Supporting Information

Penithoketone and Penithochromones A–L, Polyketides from the Deep-Sea-Derived Fungus *Penicillium thomii* YPGA3

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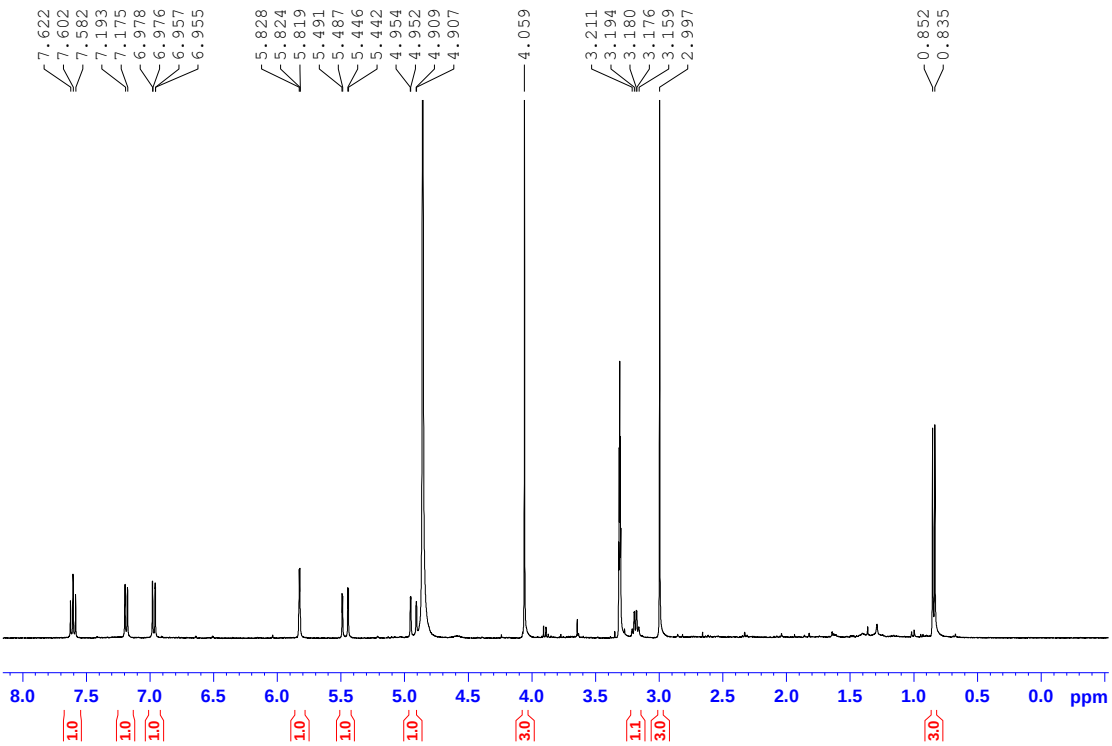

Figure S1 ^{1}H NMR Spectrum of **1** in Methanol-d_4 (400 MHz)

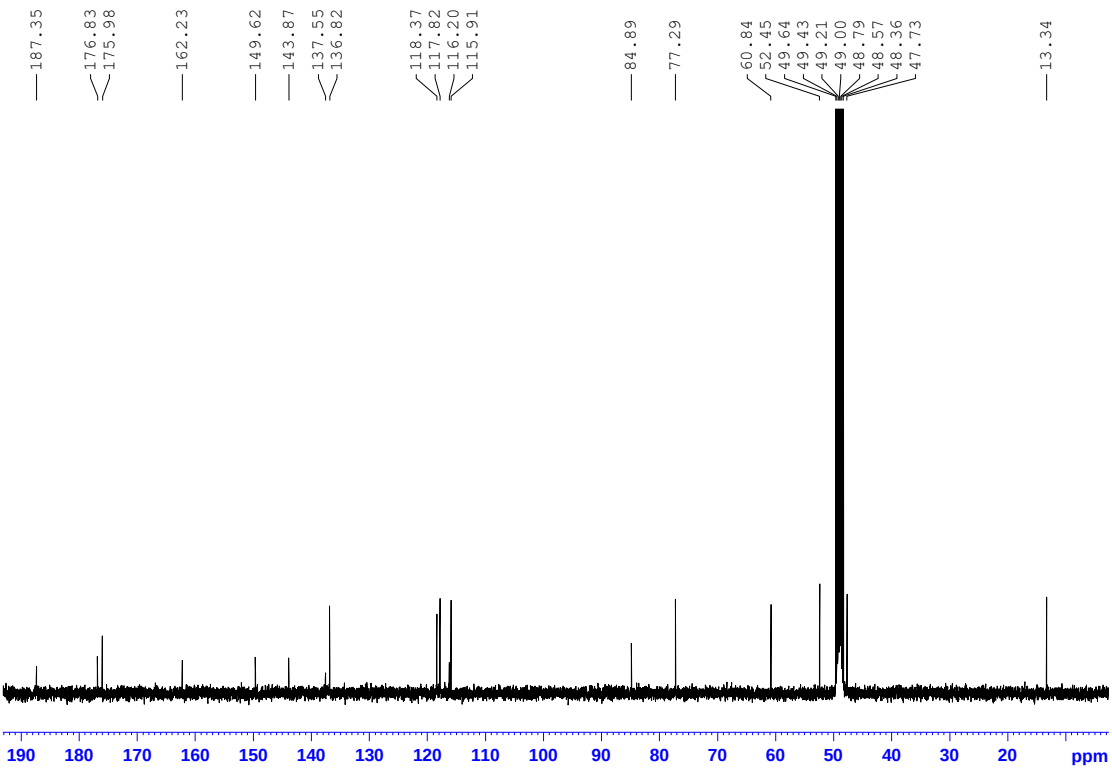

Figure S2 ^{13}C NMR Spectrum of **1** in Methanol-d_4 (100 MHz)

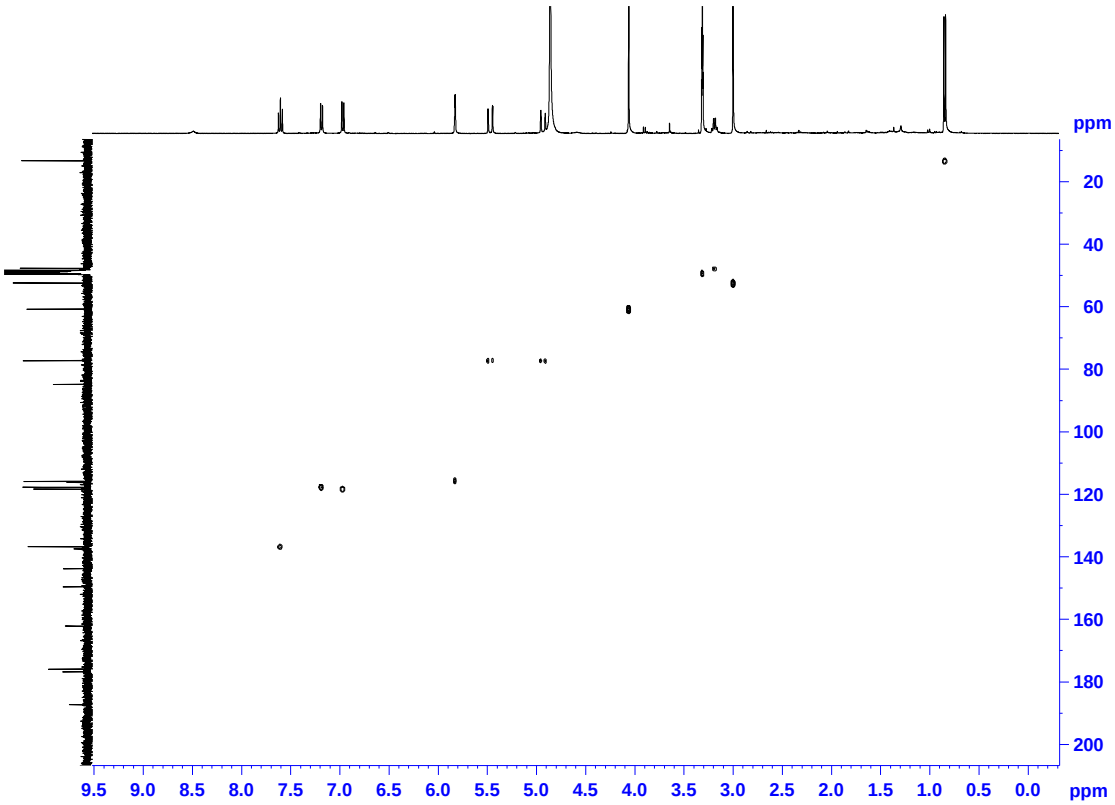

Figure S3 HSQC Spectrum of **1** in Methanol-d_4

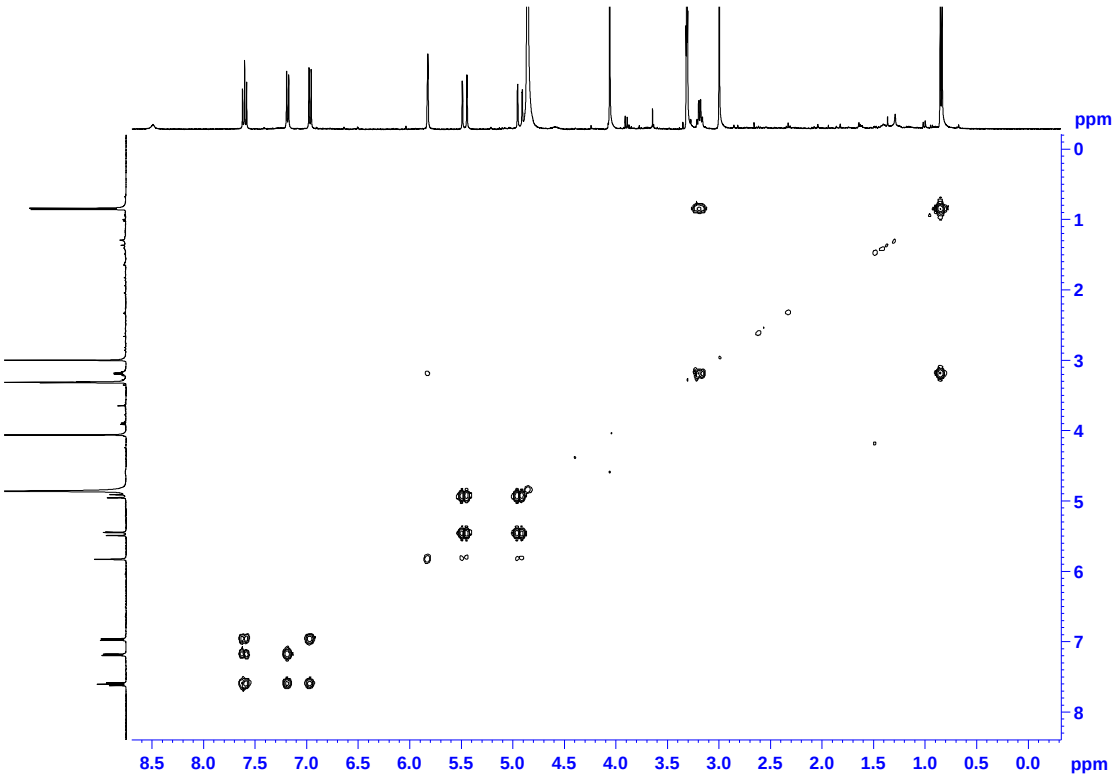

Figure S4 ^{1}H-^{1}H COSY Spectrum of **1** in Methanol-d_4

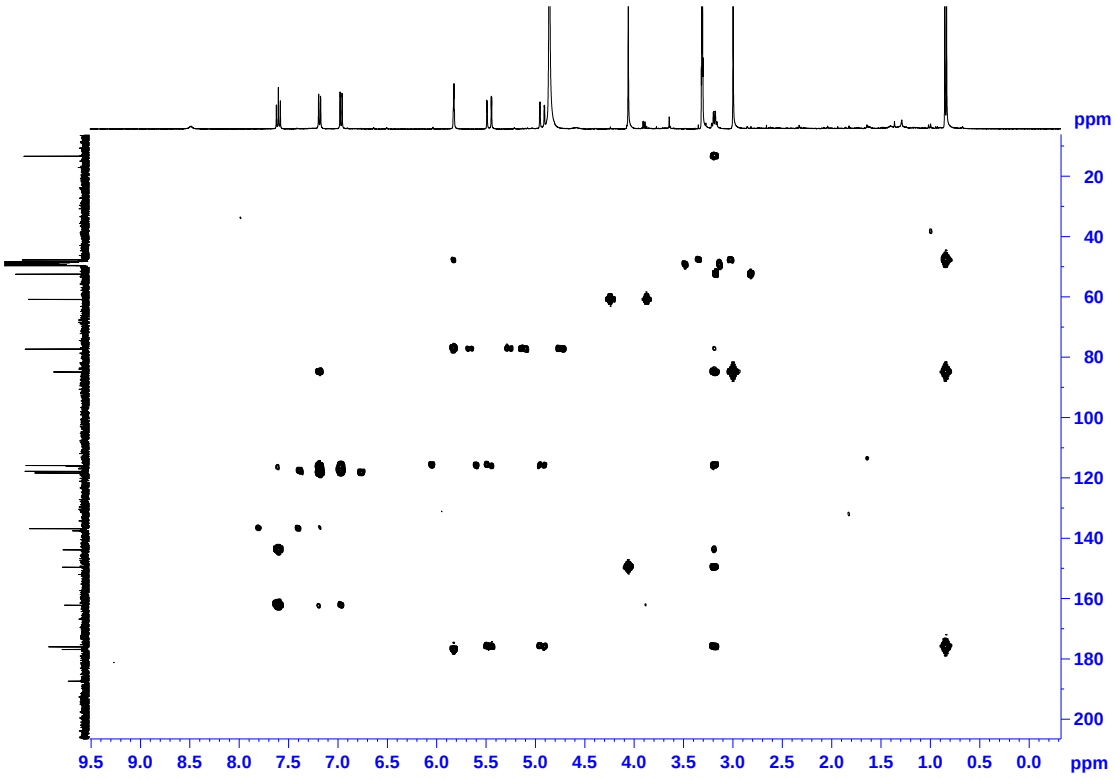

Figure S5 HMBC Spectrum of **1** in Methanol-d_4

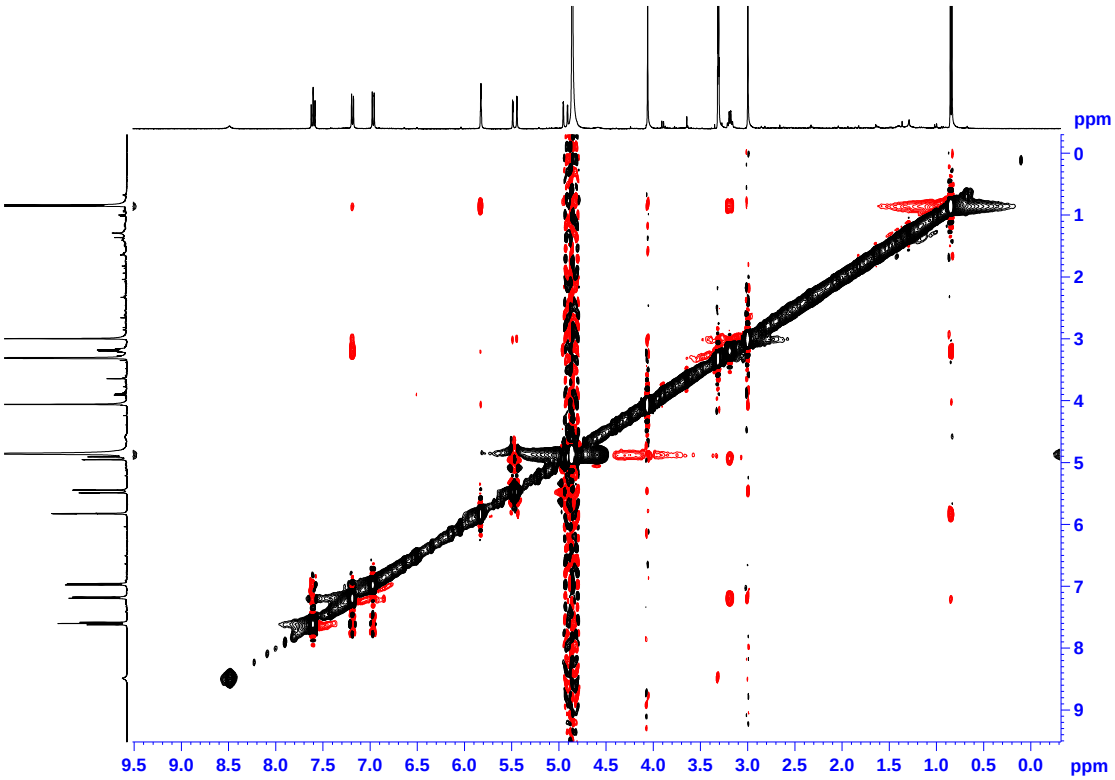

Figure S6 NOESY Spectrum of **1** in Methanol-d_4

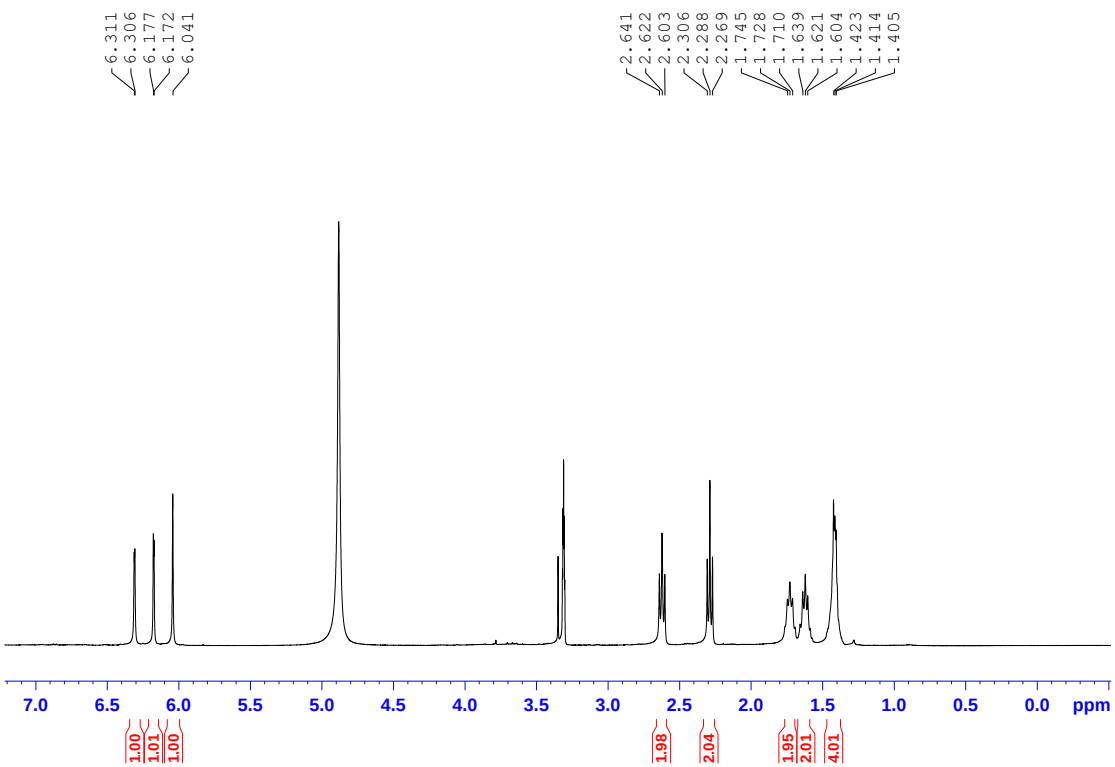

Figure S7 ^{1}H NMR Spectrum of **2** in Methanol-d_4 (400 MHz).

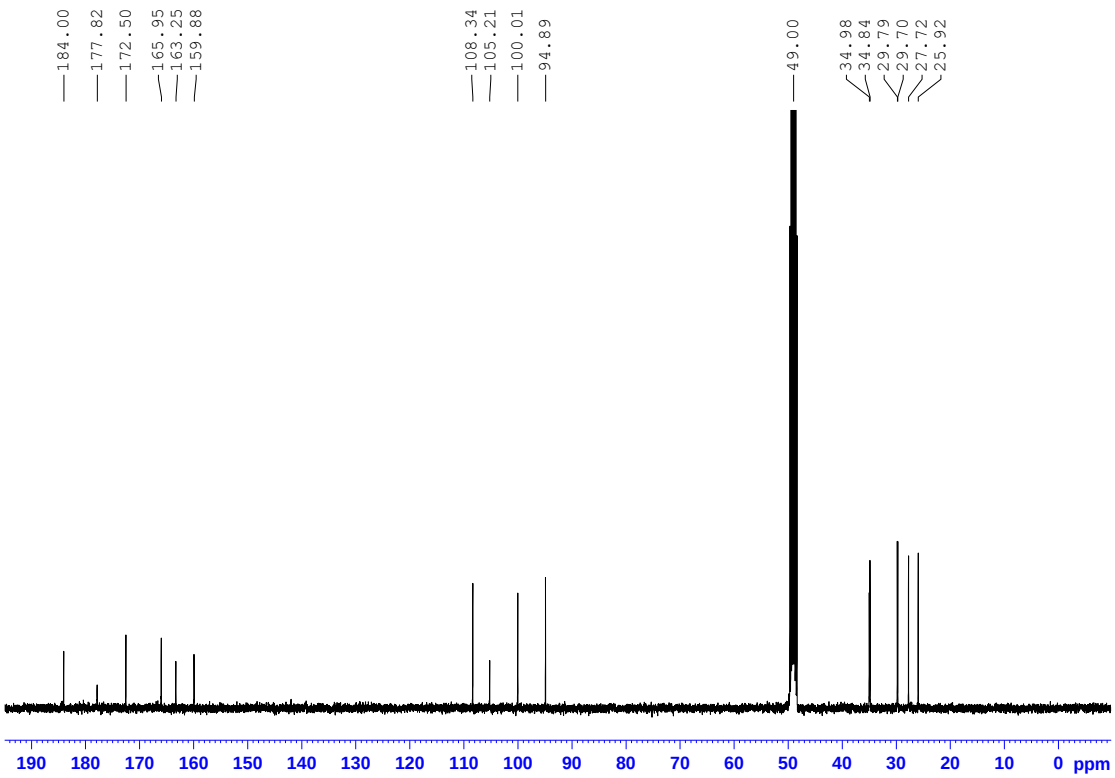

Figure S8 ^{13}C NMR Spectrum of **2** in Methanol-d_4 (100 MHz)

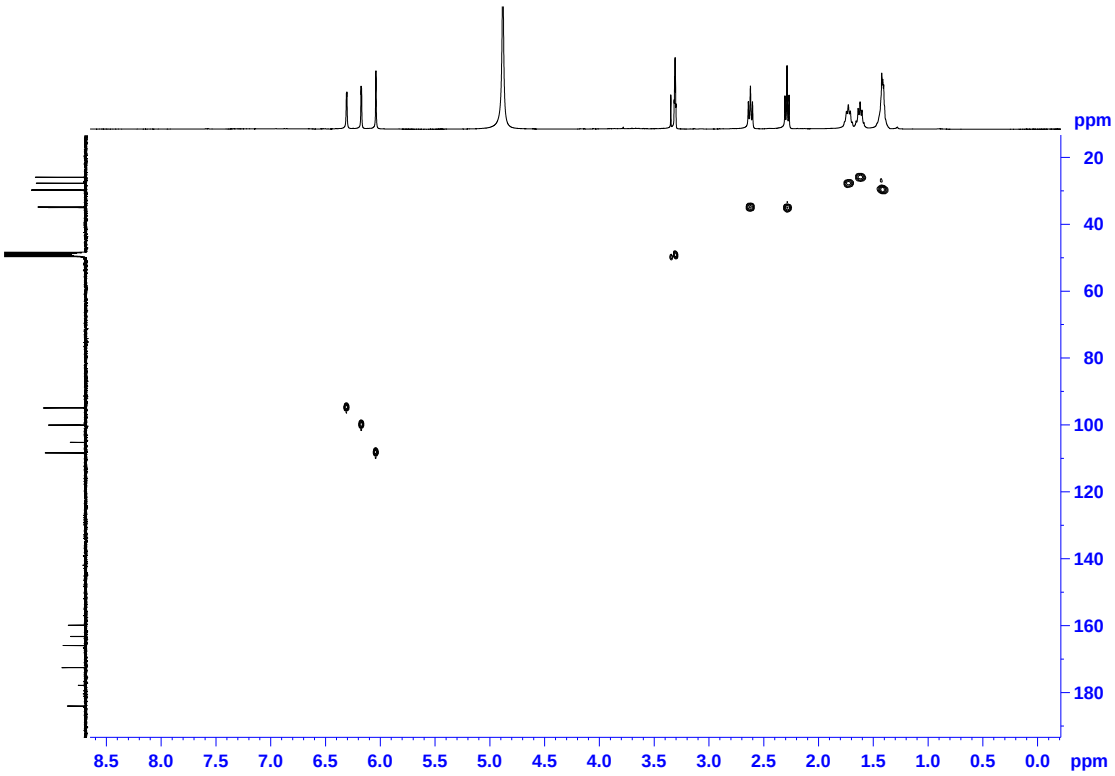

Figure S9 HSQC Spectrum of **2** in Methanol-d_4

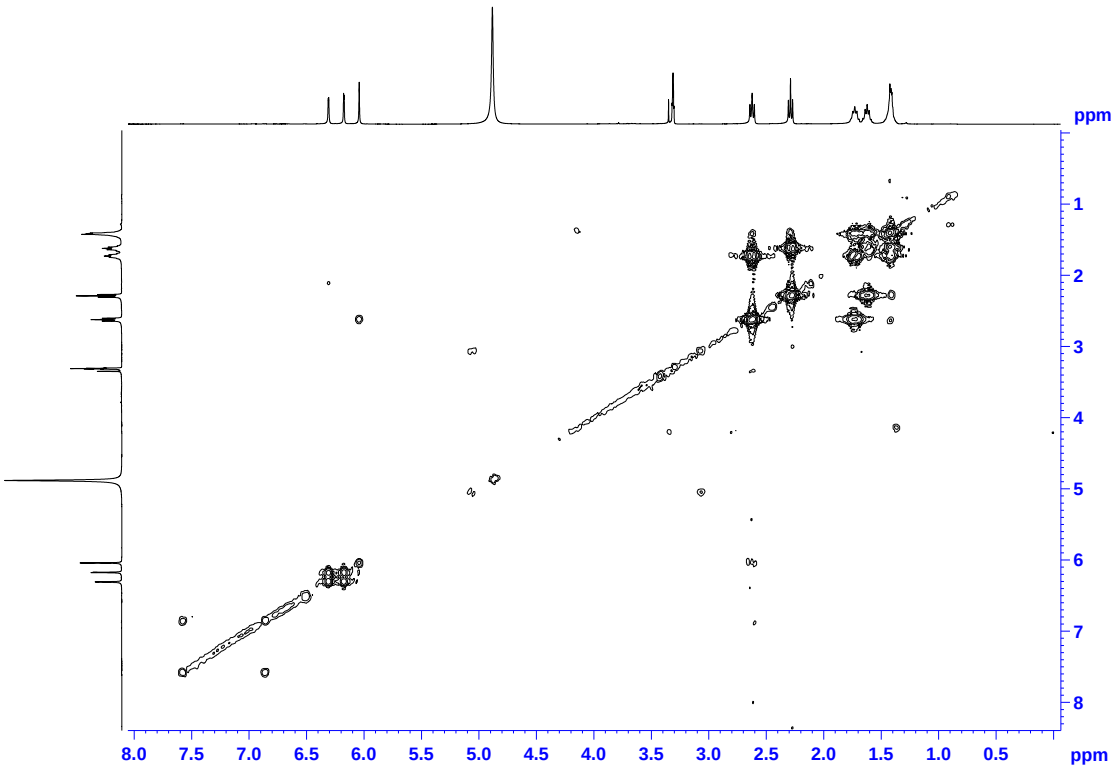

Figure S10 ^{1}H-^{1}H COSY Spectrum of **2** in Methanol-d_4

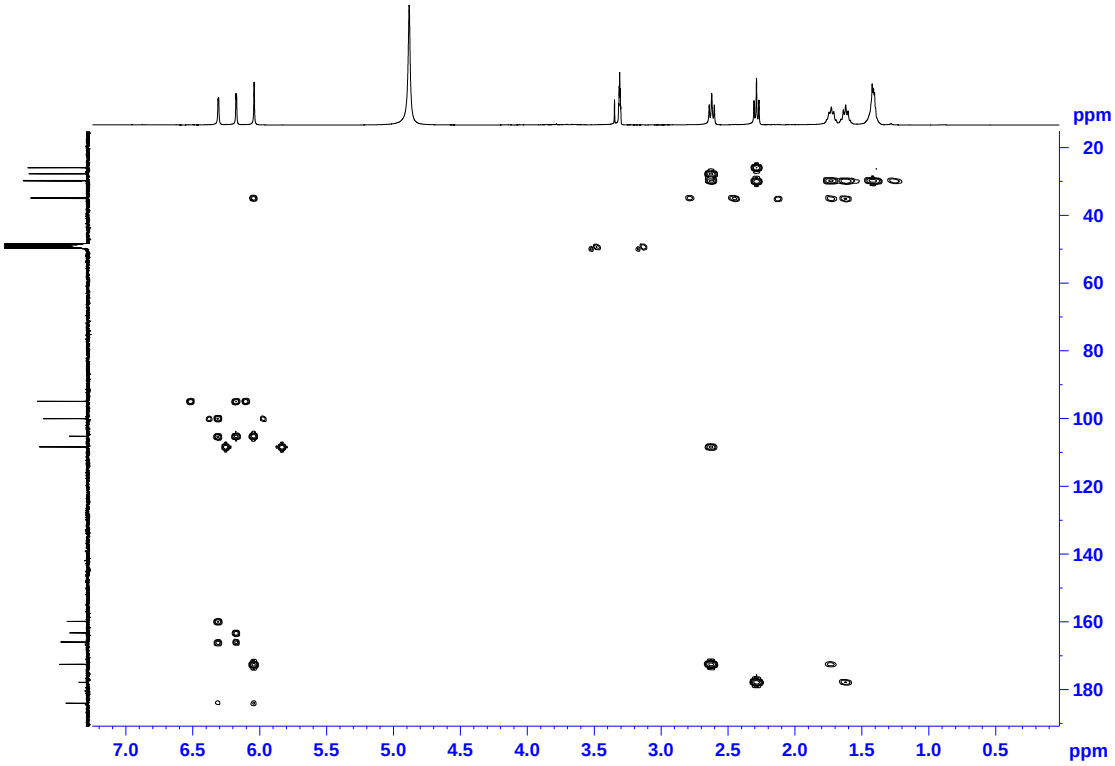

Figure S11 HMBC Spectrum of **2** in Methanol-d_4

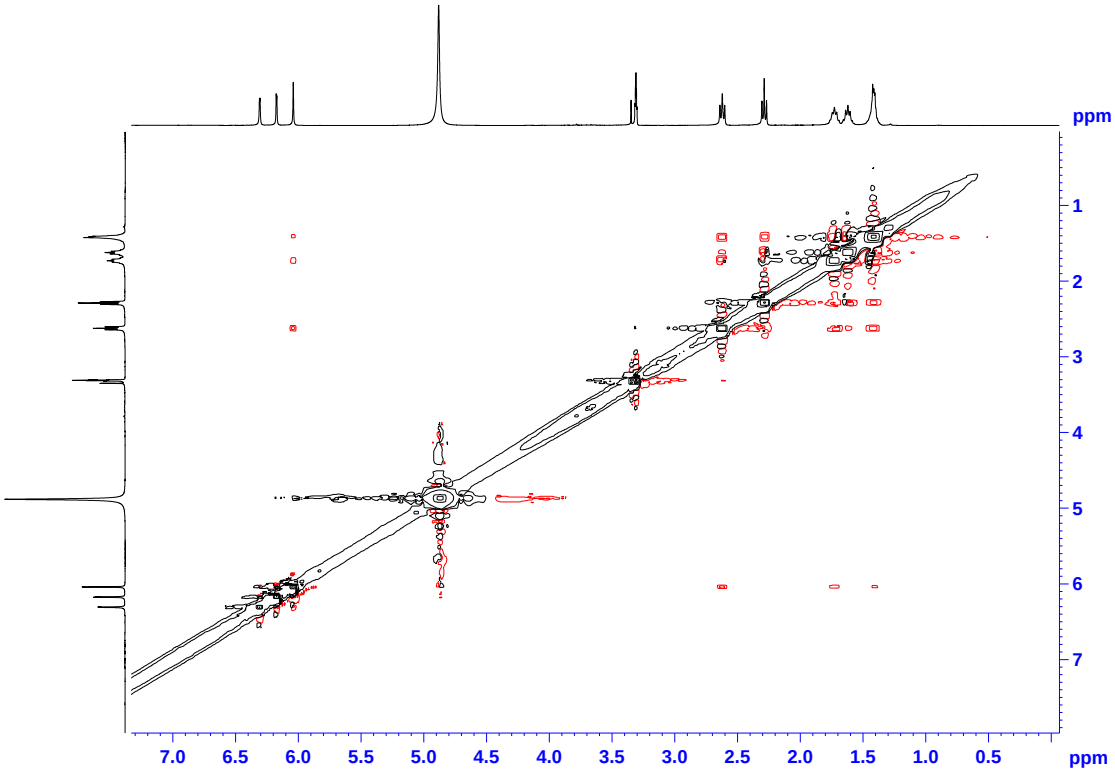

Figure S12 NOESY Spectrum of **2** in Methanol-d_4

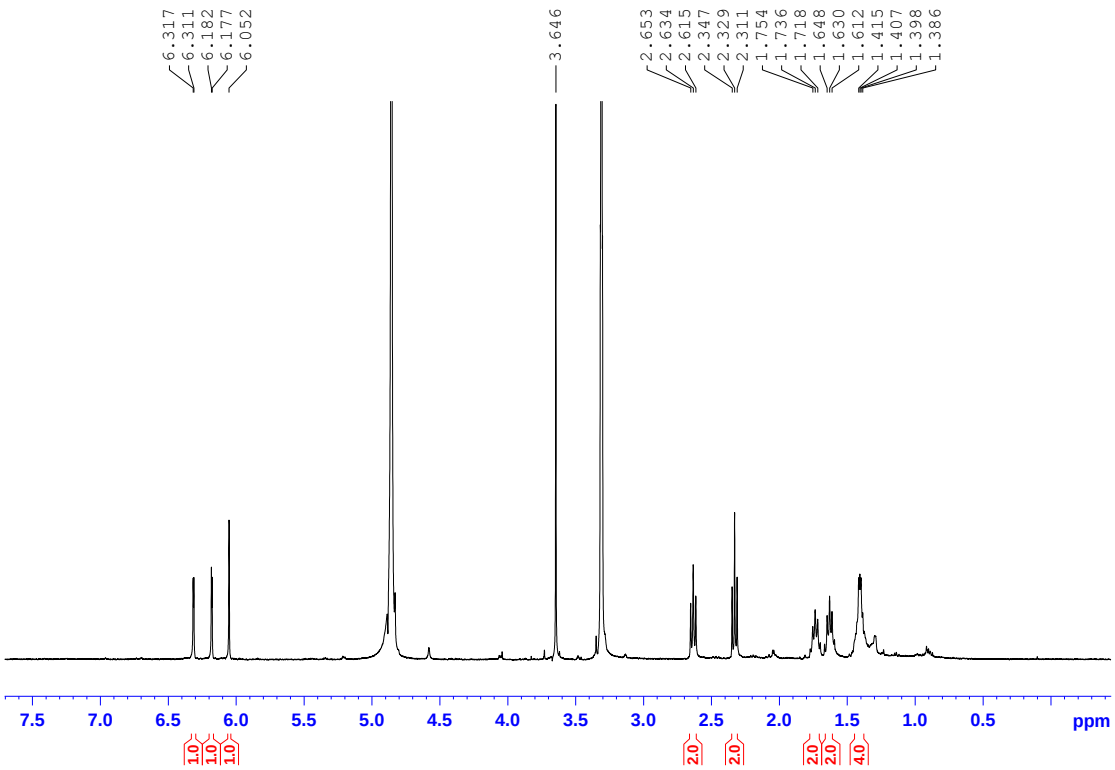

Figure S13 ^{1}H NMR Spectrum of **3** in Methanol-d_4 (400 MHz)

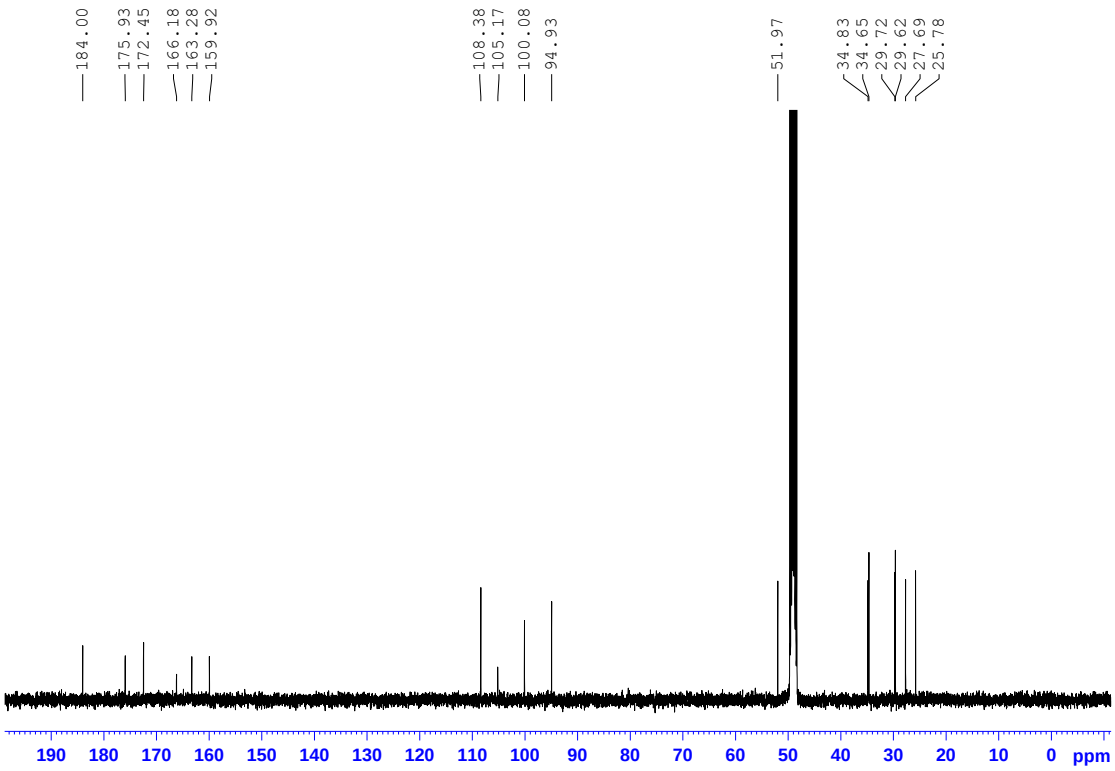

Figure S14 ^{13}C NMR Spectrum of **3** in Methanol-d_4 (100 MHz)

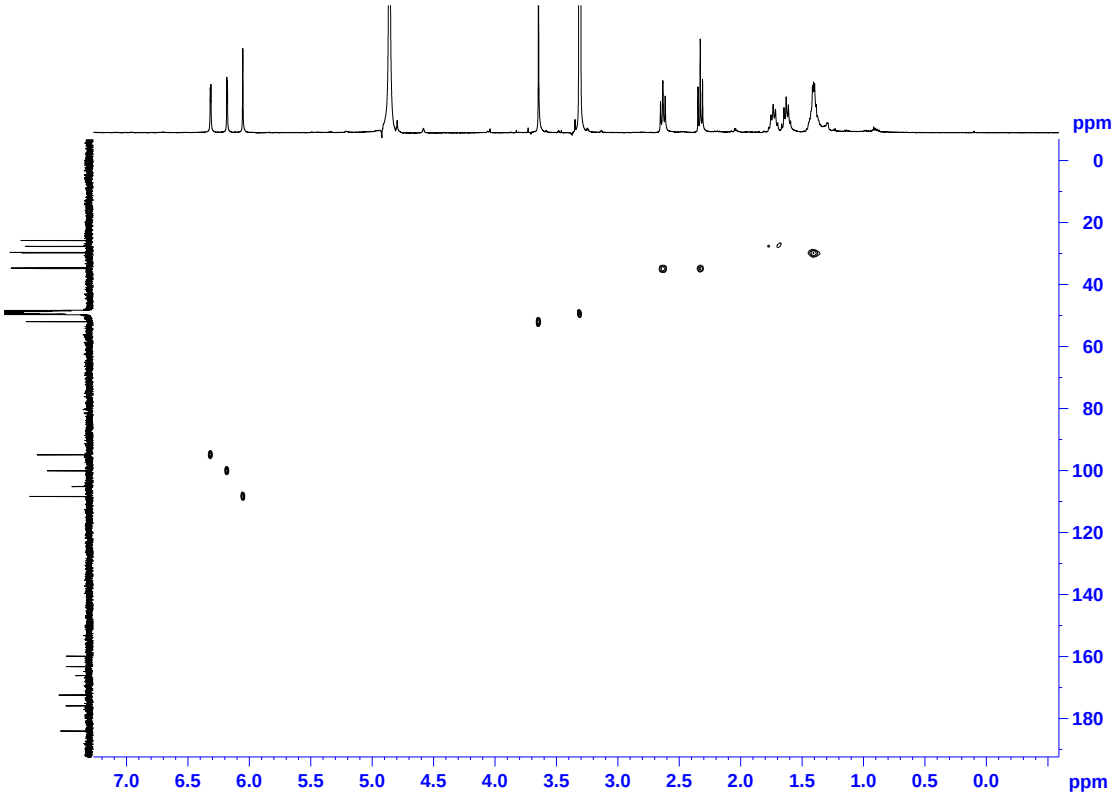

Figure S15 HSQC Spectrum of **3** in Methanol-d_4

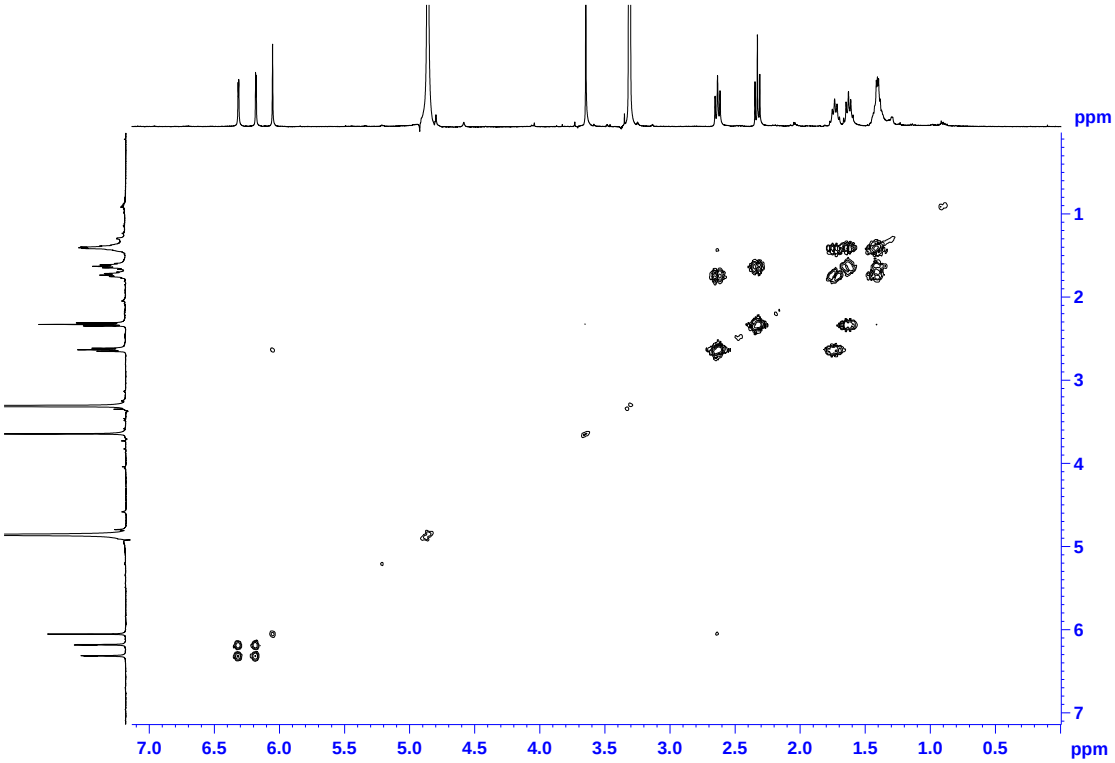

Figure S16 ^{1}H-^{1}H COSY Spectrum of **3** in Methanol-d_4

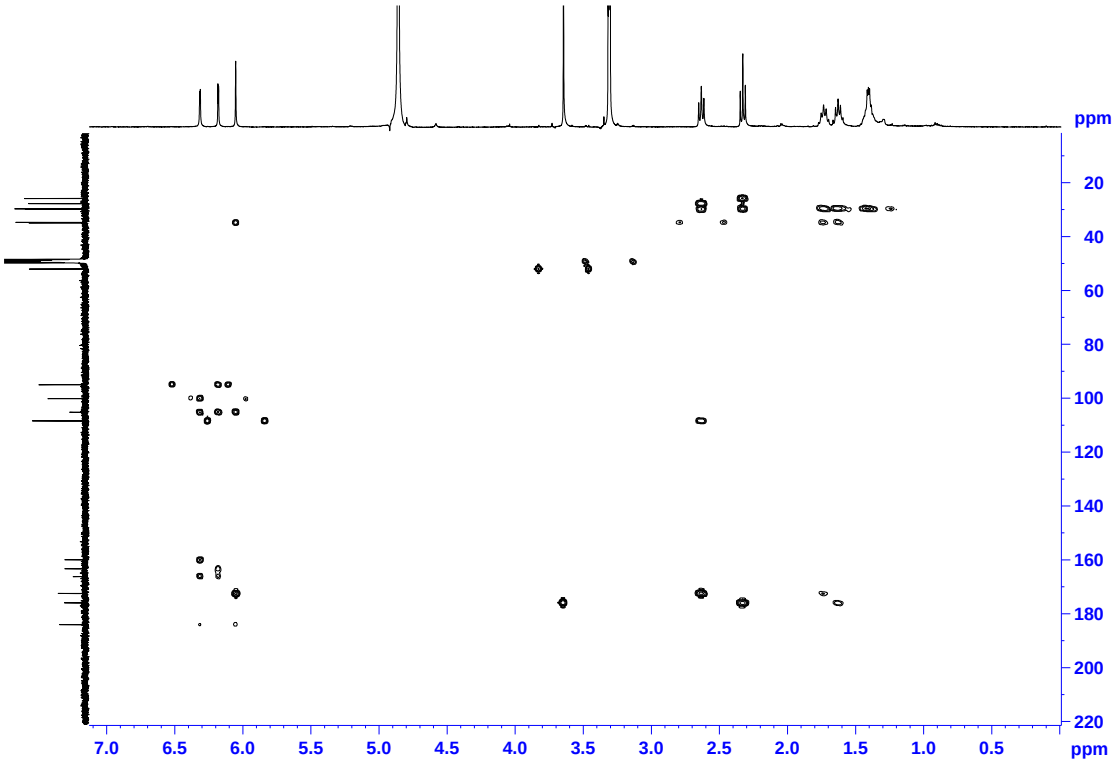

Figure S17 HMBC Spectrum of **3** in Methanol-d_4

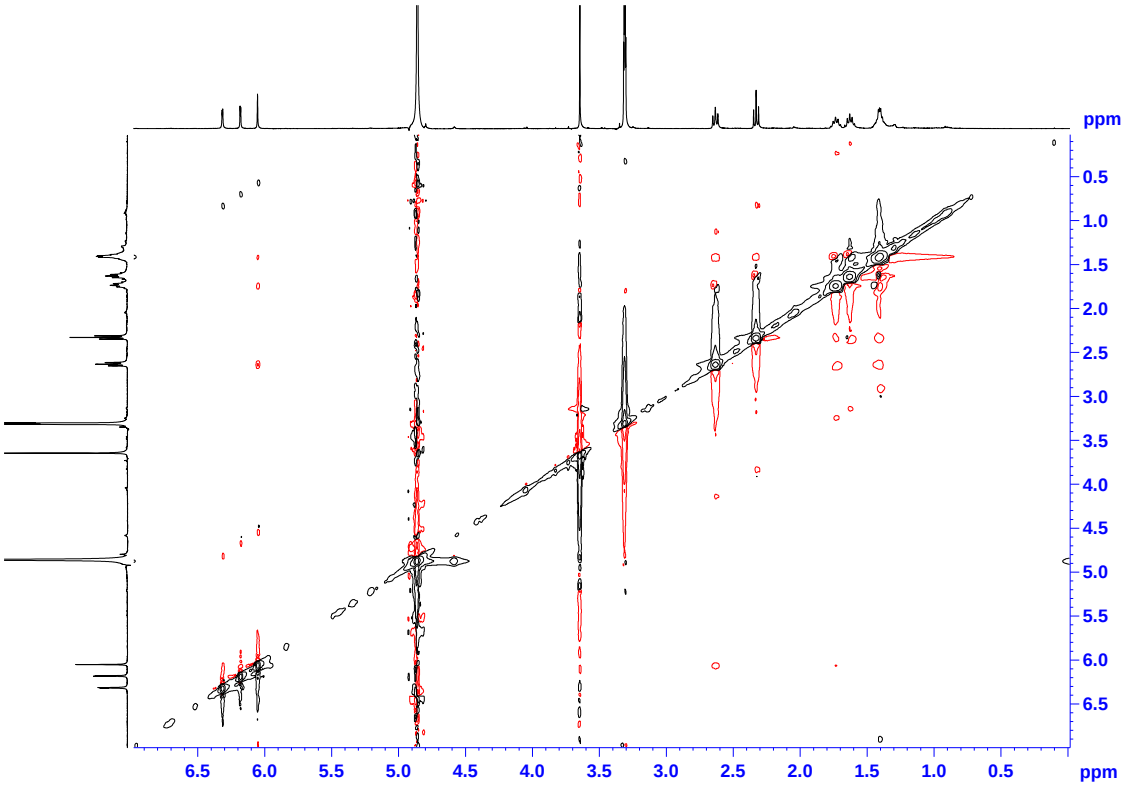

Figure S18 NOESY Spectrum of **3** in Methanol-d_4

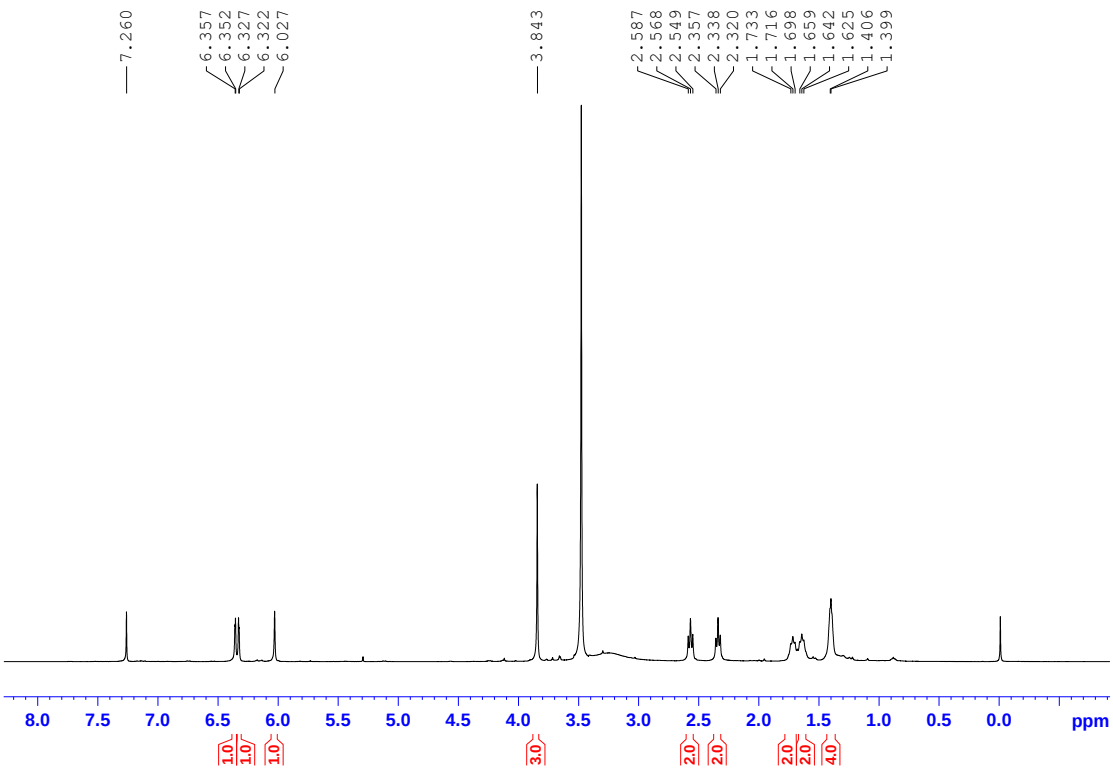

Figure S19 ^{1}H NMR Spectrum of **4** in $CDCl_3$ (400 MHz).

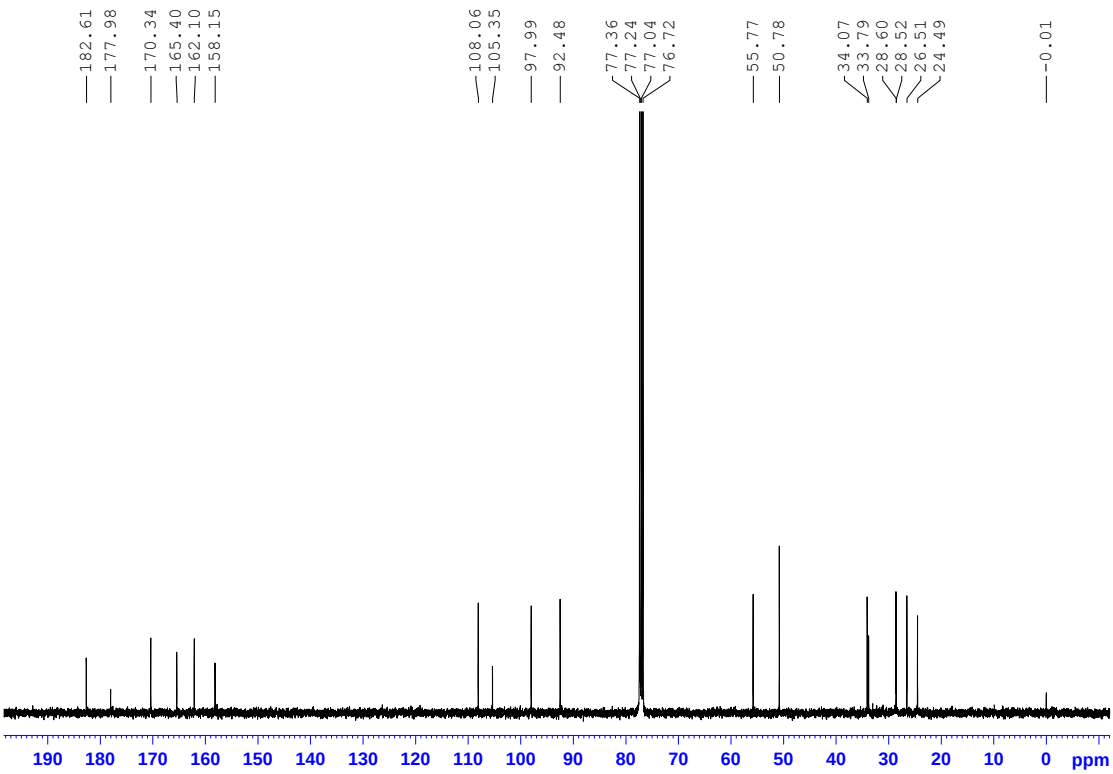

Figure S20 ^{13}C NMR Spectrum of **4** in $CDCl_3$ (100 MHz)

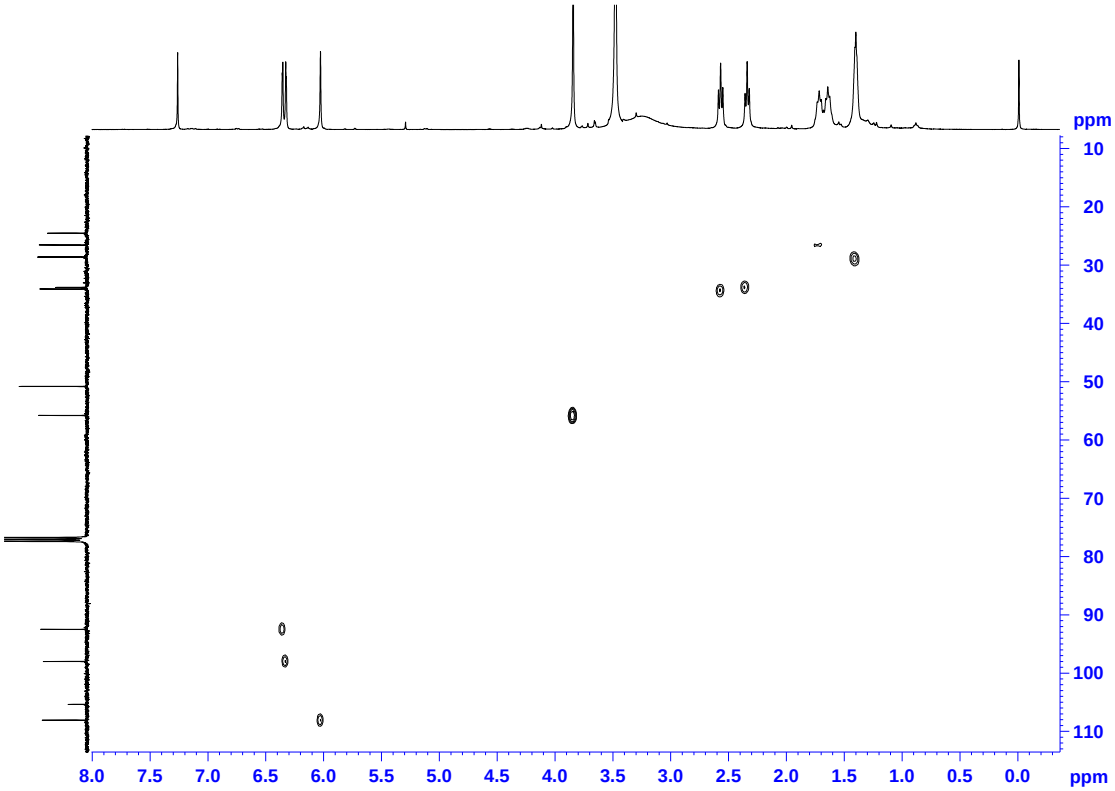

Figure S21 HSQC Spectrum of **4** in $CDCl_3$

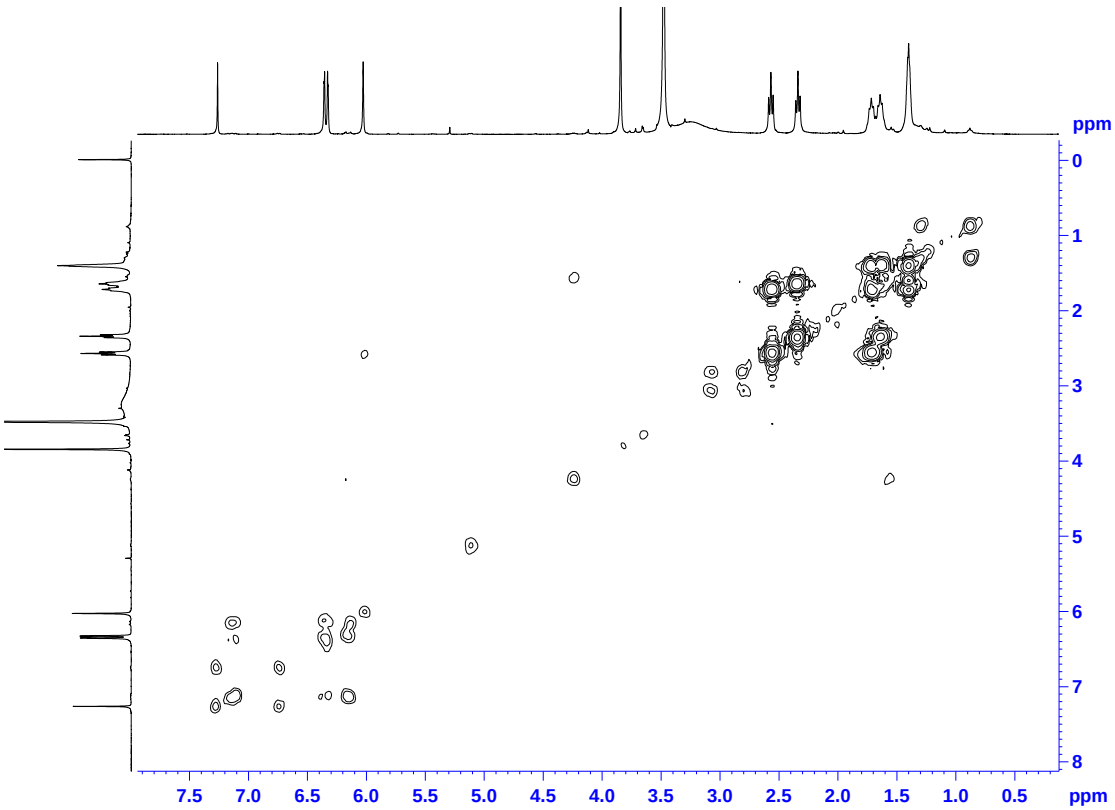

Figure S22 ^{1}H-^{1}H COSY Spectrum of **4** in $CDCl_3$

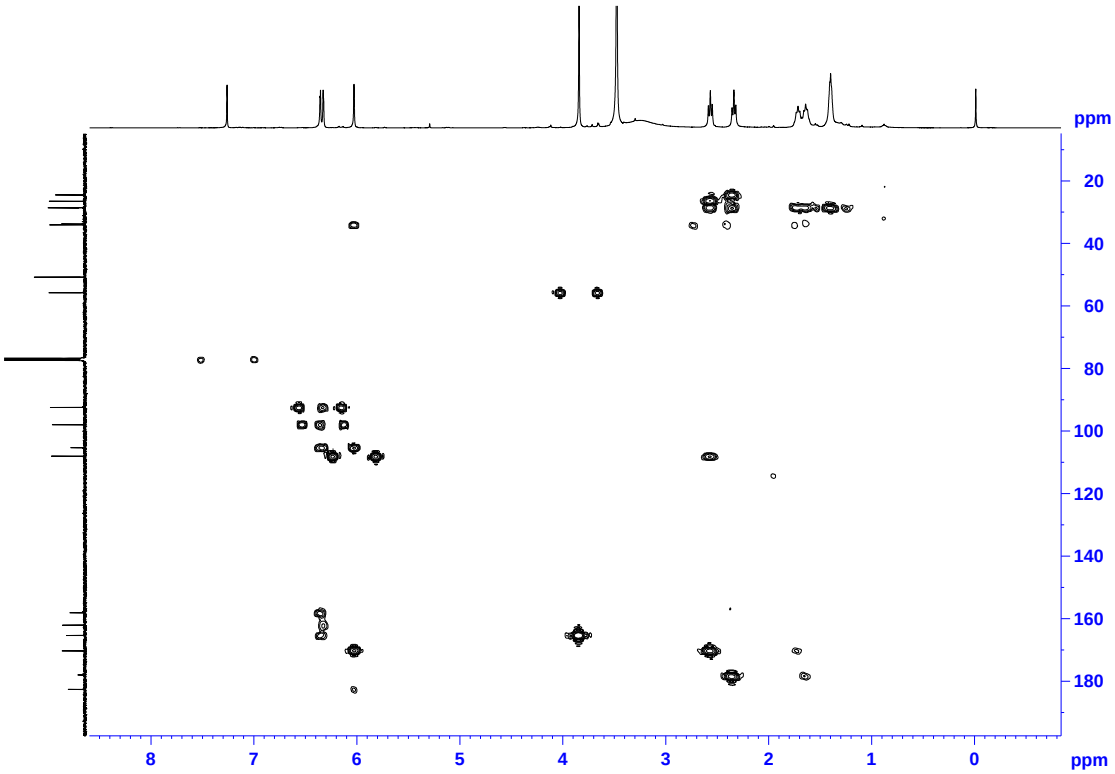

Figure S23 HMBC Spectrum of **4** in $CDCl_3$

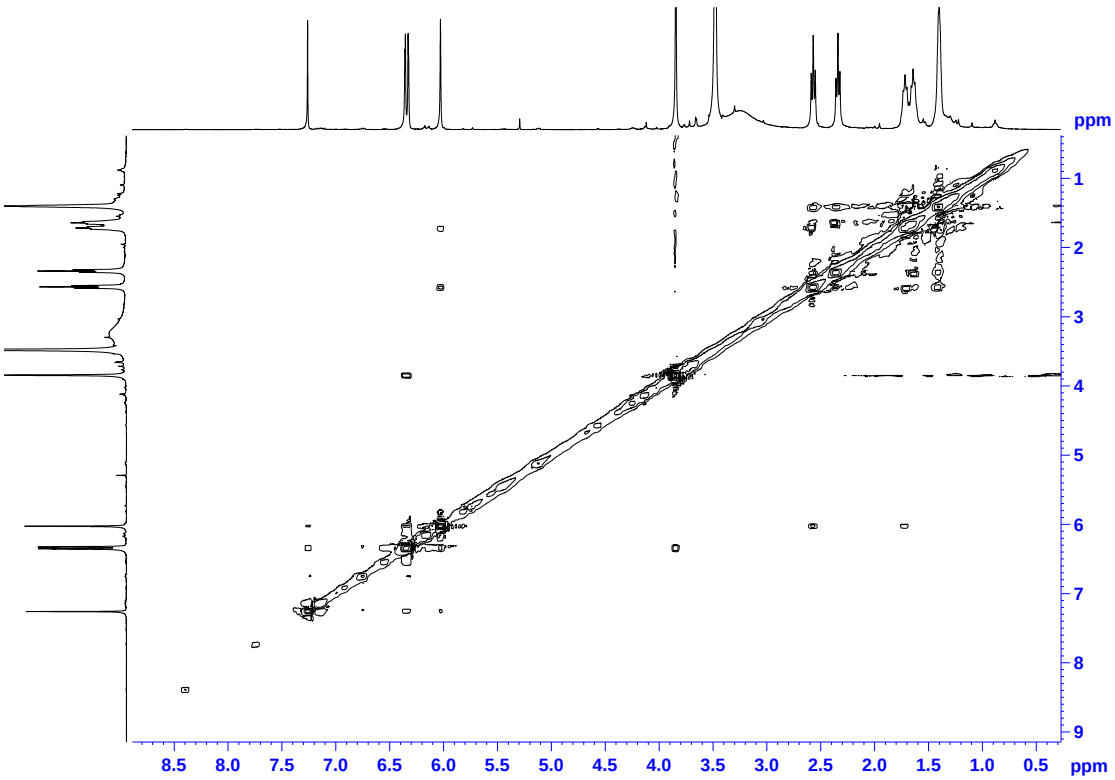

Figure S24 NOESY Spectrum of **4** in $CDCl_3$

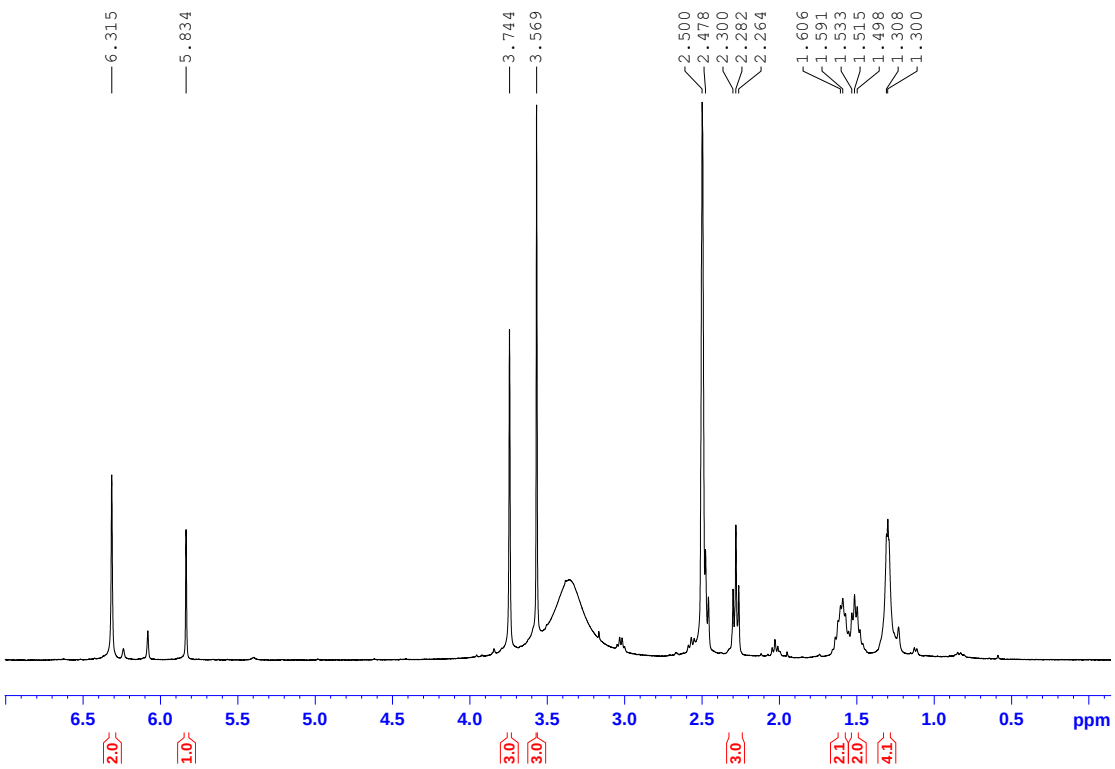

Figure S25 ^{1}H NMR Spectrum of **5** in DMSO-d_6 (400 MHz)

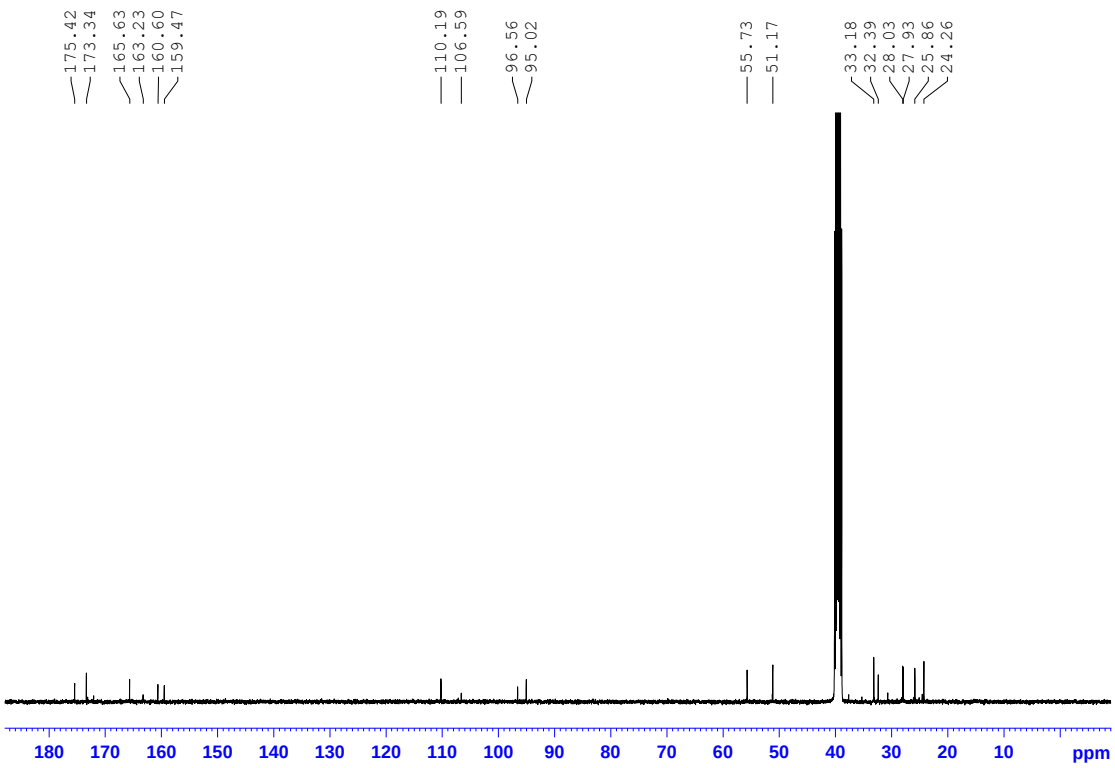

Figure S26 ^{13}C NMR Spectrum of **5** in DMSO-d_6 (100 MHz)

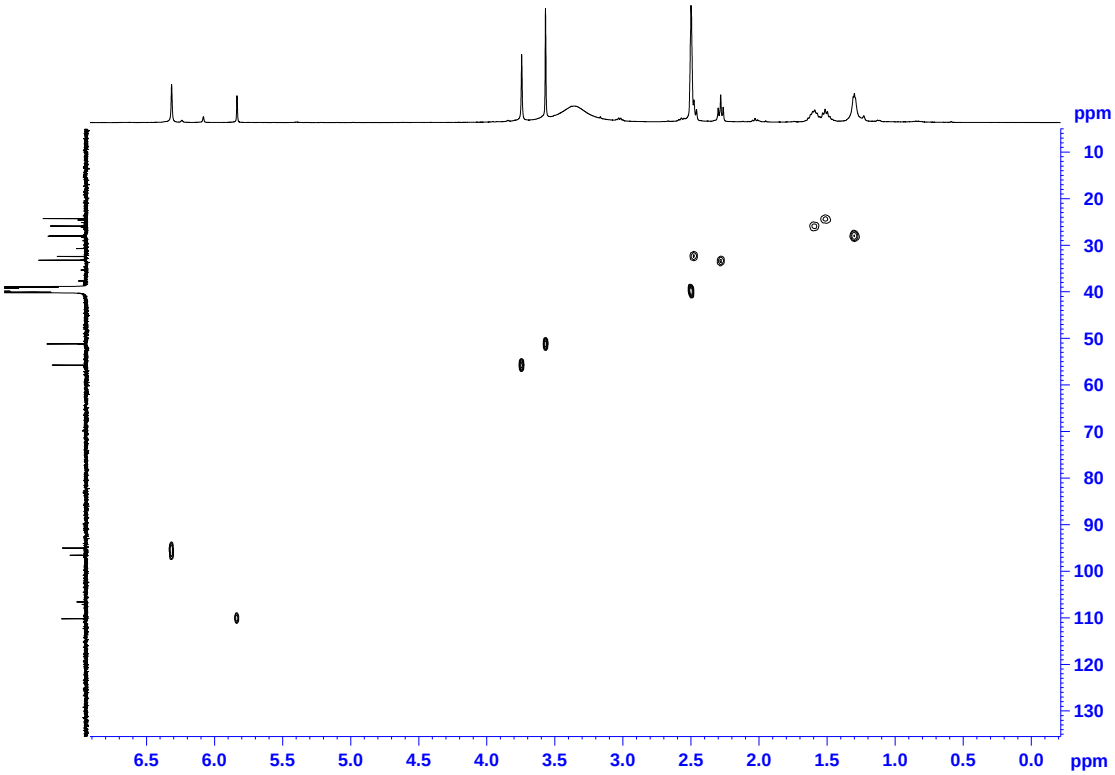

Figure S27 HSQC Spectrum of **5** in DMSO-d_6

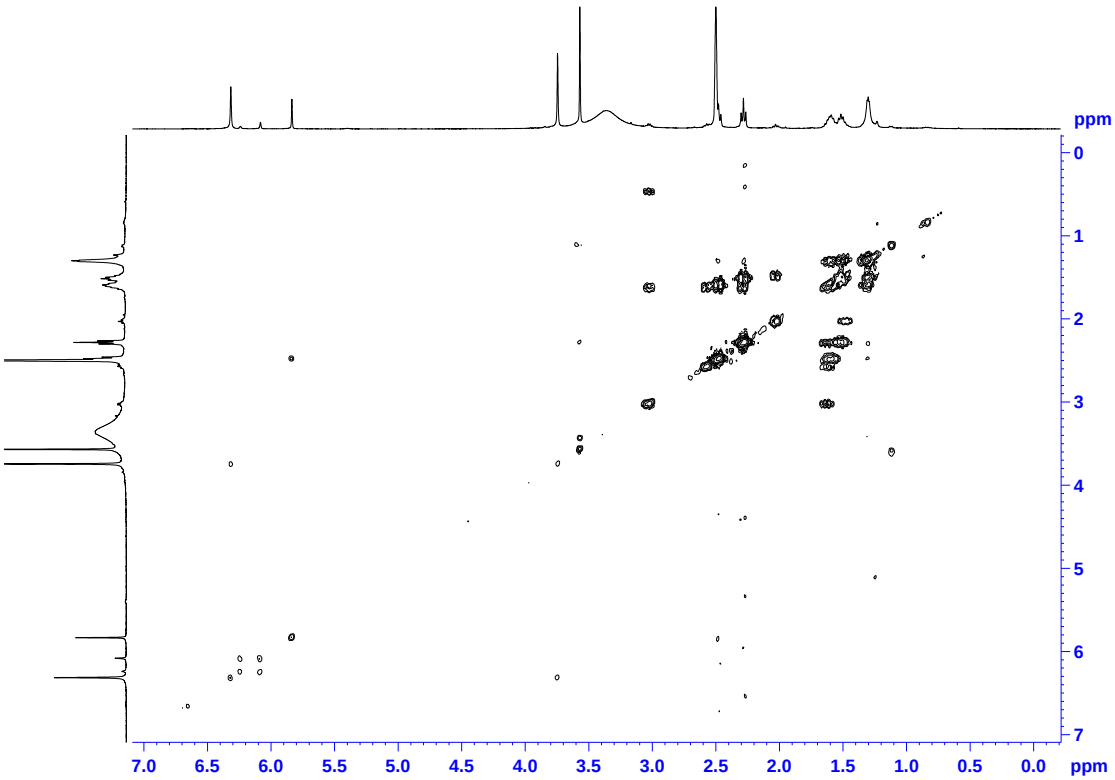

Figure S28 ^{1}H-^{1}H COSY Spectrum of **5** in DMSO-d_6

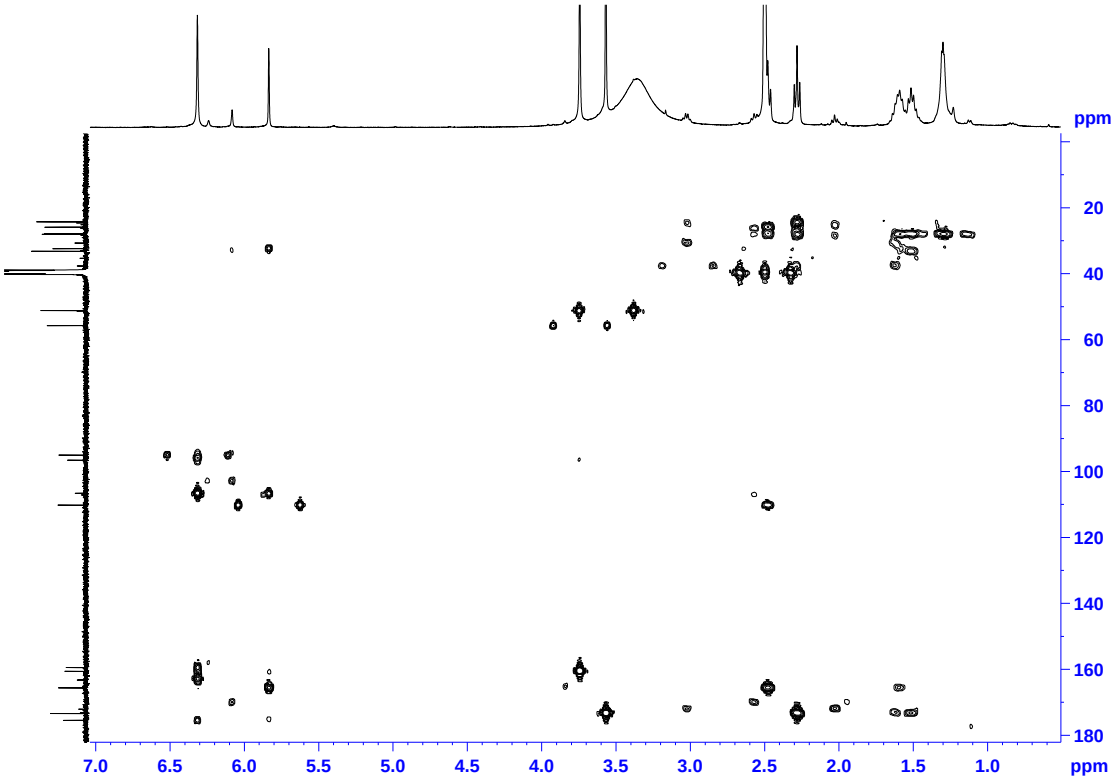

Figure S29 HMBC Spectrum of **5** in DMSO-d_6

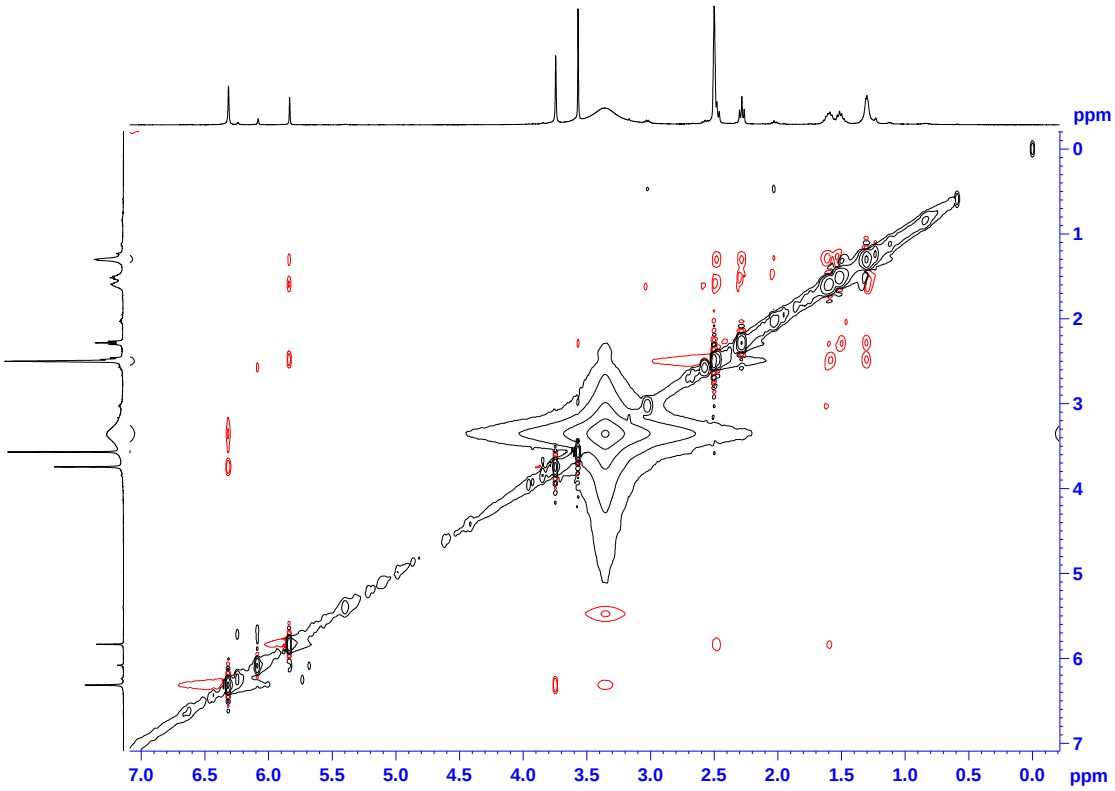

Figure S30 NOESY Spectrum of **5** in DMSO-d_6

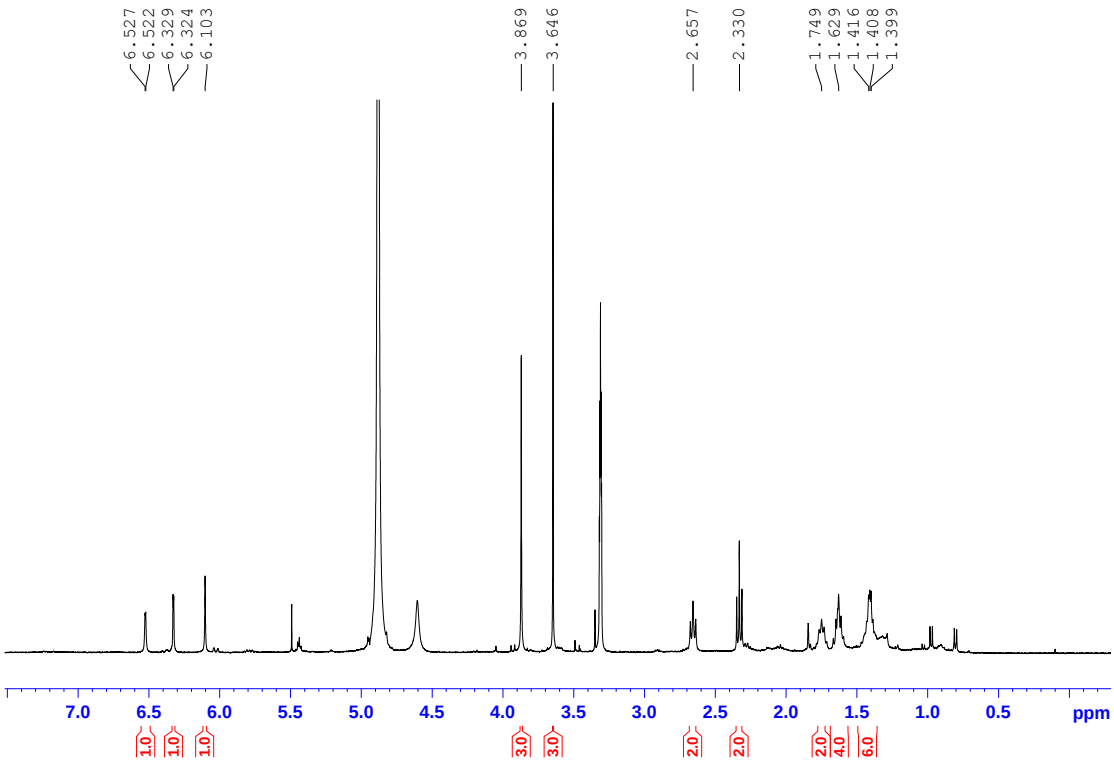

Figure S31 ^{1}H NMR Spectrum of **6** in Methanol-d_4 (400 MHz)

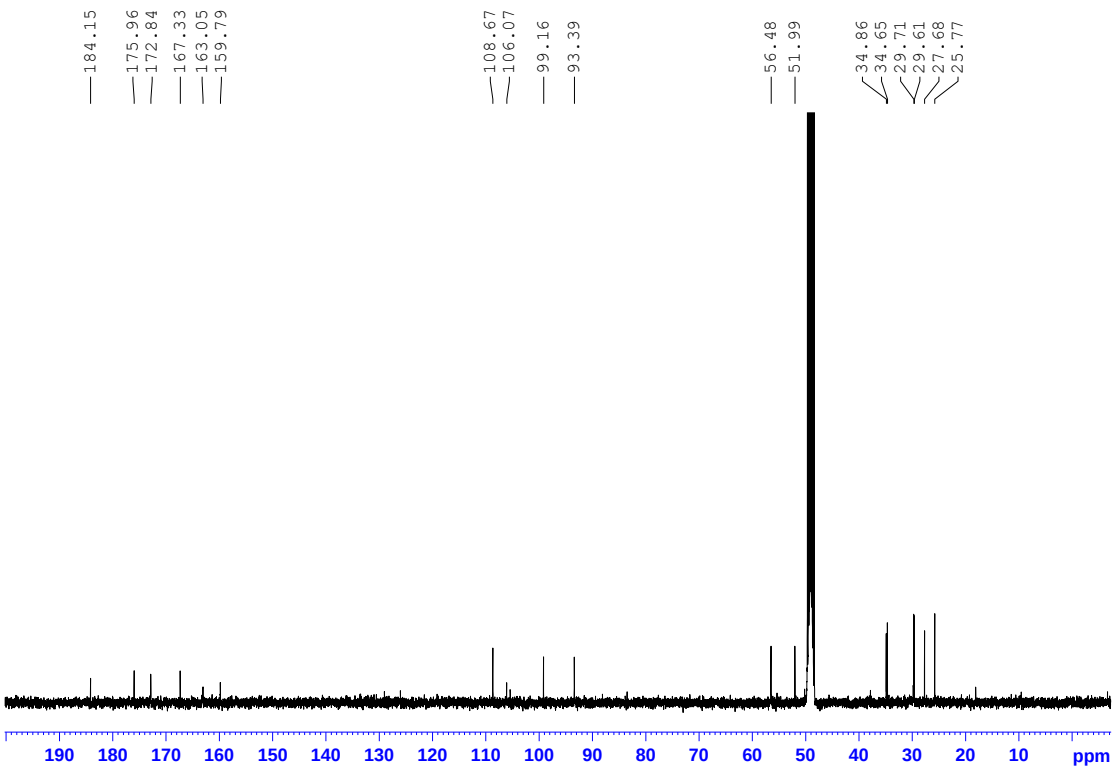

Figure S32 ^{13}C NMR Spectrum of **6** in Methanol-d_4 (100 MHz)

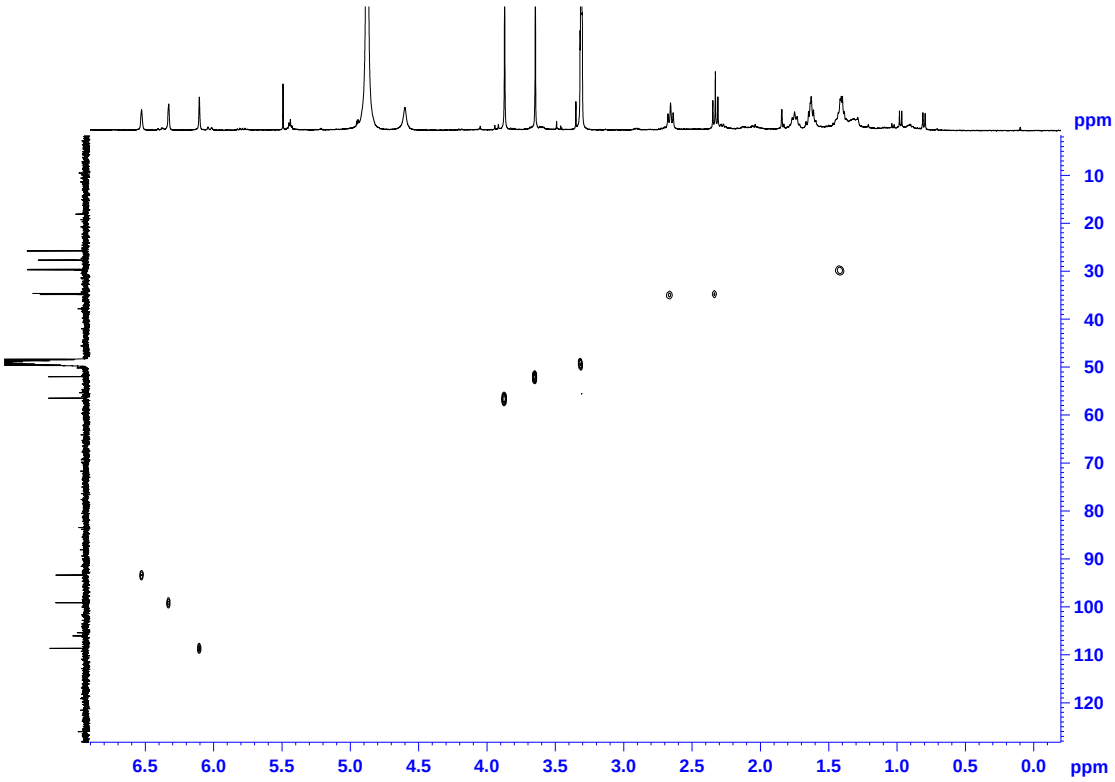

Figure S33 HSQC Spectrum of **6** in Methanol-d_4

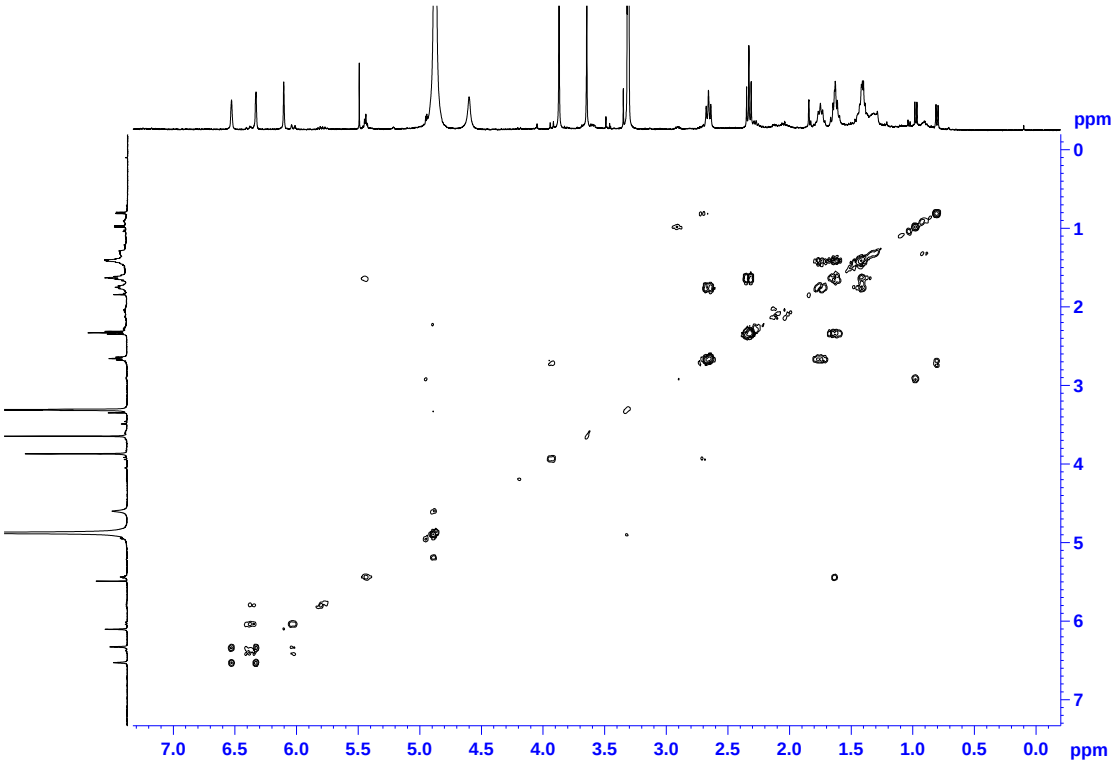

Figure S34 ^{1}H-^{1}H COSY Spectrum of **6** in Methanol-d_4

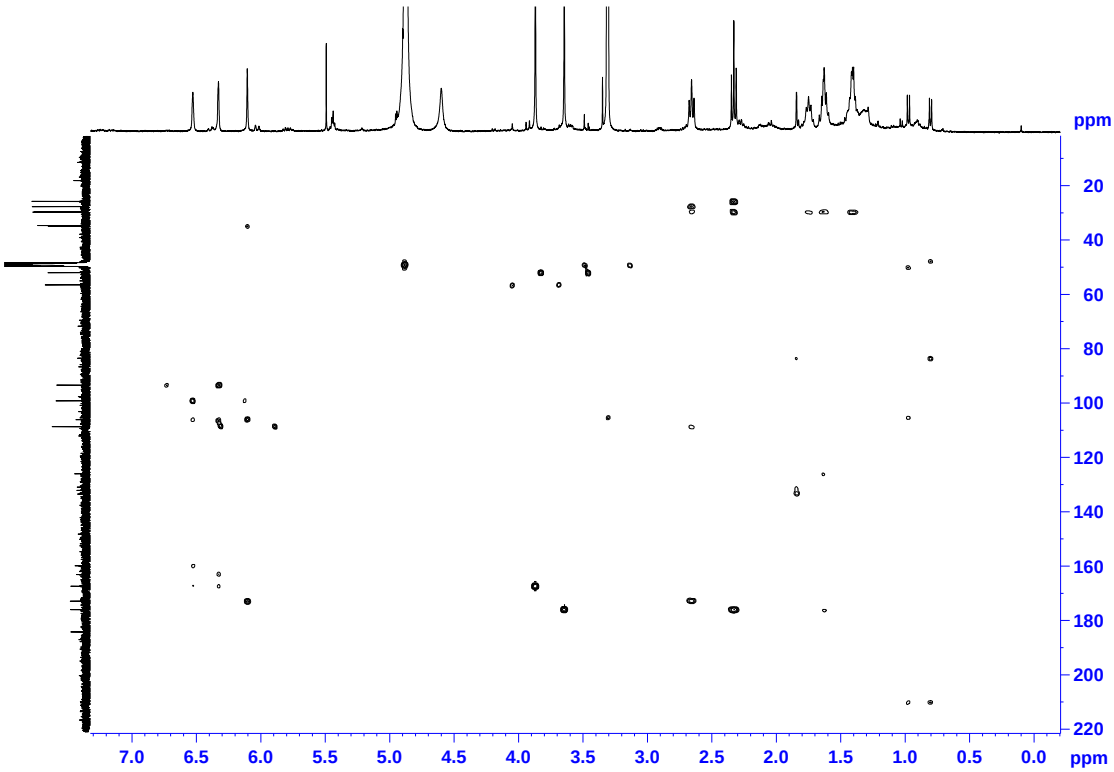

Figure S35 HMBC Spectrum of **6** in Methanol-d_4

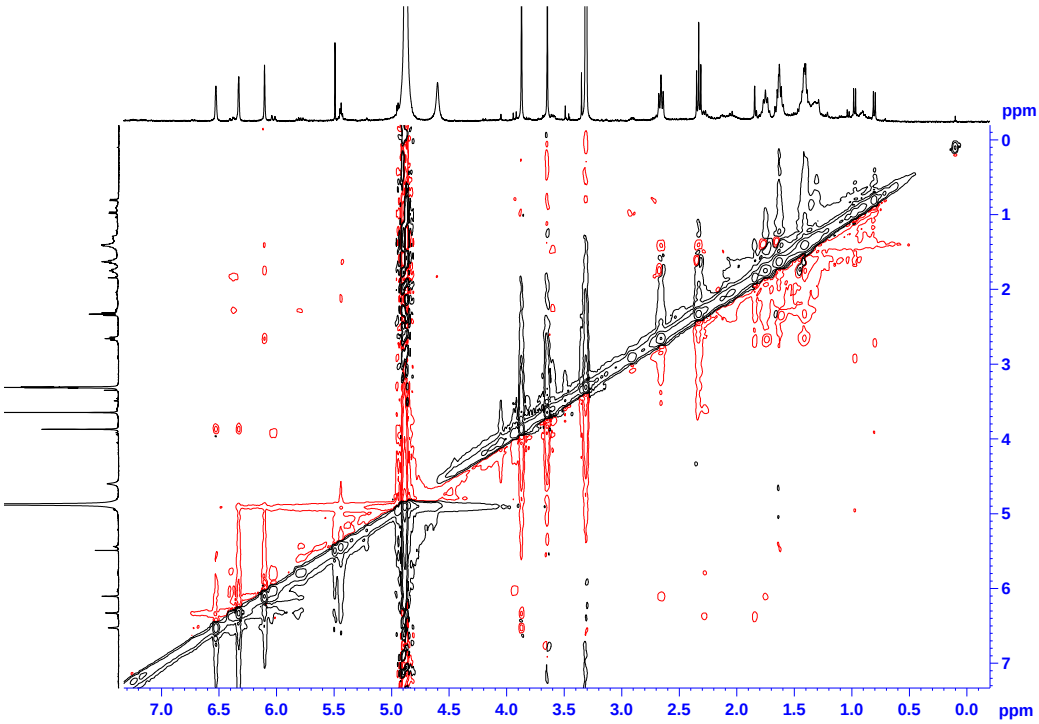

Figure S36 NOESY Spectrum of **6** in Methanol-d_4

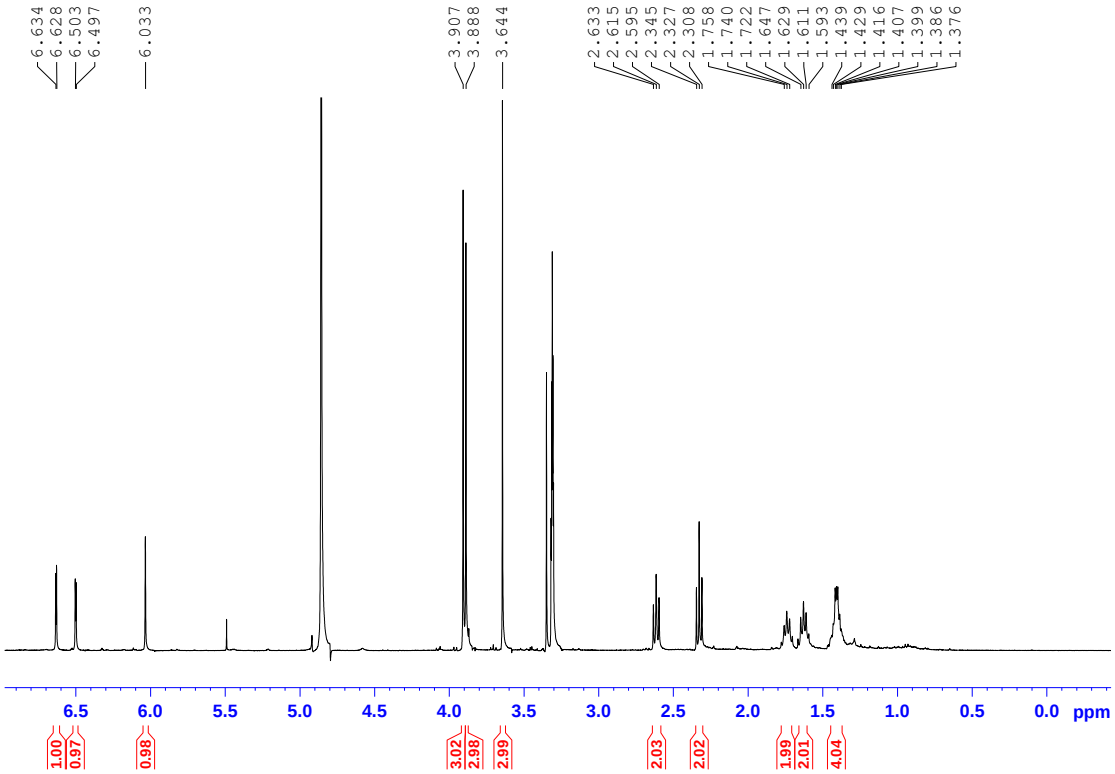

Figure S37 ^{1}H NMR Spectrum of **7** in Methanol-d_4 (400 MHz)

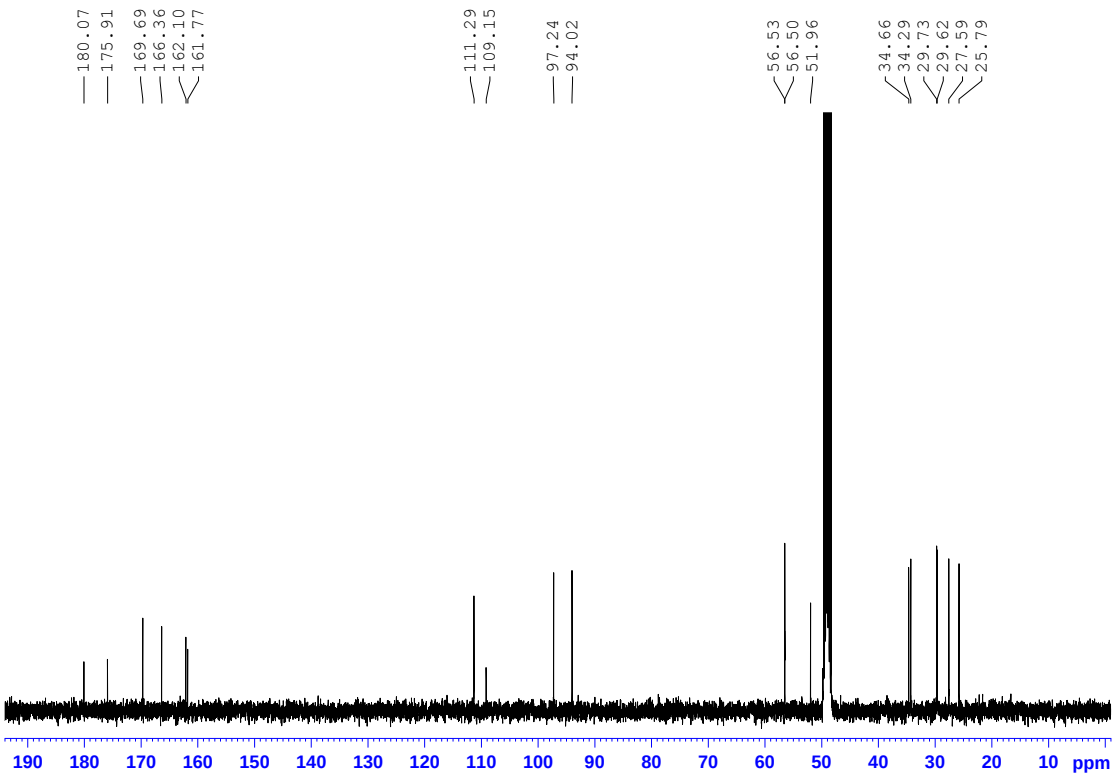

Figure S38 ^{13}C NMR Spectrum of **7** in Methanol-d_4 (100 MHz)

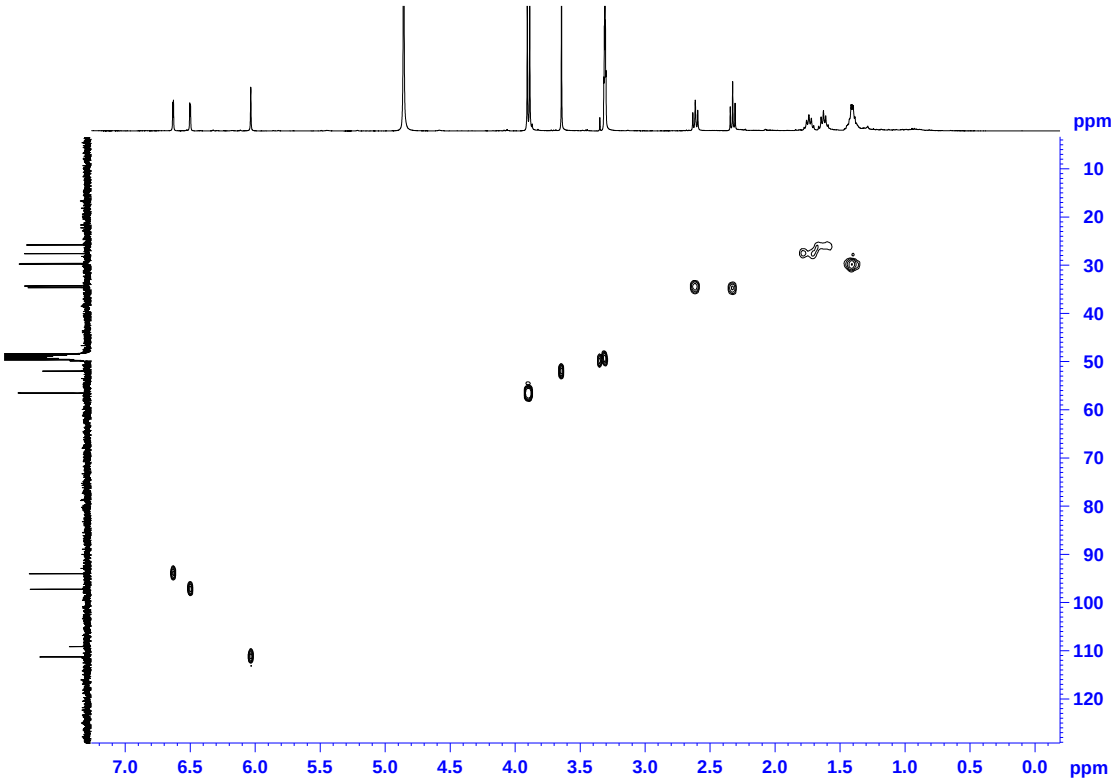

Figure S39 HSQC Spectrum of **7** in Methanol-d_4

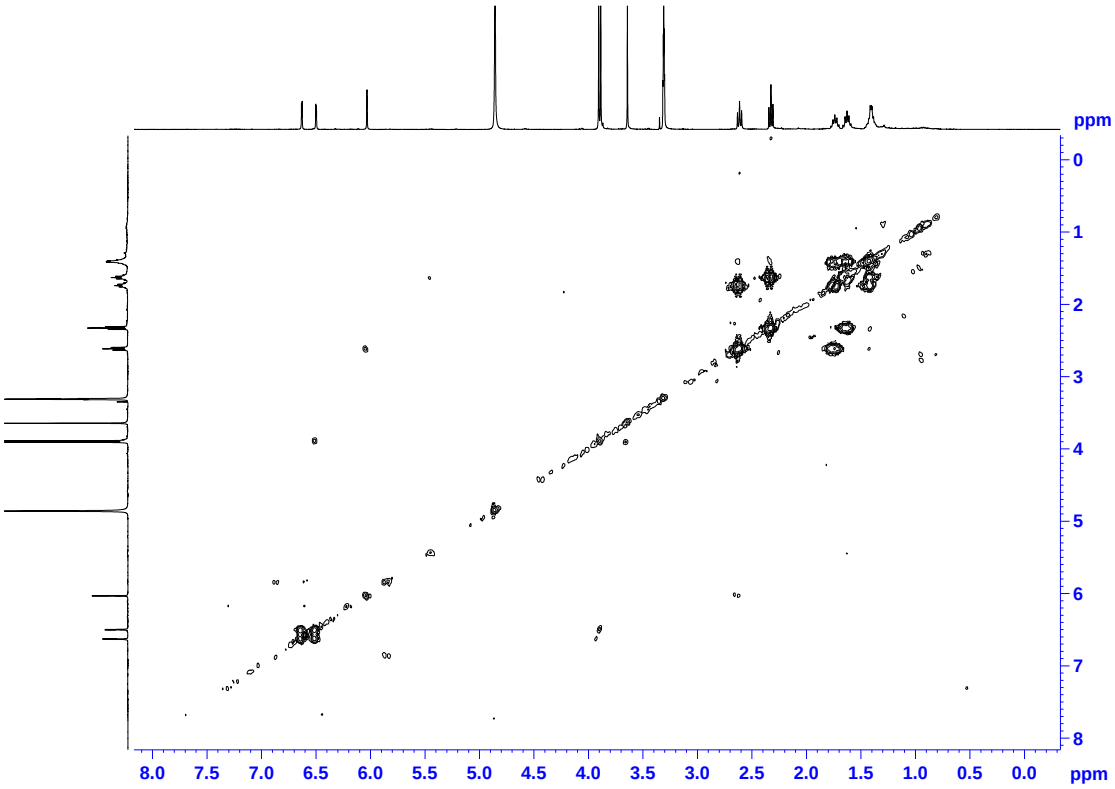

Figure S40 ^{1}H-^{1}H COSY Spectrum of **7** in Methanol-d_4

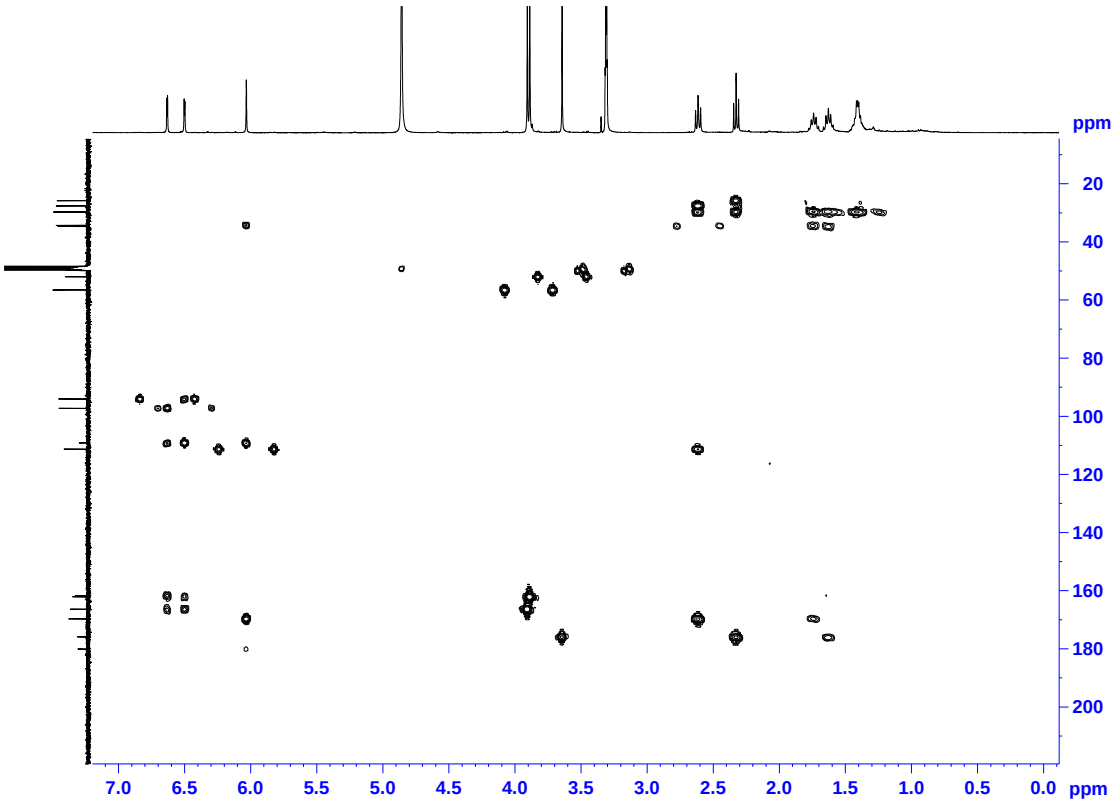

Figure S41 HMBC Spectrum of **7** in Methanol-d_4

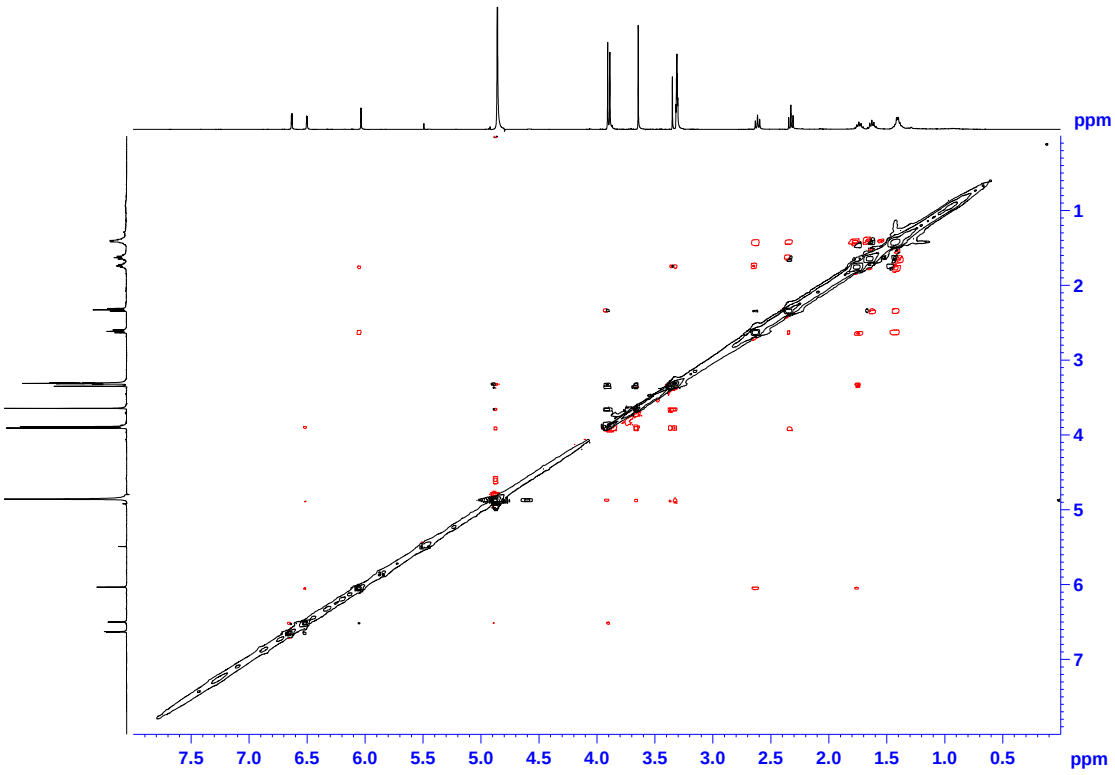

Figure S42 NOESY Spectrum of **7** in Methanol-d_4

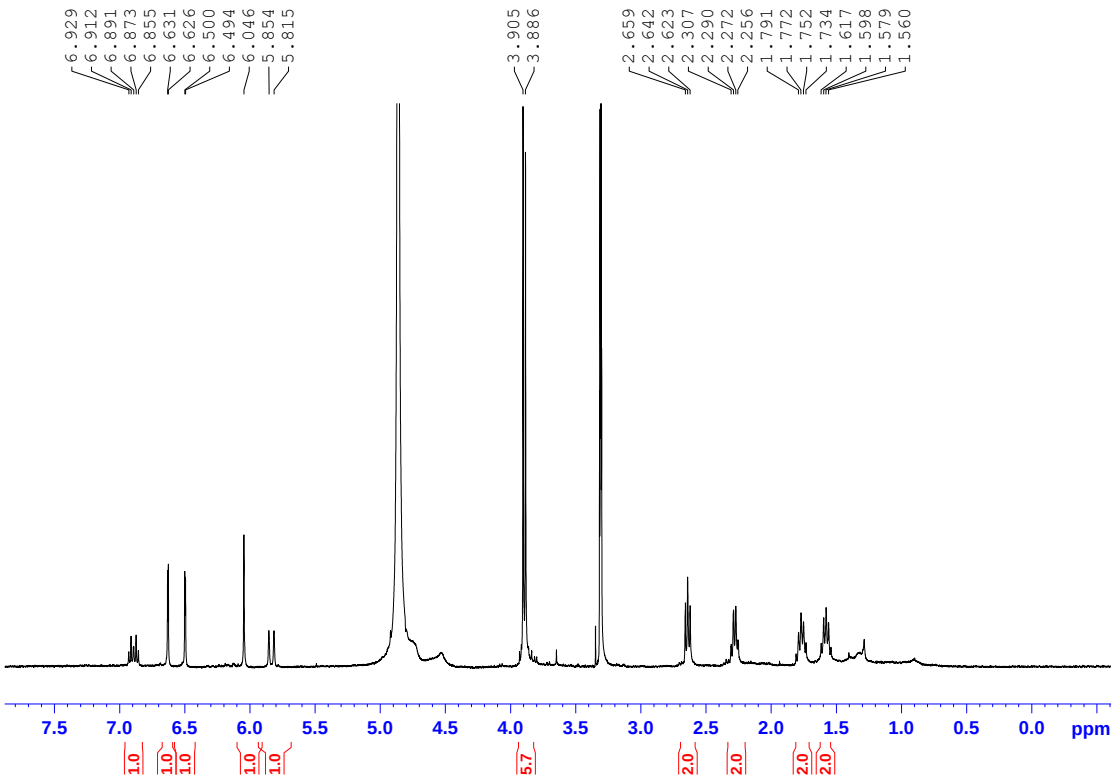

Figure S43 ^{1}H NMR Spectrum of **8** in Methanol-d_4 (400 MHz)

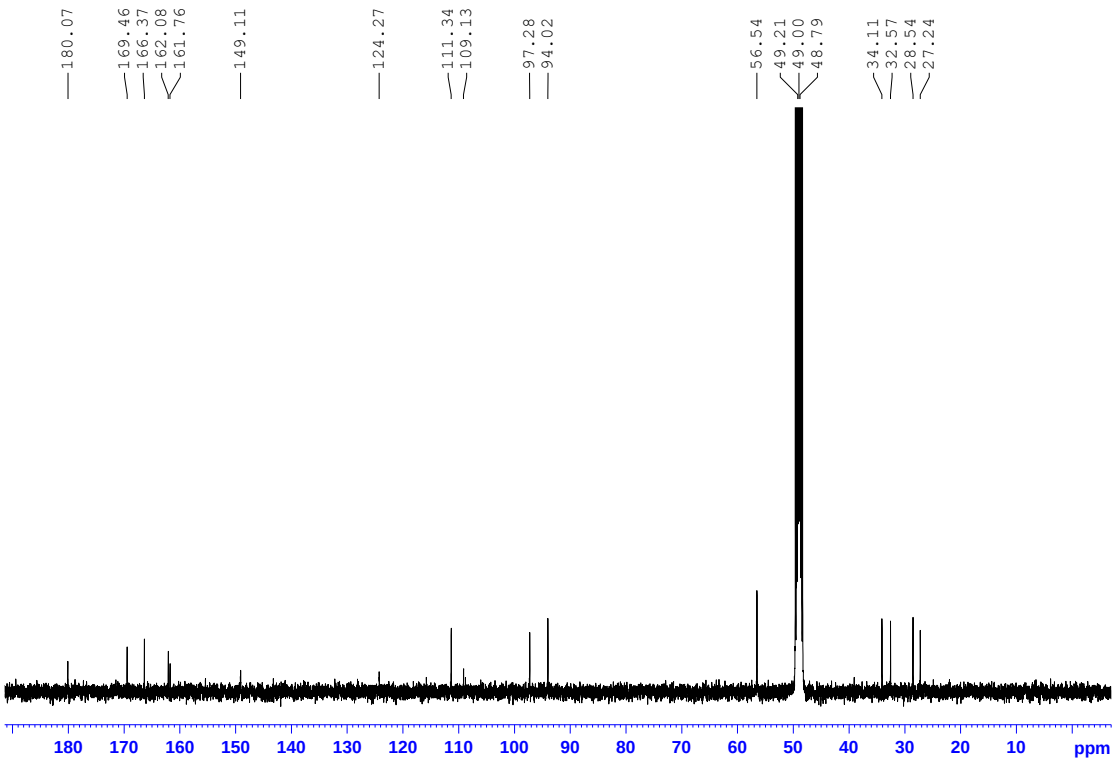

Figure S44 ^{13}C NMR Spectrum of **8** in Methanol-d_4 (100 MHz)

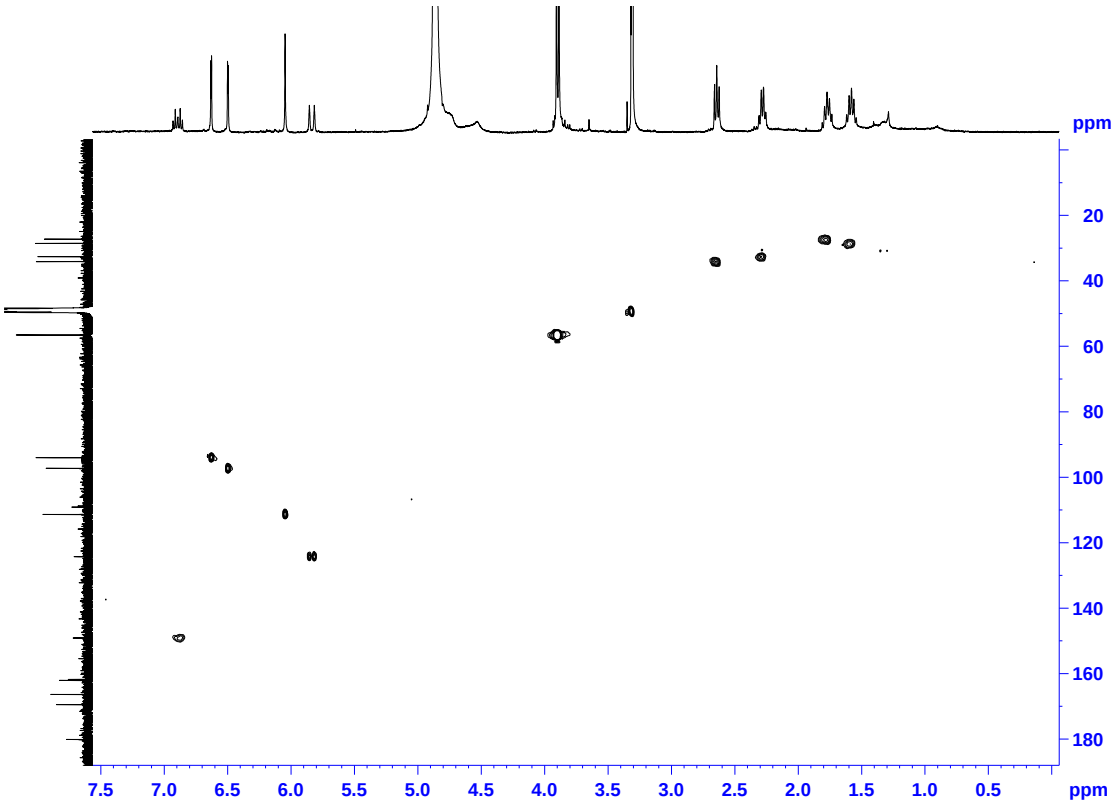

Figure S45 HSQC Spectrum of **8** in Methanol-d_4

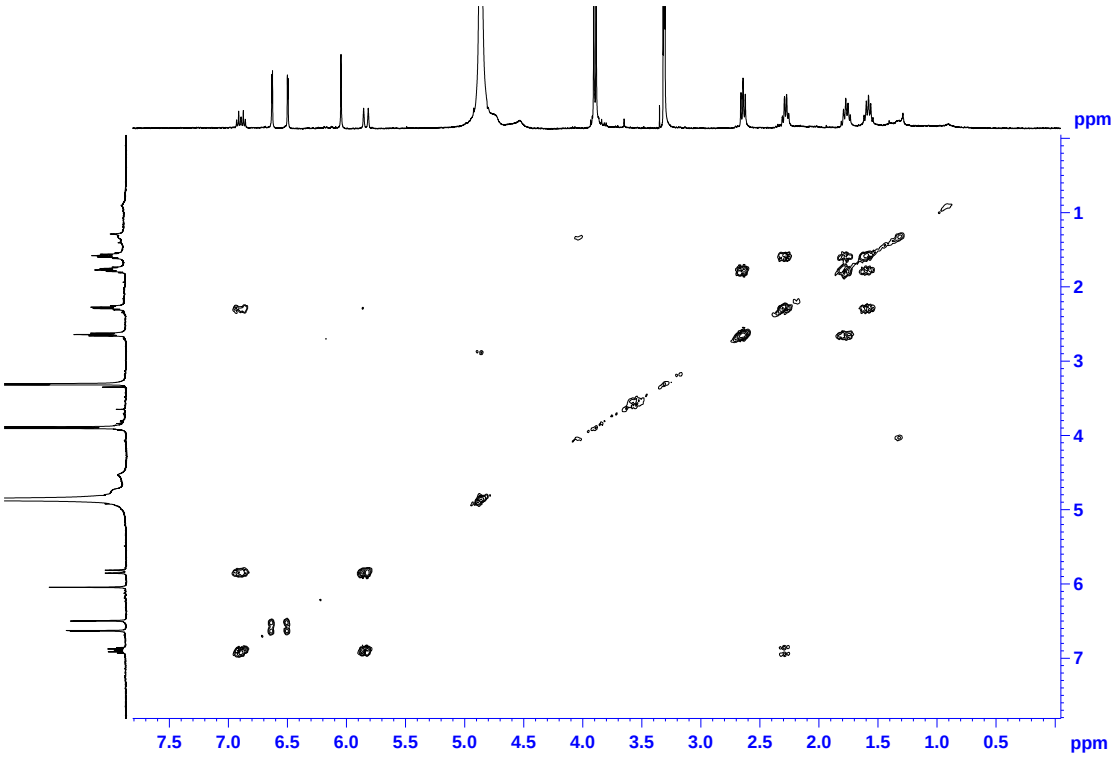

Figure S46 ^{1}H-^{1}H COSY Spectrum of **8** in Methanol-d_4

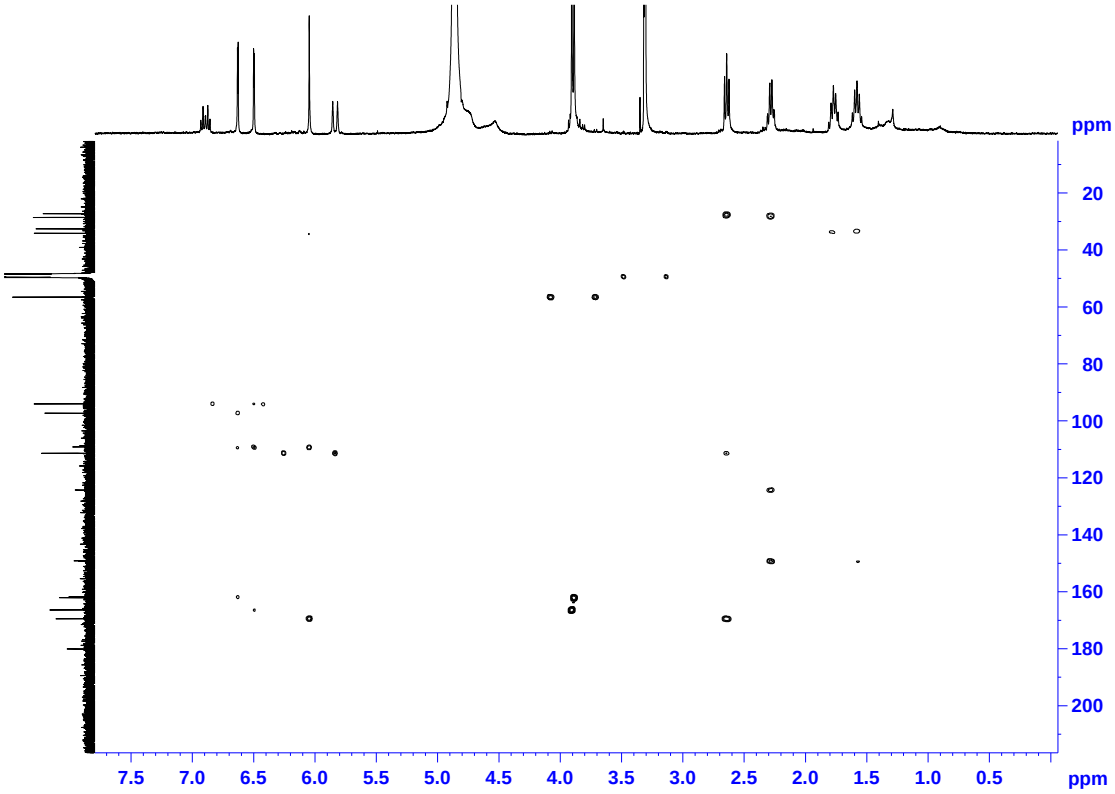

Figure S47 HMBC Spectrum of **8** in Methanol-d_4

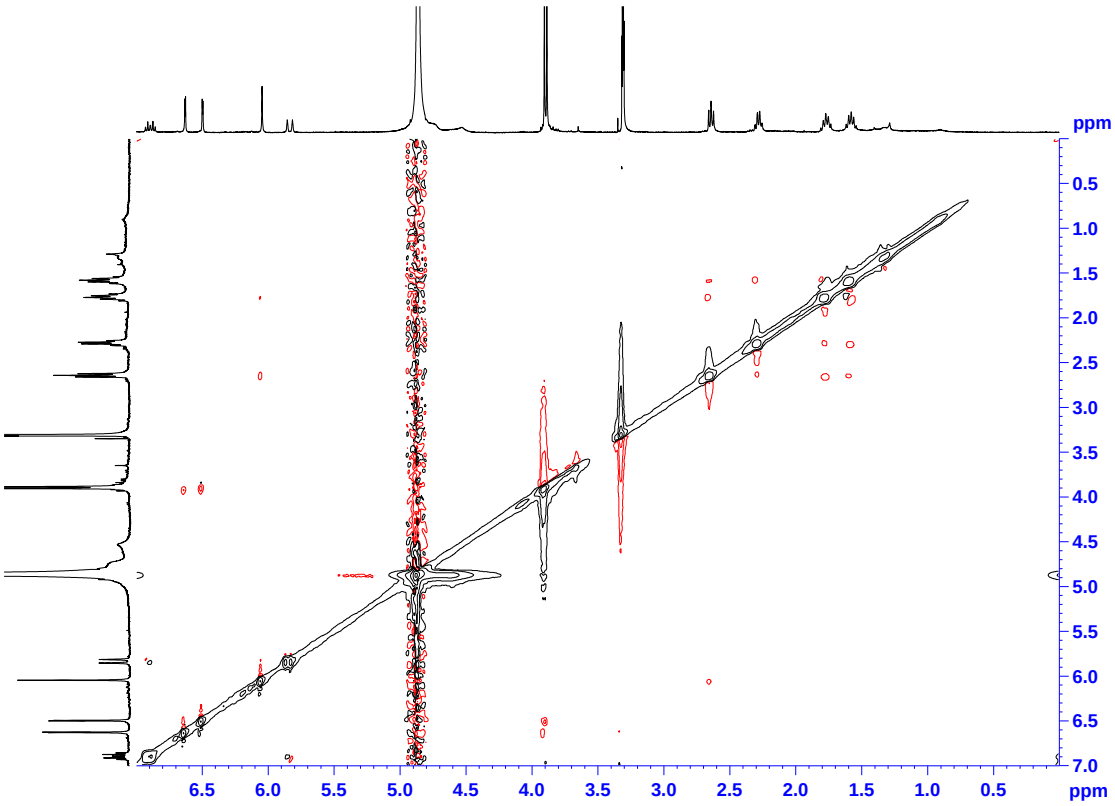

Figure S48 NOESY Spectrum of **8** in Methanol-d_4

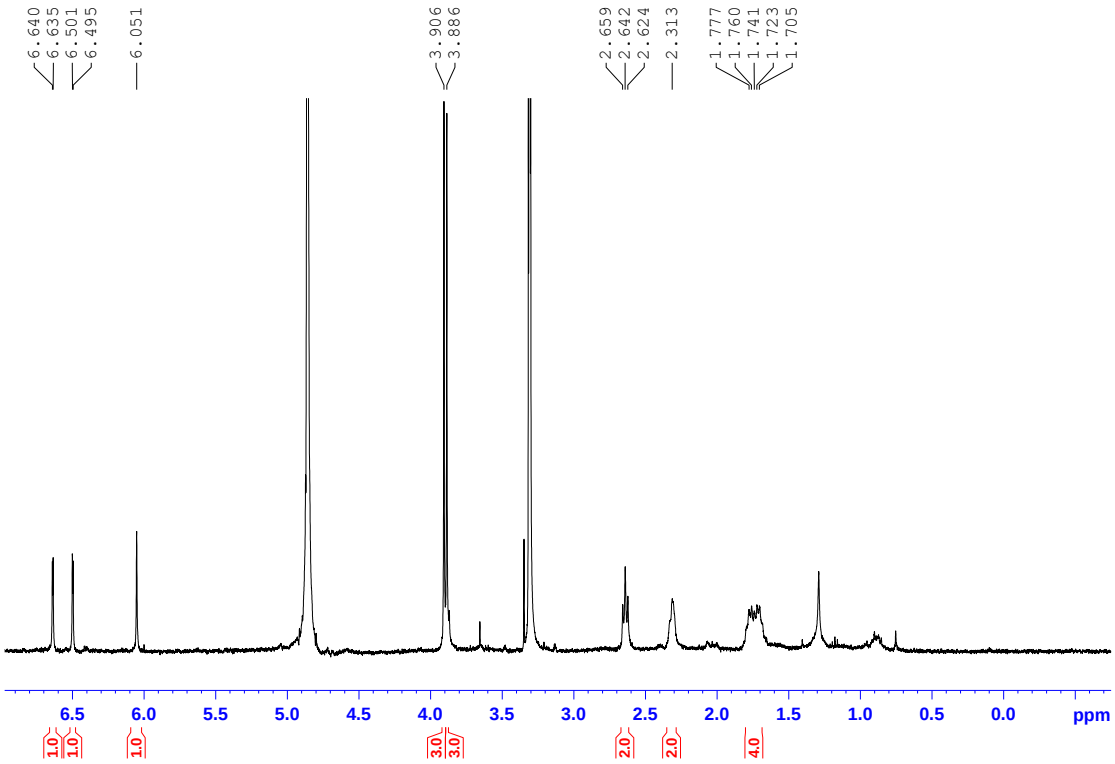

Figure S49 ^{1}H NMR Spectrum of **9** in Methanol-d_4 (400 MHz)

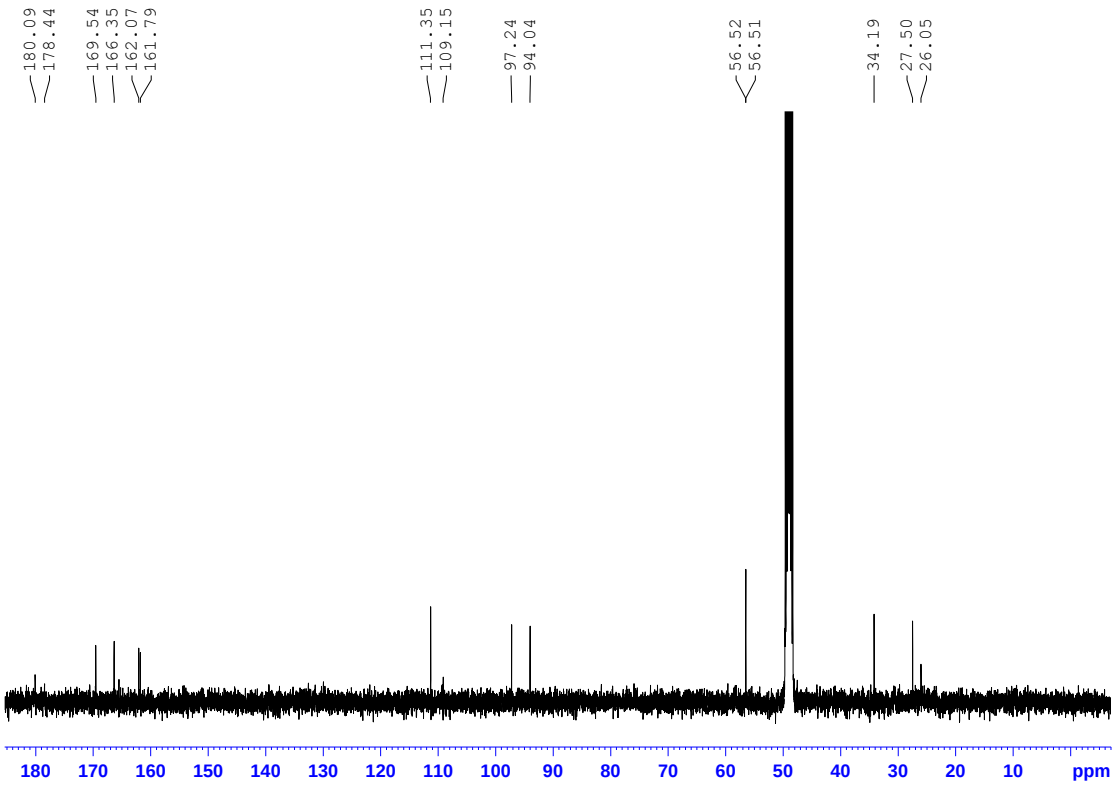

Figure S50 ^{13}C NMR Spectrum of **9** in Methanol-d_4 (100 MHz)

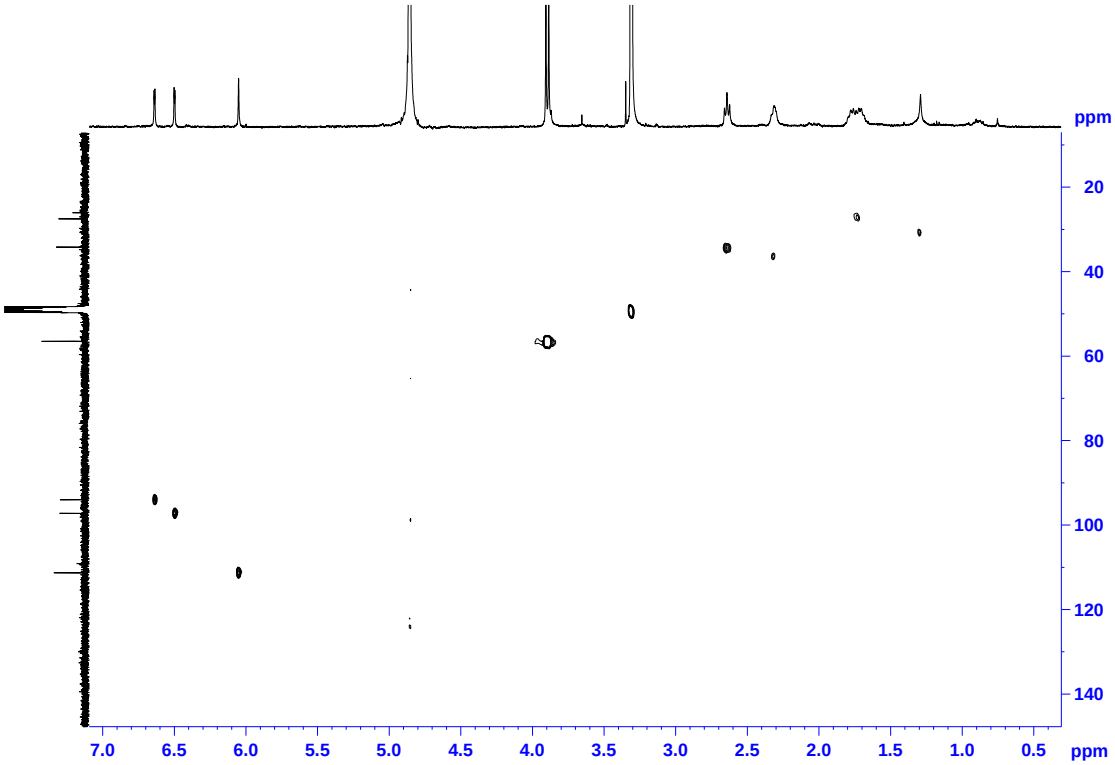

Figure S51 HSQC Spectrum of **9** in Methanol-d_4

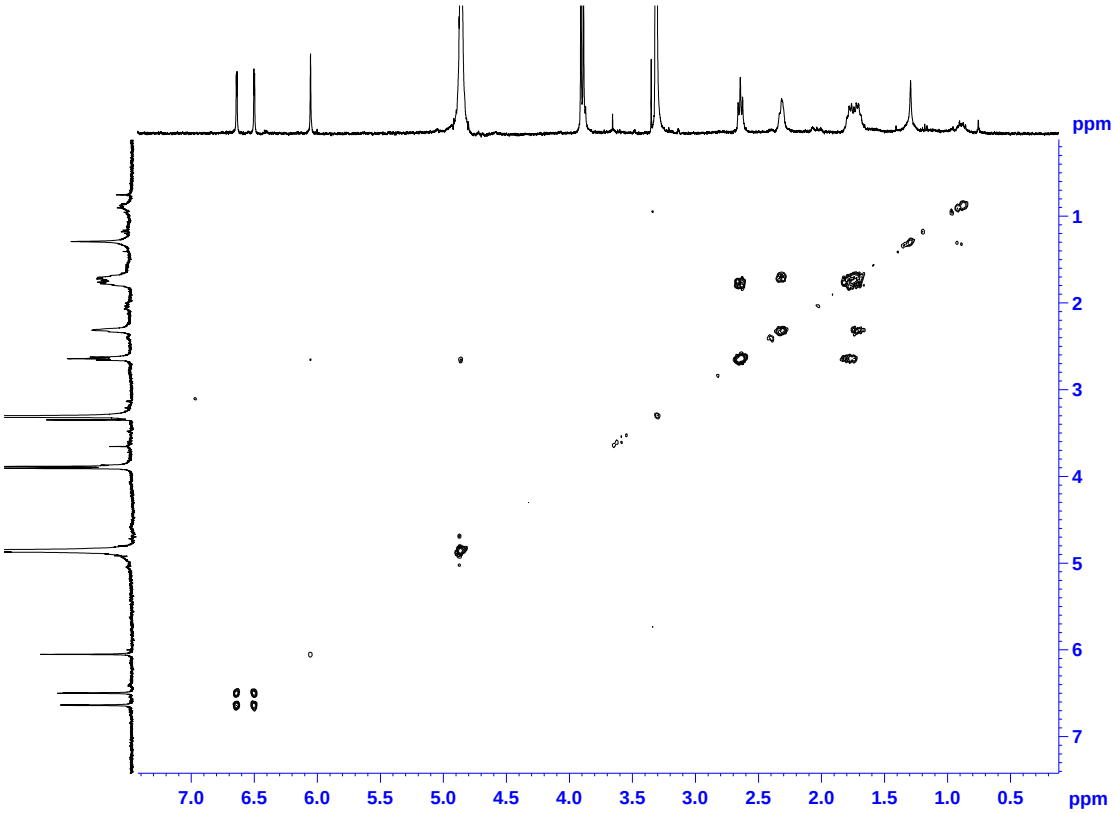

Figure S52 ^{1}H-^{1}H COSY Spectrum of **9** in Methanol-d_4

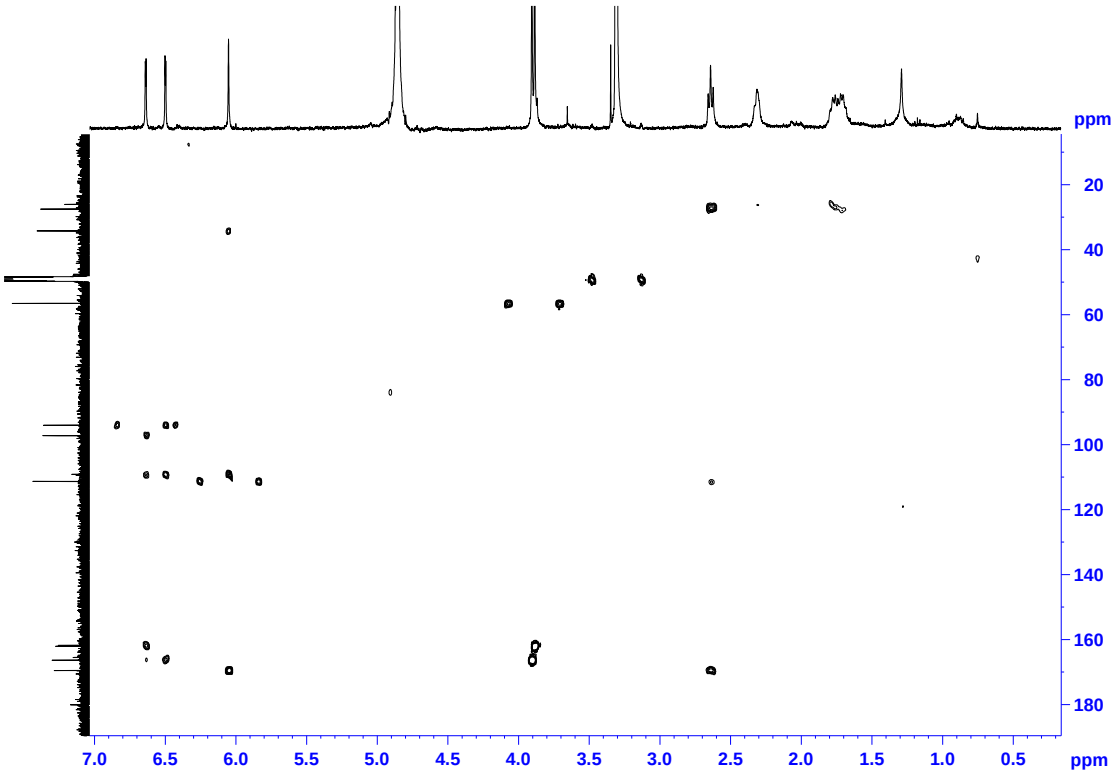

Figure S53 HMBC Spectrum of **9** in Methanol-d_4

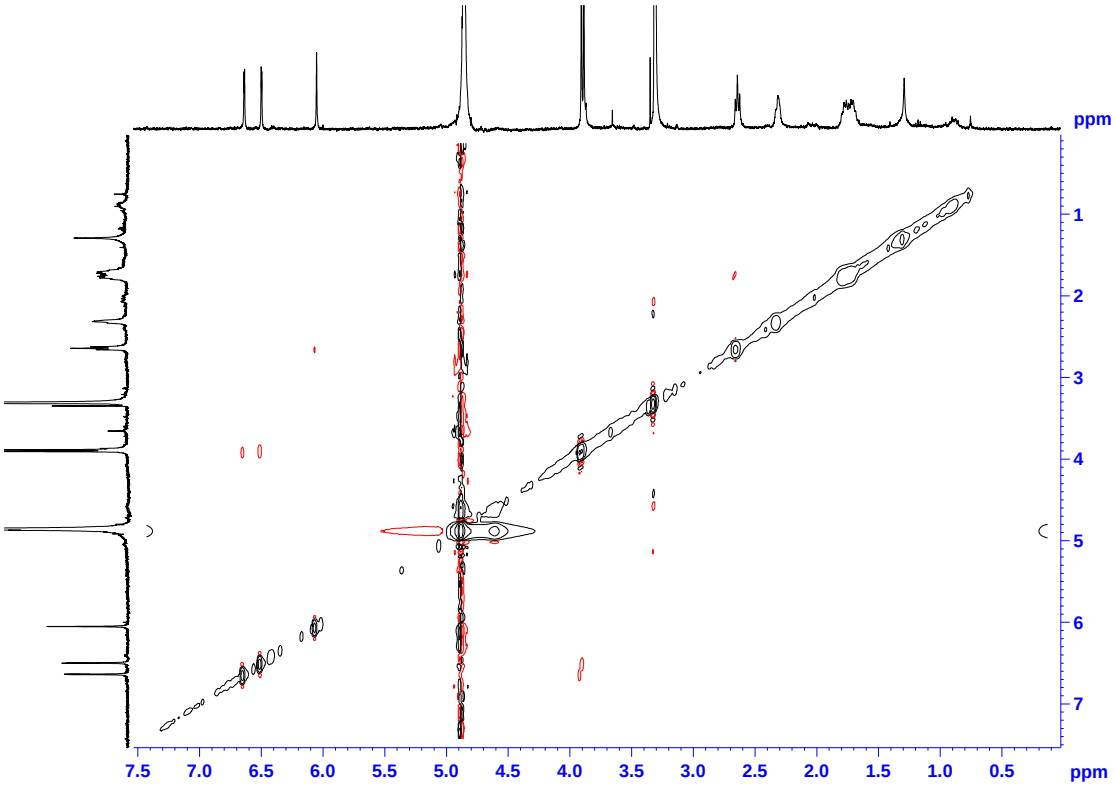

Figure S54 NOESY Spectrum of **9** in Methanol-d_4

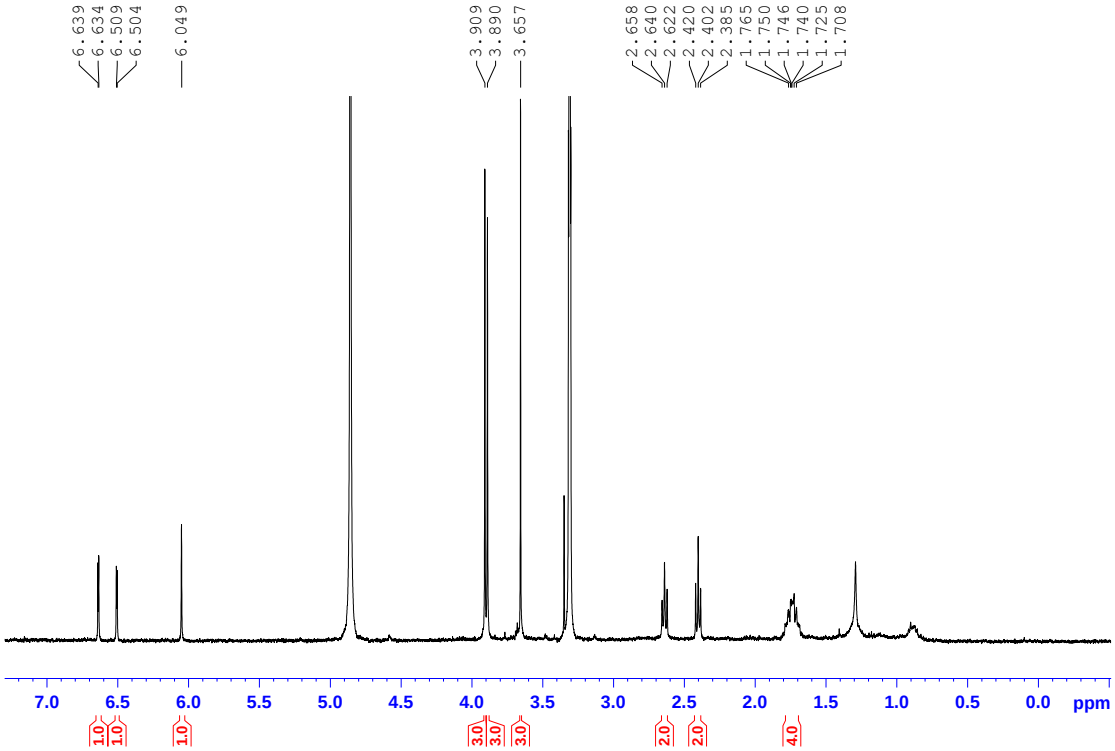

Figure S55 ^{1}H NMR Spectrum of **10** in Methanol-d_4 (400 MHz)

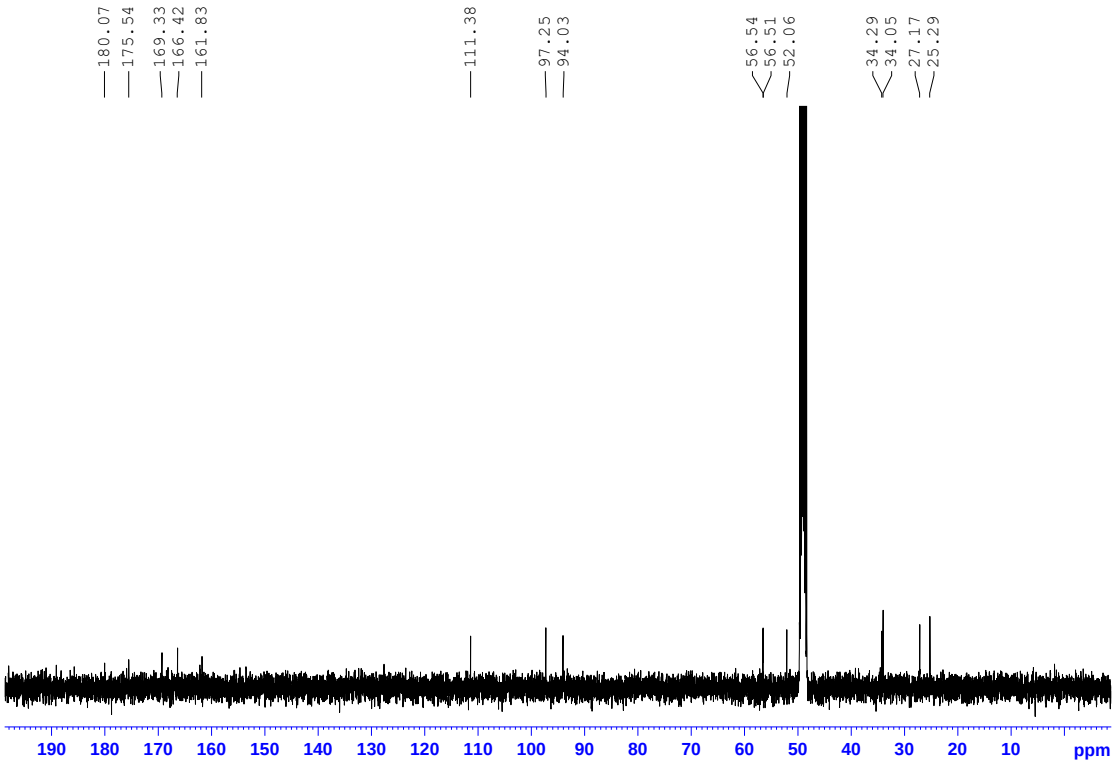

Figure S56 ^{13}C NMR Spectrum of **10** in Methanol-d_4 (100 MHz)

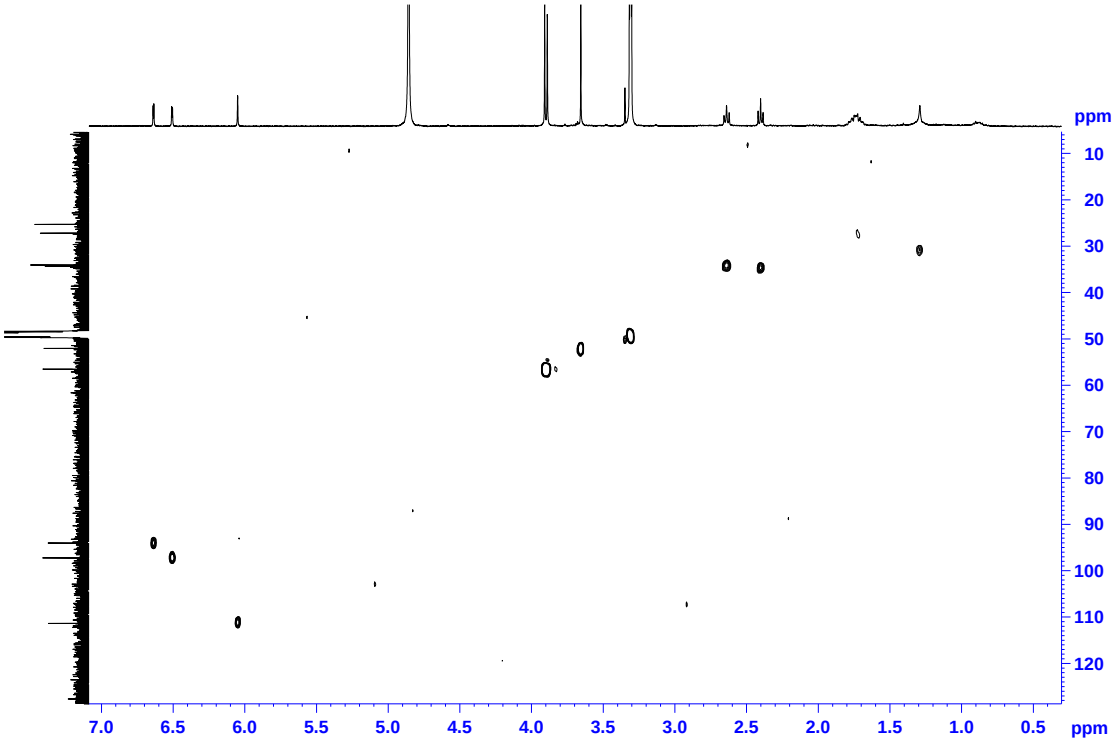

Figure S57 HSQC Spectrum of **10** in Methanol-d_4

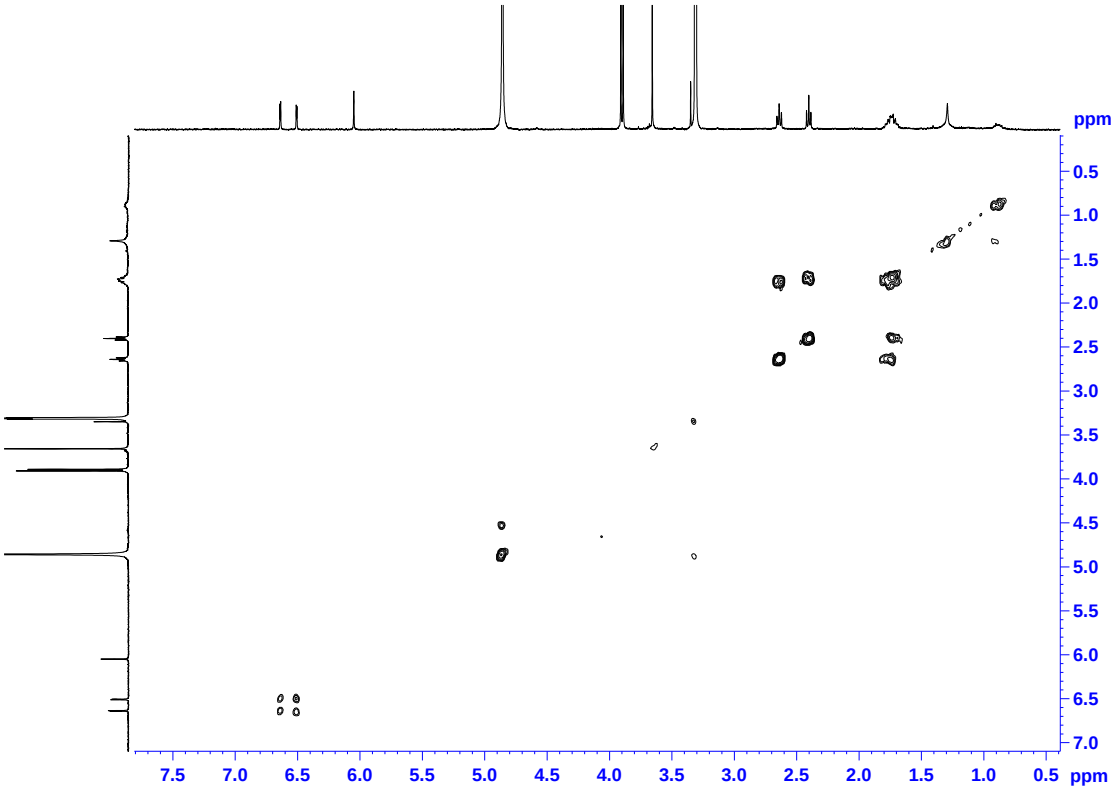

Figure S58 ^{1}H-^{1}H COSY Spectrum of **10** in Methanol-d_4

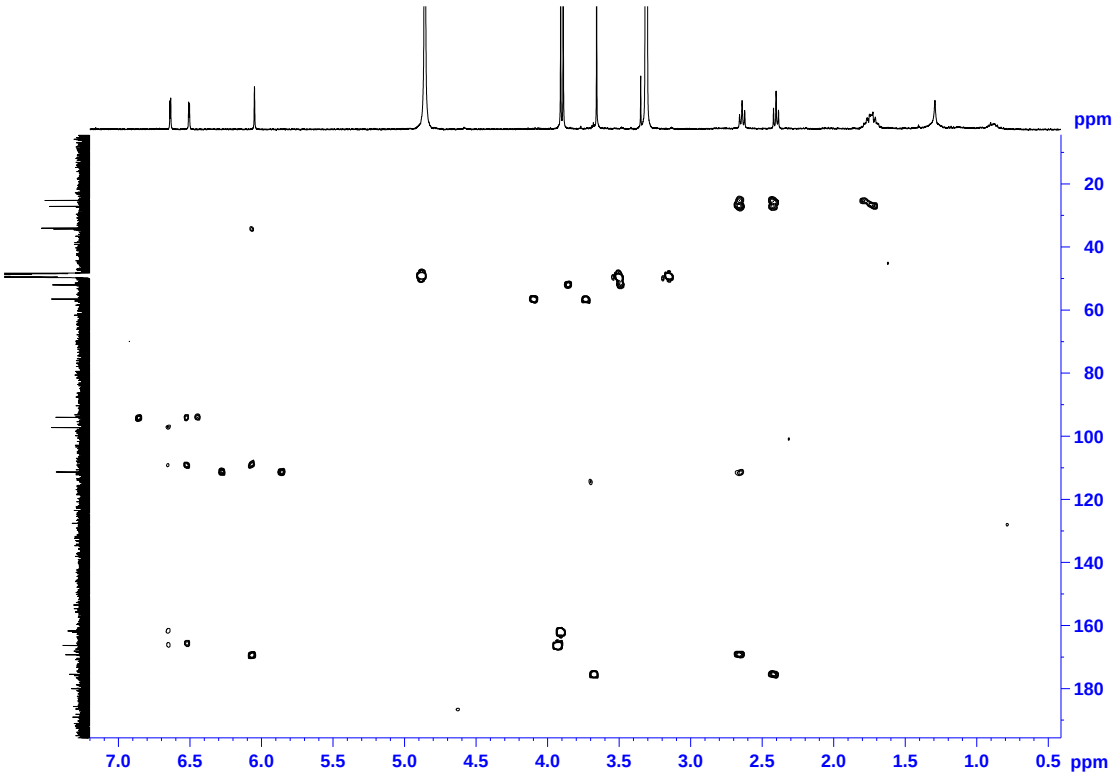

Figure S59 HMBC Spectrum of **10** in Methanol-d_4

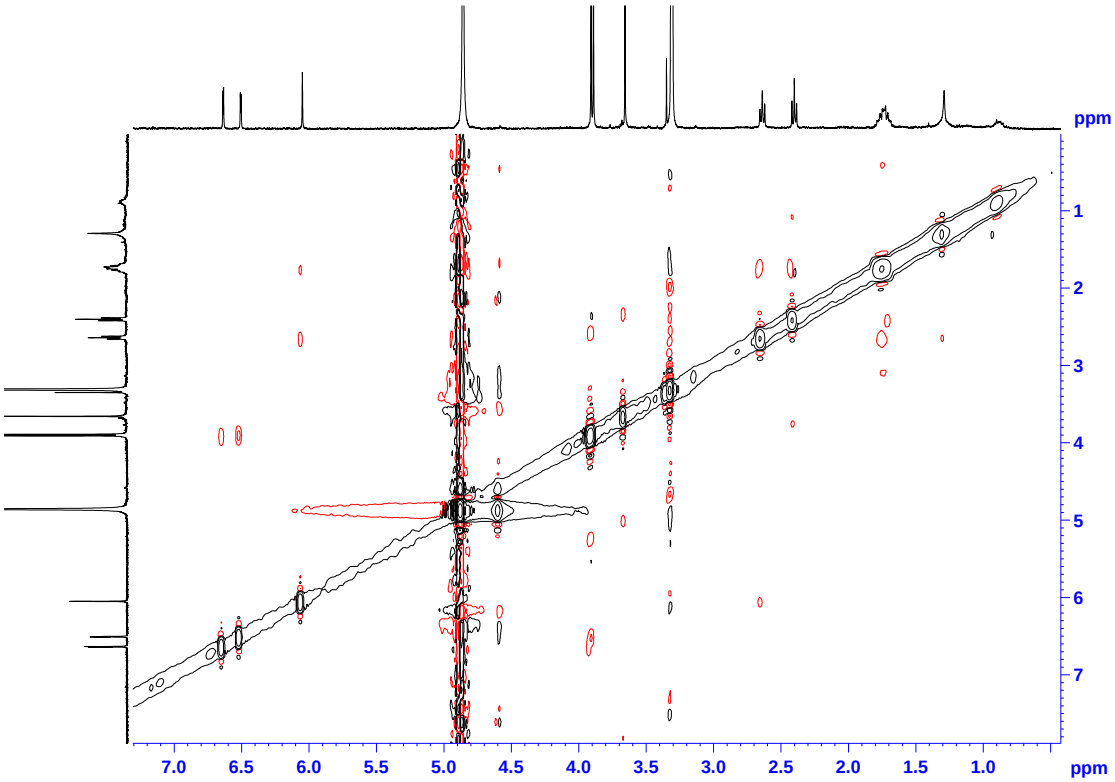

Figure S60 NOESY Spectrum of **10** in Methanol-d_4

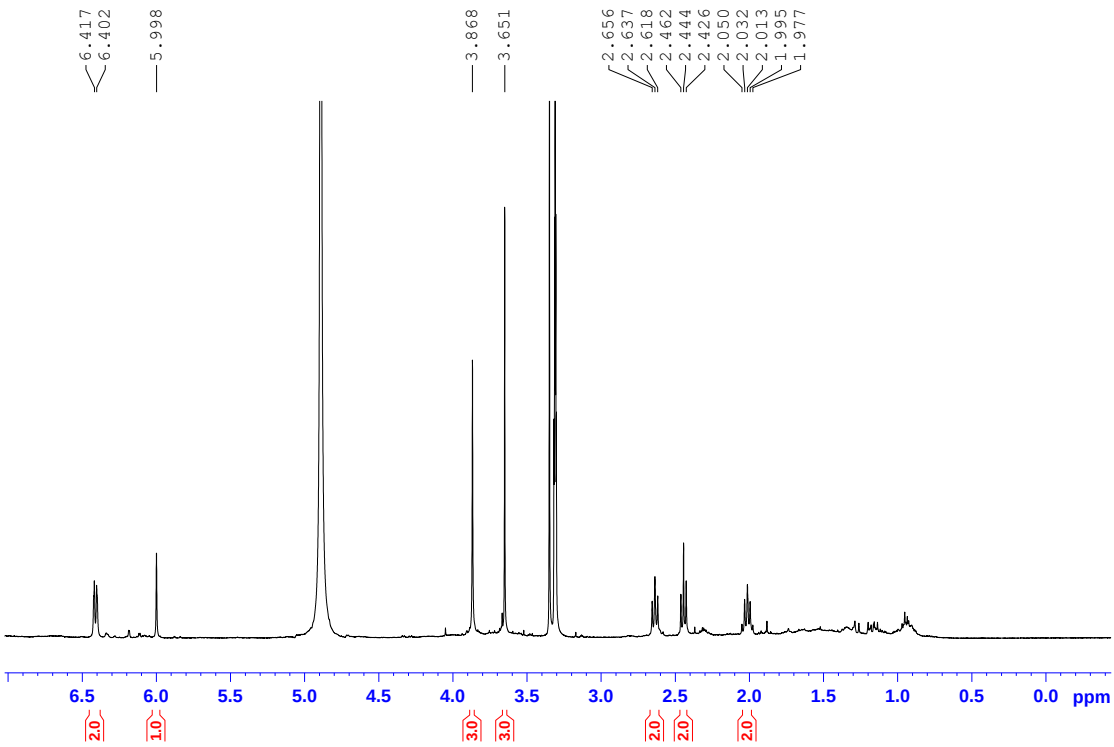

Figure S61 ^{1}H NMR Spectrum of **11** in Methanol-d_4 (400 MHz)

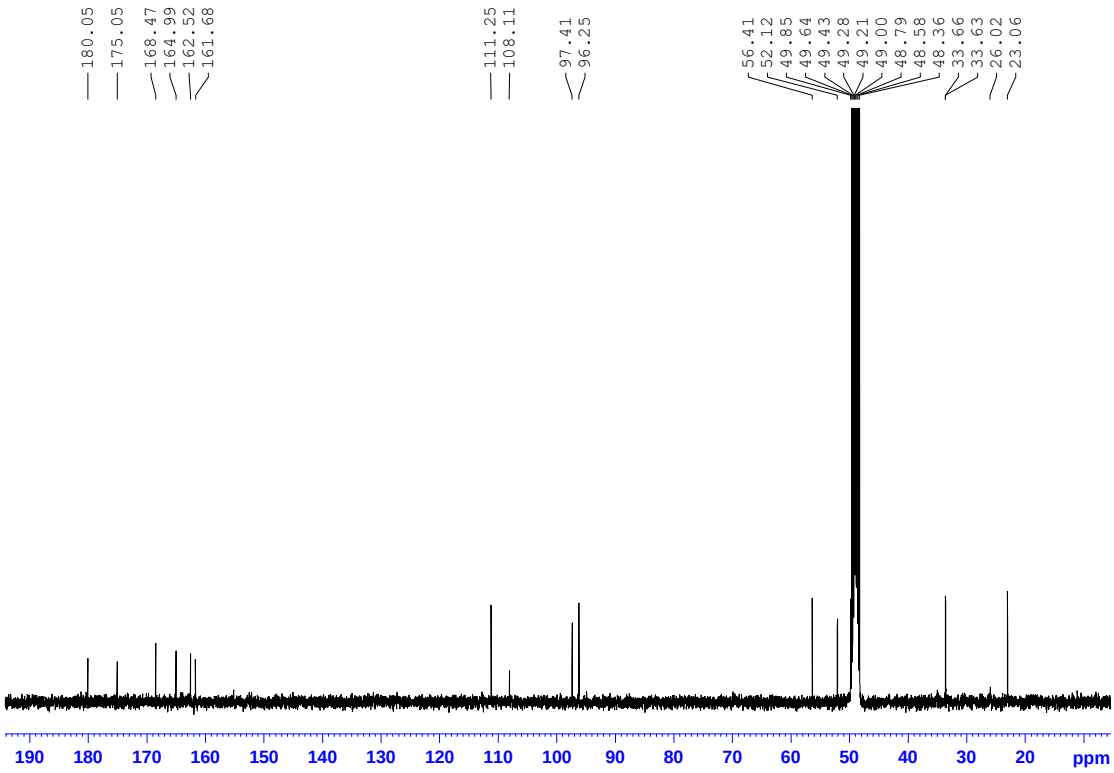

Figure S62 ^{13}C NMR Spectrum of **11** in Methanol-d_4 (100 MHz)

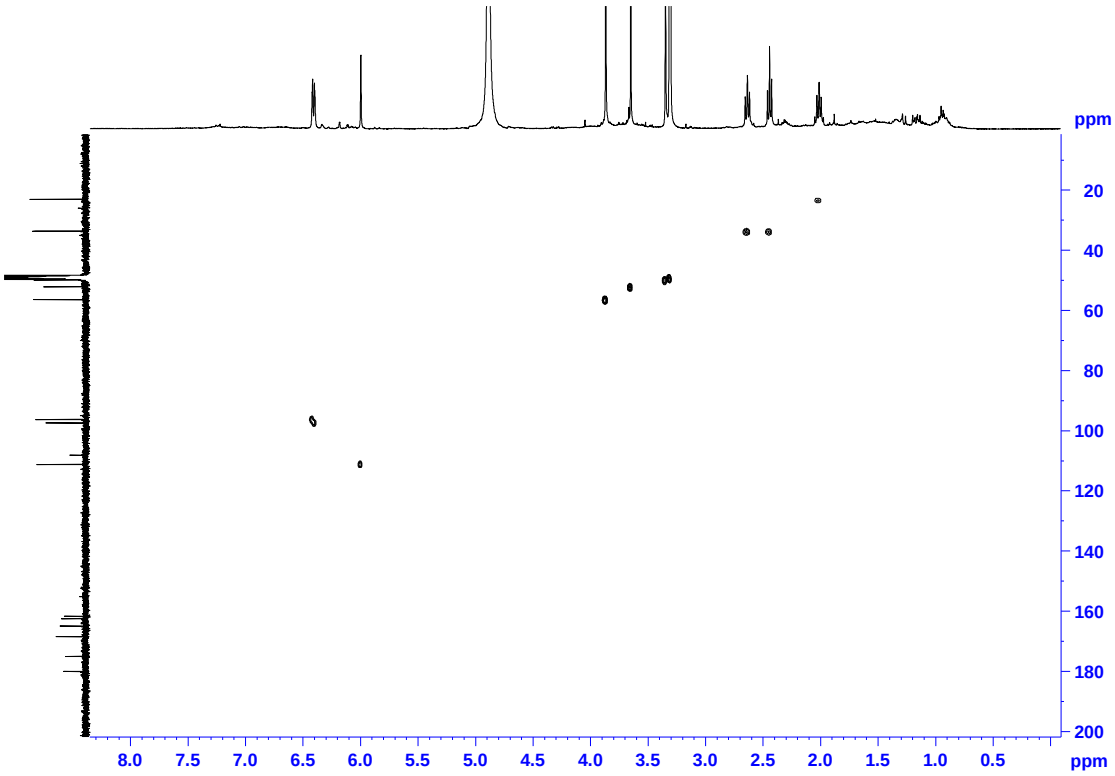

Figure S63 HSQC Spectrum of **11** in Methanol-d_4

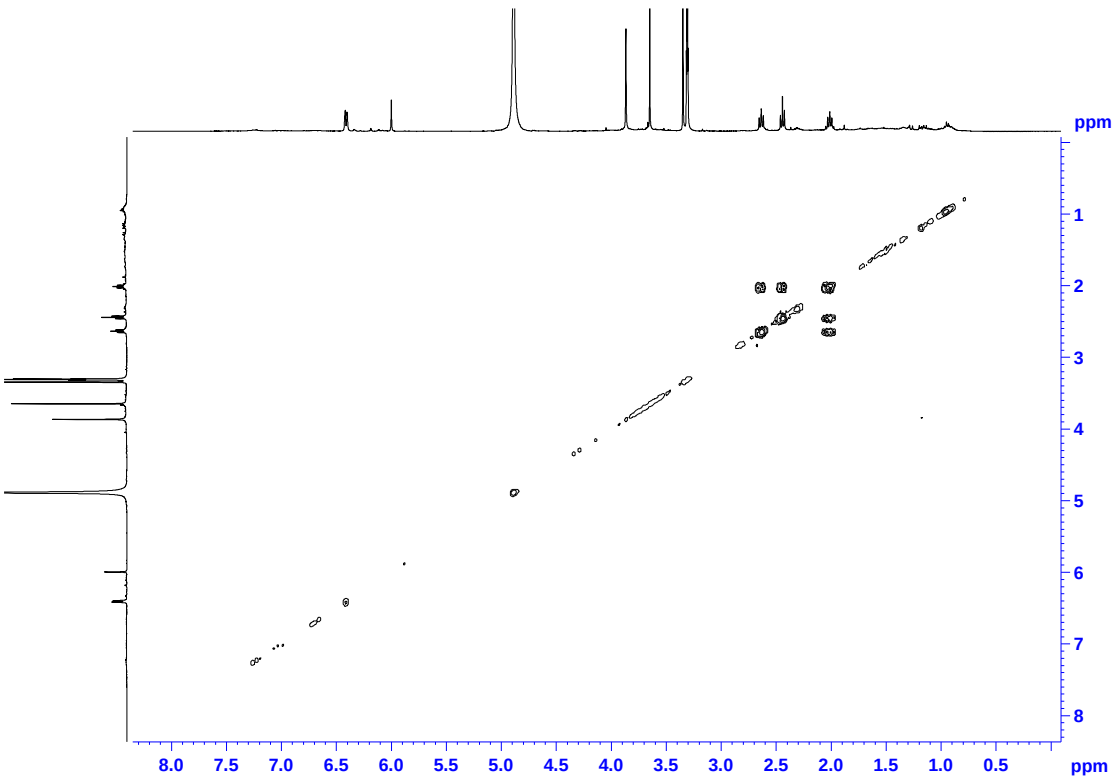

Figure S64 ^{1}H-^{1}H COSY Spectrum of **11** in Methanol-d_4

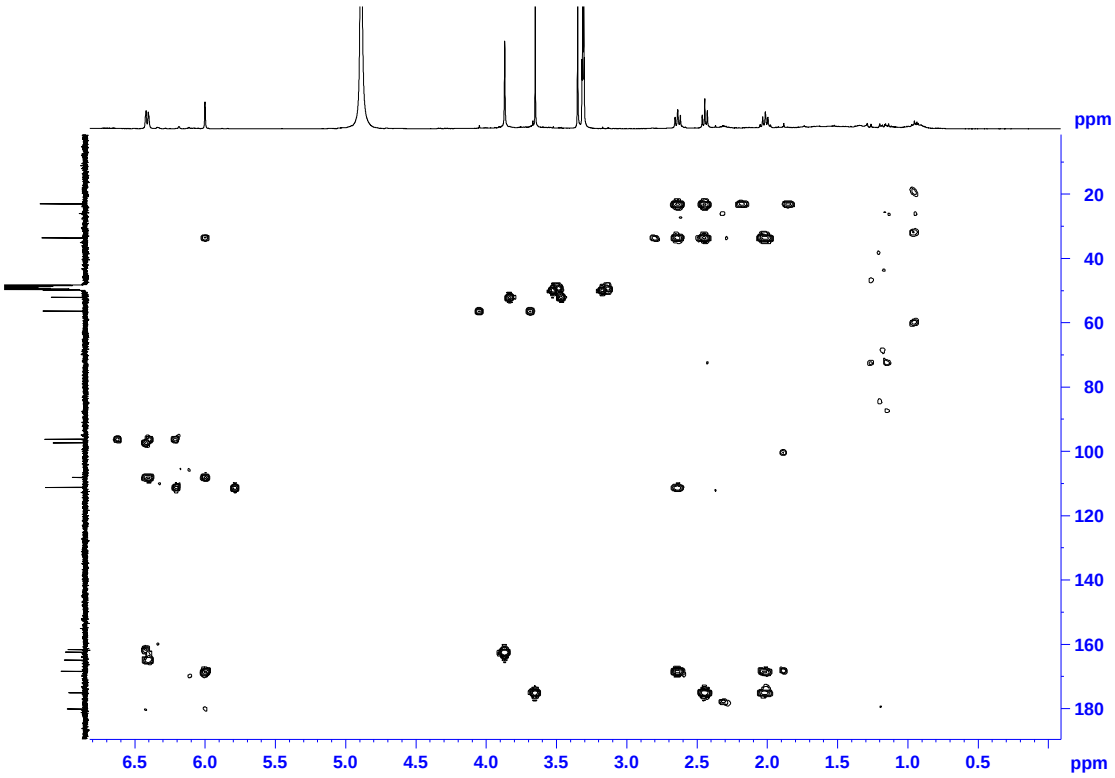

Figure S65 HMBC Spectrum of **11** in Methanol-d_4

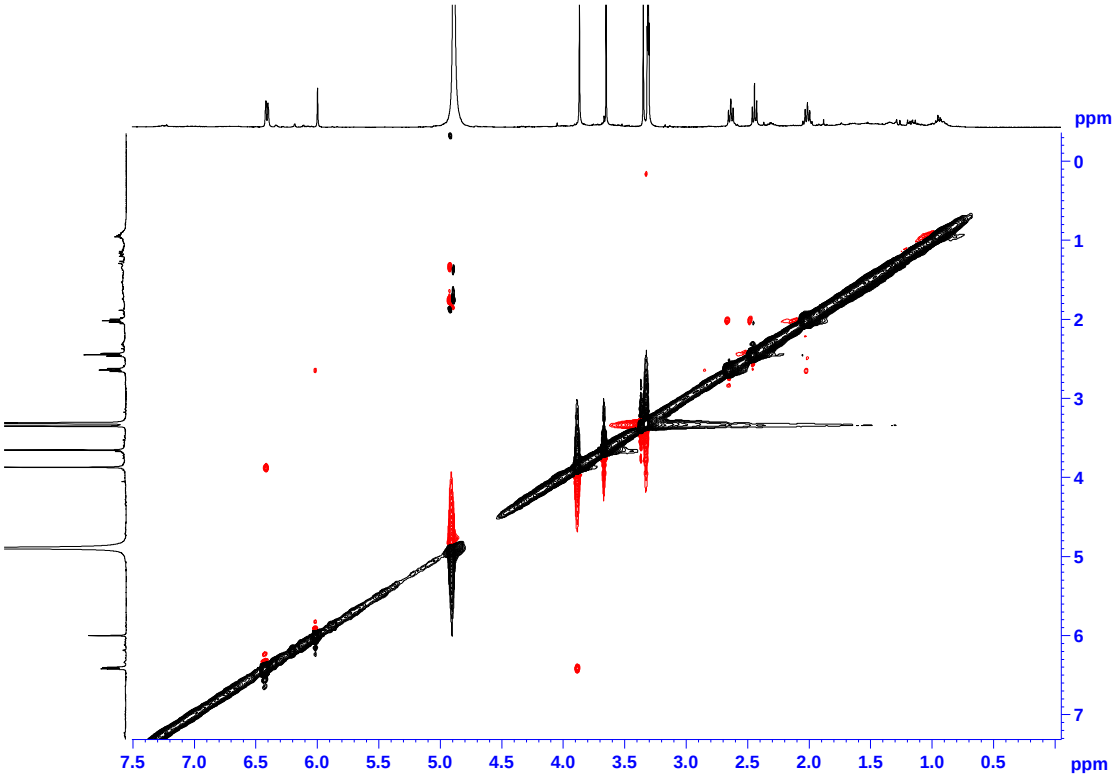

Figure S66 NOESY Spectrum of **11** in Methanol-d_4.

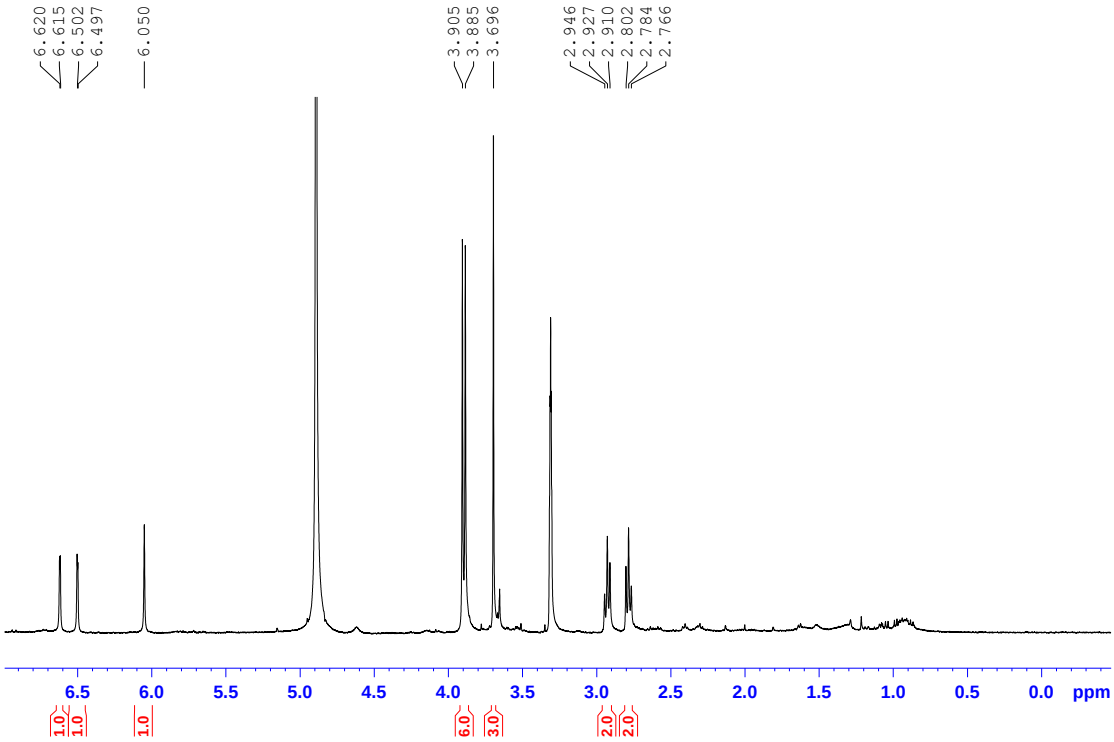

Figure S67 ^{1}H NMR Spectrum of **12** in Methanol-d_4 (400 MHz)

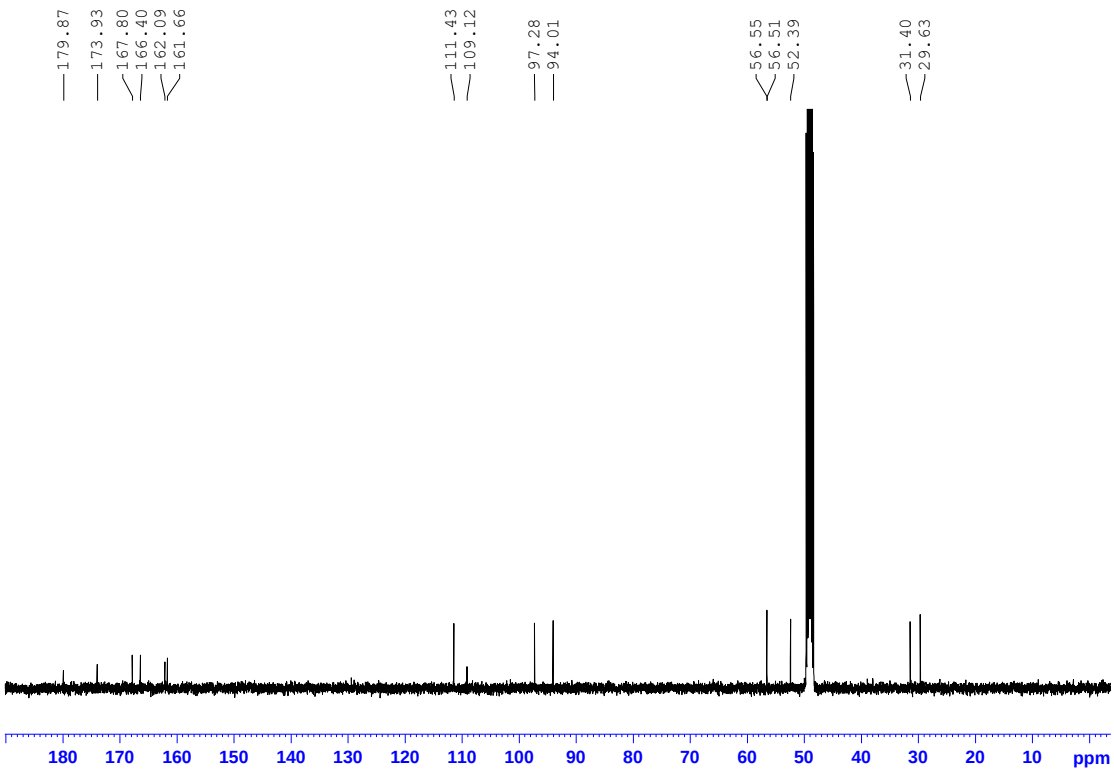

Figure S68 ^{13}C NMR Spectrum of **12** in Methanol-d_4 (100 MHz)

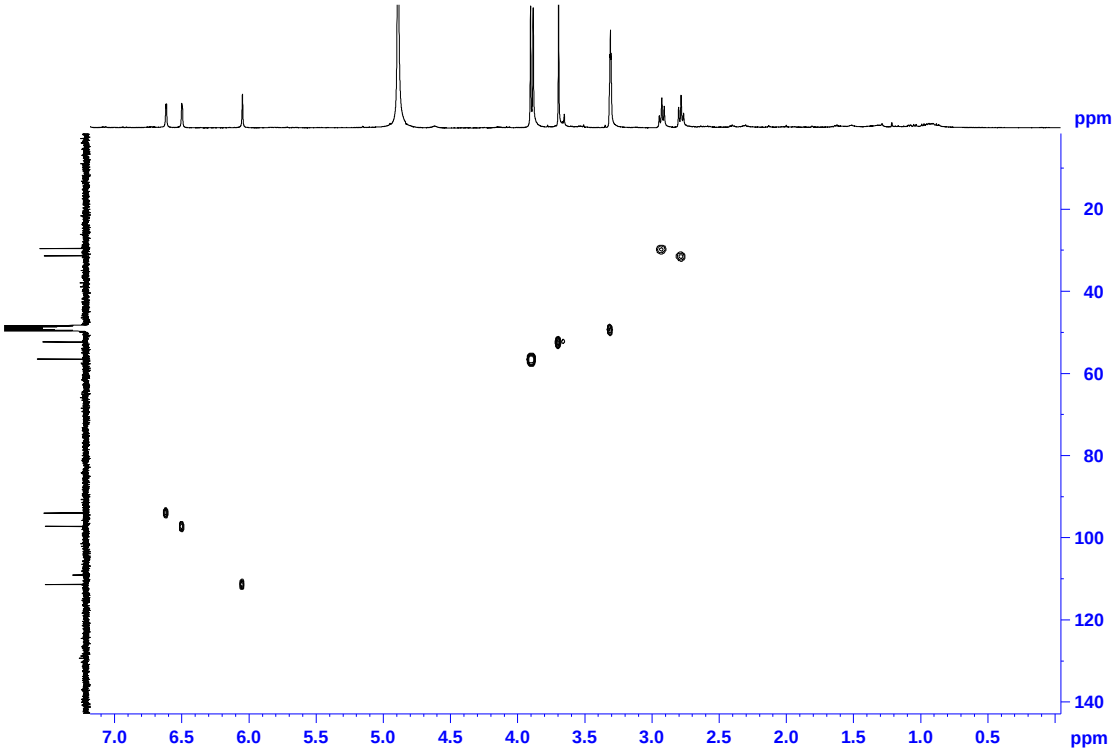

Figure S69 HSQC Spectrum of **12** in Methanol-d_4

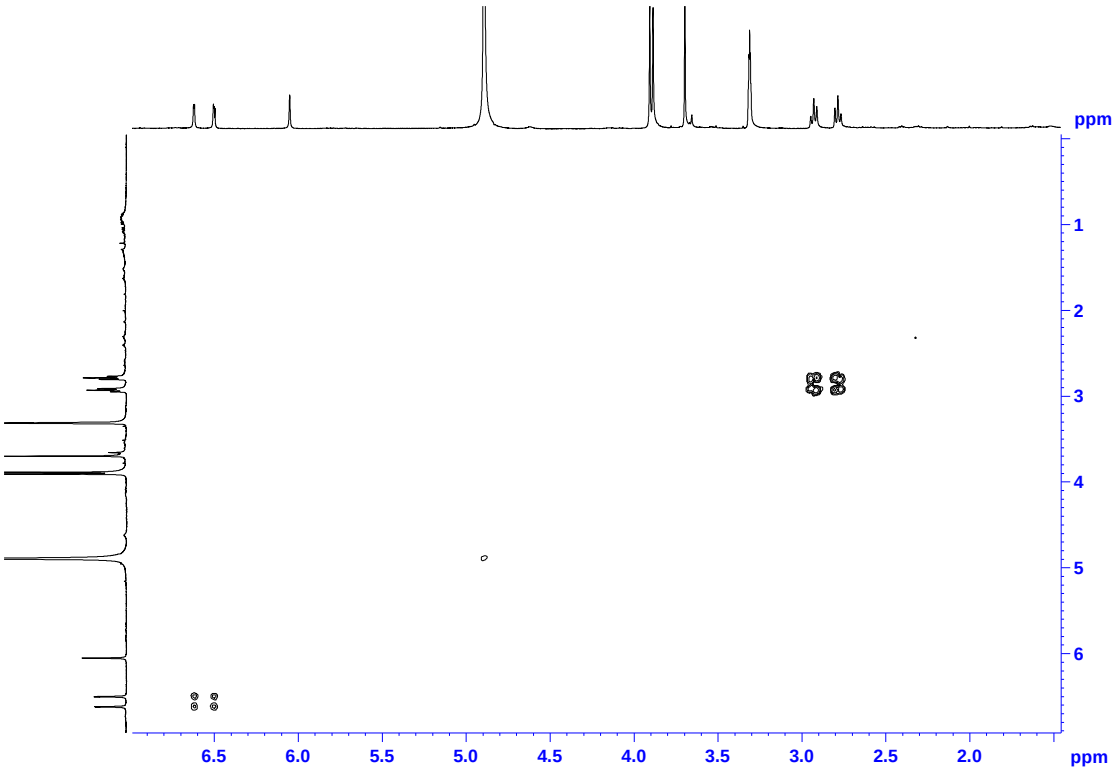

Figure S70 ^{1}H-^{1}H COSY Spectrum of **12** in Methanol-d_4

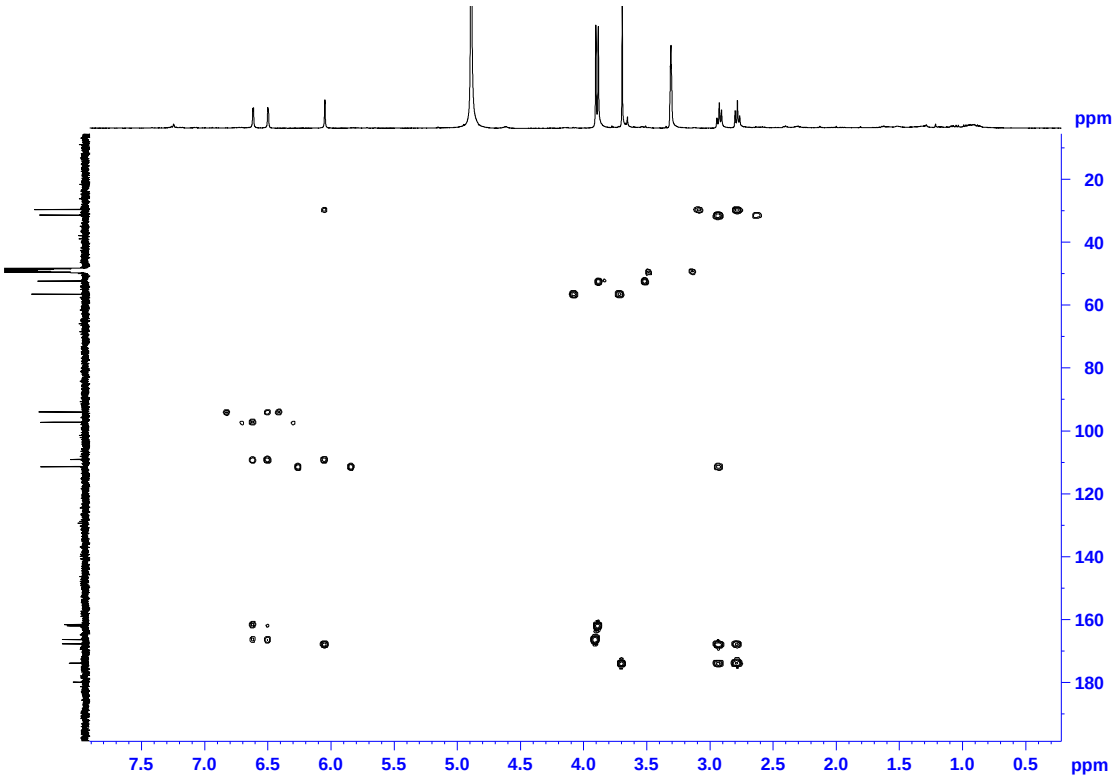

Figure S71 HMBC Spectrum of **12** in Methanol-d_4

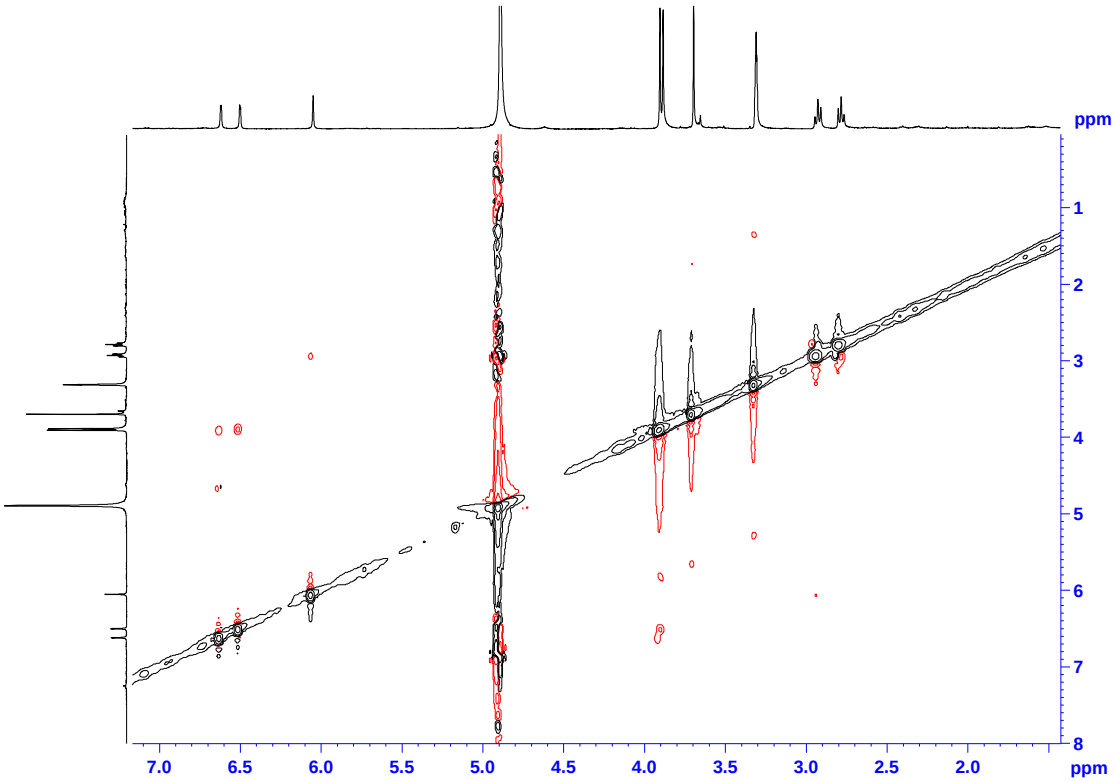

Figure S72 NOESY Spectrum of **12** in Methanol-d_4

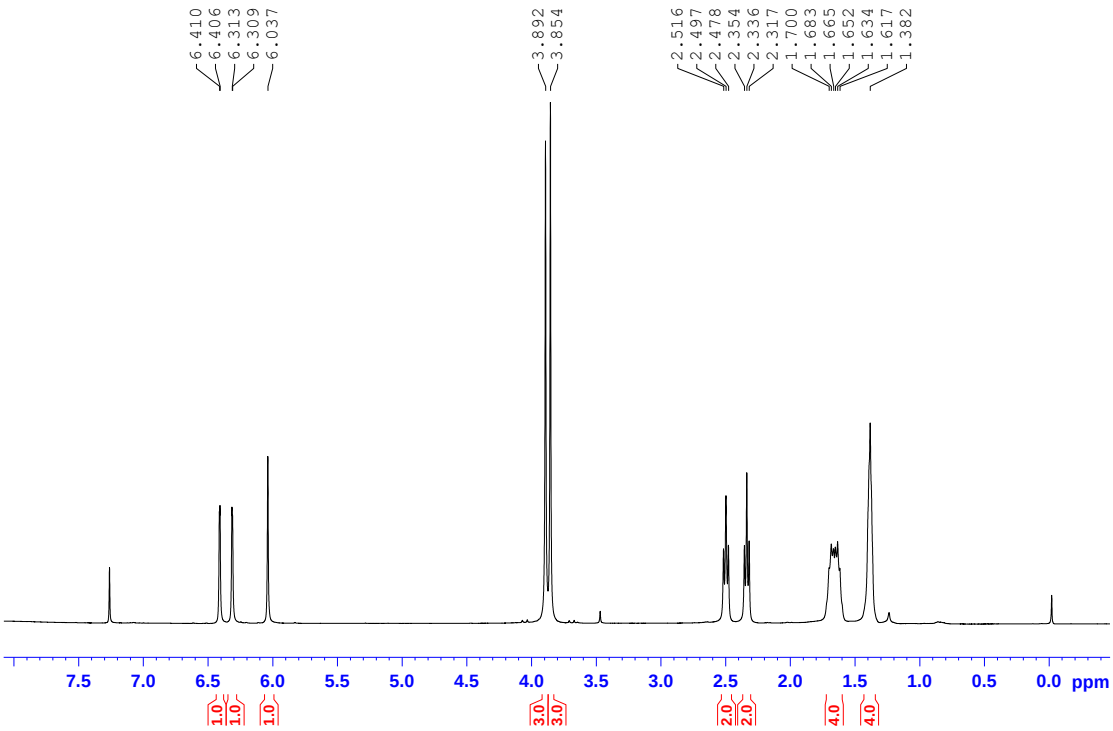

Figure S73 ^{1}H NMR Spectrum of **13** in $CDCl_3$ (400 MHz)

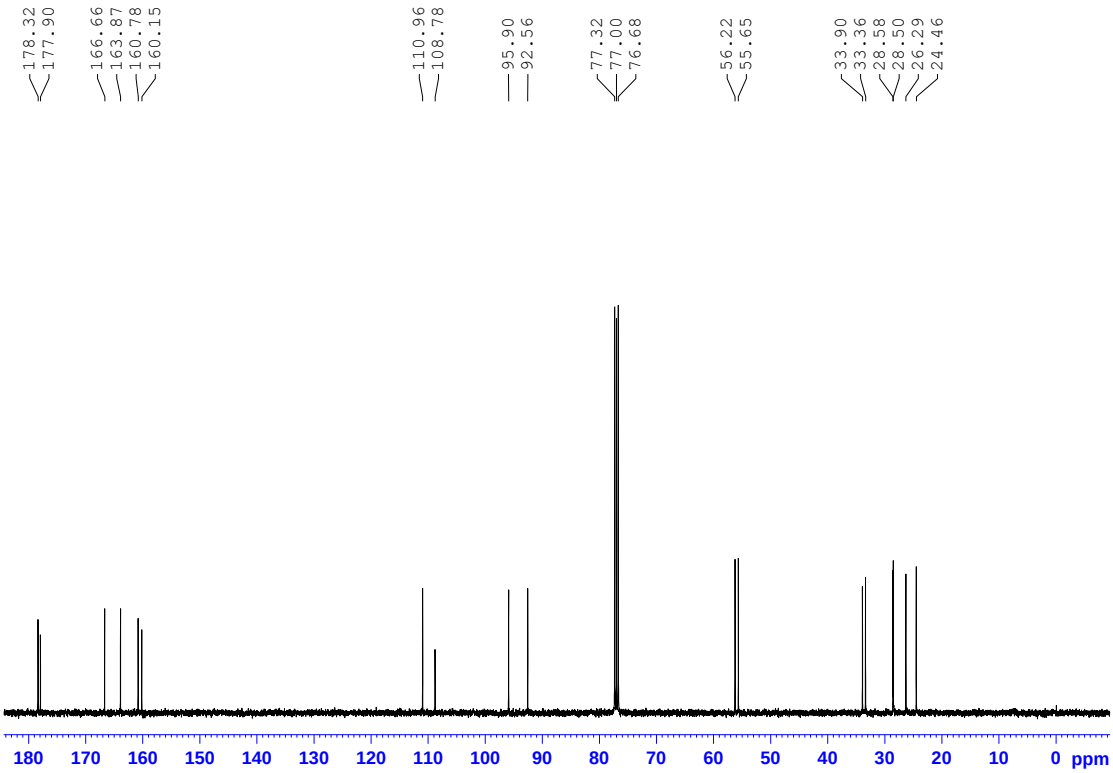

Figure S74 ^{13}C NMR Spectrum of **13** in $CDCl_3$ (100 MHz)

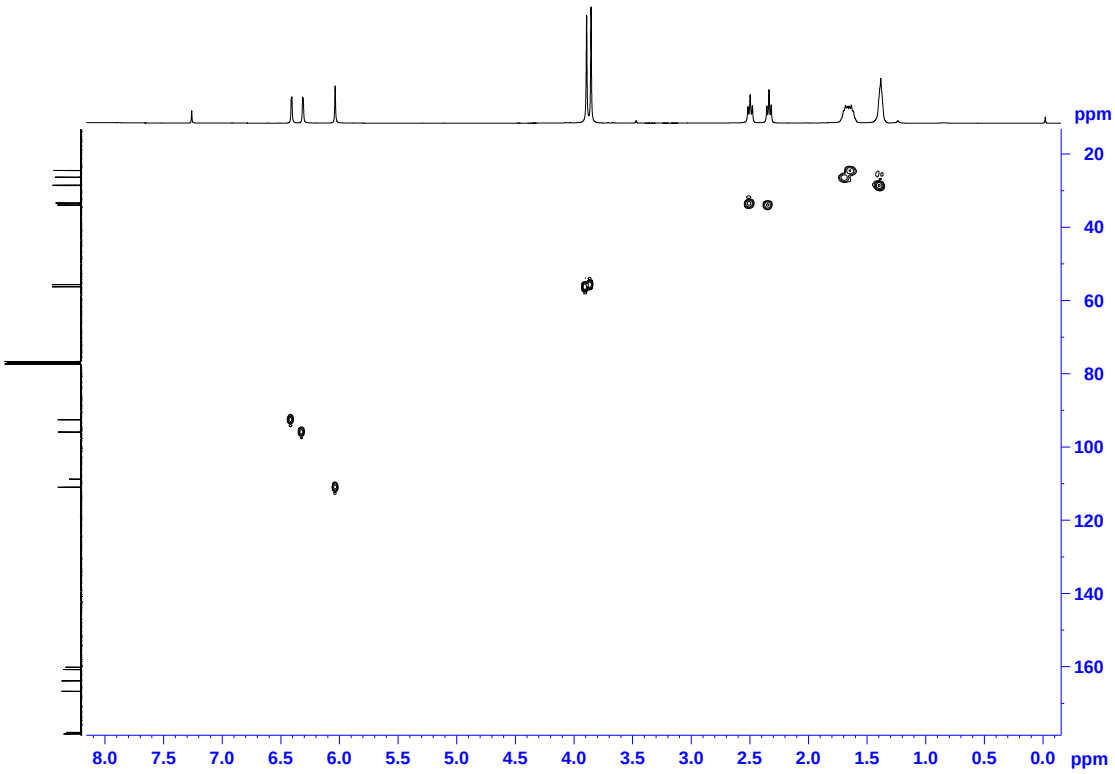

Figure S75 HSQC Spectrum of **13** in $CDCl_3$

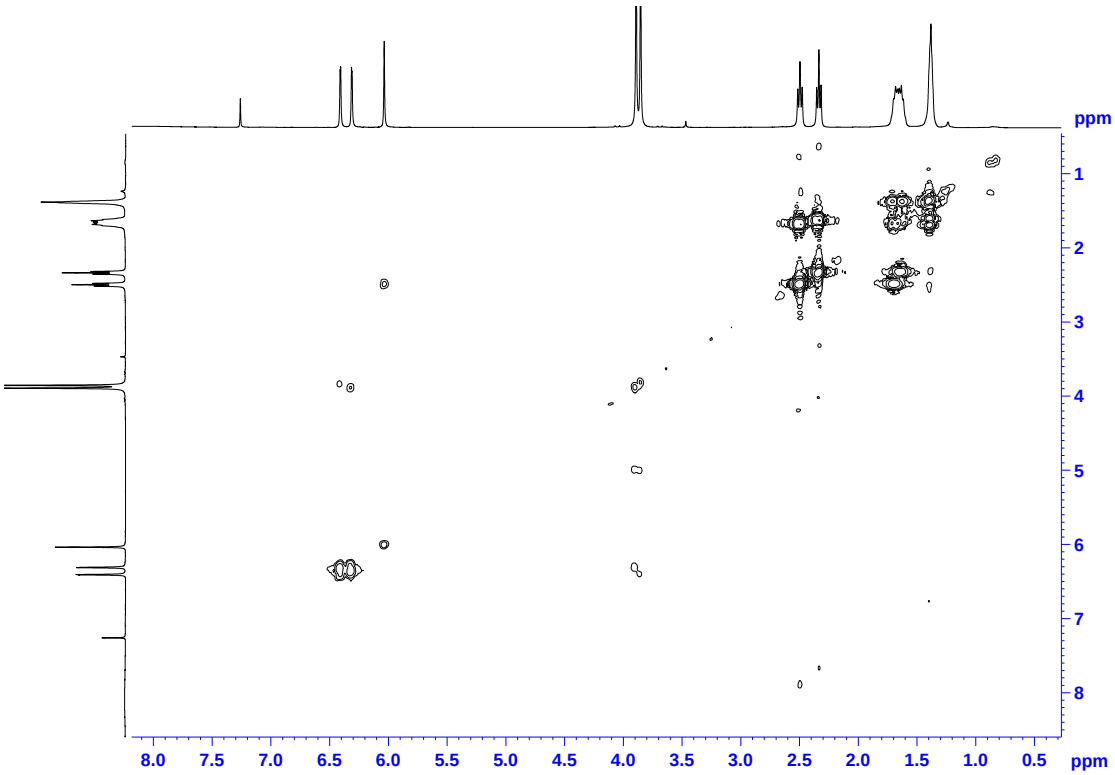

Figure S76 ^{1}H-^{1}H COSY Spectrum of **13** in $CDCl_3$

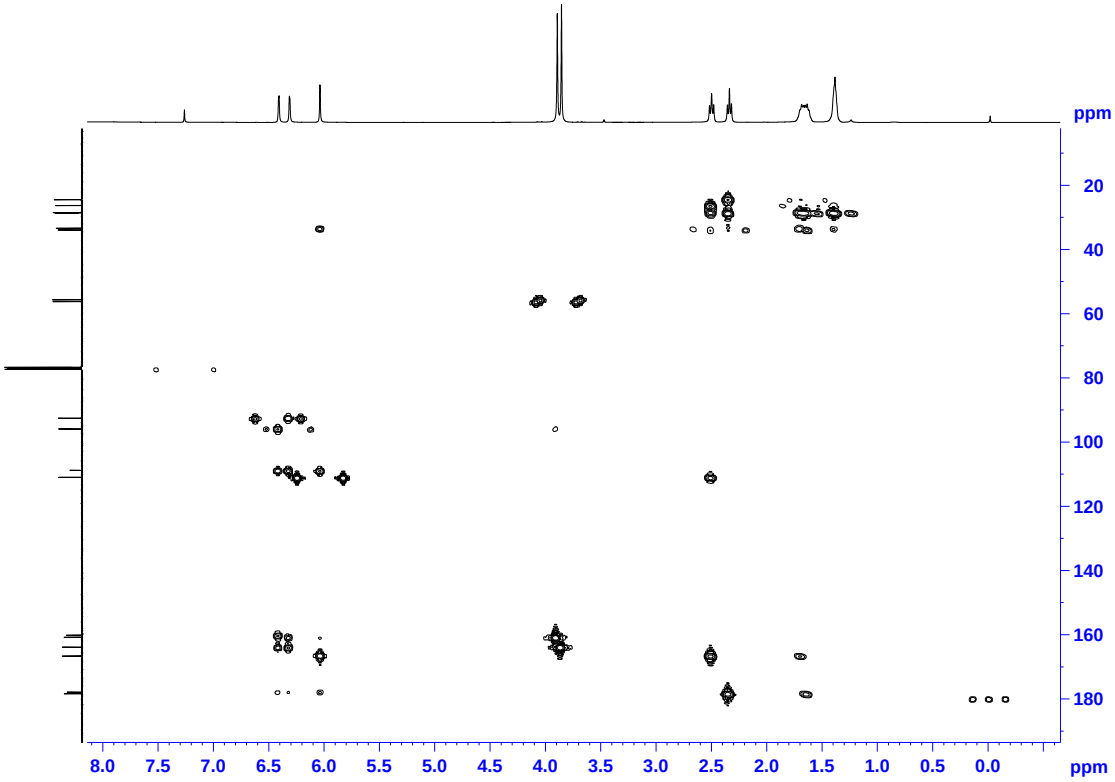

Figure S77 HMBC Spectrum of **13** in $CDCl_3$

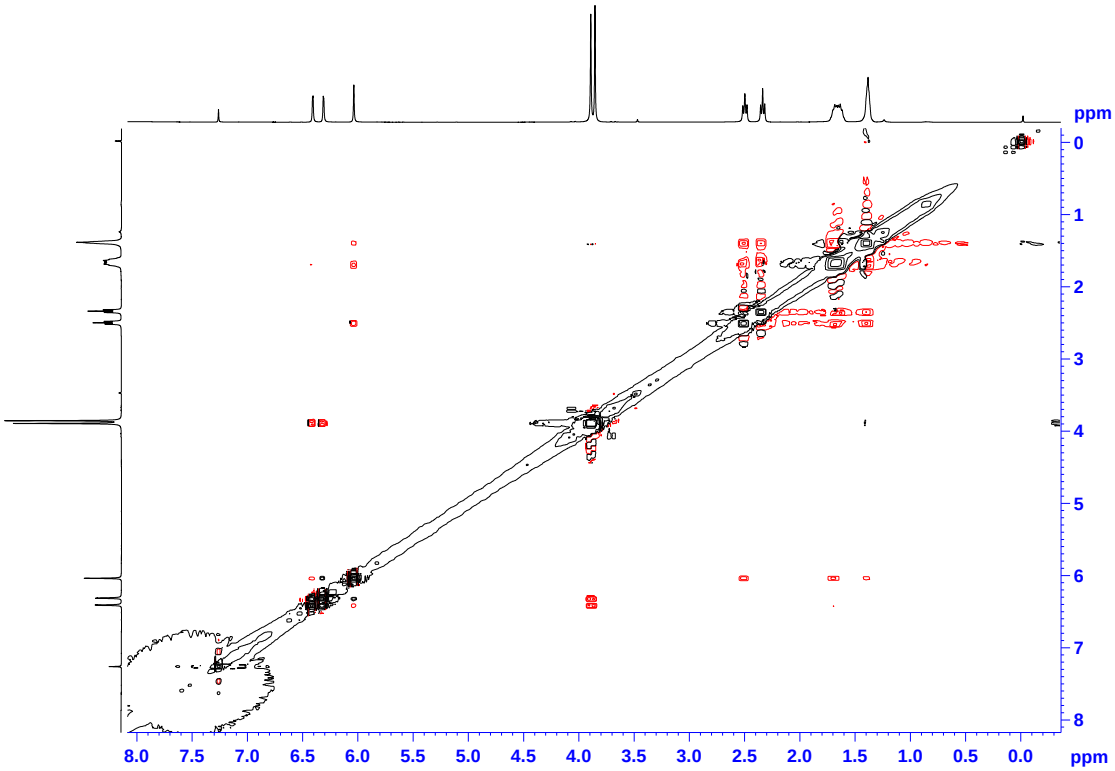

Figure S78 NOESY Spectrum of **13** in $CDCl_3$

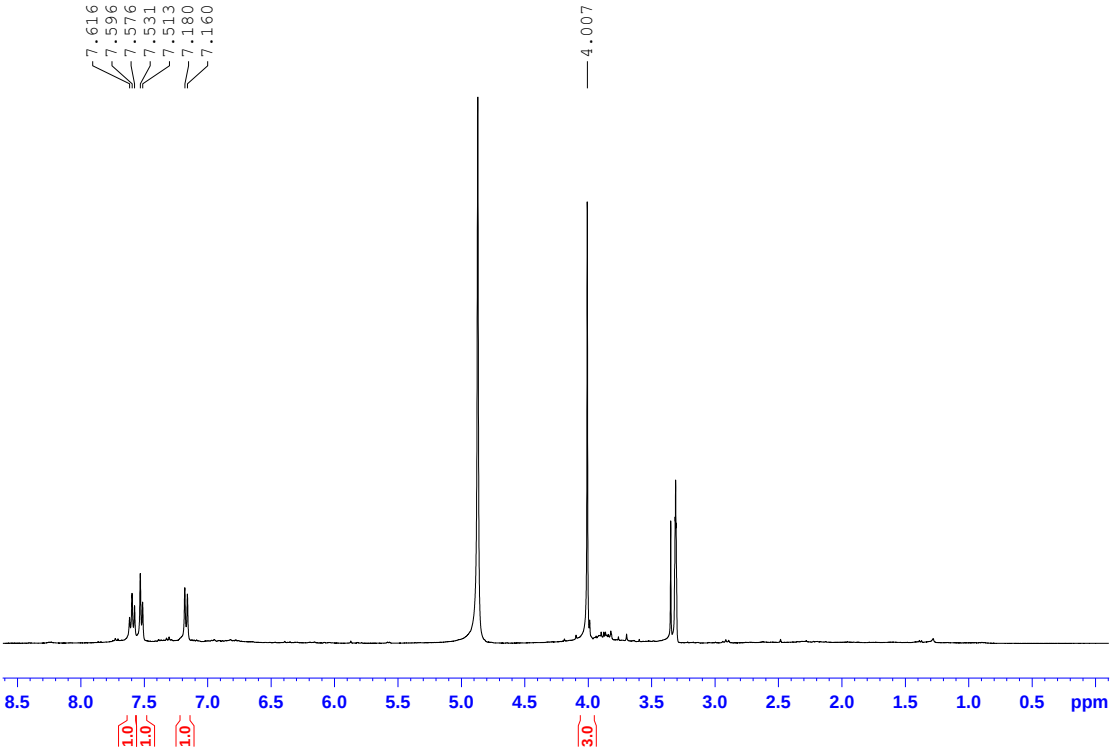

Figure S79 ^{1}H NMR Spectrum of **14** in Methanol-d_4 (400 MHz)

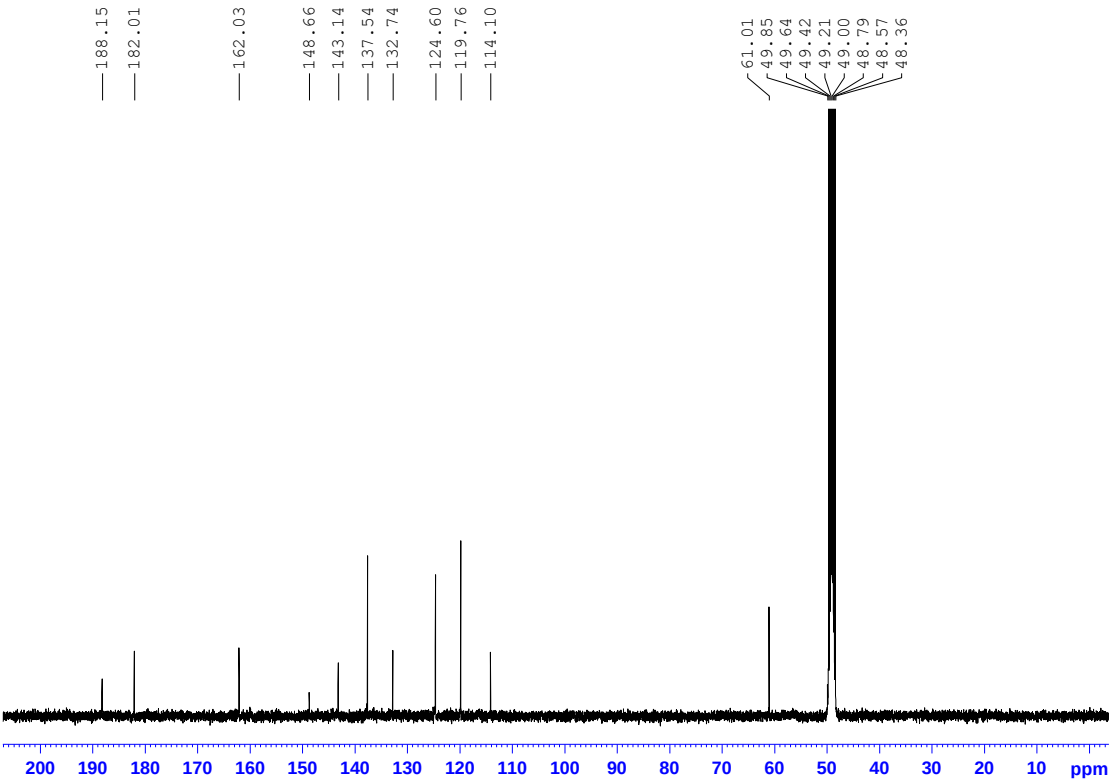

Figure S80 ^{13}C NMR Spectrum of **14** in Methanol-d_4 (100 MHz)

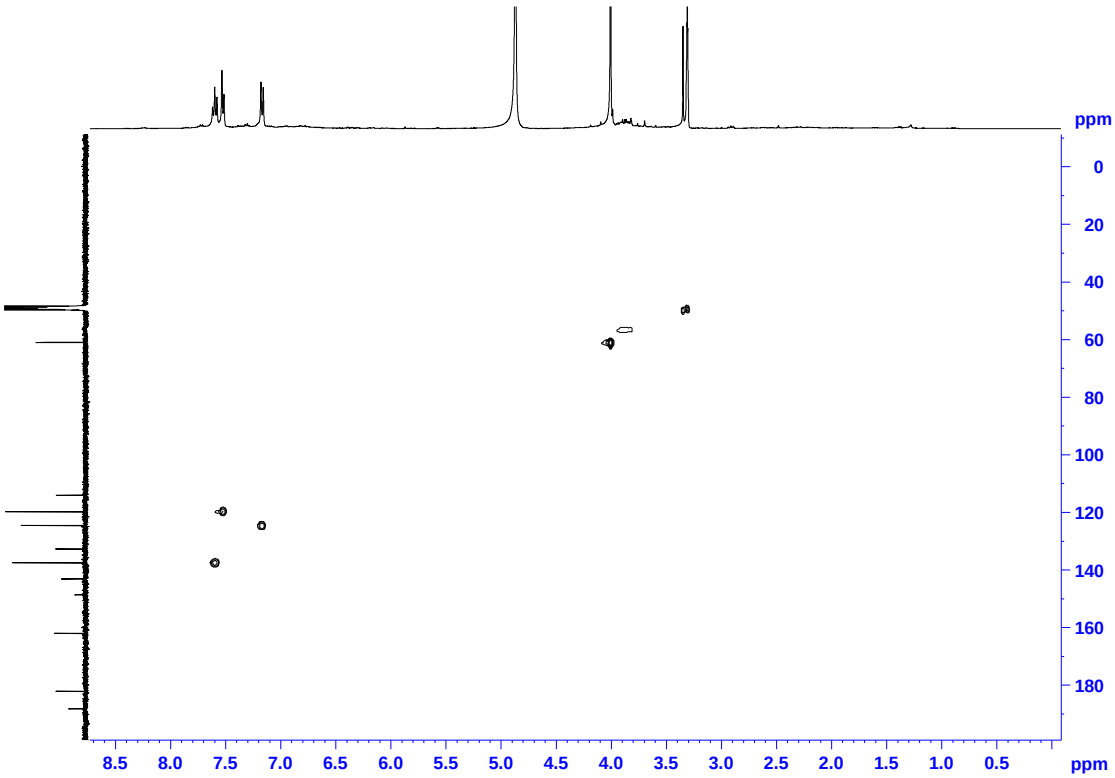

Figure S81 HSQC Spectrum of **14** in Methanol-d4

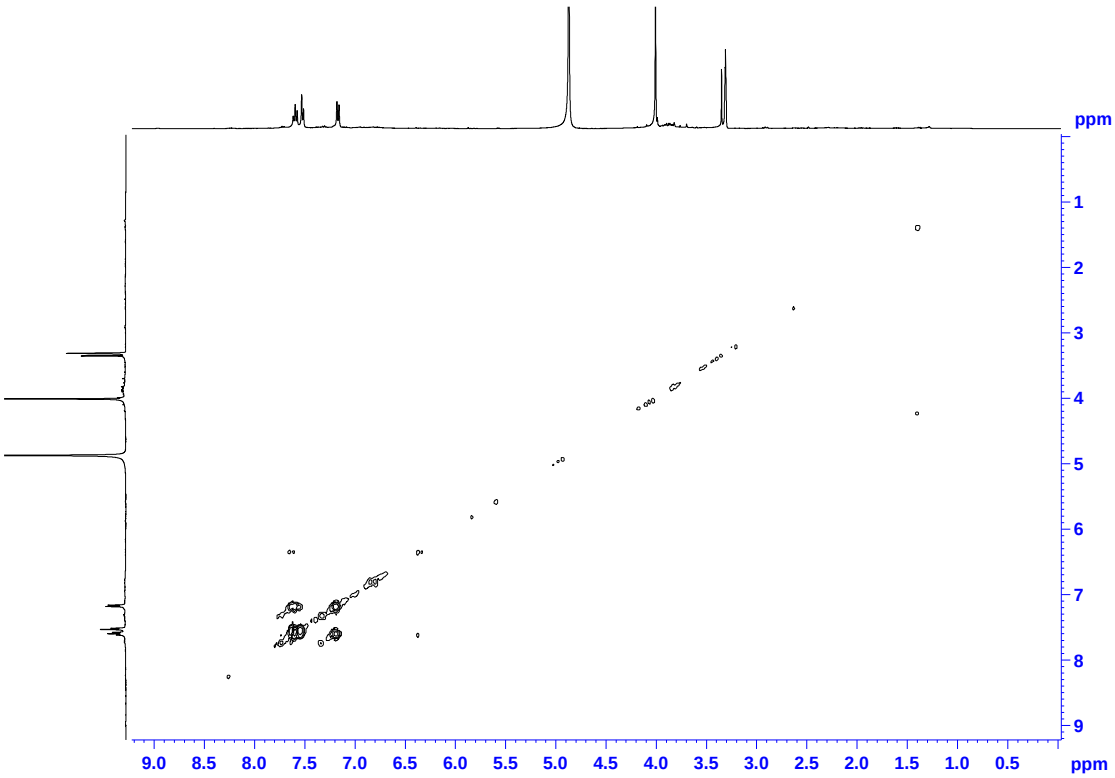

Figure S82 ^{1}H-^{1}H COSY Spectrum of **14** in Methanol-d4

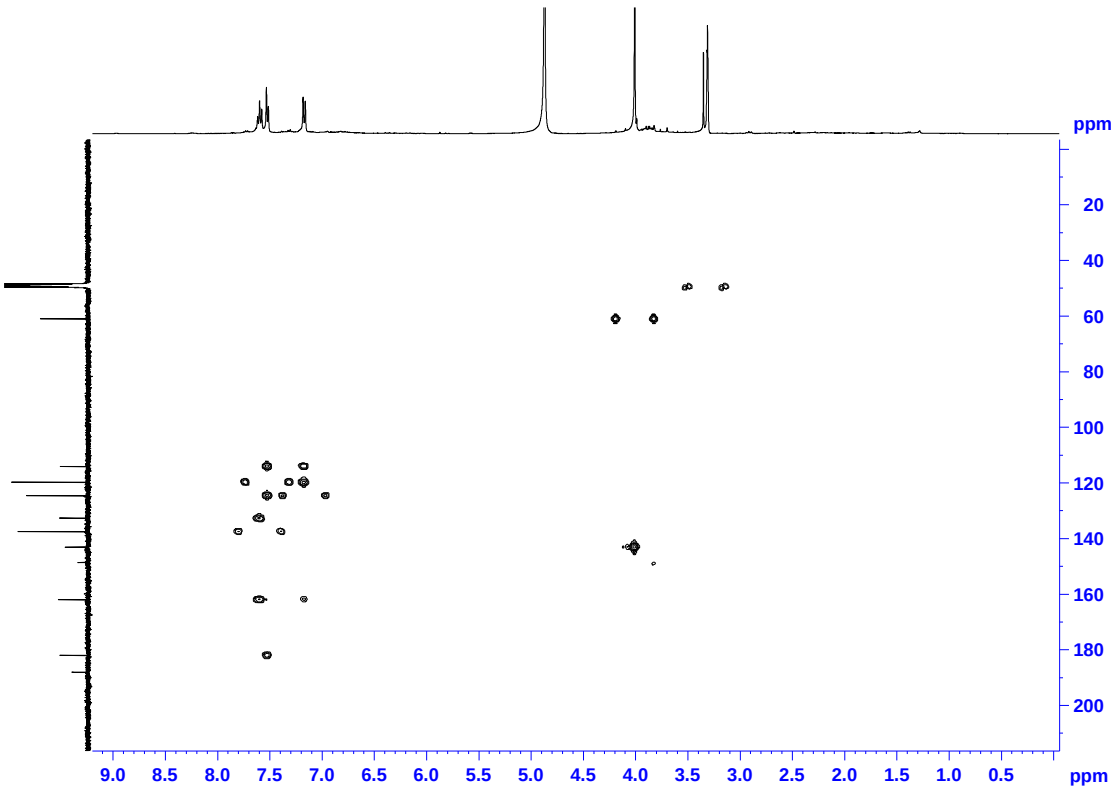

Figure S83 HMBC Spectrum of **14** in Methanol-d4

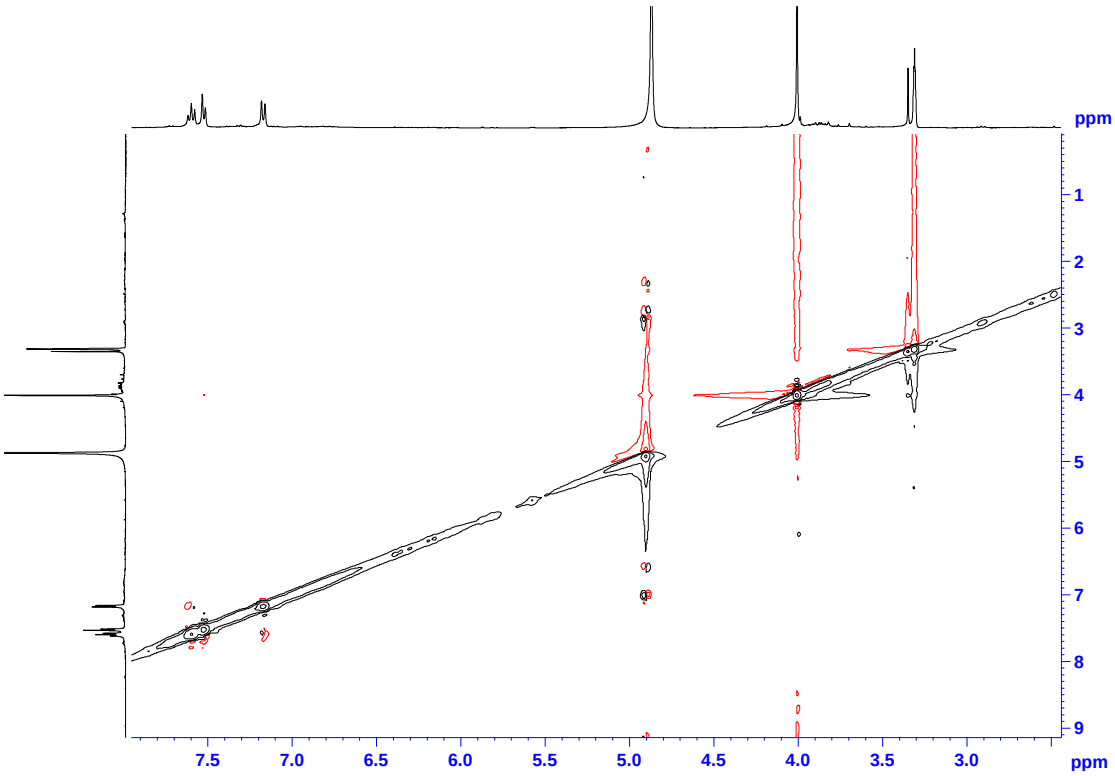

Figure S84 NOESY Spectrum of **14** in Methanol-d4

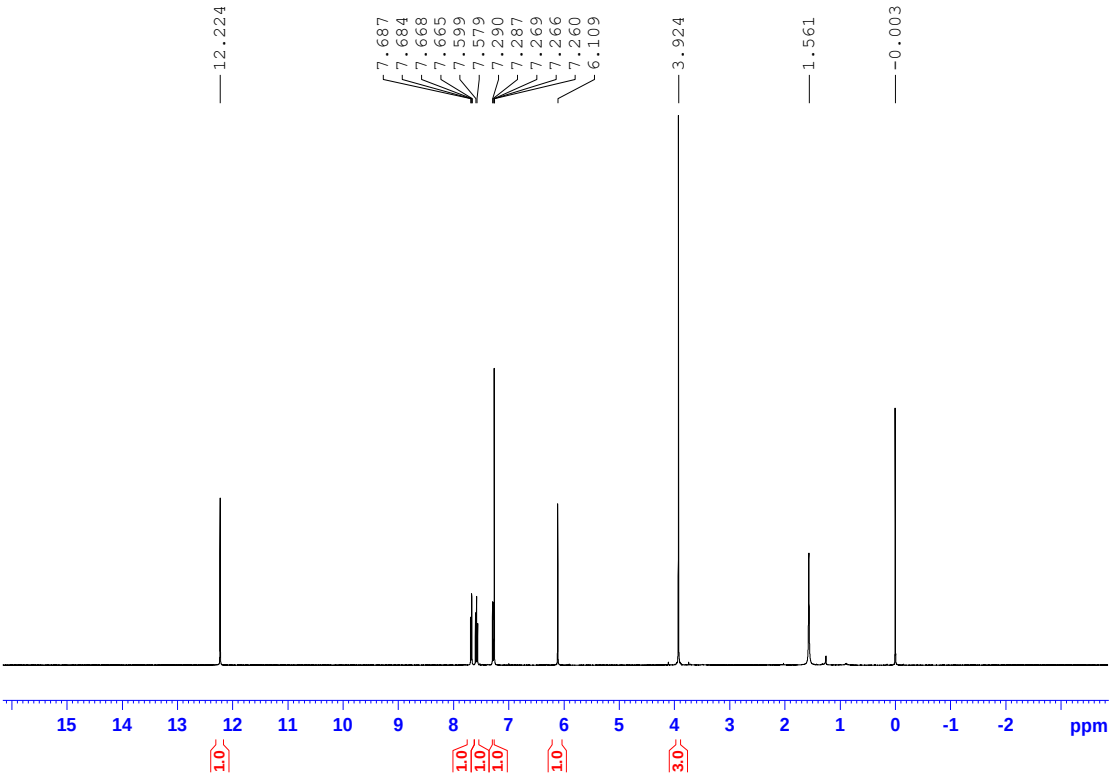

Figure S85 ^{1}H NMR Spectrum of **15** in $CDCl_3$ (400 MHz)

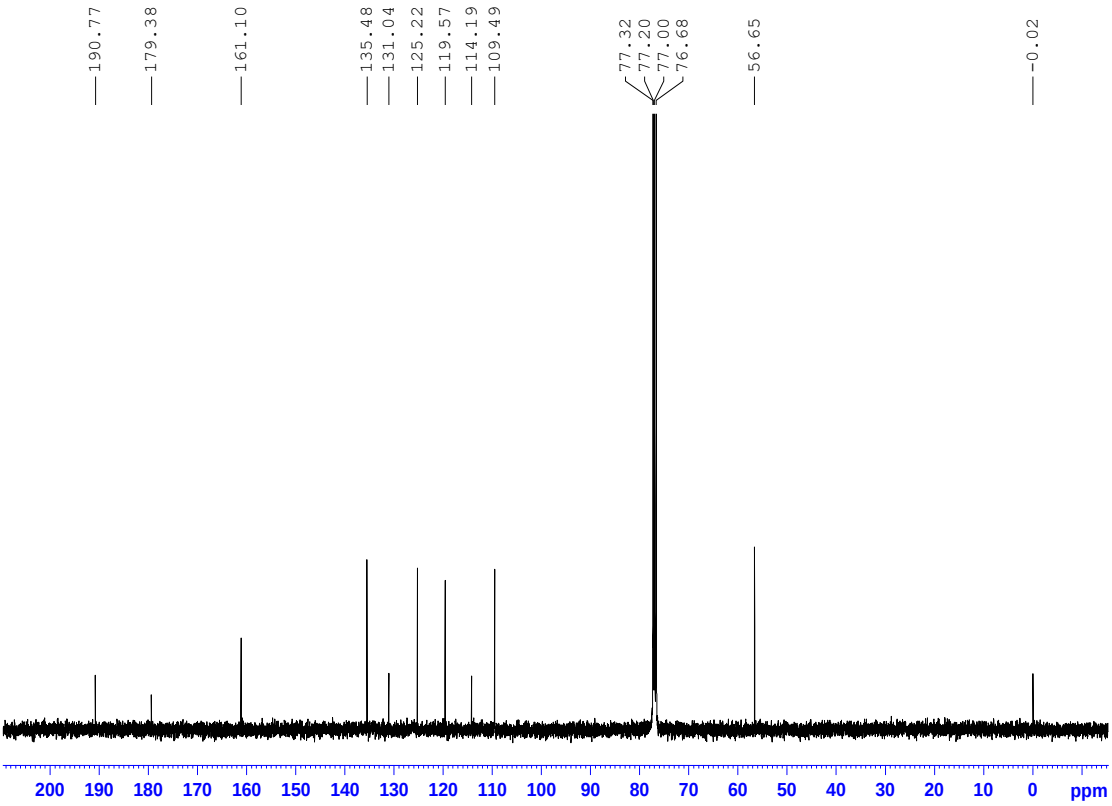

Figure S86 ^{13}C NMR Spectrum of **15** in $CDCl_3$ (100 MHz)

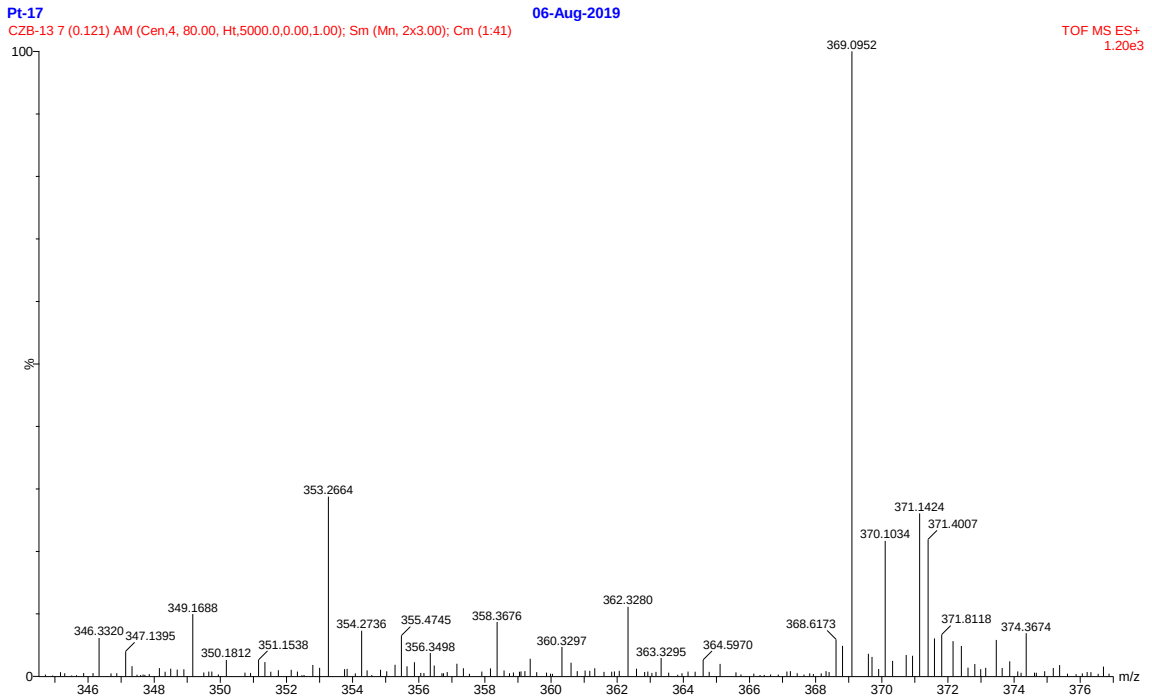

Figure S87 HRESIMS spectrum of **1**

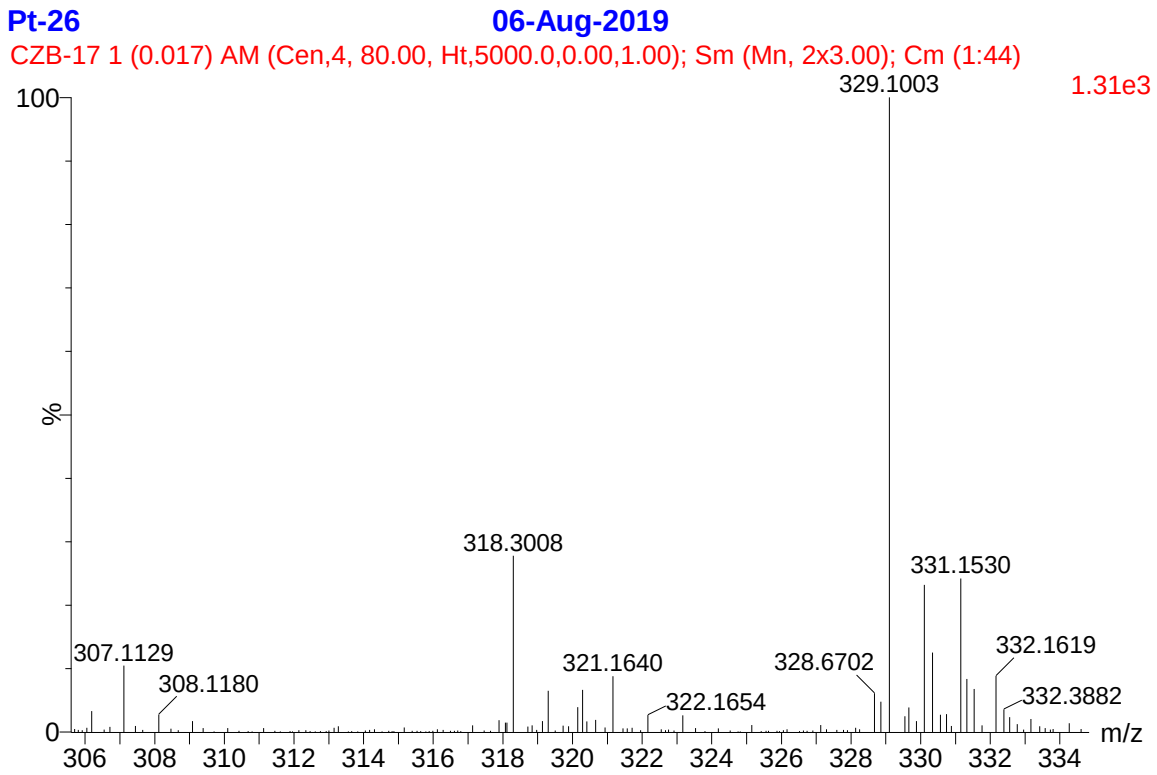

Figure S88 HRESIMS spectrum of **2**

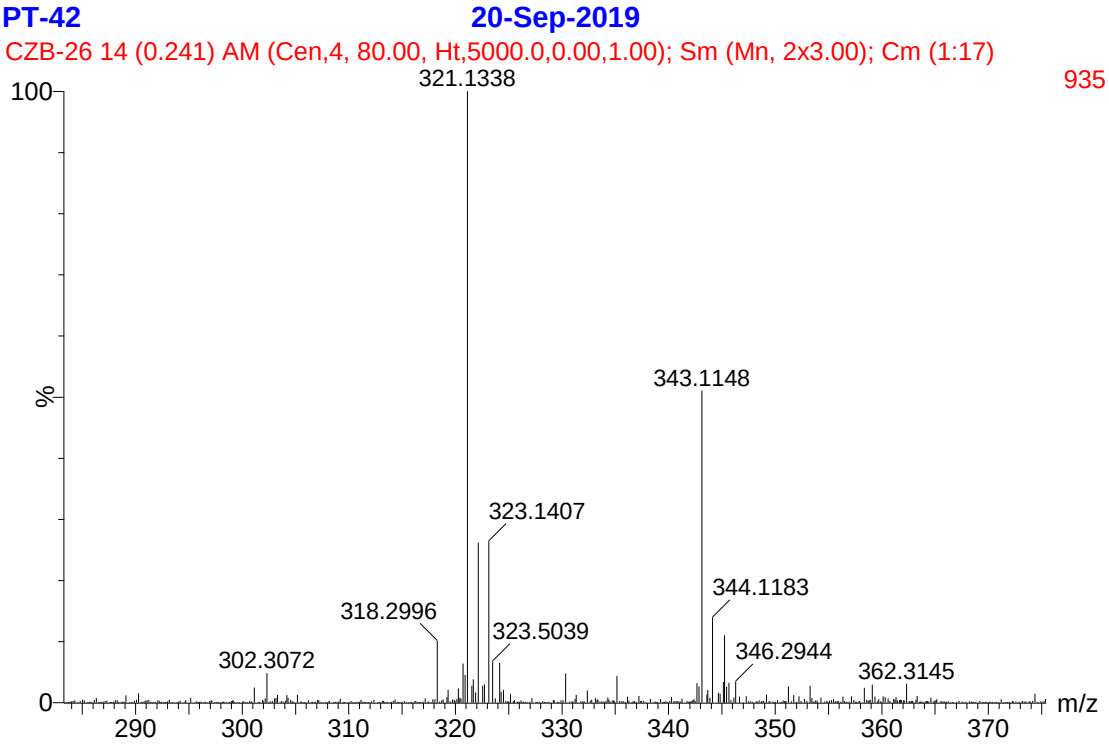

Figure S89 HRESIMS spectrum of **3**

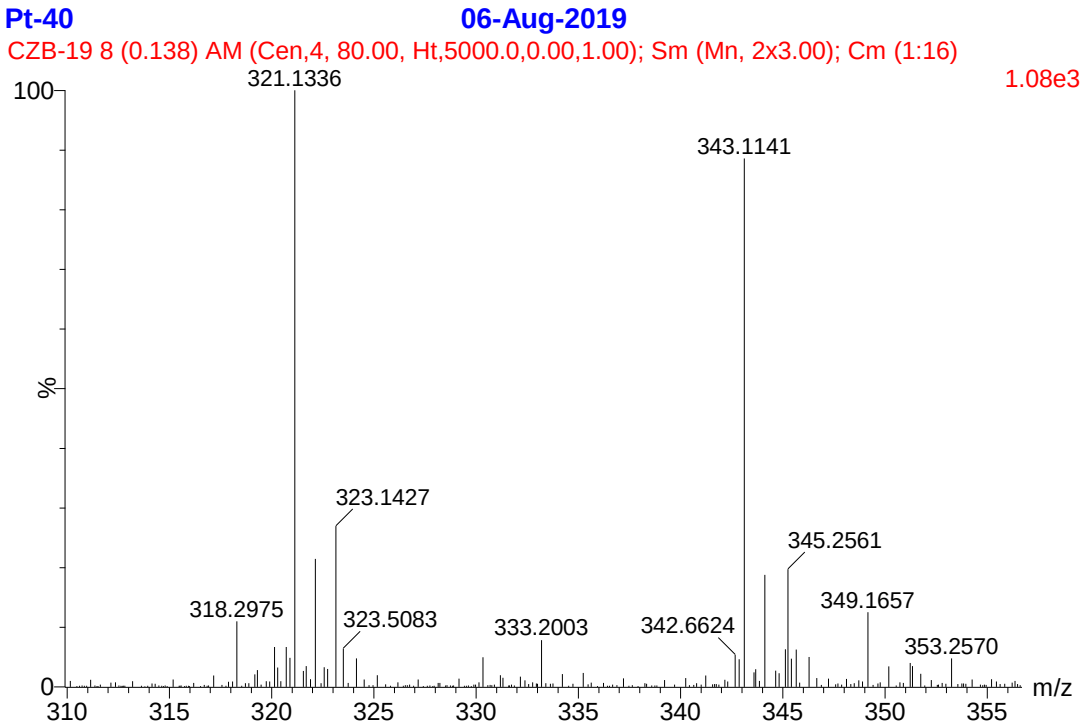

Figure S90 HRESIMS spectrum of **4**

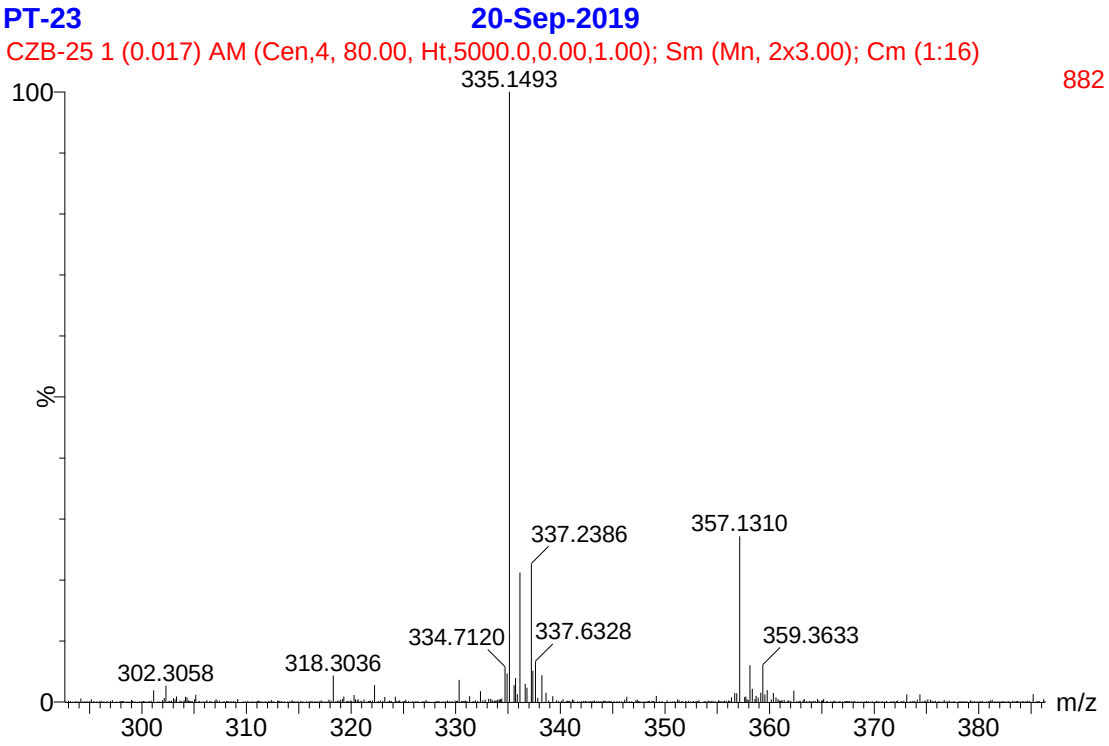

Figure S91 HRESIMS spectrum of **5**

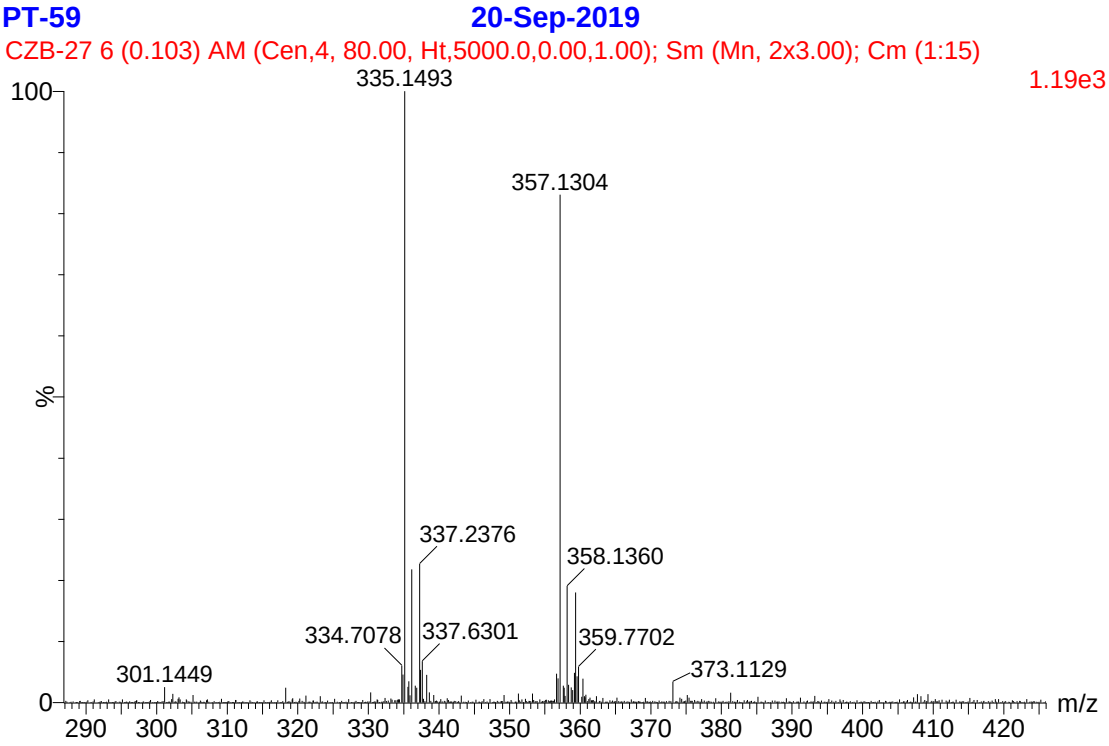

Figure S92 HRESIMS spectrum of **6**

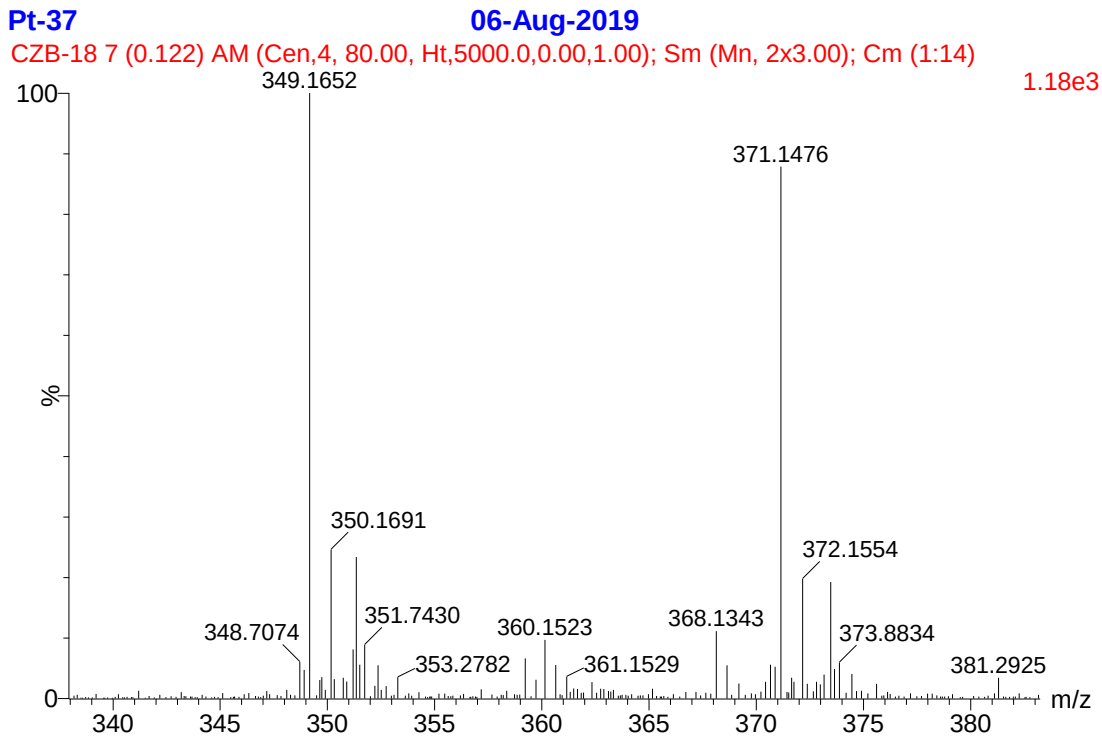

Figure S93 HRESIMS spectrum of **7**

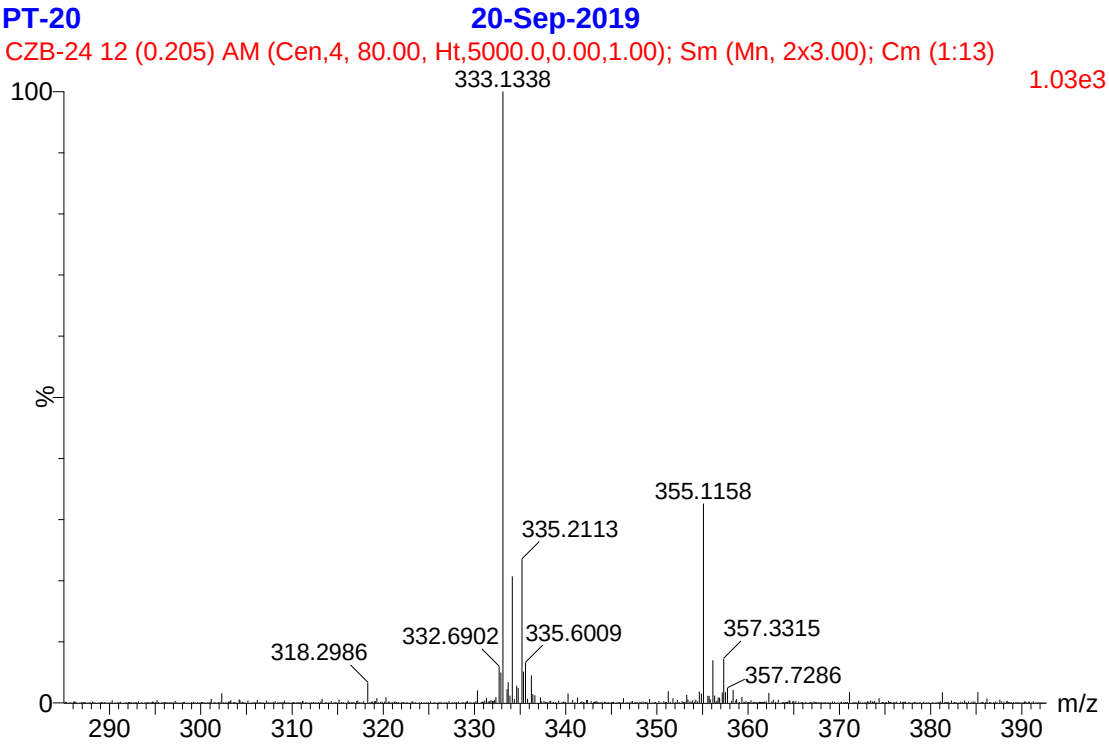

Figure S94 HRESIMS spectrum of **8**

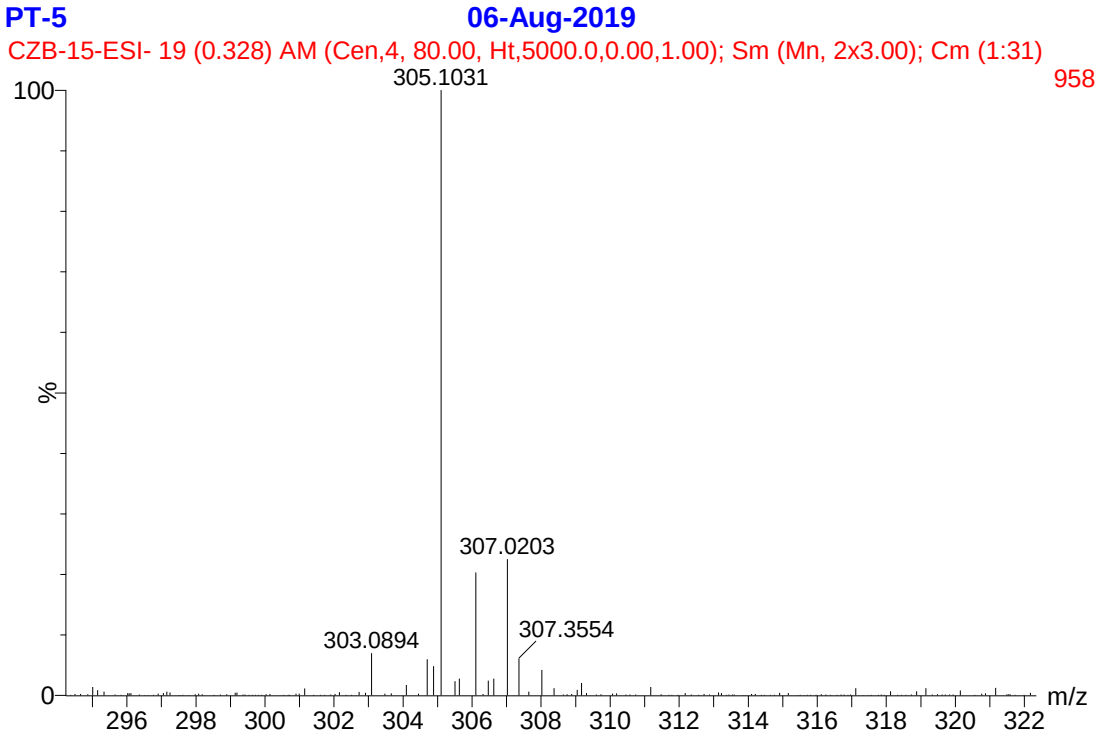

Figure S95 HRESIMS spectrum of **9**

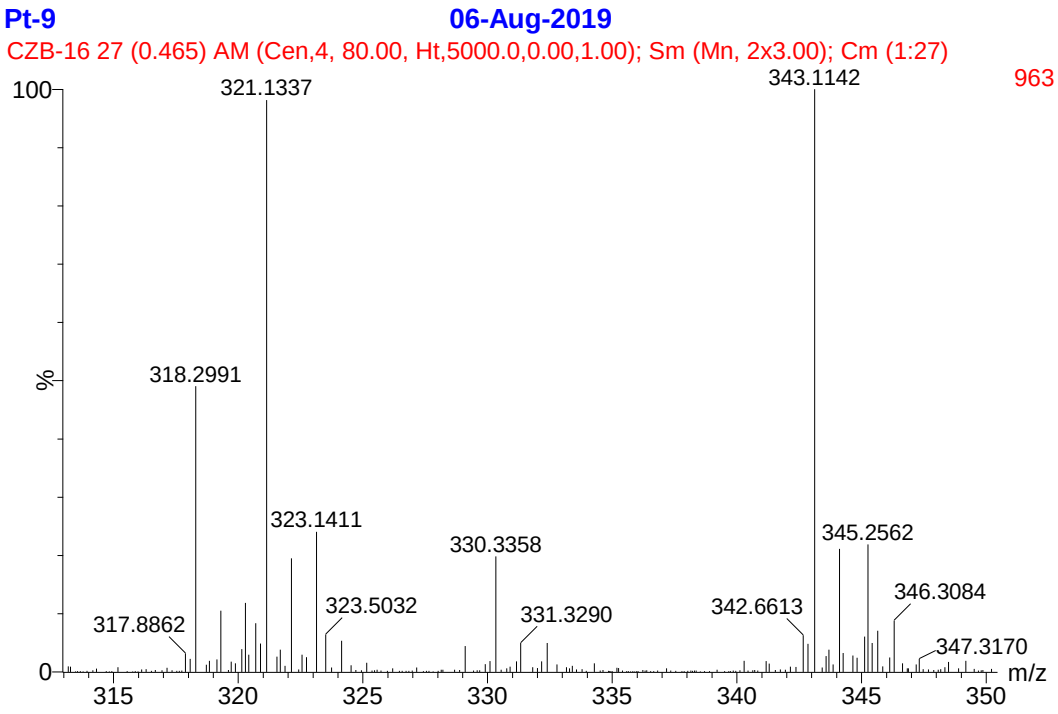

Figure S96 HRESIMS spectrum of **10**

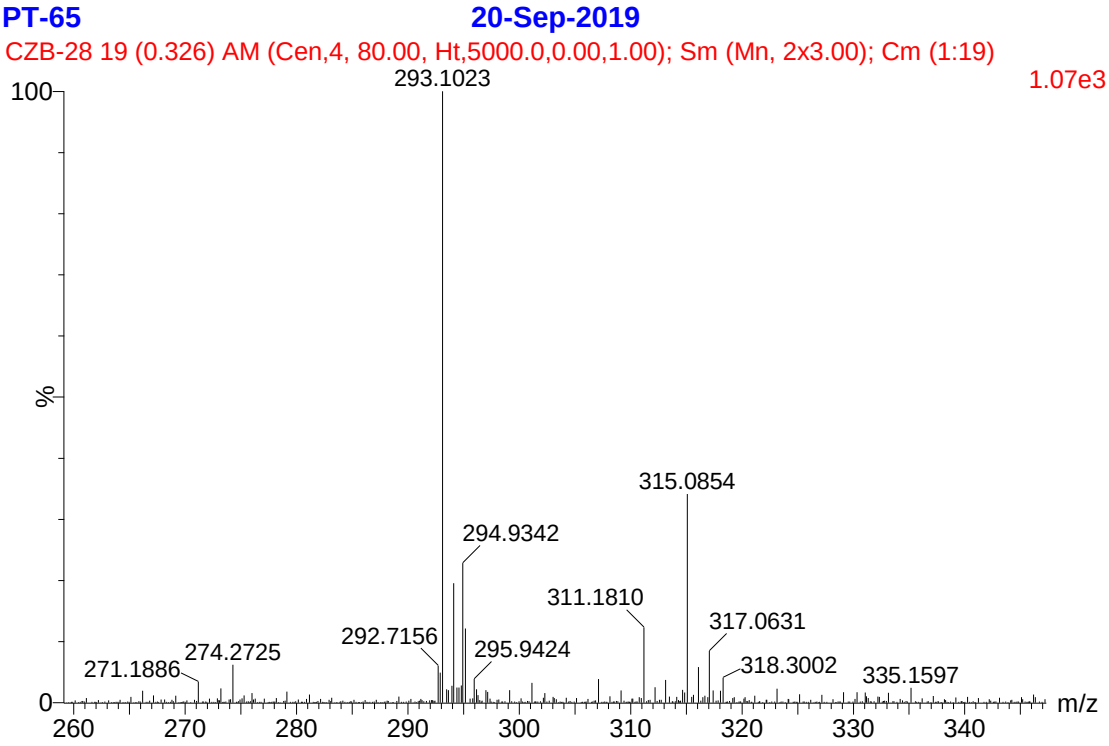

Figure S97 HRESIMS spectrum of **11**

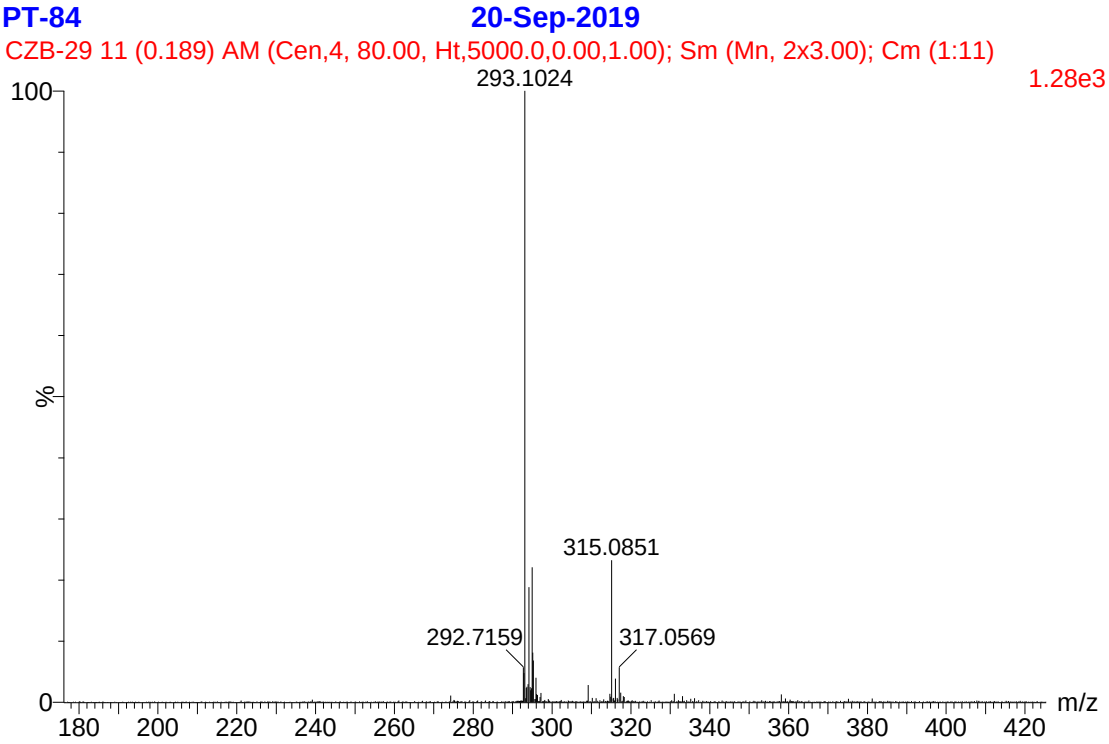

Figure S98 HRESIMS spectrum of **12**

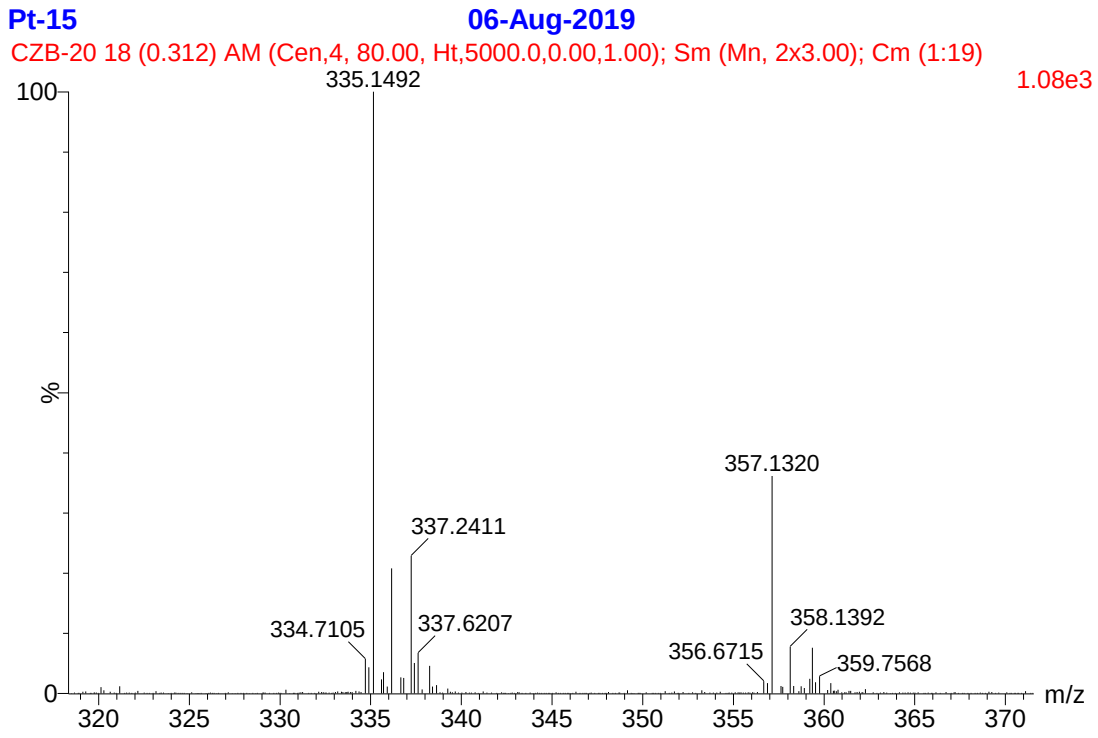

Figure S99 HRESIMS spectrum of **13**

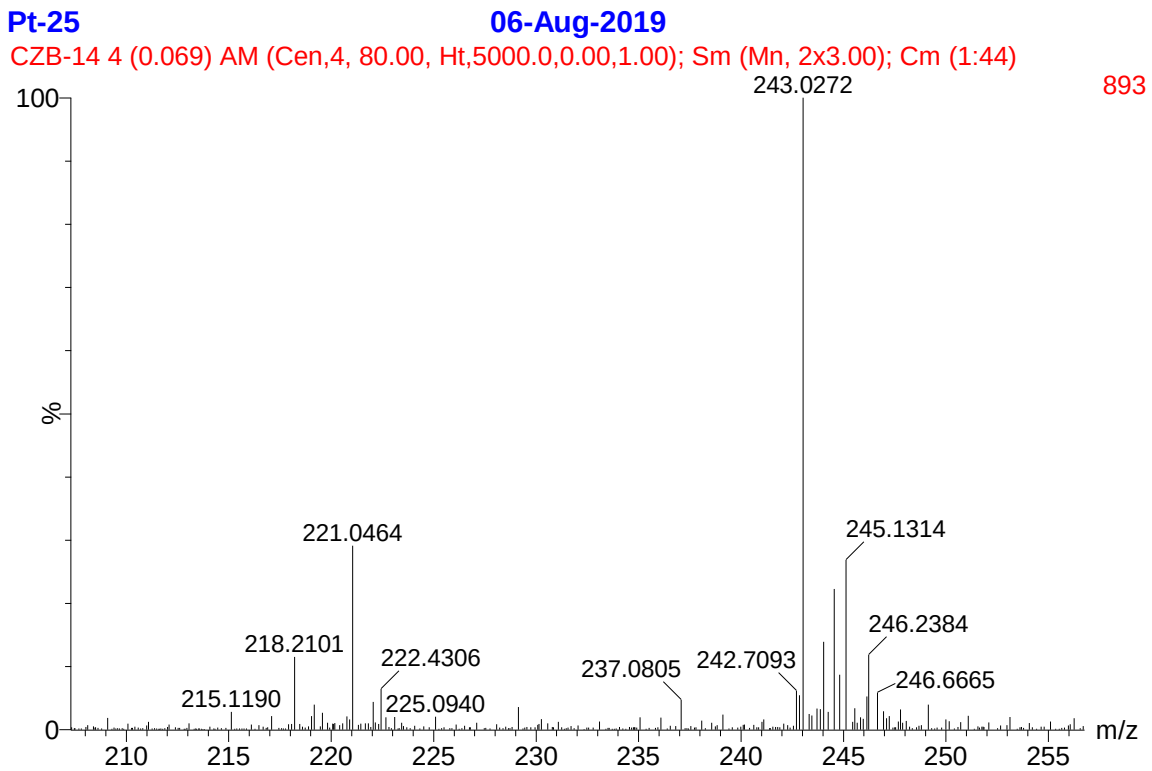

Figure S100 HRESIMS spectrum of **14.**

Table S1. DP4+ probability analysis.

Functional		Solvent?		Basis Set	Type of Data	
mPW1PW91		PCM		6-311+G(d,p)	Shielding Tensors	
		DP4+	100.00%	0.00%	-	-	-
Nuclei	sp2?	xperimenta	Isomer 1	Isomer 2	Isomer 3	Isomer 4	Isomer 5
C		84.89	98.45	98.94			
C	x	149.62	30.27	29.35			
C	x	137.55	46.92	47.73			
C	x	187.35	-2.19	-2.40			
C	x	116.2	68.21	68.96			
C	x	162.23	19.35	19.08			
C	x	118.37	64.38	64.21			
C	x	136.82	44.62	45.91			
C	x	117.82	65.75	63.67			
C	x	143.87	36.38	40.00			
C		47.73	133.35	136.73			
C	x	175.98	2.06	4.57			
C	x	115.91	65.19	61.65			
C	x	176.83	5.89	6.44			
C		77.29	174.06	172.68			
C		13.34	107.98	108.48			
C		52.45	134.33	134.08			
C		60.84	126.31	125.95			
H	x	6.97	24.48	24.48			
H	x	7.6	23.85	23.95			
H	x	7.18	24.34	24.90			
H		3.19	28.73	28.28			
H	x	5.83	25.88	26.27			
H		0.84	31.07	30.92			
H		4.93	26.84	26.99			
H		5.47	26.053	26.461			
H		3	28.686	28.733			
H		4.06	27.72	27.312			

DP4+ (H data)	100.00%	0.00%
DP4+ (C data)	99.01%	0.99%
DP4+ (all data)	100.00%	0.00%

Table S2. Shielding sensors (σ_C) of the conformers of 1*S*, 11*S*-**1** and the calculated chemical shifts (δ_C)

no.	C1 (50%)	C2 (50%)	Averaged	$\sigma_{C\ (TMS)}$	Experimental Shifts	Unscaled shifts	Scaled shifts
1	98.4547	98.4547	98.4547	187.38425	84.89	88.93	85.59
2	30.2735	30.2737	30.2736		149.62	157.11	151.73
3	46.9185	46.9185	46.9185		137.55	140.47	135.59
4	-2.1876	-2.1873	-2.18745		187.35	189.57	183.22
5	68.2135	68.2138	68.21365		116.2	119.17	114.93
6	19.3467	19.3468	19.34675		162.23	168.04	162.33
7	64.3838	64.3838	64.3838		118.37	123.00	118.64
8	44.6182	44.6181	44.61815		136.82	142.77	137.82
9	65.748	65.748	65.748		117.82	121.64	117.32
10	36.3771	36.3771	36.3771		143.87	151.01	145.81
11	133.3489	133.3488	133.3489		47.73	54.04	51.74
12	2.0573	2.0571	2.0572		175.98	185.33	179.11
13	65.1878	65.1877	65.18775		115.91	122.20	117.86
14	5.8895	5.8894	5.88945		176.83	181.49	175.39
15	174.0648	174.0648	174.0648		13.34	13.32	12.24
16	107.9832	107.9832	107.9832		77.29	79.40	76.35
17	134.329	134.329	134.329		52.45	53.06	50.79
18	126.3124	126.3126	126.3125		60.84	61.07	58.56

Table S3. Shielding sensors (σ_H) of the conformers of 1*S*, 11*S*-**1** and the calculated chemical shifts (δ_H)

no.	C1 (50%)	C2 (50%)	Averaged	$\sigma_{H\ (TMS)}$	Experimental	Unscaled shifts	Scaled shifts
7	24.4817	24.4817	24.4817	31.769067	7	7.29	7.05
8	23.8461	23.8461	23.8461		7.6	7.92	7.64
9	24.3435	24.3435	24.3435		7.18	7.43	7.18
11	28.7335	28.7335	28.7335		3.19	3.04	3.07
13	25.8831	25.883	25.88305		5.83	5.89	5.74
15	31.06697	31.067	31.06698		0.84	0.70	0.89
16a	26.8434	26.8434	26.8434		4.93	4.93	4.84
16b	26.0531	26.0531	26.0531		5.47	5.72	5.58
1-OCH_3	28.68557	28.6856	28.68558		3.00	3.08	3.11
2-OCH_3	27.7202	27.7202	27.7202		4.06	4.05	4.02

Table S4. Shielding sensors (σ_C) of the conformers of 1*S*, 11*R*-**1** and the calculated chemical shifts (δ_C)

no	C1 (77%)	C2 (5.7%)	C3 (4.9%)	C4 (4.9%)	C5 (3.8%)	C6 (3.7%)	Averaged	Unscaled shifts	Scaled shifts
1	98.4245	100.8862	100.8862	101.2943	101.302	99.4808	98.94148	88.44	85.2
2	29.6612	28.5536	28.5542	27.6985	27.7037	28.7398	29.35315	158.03	153.0
3	47.7926	47.4416	47.4417	47.491	47.4926	47.6915	47.72988	139.65	135.1
4	-2.4775	-1.868	-1.8681	-2.3281	-2.3336	-2.303	-2.39683	189.78	184.0
5	68.9722	69.6328	69.6328	68.3443	68.3679	68.5133	68.96456	118.42	114.5
6	19.0383	19.112	19.1121	19.4685	19.4611	19.0367	19.07743	168.31	163.1
7	64.1892	64.1643	64.1642	64.4827	64.46975	64.2157	64.2098	123.17	119.1
8	46.2073	44.6318	44.6319	44.773	44.7644	45.6738	45.91461	141.47	136.9
9	63.3006	65.4201	65.4201	64.4827	64.46975	64.5258	63.66633	123.72	119.6
10	40.9928	36.1055	36.1055	35.339	35.3388	39.4123	39.99971	147.38	142.7
11	138.1003	130.8306	130.8306	130.0731	130.0745	137.185	136.7337	50.65	48.4
12	4.24	4.8849	4.885	6.7173	6.7575	5.6108	4.568626	182.82	177.2
13	61.6472	62.4659	62.4658	62.5288	62.5305	59.188	61.65344	125.73	121.6
14	6.4171	6.5631	6.5631	6.7173	6.6996	6.1265	6.436704	180.95	175.4
15	107.681	110.5183	110.5182	112.0534	112.039	110.9943	108.4753	14.71	13.4
16	172.8341	169.7175	169.7175	172.9697	172.9507	175.2529	172.676	78.91	76.0
17	134.052	134.2936	134.2937	134.0566	134.0565	134.0351	134.0751	53.31	51.0
18	125.9935	125.854	125.8541	125.7097	125.7047	125.8723	125.9515	61.43	58.9

Table S5. Shielding sensors (σ_H) of the conformers of 1*S*, 11*R*-**1** and the calculated chemical shifts (δ_H)

no.	C1 (77%)	C2 (5.7%)	C3 (4.9%)	C4 (4.9%)	C5 (3.8%)	C6 (3.7%)	Averaged	Unscaled shifts	Scaled shifts
7	24.4625	24.4405	24.6373	24.6373	24.463	24.4607	24.47833	7.29	7.31
8	23.9819	24.046	23.7914	23.7914	23.8052	23.8037	23.95358	7.82	7.85
9	25.0311	24.8756	24.3354	24.3354	24.2652	24.2634	24.89655	6.87	6.88
11	28.2534	27.8593	28.7977	28.7977	28.2076	28.208	28.28086	3.49	3.43
13	26.3013	25.3989	25.9645	25.9644	26.9473	26.9416	26.26509	5.50	5.49
15	31.06127	31.05463	30.2783	30.27833	30.25093	30.25237	30.92344	0.85	0.73
16a	26.8416	27.4032	28.5844	27.333	26.8893	26.8877	26.98661	4.78	4.75
16b	26.1674	27.1212	27.333	28.5844	27.0218	27.0212	26.46137	5.31	5.29
1-OCH_3	28.74013	28.67807	28.7089	28.70893	28.7282	28.72893	28.73267	3.04	2.97
2-OCH_3	27.30363	27.31033	27.29863	27.29857	27.41763	27.4177	27.31207	4.46	4.42