Manuscript entitled:

Studies on the reactions between the DNA bases and a model α,β-unsaturated oxoaldehyde

Authors: Donata Pluskota-Karwatka, Malwina Muńko, Marcin Hoffmann, Martyna Kuta and Leif Kronberg

New Journal of Chemistry, 2015

Supplementary material

Table of contents

Section A

Tables with chemical shift assignments for protons and carbon atoms of the synthesised adducts

Section B

NMR spectra of the synthesised adducts

Section C

HRMS of the synthesised adducts

Section D

Coordinates of the studied structures

Coordinates of structures of studied substrates, transition states, intermediates and products.

Section A

Tables with chemical shift assignments for protons and carbon atoms of the synthesised adducts

Table 1. ^{1}H and ^{13}C chemical shifts (δ) and spin-spin coupling constants, $J_{H,H}$ of protons in isomeric adducts **2a** and **2b**.

Table 2. ^{1}H and ^{13}C chemical shifts (δ) and spin-spin coupling constants, $J_{H,H}$ of protons in collected together isomeric adducts **1a** and **1b**.

Table 3. ^{1}H and ^{13}C chemical shifts (δ) and spin-spin coupling constants, $J_{H,H}$ of protons in isomeric adducts **4a** and **4b**.

Table 1. ^{1}H and ^{13}C chemical shifts (δ) and spin-spin coupling constants, $J_{H,H}$ of protons in isomeric adducts 2a and 2b.

proton	δ		multiplicity		$J_{H,H}$		carbon	δ	
	2a	2b	2a	2b	2a	2b		2a	2b
H-4	7.47 7.49	7.48	d d	d	8.1 8.2	8.1	C-4	137.1 137.5	137.2 137.5
H-5	5.78 5.80	5.79 5.78	d m	d d	8.1	8.1 8.1	C-5	96.7 96.1	96.8 96.1
H-8	5.47 5.22	5.47 5.22	d d	d d	4.7 4.6	3.8 5.1	C-8	98.0 97.5	98.3 97.4
HC(OEt)$_2$	4.46 4.48	4.46 4.48	s s	s s			HC(OEt)$_2$	102.6 102.4	102.6 102.5
H-10	4.26 4.29	4.29 4.30	d d	d d	7.7 7.8	7.4 7.7	C-10	58.6 57.9	58.5 57.8
OCH_2CH$_3$	3.58 3.66	3.66 3.58	m m	m q		7.0	OCH_2CH$_3$	64.4 64.6 63.7 63.5	64.5 63.7
H-9	2.19 2.22	2.13 2.15	m m	m m			C-9	38.5	38.5
CH_3	1.10 1.05	1.10 1.05	t t	t t	7.0 7.0	7.0 7.0	CH_3	15.3 15.1	15.2 15.3
							C-12	153.7 154.0	154.0 153.7
							C-2	147.5 147.4	147.7 147.5
							C-11	111.0 108.0	110.9 108.0
H-1'	6.18 6.14	6.20 6.16	t t	t m	6.6 7.1	6.6	C-1'	83.4 83.6	83.3 83.4
H-3'	4.22	4.22	m	m			C-3'	70.4	70.7 70.5
H-4'	3.74	3.74	m	m			C-4'	87.0 87.1	87.0
H-5'	3.52	3.51	m	m			C-5'	61.5 61.4	61.5
H-2'	2.04	2.02	m	m			C-2'	38.8	38.8
H-2"	2.08	2.09	m	dd		5.9 12.6			
8-OH	6.61	6.58							
3'-OH	5.22	5.24							
5'-OH	4.97	4.95							

Table 2. ^{1}H and ^{13}C chemical shifts (δ) and spin-spin coupling constants, $J_{H,H}$ of protons in collected together isomeric adducts 1a and 1b.

proton	δ	multiplicity	$J_{H,H}$	carbon	δ
H-4	7.51	d	8.1	C-4	137.4
	7.55	dd	8.1, 2.7		137.3
	7.43	d	8.1		137.73
	7.39	dd	8.1, 2.5		137.71
H-11	5.87	d	6.5	C-11	100.3
	5.89	d	6.7		100.6
	5.94	d	6.5		100.2
	5.96	d	6.5		100.1
H-5	5.77	d	8.1	C-5	96.2
	5.76	d	8.1		96.5
	5.82	d	8.1		96.4
	5.81	d	8.1		96.1
H-10	4.51	m		C-10	58.6
	4.57	m			58.5
HC(OEt)$_2$	4.26	s		HC(OEt)$_2$	103.3
	4.21	s			102.9
OCH_2CH$_3$	3.63	q	7.1	OCH$_2$CH$_3$	63.4
	3.64	q	7.1		
H-9	2.26	m		C-9	36.5
	2.07	m			
CH_3	1.10	t	7.1	CH$_3$	14.7
	1.00	t	7.1		14.6
				C-12	154.9
					154.8
					154.7
				C-2	147.7
					147.6
					147.5
				C-8	106.3
H-1'	6.18	dm	6.6	C-1'	83.5
	6.12	d	6.9		
	6.09	d	6.8		
H-3'	4.22	m		C-3'	70.3
H-4'	3.75	m		C-4'	86.8
H-5'	3.53	m		C-5'	61.2
H-2'	2.20	m		C-2'	38.6
H-2"	2.03	m			
8-OH	6.59				
3'-OH	5.23				
5'-OH	4.97				

Table 3. ^{1}H and ^{13}C chemical shifts (δ) and spin-spin coupling constants, $J_{H,H}$ of protons in isomeric adducts 4a and 4b.

proton	δ		multiplicity		$J_{H,H}$		carbon	δ	
	4a	4b	4a	4b	4a	4b		4a	4b
H-2	8.16	8.15	s	s			C-2	137.7	137.6
H-5	8.19	8.12	s	s			C-5	143.9	143.8
H-b	5.50	5.49	d	d	4.4	4.4	C-b	97.9	97.6
H-7	4.59	4.58	d	m	6.9		C-7	59.8	59.5
HC(OEt)$_2$	4.52	4.52	s	s			HC(OEt)$_2$	102.8	102.6
OCH_2CH$_3$	3.68	3.66	m	m			OCH_2CH$_3$	64.2	63.9
	3.55	3.53	m	m				63.5	63.3
H-a	2.24	2.24	m	m			C-a	39.7	39.4
	2.21	2.21	m	m					
CH_3	1.12	1.12	t	t	7.1	7.1	CH$_3$	15.1	14.9
	1.03	0.99	t	t	7.1	7.1		15.0	14.8
							C-9a	150.4	150.0
							C-3a	144.4	144.1
							C-9b	119.4	119.1
							C-8	112.8	112.5
H-1'	6.23	6.22	m	m			C-1'	83.6	83.3
H-3'	4.35	4.36	m	m			C-3'	70.5	70.3
H-4'	3.84	3.83	m	m			C-4'	87.8	87.6
H-5'	3.56	3.56	m	m			C-5'	61.5	61.3
H-5"	3.51	3.49	m	m					
H-2'	2.57	2.59	m	m			C-2'	39.6	39.4
H-2"	2.48	2.48							

Section B

NMR spectra of the synthesised adducts

Spectra of compounds **1a** and **1b** (DMSO-d_6): ^{1}H NMR, ^{13}C NMR, HSQC, HMBC

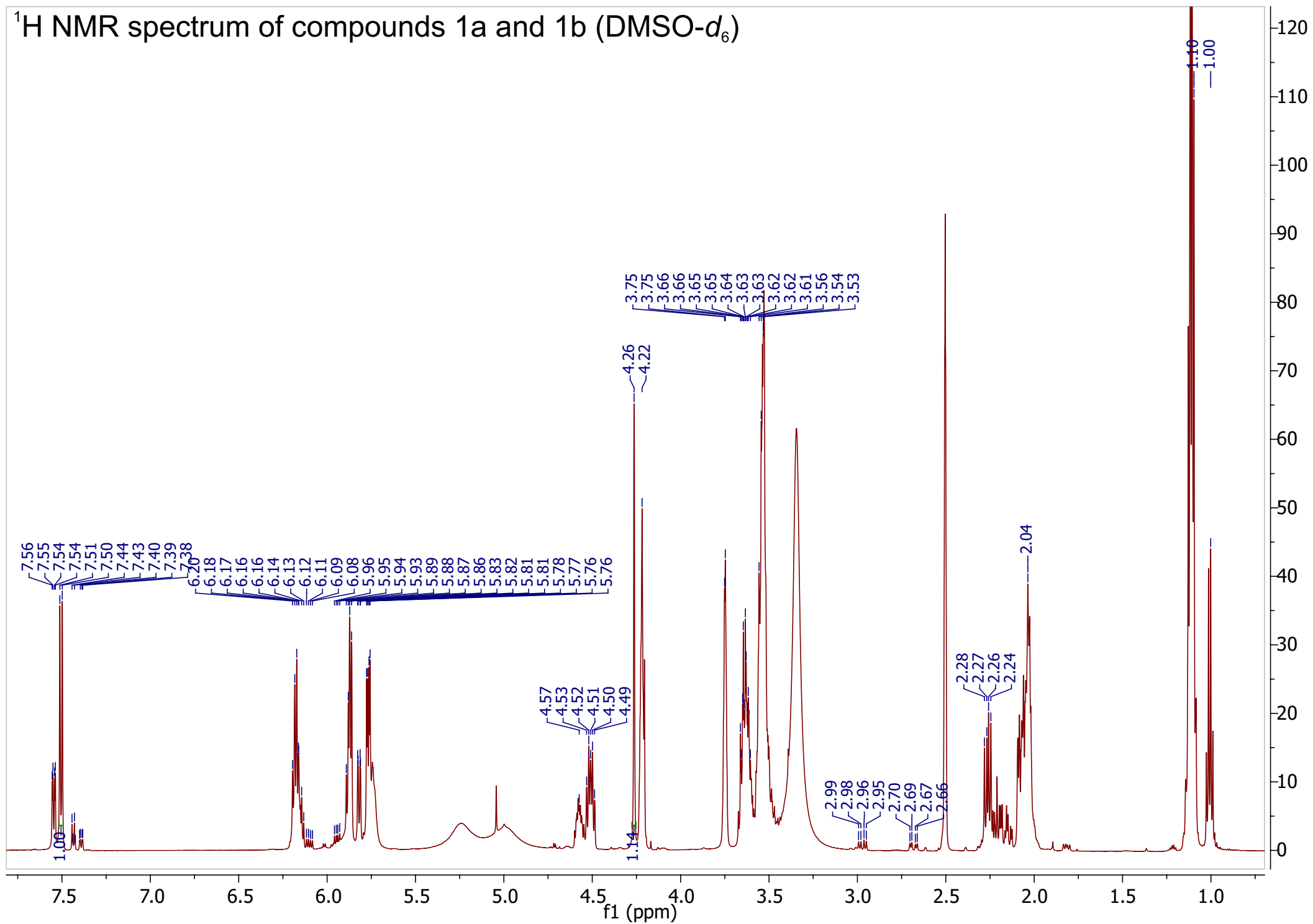Spectra of compound **2a** (DMSO-d_6): ^{1}H NMR, ^{13}C NMR, HSQC, HMBC

Spectra of compound **2b** (DMSO-d_6): ^{1}H NMR, ^{13}C NMR, HSQC, HMBC

Spectra of compound **3** (DMSO-d_6): ^{1}H NMR, HSQC,

Spectra of compound **4a** (DMSO-d_6): ^{1}H NMR, ^{13}C NMR, HSQC, HMBC

Spectra of compound **4b** (DMSO-d_6): ^{1}H NMR, HSQC, HMBC

^{1}H NMR spectrum of compounds 1a and 1b (DMSO-d_6)
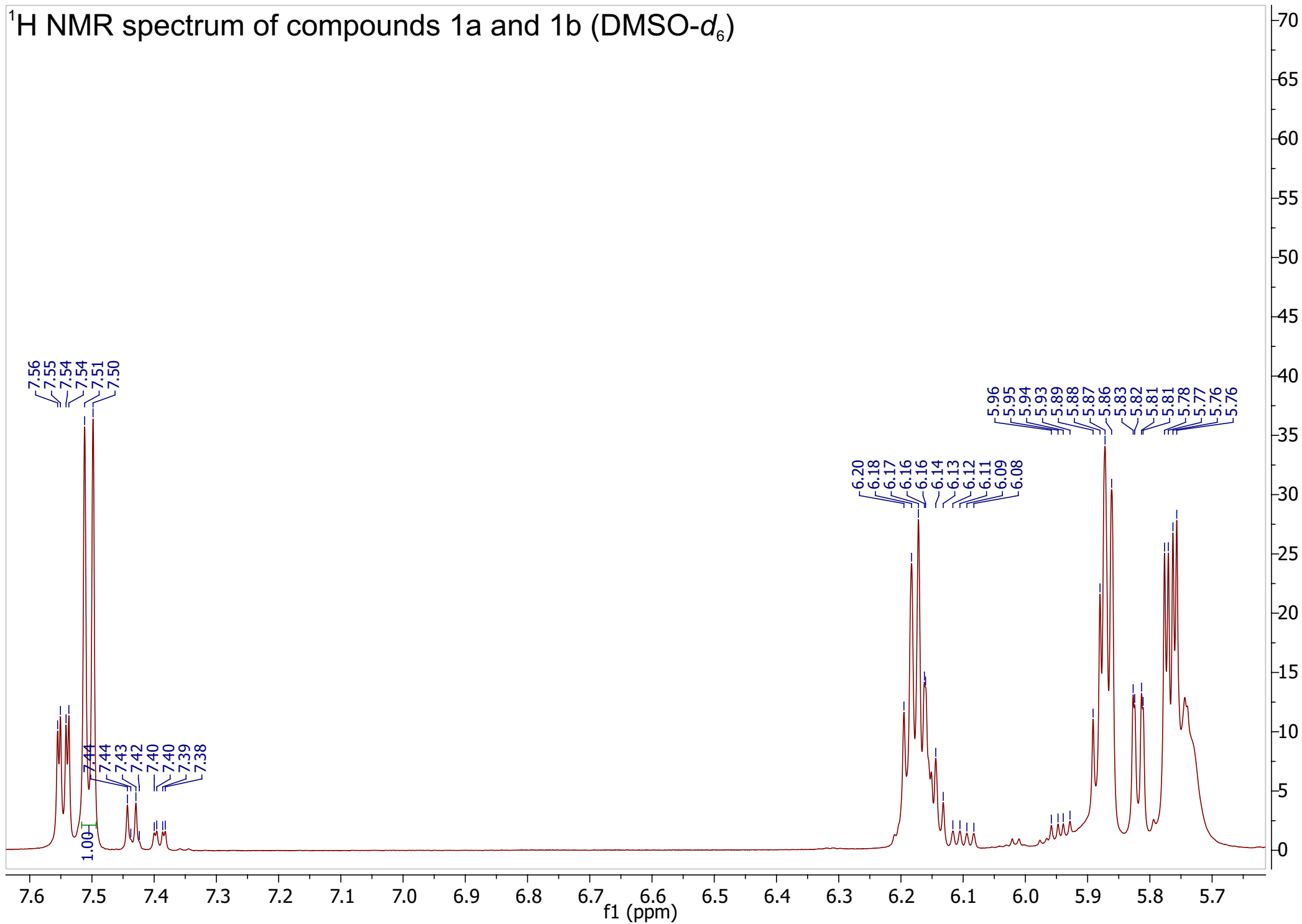
^{1}H NMR spectrum of compounds 1a and 1b (DMSO-d_6)

^{1}H NMR spectrum of compounds 1a and 1b (DMSO-d_6)

^{13}C NMR spectrum of compounds 1a and 1b (DMSO-d_6)
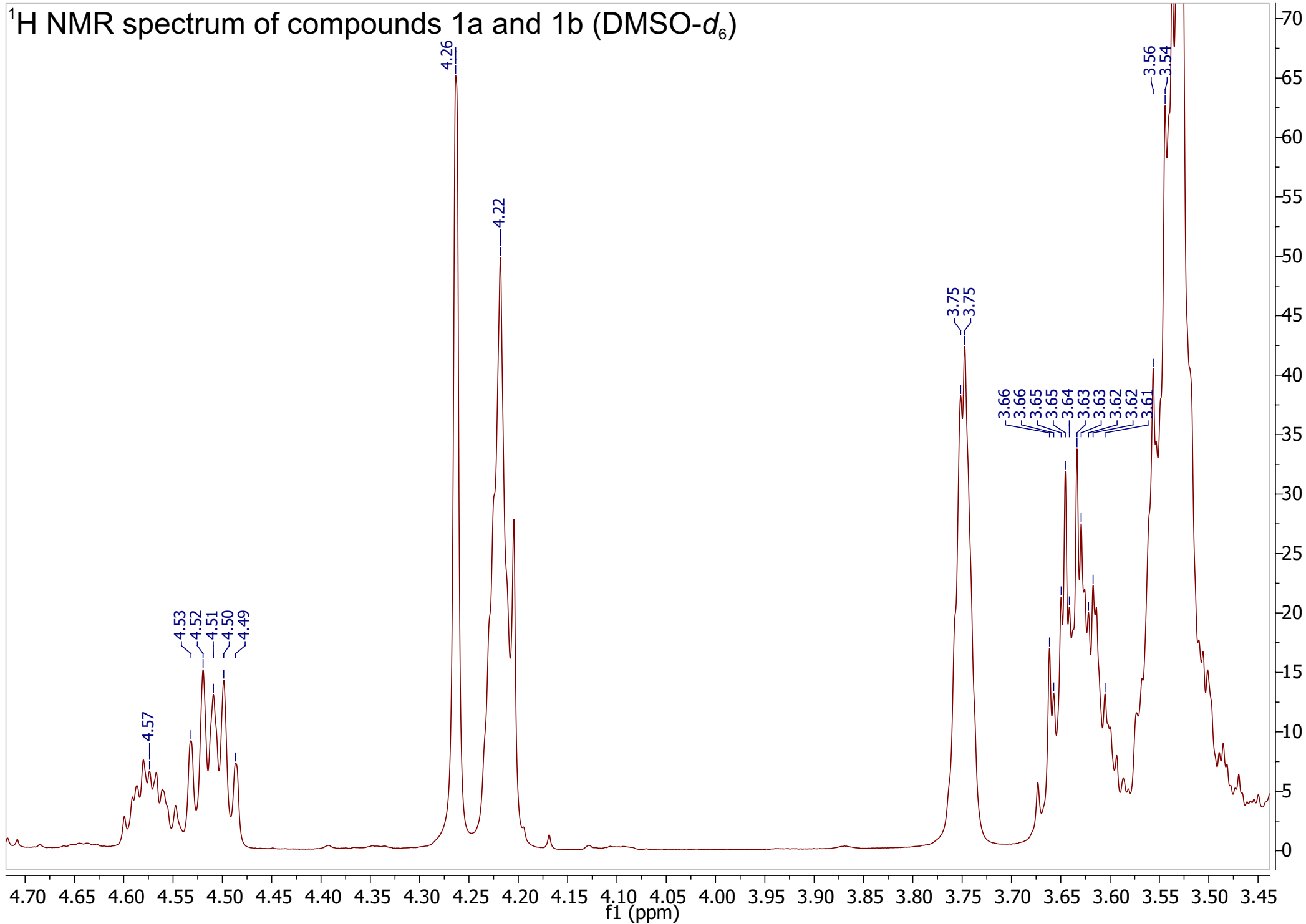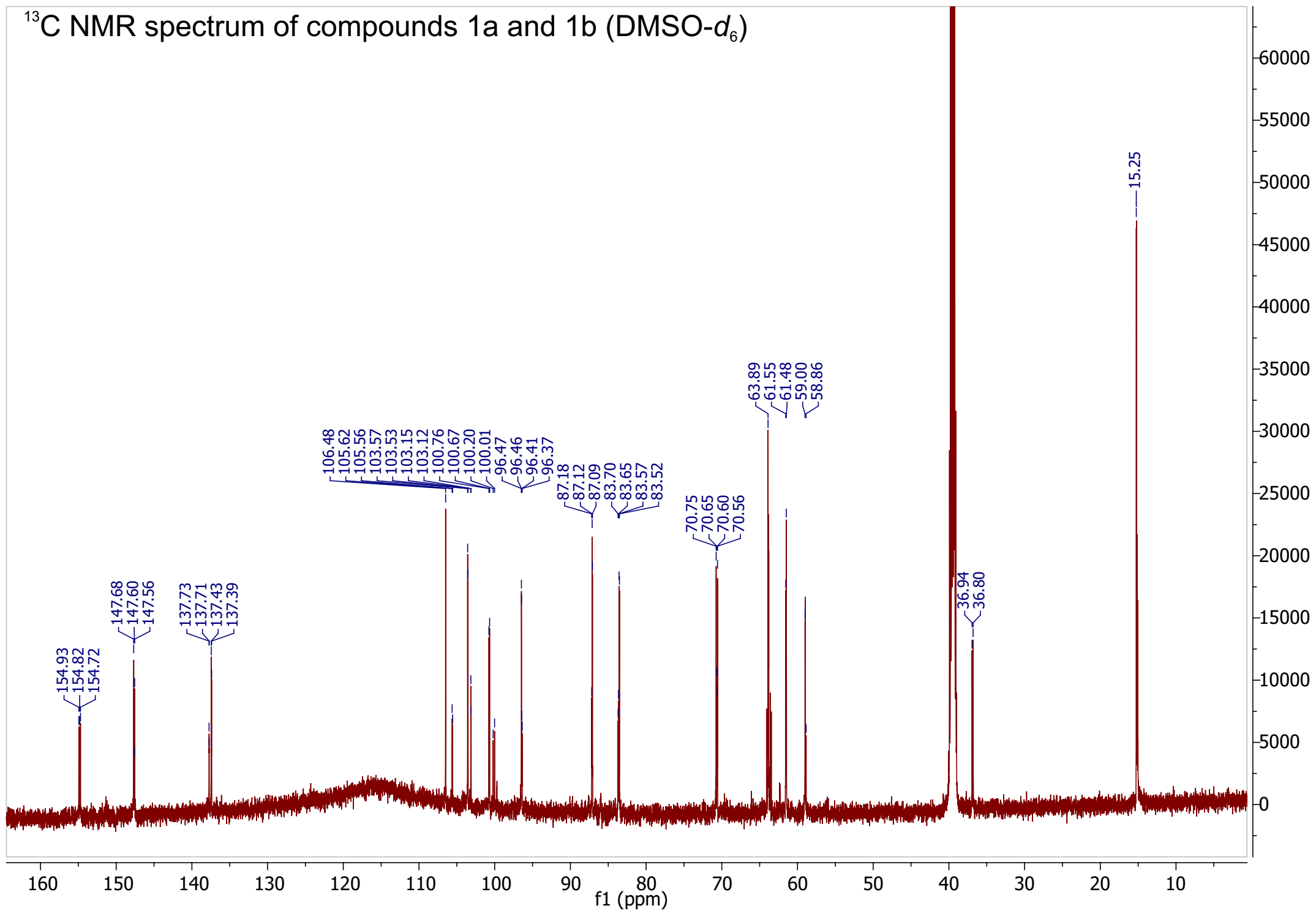
^{13}C NMR spectrum of compounds 1a and 1b (DMSO-d_6)
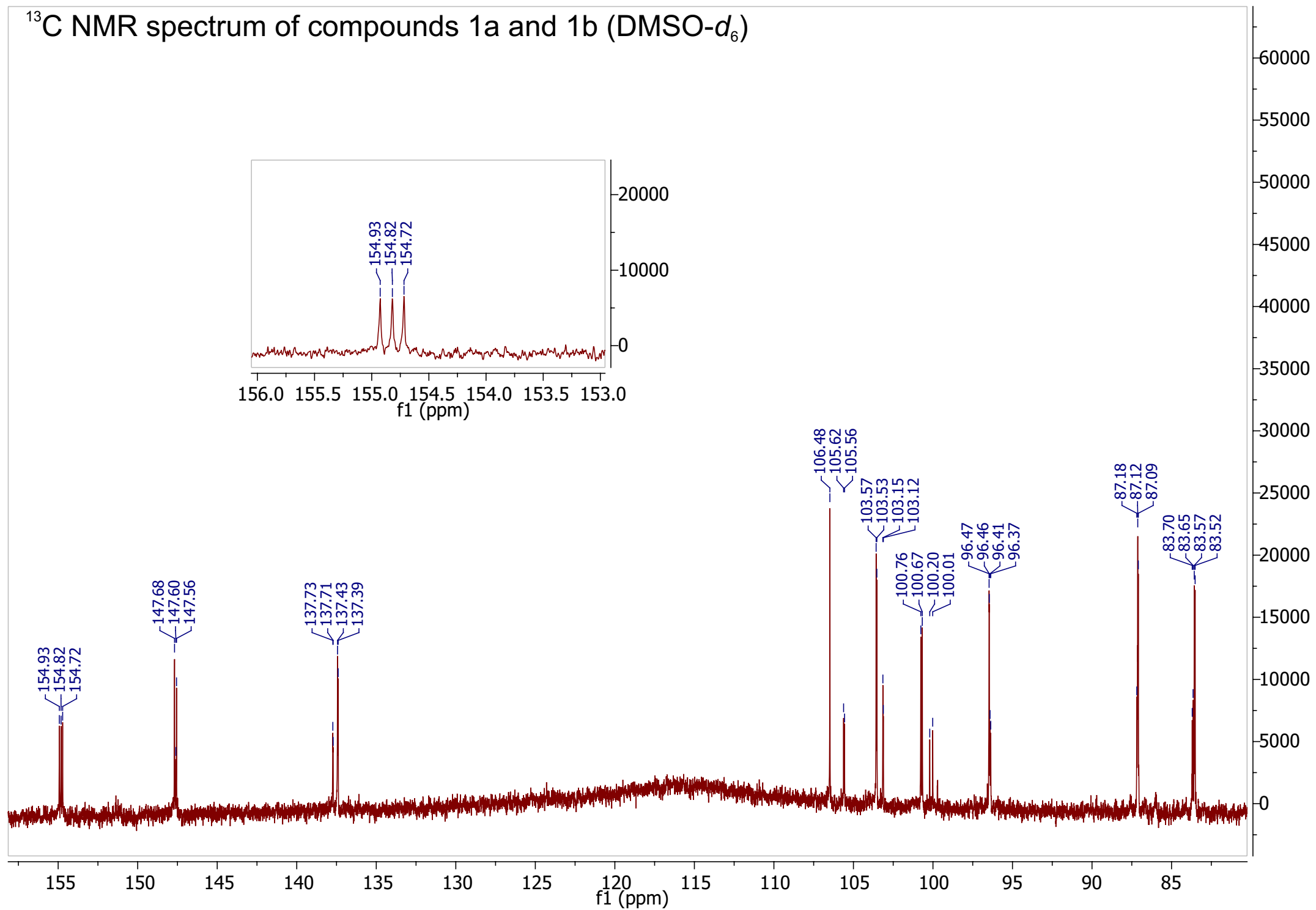
^{13}C NMR spectrum of compounds 1a and 1b (DMSO-d_6)
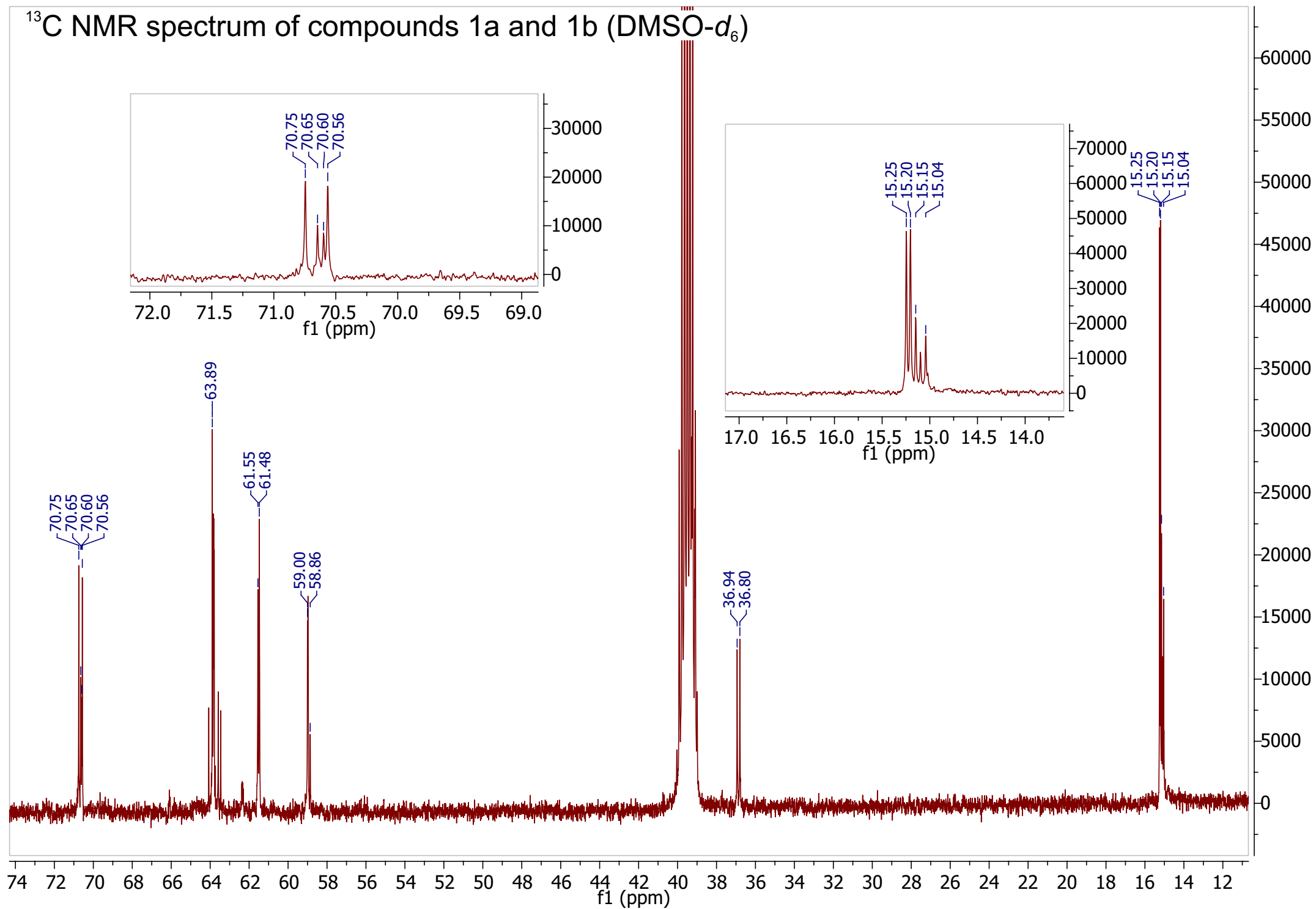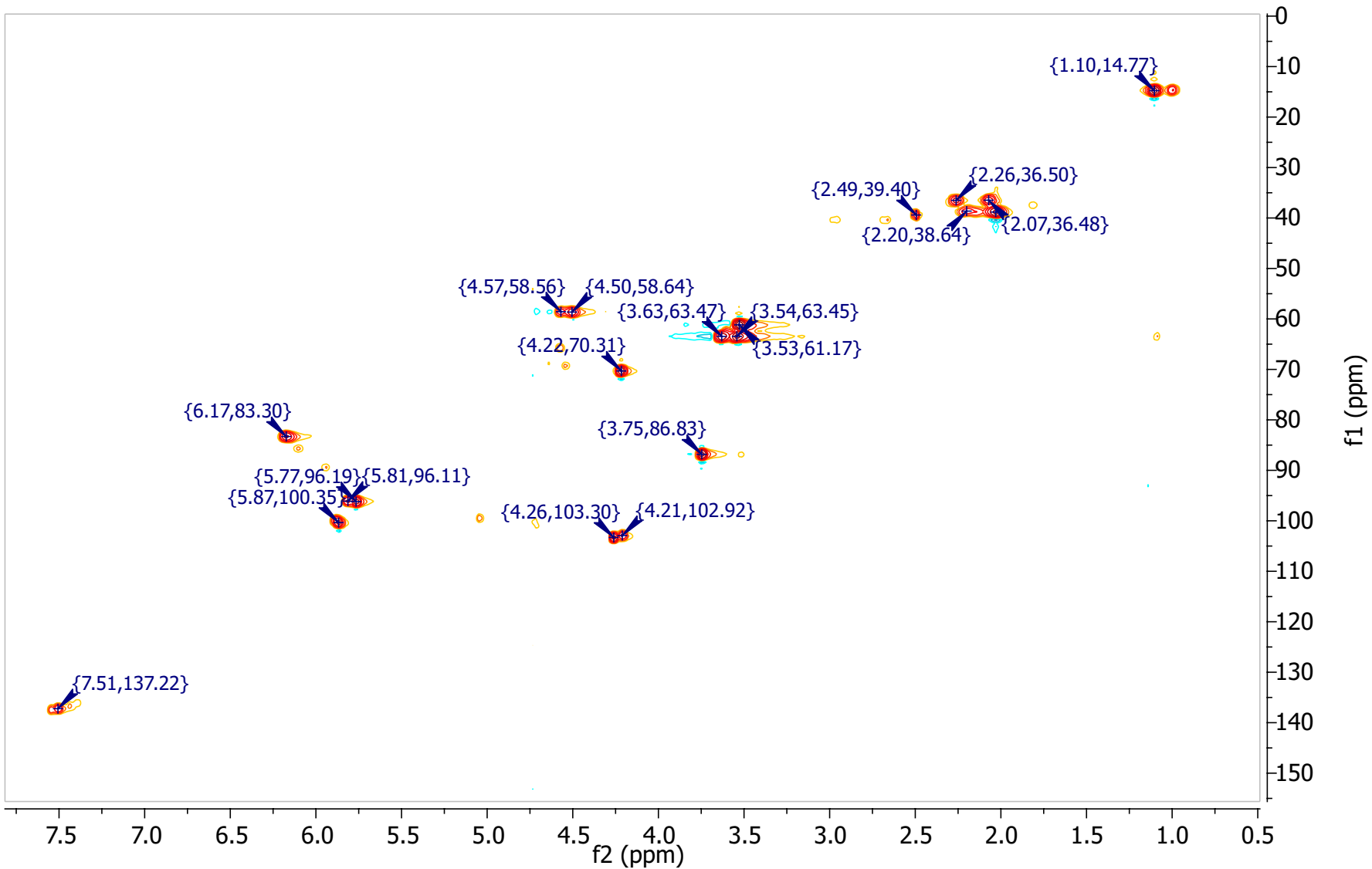
HSQC spectrum of compounds 1a and 1b (DMSO-d_6)

HMBC spectrum of compounds 1a and 1b (DMSO-d_6)
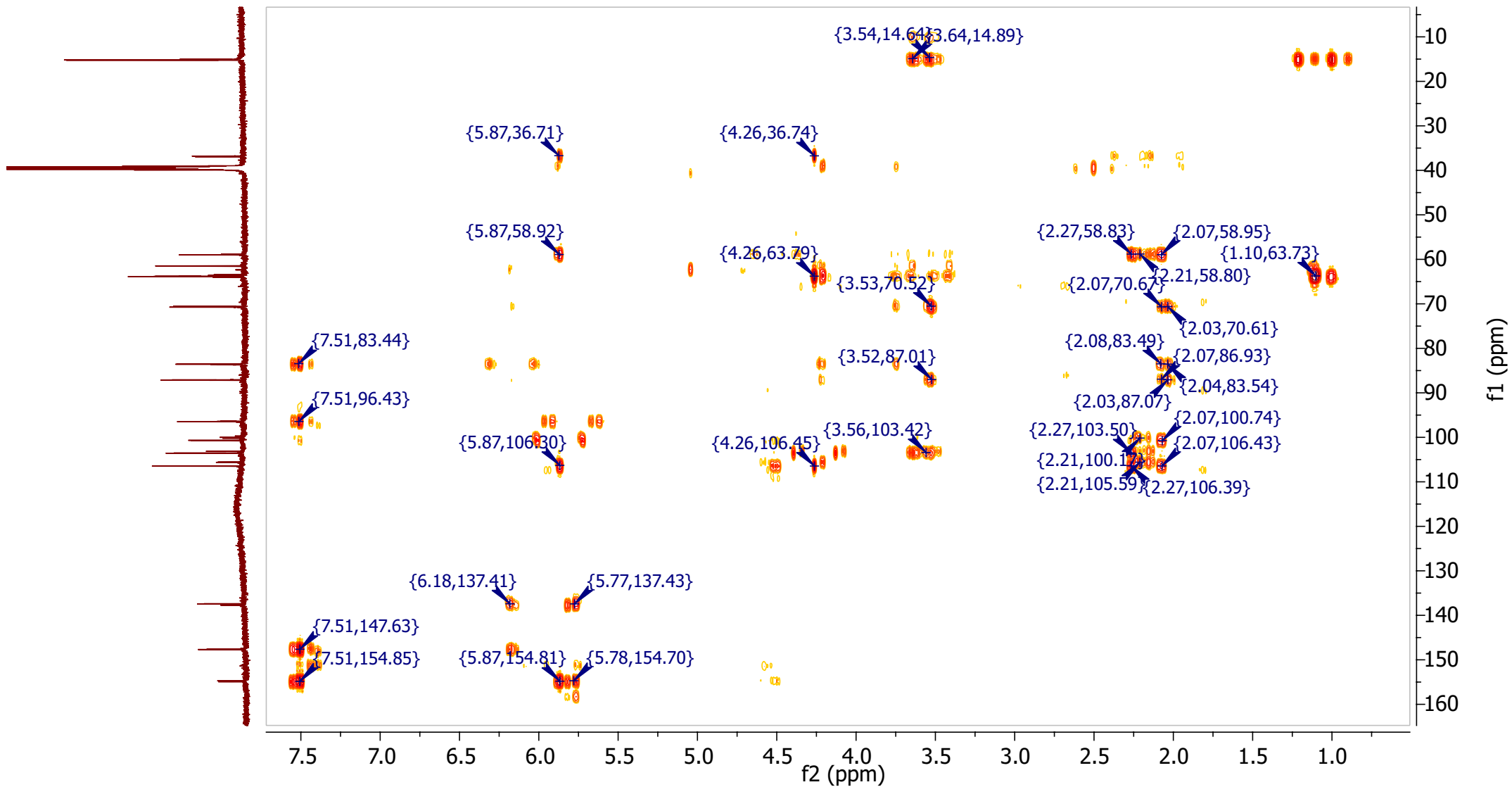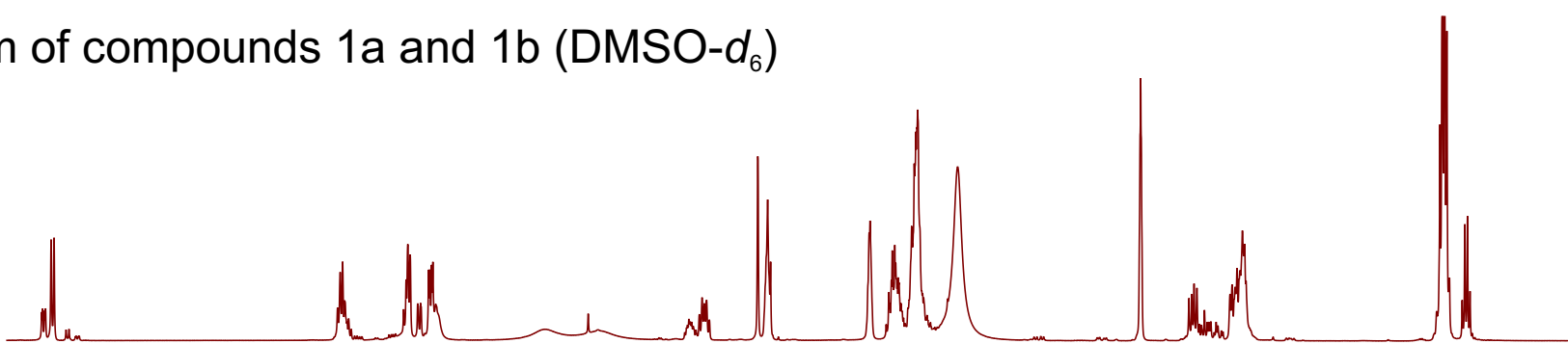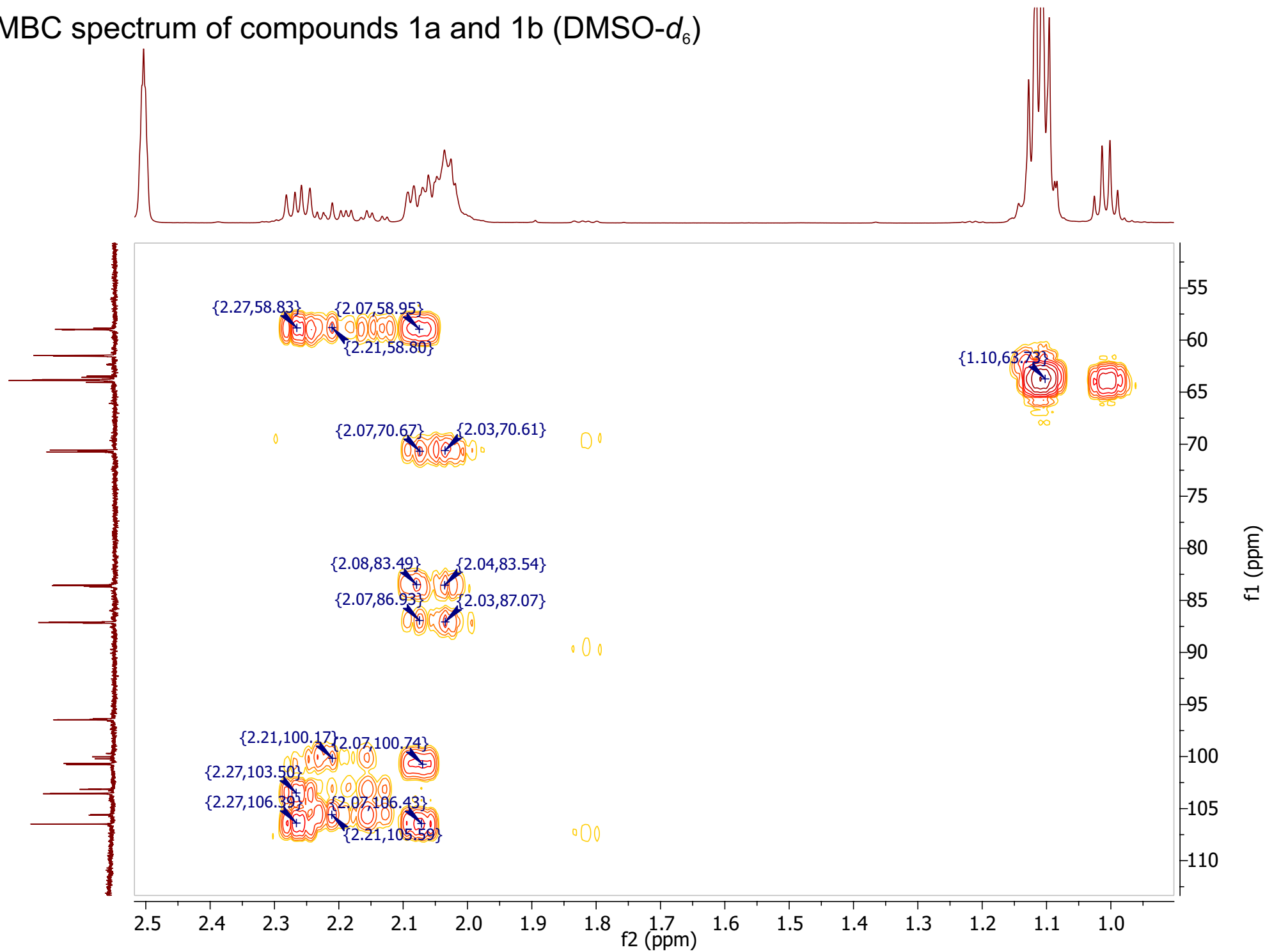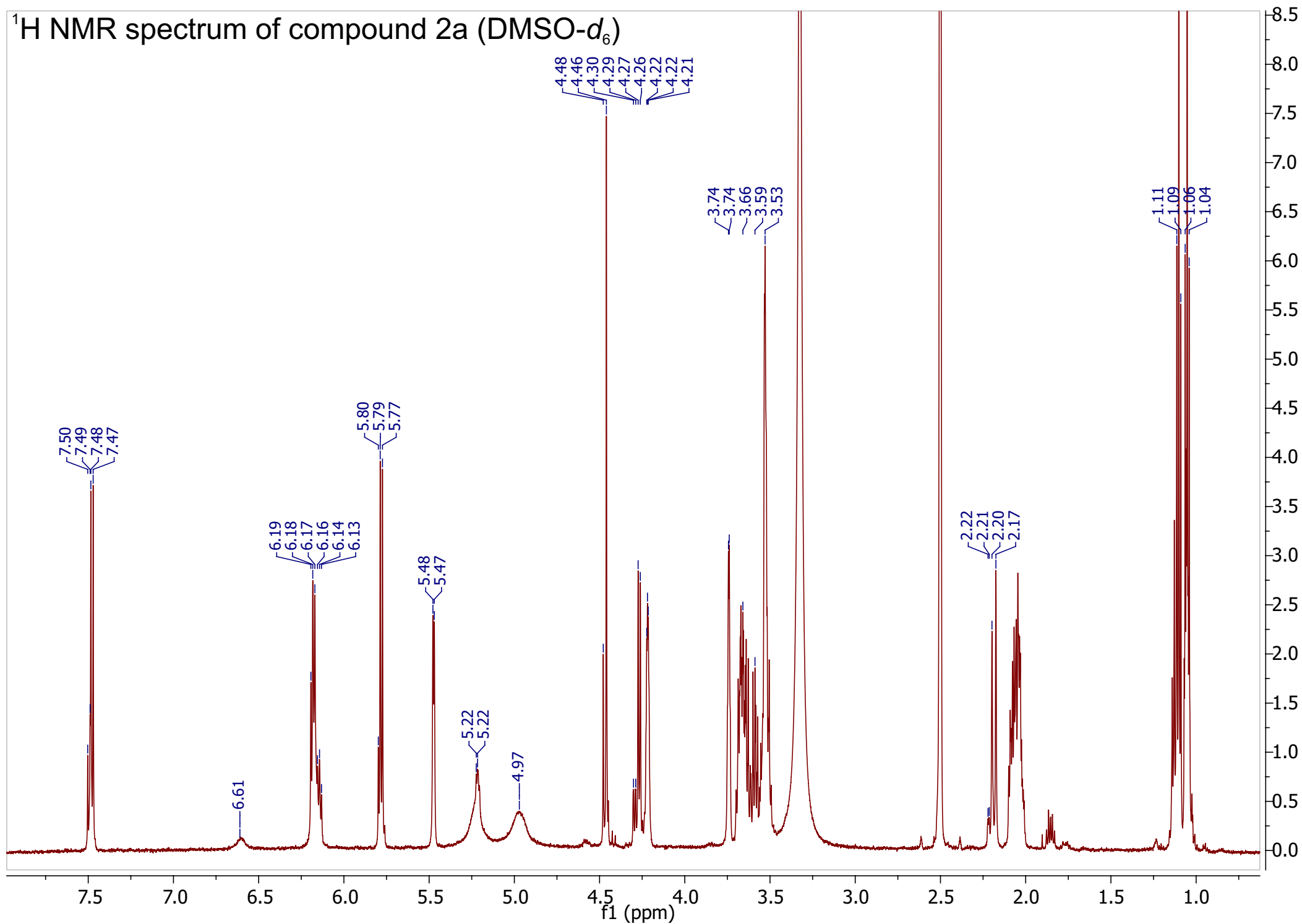
{3.54,14.64} {3.64,14.89}
{5.87,36.71} {4.26,36.74}
{5.87,58.92} {4.26,63.79} {2.27,58.83} {2.07,58.95} {1.10,63.73}
{3.53,70.52} {2.07,70.67} {2.21,58.80}
{2.03,70.61}
{7.51,83.44} {3.52,87.01} {2.08,83.49} {2.07,86.93}
{2.04,83.54}
{7.51,96.43} {2.03,87.07} {2.07,100.74}
{5.87,106.30} {4.26,106.45} {3.56,103.42} {2.27,103.50} {2.07,106.43}
{2.21,100.1}
{2.21,105.59} {2.27,106.39}
{6.18,137.41} {5.77,137.43}
{7.51,147.63}
{7.51,154.85} {5.87,154.81} {5.78,154.70}

HMBC spectrum of compounds 1a and 1b (DMSO-d_6)

{2.27,58.83}   {2.07,58.95}
{2.21,58.80}
{1.10,63.73}
{2.07,70.67}   {2.03,70.61}
{2.08,83.49}   {2.04,83.54}
{2.07,86.93}   {2.03,87.07}
{2.21,100.17}{2.07,100.74}
{2.27,103.50}
{2.27,106.39}   {2.07,106.43}
{2.21,105.59}

^{1}H NMR spectrum of compound 2a (DMSO-d_6)

^{1}H NMR spectrum of compound 2a (DMSO-d_6)
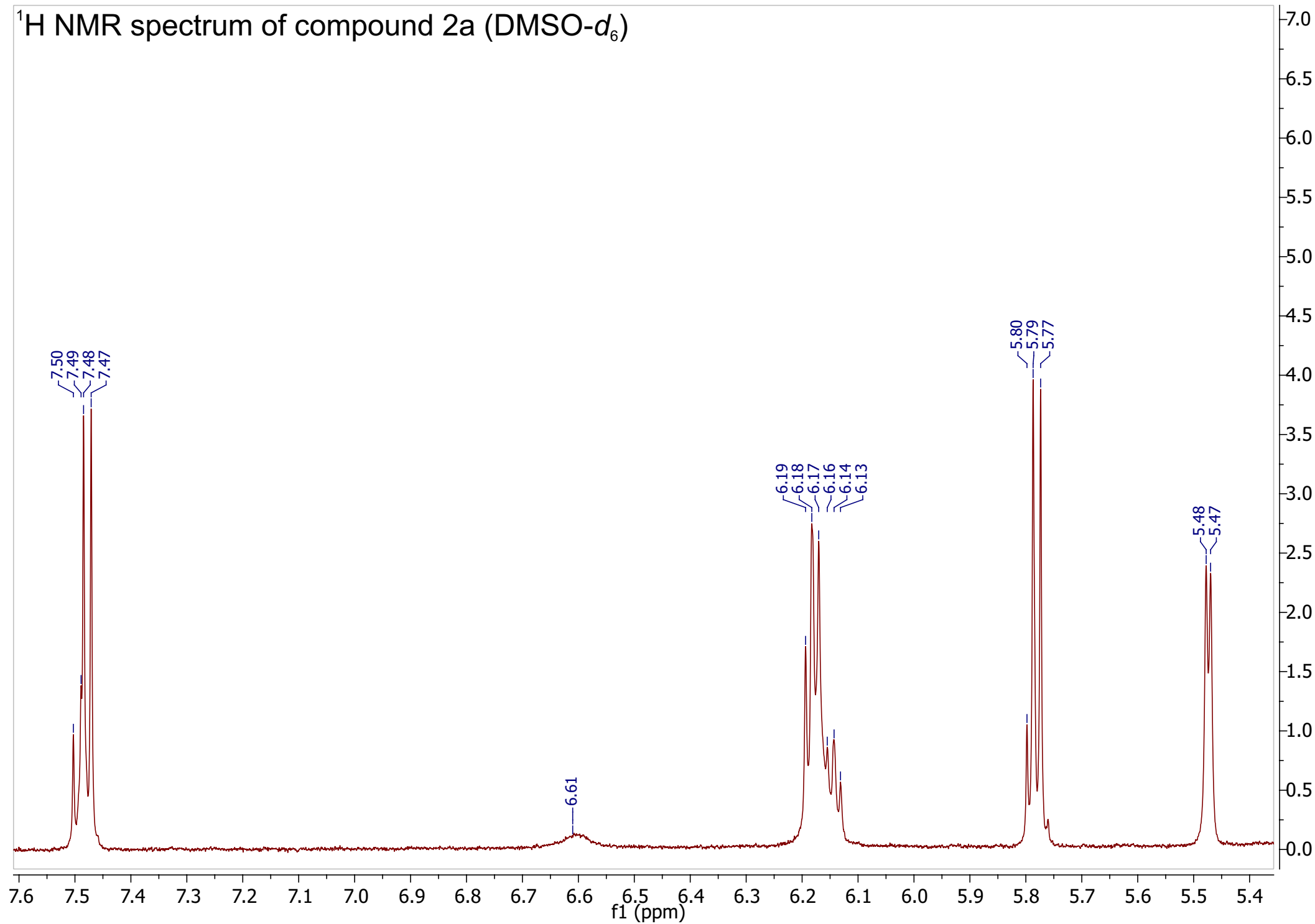
¹H NMR spectrum of compound 2a (DMSO-*d*₆)
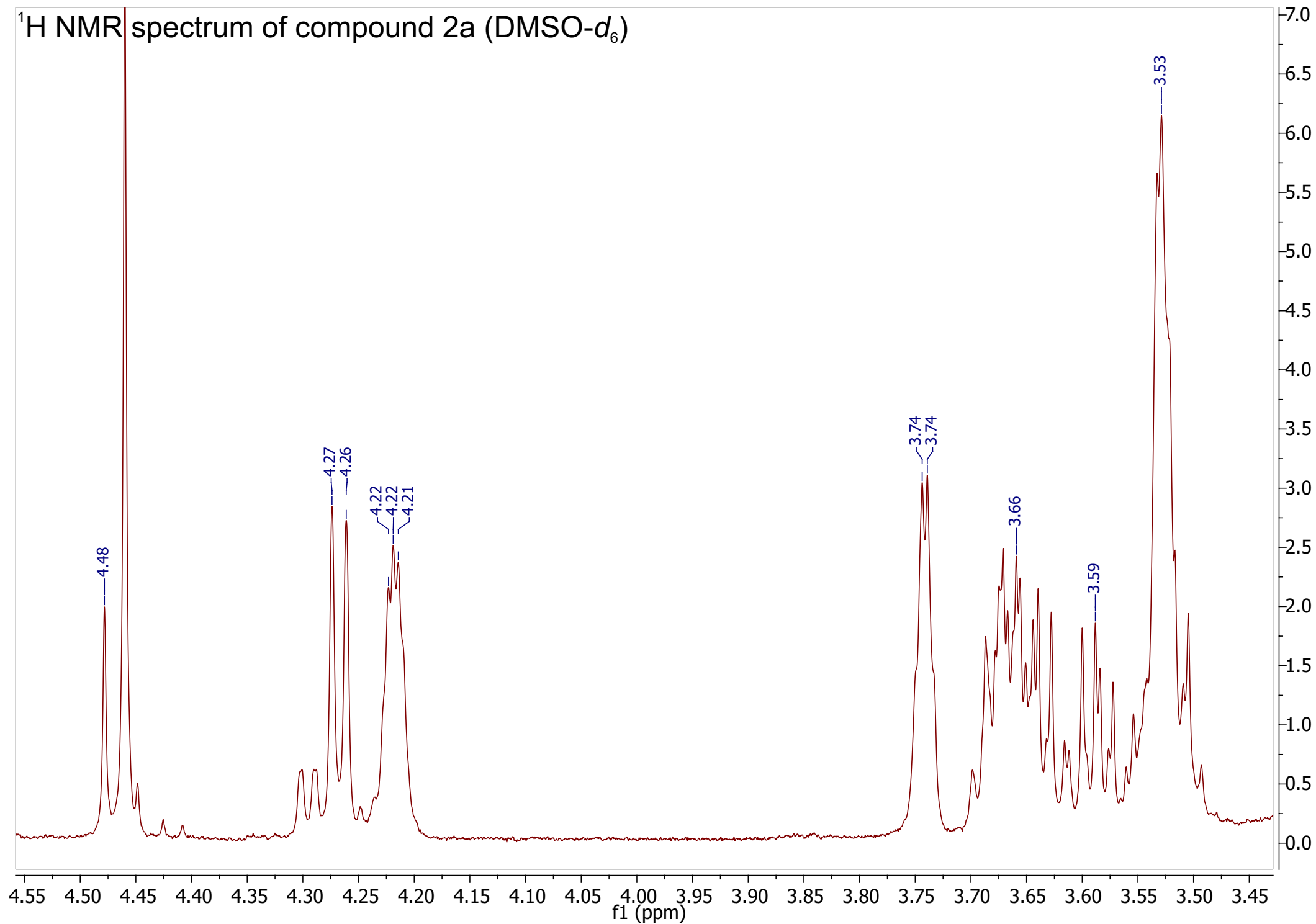
^{13}C NMR spectrum of compound 2a (DMSO-d_6)

^{13}C NMR spectrum of compound 2a (DMSO-d_6)

HSQC spectrum of compound 2a (DMSO-d_6)

{1.09,14.97} {1.04,14.89}

{2.03,38.69}{2.17,38.40}

{4.26,58.35}

{3.52,61.31}

{3.58,64.43}

{4.21,70.45}{3.51,63.49}{3.66,64.31}

{6.17,83.31}

{3.73,86.95}

{5.78,96.52}

{5.46,97.96}

{4.45,102.48}

{5.21,97.36}

{7.48,137.13}
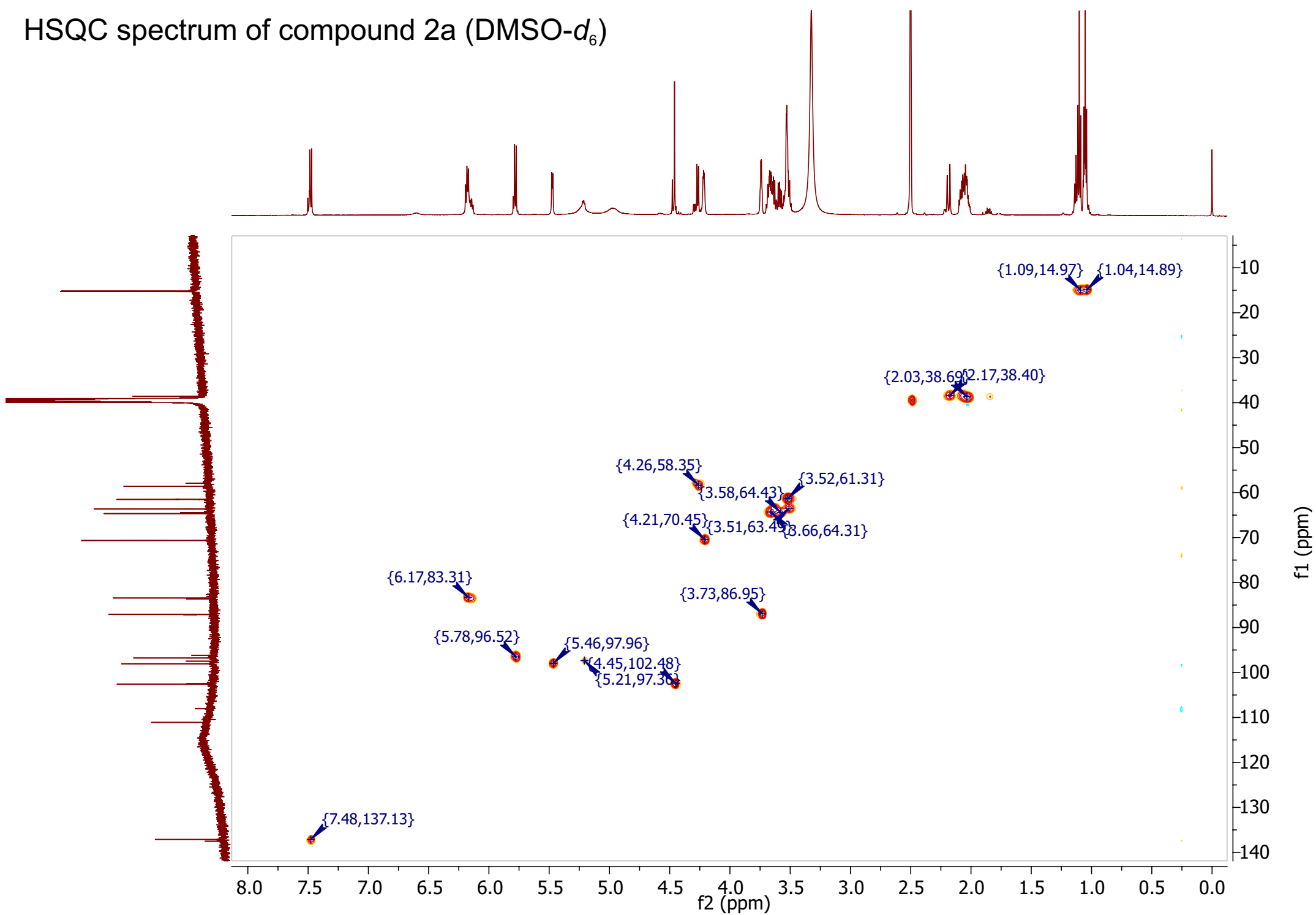
HMBC spectrum of compound 2a (DMSO-d_6)

HMBC spectrum of compound 2a (DMSO-d_6)
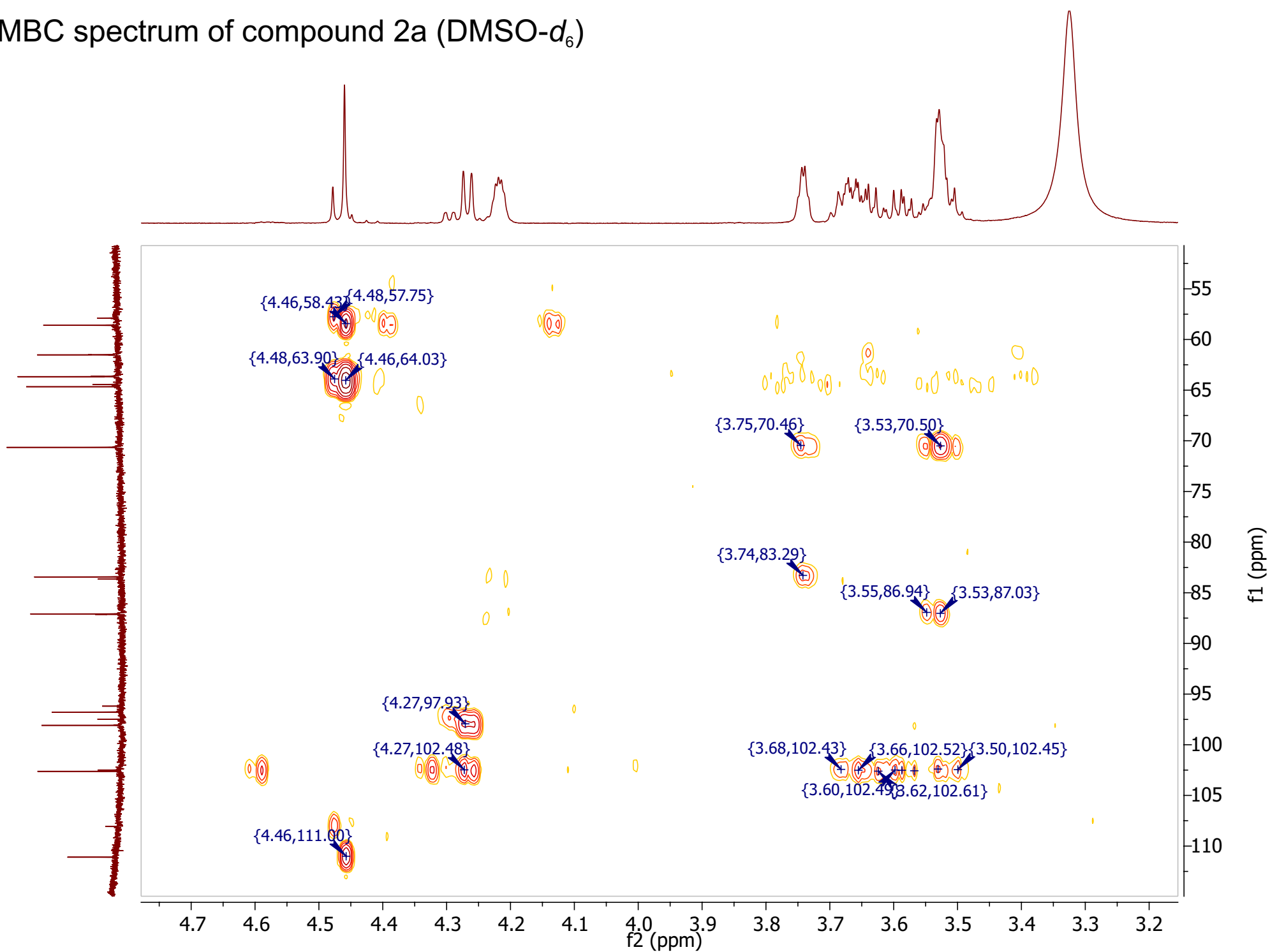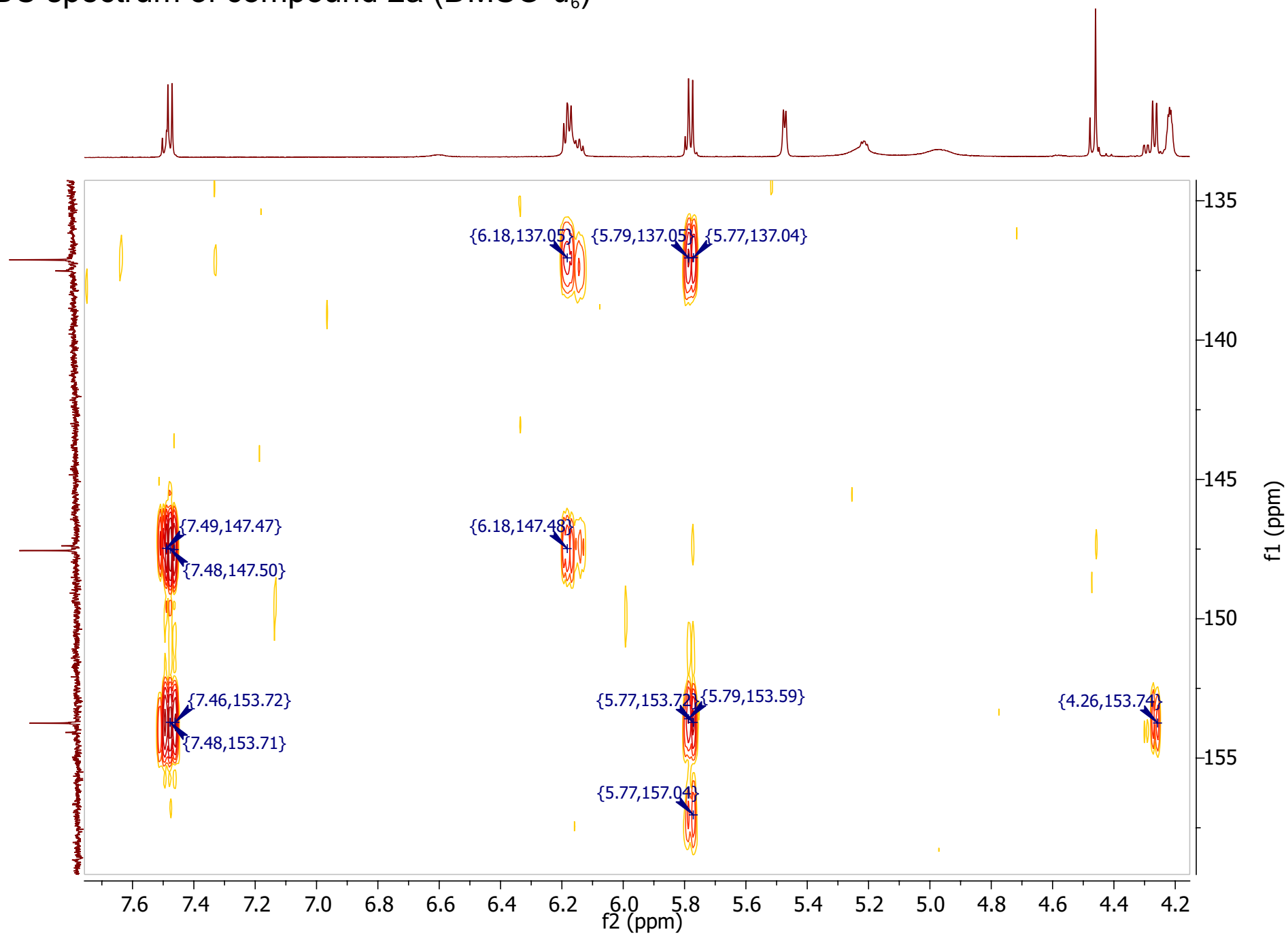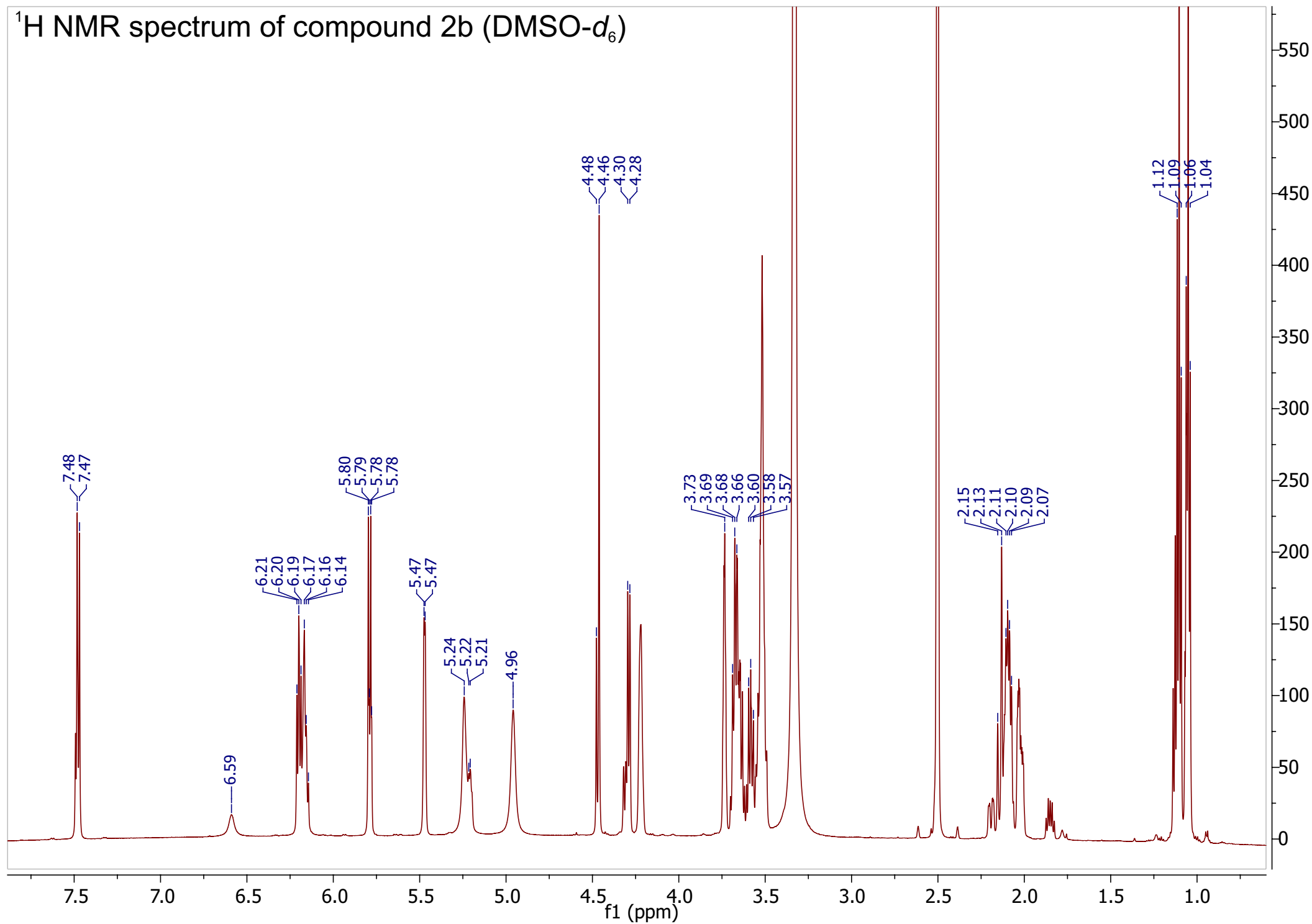
{4.46,58.43} {4.48,57.75}
{4.48,63.90} {4.46,64.03}
{3.75,70.46} {3.53,70.50}
{3.74,83.29}
{3.55,86.94} {3.53,87.03}
{4.27,97.93}
{4.27,102.48}
{3.68,102.43} {3.66,102.52} {3.50,102.45}
{3.60,102.49} {3.62,102.61}
{4.46,111.00}

HMBC spectrum of compound 2a (DMSO-d_6)

^{1}H NMR spectrum of compound 2b (DMSO-d_6)

^{1}H NMR spectrum of compound 2b (DMSO-d_6)
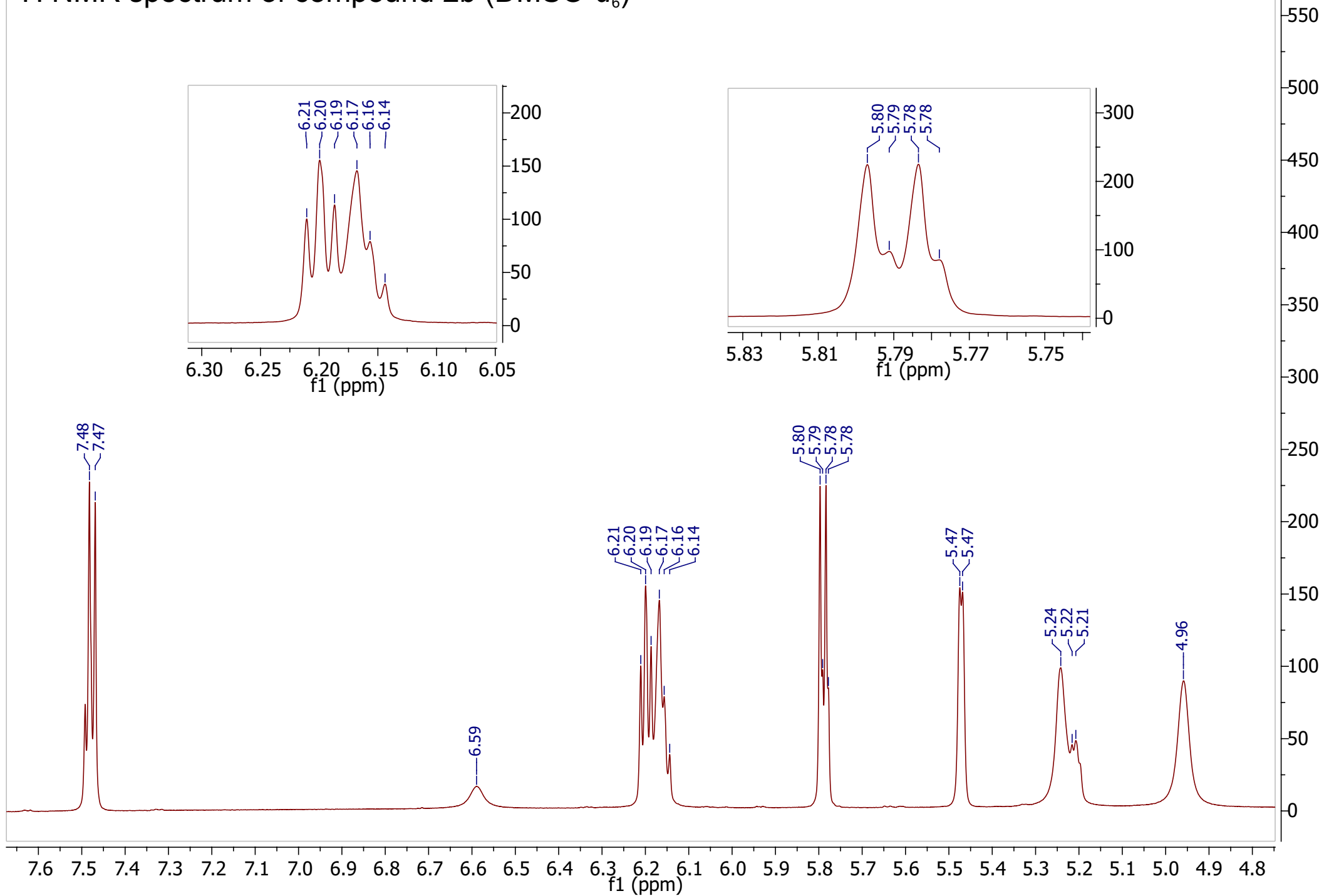
^{1}H NMR spectrum of compound 2b (DMSO-d_6)
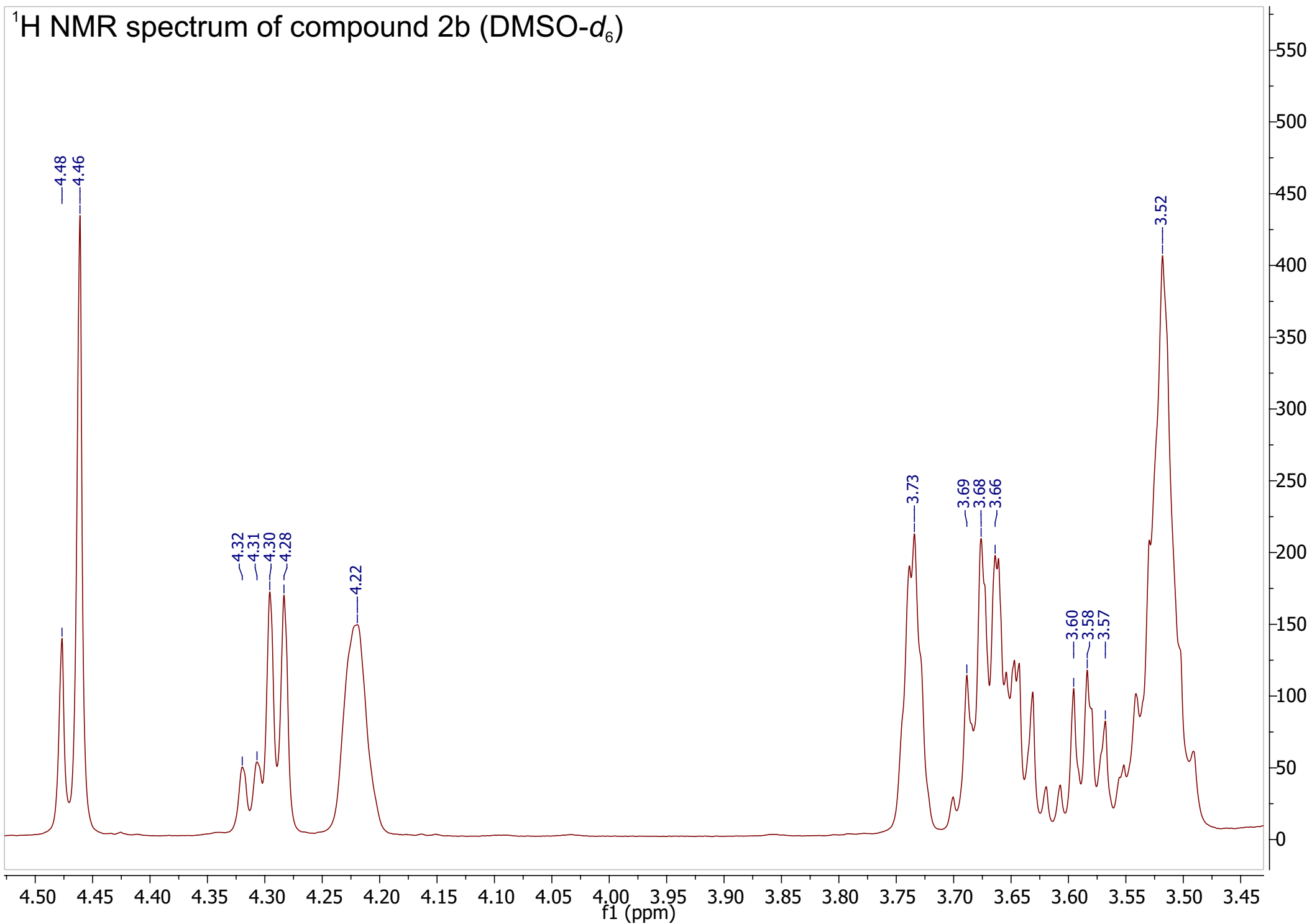
^{13}C NMR spectrum of compound 2b (DMSO-d_6)
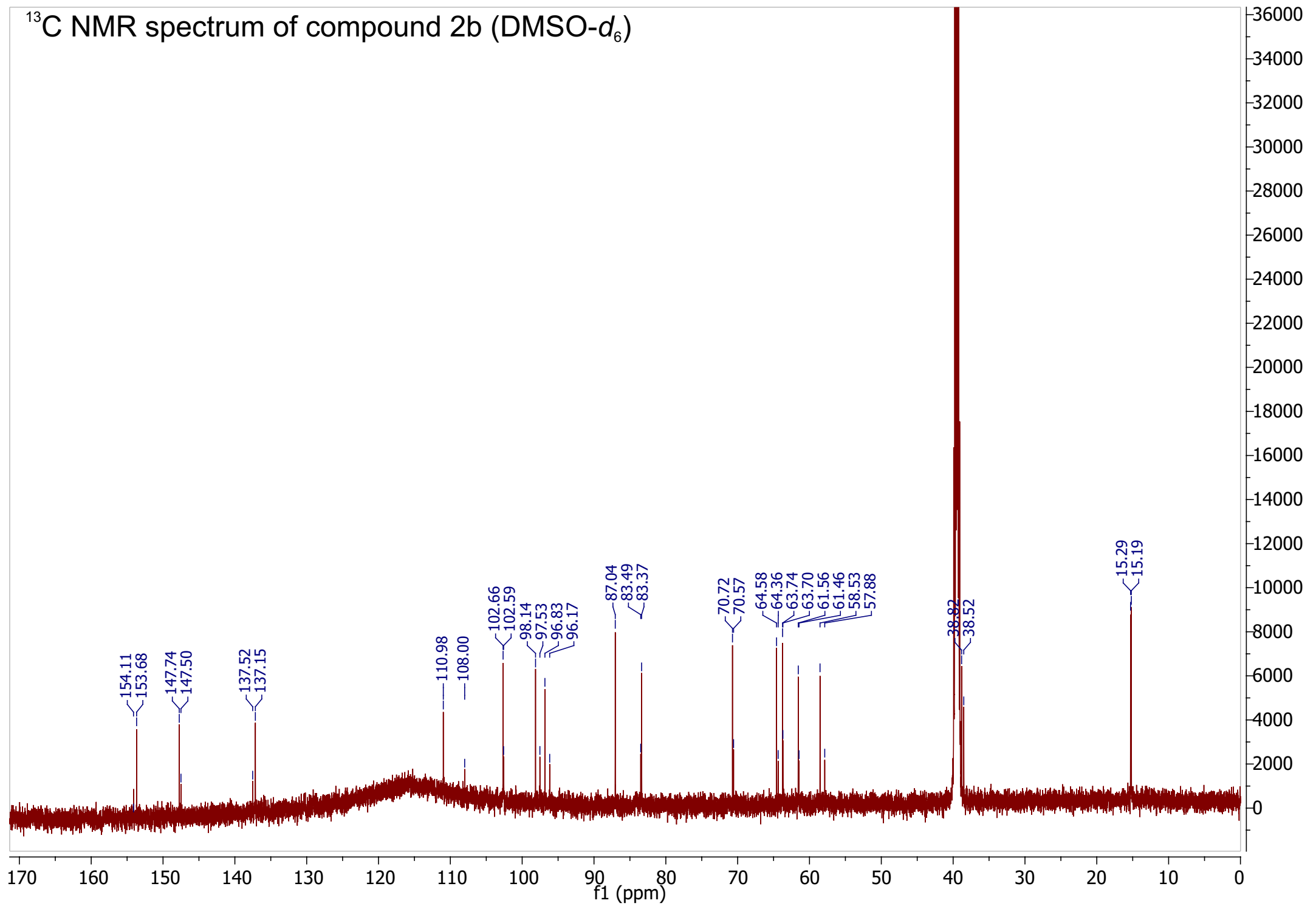
^{13}C NMR spectrum of compound 2b (DMSO-d_6)

HSQC spectrum of compound 2b (DMSO-d_6)

{1.04,15.07} {1.10,15.15}

{2.02,38.70}

{4.28,58.43}

{3.51,61.42}

{3.52,63.65}

{4.22,70.56}

{3.66,64.03}

{6.19,83.32}

{3.73,86.98}

{5.78,96.64}

{5.47,98.10}

{5.20,97.49}

{7.48,137.30}

f1 (ppm)

f2 (ppm)
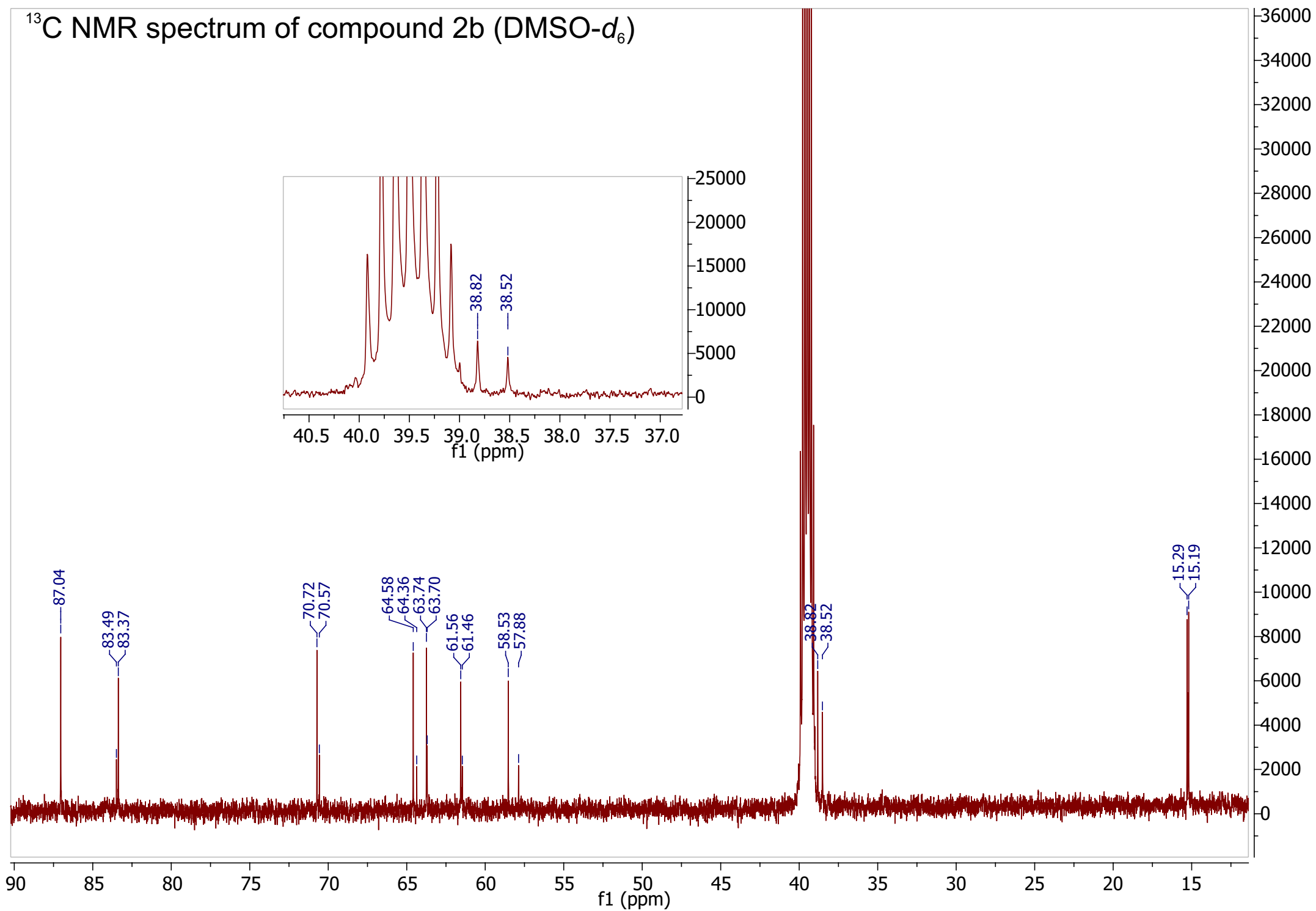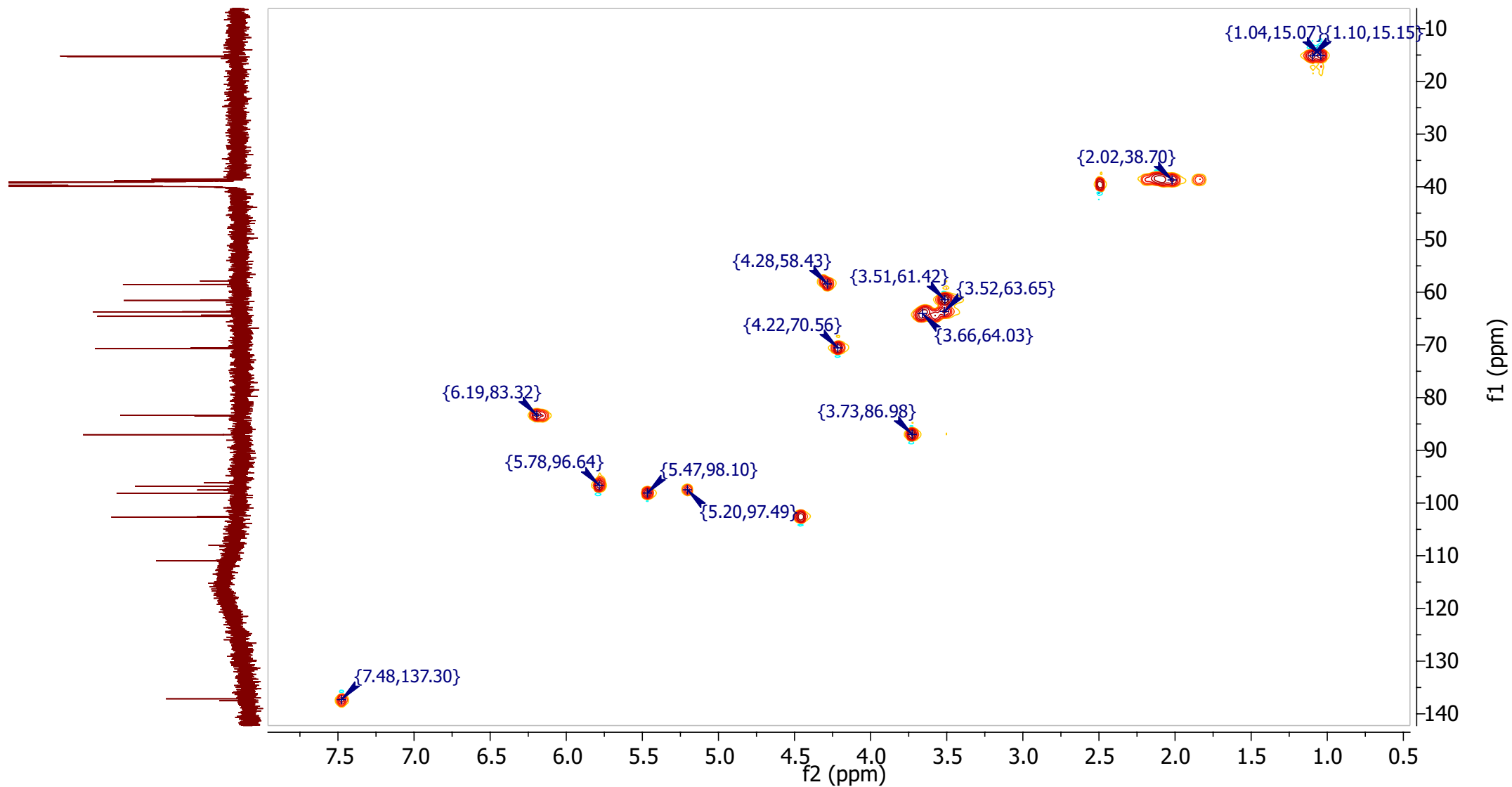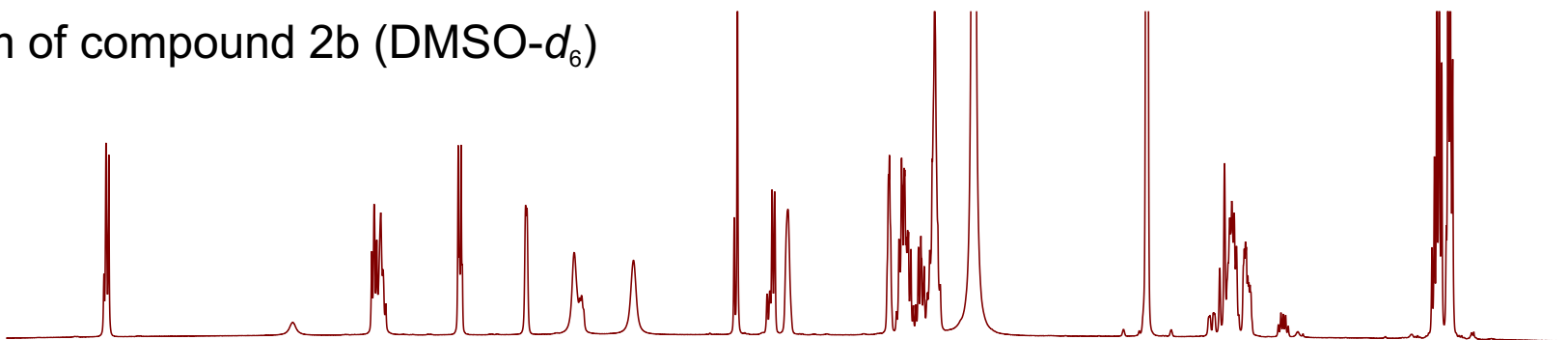
HMBC spectrum of compound 2b (DMSO-d_6)

HMBC spectrum of compound 2b (DMSO-d_6)

{4.46,58.44}
{2.13,58.56}
{4.46,64.15}
{1.10,64.54}
{1.05,63.68}
{3.51,70.67}
{2.10,70.74}
{2.02,70.67}
{3.74,70.62}
{2.09,83.30}
{3.51,87.03}
{2.02,86.99}
{4.30,98.12}
{2.13,98.07}
{4.28,102.66}
{3.66,102.51}
{3.59,102.71}
{3.53,102.57}
{4.48,108.15}
{4.46,111.08}
{2.13,110.99}
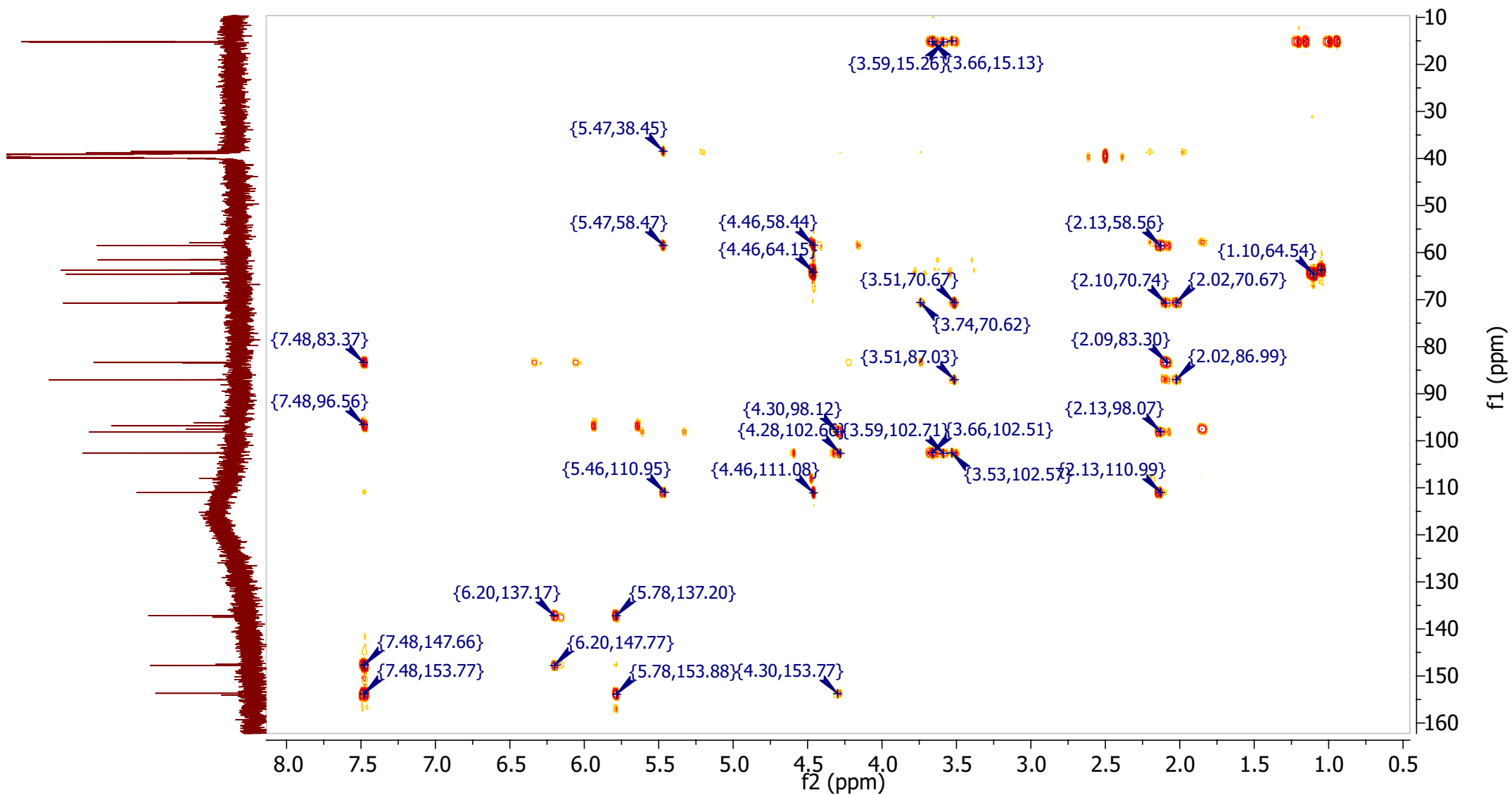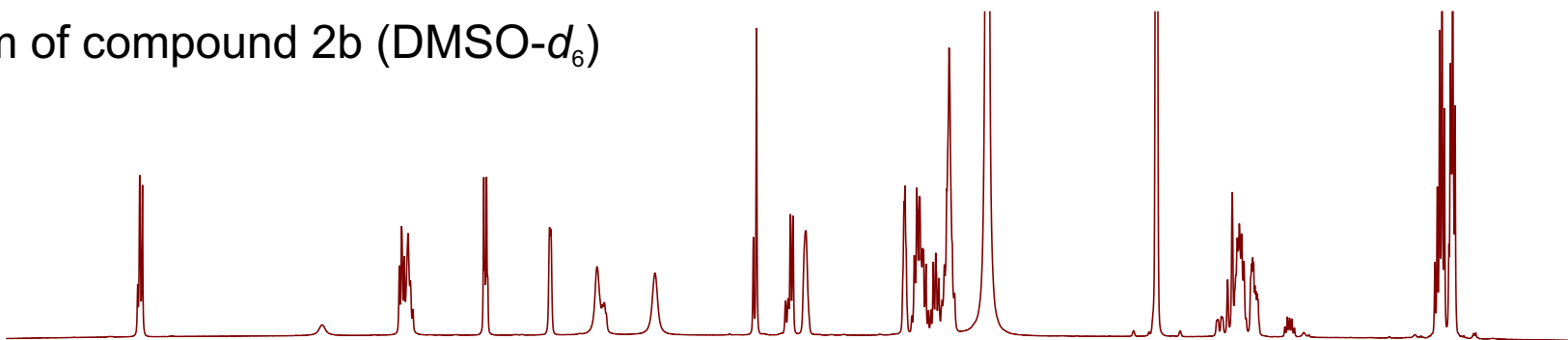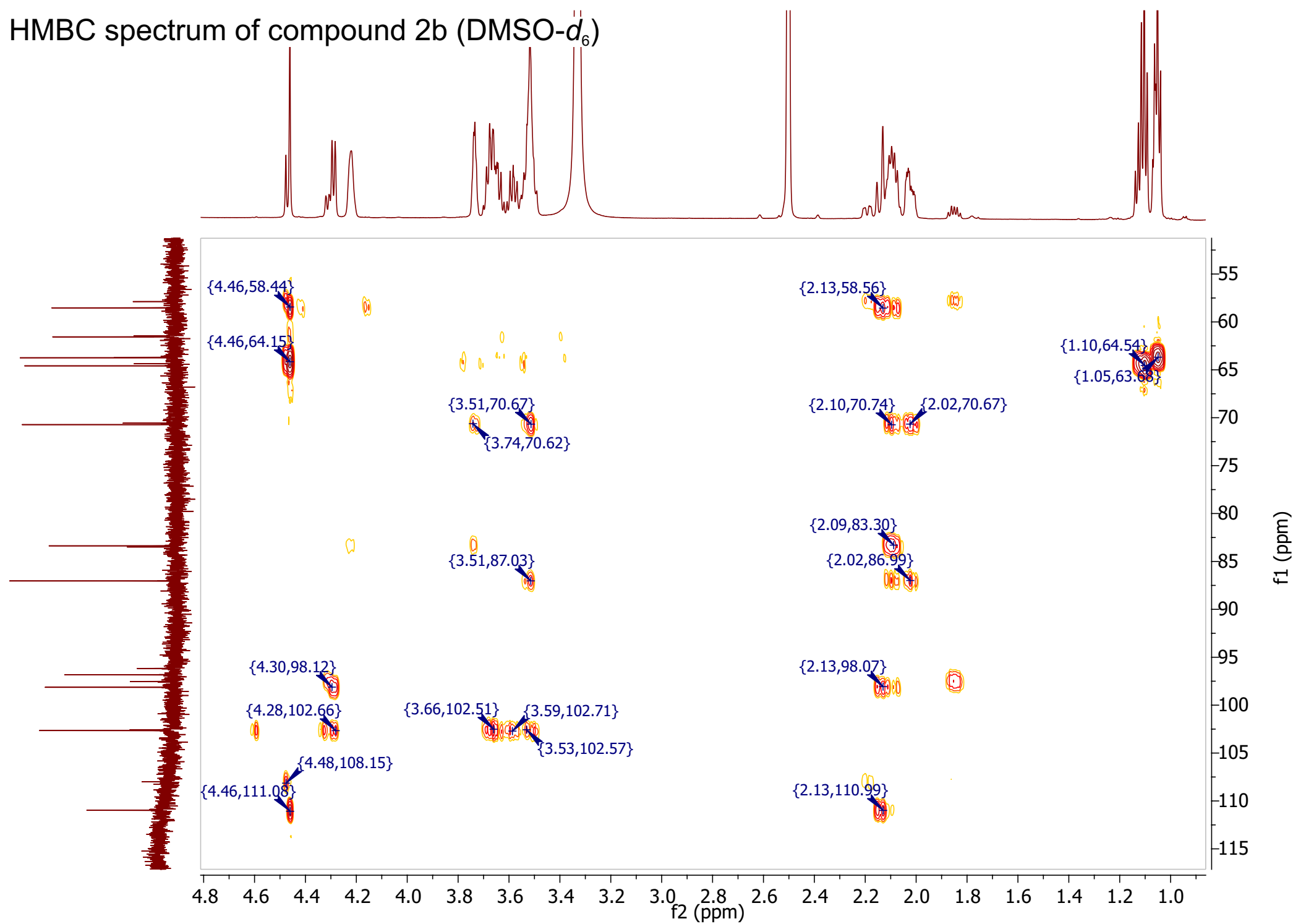
^{1}H NMR spectrum of compound 3 (DMSO-d_6)

HSQC spectrum of compound 3 (DMSO-d_6)

{1.11,15.32}

{2.25,39.83}   {2.13,39.45}

{4.77,60.71}   {3.57,61.84}   {3.51,61.85}

{3.55,63.99}{3.64,64.01}

{4.36,70.88}

{6.24,83.83}

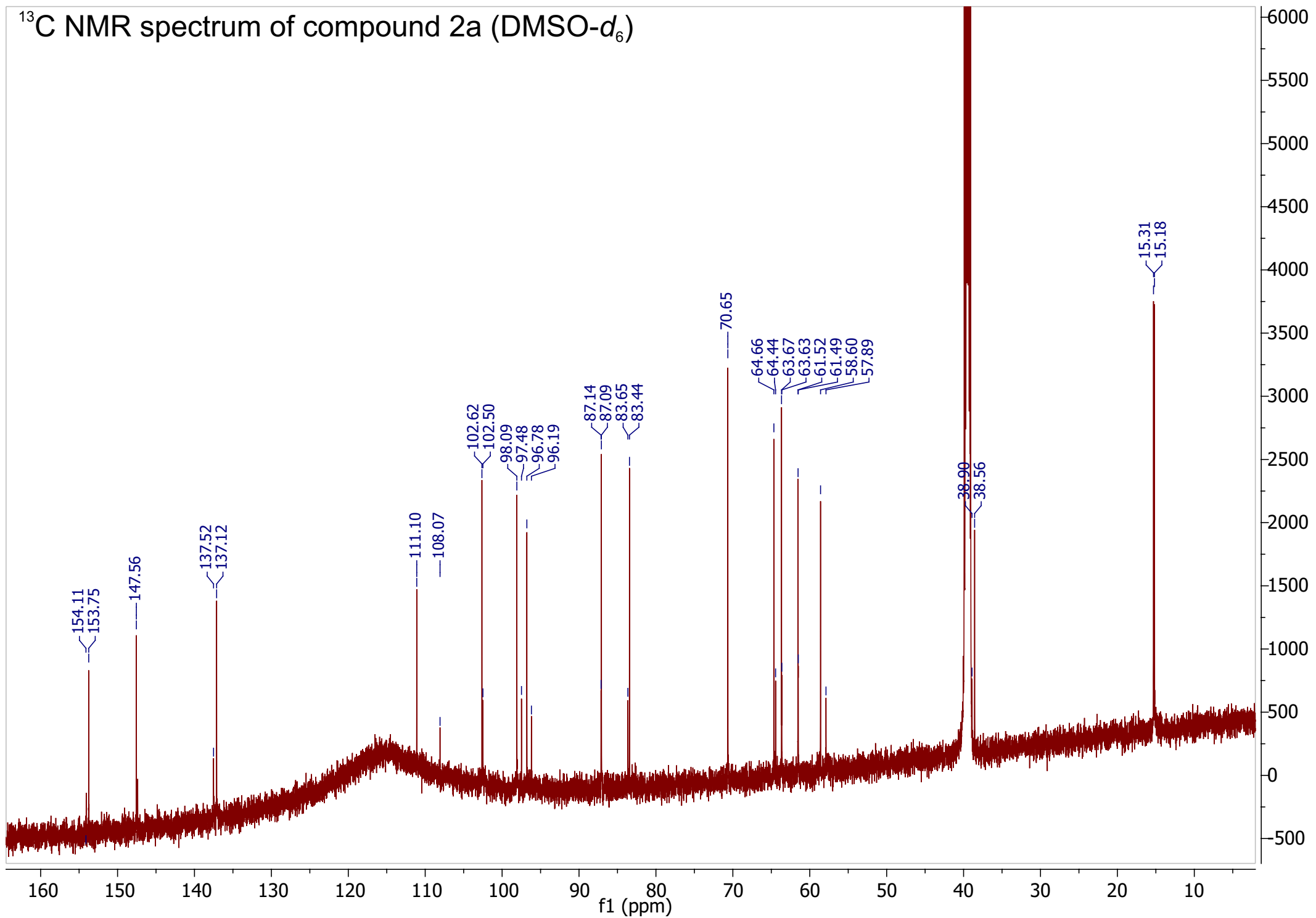{3.85,88.13}

{6.00,102.30}

{4.27,103.76}
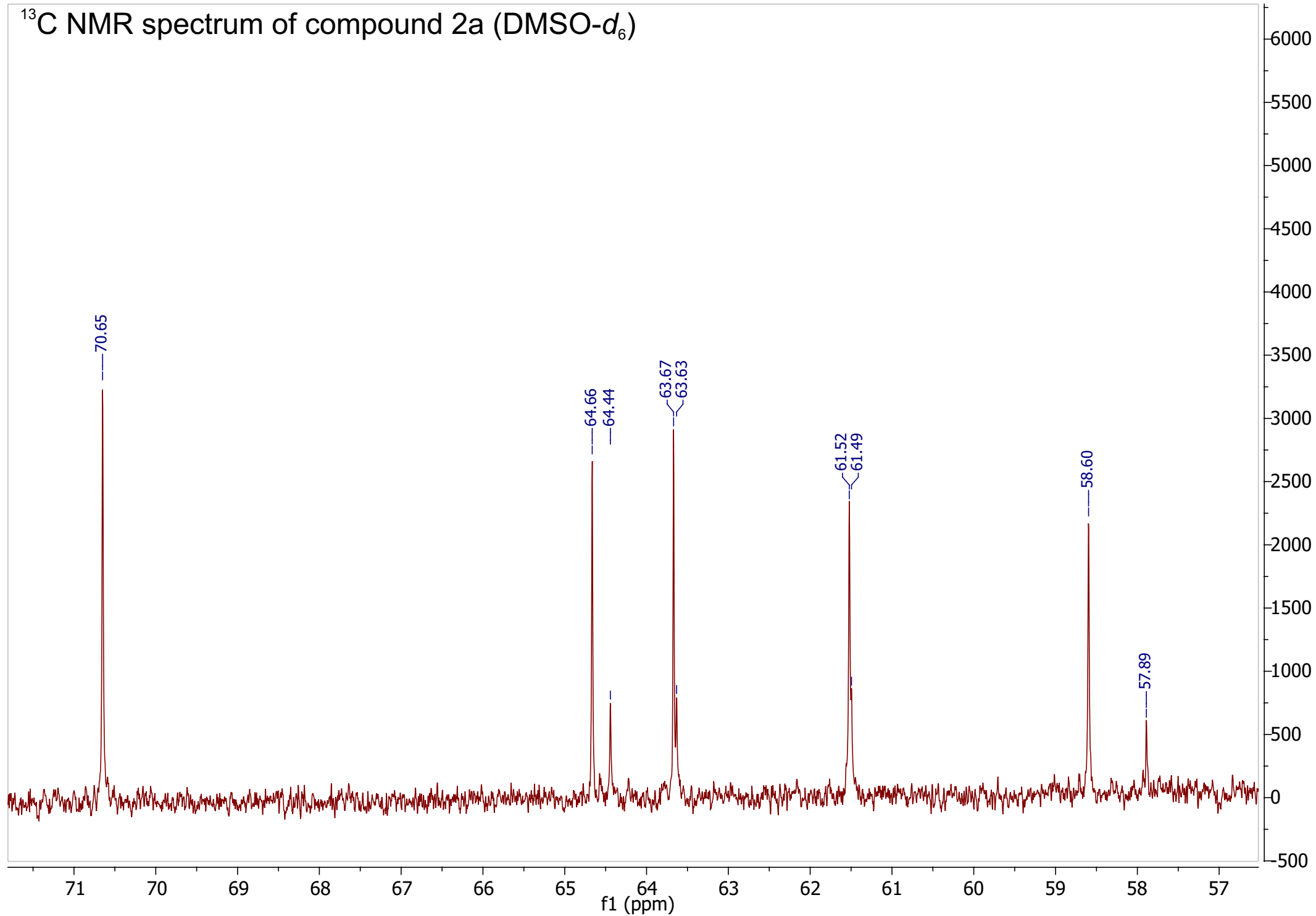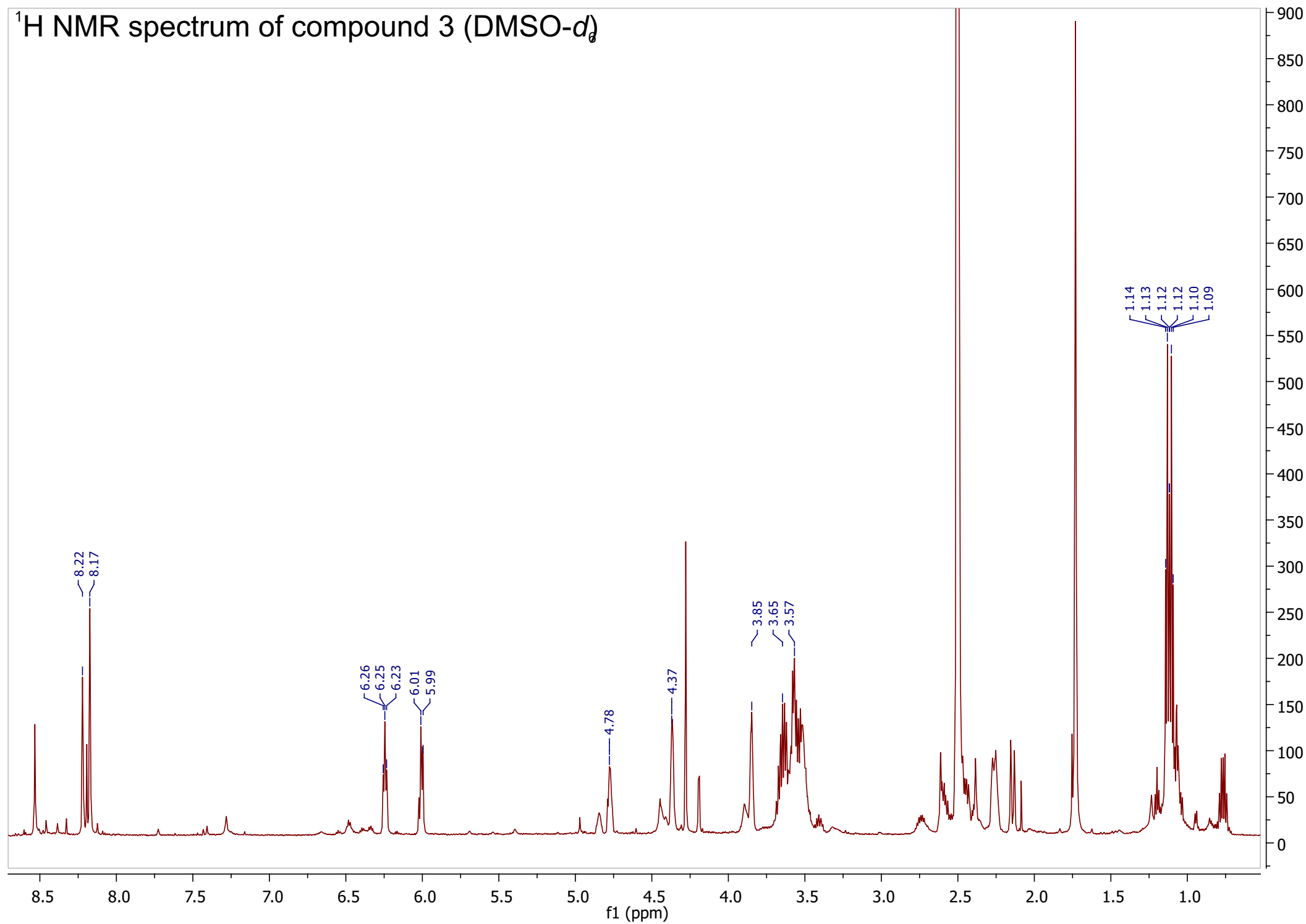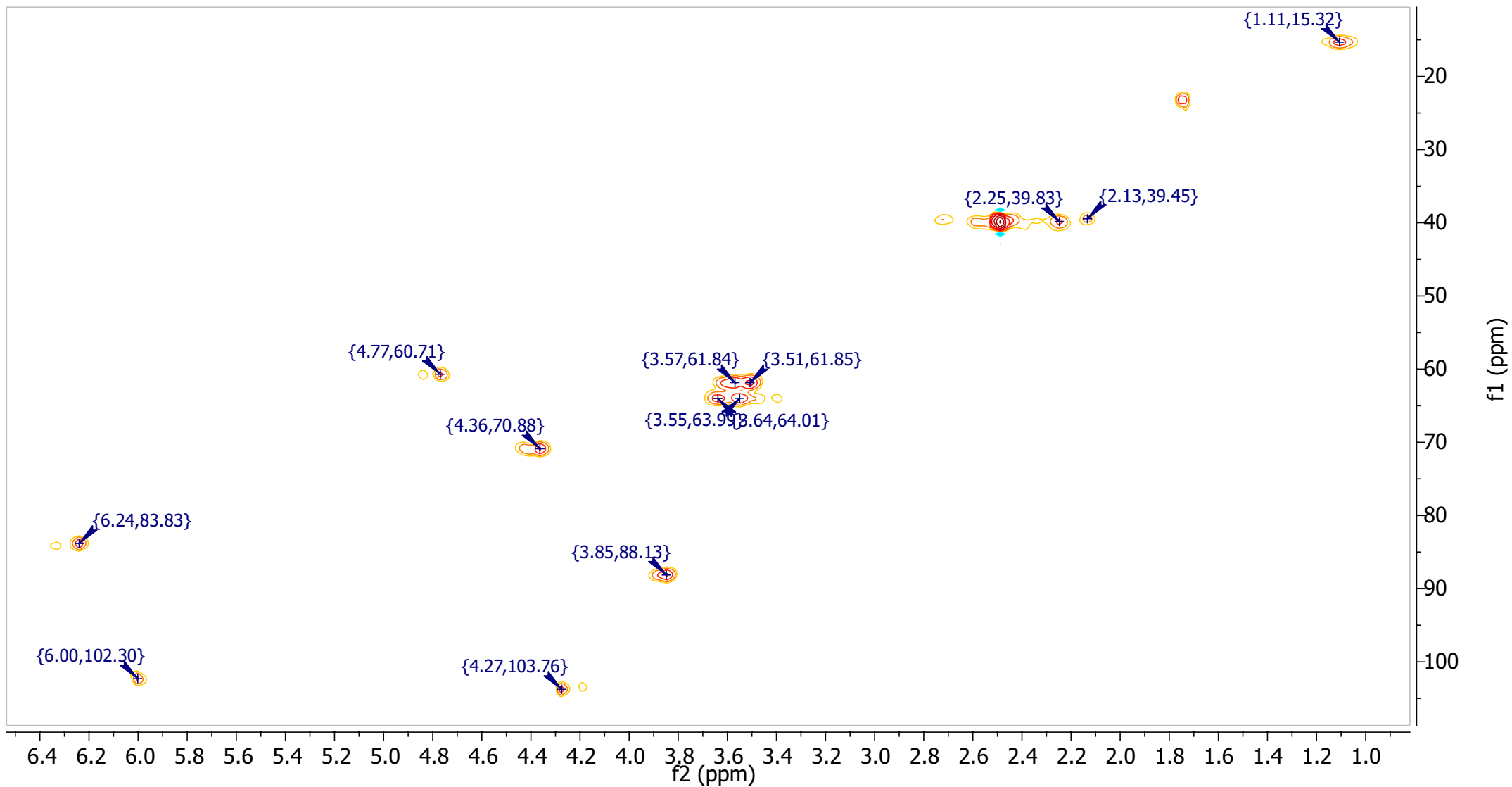
^{1}H NMR spectrum of compound 4a (DMSO-d_6)

^{1}H NMR spectrum of compound 4a (DMSO-d_6)
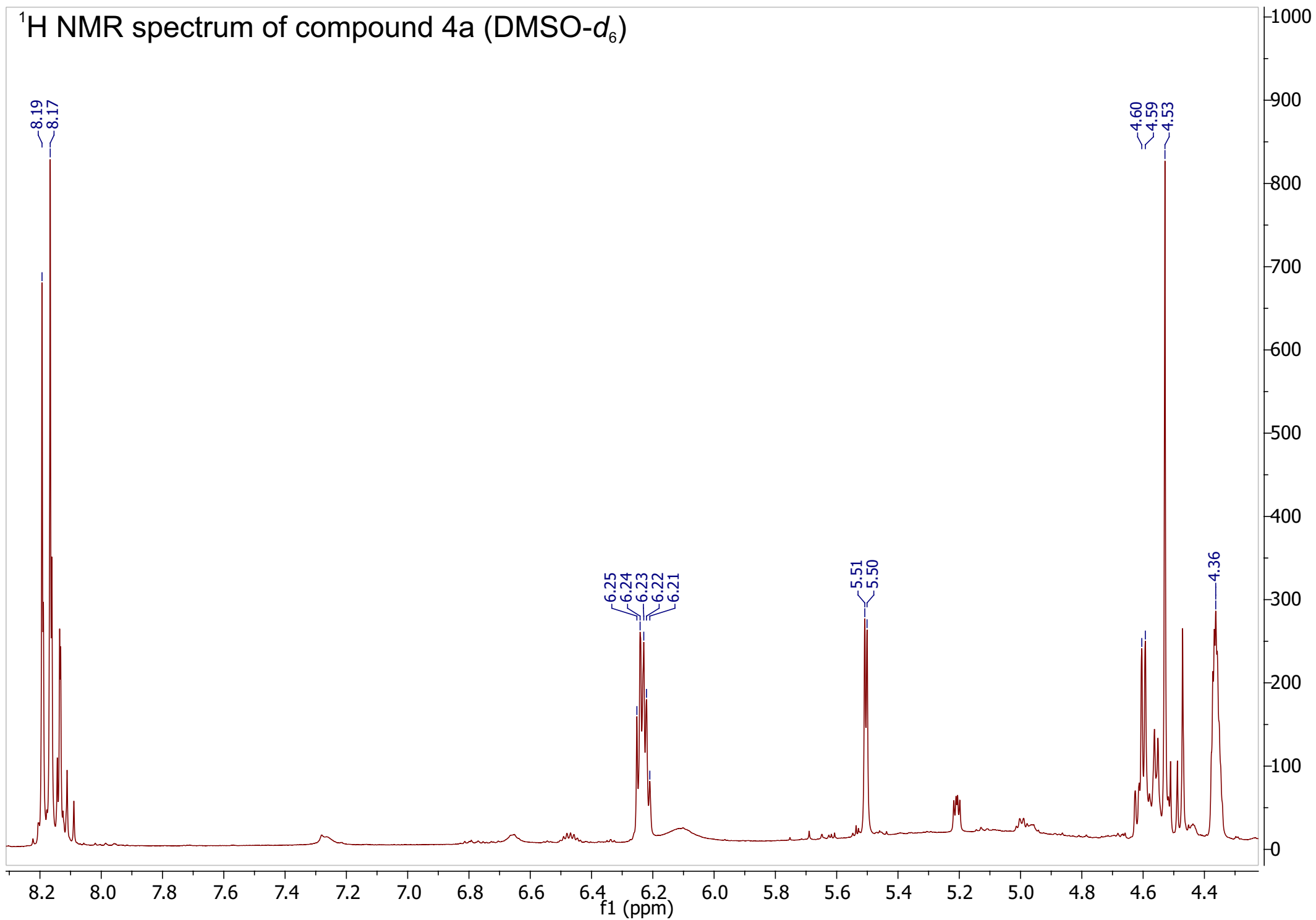
^{13}C NMR spectrum of compound 4a (DMSO-d_6)
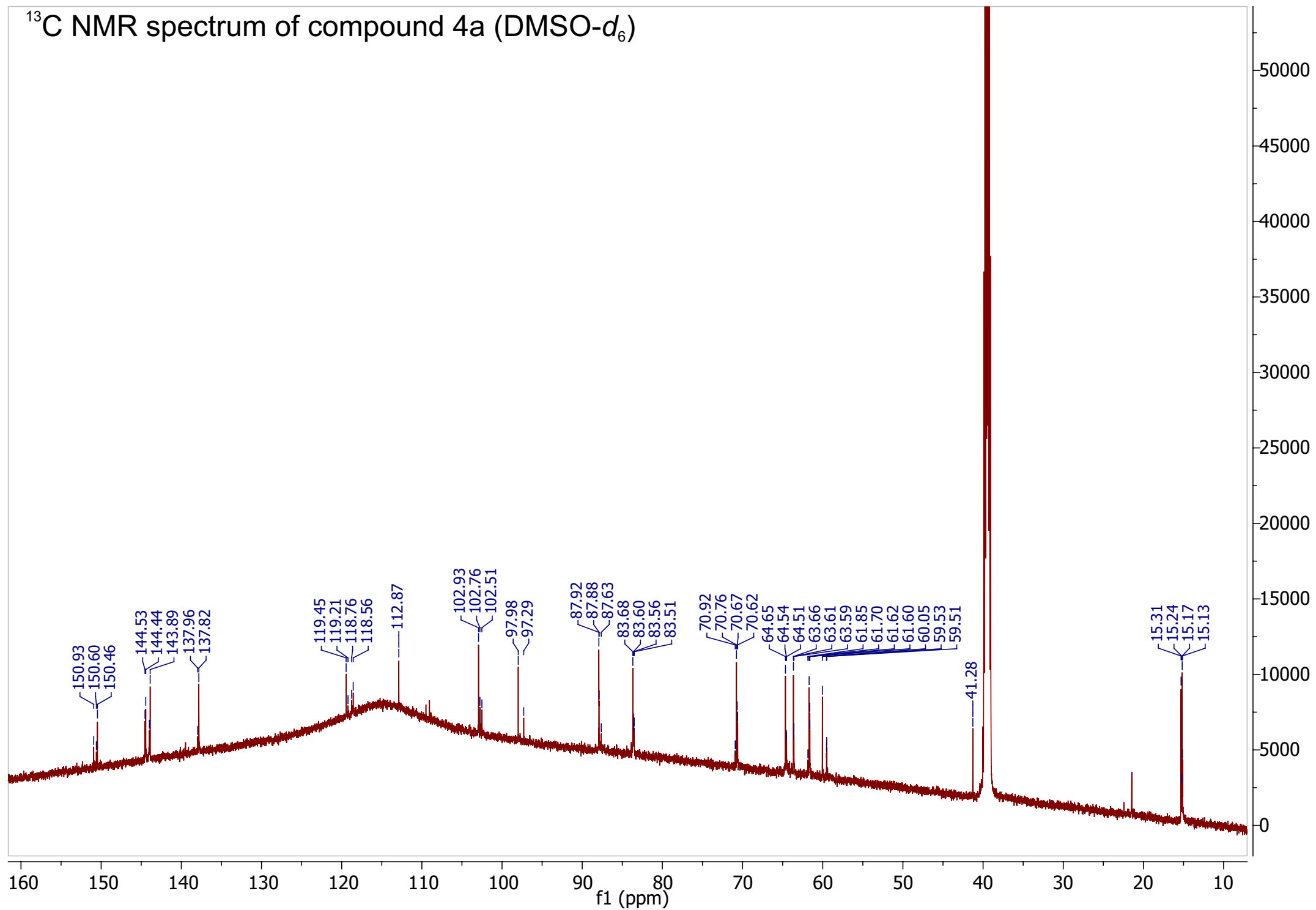
^{13}C NMR spectrum of compound 4a (DMSO-d_6)

HSQC spectrum of compound 4a (DMSO-d_6)

{1.12,15.14} {1.03,15.06}

{2.57,39.69} {2.49,39.63}
{2.24,39.74}

{4.60,59.82} {3.57,61.56} {3.51,61.53}
{4.36,70.59}
{3.56,63.59}{3.68,64.29}

{6.23,83.57} {4.98,87.14} {4.56,87.60}{3.84,87.85}

{5.50,97.94} {5.20,97.24}
{4.53,102.83}

{8.17,137.69}
{8.19,144.00}
{8.13,144.12}

f1 (ppm)

f2 (ppm)

HMBC spectrum of compound 4a (DMSO-d_6)

{3.63,15.14} {3.66,15.25}

{5.51,59.98}
{4.53,60.08}
{4.53,64.04}
{2.26,59.78} {2.22,59.91}
{2.19,59.98}

{3.59,70.67} {3.51,70.72}

{2.60,83.59} {2.56,83.49}

{4.61,97.89}
{2.22,97.90} {2.19,98.00}

{3.68,102.66} {3.55,102.99}
{3.72,102.71} {3.55,102.99}

{5.50,112.86}
{4.53,112.86}
{2.21,112.83} {2.19,112.93}

f1 (ppm)

f2 (ppm)
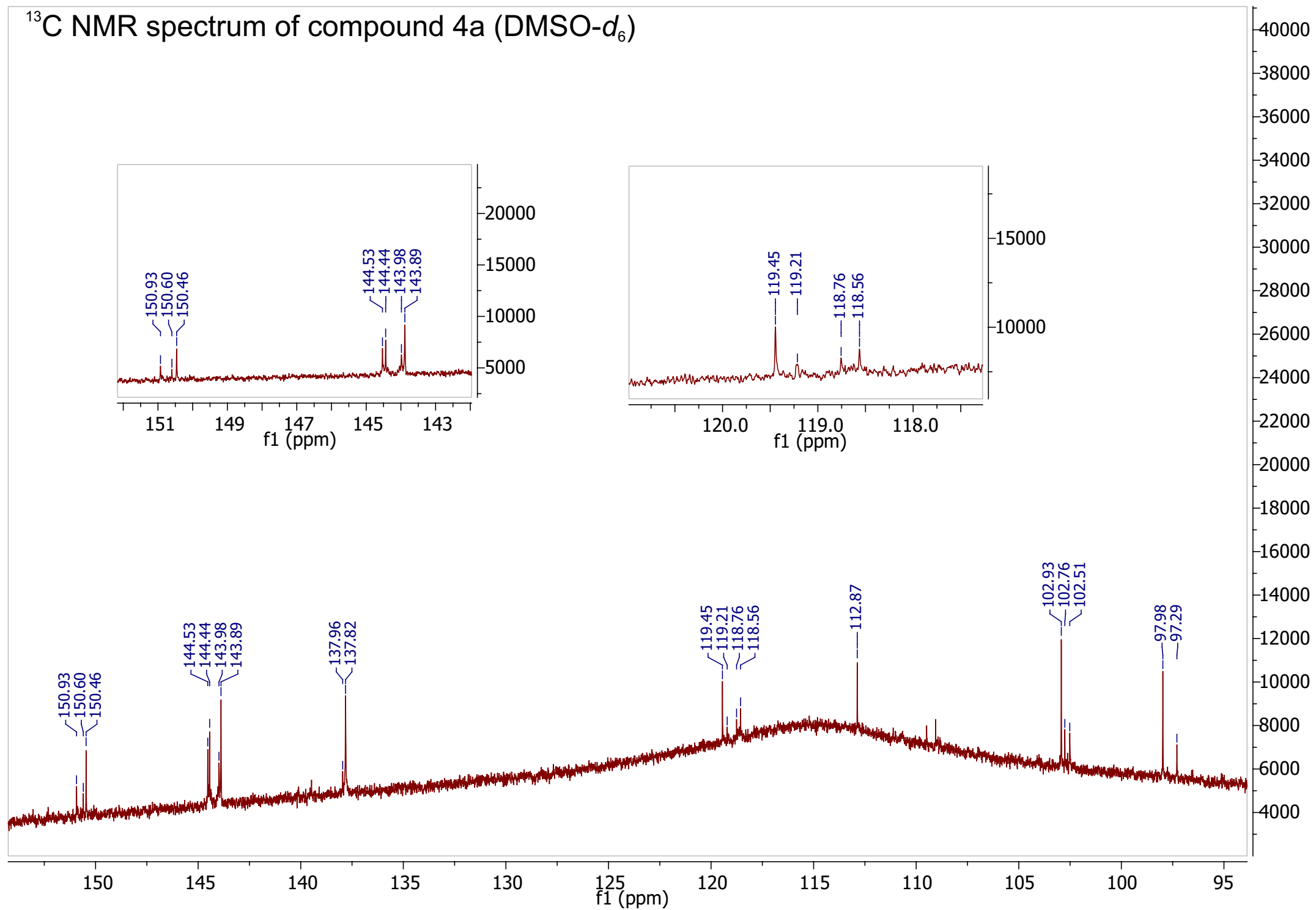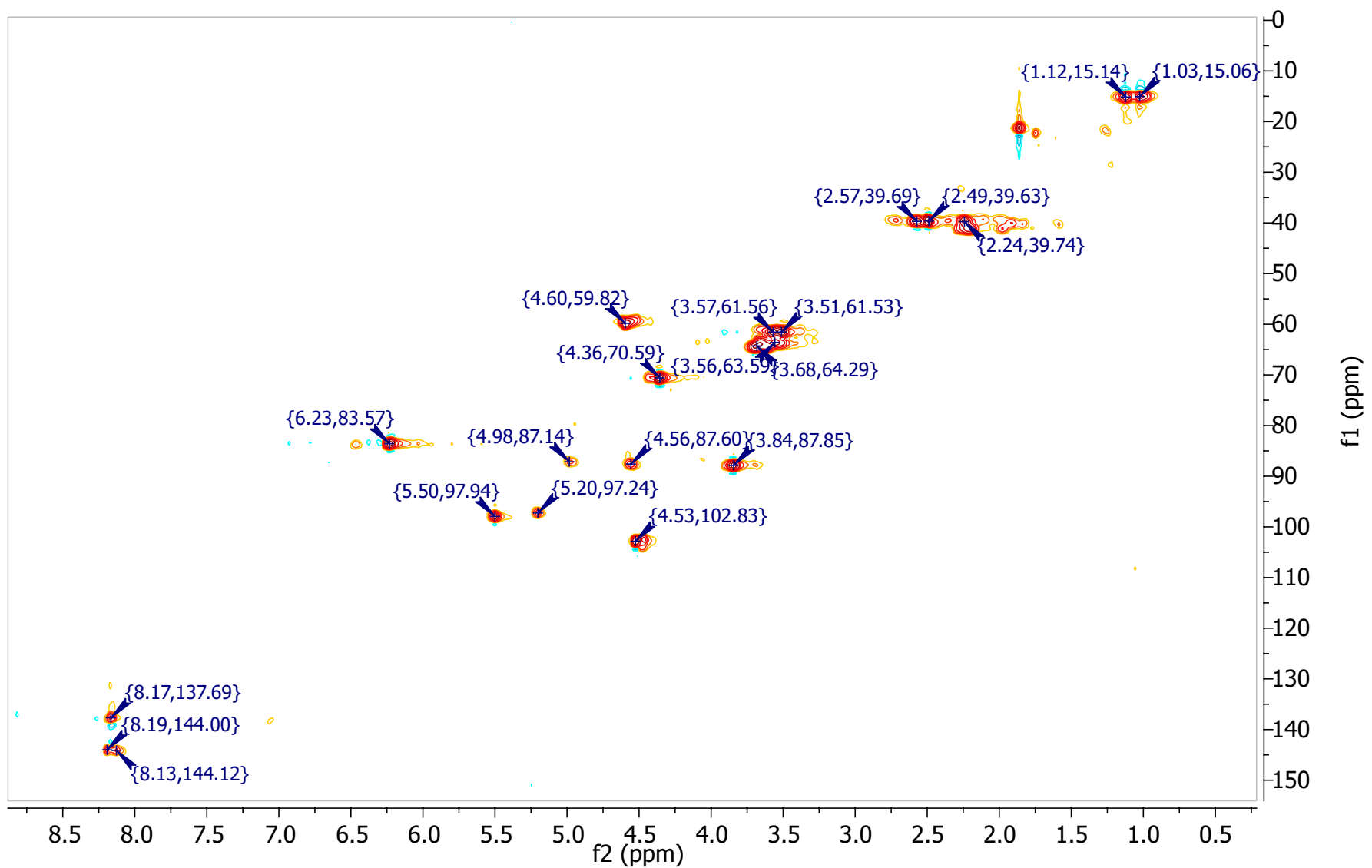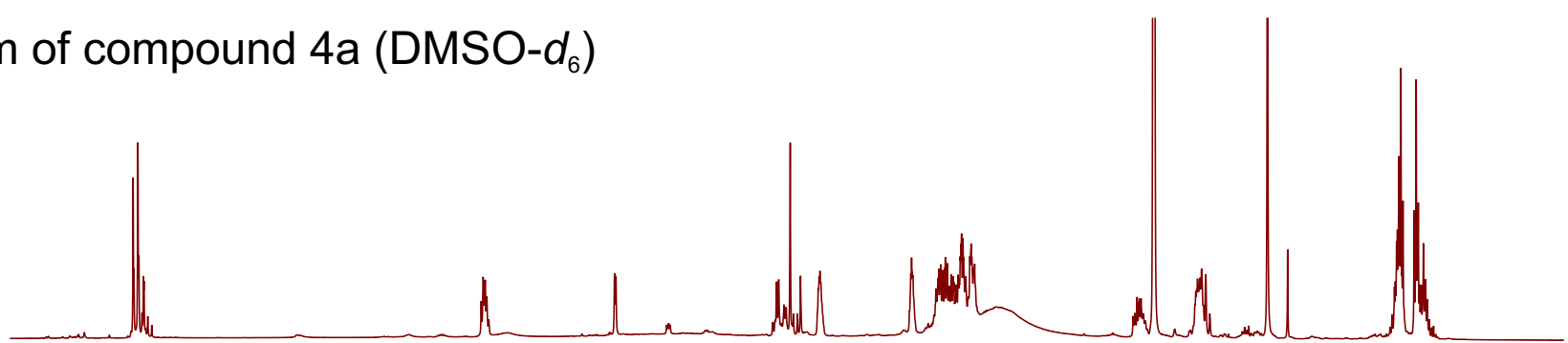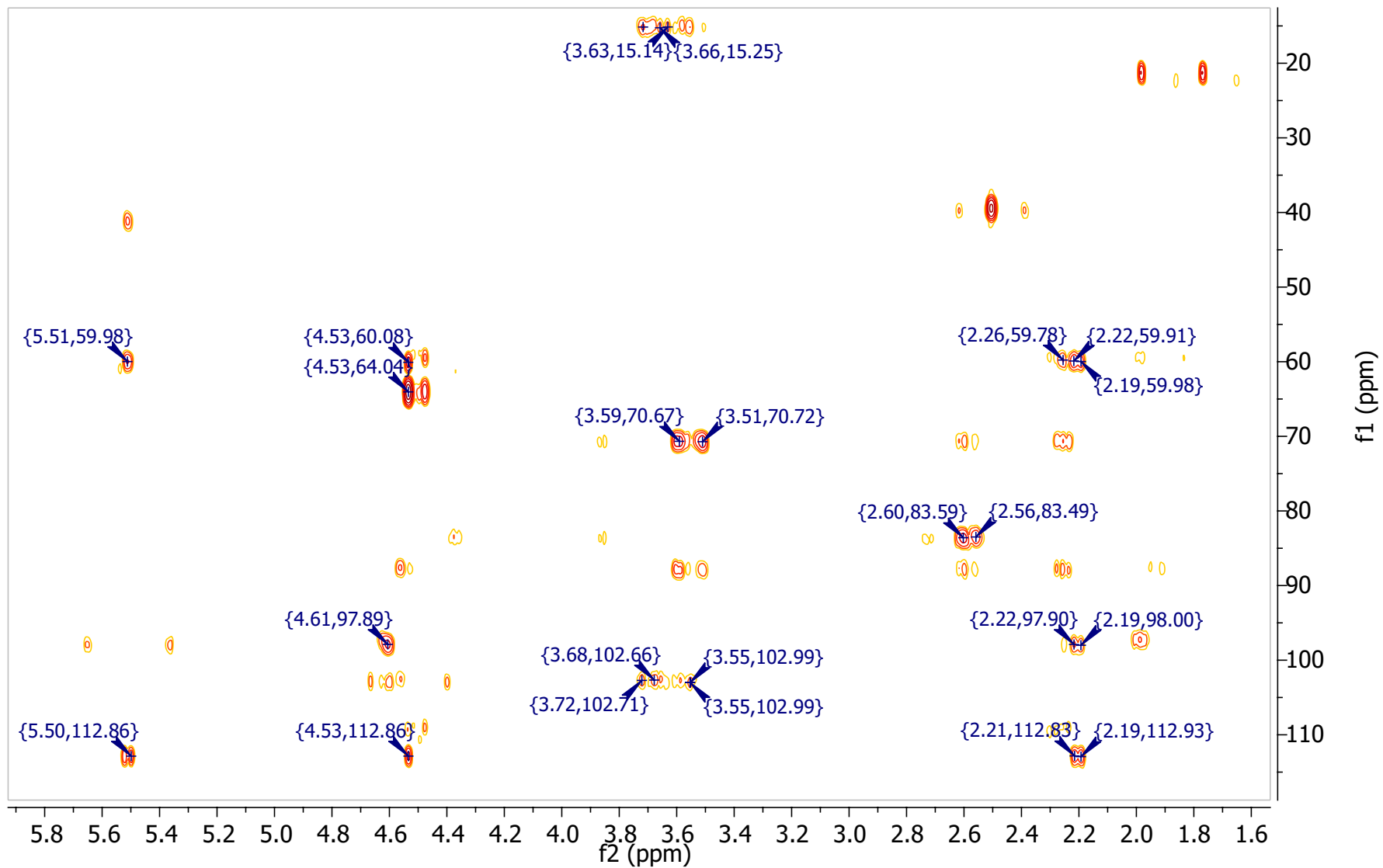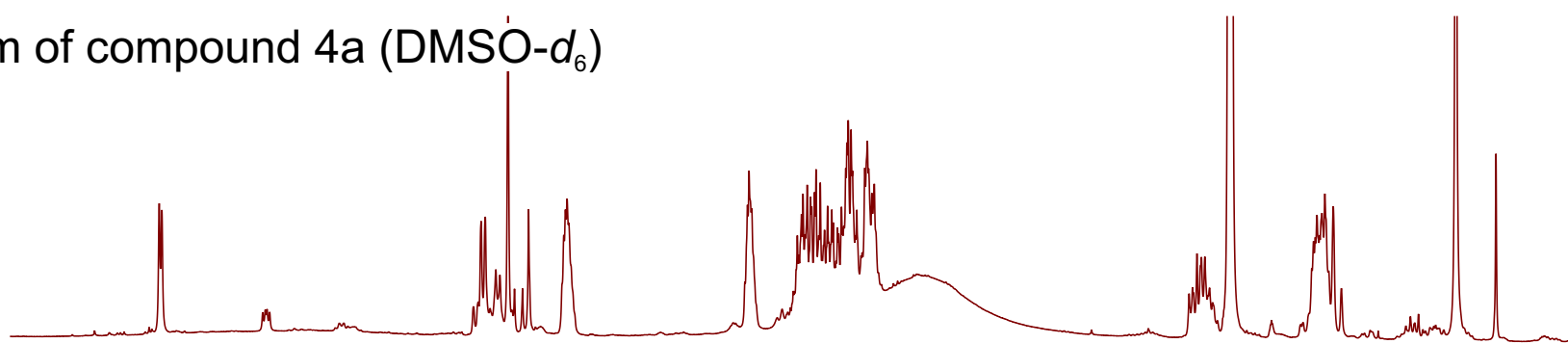
^{1}H NMR spectrum of compound 4b (DMSO-d_6)

HSQC spectrum of compound 4b (DMSO-d_6)

{1.12,14.91}   {0.99,14.80}

{2.49,39.40}   {2.25,39.40}

{2.21,40.92}

{4.58,59.49}   {3.56,61.28}   {3.50,61.27}

{4.36,70.33}   {3.54,63.36}{3.67,63.89}

{6.22,83.36}   {4.99,86.92}   {4.58,87.19}{3.84,87.61}

{5.50,97.69}   {5.20,96.97}

{4.52,102.58}

{8.16,137.55}

{8.12,143.87}

f1 (ppm)

f2 (ppm)
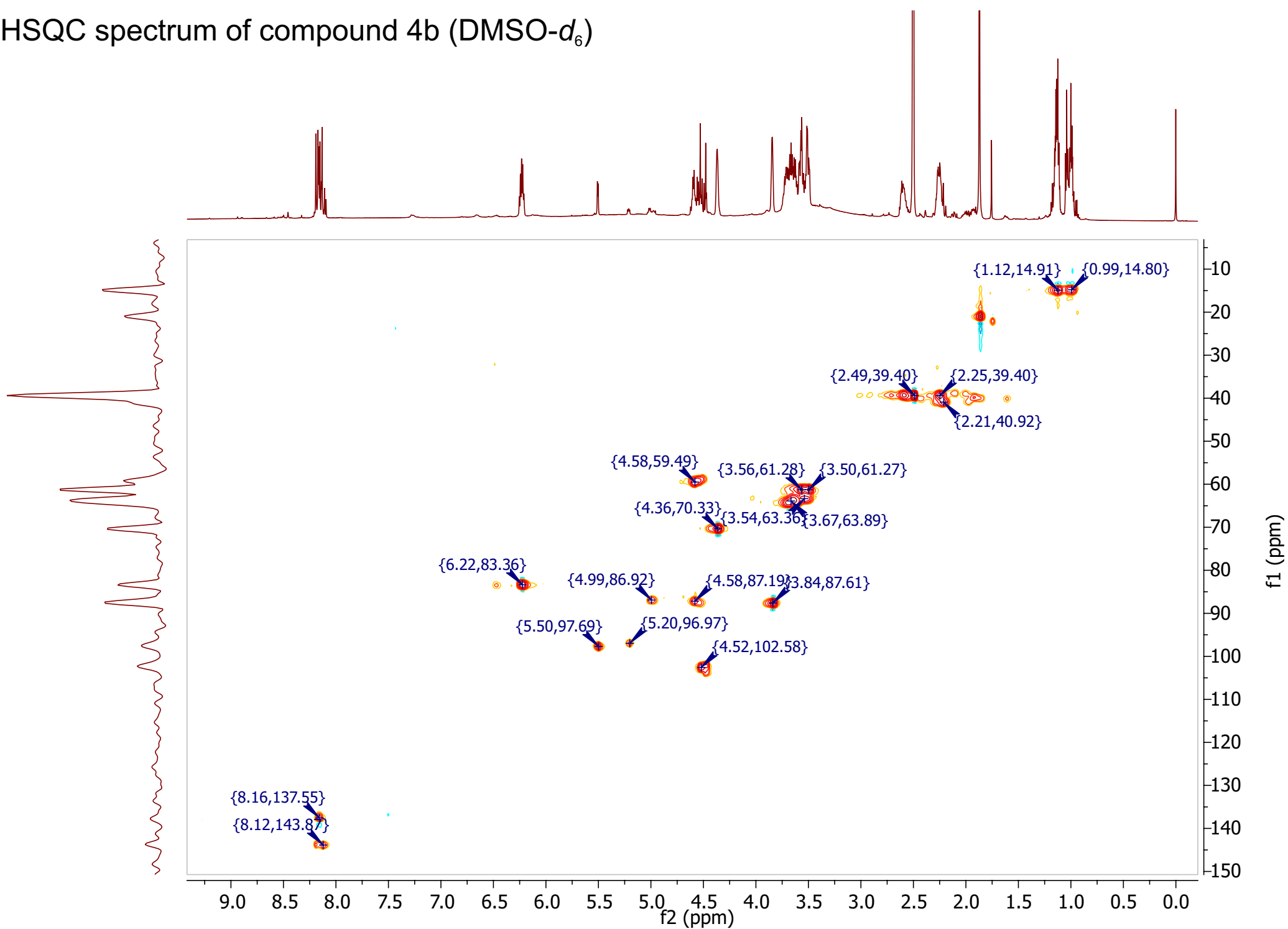
HMBC spectrum of compound 4b (DMSO-d_6)

HMBC spectrum of compound 4b (DMSO-d_6)

{4.53,63.65} {4.48,63.56}

{2.22,59.54} {2.25,59.31}

{3.59,70.17} {3.49,70.29}

{2.61,69.95}

{4.55,86.92}

{3.59,87.48} {3.49,87.47}

{2.61,83.28}

{4.59,97.61}

{2.22,97.65}

{3.65,102.21}

{4.53,112.52}

{2.22,112.60}

f1 (ppm)

f2 (ppm)
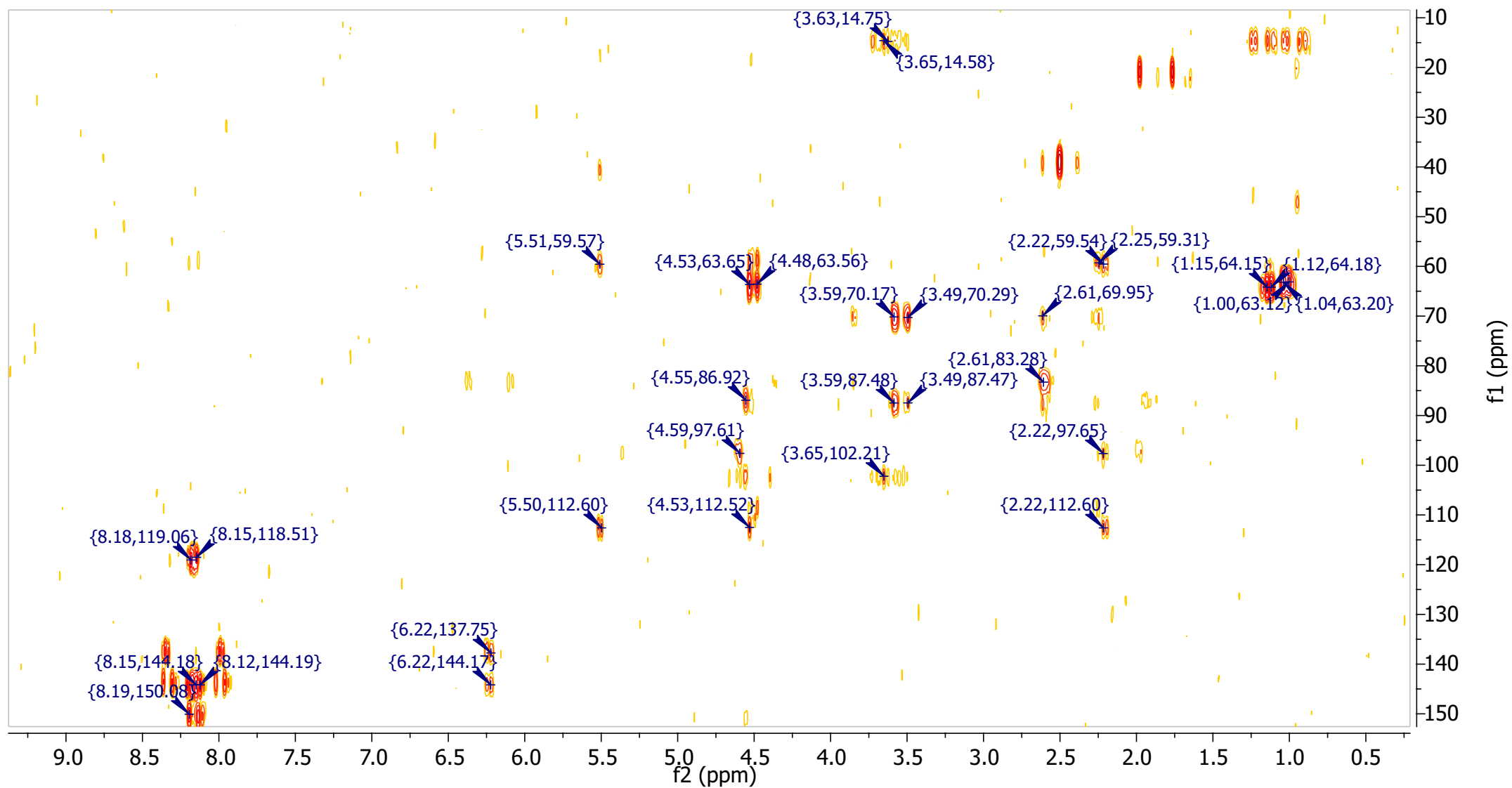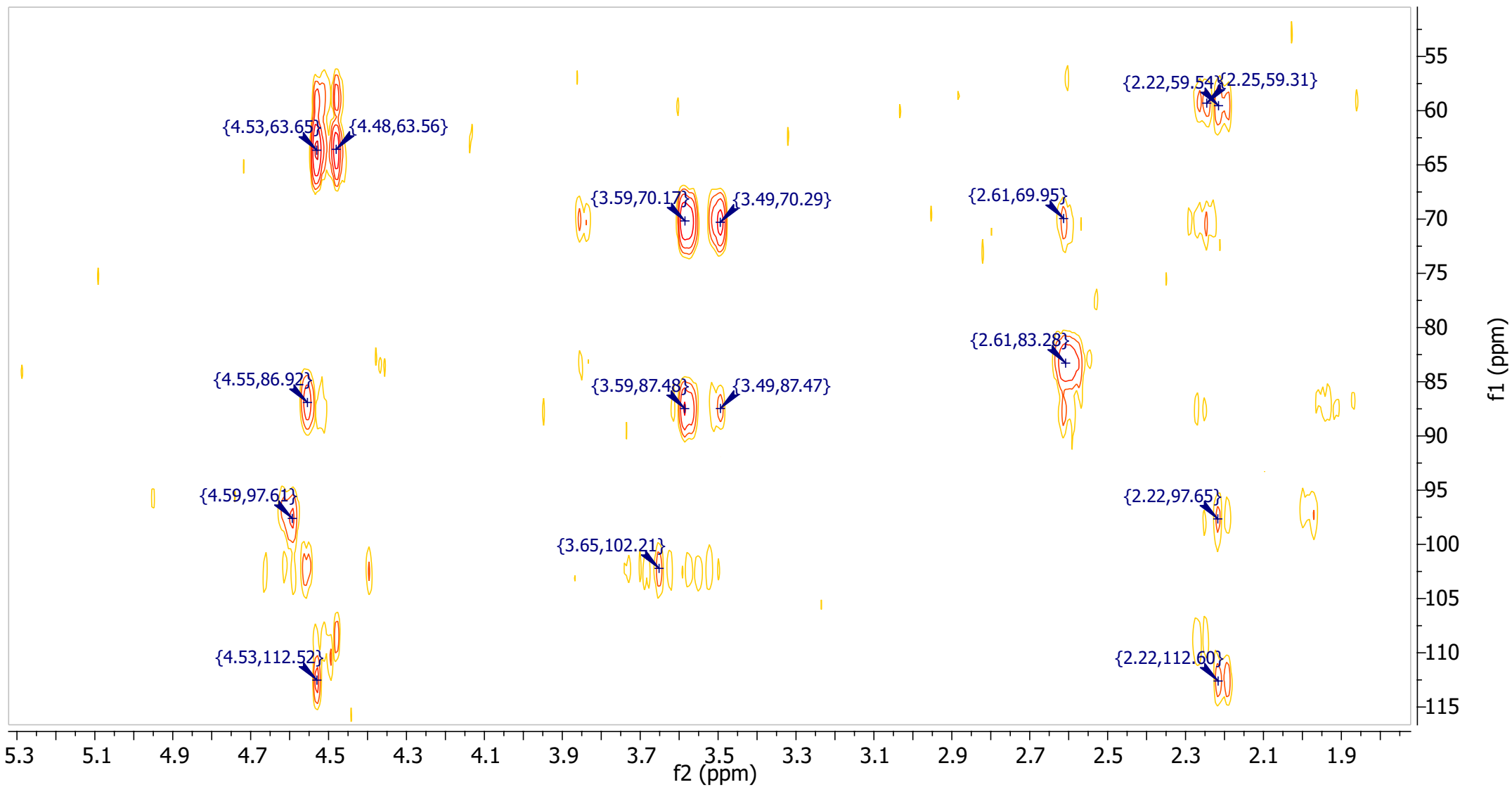
Section C

HRMS of the synthesised adducts

HRMS of compound **1a**

HRMS of compound **1b**

HRMS of compound **2a**

HRMS of compound **2b**

HRMS of compound **4a**

HRMS of compound **4b**

HRMS of compound 1a

Analysis Info

Analysis Name	D:\Data\SabineRendon\130912\Donata 1a and 1b_1-A,3_01_5604.d	Acquisition Date	9/12/2013 4:20:10 PM
Method	130912Donata.m	Operator	Bruker07
Sample Name	Donata 1a and 1b	Instrument	micrOTOF-Q
Comment			

TIC +All MS

UV, 4.5-5.3min #(1295-1544),

+MS, 4.5-5.3min #(267-316)

298.1379

414.1879

HRMS of compound 1b

Analysis Info

Analysis Name	D:\Data\SabineRendon\130912\Donata 1a and 1b_1-A,3_01_5604.d		
Method	130912Donata.m	Operator	Bruker07
Sample Name	Donata 1a and 1b	Instrument	micrOTOF-Q
Comment			

Acquisition Date 9/12/2013 4:20:10 PM

TIC +All MS

UV, 5.4-5.9min #(1563-1727),

+MS, 5.4-5.9min #(321-353)

298.1381

414.1880

HRMS of compound 2a

Analysis Info

Analysis Name	D:\Data\SabineRendon\130912 Donata 2a.d	Acquisition Date	9/12/2013 2:21:40 PM
Method	tune_wide pos021112.m	Operator	Bruker07
Sample Name	130912 Donata 2a	Instrument	micrOTOF-Q
Comment			

+MS, 0.1-0.7min #(3-26)

Peaks labeled: 436.1696, 414.1869, 298.1396, 320.1222, 353.2628, 849.3487
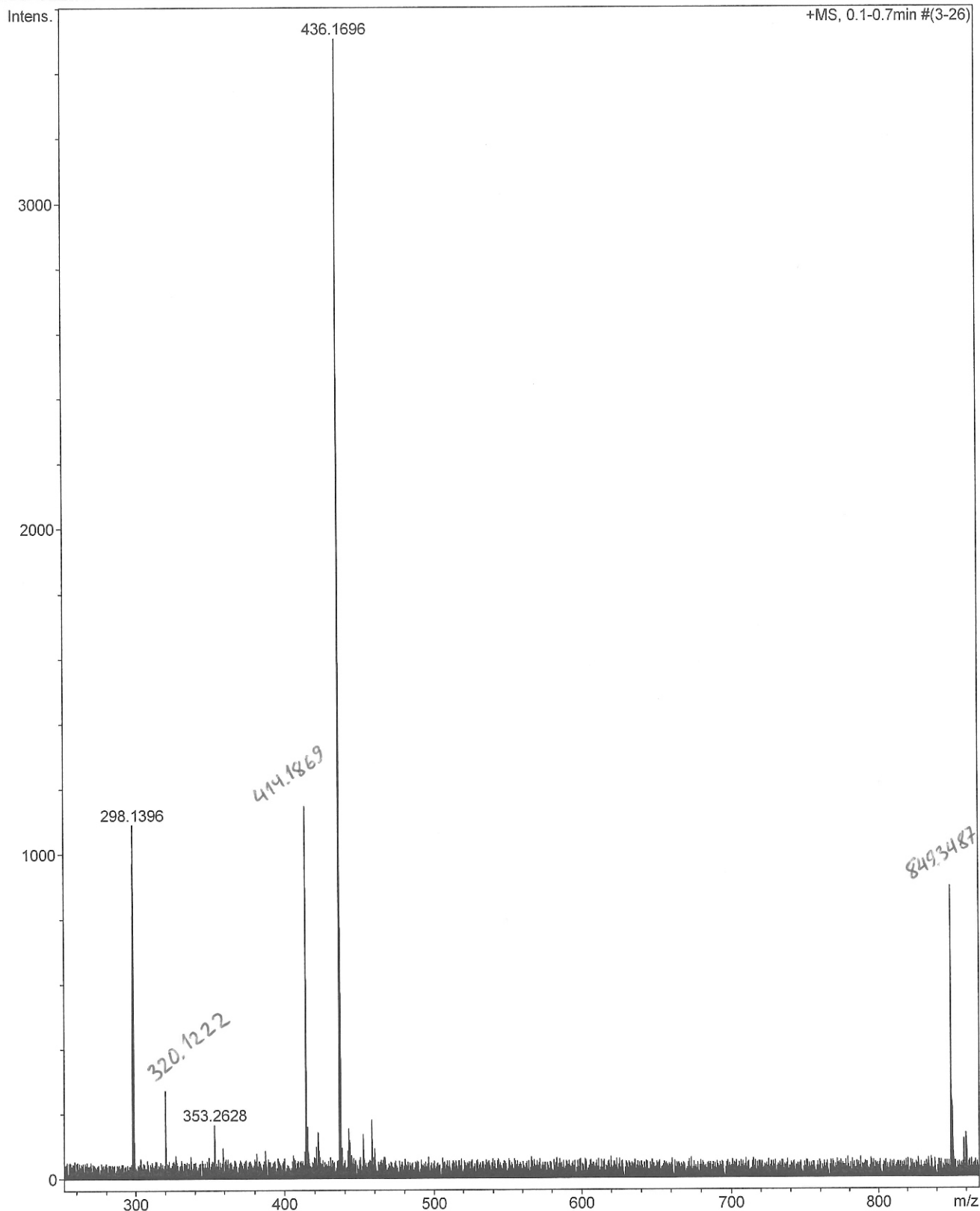
HRMS of compound 2b

Analysis Info

		Acquisition Date	9/12/2013 2:34:11 PM
Analysis Name	D:\Data\SabineRendon\130912 Donata 2b.d		
Method	tune_wide pos021112.m	Operator	Bruker07
Sample Name	130912 Donata 2b	Instrument	micrOTOF-Q
Comment			

+MS, 0.1-0.5min #(3-20)

Peaks labeled: 414.1854, 436.1686, 298.1387, 320.1387, 849.3441, 827.3490

HRMS of compound 4a

Analysis Info

Analysis Name	D:\Data\SabineRendon\130912 Donata 4a.d	Acquisition Date	9/12/2013 3:05:21 PM
Method	tune_wide pos021112.m	Operator	Bruker07
Sample Name	130912 Donata 4a	Instrument	micrOTOF-Q
Comment			

+MS, 0.1-0.2min #(2-9)

Peaks: 438.1993, 322.1502, 460.1805, 423.2024, 444.6523, 897.3553
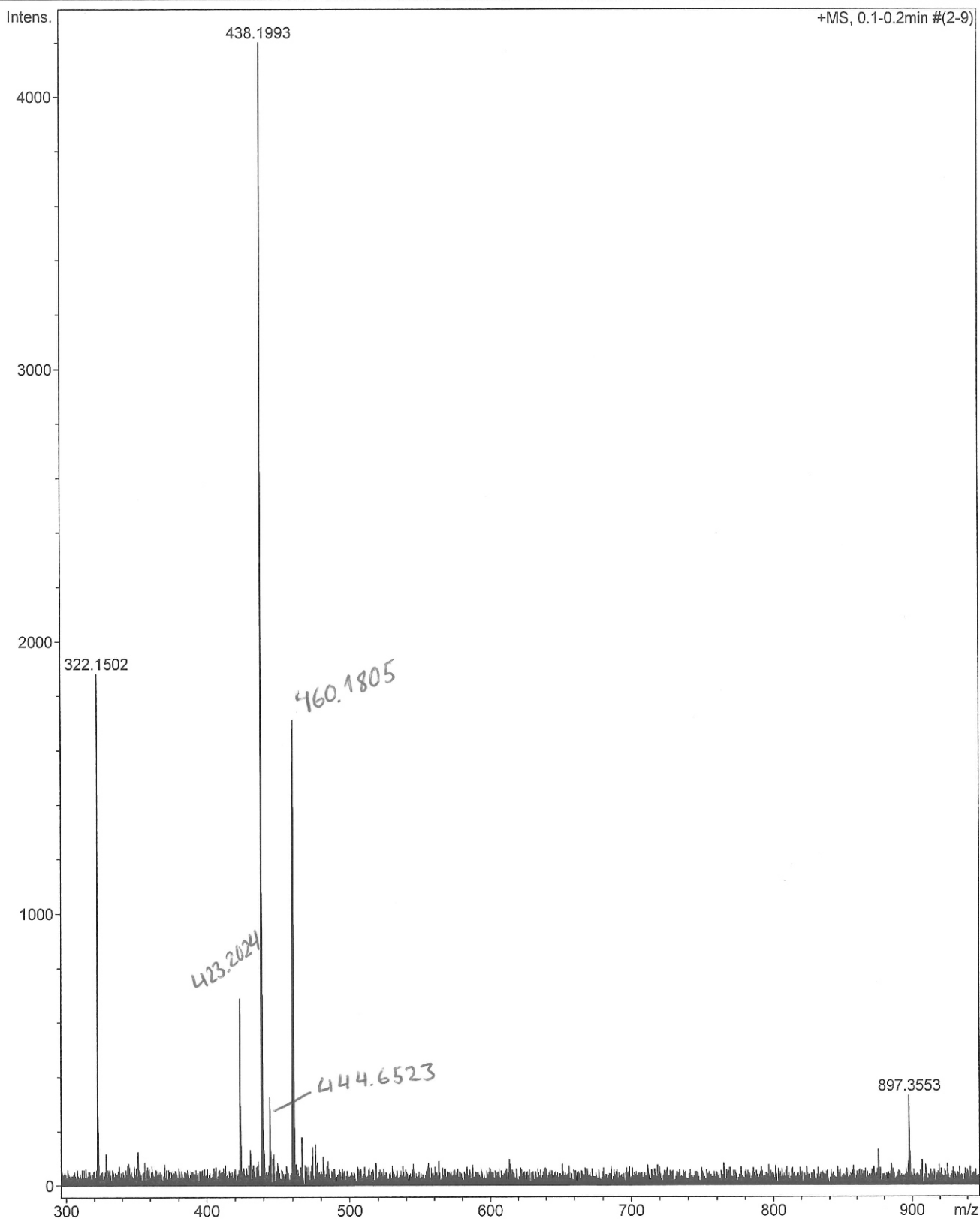
HRMS of compound 4b

Analysis Info

		Acquisition Date	9/12/2013 2:54:20 PM
Analysis Name	D:\Data\SabineRendon\130912 Donata 4b.d		
Method	tune_wide pos021112.m	Operator	Bruker07
Sample Name	130912 Donata 4b	Instrument	micrOTOF-Q
Comment			
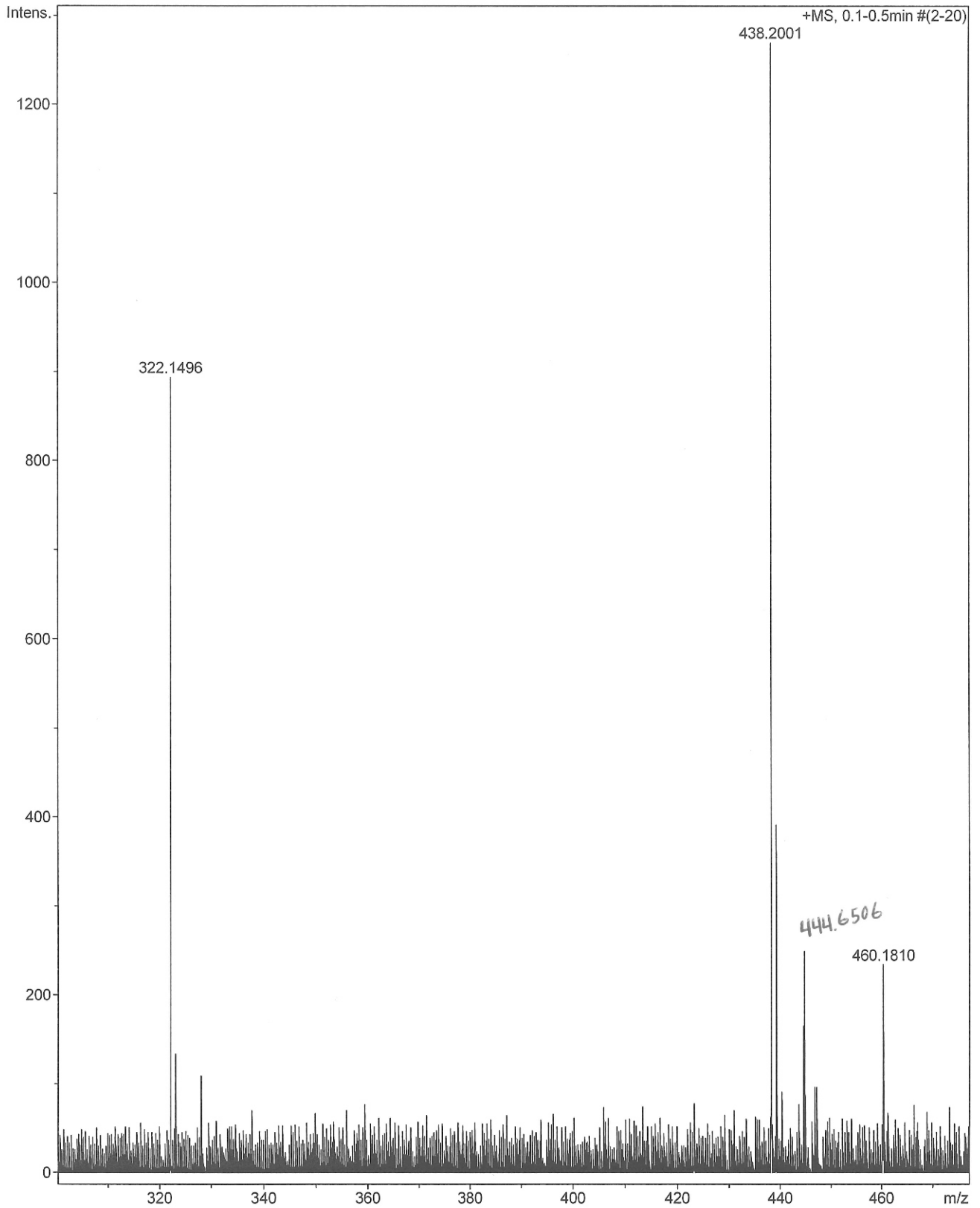
+MS, 0.1-0.5min #(2-20)

438.2001

322.1496

444.6506

460.1810

Section D

Coordinates of the studied structures

Coordinates of structures of studied substrates, transition states, intermediates and products.

Coordinates of structures of studied substrates, transition states, intermediates and products

A1.S				A1.TS1			
C	0.852861	-1.392458	-0.854239	C	0.747682	1.374731	0.183610
C	0.346375	-2.545967	-0.151166	C	0.106750	2.495831	-0.507480
C	1.260342	-3.322459	0.461708	C	0.837605	3.593107	-0.674950
N	2.587637	-3.014736	0.381365	N	2.150622	3.634242	-0.200260
C	3.067210	-1.831090	-0.221639	C	2.777102	2.533547	0.471270
N	2.144272	-1.040036	-0.843532	N	1.969249	1.339708	0.640030
N	-0.025768	-0.644836	-1.521110	N	-0.066525	0.184735	0.363430
O	4.259818	-1.577925	-0.139354	O	3.931302	2.619033	0.863490
C	-0.034571	0.515178	1.532915	C	-0.142403	-0.682666	-0.986240
C	-0.709071	1.616441	0.831841	C	-0.397312	-2.143228	-0.498500
C	-0.176915	2.374324	-0.138124	C	0.401031	-2.898950	0.221800
C	1.166143	2.333859	-0.786961	C	1.748288	-2.499569	0.829080
C	2.458995	2.553709	0.005161	C	2.995006	-2.318834	-0.130920
O	2.277204	3.428284	1.069323	O	2.997865	-3.287642	-1.178340
O	2.941353	1.342408	0.478018	O	3.047395	-1.027608	-0.742390
O	1.226846	2.170192	-1.992383	O	1.901141	-2.370546	2.052210
O	-0.633647	-0.239216	2.278500	O	-1.051567	-0.162021	-1.839220
H	-0.727092	-2.711298	-0.105258	H	-0.922991	2.392827	-0.817630
H	1.000211	-4.210839	1.033118	H	0.480705	4.496489	-1.161700
H	3.289822	-3.549123	0.874837	H	2.714102	4.472701	-0.337720
H	-1.775156	1.710875	1.044359	H	-1.350393	-2.548030	-0.826340
H	-0.861688	3.037957	-0.670177	H	0.091137	-3.902550	0.490300
H	3.162571	3.047499	-0.687631	H	3.892401	-2.510631	0.483700
H	1.803312	2.931547	1.754646	H	2.305849	-2.952387	-1.802340
H	2.853249	0.629889	-0.206350	H	2.928237	-0.371054	-0.009750
H	-3.981230	1.365512	-1.303271	H	-2.981401	-1.647062	1.088300
P	-3.560678	-0.355139	-0.147152	P	-3.778799	0.149392	0.189990
O	-3.152883	1.075372	-0.897842	O	-3.560827	-0.944917	1.478350
O	-2.422541	-1.310671	-0.419928	O	-2.646688	1.306365	0.532500
O	-4.978254	-0.627727	-0.502646	O	-5.276611	0.677291	0.138390
O	-3.444382	0.068067	1.433433	O	-3.236688	-0.802463	-1.027200
H	-2.598447	-0.266181	1.784671	H	-1.998132	-0.345917	-1.563630
H	0.308748	0.188980	-1.991847	H	0.369043	-0.368112	1.120060
H	-1.039025	-0.780138	-1.324434	H	-1.404751	0.792474	0.555800
H	1.055579	0.390156	1.353624	H	0.899686	-0.644179	-1.359670

A1.I1′			
C	0.793213	1.291608	-0.035733
C	0.433942	2.146441	-1.124061
C	1.085400	3.331460	-1.176392
N	2.017894	3.636678	-0.238675
C	2.397067	2.762305	0.810310
N	1.731631	1.565053	0.856313
N	0.119520	0.108779	0.117787
O	3.280446	3.113622	1.569399
C	-0.061245	-0.791100	-1.069415
C	-0.276096	-2.184791	-0.517760
C	0.558197	-2.936834	0.214678
C	1.921470	-2.665620	0.757160
C	3.044658	-2.123780	-0.141696
O	3.089969	-2.844897	-1.325033
O	2.904520	-0.768417	-0.447030
O	2.181978	-2.987550	1.901580
O	-1.055952	-0.392801	-1.914786
H	-0.351042	1.854672	-1.813713
H	0.892274	4.085318	-1.936249
H	2.524551	4.512596	-0.258930
H	-1.287287	-2.553244	-0.696681
H	0.165096	-3.875130	0.611733
H	3.987931	-2.331685	0.388983
H	2.223063	-2.750364	-1.751992
H	2.832099	-0.214438	0.356414
H	-3.533964	-1.338479	1.792536
P	-3.787163	0.070216	0.238345
O	-3.825502	-0.417813	1.817295
O	-2.733402	1.318993	0.311559
O	-5.101908	0.578390	-0.211180
O	-3.067981	-1.081662	-0.465233
H	-1.940521	-0.576558	-1.448072
H	0.423783	-0.374662	0.959586
H	-1.852850	0.959339	0.513548
H	0.884023	-0.745227	-1.635417

A1.I1″			
C	-0.781148	1.175050	0.820539
C	-1.654848	2.201539	0.363325
C	-1.086537	3.175359	-0.373338
N	0.261917	3.179285	-0.630105
C	1.147761	2.181431	-0.229742
N	0.540857	1.199830	0.521061
N	-1.097558	0.143321	1.568594
O	2.327574	2.231660	-0.510305
C	0.013850	-0.808345	1.670027
C	1.183525	-0.141021	0.850891
C	1.542295	-0.884094	-0.367466
C	2.857519	-1.192158	-0.742645
C	4.029638	-1.024368	0.274665
O	5.188216	-1.444677	-0.347458
O	4.126640	0.299013	0.758594
O	3.203030	-1.630048	-1.862043
O	-0.321288	-2.042525	1.139350
H	0.687321	3.898941	-1.199694
H	0.274388	-0.923379	2.732250
H	3.854435	-1.636611	1.177584
H	4.863973	-1.643093	-1.261164
H	3.778856	0.905176	0.081629
H	0.337229	-2.143754	0.390361
H	-2.128590	-0.114512	1.597260
P	-3.372036	-0.762339	-0.385750
O	-2.975430	-2.330369	-0.182218
O	-3.645268	-0.149167	0.977355
O	-4.803855	-0.937407	-1.149200
H	-2.090018	-2.368167	0.228490
O	-2.390647	-0.077966	-1.289631
H	0.799608	-0.876582	-1.172014
H	-1.651498	3.991908	-0.813162
H	-2.719565	2.097903	0.544524
H	2.052435	0.063764	1.484125
H	-4.598662	-0.922034	-2.093865

A1.TS2

C	-1.516243	0.950289	1.013270
C	-2.863647	1.336444	0.728101
C	-3.045079	2.333734	-0.152847
N	-1.976873	2.981396	-0.727436
C	-0.643131	2.613643	-0.550095
N	-0.483454	1.621114	0.388040
N	-1.122788	0.019886	1.829069
O	0.259213	3.163247	-1.146613
C	0.362283	0.011194	1.844827
C	0.775902	0.873345	0.602679
C	1.141611	0.072045	-0.651905
C	2.554322	-0.221533	-0.862053
C	3.546669	-0.274454	0.318486
O	4.666382	-0.979480	-0.073028
O	3.857211	1.074804	0.647818
O	3.049067	-0.435960	-1.970485
O	0.888487	-1.252024	1.915280
H	-2.112500	3.685168	-1.439842
H	0.676485	0.535692	2.762502
H	3.107238	-0.705350	1.225782
H	4.566365	-1.025415	-1.049906
H	4.238630	1.456680	-0.158101
H	1.496650	-1.275368	2.711953
H	-1.787096	-1.128069	1.622708
P	-1.715238	-1.939636	-0.472079
O	-0.170644	-2.059058	-0.344636
O	-2.353145	-2.076415	0.962373
O	-2.255435	-3.281890	-1.245654
H	0.555107	-0.953627	-0.612533
O	-2.161697	-0.736679	-1.259079
H	0.747170	0.551312	-1.555625
H	-4.026359	2.680638	-0.463821
H	-3.678438	0.768772	1.160414
H	1.561725	1.584633	0.879398
H	-2.646249	-2.937914	-2.060040

A1.I2'

C	-1.293042	1.005076	1.197968
C	-2.677104	1.392549	1.121892
C	-3.042937	2.232780	0.143382
N	-2.121455	2.772163	-0.725845
C	-0.770281	2.437256	-0.734414
N	-0.406274	1.642406	0.319309
N	-0.766040	0.149092	1.997963
O	-0.009713	2.882026	-1.575121
C	0.671753	0.097970	1.714635
C	0.912685	1.023473	0.467787
C	1.323494	0.242175	-0.771105
C	2.604506	-0.517357	-0.632575
C	3.714106	-0.009584	0.312047
O	4.791553	-0.866256	0.229874
O	4.053612	1.303473	-0.093160
O	2.896755	-1.440182	-1.375127
O	1.162927	-1.181743	1.547445
H	-2.414298	3.291350	-1.541261
H	1.203285	0.519266	2.585950
H	3.362655	0.084254	1.346526
H	4.522289	-1.511594	-0.460133
H	4.513619	1.204463	-0.940441
H	0.541204	-1.687825	0.938241
H	-2.082733	-1.475645	1.646282
P	-1.864854	-1.826592	-0.435189
O	-0.486723	-2.370395	-0.145592
O	-2.701906	-1.820691	0.974461
O	-2.745671	-2.943400	-1.250403
H	0.536730	-0.465567	-1.068701
O	-2.005422	-0.525009	-1.172031
H	1.455709	0.952682	-1.600155
H	-4.072752	2.538285	-0.020798
H	-3.392609	0.924111	1.786586
H	1.653870	1.805373	0.680192
H	-3.100152	-2.454526	-2.004910

A1.I2''

C	-1.511319	-1.236876	1.203660
C	-2.948795	-1.162227	1.300924
C	-3.676056	-1.399053	0.196827
N	-3.087175	-1.752767	-0.997895
C	-1.706411	-1.850440	-1.189809
N	-0.994976	-1.612137	-0.051762
N	-0.648562	-1.016132	2.120590
O	-1.231522	-2.150239	-2.269580
C	0.670632	-1.113888	1.501066
C	0.462477	-1.594159	0.024975
C	1.125540	-0.596809	-0.916559
C	2.236088	0.191281	-0.248019
C	3.505911	-0.540422	0.202255
O	4.527471	-0.202902	-0.700937
O	3.337165	-1.925844	0.178030
O	2.446014	1.380641	-0.543240
O	1.336531	0.106739	1.499158
H	-3.397422	-0.865588	2.241535
H	-4.760993	-1.330377	0.178434
H	-3.630762	-1.874178	-1.840134
H	0.393896	0.128271	-1.295957
H	1.558683	-1.110536	-1.786040
H	4.226086	-2.305116	0.210032
H	3.762312	-0.187126	1.217971
H	4.342197	0.730620	-0.915983
H	1.285805	-1.837269	2.057495
H	0.846182	-2.609211	-0.130863
H	0.593503	0.969055	1.352394
P	-0.916611	2.518169	-0.026270
O	-0.221751	1.918454	1.193152
O	0.214498	2.853847	-1.122401
O	-1.882026	3.634388	0.130005
H	1.041925	2.347422	-0.932146
O	-1.741635	1.263445	-0.740514
H	-2.623613	1.626084	-0.900527

A1.TS3

C	-1.405588	-1.283187	1.209413
C	-2.880195	-1.279600	1.327465
C	-3.603350	-1.672879	0.294795
N	-3.032196	-2.195986	-0.894981
C	-1.619418	-2.111250	-1.163188
N	-0.866488	-1.827660	0.004288
N	-0.553505	-0.875418	2.085213
O	-1.148059	-2.353188	-2.261250
C	0.800860	-1.030824	1.453004
C	0.601379	-1.681458	0.039897
C	1.237208	-0.668973	-0.939712
C	2.127934	0.240648	-0.020870
C	3.563370	-0.394887	0.237168
O	4.446821	-0.145959	-0.860279
O	3.472980	-1.814466	0.406411
O	2.343711	1.545916	-0.463386
O	1.392023	0.265892	1.250138
H	-3.323865	-0.907238	2.237004
H	-4.689136	-1.663275	0.297864
H	-3.610403	-2.149165	-1.736235
H	0.480542	-0.029781	-1.395516
H	1.819911	-1.157143	-1.713242
H	4.413455	-2.119620	0.335024
H	3.968077	0.069639	1.158265
H	4.160129	0.740295	-1.191819
H	1.445355	-1.638889	2.103878
H	1.079517	-2.659930	-0.031967
H	0.593400	1.547603	1.301956
P	-1.034153	2.631138	-0.234961
O	-0.254066	2.601373	1.254190
O	-0.104920	2.199808	-1.409959
O	-1.924283	3.938341	-0.387036
H	1.452331	1.842525	-0.890306
O	-2.108918	1.324267	-0.046222
H	-2.967212	1.749939	0.199180

A1.P

C	-1.347814	-1.231770	1.200763
C	-2.783808	-1.233015	1.335065
C	-3.519898	-1.617576	0.278088
N	-2.938861	-2.029445	-0.899356
C	-1.558824	-2.055123	-1.122448
N	-0.839006	-1.710271	-0.015825
N	-0.475185	-0.893471	2.077257
O	-1.086404	-2.403800	-2.186423
C	0.824238	-1.057361	1.456991
C	0.617218	-1.615548	0.018980
C	1.228025	-0.565662	-0.896432
C	2.121120	0.264503	0.029898
C	3.539613	-0.296755	0.180589
O	4.277820	-0.045051	-0.980234
O	3.501434	-1.679160	0.387978
O	2.318109	1.563410	-0.336634
O	1.458153	0.200663	1.309404
H	-3.226752	-0.897854	2.265508
H	-4.607015	-1.631097	0.290763
H	-3.492857	-2.217506	-1.722748
H	0.456327	0.102571	-1.302709
H	1.799274	-0.996757	-1.724936
H	4.382449	-2.003901	0.158025
H	3.999527	0.212566	1.052204
H	3.954076	0.827841	-1.272072
H	1.460461	-1.709715	2.073541
H	1.056777	-2.608520	-0.121757
H	0.077185	1.650580	1.375445
P	-1.113590	2.521586	-0.241252
O	-0.588343	2.361058	1.290924
O	0.065626	2.391327	-1.183595
O	-2.080446	3.646964	-0.295216
H	1.436893	1.967285	-0.669460
O	-1.954342	1.101219	-0.469106
H	-2.833190	1.269812	-0.103301

B1.S

C	1.363378	0.326470	0.657267
C	2.121684	1.546769	0.638332
C	3.316542	1.541296	0.033851
N	3.792934	0.389377	-0.544731
C	3.056081	-0.769850	-0.681715
N	1.793831	-0.736178	-0.089823
O	3.496829	-1.725762	-1.289623
N	0.284909	0.270086	1.395546
C	0.865603	-1.879683	-0.460443
C	0.884001	-2.923683	0.638791
O	1.637160	-2.942036	1.578763
C	-0.492480	-1.494571	-0.915778
C	-1.553401	-1.686258	-0.058149
O	-1.444894	-1.956779	1.182765
C	-2.993968	-1.594436	-0.579333
O	-3.252874	-2.824794	-1.235214
O	-3.853816	-1.401823	0.483315
H	4.687993	0.358083	-1.013722
H	0.204511	-3.769776	0.400499
H	-3.136837	-0.761930	-1.288960
H	-4.218729	-2.884386	-1.256397
H	-3.303380	-1.708054	1.239229
H	-0.291676	-0.575325	1.457948
H	-0.112171	1.199809	1.666257
P	-0.928390	2.801838	-0.087731
O	-1.940157	4.059163	-0.368466
O	-2.053412	1.615886	-0.322920
O	-0.532333	2.802566	1.380746
H	-2.820148	3.681587	-0.496212
H	-0.647297	-1.311333	-1.978184
O	0.151025	2.705535	-1.115266
H	1.656845	2.426438	1.076663
H	3.961172	2.411914	-0.031333
H	1.400946	-2.365683	-1.289724
H	-1.621956	0.756127	-0.486790

B1.TS1

C	-1.544751	-1.530538	0.038334
C	-2.117119	-2.231598	-1.145716
C	-3.294544	-1.877529	-1.615546
N	-4.049528	-0.845381	-0.994426
C	-3.379385	0.152378	-0.202046
N	-2.142512	-0.268541	0.386154
O	-3.883035	1.248125	-0.015086
N	-0.511775	-2.114893	0.667574
C	-1.289912	0.852818	0.905724
C	-0.918046	0.662106	2.401964
O	-0.649031	-0.413106	2.928164
C	-0.009873	1.062590	0.045104
C	0.562788	2.424809	0.230104
O	0.402266	3.186462	1.183624
C	1.550302	2.946363	-0.878956
O	0.786952	3.145838	-2.079866
O	2.112835	4.173575	-0.427126
H	-4.806721	-0.444775	-1.554076
H	-0.870553	1.608196	2.968744
H	2.352132	2.206613	-1.052656
H	1.452408	3.507686	-2.718416
H	1.577865	4.339350	0.394774
H	-0.301719	-1.508390	1.518304
H	0.649381	-2.586034	-0.078806
P	2.601610	-1.719127	-0.273096
O	3.676816	-2.682916	0.624354
O	1.959116	-0.847456	0.954254
O	1.454034	-2.844850	-0.711226
H	3.426225	-2.495283	1.563774
H	-0.244446	0.903990	-1.002796
O	3.341535	-1.023969	-1.495196
H	-1.538397	-3.041222	-1.563486
H	-3.782058	-2.364316	-2.453976
H	-1.948604	1.724072	0.865224
H	0.968387	0.236730	0.425824

B1.I1′

C	-1.978461	-1.287143	-0.166343
C	-3.067569	-2.016723	-0.800197
C	-4.239553	-1.425310	-1.051900
N	-4.434323	-0.099025	-0.731305
C	-3.451536	0.722333	-0.202801
N	-2.236241	0.102765	0.042632
O	-3.680713	1.901337	-0.001548
N	-0.906184	-1.897859	0.141248
C	-1.162297	0.969466	0.526078
C	-0.709377	0.588658	1.926666
O	-1.407505	-0.012539	2.704823
C	-0.040333	1.144697	-0.490912
C	0.916058	2.231986	-0.081400
O	0.555557	3.233143	0.518262
C	2.377445	2.032150	-0.472191
O	2.449177	1.595150	-1.783097
O	3.069947	3.225201	-0.278940
H	-5.304538	0.377152	-0.919940
H	0.294140	0.975745	2.202545
H	2.757150	1.245991	0.212382
H	2.665573	0.626089	-1.739687
H	2.417780	3.837086	0.106423
H	-0.179128	-1.343893	0.616591
H	0.732734	-2.995262	-0.246241
P	2.428248	-1.679809	0.004546
O	3.824042	-2.183622	0.686919
O	1.638891	-0.903259	1.038586
O	1.702290	-3.121059	-0.231054
H	3.629055	-2.340785	1.620668
H	-0.475175	1.465242	-1.450396
O	2.758904	-1.027406	-1.305346
H	-2.882345	-3.060791	-1.025419
H	-5.087110	-1.932305	-1.505271
H	-1.624061	1.959540	0.664889
H	0.518445	0.225913	-0.683599

B1.I1''

C	3.485738	0.250468	0.240284
N	4.151449	-0.883860	0.717393
C	3.620386	-2.157225	0.696701
C	2.431108	-2.416237	0.128771
C	1.701592	-1.320212	-0.464712
N	2.294124	-0.042706	-0.357779
N	0.583095	-1.354878	-1.075485
O	3.965232	1.362611	0.356282
C	1.328394	0.946766	-0.836339
C	0.209666	0.046439	-1.483955
O	-1.015800	0.406256	-1.083933
C	0.725203	1.746479	0.307365
C	-0.376324	2.617826	-0.221238
O	-0.222231	3.349984	-1.185170
C	-1.654570	2.762354	0.606726
O	-1.195750	3.296822	1.835851
O	-2.537328	3.599776	-0.043828
H	5.028591	-0.684861	1.177234
H	-2.135321	1.786806	0.769156
H	-1.964135	3.328786	2.420836
H	-1.993687	4.031902	-0.734042
H	0.329895	0.061939	-2.590165
P	-2.508119	-2.127932	0.279229
O	-1.335388	-3.165746	-0.092742
O	-2.932326	-1.465991	-1.117045
O	-1.778724	-0.924833	1.051583
H	-1.378335	-0.314779	0.358208
H	-2.306656	-0.721484	-1.345816
O	-3.598327	-2.775802	1.023063
H	1.802082	1.617346	-1.561729
H	1.488527	2.395896	0.759496
H	0.344212	1.073844	1.087824
H	4.230418	-2.924350	1.166782
H	1.992097	-3.407800	0.117410
H	-0.638592	-2.678730	-0.596648

B1.TS2

C	-2.856909	-2.213410	0.408618
N	-2.780710	-3.531390	-0.157356
C	-1.651742	-3.995129	-0.874989
C	-0.513772	-3.326270	-0.921129
C	-0.425193	-2.018344	-0.233675
N	-1.593213	-1.579663	0.469753
N	0.568856	-1.216261	-0.182502
O	-3.903302	-1.746439	0.829788
C	-1.370300	-0.189112	0.918466
C	0.177661	0.008746	0.645688
O	0.405013	1.216453	-0.015898
C	-2.187671	0.843913	0.101197
C	-1.697502	2.275143	0.401399
O	-1.541868	2.735535	1.522276
C	-1.546613	3.266792	-0.804667
O	-2.813225	3.309145	-1.483416
O	-1.209555	4.554506	-0.299868
H	-3.681846	-3.969286	-0.347997
H	-0.754066	2.903719	-1.482424
H	-2.707837	4.067935	-2.111237
H	-1.204139	4.400678	0.680669
H	0.736265	-0.103063	1.592486
P	3.897001	-0.017791	-0.087352
O	3.298196	-1.345336	-0.913839
O	3.286183	-0.339263	1.471072
O	3.111589	1.320537	-0.575165
H	1.511329	1.271318	-0.131092
H	4.096418	-0.534434	2.011536
O	5.484253	-0.043869	0.030359
H	-1.610873	-0.091119	1.979385
H	-3.245847	0.768486	0.348662
H	-2.070475	0.649963	-0.961052
H	-1.793274	-4.956711	-1.359056
H	0.353381	-3.691987	-1.448389
H	2.045395	-1.361576	-0.738386

B1.I2'

C	2.363521	2.491271	0.596792
N	2.252174	3.748502	-0.004788
C	1.219243	4.115338	-0.843559
C	0.200405	3.284172	-1.119013
C	0.190844	1.979938	-0.498787
N	1.288275	1.689182	0.349635
N	-0.673678	1.050617	-0.596910
O	3.332066	2.189627	1.268811
C	1.186734	0.283088	0.740241
C	-0.274627	-0.038047	0.334206
O	-0.338012	-1.282544	-0.236443
C	2.173756	-0.572692	-0.044270
C	2.071538	-2.011852	0.364692
O	2.096793	-2.370612	1.526430
C	2.075844	-3.076299	-0.731227
O	3.316644	-2.881870	-1.387077
O	1.965736	-4.332104	-0.173833
H	3.029919	4.366425	0.177826
H	1.238339	-2.909888	-1.426112
H	3.402183	-3.617522	-2.008575
H	2.111911	-4.193509	0.783860
H	-0.963360	0.045749	1.193451
P	-3.845564	-0.453425	0.063851
O	-3.522884	0.596314	-1.144028
O	-3.376132	0.430148	1.396494
O	-2.858275	-1.595863	-0.008901
H	-1.327629	-1.538626	-0.199379
H	-4.192250	0.832816	1.721259
O	-5.314951	-0.659877	0.144026
H	1.362777	0.171590	1.815181
H	3.198365	-0.237388	0.172920
H	1.994727	-0.467076	-1.121754
H	1.290717	5.117942	-1.257442
H	-0.620871	3.564971	-1.767980
H	-2.560194	0.772520	-1.154855

B1.I2''

C	-1.511319	-1.236876	1.203660
C	-2.948795	-1.162227	1.300924
C	-3.676056	-1.399053	0.196827
N	-3.087175	-1.752767	-0.997895
C	-1.706411	-1.850440	-1.189809
N	-0.994976	-1.612137	-0.051762
N	-0.648562	-1.016132	2.120590
O	-1.231522	-2.150239	-2.269580
C	0.670632	-1.113888	1.501066
C	0.462477	-1.594159	0.024975
C	1.125540	-0.596809	-0.916559
C	2.236088	0.191281	-0.248019
C	3.505911	-0.540422	0.202255
O	4.527471	-0.202902	-0.700937
O	3.337165	-1.925844	0.178030
O	2.446014	1.380641	-0.543240
O	1.336531	0.106739	1.499158
H	-3.397422	-0.865588	2.241535
H	-4.760993	-1.330377	0.178434
H	-3.630762	-1.874178	-1.840134
H	0.393896	0.128271	-1.295957
H	1.558683	-1.110536	-1.786040
H	4.226086	-2.305116	0.210032
H	3.762312	-0.187126	1.217971
H	4.342197	0.730620	-0.915983
H	1.285805	-1.837269	2.057495
H	0.846182	-2.609211	-0.130863
H	0.593503	0.969055	1.352394
P	-0.916611	2.518169	-0.026270
O	-0.221751	1.918454	1.193152
O	0.214498	2.853847	-1.122401
O	-1.882026	3.634388	0.130005
H	1.041925	2.347422	-0.932146
O	-1.741635	1.263445	-0.740514
H	-2.623613	1.626084	-0.900527

B1.TS3

C	-1.405588	-1.283187	1.209413
C	-2.880195	-1.279600	1.327465
C	-3.603350	-1.672879	0.294795
N	-3.032196	-2.195986	-0.894981
C	-1.619418	-2.111250	-1.163188
N	-0.866488	-1.827660	0.004288
N	-0.553505	-0.875418	2.085213
O	-1.148059	-2.353188	-2.261250
C	0.800860	-1.030824	1.453004
C	0.601379	-1.681458	0.039897
C	1.237208	-0.668973	-0.939712
C	2.127934	0.240648	-0.020870
C	3.563370	-0.394887	0.237168
O	4.446821	-0.145959	-0.860279
O	3.472980	-1.814466	0.406411
O	2.343711	1.545916	-0.463386
O	1.392023	0.265892	1.250138
H	-3.323865	-0.907238	2.237004
H	-4.689136	-1.663275	0.297864
H	-3.610403	-2.149165	-1.736235
H	0.480542	-0.029781	-1.395516
H	1.819911	-1.157143	-1.713242
H	4.413455	-2.119620	0.335024
H	3.968077	0.069639	1.158265
H	4.160129	0.740295	-1.191819
H	1.445355	-1.638889	2.103878
H	1.079517	-2.659930	-0.031967
H	0.593400	1.547603	1.301956
P	-1.034153	2.631138	-0.234961
O	-0.254066	2.601373	1.254190
O	-0.104920	2.199808	-1.409959
O	-1.924283	3.938341	-0.387036
H	1.452331	1.842525	-0.890306
O	-2.108918	1.324267	-0.046222
H	-2.967212	1.749939	0.199180

B1.P

C	-1.347814	-1.231770	1.200763
C	-2.783808	-1.233015	1.335065
C	-3.519898	-1.617576	0.278088
N	-2.938861	-2.029445	-0.899356
C	-1.558824	-2.055123	-1.122448
N	-0.839006	-1.710271	-0.015825
N	-0.475185	-0.893471	2.077257
O	-1.086404	-2.403800	-2.186423
C	0.824238	-1.057361	1.456991
C	0.617218	-1.615548	0.018980
C	1.228025	-0.565662	-0.896432
C	2.121120	0.264503	0.029898
C	3.539613	-0.296755	0.180589
O	4.277820	-0.045051	-0.980234
O	3.501434	-1.679160	0.387978
O	2.318109	1.563410	-0.336634
O	1.458153	0.200663	1.309404
H	-3.226752	-0.897854	2.265508
H	-4.607015	-1.631097	0.290763
H	-3.492857	-2.217506	-1.722748
H	0.456327	0.102571	-1.302709
H	1.799274	-0.996757	-1.724936
H	4.382449	-2.003901	0.158025
H	3.999527	0.212566	1.052204
H	3.954076	0.827841	-1.272072
H	1.460461	-1.709715	2.073541
H	1.056777	-2.608520	-0.121757
H	0.077185	1.650580	1.375445
P	-1.113590	2.521586	-0.241252
O	-0.588343	2.361058	1.290924
O	0.065626	2.391327	-1.183595
O	-2.080446	3.646964	-0.295216
H	1.436893	1.967285	-0.669460
O	-1.954342	1.101219	-0.469106
H	-2.833190	1.269812	-0.103301

A2.S

C	1.063481	-1.488636	-1.037033
C	0.233337	-2.390274	-0.275385
C	0.891662	-3.264710	0.514901
N	2.252533	-3.276251	0.538421
C	3.055638	-2.398699	-0.239580
N	2.391276	-1.502319	-1.019573
N	0.452871	-0.555199	-1.783811
C	0.247448	1.626276	0.404887
O	-0.618687	2.359684	-0.044733
C	-0.146515	0.490388	1.353123
O	1.014717	-0.012279	1.937391
O	-1.037551	0.933119	2.320494
C	1.679694	1.767672	0.033265
C	2.275025	2.930853	-0.278360
C	1.655203	4.264970	-0.241477
O	2.262165	5.262687	-0.580205
O	4.268034	-2.512121	-0.149740
H	-0.854900	-2.313700	-0.279298
H	0.381533	-3.983221	1.153784
H	2.773398	-3.927664	1.109942
H	-0.634463	-0.282476	0.731050
H	0.768333	-0.851806	2.350260
H	-1.933050	0.825984	1.933487
H	2.267408	0.847703	0.041347
H	3.332825	2.939868	-0.547388
H	0.610193	4.316049	0.122433
H	-0.579608	-0.453429	-1.816559
H	1.048186	0.051937	-2.330770
P	-3.075921	-0.440638	-0.363852
O	-2.295635	-0.207893	-1.625240
O	-4.657427	-0.646995	-0.729030
O	-3.118318	0.996384	0.453018
H	-2.498117	1.616546	0.022716
H	-4.966384	-1.340232	-0.130515
O	-2.690191	-1.513416	0.611293

A2.TS1

C	-1.119890	-0.279927	-1.182649
C	-2.413839	0.210555	-1.535599
C	-3.472680	-0.383544	-0.960849
N	-3.314892	-1.439254	-0.093549
C	-2.082952	-1.925456	0.344761
N	-1.022261	-1.322168	-0.290839
N	0.033051	0.128751	-1.641219
C	1.040849	-0.771751	-1.111349
O	1.260608	-1.749671	-2.134339
C	2.375830	-0.063443	-0.903499
O	3.250369	-1.108024	-0.488299
O	2.809711	0.497767	-2.098679
C	0.391728	-1.448670	0.127871
C	0.600509	-0.801120	1.499851
C	1.644608	-1.450162	2.300491
O	1.743608	-1.411162	3.514161
O	-1.992544	-2.819246	1.172301
H	-4.105462	-1.841153	0.391101
H	2.024957	-2.260242	-1.814029
H	2.297202	0.739747	-0.158209
H	4.108780	-0.696665	-0.321939
H	2.524350	-0.125643	-2.789969
H	2.427228	-1.989443	1.700541
H	-2.493708	1.076465	-2.180869
H	-4.497550	-0.069732	-1.136559
H	0.185643	1.555131	-1.517549
H	-0.337311	-0.795369	2.070261
H	0.658087	-2.516390	0.121011
P	-0.237776	2.381451	0.546071
O	0.072555	2.746481	-0.966449
O	-1.567807	1.691353	0.735721
O	0.962263	1.646039	1.164851
H	0.808021	0.358240	1.387401
O	-0.343874	3.864641	1.247841
H	-1.248994	3.887653	1.586001

A2.I1′				A2.I1′′		
C	-1.294261	-0.685556	-0.185999	C	-0.060555	0.947324	-0.913307
C	-2.319935	-0.278836	-1.110767	C	0.784950	2.091290	-0.884734
C	-3.336376	-1.150210	-1.297306	C	0.176844	3.261617	-0.590439
N	-3.357089	-2.332009	-0.635519	N	-1.173638	3.333824	-0.381644
C	-2.318769	-2.744885	0.249537	C	-2.039145	2.230252	-0.386347
N	-1.303654	-1.859889	0.434272	N	-1.381995	1.047350	-0.639808
N	-0.238137	0.107078	0.109790	N	0.294320	-0.300851	-1.143908
C	0.115538	1.479669	-0.291614	C	-0.812944	-1.208693	-0.970879
O	1.050096	1.958912	0.617901	O	-1.224286	-1.658820	-2.256207
C	0.784043	1.490493	-1.681820	C	-0.392044	-2.455647	-0.182621
O	-0.148990	1.138873	-2.654976	O	-1.553944	-3.240114	-0.023882
O	1.238659	2.787518	-1.959427	O	0.560964	-3.156446	-0.894828
C	-1.069101	2.426968	-0.291470	C	-1.937164	-0.377848	-0.286877
C	-1.753446	2.838697	0.781492	C	-2.169054	-0.581793	1.133201
C	-1.507520	2.437055	2.174802	C	-3.475451	-0.493209	1.663861
O	-2.188556	2.858068	3.090461	O	-3.830018	-0.515598	2.844373
O	-2.423873	-3.842576	0.768072	O	-3.227570	2.349765	-0.198550
H	-2.260557	0.647647	-1.665918	H	-1.628377	4.212855	-0.170366
H	-4.164458	-0.951827	-1.975126	H	-1.876128	-2.353322	-2.044440
H	-4.100687	-3.005887	-0.761479	H	0.057674	-2.176713	0.780694
H	1.631315	0.782726	-1.651724	H	-2.102086	-2.697646	0.592373
H	0.317007	1.152032	-3.502055	H	0.277584	-3.115130	-1.824390
H	1.754354	3.039241	-1.174043	H	-4.261678	-0.433561	0.851868
H	-1.341635	2.816781	-1.272521	H	1.857462	1.982902	-1.012734
H	-2.579986	3.542322	0.662511	H	0.722676	4.196895	-0.503441
H	-0.664923	1.738709	2.347644	H	1.325281	-0.542642	-1.127036
H	1.355476	-1.437415	-0.944994	H	-1.312927	-0.531107	1.813121
H	0.389424	-0.294112	0.822954	H	-2.869506	-0.473170	-0.860388
P	3.028574	-1.091665	0.395784	P	3.246478	0.138688	0.525911
O	2.235956	-1.831133	-0.844104	O	2.919152	-0.215005	-0.900624
O	1.850744	-1.228877	1.570871	O	3.453595	1.550883	0.975757
O	3.062050	0.401519	0.147525	O	2.024451	-0.519062	1.418407
H	1.873470	1.361577	0.557219	H	1.936109	0.015184	2.219325
H	1.562731	-2.151461	1.641136	O	4.558473	-0.732023	0.982675
O	4.235287	-1.886304	0.706015	H	5.106769	-0.115525	1.486151

A2.TS2				A2.I2'			
C	-1.119890	-0.279927	-1.182649	C	-0.817901	-0.820039	-1.238474
C	-2.413839	0.210555	-1.535599	C	-2.201111	-0.928868	-1.610279
C	-3.472680	-0.383544	-0.960849	C	-2.985527	-1.732828	-0.877217
N	-3.314892	-1.439254	-0.093549	N	-2.481646	-2.480161	0.163739
C	-2.082952	-1.925456	0.344761	C	-1.169567	-2.393233	0.617633
N	-1.022261	-1.322168	-0.290839	N	-0.377737	-1.613555	-0.179592
N	0.033051	0.128751	-1.641219	N	0.085702	-0.085437	-1.788957
C	1.040849	-0.771751	-1.111349	C	1.333675	-0.398137	-1.132526
O	1.260608	-1.749671	-2.134339	O	2.082010	-1.212264	-2.046786
C	2.375830	-0.063443	-0.903499	C	2.164432	0.858874	-0.892392
O	3.250369	-1.108024	-0.488299	O	3.349660	0.361229	-0.265508
O	2.809711	0.497767	-2.098679	O	2.457207	1.482839	-2.096159
C	0.391728	-1.448670	0.127871	C	0.994640	-1.223902	0.146915
C	0.600509	-0.801120	1.499851	C	1.111277	-0.520790	1.498153
C	1.644608	-1.450162	2.300491	C	2.492366	-0.637785	2.066366
O	1.743608	-1.411162	3.514161	O	3.001691	0.124693	2.853913
O	-1.992544	-2.819246	1.172301	O	-0.784605	-3.009054	1.595640
H	-4.105462	-1.841153	0.391101	H	-3.096926	-2.969842	0.797836
H	2.024957	-2.260242	-1.814029	H	2.957863	-1.301439	-1.632588
H	2.297202	0.739747	-0.158209	H	1.629421	1.577667	-0.254759
H	4.108780	-0.696665	-0.321939	H	3.761250	1.091485	0.215640
H	2.524350	-0.125643	-2.789969	H	2.522497	0.761647	-2.746482
H	2.427228	-1.989443	1.700541	H	3.040106	-1.566993	1.748994
H	-2.493708	1.076465	-2.180869	H	-2.581937	-0.301905	-2.406719
H	-4.497550	-0.069732	-1.136559	H	-4.050459	-1.848172	-1.059623
H	0.185643	1.555131	-1.517549	H	-0.924350	1.879562	-1.546793
H	-0.337311	-0.795369	2.070261	H	0.453535	-1.053527	2.203720
H	0.658087	-2.516390	0.121011	H	1.620854	-2.130642	0.154216
P	-0.237776	2.381451	0.546071	P	-1.415968	1.990401	0.522136
O	0.072555	2.746481	-0.966449	O	-1.712961	2.211590	-1.081229
O	-1.567807	1.691353	0.735721	O	-1.931733	0.653342	0.980777
O	0.962263	1.646039	1.164851	O	0.009371	2.384548	0.787591
H	0.808021	0.358240	1.387401	H	0.765987	0.525900	1.482685
O	-0.343874	3.864641	1.247841	O	-2.454110	3.118514	1.119320
H	-1.248994	3.887653	1.586001	H	-3.108486	2.591060	1.595939

A2.I2''

C	0.985537	0.947668	-1.089559
C	0.877122	2.264241	-1.673613
C	1.416721	3.303675	-1.015366
N	2.097387	3.134094	0.169528
C	2.237659	1.903837	0.825554
N	1.663366	0.873719	0.143325
O	2.823820	1.813068	1.886739
N	0.523603	-0.155240	-1.542294
C	1.625519	-0.508605	0.613111
C	0.841539	-1.203597	-0.550137
O	-0.289189	-1.779911	-0.055580
C	1.657315	-2.313917	-1.243419
O	2.390377	-2.995642	-0.237875
O	0.803815	-3.179682	-1.892391
C	0.847520	-0.678946	1.908012
C	-0.206713	-1.780191	1.827251
O	-1.352676	-1.605795	2.288273
H	0.344319	2.385018	-2.611870
H	1.344926	4.326997	-1.371031
H	2.490415	3.919533	0.671613
H	2.652196	-0.882816	0.692352
H	2.348745	-1.892881	-1.994780
H	2.434313	-3.906316	-0.559952
H	-0.014897	-3.095144	-1.351823
H	1.529110	-0.918515	2.734942
H	0.334380	0.254690	2.161352
H	-1.805950	-1.244487	-0.419899
H	0.216864	-2.806076	1.850312
P	-2.970348	0.544265	-0.078091
O	-1.940683	0.701723	1.132668
H	-1.874406	-0.138460	1.687819
O	-2.294433	1.567493	-1.141715
O	-4.384748	0.891560	0.156261
O	-2.725868	-0.919750	-0.640869
H	-1.371919	1.316956	-1.286666

A2.TS3

C	0.069395	1.382023	-1.103351
C	-1.099738	1.921173	-1.743677
C	-2.060309	2.447269	-0.956891
N	-1.894712	2.589682	0.394201
C	-0.758425	2.168457	1.093385
N	0.174664	1.585917	0.278751
O	-0.629914	2.359628	2.284219
N	1.026704	0.713134	-1.640291
C	1.430233	0.987561	0.739955
C	1.798928	0.192073	-0.532552
O	1.376000	-1.144309	-0.272473
C	3.287521	0.159427	-0.875000
O	4.014174	0.079199	0.335887
O	3.575295	-0.914338	-1.698656
C	1.287782	-0.026834	1.862103
C	1.459681	-1.439875	1.272476
O	0.599396	-2.357268	1.611079
H	-1.218784	1.804339	-2.814791
H	-3.015785	2.788512	-1.347041
H	-2.675315	2.830006	0.989904
H	2.149892	1.787372	0.961987
H	3.557173	1.079004	-1.422077
H	4.838641	-0.368247	0.100001
H	2.921150	-1.597397	-1.448320
H	2.048350	0.146813	2.631711
H	0.303412	0.050714	2.332129
H	-0.061879	-1.450088	-0.829483
H	2.507271	-1.783339	1.361641
P	-2.288744	-1.554161	-0.169928
O	-1.695622	-0.851494	1.102554
H	-0.434354	-1.845323	1.461816
O	-3.273602	-0.410252	-0.835511
O	-3.036113	-2.817725	0.031637
O	-1.126391	-1.588511	-1.268107
H	-2.651403	0.061825	-1.520897

A2.P			
C	0.130355	1.303660	-1.098484
C	-1.028961	1.834244	-1.761176
C	-1.973929	2.420691	-1.009476
N	-1.819089	2.584460	0.352606
C	-0.695055	2.168813	1.069125
N	0.211877	1.512892	0.285030
O	-0.558474	2.402832	2.253624
N	1.102463	0.638790	-1.614310
C	1.434955	0.889127	0.785800
C	1.880916	0.147190	-0.497340
O	1.531254	-1.212275	-0.290483
C	3.377153	0.209745	-0.798449
O	4.065297	0.097009	0.433466
O	3.740348	-0.810754	-1.660912
C	1.227630	-0.193900	1.834586
C	1.525373	-1.533019	1.137573
O	0.648278	-2.531940	1.385816
H	-1.170711	1.630374	-2.815149
H	-2.920454	2.765288	-1.415231
H	-2.501984	3.085991	0.903609
H	2.139396	1.669189	1.102029
H	3.624606	1.165391	-1.291253
H	4.919588	-0.294104	0.203597
H	3.115128	-1.534145	-1.452676
H	1.894519	-0.043192	2.690089
H	0.190688	-0.207373	2.186456
H	-0.587291	-1.363976	-1.221413
H	2.535596	-1.896033	1.384437
P	-2.453808	-1.450144	-0.153934
O	-1.550590	-1.118933	1.030183
H	-0.272216	-2.138565	1.297149
O	-3.435782	-0.124406	-0.288770
O	-3.270639	-2.684807	-0.219827
O	-1.518170	-1.288951	-1.494269
H	-3.109306	0.458817	0.410514

B2.S			
C	-0.280426	-0.291446	-0.014678
C	-1.160533	-1.366989	-0.388882
C	-0.827138	-2.621285	-0.054754
N	0.331858	-2.868555	0.631230
C	1.256226	-1.891866	0.952103
N	0.891440	-0.584329	0.642681
O	2.310806	-2.189000	1.482951
N	-0.608980	0.933215	-0.327926
C	1.994420	0.461941	1.048278
C	3.175605	0.237510	0.131076
O	4.322189	0.286127	0.540025
C	2.980782	-0.150514	-1.348446
O	4.101353	0.236633	-2.052551
O	2.756364	-1.545926	-1.404886
C	1.612527	1.884755	1.144283
C	2.138125	2.851048	0.265504
O	2.076935	4.078925	0.350622
H	0.637190	-3.807971	0.848222
H	2.086931	0.305071	-1.793528
H	4.797158	0.338701	-1.372761
H	3.474241	-1.964358	-0.902582
H	2.663148	2.397865	-0.633828
P	-4.218947	0.487734	-0.246457
O	-3.142753	0.768096	-1.262264
O	-5.499669	1.238090	-0.123230
H	-4.052055	1.006372	1.808519
O	-4.567517	-1.117683	-0.420292
H	-5.503091	-1.205939	-0.195175
H	2.303340	0.069317	2.023328
H	1.199476	2.223354	2.095784
H	-1.443445	-3.482785	-0.293768
H	-1.579071	1.076760	-0.707057
H	-0.001528	1.681841	0.045315
H	-2.070847	-1.108234	-0.925081
O	-3.465834	0.508833	1.223457

B2.TS1

C	-0.120860	1.243690	-0.772919
C	0.320631	2.648919	-0.966639
C	-0.168588	3.618800	-0.218989
N	-1.180798	3.378770	0.738291
C	-1.468219	2.043391	1.183501
N	-1.055440	1.012480	0.279011
O	-2.086809	1.835151	2.213051
N	0.256720	0.241039	-1.505219
C	-1.263881	-0.378820	0.783271
C	-1.689441	-1.291549	-0.400099
O	-1.325692	-2.439950	-0.584969
C	-2.818481	-0.752329	-1.366379
O	-3.147492	-1.792758	-2.280709
O	-3.985371	-0.349008	-0.634919
C	-0.085111	-0.871070	1.685481
C	0.178018	-2.381111	1.630411
O	-0.216993	-3.179970	2.467391
H	-1.297948	4.081030	1.471761
H	-2.460020	0.142521	-1.897059
H	-2.518272	-2.514059	-2.015949
H	-4.435921	-1.207917	-0.430049
H	0.822518	-2.699201	0.791441
P	3.189459	-0.301063	-0.129629
O	2.161528	-1.503932	-0.716659
O	4.706039	-0.777274	-0.124879
H	1.056569	-0.255871	1.383761
O	3.058610	0.787397	-1.452479
H	3.918800	0.687627	-1.930379
H	-2.167261	-0.294679	1.396341
H	-0.354731	-0.612570	2.706981
H	0.137193	4.656499	-0.312569
H	0.929500	0.603859	-2.205269
H	1.135699	-0.855321	-1.025619
H	1.084121	2.825159	-1.708329
O	2.443690	0.452008	1.087801

B2.I1′

C	0.240584	1.087216	-0.743995
C	1.137805	2.220867	-0.754737
C	1.314972	2.932743	0.364337
N	0.595070	2.653320	1.499708
C	-0.257800	1.569116	1.614543
N	-0.518266	0.911857	0.420369
O	-0.767356	1.271679	2.676362
N	0.016277	0.266689	-1.712893
C	-1.320064	-0.306106	0.541721
C	-2.172361	-0.543745	-0.678071
O	-2.462205	-1.666503	-1.053607
C	-2.981896	0.618476	-1.269159
O	-3.502727	0.225757	-2.484755
O	-3.980470	0.913661	-0.312073
C	-0.507348	-1.528845	0.933574
C	-1.281491	-2.479656	1.777337
O	-2.420119	-2.321803	2.159504
H	0.849606	3.057259	2.390489
H	-2.408361	1.543245	-1.381093
H	-3.397037	-0.747722	-2.489201
H	-4.521160	0.112146	-0.230217
H	-0.715096	-3.400719	2.058448
P	3.043770	-0.833885	-0.228653
O	2.053262	-1.812984	-1.111527
O	4.296580	-1.585967	0.050992
H	-0.134911	-2.078527	0.056497
O	3.406183	0.329757	-1.378948
H	4.226779	0.010491	-1.778079
H	-2.038095	-0.103490	1.351578
H	0.422196	-1.222164	1.446436
H	2.025748	3.750169	0.444665
H	0.597505	0.513449	-2.514285
H	1.254117	-1.302967	-1.346679
H	1.761764	2.372675	-1.627997
O	2.218653	-0.133477	0.814756

B2.I1''

C	0.246792	1.261141	-0.601315
C	-0.373135	2.503721	-0.940387
C	0.282321	3.621208	-0.575299
N	1.501175	3.564380	0.066144
C	2.131959	2.386234	0.464705
N	1.437965	1.261284	0.094781
O	3.189730	2.386393	1.061775
N	-0.179055	0.060254	-0.818697
C	1.836805	-0.122884	0.407544
C	0.460010	-0.875540	0.272813
O	-0.220752	-0.838174	1.381542
C	0.528051	-2.299413	-0.303474
O	1.044945	-3.078802	0.754212
O	-0.696337	-2.712682	-0.775726
C	2.985096	-0.553558	-0.487812
C	3.635613	-1.845405	-0.059792
O	4.195915	-2.594507	-0.822179
H	-1.368132	2.470029	-1.378114
H	-0.108879	4.620278	-0.746795
H	1.986028	4.405912	0.347308
H	2.122719	-0.170157	1.465792
H	1.238955	-2.408031	-1.136740
H	0.552625	-2.718835	1.521617
H	-1.451276	-2.360857	-0.236163
H	3.779164	0.210628	-0.424255
H	2.686741	-0.629389	-1.542724
H	3.619837	-2.037887	1.038494
P	-3.250584	-0.159140	0.001416
O	-2.542815	0.546062	1.279472
O	-2.767912	0.524906	-1.264565
H	-1.710466	0.032659	1.463504
O	-4.813440	0.270580	0.221198
O	-3.130010	-1.653871	0.115695
H	-1.171720	-0.019200	-1.171282
H	-5.213105	-0.461738	0.709256

B2.TS2

C	-0.386299	1.338011	0.656040
C	-0.011238	2.693841	1.092580
C	-0.837067	3.688841	0.806980
N	-2.066267	3.485322	0.147460
C	-2.430318	2.230562	-0.447620
N	-1.642099	1.146502	0.040570
O	-3.352798	2.123503	-1.236230
N	0.302390	0.254111	0.746330
C	-1.689750	-0.222288	-0.544800
C	-0.395431	-0.942619	0.067780
O	0.403909	-1.549090	-0.857180
C	-0.646571	-2.073199	1.215880
O	0.049368	-3.184239	0.732100
O	-0.165171	-1.643349	2.499790
C	-3.074650	-0.874907	-0.321220
C	-3.153051	-2.288057	-0.941520
O	-3.968012	-3.126866	-0.603380
H	0.930892	2.832550	1.598970
H	-0.632246	4.721711	1.075900
H	-2.540257	4.299603	-0.244630
H	-1.528980	-0.143538	-1.625880
H	-1.722381	-2.257518	1.355920
H	0.424228	-2.713280	-0.130560
H	0.797679	-1.869990	2.462000
H	-3.822870	-0.248327	-0.807370
H	-3.326300	-0.920357	0.734900
H	-2.417022	-2.480988	-1.741260
P	3.466830	-0.106192	-0.440850
O	2.199420	0.085479	-1.508360
O	2.932300	0.335769	1.037910
H	1.463240	-0.675510	-1.283260
O	4.344761	1.286888	-0.876520
O	4.349299	-1.405992	-0.647590
H	1.446440	0.258950	0.975530
H	4.168602	1.910098	-0.126930

B2.I2′

C	0.228453	0.524538	1.268153
C	1.334374	1.115877	1.979437
C	1.895052	2.220513	1.451026
N	1.389490	2.828426	0.327559
C	0.275861	2.363575	-0.372407
N	-0.324288	1.296319	0.240545
O	-0.134578	2.908681	-1.376721
N	-0.299326	-0.632487	1.442304
C	-1.406039	0.532229	-0.372955
C	-1.181218	-0.862700	0.291435
O	-0.567276	-1.752115	-0.597750
C	-2.466933	-1.595513	0.679207
O	-3.216736	-1.781507	-0.498952
O	-2.165443	-2.790111	1.315153
C	-2.726802	1.243545	-0.109545
C	-3.911211	0.773802	-0.911223
O	-5.052212	0.860713	-0.526778
H	1.750759	0.604636	2.839955
H	2.776807	2.693639	1.877175
H	1.909558	3.549514	-0.153400
H	-1.219022	0.454071	-1.453231
H	-3.099563	-1.008123	1.356842
H	-2.564221	-2.117098	-1.141021
H	-1.324925	-3.087388	0.925788
H	-2.578903	2.295460	-0.408577
H	-2.988828	1.252705	0.957709
H	-3.668072	0.424970	-1.943011
P	2.898175	-0.989699	-0.699398
O	1.561486	-0.402964	-1.144860
O	2.593672	-1.688248	0.767964
H	0.296020	-1.317570	-0.922555
O	3.847316	0.250479	-0.169025
O	3.697277	-1.860843	-1.588880
H	1.634249	-1.691064	0.929031
H	3.485133	0.498049	0.693437

B2.I2′′

C	0.985537	0.947668	-1.089559
C	0.877122	2.264241	-1.673613
C	1.416721	3.303675	-1.015366
N	2.097387	3.134094	0.169528
C	2.237659	1.903837	0.825554
N	1.663366	0.873719	0.143325
O	2.823820	1.813068	1.886739
N	0.523603	-0.155240	-1.542294
C	1.625519	-0.508605	0.613111
C	0.841539	-1.203597	-0.550137
O	-0.289189	-1.779911	-0.055580
C	1.657315	-2.313917	-1.243419
O	2.390377	-2.995642	-0.237875
O	0.803815	-3.179682	-1.892391
C	0.847520	-0.678946	1.908012
C	-0.206713	-1.780191	1.827251
O	-1.352676	-1.605795	2.288273
H	0.344319	2.385018	-2.611870
H	1.344926	4.326997	-1.371031
H	2.490415	3.919533	0.671613
H	2.652196	-0.882816	0.692352
H	2.348745	-1.892881	-1.994780
H	2.434313	-3.906316	-0.559952
H	-0.014897	-3.095144	-1.351823
H	1.529110	-0.918515	2.734942
H	0.334380	0.254690	2.161352
H	-1.805950	-1.244487	-0.419899
H	0.216864	-2.806076	1.850312
P	-2.970348	0.544265	-0.078091
O	-1.940683	0.701723	1.132668
H	-1.874406	-0.138460	1.687819
O	-2.294433	1.567493	-1.141715
O	-4.384748	0.891560	0.156261
O	-2.725868	-0.919750	-0.640869
H	-1.371919	1.316956	-1.286666

B2.TS3

C	0.069395	1.382023	-1.103351
C	-1.099738	1.921173	-1.743677
C	-2.060309	2.447269	-0.956891
N	-1.894712	2.589682	0.394201
C	-0.758425	2.168457	1.093385
N	0.174664	1.585917	0.278751
O	-0.629914	2.359628	2.284219
N	1.026704	0.713134	-1.640291
C	1.430233	0.987561	0.739955
C	1.798928	0.192073	-0.532552
O	1.376000	-1.144309	-0.272473
C	3.287521	0.159427	-0.875000
O	4.014174	0.079199	0.335887
O	3.575295	-0.914338	-1.698656
C	1.287782	-0.026834	1.862103
C	1.459681	-1.439875	1.272476
O	0.599396	-2.357268	1.611079
H	-1.218784	1.804339	-2.814791
H	-3.015785	2.788512	-1.347041
H	-2.675315	2.830006	0.989904
H	2.149892	1.787372	0.961987
H	3.557173	1.079004	-1.422077
H	4.838641	-0.368247	0.100001
H	2.921150	-1.597397	-1.448320
H	2.048350	0.146813	2.631711
H	0.303412	0.050714	2.332129
H	-0.061879	-1.450088	-0.829483
H	2.507271	-1.783339	1.361641
P	-2.288744	-1.554161	-0.169928
O	-1.695622	-0.851494	1.102554
H	-0.434354	-1.845323	1.461816
O	-3.273602	-0.410252	-0.835511
O	-3.036113	-2.817725	0.031637
O	-1.126391	-1.588511	-1.268107
H	-2.651403	0.061825	-1.520897

B2.P

C	0.130355	1.303660	-1.098484
C	-1.028961	1.834244	-1.761176
C	-1.973929	2.420691	-1.009476
N	-1.819089	2.584460	0.352606
C	-0.695055	2.168813	1.069125
N	0.211877	1.512892	0.285030
O	-0.558474	2.402832	2.253624
N	1.102463	0.638790	-1.614310
C	1.434955	0.889127	0.785800
C	1.880916	0.147190	-0.497340
O	1.531254	-1.212275	-0.290483
C	3.377153	0.209745	-0.798449
O	4.065297	0.097009	0.433466
O	3.740348	-0.810754	-1.660912
C	1.227630	-0.193900	1.834586
C	1.525373	-1.533019	1.137573
O	0.648278	-2.531940	1.385816
H	-1.170711	1.630374	-2.815149
H	-2.920454	2.765288	-1.415231
H	-2.501984	3.085991	0.903609
H	2.139396	1.669189	1.102029
H	3.624606	1.165391	-1.291253
H	4.919588	-0.294104	0.203597
H	3.115128	-1.534145	-1.452676
H	1.894519	-0.043192	2.690089
H	0.190688	-0.207373	2.186456
H	-0.587291	-1.363976	-1.221413
H	2.535596	-1.896033	1.384437
P	-2.453808	-1.450144	-0.153934
O	-1.550590	-1.118933	1.030183
H	-0.272216	-2.138565	1.297149
O	-3.435782	-0.124406	-0.288770
O	-3.270639	-2.684807	-0.219827
O	-1.518170	-1.288951	-1.494269
H	-3.109306	0.458817	0.410514