Supplementary Materials

4-Substituted Pyridine-3-Sulfonamides as Carbonic Anhydrase Inhibitors Modified by Click Tailing: Synthesis, Activity, and Docking Studies

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Table S1. Experimental details on X-ray diffraction structural analyses for **8** and **18**

	18	**8**
Crystal data		
Chemical formula	$C_{14}H_{19}N_5O_2S_2$	$C_{13}H_{11}N_5O_2S$
M_r	353.46	301.33
Crystal system, space group	Monoclinic, $P2_1/c$	Triclinic, $P\bar{1}$
Temperature (K)	120	120
a, *b*, *c* (Å)	13.2431 (7), 9.3471 (3), 12.8715 (7)	10.9590 (14), 14.6972 (17), 16.8438 (18)
α, β, γ (°)	90, 99.184 (4), 90	93.358 (9), 98.724 (9), 101.205 (10)
V (Å^3)	1572.87 (13)	2619.6 (5)
Z	4	8
Radiation type	Cu *K*α	Cu *K*α
μ (mm^{-1})	3.23	2.33
Crystal size (mm)	0.32 × 0.11 × 0.03	0.31 × 0.09 × 0.04
Data collection		
Diffractometer	STOE *IPDS* 2T	STOE *IPDS* 2T
Absorption correction	Integration STOE *X-RED32*, absorption correction by Gaussian integration	Integration STOE *X-RED32*, absorption correction by Gaussian integration
T_{min}, T_{max}	0.503, 0.915	0.518, 0.894
No. of measured, independent and observed [$I > 2\sigma(I)$] reflections	7169, 2532, 2311	22493, 8301, 6936
R_{int}	0.018	0.023
$(\sin\theta/\lambda)_{max}$ (Å^{-1})	0.583	0.582
Refinement		
$R[F^2 > 2\sigma(F^2)]$, $wR(F^2)$, *S*	0.032, 0.085, 1.07	0.038, 0.108, 1.04
No. of reflections	2532	8301
No. of parameters	216	789
H-atom treatment	H atoms treated by a mixture of independent and constrained refinement	H atoms treated by a mixture of independent and constrained refinement

$\Delta\rangle_{max}$, $\Delta\rangle_{min}$ (e Å^{-3})	0.23, -0.38	0.26, -0.53

Table S2. Dihedral acute angles (º) between rings in conformers A, B, C, D in **8**. Symbols scheme: A1, A2 and A3 denote pyridine, triazol and phenyl ring planes in molecule A, respectively.

Definition	Angle	Definition	Angle
A1-A2	43.07(11)	C1-C2	21.89(12)
A2-A3	7.78(11)	C2-C3	33.65(12)
A1-A3	44.54(10)	C1-C3	55.32(10)
B1-B2	45.31(11)	D1-D2	12.19(12)
B2-B3	7.32(11)	D2-D3	14.51(12)
B1-B3	49.55(10)	D1-D3	2.32(11)

Namely: A1: C1-C5, N2; A2: N3-N5, C6-C7; A3: C8-C13. Indexes for next molecules (B,C,D) are obtained by adding +5 to N-atom labels and +13 to C-atom labels.

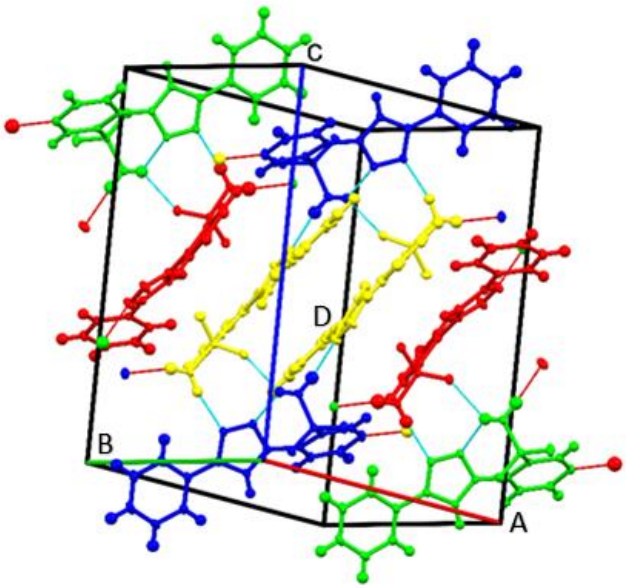
Table S3. Hydrogen-bond geometry (Å, º) for **8**) and 1**8**

18				
D—H···*A*	*D*—H	H···*A*	*D*···*A*	*D*—H···*A*
N1—H1*A*···O2^{i}	0.89 (3)	2.34 (3)	3.196 (2)	162 (2)
N1—H1*B*···N2^{ii}	0.87 (3)	2.08 (3)	2.914 (2)	161 (3)
C6—H6*A*···N3^{iii}	0.99	2.47	3.330 (3)	145
C6—H6*A*···N4^{iii}	0.99	2.37	3.311 (3)	158
Symmetry codes: (i) -*x*, *y*+1/2, -*z*+1/2; (ii) *x*, -*y*+3/2, *z*-1/2; (iii) -*x*+1, *y*+1/2, -*z*+1/2.				
8				

D—H···*A*	*D*—H	H···*A*	*D*···*A*	*D*—H···*A*
N1—H1*A*···N4	0.85 (3)	2.39 (3)	3.023 (3)	131 (2)
N1—H1*A*···O6	0.85 (3)	2.29 (3)	2.942 (2)	134 (2)
N1—H1*B*···N15^{i}	0.90 (3)	2.07 (3)	2.965 (3)	172 (2)
C6—H6···O1^{ii}	0.95	2.61	3.452 (3)	148
N11—H11*A*···N5	0.87 (3)	2.08 (3)	2.945 (3)	170 (3)
N11—H11*B*···N2^{iii}	0.86 (3)	2.03 (3)	2.873 (3)	168 (3)
C30—H30···O7^{iv}	0.95	2.38	3.147 (3)	138
C31—H31···N11	0.95	2.41	2.907 (3)	112
C31—H31···O4	0.95	2.41	3.180 (3)	138
C32—H32···O5	0.95	2.30	3.051 (3)	136
N16—H16*A*···N7^{iii}	0.85 (3)	2.08 (3)	2.898 (3)	163 (3)
N16—H16*B*···N10	0.89 (3)	2.13 (3)	2.995 (3)	164 (2)
C43—H43···O5^{v}	0.95	2.47	3.302 (3)	146
C44—H44···O2^{vi}	0.95	2.53	3.281 (3)	136
C44—H44···N16	0.95	2.39	2.899 (3)	113
C45—H45···O8	0.95	2.27	2.984 (3)	132
N6—H6*A*···O8	0.86 (3)	2.21 (3)	2.913 (2)	138 (2)
N6—H6*A*···N9	0.86 (3)	2.43 (3)	3.061 (3)	130 (2)
N6—H6*B*···N20^{vii}	0.92 (3)	2.06 (3)	2.970 (3)	172 (2)
C18—H18···N12	0.95	2.59	3.515 (3)	165
C19—H19···O3^{viii}	0.95	2.64	3.426 (3)	141

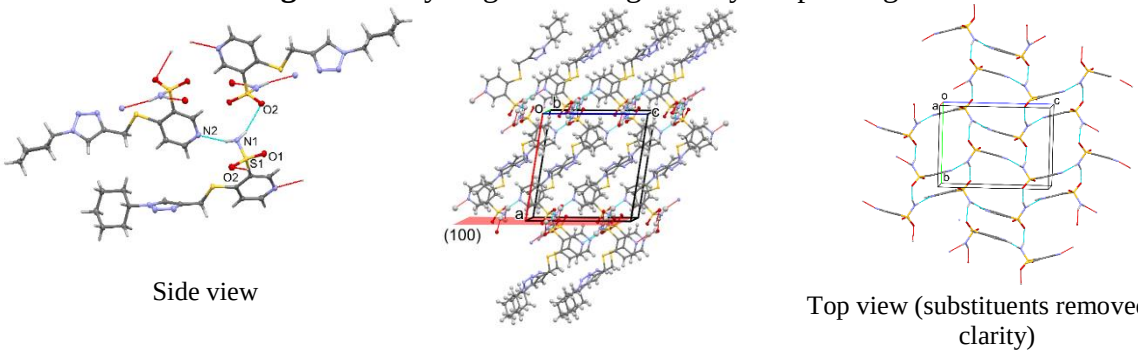
Symmetry codes: (i) -*x*+2, -*y*, -*z*+1; (ii) -*x*+2, -*y*, -*z*; (iii) *x*-1, *y*, *z*; (iv) *x*+1, *y*, *z*; (v) *x*, *y*+1, *z*; (vi) *x*-1, *y*+1, *z*; (vii) -*x*+1, -*y*+1, -*z*+1; (viii) -*x*+1, -*y*+1, -*z*.

Figure S1. View of the crystal packing in **8**.



Colouring code for conformers: green A, blue B, red C, yellow D. Hydrogen bonding shown as dotted cyan lines (red lines for hanging interactions).

Figure S2. Hydrogen bonding and crystal packing in **18**.



Side view

Top view (substituents removed for clarity)

Molecules are linked by hydrogen bonding of the NH..O and NH…N type (on the left), forming infinite layers of fused ring motifs $R_4^4(16)$ and $R_4^4(20)$ (on the right) propagating along crystallographic (100) plane. Mainly donor type -SO_2NH_2 is used in hydrogen bonding (drawn as dashed cyan lines or red lines if hanging i.e. are linking to invisible molecules).

Table S4. hCA II (PDB id: 6RH4) cross-docking validation results

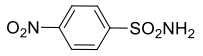
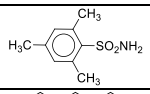
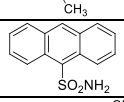
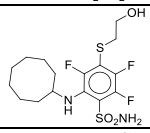
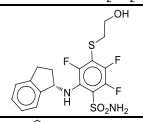
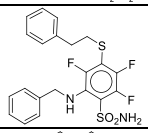
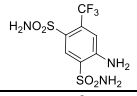
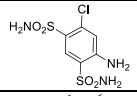
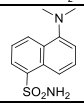
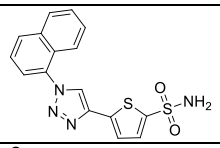
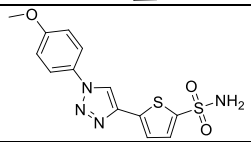
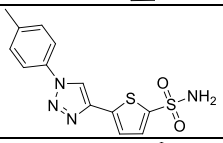
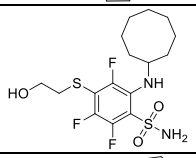
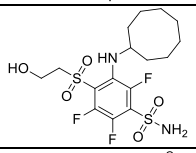
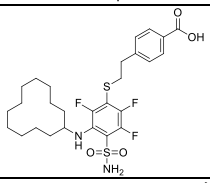
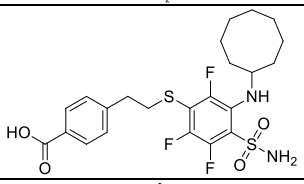
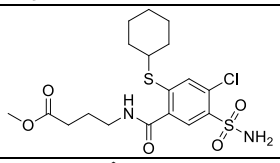
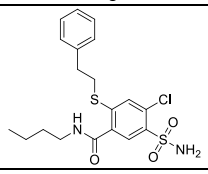
Protein PDB code	Ligand structure	m.w.	No. of heavy atoms	No. of rotatable bonds	First ranked pose RMSD	First ranked pose S [kcal/mol]	Best fitted pose RMSD	Best fitted pose [kcal/mol]
6RH4 (original ligand)		202.19	13	3	0.38	-7.45	0.38	-7.45
6T4N		199.27	13	2	0.93	-9.07	0.93	-9.07
6T5C		257.31	18	2	1.33	-9.23	1.15	-8.66
4PYX		412.50	26	6	1.56	-10.86	0.86	-10.58
5DOH		418.46	27	6	1.53	-10.35	1.34	-9.74
5DOG		452.52	30	8	1.91	-11.08	0.98	-10.48
6T4P		207.25	14	2	4.26	-8.62	2.36	-7.72
2POW		319.28	19	5	3.40	-10.85	1.15	-8.37
2POV		285.72	16	4	2.47	-9.25	1.24	-8.13
1OKL		250.32	17	3	3.00	-8.957	2.1	-8.09

Table S5. hCA IX (PDB id: 5DVX) cross-docking validation results

Protein PDB code	Ligand structure	m.w.	No. of heavy atoms	No. of rotatable bonds	First ranked pose RMSD	First ranked pose S [kcal/mol]	Best fitted pose RMSD	Best fitted pose [kcal/mol]
5FL4		**355.42**	24	3	6.40	-8.70	1.75	-8.19
5FL5		**335.39**	22	4	6.12	-8.59	0.64	-8.17
5FL6		**319.39**	21	3	5.67	-8.44	0.30	-8.11
6FE0		**411.49**	26	6	1.53	-9.67	1.18	-9.21
6FE1		**443.49**	28	6	5.36	-9.51	1.96	-9.40
6G98		**571.71**	38	8	2.33	-10.13	2.33	-10.13
6G9U		**515.60**	34	8	1.97	-10.20	1.64	-9.88
6QN2		**447.98**	28	8	2.20	-9.76	2.20	-9.76
6QN6		**425.98**	27	9	3.94	-10.21	3.94	-10.21

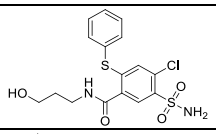
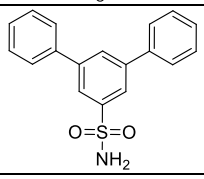
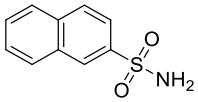
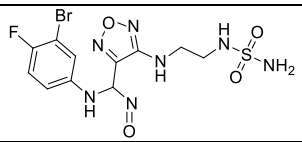
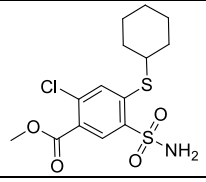
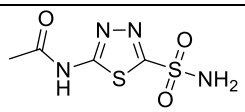
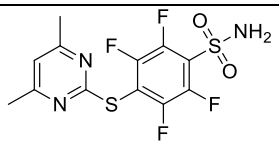
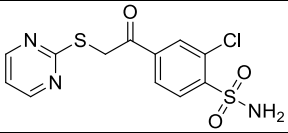
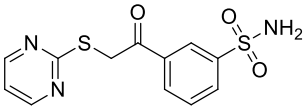
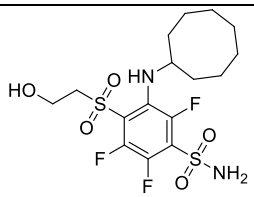
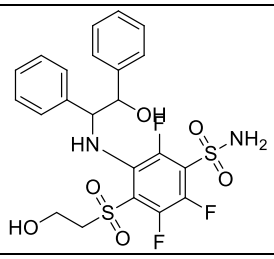
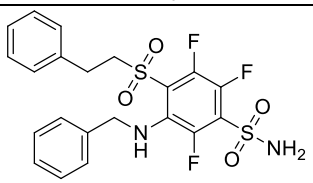
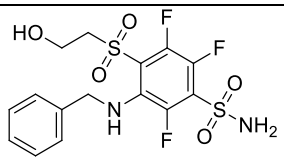
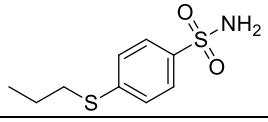
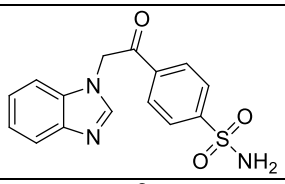
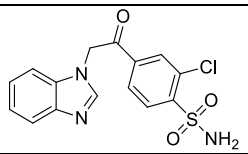
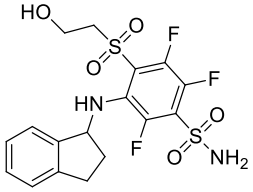
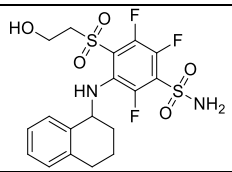
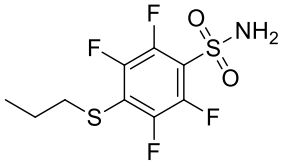
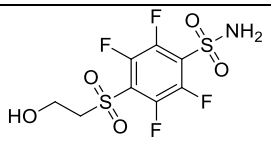
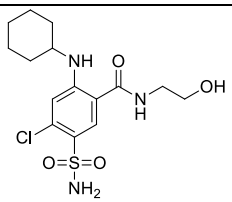
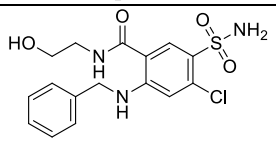
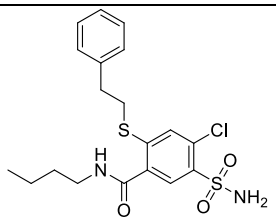
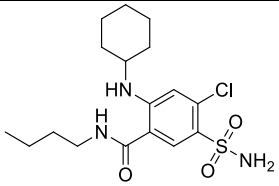
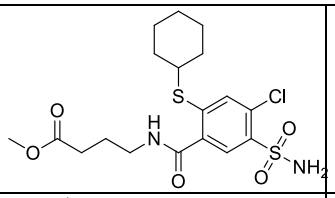
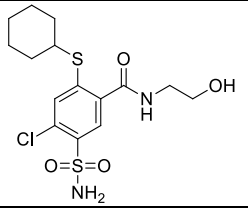
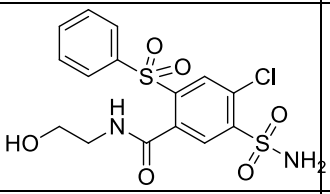
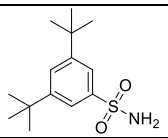
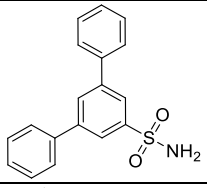
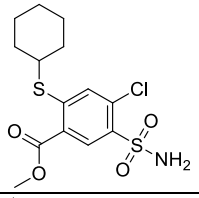
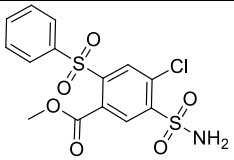
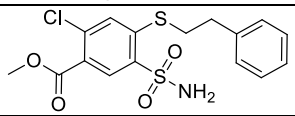
6QUT		**399.90**	25	7	1.61	-9.99	2.86	-9.00
6TL5		**308.38**	22	3	0.57	-9.07	0.57	-9.07
6TL6		**206.25**	14	1	2.33	-7.56	0.51	-7.16
6VKG		**437.23**	25	9	4.90	-9.81	2.74	-8.98
7POM		**362.88**	22	4	5.87	-9.31	1.47	-8.96
				Mean:	3.63		1.61	

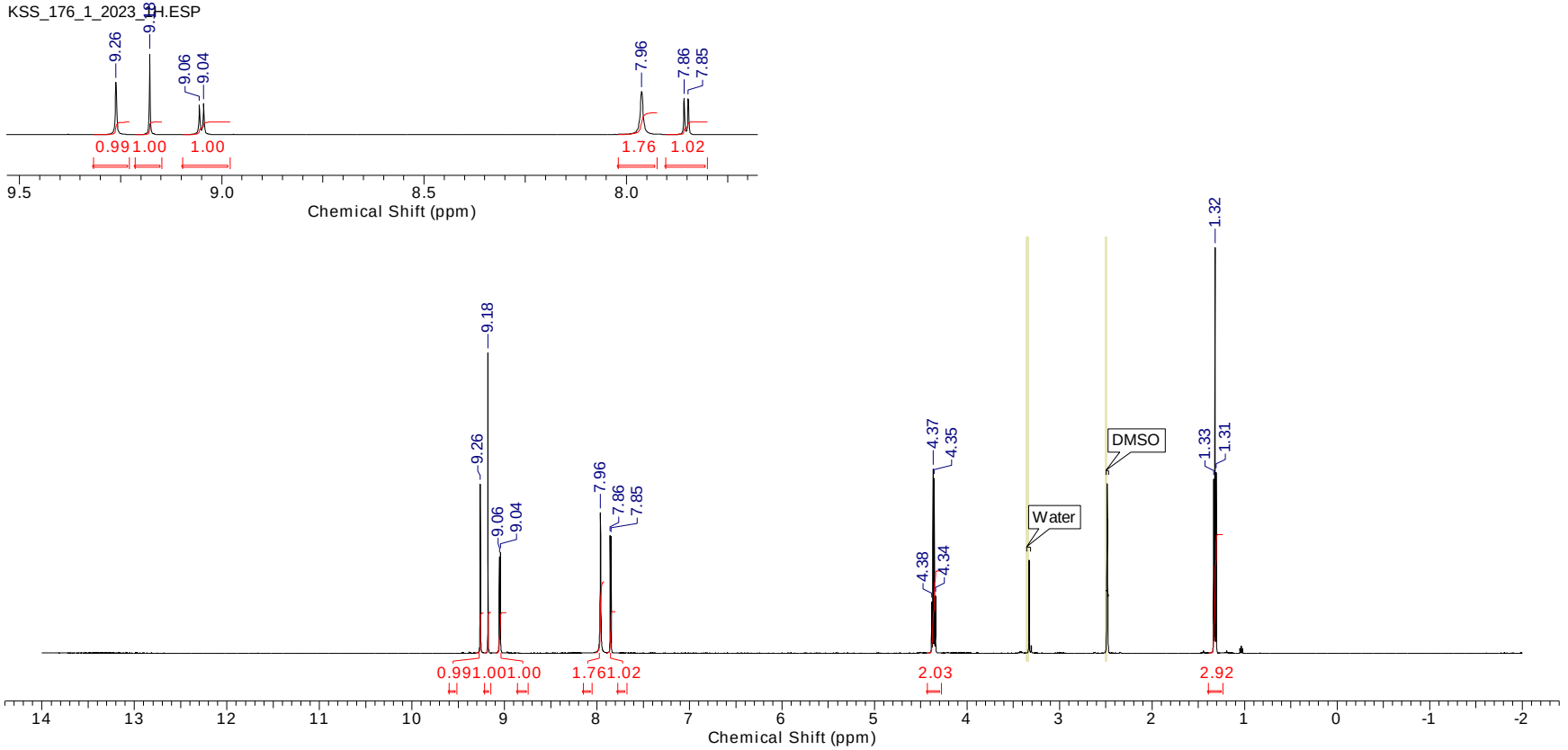
Table S6. hCA XII (PDB id: 6QNG) cross-docking validation results

Protein PDB code	Ligand structure	m.w.	No. of heavy atoms	No. of rotatable bonds	First ranked pose RMSD	First ranked pose S [kcal/mol]	Best fitted pose RMSD	Best fitted pose [kcal/mol]
1JD0.A		221.24	13	3	4.13	-7.34	1.40	-7.24
4HT2.A		366.34	23	3	2.35	-8.89	1.36	-8.71
4KP5.A		342.81	21	5	5.00	-9.07	0.85	-8.53
4KP8.A		308.36	20	5	5.61	-8.89	3.33	-8.48
4Q0L.A		443.49	28	6	5.16	-10.16	1.66	-9.66
4QJ0.A		529.54	35	9	2.24	-10.26	1.17	-9.47
4QJO.A		483.51	32	8	5.66	-10.18	2.57	-9.71
4QJW.A		423.41	27	7	5.77	-9.76	5.35	-9.30
4WW8.A		230.33	14	4	0.79	-8.05	0.79	-8.05

5LL5.A		314.35	22	4	4.99	-8.66	2.26	-8.33
5LL9.A		348.79	23	4	4.93	-9.12	2.18	-8.71
5LLO.A		449.45	29	6	5.48	-9.56	1.56	-9.11
5LLP.A		463.48	30	6	5.72	-10.07	5.21	-9.36
5MSA.A		302.29	18	4	0.53	-8.11	0.53	-8.11
5MSB.A		336.26	20	4	1.21	-8.00	1.21	-8.00
6G5L.A		374.87	24	7	1.28	-9.96	0.93	-9.87
6G7A.A		382.85	25	8	1.79	-9.95	1.66	-9.79
6QN0.A		425.98	27	10	3.17	-11.10	2.21	-10.52
6QNG.A		386.92	25	8	1.28	-10.88	0.74	-10.57

6QNL.A		447.98	28	10	3.91	-11.01	1.58	-10.34
6R6Y.A		391.92	24	7	1.75	-10.20	0.97	-9.90
6R71.A		417.87	26	7	1.91	-9.86	1.17	-9.49
6T5P.A		268.40	18	3	1.17	-8.11	0.74	-7.93
6T5Q.A		308.38	22	3	1.71	-9.06	0.56	-8.79
7PUU.A		362.88	22	5	0.72	-9.42	0.44	-9.21
7PUV.A		388.83	24	5	2.18	-9.08	1.01	-8.75
7PUW.A		384.88	24	7	1.05	-10.01	0.80	-9.97
				Mean:	3.02		1.64	

Spectrum S1. ^{1}H-NMR of compound **3** (500 MHz, DMSO-d_6).



No.	(ppm)	(Hz)	Height
1	1.31	652.5	0.4455
2	1.32	659.8	1.0000
3	1.33	666.7	0.4286

No.	(ppm)	(Hz)	Height
4	4.34	2169.1	0.1407
5	4.35	2175.9	0.4305
6	4.37	2183.3	0.4535

No.	(ppm)	(Hz)	Height
7	4.38	2190.1	0.1263
8	7.85	3921.9	0.2875
9	7.86	3926.8	0.2901

No.	(ppm)	(Hz)	Height
10	7.96	3979.5	0.3456
11	9.04	4520.4	0.2478
12	9.06	4525.7	0.2375

No.	(ppm)	(Hz)	Height
13	9.18	4586.7	0.7407
14	9.26	4628.7	0.4166

Spectrum S2. ^{13}C-NMR of compound **3** (125 MHz, DMSO- d_6).

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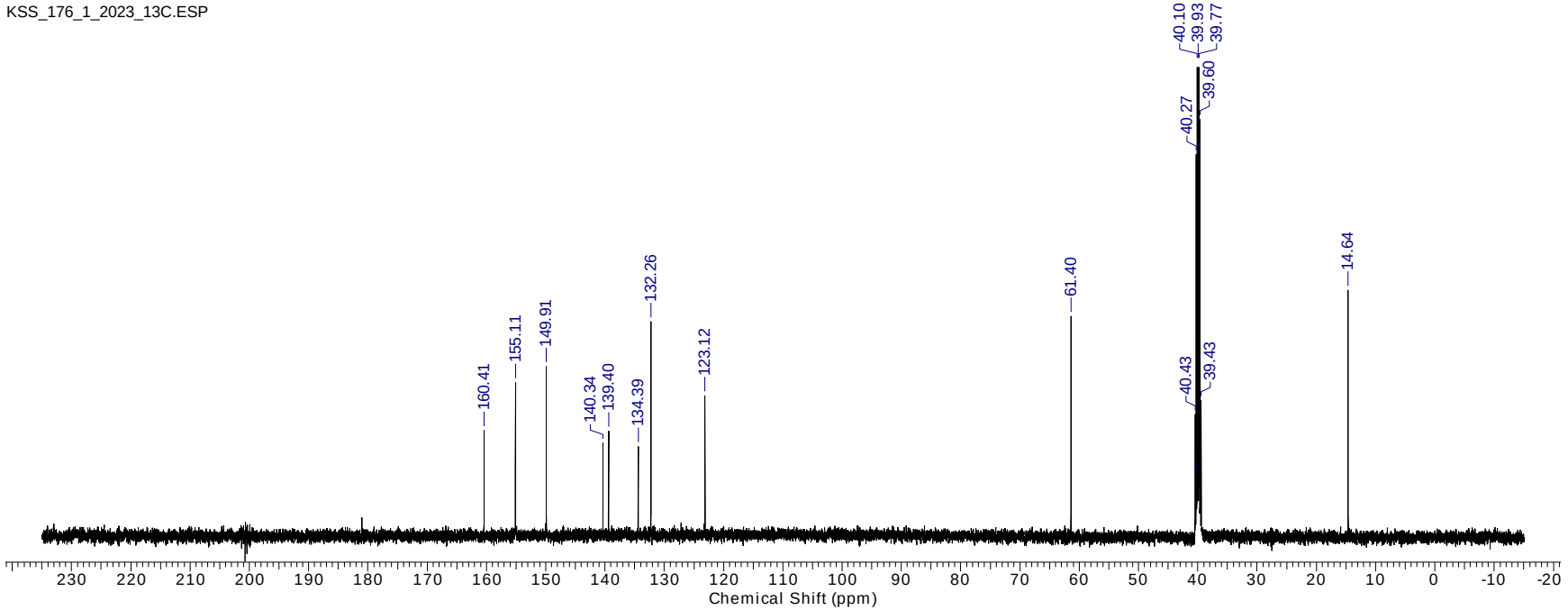


No.	(ppm)	(Hz)	Height
1	14.64	1840.0	0.2597
2	39.43	4955.6	0.1436
3	39.60	4976.7	0.4397
4	39.77	4997.8	0.8566

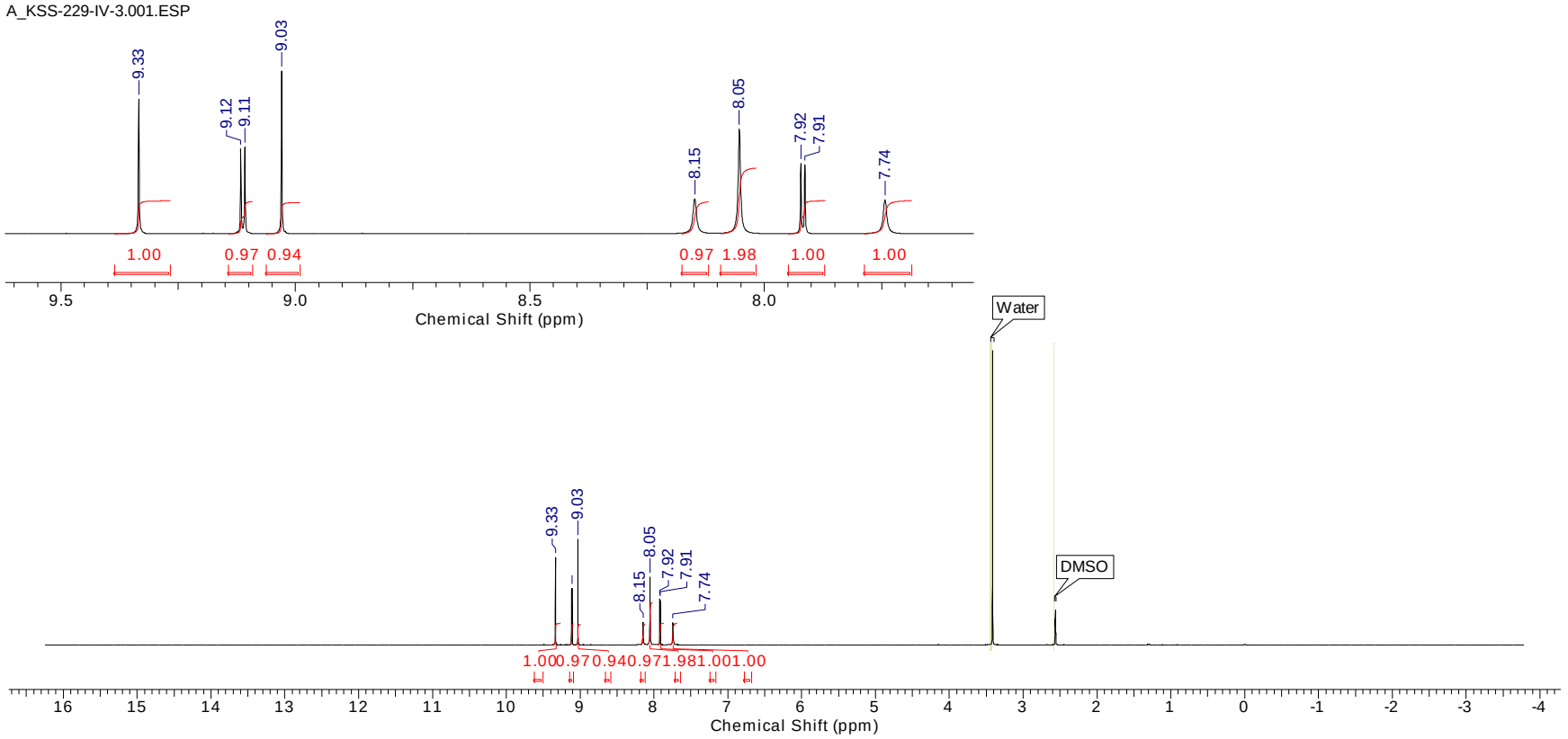
No.	(ppm)	(Hz)	Height
5	39.93	5018.9	1.0000
6	40.10	5040.0	0.8347
7	40.19	5050.6	0.0654
8	40.27	5061.1	0.4023

No.	(ppm)	(Hz)	Height
9	40.35	5071.7	0.0394
10	40.43	5081.3	0.1287
11	61.40	7716.5	0.2323
12	123.12	15474.3	0.1487

No.	(ppm)	(Hz)	Height
13	132.26	16623.2	0.2264
14	134.39	16890.7	0.0952
15	139.40	17520.7	0.1113
16	140.34	17638.7	0.0983

No.	(ppm)	(Hz)	Height
17	149.91	18841.2	0.1792
18	155.11	19495.2	0.1620
19	160.41	20160.7	0.1116

Spectrum S3. ^{1}H-NMR of compound **4** (600 MHz, DMSO-d_6).



No.	(ppm)	(Hz)	Height
1	7.74	4646.9	0.0749
2	7.91	4749.6	0.1517
3	7.92	4754.7	0.1557
4	8.05	4833.6	0.2309

No.	(ppm)	(Hz)	Height
5	8.15	4890.4	0.0775
6	9.03	5419.4	0.3593
7	9.11	5466.3	0.1920
8	9.12	5471.5	0.1879

No.	(ppm)	(Hz)	Height
9	9.33	5602.0	0.2972

Spectrum S4. ^{13}C-NMR of compound **4** (150 MHz, DMSO- d_6).

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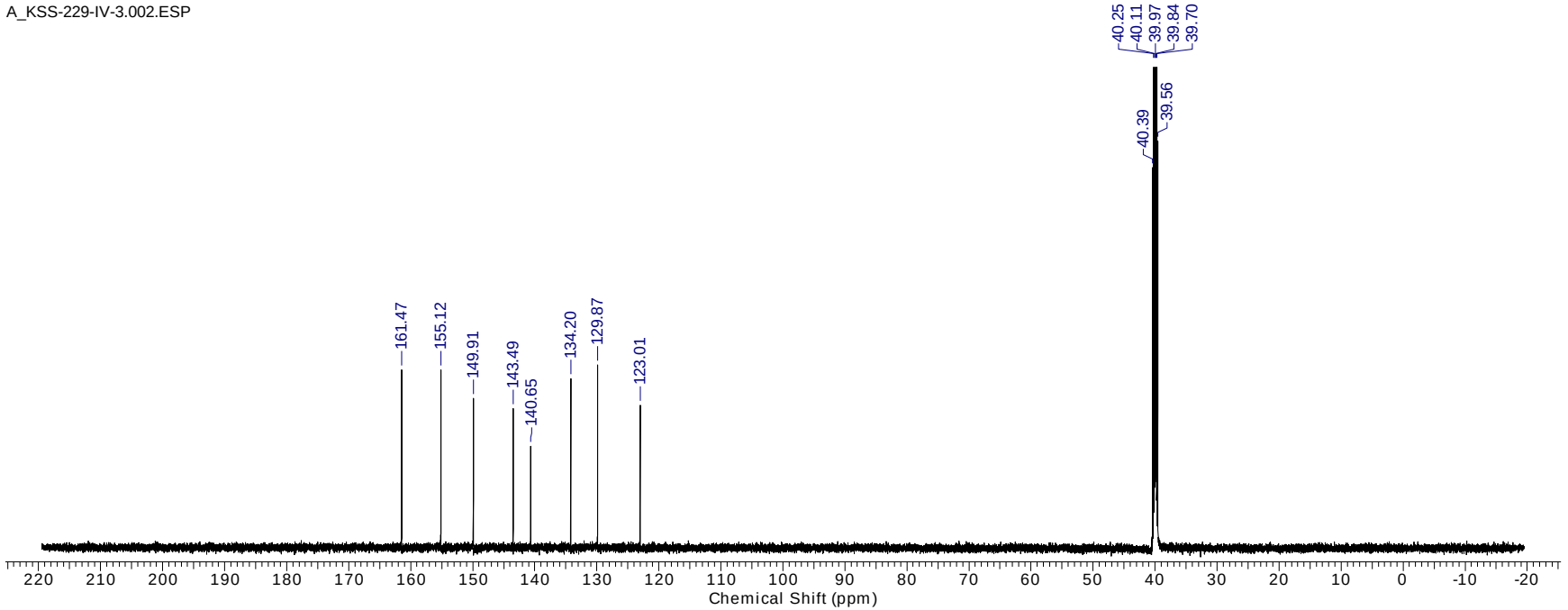


No.	(ppm)	(Hz)	Height
1	39.56	5969.7	0.1401
2	39.70	5990.6	0.4338
3	39.84	6011.5	0.8585

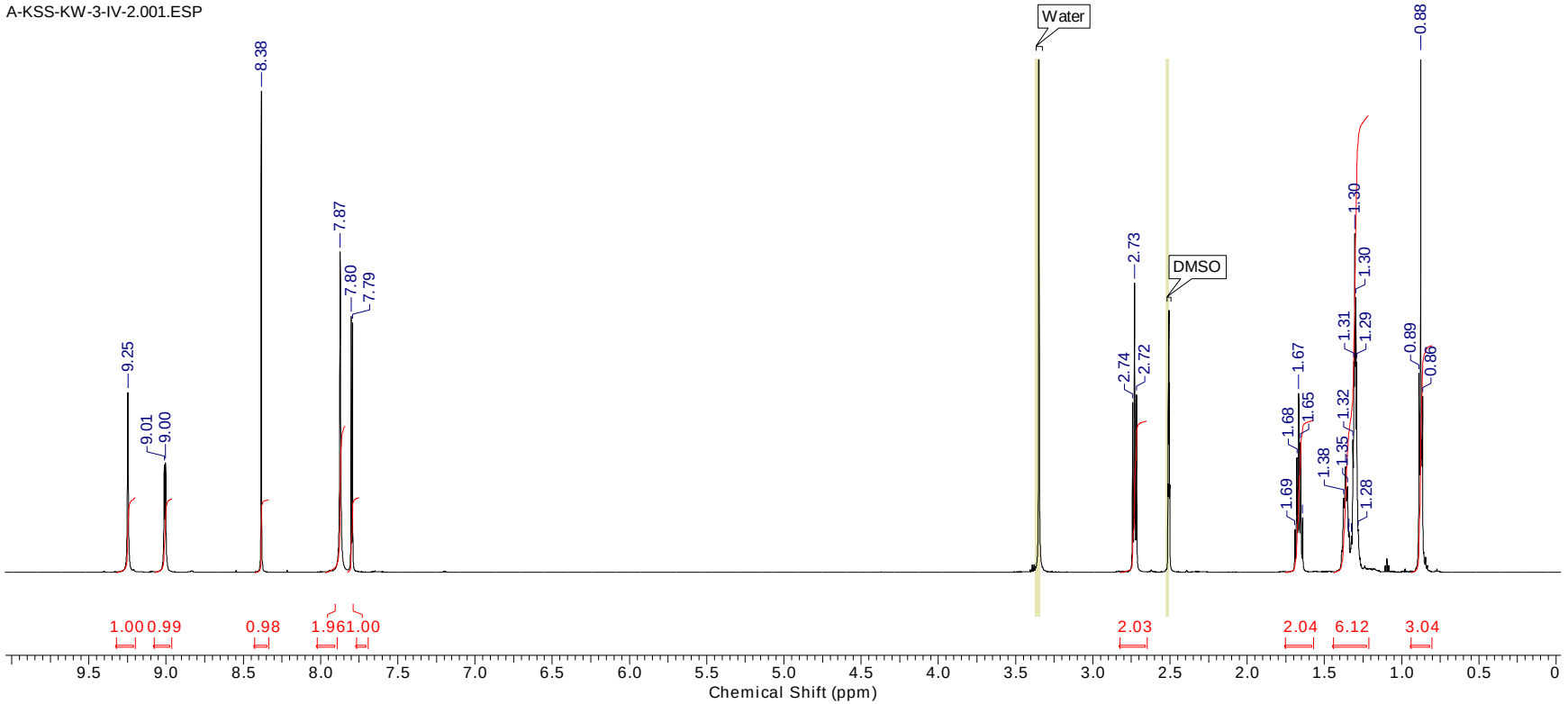
No.	(ppm)	(Hz)	Height
4	39.97	6032.4	1.0000
5	40.11	6053.4	0.8379
6	40.25	6074.3	0.4112

No.	(ppm)	(Hz)	Height
7	40.39	6095.2	0.1309
8	123.01	18563.7	0.0492
9	129.87	19599.2	0.0631

No.	(ppm)	(Hz)	Height
10	134.20	20252.8	0.0584
11	140.65	21225.6	0.0351
12	143.49	21654.7	0.0481

No.	(ppm)	(Hz)	Height
13	149.91	22623.1	0.0516
14	155.12	23409.9	0.0614
15	161.47	24367.2	0.0613

Spectrum S5. ^{1}H-NMR of compound **5** (600 MHz, DMSO-d_6).



No.	(ppm)	(Hz)	Height
1	0.86	518.9	0.0976
2	0.87	521.5	0.0631
3	0.88	526.3	0.2855
4	0.88	530.7	0.0626
5	0.89	533.2	0.1102
6	1.28	769.1	0.0236
7	1.29	775.0	0.1163

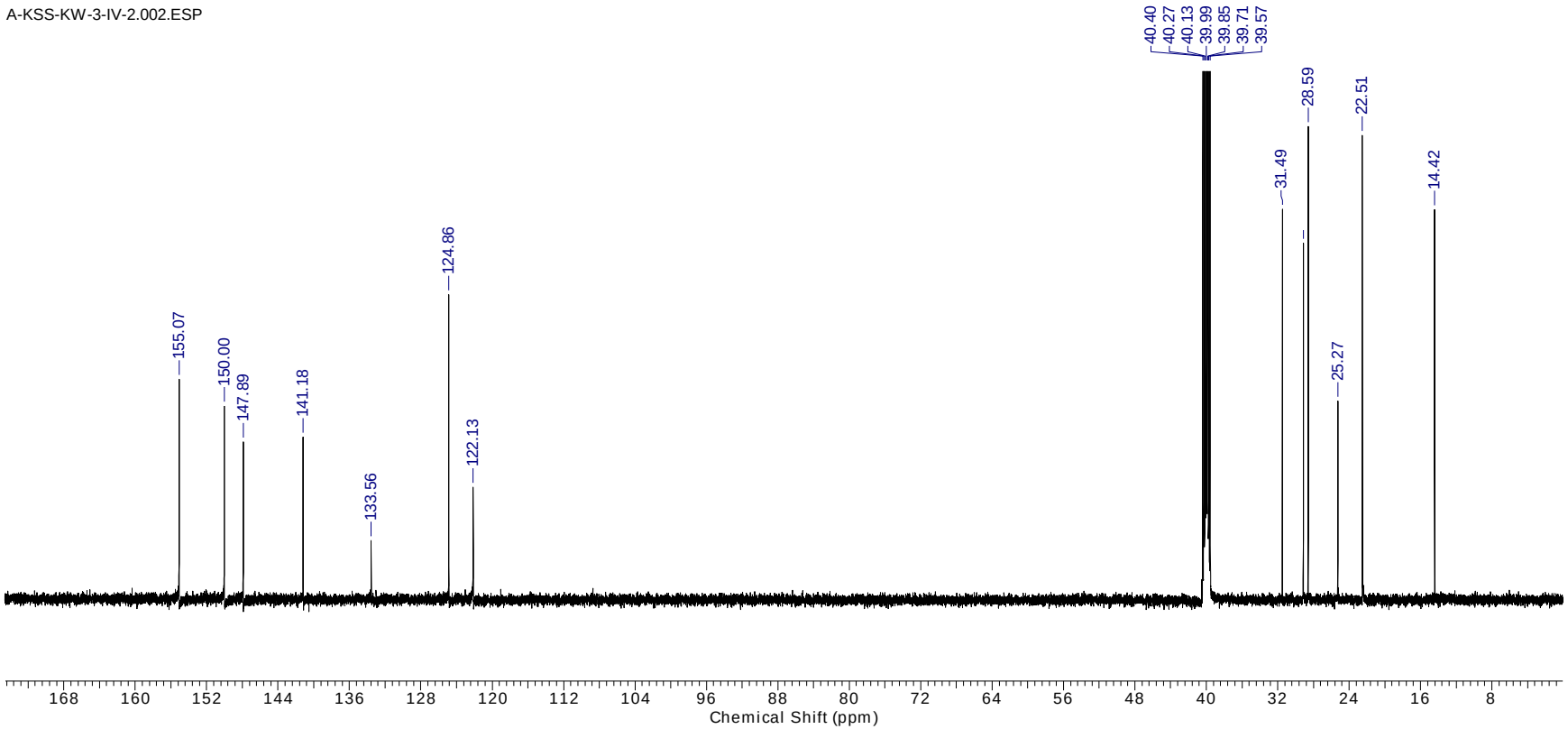
No.	(ppm)	(Hz)	Height
8	1.30	778.3	0.1522
9	1.30	782.3	0.1877
10	1.31	785.2	0.1167
11	1.32	789.3	0.0734
12	1.32	795.1	0.0201
13	1.34	804.7	0.0228
14	1.34	806.5	0.0204

No.	(ppm)	(Hz)	Height
15	1.35	810.9	0.0475
16	1.36	813.5	0.0414
17	1.36	818.6	0.0587
18	1.38	826.0	0.0410
19	1.64	985.1	0.0305
20	1.65	992.8	0.0720
21	1.67	1000.2	0.0993

No.	(ppm)	(Hz)	Height
22	1.68	1007.5	0.0637
23	1.69	1015.2	0.0239
24	2.72	1630.7	0.0984
25	2.73	1638.0	0.1602
26	2.74	1645.7	0.0941
27	7.79	4677.3	0.1382
28	7.80	4682.5	0.1418

No.	(ppm)	(Hz)	Height
29	7.87	4725.0	0.1773
30	8.38	5031.7	0.2663
31	9.00	5403.6	0.0608
32	9.01	5408.7	0.0596
33	9.25	5549.9	0.0997

Spectrum S6. ^{13}C-NMR of compound **5** (125 MHz, DMSO- d_6).



No.	(ppm)	(Hz)	Height
1	14.42	2176.7	0.0952
2	22.51	3397.0	0.1132
3	25.27	3813.0	0.0485
4	28.59	4314.7	0.1154

No.	(ppm)	(Hz)	Height
5	29.14	4397.3	0.0869
6	31.49	4751.6	0.0952
7	39.57	5971.9	0.1345
8	39.71	5992.8	0.4175

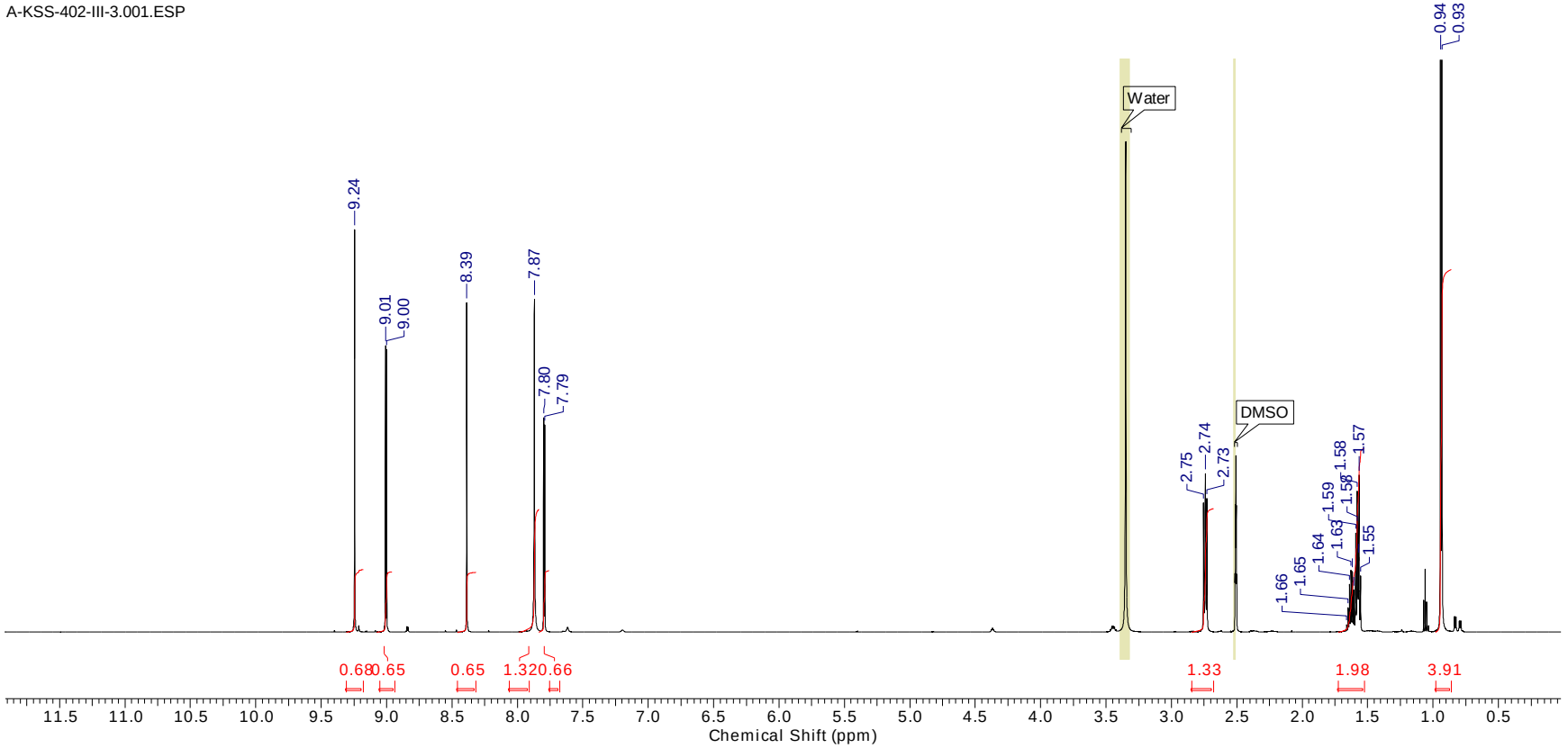
No.	(ppm)	(Hz)	Height
9	39.85	6013.7	0.8430
10	39.99	6034.6	1.0000
11	40.13	6055.6	0.8519
12	40.27	6076.5	0.4251

No.	(ppm)	(Hz)	Height
13	40.40	6097.4	0.1368
14	122.13	18430.6	0.0275
15	124.86	18842.1	0.0743
16	133.56	20156.0	0.0144

No.	(ppm)	(Hz)	Height
17	141.18	21304.8	0.0396
18	147.89	22318.3	0.0385
19	150.00	22636.3	0.0472
20	155.07	23401.1	0.0538

Spectrum S7. ^{1}H-NMR of compound **6** (600 MHz, DMSO-d_6).

A-KSS-402-III-3.001.ESP



No.	(ppm)	(Hz)	Height
1	0.93	559.3	0.8763
2	0.94	565.9	1.0000
3	1.55	933.1	0.0406
4	1.57	939.7	0.1134
5	1.57	941.1	0.0544

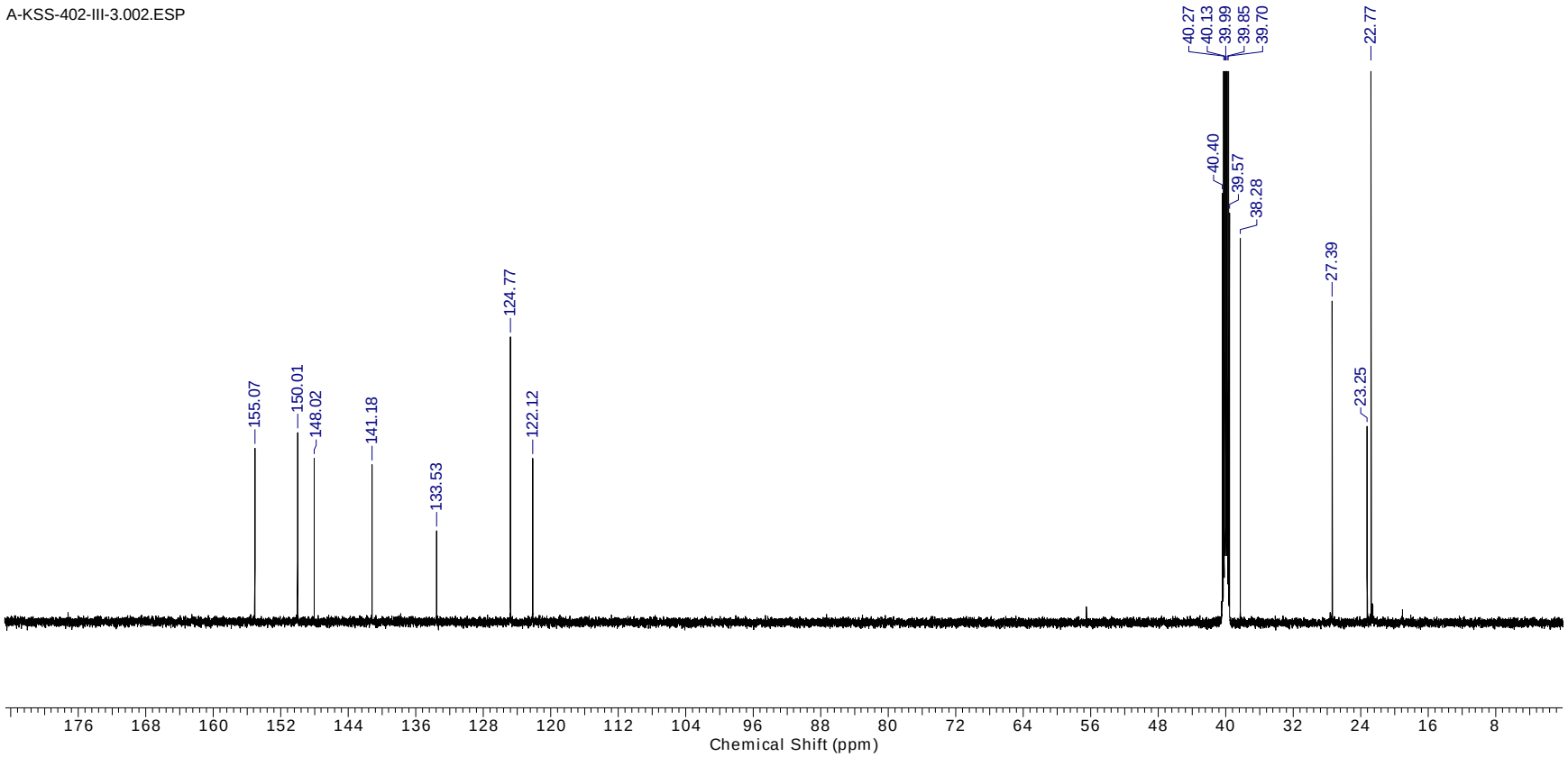
No.	(ppm)	(Hz)	Height
6	1.58	947.4	0.1017
7	1.58	948.8	0.0771
8	1.59	955.1	0.0715
9	1.60	963.1	0.0303
10	1.62	969.7	0.0438

No.	(ppm)	(Hz)	Height
11	1.63	976.0	0.0450
12	1.64	982.9	0.0348
13	1.65	989.5	0.0180
14	1.66	996.1	0.0057
15	2.73	1637.7	0.0964

No.	(ppm)	(Hz)	Height
16	2.74	1645.4	0.1143
17	2.75	1653.1	0.0934
18	7.79	4675.9	0.1495
19	7.80	4681.4	0.1547
20	7.87	4723.5	0.2403

No.	(ppm)	(Hz)	Height
21	8.39	5033.9	0.2378
22	9.00	5401.8	0.2039
23	9.01	5406.9	0.2068
24	9.24	5548.1	0.2904

Spectrum S8. ^{13}C-NMR of compound **6** (150 MHz, DMSO- d_6).



No.	(ppm)	(Hz)	Height
1	22.77	3436.6	0.1989
2	23.25	3508.1	0.0663
3	27.39	4133.2	0.1088
4	38.28	5777.2	0.1301

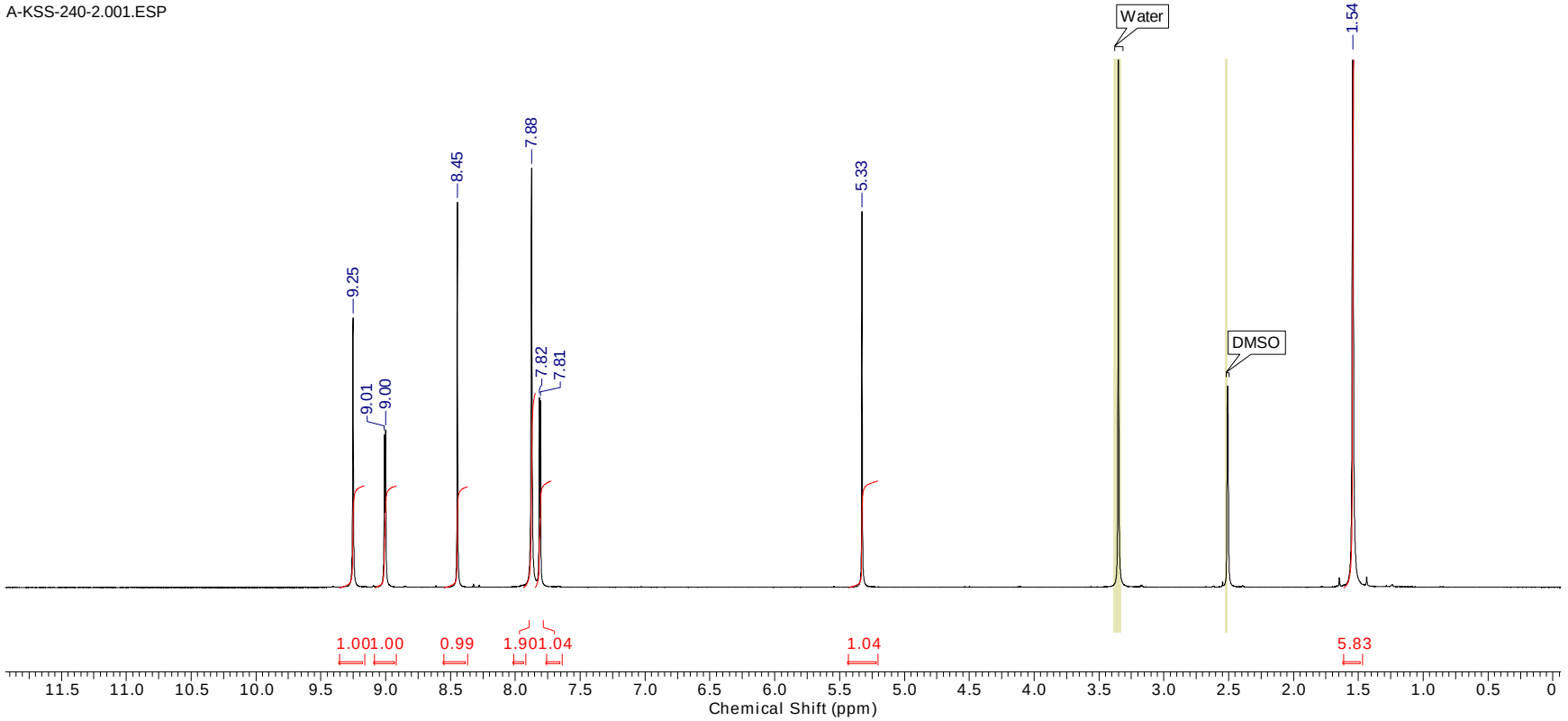
No.	(ppm)	(Hz)	Height
5	39.57	5970.8	0.1386
6	39.70	5991.7	0.4221
7	39.85	6013.7	0.8306
8	39.99	6034.6	1.0000

No.	(ppm)	(Hz)	Height
9	40.13	6055.6	0.8647
10	40.27	6076.5	0.4401
11	40.40	6097.4	0.1452
12	122.12	18429.5	0.0554

No.	(ppm)	(Hz)	Height
13	124.77	18828.9	0.0965
14	133.53	20151.6	0.0308
15	141.18	21304.8	0.0534
16	148.02	22338.1	0.0554

No.	(ppm)	(Hz)	Height
17	150.01	22637.4	0.0641
18	155.07	23402.2	0.0589

Spectrum SS9. ^{1}H-NMR of compound **7** (600 MHz, DMSO-d_6).

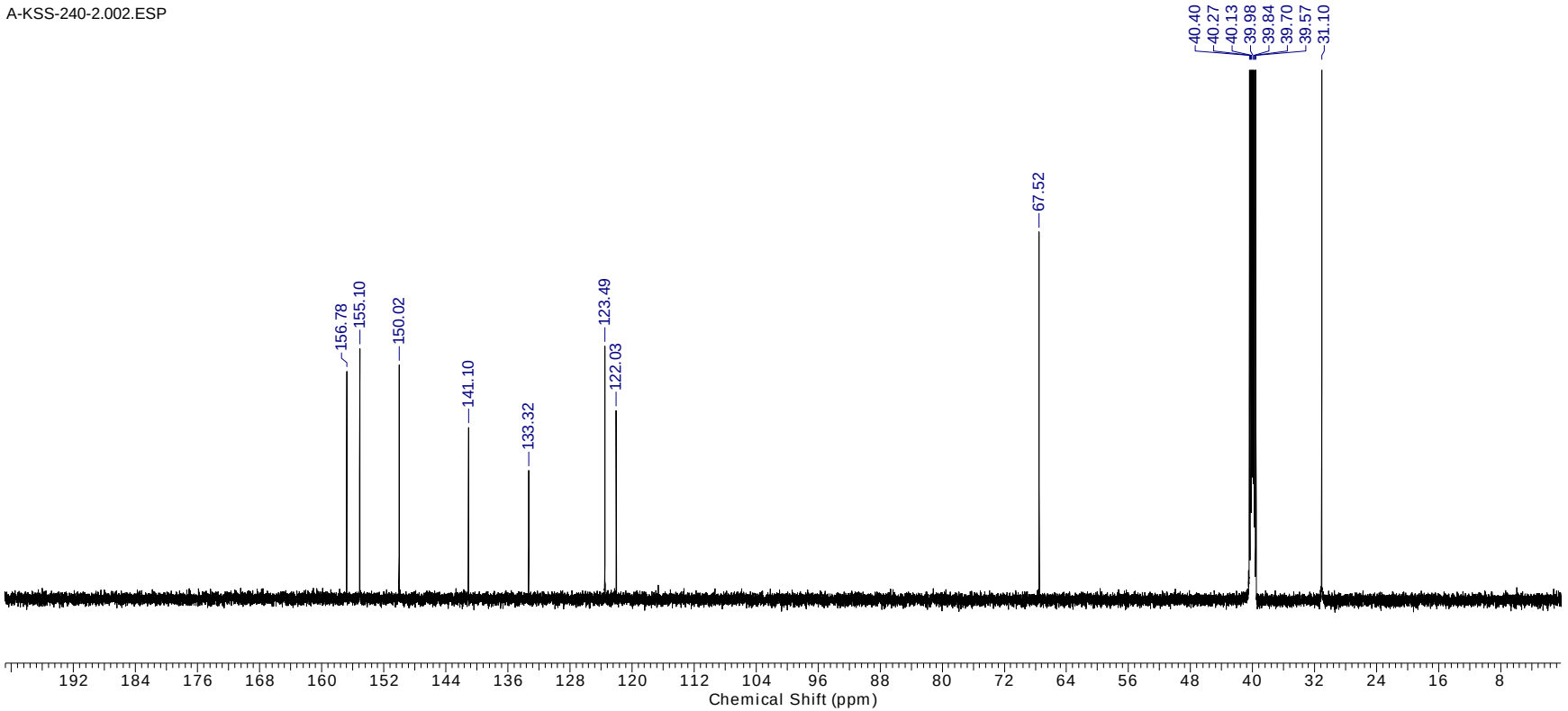


No.	(ppm)	(Hz)	Height
1	1.54	926.1	1.0000
2	5.33	3197.3	0.2021
3	7.81	4685.4	0.1005

No.	(ppm)	(Hz)	Height
4	7.82	4690.5	0.1023
5	7.88	4726.5	0.2254
6	8.45	5069.8	0.2071

No.	(ppm)	(Hz)	Height
7	9.00	5402.1	0.0849
8	9.01	5407.3	0.0824
9	9.25	5552.9	0.1449

Spectrum S10. ^{13}C-NMR of compound **7** (150 MHz, DMSO- d_6).



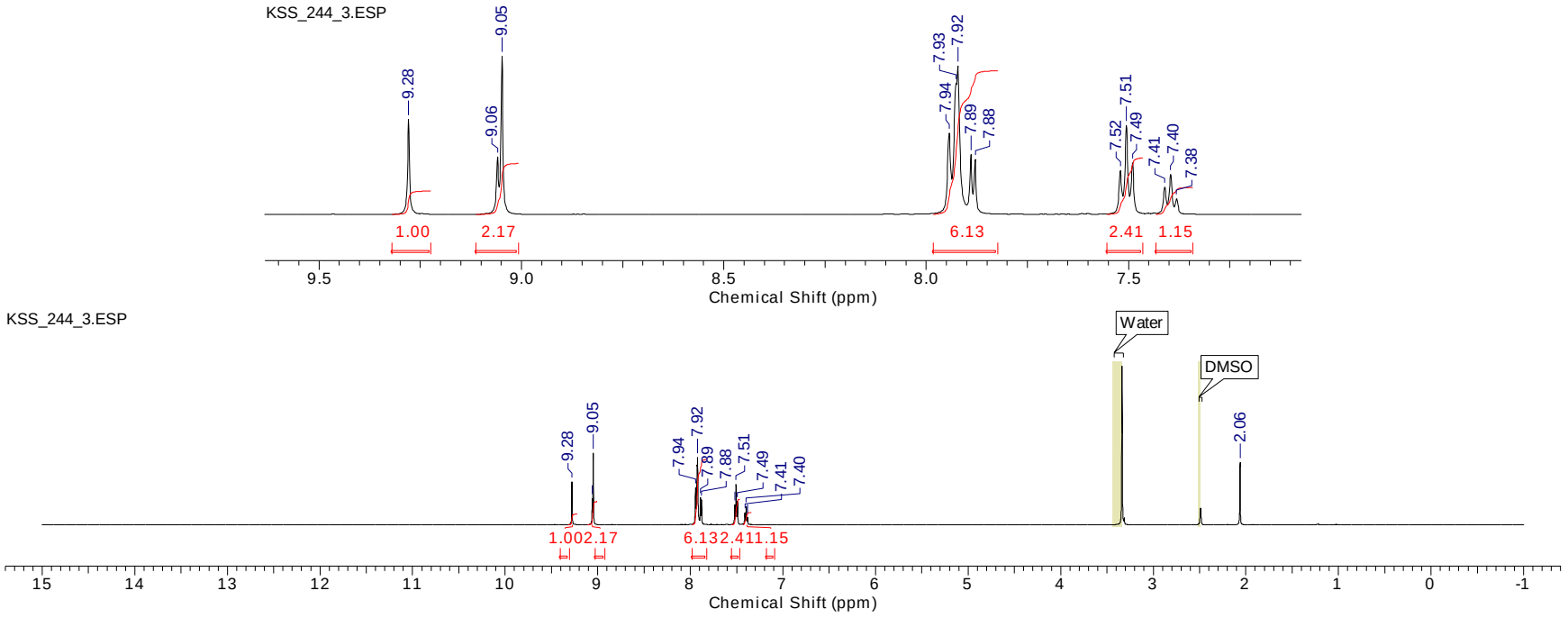
No.	(ppm)	(Hz)	Height
1	31.10	4693.3	0.1922
2	39.57	5970.8	0.1440
3	39.70	5991.7	0.4385
4	39.84	6012.6	0.8657

No.	(ppm)	(Hz)	Height
5	39.98	6033.5	1.0000
6	40.13	6055.6	0.8476
7	40.27	6076.5	0.4339
8	40.40	6097.4	0.1439

No.	(ppm)	(Hz)	Height
9	67.52	10189.7	0.0951
10	122.03	18416.3	0.0488
11	123.49	18636.4	0.0655
12	133.32	20119.7	0.0333

No.	(ppm)	(Hz)	Height
13	141.10	21292.7	0.0444
14	150.02	22639.6	0.0606
15	155.10	23405.5	0.0649
16	156.78	23659.6	0.0590

Spectrum S11. ^{1}H-NMR of compound 8 (500 MHz, DMSO-d_6).



No.	(ppm)	(Hz)	Height
1	2.06	1030.5	0.3930
2	7.38	3689.4	0.0449
3	7.40	3696.7	0.1140

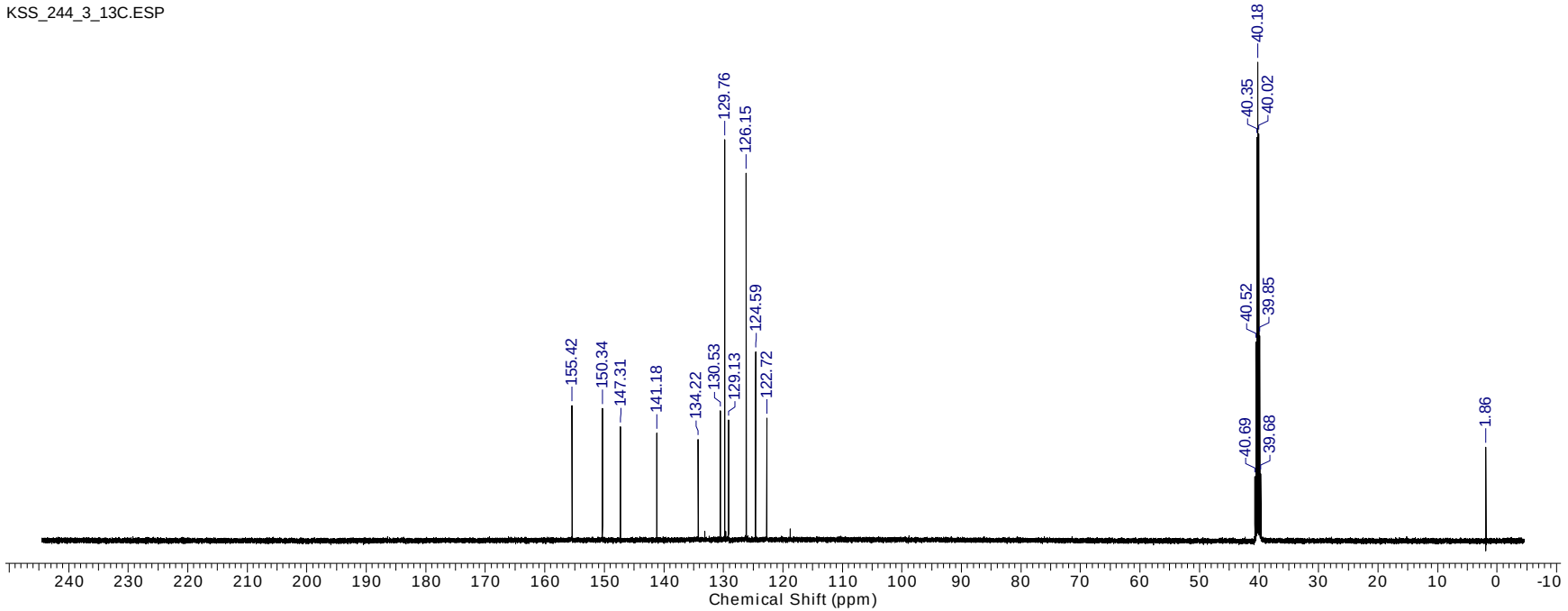
No.	(ppm)	(Hz)	Height
4	7.41	3704.0	0.0772
5	7.49	3743.6	0.1474
6	7.51	3751.4	0.2541

No.	(ppm)	(Hz)	Height
7	7.52	3758.7	0.1245
8	7.88	3937.9	0.1571
9	7.89	3943.3	0.1708

No.	(ppm)	(Hz)	Height
10	7.92	3959.4	0.4244
11	7.93	3961.9	0.3744
12	7.94	3970.2	0.2325

No.	(ppm)	(Hz)	Height
13	9.05	4522.5	0.4519
14	9.06	4527.8	0.1641
15	9.28	4637.7	0.2708

Spectrum S12. ^{13}C-NMR of compound **8** (125 MHz, DMSO- d_6).



No.	(ppm)	(Hz)	Height
1	1.86	233.9	0.1949
2	39.68	4987.8	0.1389
3	39.85	5008.8	0.4281
4	40.02	5029.8	0.8500

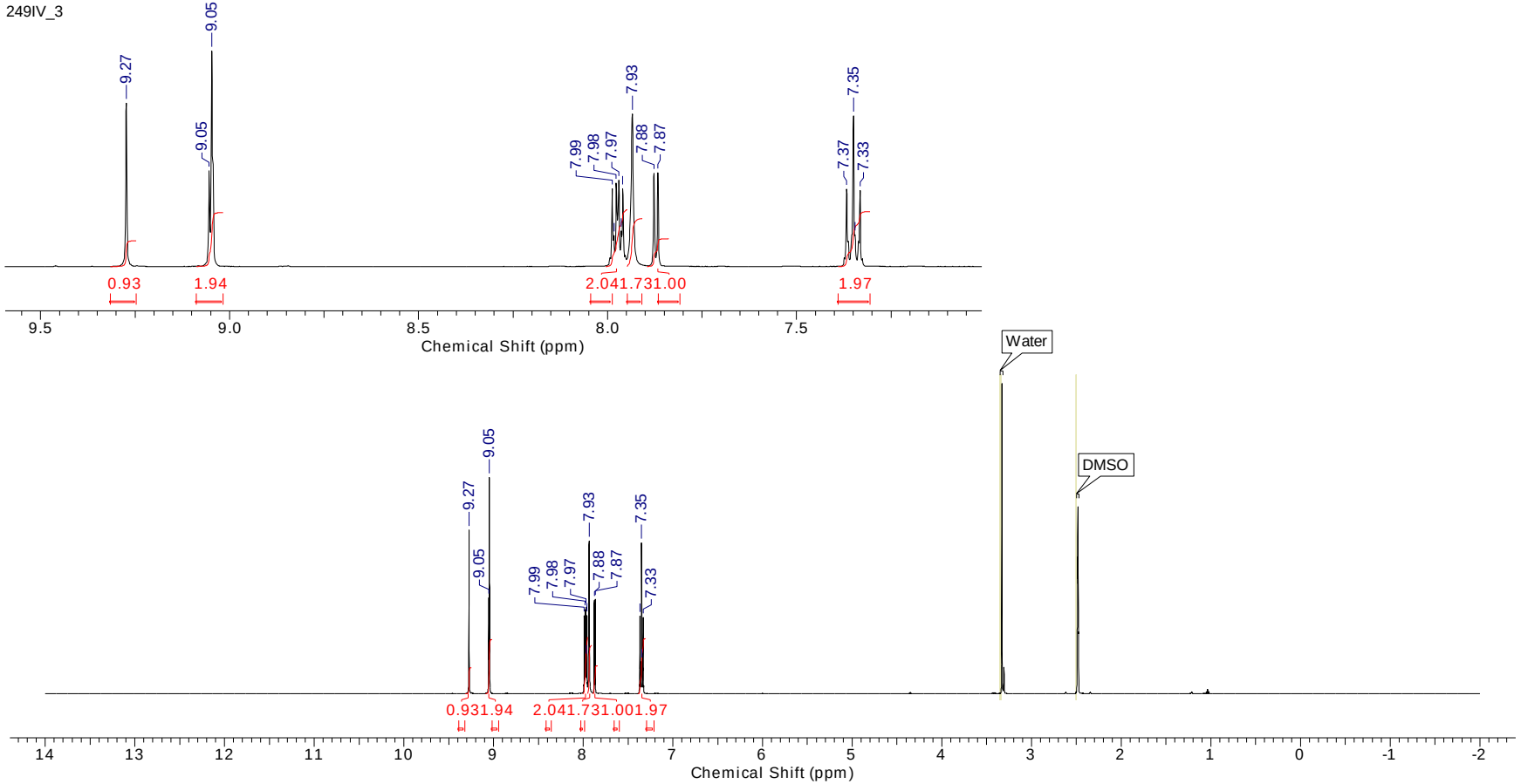
No.	(ppm)	(Hz)	Height
5	40.18	5050.8	1.0000
6	40.35	5071.9	0.8432
7	40.52	5092.9	0.4148
8	40.69	5113.9	0.1330

No.	(ppm)	(Hz)	Height
9	122.72	15425.5	0.2553
10	124.59	15660.5	0.3944
11	126.15	15856.3	0.7687
12	129.13	16230.8	0.2511

No.	(ppm)	(Hz)	Height
13	129.76	16309.6	0.8385
14	130.53	16407.0	0.2712
15	134.22	16870.7	0.2107
16	141.18	17745.7	0.2237

No.	(ppm)	(Hz)	Height
17	147.31	18516.0	0.2377
18	150.34	18896.2	0.2761
19	155.42	19534.7	0.2824

Spectrum S13. ^{1}H-NMR of compound **9** (500 MHz, DMSO-d_6).



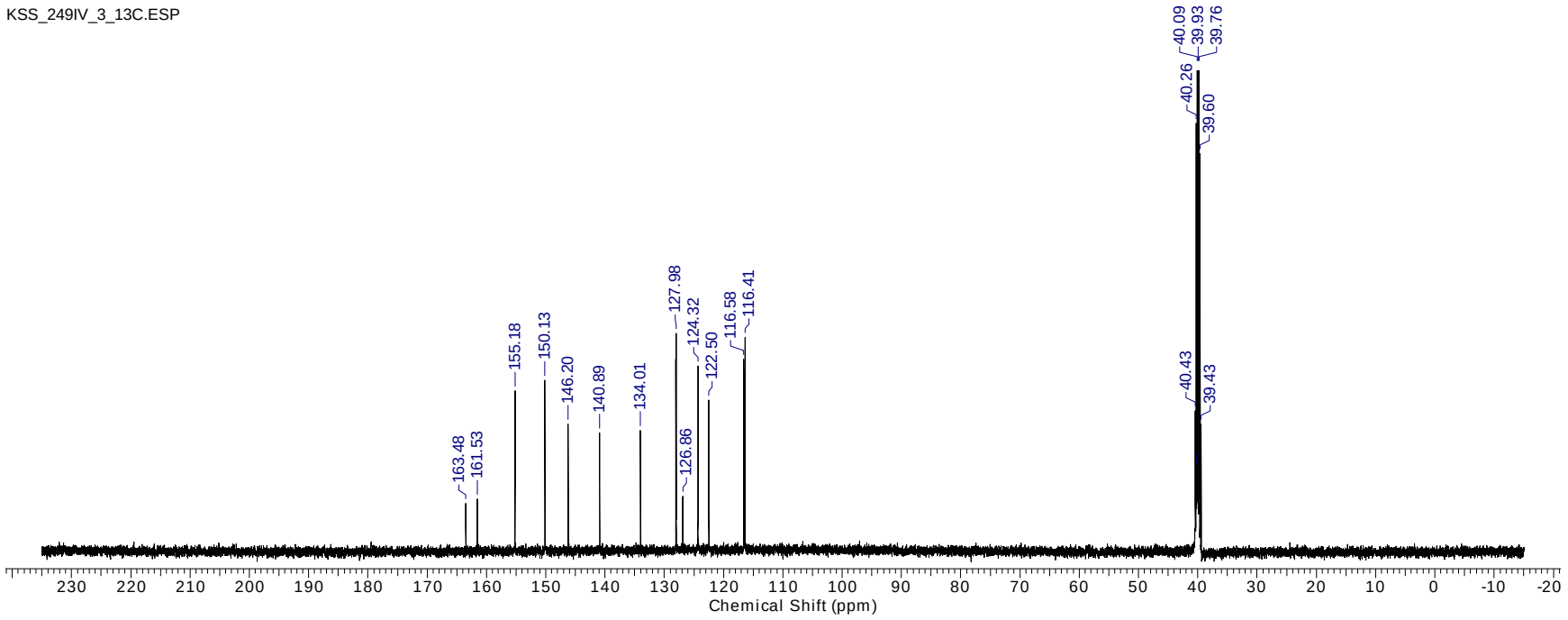
No.	(ppm)	(Hz)	Height
1	7.33	3664.1	0.2461
2	7.35	3671.0	0.1026
3	7.35	3672.9	0.4859
4	7.37	3682.2	0.2498

No.	(ppm)	(Hz)	Height
5	7.87	3931.6	0.3037
6	7.88	3936.5	0.3015
7	7.93	3965.3	0.4923
8	7.96	3978.0	0.2515

No.	(ppm)	(Hz)	Height
9	7.96	3979.9	0.1155
10	7.97	3983.3	0.2788
11	7.98	3986.7	0.2704
12	7.98	3989.7	0.1001

No.	(ppm)	(Hz)	Height
13	7.99	3992.1	0.2518
14	9.05	4521.7	0.6962
15	9.05	4525.1	0.3093
16	9.27	4634.4	0.5271

Spectrum S14. ^{13}C-NMR of compound **9** (125 MHz, DMSO- d_6).



No.	(ppm)	(Hz)	Height
1	39.43	4955.6	0.1305
2	39.60	4976.7	0.4087
3	39.76	4996.9	0.8341
4	39.93	5018.0	1.0000
5	40.02	5029.5	0.0753

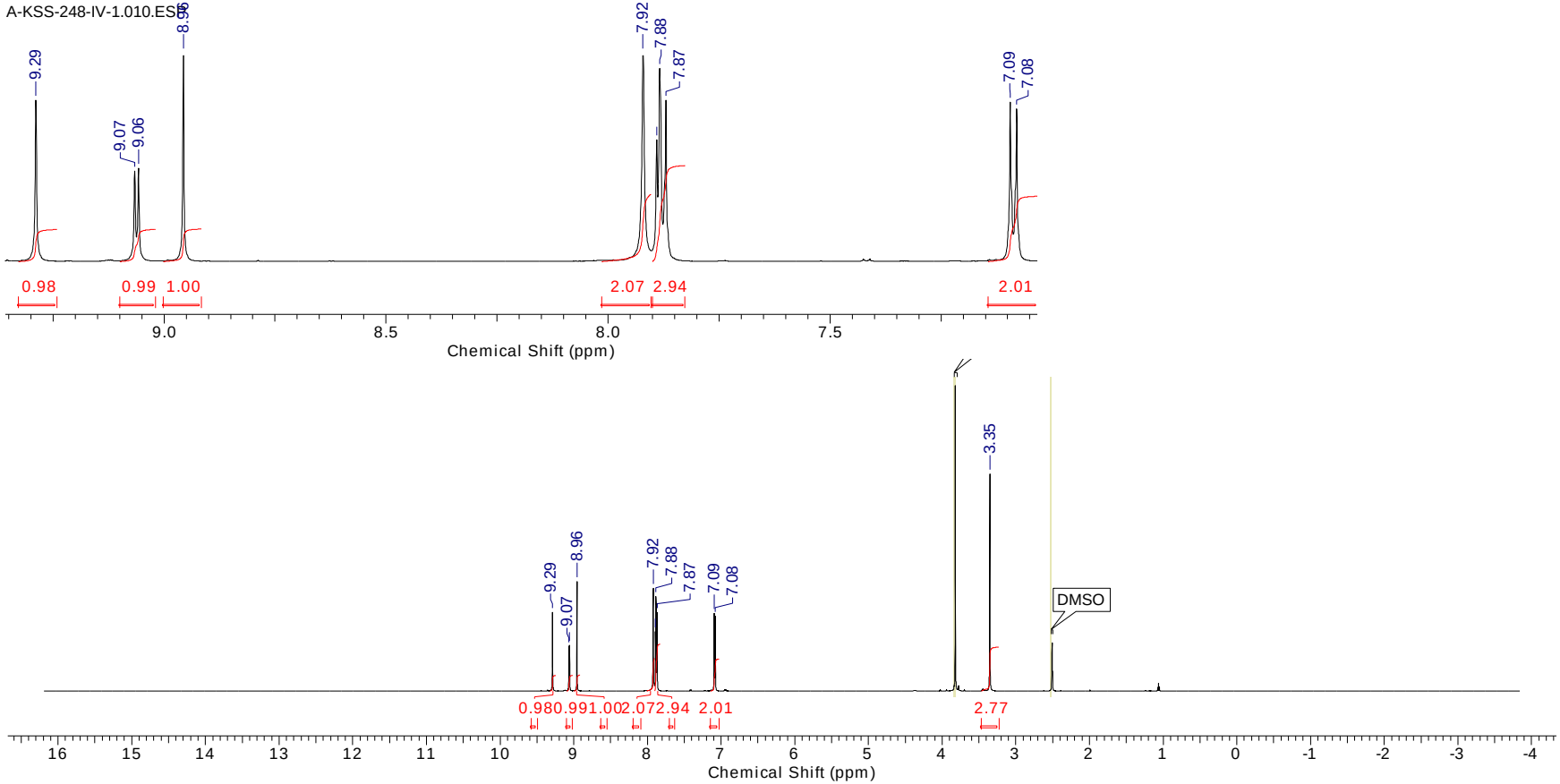
No.	(ppm)	(Hz)	Height
6	40.09	5039.1	0.8683
7	40.19	5050.6	0.0859
8	40.26	5060.2	0.4398
9	40.35	5071.7	0.0514
10	40.43	5081.3	0.1441

No.	(ppm)	(Hz)	Height
11	116.41	14630.5	0.2200
12	116.58	14652.5	0.1972
13	122.50	15396.7	0.1554
14	124.32	15624.9	0.1902
15	126.86	15944.2	0.0564

No.	(ppm)	(Hz)	Height
16	126.89	15948.1	0.0557
17	127.98	16084.2	0.2236
18	128.04	16092.9	0.1973
19	134.01	16842.8	0.1241
20	140.89	17707.7	0.1219

No.	(ppm)	(Hz)	Height
21	146.20	18375.2	0.1308
22	150.13	18869.0	0.1758
23	155.18	19502.9	0.1647
24	161.53	20301.7	0.0536
25	163.48	20547.2	0.0492

Spectrum S15. ^{1}H-NMR of compound **10** (600 MHz, DMSO-d_6).



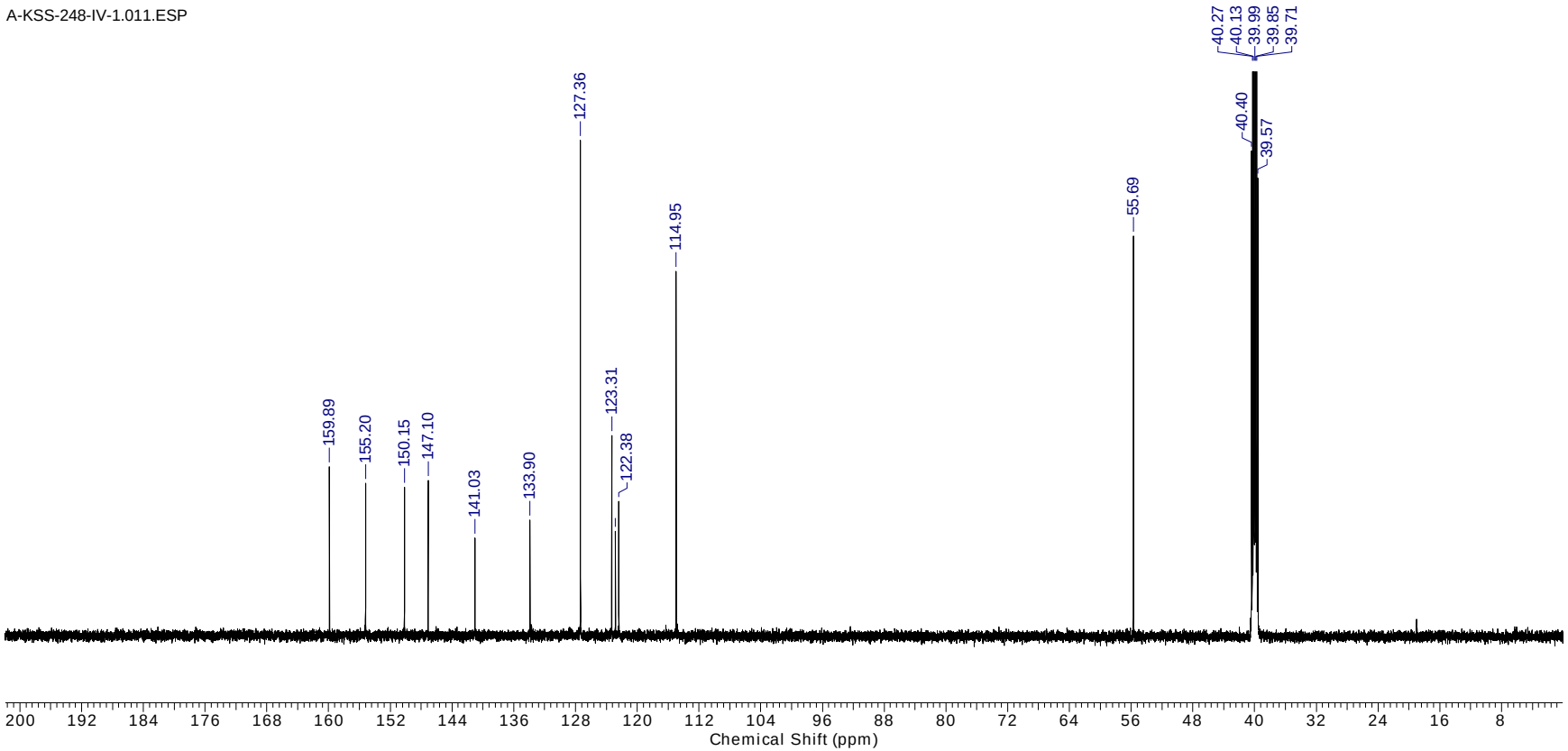
No.	(ppm)	(Hz)	Height
1	3.35	2012.5	0.7115
2	7.08	4248.9	0.2448
3	7.09	4257.7	0.2552

No.	(ppm)	(Hz)	Height
4	7.87	4722.8	0.2582
5	7.88	4731.6	0.3096
6	7.89	4735.6	0.1950

No.	(ppm)	(Hz)	Height
7	7.92	4754.0	0.3369
8	8.96	5375.3	0.3589
9	9.06	5435.9	0.1498

No.	(ppm)	(Hz)	Height
10	9.07	5441.0	0.1451
11	9.29	5574.5	0.2584

Spectrum S16. ^{13}C-NMR of compound **10** (150 MHz, DMSO- d_6).



No.	(ppm)	(Hz)	Height
1	39.57	5970.8	0.1351
2	39.71	5992.8	0.4112
3	39.85	6013.7	0.8363
4	39.99	6034.6	1.0000

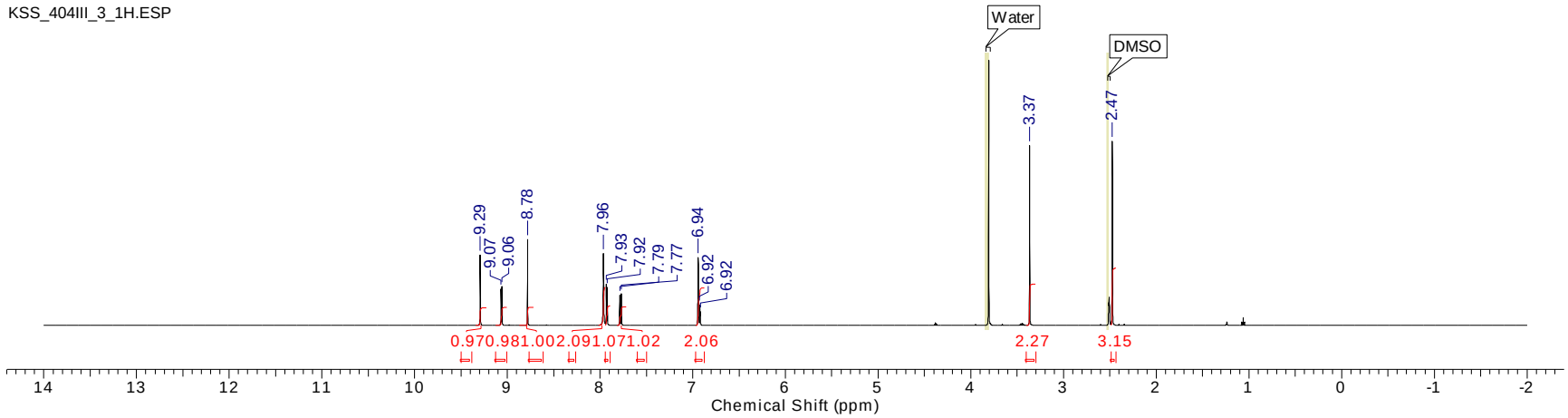
No.	(ppm)	(Hz)	Height
5	40.13	6055.6	0.8618
6	40.27	6076.5	0.4346
7	40.40	6097.4	0.1431
8	55.69	8404.9	0.1180

No.	(ppm)	(Hz)	Height
9	114.95	17346.7	0.1077
10	122.38	18469.1	0.0397
11	122.82	18535.1	0.0309
12	123.31	18608.8	0.0592

No.	(ppm)	(Hz)	Height
13	127.36	19219.6	0.1462
14	133.90	20206.6	0.0342
15	141.03	21282.8	0.0288
16	147.10	22198.3	0.0458

No.	(ppm)	(Hz)	Height
17	150.15	22659.4	0.0438
18	155.20	23420.9	0.0449
19	159.89	24128.4	0.0500

Spectrum S17. ^{1}H-NMR of compound **11** (500 MHz, DMSO-d_6).



No.	(ppm)	(Hz)	Height
1	2.47	1236.4	0.6948
2	3.37	1682.0	0.6781
3	6.92	3457.8	0.0518

No.	(ppm)	(Hz)	Height
4	6.92	3460.7	0.0768
5	6.94	3469.0	0.2560
6	7.77	3883.4	0.1182

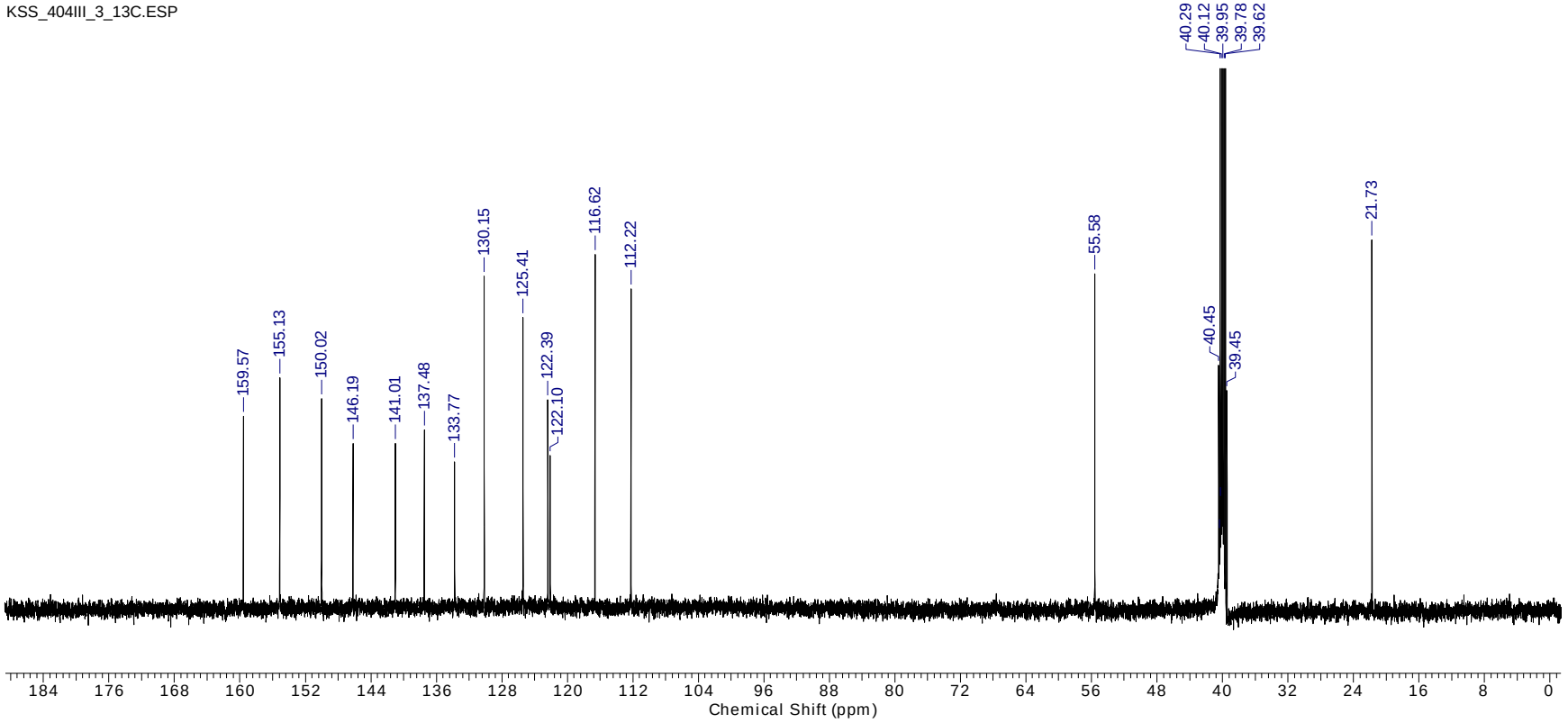
No.	(ppm)	(Hz)	Height
7	7.79	3891.7	0.1131
8	7.92	3959.1	0.1419
9	7.93	3964.0	0.1547

No.	(ppm)	(Hz)	Height
10	7.96	3980.1	0.2713
11	8.78	4389.1	0.3235
12	9.06	4526.8	0.1466

No.	(ppm)	(Hz)	Height
13	9.07	4531.6	0.1370
14	9.29	4644.4	0.2646

Spectrum S18. ^{13}C-NMR of compound **11** (125 MHz, DMSO- d_6).

KSS_404III_3_13C.ESP



No.	(ppm)	(Hz)	Height
1	21.73	2731.2	0.2165
2	39.45	4958.9	0.1280
3	39.62	4980.0	0.4144
4	39.78	5000.1	0.8256
5	39.95	5021.2	1.0000

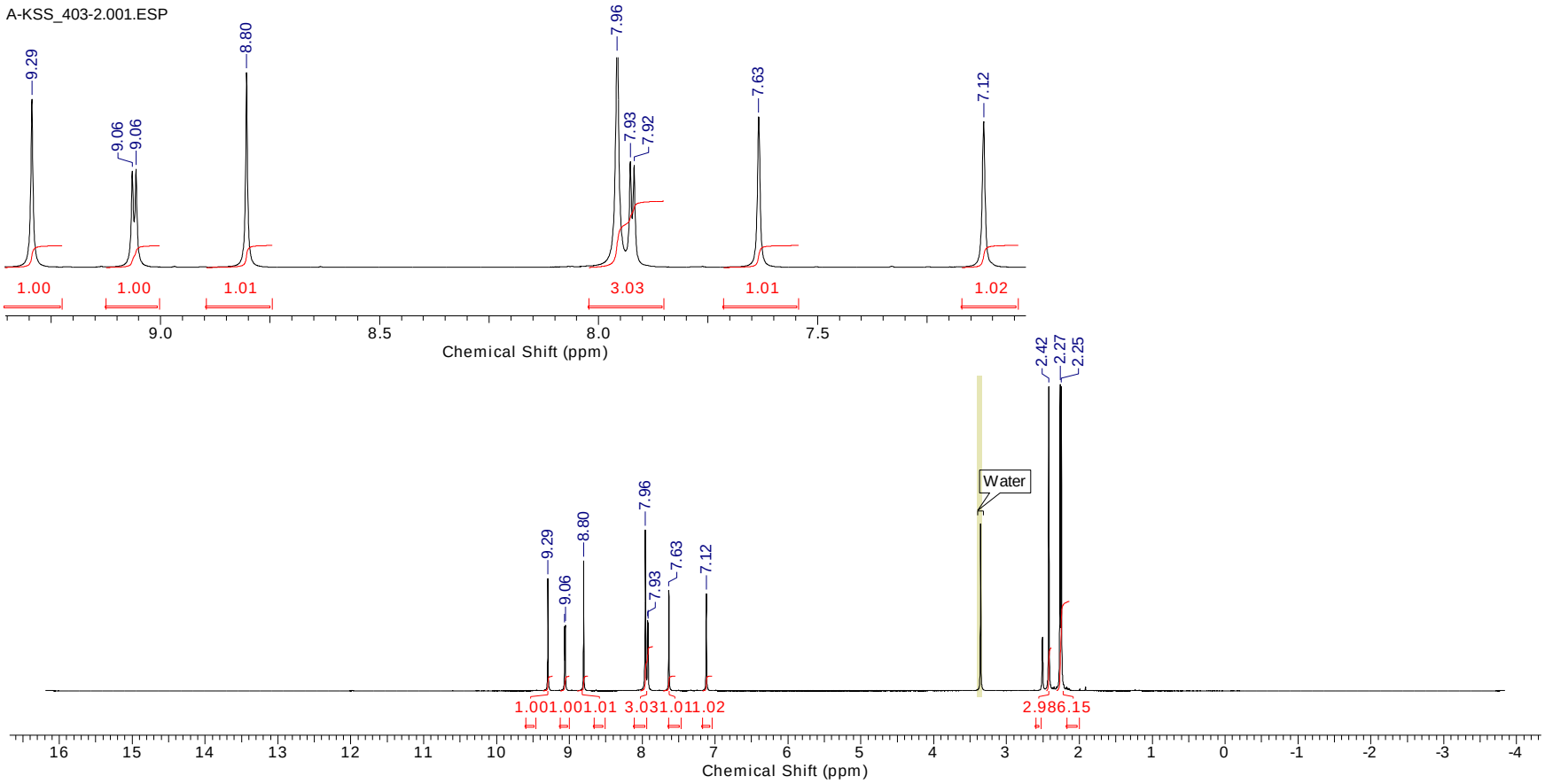
No.	(ppm)	(Hz)	Height
6	40.12	5042.3	0.8669
7	40.21	5053.8	0.0638
8	40.29	5063.4	0.4452
9	40.38	5074.9	0.0449
10	40.45	5084.5	0.1430

No.	(ppm)	(Hz)	Height
11	55.58	6986.1	0.1964
12	112.22	14104.3	0.1875
13	116.62	14657.7	0.2079
14	122.10	15346.2	0.0901
15	122.39	15382.6	0.1227

No.	(ppm)	(Hz)	Height
16	125.41	15762.4	0.1708
17	130.15	16357.9	0.1951
18	133.77	16812.4	0.0863
19	137.48	17279.4	0.1051
20	141.01	17723.4	0.0971

No.	(ppm)	(Hz)	Height
21	146.19	18373.6	0.0970
22	150.02	18855.0	0.1233
23	155.13	19497.5	0.1354
24	159.57	20055.6	0.1132

Spectrum S19. ^{1}H-NMR of compound **12** (600 MHz, DMSO-d_6).



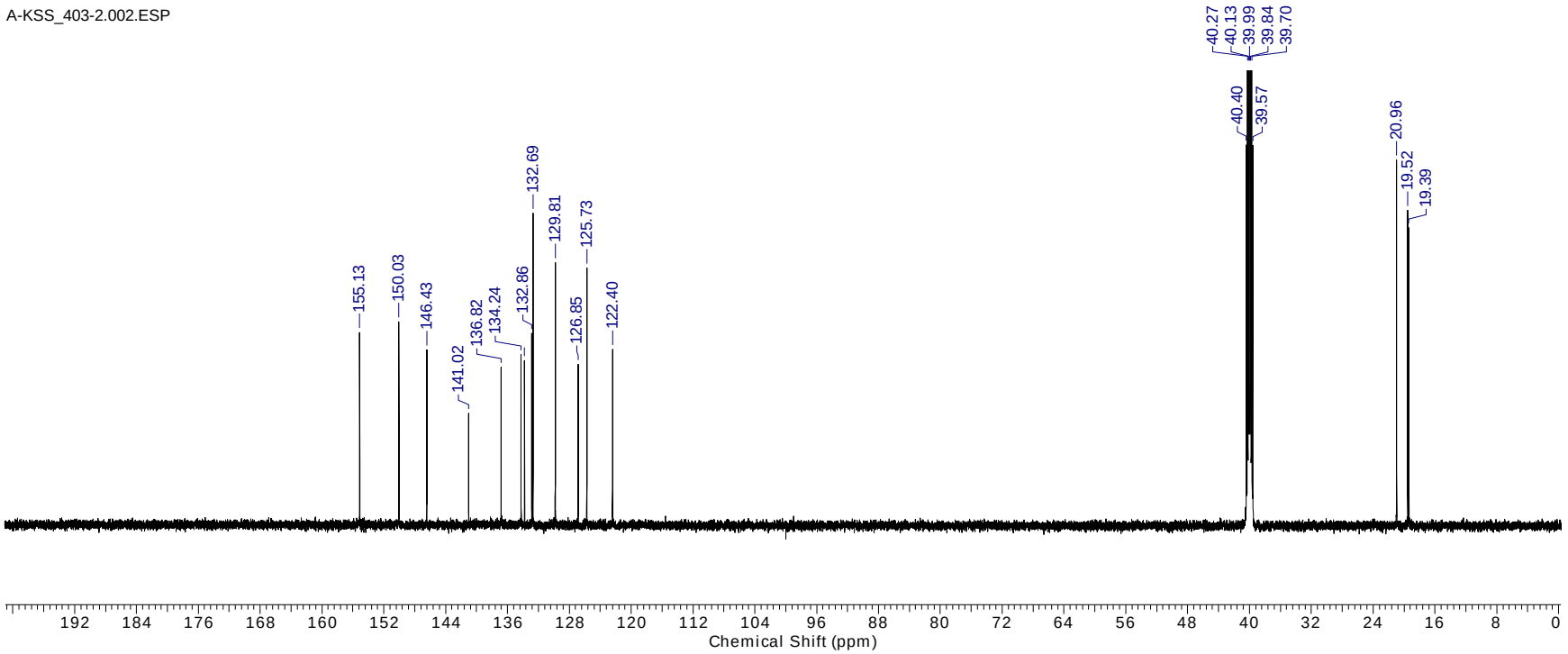
No.	(ppm)	(Hz)	Height
1	2.25	1349.0	0.9919
2	2.27	1359.6	1.0000
3	2.42	1452.1	0.9916

No.	(ppm)	(Hz)	Height
4	7.12	4273.5	0.3172
5	7.63	4582.0	0.3274
6	7.92	4752.5	0.2223

No.	(ppm)	(Hz)	Height
7	7.93	4757.7	0.2304
8	7.96	4775.6	0.5252
9	8.80	5283.6	0.4242

No.	(ppm)	(Hz)	Height
10	9.06	5435.1	0.2137
11	9.06	5440.3	0.2097
12	9.29	5577.8	0.3657

Spectrum S20. ^{13}C-NMR of compound **12** (150 MHz, DMSO- d_6).



No.	(ppm)	(Hz)	Height
1	19.39	2926.0	0.1143
2	19.52	2945.8	0.1210
3	20.96	3163.7	0.1404
4	39.57	5970.8	0.1460
5	39.70	5991.7	0.4408

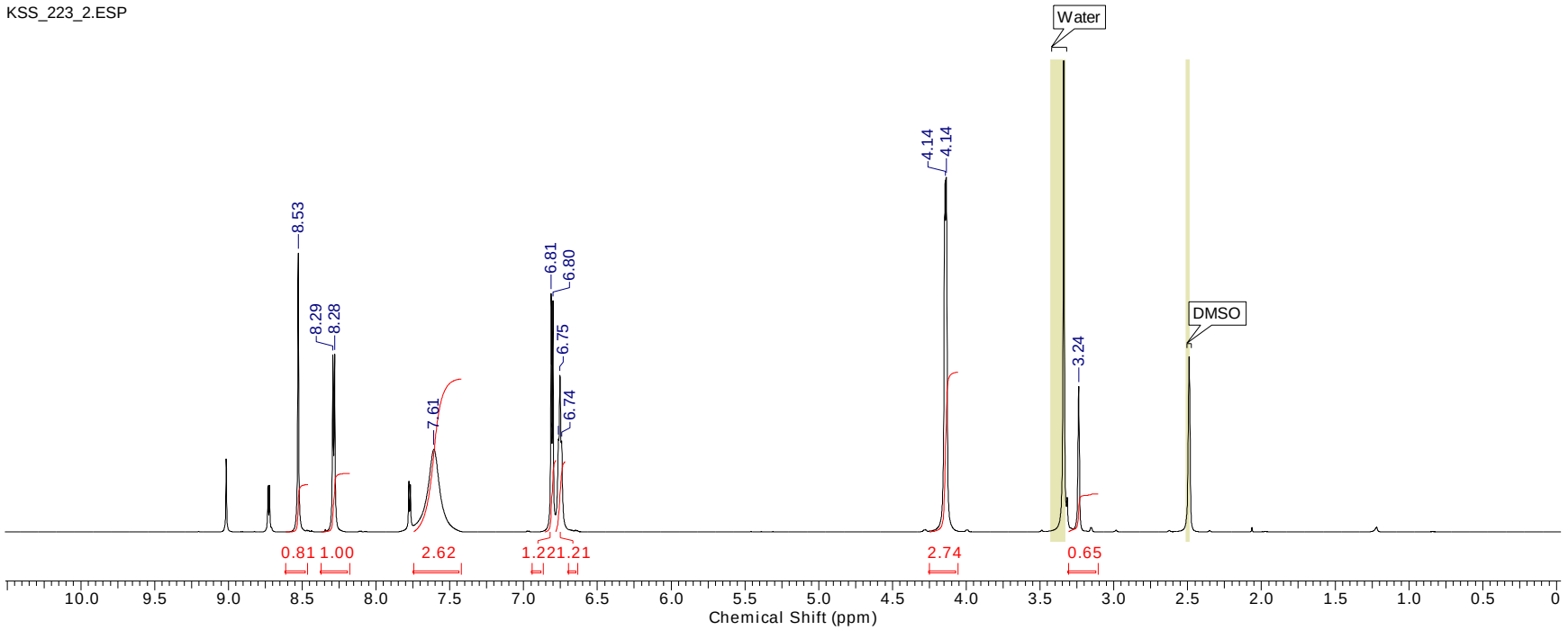
No.	(ppm)	(Hz)	Height
6	39.84	6012.6	0.8655
7	39.99	6034.6	1.0000
8	40.13	6055.6	0.8674
9	40.27	6076.5	0.4431
10	40.40	6097.4	0.1461

No.	(ppm)	(Hz)	Height
11	122.40	18471.3	0.0676
12	125.73	18974.2	0.0989
13	126.85	19142.5	0.0617
14	129.81	19589.3	0.1008
15	132.69	20023.9	0.1199

No.	(ppm)	(Hz)	Height
16	132.86	20049.3	0.0737
17	133.79	20190.1	0.0633
18	134.24	20258.3	0.0655
19	136.82	20647.9	0.0607
20	141.02	21281.7	0.0430

No.	(ppm)	(Hz)	Height
21	146.43	22097.1	0.0674
22	150.03	22641.8	0.0782
23	155.13	23411.0	0.0741

Spectrum S21. ^{1}H-NMR of compound **13** (500 MHz, DMSO-d_6).



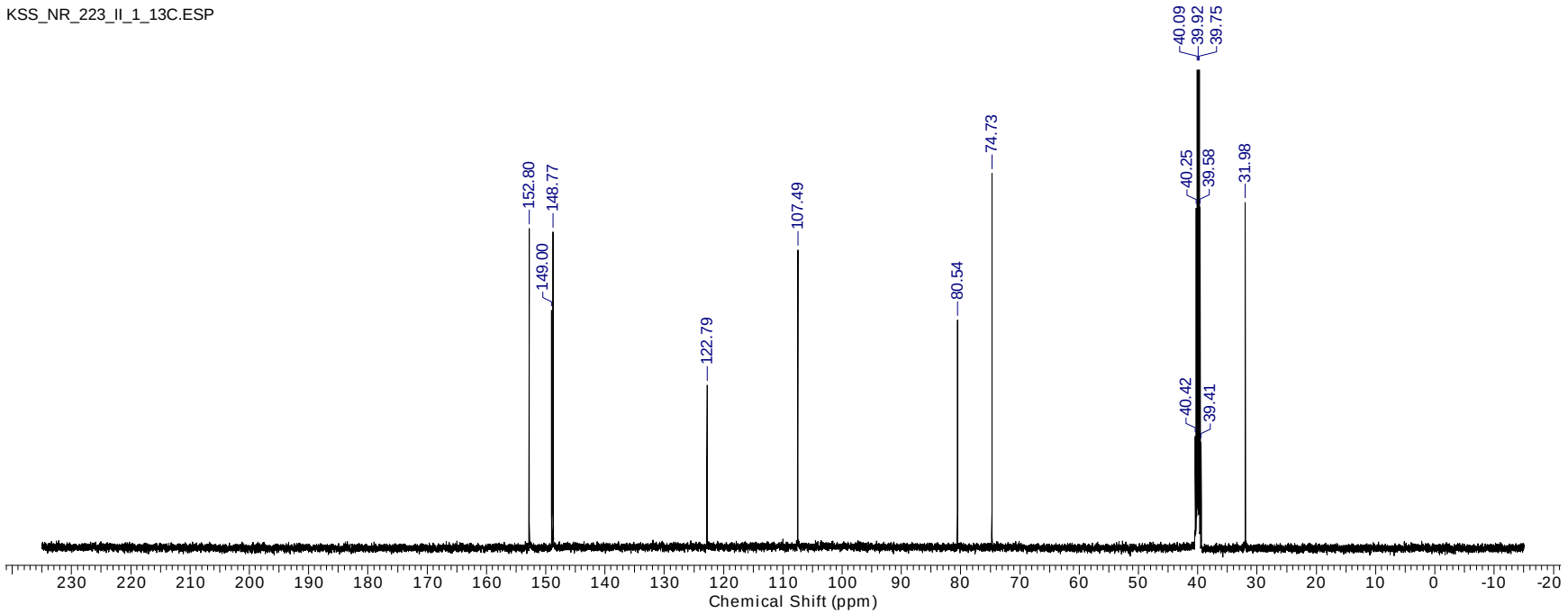
No.	(ppm)	(Hz)	Height
1	3.24	1618.5	0.2194
2	4.14	2067.2	0.5357

No.	(ppm)	(Hz)	Height
3	4.14	2070.6	0.5308
4	6.74	3370.0	0.1377

No.	(ppm)	(Hz)	Height
5	6.75	3375.4	0.2365
6	6.76	3380.3	0.1407

No.	(ppm)	(Hz)	Height
7	6.80	3399.3	0.3486
8	6.81	3405.2	0.3600

Spectrum S22. ^{13}C-NMR of compound **13** (125 MHz, DMSO-d_6).



No.	(ppm)	(Hz)	Height
1	31.98	4019.7	0.4285
2	39.41	4953.7	0.1306
3	39.58	4974.8	0.4217

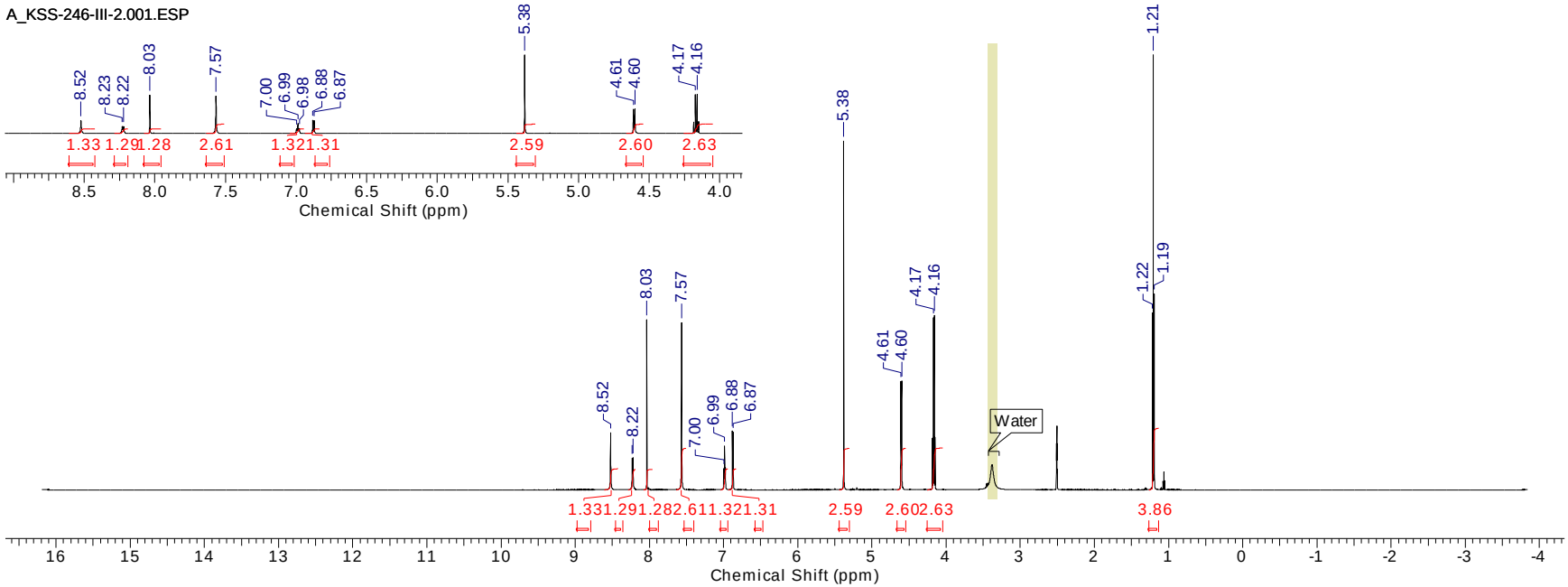
No.	(ppm)	(Hz)	Height
4	39.75	4995.9	0.8428
5	39.92	5017.0	1.0000
6	40.09	5038.1	0.8466

No.	(ppm)	(Hz)	Height
7	40.25	5059.2	0.4211
8	40.42	5080.3	0.1378
9	74.73	9392.7	0.4644

No.	(ppm)	(Hz)	Height
10	80.54	10122.4	0.2824
11	107.49	13509.5	0.3699
12	122.79	15432.1	0.2015

No.	(ppm)	(Hz)	Height
13	148.77	18697.4	0.3919
14	149.00	18726.1	0.2941
15	152.80	19203.7	0.3960

Spectrum S23. ^{1}H-NMR of compound **15** (500 MHz, DMSO-d_6).



No.	(ppm)	(Hz)	Height
1	1.19	716.3	0.4509
2	1.21	723.2	1.0000
3	1.22	730.6	0.4073
4	4.16	2496.3	0.4016

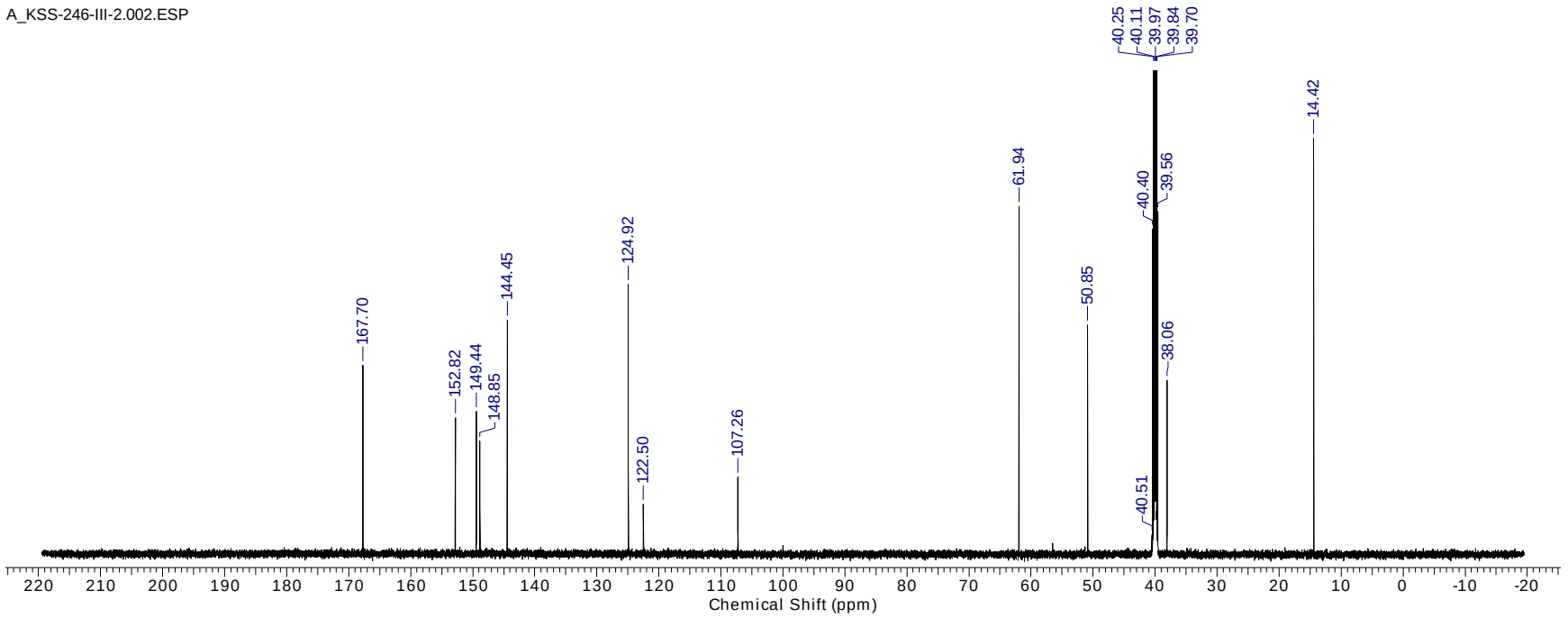
No.	(ppm)	(Hz)	Height
5	4.17	2503.3	0.3959
6	4.60	2760.1	0.2509
7	4.61	2765.9	0.2501
8	5.38	3228.8	0.8022

No.	(ppm)	(Hz)	Height
9	6.87	4123.5	0.1331
10	6.88	4129.3	0.1354
11	6.98	4186.9	0.0521
12	6.99	4192.8	0.1012

No.	(ppm)	(Hz)	Height
13	7.00	4198.3	0.0487
14	7.57	4540.9	0.3847
15	8.03	4822.2	0.3913
16	8.22	4933.7	0.0744

No.	(ppm)	(Hz)	Height
17	8.23	4939.6	0.0730
18	8.52	5114.9	0.1316

Spectrum S24. ^{13}C-NMR of compound **15** (125 MHz, DMSO- d_6).



No.	(ppm)	(Hz)	Height
1	14.42	2176.7	0.1707
2	38.06	5744.1	0.0712
3	39.56	5969.7	0.1406
4	39.70	5990.6	0.4345

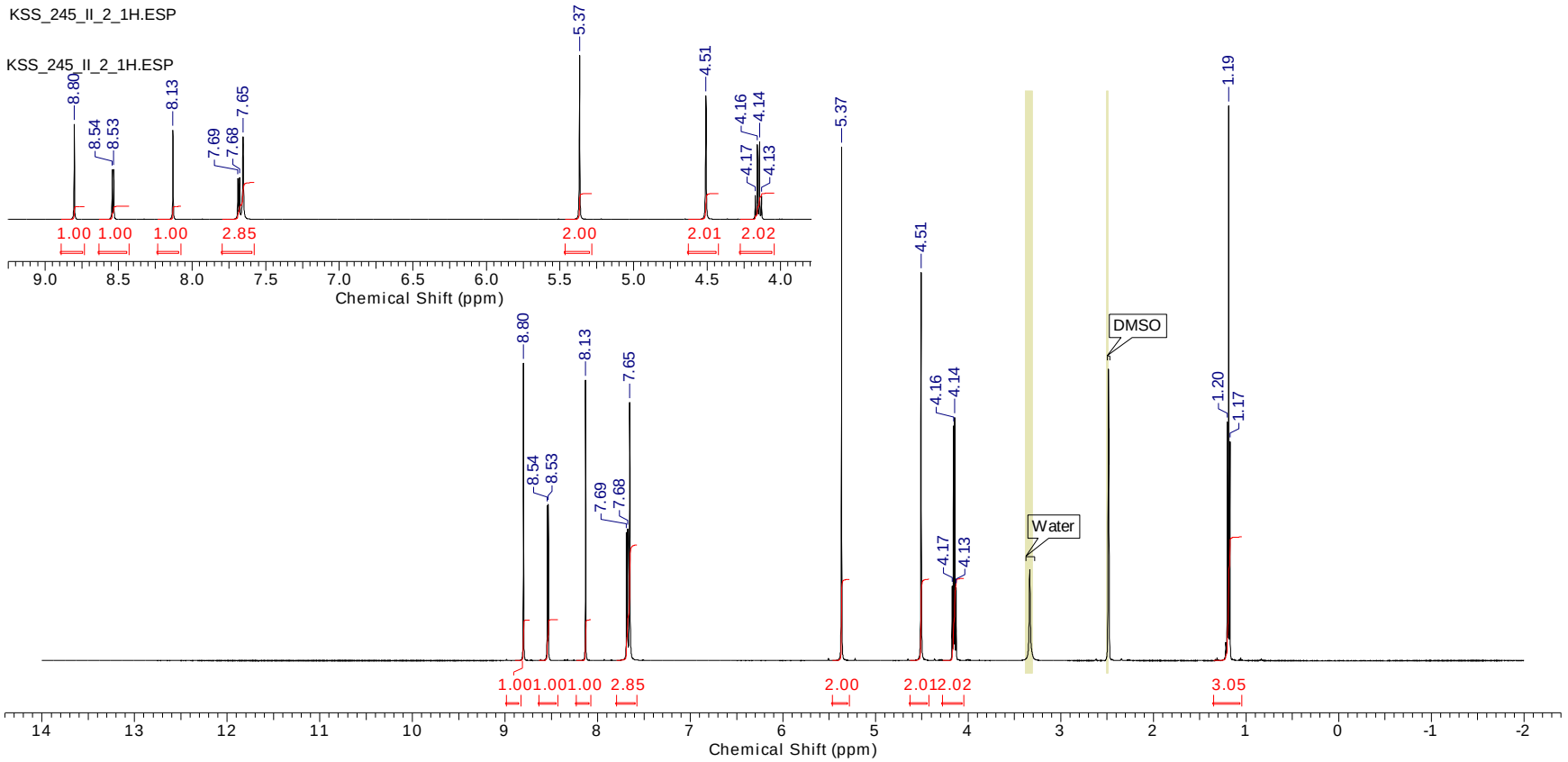
No.	(ppm)	(Hz)	Height
5	39.84	6011.5	0.8613
6	39.97	6032.4	1.0000
7	40.11	6053.4	0.8360
8	40.25	6074.3	0.4097

No.	(ppm)	(Hz)	Height
9	40.40	6096.3	0.1334
10	40.51	6113.9	0.0080
11	50.85	7674.2	0.0941
12	61.94	9346.8	0.1428

No.	(ppm)	(Hz)	Height
13	107.26	16186.9	0.0315
14	122.50	18486.7	0.0204
15	124.92	18852.0	0.1105
16	144.45	21798.9	0.0961

No.	(ppm)	(Hz)	Height
17	148.85	22463.5	0.0462
18	149.44	22551.6	0.0586
19	152.82	23062.1	0.0560
20	167.70	25306.9	0.0774

Spectrum S25. ^{1}H-NMR of compound **16** (500 MHz, DMSO-d_6).



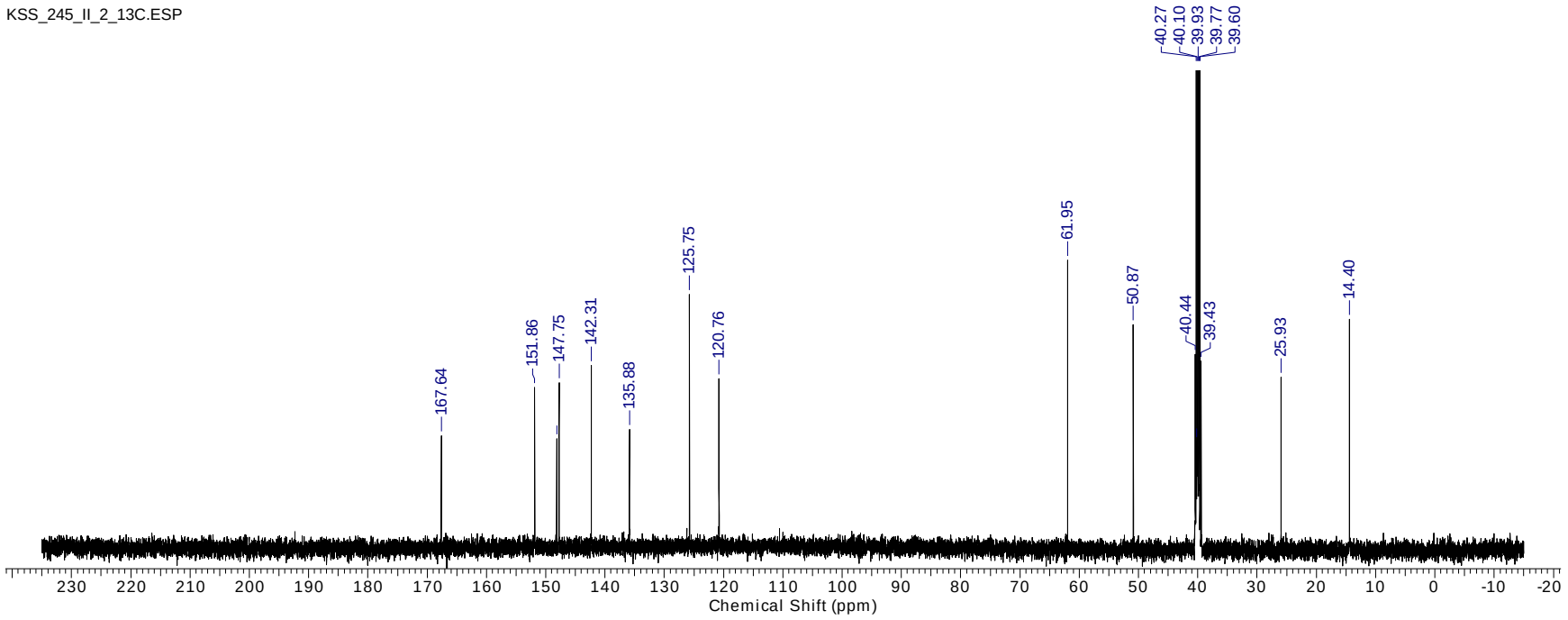
No.	(ppm)	(Hz)	Height
1	1.17	586.1	0.3946
2	1.19	593.5	1.0000
3	1.20	600.8	0.4296
4	4.13	2064.2	0.1315

No.	(ppm)	(Hz)	Height
5	4.14	2071.0	0.4375
6	4.16	2078.3	0.4226
7	4.17	2085.1	0.1338
8	4.51	2253.1	0.6990

No.	(ppm)	(Hz)	Height
9	5.37	2682.1	0.9256
10	7.65	3825.3	0.4653
11	7.68	3837.0	0.2365
12	7.69	3842.9	0.2311

No.	(ppm)	(Hz)	Height
13	8.13	4063.5	0.5055
14	8.53	4264.6	0.2818
15	8.54	4270.0	0.2789
16	8.80	4398.3	0.5361

Spectrum S26. ^{13}C-NMR of compound **16** (125 MHz, DMSO- d_6).



No.	(ppm)	(Hz)	Height
1	14.40	1810.3	0.1647
2	25.93	3259.3	0.1229
3	39.43	4955.6	0.1347
4	39.60	4976.7	0.4190
5	39.77	4997.8	0.8479

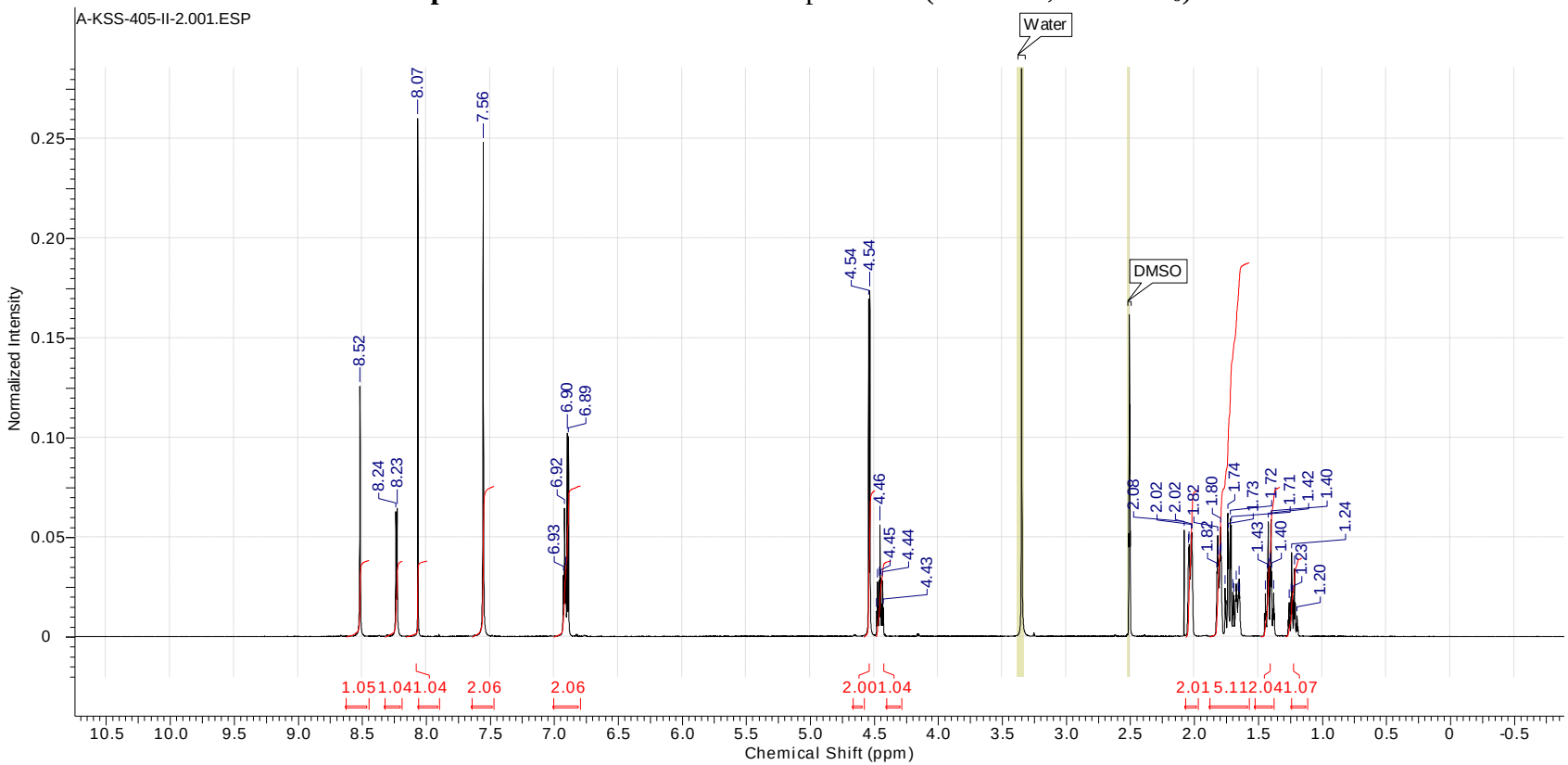
No.	(ppm)	(Hz)	Height
6	39.93	5018.9	1.0000
7	40.10	5040.0	0.8469
8	40.19	5051.5	0.0768
9	40.27	5061.1	0.4221
10	40.35	5071.7	0.0505

No.	(ppm)	(Hz)	Height
11	40.44	5082.2	0.1394
12	50.87	6394.1	0.1609
13	61.95	7786.5	0.2071
14	120.76	15178.0	0.1221
15	125.75	15804.2	0.1824

No.	(ppm)	(Hz)	Height
16	135.88	17077.7	0.0855
17	142.31	17886.1	0.1314
18	147.75	18569.8	0.1190
19	148.16	18620.6	0.0790
20	151.86	19085.7	0.1158

No.	(ppm)	(Hz)	Height
21	167.64	21068.8	0.0811

Spectrum S27. ^{1}H-NMR of compound **17** (500 MHz, DMSO-d_6).



No.	(ppm)	(Hz)	Height
1	1.20	718.8	0.0108
2	1.22	731.7	0.0344
3	1.23	740.5	0.0211
4	1.24	744.2	0.0423
5	1.25	747.8	0.0204
6	1.26	757.4	0.0174
7	1.38	828.9	0.0220
8	1.40	838.4	0.0328
9	1.40	841.7	0.0589
10	1.41	845.0	0.0355
11	1.42	851.3	0.0331

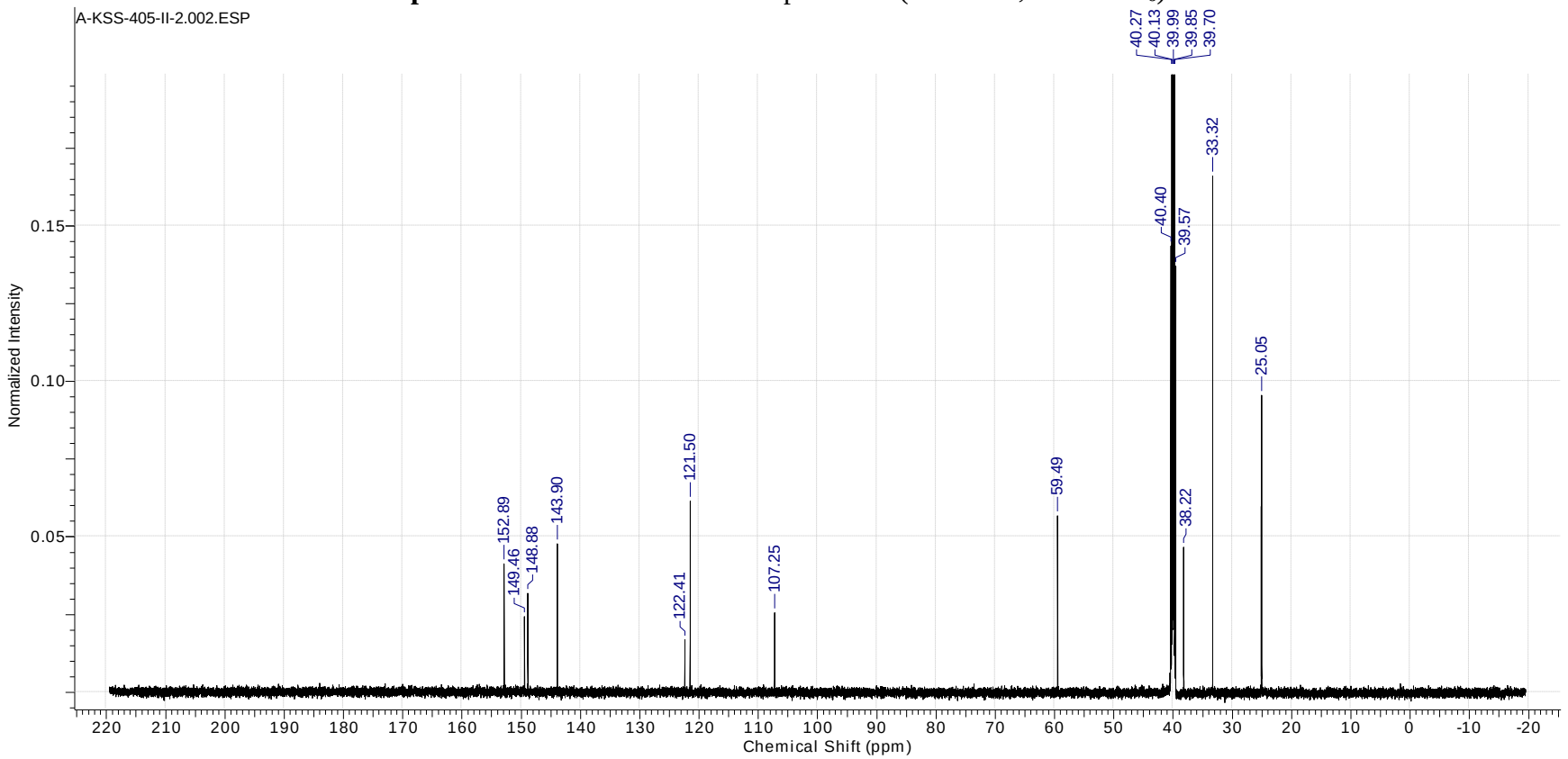
No.	(ppm)	(Hz)	Height
12	1.42	854.9	0.0578
13	1.43	858.2	0.0323
14	1.45	867.8	0.0219
15	1.65	988.1	0.0204
16	1.65	991.4	0.0291
17	1.66	994.7	0.0211
18	1.67	1004.6	0.0268
19	1.69	1016.0	0.0206
20	1.70	1019.6	0.0226
21	1.71	1028.4	0.0560
22	1.72	1032.1	0.0594

No.	(ppm)	(Hz)	Height
23	1.73	1040.5	0.0527
24	1.74	1044.2	0.0623
25	1.76	1056.7	0.0244
26	1.79	1074.6	0.0409
27	1.80	1077.9	0.0555
28	1.80	1080.9	0.0397
29	1.81	1088.2	0.0392
30	1.82	1091.5	0.0510
31	1.82	1094.8	0.0329
32	2.02	1212.6	0.0524
33	2.02	1215.1	0.0521

No.	(ppm)	(Hz)	Height
34	2.04	1224.7	0.0467
35	2.05	1227.6	0.0450
36	2.08	1249.2	0.0537
37	4.43	2658.8	0.0146
38	4.44	2662.5	0.0285
39	4.45	2670.6	0.0294
40	4.46	2674.2	0.0563
41	4.46	2678.3	0.0288
42	4.48	2686.0	0.0276
43	4.48	2690.0	0.0131
44	4.54	2721.9	0.1738

No.	(ppm)	(Hz)	Height
45	4.54	2727.4	0.1697
46	6.89	4134.8	0.1007
47	6.90	4141.1	0.1025
48	6.91	4147.7	0.0339
49	6.92	4153.5	0.0646
50	6.93	4159.0	0.0312
51	7.56	4535.0	0.2485
52	8.07	4840.9	0.2603
53	8.23	4938.1	0.0647
54	8.24	4944.0	0.0629
55	8.52	5112.7	0.1260

Spectrum S28. ^{13}C-NMR of compound **17** (125 MHz, DMSO- d_6).



No.	(ppm)	(Hz)	Height
1	25.05	3781.0	0.0956
2	25.13	3792.0	0.0598
3	33.32	5028.9	0.1660
4	38.22	5767.2	0.0467

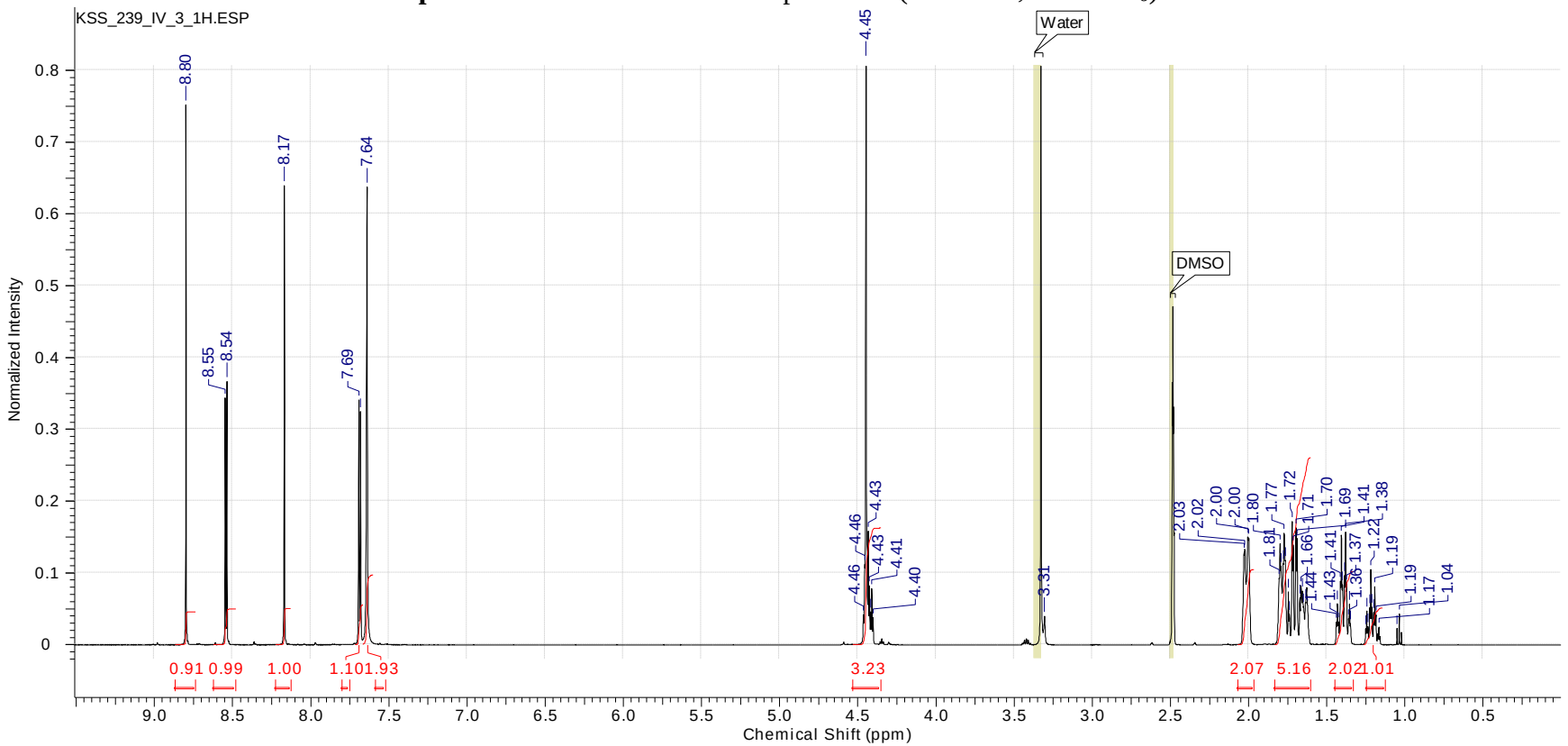
No.	(ppm)	(Hz)	Height
5	39.57	5970.8	0.1370
6	39.70	5991.7	0.4196
7	39.85	6013.7	0.8299
8	39.99	6034.6	1.0000

No.	(ppm)	(Hz)	Height
9	40.13	6055.6	0.8636
10	40.27	6076.5	0.4420
11	40.40	6097.4	0.1435
12	59.49	8977.1	0.0568

No.	(ppm)	(Hz)	Height
13	107.25	16184.7	0.0255
14	121.50	18335.9	0.0614
15	122.41	18472.4	0.0168
16	143.90	21715.3	0.0478

No.	(ppm)	(Hz)	Height
17	148.88	22466.8	0.0318
18	149.46	22554.9	0.0243
19	152.89	23073.1	0.0413

Spectrum S29. ^{1}H-NMR of compound **18** (500 MHz, DMSO-d_6).



No.	(ppm)	(Hz)	Height
1	1.04	517.8	0.0430
2	1.05	524.9	0.0223
3	1.17	583.2	0.0246
4	1.19	592.5	0.0413
5	1.19	595.8	0.0812
6	1.20	599.6	0.0450
7	1.21	605.1	0.0527
8	1.22	609.0	0.1046
9	1.23	612.3	0.0517
10	1.24	617.7	0.0256
11	1.24	621.6	0.0468
12	1.25	624.9	0.0224
13	1.35	673.8	0.0295

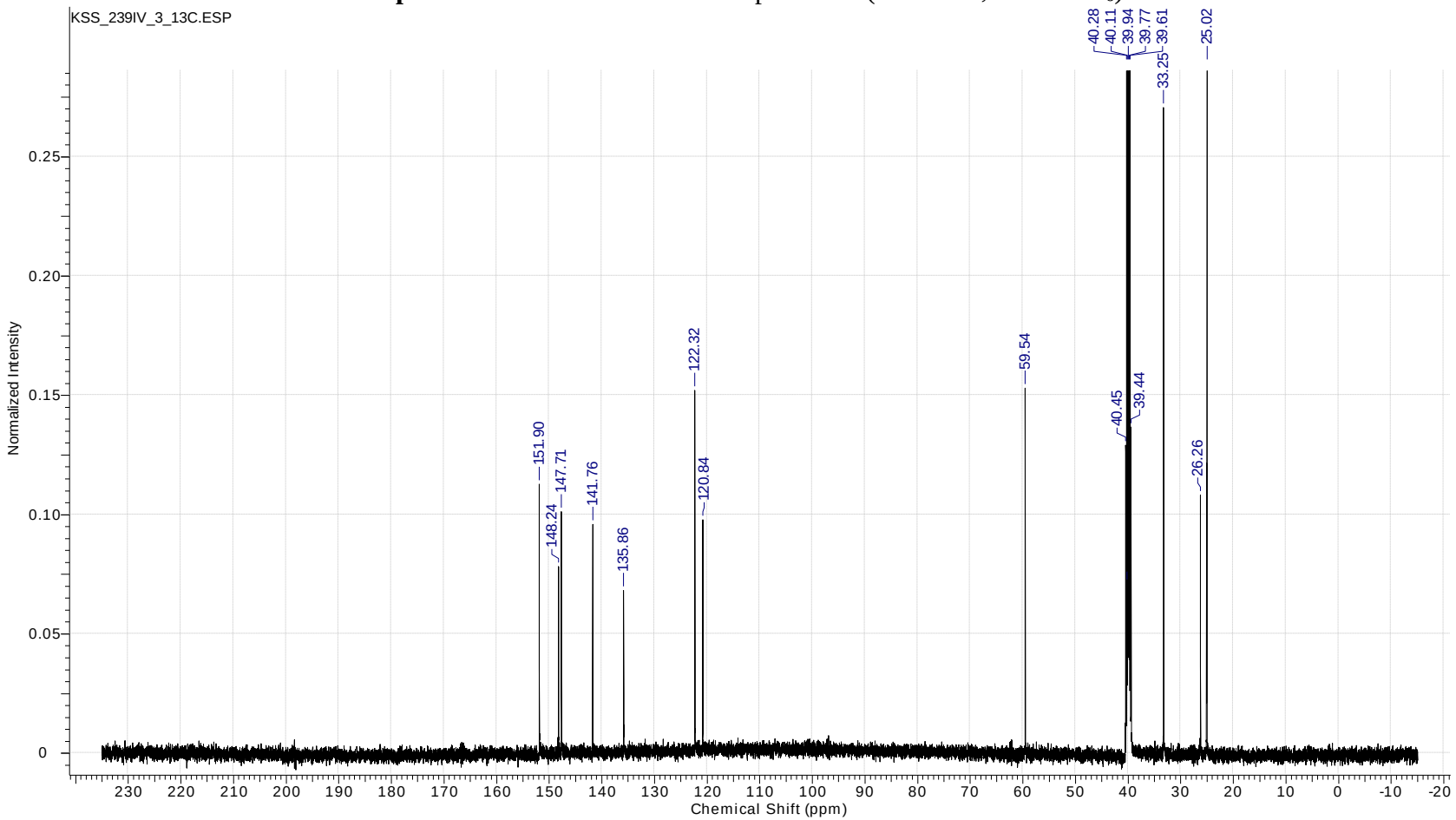
No.	(ppm)	(Hz)	Height
14	1.35	677.0	0.0564
15	1.36	680.3	0.0364
16	1.37	686.4	0.0851
17	1.38	689.7	0.1567
18	1.39	693.0	0.0963
19	1.40	699.6	0.0834
20	1.41	702.9	0.1528
21	1.41	706.1	0.0886
22	1.43	712.2	0.0320
23	1.43	715.5	0.0574
24	1.44	718.8	0.0317
25	1.63	813.8	0.0793
26	1.63	817.1	0.0594

No.	(ppm)	(Hz)	Height
27	1.65	823.7	0.0531
28	1.65	827.0	0.0746
29	1.66	831.9	0.0821
30	1.67	835.7	0.0653
31	1.69	844.5	0.1481
32	1.70	848.4	0.1625
33	1.71	856.6	0.1394
34	1.72	860.4	0.1718
35	1.74	868.7	0.0422
36	1.75	872.5	0.0732
37	1.77	882.4	0.1177
38	1.77	885.7	0.1551
39	1.78	888.4	0.1130

No.	(ppm)	(Hz)	Height
40	1.79	895.6	0.1090
41	1.80	898.9	0.1403
42	1.81	902.2	0.0925
43	2.00	999.4	0.1484
44	2.00	1001.6	0.1500
45	2.02	1011.4	0.1332
46	2.03	1014.2	0.1286
47	3.31	1652.2	0.0394
48	4.40	2200.2	0.0375
49	4.41	2204.1	0.0783
50	4.42	2207.9	0.0457
51	4.43	2211.8	0.0824
52	4.43	2215.6	0.1579

No.	(ppm)	(Hz)	Height
53	4.45	2223.3	1.0000
54	4.46	2227.1	0.1118
55	4.46	2231.0	0.0417
56	7.64	3818.4	0.6374
57	7.68	3839.3	0.3249
58	7.69	3844.8	0.3407
59	8.17	4082.5	0.6394
60	8.54	4266.5	0.3667
61	8.55	4272.0	0.3433
62	8.80	4397.2	0.7519

Spectrum S30. ^{13}C-NMR of compound **18** (125 MHz, DMSO- d_6).



No.	(ppm)	(Hz)	Height
1	25.02	3144.3	0.3088
2	25.09	3153.9	0.1216
3	26.26	3300.6	0.1081
4	33.25	4179.0	0.2706
5	39.44	4956.7	0.1366

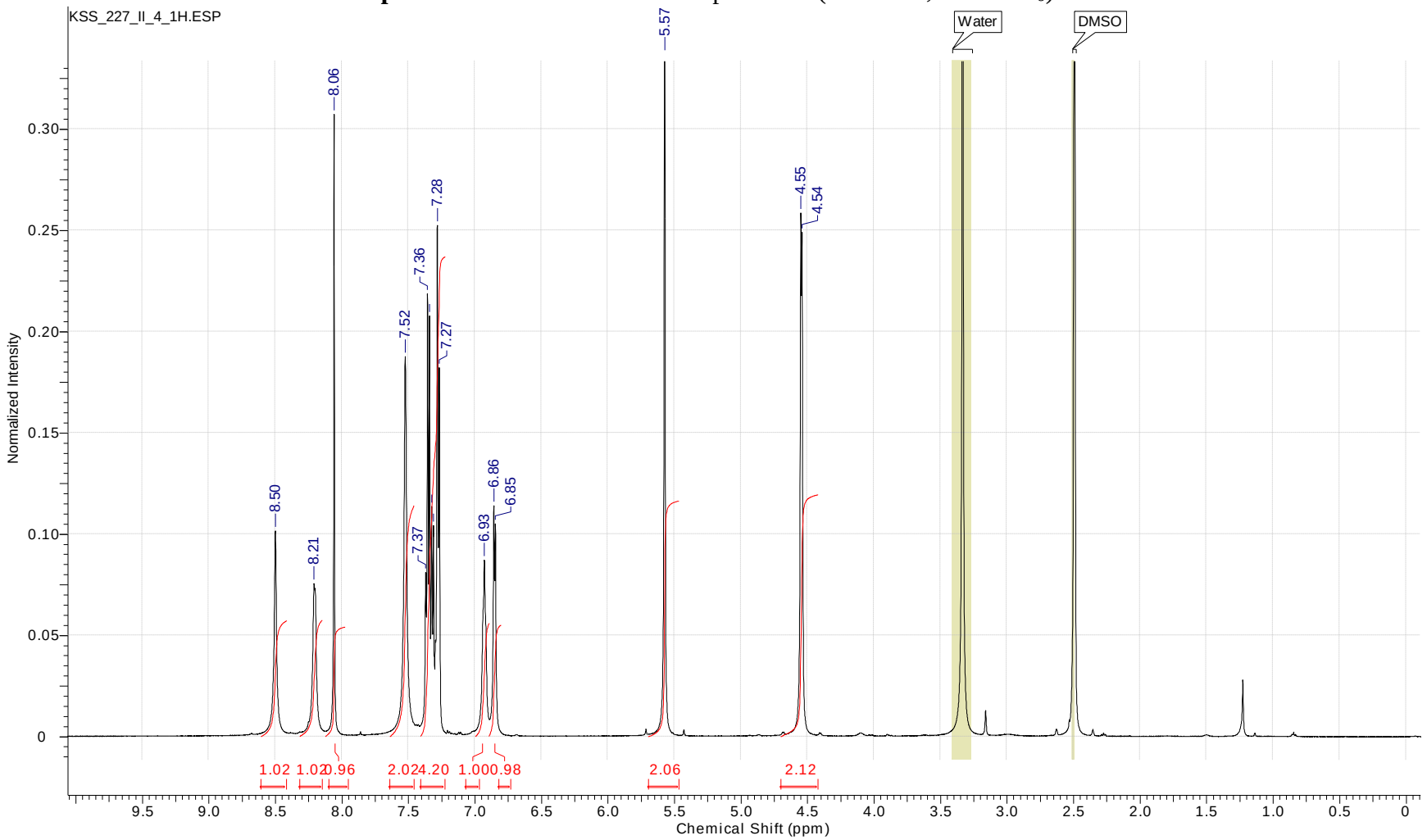
No.	(ppm)	(Hz)	Height
6	39.61	4977.8	0.4286
7	39.77	4998.9	0.8535
8	39.94	5020.0	1.0000
9	40.03	5031.5	0.0641
10	40.11	5041.1	0.8406

No.	(ppm)	(Hz)	Height
11	40.20	5052.6	0.0711
12	40.28	5062.2	0.4114
13	40.45	5083.3	0.1291
14	59.54	7483.5	0.1530
15	120.84	15187.7	0.0978

No.	(ppm)	(Hz)	Height
16	122.32	15373.7	0.1521
17	135.86	17074.9	0.0682
18	141.76	17817.1	0.0960
19	147.71	18564.2	0.1013
20	148.24	18631.3	0.0782

No.	(ppm)	(Hz)	Height
21	151.90	19090.6	0.1128

Spectrum S31. ^{1}H-NMR of compound **19** (500 MHz, DMSO-d_6).



No.	(ppm)	(Hz)	Height
1	4.54	2269.8	0.2491
2	4.55	2274.2	0.2588
3	5.57	2786.3	0.5969
4	6.85	3421.8	0.1052

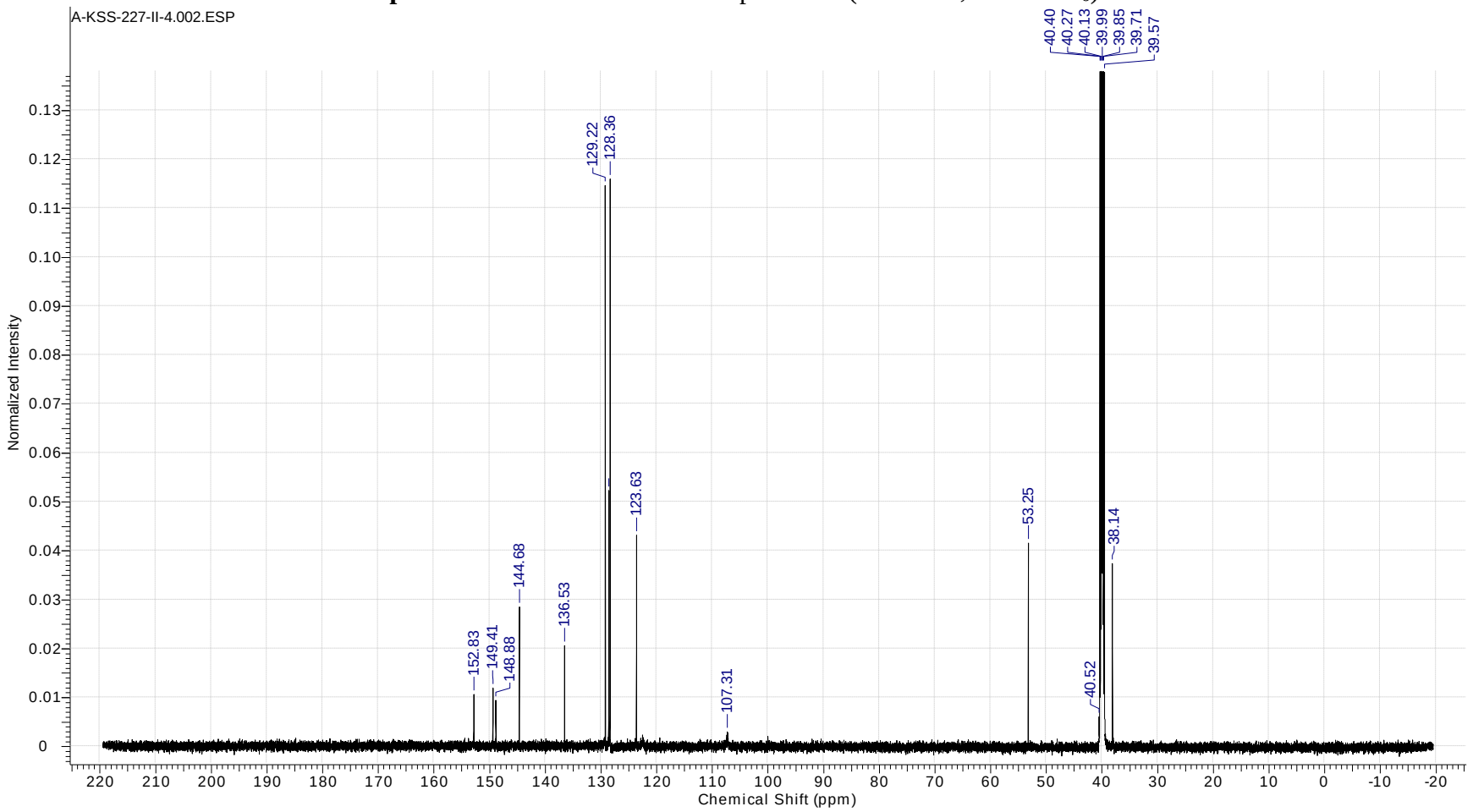
No.	(ppm)	(Hz)	Height
5	6.86	3427.7	0.1141
6	6.93	3463.3	0.0874
7	7.27	3632.7	0.1823
8	7.28	3640.0	0.2527

No.	(ppm)	(Hz)	Height
9	7.31	3654.6	0.1042
10	7.33	3661.5	0.1137
11	7.34	3669.8	0.2078
12	7.36	3677.1	0.2186

No.	(ppm)	(Hz)	Height
13	7.37	3683.9	0.0812
14	7.52	3760.5	0.1877
15	8.06	4028.0	0.3073
16	8.21	4103.2	0.0757

No.	(ppm)	(Hz)	Height
17	8.50	4248.7	0.1016

Spectrum S32. ^{13}C-NMR of compound **19** (125 MHz, DMSO- d_6)



No.	(ppm)	(Hz)	Height
1	38.14	5756.2	0.0374
2	39.57	5971.9	0.1378
3	39.71	5992.8	0.4224
4	39.85	6013.7	0.8466

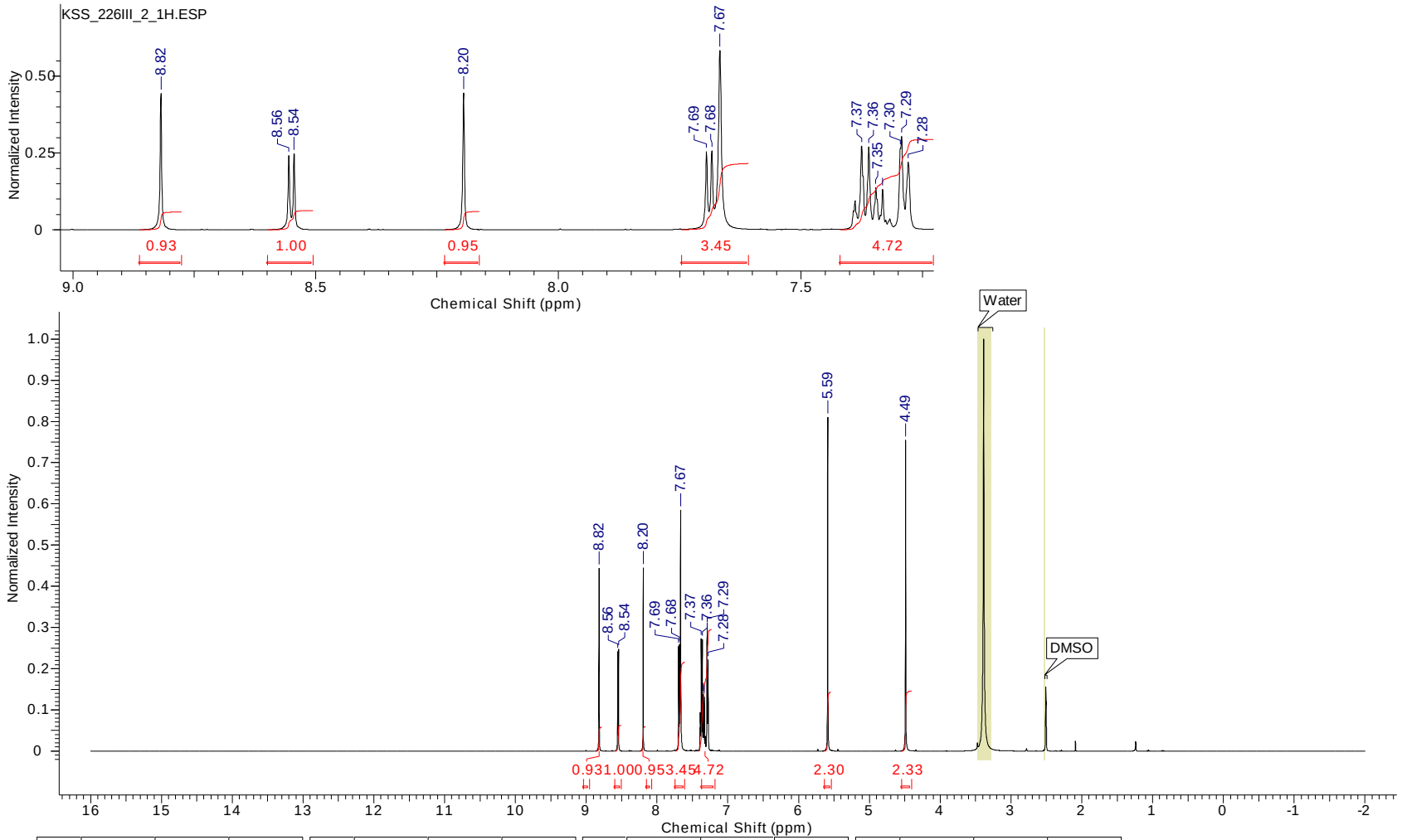
No.	(ppm)	(Hz)	Height
5	39.99	6034.6	1.0000
6	40.13	6055.6	0.8502
7	40.27	6076.5	0.4261
8	40.40	6097.4	0.1395

No.	(ppm)	(Hz)	Height
9	40.52	6115.0	0.0061
10	53.25	8036.3	0.0416
11	107.31	16193.5	0.0030
12	123.63	18657.3	0.0432

No.	(ppm)	(Hz)	Height
13	128.36	19371.4	0.1160
14	128.60	19407.7	0.0523
15	129.22	19501.3	0.1147
16	136.53	20603.9	0.0207

No.	(ppm)	(Hz)	Height
17	144.68	21834.1	0.0285
18	148.88	22467.9	0.0095
19	149.41	22548.2	0.0120
20	152.83	23064.3	0.0107

Spectrum S33. ^{1}H-NMR of compound **20** (500 MHz, DMSO-d_6).



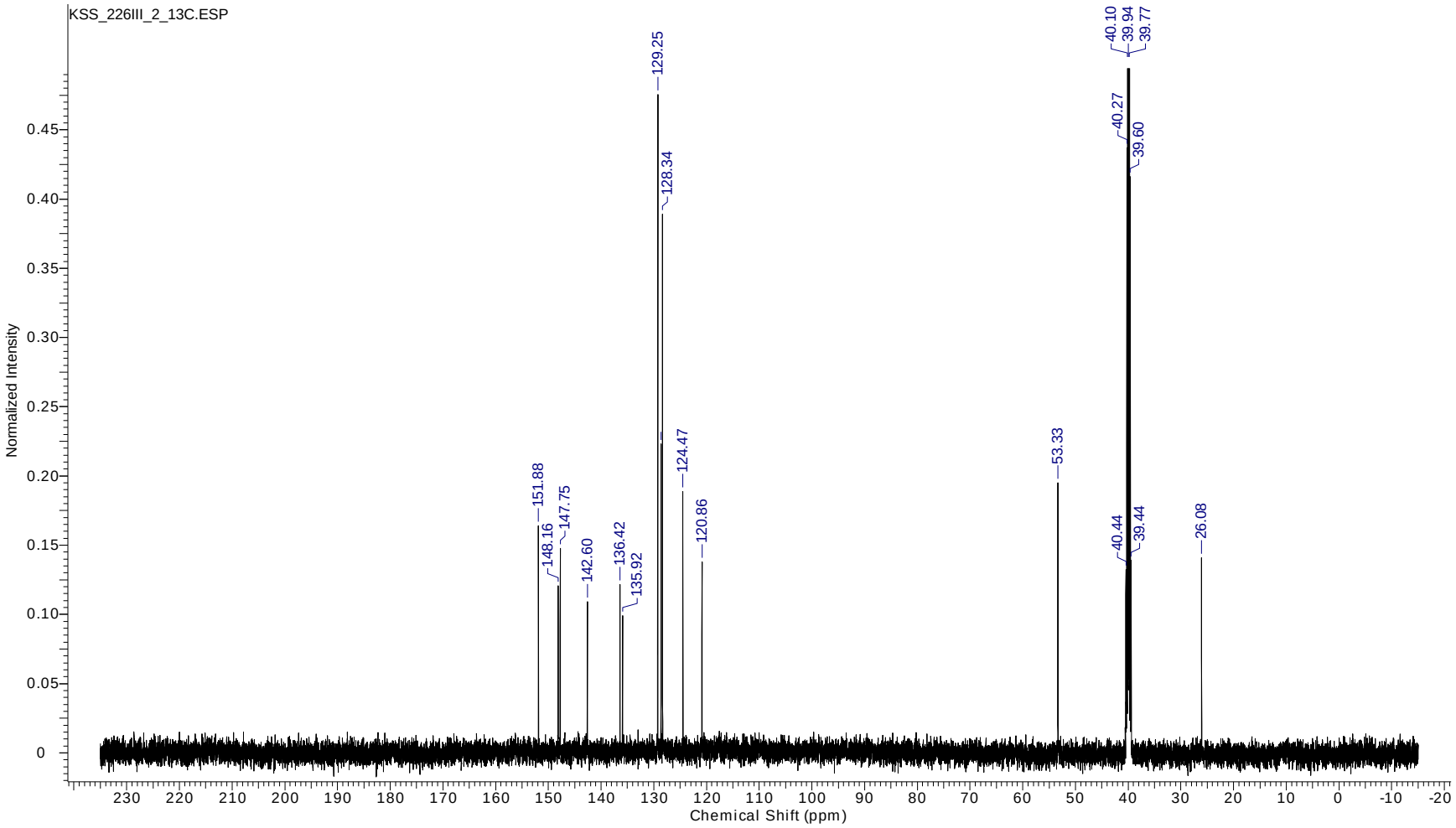
No.	(ppm)	(Hz)	Height
1	4.49	2243.3	0.7544
2	5.59	2793.3	0.8100
3	7.28	3637.9	0.2212
4	7.29	3644.7	0.3036

No.	(ppm)	(Hz)	Height
5	7.30	3646.1	0.2662
6	7.33	3664.2	0.1312
7	7.35	3671.4	0.1371
8	7.36	3678.5	0.2708

No.	(ppm)	(Hz)	Height
9	7.37	3685.9	0.2732
10	7.67	3832.0	0.5843
11	7.68	3840.2	0.2577
12	7.69	3845.7	0.2541

No.	(ppm)	(Hz)	Height
13	8.20	4095.8	0.4448
14	8.54	4270.5	0.2473
15	8.56	4275.7	0.2415
16	8.82	4407.5	0.4437

Spectrum S34. ^{13}C-NMR of compound **20** (125 MHz, DMSO- d_6).



No.	(ppm)	(Hz)	Height
1	26.08	3277.8	0.1409
2	39.44	4956.9	0.1389
3	39.60	4977.1	0.4162
4	39.77	4998.2	0.8407

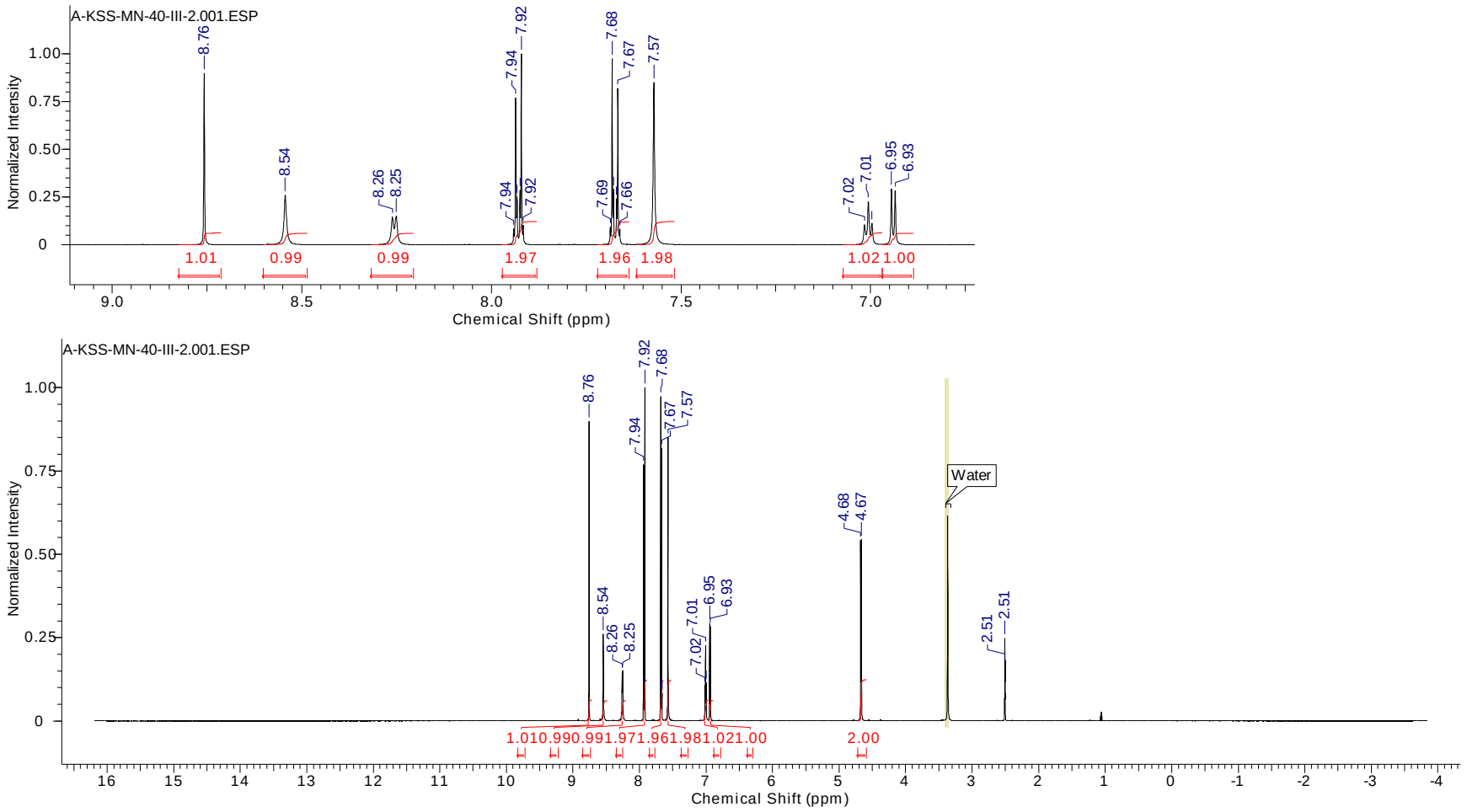
No.	(ppm)	(Hz)	Height
5	39.94	5019.3	1.0000
6	40.10	5040.4	0.8562
7	40.27	5061.5	0.4371
8	40.44	5082.6	0.1325

No.	(ppm)	(Hz)	Height
9	53.33	6702.2	0.1951
10	120.86	15190.8	0.1379
11	124.47	15644.4	0.1888
12	128.34	16130.6	0.3890

No.	(ppm)	(Hz)	Height
13	128.64	16168.0	0.2230
14	129.25	16244.7	0.4756
15	135.92	17082.8	0.0991
16	136.42	17146.1	0.1215

No.	(ppm)	(Hz)	Height
17	142.60	17922.9	0.1091
18	147.75	18570.2	0.1476
19	148.16	18621.0	0.1208
20	151.88	19089.0	0.1639

Spectrum S35. ^{1}H-NMR of compound **21** (500 MHz, DMSO-d_6).



No.	(ppm)	(Hz)	Height
1	2.50	1501.2	0.0826
2	2.50	1503.1	0.1801
3	2.51	1504.9	0.2480
4	2.51	1506.7	0.1762
5	2.51	1508.6	0.0786
6	4.67	2800.1	0.5430

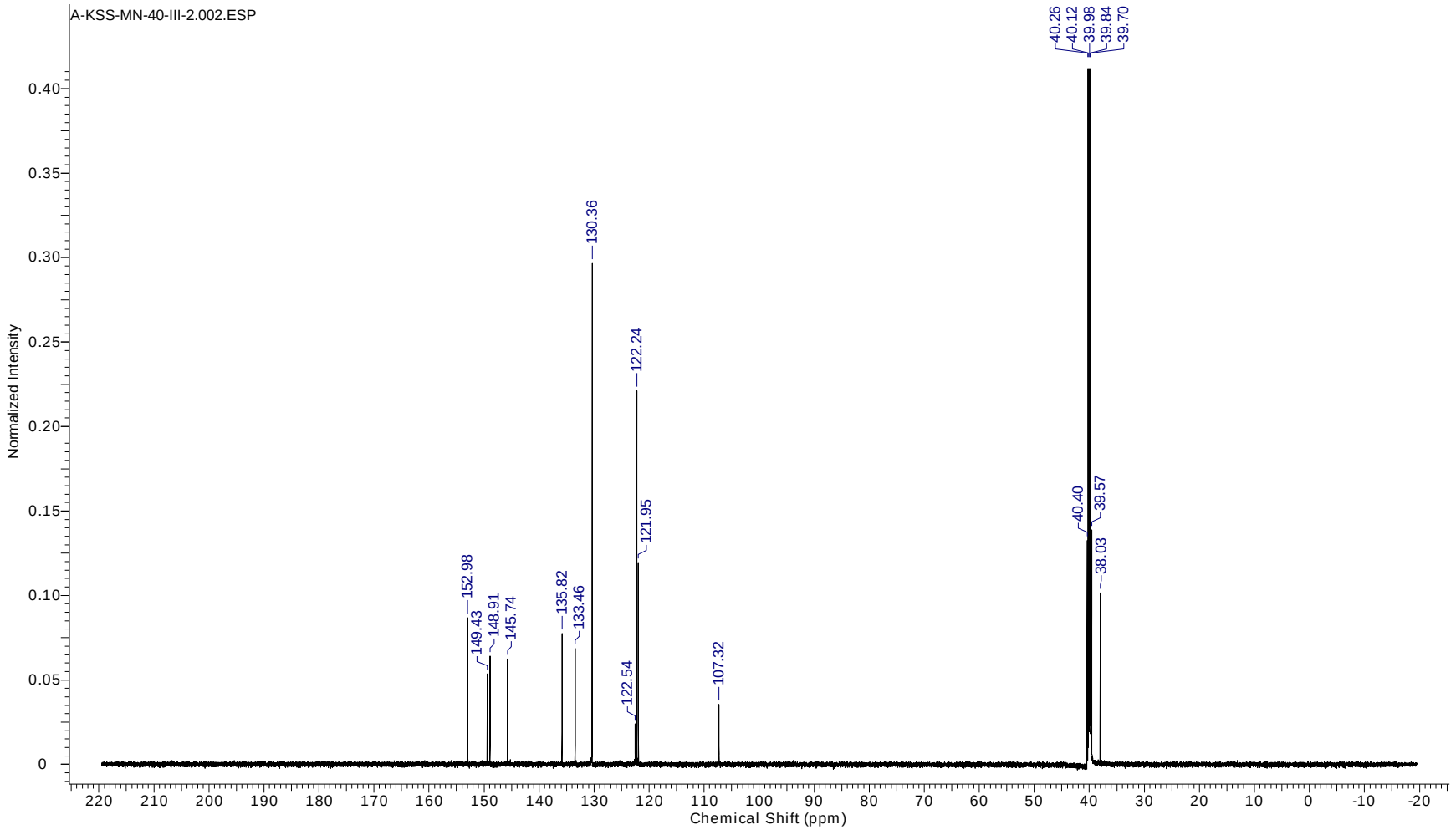
No.	(ppm)	(Hz)	Height
7	4.68	2805.9	0.5405
8	6.93	4162.0	0.2829
9	6.95	4168.2	0.2931
10	7.00	4199.0	0.1139
11	7.01	4204.9	0.2263
12	7.02	4210.8	0.1062

No.	(ppm)	(Hz)	Height
13	7.57	4544.2	0.8497
14	7.66	4598.1	0.0830
15	7.67	4601.4	0.8172
16	7.67	4603.6	0.2400
17	7.68	4608.0	0.2900
18	7.68	4610.2	0.9722

No.	(ppm)	(Hz)	Height
19	7.69	4613.1	0.0934
20	7.92	4751.1	0.1029
21	7.92	4754.0	1.0000
22	7.92	4756.2	0.2852
23	7.93	4761.0	0.2506
24	7.94	4762.8	0.7683

No.	(ppm)	(Hz)	Height
25	7.94	4766.1	0.0840
26	8.25	4952.1	0.1502
27	8.26	4957.9	0.1471
28	8.54	5127.8	0.2594
29	8.76	5256.1	0.8971

Spectrum S36. ^{13}C-NMR of compound **21** (125 MHz, DMSO- d_6).



No.	(ppm)	(Hz)	Height
1	38.03	5739.7	0.1016
2	39.57	5970.8	0.1387
3	39.70	5991.7	0.4229
4	39.84	6012.6	0.8490

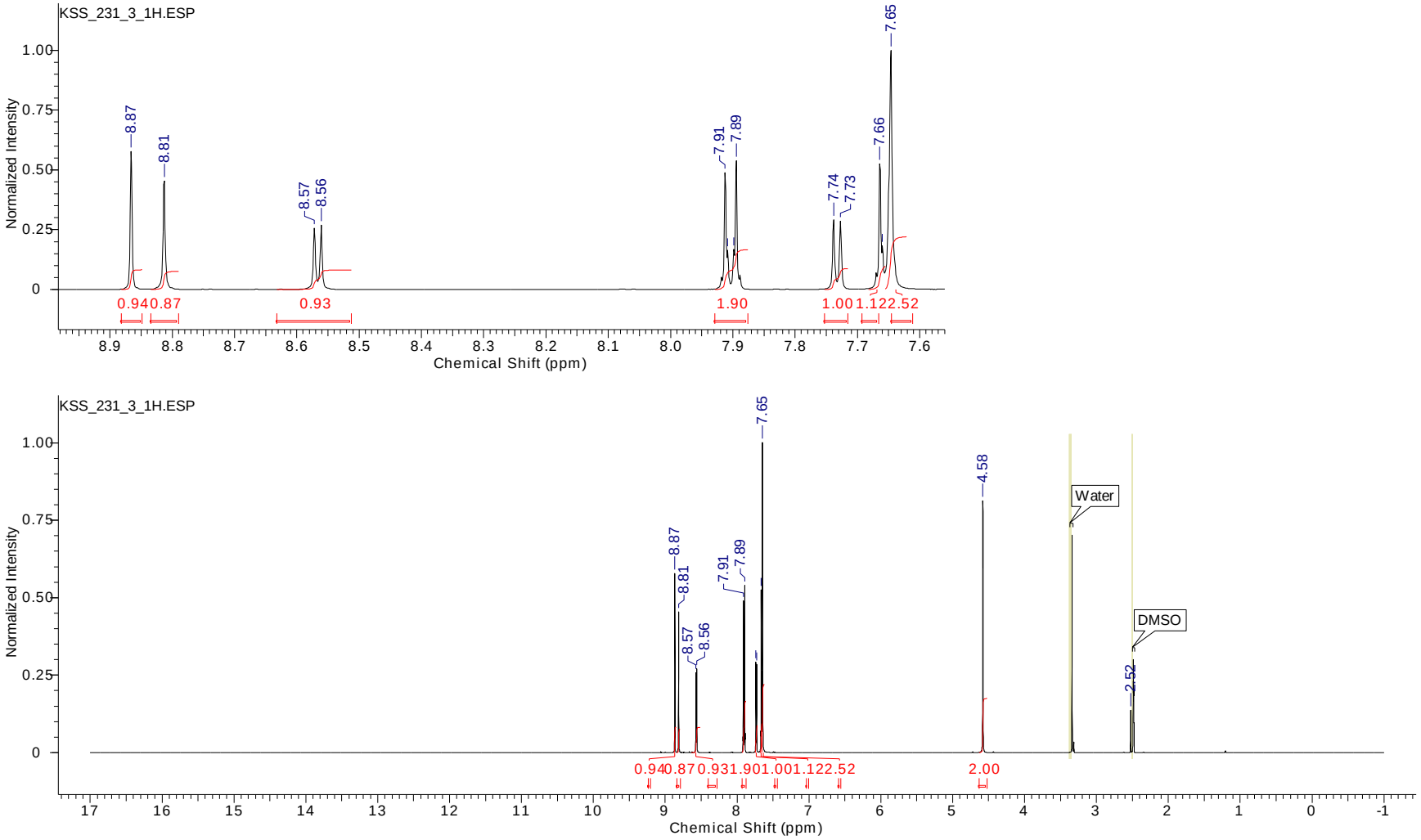
No.	(ppm)	(Hz)	Height
5	39.98	6033.5	1.0000
6	40.12	6054.5	0.8454
7	40.26	6075.4	0.4185
8	40.40	6096.3	0.1326

No.	(ppm)	(Hz)	Height
9	107.32	16195.7	0.0355
10	121.95	18403.1	0.1196
11	122.24	18447.1	0.2212
12	122.54	18493.3	0.0239

No.	(ppm)	(Hz)	Height
13	130.36	19672.9	0.2965
14	133.46	20140.6	0.0687
15	135.82	20497.1	0.0774
16	145.74	21993.7	0.0624

No.	(ppm)	(Hz)	Height
17	148.91	22472.3	0.0640
18	149.43	22550.5	0.0537
19	152.98	23086.3	0.0867

Spectrum S37. ^{1}H-NMR of compound **22** (500 MHz, DMSO-d_6).



No.	(ppm)	(Hz)	Height
1	2.52	1260.7	0.1371
2	4.58	2289.2	0.8117
3	7.65	3821.2	1.0000

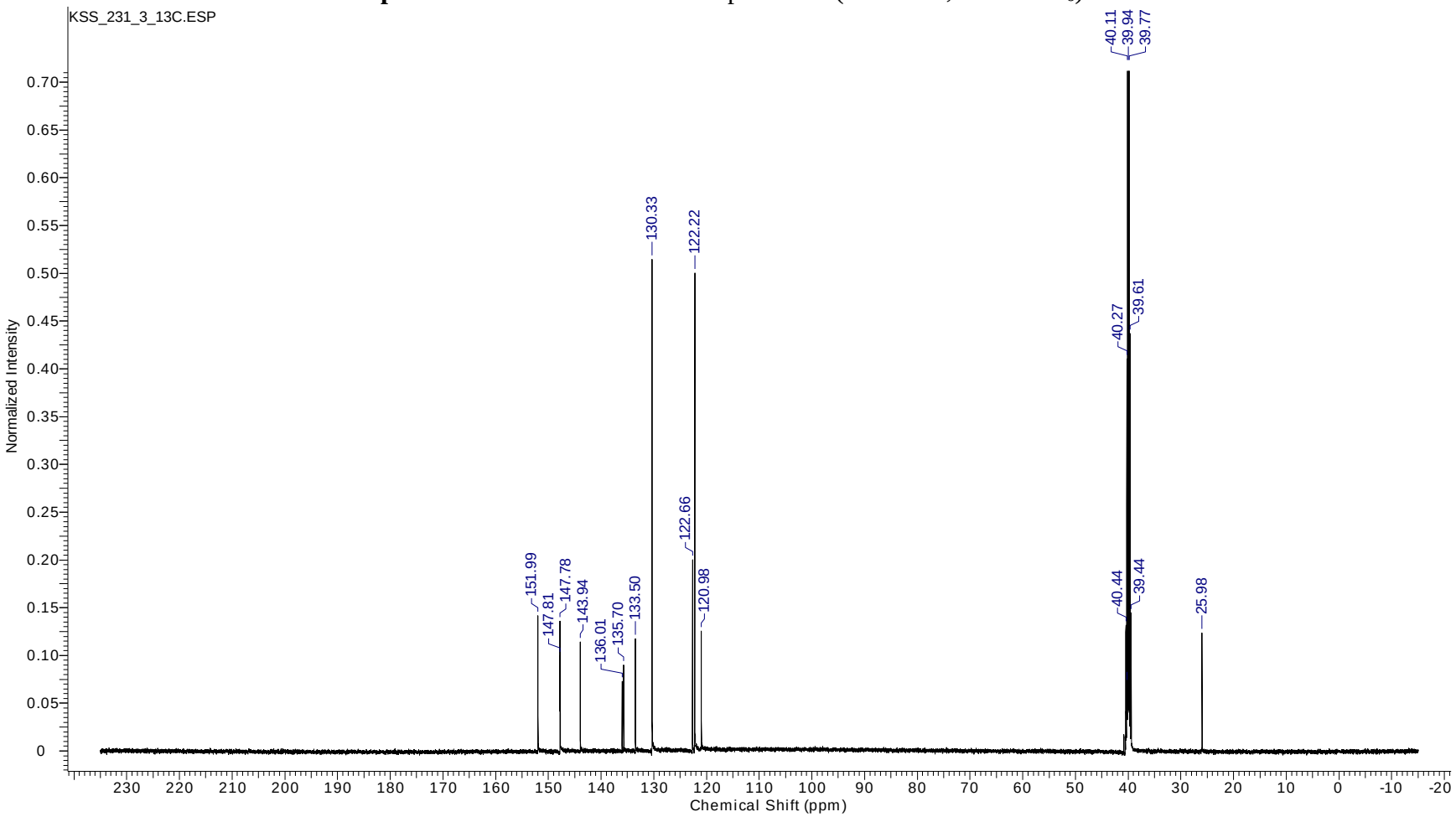
No.	(ppm)	(Hz)	Height
4	7.66	3828.3	0.1818
5	7.66	3830.5	0.5253
6	7.73	3861.8	0.2850

No.	(ppm)	(Hz)	Height
7	7.74	3867.3	0.2920
8	7.89	3945.3	0.5387
9	7.90	3947.5	0.1682

No.	(ppm)	(Hz)	Height
10	7.91	3952.4	0.1651
11	7.91	3954.6	0.4887
12	8.56	4278.6	0.2698

No.	(ppm)	(Hz)	Height
13	8.57	4284.1	0.2571
14	8.81	4404.3	0.4541
15	8.87	4431.2	0.5779

Spectrum S38. ^{13}C-NMR of compound **22** (125 MHz, DMSO- d_6).



No.	(ppm)	(Hz)	Height
1	25.98	3265.1	0.1235
2	39.44	4956.7	0.1445
3	39.61	4977.8	0.4370
4	39.77	4998.9	0.8619
5	39.94	5020.0	1.0000

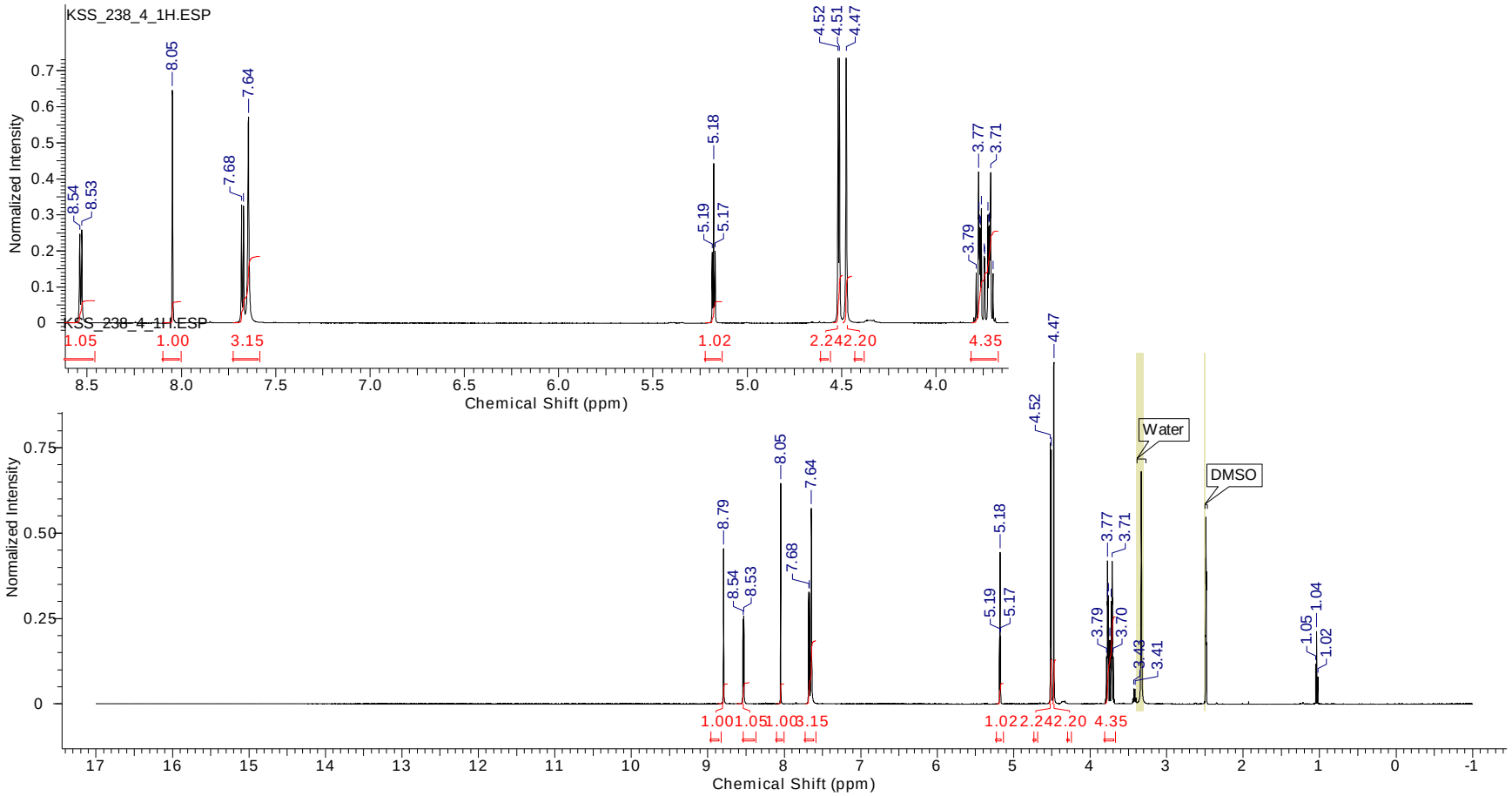
No.	(ppm)	(Hz)	Height
6	40.03	5030.5	0.0679
7	40.11	5041.1	0.8283
8	40.19	5051.6	0.0702
9	40.27	5061.2	0.4102
10	40.44	5082.3	0.1318

No.	(ppm)	(Hz)	Height
11	120.98	15205.0	0.1253
12	122.22	15360.3	0.5005
13	122.66	15415.9	0.2005
14	130.33	16380.6	0.5147
15	133.50	16778.6	0.1174

No.	(ppm)	(Hz)	Height
16	135.70	17055.7	0.0899
17	136.01	17094.1	0.0730
18	143.94	18090.4	0.1140
19	147.78	18572.8	0.1358
20	147.81	18577.6	0.0994

No.	(ppm)	(Hz)	Height
21	151.99	19103.1	0.1415

Spectrum S39. ^{1}H-NMR of compound **23** (500 MHz, DMSO-d_6).



No.	(ppm)	(Hz)	Height
1	1.02	510.7	0.0786
2	1.04	517.8	0.2126
3	1.05	524.9	0.1153
4	3.41	1706.1	0.0437
5	3.43	1713.2	0.0445
6	3.70	1847.7	0.1374
7	3.71	1854.3	0.4176

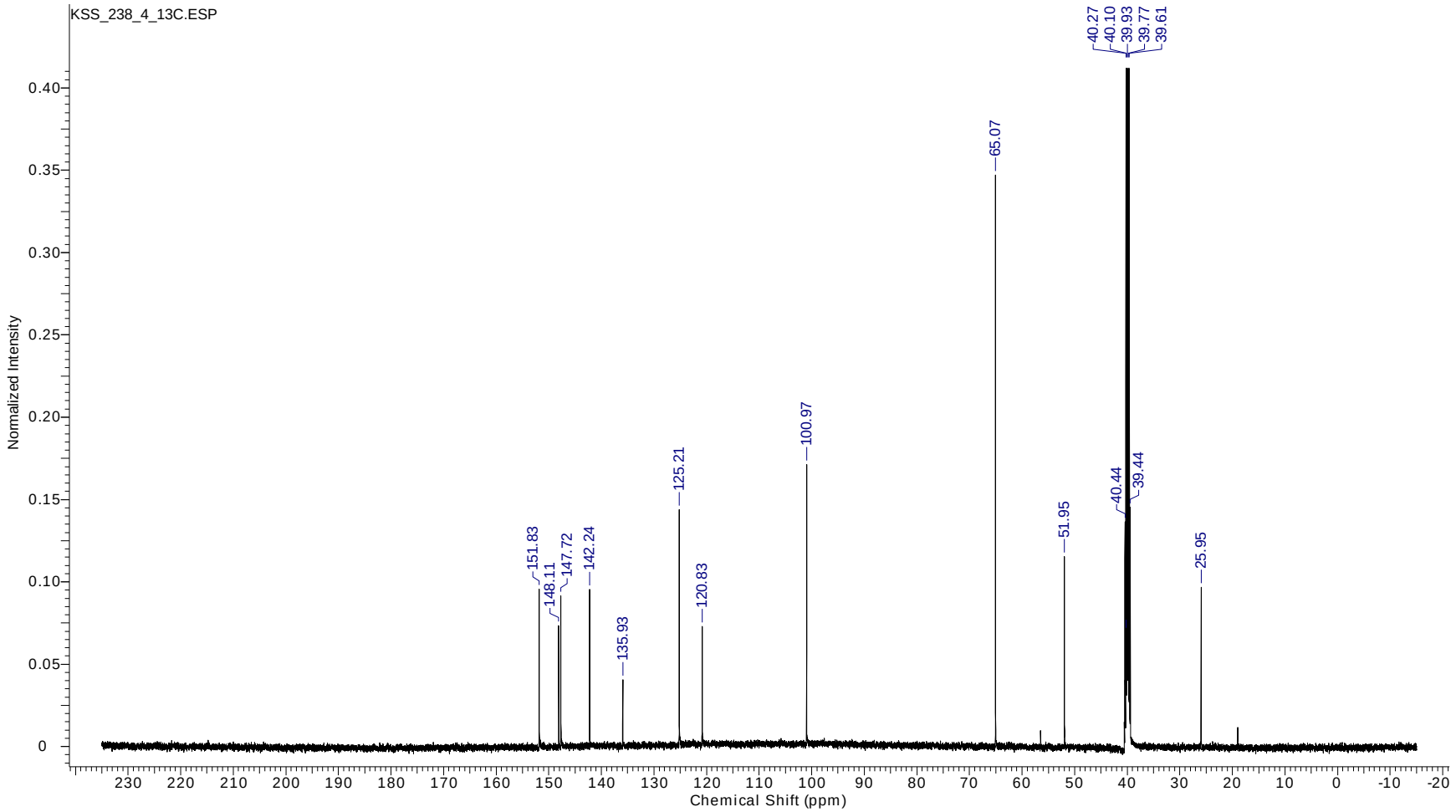
No.	(ppm)	(Hz)	Height
8	3.71	1855.4	0.3114
9	3.72	1857.1	0.2708
10	3.72	1859.3	0.2674
11	3.72	1861.4	0.3004
12	3.74	1869.7	0.1789
13	3.74	1870.8	0.1860
14	3.76	1879.0	0.3169

No.	(ppm)	(Hz)	Height
15	3.76	1881.2	0.2615
16	3.77	1883.4	0.2655
17	3.77	1885.1	0.3003
18	3.77	1886.2	0.4188
19	3.79	1892.7	0.1385
20	4.47	2236.5	1.0000
21	4.51	2254.6	0.7429

No.	(ppm)	(Hz)	Height
22	4.52	2258.4	0.7630
23	5.17	2584.1	0.1983
24	5.18	2587.9	0.4427
25	5.19	2591.7	0.1961
26	7.64	3820.6	0.5722
27	7.67	3833.3	0.3253
28	7.68	3838.7	0.3277

No.	(ppm)	(Hz)	Height
29	8.05	4022.1	0.6457
30	8.53	4262.1	0.2582
31	8.54	4267.6	0.2476
32	8.79	4395.0	0.4540

Spectrum S40. ^{13}C-NMR of compound **23** (125 MHz, DMSO- d_6).



No.	(ppm)	(Hz)	Height
1	25.95	3261.3	0.0966
2	39.44	4956.7	0.1452
3	39.61	4977.8	0.4346
4	39.77	4998.9	0.8421
5	39.93	5019.0	1.0000

No.	(ppm)	(Hz)	Height
6	40.03	5030.5	0.0676
7	40.10	5040.1	0.8590
8	40.19	5051.6	0.0696
9	40.27	5061.2	0.4316
10	40.36	5072.7	0.0402

No.	(ppm)	(Hz)	Height
11	40.44	5082.3	0.1364
12	51.95	6529.4	0.1154
13	65.07	8177.8	0.3470
14	100.97	12689.7	0.1711
15	120.83	15186.8	0.0729

No.	(ppm)	(Hz)	Height
16	125.21	15736.2	0.1439
17	135.93	17084.5	0.0407
18	142.24	17877.6	0.0955
19	147.72	18566.1	0.0916
20	148.11	18615.0	0.0734

No.	(ppm)	(Hz)	Height
21	151.83	19083.0	0.0956