Supporting Information

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Chemical Constituents of *Tectus maximus* Koch, 1844

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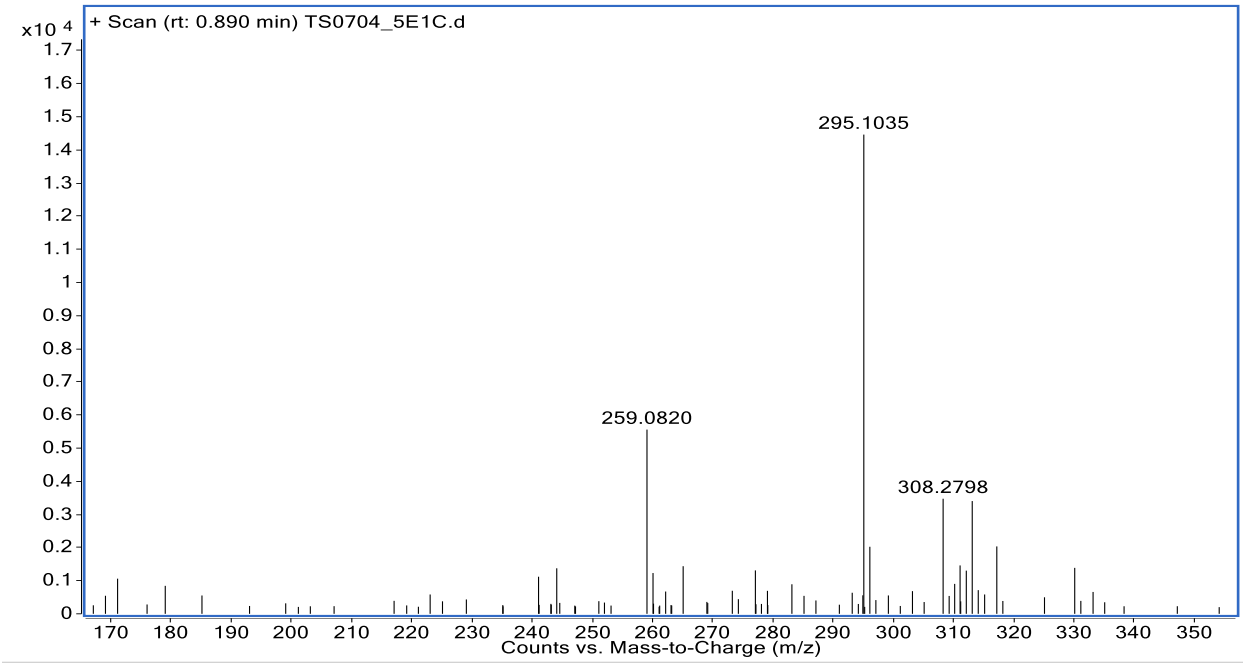


Formula (M)	Score (MFG	Mass	Mass (MFG)	m/z (Calc)	Diff (ppm)	DBE	m/z
C12 H14 N4 O5	99.86	294.0962	294.0964	295.1037	0.67	8	295.1035
C11 H18 O9	95.56	294.0962	294.0951	295.1024	-3.88	3	295.1035
C13 H10 N8 O	92.28	294.0962	294.0978	295.105	5.21	13	295.1035

Figure S1: HR-ESI-MS of compound **1**

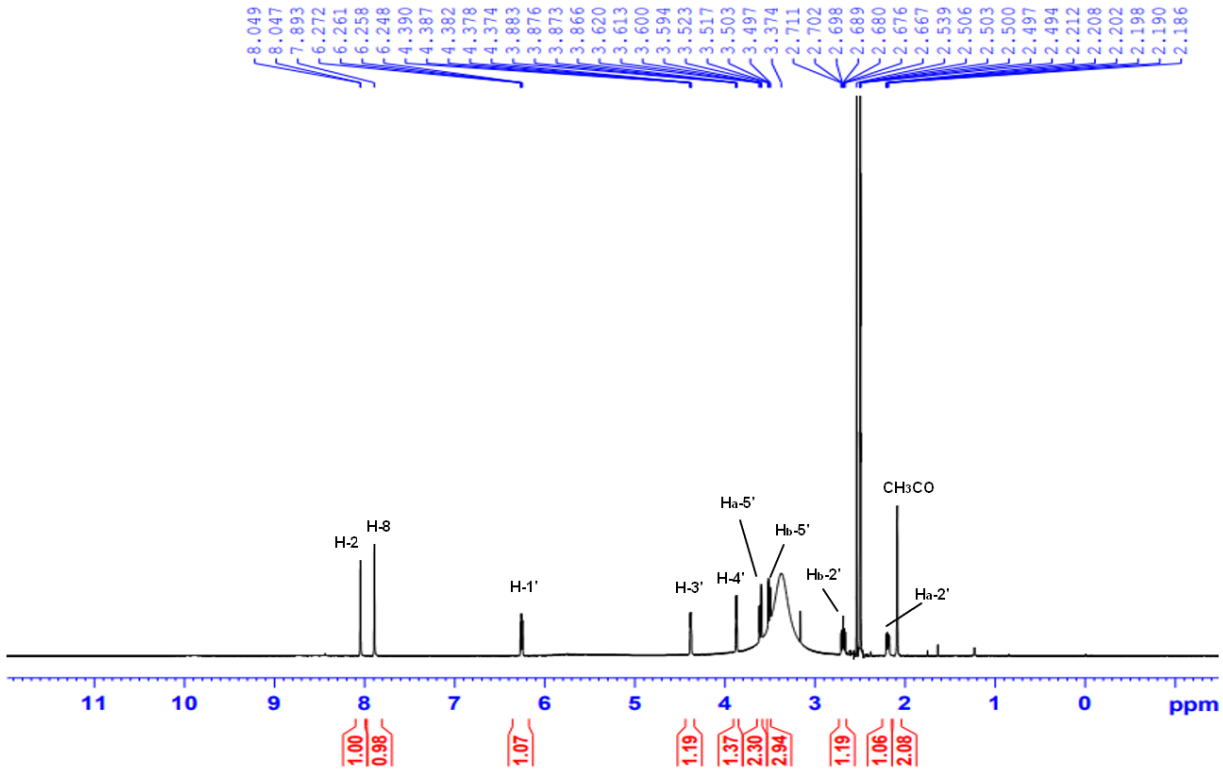


Figure S2: ^{1}H NMR spectrum of compound **1** in DMSO-d_6

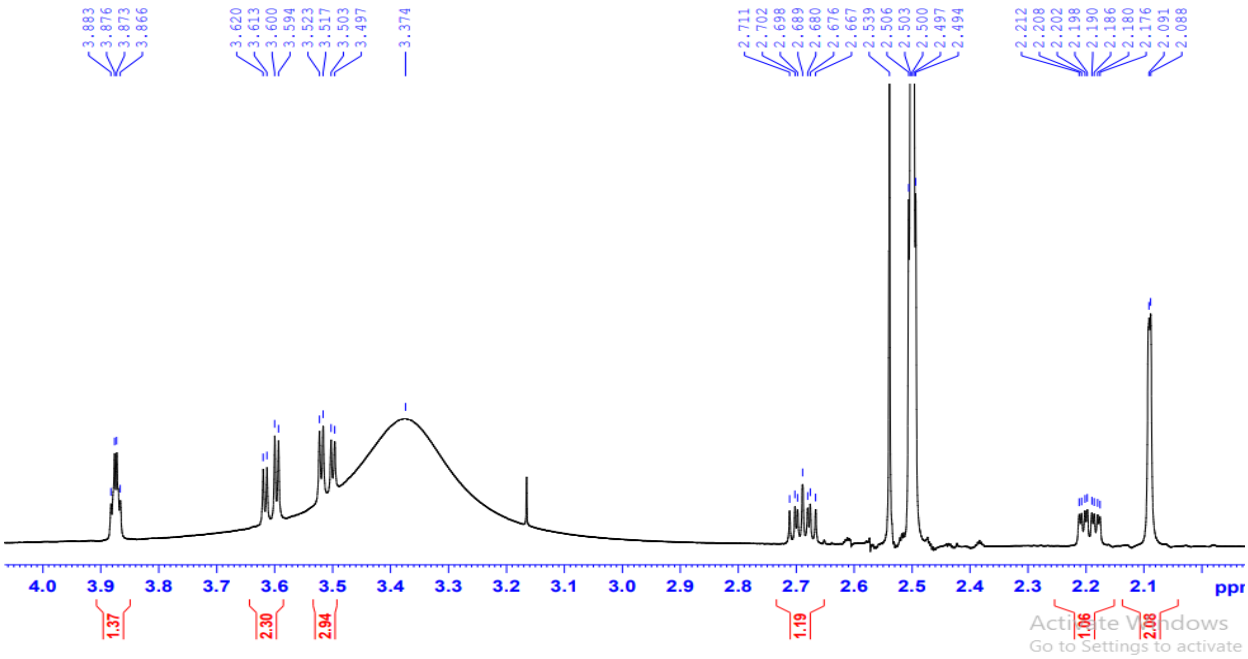


Figure S3: Extended ^{1}H NMR spectrum of compound **1** in DMSO-d_6

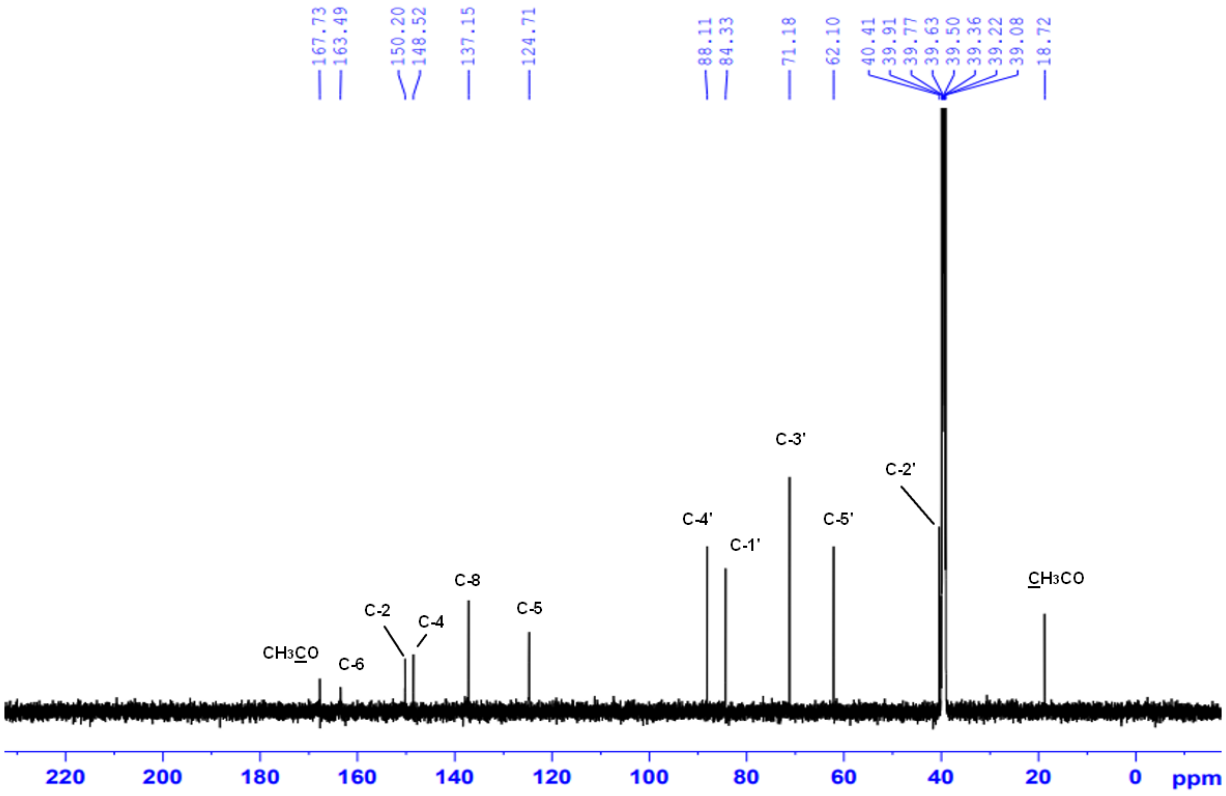


Figure S4: ^{13}C NMR spectrum of compound **1** in DMSO-d_6

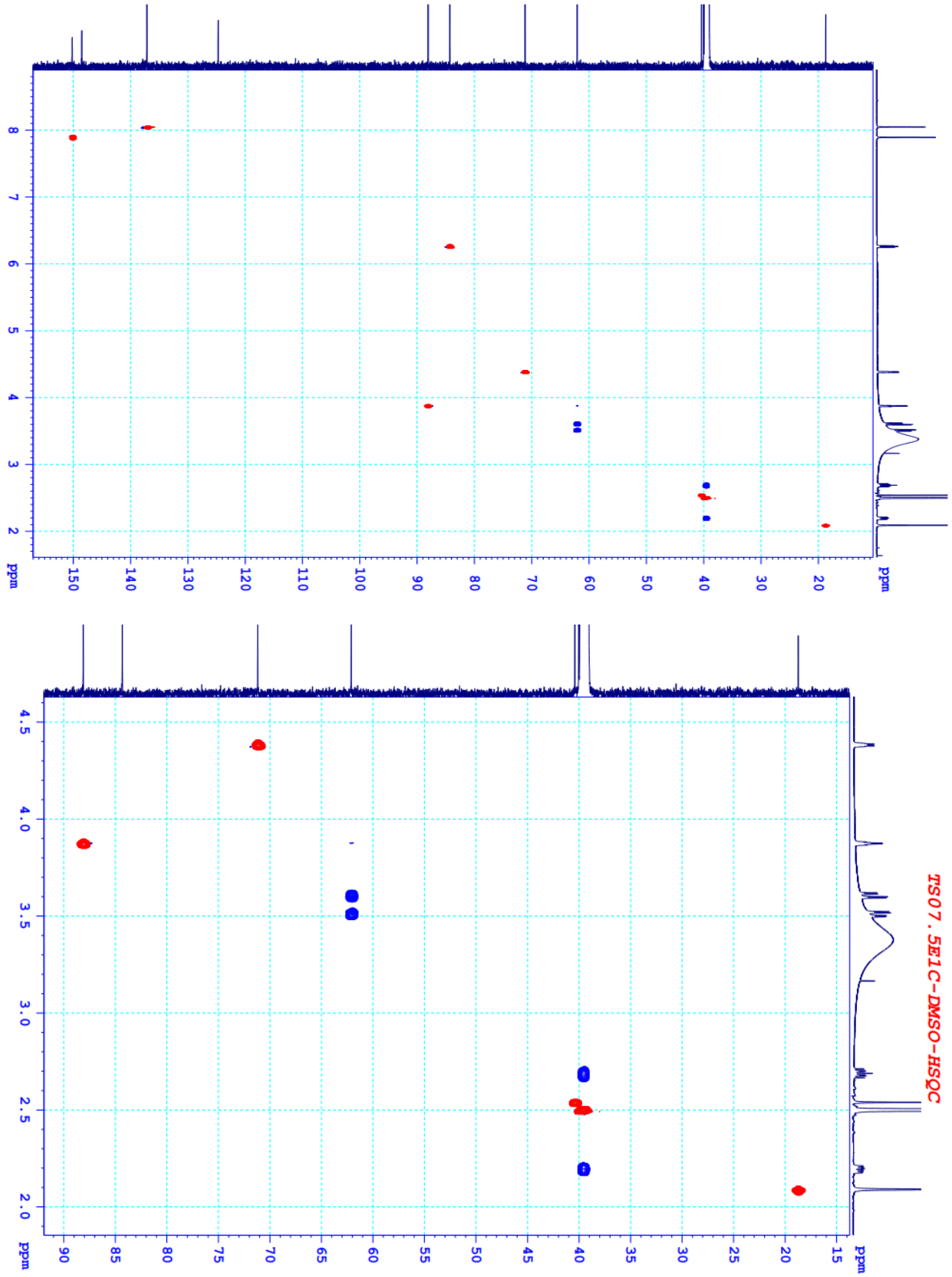


Figure S5: HSQC spectrum of compound **1** in DMSO-d_6

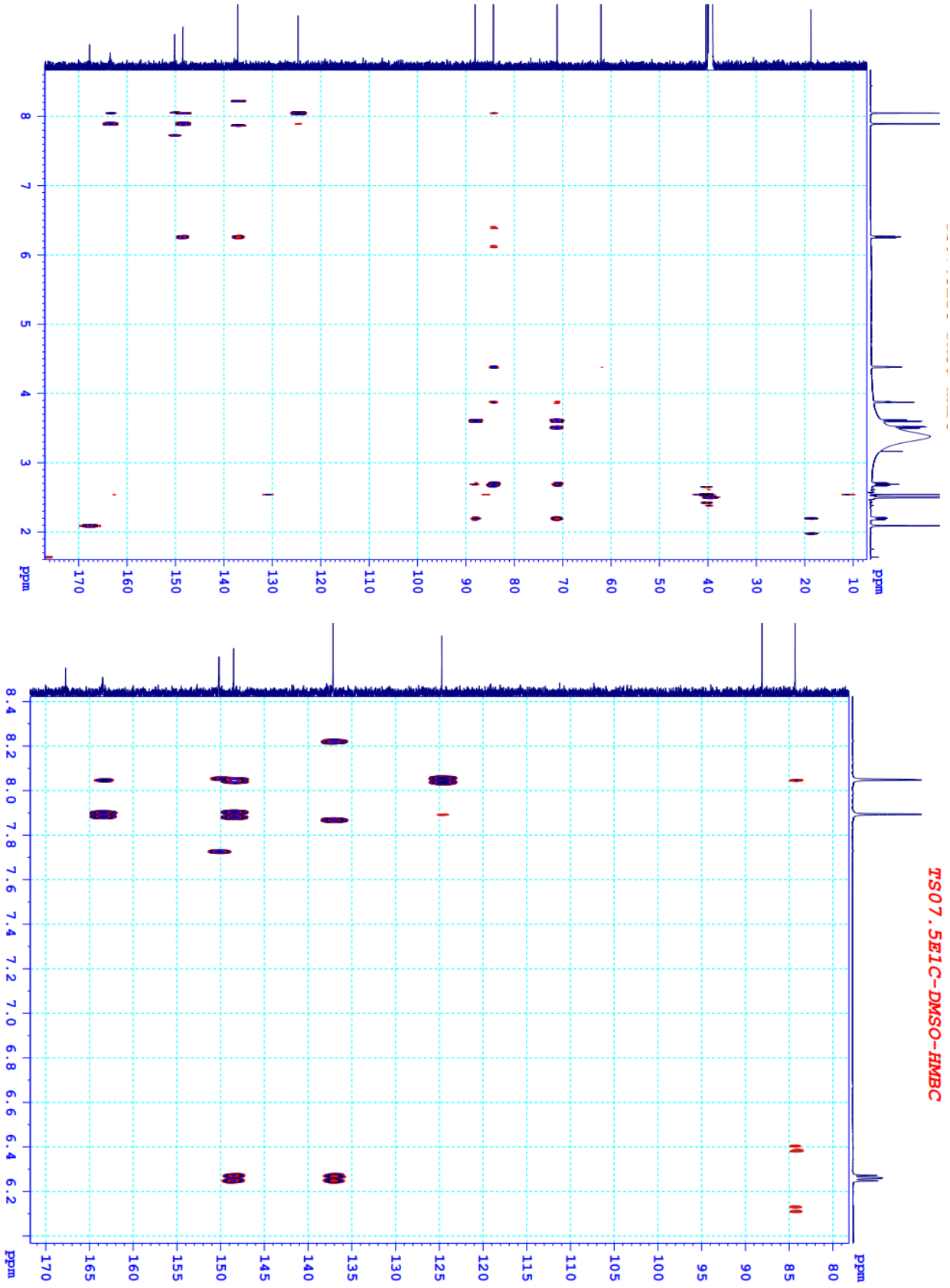


Figure S6:HMBC spectrum of compound **1** in DMSO-d_6

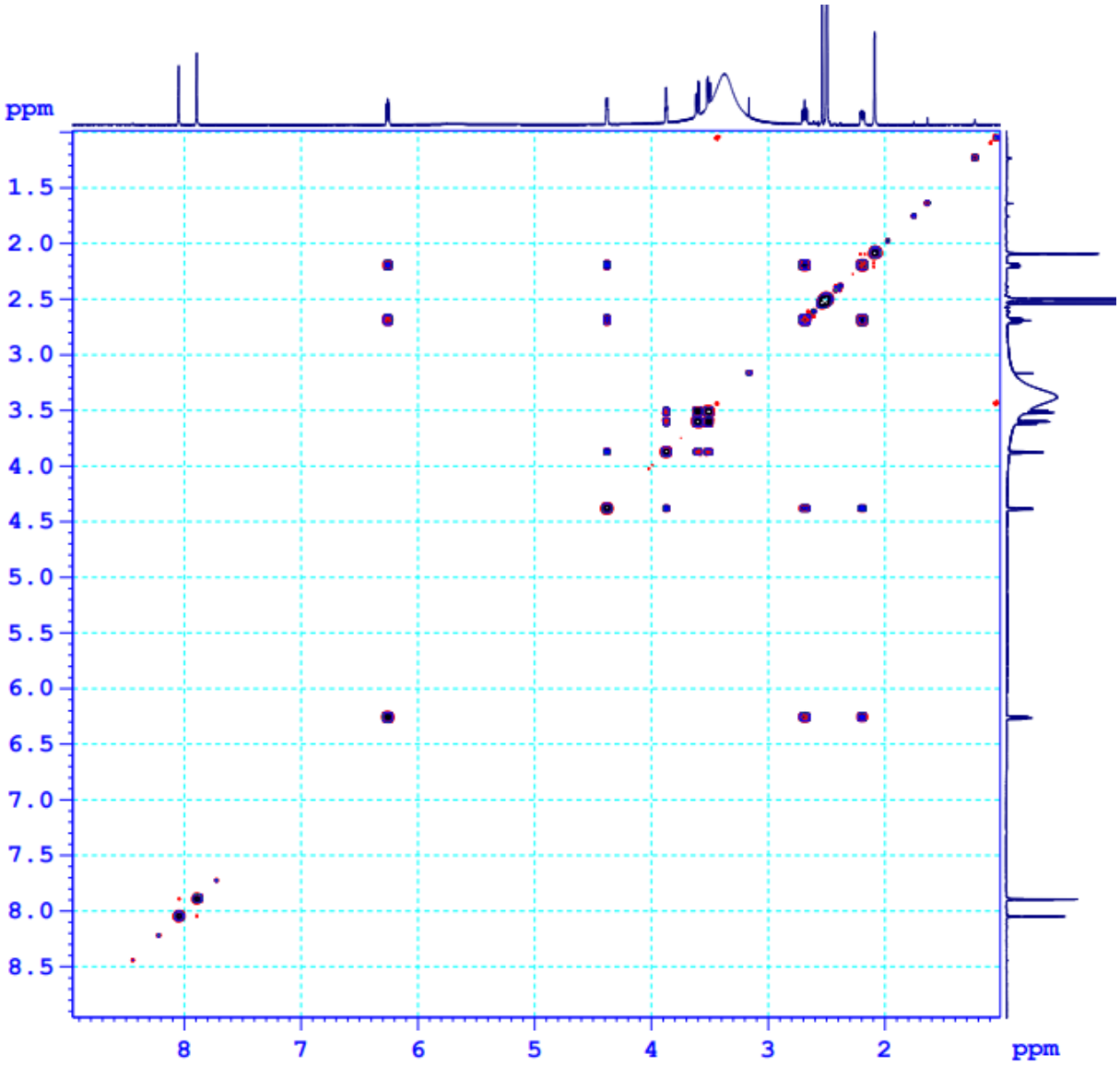


Figure S7: ^{1}H-^{1}H COSY spectrum of compound **1** in DMSO-d_6

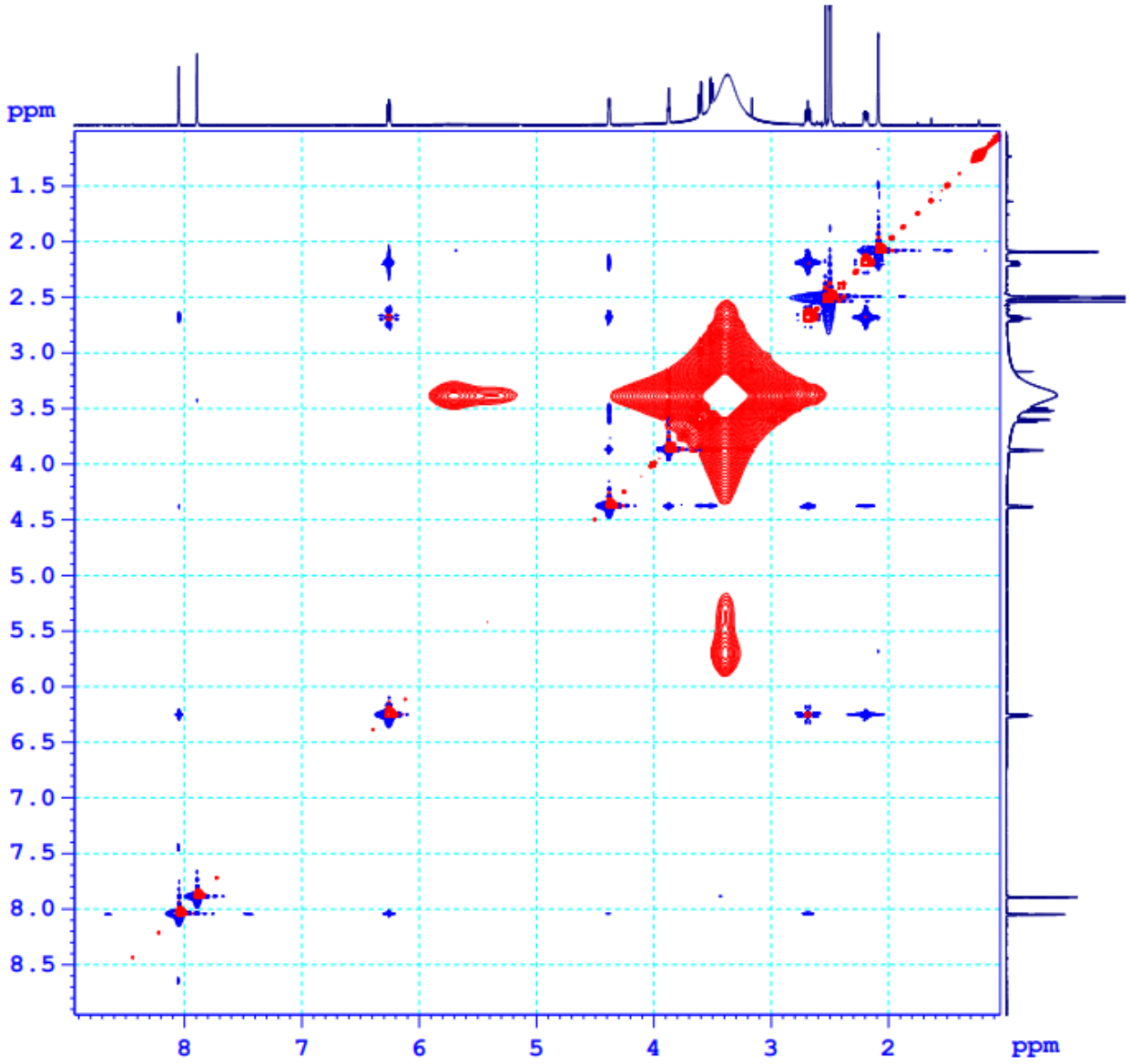
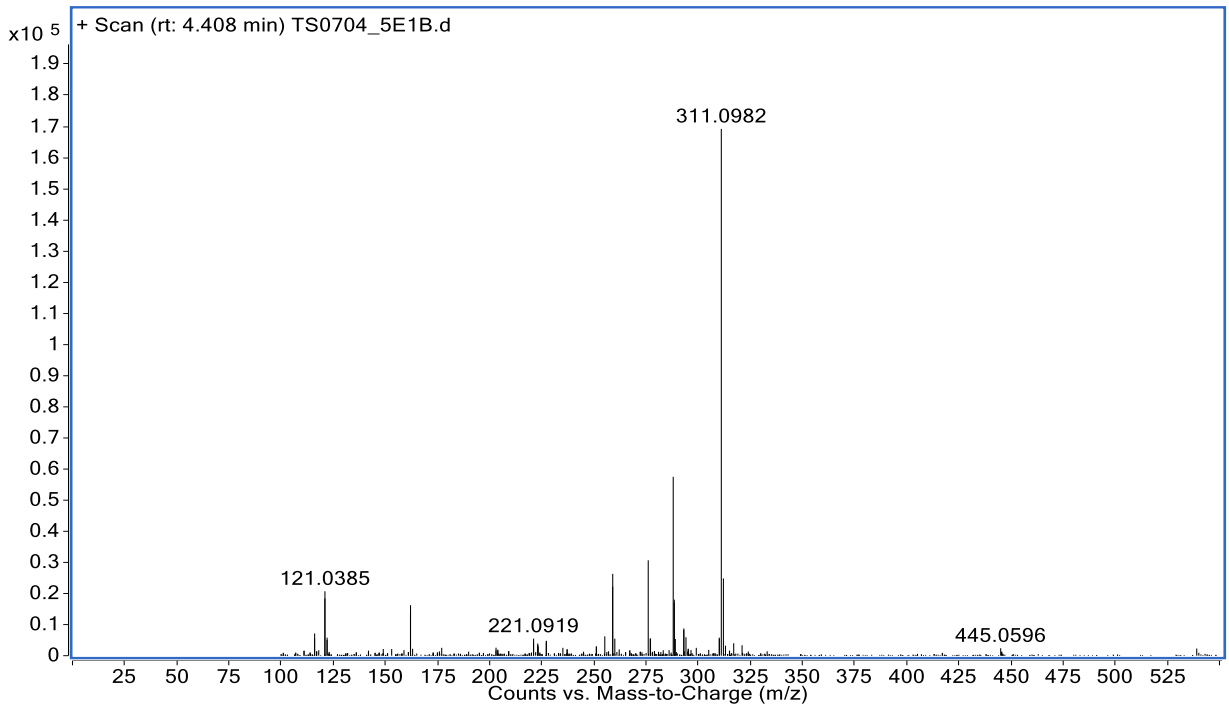


Figure S8: NOESY spectrum of compound **1** in DMSO-d_6



Formula (M)	Score (MFG	Mass	Mass (MFG)	m/z (Calc)	Diff (ppm)	DBE	m/z
C12 H14 N4 O6	99.43	310.0909	310.0913	311.0986	1.32	8	311.0982
C11 H18 O10	97.16	310.0909	310.09	311.0973	-2.99	3	311.0982
C13 H10 N8 O2	90.64	310.0909	310.0927	311.0999	5.64	13	311.0982

Figure S9: HRESIMS spectrum of compound **2**

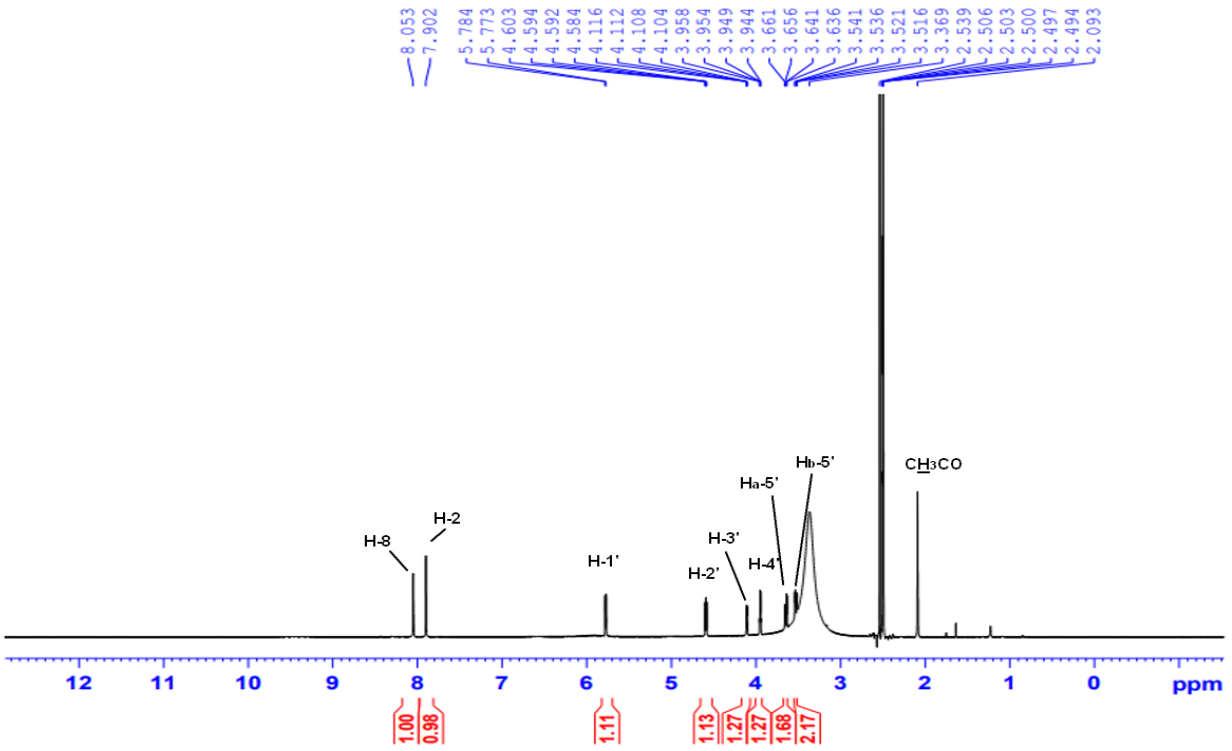


Figure S10: ^{1}H NMR spectrum of compound **2** in DMSO-d_6

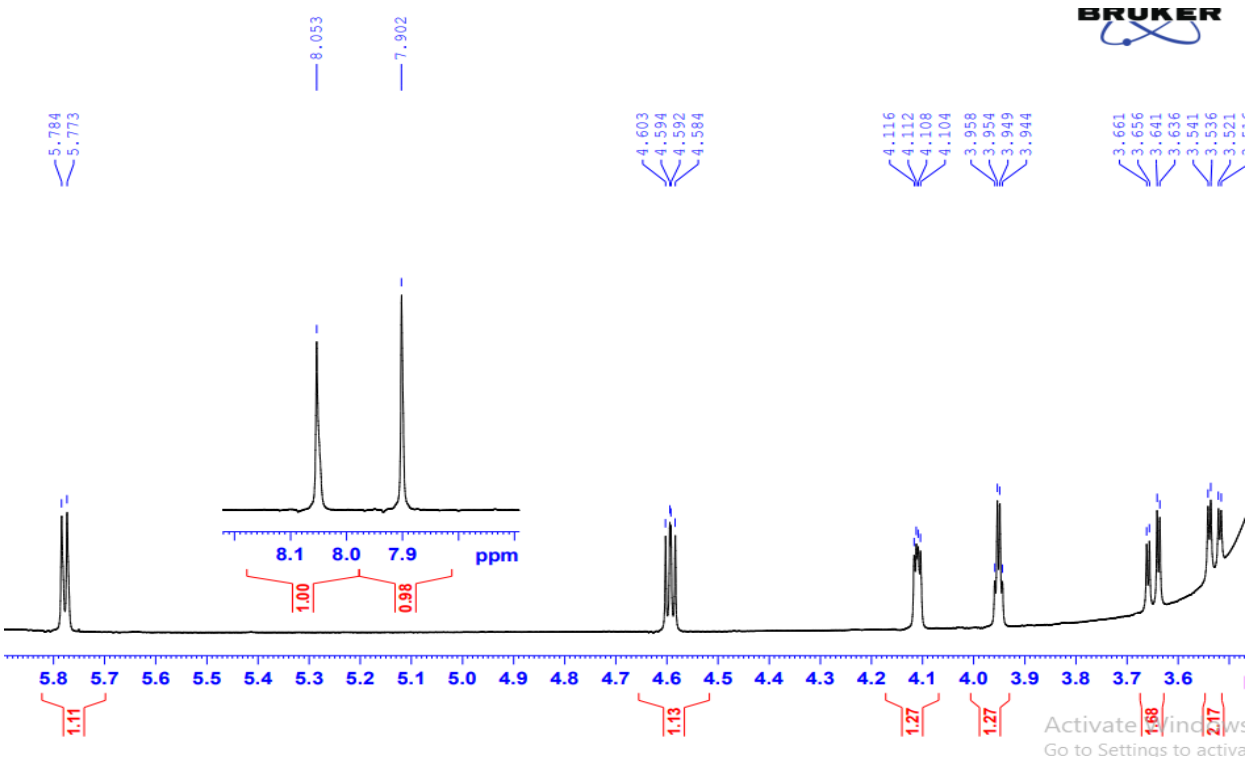


Figure S11: Extended ^{1}H NMR spectrum of compound **2** in DMSO-d_6

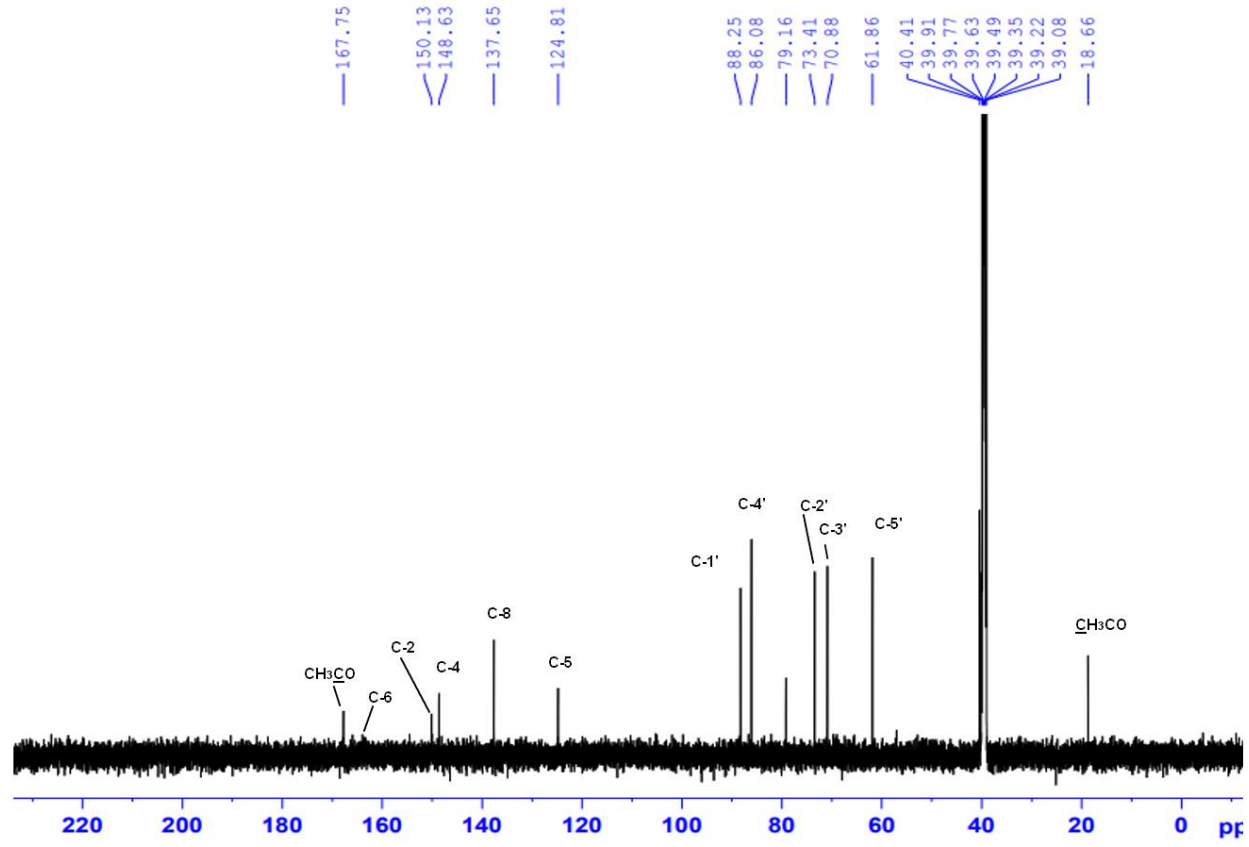


Figure S12: ^{13}C NMR spectrum of compound **2** in DMSO-d_6

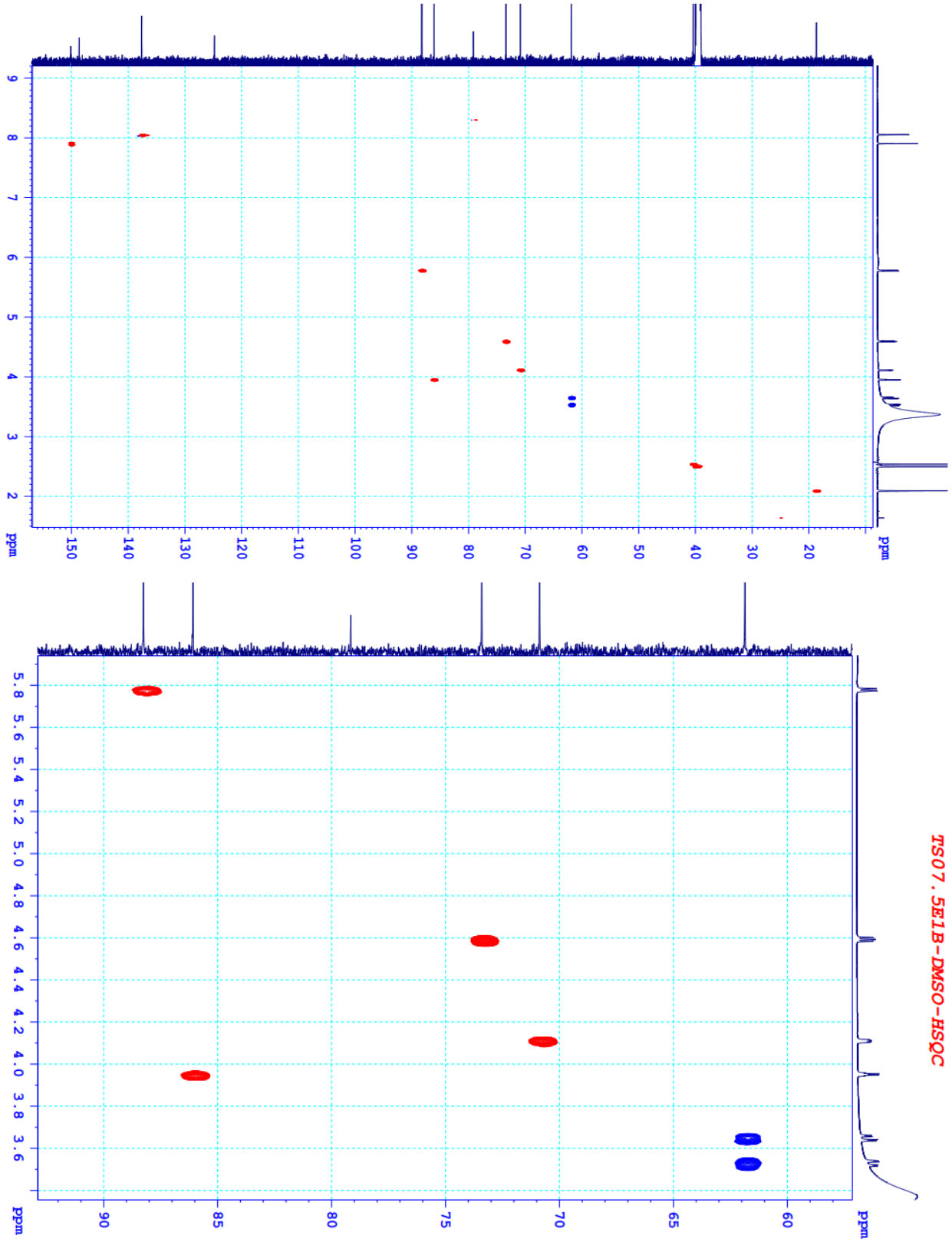


Figure S13: HSQC spectrum of compound **2** in DMSO-d_6

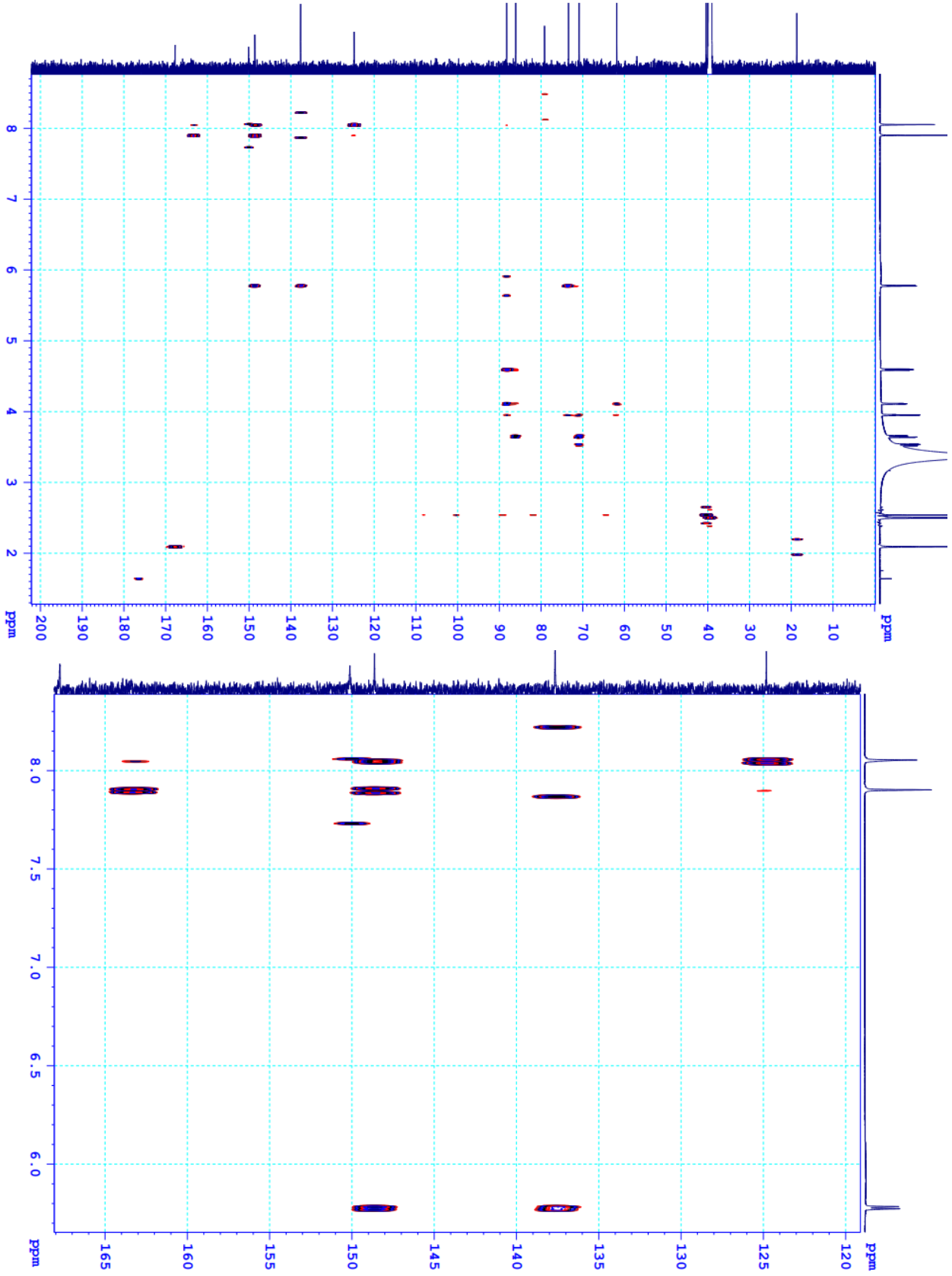


Figure S14: HMBC spectrum of compound **2** in DMSO-d_6

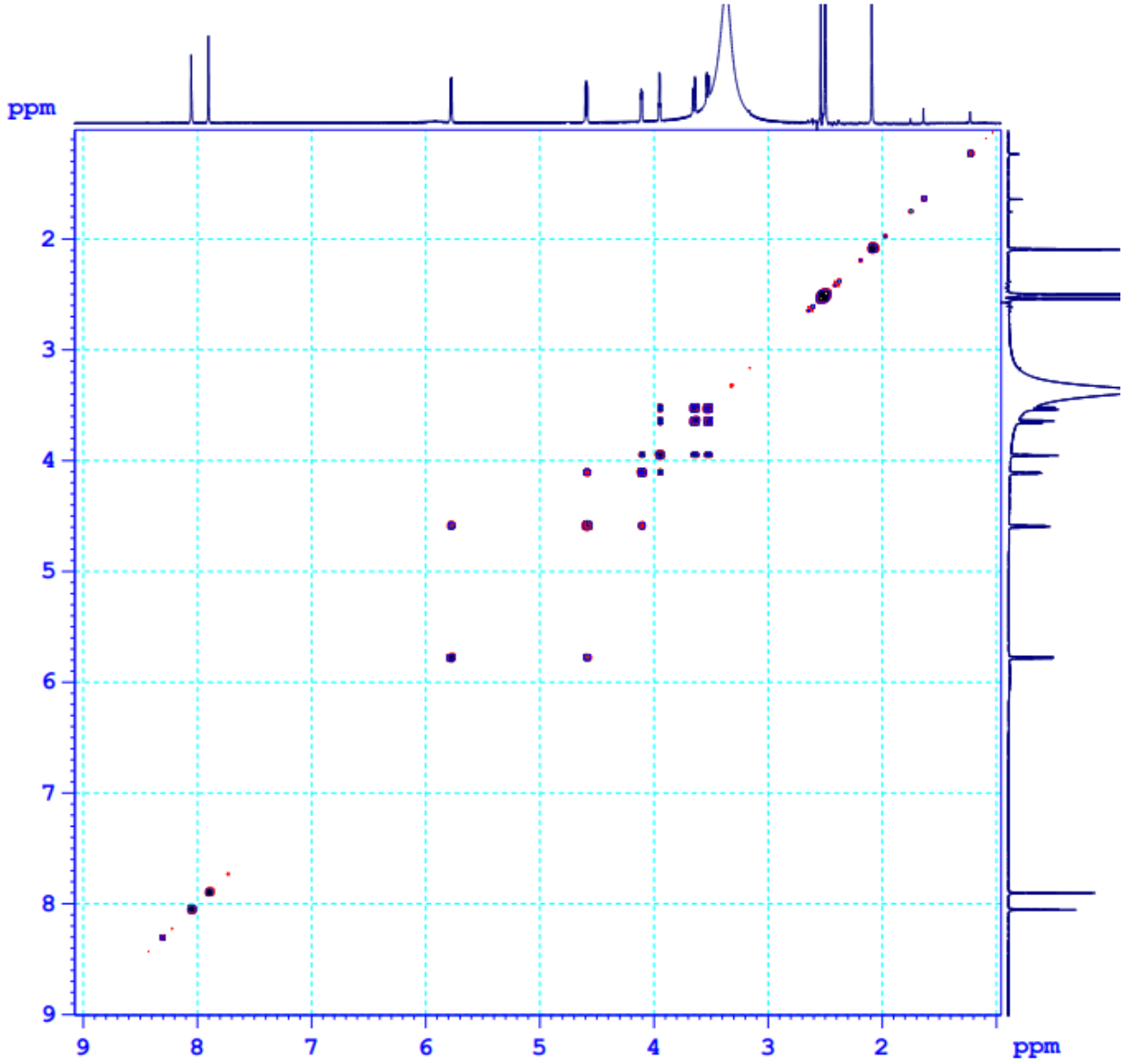


Figure S15: ^{1}H-^{1}H COSY spectrum of compound **2** in DMSO-d_6

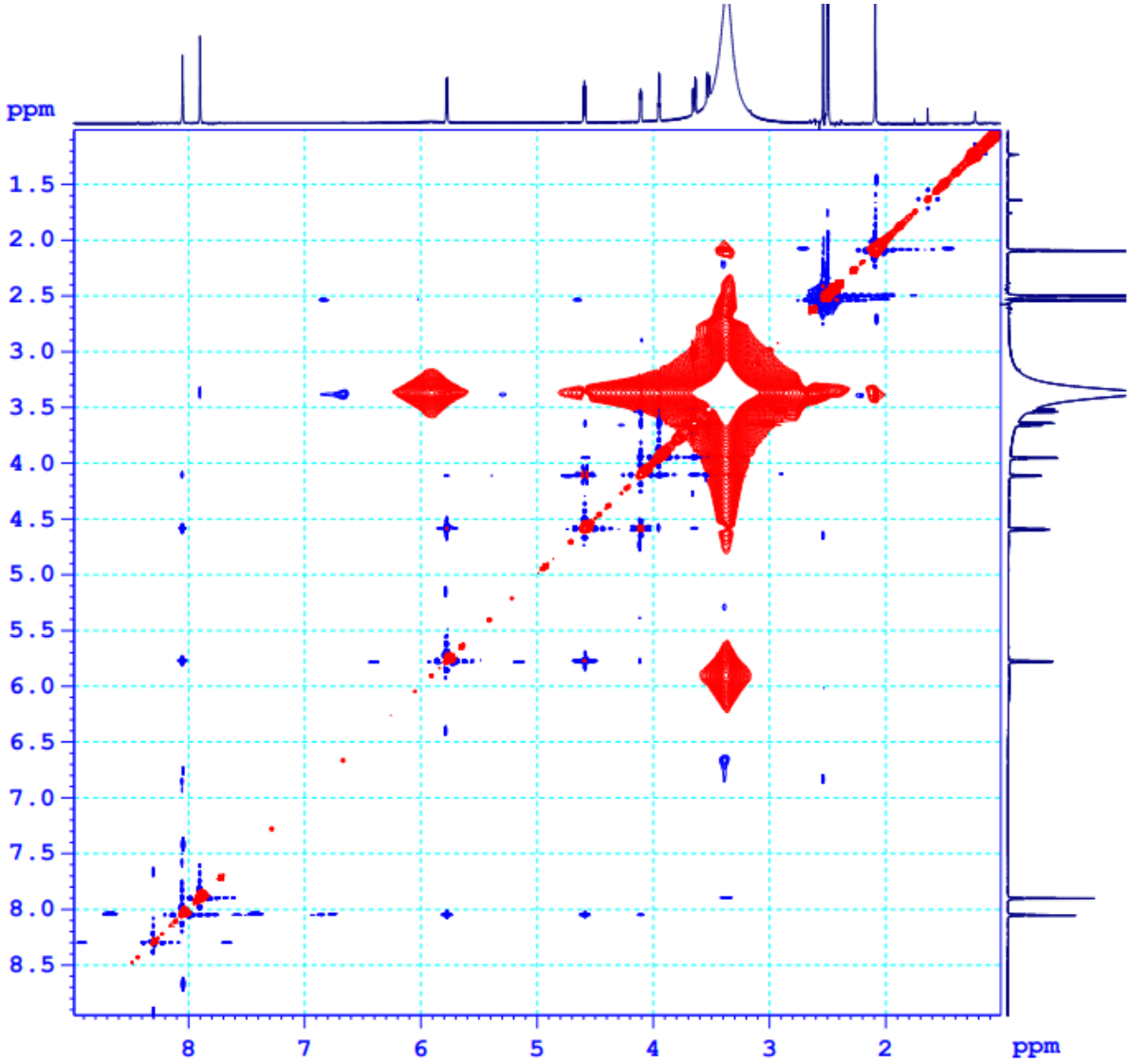


Figure S16: NOESY spectrum of compound **2** in DMSO-d_6

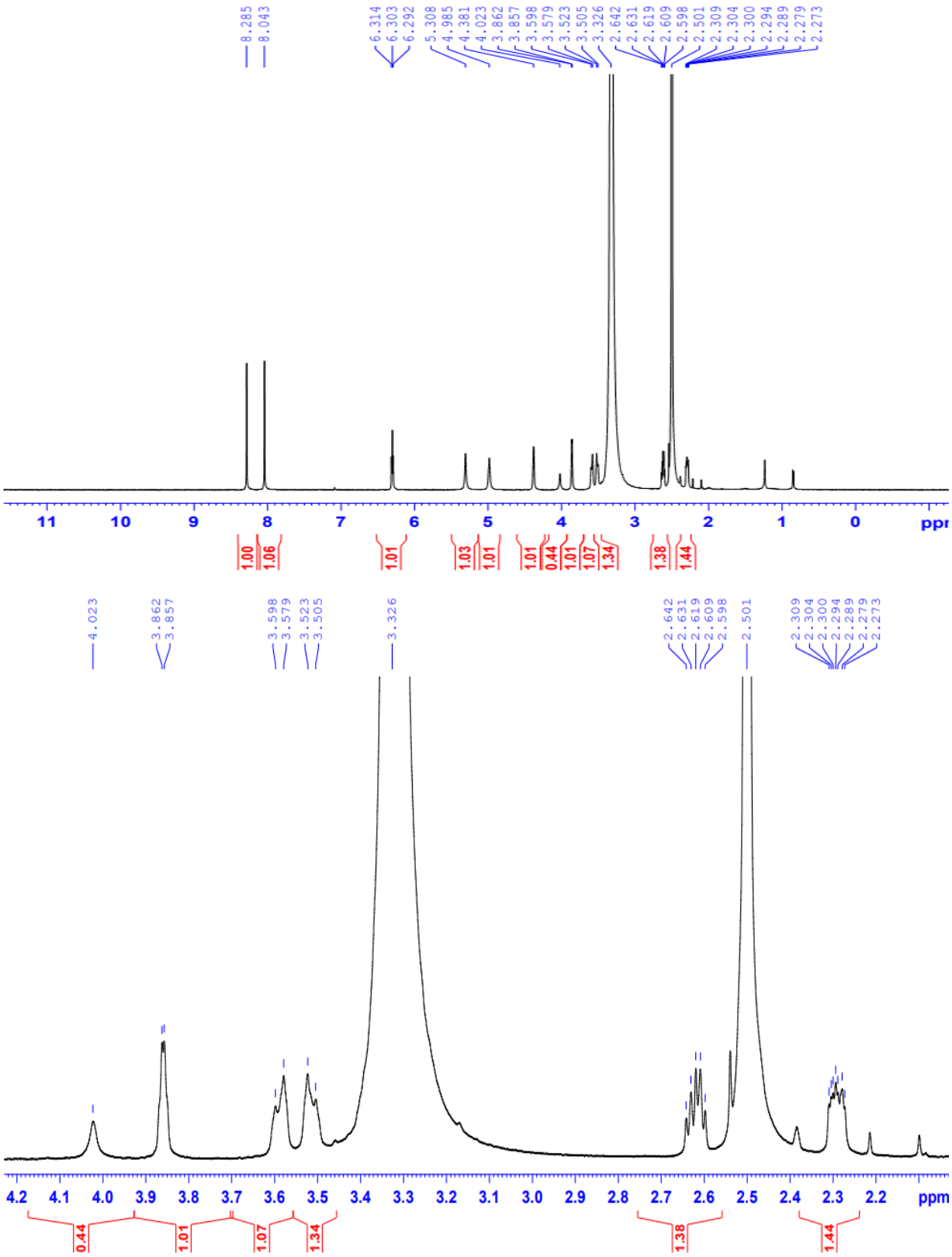


Figure S17: ^{1}H NMR spectrum of compound **3** in DMSO-d_6

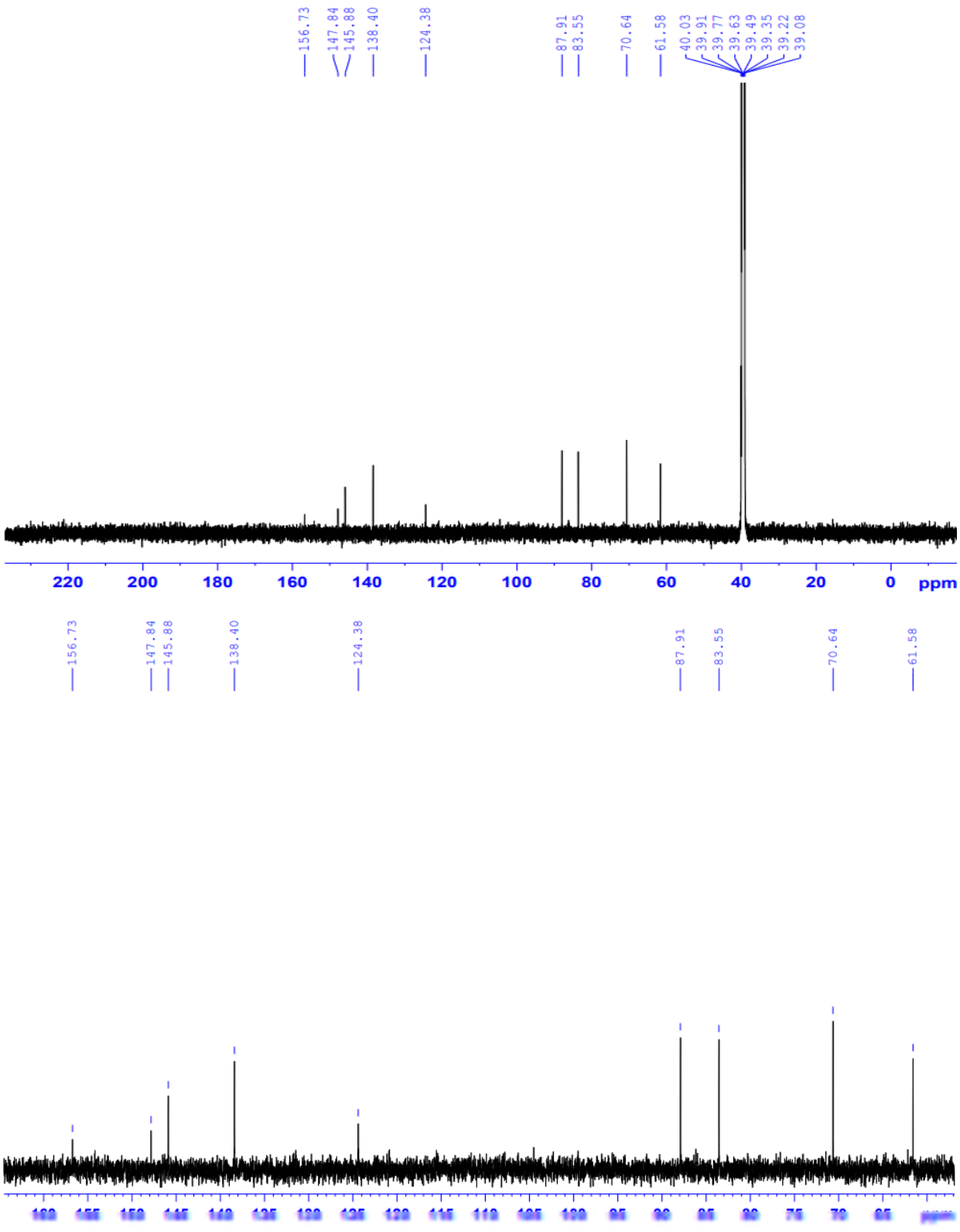


Figure S18: ^{13}C NMR spectrum of compound **3** in DMSO-d_6

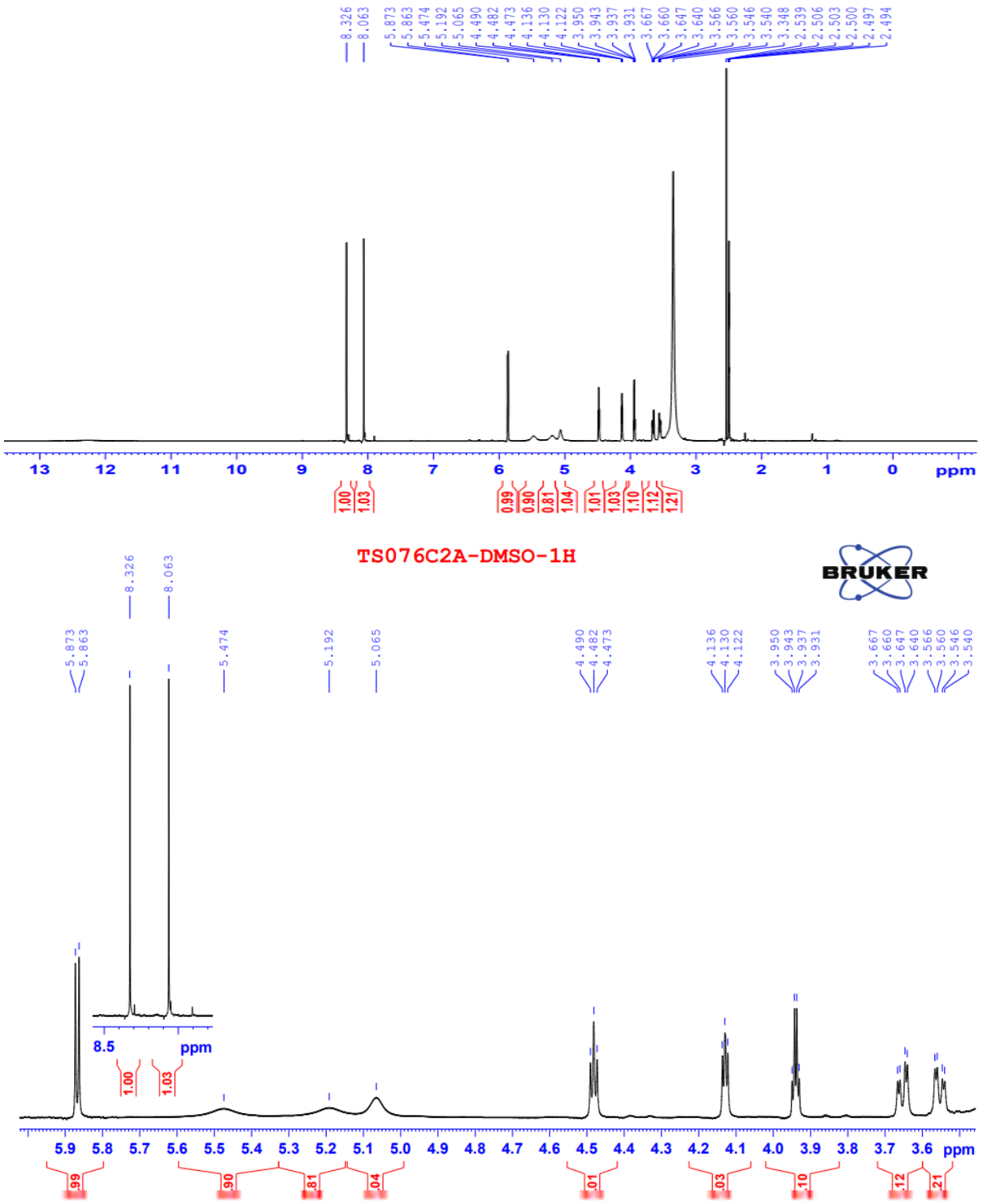


Figure S19: ^{1}H NMR spectrum of compound **4** in DMSO-d_6

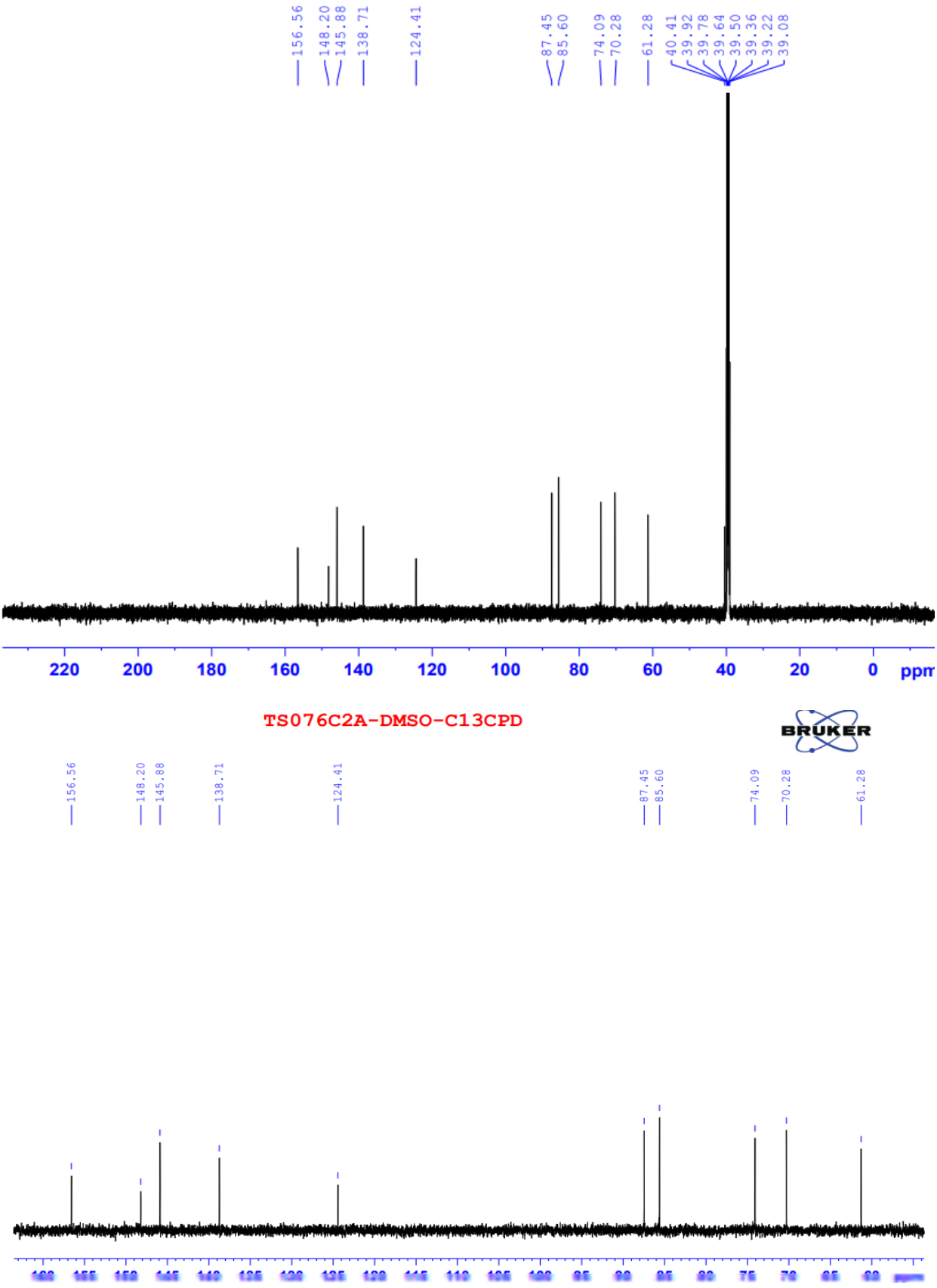


Figure S20: ^{13}C NMR spectrum of compound **4** in DMSO-d_6

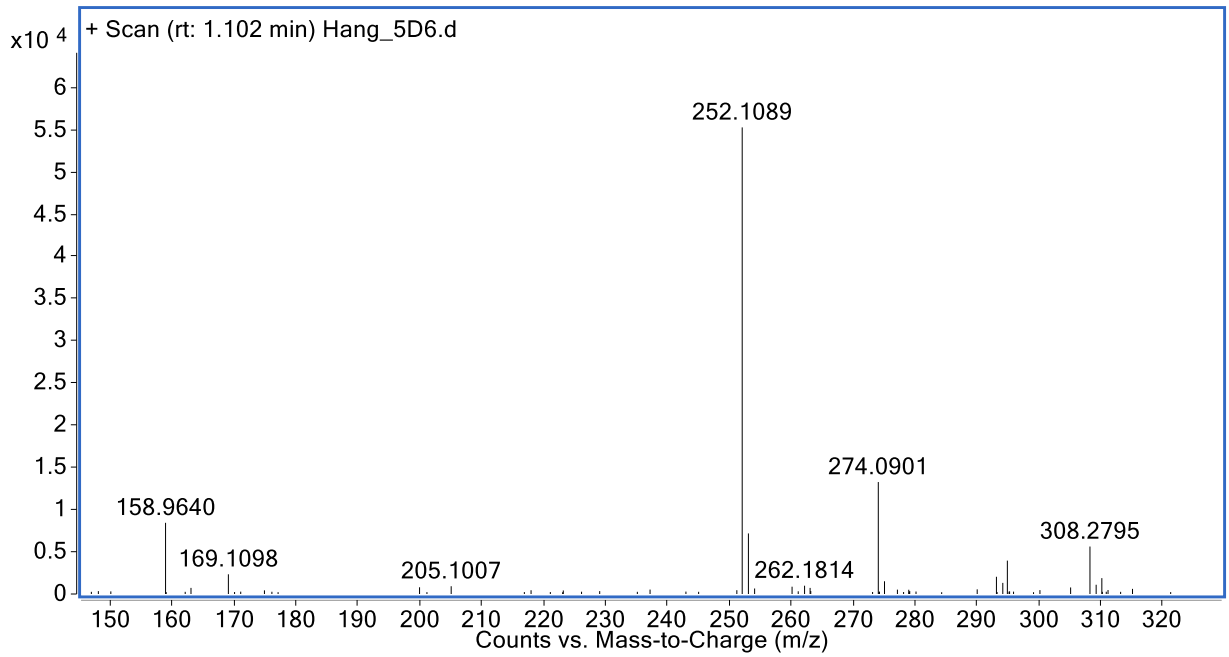


Figure S21: HRESIMS spectrum of compound **5**

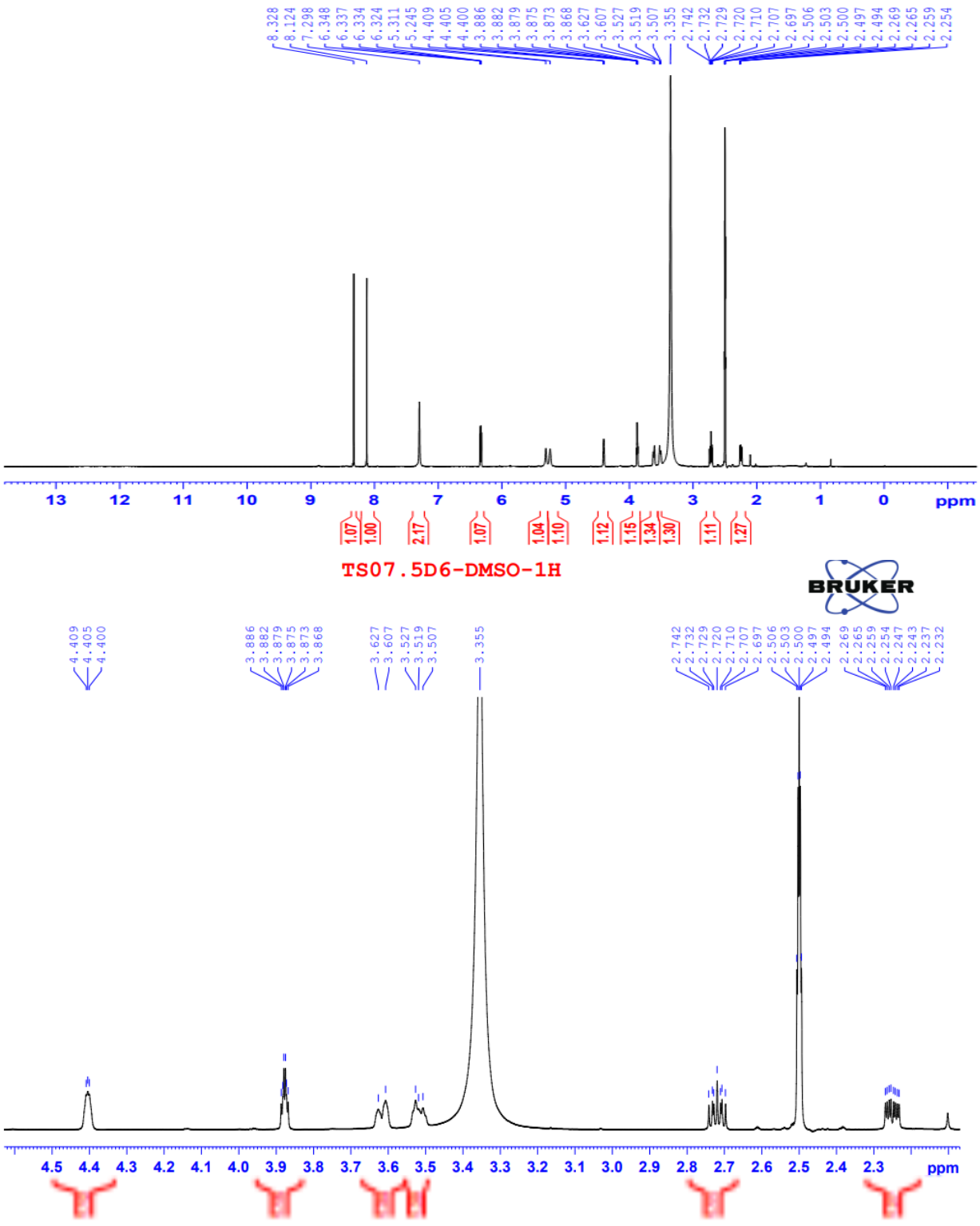


Figure S22: ^{1}H NMR spectrum of compound **5** in DMSO-d_6

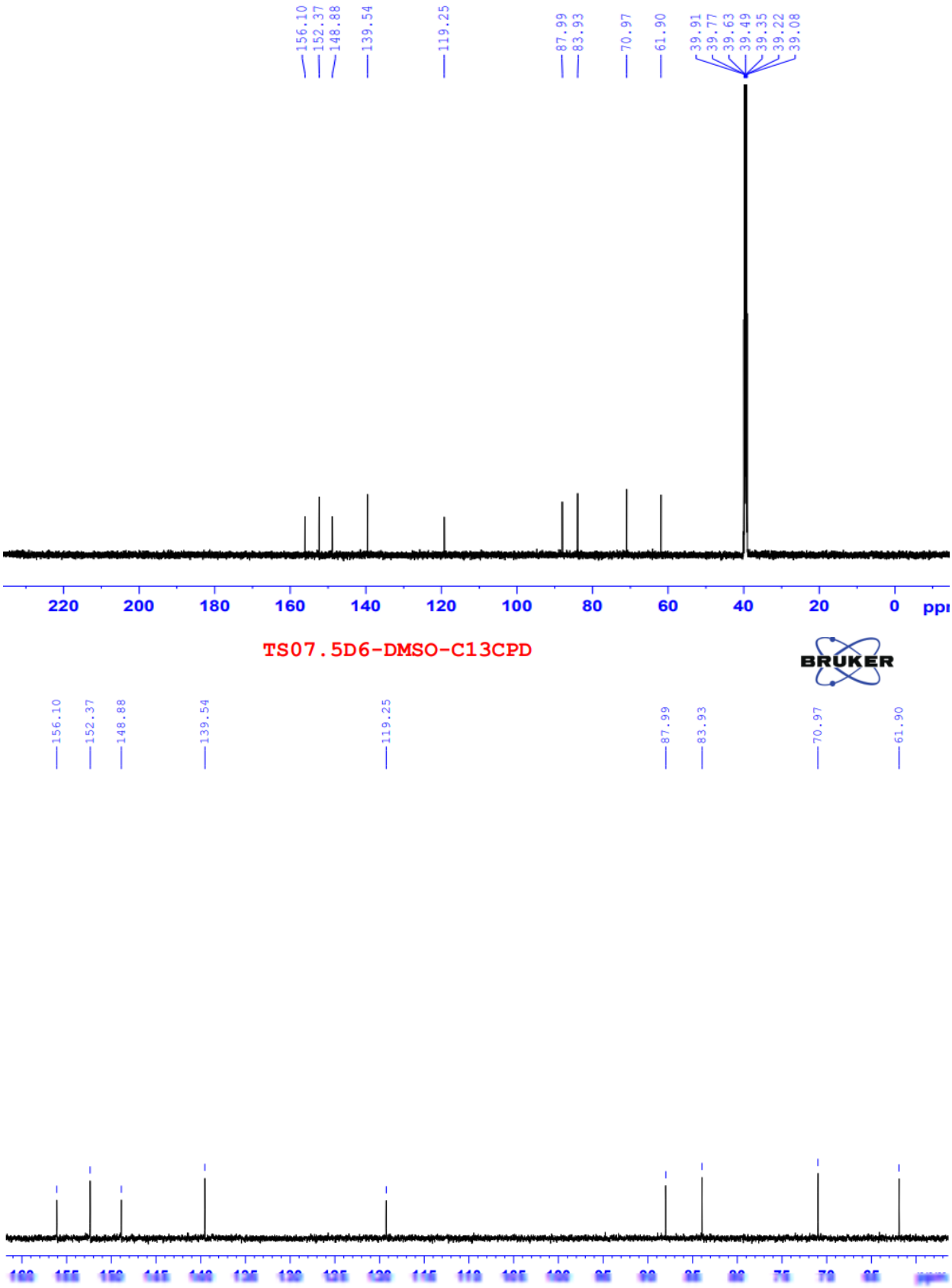


Figure S23: ^{13}C NMR spectrum of compound **5** in DMSO-d_6

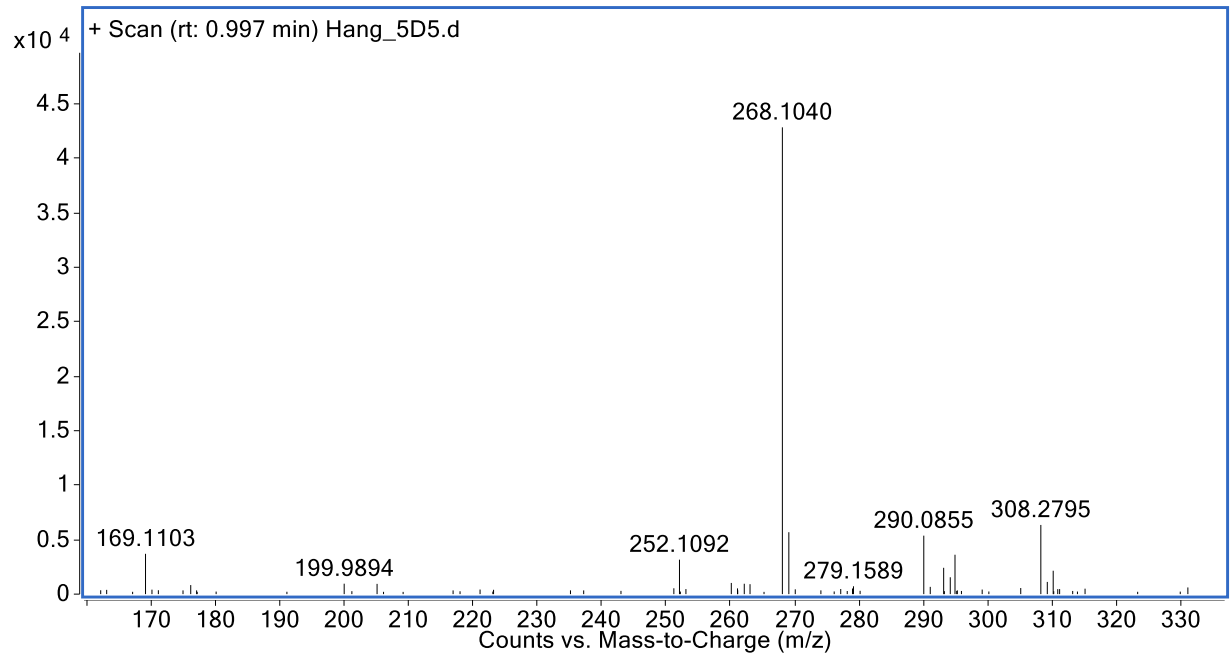


Figure S24: HRESIMS spectrum of compound **6**

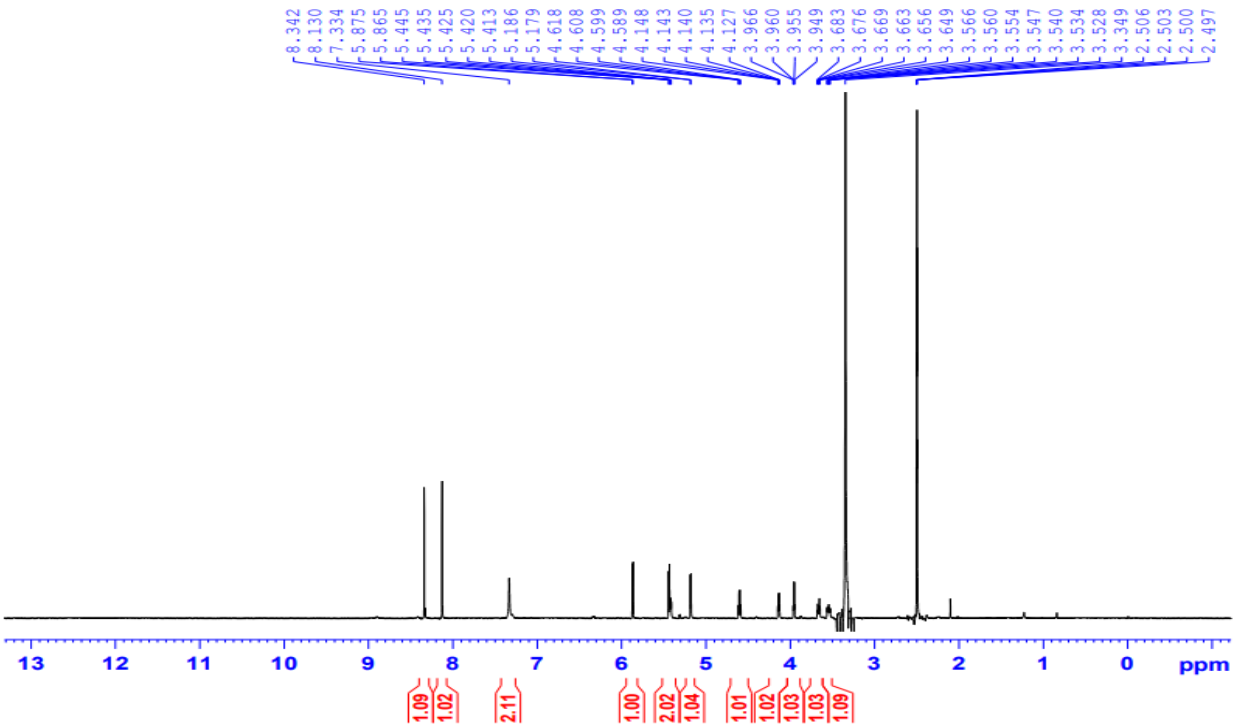


Figure S25: ^{1}H NMR spectrum of compound **6** in DMSO-d_6

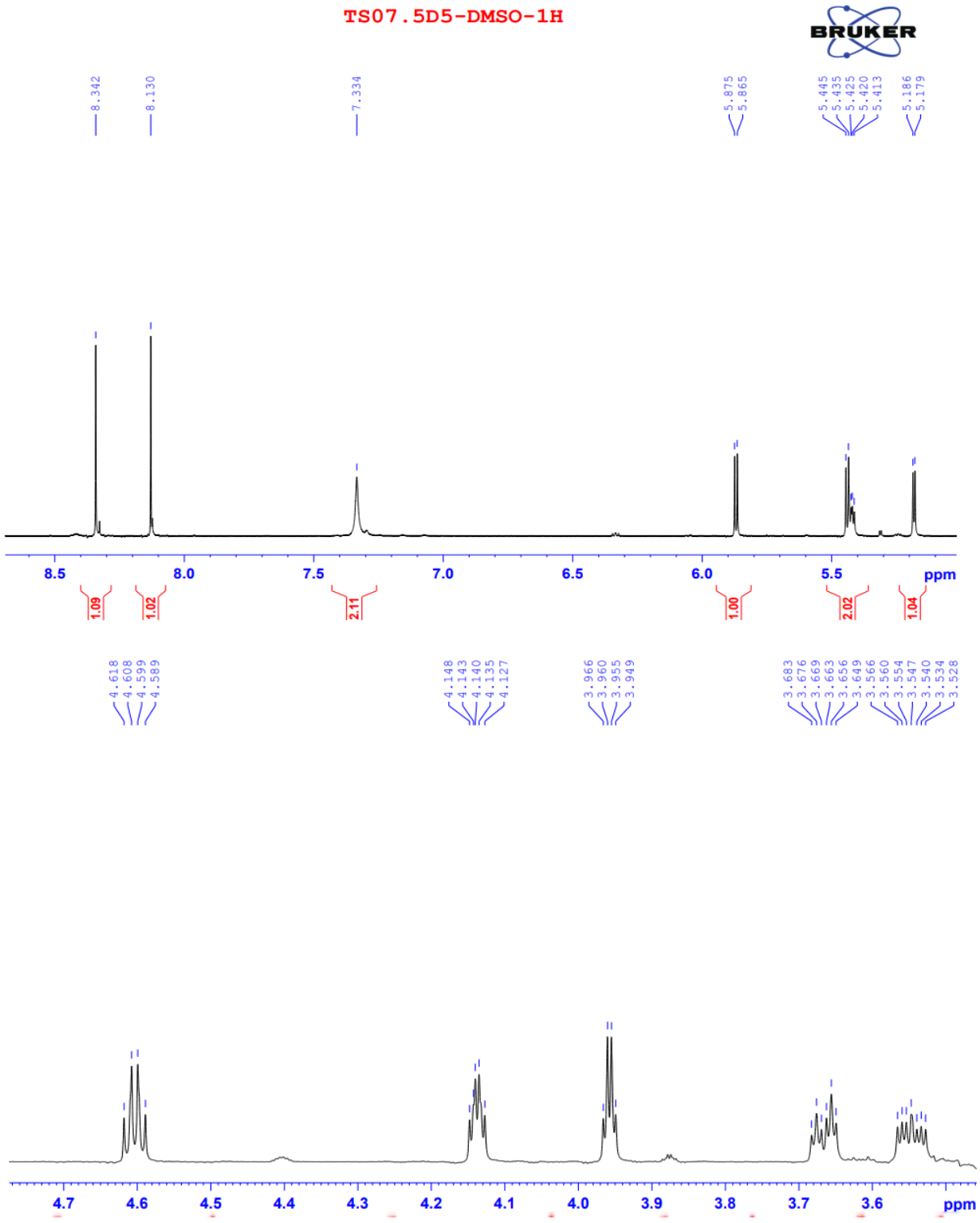


Figure S26: Extened ^{1}H NMR spectrum of compound **6** in DMSO-d_6

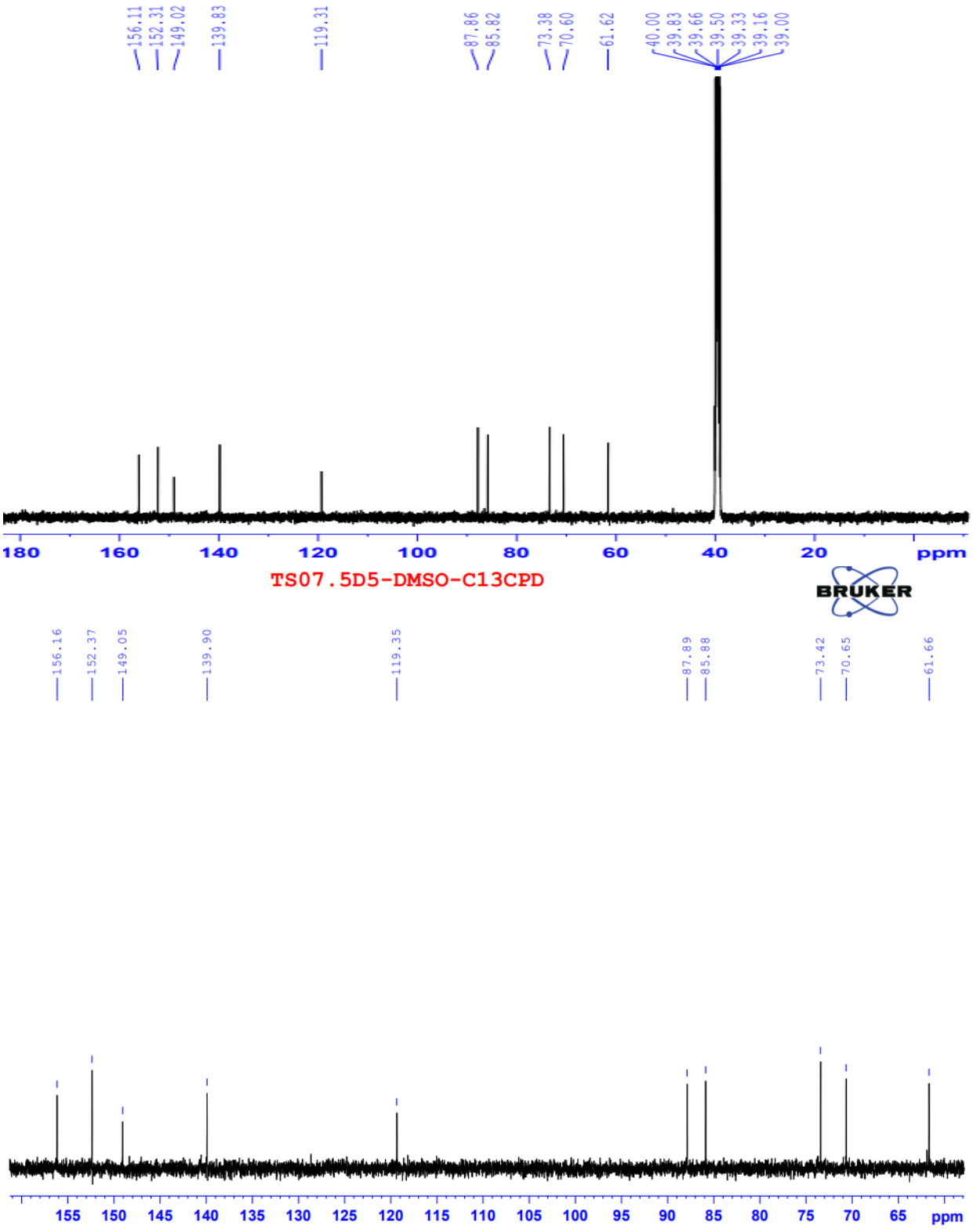


Figure S27: ^{13}C NMR spectrum of compound **6** in DMSO-d_6

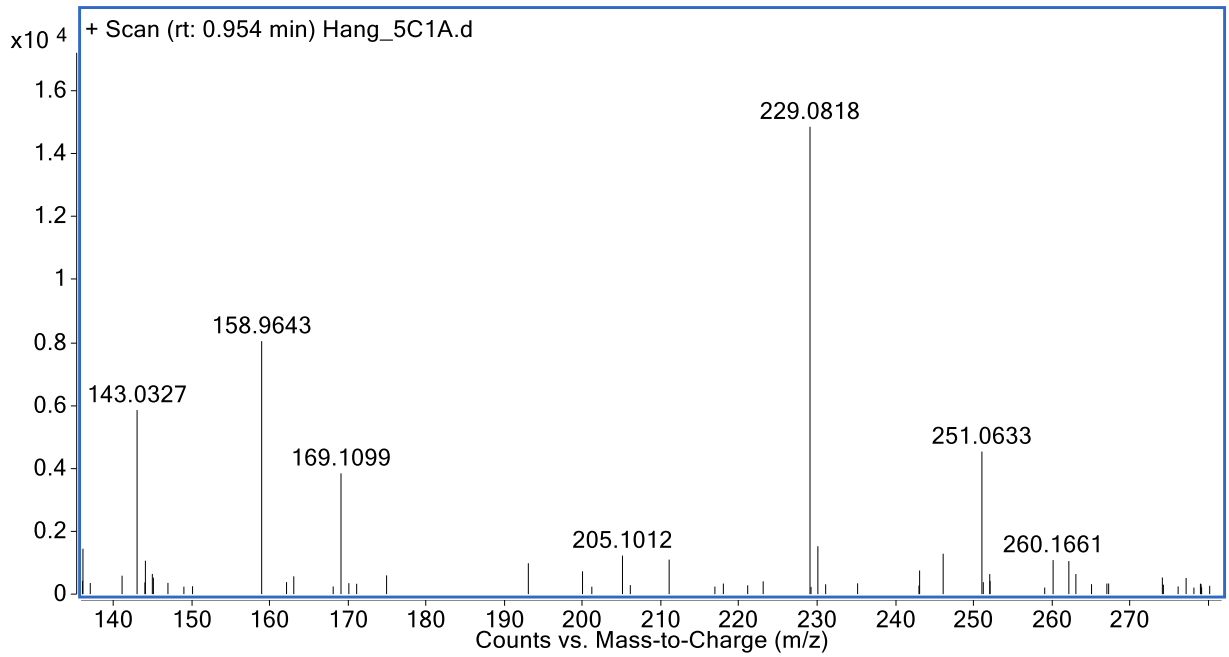


Figure S28: HRESIMS spectrum of compound **7**

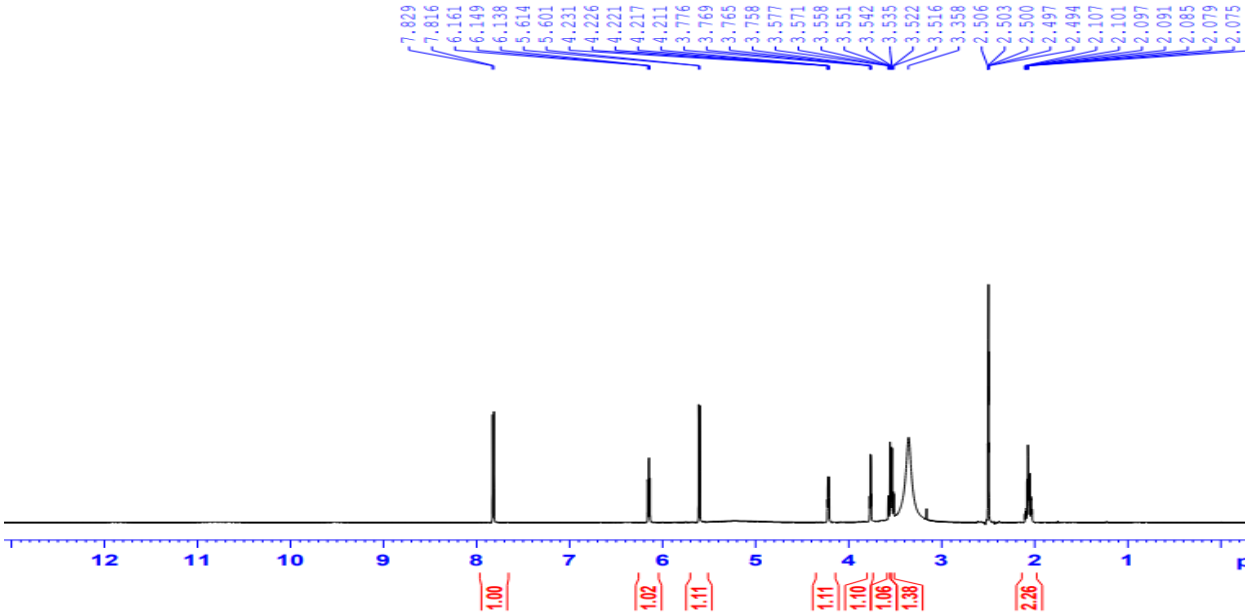


Figure S29: ^{1}H NMR spectrum of compound **7** in DMSO-d_6

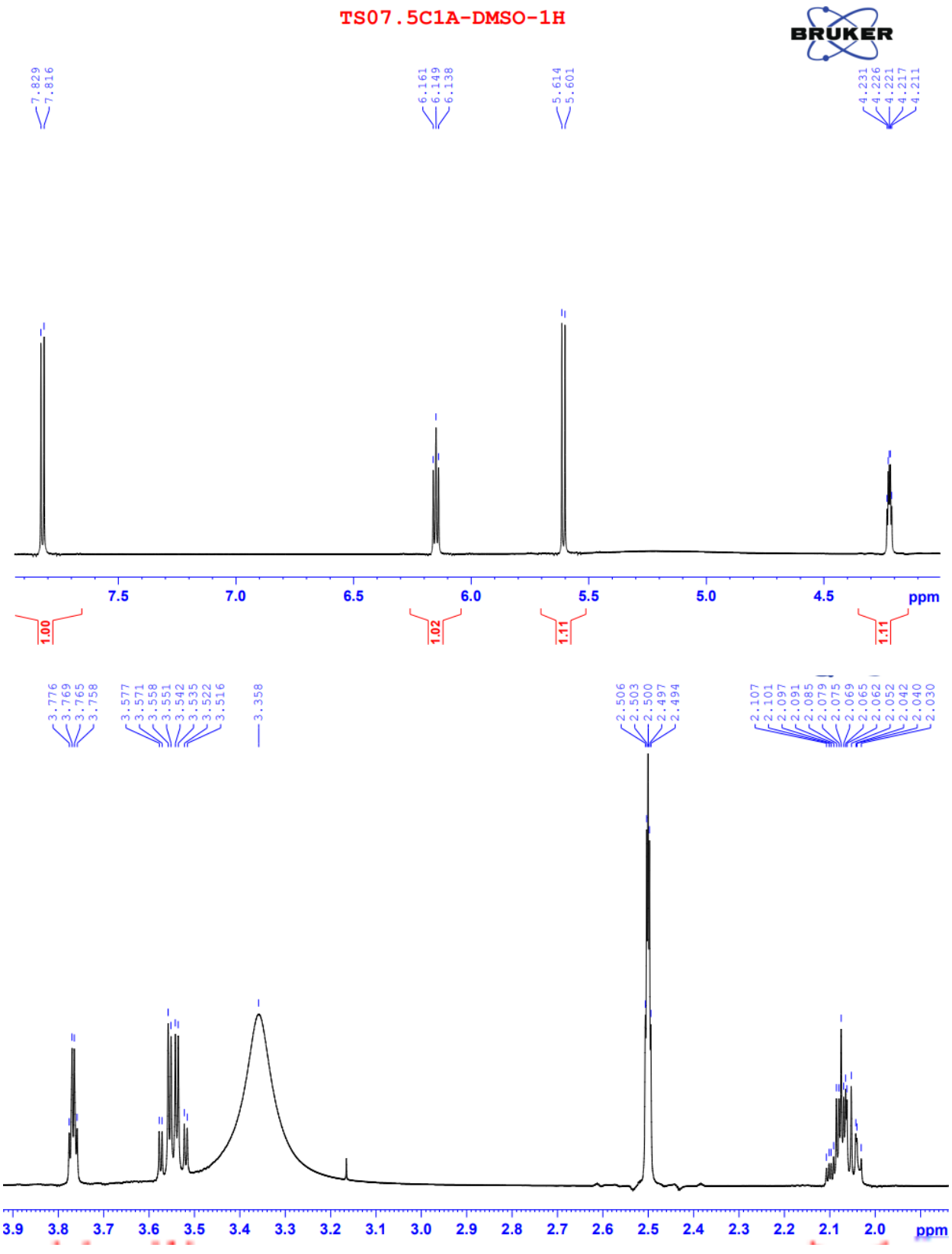


Figure S30: Extended ^{1}H NMR spectrum of compound **7** in DMSO-d_6

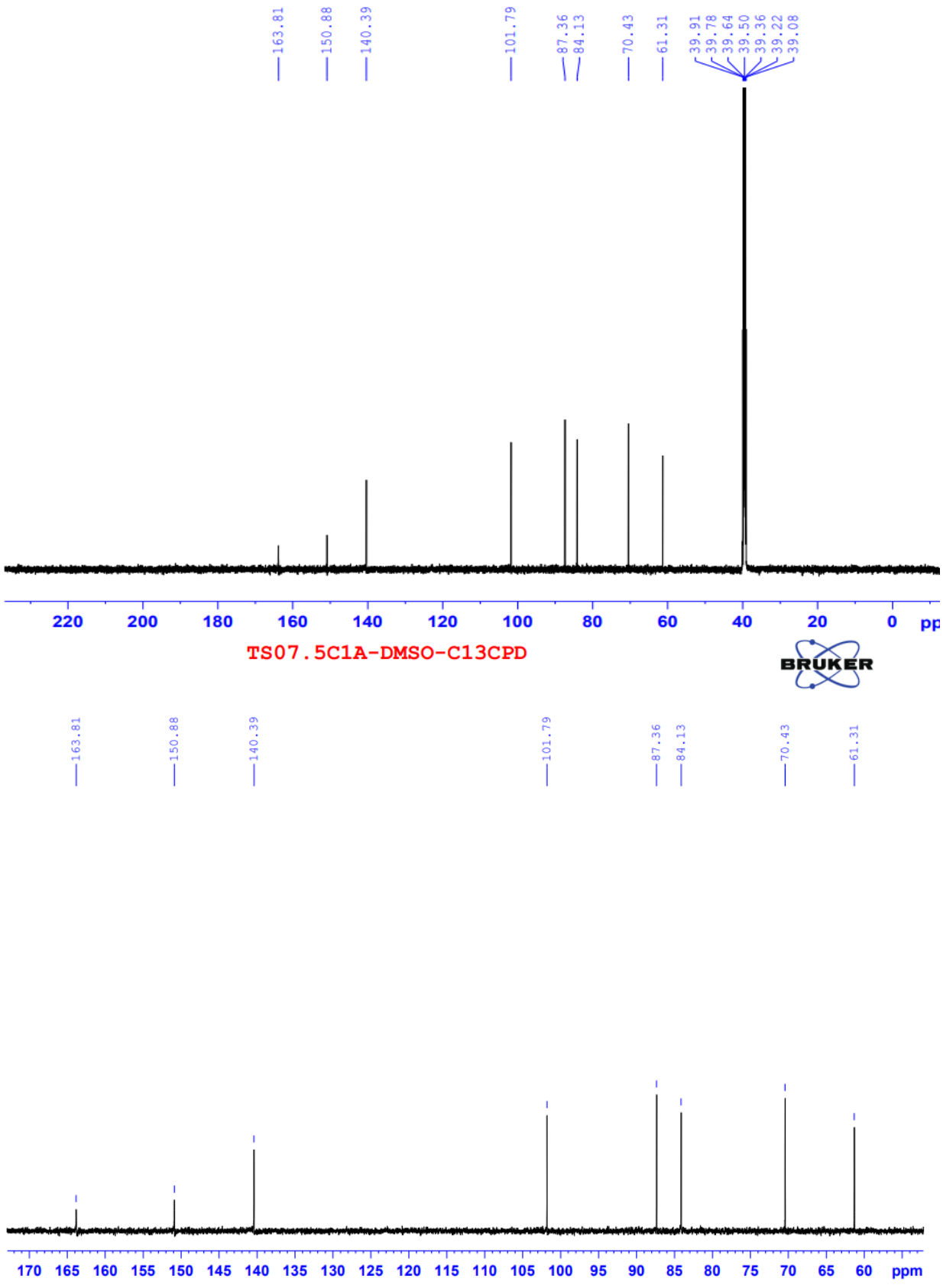


Figure S31: ^{13}C NMR spectrum of compound **7** in DMSO-d_6

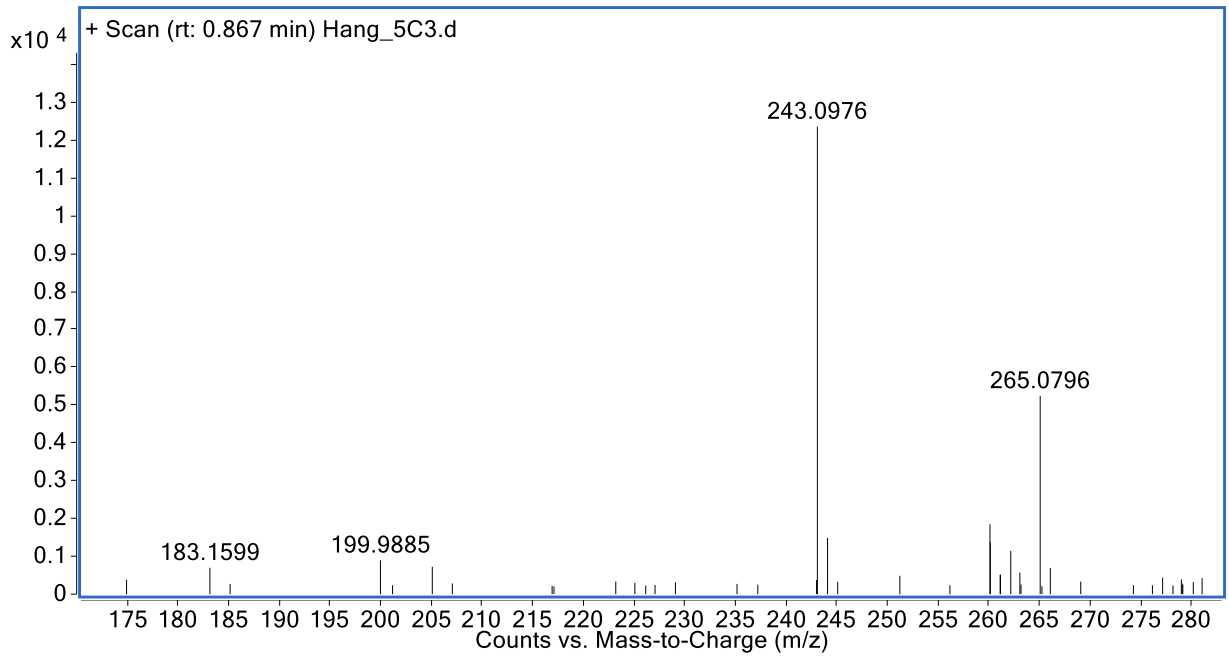


Figure S32: HRESIMS spectrum of compound **8**

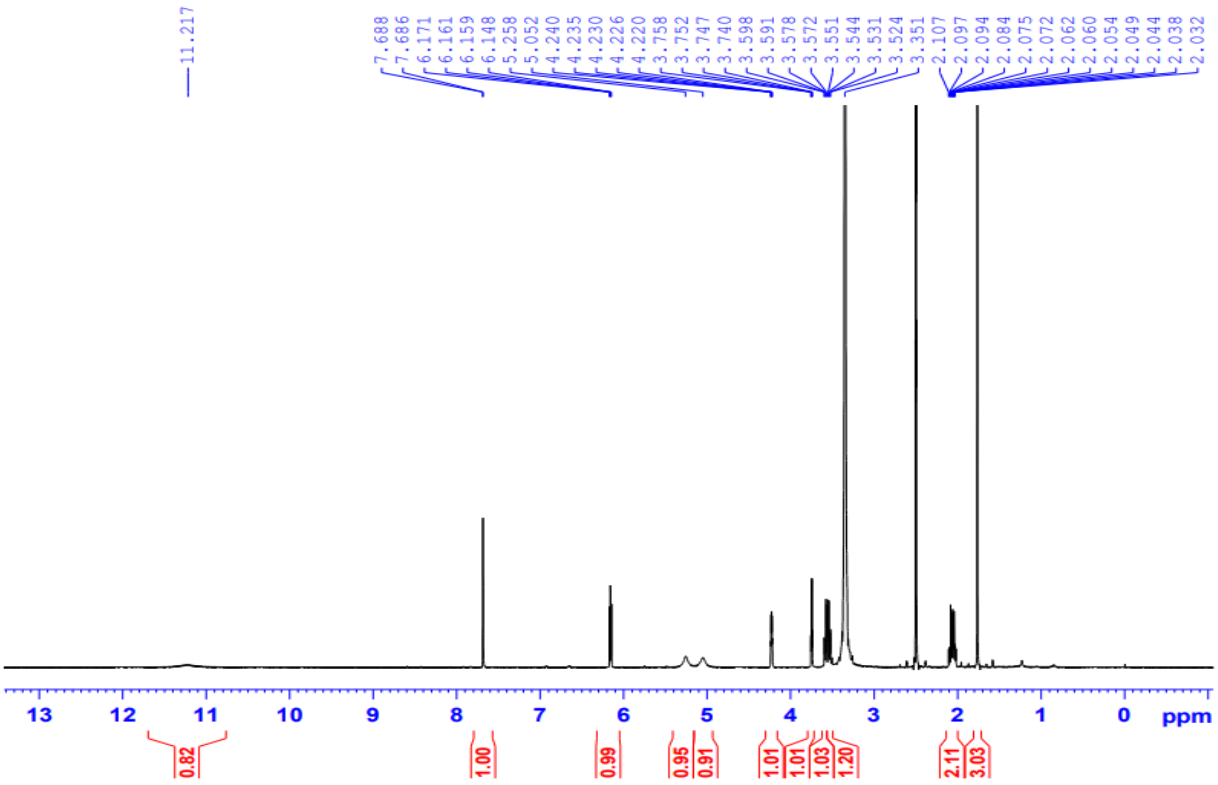


Figure S33: ^{1}H NMR spectrum of compound **8** in DMSO-d_6

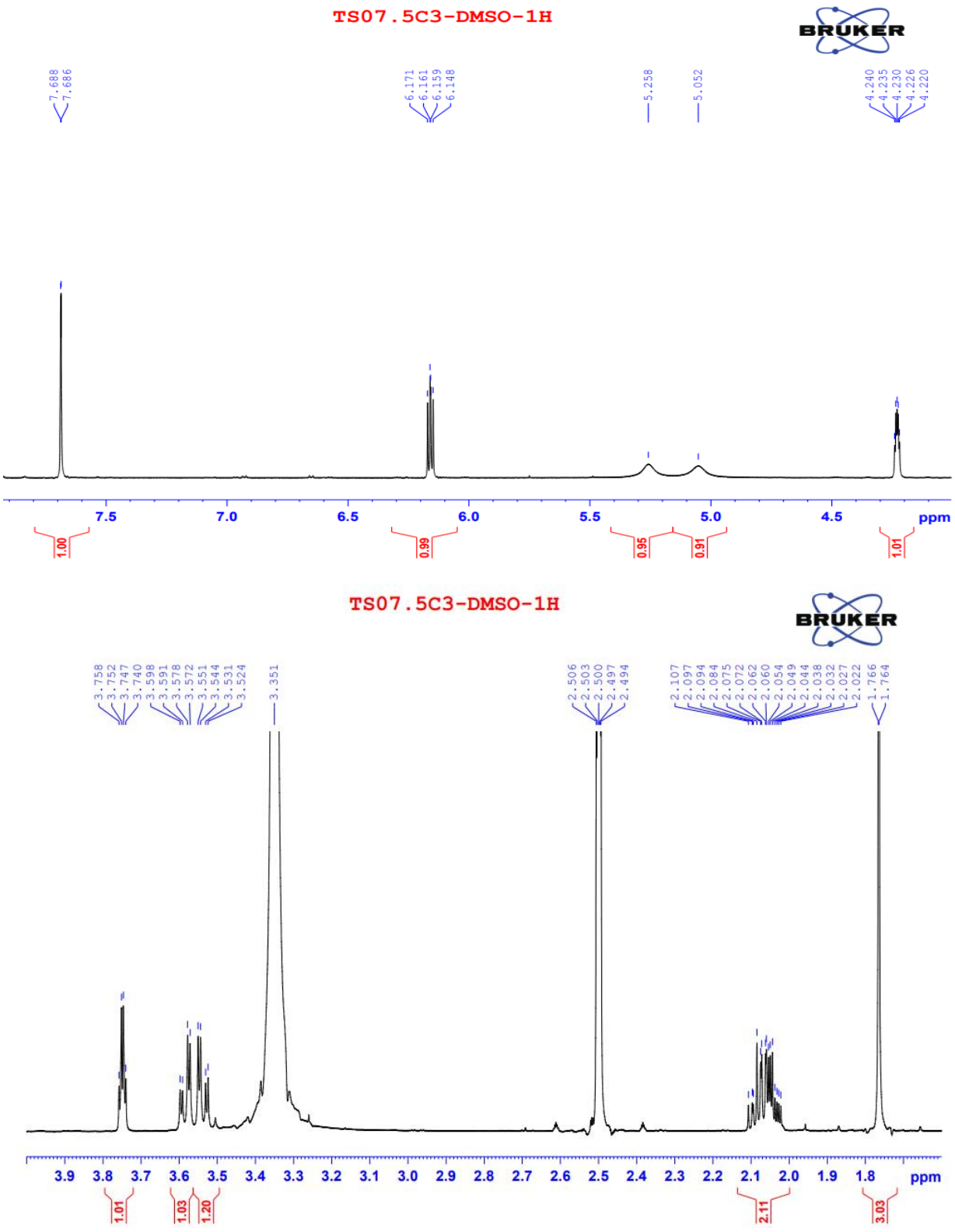


Figure S34: Extended ^{1}H NMR spectrum of compound **8** in DMSO-d_6

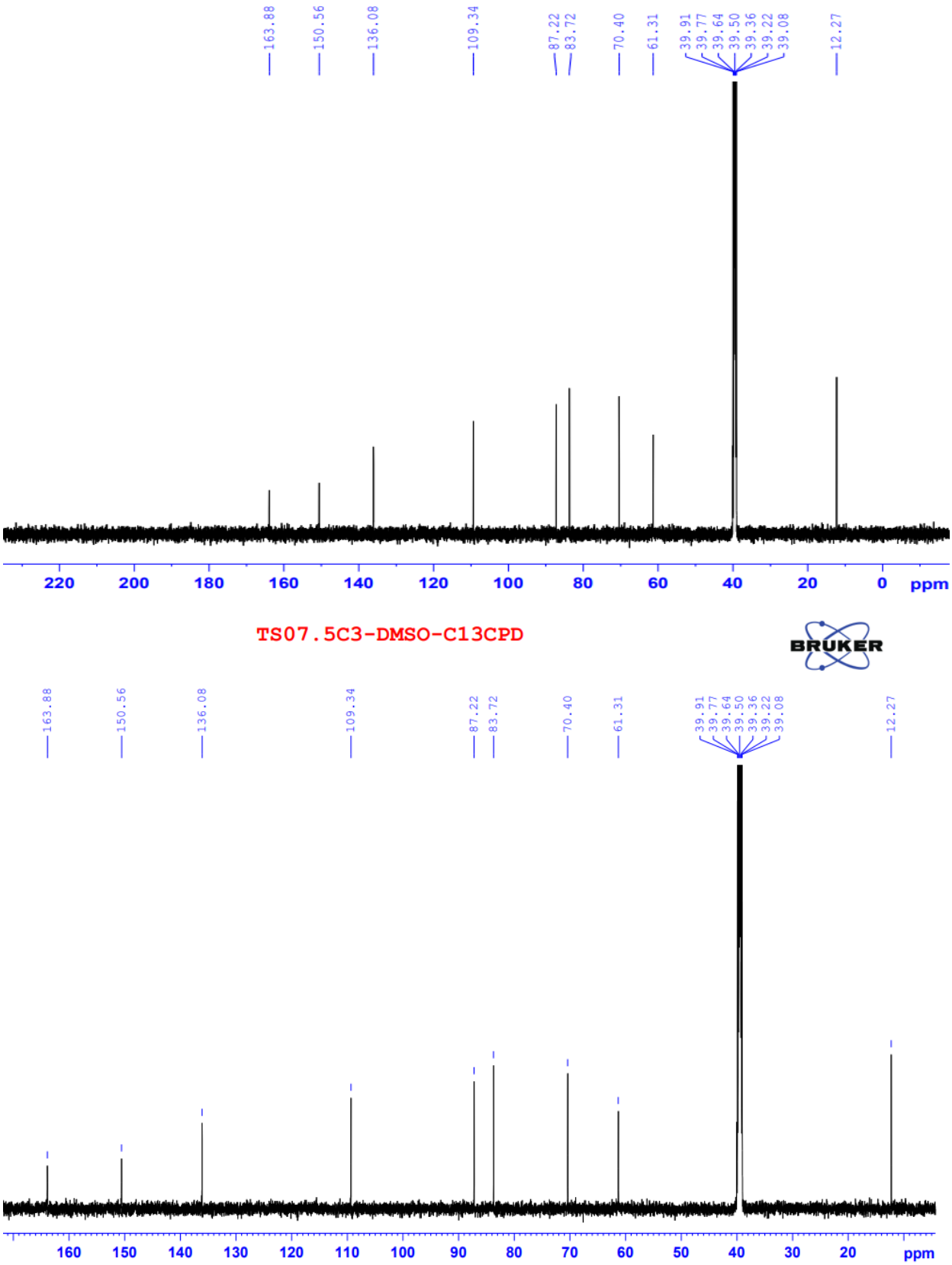


Figure S35: ^{13}C NMR spectrum of compound **8** in DMSO-d_6

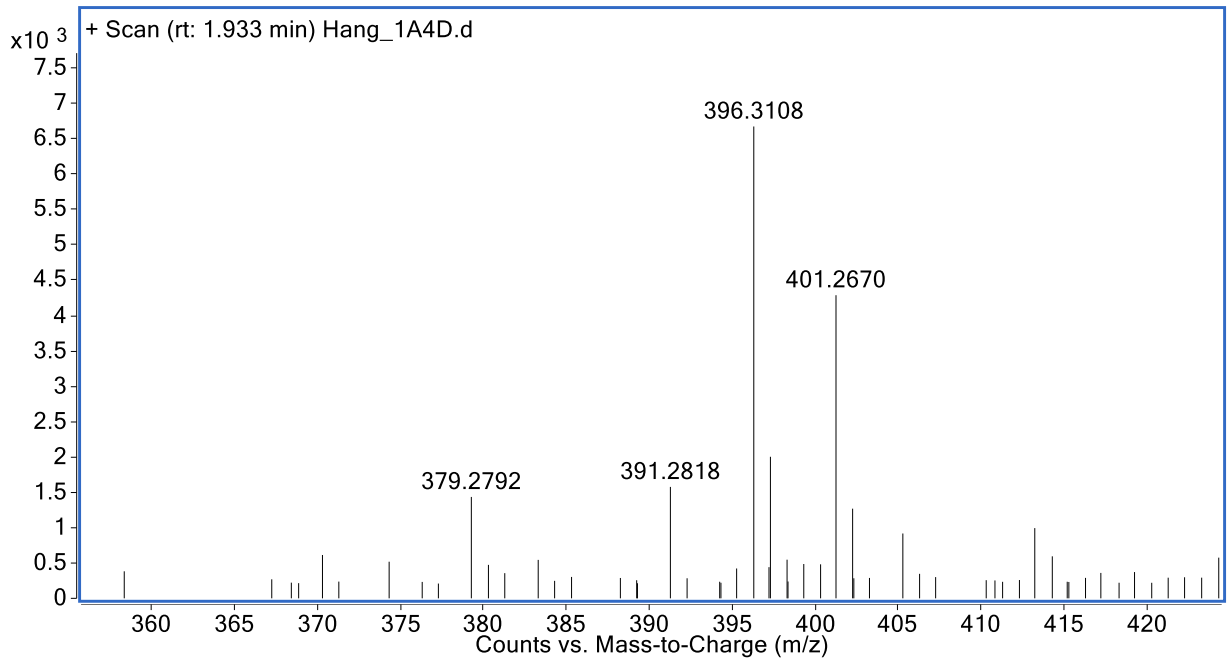


Figure S36: HRESIMS spectrum of compound **9**

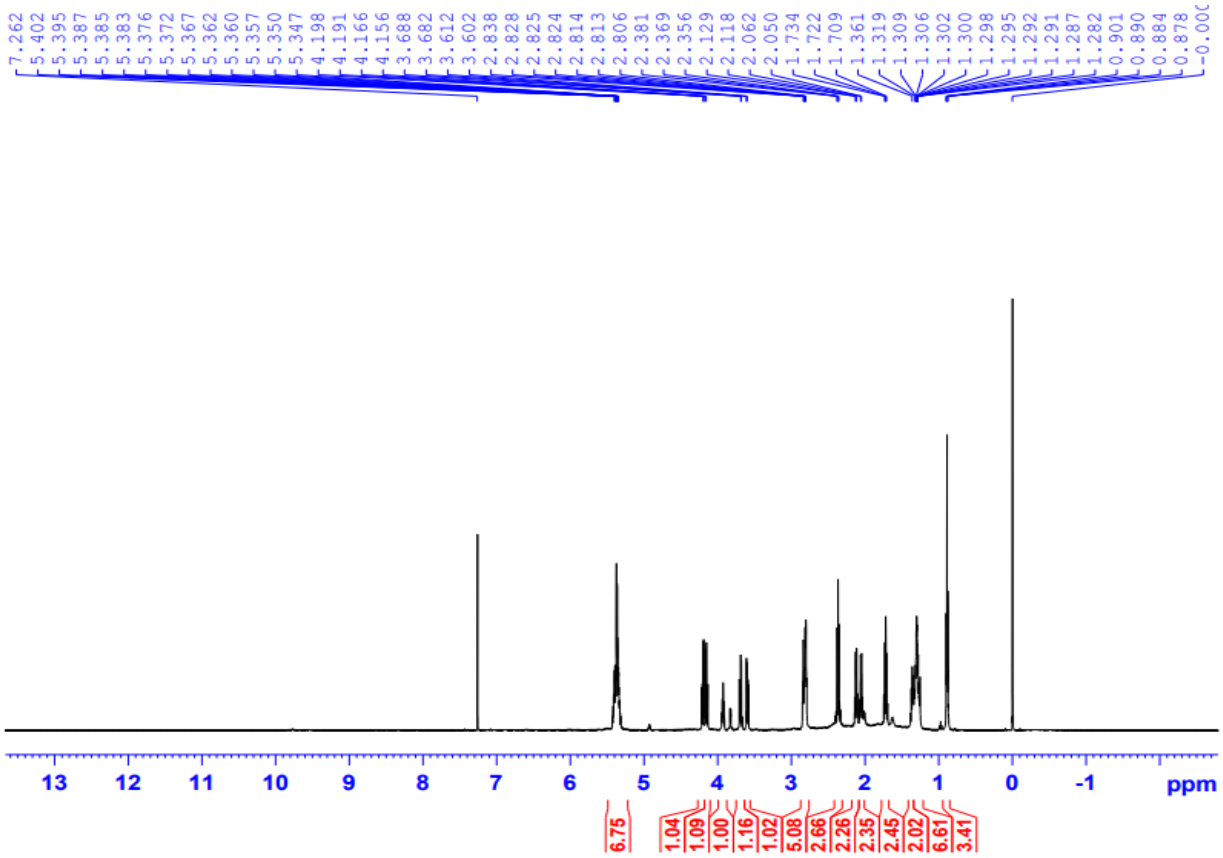


Figure S37: ^{1}H NMR spectrum of compound **9** in $CDCl_3$

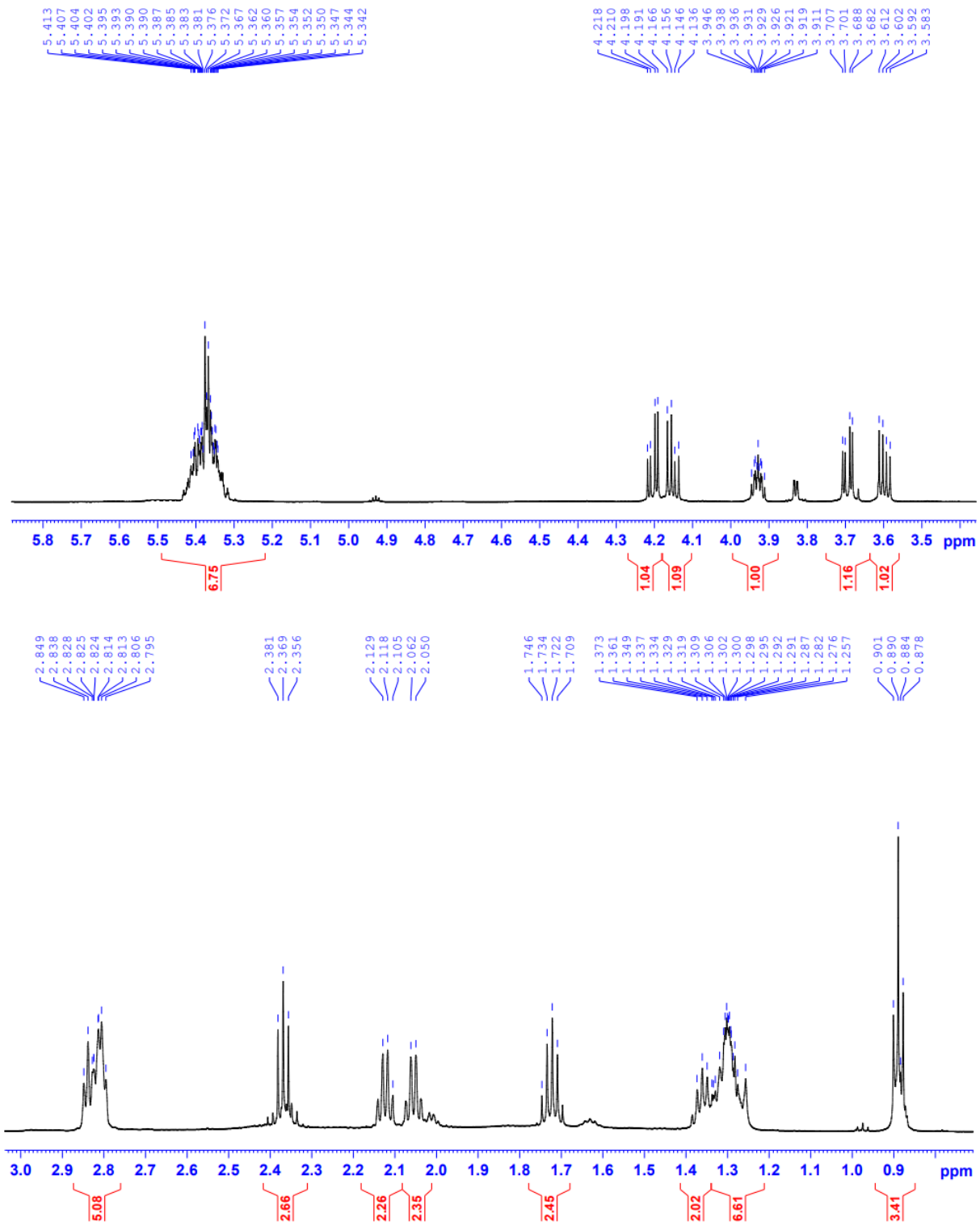


Figure S38: Extened ^{1}H NMR spectrum of compound **9** in $CDCl_3$

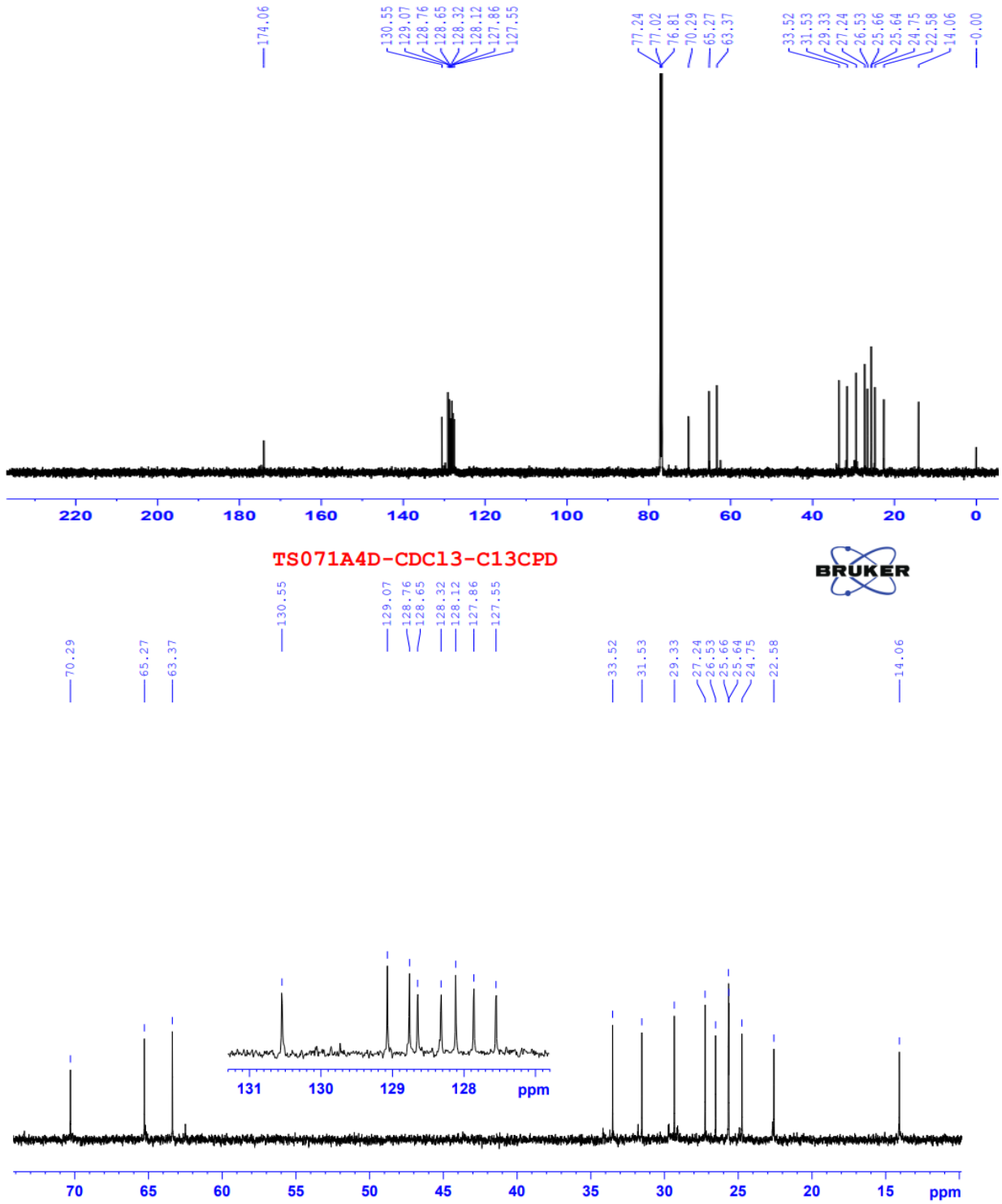


Figure S39: ^{1}H NMR spectrum of compound **9** in $CDCl_3$

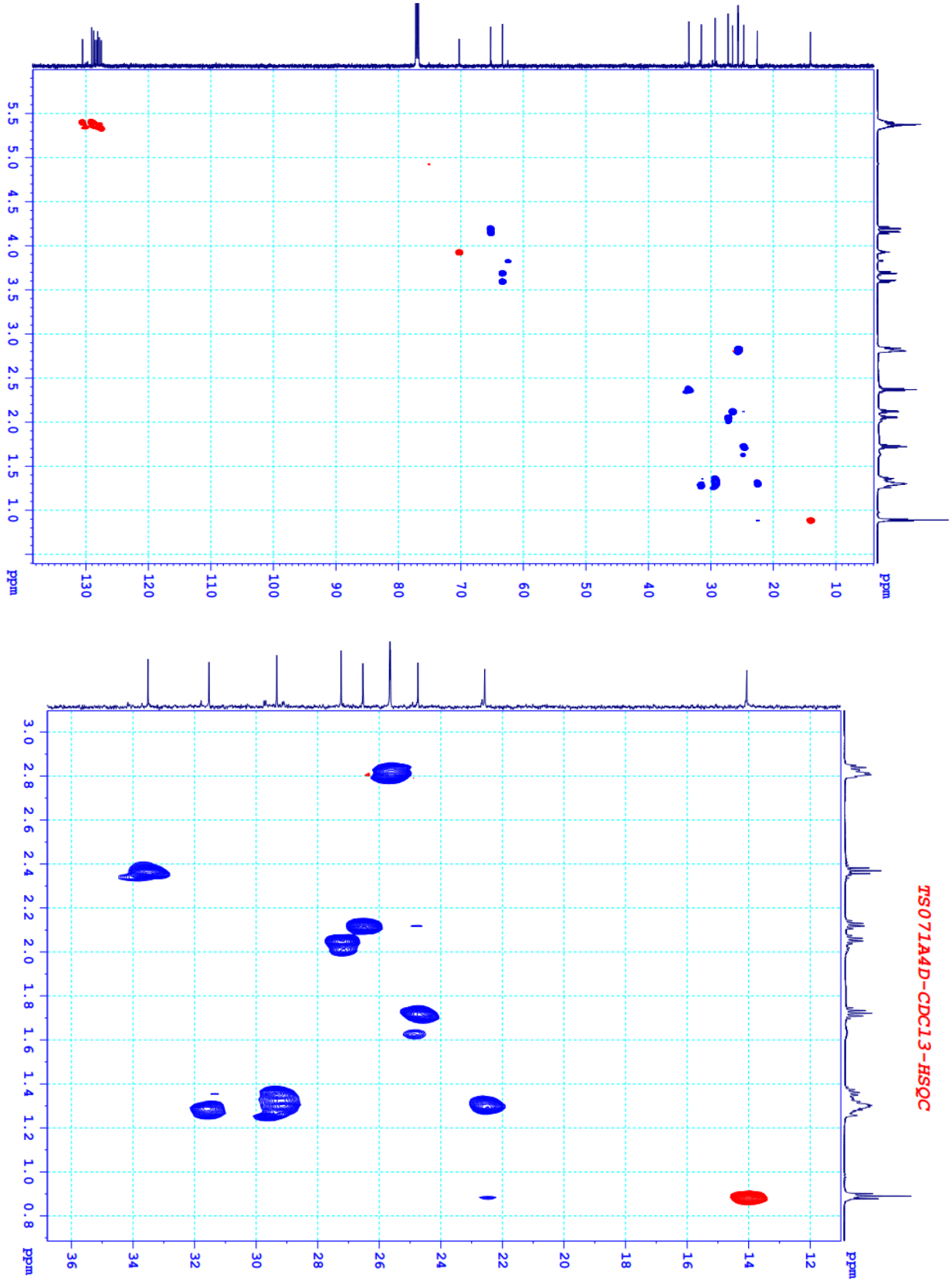


Figure S40: ^{1}H NMR spectrum of compound **9** in $CDCl_3$

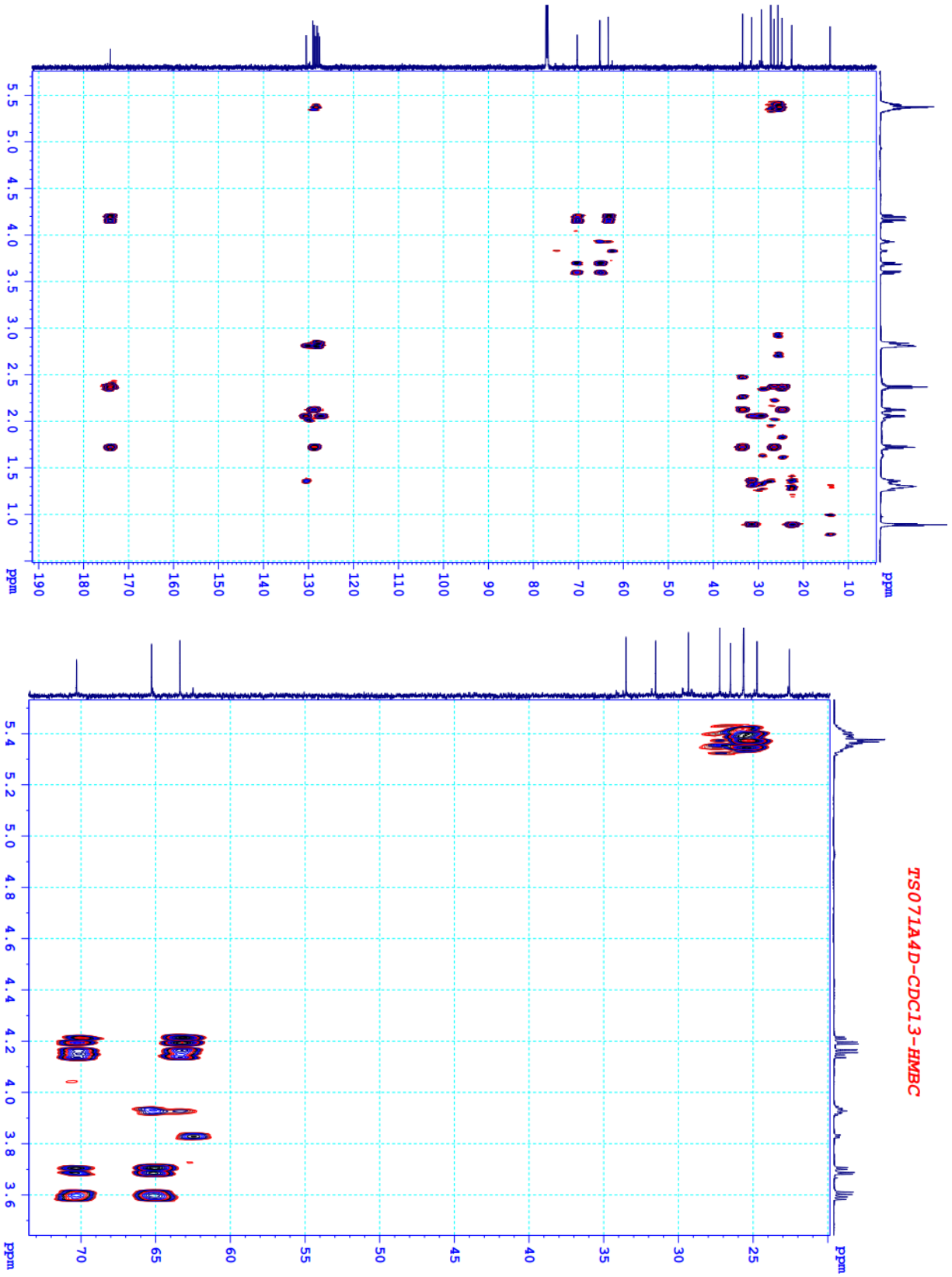


Figure S41: ^{1}H NMR spectrum of compound **9** in $CDCl_3$

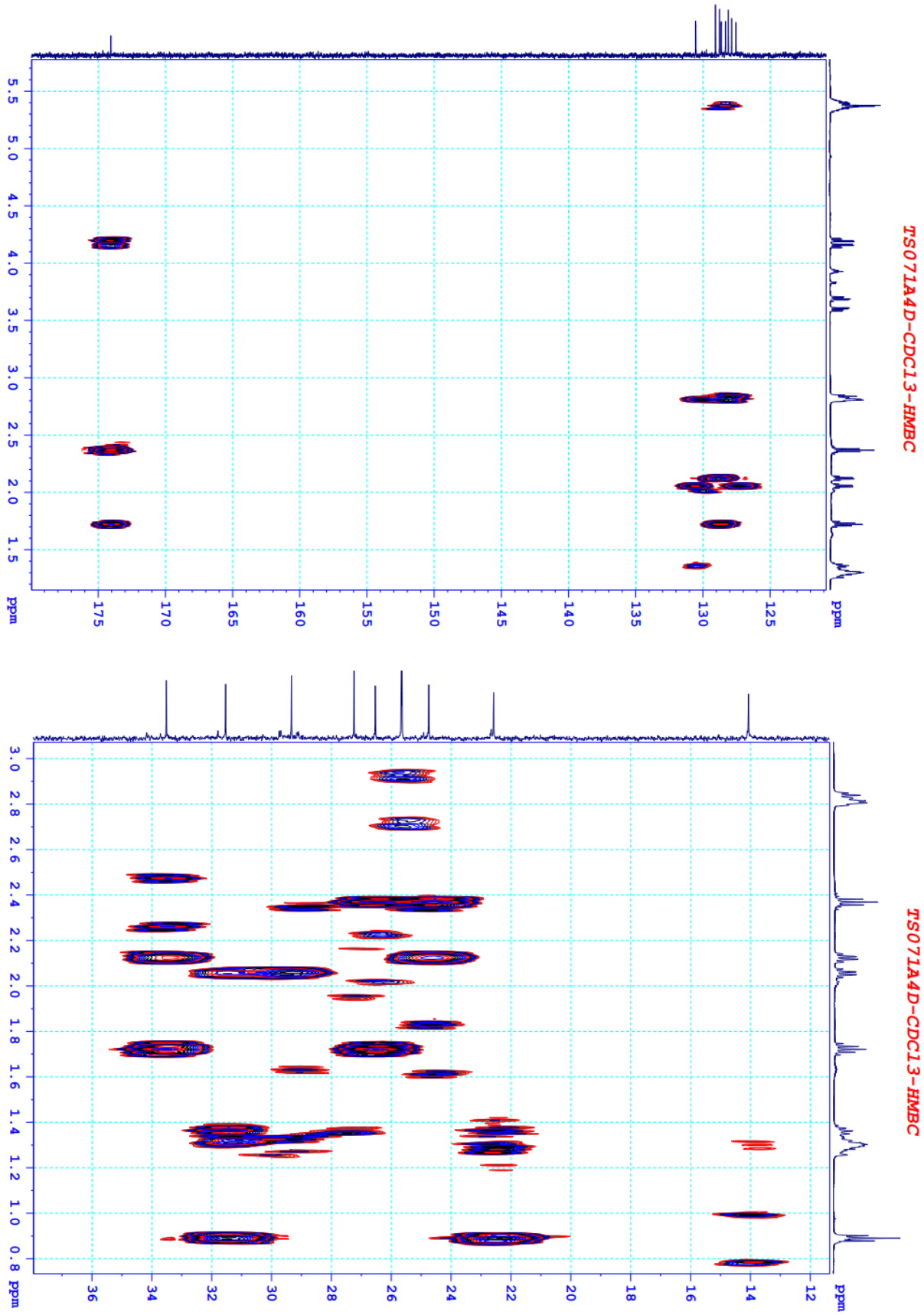


Figure S42: Extended ^{1}H NMR spectrum of compound **9** in $CDCl_3$

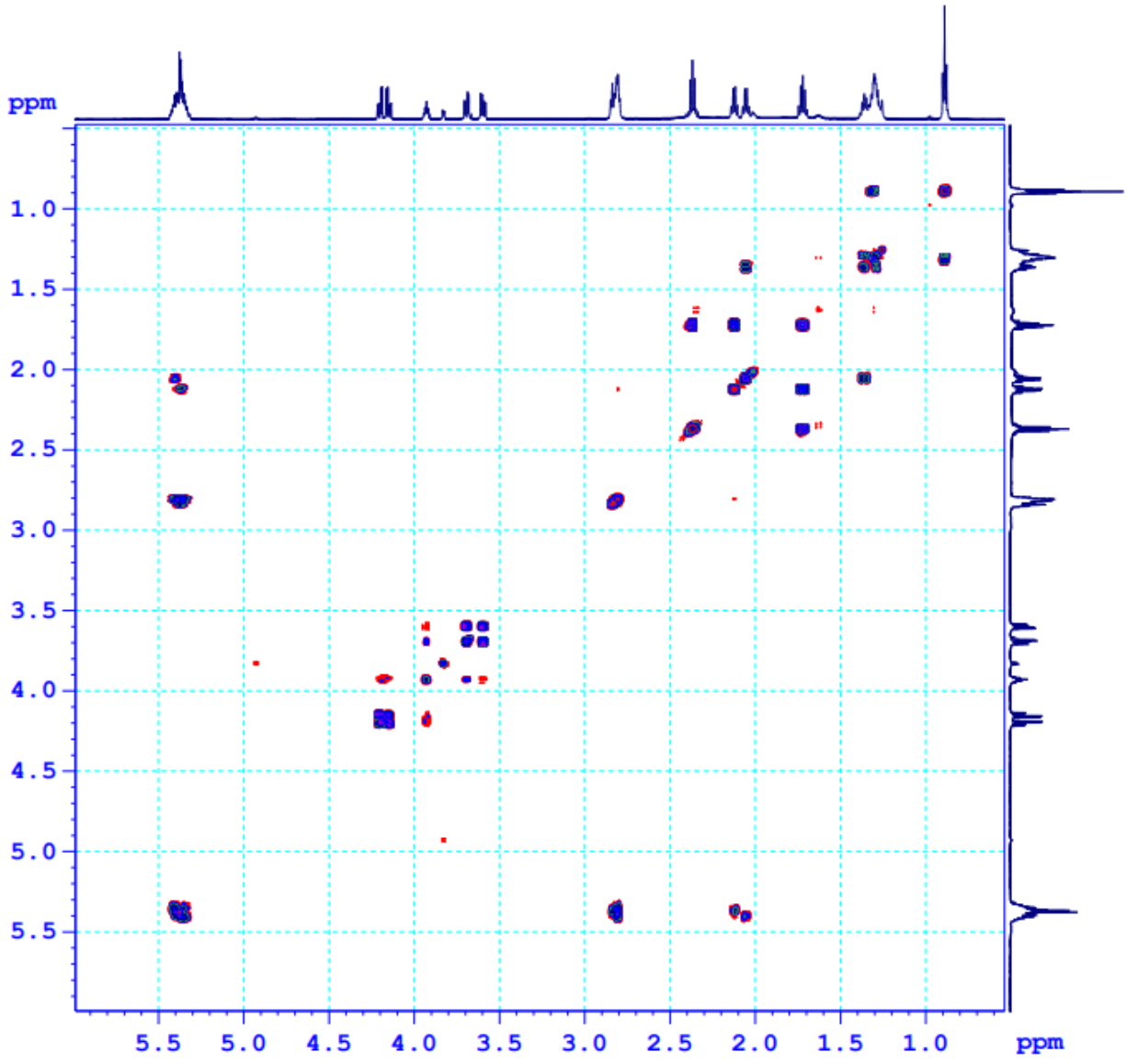


Figure S43: ^{1}H-^{1}H COSY spectrum of compound **9** in $CDCl_3$

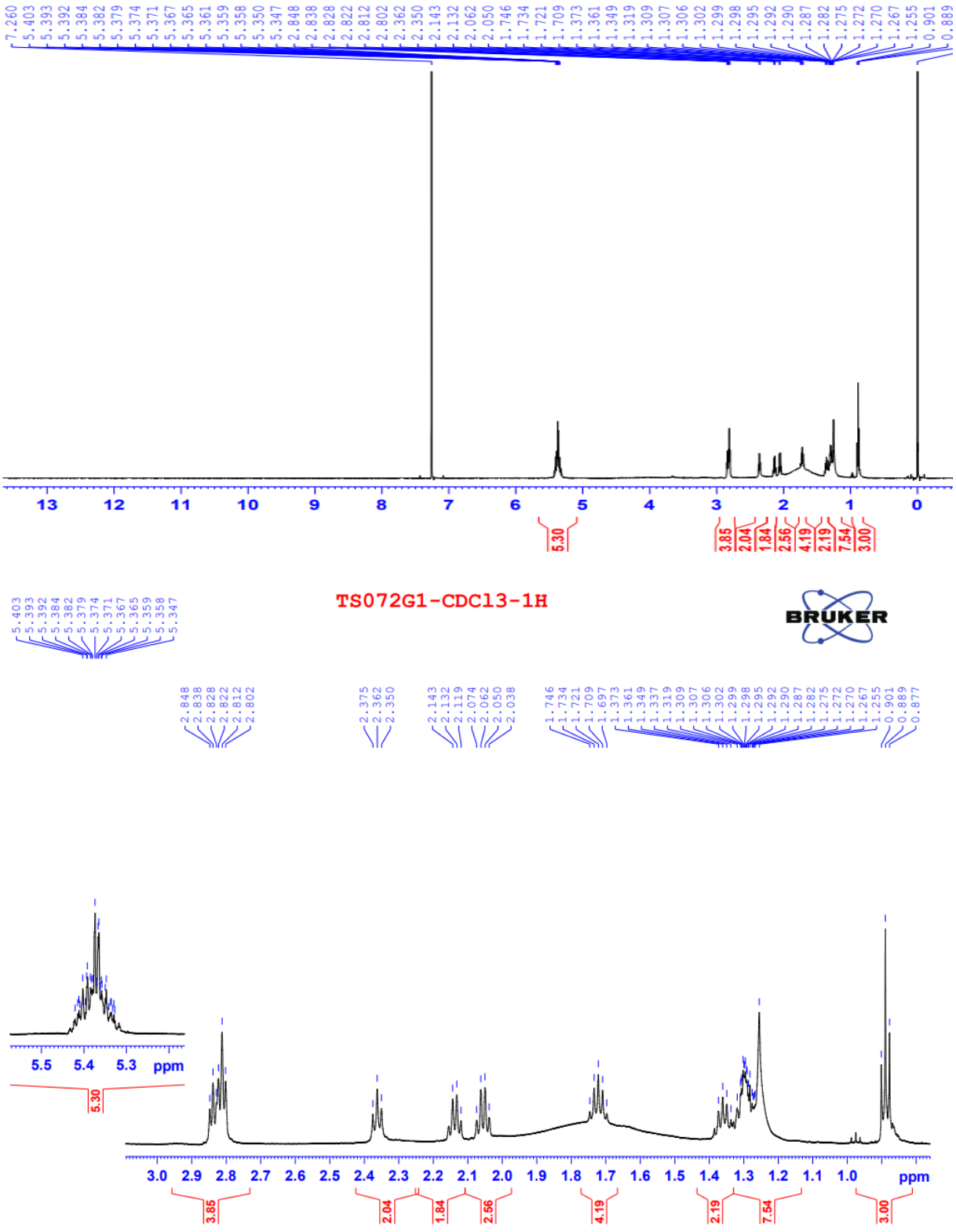


Figure S44: ^{1}H NMRspectrum of compound **10** in $CDCl_3$

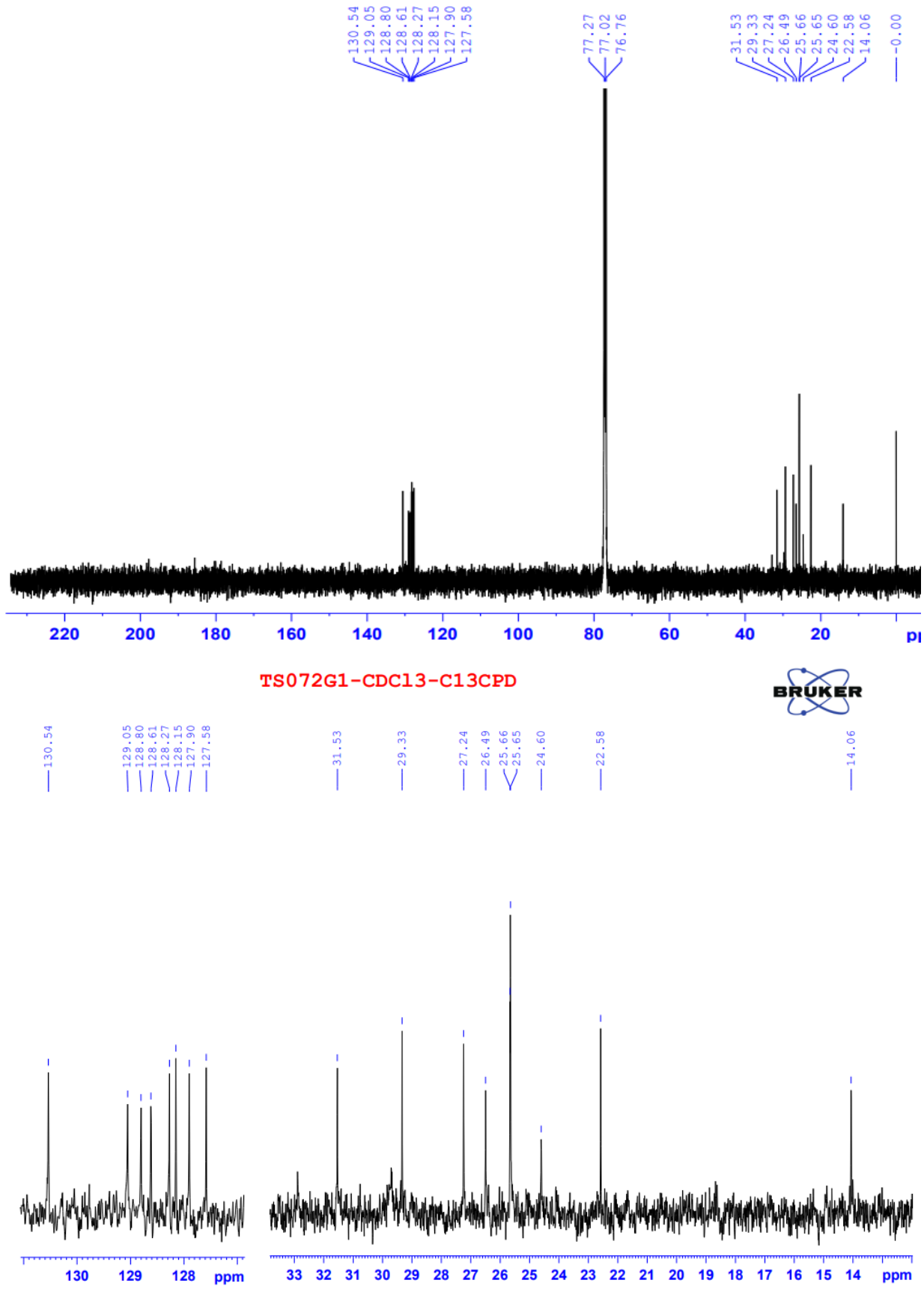


Figure S45: ^{13}C NMRspectrum of compound **10** in $CDCl_3$

S1: *Experimental: The NMR Data of Compounds* **3-10**

*Deoxyinosine (**3**):*A dark yellow solid. ^{1}H NMR (DMSO-d_6, 600 MHz) δ (ppm): 8.04 (1H, s, H-2), 8.28 (1H, s, H-8), 6.30 (1H, dd, J = 6.6, 6.0 Hz, H-1′), 2.29 (1H, ddd, J = 10.4, 6.0, 2.4 Hz, H_a-2′), 2.62 (1H, ddd, J = 10.4, 8.4, 5.4 Hz, H_b-2′), 4.38 (1H, ddd, J = 5.4, 2.4, 2.4 Hz, H-3′), 3.86 (1H, m, H-4′), 3.58 (1H, dd, 12.0, 4.2 Hz, H_a-5′), 3.51 (1H, dd, 12.0, 3.6 Hz, H_b-5′). ^{13}C NMR (DMSO-d_6, 150 MHz) δ (ppm) data shown in Table S1.

*Inosine (**4**):* A dark yellow solid. ^{1}H NMR (DMSO-d_6, 600 MHz) δ (ppm), 8.06 (1H, s, H-2), 8.33 (1H, s, H-8), 5.87 (1H, d, J = 6.0 Hz, H-1′), 4.48 (1H, dd, J = 6.0, 4.8 Hz, H-2′), 4.13 (1H, dd, J = 4.8, 3.6 Hz, H-3′), 3.94 (1H, m, H-4′), 3.65 (1H, dd, 12.0, 3.6 Hz, H_a-5′), 3.54 (1H, dd, 12.0, 3.6 Hz, H_b-5′). ^{13}C NMR (DMSO-d_6, 150 MHz) δ (ppm) data shown in Table S1.

*Adenosine (**5**):*A dark yellow solid. HRESIMS *m/z* 252.1089 $[M+H]^+$ (calcd. for $[C_{10}H_{13}N_5O_3]^-$: 252.1091, Δ = -0.8 ppm); *m/z* 274.0901 $[M+Na]^+$ (calcd. for $[C_{10}H_{12}N_5O_3Na]^-$: 274.0911, Δ = -3.7 ppm); ^{1}H NMR (DMSO-d_6, 600 MHz) δ (ppm): 8.12 (1H, s, H-2), 8.33 (1H, s, H-8), 6.35 (2H, s, NH_2), 6.34 (1H, dd, J = 6.6, 6.0 Hz, H-1′), 2.25 (1H, ddd, J = 13.2, 6.0, 2.4 Hz, H_a-2′), 2.72 (1H, ddd, J = 13.2, 8.0, 6.0 Hz, H_b-2′), 4.41 (1H, ddd, J = 8.0, 6.0, 6.0 Hz, H-3′), 3.88 (1H, m, H-4′), 3.62 (1H, dd, 12.0, 6.5 Hz, H_a-5′), 3.52 (1H, dd, 12.0, 5.0 Hz, H_b-5′). ^{13}C NMR (DMSO-d_6, 150 MHz) δ (ppm) data shown in Table S1.

*Deoxyadenosine (**6**):*A dark yellow solid. HRESIMS *m/z* 268.1040 $[M+H]^+$ (calcd. for $[C_{10}H_{13}N_5O_4]^-$: 268.1040, Δ = 0.0 ppm); *m/z* 290.0855 $[M+Na]^+$ (calcd. for $[C_{10}H_{12}N_5O_4Na]^-$: 290.0860, Δ = -1.9 ppm); ^{1}H NMR (DMSO-d_6, 600 MHz) δ (ppm): 8.13 (1H, s, H-2), 8.34 (1H, s, H-8), 7.33 (2H, s, NH_2), 5.87 (1H, dd, J = 6.6, 6.0 Hz, H-1′), 4.61 (1H, ddd, J = 6.6, 6.0, 5.4 Hz, H-2′), 4.14 (1H, ddd, J = 6.0, 6.0, 3.0 Hz, H-3′), 3.96 (1H, m, H-4′), 3.67 (1H, ddd, 12.0, 6.0, 4.2 Hz, H_a-5′), 3.55 (1H, ddd, 12.0, 6.0, 3.6 Hz, H_b-5′), 5.42 (1H, d, J = 6.0 Hz, 5′-O<u>H</u>). ^{13}C NMR (DMSO-d_6, 150 MHz) δ (ppm) data data shown in Table S1.

*Deoxyuridine (**7**):*A dark yellow solid. HRESIMS *m/z* 229.0818 $[M+H]^+$ (calcd. for $[C_9H_{13}N_2O_5]^+$: 229.0819, Δ = -0.4 ppm); *m/z* 251.0633 $[M+Na]^+$ (calcd. for $[C_9H_{12}N_2O_5Na]^+$: 251.0638, Δ = -2.0 ppm); ^{1}H NMR (DMSO-d_6, 600 MHz) δ (ppm): 5.61 (1H, d, J = 7.8 Hz, H-5), 7.82 (1H, d, J = 7.8 Hz, H-4), 6.15 (1H, dd, J = 6.6, 6.0 Hz, H-1′), 2.07 (2H, m, H-2′), 4.22 (1H, m, H-3′), 3.76 (1H, m, H-4′), 3.52 (1H, dd, 12.0, 3.6 Hz, H_a-5′), 3.56 (1H, dd, 12.0, 3.6 Hz, H_b-5′), ^{13}C NMR (DMSO-d_6, 150 MHz) δ (ppm) data shown in Table S1.

*Thymidine (**8**):*A dark yellow solid. HRESIMS *m/z* 243.0976 $[M+H]^+$ (calcd. for $[C_{10}H_{16}N_2O_5]^+$: 243.0975, Δ = +0.3 ppm); *m/z* 265.0796 $[M+Na]^+$ (calcd. for [C $C_{10}H_{15}N_2O_5Na]^+$: 265.0795, Δ = +0.3 ppm); ^{1}H NMR

(DMSO-d_6, 600 MHz) δ (ppm): 7.68 (1H, s, H-4), 1.76 (3H, s, 5-CH_3), 6.16 (1H, dd, J = 6.6, 6.0 Hz, H-1′), 2.06 (2H, m, H-2′), 4.23 (1H, m, H-3′), 3.53 (1H, dd, J = 12.0, 3.6 Hz, H-5′$_a$), 3.56 (1H, dd, J = 12.0, 3.6 Hz, H-5′$_b$). ^{13}C NMR (DMSO-d_6, 150 MHz) δ (ppm) data shown in Table S1.

Glycerol arachidonate ***(9)****:*Colorless solid; HRESIMS m/z 396.3108 $[M+NH_4]^+$, calcd for $C_{23}H_{42}NO_4$: 396.3108, Δ=0; *m/z* 401.2670 [M+Na]+, calcd. for $C_{23}H_{38}O_4Na$: 401.2662, Δ=+2.0 ppm. ^{1}H NMR ($CDCl_3$, 600 MHz) δ (ppm), ^{13}C NMR ($CDCl_3$, 150 MHz) δ (ppm) data shown in Table S2.

Arachidonic acid ***(10)****:*Colorless solid. ^{1}H NMR ($CDCl_3$, 600 MHz) δ (ppm), ^{13}C NMR ($CDCl_3$, 150 MHz) δ (ppm) data shown in Table S2.

Table S1: ^{13}C NMR data for compounds **1-8** in DMSO-d_6 and reference compounds

Pos.	3		4		5		6		7		8	
	δ_C[a]	δ_C	δ_C[b]	δ_C	δ_C[c]	δ_C	δ_C[d]	δ_C	δ_C[e]	δ_C	δ_C[f]	δ_C
2	145.8	145.9	145.8	145.9	152.4	152.4	152.4	152.4	151.96	150.9	150.6	150.6
4	147.8	147.8	148.2	148.2	148.9	148.9	149.0	149.1	141.43	140.4	136.2	136.1
5	124.4	124.4	124.5	124.4	119.3	119.3	119.3	119.4	102.68	101.8	109.4	109.3
6	156.6	156.7	156.6	156.6	156.1	156.1	156.2	156.2	163.57	163.8	163.8	163.9
8	138.5	138.4	138.7	138.7	139.5	139.5	139.9	139.9				
1′	83.5	83.6	87.6	87.5	83.9	83.9	87.9	87.9	86.03	84.1	83.8	83.7
2′	39.5	39.4	74.1	74.1	39.4	39.4	73.4	73.4	39.34	39.1	39.5	39.4
3′	70.6	70.6	70.3	70.3	71.0	71.0	70.6	70.7	71.05	70.4	70.5	70.4
4′	87.9	87.9	85.6	85.6	88.0	88.0	85.9	85.9	87.26	87.4	87.3	87.2
5′	61.6	61.6	61.3	61.3	61.9	61.9	61.6	61.7	61.81	61.3	61.5	61.3

a: δ_C of deoxyinosine in DMSO-d_6 [1]
b: δ_C of inosine in DMSO-d_6 [2]
c: δ_C of deoxyadenosine in DMSO-d_6 [3]
d: δ_C of adenosine in DMSO-d_6 [3]
e: δ_C of deoxyuridine in $CDCl_3$ [4]
f: δ_C of thymidine in DMSO-d_6 [5]

Table S2: NMR spectroscopic data for **9** and **10** (in $CDCl_3$) and reference compounds

Pos.	**9** (glycerol arachidonate)		**10** (arachidonic acid)			
	δ_C	δ_H **(mult, *J* in Hz)**	**Pos.**	δ_C[a]	δ_C	δ_H **(mult, *J* in Hz)**
1′	174.1, C	-	1	180.23	nd	-
2′	33.5, CH_2	2.37 (t, 7.2)	2	33.43, CH_2	33.5, CH_2	2.37 (t, 7.2)
3′	24.8, CH_2	1.72 (m)	3	24.52, CH_2	24.6, CH_2	1.72 (m)
4′	26.5, CH_2	2.11 (q, 7.2)	4	26.50, CH_2	26.5, CH_2	2.11 (q, 7.2)
5′	128.3, CH	5.32 - 5.42	5	129.08, CH	129.1, CH	5.32 - 5.42
6′	129.1, CH	5.32 - 5.42	6	128.70,CH	128.3,CH	5.32 - 5.42
7′,10′,13′	25.6, CH_2	2.82 (m)	7	25.66, CH_2	25.6, CH_2	2.82 (m)
8′, 9′, 11′, 12′	128.8, 128.7, 128.1, 127.9, CH	5.32 - 5.42	8, 9,	128.21, 128.06, CH	128.8, 128.6, CH	5.32 - 5.42
14′	127.6, CH	5.32 - 5.42	10	25.66	25.6, CH_2	2.82 (m)
15′	130.6, CH	5.32 - 5.42	11, 12	128.52, 127.85, CH	128.2, 127.9, CH	5.32 - 5.42
16′	27.2, CH_2	2.06 (q, 7.2)	13	25.66	25.6, CH_2	2.82 (m)
17′	29.3, CH_2	1.30 (m)	14	127.61, CH	127.6, CH	5.32 - 5.42
18′	31.5, CH_2	1.28 (m)	15	130.34, CH	130.5, CH	5.32 - 5.42
19′	22.6, CH_2	1.30 (m)	16	27.25, CH_2	27.2, CH_2	2.06 (q, 7.2)
20′	14.1, CH_3	0.89 (t, 7.2)	17	29.39, CH_2	29.3, CH_2	1.30 (m)
1	65.3, CH_2	4.16 (dd, 12.0, 6.0) 4.20 (dd, 12.0, 4.8)	18	31.57, CH_2	31.5, CH_2	1.28 (m)
2	70.3, CH	3.92 (m)	19	22.63, CH_2	22.6, CH_2	1.30 (m)
3	63.4, CH_2	3.60 (dd, 12.0, 5.4) 3.70 (dd. 12.0, 2.4)	20	14.05, CH_3	14.1, CH_3	0.89 (t, 7.2)

The signals without multiples are overlapped, nd: none detected.

Glycerol arachidonate [6]: NMR ^{1}H (400 MHz, $CDCl_3$): 0.89 (3H, t, *J* = 6,8 Hz), 1.30 (8H, m), 1.70 (2H, m), 2.09 (4H, m), 2.37 (2H, t, J = 7,8 Hz), 2.81 (6H, m), 3.60 (1H, dd, *J*= 11.7, 5.8 Hz), 3.70 (1H, dd, *J* = 11.7, 3.9 Hz), 3.93 (1H, m), 4.15 (1H, dd, *J* = 11.7, 6.8 Hz), 4.21 (1H, dd, *J* = 11.7, 4.4 Hz), 5.38 (8H, m)

a: δ_C of arachidonic acid in $CDCl_3$ [7]

S2: Cytotoxicity Assay

Human lung carcinoma (SK-LU-1) and human hepatocellular carcinoma (HepG2) cell lines were kindly provided by the Milan University, Italy and Long Island University, USA. The cells were maintained and cultured in DMEM supplemented with FBS, trypsin-EDTA, L-glutamine, sodium piruvat, $NaHCO_3$, and penicillin/streptomycin at 37°C in a humidified atmosphere of 5% CO2. Cytotoxic effects of compounds were determined using Sulforhodamine B (SRB) assay as previously described by Skehan et al. In brief, the cells were incubated with/without compounds for 72h in 96-well culture plate. After incubation, cells were stained with sulforhodamine B and measured optical density (OD) at 540 nm [8]. Difference of OD between samples and vehicle well during experiments indicated cells situation induced by compounds. Results are expressed as percentage of cells death in comparison with vehicle well. Ellipticine was used as a positive control throughout experiments.

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