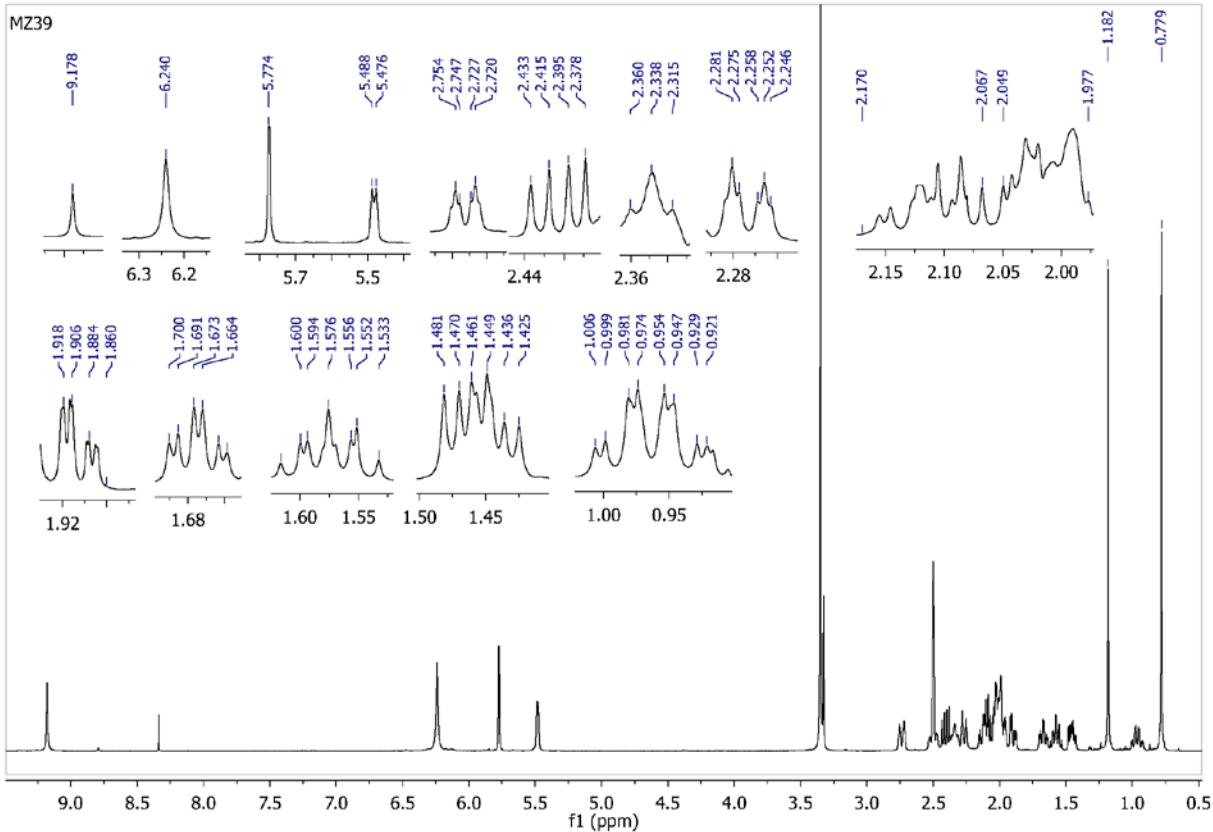


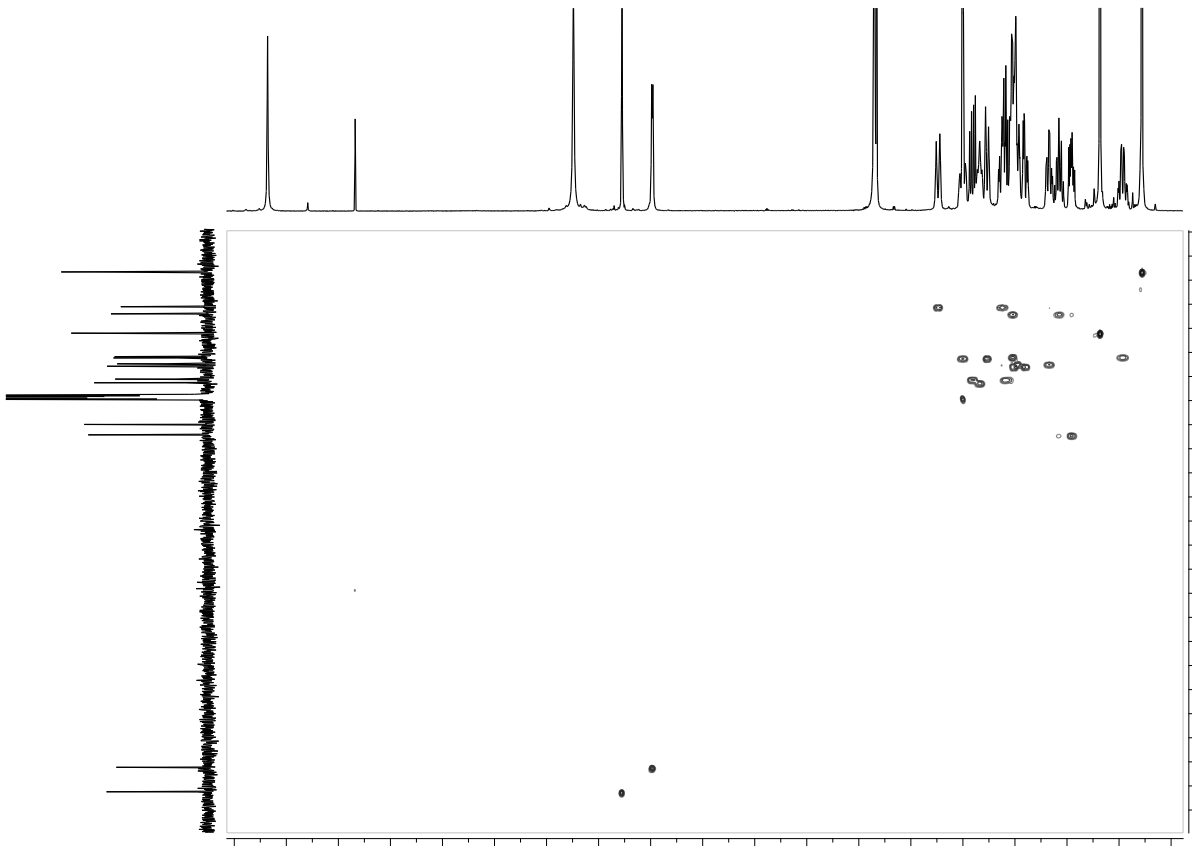
Formula	Compound name	Mass	Peak RT (min)	Peak area	Description
C20H29N3O2	--	343.22598	0.40	2.66521 E7	--

Species	Abundance (counts)	Ion Mass	Measured Mass	Error (mDa)	Error (ppm)	Ret. Time Error (min)
[M+H] ⁺	1616774.51	344.23325	344.23283	-0.42258	-1.23	--

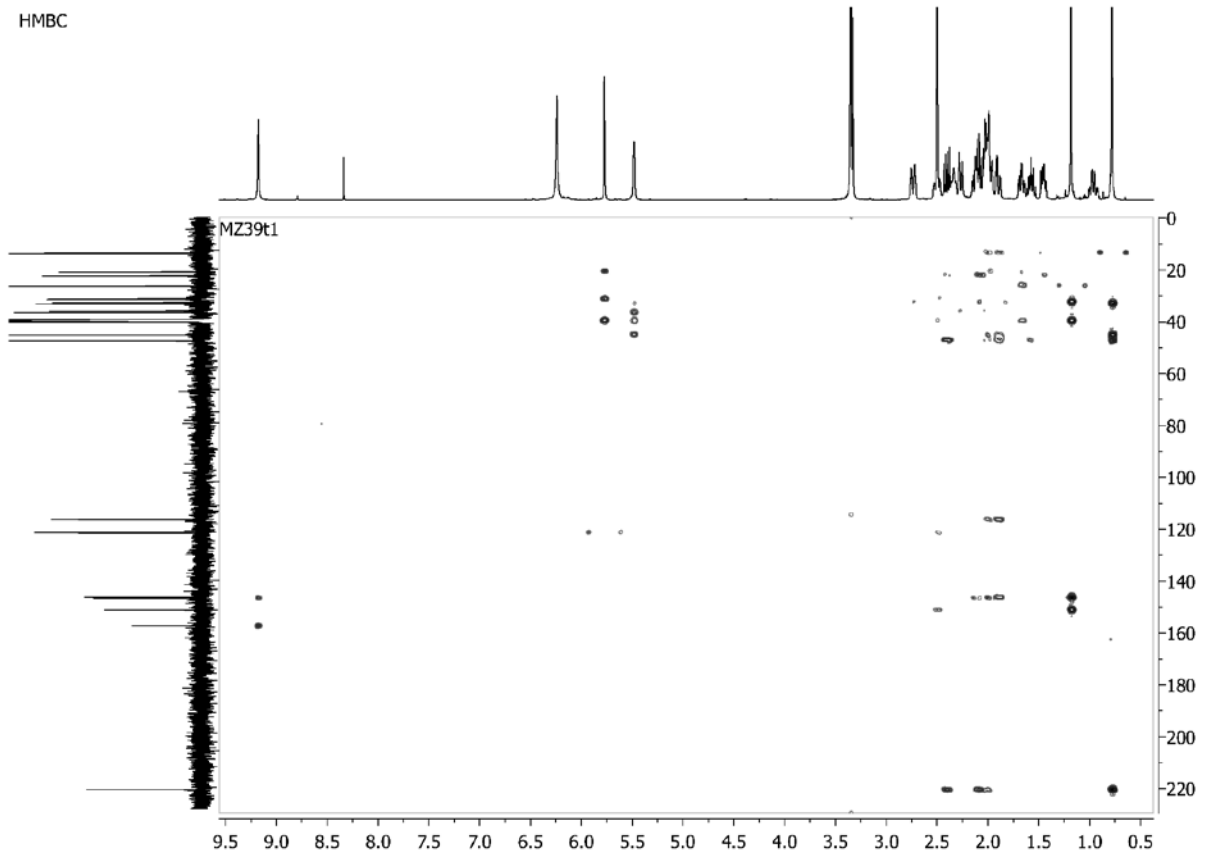
Compound 2c



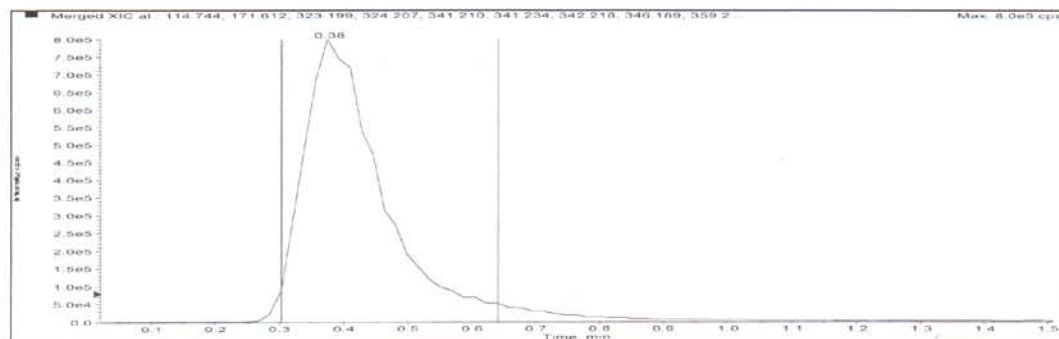




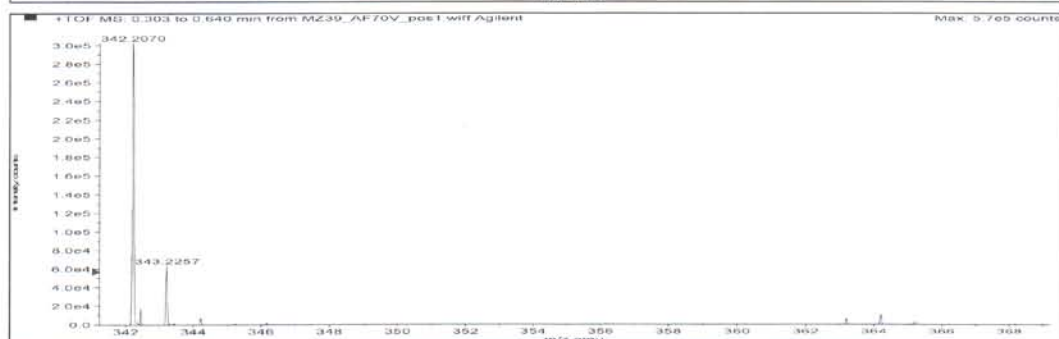
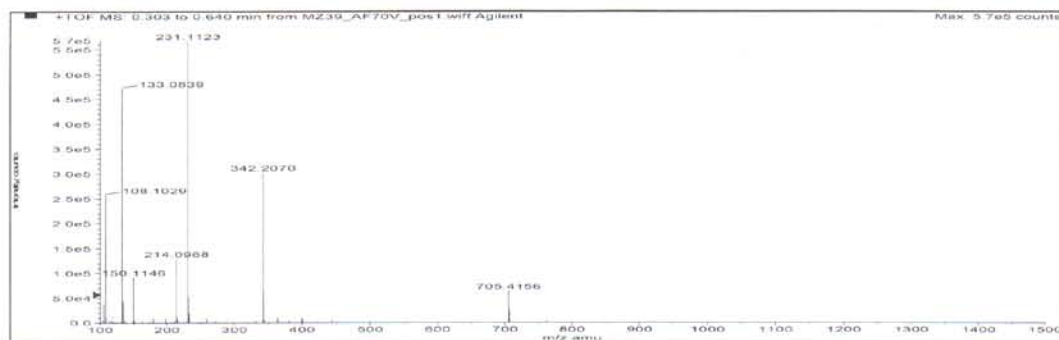
HMBC



Sample Name: MZ39 Sample Location: P1-C8 Sample Id: Operator: Milka
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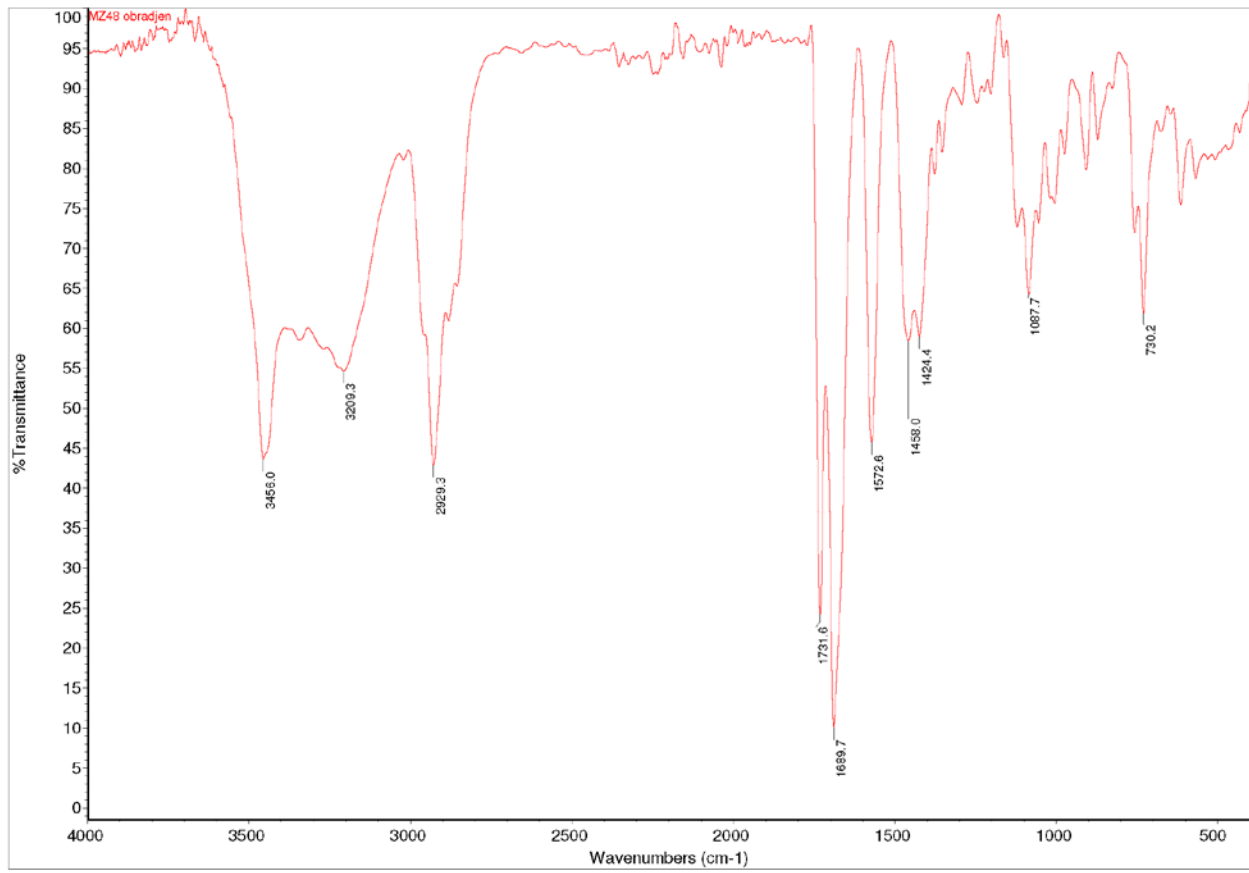
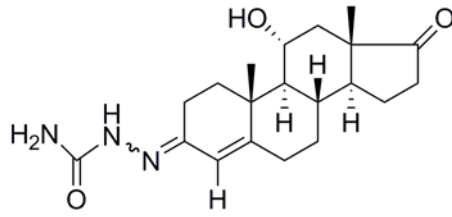
Merged XIC, Period# : 1 Experiment# : 1

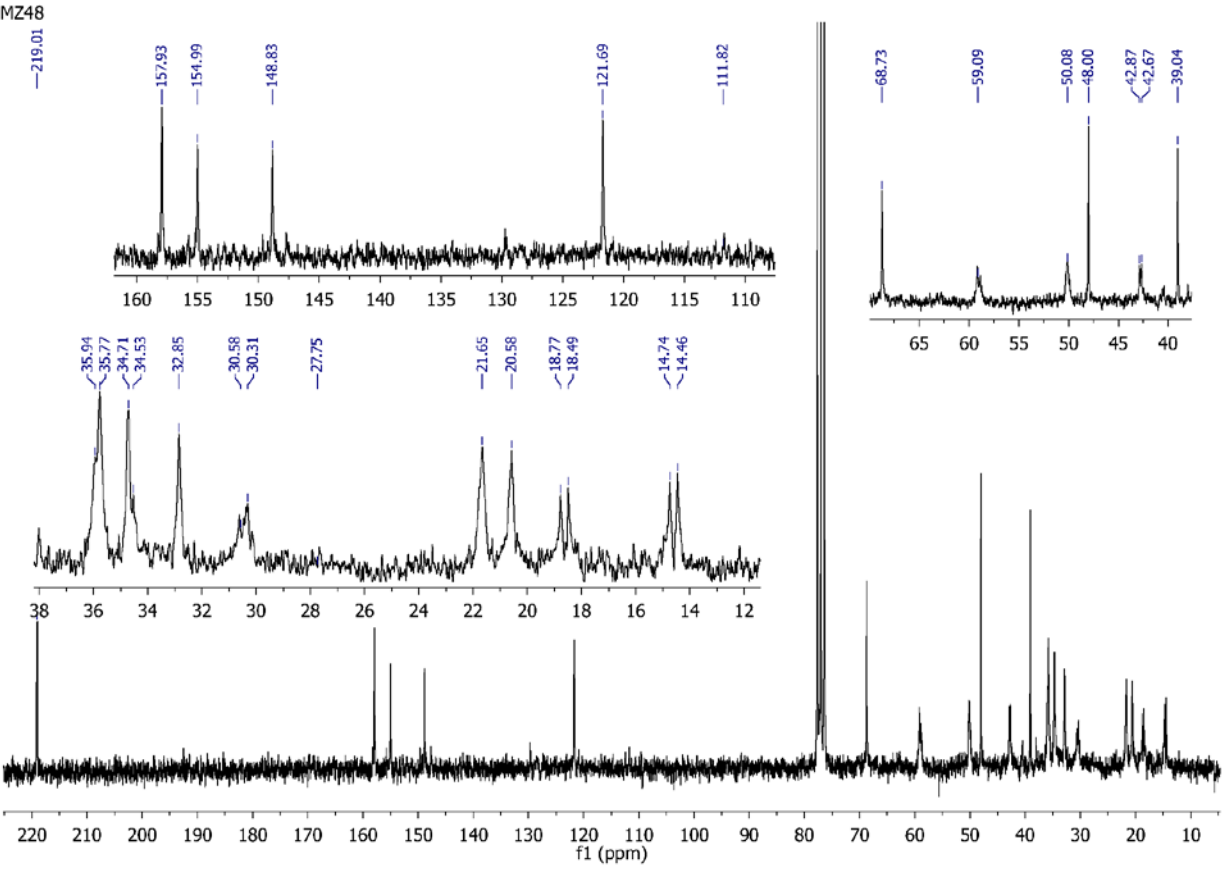
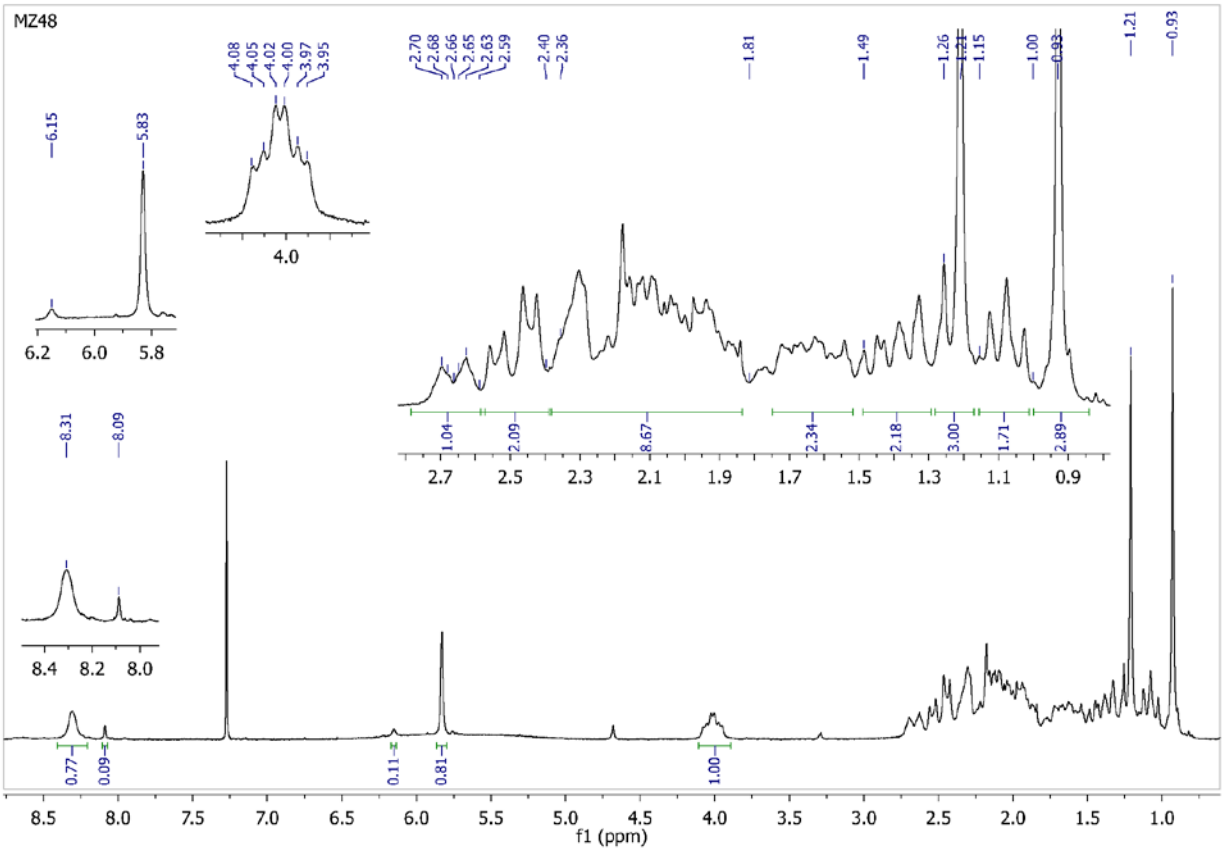


Formula	Compound name	Mass	Peak RT (min)	Peak area	Description
C20H27N3O2	--	341.21033	0.38	6.87142 E6	--

Species	Abundance (counts)	Ion Mass	Measured Mass	Error (mDa)	Error (ppm)	Ret. Time Error (min)
[M+H] ⁺	326525.54	342.21760	342.21731	-0.29466	-0.86	--
[M+Na] ⁺	10294.66	364.19955	364.20002	0.47177	1.30	--

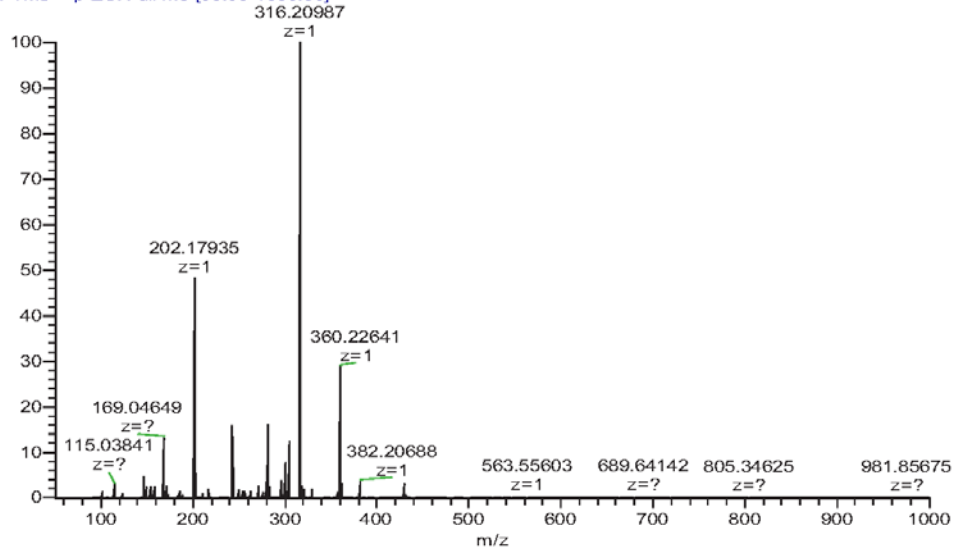
Compound 2d





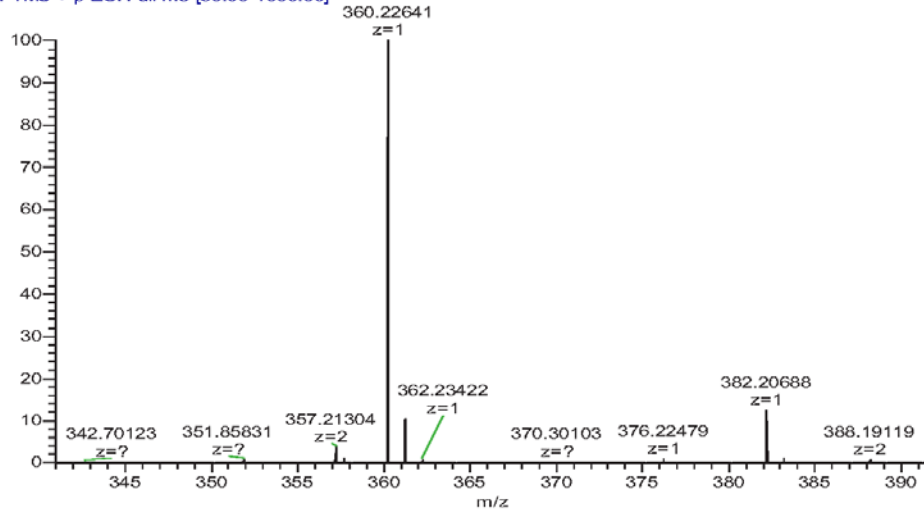
OB5266 MZ48

OB5266 #4 RT: 0.04 AV: 1 NL: 3.15E6
 T: FTMS + p ESI Full ms [50.00-1000.00]



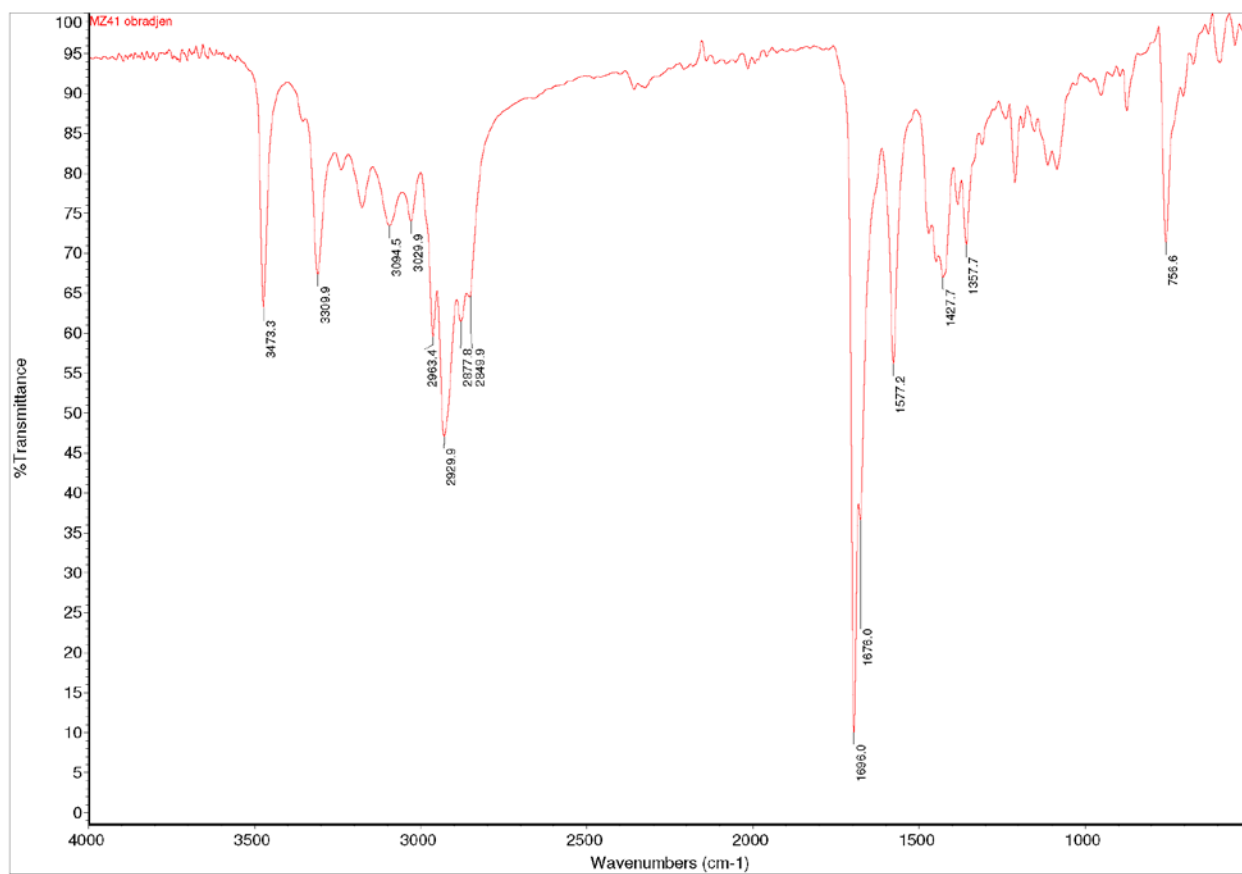
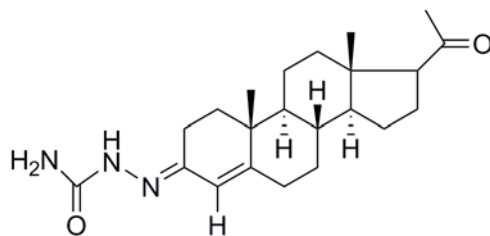
Zumirani spektri

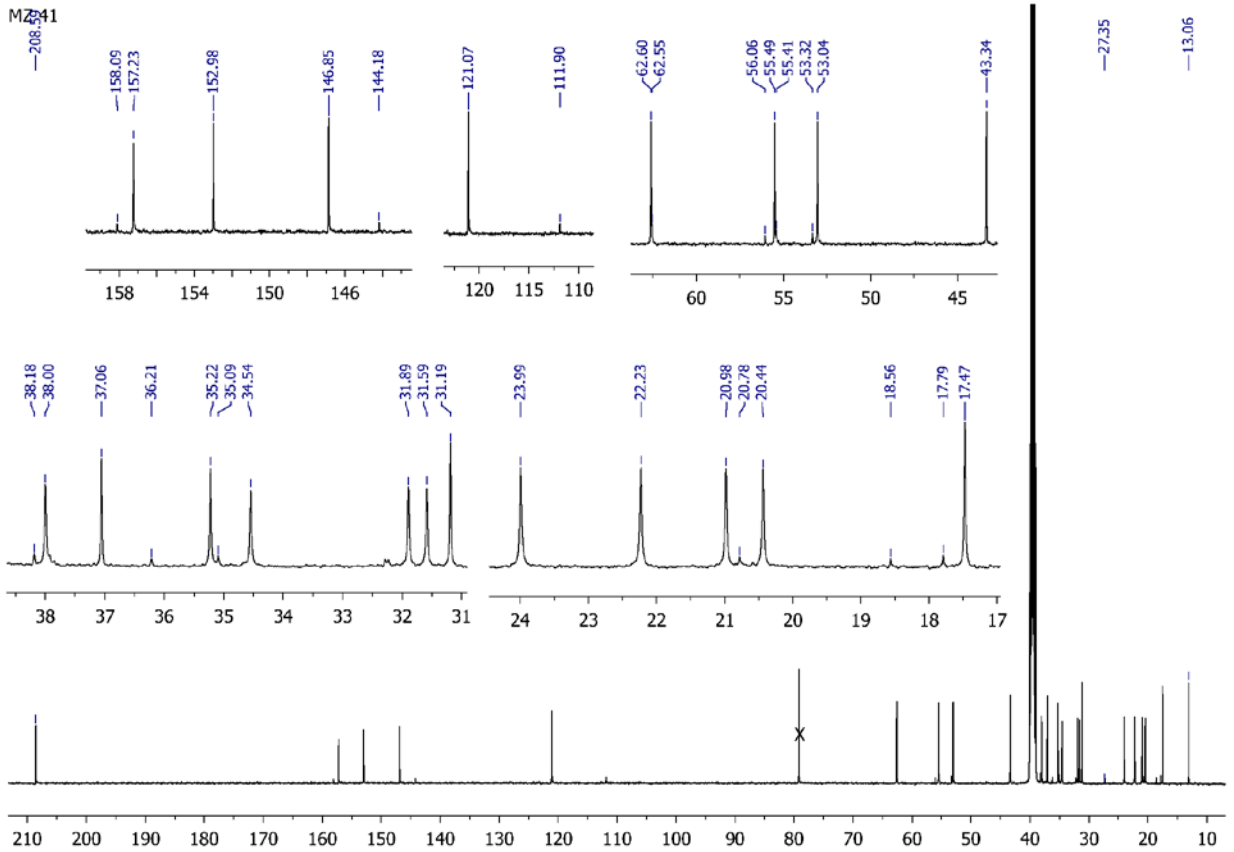
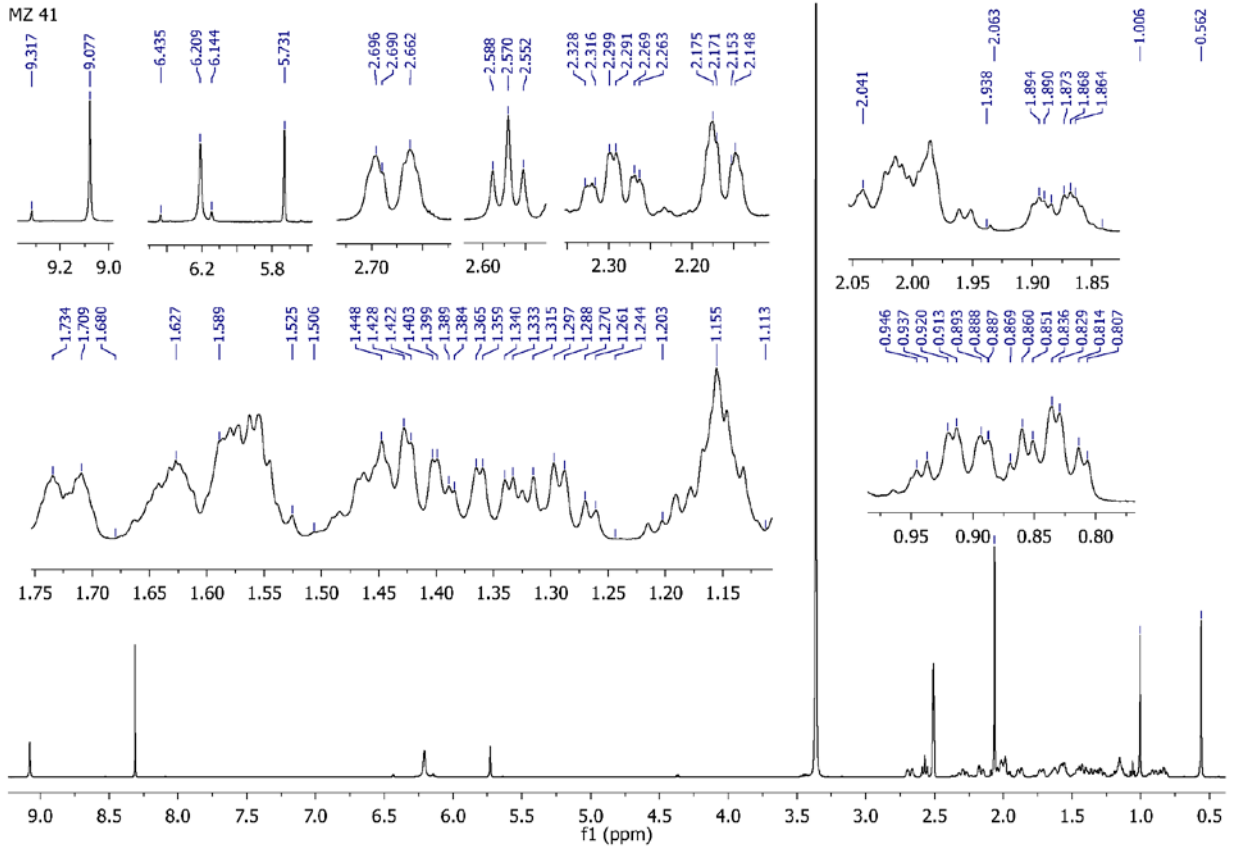
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 T: FTMS + p ESI Full ms [50.00-1000.00]



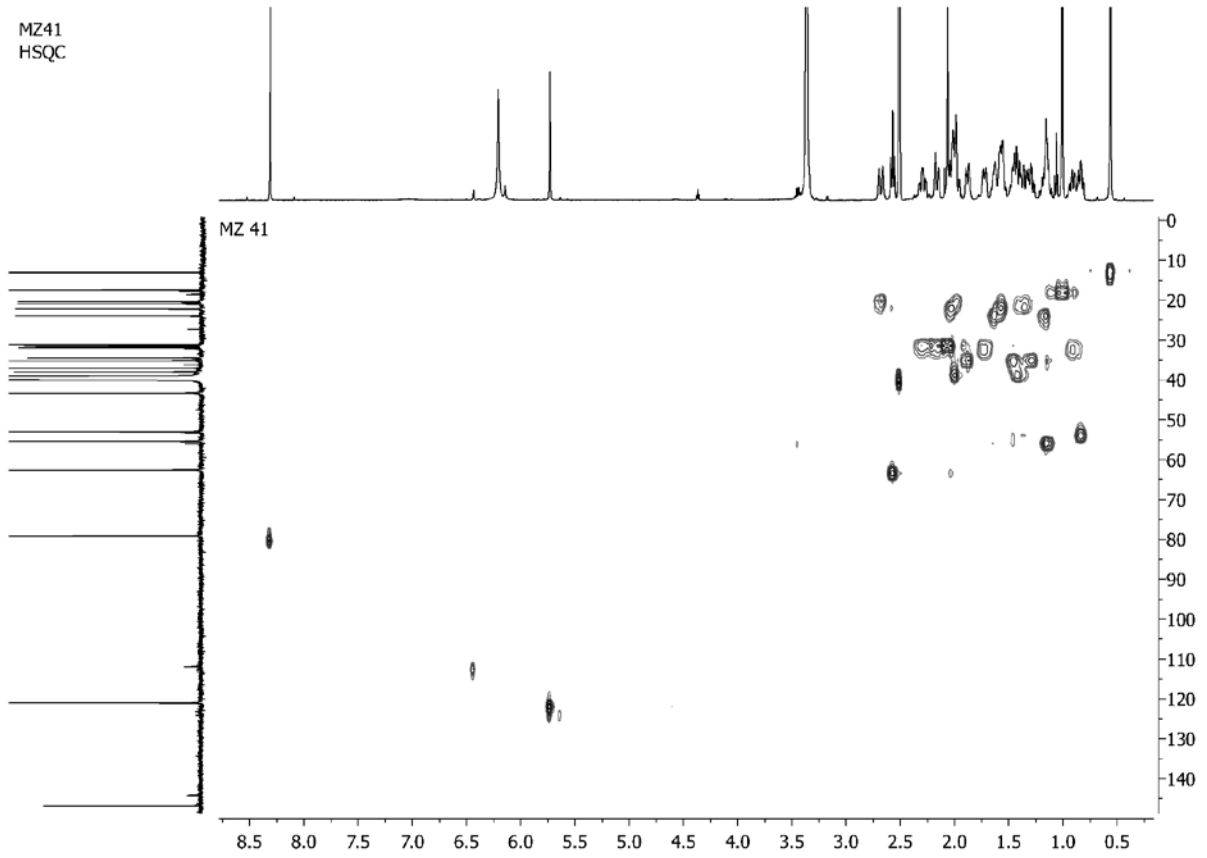
Exact mass	Observed m/z	Error (ppm)
360.2282	360.2264	4.87

Compound 2e

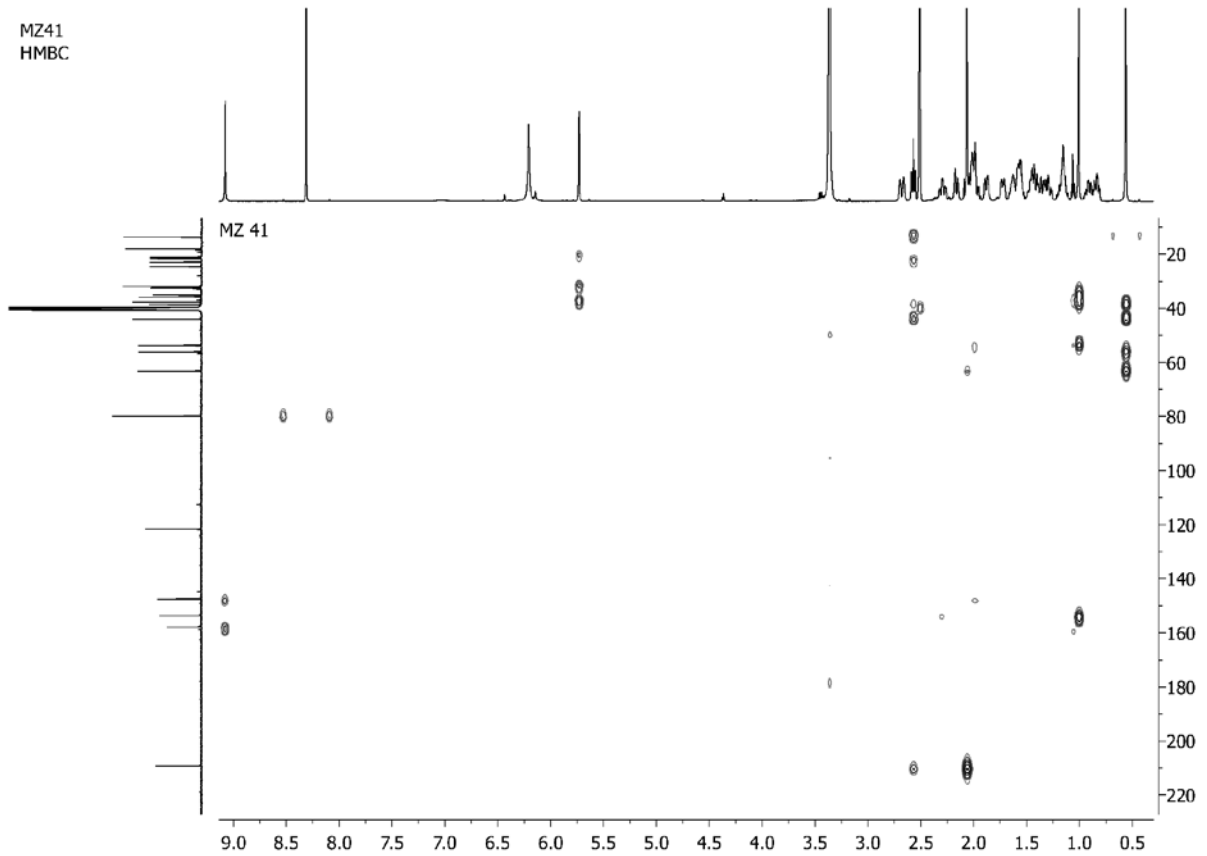




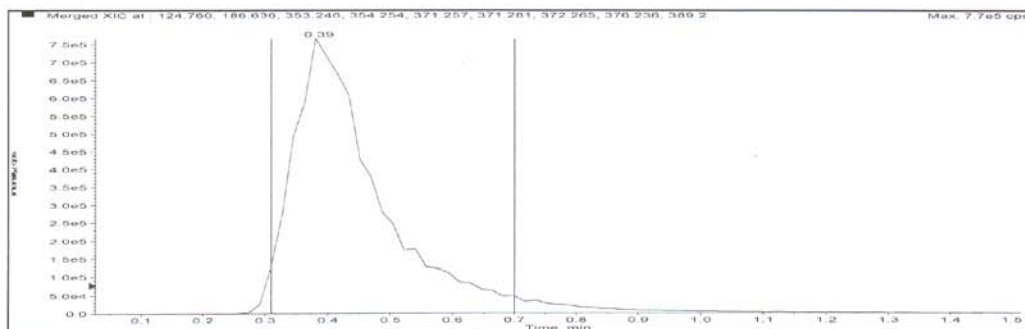
MZ41
HSQC



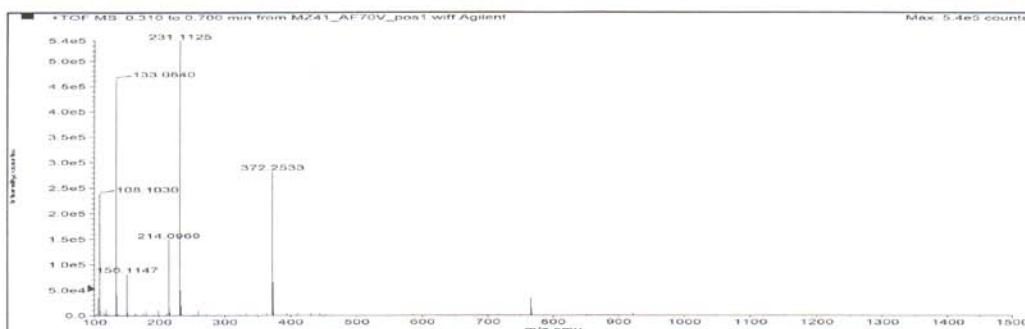
MZ41
HMBC



Sample Name: MZ41 Sample Location: P1-D1 Sample Id: Operator: Milka
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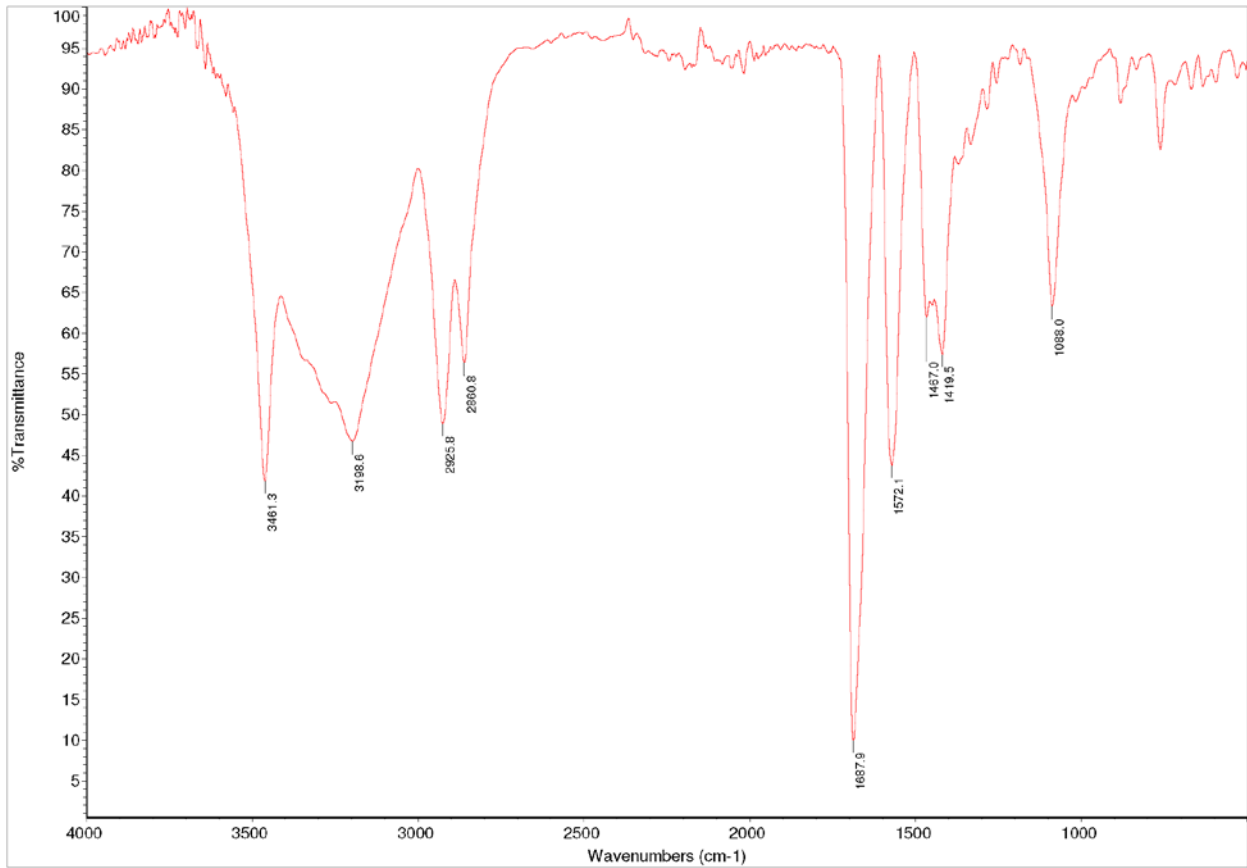
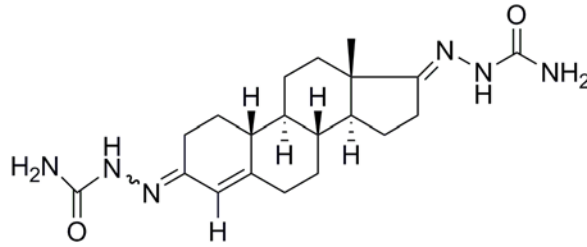
Merged XIC, Period# : 1 Experiment# : 1

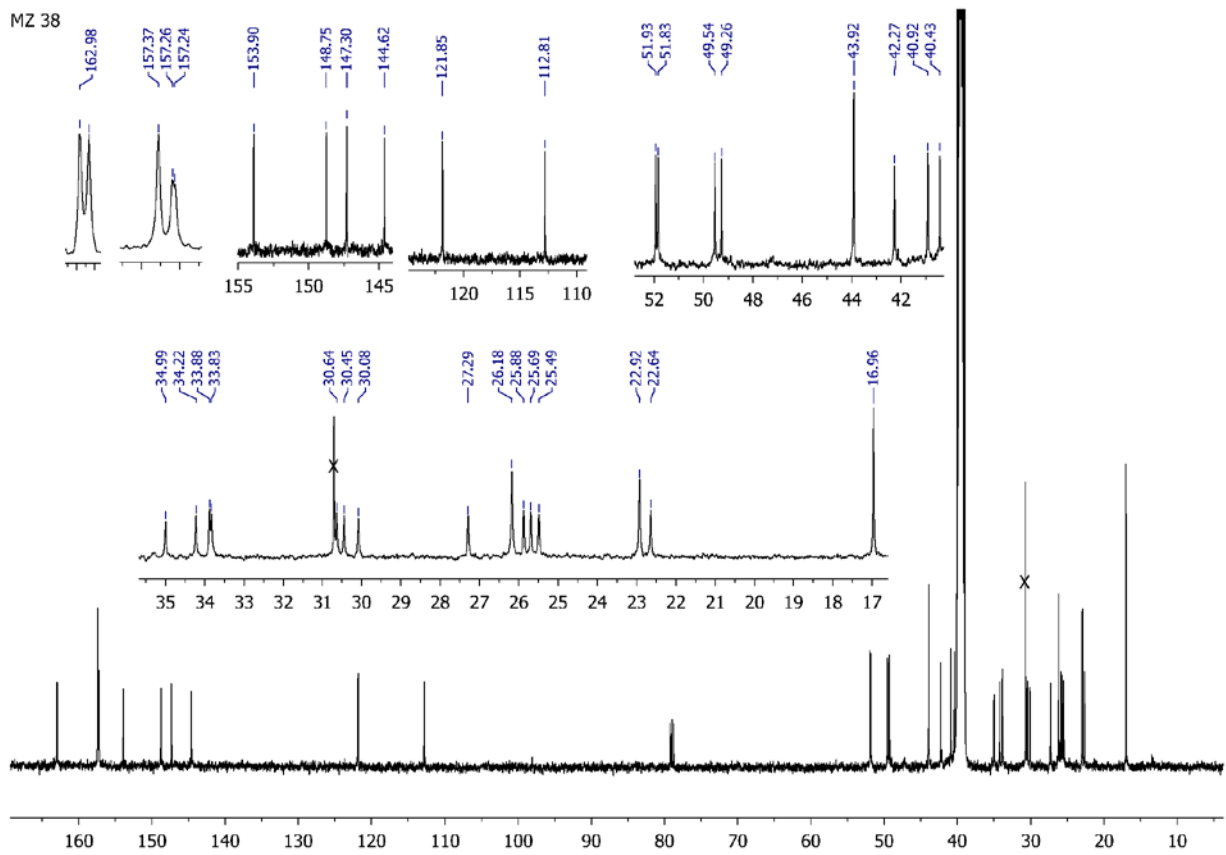
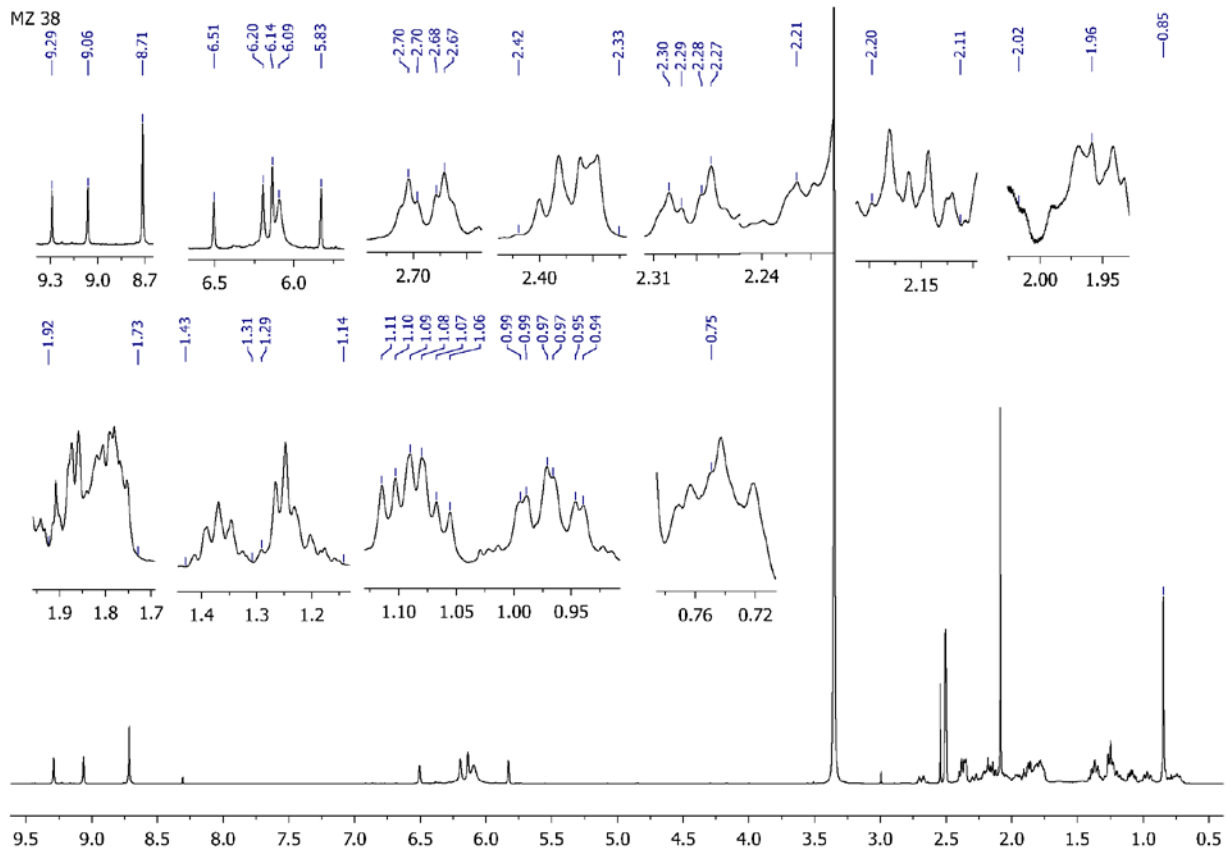


Formula	Compound name	Mass	Peak RT (min)	Peak area	Description
C22H33N3O2	--	371.25728	0.39	7.29835 E6	--

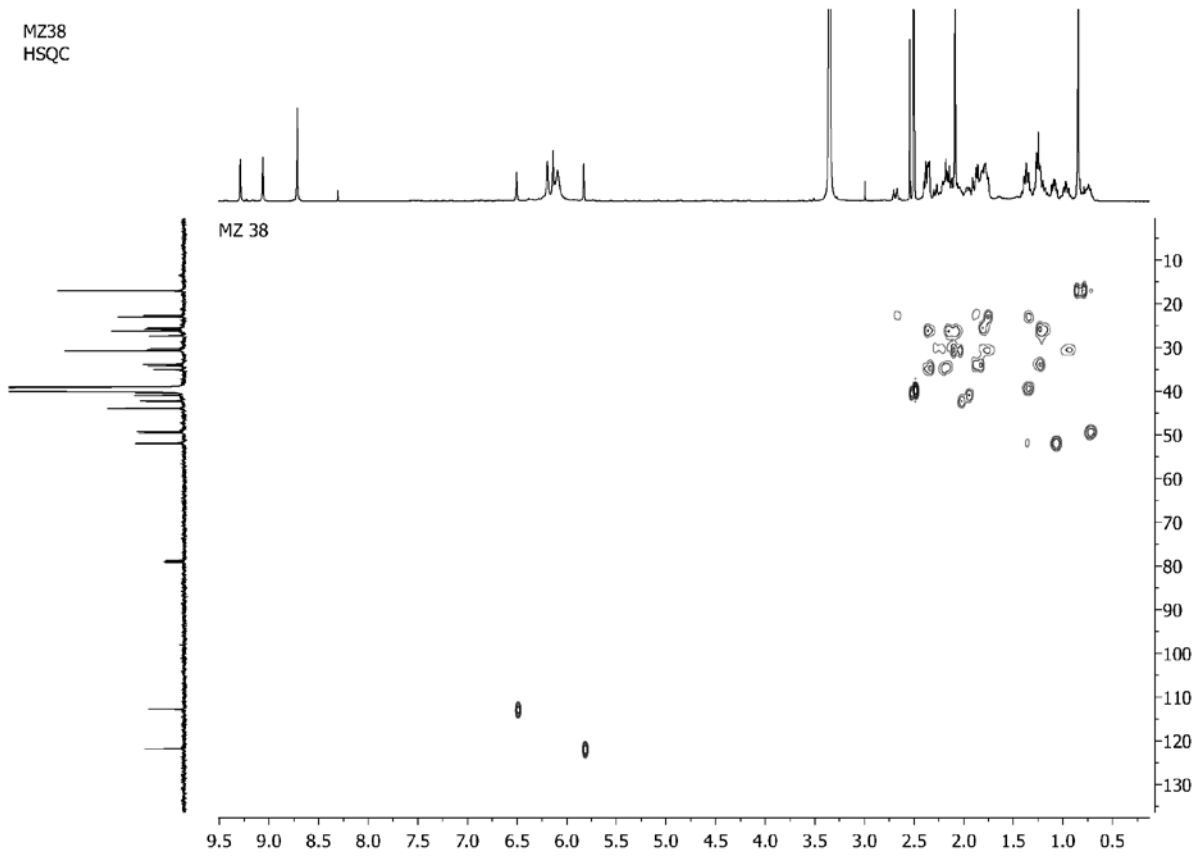
Species	Abundance (counts)	Ion Mass	Measured Mass	Error (mDa)	Error (ppm)	Ret. Time Error (min)
[M+H] ⁺	305533.71	372.26455	372.26441	-0.14749	-0.40	--
[M+Na] ⁺	5926.01	394.24650	394.24726	0.76344	1.94	--

Compound 3a

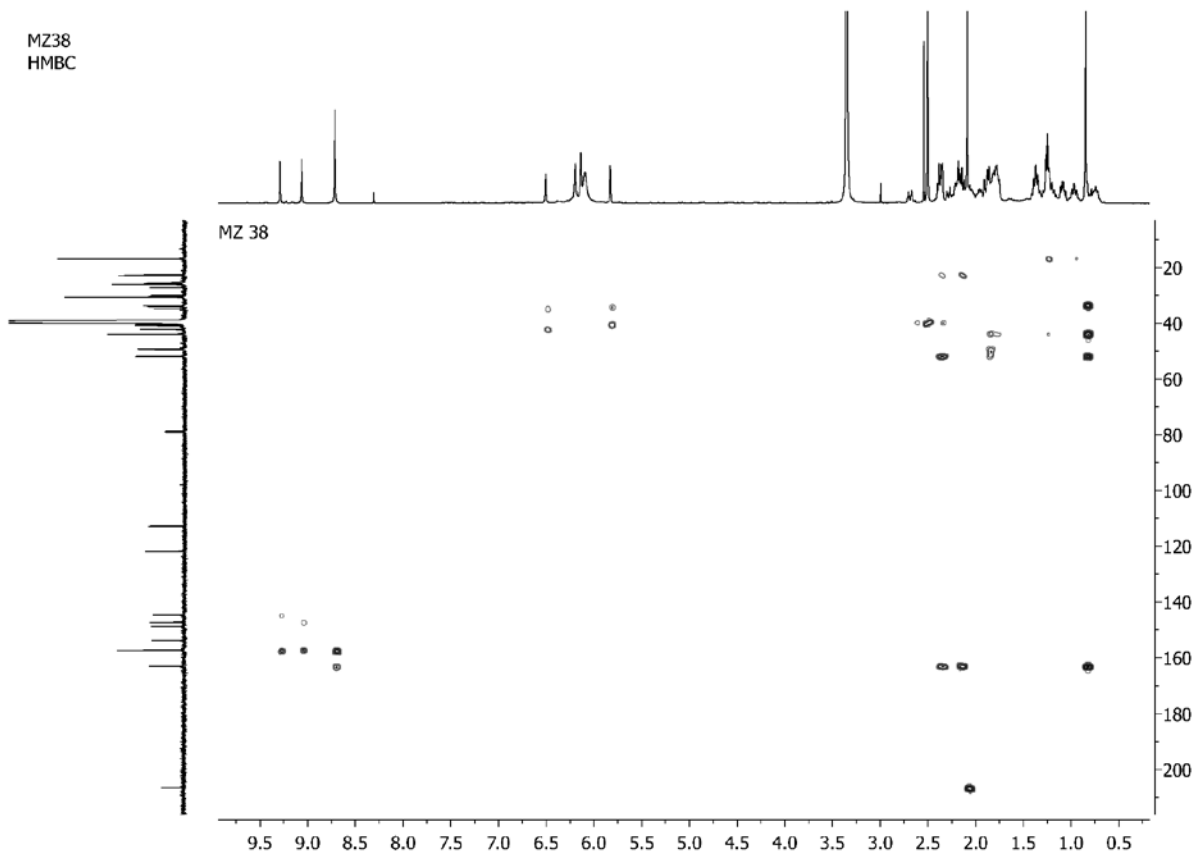




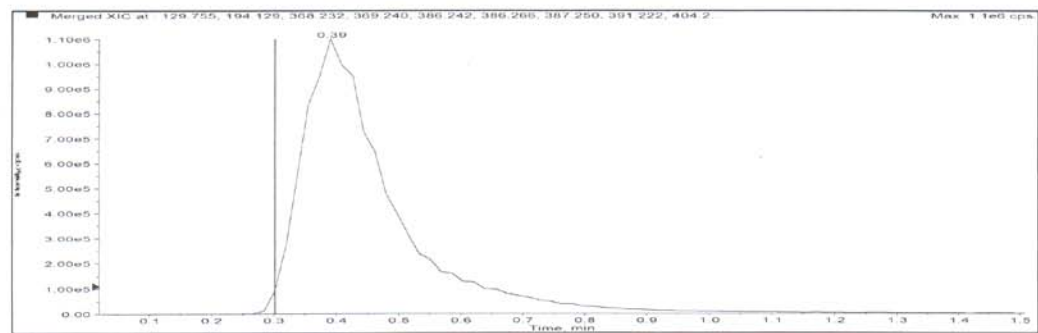
MZ38
HSQC



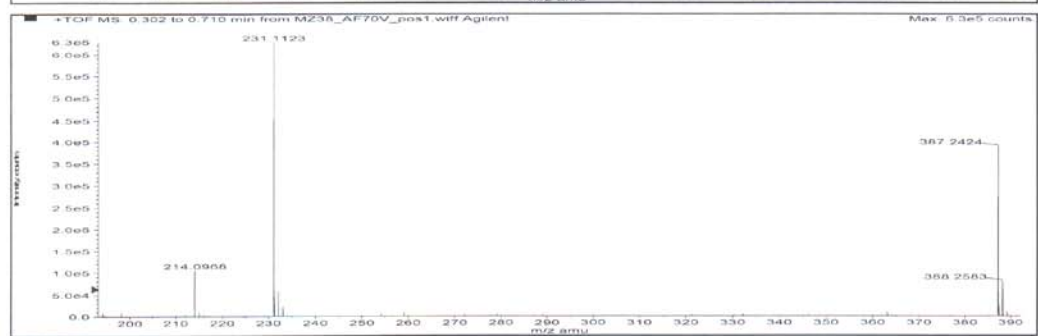
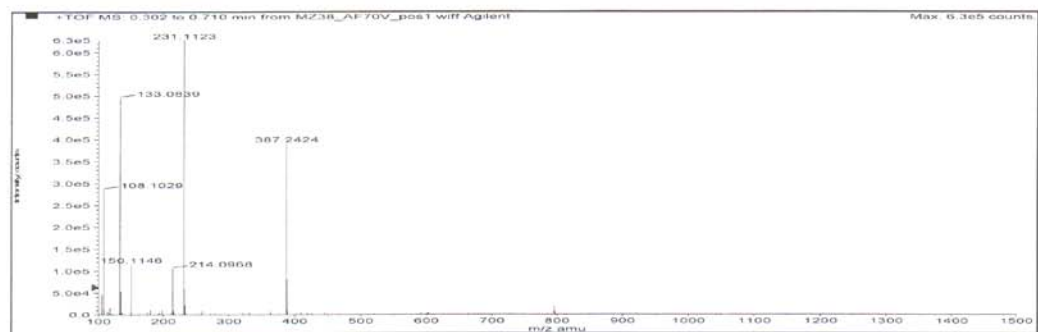
MZ38
HMBC



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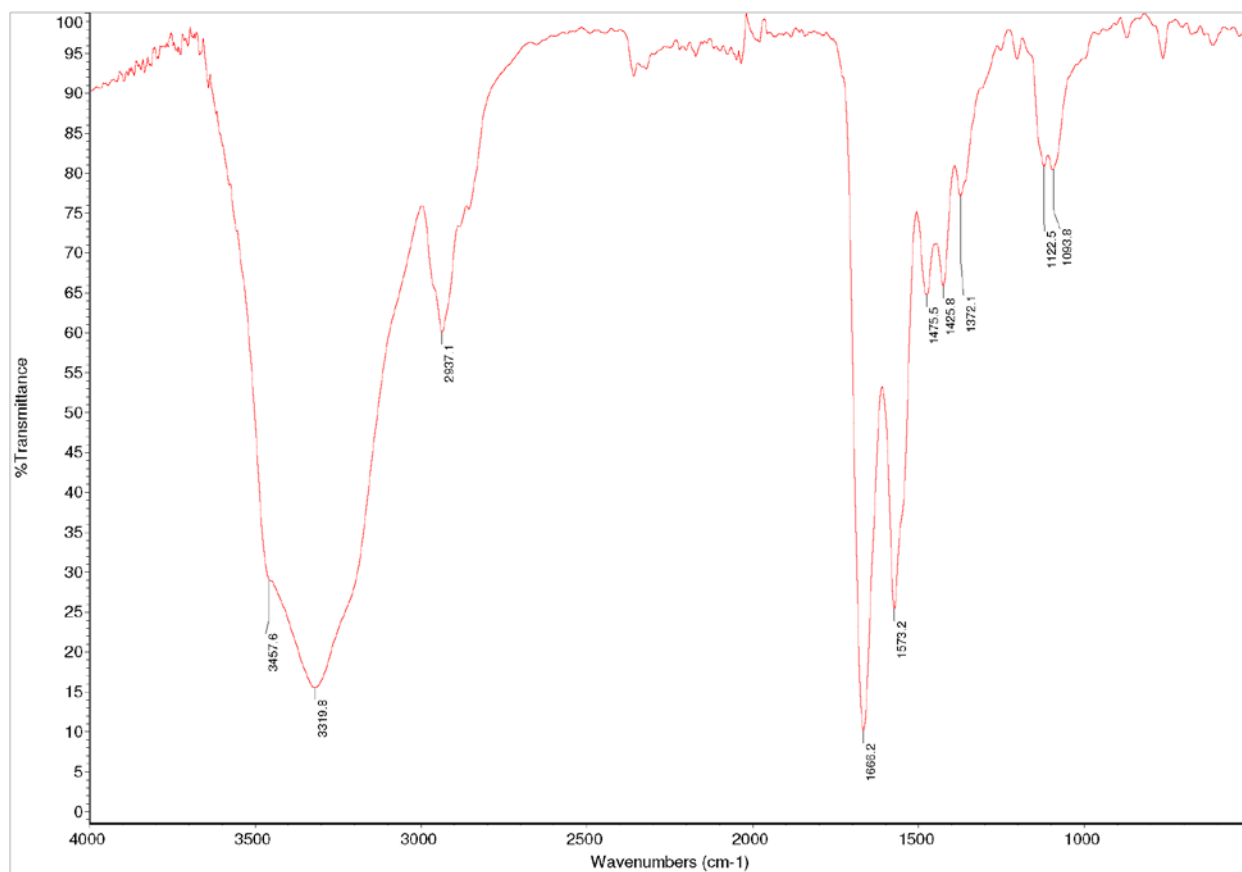
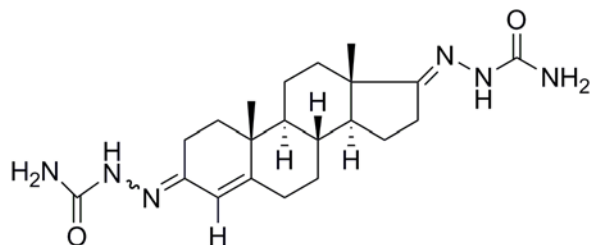
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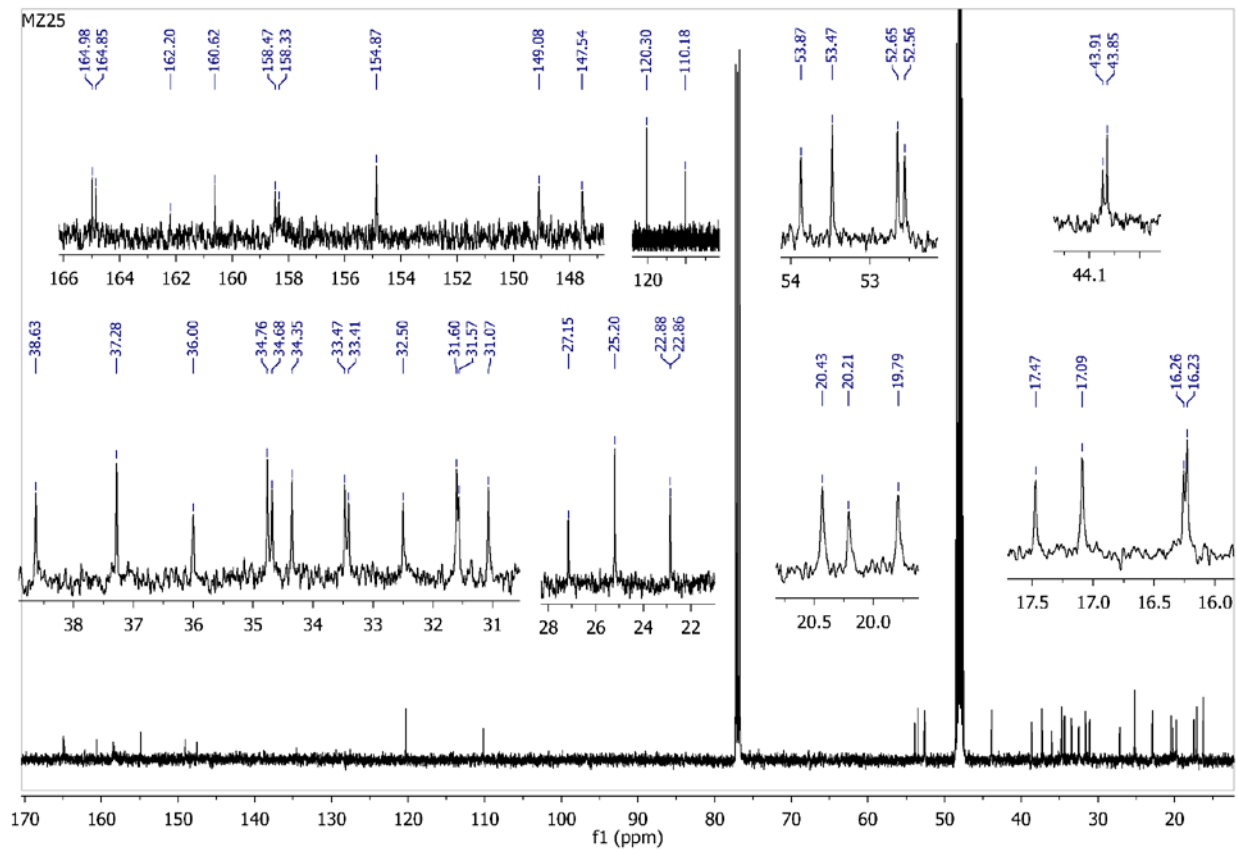
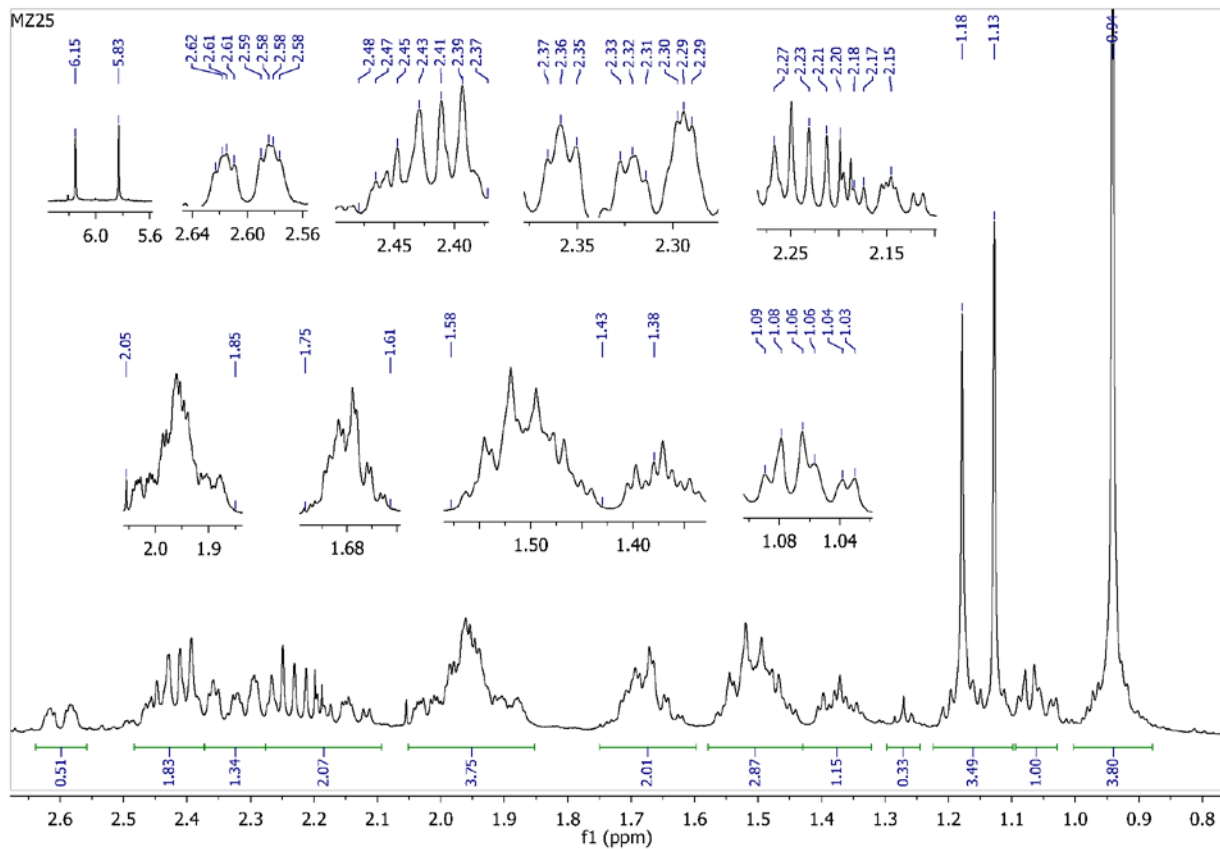


Formula	Compound name	Mass	Peak RT (min)	Peak area	Description
C20H30N6O2	--	386.24302	0.39	1.06090 E7	--

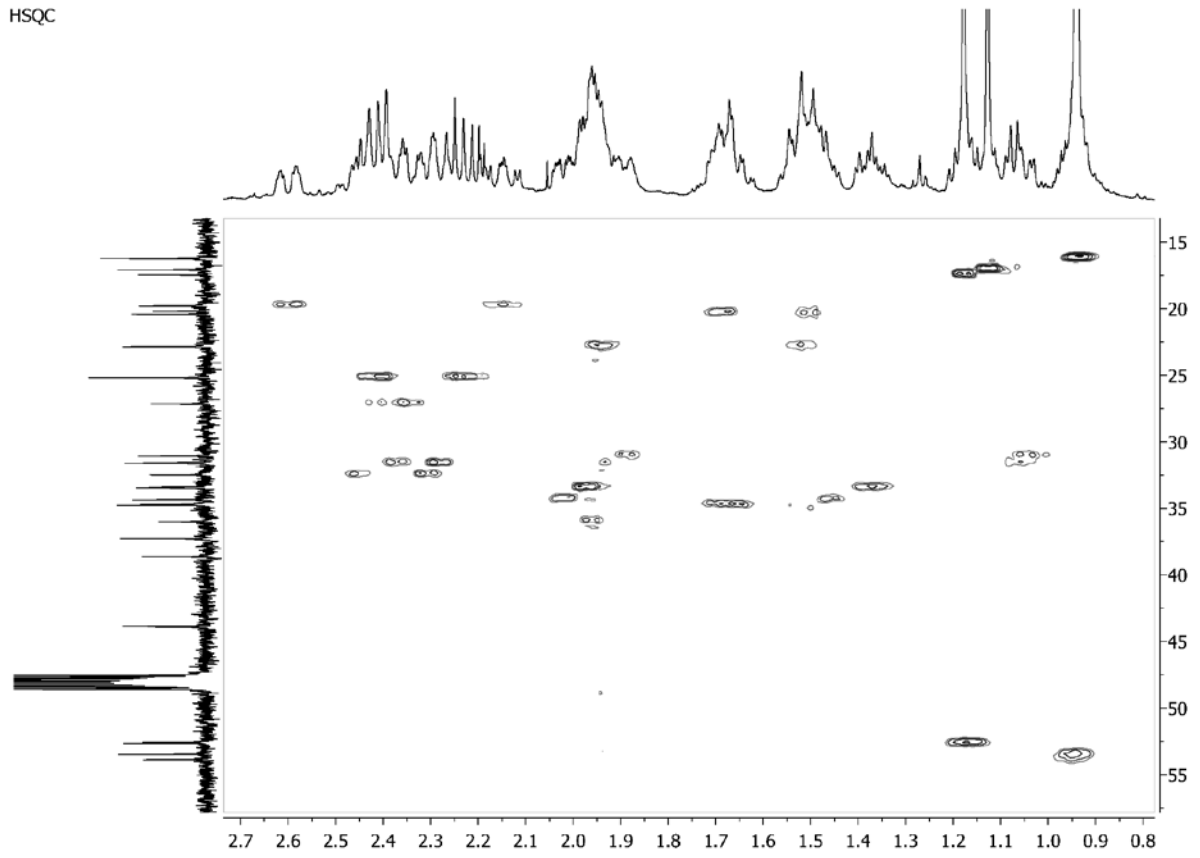
Species	Abundance (counts)	Ion Mass	Measured Mass	Error (mDa)	Error (ppm)	Ret. Time Error (min)
[M+2H] ²⁺	8512.22	194.12879	194.12894	0.15318	0.79	--
[M+H] ⁺	402059.98	387.25030	387.24978	-0.52376	-1.35	--

Compound 3b

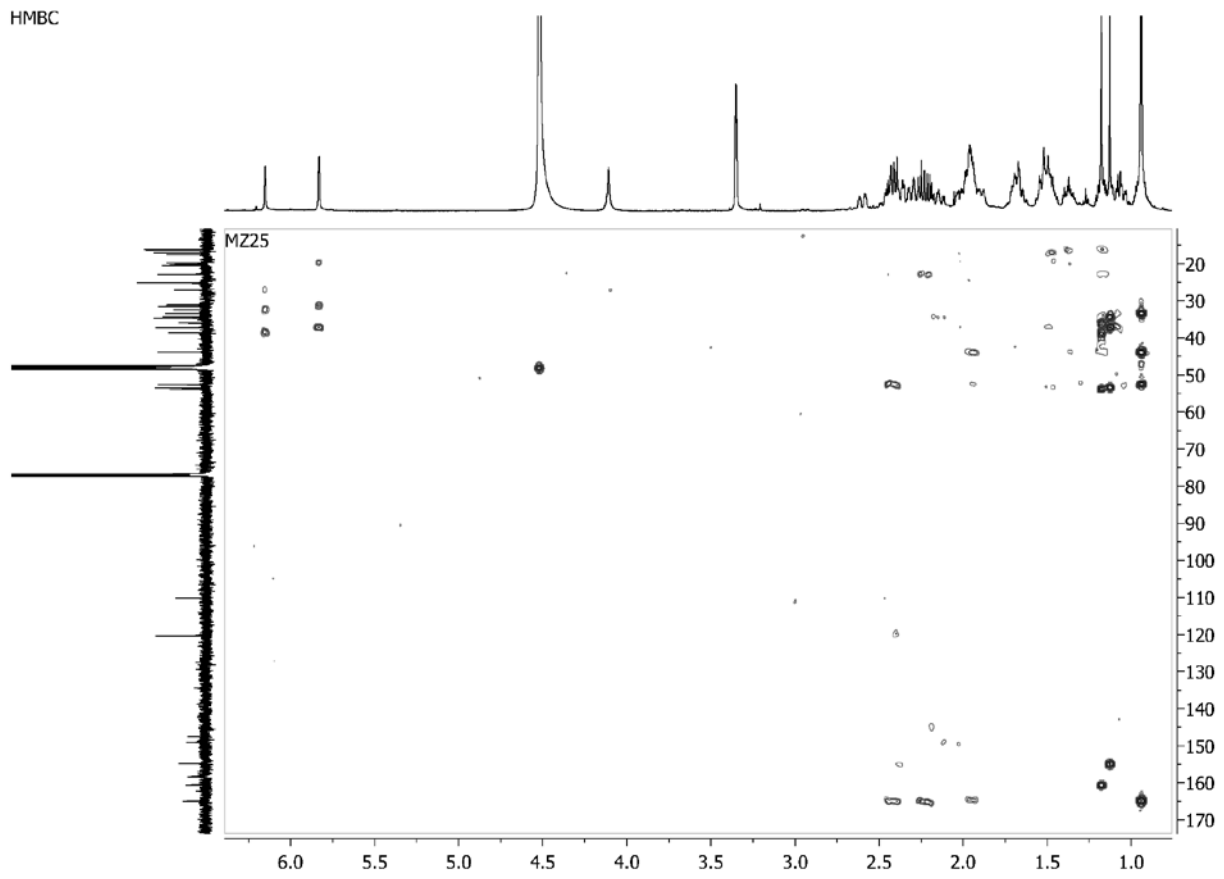




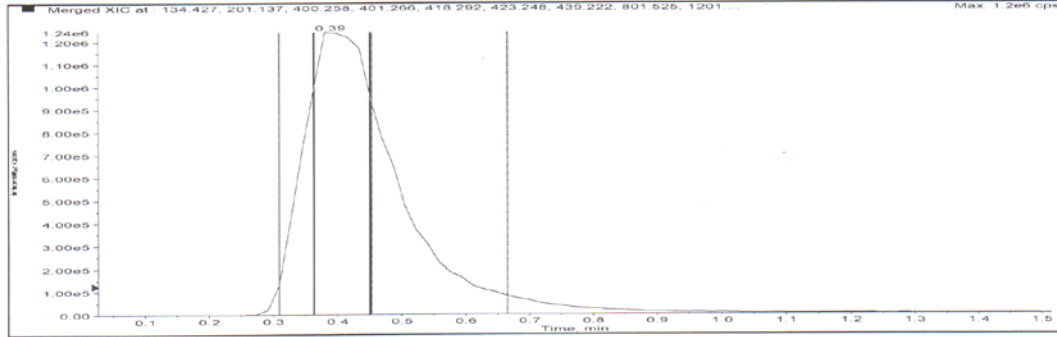
HSQC



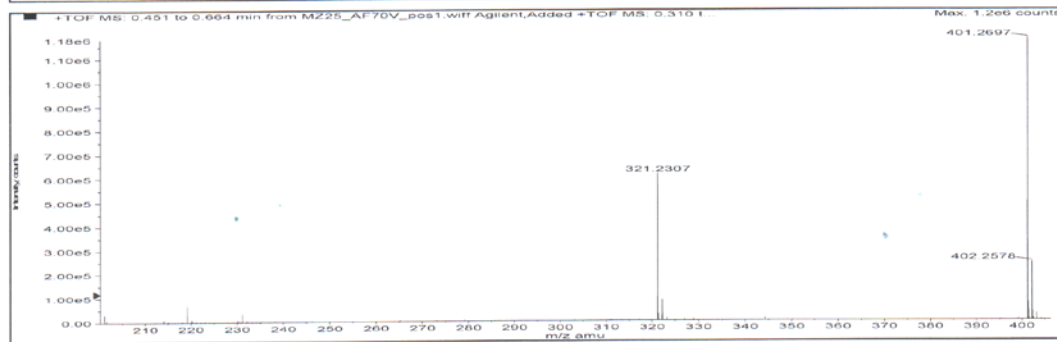
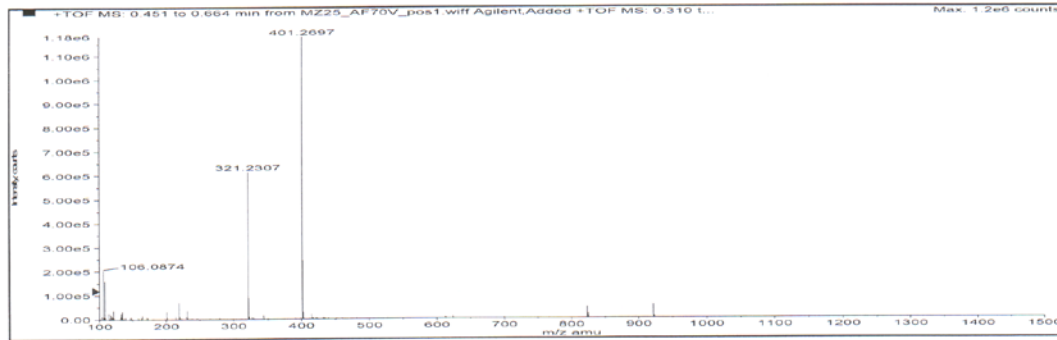
HMBC



Sample Name: MZ25 Sample Location: P1-D8 Sample Id: Operator: Milka
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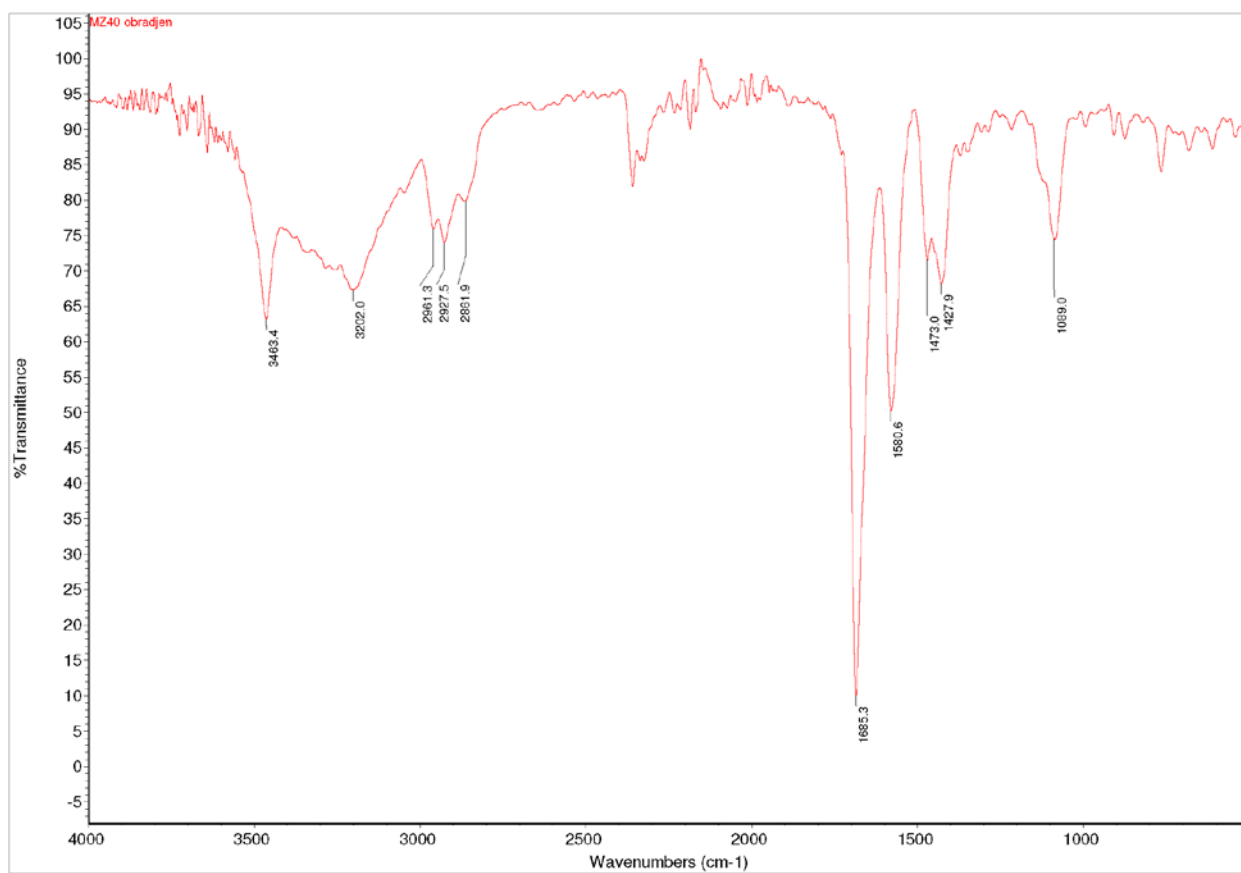
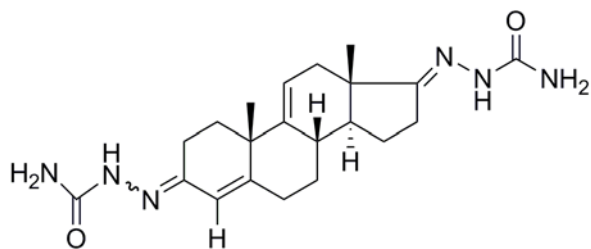
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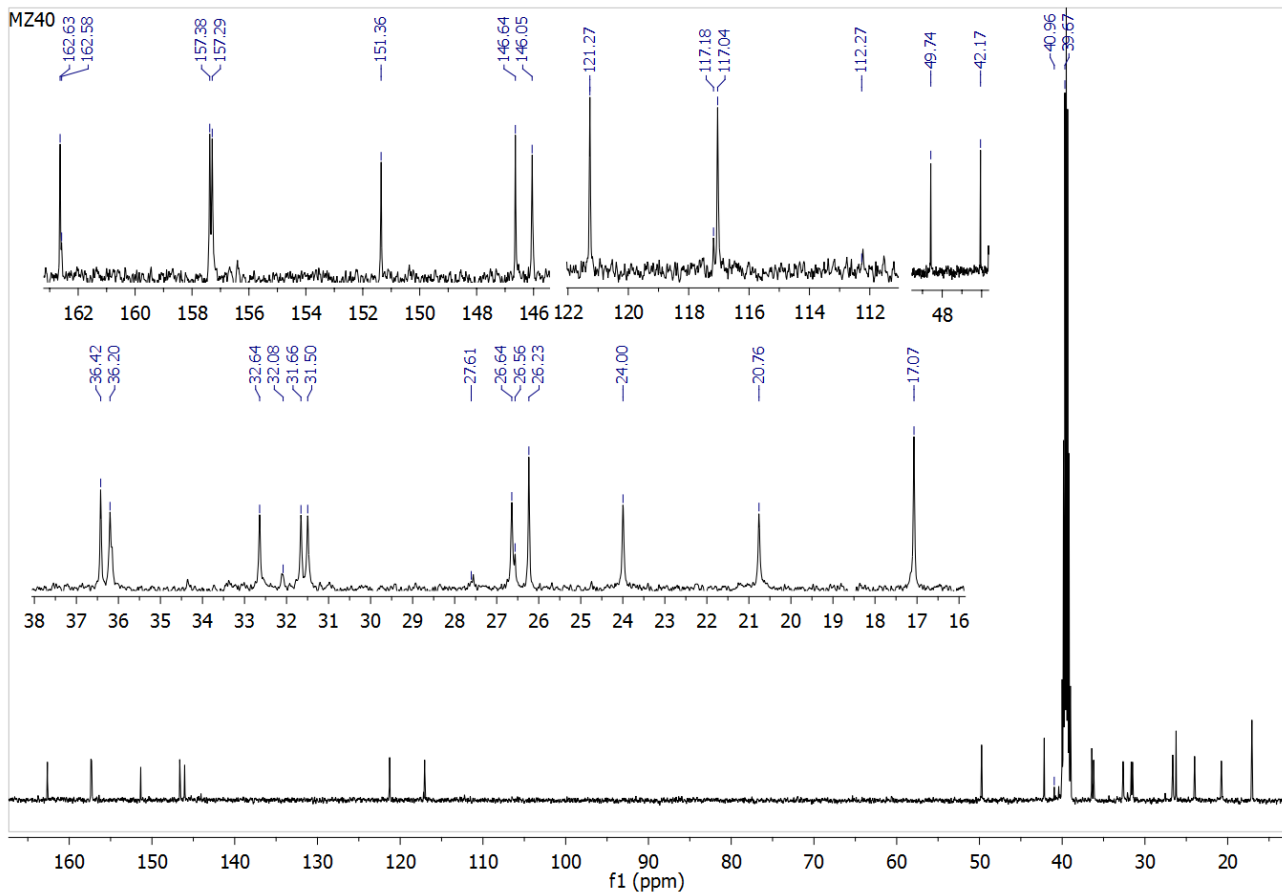
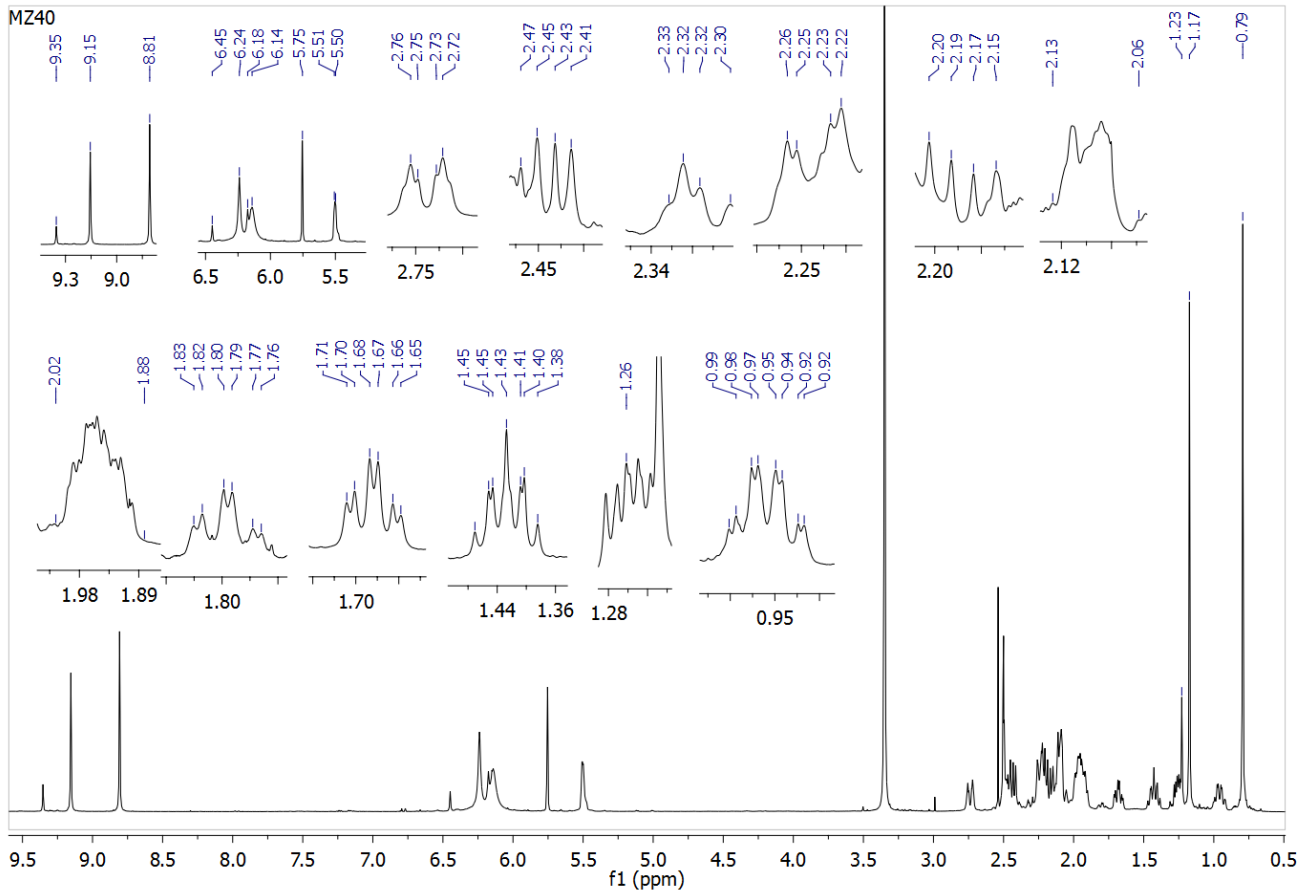


Formula	Compound name	Mass	Peak RT (min)	Peak area	Description
C21H32N6O2	--	400.25867	0.39	1.27046 E7	--

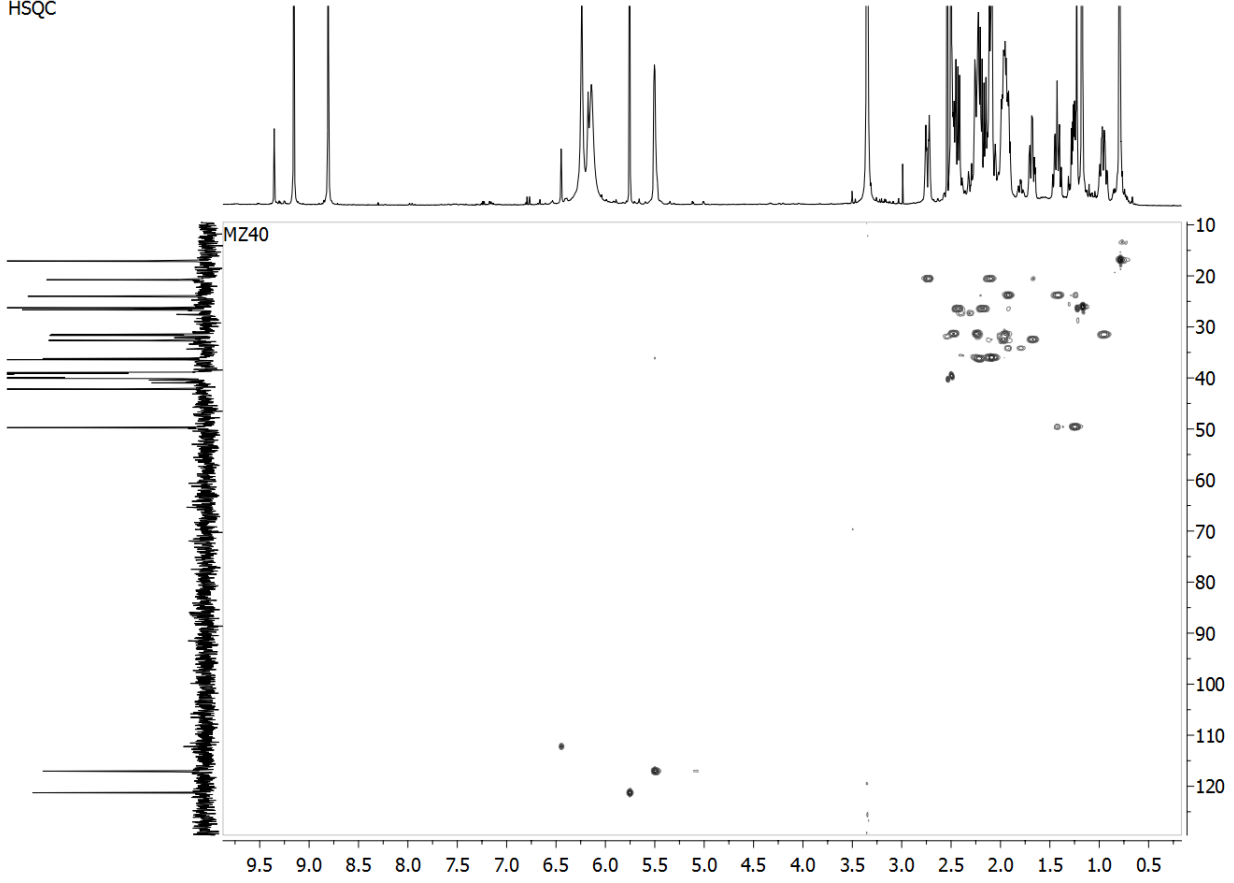
Species	Abundance (counts)	Ion Mass	Measured Mass	Error (mDa)	Error (ppm)	Ret. Time Error (min)
[M+2H] ²⁺	31682.44	201.13661	201.13684	0.22849	1.14	--
[M+H] ⁺	1191709.72	401.26595	401.26542	-0.52774	-1.32	--

Compound 3c

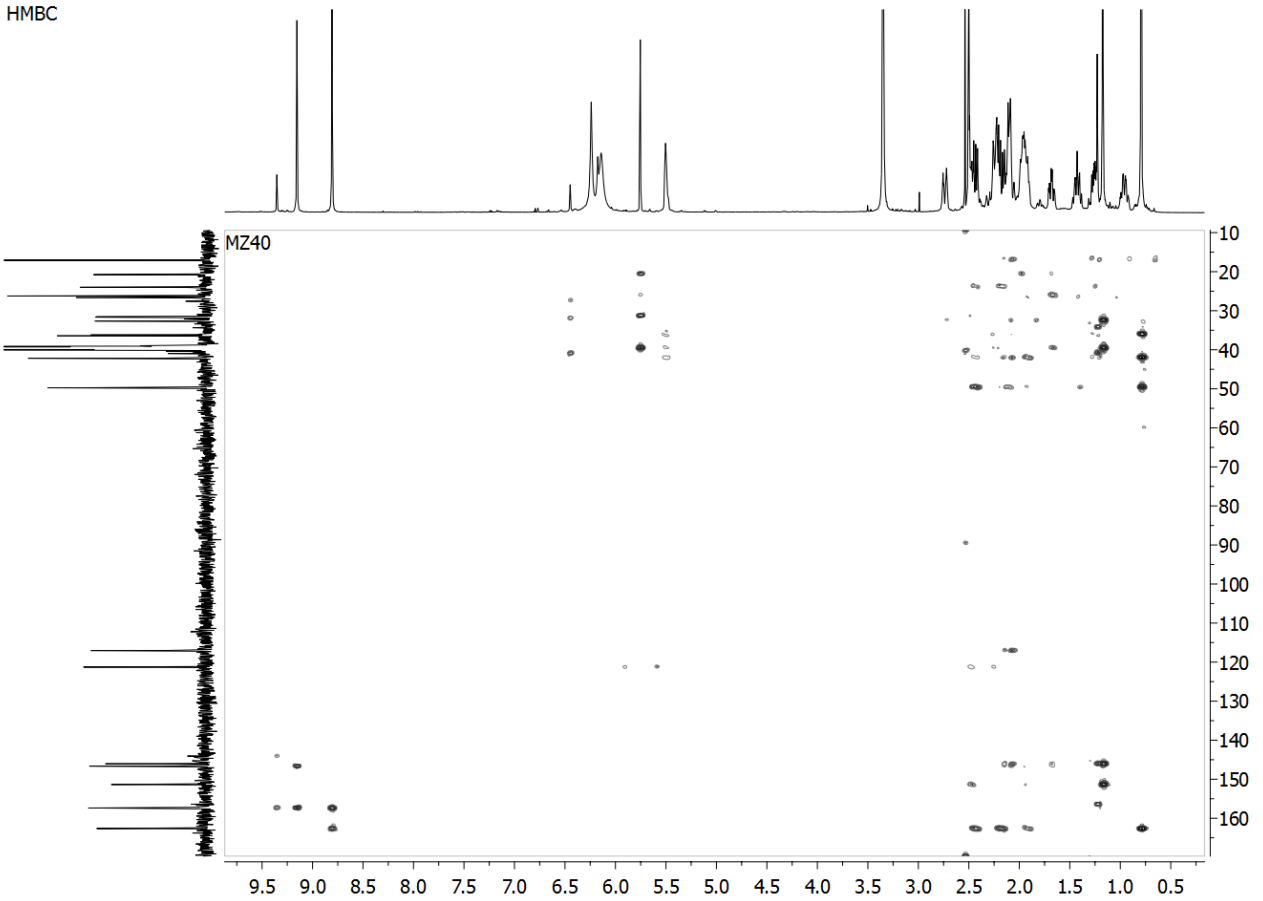




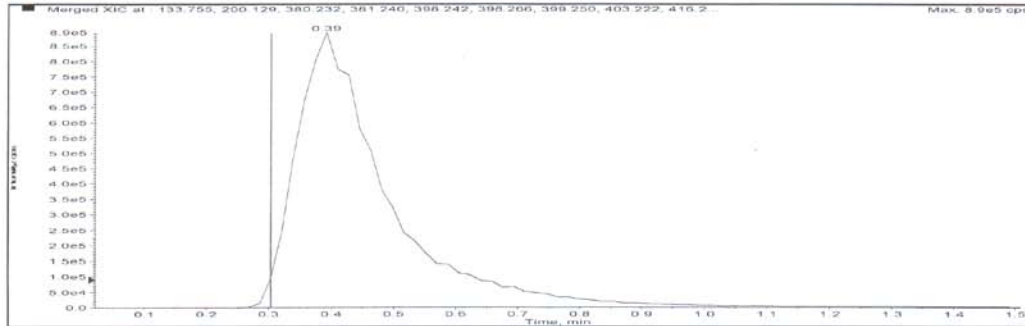
HSQC



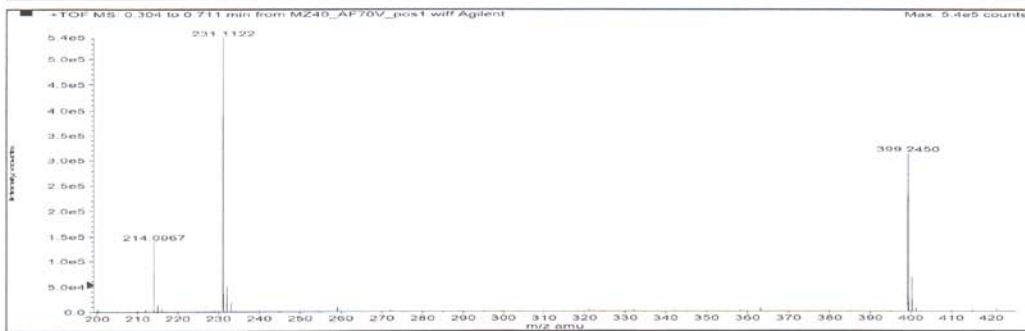
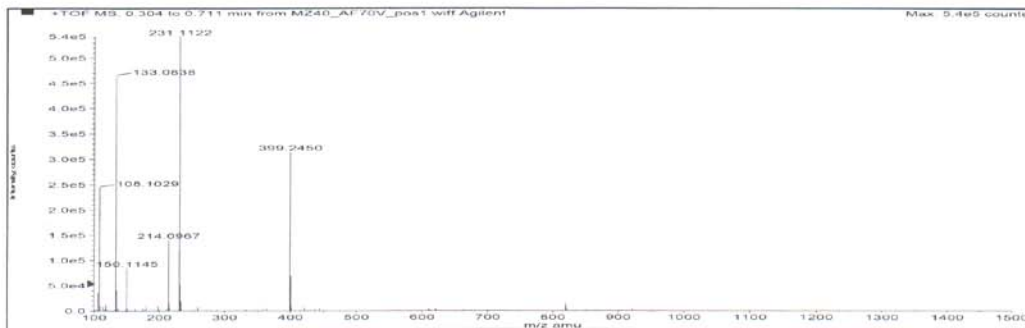
HMBC



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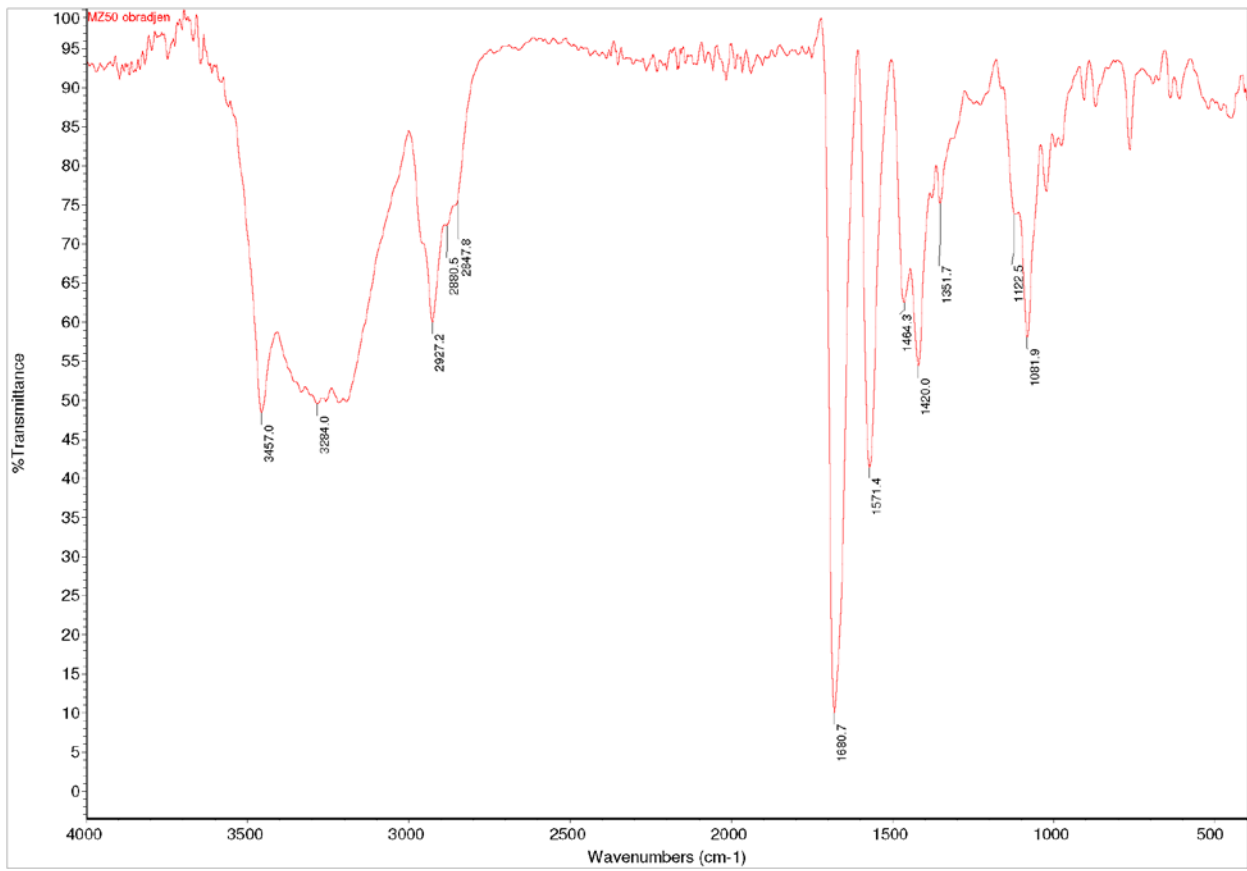
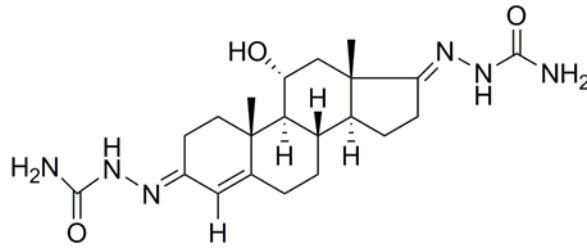
Merged XIC, Period# : 1 Experiment# : 1

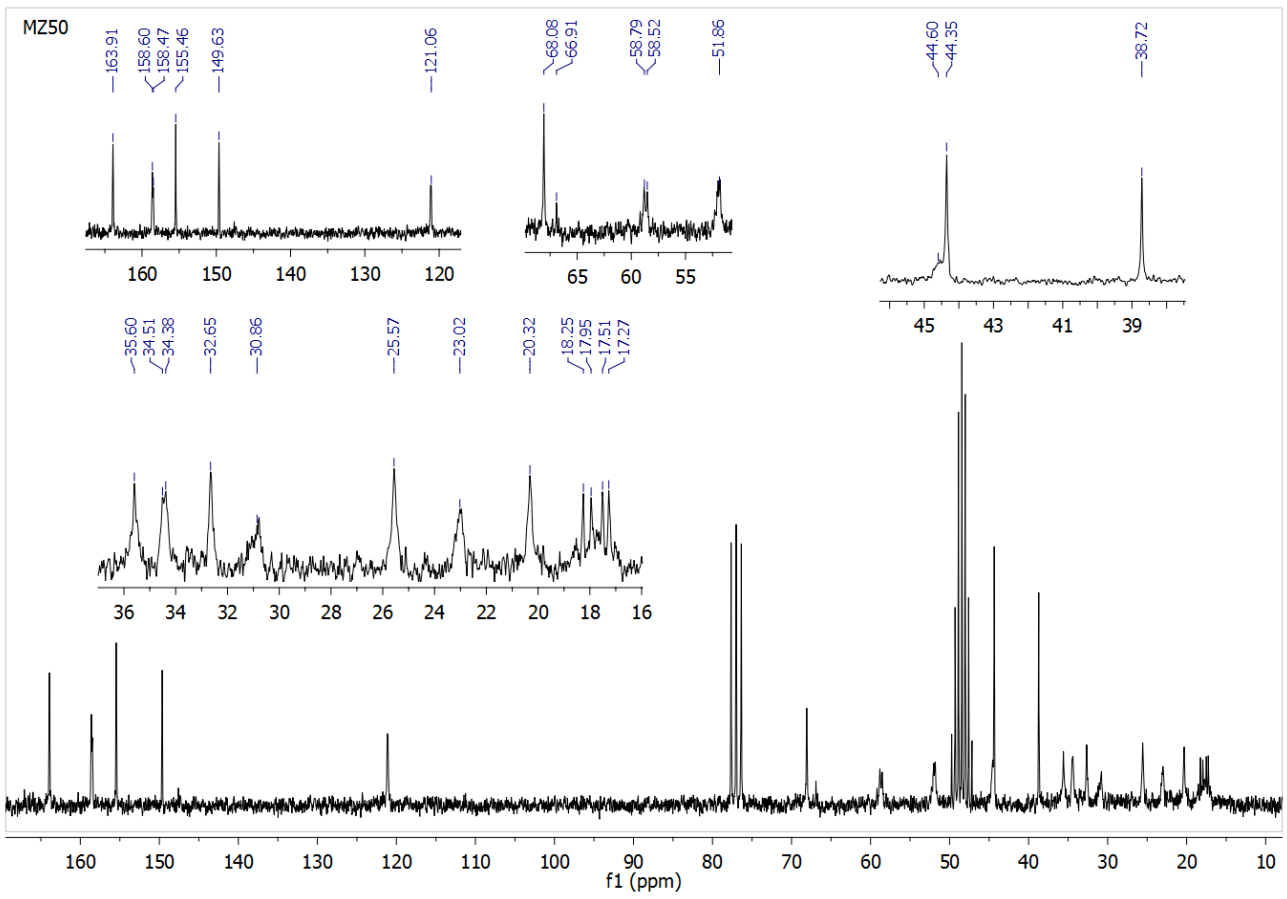
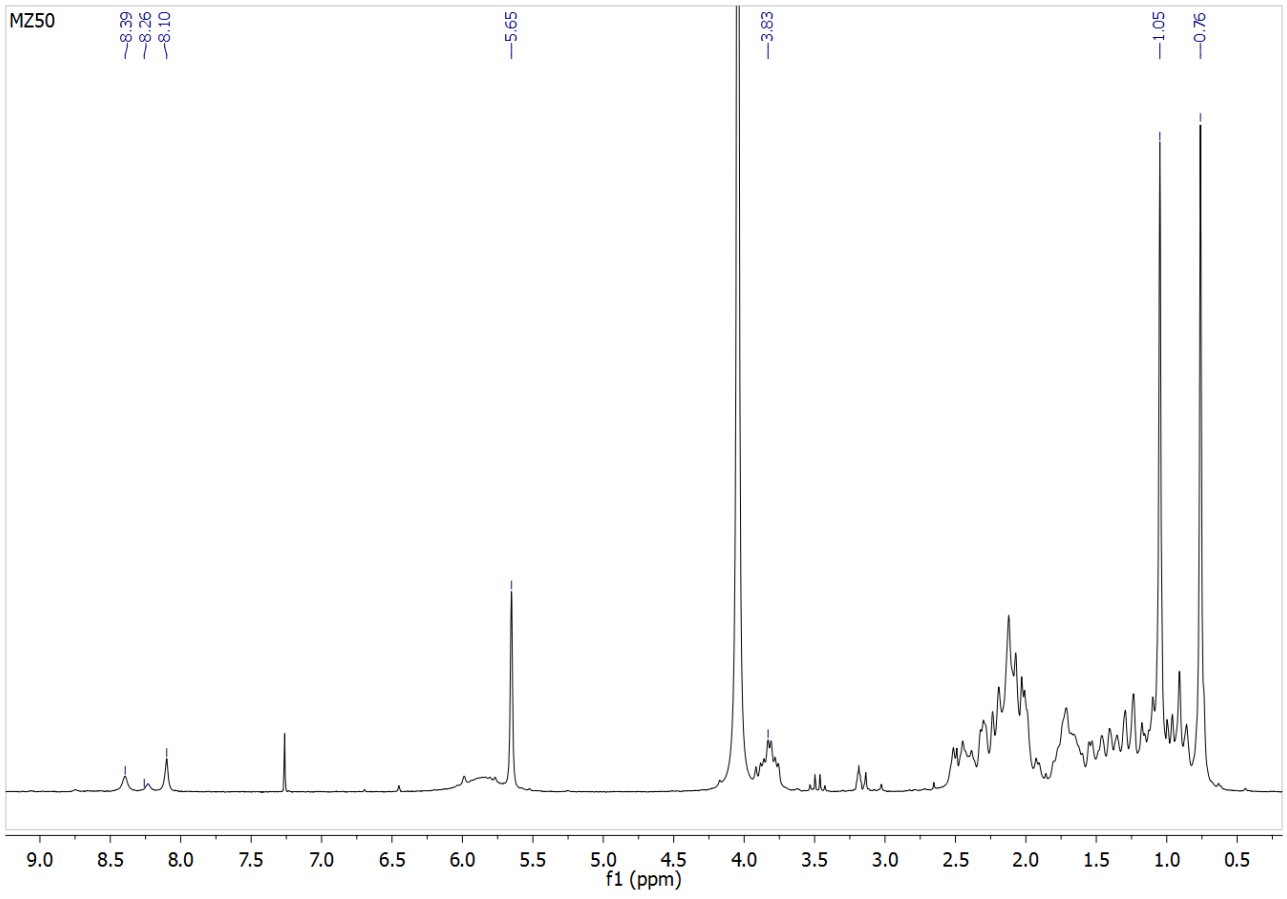


Formula	Compound name	Mass	Peak RT (min)	Peak area	Description
C21H30N6O2	--	398.24302	0.39	8.75311 E6	--

Species	Abundance (counts)	Ion Mass	Measured Mass	Error (mDa)	Error (ppm)	Ret. Time Error (min)
[M+2H] ²⁺	5719.56	200.12879	200.12900	0.21110	1.05	--
[M+H] ⁺	317278.15	399.25030	399.24961	-0.69054	-1.73	--
[M+Na] ⁺	6677.55	421.23225	421.23209	-0.15152	-0.36	--

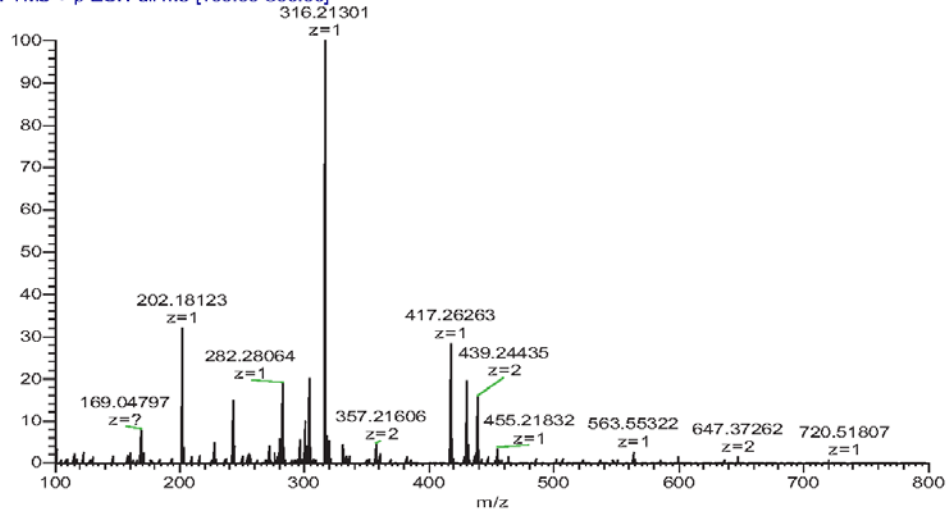
Compound 3d





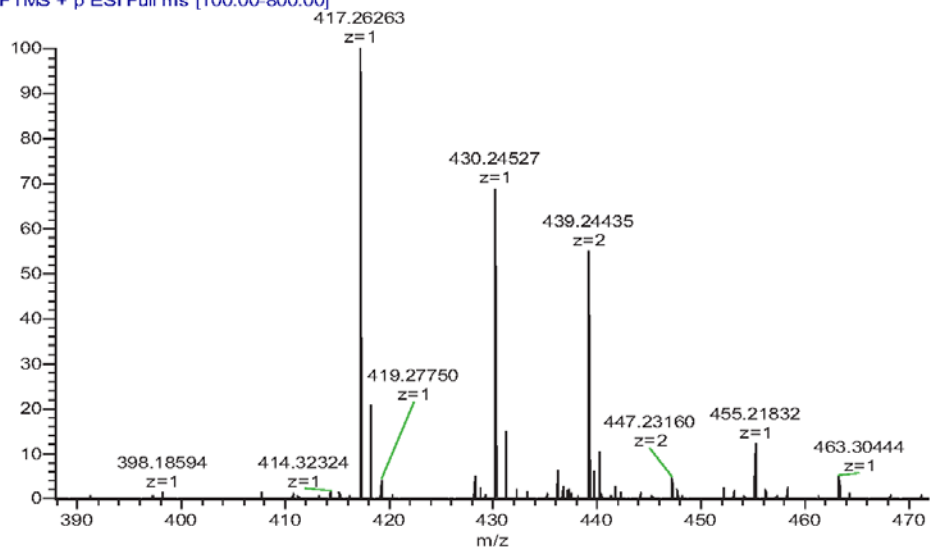
OB5268 MZ50

OB5268 #21 RT: 0.30 AV: 1 NL: 2.45E6
 T: FTMS + p ESI Full ms [100.00-800.00]



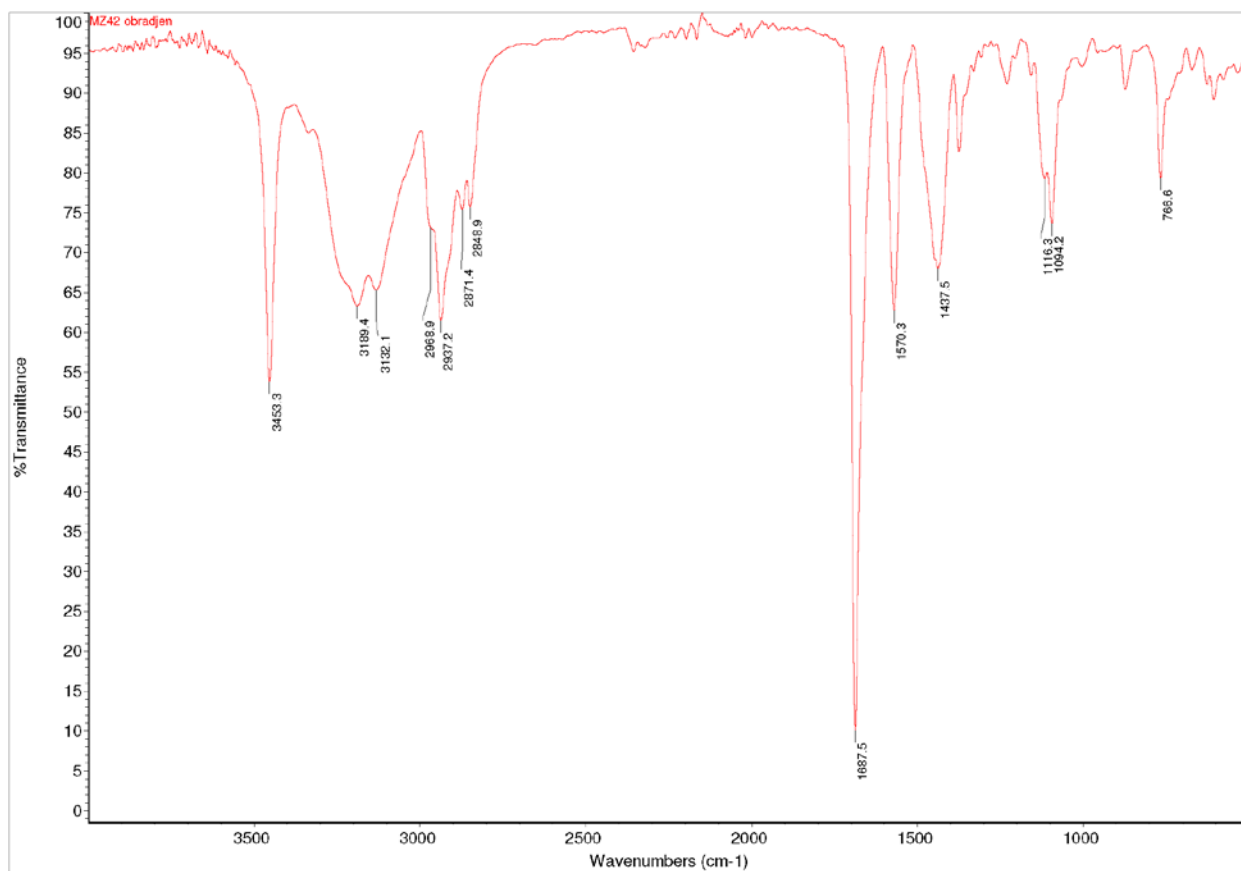
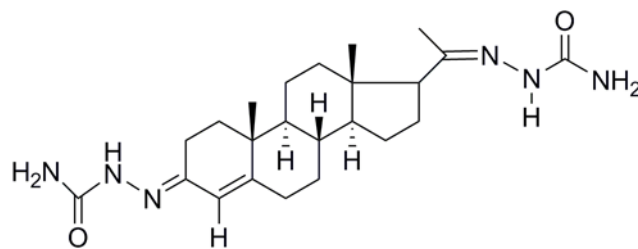
Zumirani spektri

OB5268 #21 RT: 0.30 AV: 1 NL: 6.92E5
 T: FTMS + p ESI Full ms [100.00-800.00]

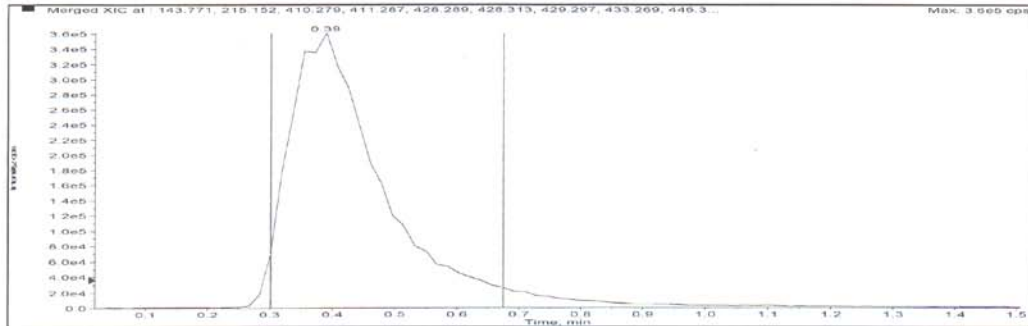


Exact mass	Observed m/z	Error (ppm)
417.2609	417.2626	-4.23

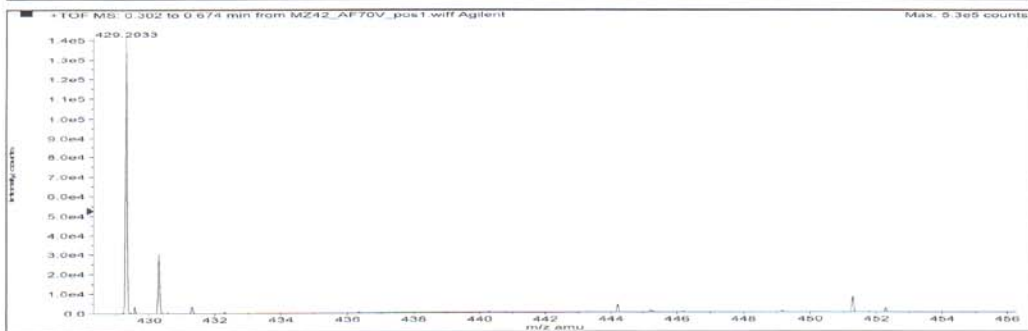
Compound 3e



Sample Name: MZ42 Sample Location: P1-D2 Sample Id: Operator: Milka
 Data File Name: D:\PE Sclex Data\Projects\Sladlc\Data\MZ42_AF70V_pos1.wiff Acq Time: June 27 2016, 10:53:00 AM
 Method: d:\TOF_Data\damethods\Night_Seq_Comp_ident1.anml\efc.xml



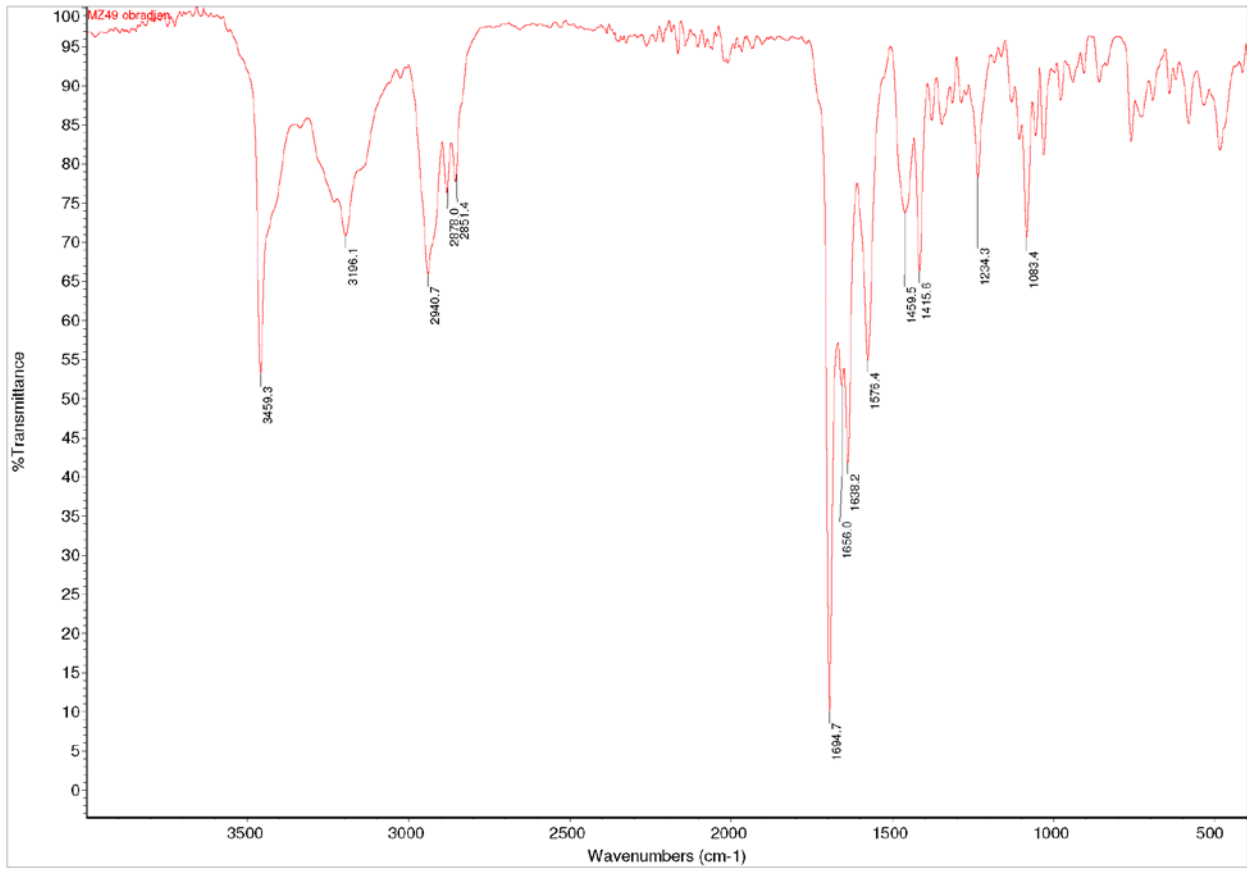
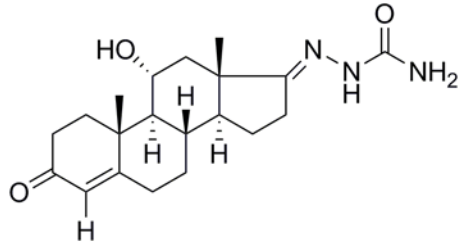
Merged XIC, Period# : 1 Experiment# : 1

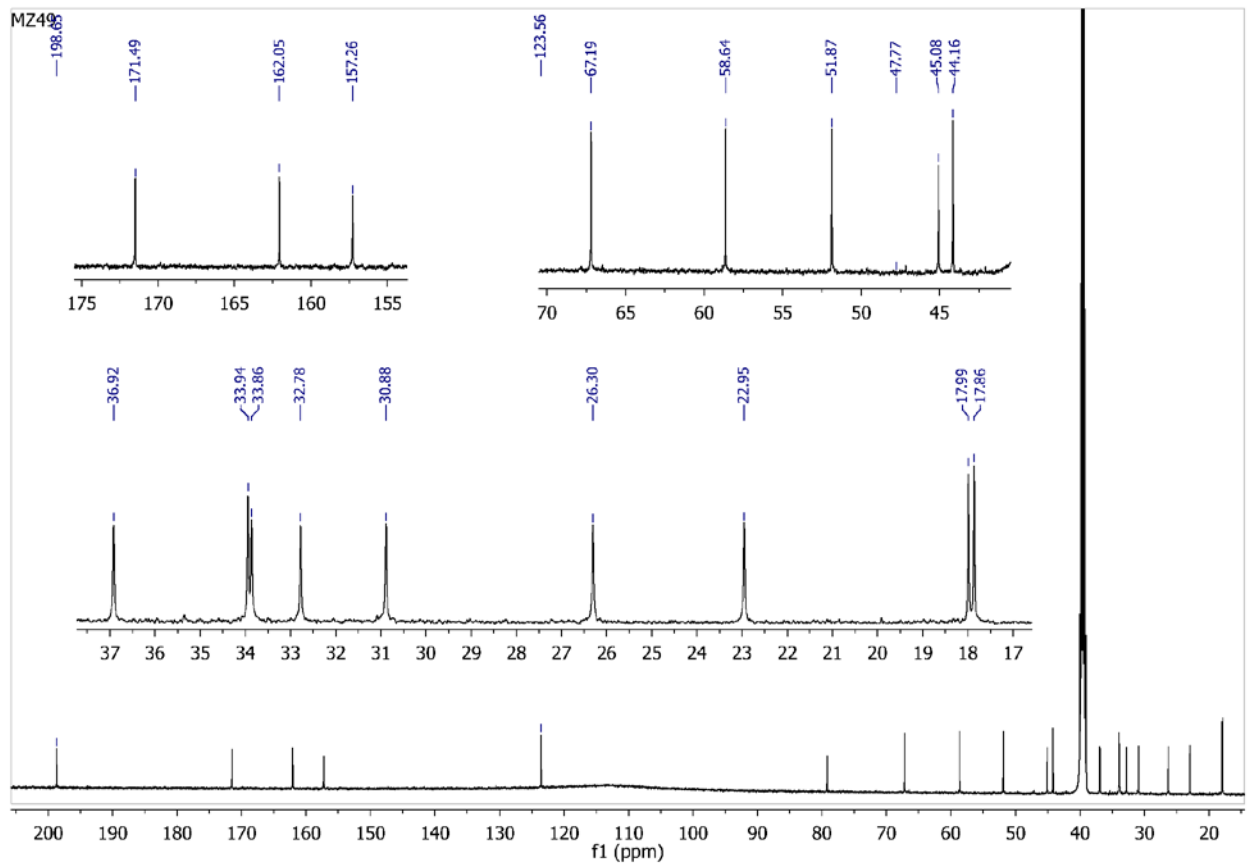
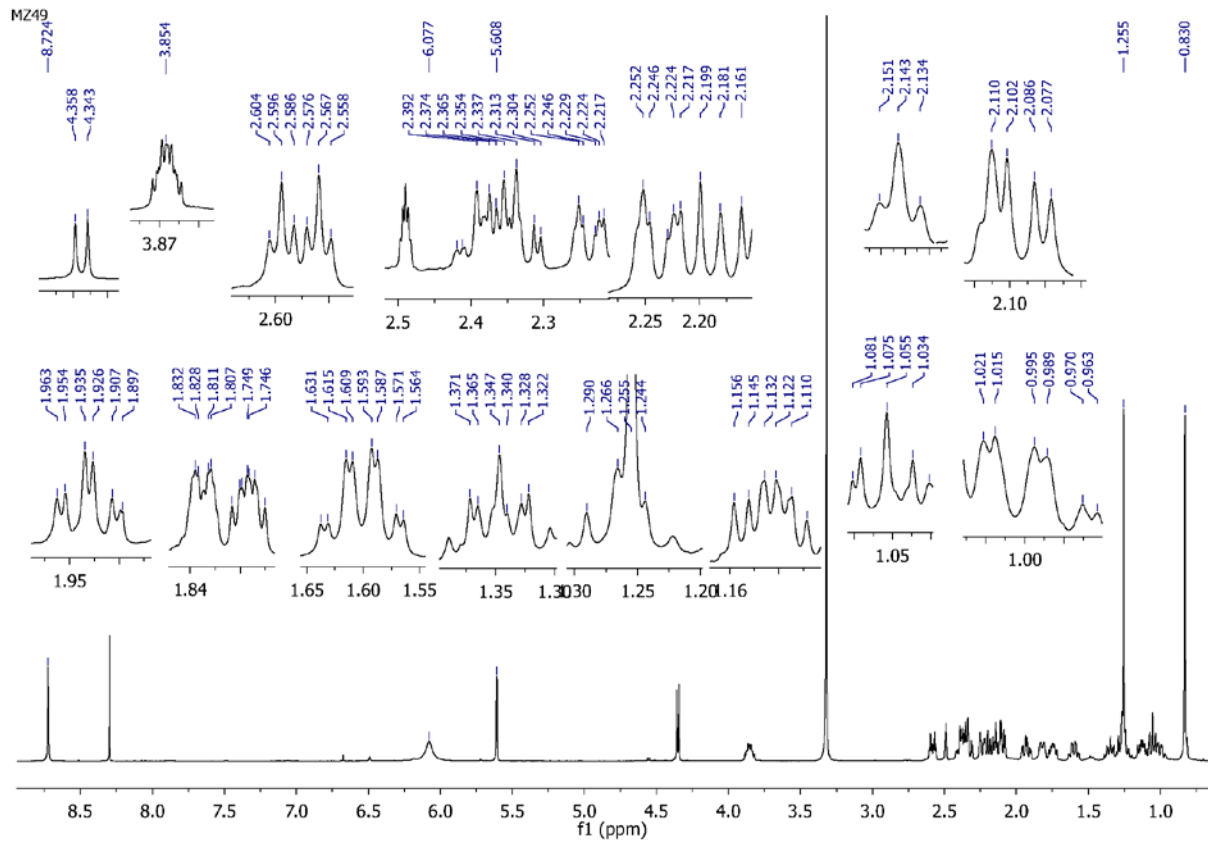


Formula	Compound name	Mass	Peak RT (min)	Peak area	Description
C23H36N6O2	--	428.28997	0.39	3.70878 E6	--

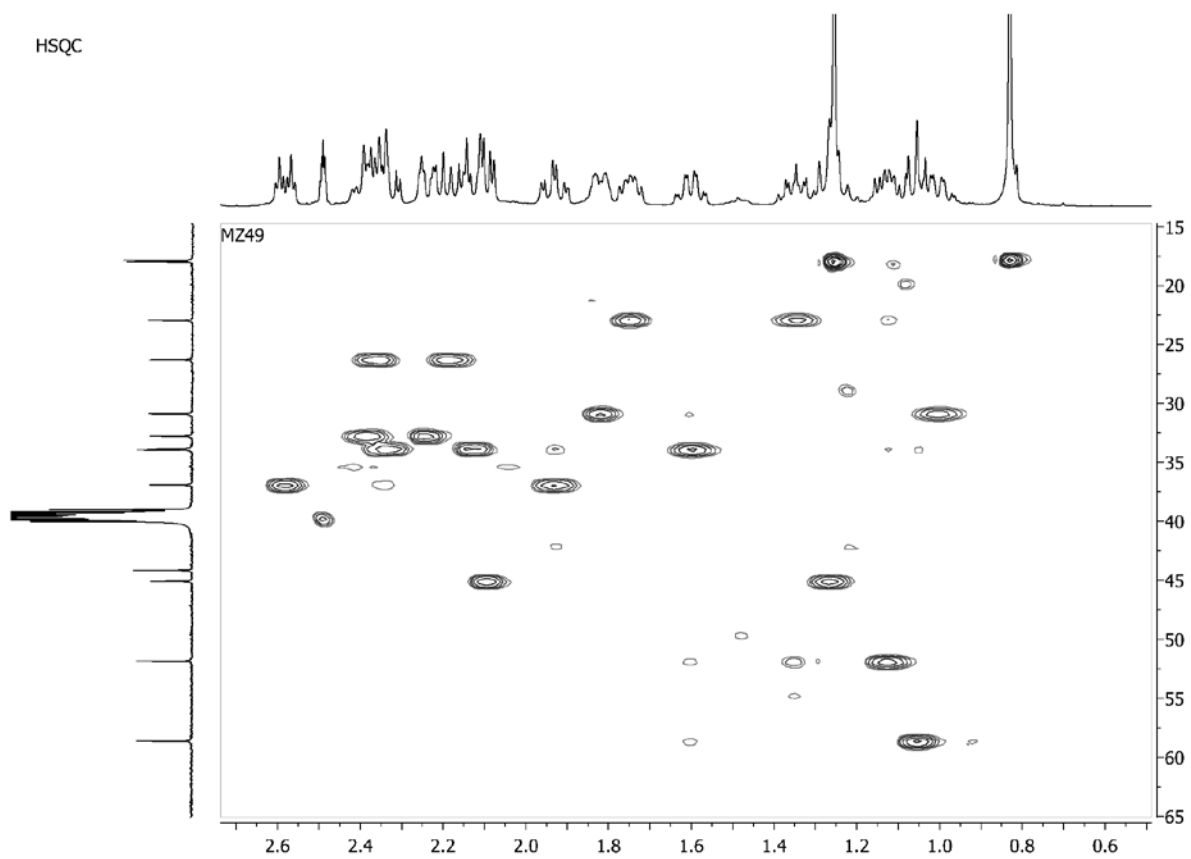
Species	Abundance (counts)	Ion Mass	Measured Mass	Error (mDa)	Error (ppm)	Ret. Time Error (min)
[M+H] ⁺	141809.19	429.29725	429.29678	-0.47110	-1.10	--
[M+Na] ⁺	7978.55	451.27920	451.27953	0.32977	0.73	--

Compound 4d

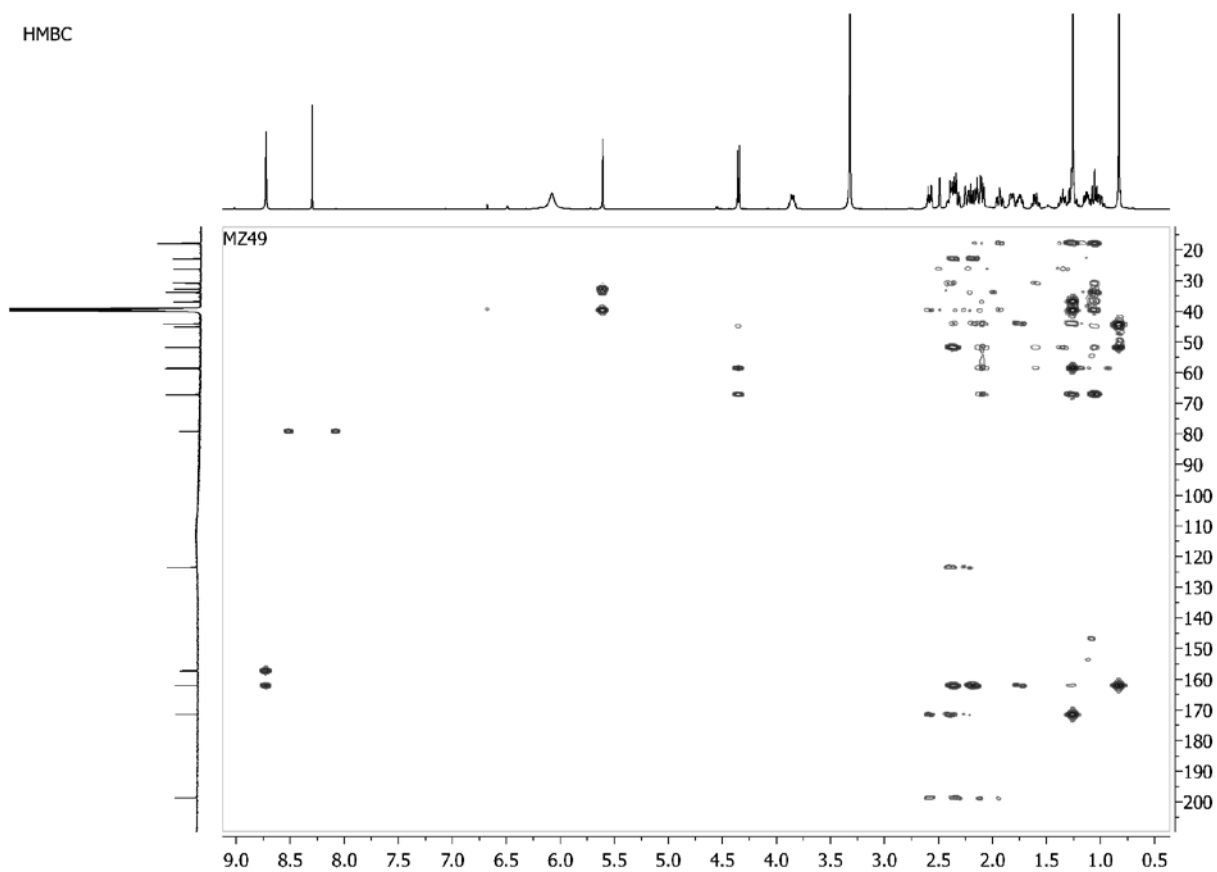




HSQC

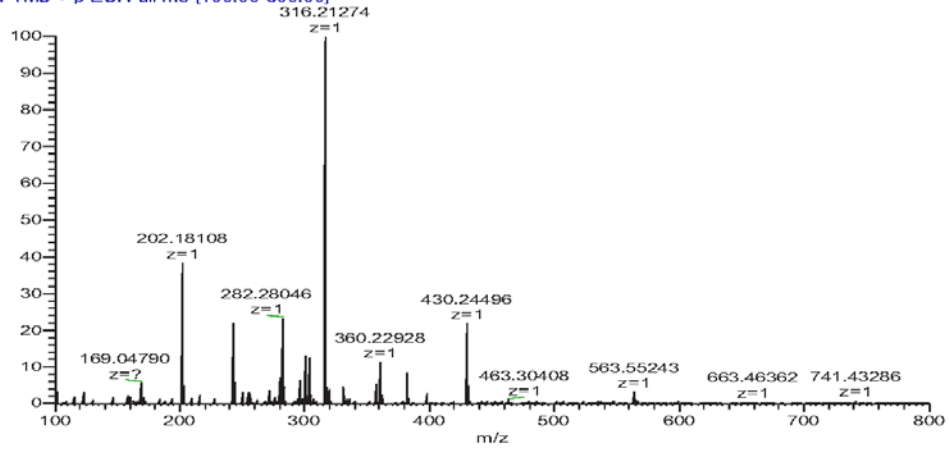


HMBC



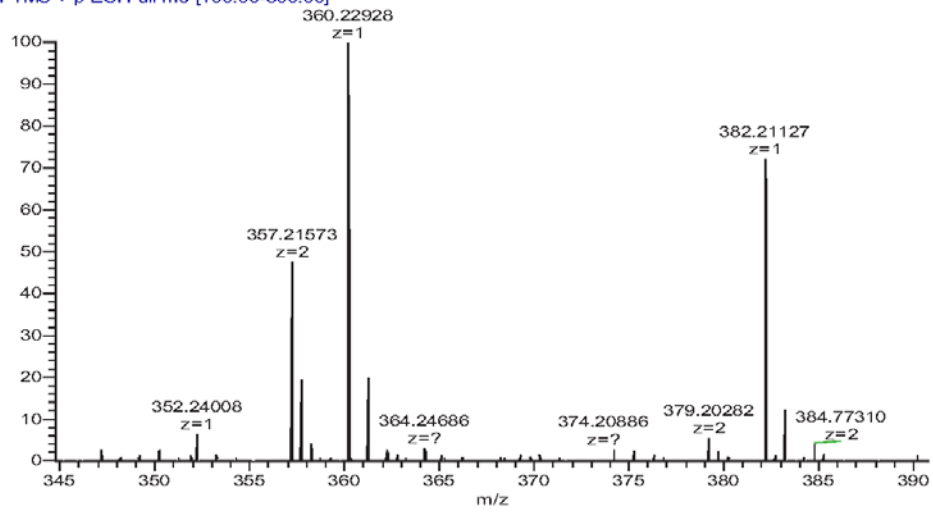
OBS267 MZ49

OBS267 #16 RT: 0.31 AV: 1 NL: 1.80E6
 T: FTMS + p ESI Full ms [100.00-800.00]



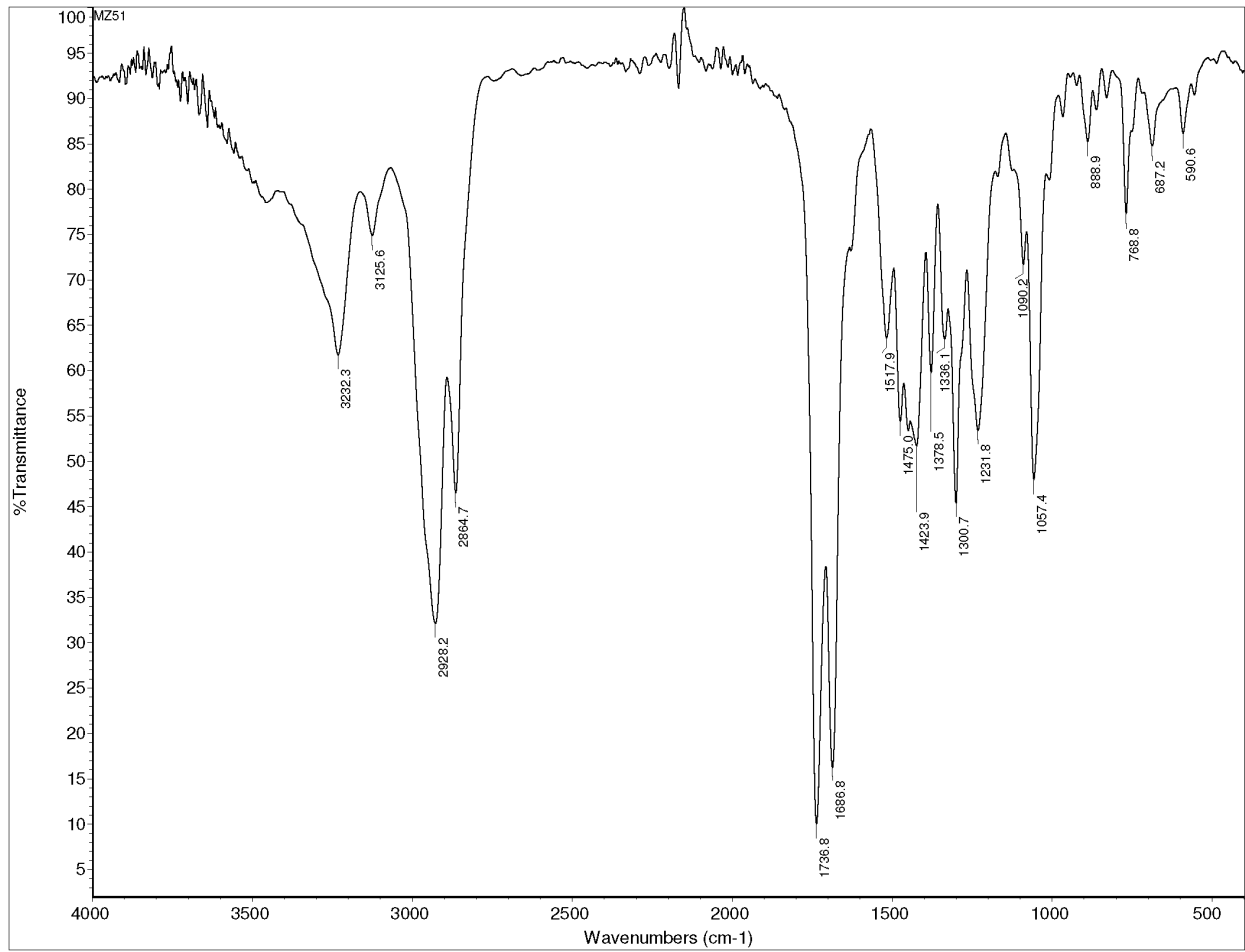
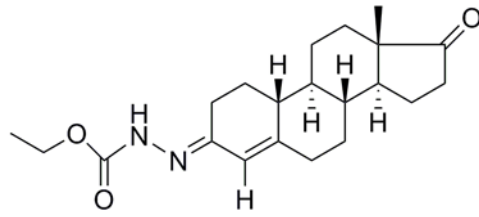
Zumirani spektri

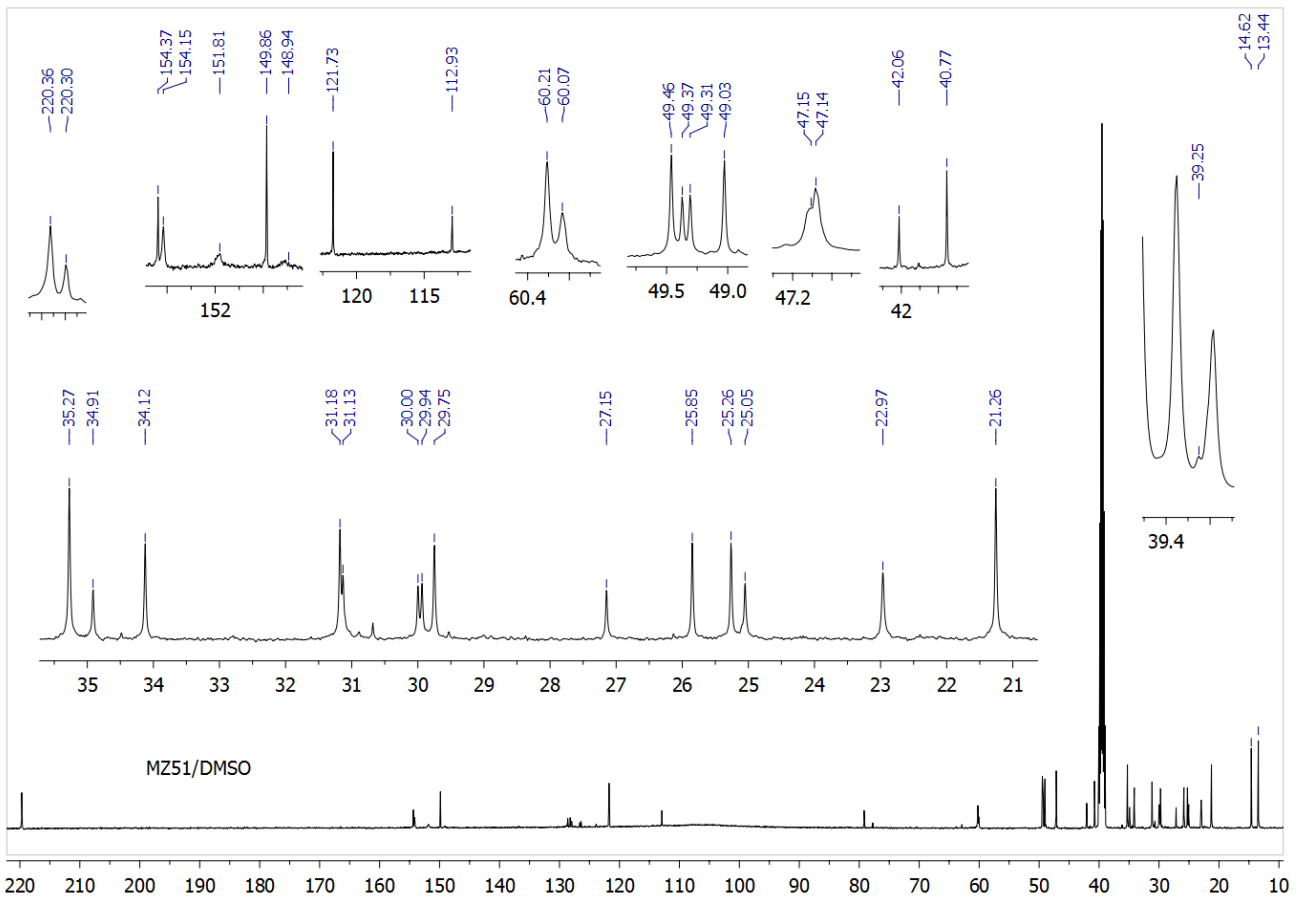
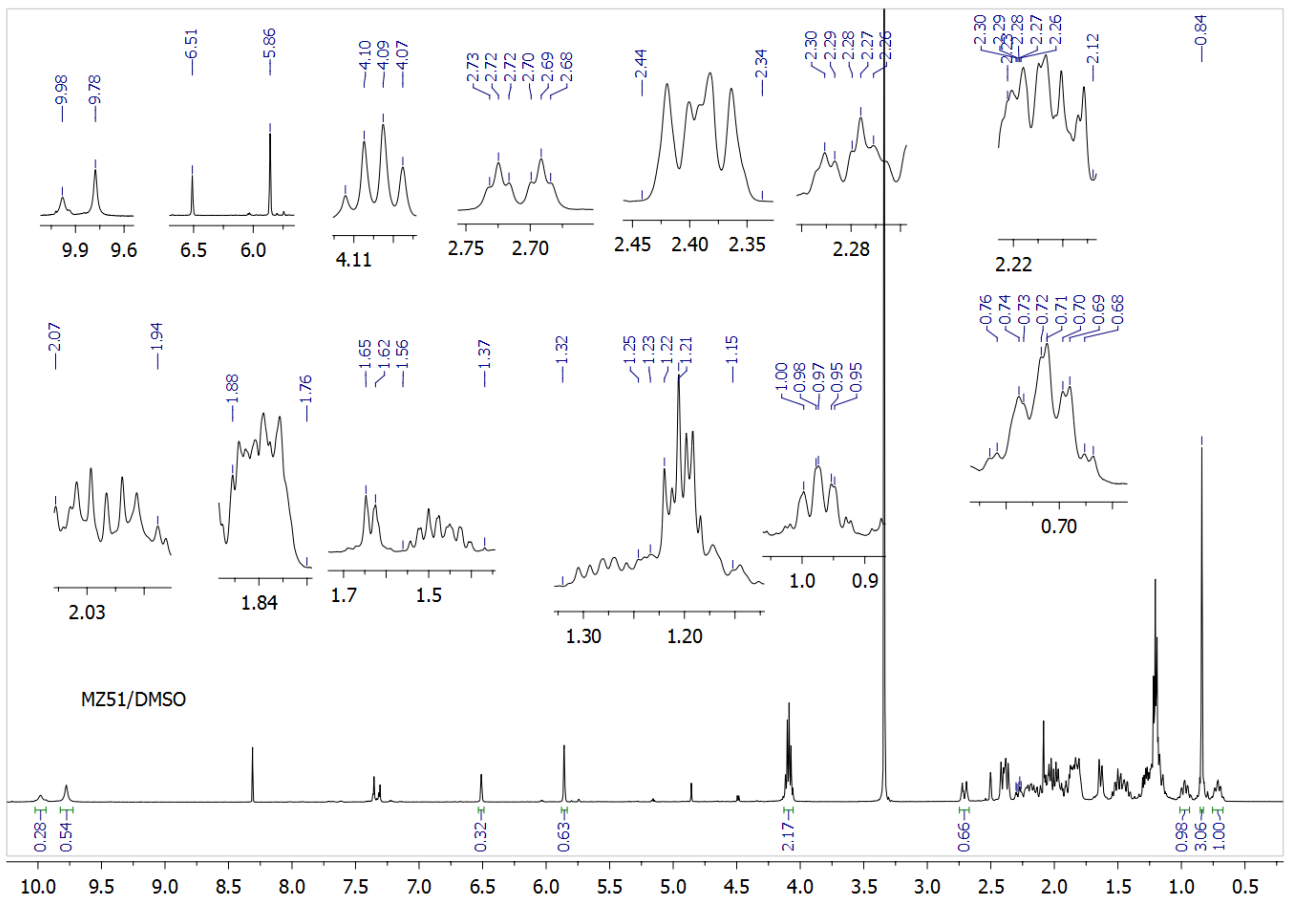
OBS267 #16 RT: 0.31 AV: 1 NL: 2.02E5
 T: FTMS + p ESI Full ms [100.00-800.00]

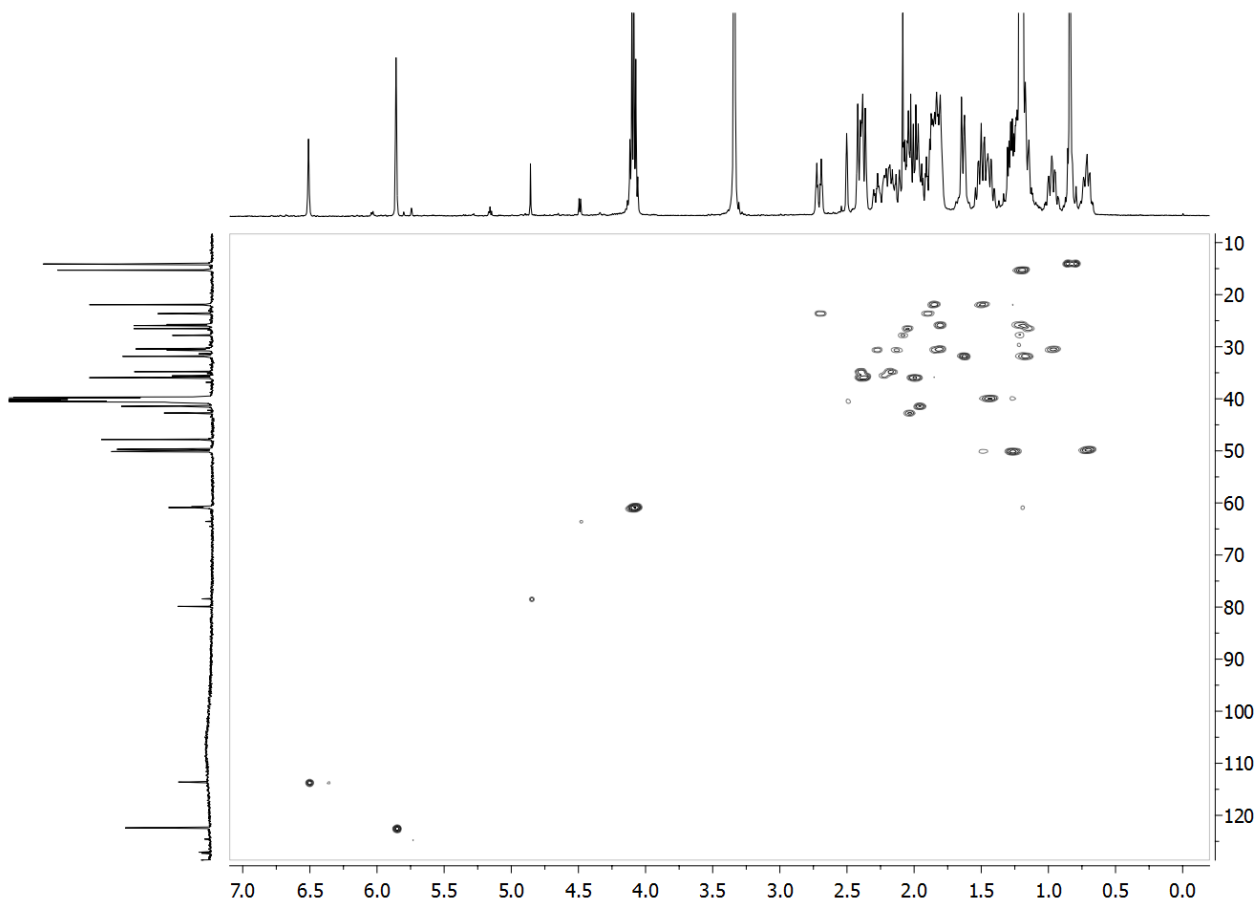


Exact mass	Observed m/z	Error (ppm)
360.2282	360.2293	-3.09

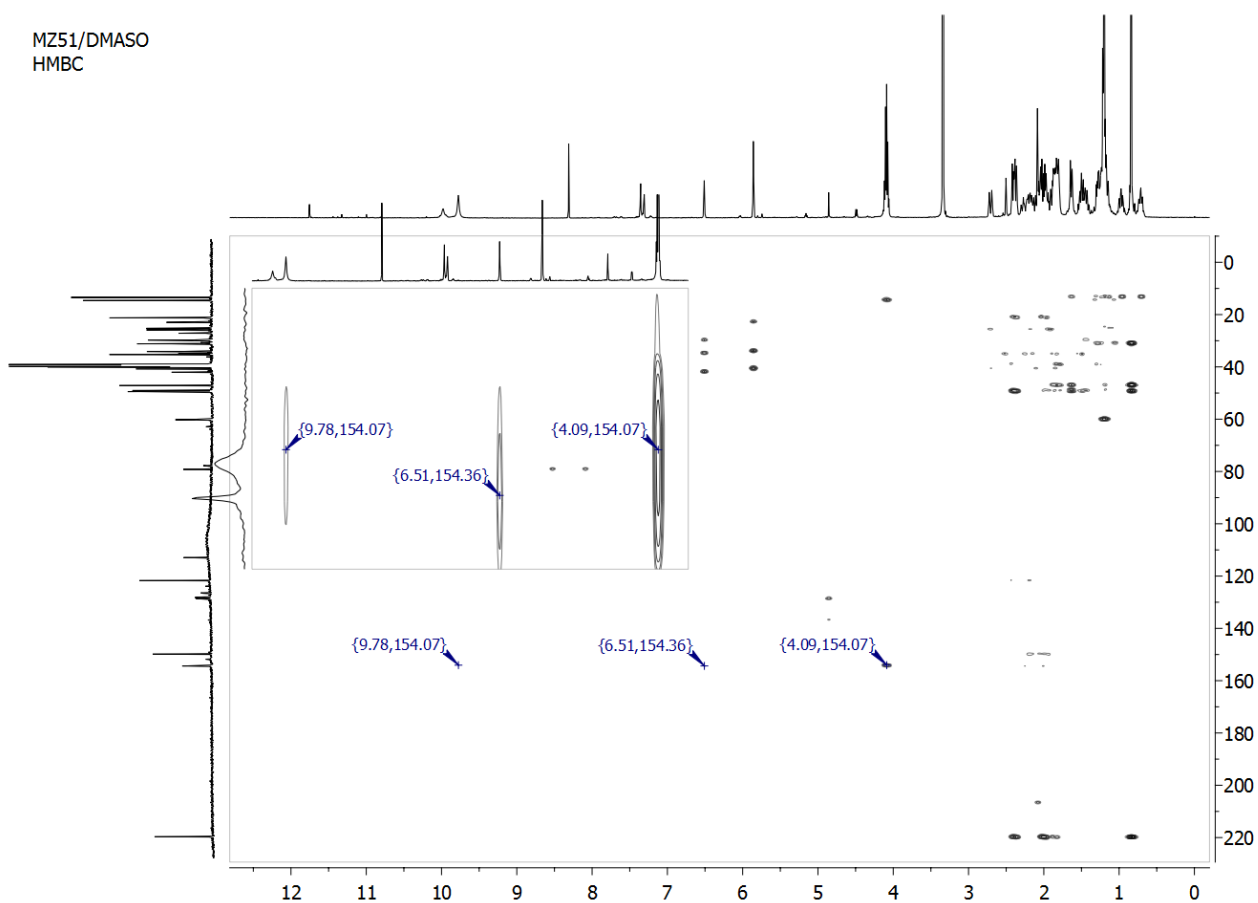
Compound 5a



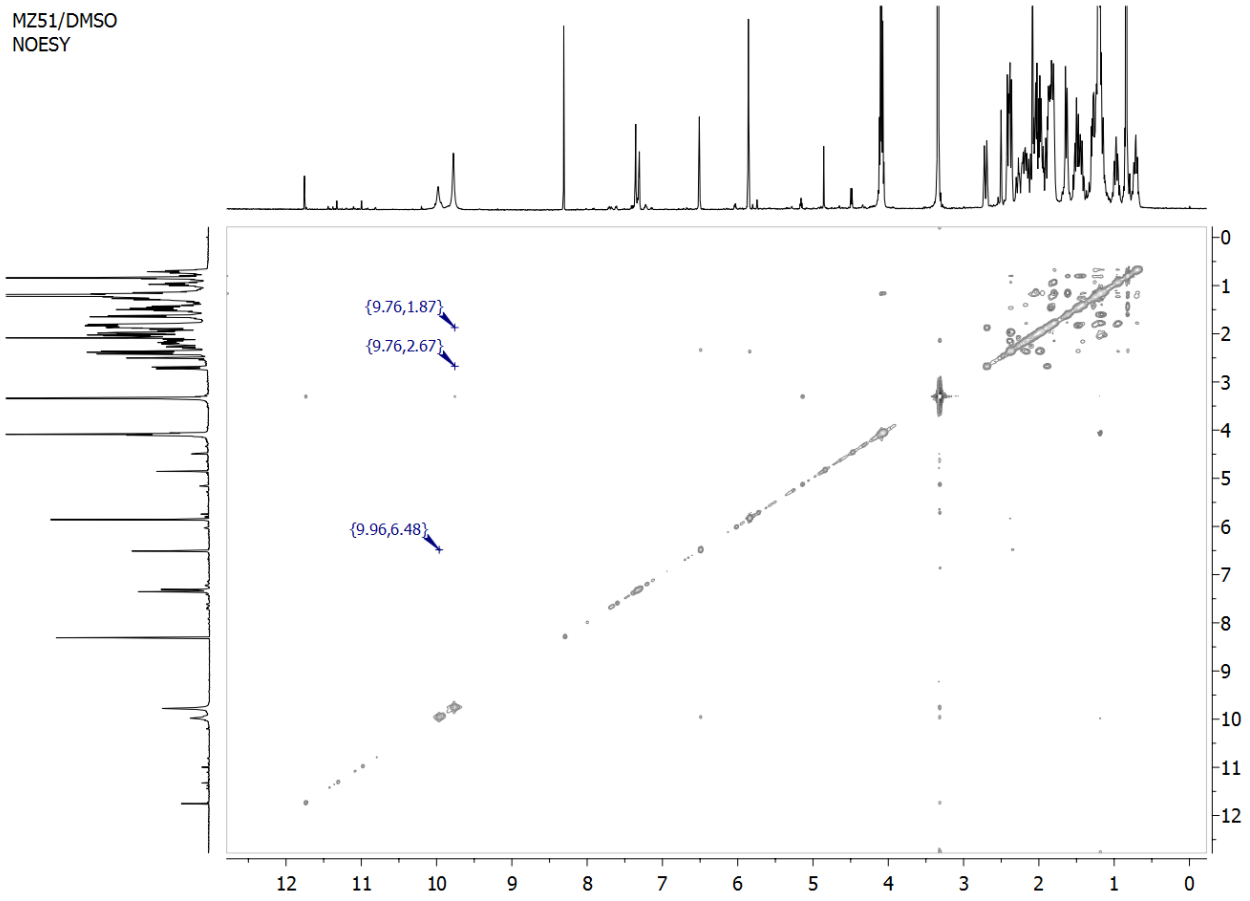




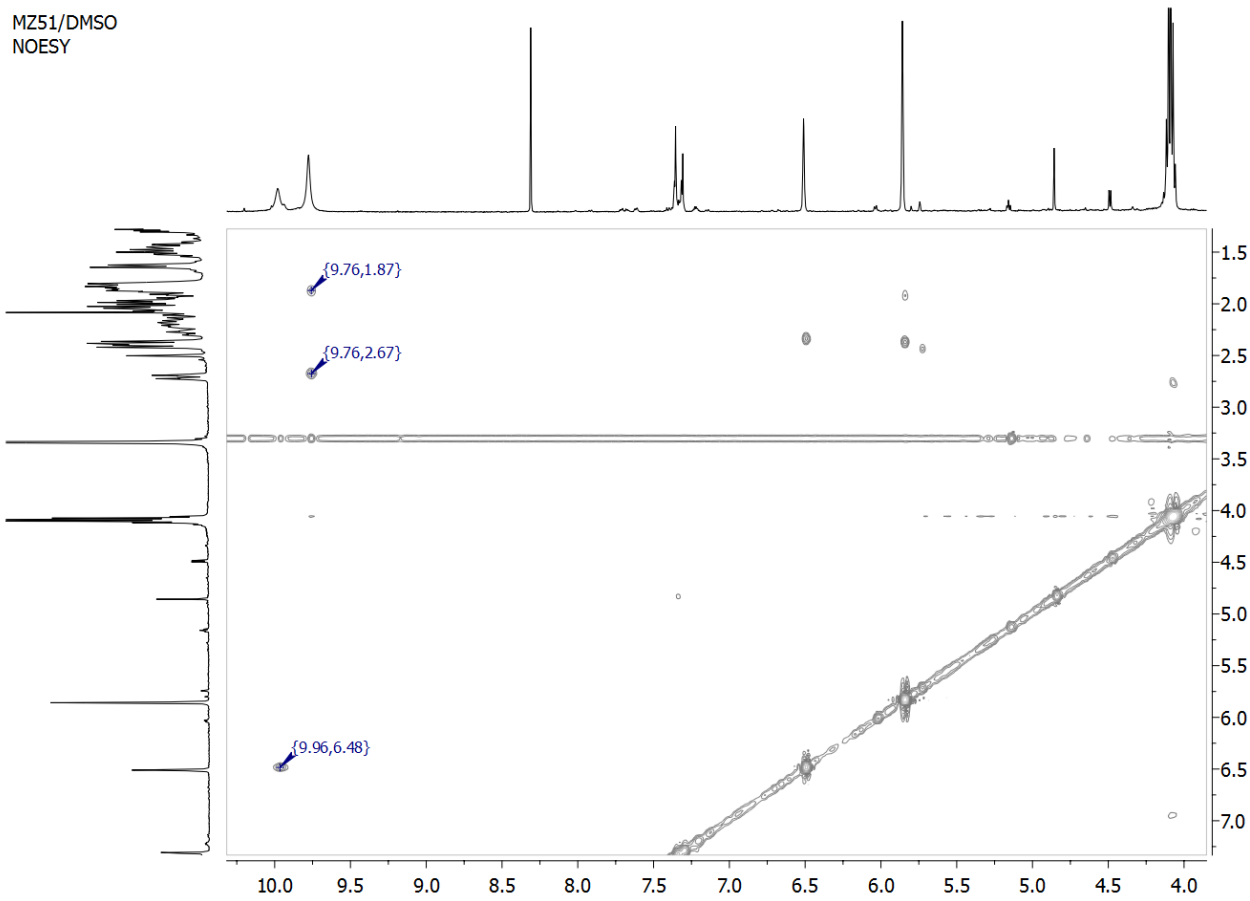
MZ51/DMSO
HMBC



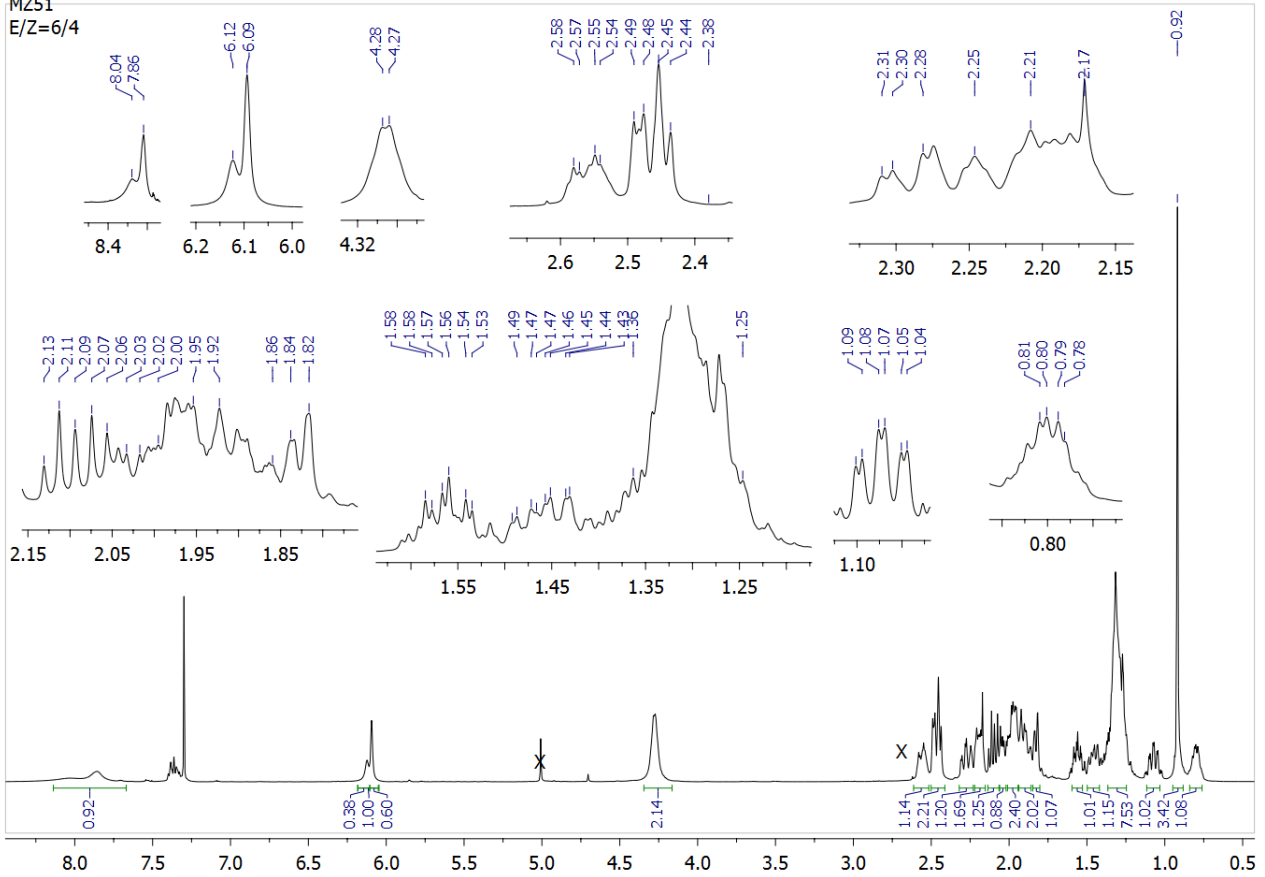
MZ51/DMSO
NOESY



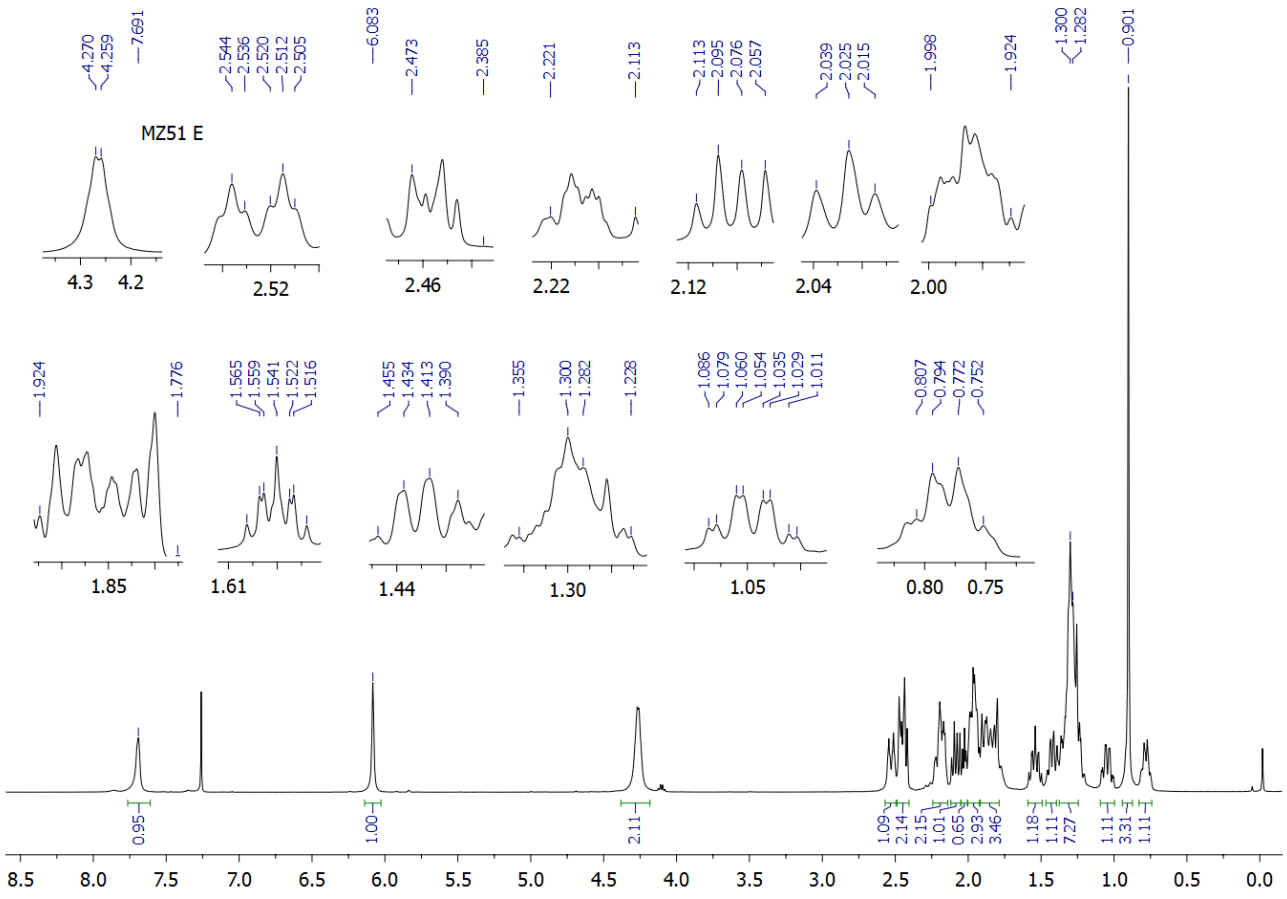
MZ51/DMSO
NOESY

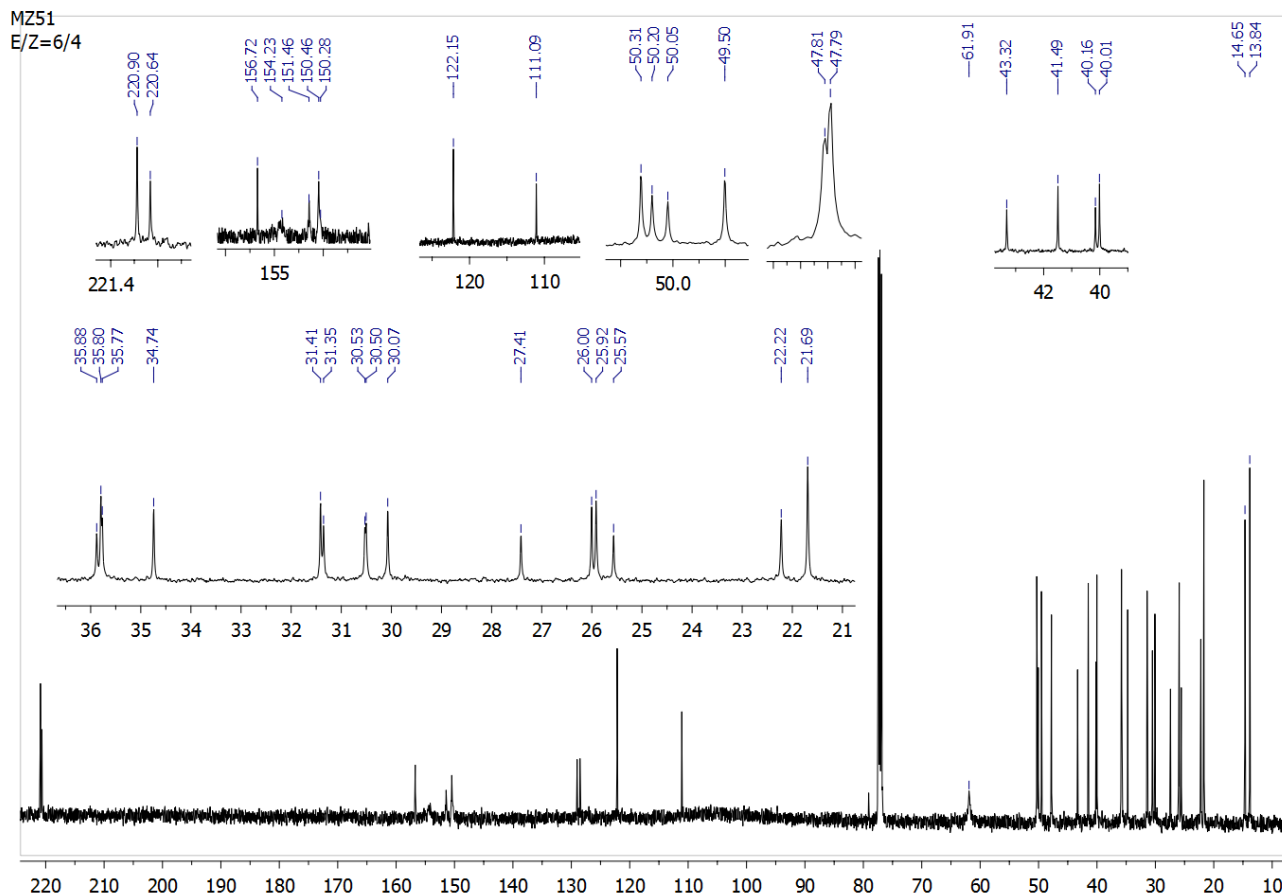
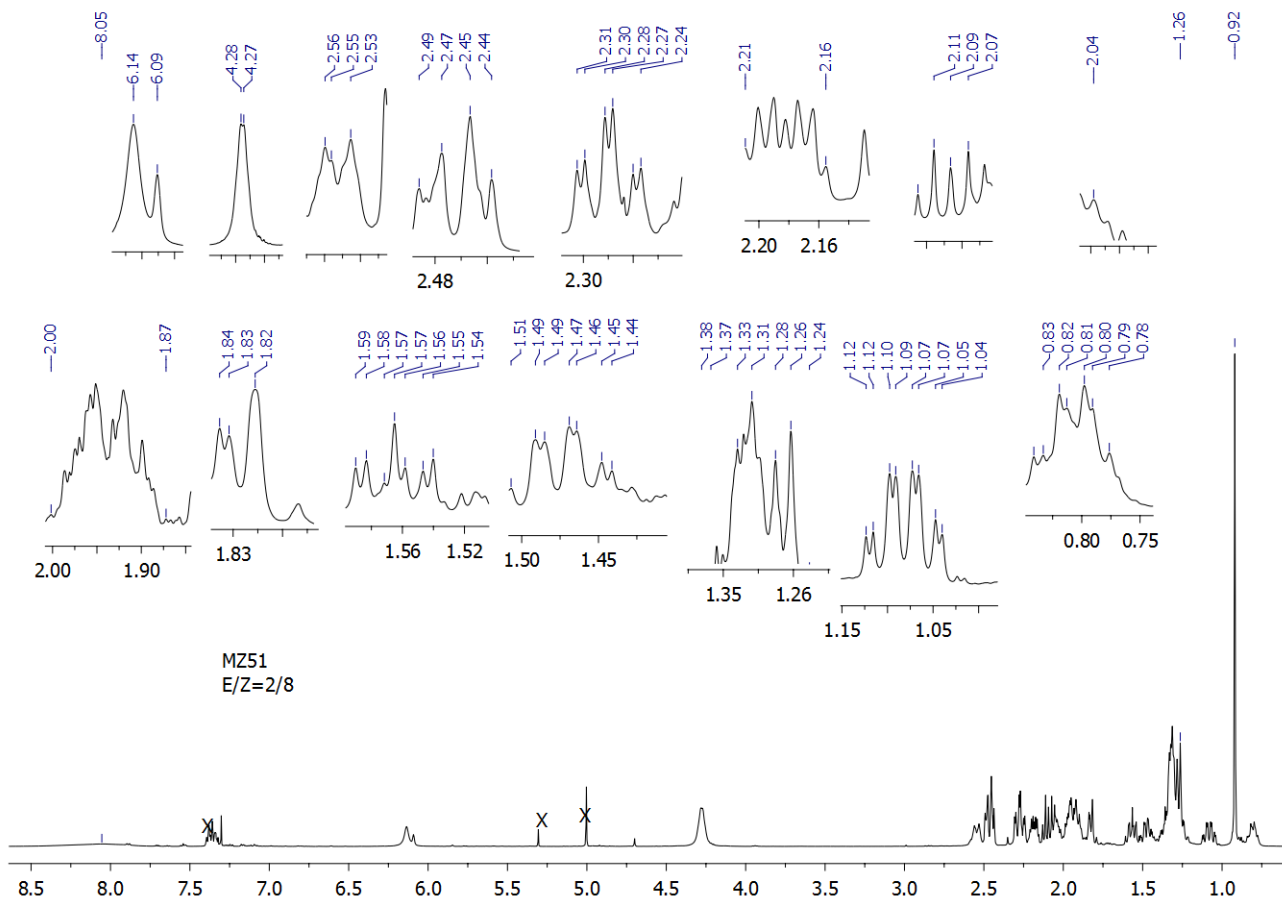


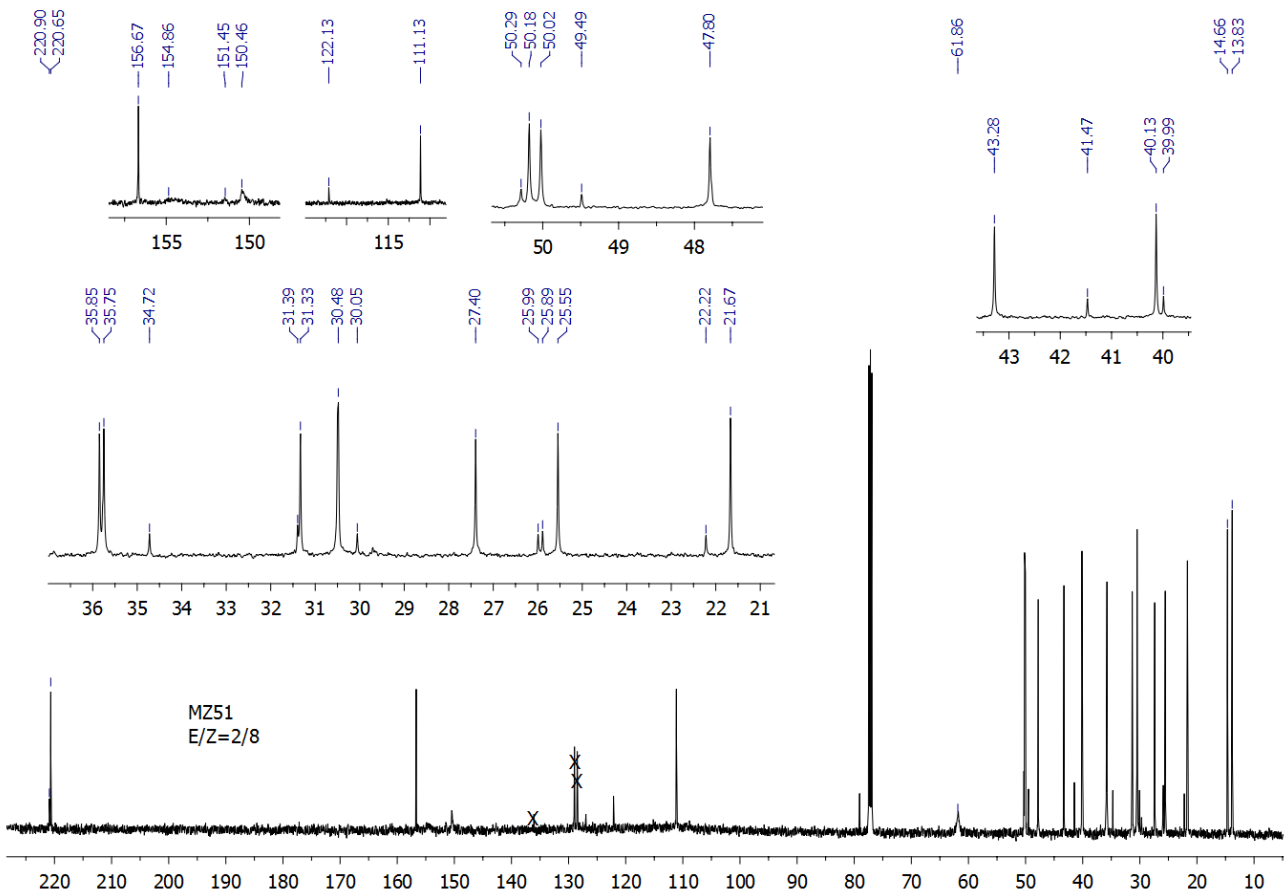
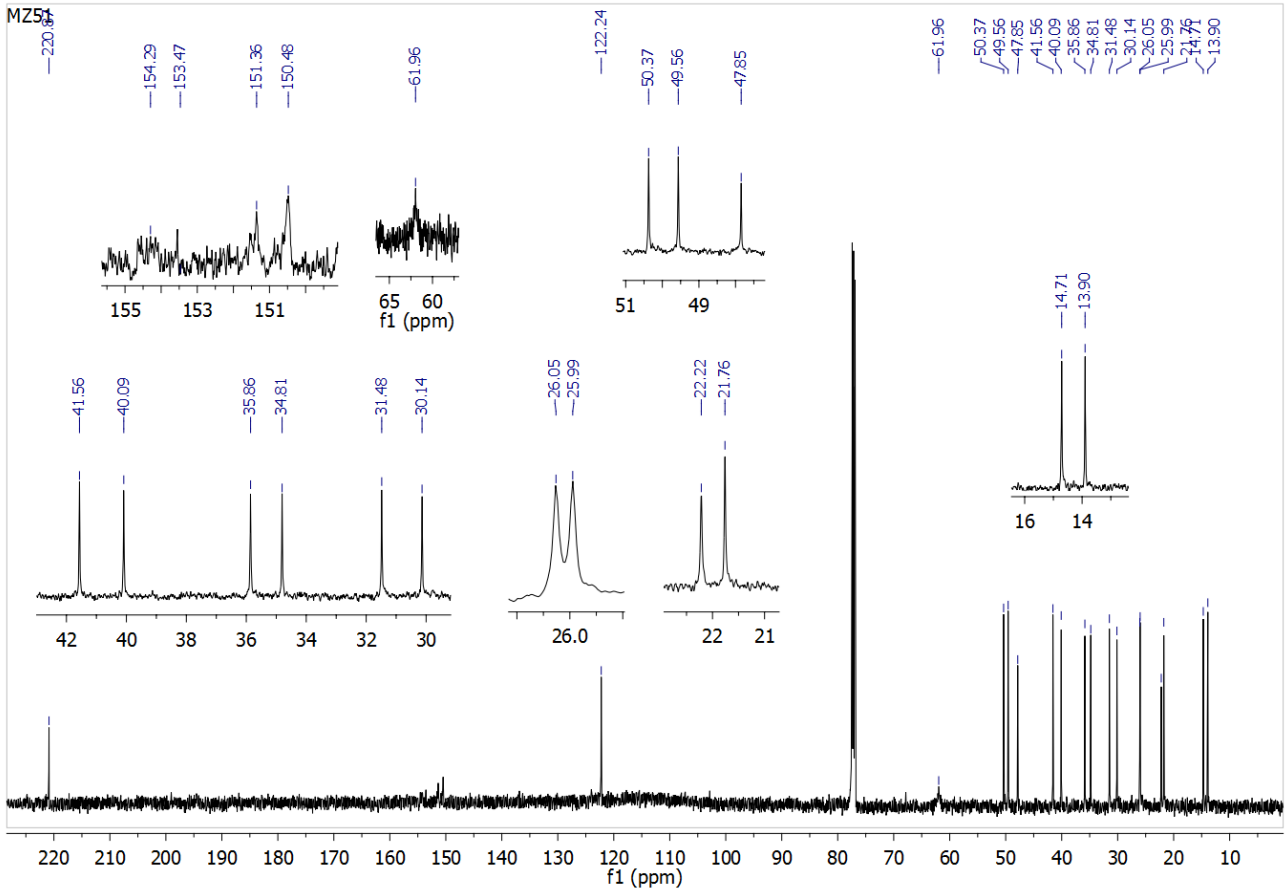
MZ51
E/Z=6/4



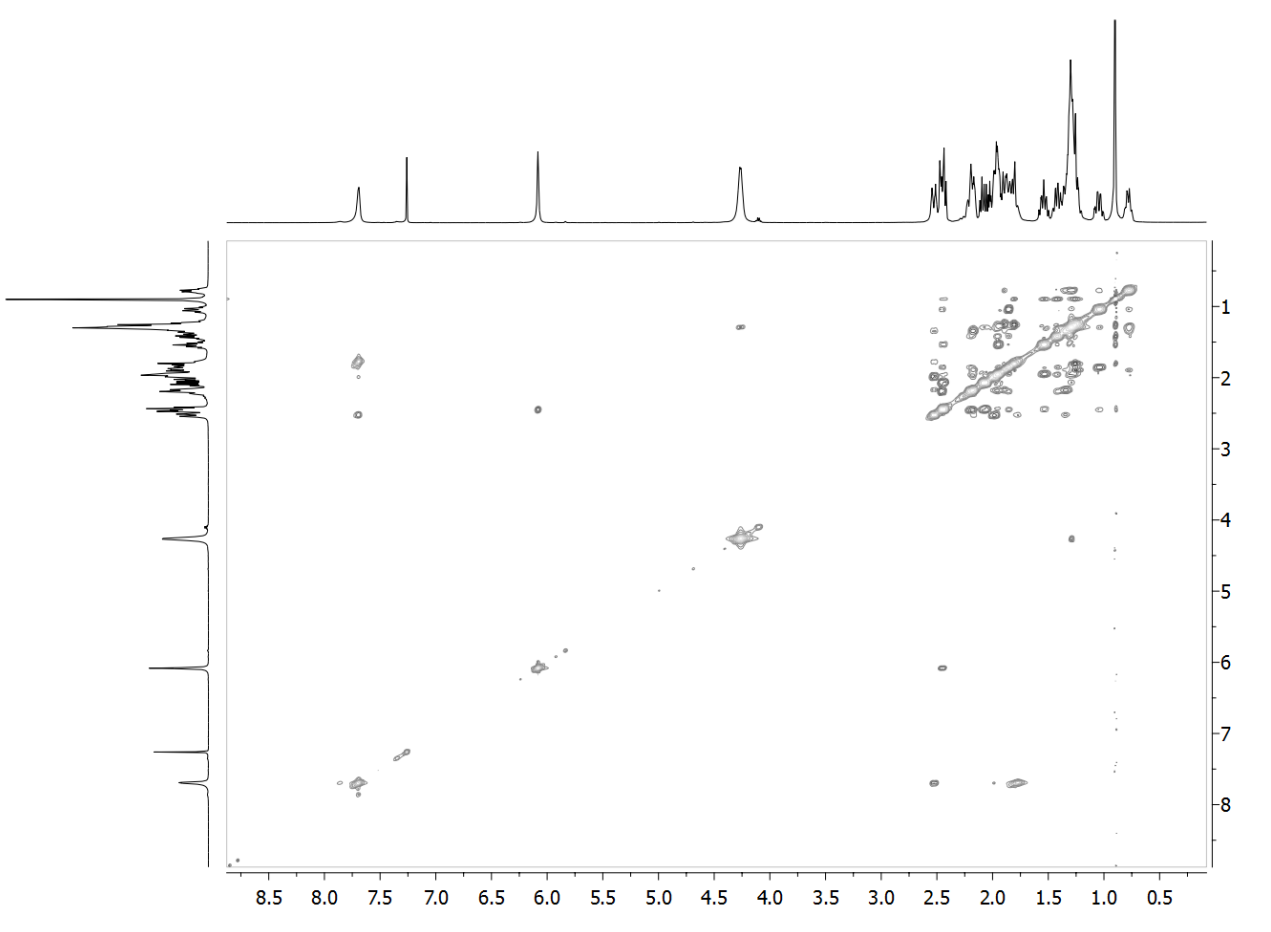
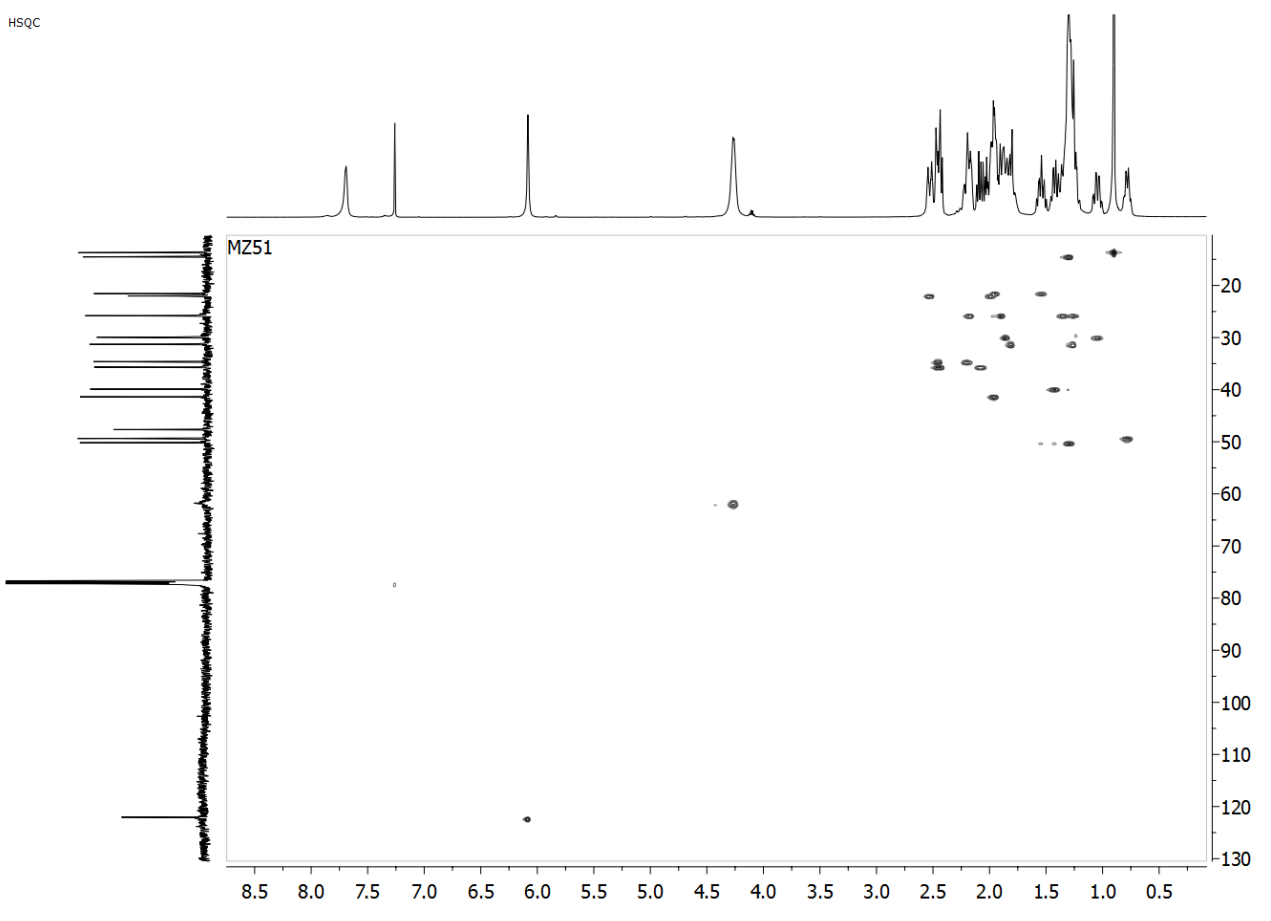
MZ51 E



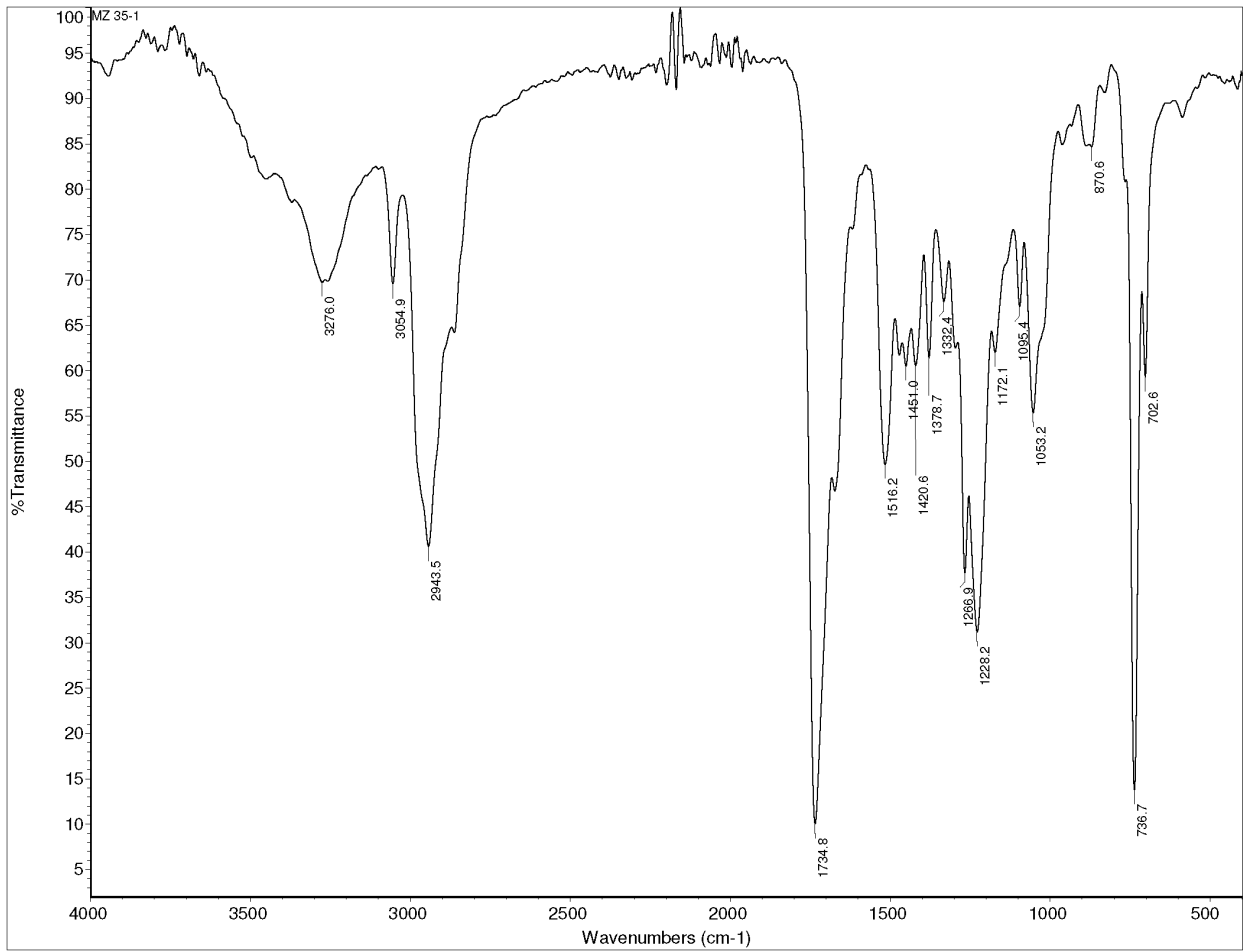
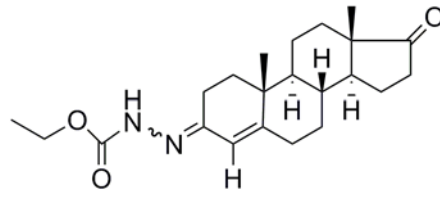


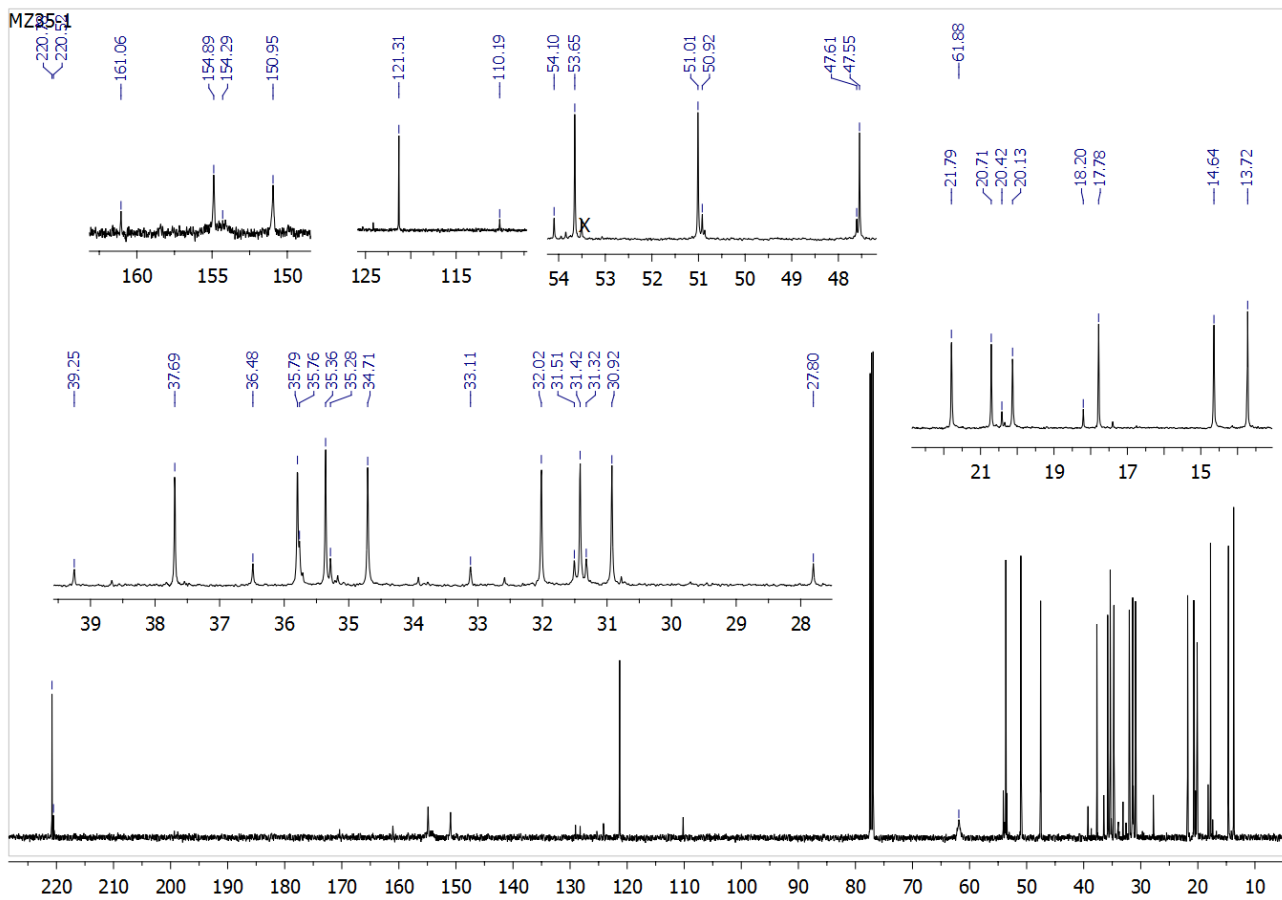
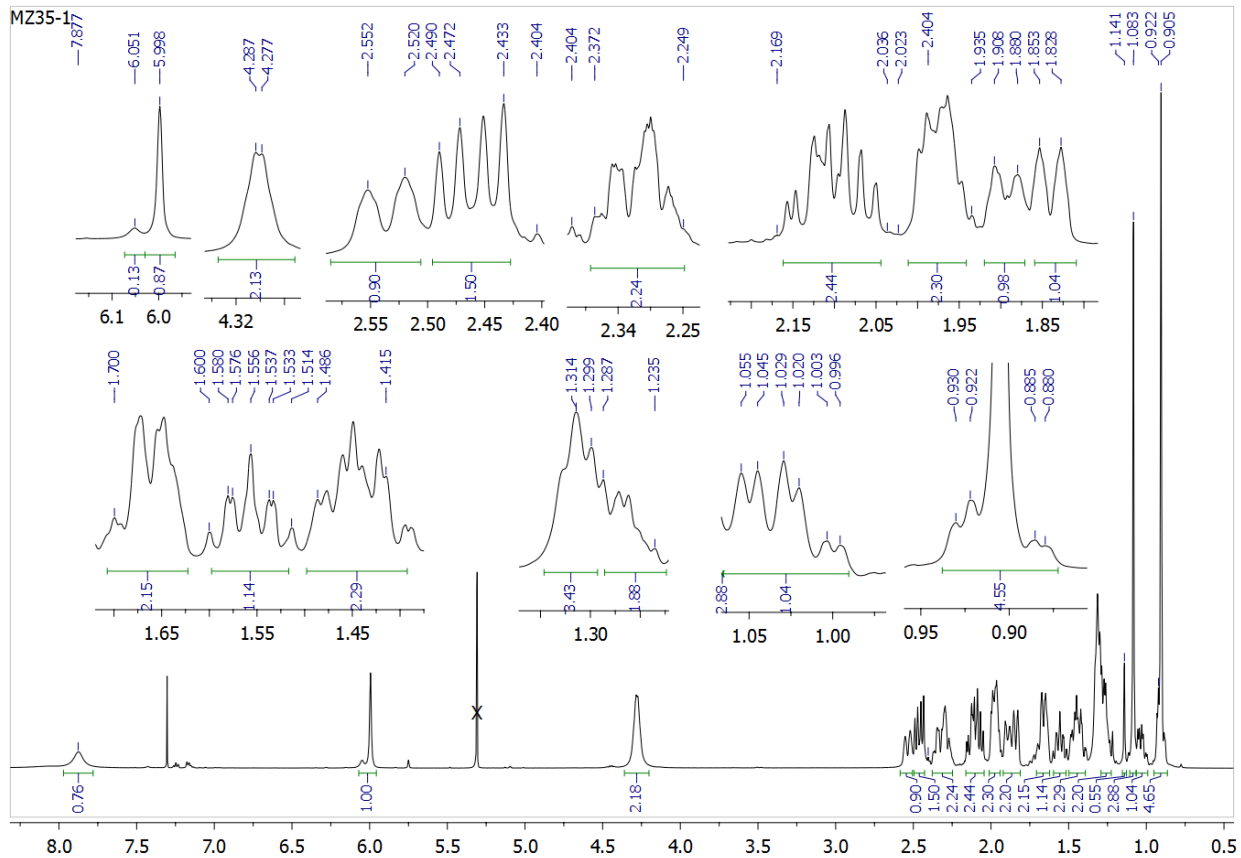


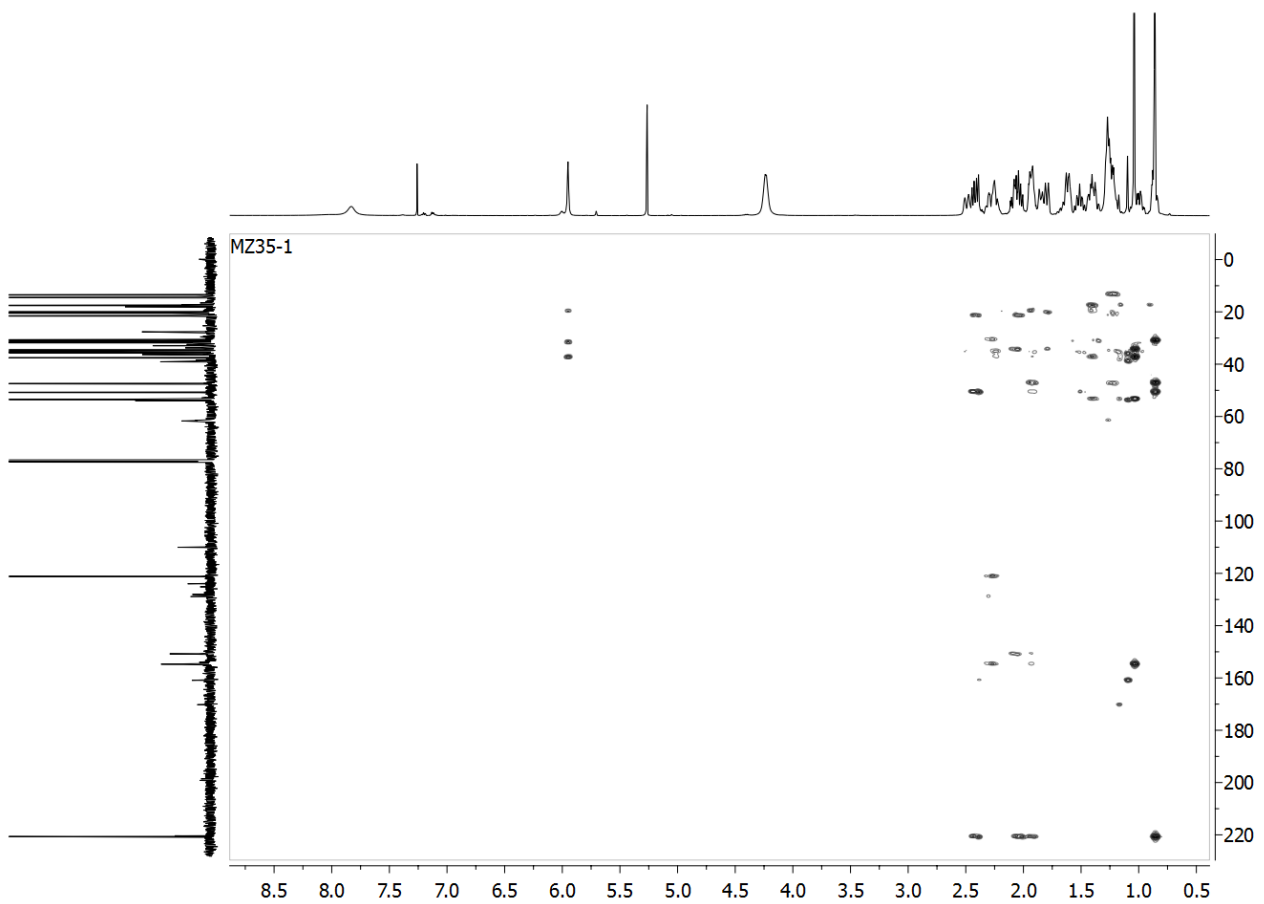
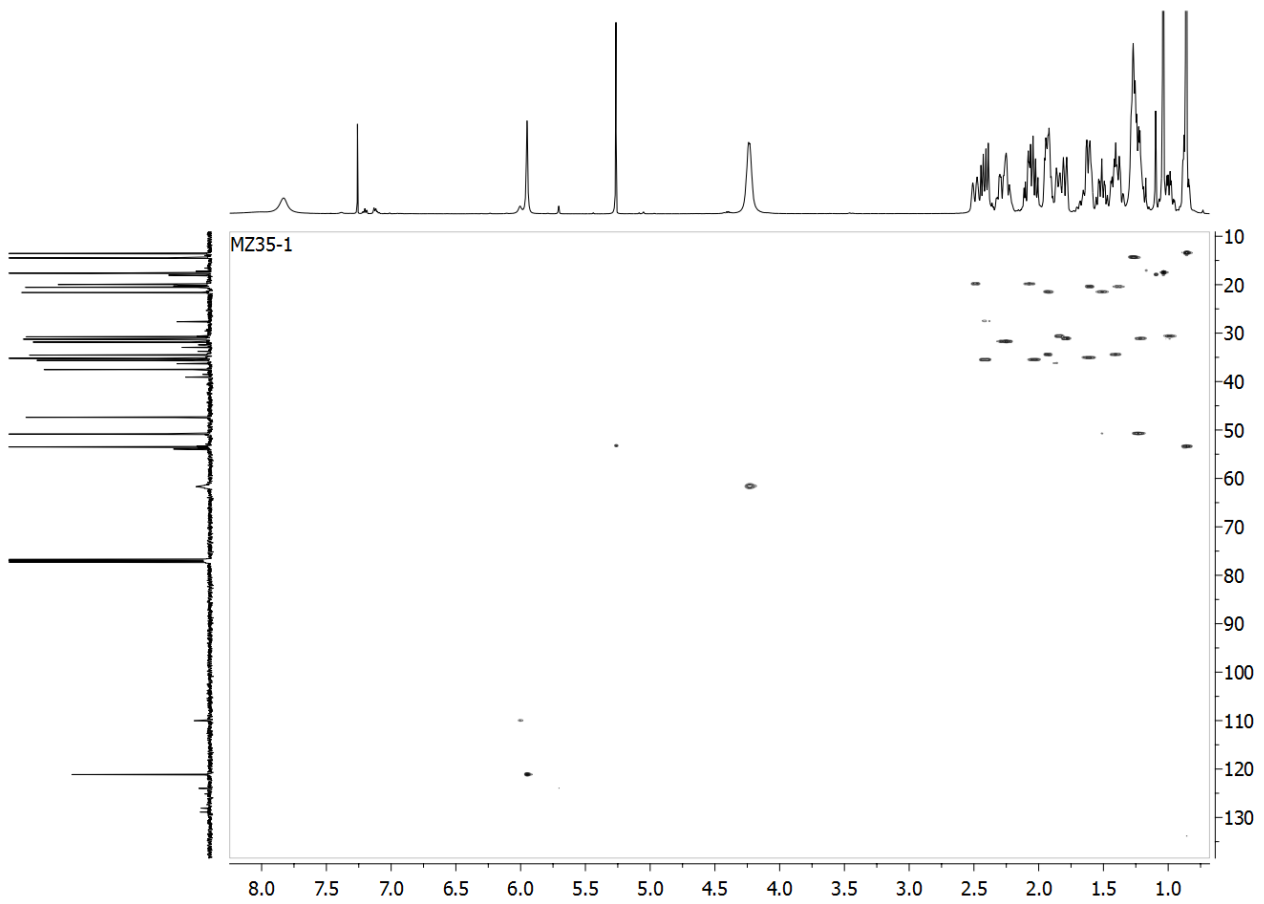
HSQC



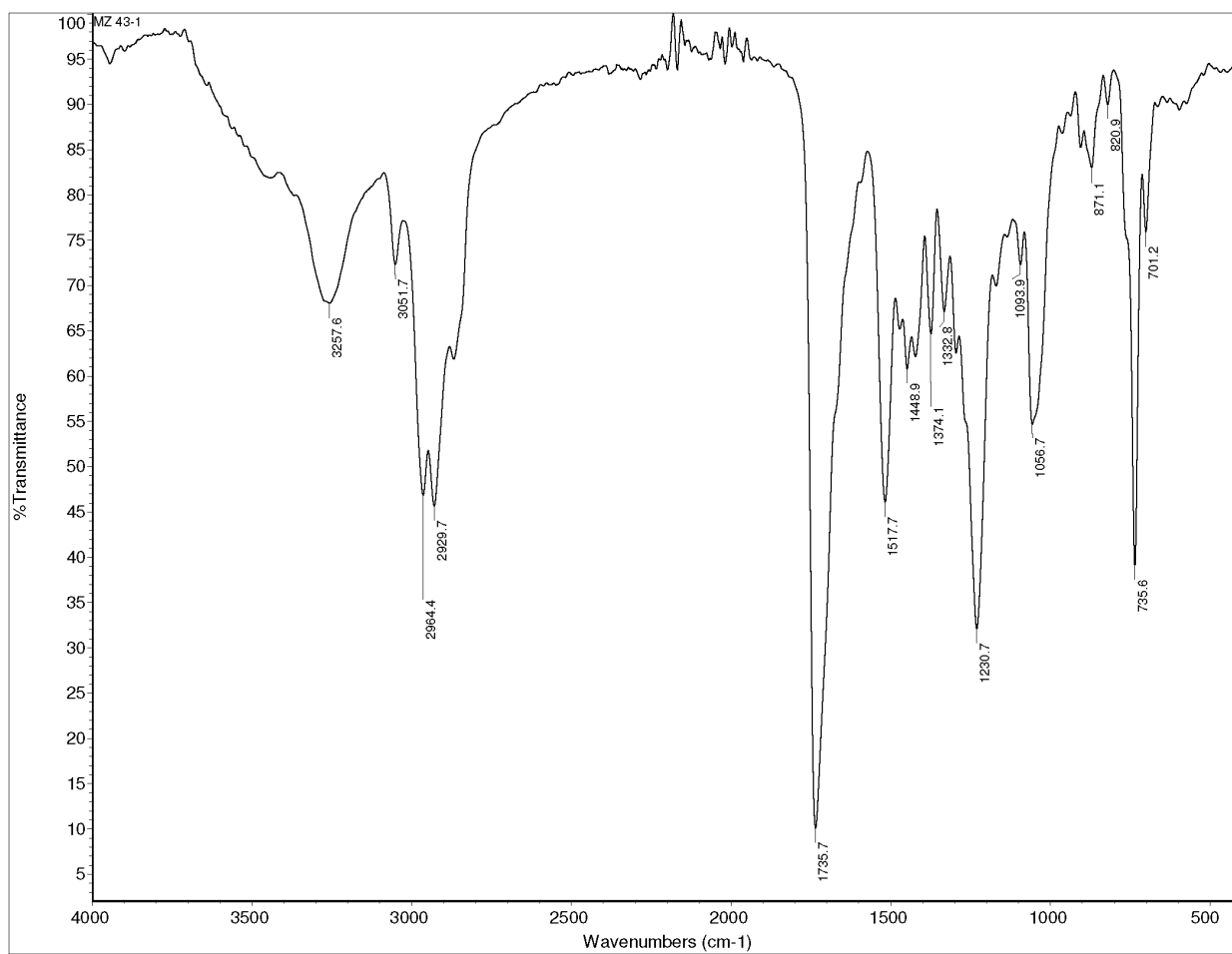
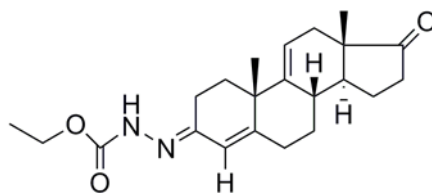
Compound 5b

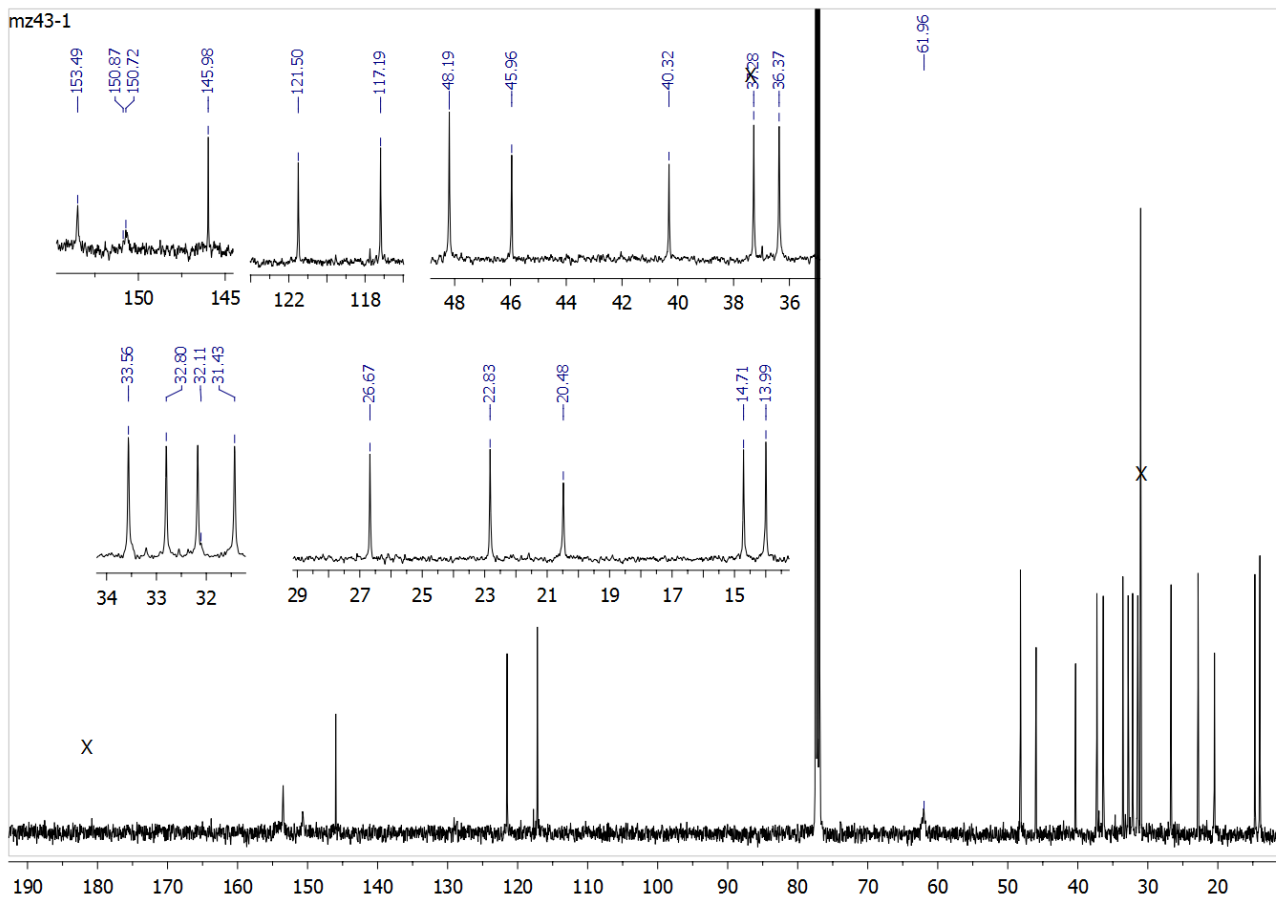
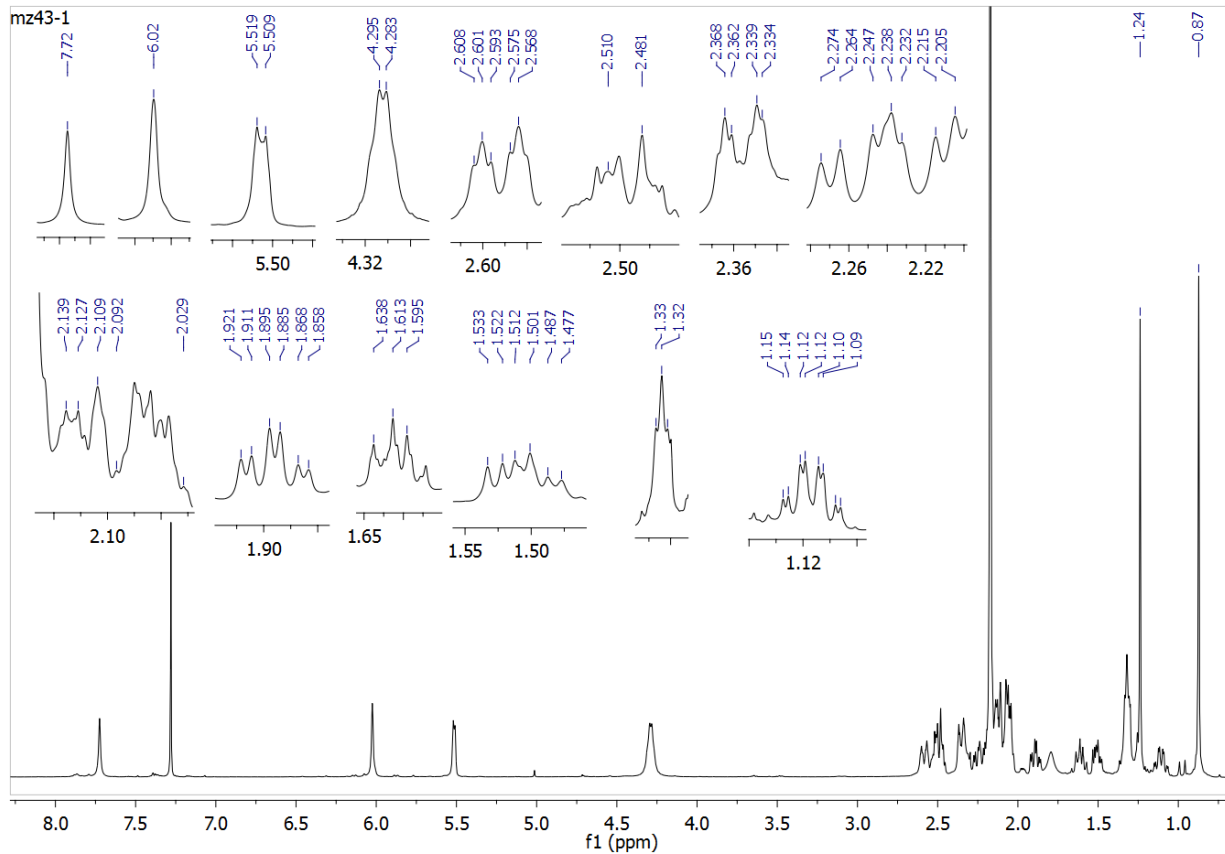




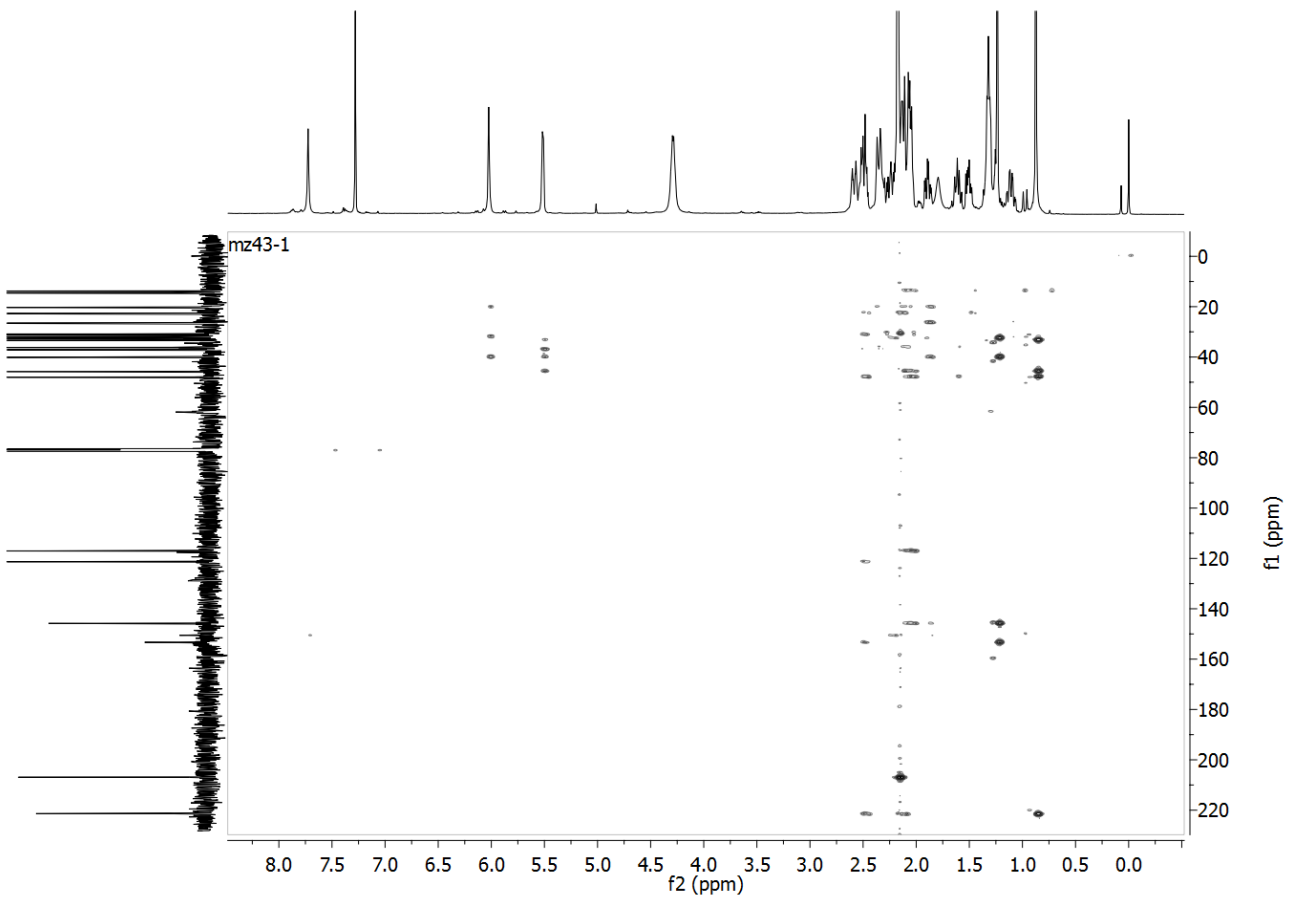
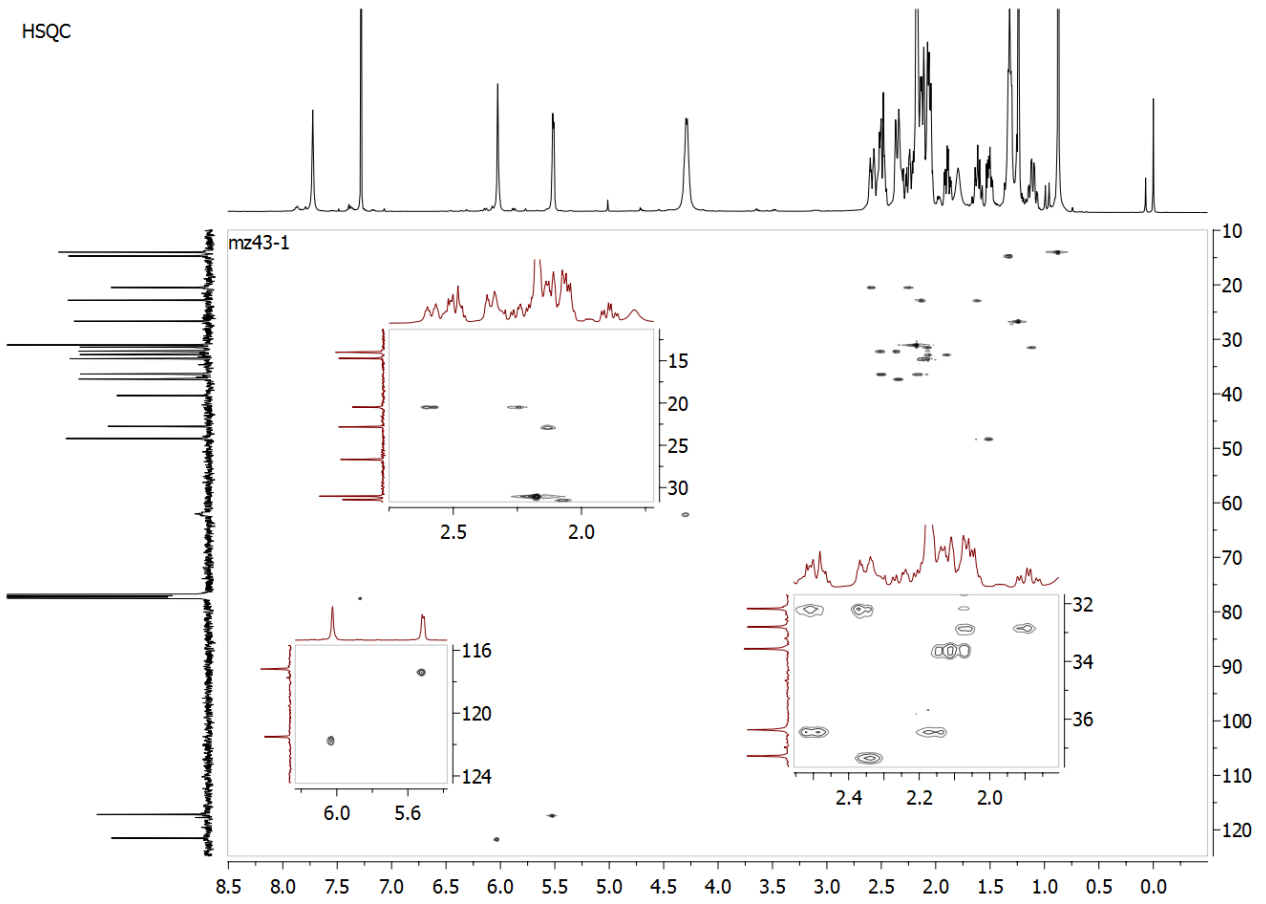


Compound 5c

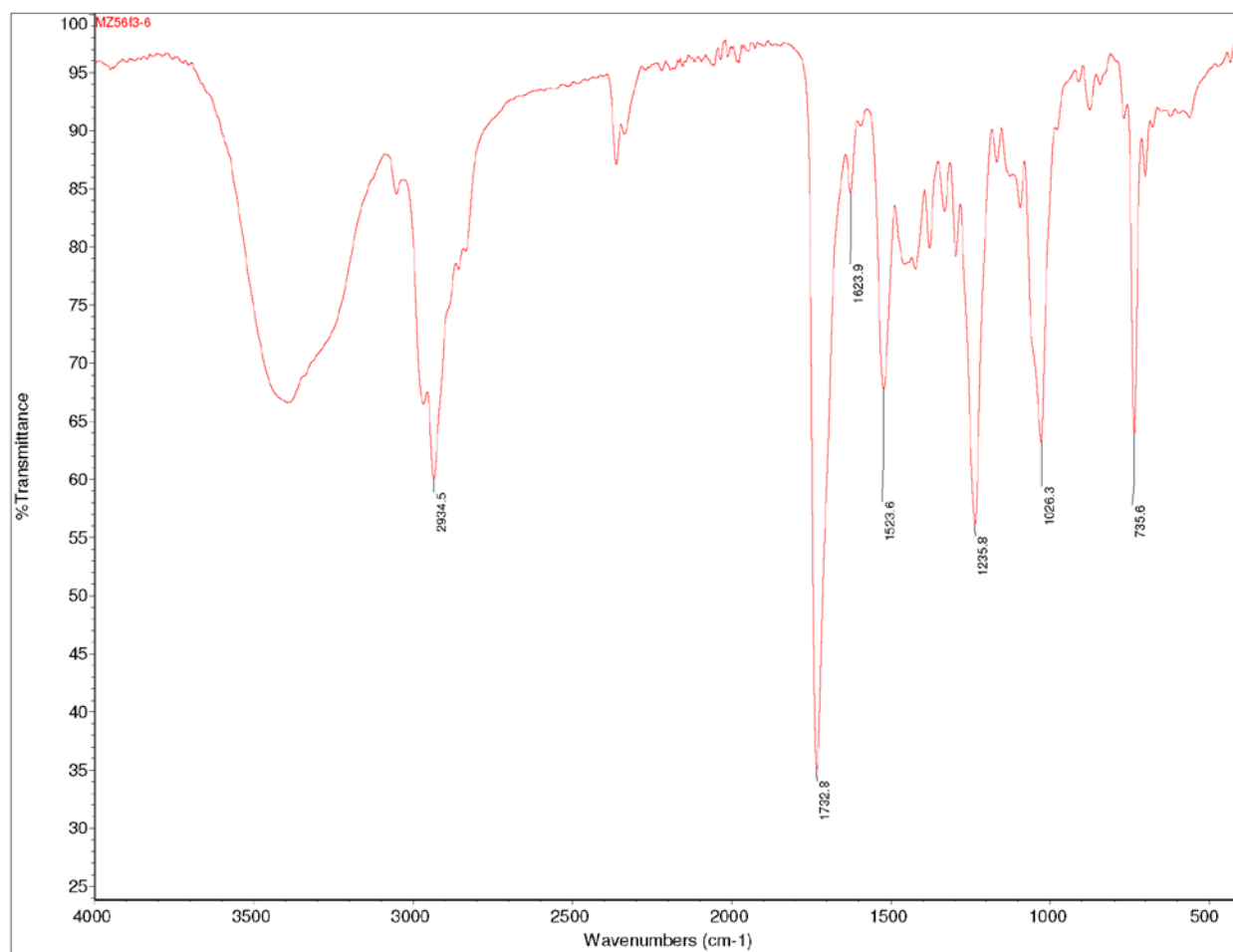




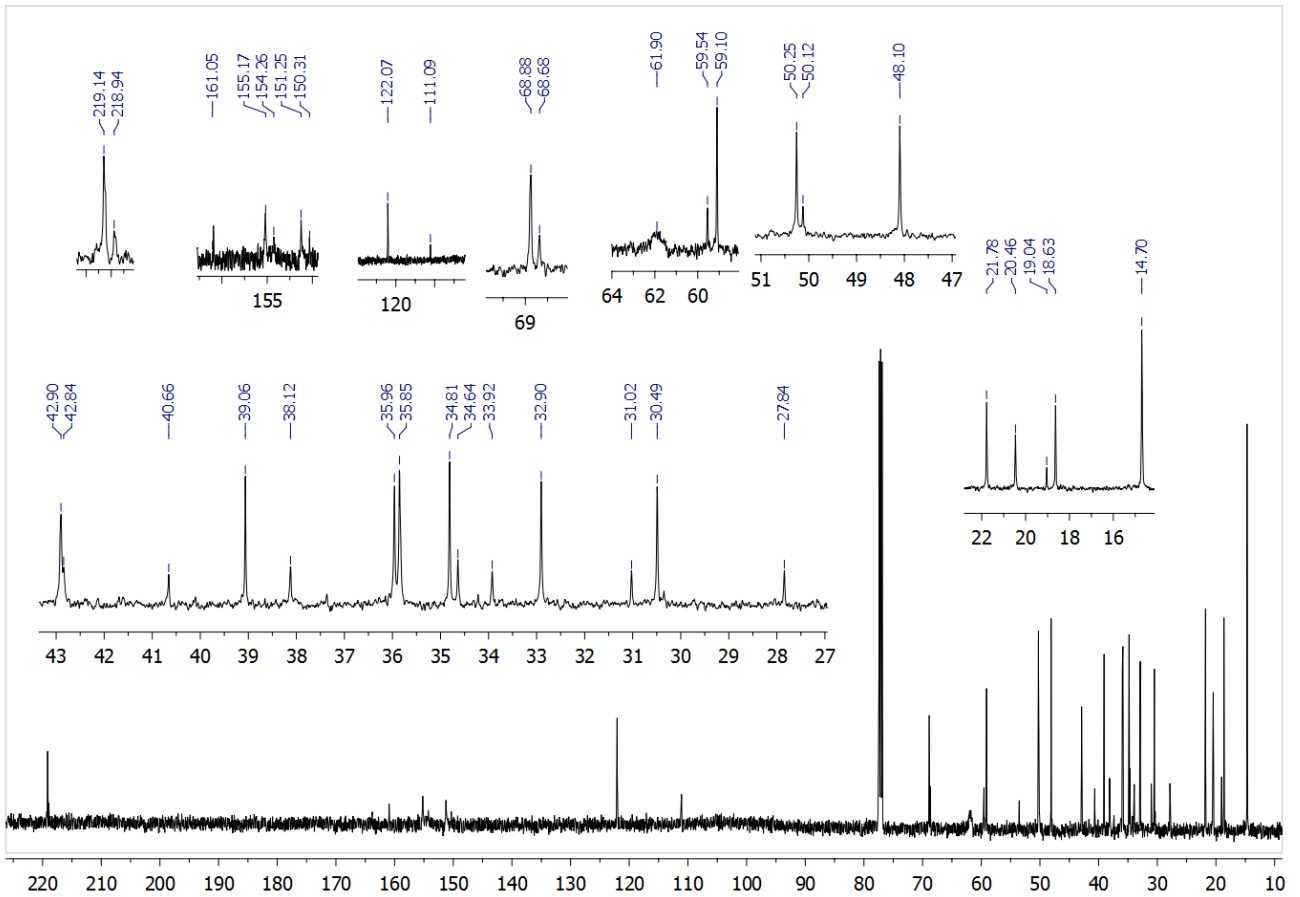
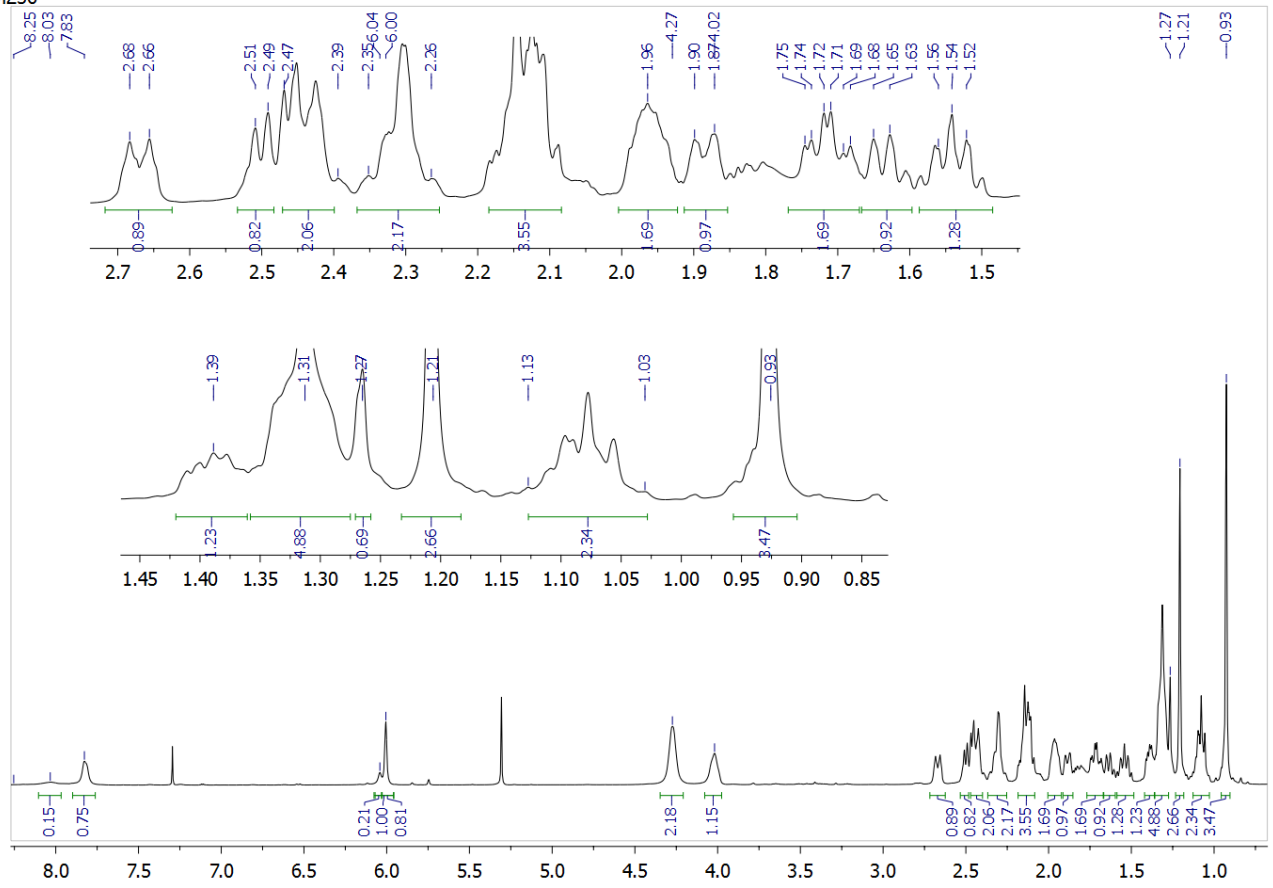
HSQC

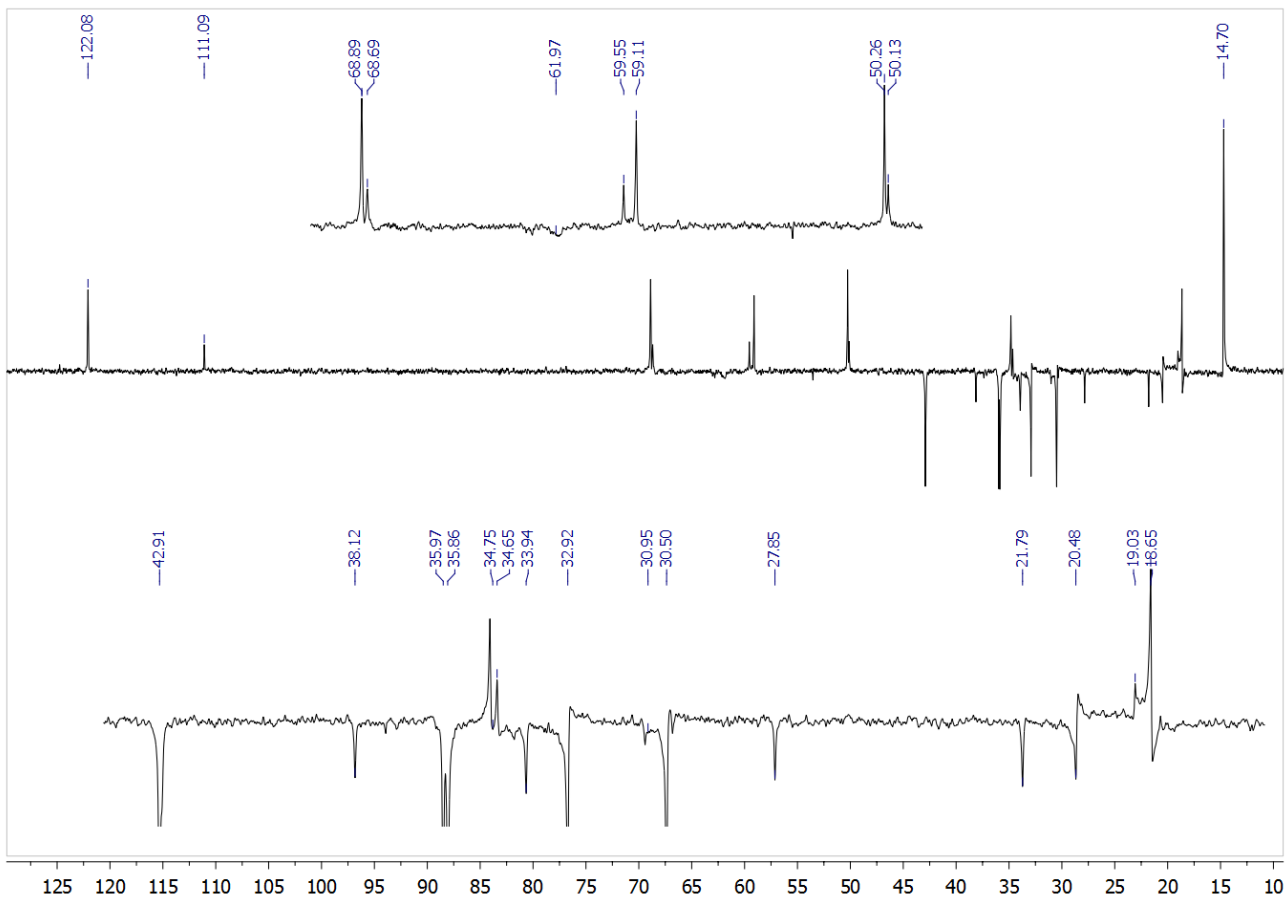


Compound 5d

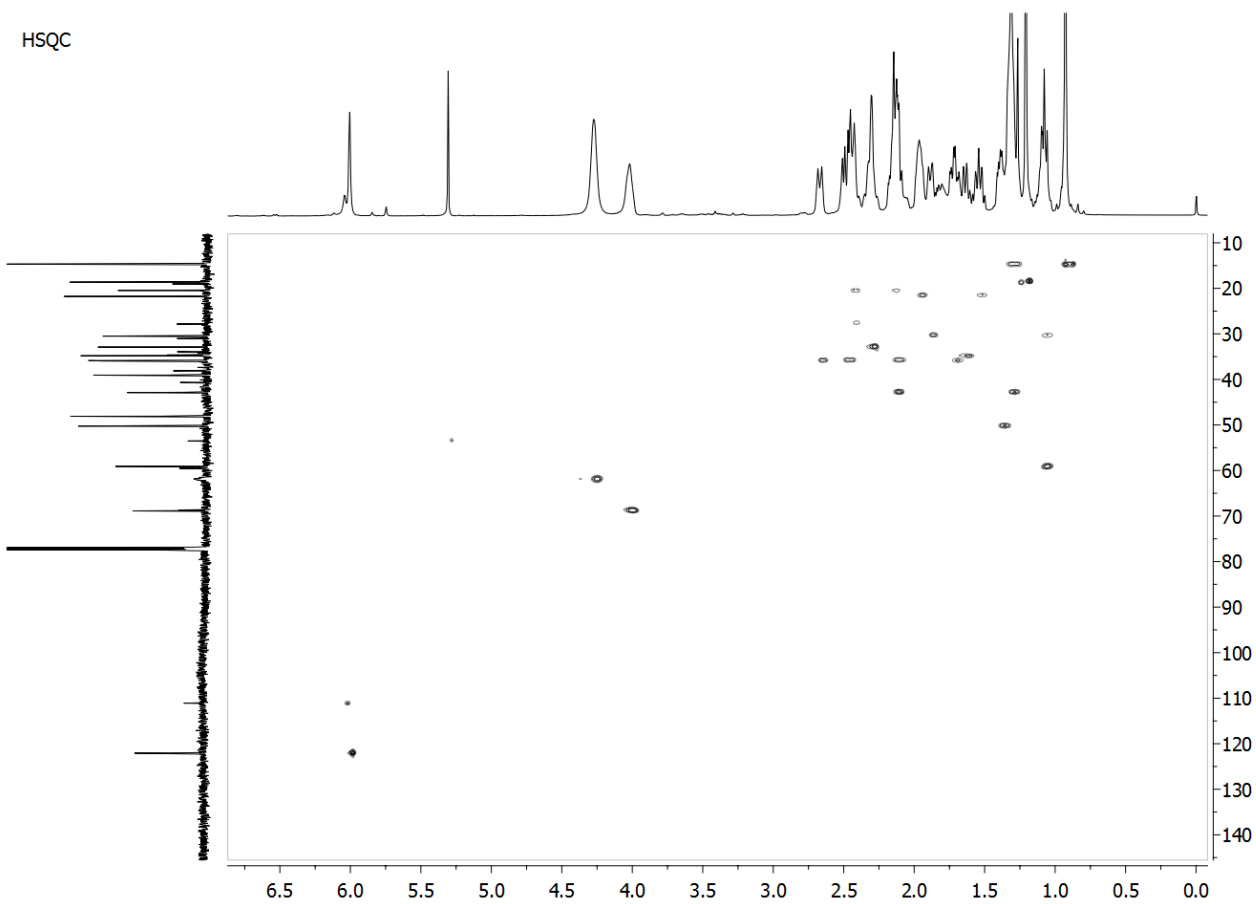


MZ56

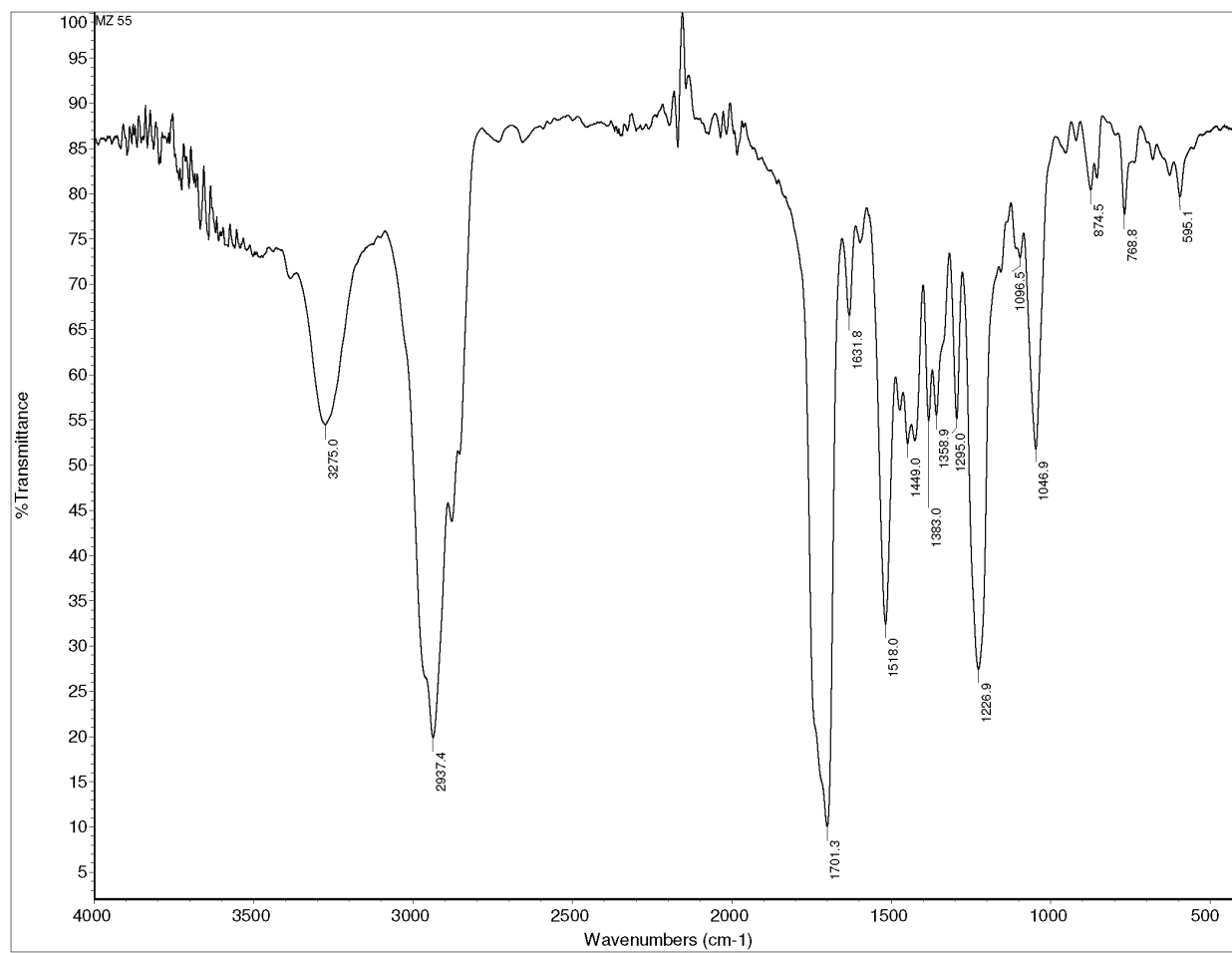
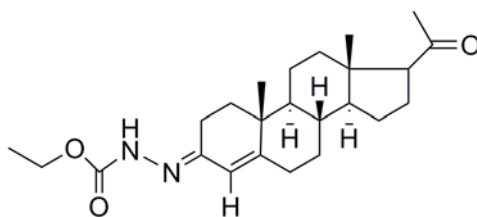


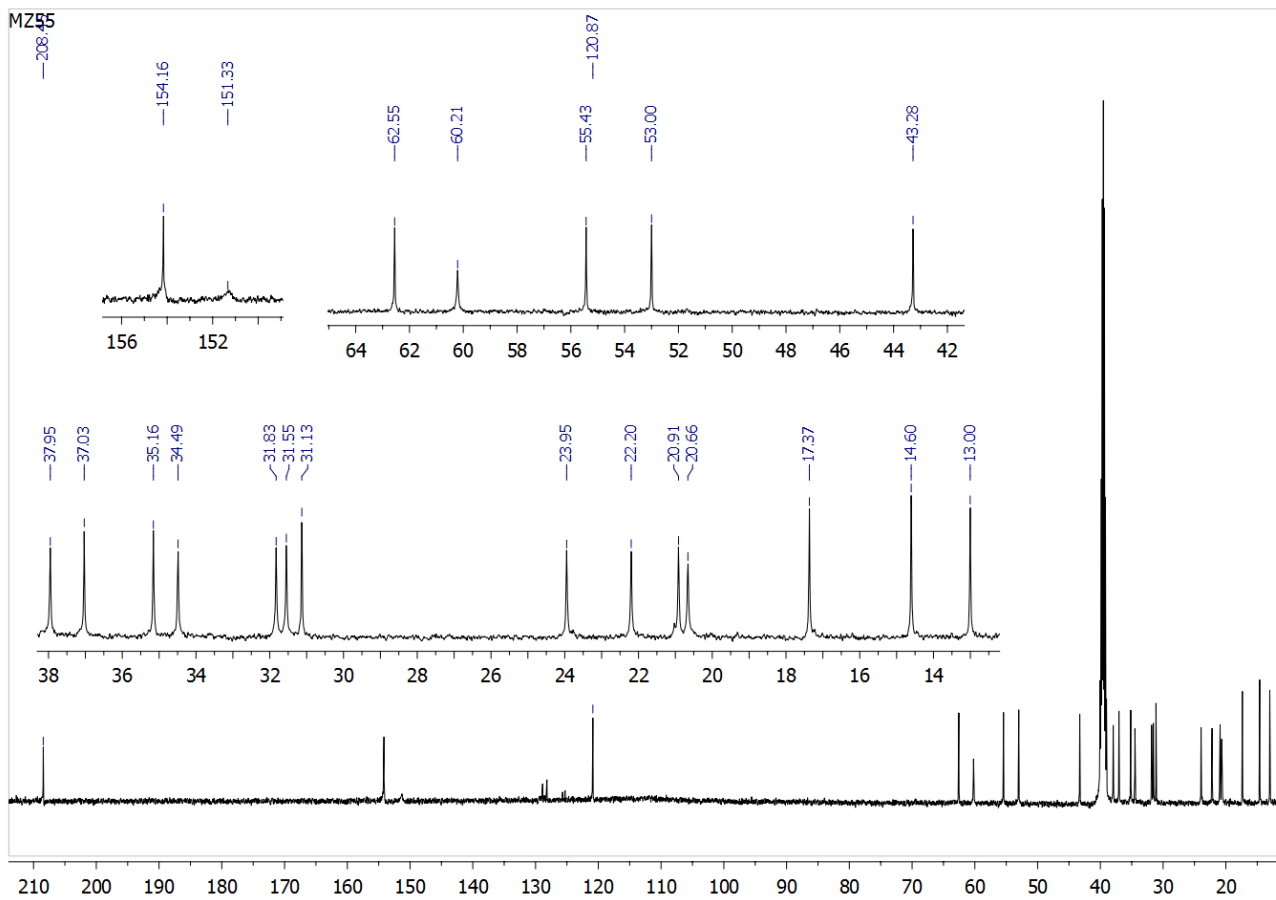
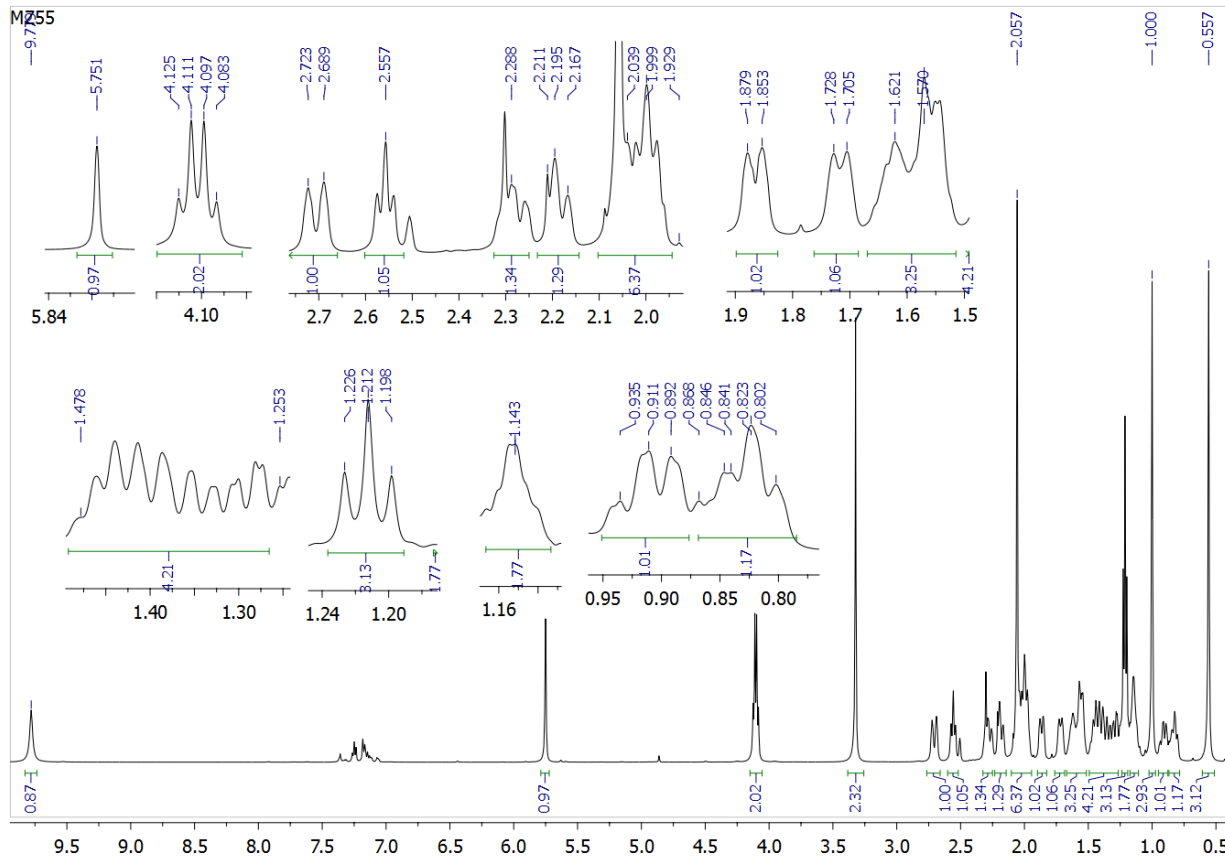


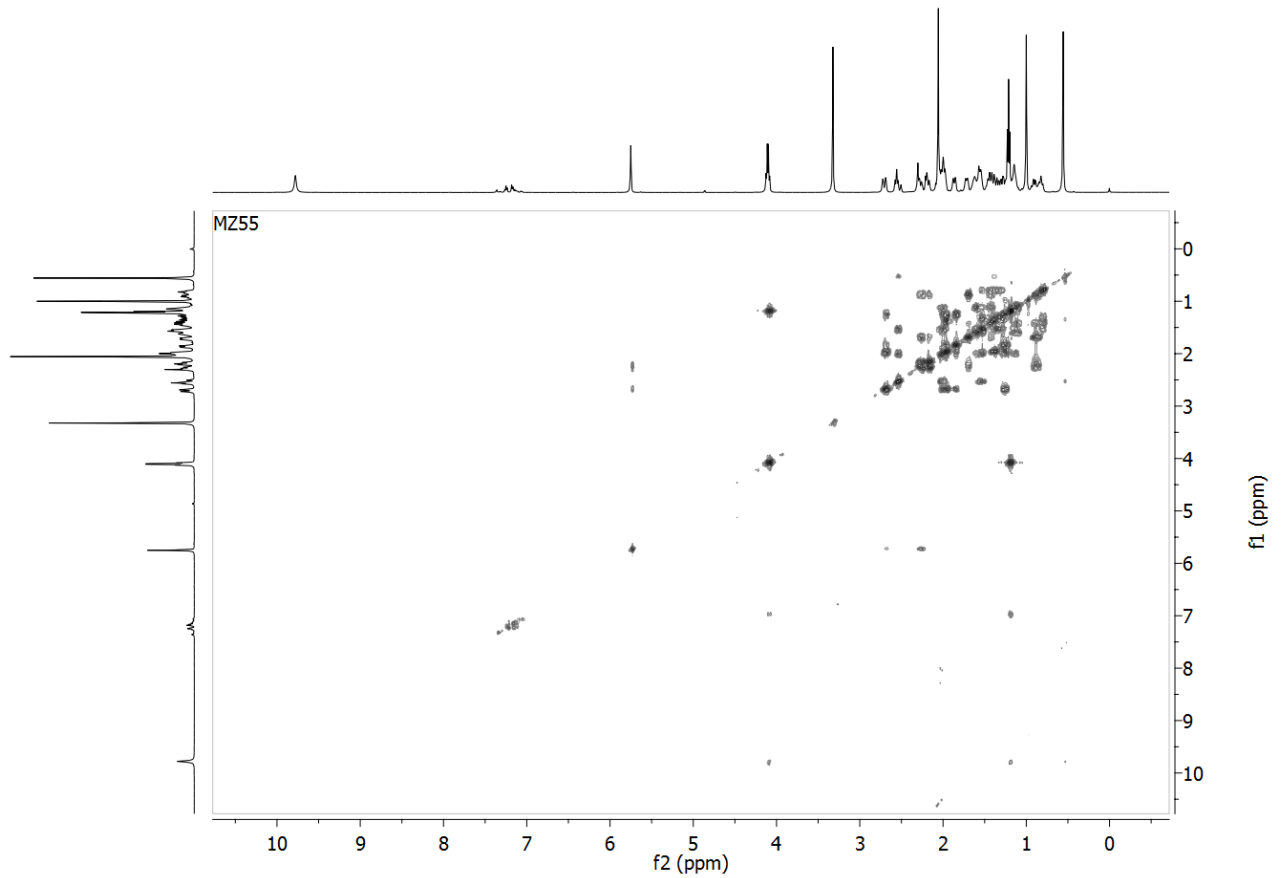
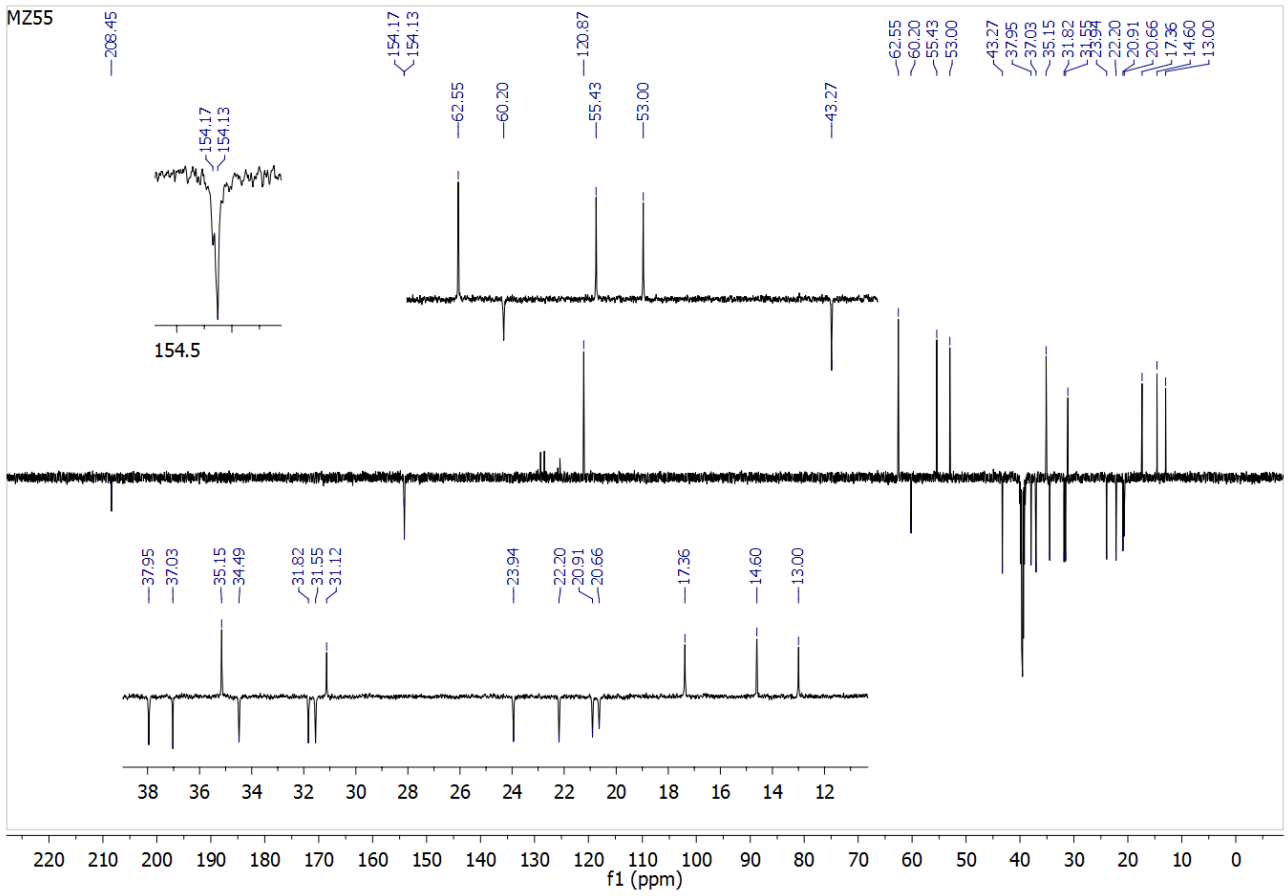
HSQC



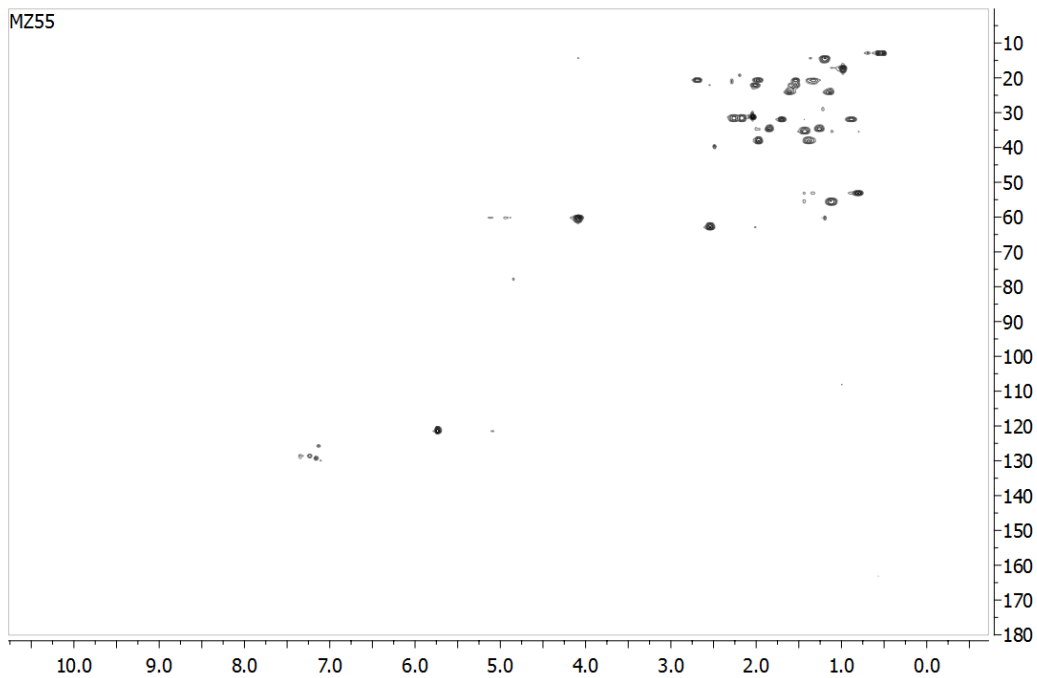
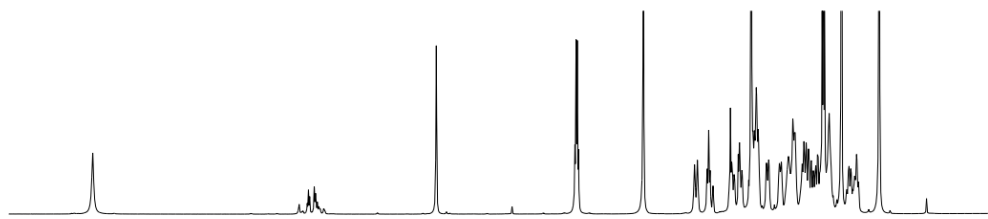
Compound 5e







HSQC



HMBC

