Supplementary Material

Synthesis and exploratory biological evaluation of 3-[(*N*-4-benzyloxyphenyl)iminoethyl]- and 3-(1-hydrazonoethyl)-4-hydroxycoumarins

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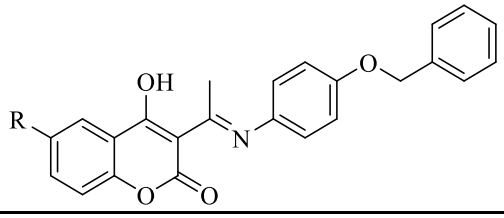
Table of Contents

Biological studies

To assess antimalarial activity, percentage viability of *Plasmodium falciparum* (3D7 strain) parasites incubated for 48 hours with 20 µM of the test compounds was determined by detecting plasmodium lactate dehydrogenase (pLDH) activity as described previously by Lunga *et al.*(*ChemMedChem* **2018**, *13*, 1352-1362). For anti-trypanosomal and cytotoxicity evaluation, percentage viability of *Trypanosoma brucei brucei* (427 strain) parasites or HeLa cells incubated with 20 µM of the test compounds for 48 hours was determined using resazurin, as previously described by Veale and Hoppe (*Med. Chem. Commun.* **2018**, *9*, 2037).

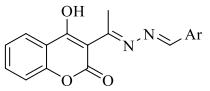
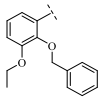
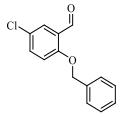
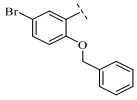
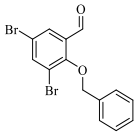
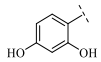
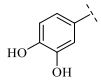
Table 1. Bioassay data for compounds **9a-f** showing % viability of pLDH, *T.b. brucei* and HeLa cells at 20 µM concentrations



Compound	R	PLDH % parasite viability	*T.b. brucei* % parasite viability	Cytotoxicity % HeLa cells viability
9a	H	93.0	33.5	82.6
9b	F	100.0	37.9	77.7
9c	Cl	94.2	31.3	96.3
9d	Br	100.0	23.3	100.0
9e	Me	100.0	96.4	100.0
9f	MeO	71.1	89.1	100.0
Control		IC_{50} = 0.010µM[a]	IC_{50} = 0.022 µM [b]	IC_{50} = 0.019 µM [c]

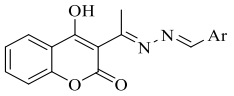
Controls: [a] chloroquine; [b] pentamidine and [c] emetine

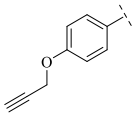
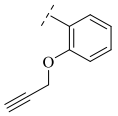
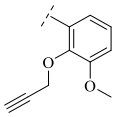
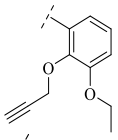
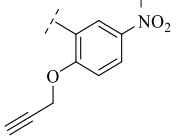
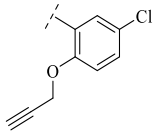
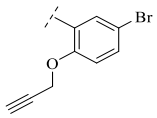
Table 2. Bioassay data for compounds **13a-g**, showing % viability of pLDH, *T.b. brucei* and HeLa and activity against mycobacterial cells at 20 µM concentrations.

	Ar	PLDH % viability[a]	*T.b. brucei* % viability [b]	% HeLa cells viability [c]	Visual MIC90 7D 7H9 GLU CAS Tx(µM)	Calculated MIC90 7D 7H9 GLU CAS Tx (µM)
13a		100.00	97.40	96.98	>125	>125
13b		100.00	52.34	92.26	>125	>125
13c		100.00	80.86	89.75	125	>125
13d		100.00	100.00	83.50	-	-
13e		63.93	100.22	67.78	>125	>125
13f		81.62	58.11	59.80	>125	>125
13g		86.51	**1.53 (IC_{50} 0.90)**	65.25	62.50	62.44
Control		IC_{50} = 0.01 µM [a]	IC_{50} = 0.022 µM [b]	IC_{50} = 0.021 µM [c]	0.019 [d]	0.007 [d]

Controls. [a] Chloroquine [b] Pentamidine [c] emetine [d] Rifampicin [e] IC_{50} value

Table 3. Bioassay data for compounds **15a-g**, showing % activity against pLDH, *T.b. brucei* and HeLa cells at 20 µM concentrations



Compound	Ar	PLDH % viability [a]	*T.b. brucei* % viability [b]	Cytotoxicity % HeLa cells viability
15a		100.00	96.35	78.49
15b		100.00	100.00	78.04
15c		100.00	94.57	84.71
15d		100.00	90.96	80.70
15e		100.00	64.77	72.24
15f		100.00	90.01	89.55
15g		100.00	80.49	79.38
Control		IC_{50} = 0.01µM [a]	IC_{50} = 0.022 µM	IC_{50} = 0.021 µM [c]

Controls. [a] chloroquine [b] pentamidine [c] emetine

NMR Spectra

3-[(*N*-4-benzyloxyphenyl)iminoethyl]-4-hydroxycoumarins 9a-f

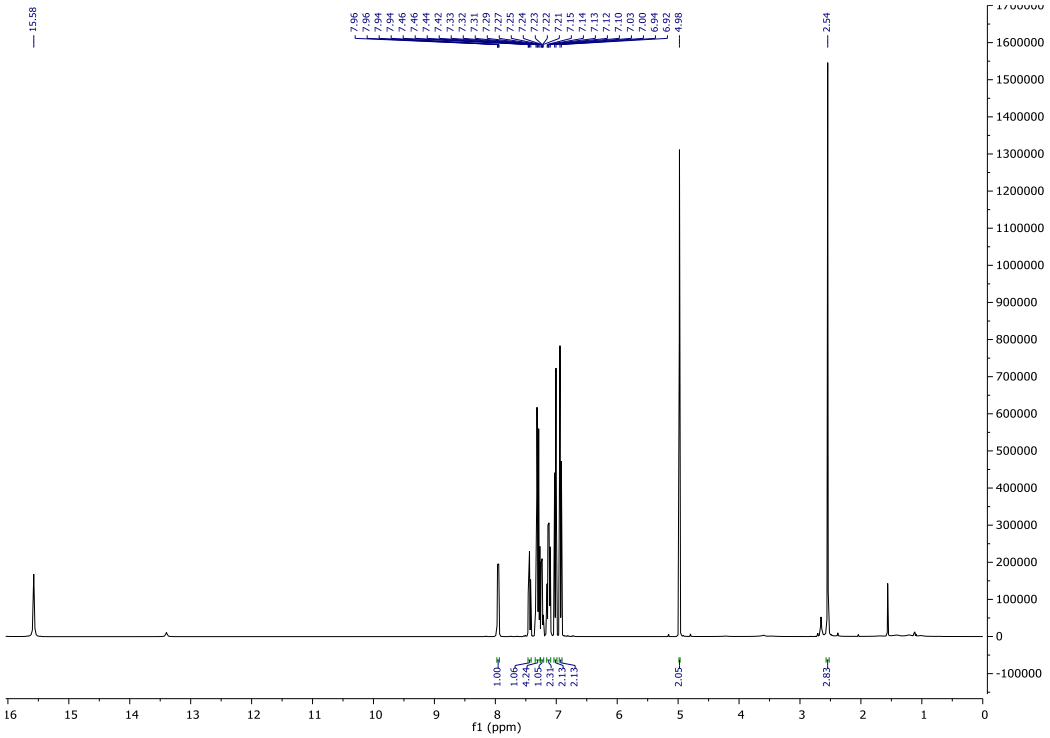


Figure 1. 400 MHz ^{1}H NMR spectrum of compound **9a** in $CDCl_3$.

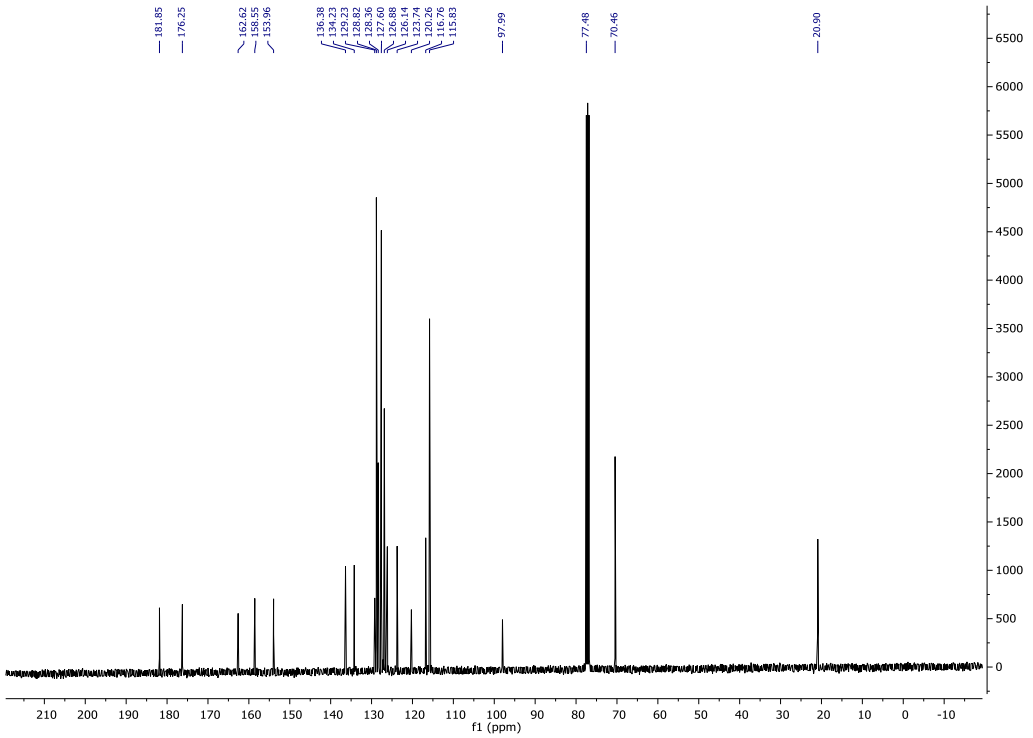


Figure 2. 100 MHz ^{13}C NMR spectrum of compound **9a** in $CDCl_3$.

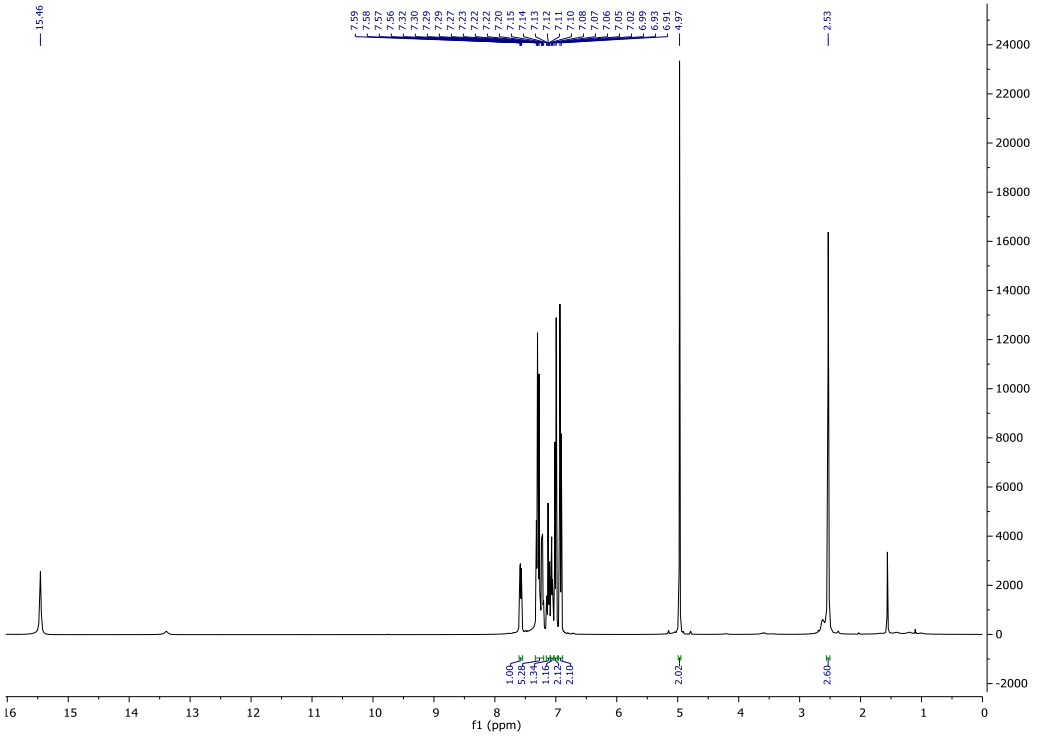


Figure 3. 400 MHz ^{1}H NMR spectrum of compound **9b** in $CDCl_3$.

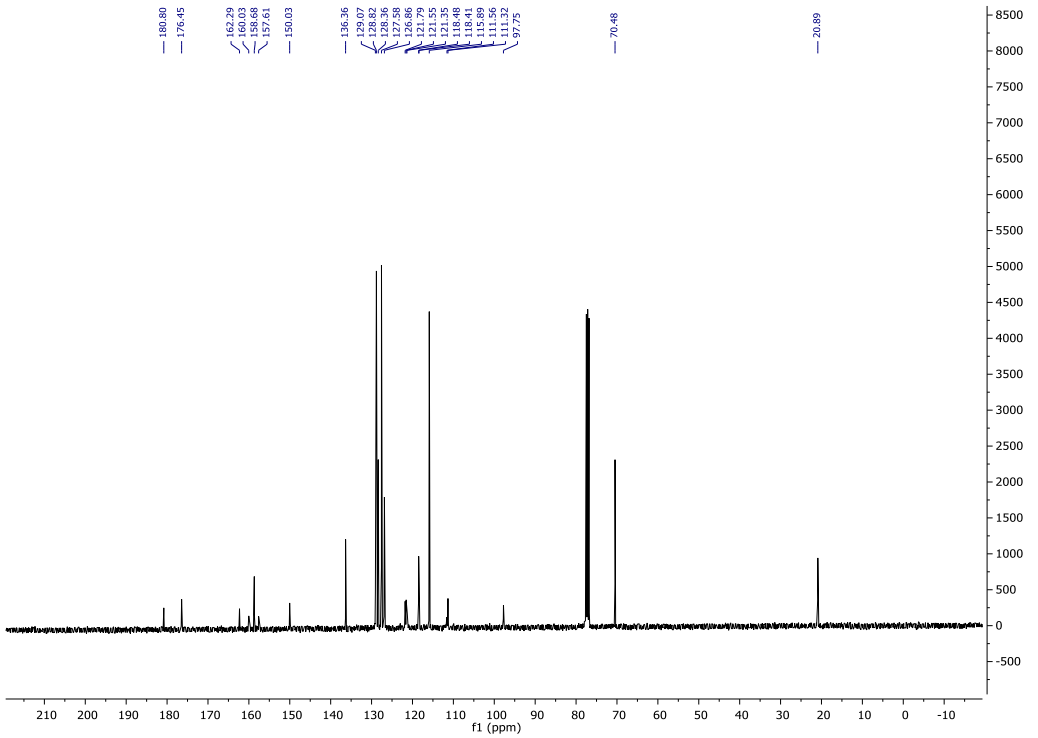


Figure 4. 100 MHz ^{13}C NMR spectrum of compound **9b** in $CDCl_3$.

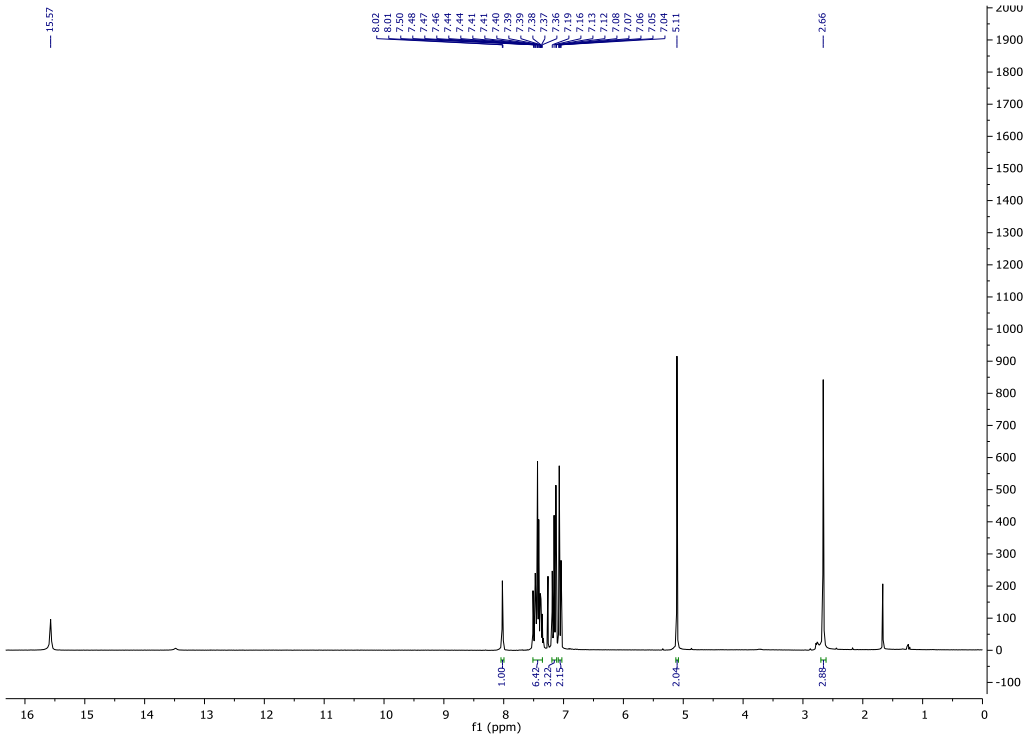


Figure 5. 400 MHz ^{1}H NMR spectrum of compound **9c** in $CDCl_3$.

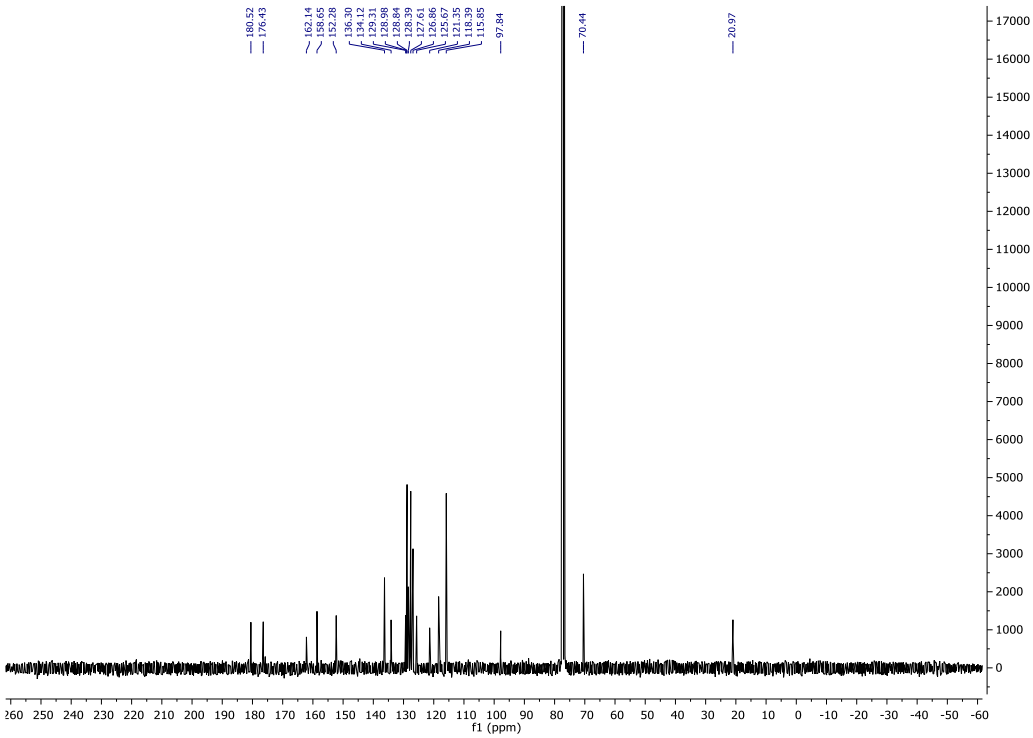


Figure 6. 100 MHz ^{13}C NMR spectrum of compound **9c** in $CDCl_3$.

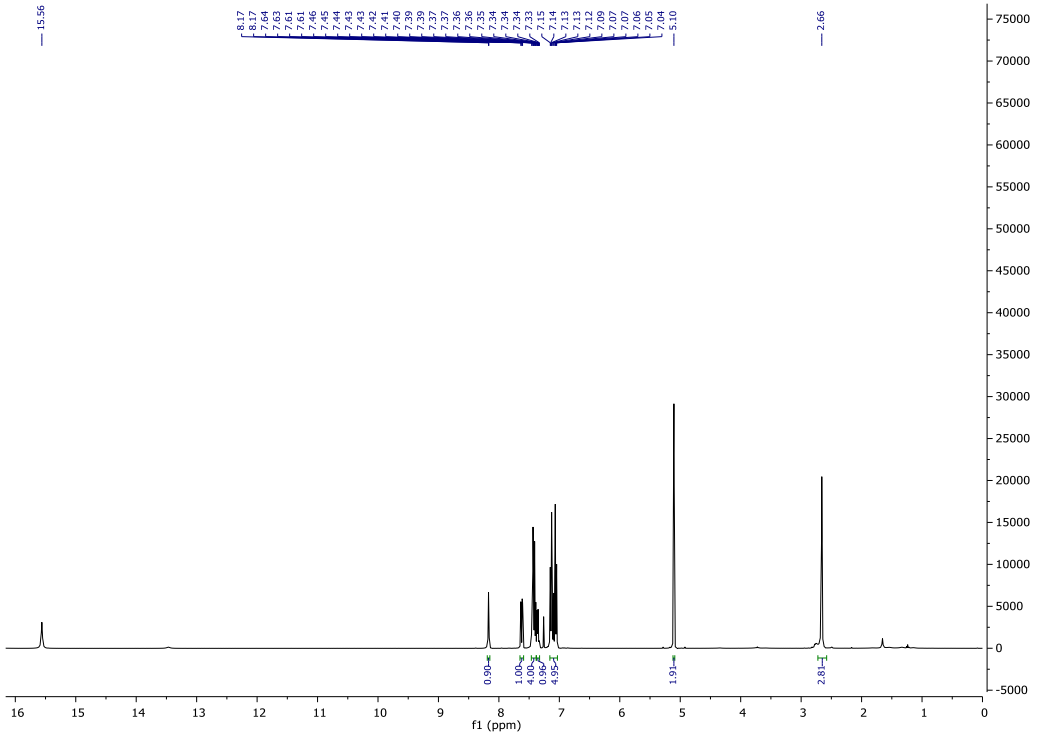


Figure 7. 400 MHz ^{1}H NMR spectrum of compound **9d** in $CDCl_3$.

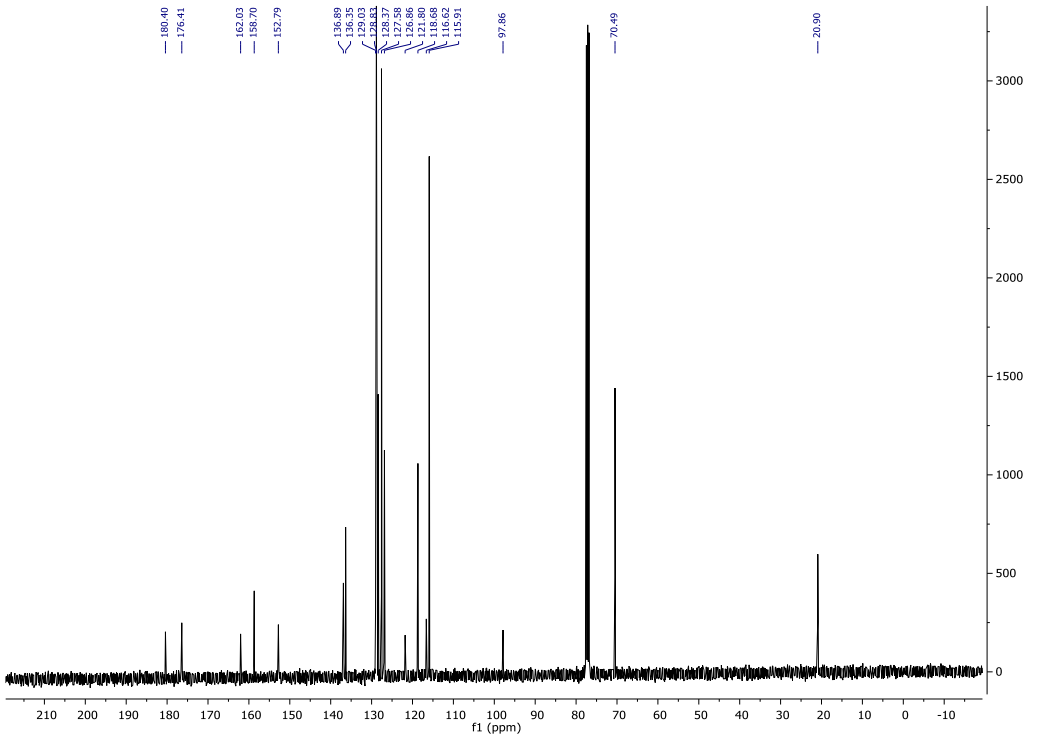


Figure 8. 100 MHz ^{13}C NMR spectrum of compound **9d** in $CDCl_3$.

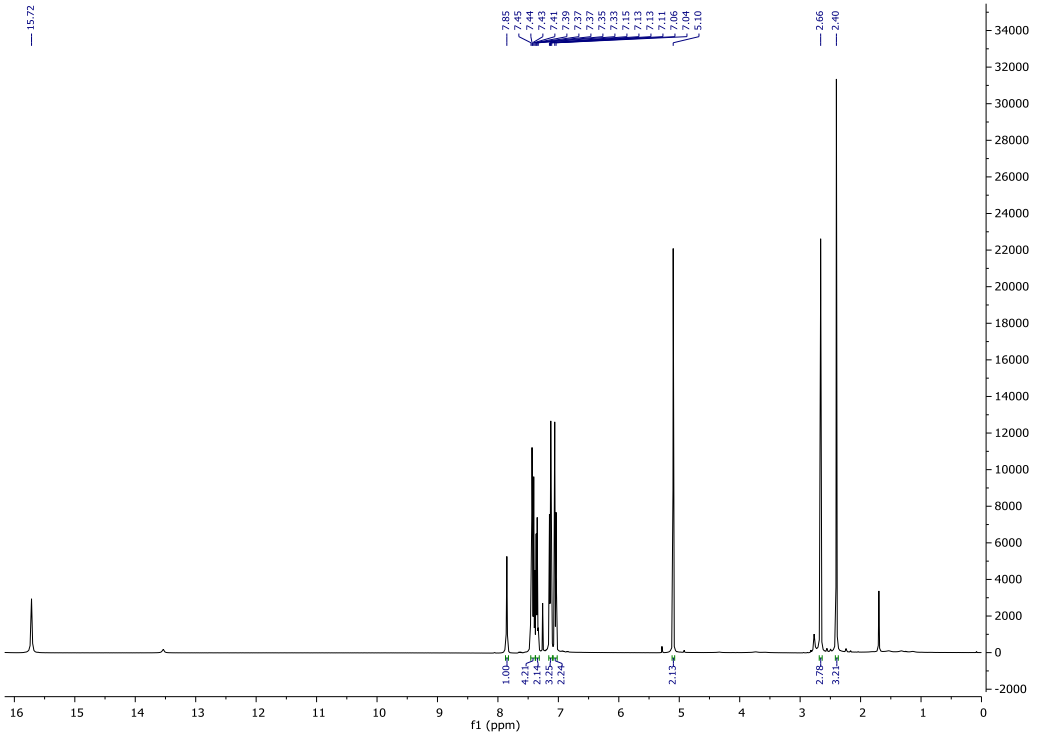


Figure 9. 400 MHz ^{1}H NMR spectrum of compound **9e** in $CDCl_3$.

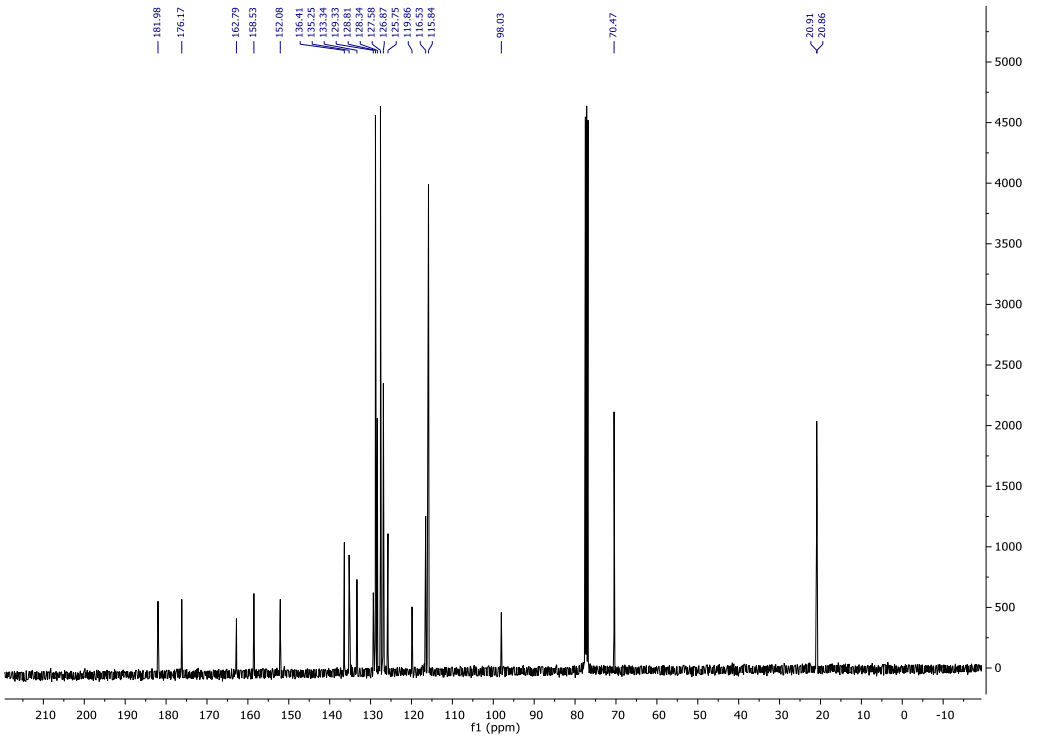


Figure 10. 100 MHz ^{13}C NMR spectrum of compound **9e** in $CDCl_3$.

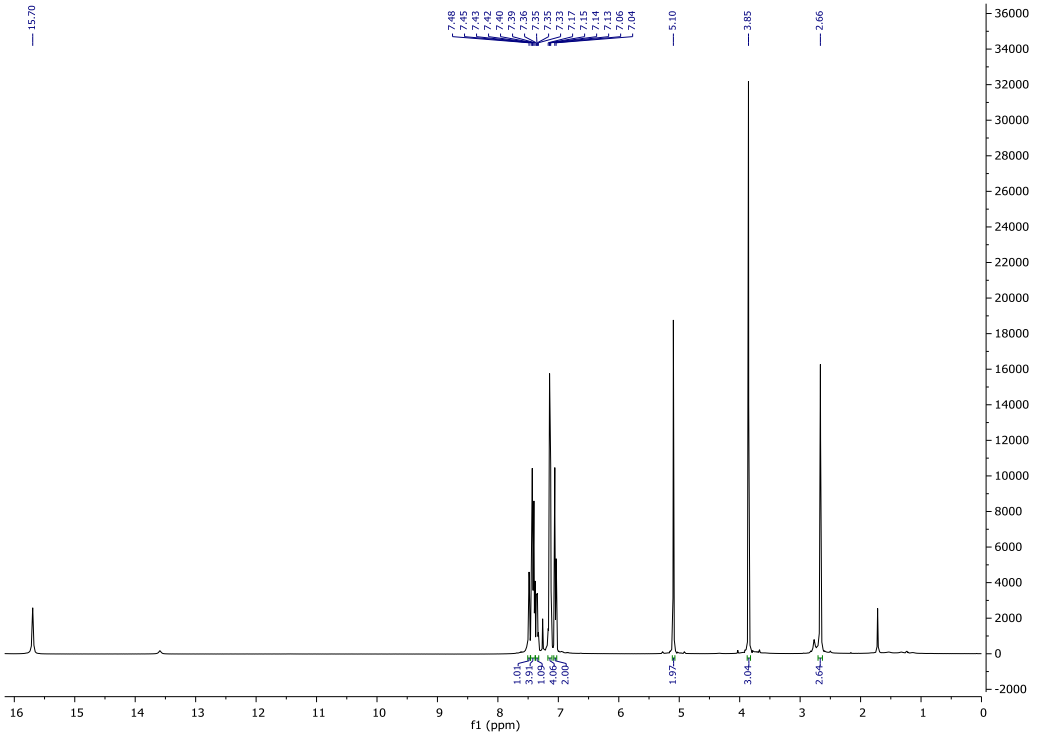


Figure 11. ^{1}H 400 MHz NMR spectrum of compound **9f** in $CDCl_3$.

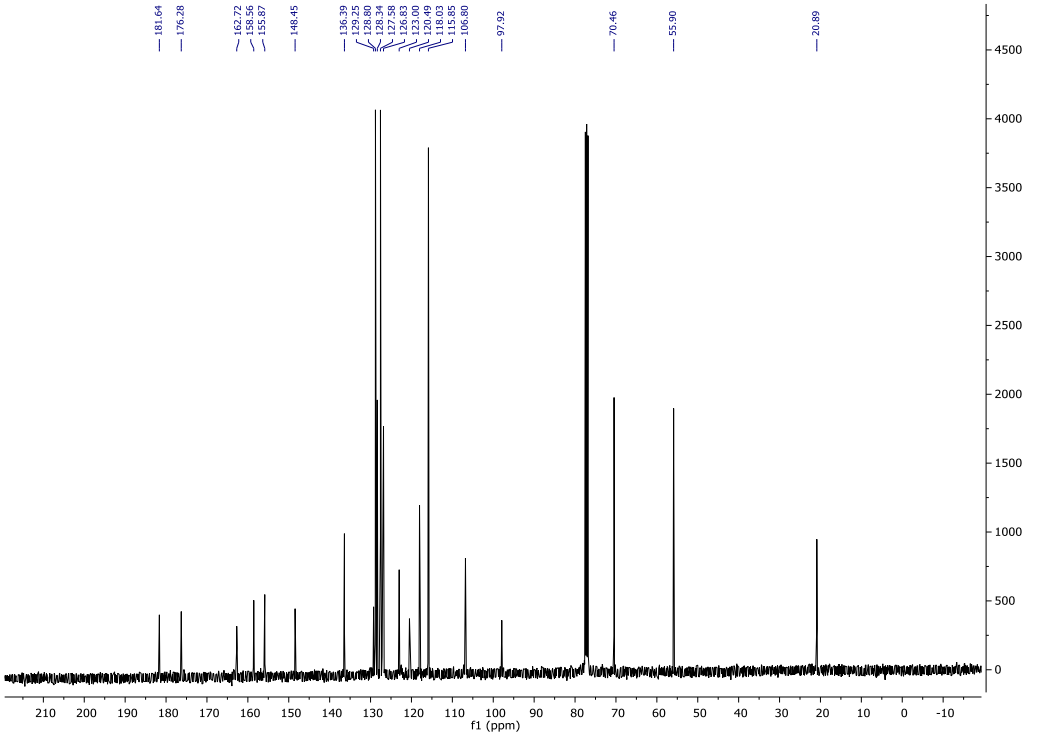


Figure 12. 100 MHz ^{13}C NMR spectrum of compound **9f** in $CDCl_3$.

3-[1-(Benzylidenehydrazono)ethyl]-4-hydroxycoumarins 13a-g

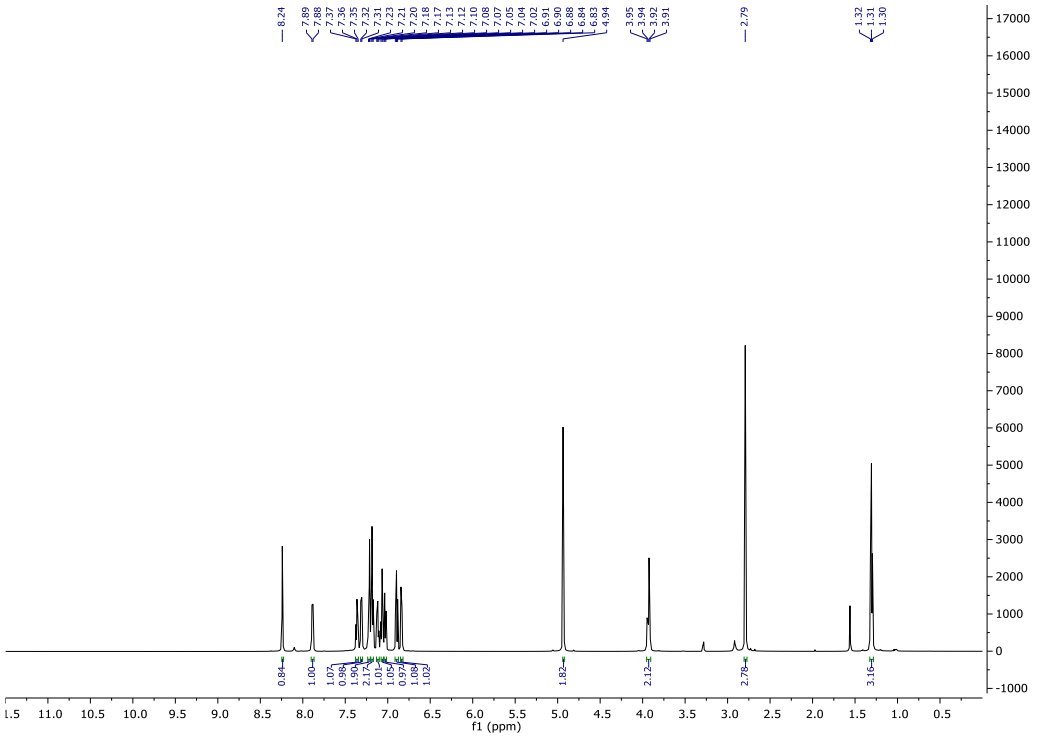


Figure 13. ^{1}H 600 MHz NMR spectrum of compound **13a** in $CDCl_3$.

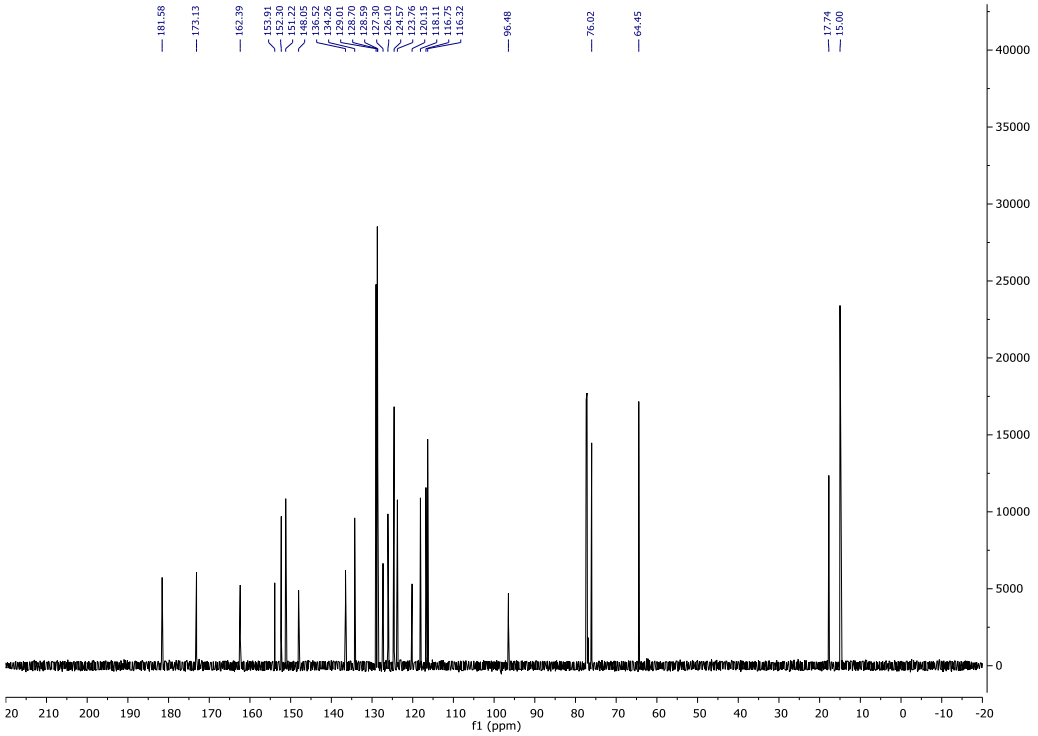


Figure 14. 150 MHz ^{13}C NMR spectrum of compound **13a** in $CDCl_3$.

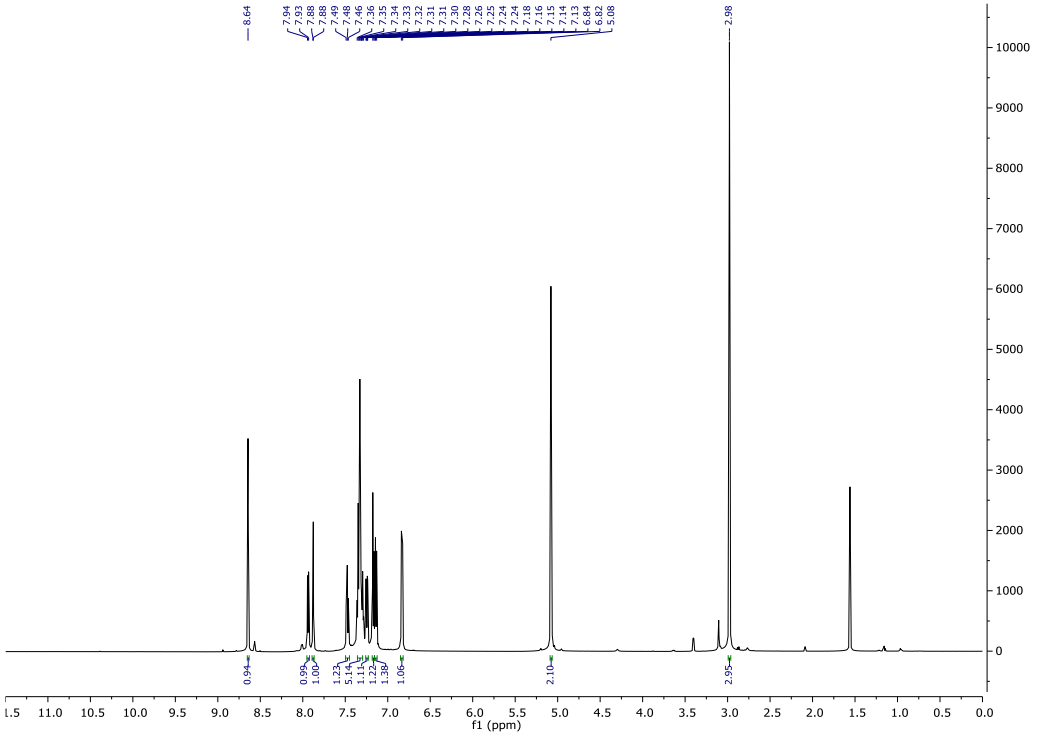


Figure 15. ^{1}H 600 MHz NMR spectrum of compound **13b** in $CDCl_3$.

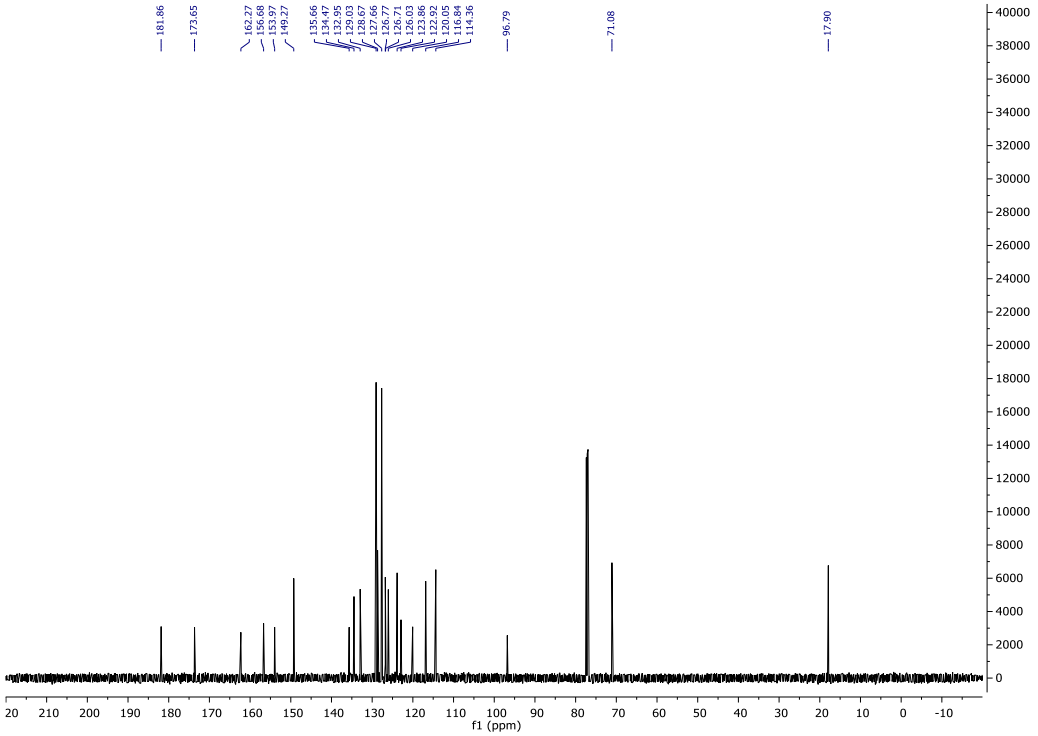


Figure 16. 150 MHz ^{13}C NMR spectrum of compound **13b** in $CDCl_3$.

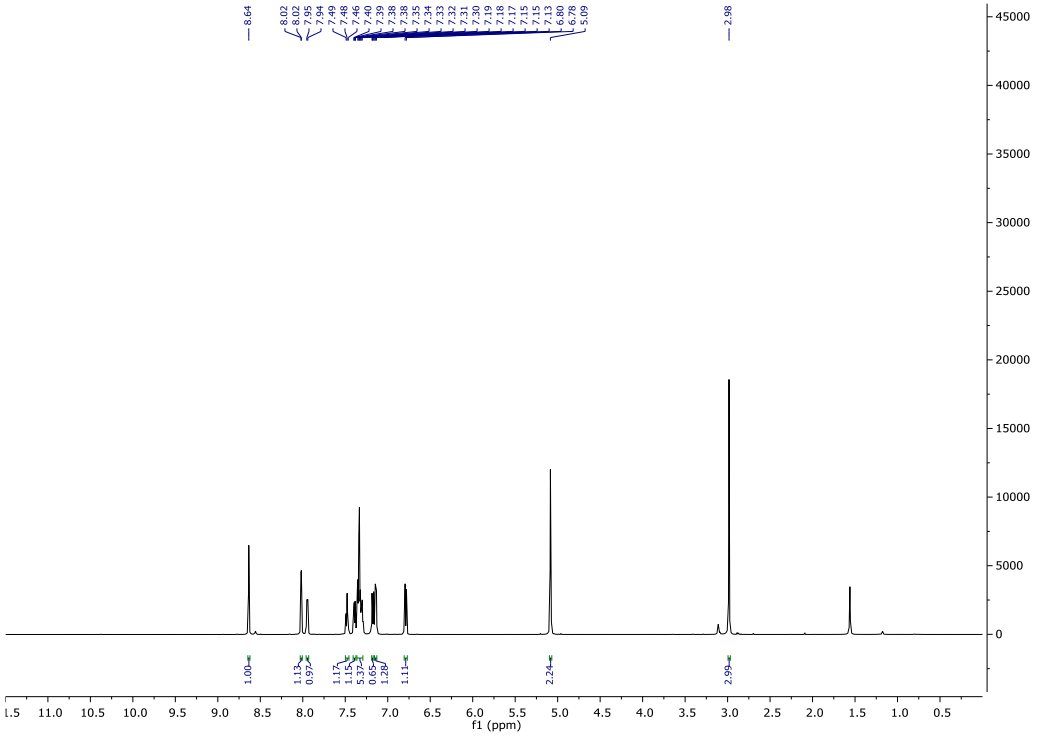


Figure 17. ^{1}H 600 MHz NMR spectrum of compound **13c** in $CDCl_3$.

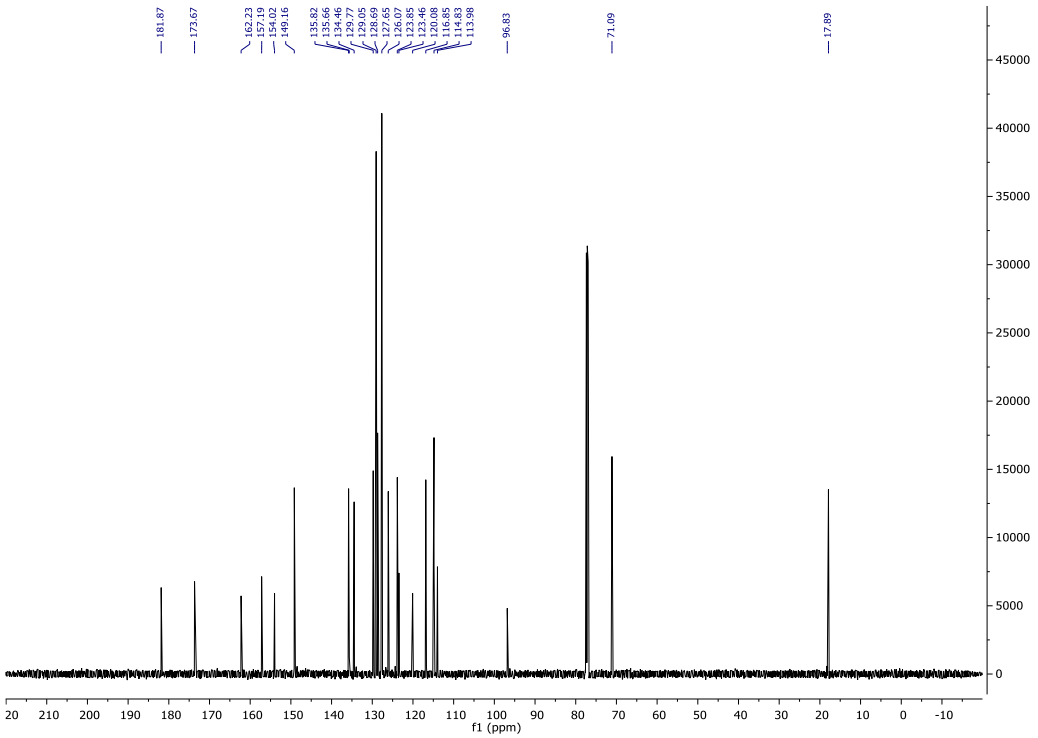


Figure 18. 150 MHz ^{13}C NMR spectrum of compound **13c** in $CDCl_3$.

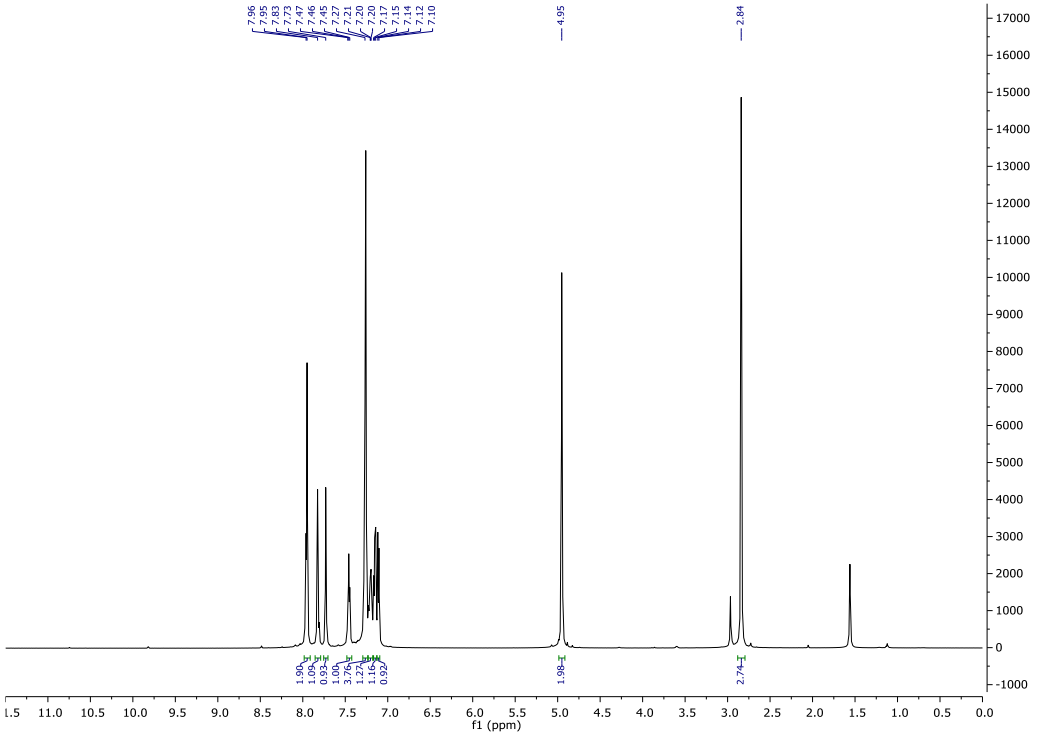


Figure 19. ^{1}H 600 MHz NMR spectrum of compound **13d** in $CDCl_3$.

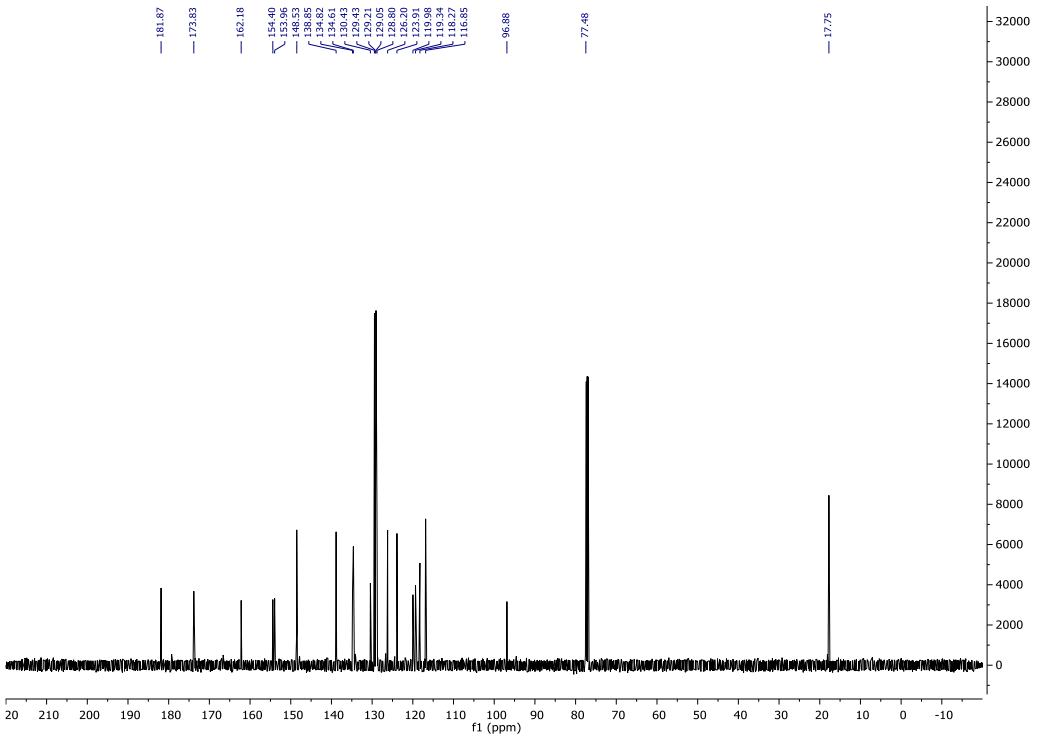


Figure 20. 150 MHz ^{13}C NMR spectrum of compound **13d** in $CDCl_3$.

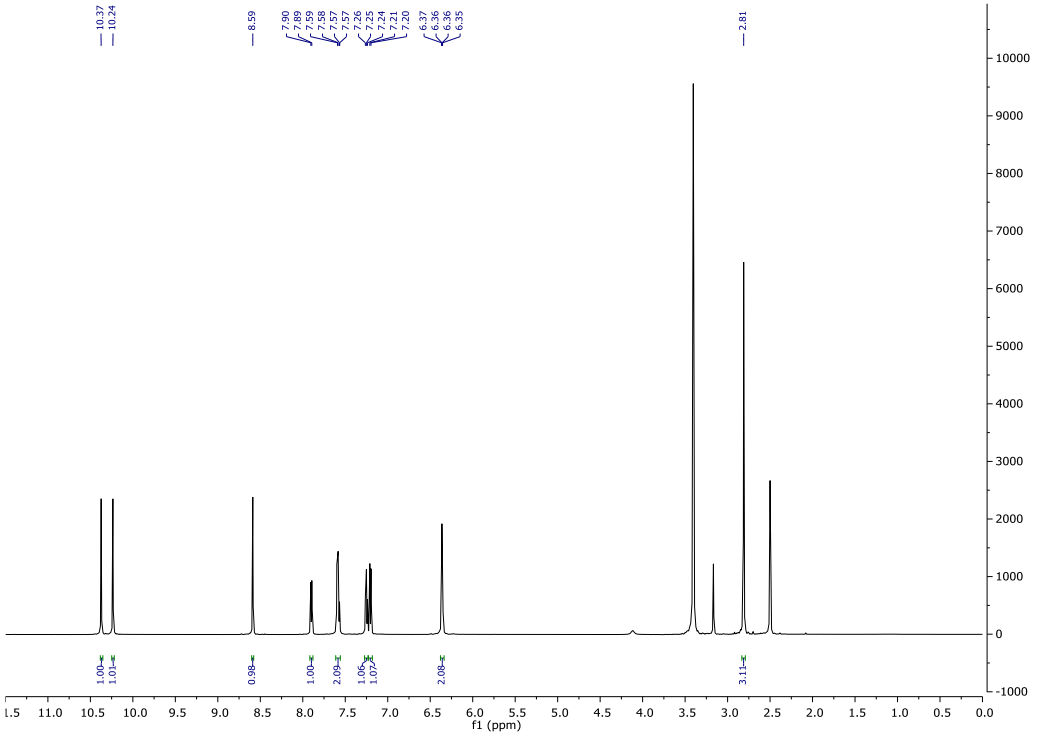


Figure 21. ^{1}H 600 MHz NMR spectrum of compound **13e** in DMSO-d_6.

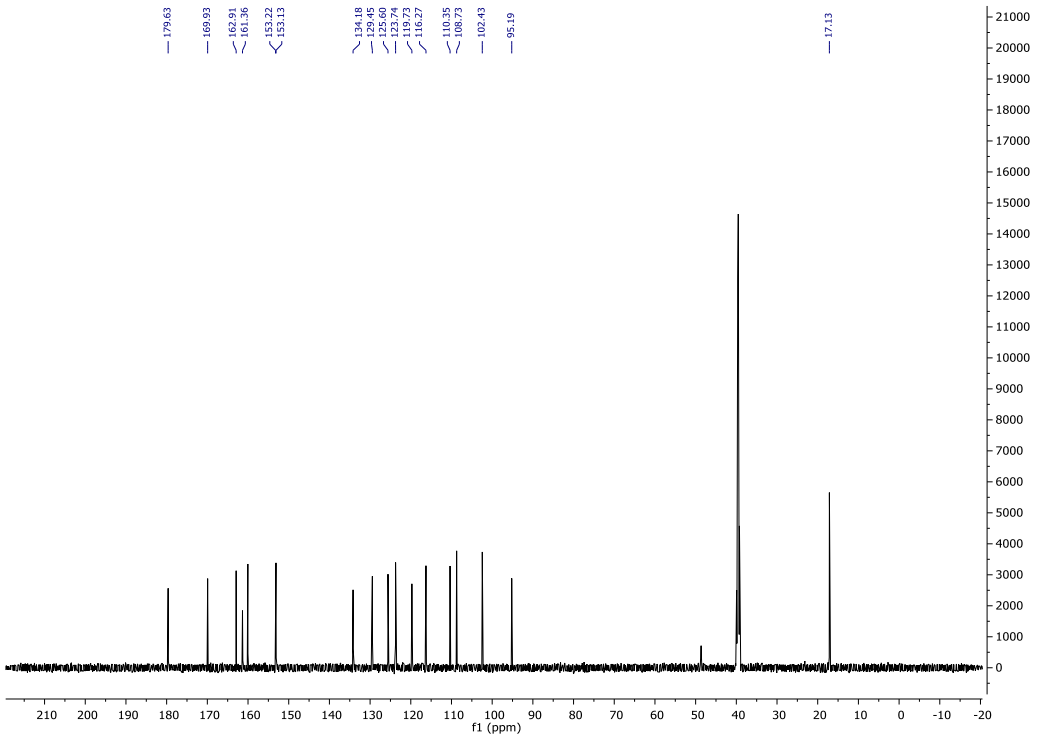


Figure 22. 150 MHz ^{13}C NMR spectrum of compound **13e** in DMSO-d_6.

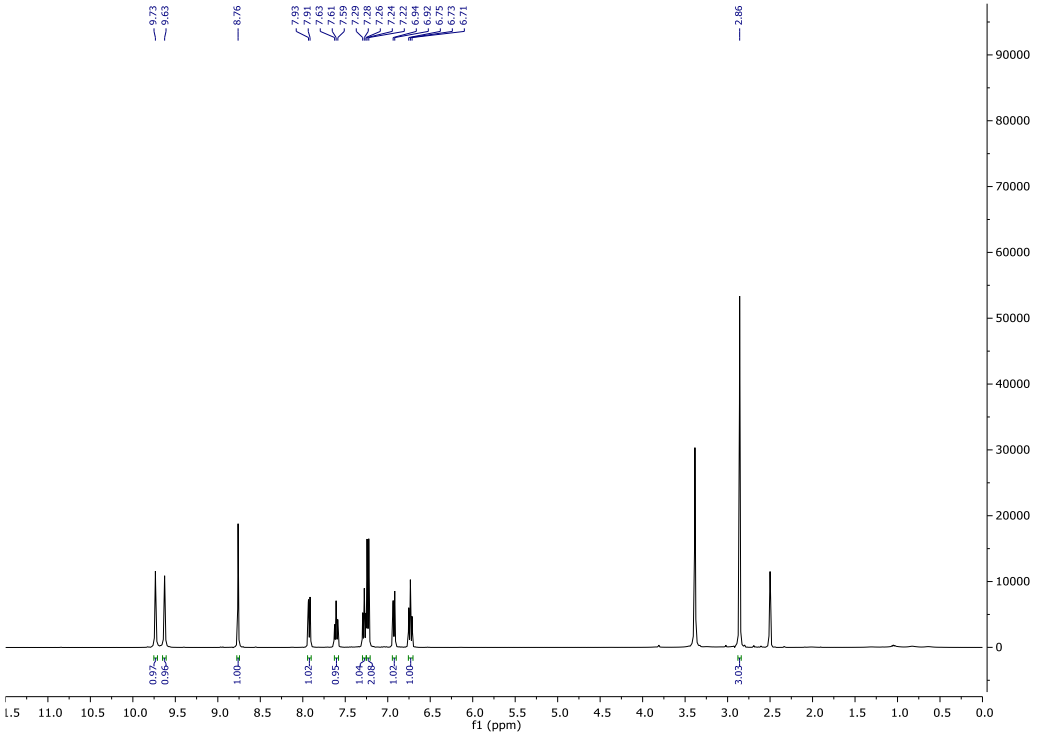


Figure 23. ^{1}H 400 MHz NMR spectrum of compound **13f** in DMSO-d_6.

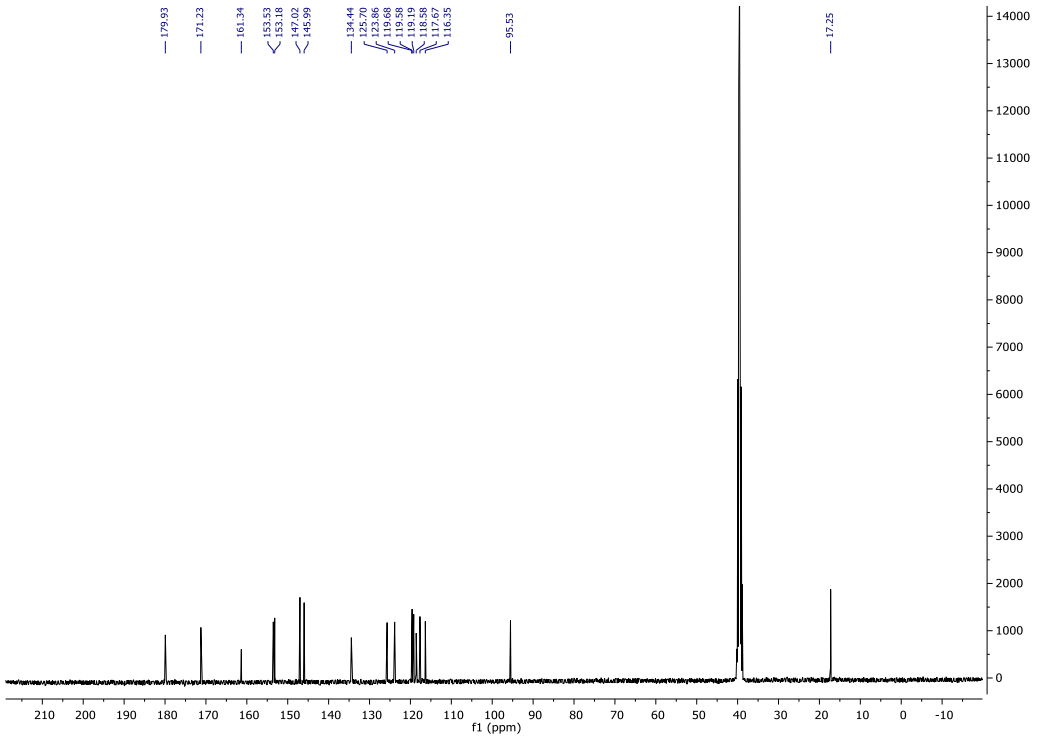


Figure 24. 100 MHz ^{13}C NMR spectrum of compound **13f** in DMSO-d_6.

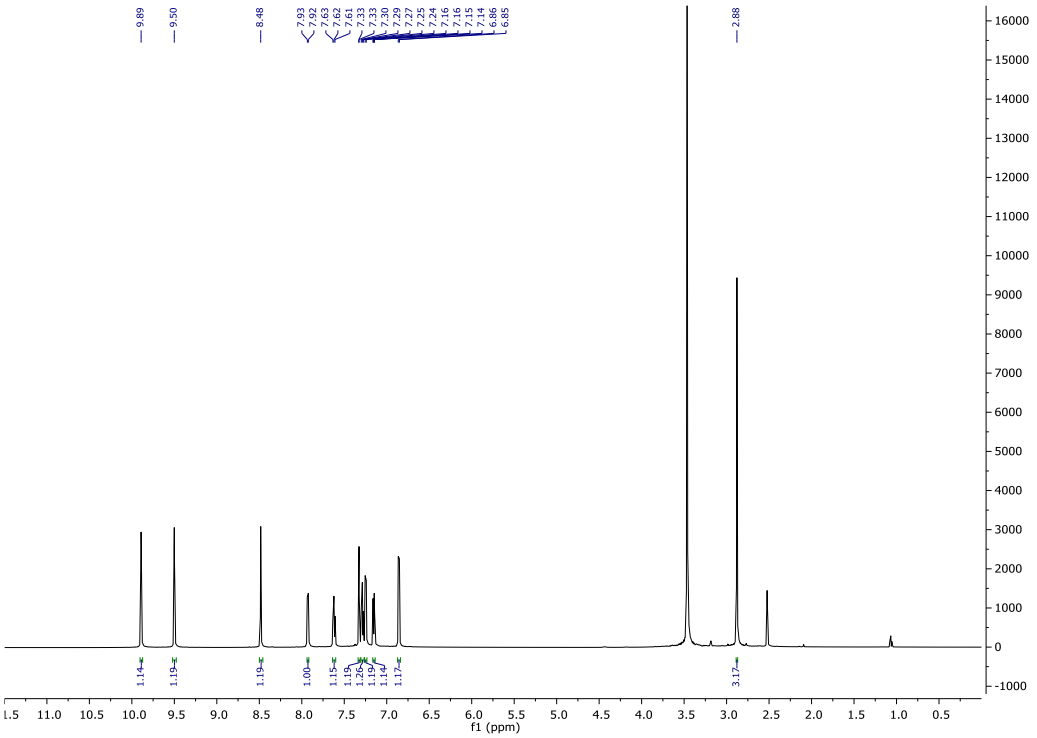


Figure 25. ^{1}H 400 MHz NMR spectrum of compound **13g** in DMSO-d_6.

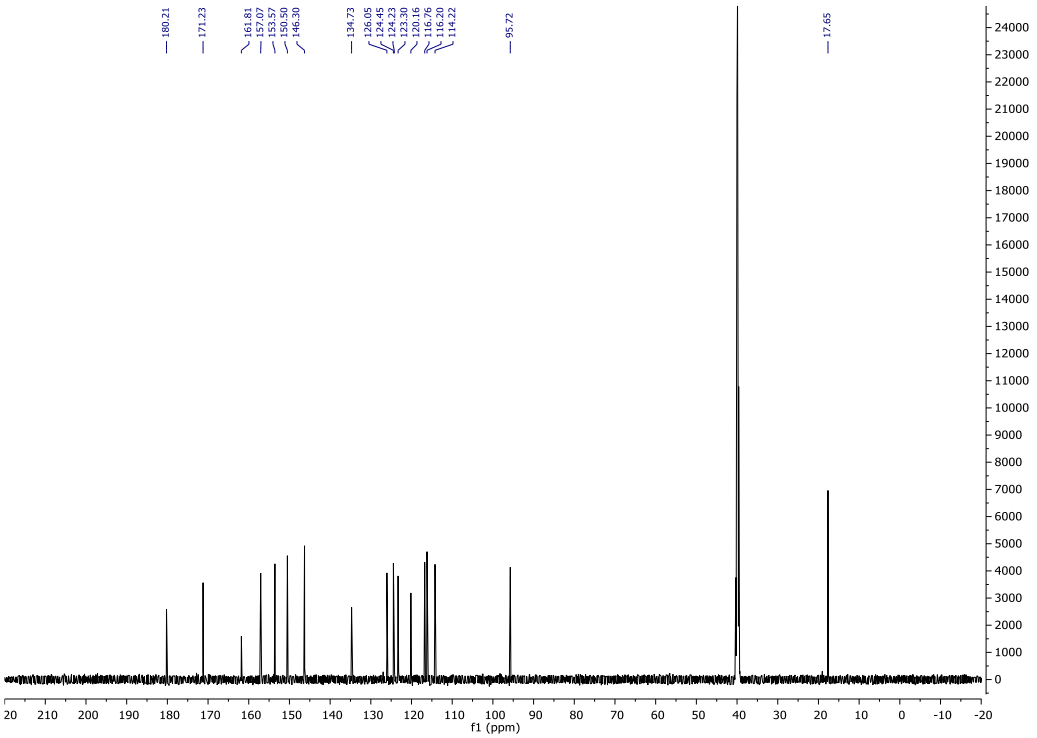


Figure 26. 100 MHz ^{13}C NMR spectrum of compound **13g** in DMSO-d_6.

3-{1-[(prop-2-yn-1-yloxy)benzylidenehydrazono]ethyl}-4-hydroxycoumarins 15a-g

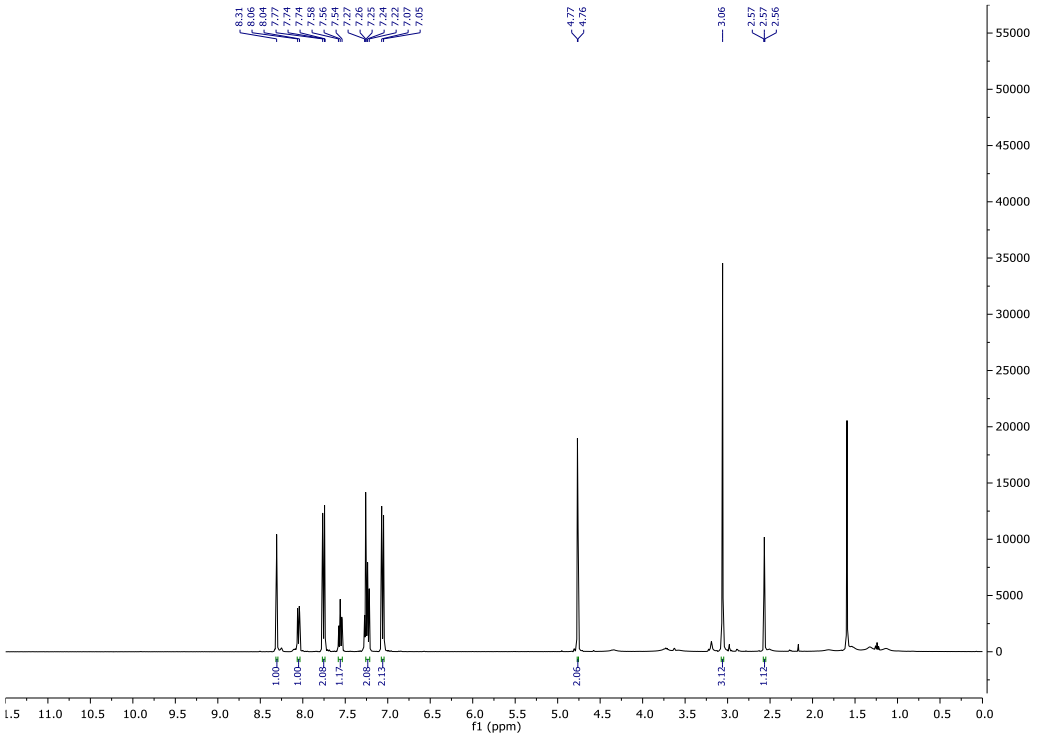


Figure 27. ^{1}H 400 MHz NMR spectrum of compound **15a** in $CDCl_3$.

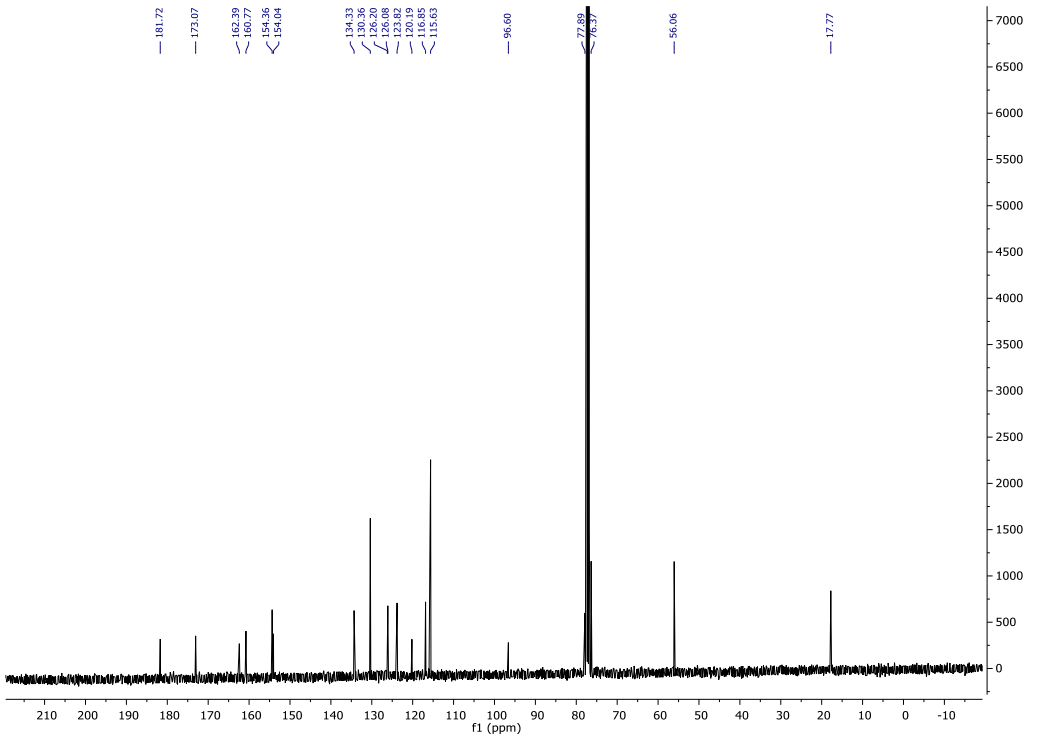


Figure 28. 100 MHz ^{13}C NMR spectrum of compound **15a** in $CDCl_3$.

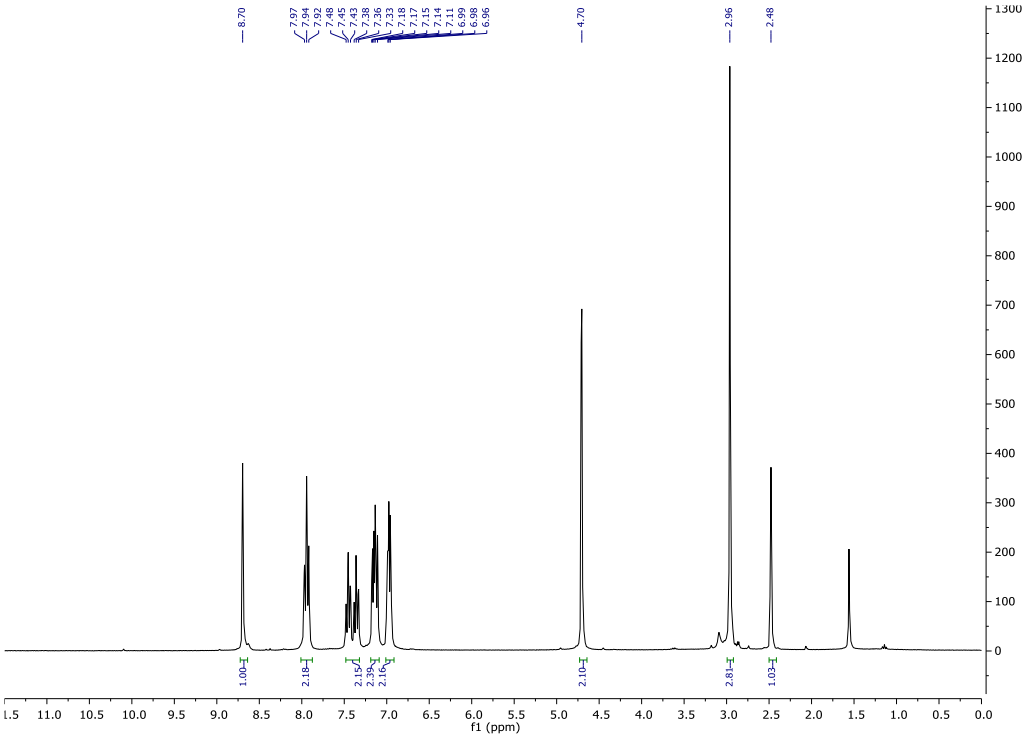


Figure 29. ^{1}H 300 MHz NMR spectrum of compound **15b** in $CDCl_3$.

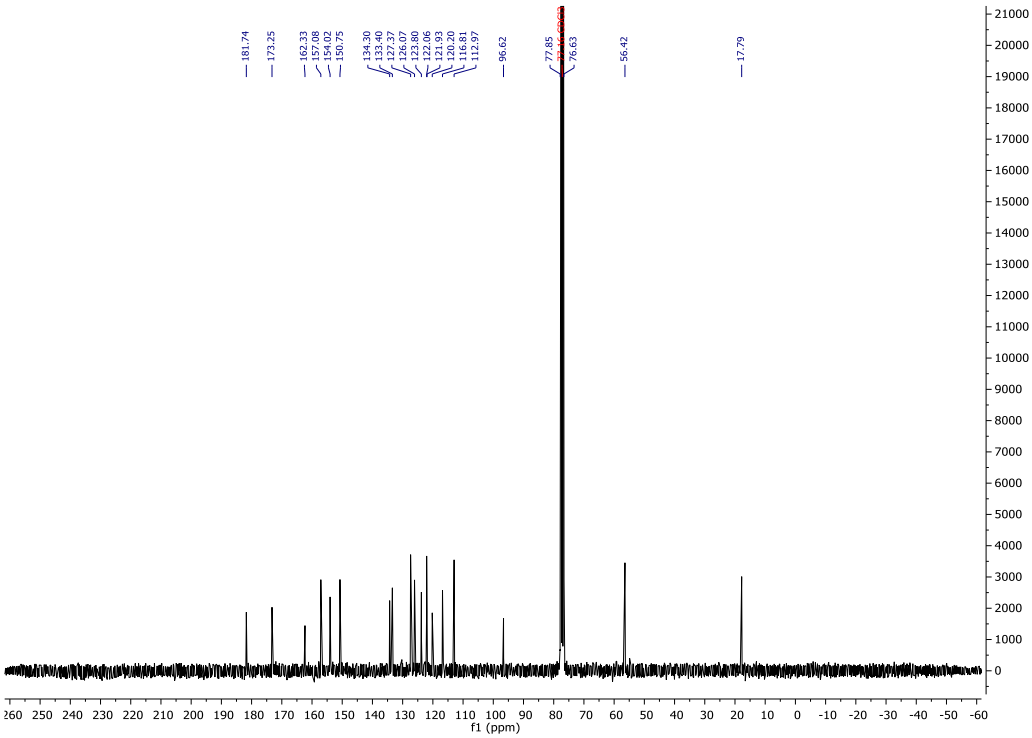


Figure 30. 75 MHz ^{13}C NMR spectrum of compound **15b** in $CDCl_3$.

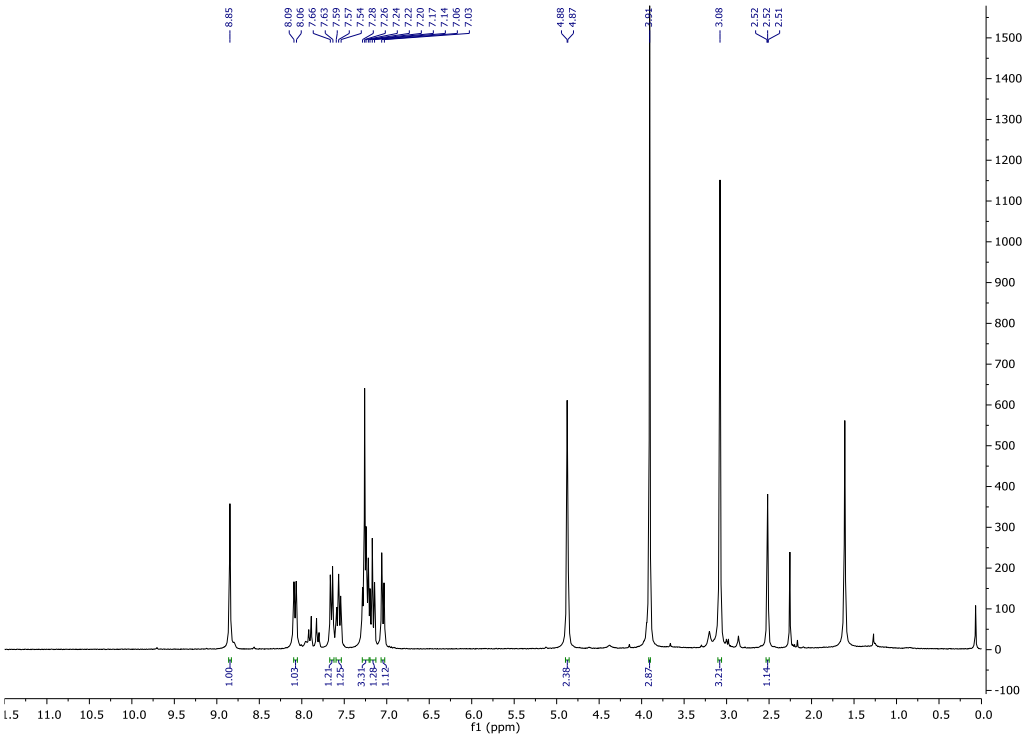


Figure 31. ^{1}H 300 MHz NMR spectrum of compound **15c** in $CDCl_3$.

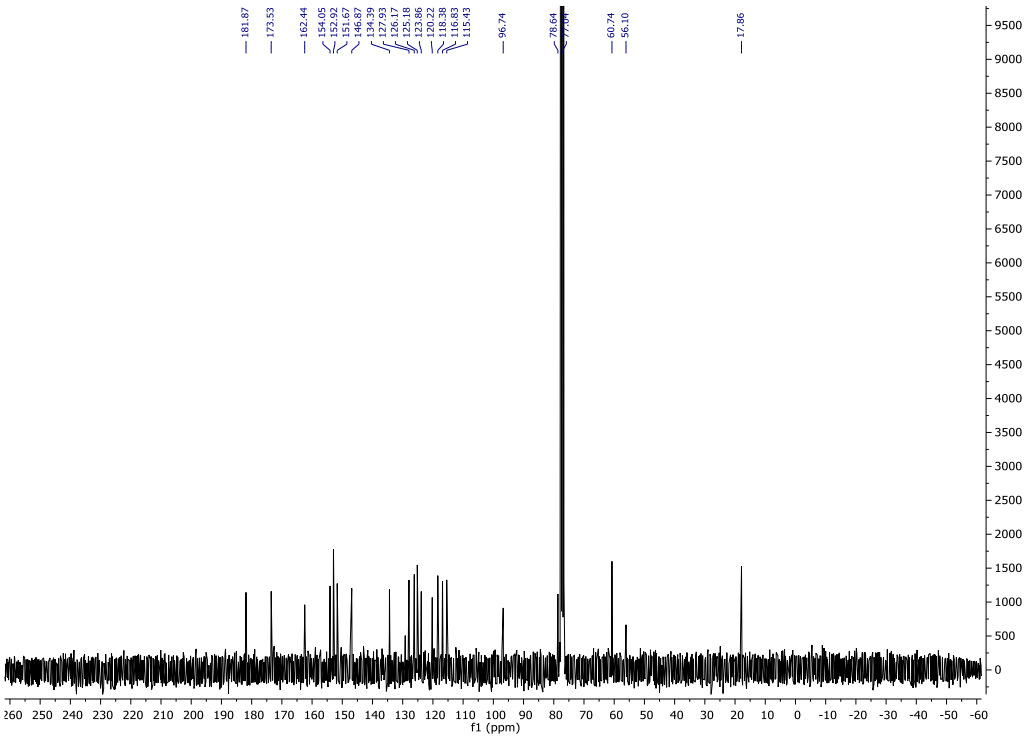


Figure 32. 75 MHz ^{13}C NMR spectrum of compound **15c** in $CDCl_3$.

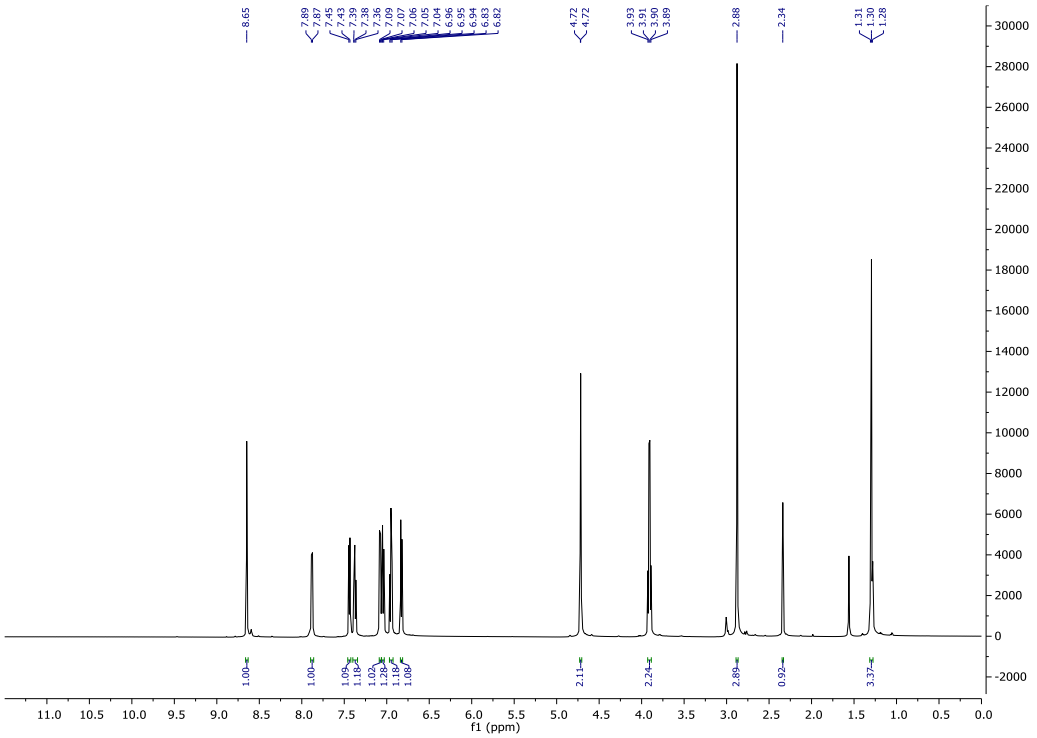


Figure 33. ^{1}H 600 MHz NMR spectrum of compound **15d** in $CDCl_3$.

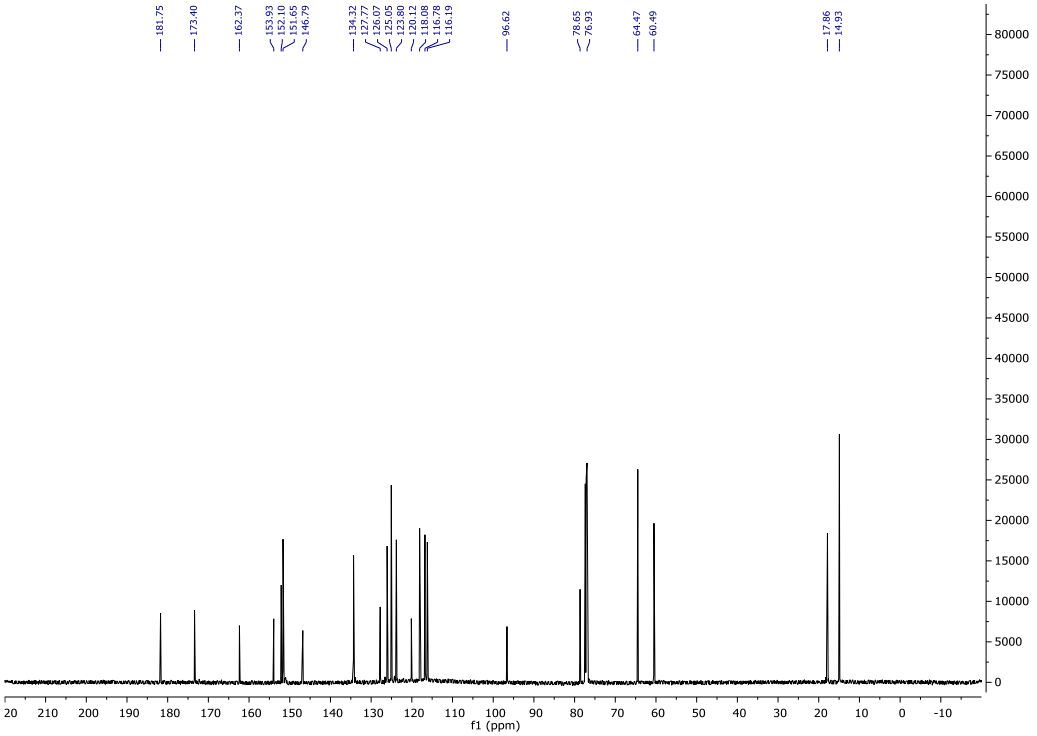


Figure 34. 150 MHz ^{13}C NMR spectrum of compound **15d** in $CDCl_3$.

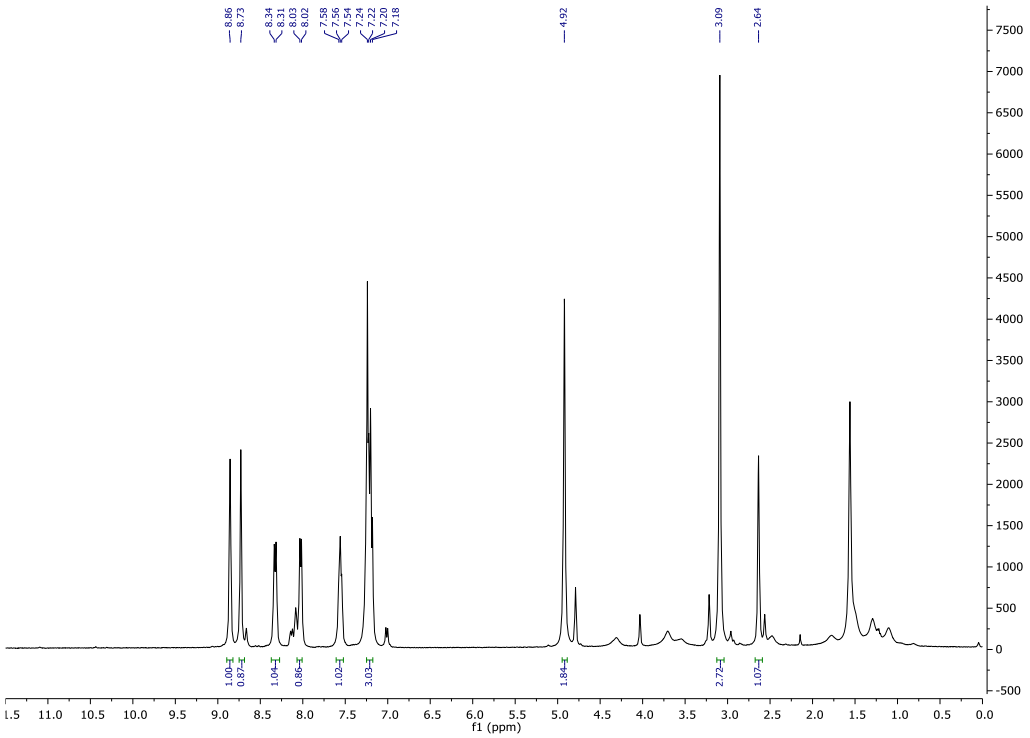


Figure 35. ^{1}H 400 MHz NMR spectrum of compound **15e** in $CDCl_3$.

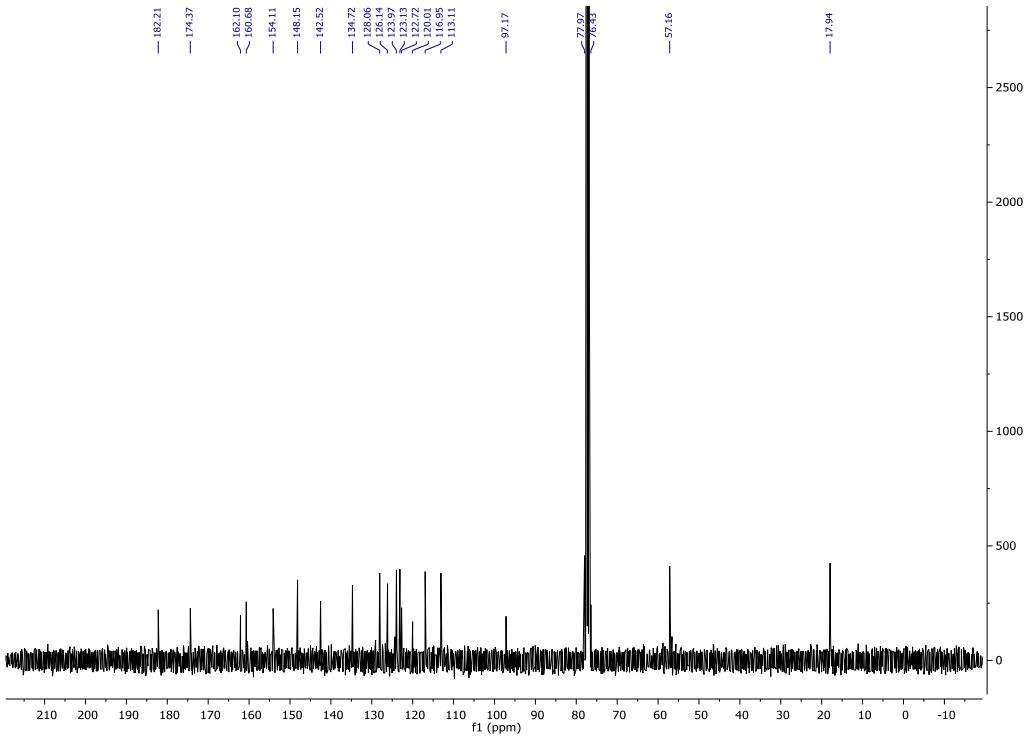


Figure 36. 100 MHz ^{13}C NMR spectrum of compound **15e** in $CDCl_3$.

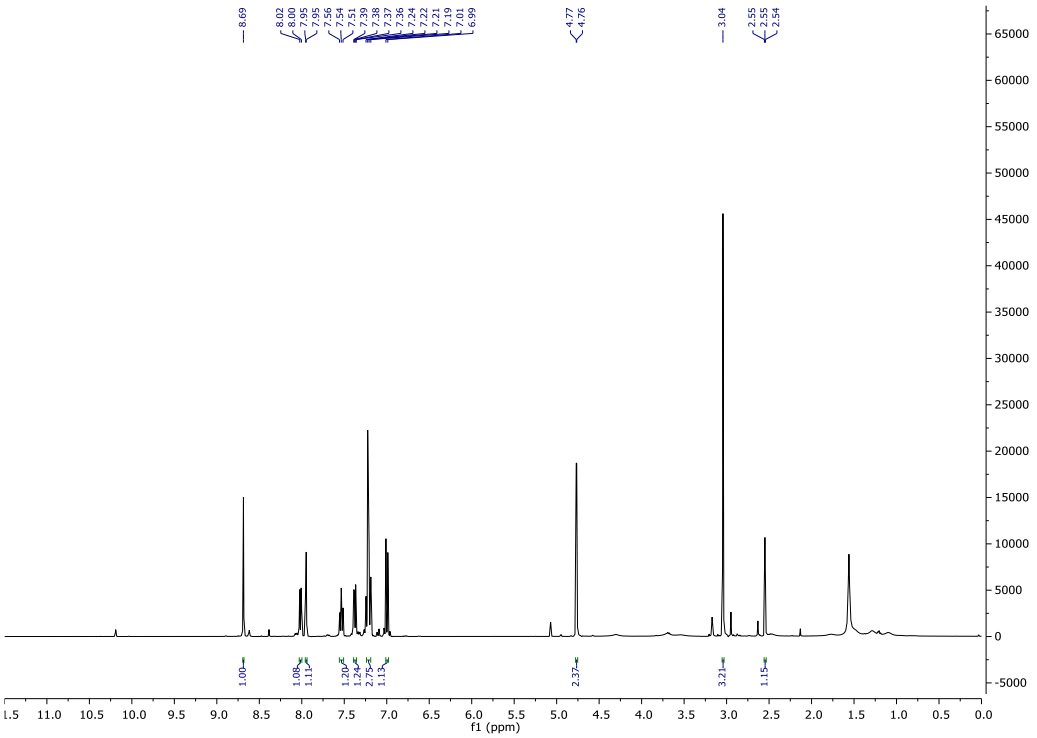


Figure 37. ^{1}H 600 MHz NMR spectrum of compound **15f** in $CDCl_3$.

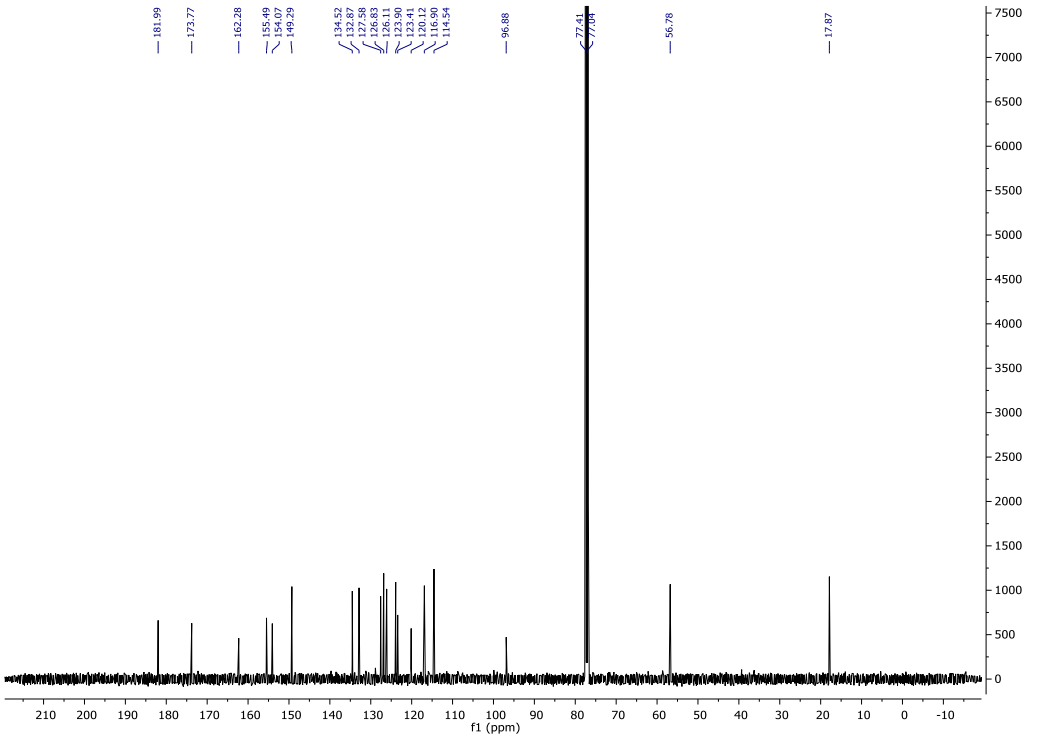


Figure 38. 150 MHz ^{13}C NMR spectrum of compound **15f** in $CDCl_3$.

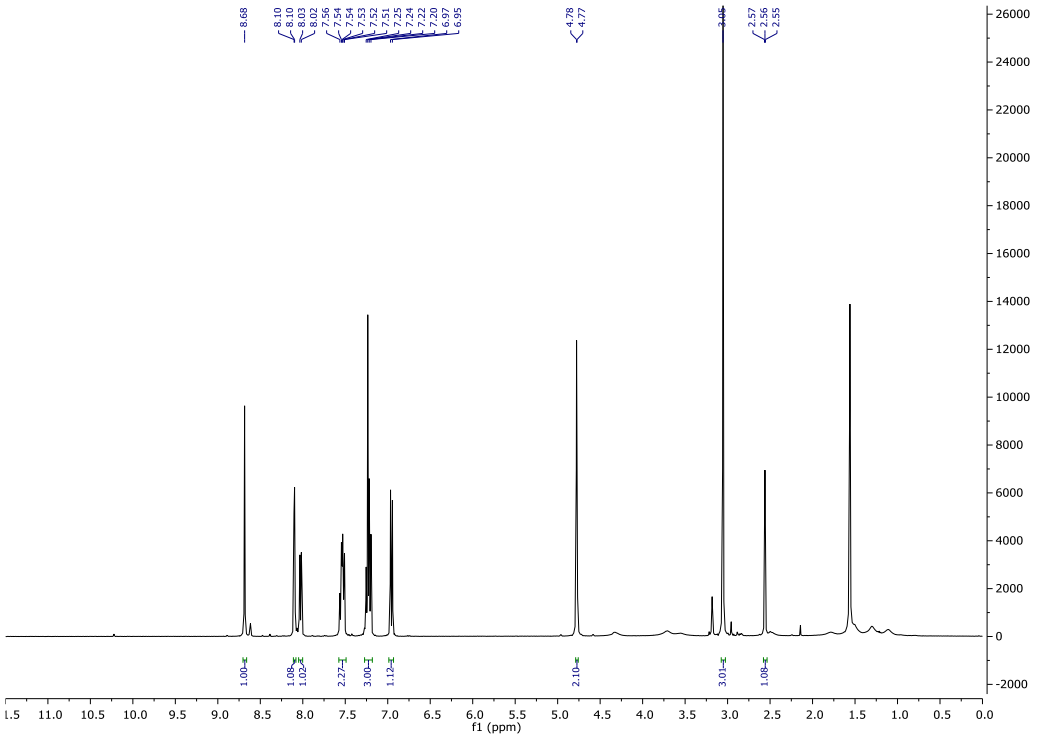


Figure 39. ^{1}H 400 MHz NMR spectrum of compound **15g** in $CDCl_3$.

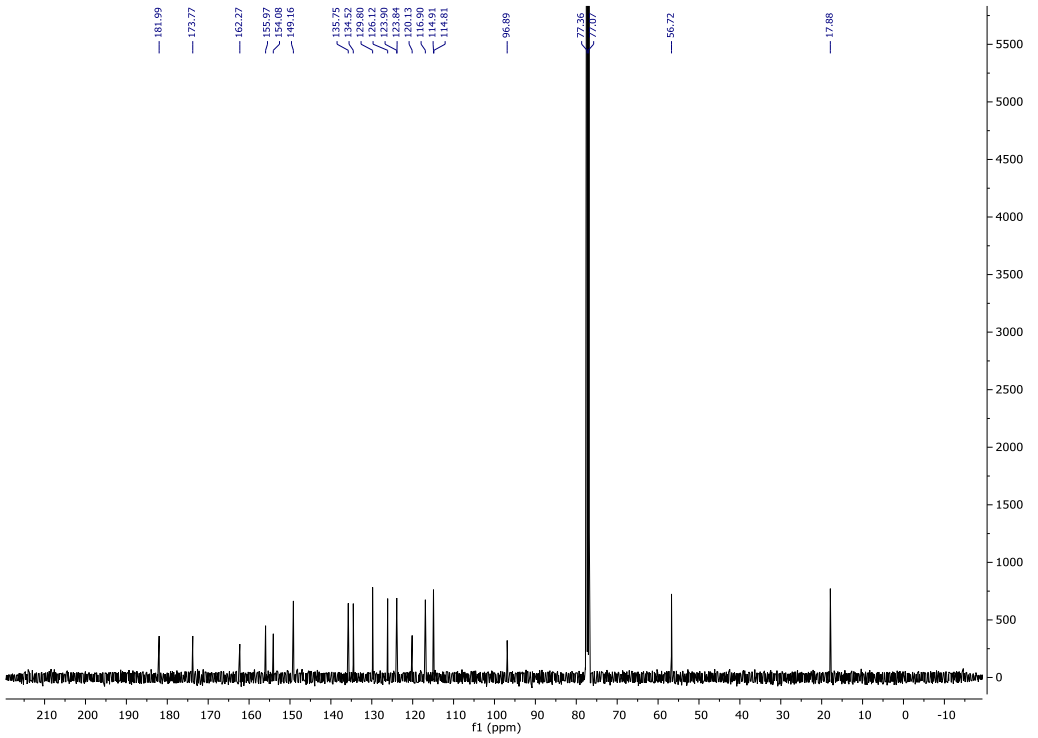
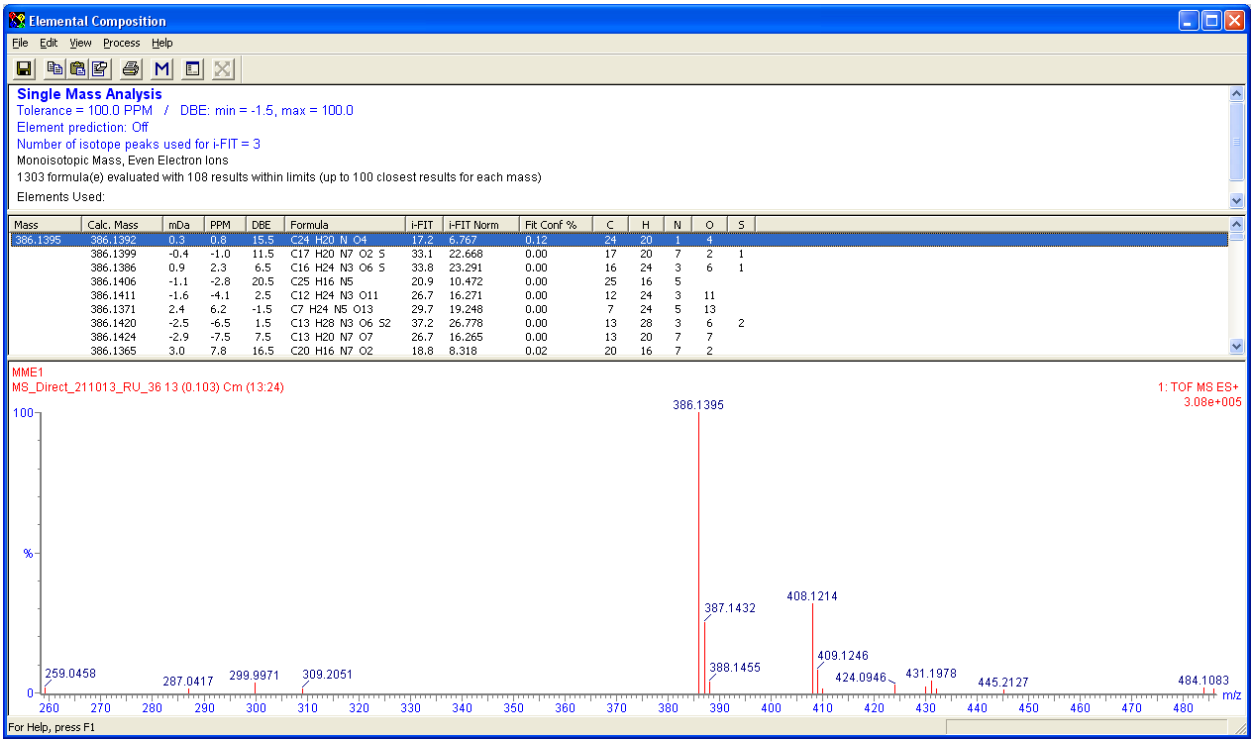


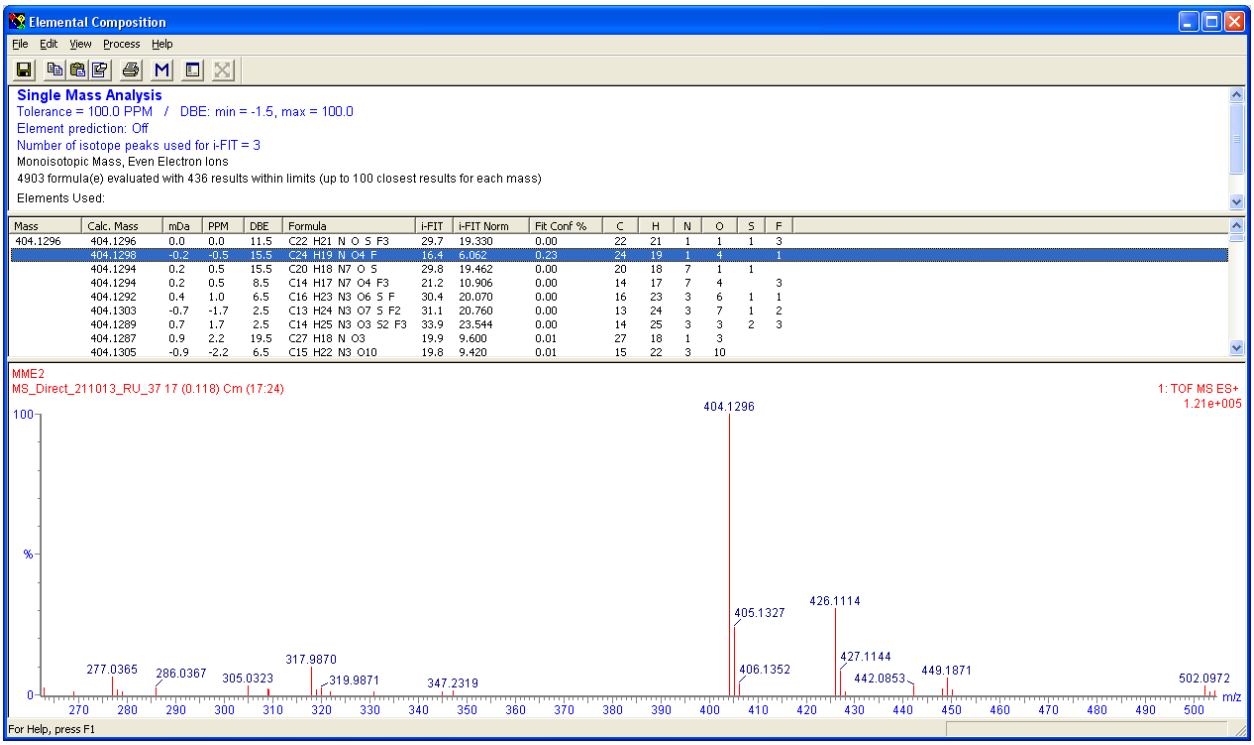
Figure 40. 100 MHz ^{13}C NMR spectrum of compound **15g** in $CDCl_3$.

HRMS Spectrometric data

9a



9b



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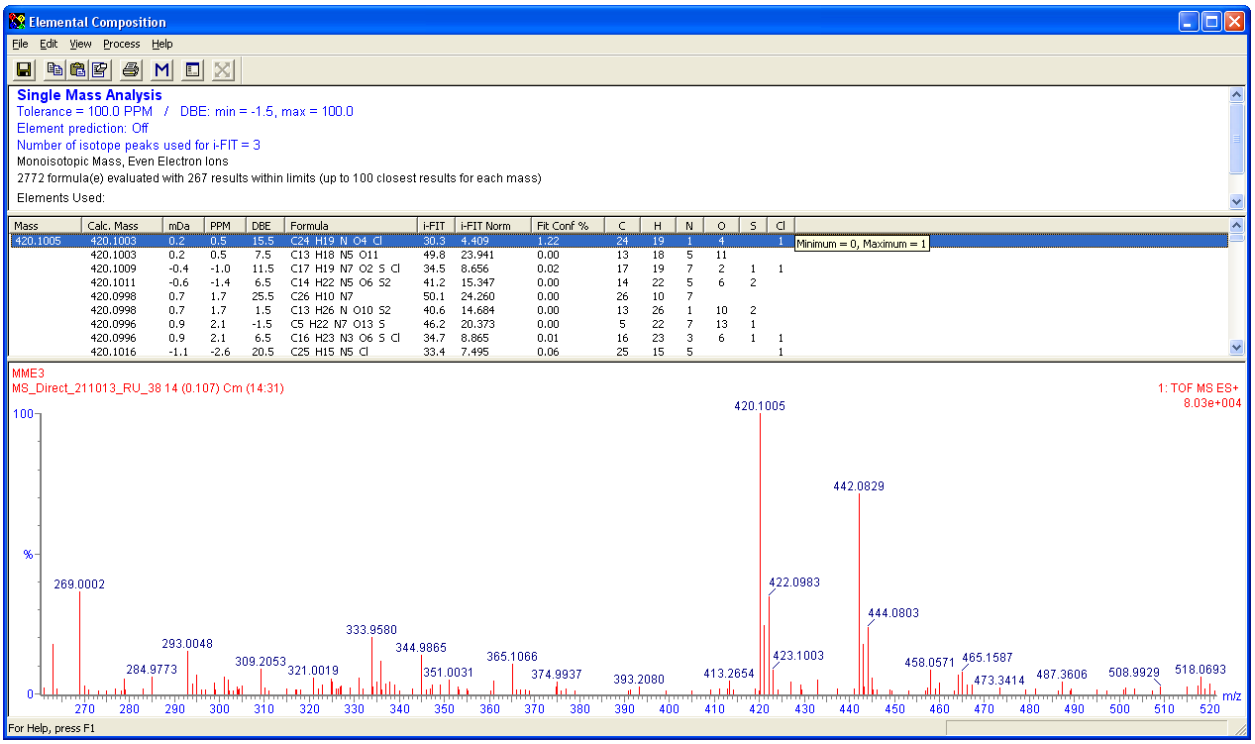

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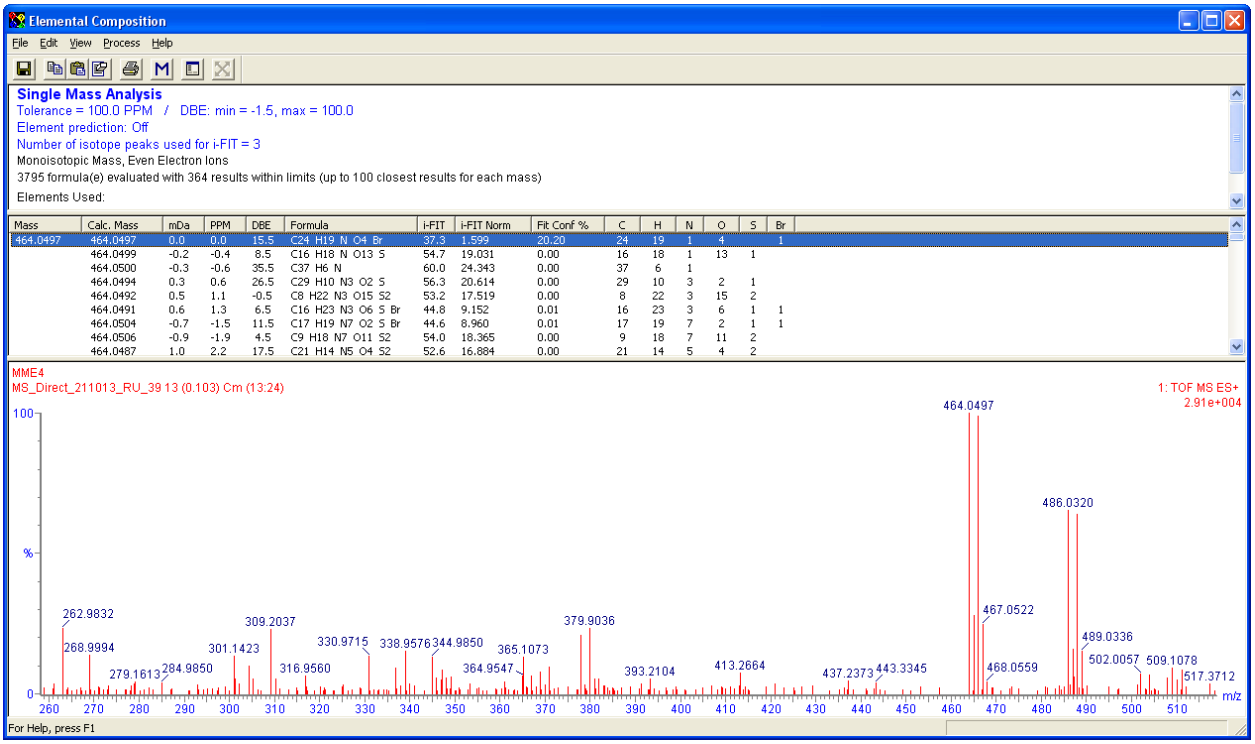
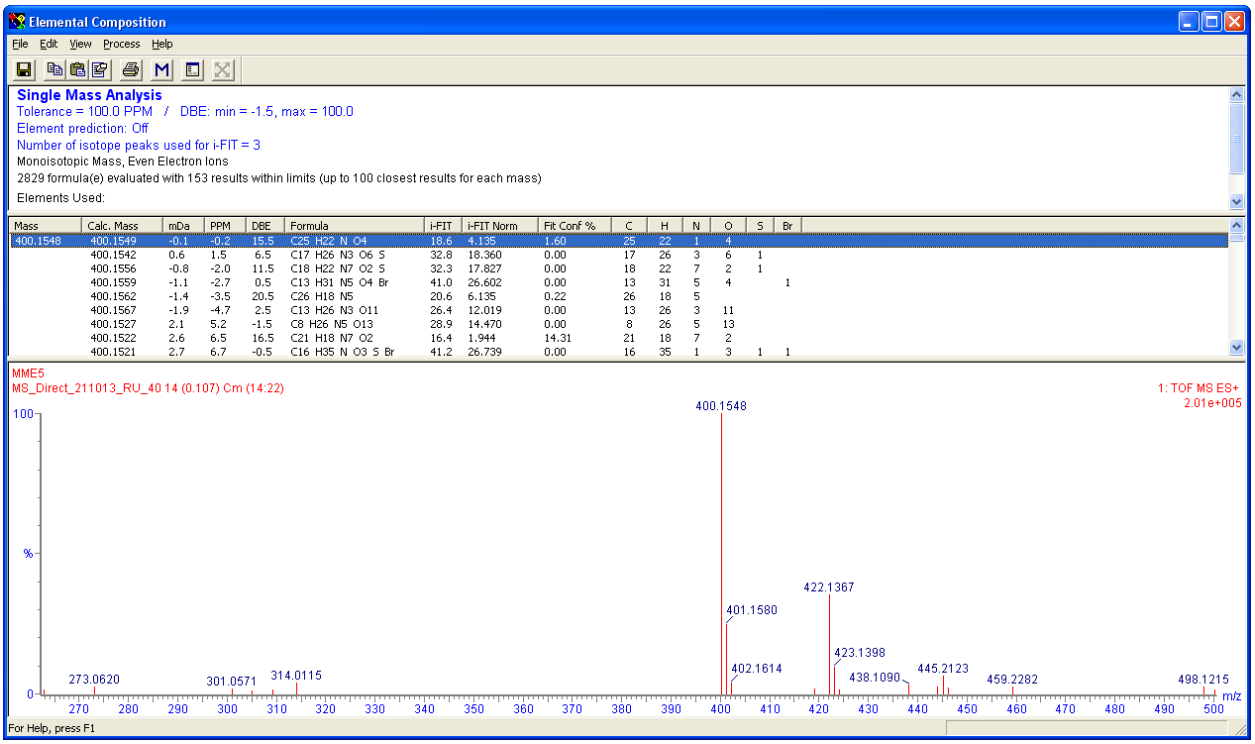


9e


Elemental Composition
File Edit View Process Help
Single Mass Analysis
Tolerance = 100.0 PPM / DBE: min = -1.5, max = 100.0
Element prediction: Off
Number of isotope peaks used for i-FIT = 3
Monoisotopic Mass, Even Electron Ions
2829 formula(e) evaluated with 153 results within limits (up to 100 closest results for each mass)
Elements Used:
Mass Calc. Mass mDa PPM DBE Formula i-FIT i-FIT Norm Fit Conf % C H N O S Br
400.1548 400.1549 -0.1 -0.2 15.5 C25 H22 N O4 18.6 4.135 1.60 25 22 1 4
400.1542 0.6 1.5 6.5 C17 H26 N3 O6 S 32.8 18.360 0.00 17 26 3 6 1
400.1556 -0.8 -2.0 11.5 C18 H22 N7 O2 S 32.3 17.827 0.00 18 22 7 2 1
400.1559 -1.1 -2.7 0.5 C13 H31 N5 O4 Br 41.0 26.602 0.00 13 31 5 4 1
400.1562 -1.4 -3.5 20.5 C26 H18 N5 20.6 6.135 0.22 26 18 5
400.1567 -1.9 -4.7 2.5 C13 H26 N3 O11 26.4 12.019 0.00 13 26 3 11
400.1527 2.1 5.2 -1.5 C8 H26 N5 O13 28.9 14.470 0.00 8 26 5 13
400.1522 2.6 6.5 16.5 C21 H18 N7 O2 16.4 1.944 14.31 21 18 7 2
400.1521 2.7 6.7 -0.5 C16 H35 N O3 S Br 41.2 26.739 0.00 16 35 1 3 1 1
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401.1580
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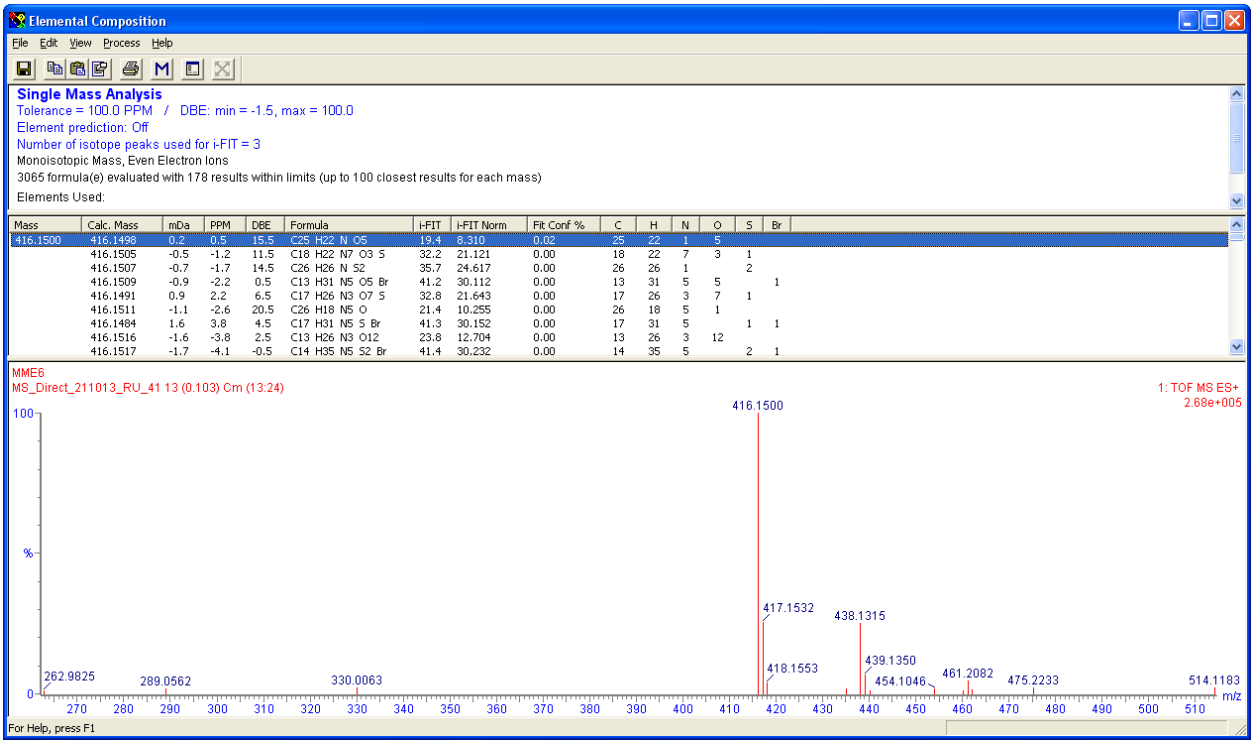
314.0115
m/z
For Help, press F1

9f


Elemental Composition
File Edit View Process Help
Single Mass Analysis
Tolerance = 100.0 PPM / DBE: min = -1.5, max = 100.0
Element prediction: Off
Number of isotope peaks used for i-FIT = 3
Monoisotopic Mass, Even Electron Ions
3065 formula(e) evaluated with 178 results within limits (up to 100 closest results for each mass)
Elements Used:
Mass Calc. Mass mDa PPM DBE Formula i-FIT i-FIT Norm Fit Conf % C H N O S Br
416.1500 416.1498 0.2 0.5 15.5 C25 H22 N O5 19.4 8.310 0.02 25 22 1 5
416.1505 -0.5 -1.2 11.5 C18 H22 N7 O3 S 32.2 21.121 0.00 18 22 7 3 1
416.1507 -0.7 -1.7 14.5 C26 H26 N S2 35.7 24.617 0.00 26 26 1 2
416.1509 -0.9 -2.2 0.5 C13 H31 N5 O5 Br 41.2 30.112 0.00 13 31 5 5 1
416.1491 0.9 2.2 6.5 C17 H26 N3 O7 S 32.8 21.643 0.00 17 26 3 7 1
416.1511 -1.1 -2.6 20.5 C26 H18 N5 O 21.4 10.255 0.00 26 18 5 1
416.1484 1.6 3.8 4.5 C17 H31 N5 S Br 41.3 30.152 0.00 17 31 5 1 1
416.1516 -1.6 -3.8 2.5 C13 H26 N3 O12 23.8 12.704 0.00 13 26 3 12
416.1517 -1.7 -4.1 -0.5 C14 H35 N5 S2 Br 41.4 30.232 0.00 14 35 5 2 1
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439.1350
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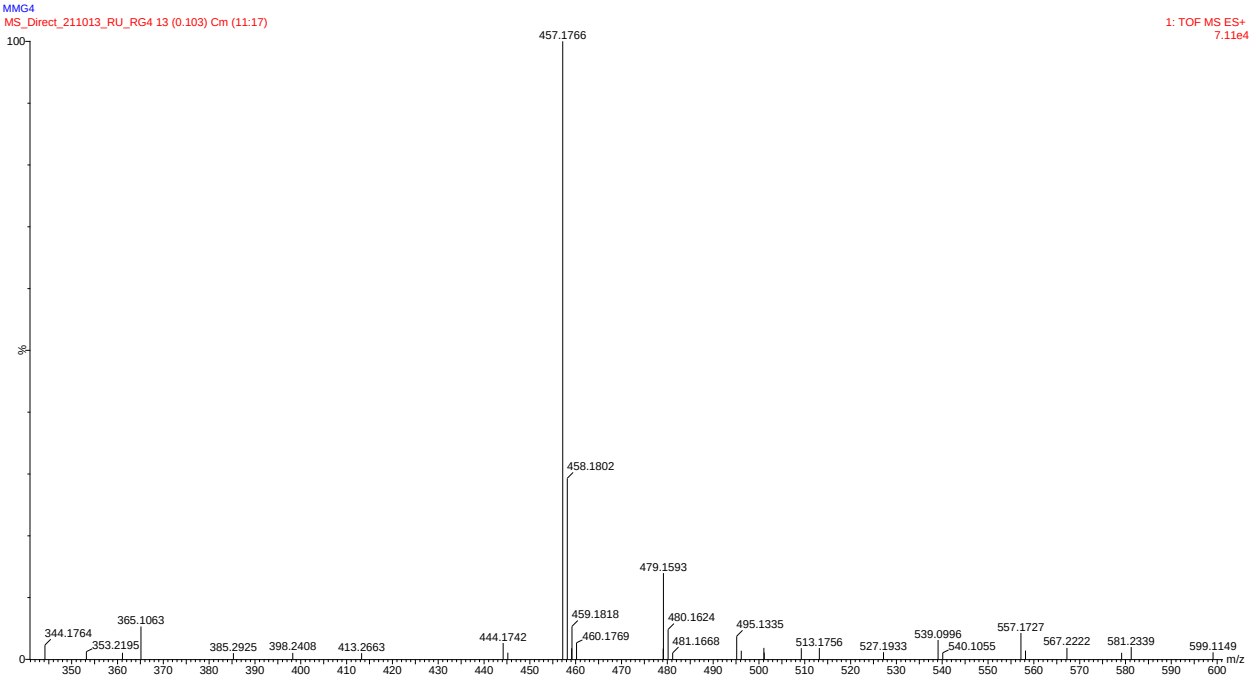
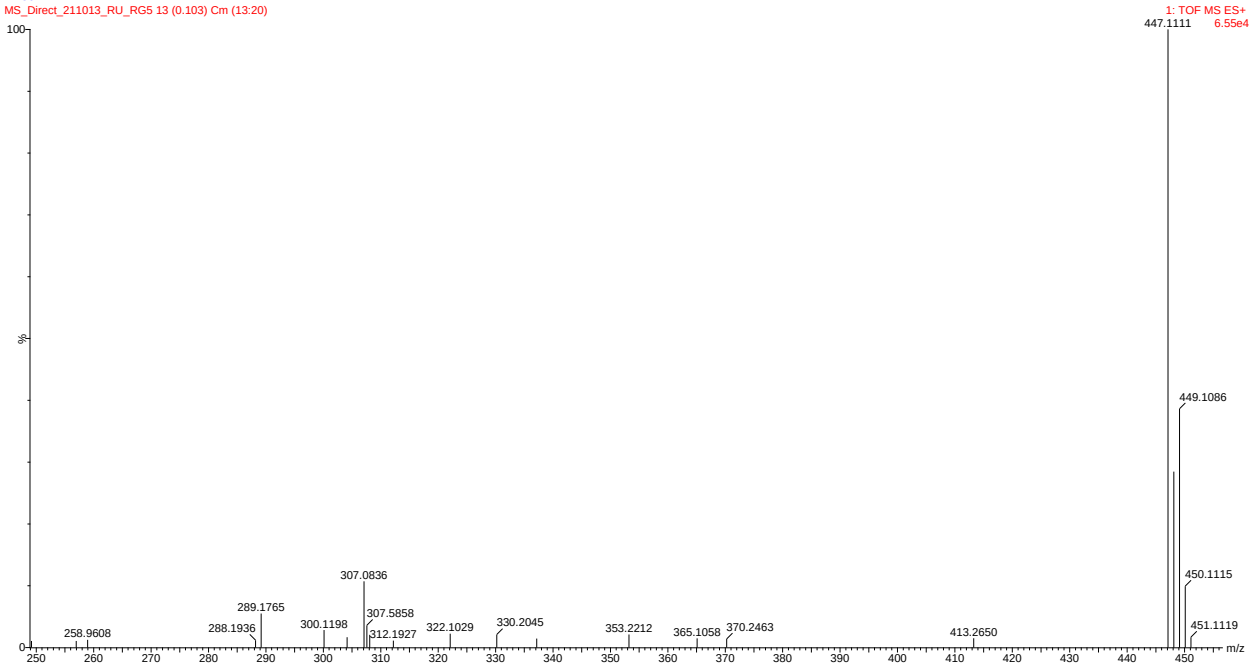
461.2082
475.2233
514.1183
262.9825
289.0562
330.0063
m/z
For Help, press F1

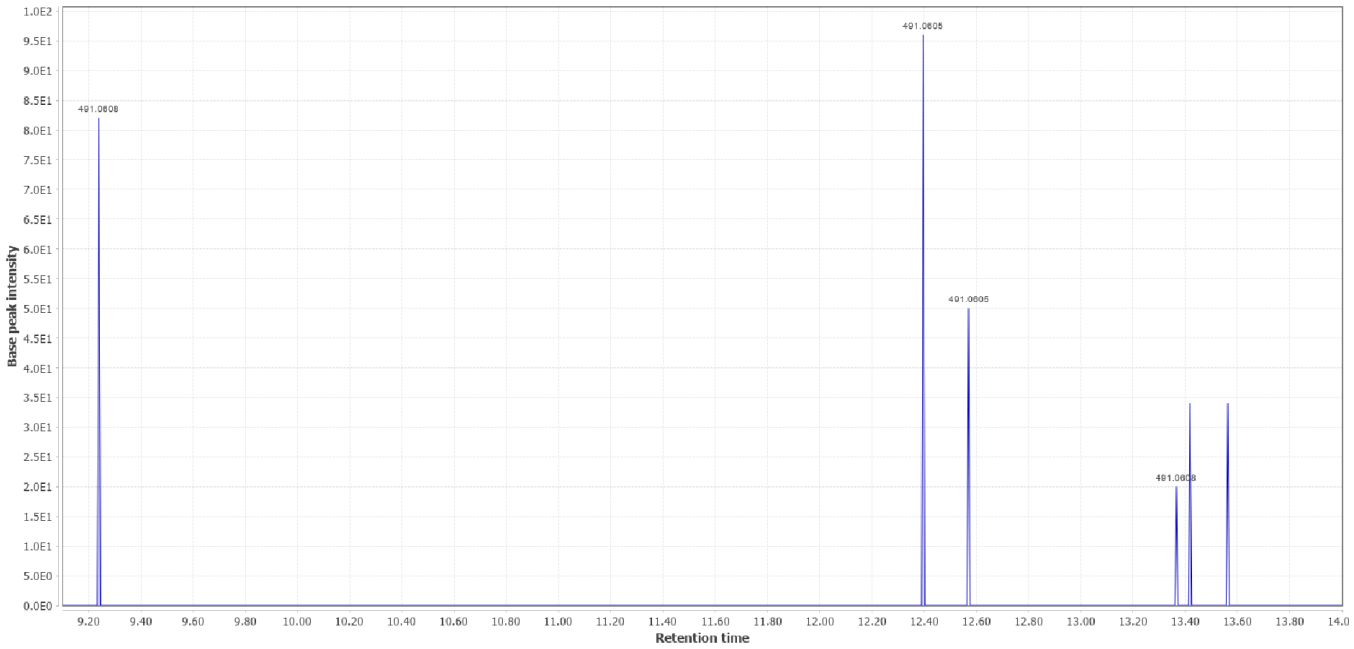
13a



13b



13c



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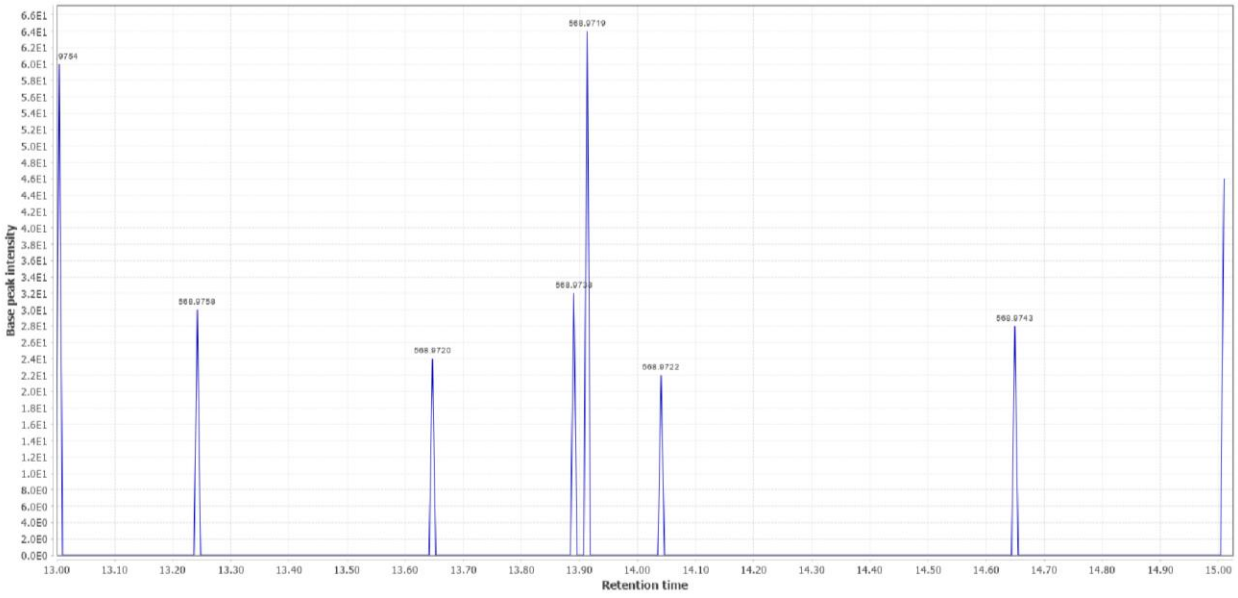
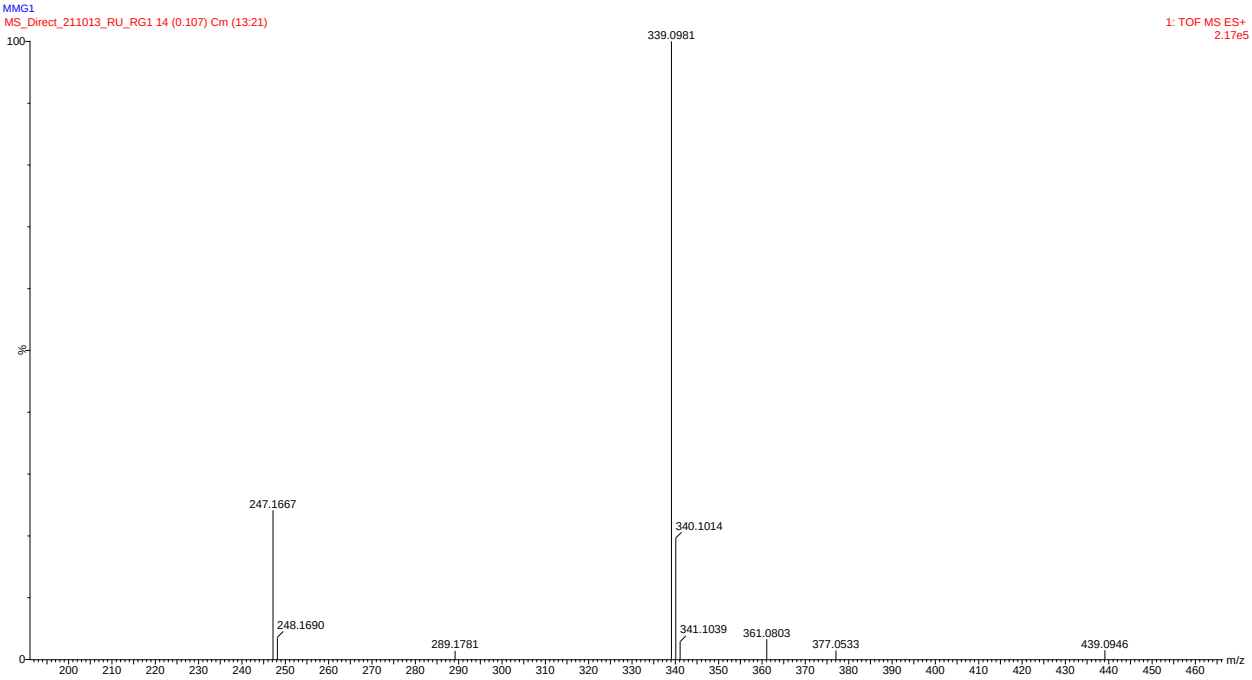


13e



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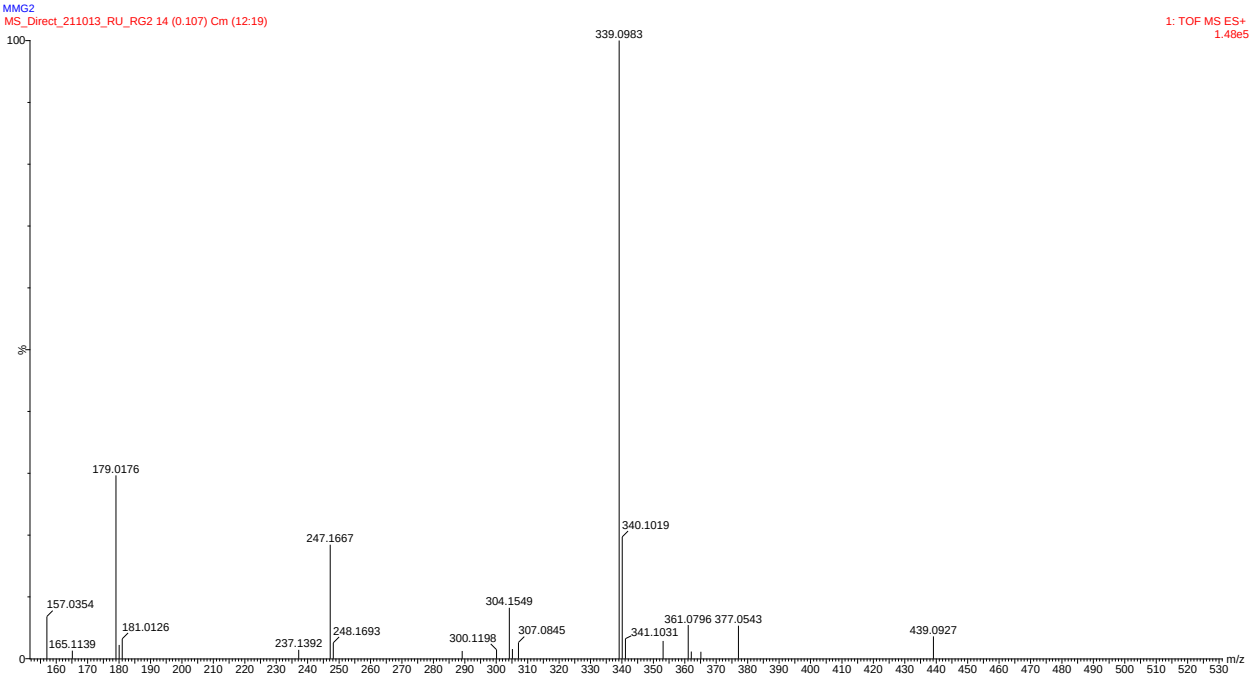
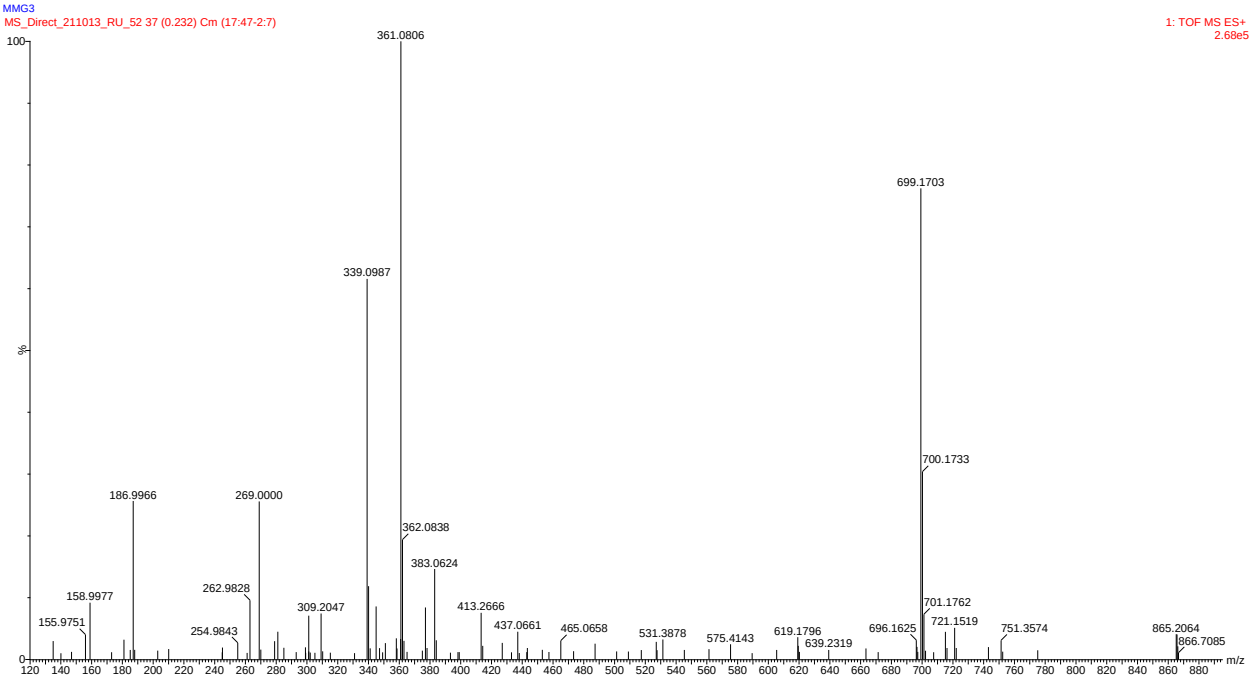


13g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100
%
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700.1733
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269.0000
362.0838
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158.9977
262.9828
309.2047
413.2666
701.1762
155.9751
254.9843
437.0661
465.0658
721.1519
751.3574
531.3878
575.4143
619.1796
639.2319
696.1625
865.2064
866.7085
m/z

15a

Elemental Composition

File Edit View Process Help

Single Mass Analysis

Tolerance = 100.0 PPM / DBE: min = -1.5, max = 100.0

Element prediction: Off

Number of isotope peaks used for i-FIT = 3

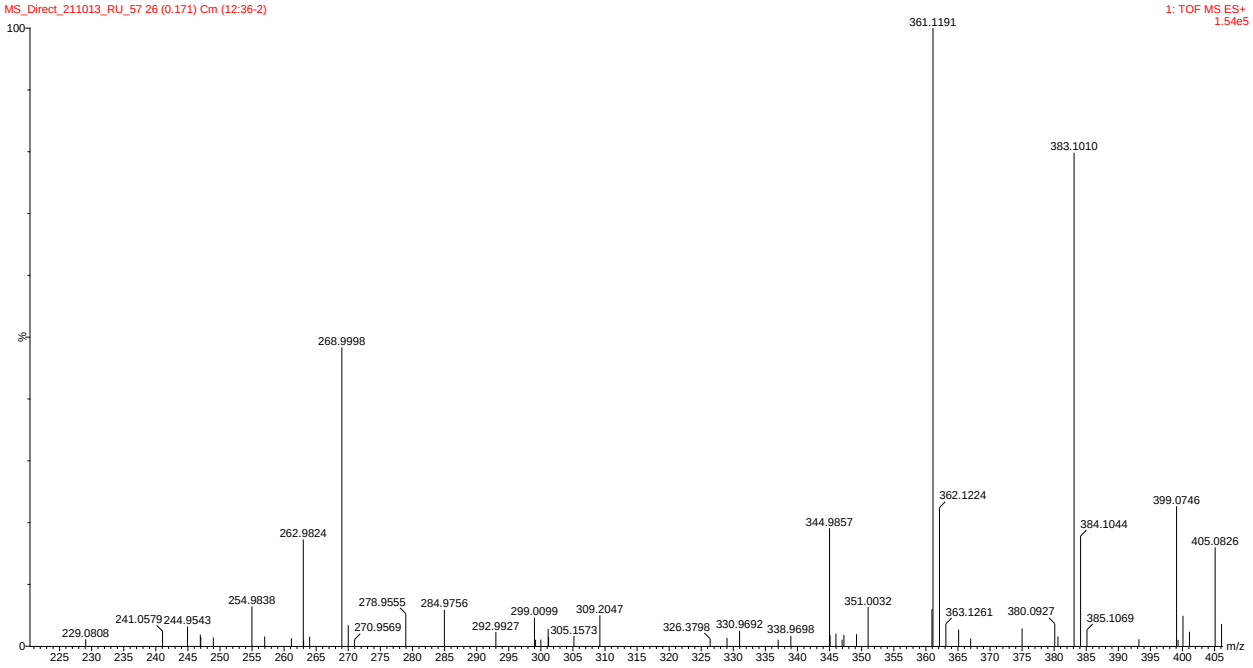
Monoisotopic Mass, Even Electron Ions

2304 formula(e) evaluated with 135 results within limits (up to 100 closest results for each mass)

Elements Used:

Mass	Calc. Mass	mDa	PPM	DBE	Formula	i-FIT	i-FIT Norm	Fit Conf %	C	H	N	O	S	Br
361.1191	361.1188	0.3	0.8	14.5	C21 H17 N2 O4	16.3	1.157	31.45	21	17	2	4		
	361.1199	-0.8	-2.2	-0.5	C9 H26 N6 O4 Br	40.3	25.166	0.00	9	26	6	4		1
	361.1182	0.9	2.5	5.5	C13 H21 N4 O6 S	32.5	17.389	0.00	13	21	4	6	1	
	361.1201	-1.0	-2.8	2.5	C17 H30 O S Br	40.5	25.355	0.00	17	30		1	1	1
	361.1202	-1.1	-3.0	19.5	C22 H13 N6	20.7	5.589	0.37	22	13	6			
	361.1207	-1.6	-4.4	1.5	C9 H21 N4 O11	27.8	12.630	0.00	9	21	4	11		
	361.1168	2.3	6.4	0.5	C12 H25 O10 S	33.3	18.118	0.00	12	25		10	1	
	361.1167	2.4	6.6	7.5	C20 H26 O Br	40.4	25.267	0.00	20	26		1		1
	361.1216	-2.5	-6.9	0.5	C10 H25 N4 O6 S2	35.8	20.652	0.00	10	25	4	6	2	
	361.1161	3.0	8.3	-1.5	C12 H30 N2 O3 S Br	40.5	25.332	0.00	12	30	2	3	1	1
	361.1222	-3.1	-8.6	9.5	C18 H21 N2 O4 S	31.9	16.755	0.00	18	21	2	4	1	
	361.1157	3.4	9.4	9.5	C17 H21 N4 O S2	35.3	20.125	0.00	17	21	4	1	2	
	361.1226	-3.5	-9.7	-1.5	C13 H30 O6 Br	40.5	25.360	0.00	13	30		6		1
	361.1229	-3.8	-10.5	18.5	C26 H17 O2	20.1	4.965	0.70	26	17		2		
	361.1148	4.3	11.9	10.5	C16 H17 N4 O6	21.9	6.743	0.12	16	17	4	6		
	361.1235	-4.4	-12.2	14.5	C19 H17 N6 S	31.6	16.431	0.00	19	17	6		1	
	361.1143	4.8	13.3	4.5	C16 H25 O5 S2	35.5	20.363	0.00	16	25		5	2	
	361.1239	-4.8	-13.3	3.5	C14 H26 N4 O2 Br	40.4	25.223	0.00	14	26	4	2		1
	361.1142	4.9	13.6	1.5	C8 H21 N6 O8 S	33.6	18.438	0.00	8	21	6	8	1	

MMH1



15b

Elemental Composition

File Edit View Process Help

Single Mass Analysis

Tolerance = 100.0 PPM / DBE: min = -1.5, max = 100.0

Element prediction: Off

Number of isotope peaks used for i-FIT = 3

Monoisotopic Mass, Even Electron Ions

2304 formula(e) evaluated with 135 results within limits (up to 100 closest results for each mass)

Elements Used:

Mass	Calc. Mass	mDa	PPM	DBE	Formula	i-FIT	i-FIT Norm	Fit Conf %	C	H	N	O	S	Br
361.1190	361.1188	0.2	0.6	14.5	C21 H17 N2 O4	70.3	0.254	77.57	21	17	2	4		
	361.1182	0.8	2.2	5.5	C13 H21 N4 O6 S	89.5	19.513	0.00	13	21	4	6	1	
	361.1199	-0.9	-2.5	-0.5	C9 H26 N6 O4 Br	97.3	27.264	0.00	9	26	6	4		1
	361.1201	-1.1	-3.0	2.5	C17 H30 O 5 Br	97.5	27.488	0.00	17	30		1	1	1
	361.1202	-1.2	-3.3	19.5	C22 H13 N6	77.0	6.945	0.10	22	13	6			
	361.1207	-1.7	-4.7	1.5	C9 H21 N4 O11	81.9	11.865	0.00	9	21	4	11		
	361.1168	2.2	6.1	0.5	C12 H25 O10 S	90.2	20.166	0.00	12	25		10	1	
	361.1167	2.3	6.4	7.5	C20 H26 O Br	97.4	27.387	0.00	20	26		1		1
	361.1216	-2.6	-7.2	0.5	C10 H25 N4 O6 S2	92.9	22.886	0.00	10	25	4	6	2	
	361.1161	2.9	8.0	-1.5	C12 H30 N2 O3 S Br	97.5	27.457	0.00	12	30	2	3	1	1
	361.1222	-3.2	-8.9	9.5	C18 H21 N2 O4 S	88.7	18.718	0.00	18	21	2	4	1	
	361.1157	3.3	9.1	9.5	C17 H21 N4 O S2	92.3	22.309	0.00	17	21	4	1	2	
	361.1226	-3.6	-10.0	-1.5	C13 H30 O6 Br	97.5	27.492	0.00	13	30		6		1
	361.1229	-3.9	-10.8	18.5	C26 H17 O2	80.5	10.462	0.00	26	17		2		
	361.1148	4.2	11.6	10.5	C16 H17 N4 O6	76.9	6.883	0.10	16	17	4	6		
	361.1235	-4.5	-12.5	14.5	C19 H17 N6 S	88.4	18.390	0.00	19	17	6		1	
	361.1143	4.7	13.0	4.5	C16 H25 O5 S2	92.6	22.535	0.00	16	25		5	2	
	361.1142	4.8	13.3	1.5	C8 H21 N6 O8 S	90.6	20.587	0.00	8	21	6	8	1	
	361.1239	-4.9	-13.6	3.5	C14 H26 N4 O2 Br	97.4	27.332	0.00	14	26	4	2		1

MMH2

2 Microsoft... | Iperius Back... | ACQUITY UP... | Phenolics_T3... | Data | System (C:) | MULTIBOOT ... | SYNAPT G2 ... | Experiment ... | MM_RU_211... | Elemental C

MMH2

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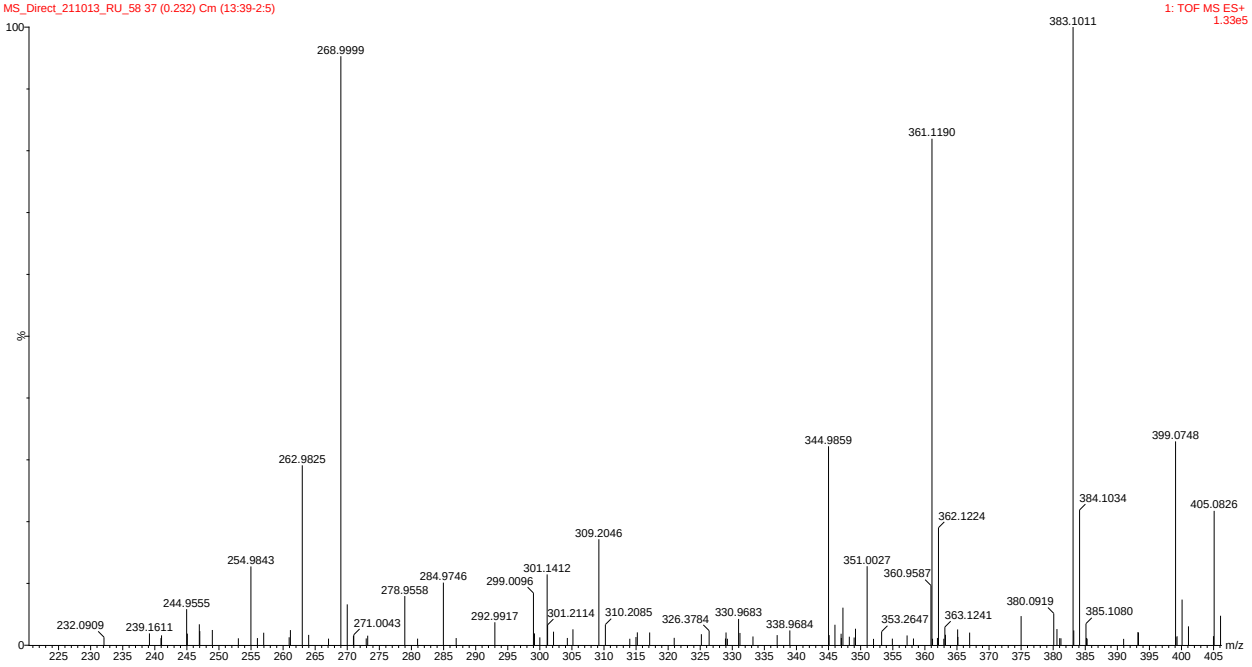

15c

Elemental Composition

File Edit View Process Help

Single Mass Analysis

Tolerance = 100.0 PPM / DBE: min = -1.5, max = 100.0

Element prediction: Off

Number of isotope peaks used for i-FIT = 3

Monoisotopic Mass, Even Electron Ions

2733 formula(e) evaluated with 165 results within limits (up to 100 closest results for each mass)

Elements Used:

Mass	Calc. Mass	mDa	PPM	DBE	Formula	i-FIT	i-FIT Norm	Fit Conf %	C	H	N	O	S	Br
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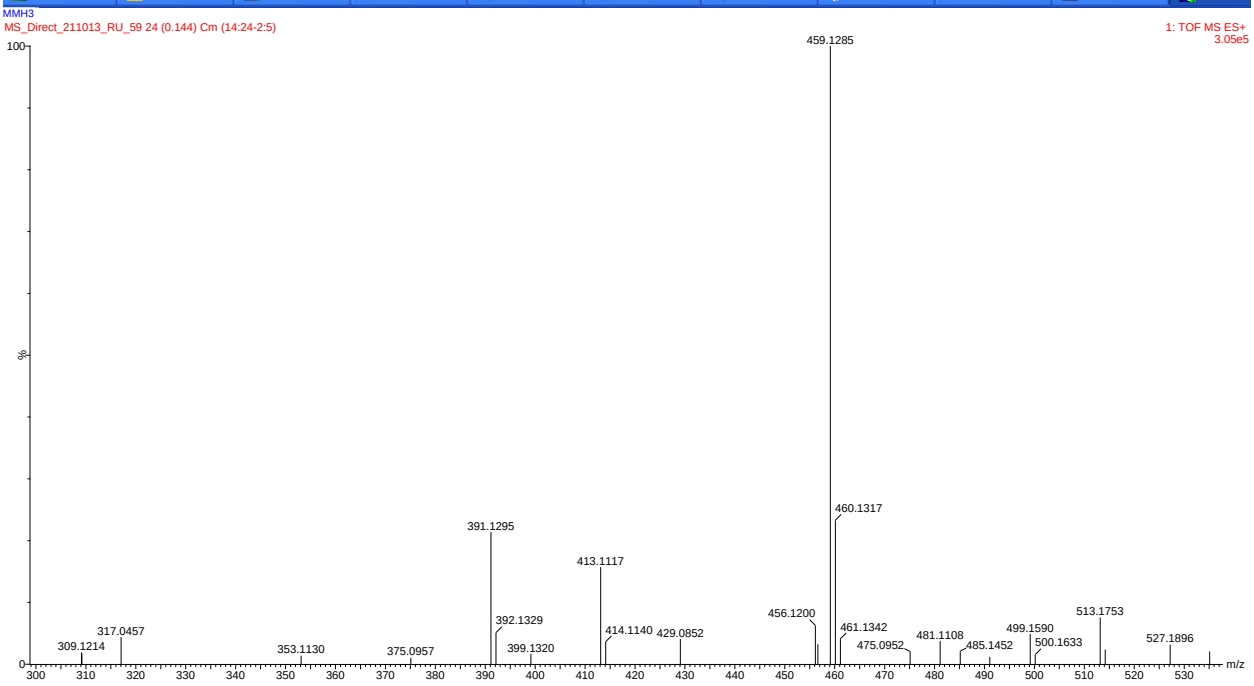
	391.1287	0.8	2.0	5.5	C14 H23 N4 O7 S	32.8	4.683	0.93	14	23	4	7	1	
	391.1303	-0.8	-2.0	13.5	C23 H23 N2 S2	32.7	4.581	1.02	23	23	2		2	
	391.1305	-1.0	-2.6	-0.5	C10 H28 N6 O5 Br	35.6	7.536	0.05	10	28	6	5		1
	391.1306	-1.1	-2.8	2.5	C18 H32 O2 S Br	33.9	5.837	0.29	18	32		2	1	1
	391.1307	-1.2	-3.1	19.5	C23 H15 N6 O	31.7	3.612	2.70	23	15	6	1		
	391.1280	1.5	3.8	3.5	C14 H28 N6 S Br	35.5	7.369	0.06	14	28	6		1	1
	391.1312	-1.7	-4.3	1.5	C10 H23 N4 O12	32.0	3.931	1.96	10	23	4	12		
	391.1313	-1.8	-4.6	-1.5	C11 H32 N6 S2 Br	36.3	8.172	0.03	11	32	6		2	1
	391.1274	2.1	5.4	0.5	C13 H27 O11 S	32.0	3.875	2.07	13	27		11	1	
	391.1273	2.2	5.6	7.5	C21 H28 O2 Br	33.9	5.764	0.31	21	28		2		1
	391.1269	2.6	6.6	18.5	C26 H19 N2 S	32.1	4.000	1.83	26	19	2		1	
	391.1321	-2.6	-6.6	0.5	C11 H27 N4 O7 S2	33.9	5.837	0.29	11	27	4	7	2	
	391.1266	2.9	7.4	-1.5	C13 H32 N2 O4 S Br	34.4	6.252	0.19	13	32	2	4	1	1
	391.1262	3.3	8.4	9.5	C18 H23 N4 O2 S2	33.2	5.094	0.61	18	23	4	2	2	
	391.1328	-3.3	-8.4	9.5	C19 H23 N2 O5 S	32.2	4.071	1.71	19	23	2	5	1	
	391.1331	-3.6	-9.2	-1.5	C14 H32 O7 Br	33.9	5.822	0.30	14	32		7		1
	391.1334	-3.9	-10.0	18.5	C27 H19 O3	31.4	3.259	3.84	27	19		3		
	391.1254	4.1	10.5	10.5	C17 H19 N4 O7	31.5	3.405	3.32	17	19	4	7		

MMH3



15d

Elemental Composition

File Edit View Process Help

Single Mass Analysis

Tolerance = 100.0 PPM / DBE: min = -1.5, max = 100.0

Element prediction: Off

Number of isotope peaks used for i-FIT = 3

Monoisotopic Mass, Even Electron Ions

2932 formula(e) evaluated with 170 results within limits (up to 100 closest results for each mass)

Elements Used:

Mass	Calc. Mass	mDa	PPM	DBE	Formula	i-FIT	i-FIT Norm	Fit Conf %	C	H	N	O	S	Br
405.1457	405.1459	-0.2	-0.5	13.5	C24 H25 N2 S2	73.2	23.875	0.00	24	25	2		2	
	405.1461	-0.4	-1.0	-0.5	C11 H30 N6 O5 Br	78.5	29.140	0.00	11	30	6	5		1
	405.1463	-0.6	-1.5	2.5	C19 H34 O2 S Br	78.7	29.380	0.00	19	34		2	1	1
	405.1450	0.7	1.7	14.5	C23 H21 N2 O5	56.6	7.240	0.07	23	21	2	5		
	405.1464	-0.7	-1.7	19.5	C24 H17 N6 O	58.7	9.383	0.01	24	17	6	1		
	405.1469	-1.2	-3.0	1.5	C11 H25 N4 O12	61.3	11.982	0.00	11	25	4	12		
	405.1470	-1.3	-3.2	-1.5	C12 H34 N6 S2 Br	78.6	29.261	0.00	12	34	6		2	1
	405.1444	1.3	3.2	5.5	C15 H25 N4 O7 S	70.4	21.069	0.00	15	25	4	7	1	
	405.1436	2.1	5.2	3.5	C15 H30 N6 S Br	78.5	29.206	0.00	15	30	6		1	1
	405.1478	-2.1	-5.2	0.5	C12 H29 N4 O7 S2	73.9	24.549	0.00	12	29	4	7	2	
	405.1431	2.6	6.4	0.5	C14 H29 O11 S	71.0	21.683	0.00	14	29		11	1	
	405.1484	-2.7	-6.7	9.5	C20 H25 N2 O5 S	69.8	20.475	0.00	20	25	2	5	1	
	405.1429	2.8	6.9	7.5	C22 H30 O2 Br	78.6	29.269	0.00	22	30		2		1
	405.1488	-3.1	-7.7	-1.5	C15 H34 O7 Br	78.7	29.380	0.00	15	34		7		1
	405.1425	3.2	7.9	18.5	C27 H21 N2 S	69.7	20.352	0.00	27	21	2		1	
	405.1491	-3.4	-8.4	18.5	C28 H21 O3	62.7	13.391	0.00	28	21		3		
	405.1423	3.4	8.4	-1.5	C14 H34 N2 O4 S Br	78.7	29.325	0.00	14	34	2	4	1	1
	405.1419	3.8	9.4	9.5	C19 H25 N4 O2 S2	73.4	24.042	0.00	19	25	4	2	2	
	405.1498	-4.1	-10.1	14.5	C21 H21 N6 O S	69.6	20.245	0.00	21	21	6	1	1	

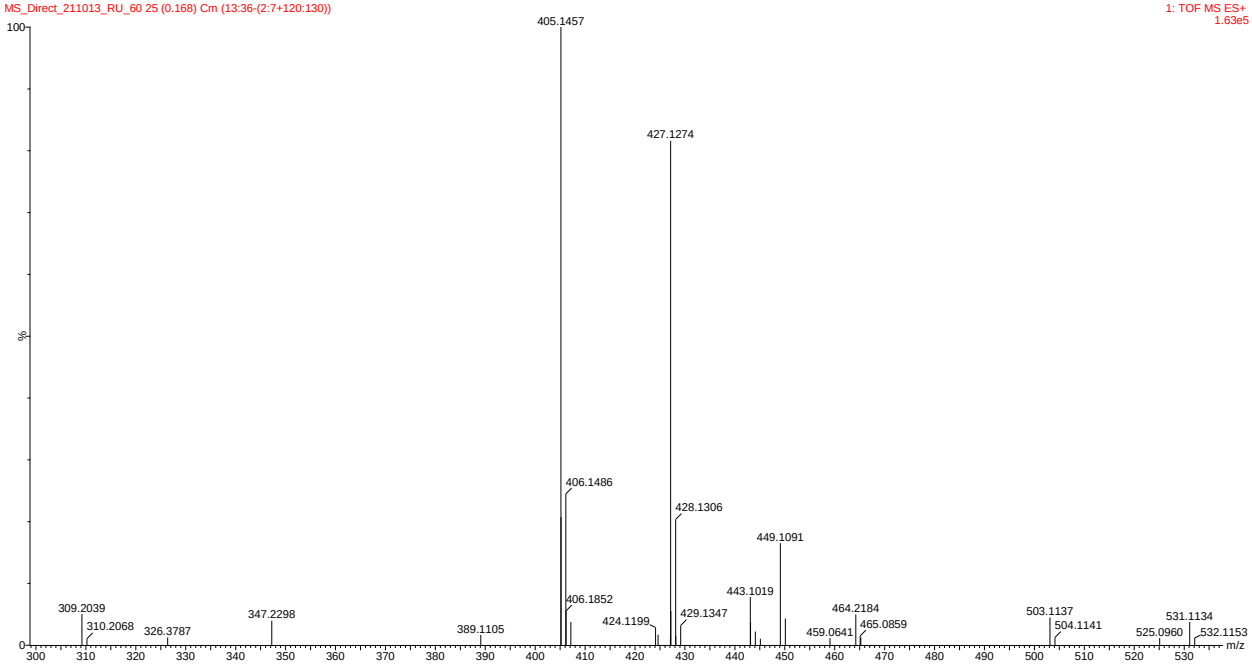
MMH4

2 Microsoft... | Iperius Back... | ACQUITY UP... | Phenolics_T3... | Data | System (C:) | MULTIBOOT ... | SYNAPT G2 ... | Experiment ... | MM_RU_211... | Elemental C

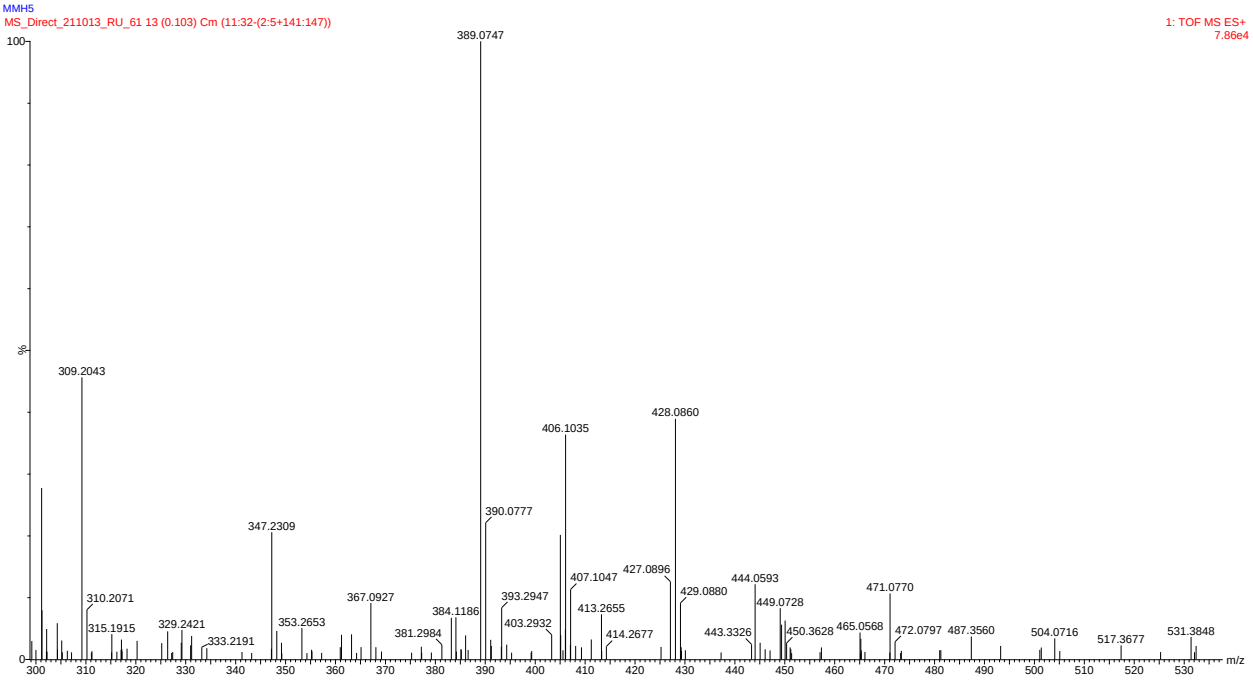
MMH4

MS_Direct_211013_RU_60 25 (0.168) Cm (13:36-(2:7+120:130))

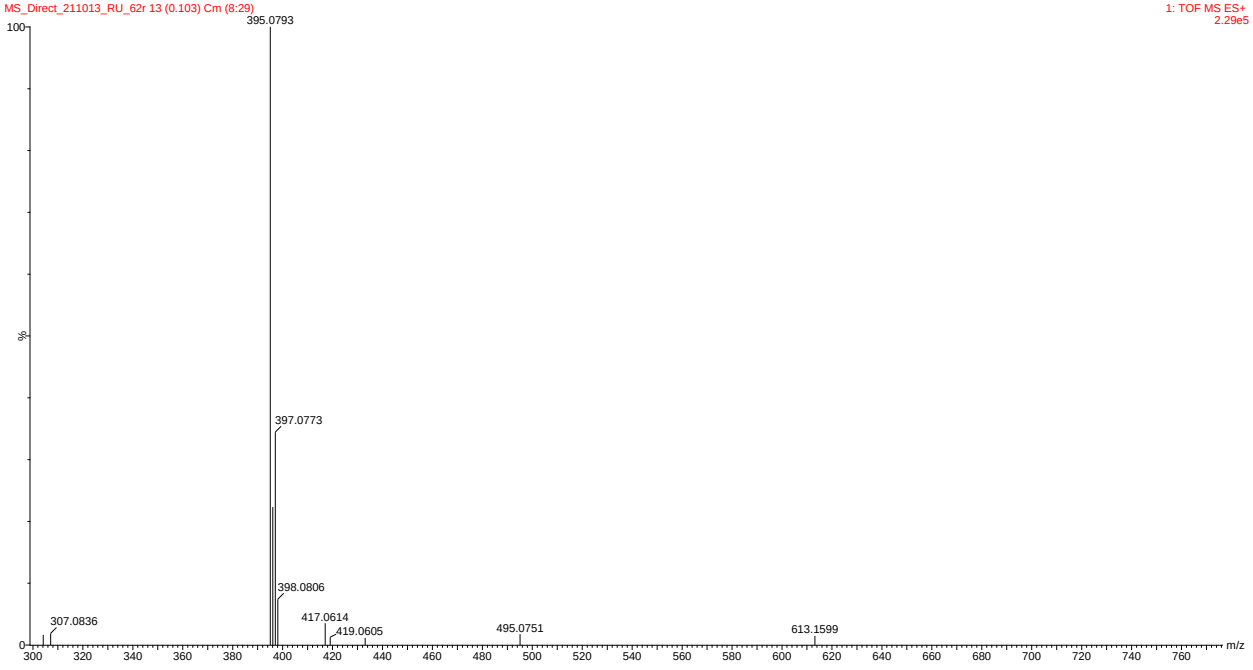
1: TOF MS ES+
1.63e5



15e



15f



15g

Elemental Composition

File Edit View Process Help

Single Mass Analysis

Tolerance = 100.0 PPM / DBE: min = -1.5, max = 100.0

Element prediction: Off

Number of isotope peaks used for i-FIT = 3

Monoisotopic Mass, Even Electron Ions

1318 formula(e) evaluated with 132 results within limits (up to 100 closest results for each mass)

Elements Used:

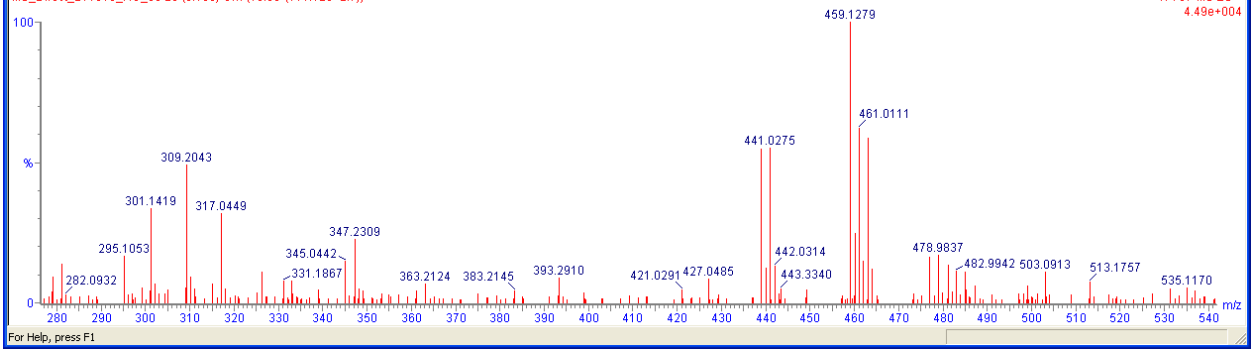
Mass	Calc. Mass	mDa	PPM	DBE	Formula	i-FIT	i-FIT Norm	Fit Conf %	C	H	N	O	Br
439.0298	439.0296	0.2	0.5	34.5	C34 H3 N2	59.8	27.739	0.00	34	3	2		
	439.0301	-0.3	-0.7	16.5	C21 H11 O11	59.3	27.170	0.00	21	11		11	
	439.0293	0.5	1.1	14.5	C21 H16 N2 O4 Br	34.9	2.770	6.27	21	16	2	4	1
	439.0304	-0.6	-1.4	-0.5	C9 H25 N6 O4 Br2	47.0	14.893	0.00	9	25	6	4	2
	439.0307	-0.9	-2.0	19.5	C22 H12 N6 Br	39.1	6.962	0.09	22	12	6		1
	439.0312	-1.4	-3.2	1.5	C9 H20 N4 O11 Br	43.7	11.627	0.00	9	20	4	11	1
	439.0315	-1.7	-3.9	21.5	C22 H7 N4 O7	59.3	27.193	0.00	22	7	4	7	
	439.0275	2.3	5.2	17.5	C17 H7 N6 O9	59.0	26.948	0.00	17	7	6	9	
	439.0272	2.6	5.9	7.5	C20 H25 O Br2	48.4	16.302	0.00	20	25		1	2

MMH7

MS_Direct_211013_RU_63 25 (0.168) Cm (10:35-(111:120+2:7))

1: TOF MS ES+

4.49e+004



For Help, press F1