



Supporting Information

for

Discovery of sugarnitriles A and B, and structural reassignment of SF-2140, from a sugarcane endophytic actinomycete *Amycolatopsis* sp. JS-O27

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NMR data and copies of NMR and MS spectra

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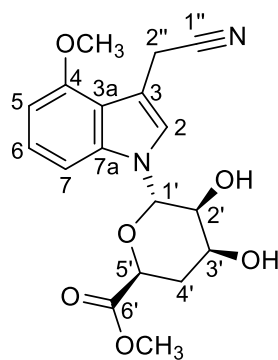
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Table S1: Comparison of ¹H NMR data for reported SF-2140 and compound **1**.



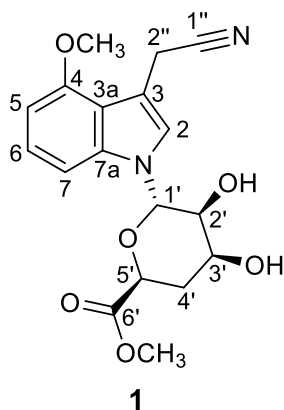
SF-2140 (**1**)

NO.	SF-2140 (acetone- <i>d</i> ₆)		compound 1 (DMSO- <i>d</i> ₆)
	δ_{H} (J in Hz) ^a	δ_{H} (J in Hz) ^b	δ_{H} (J in Hz)
2	lack	7.36, s	7.38, s
3	-	-	-
3a	-	-	-
4	-	-	-
4-OMe	lack	3.90, s	3.87, s
5	lack	6.57, d, 7.5	6.60, d, 7.8
6	lack	7.11, t, 8.0	7.13, t, 8.1
7	lack	7.42, d, 8.0	7.36, d, 8.5
7a	-	-	-
1'	6.33, d, 9.3	6.29, d, 9.4	6.13, d, 9.4
2'	4.16, ddd, 2.7	4.12, dd, 9.4, 2.8	3.96, dd, 9.3, 2.5
2'-OH	4.36, d, 7.1	-	-
3'	4.29, ddd, 3.7, 2.2	4.26, m	4.08, br s
3'-OH	4.21, dd, 2.7, 1.2	-	-
4'a	2.28, dddd, 14.4, 6.8	2.28, ddd, 14.3, 7.0	2.17, ddd, 14.0, 7.0, 1.9
4'b	2.51, dddd, 1.2	2.50, ddd, 1.3	2.30, dd, 13.1, 1.9
5'	4.45, br d	4.42, br d	4.49, d, 6.5
6'	-	-	-
6'-OMe	3.75, s	3.75, s	3.70, s
1''	-	-	-
2''	lack	4.02, s	4.04, s

^aJ. Antibiot. **1984**, 37, 931-934.

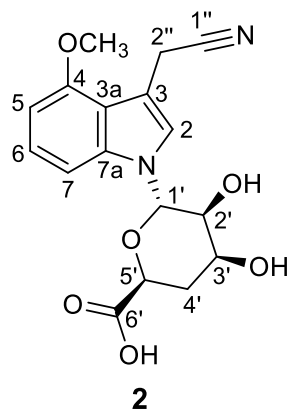
^bJ. Chem. Soc., Perkin Trans. 1 **1994**, 1417-1426.

Table S2: 1D and 2D NMR data for **1** in DMSO-*d*₆.



No.	δ_{H} , m, <i>J</i> (Hz)	δ_{C} , type	COSY	HMBC	NOESY
2	7.38, s	123.0, CH	2''	2'', 3, 7a	2''
3	-	104.4, C			
3a	-	116.4, C			
4	-	153.7, C			
4-OMe	3.87, s	55.3, CH ₃		4	5
5	6.60, d, 7.8	100.5, CH	6	3a, 4, 7	4-OMe, 6
6	7.13, t, 8.1	123.2, CH	5, 7	4, 5, 7, 7a	5, 7
7	7.36, d, 8.5	104.3, CH	6	3a, 5	1', 6
7a	-	138.8, C			
1'	6.13, d, 9.4	78.1, CH	2'	2, 2', 7a	2', 7
2'	3.96, dd, 9.3, 2.5	68.5, CH	1'	1'	1', 3', 4'a
3'	4.08, br s	67.0, CH	4'b		2', 4'a, 4'b
4'a	2.17, ddd, 14.0, 7.0, 1.9	33.6, CH ₂	5'	5', 6'	2', 3', 4'b, 5'
4'b	2.30, dd, 13.1, 1.9	-	3'		3', 4'a, 5'
5'	4.49, d, 6.5	69.3, CH	4'a	1', 3', 4', 6'	4'a, 4'b
6'	-	172.4, C			
6'-OMe	3.70, s	51.5, CH ₃		6'	
1''	-	119.6, C			
2''	4.04, s	15.2, CH ₂	2	1'', 2, 3, 3a	2

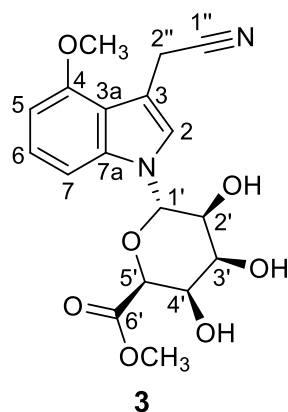
Table S3: 1D and 2D NMR data for **2** in DMSO-*d*₆.



No.	δ_{H} , m, <i>J</i> (Hz)	δ_{C} , type	COSY	HMBC	NOESY
2	7.35, s	123.2, CH	2''	2''	2', 2''
3	-	104.0, C			
3a	-	116.3, C			
4	-	153.6, C			
4-OMe	3.87, s	55.3, CH ₃		4	5
5	6.57, d, 7.8	100.3, CH	6	3a, 4, 7	4-OMe, 6
6	7.08, t, 8.1	122.9, CH	5, 7	4, 7a	5, 7
7	7.36, d, 8.0	104.8, CH	6	3a, 5, 7a	1', 6
7a	-	138.8, C			
1'	6.15, d, 9.3	78.4, CH	2'	2, 2', 7a	7
2'	3.90, dd, 9.2, 2.9	69.1, CH	1', 3'		2
3'	4.03, s	67.3, CH	2', 4'b		
4'a	2.07, ddd, 14.0, 7.1, 2.2	33.1, CH ₂	5'		
4'b	2.29, dd, 13.5, 1.8	-	3'		
5'	4.18, d, 6.9	71.9, CH	4'a	1', 3', 6'	
6'	-	174.7, C*			
1''	-	119.7, C			
2''	4.05, s	15.2, CH ₂	2	1'', 2, 3, 3a	2

Note: * Assignment made by HMBC.

Table S4: 1D and 2D NMR data for **3** in DMSO-*d*₆.



No.	δ_{H} , m, <i>J</i> (Hz)	δ_{C} , type	COSY	HMBC	NOESY
2	7.36, s	123.4, CH	2''	2'', 1', 3	2', 2''
3	-	104.3, C			
3a	-	116.5, C			
4	-	153.8, C			
4-OMe	3.87, s	55.4, CH ₃		4	5
5	6.60, d, 7.8	100.5, CH	6	3a, 4, 6	4-OMe, 6
6	7.12, t, 8.1	123.1, CH	5, 7	4, 5, 7, 7a	5, 7
7	7.36, d, 8.4	104.5, CH	6	4, 5, 3a, 7a	1', 6
7a	-	138.6, C			
1'	6.11, d, 9.6	78.7, CH	2'	2, 2', 3', 7a	2', 7
2'	4.28, d, 9.0	64.8, CH	1', 2'-OH, 3'		1', 2, 3'
2'-OH	5.08, s	-	2'		3'-OH, 4'-OH
3'	3.94, br s	71.2, CH	2', 3'-OH, 4'		2', 4'
3'-OH	5.50, s	-	3'		2'-OH, 4'-OH
4'	4.21, d, 2.9	70.9, CH	3'	2', 3'	3', 5'
4'-OH	5.63, s	-			2'-OH, 3'-OH
5'	4.36, s	76.0, CH		1', 3', 6'	4'
6'	-	170.2, C			
6'-OMe	3.70, s	51.6, CH ₃		6'	
1''	-	119.7, C			
2''	4.05, s	15.2, CH ₂	2	1'', 2, 3, 3a,	2

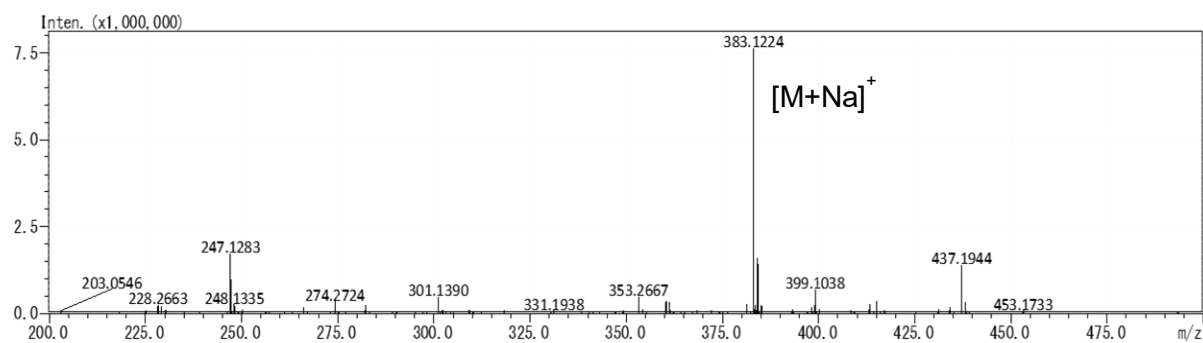


Figure S1: HRESIMS spectrum of **1**.

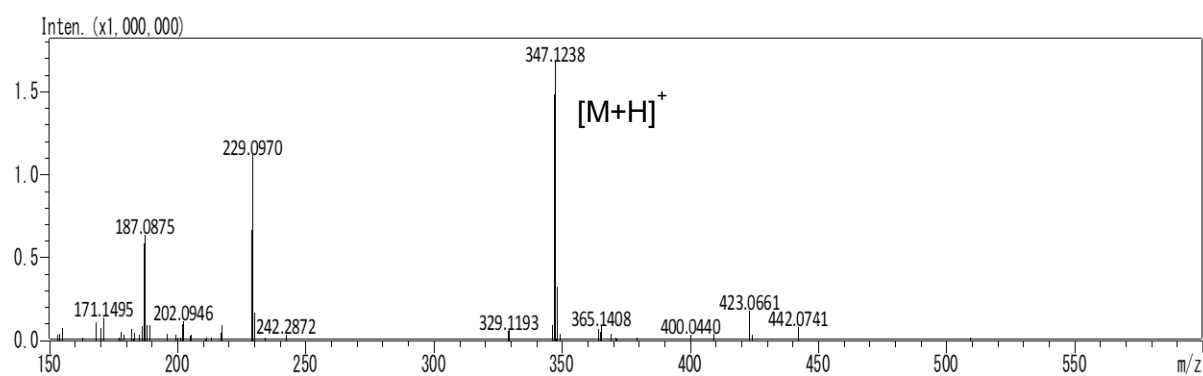


Figure S2: HRESIMS spectrum of **2**.

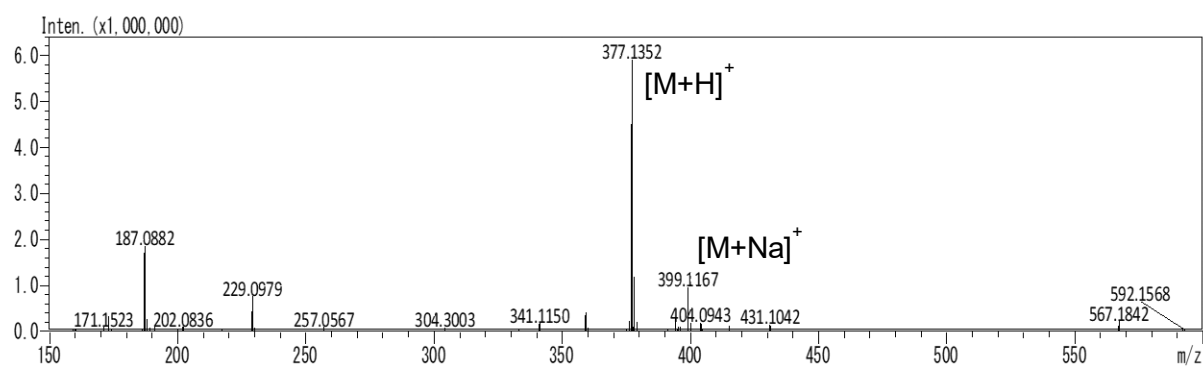


Figure S3: HRESIMS spectrum of **3**.

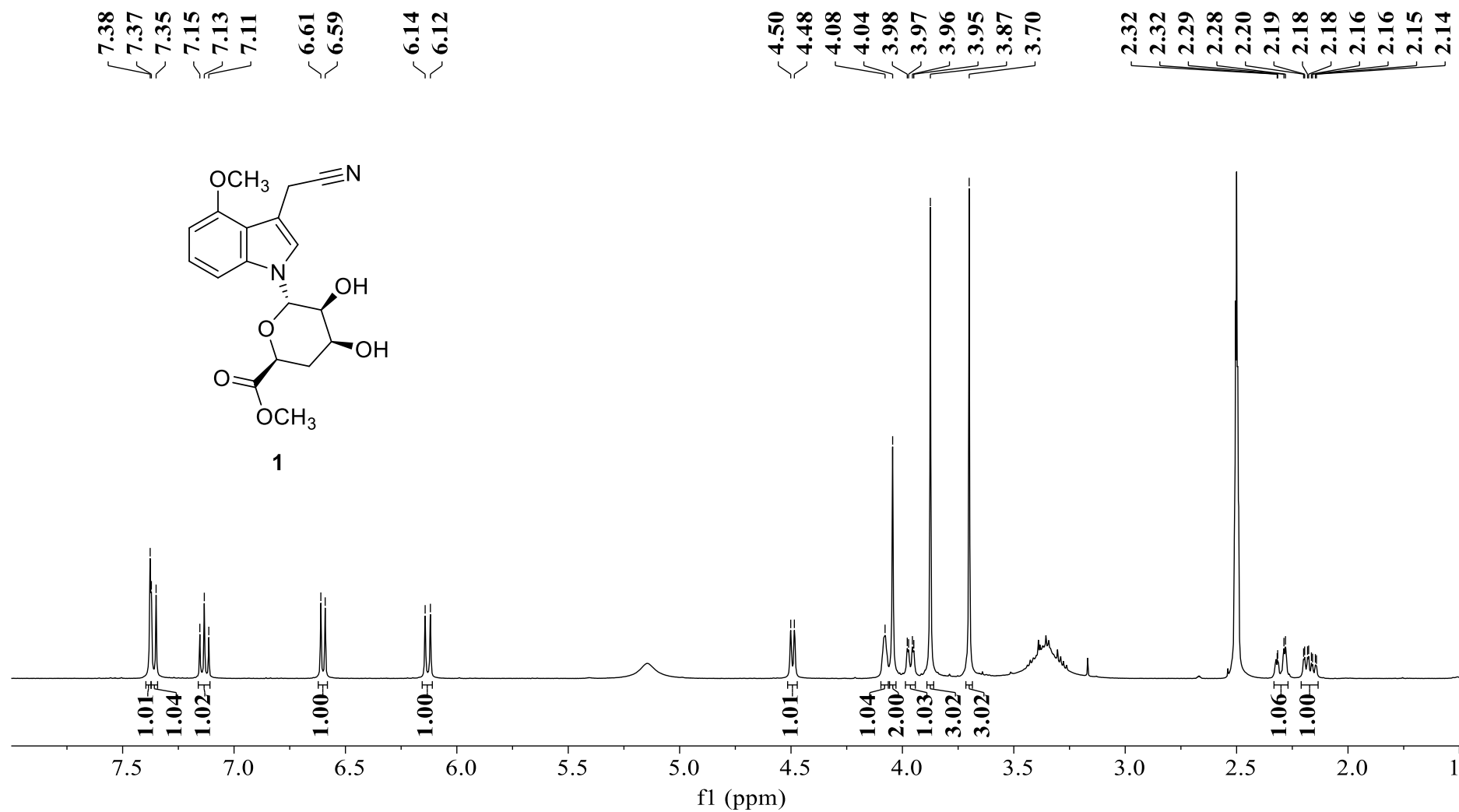


Figure S4: ¹H NMR spectrum (400 MHz) of **1** in DMSO-*d*₆.

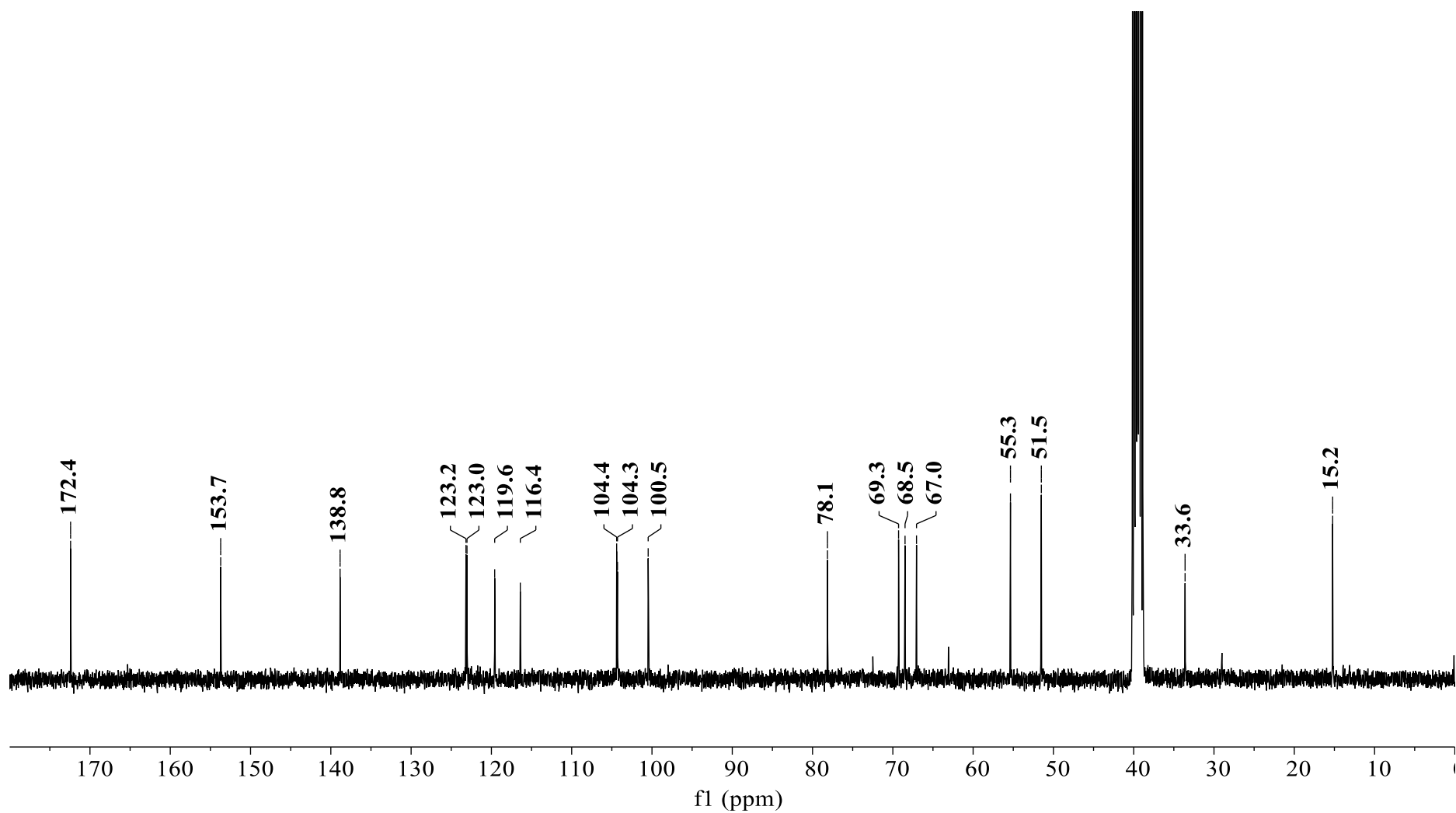


Figure S5: ¹³C NMR spectrum (100 MHz) of **1** in DMSO-*d*₆.

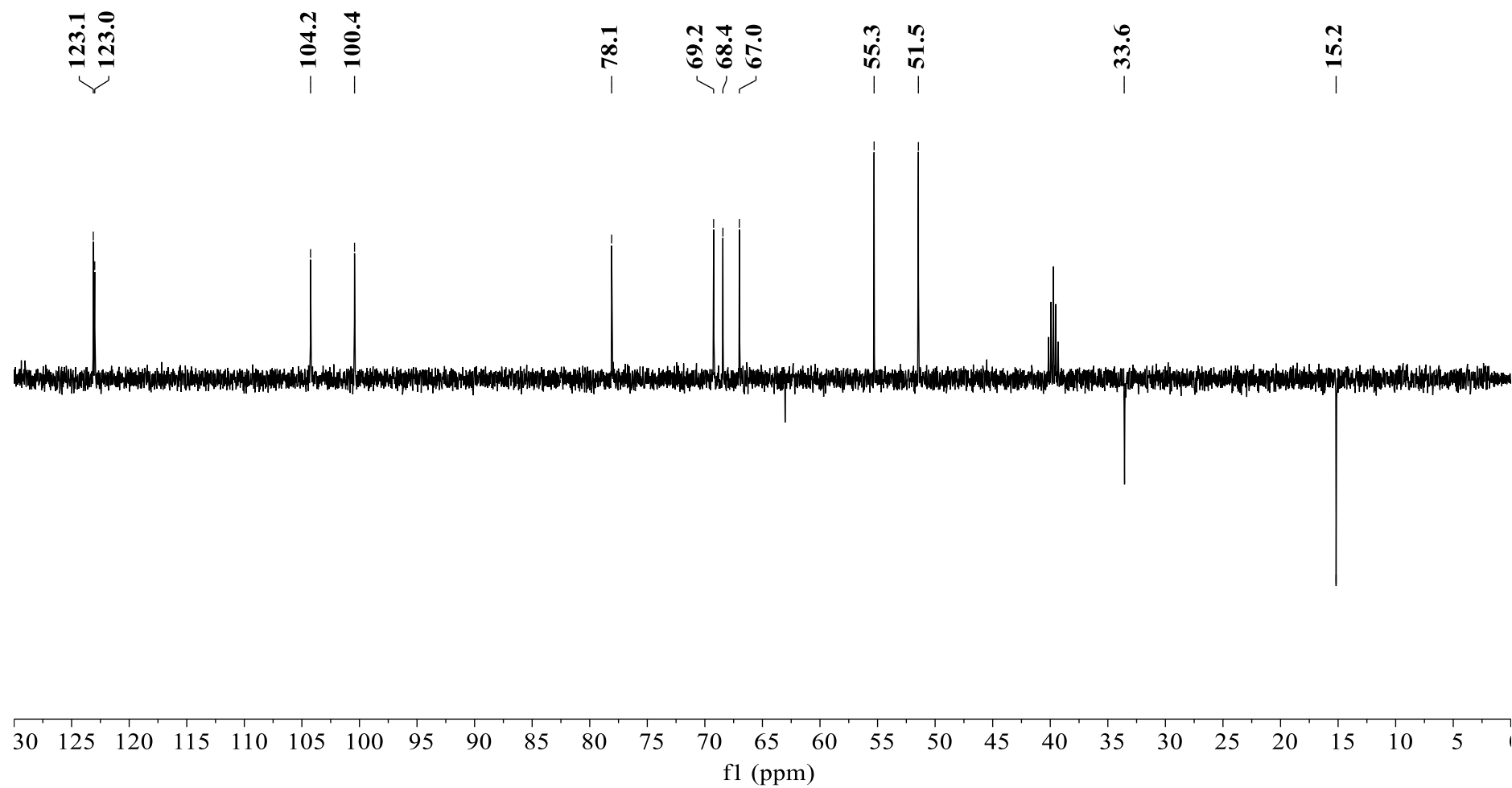


Figure S6: DEPT135 spectrum of **1** in DMSO- d_6 .

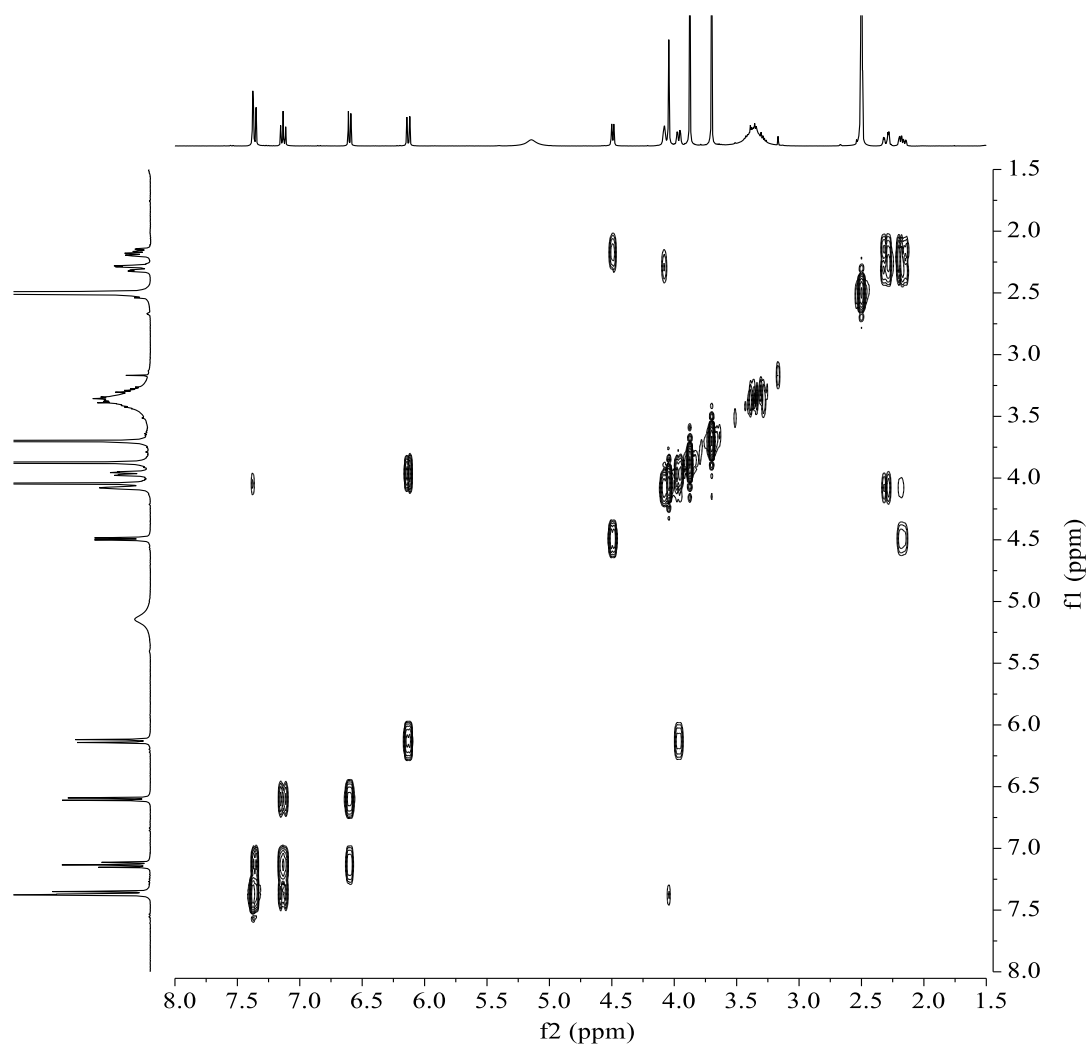


Figure S7: ^1H , ^1H COSY spectrum of **1** in $\text{DMSO}-d_6$.

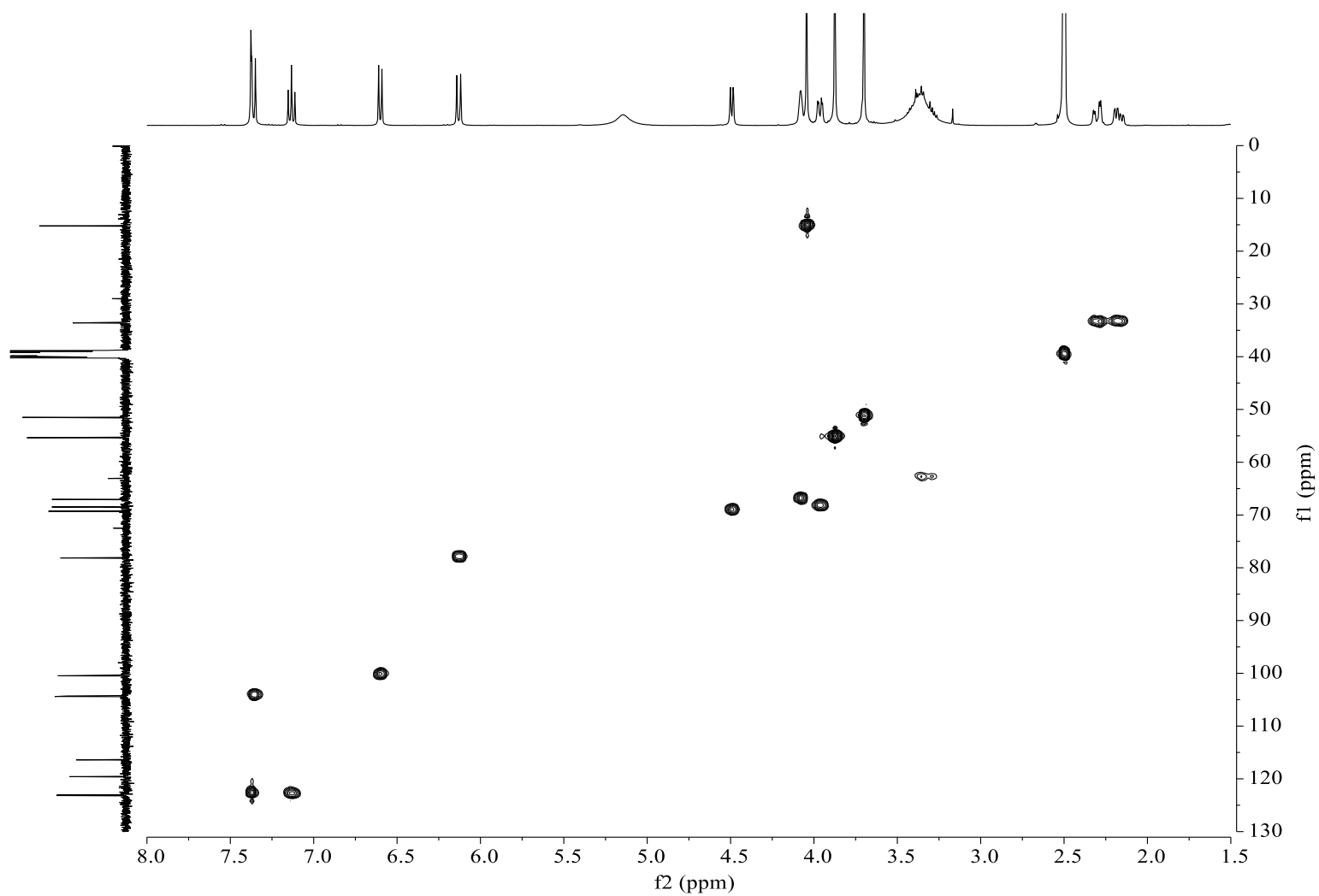


Figure S8: HSQC spectrum of **1** in DMSO- d_6 .

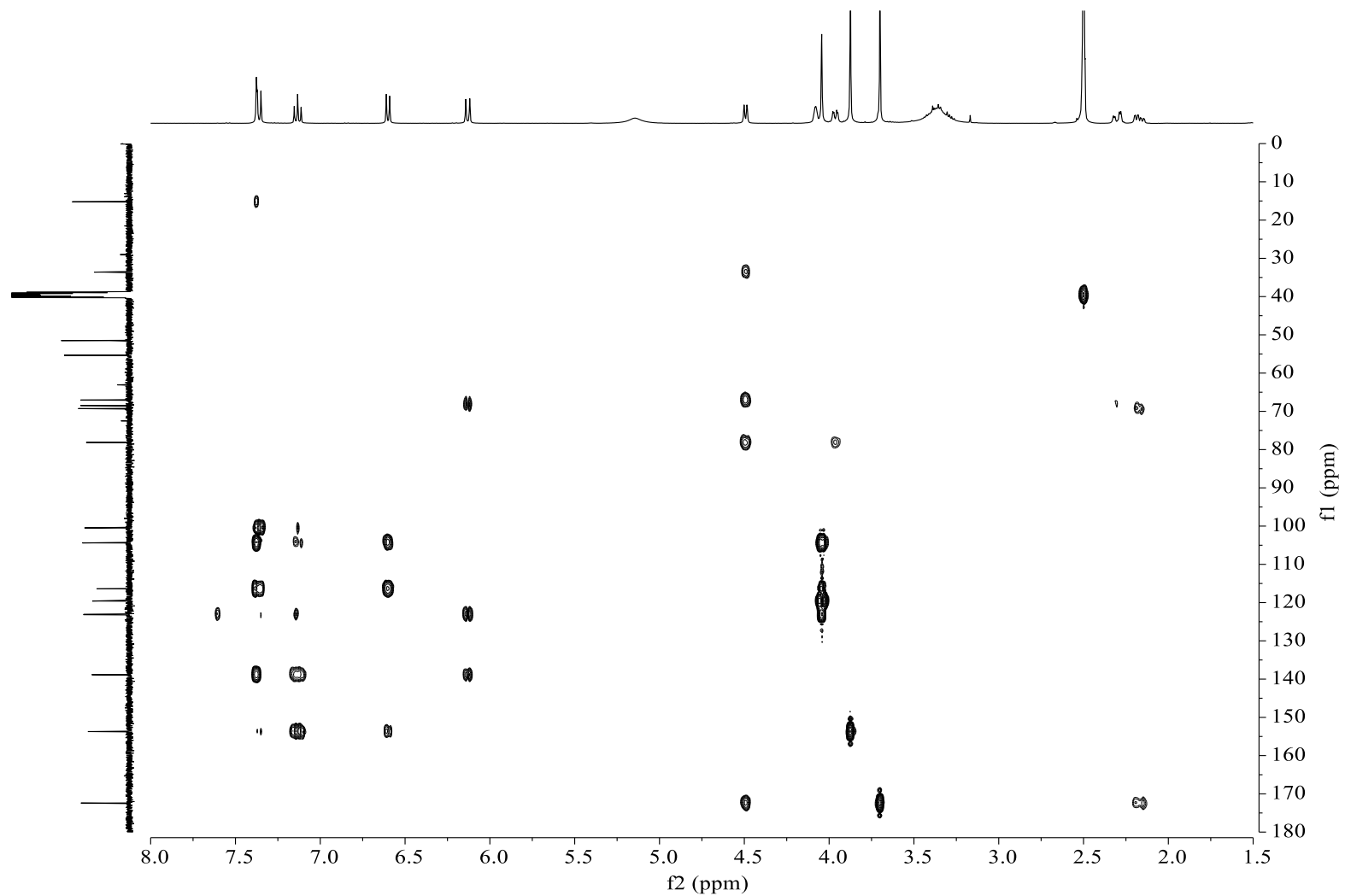


Figure S9: HMBC spectrum of **1** in DMSO-*d*₆.

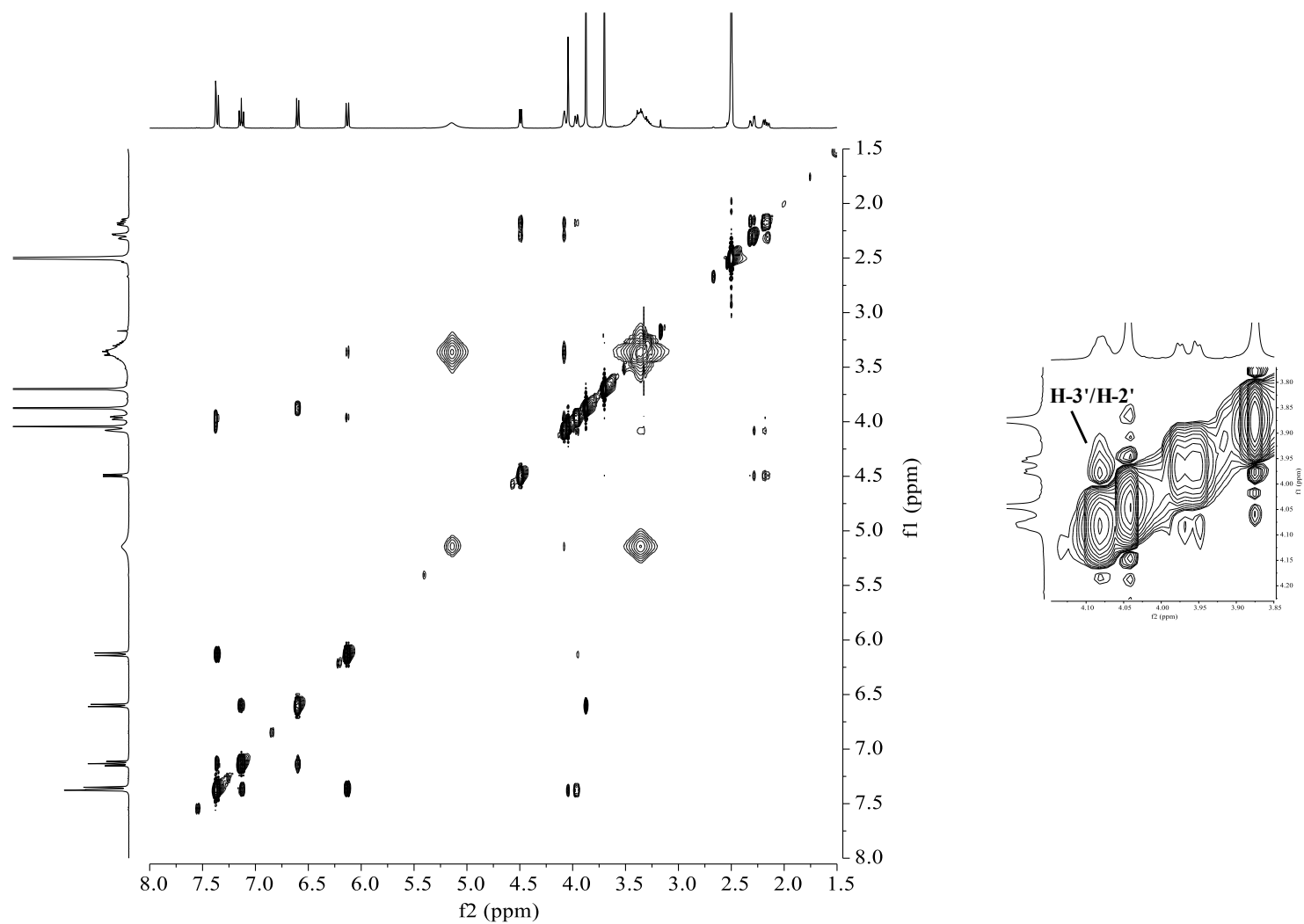


Figure S10: NOESY spectrum of **1** in DMSO-*d*₆.

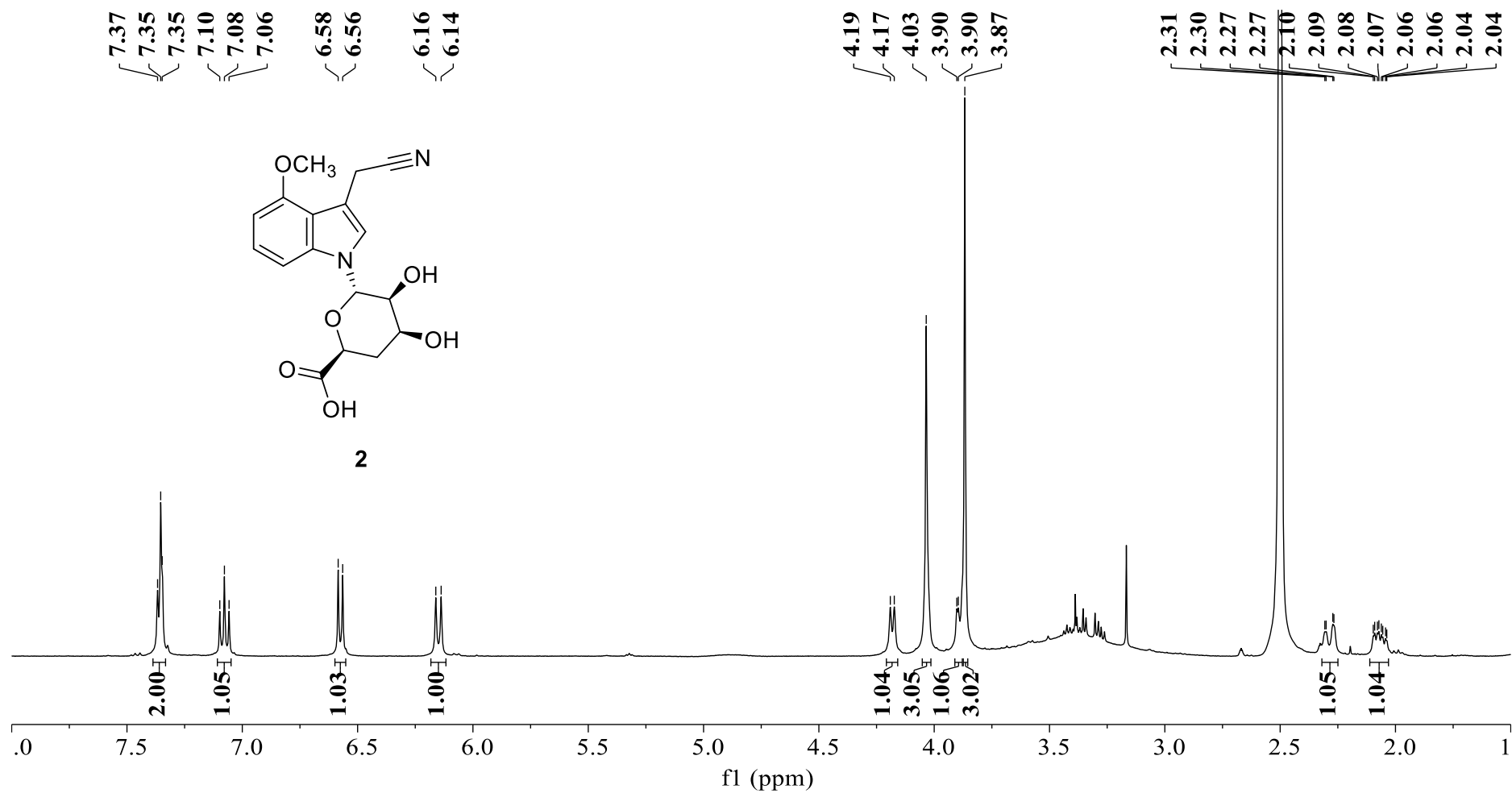


Figure S11: ¹H NMR spectrum (400 MHz) of **2** in DMSO-*d*₆.

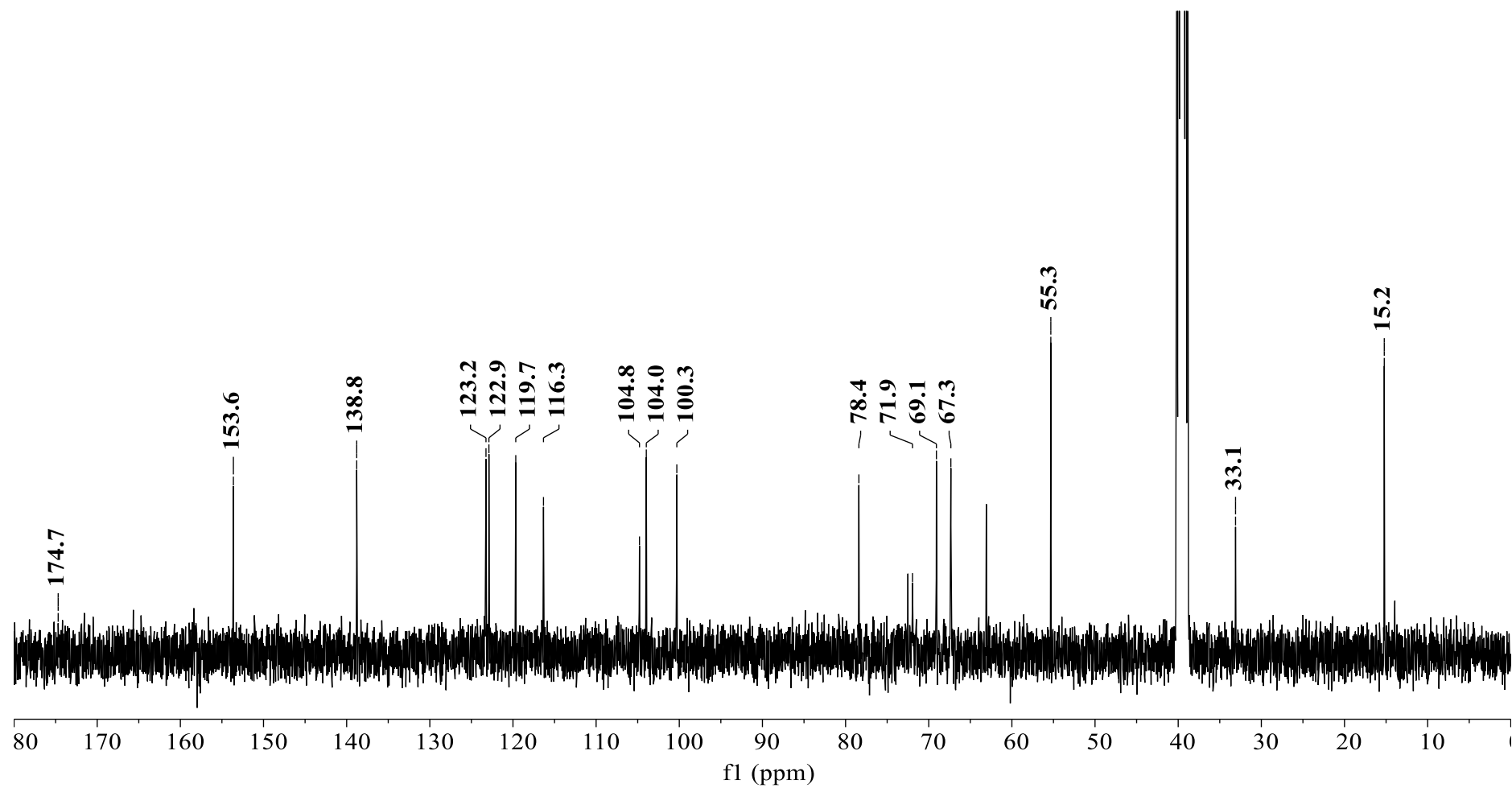


Figure S12: ¹³C NMR spectrum (100 MHz) of **2** in DMSO-*d*₆.

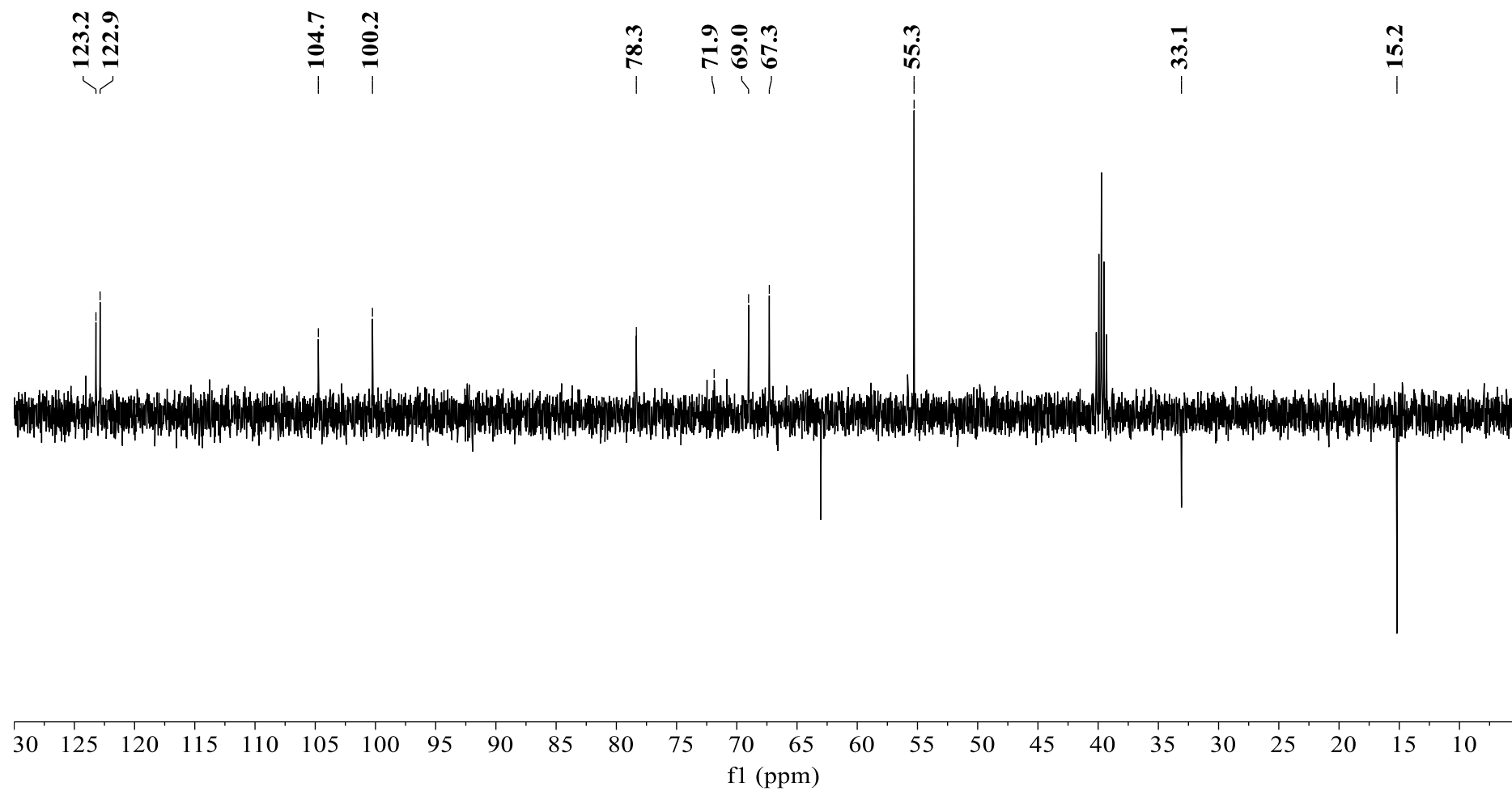


Figure S13: DEPT135 spectrum of **2** in DMSO- d_6 .

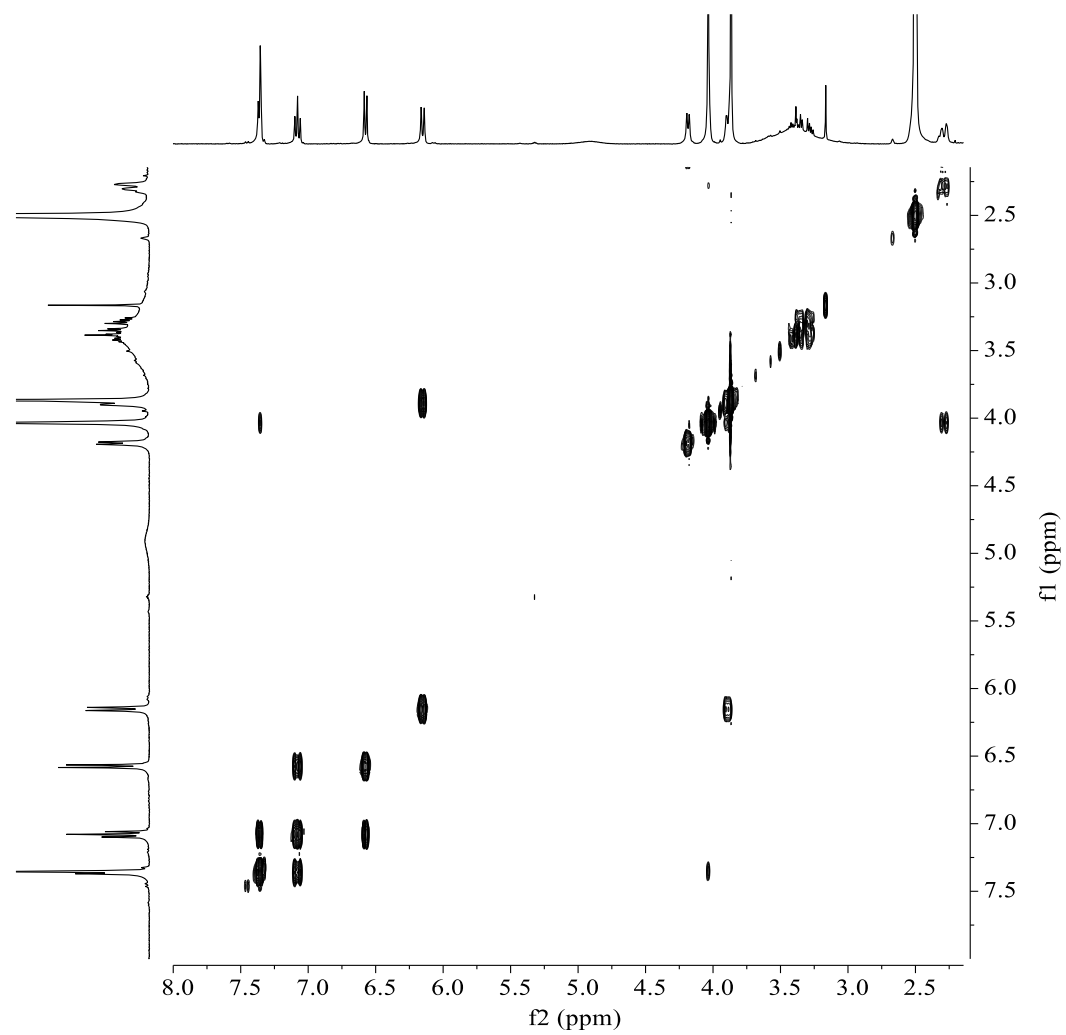


Figure S14: ^1H , ^1H COSY spectrum of **2** in $\text{DMSO}-d_6$.

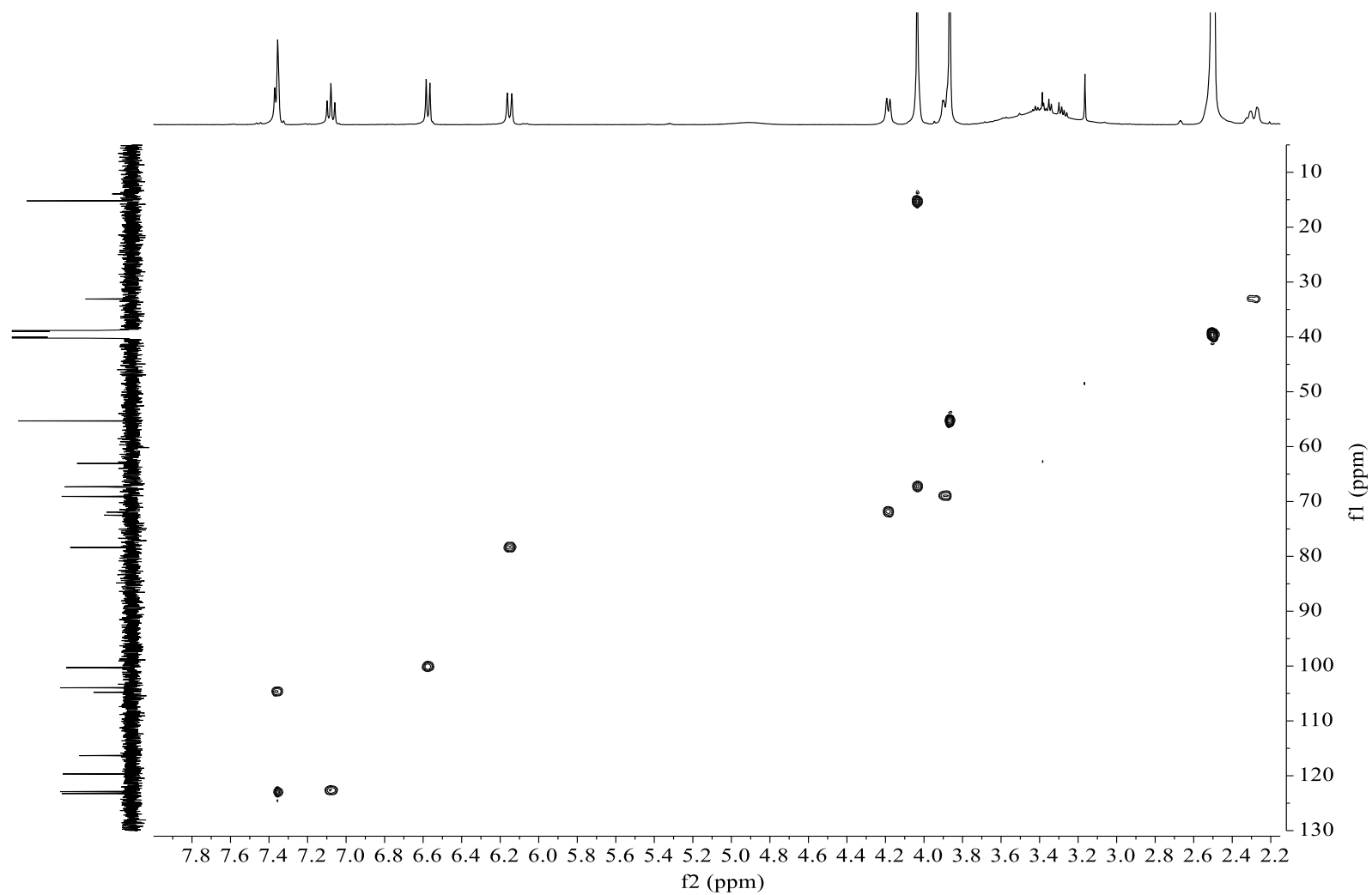


Figure S15: HSQC spectrum of **2** in DMSO- d_6 .

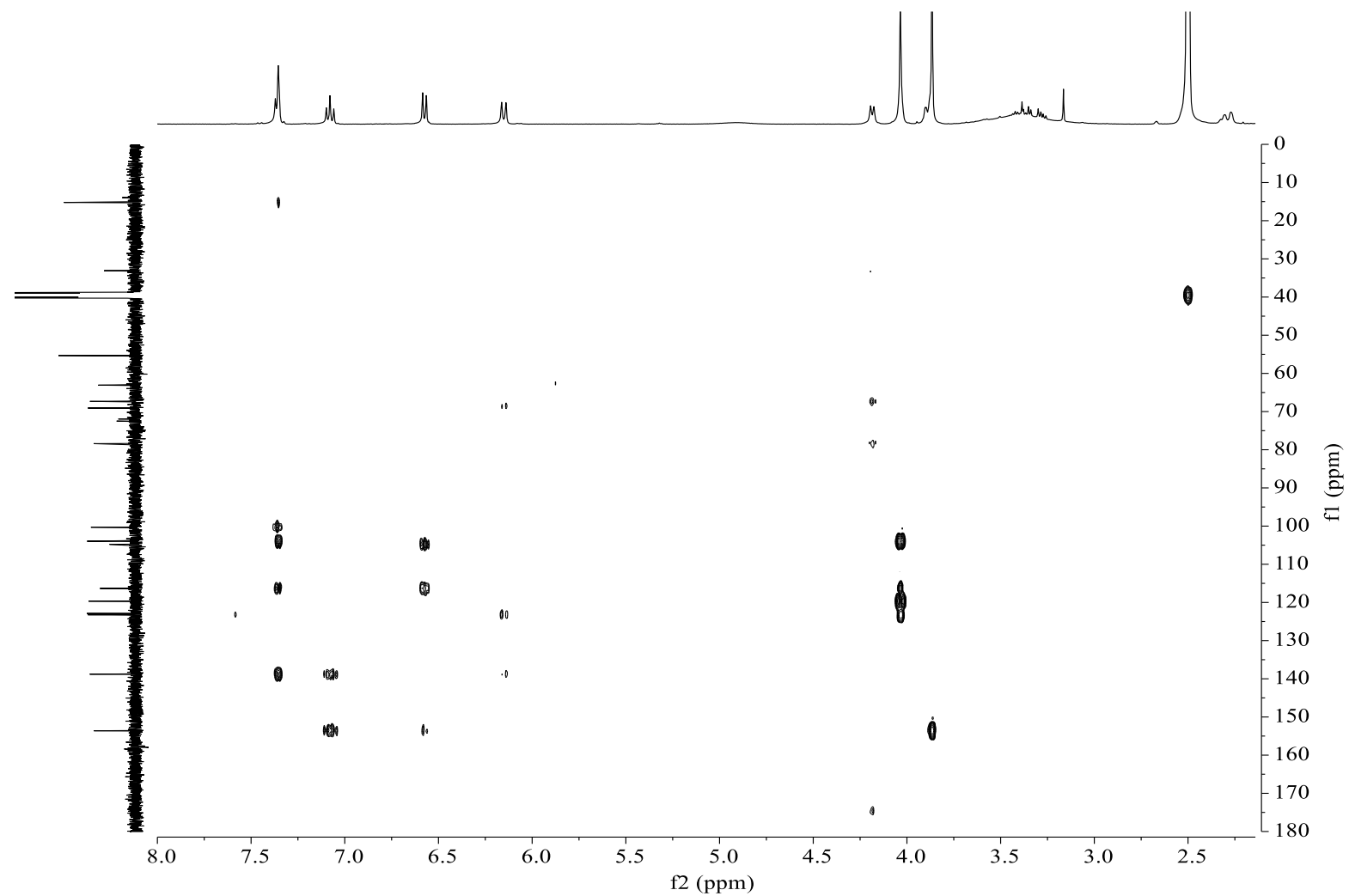


Figure S16: HMBC spectrum of **2** in DMSO- d_6 .

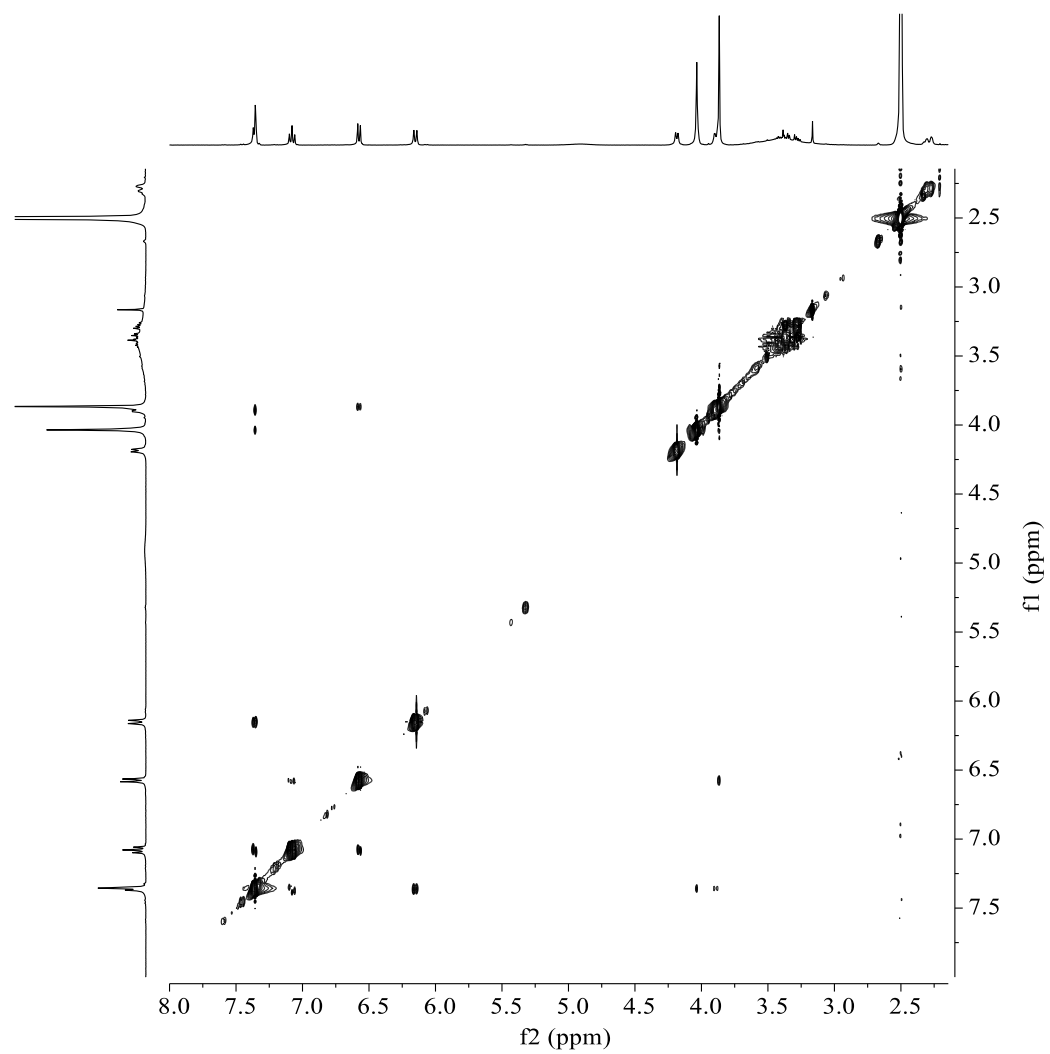


Figure S17: NOESY spectrum of **2** in DMSO-*d*₆.

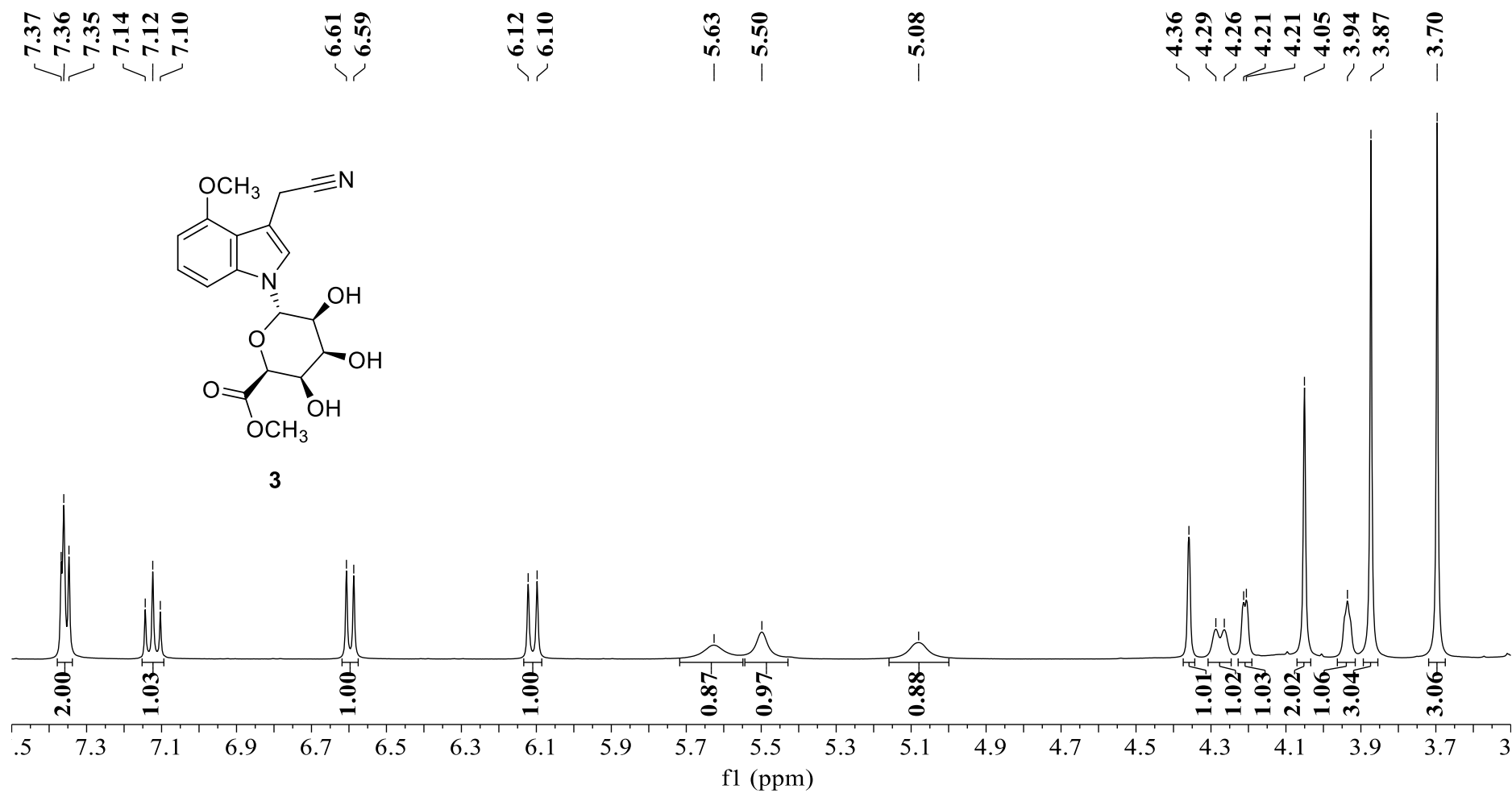


Figure S18: ¹H NMR spectrum (400 MHz) of **3** in DMSO-*d*₆.

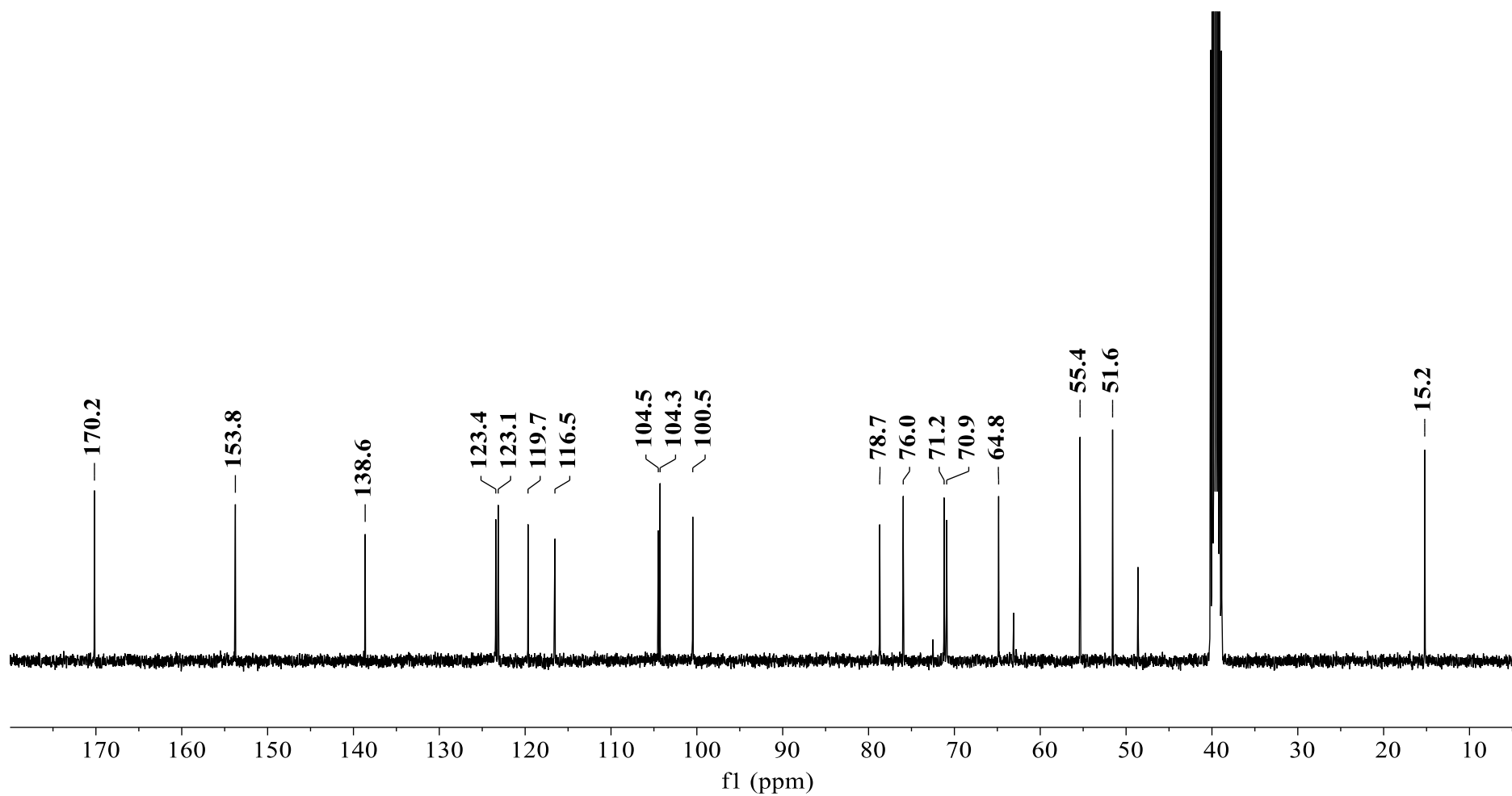


Figure S19: ^{13}C NMR spectrum (100 MHz) of **3** in $\text{DMSO-}d_6$.

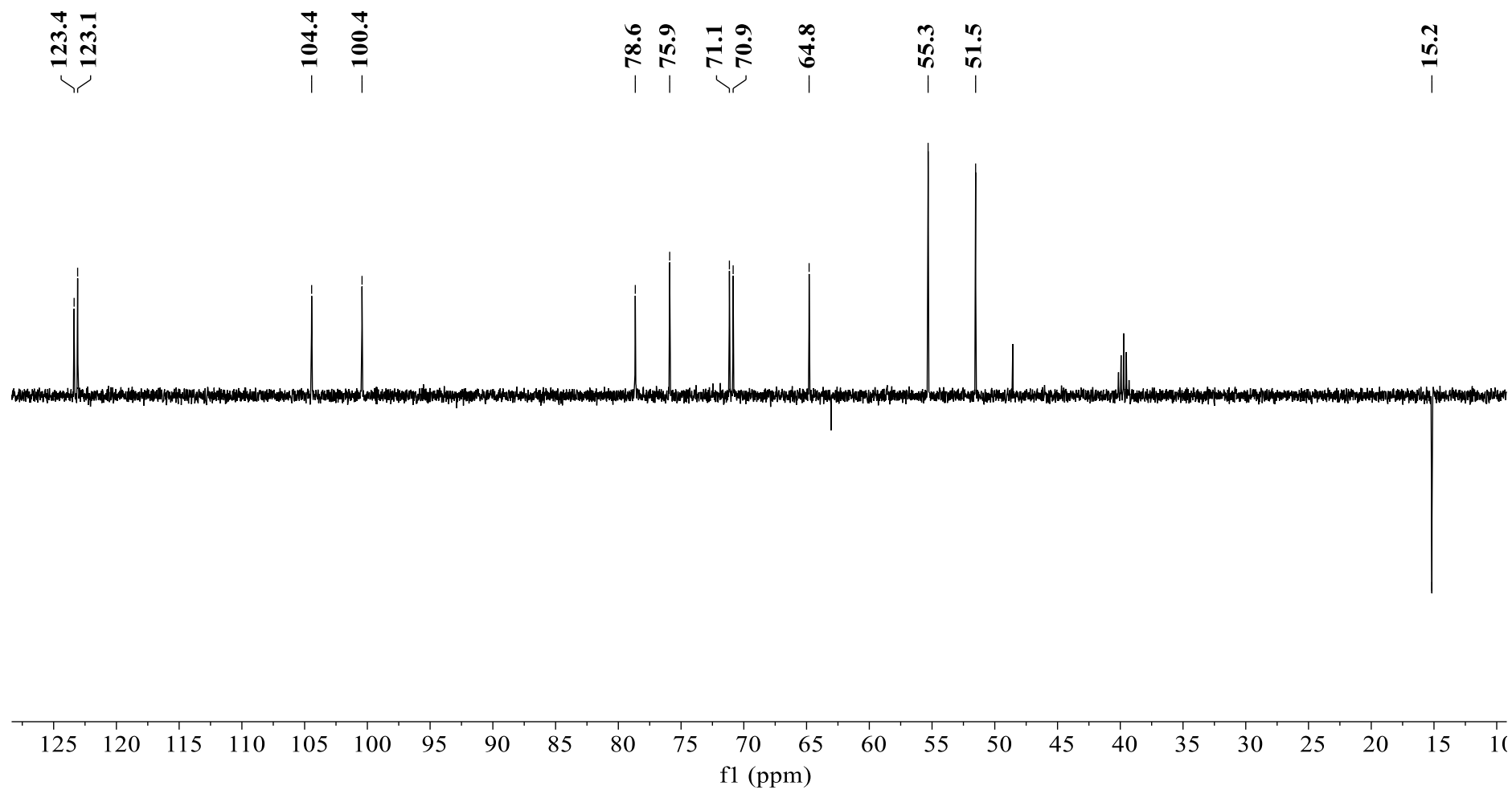


Figure S20: DEPT135 spectrum of **3** in DMSO- d_6 .

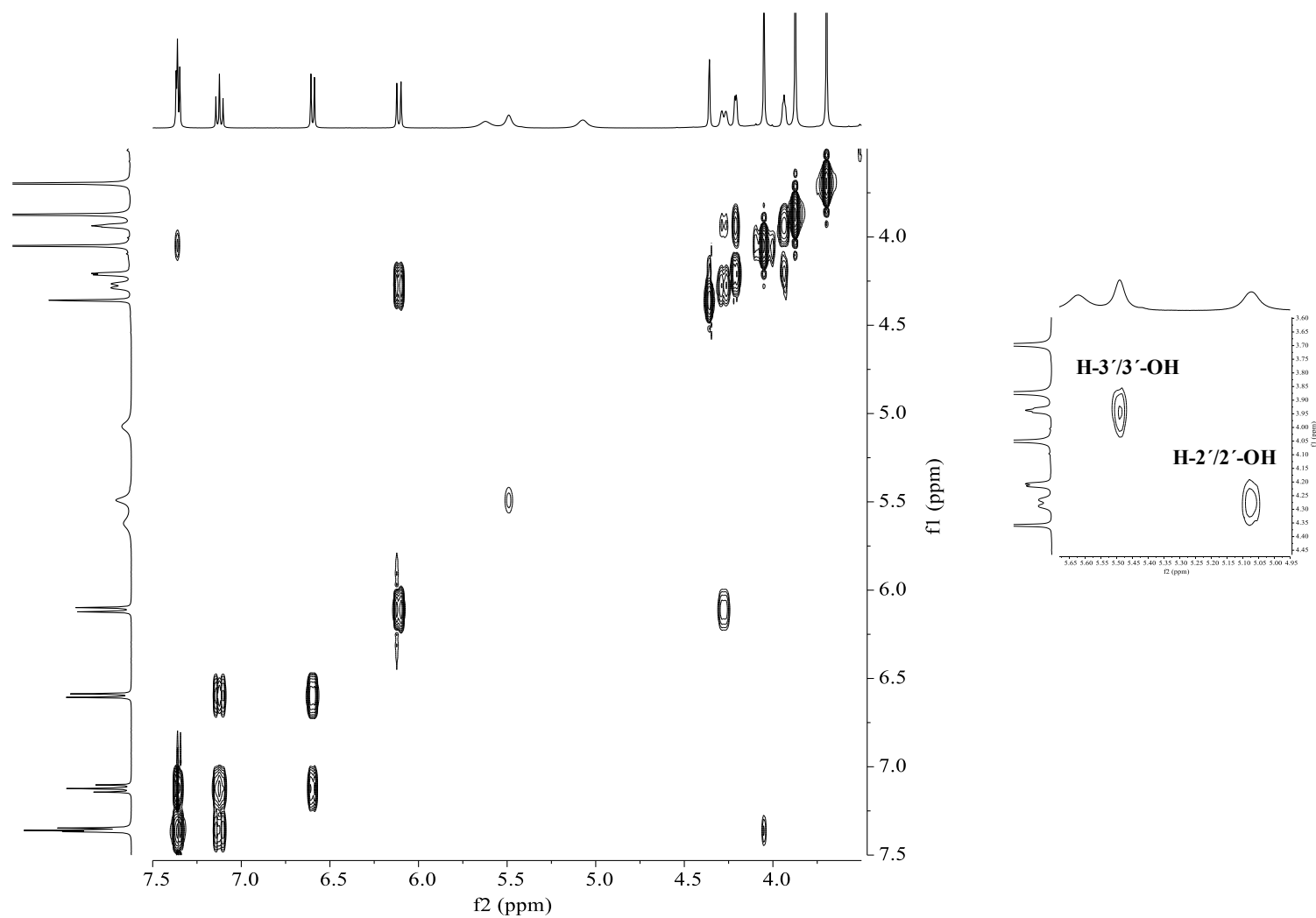


Figure S21: ^1H , ^1H COSY spectrum of **3** in $\text{DMSO}-d_6$.

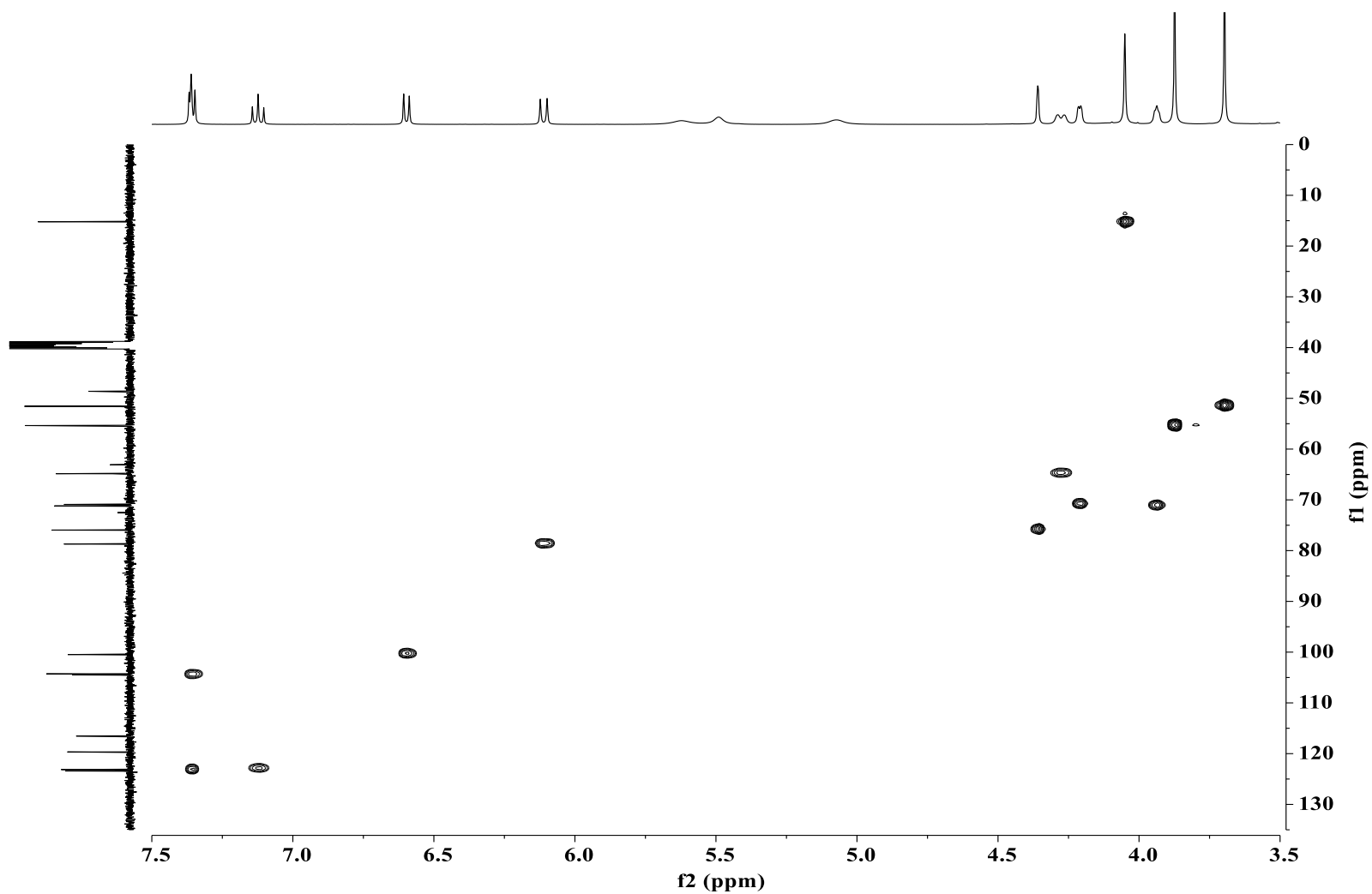


Figure S22: HSQC spectrum of **3** in DMSO- d_6 .

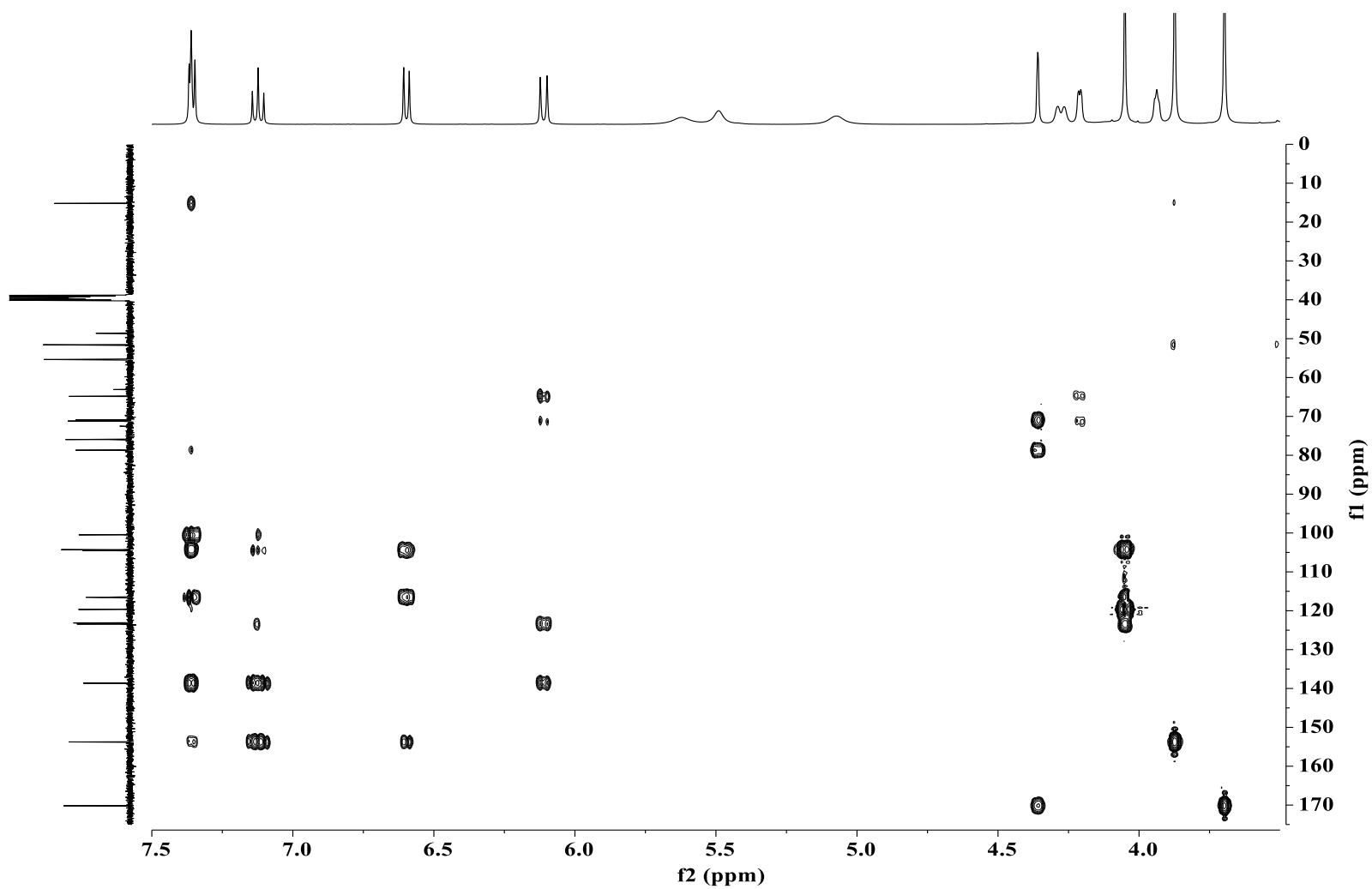


Figure S23: HMBC spectrum of **3** in DMSO- d_6 .

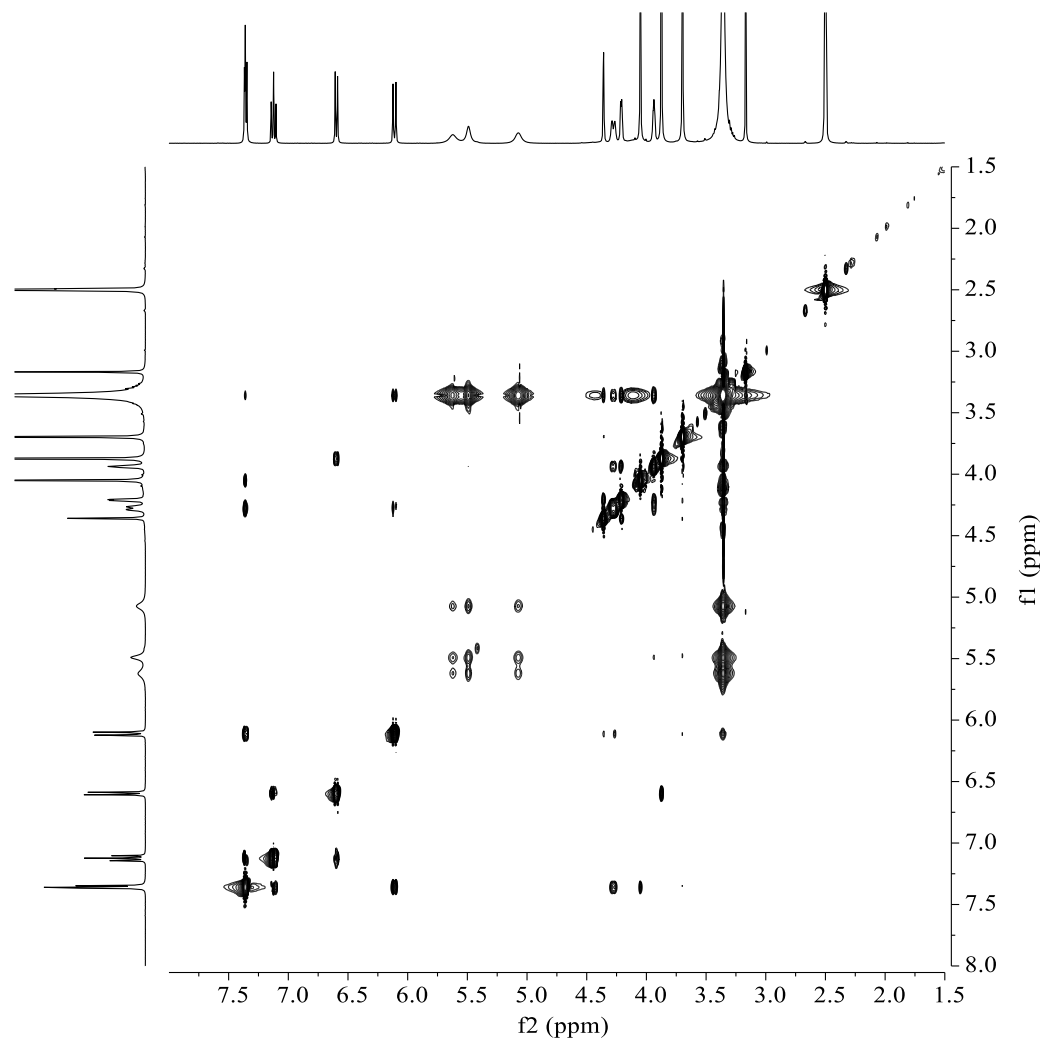


Figure S24: NOESY spectrum of **3** in DMSO- d_6 .