

Supporting Information

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The Limonoid and Other Constituents from The Fruits of *Melia azedarach* and Their Biological Activity

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Table S1: Comparison table of the NMR data of trichilin G and E

Position	trichilin G		trichilin E	
	δ_{H} (ppm, multi., J in Hz)	δ_{C} (ppm)	δ_{H} (ppm, multi., J in Hz)	δ_{C} (ppm)
1	3.56 (br s)	71.8	5.06 (br t, 2.9)	71.1
2	1.53 (m), 2.27 (m)	24.3	2.22 (dt, 16.3, 2.6), 2.34 (dt, 6.3, 3.1)	30.5
3	3.56 (br s)	72.8	3.88 (m)	74.0
4	-	42.3	-	43.8
5	2.55 (d, 12.5)	40.3	2.85 (d, 12.3)	38.6
6	4.27 (dd, 12.5, 3.0)	73.6	4.23 (dd, 12.3, 3.1)	73.9
7	5.85 (d, 3.0)	74.2	4.26 (d, 3.1)	72.7
8	-	51.7	-	45.3
9	3.15 (dd, 13.0, 7.5)	36.2	2.87 (dd, 12.7, 7.5)	34.6
10	-	44.1	-	39.9
11	2.04 (m), 2.36 (m)	30.0	1.12 (br dt, 14.5, 7.2), 2.19 (m)	24.6
12	5.08 (m)	77.8	5.03 (dd, 9.1, 6.7)	77.1
13	-	40.2	-	51.3
14	-	155.7	-	157.2
15	5.70 (br s)	122.7	5.70 (br dd, 3.1, 1.6)	122.7
16	2.32 (m)	36.6	2.51 (ddd, 16.4, 10.9, 1.6), 2.42 (ddd, 16.4, 7.7, 3.4)	36.6
17	2.97 (dd, 10.8, 7.5)	50.4	2.96 (dd, 10.9, 7.8)	50.5
18	1.18 (s)	18.8	1.20 (s)	20.2
19	3.13 (m), 3.45 (d, 7.5)	77.9	4.18 (d br, 7.4), 3.67 (d, 7.4)	78.2
20	1.00 (s)	15.8	1.08 (s)	15.3
21	1.25 (s)	27.1	0.70 (s)	26.9
22	1.00 (s)	15.4	1.15 (s)	15.4
23	-	124.6	-	124.5
24	7.13 (br s)	140.2	7.12 (br s)	140.2
25	7.28 (br s)	141.9	7.25 (br t, 1.8)	142.0
26	6.16 (br s)	111.8	6.14 (m)	111.7
27	-	169.0	-	-
28	1.91 (s)	20.8	-	-
29	-	171.0	-	170.3
30	1.90 (s)	21.3	-	21.3
1'	-	165.0	-	165.3
2'	-	130.6	-	130.5
3'	8.08 (d, 7.5)	129.5	8.03 (dd, 8.4, 1.1)	129.6
4'	7.43 (t, 7.5)	128.3	7.43 (dd, 8.4, 7.4)	128.8
5'	7.56 (t, 7.5)	132.9	7.57 (dt, 7.4, 1.1)	133.7
6'	7.43 (t, 7.5)	128.3	7.43 (dd, 8.4, 7.4)	128.8
7'	8.08 (d, 7.5)	129.5	8.03 (dd, 8.4, 1.1)	129.6

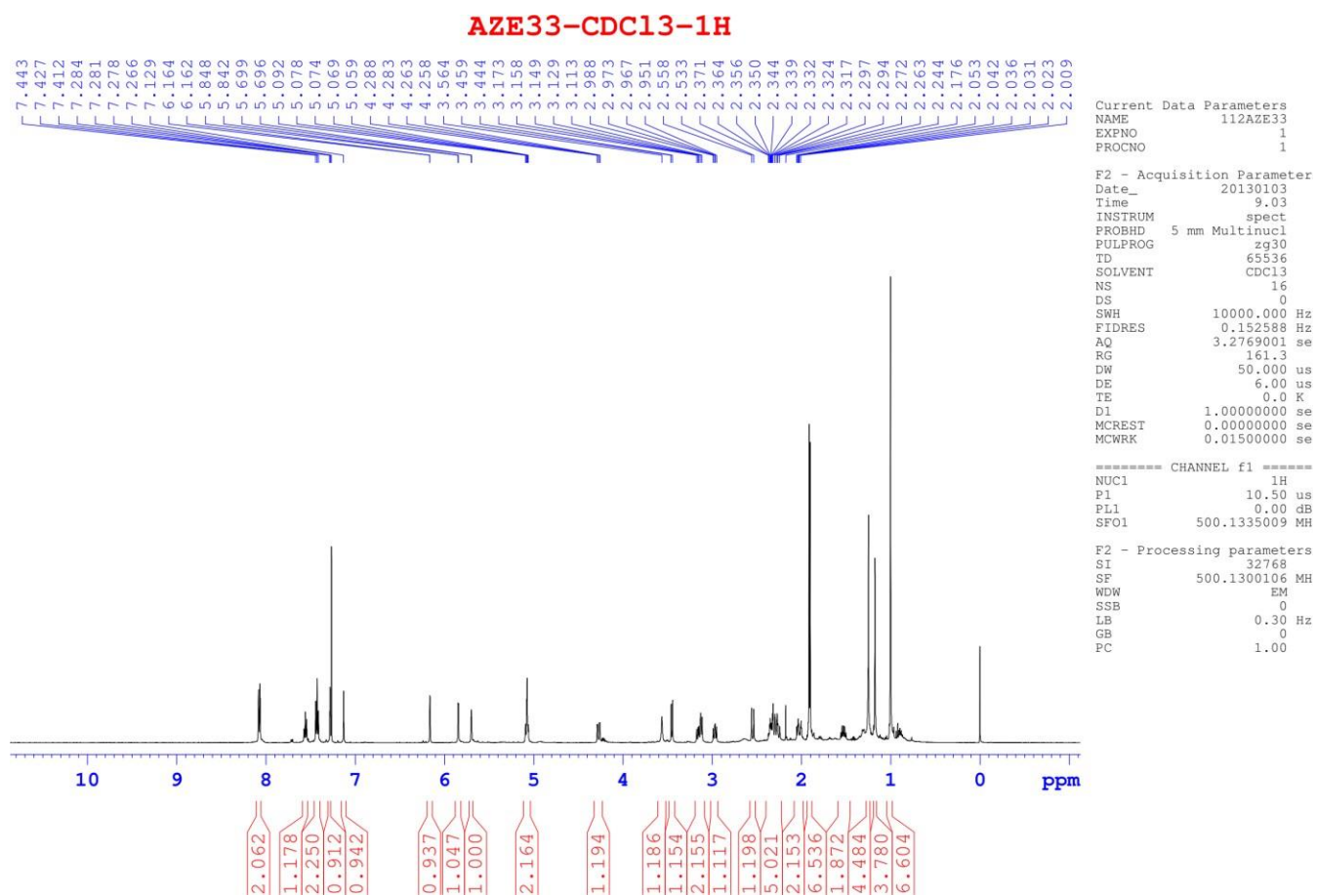


Figure S1: ^1H NMR spectrum of compound **1**.

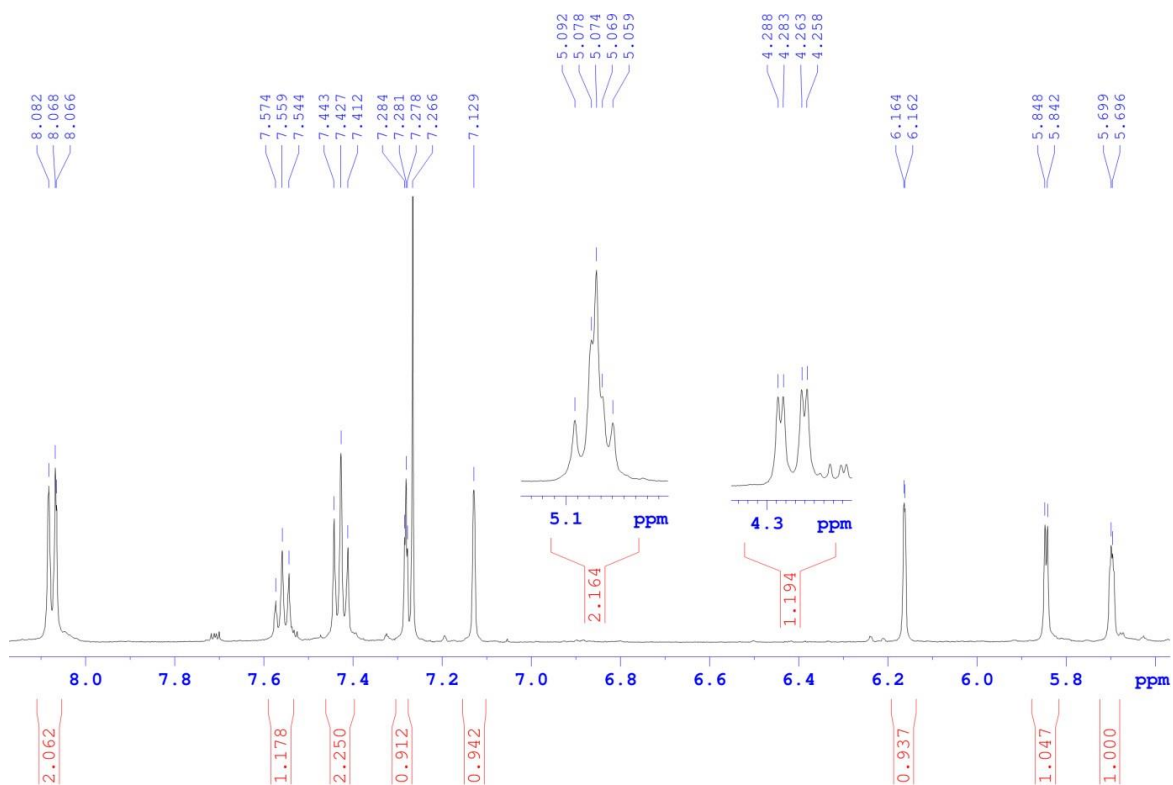


Figure S2: ^1H NMR spectrum of compound **1**.

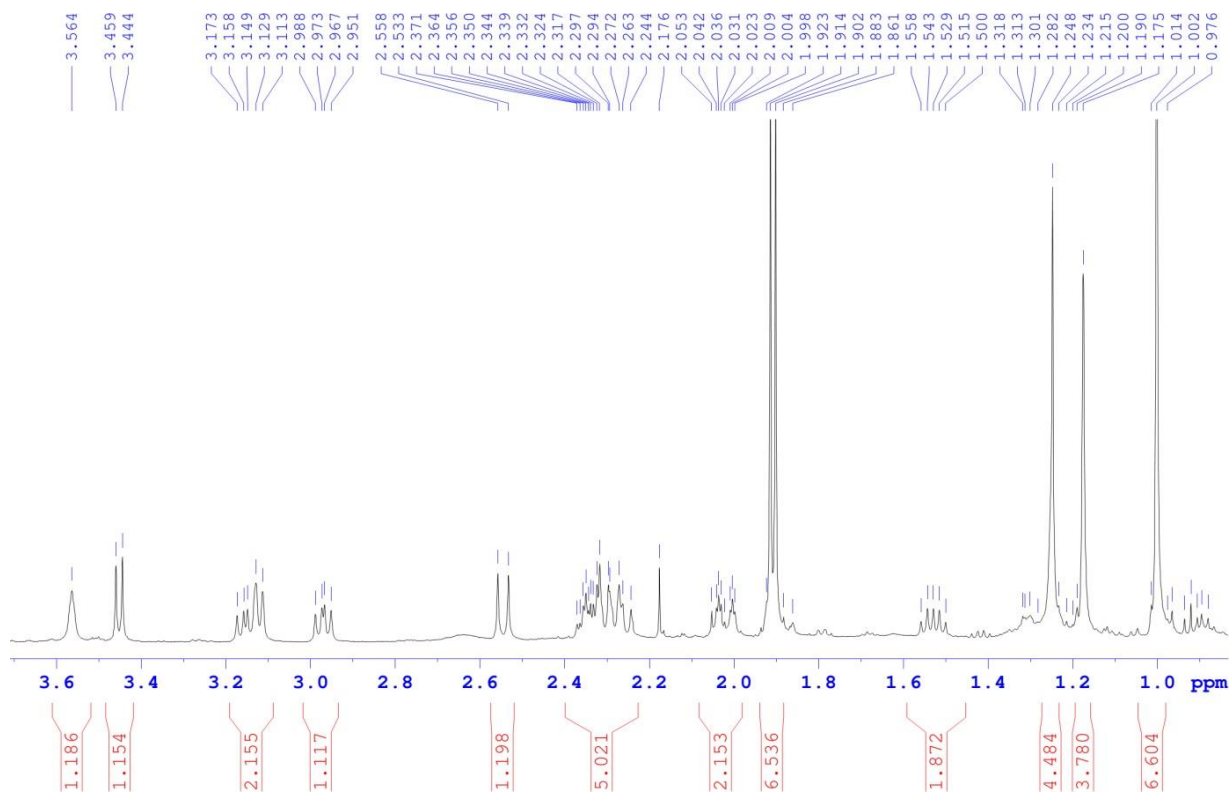


Figure S3: ^1H NMR spectrum of compound **1**.

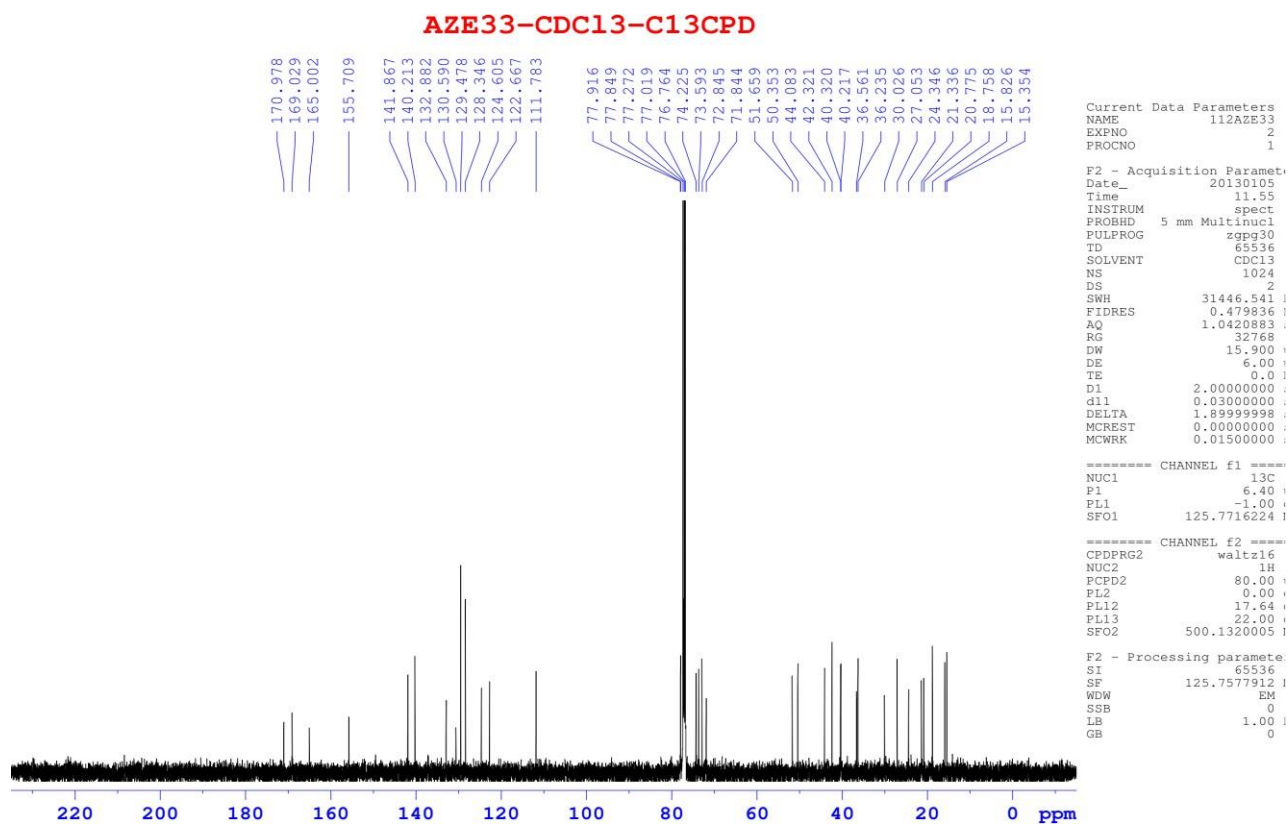


Figure S4: ^{13}C NMR spectrum of compound **1**.

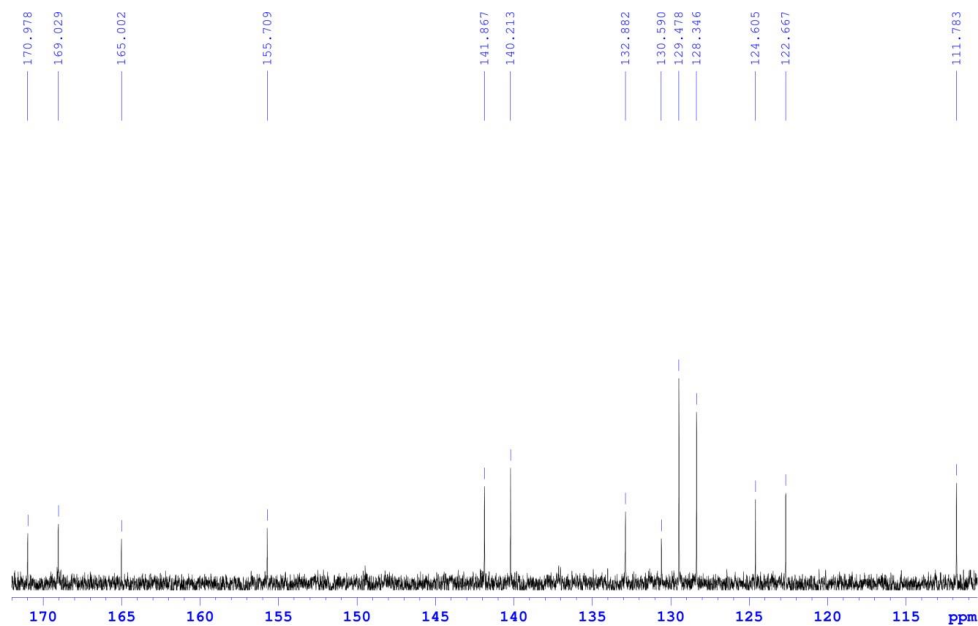


Figure S5: ^{13}C NMR spectrum of compound **1**.

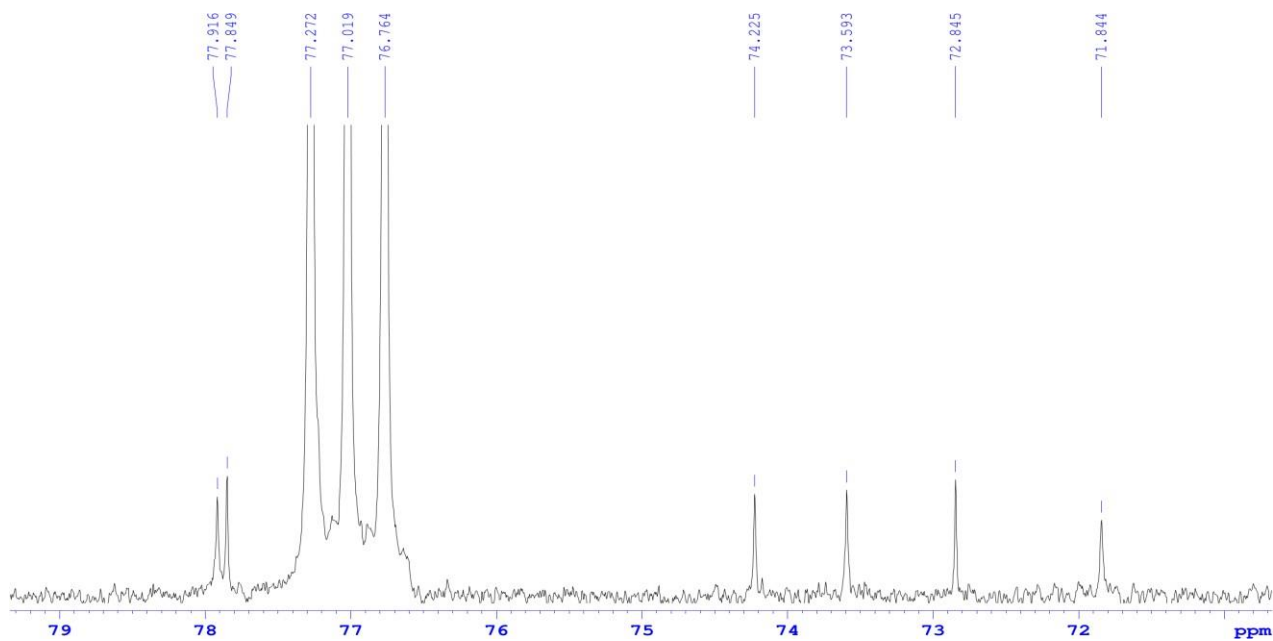


Figure S6: ^{13}C NMR spectrum of compound 1.

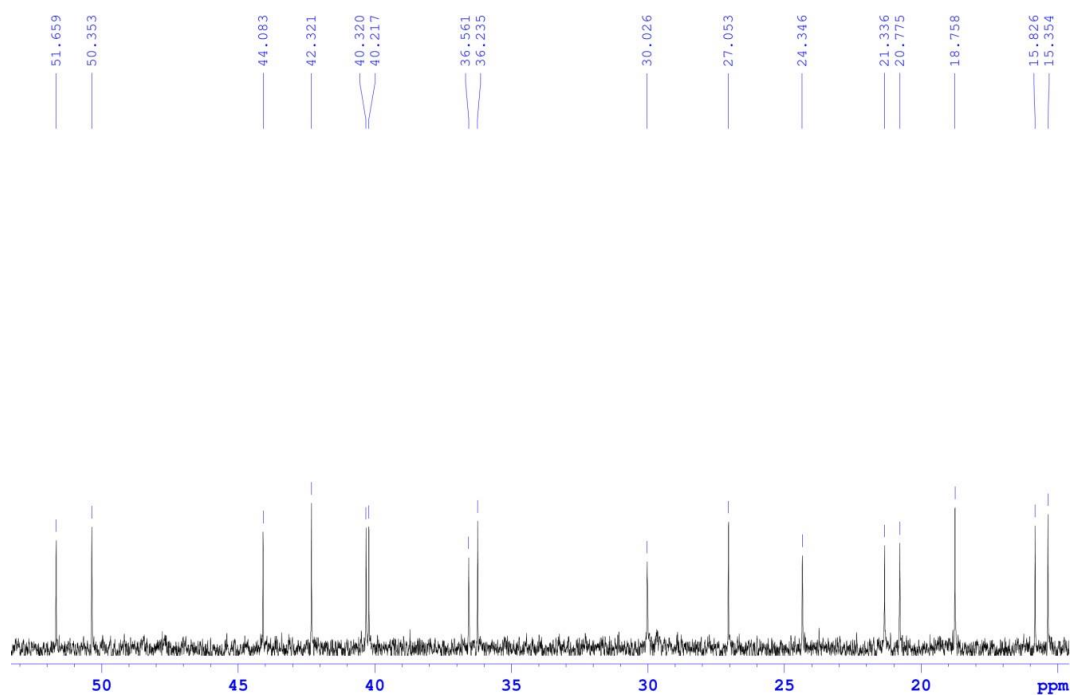
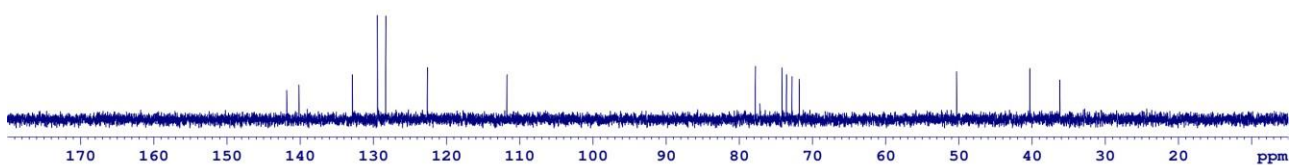


Figure S7: ^{13}C NMR spectrum of compound 1.

AZE33-CDC13-C13CPD&DEPT

DEPT90



DEPT135

CH&CH3

CH2



C13CPD

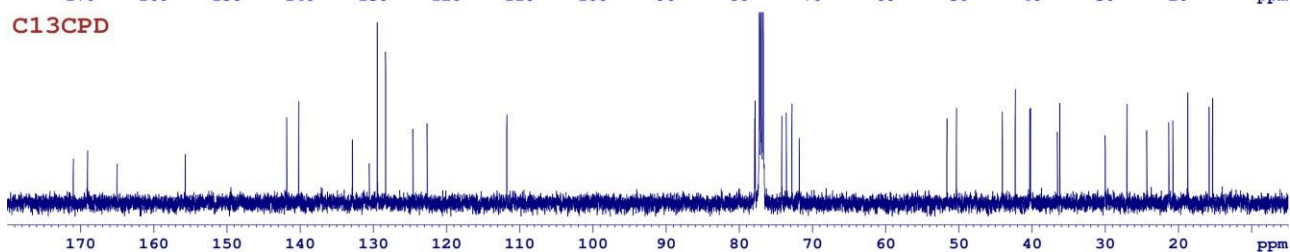
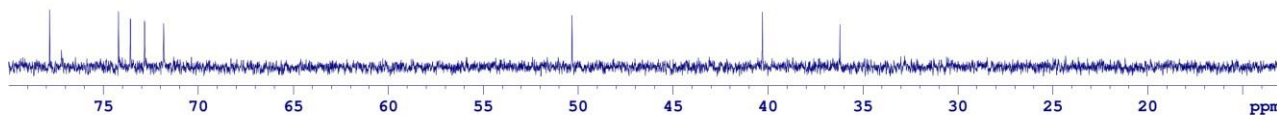


Figure S8: DEPT spectrum of compound 1.

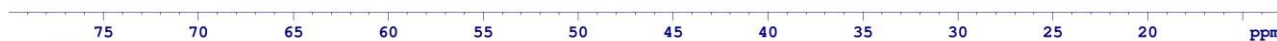
DEPT90



DEPT135

CH&CH3

CH2



C13CPD

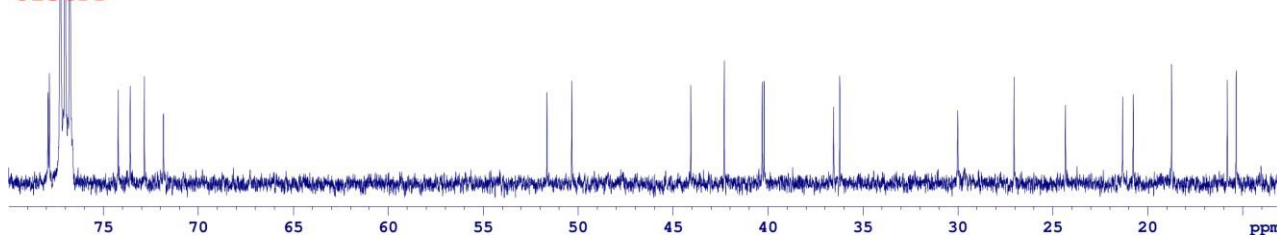


Figure S9: DEPT spectrum of compound 1.

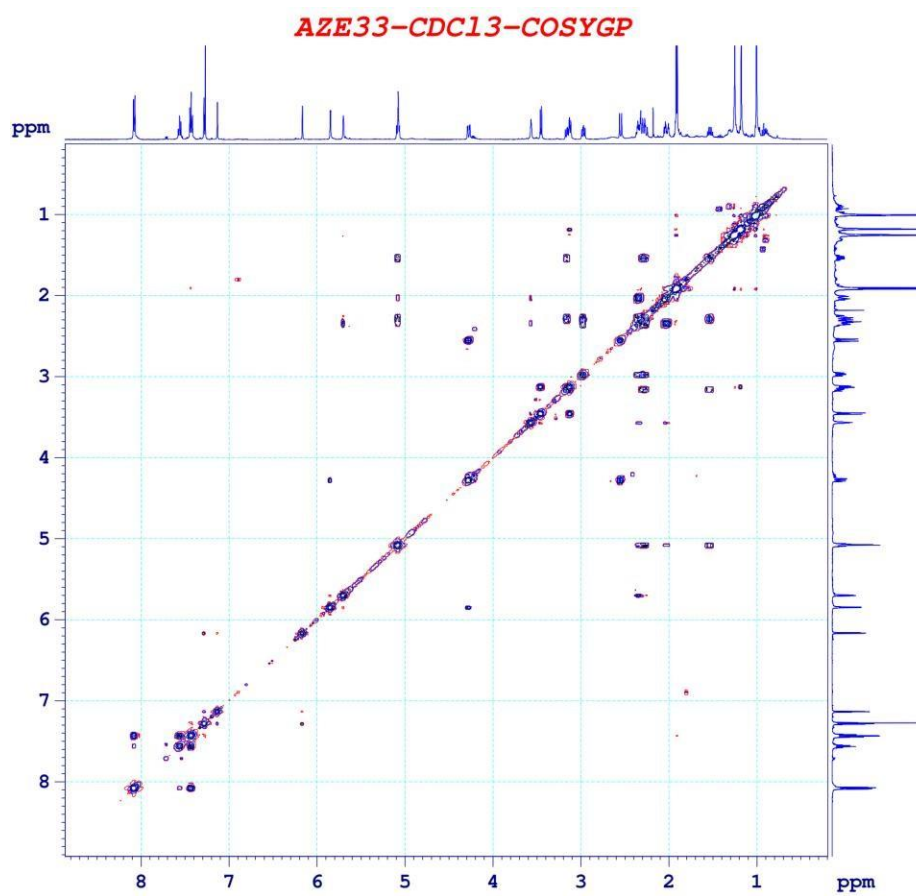
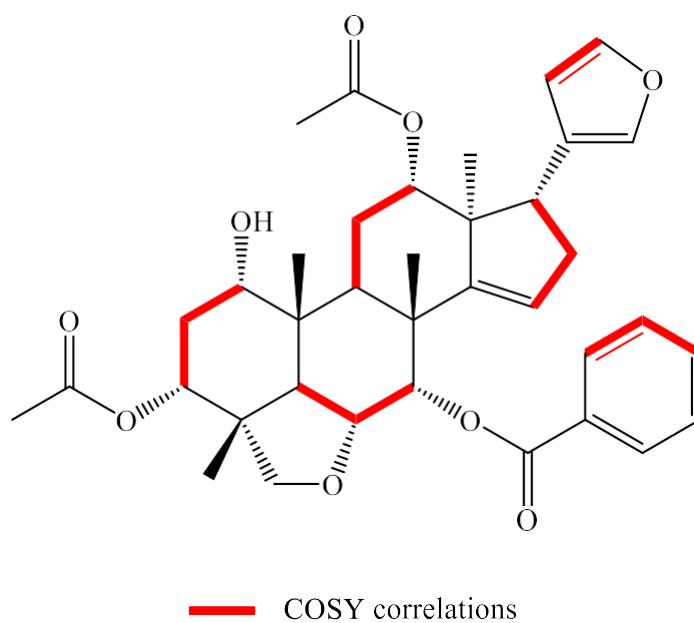


Figure S10: COSY spectrum of compound 1.



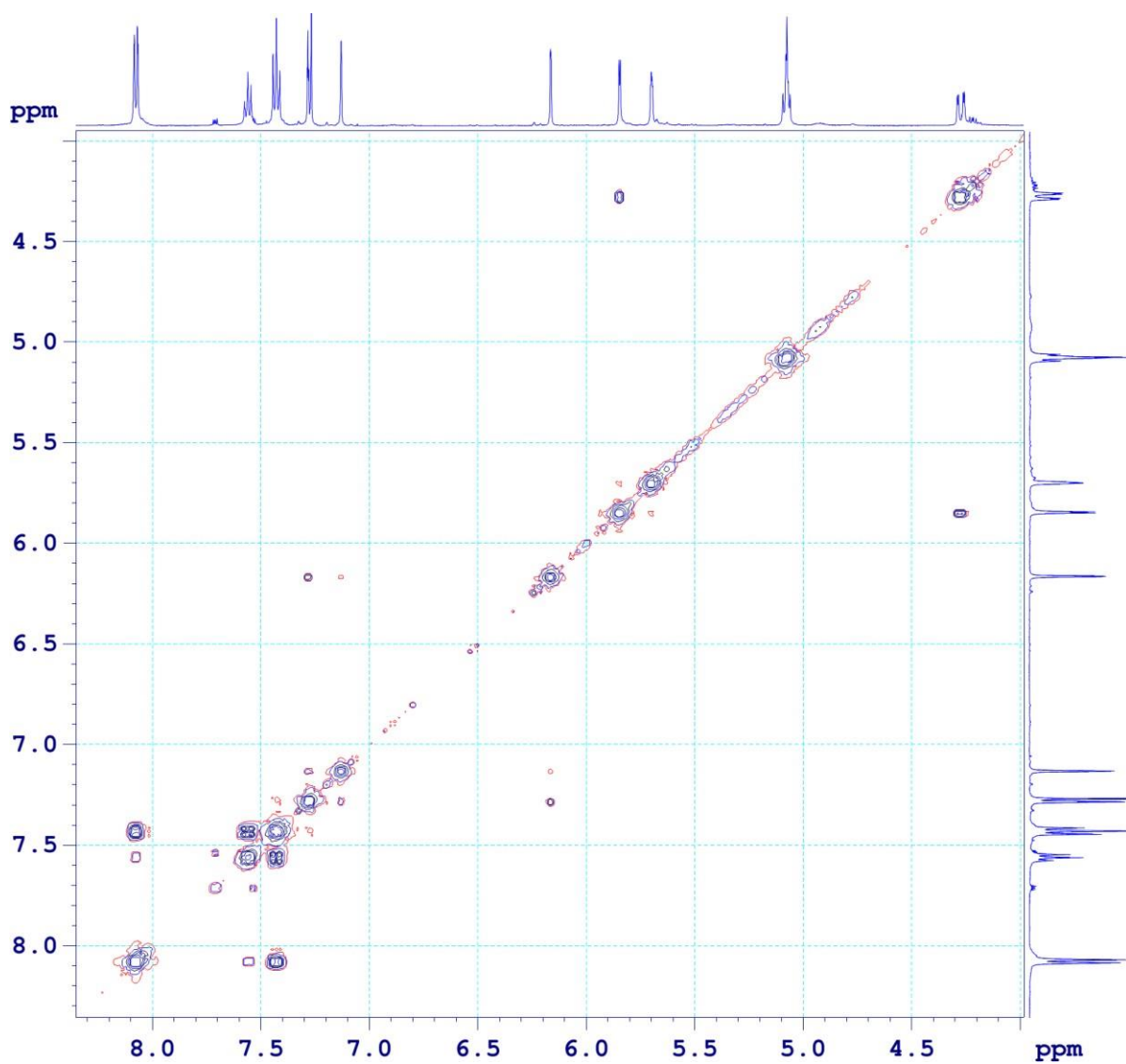


Figure S11: COSY spectrum of compound **1**.

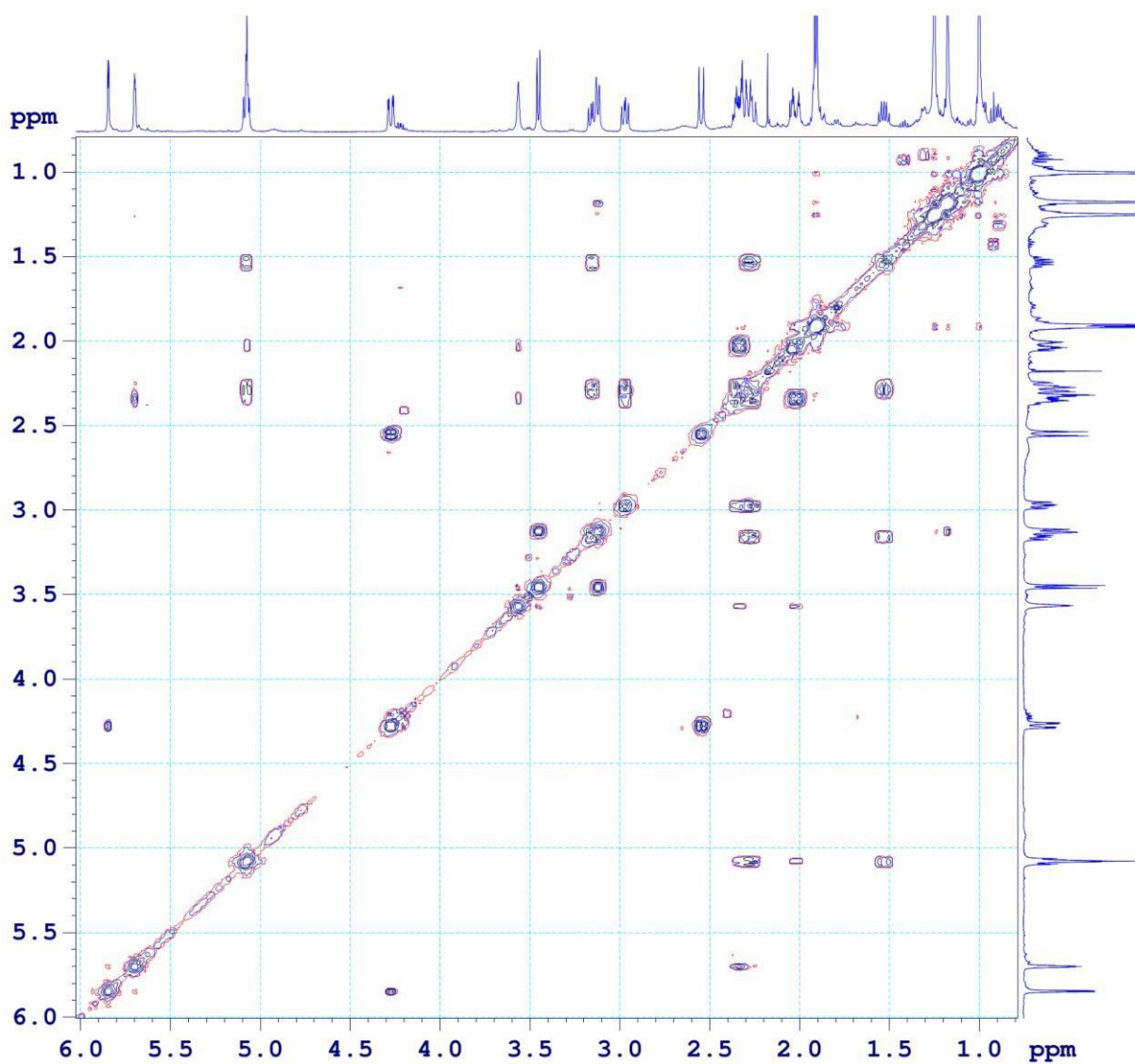


Figure S12: COSY spectrum of compound **1**.

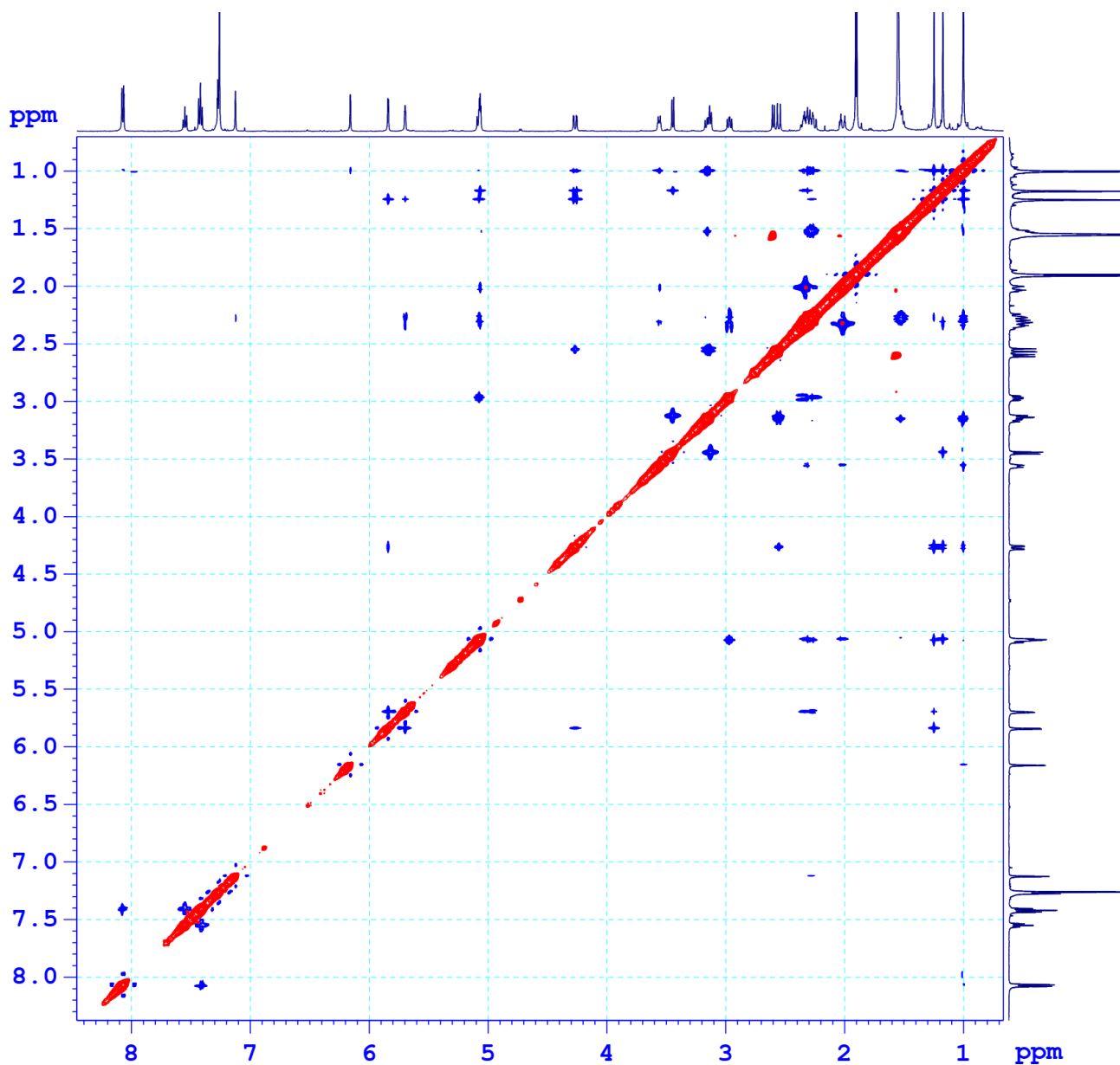
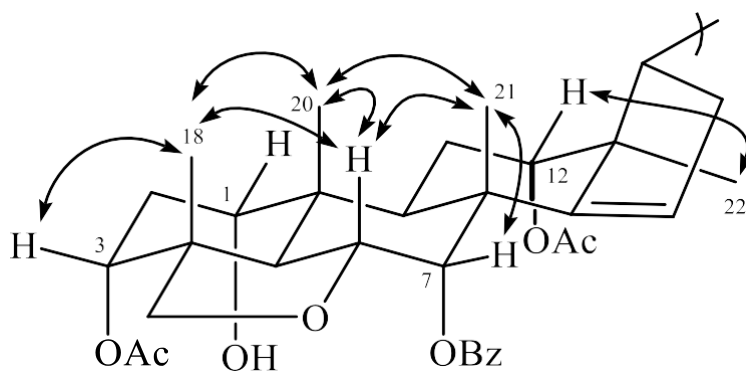


Figure S13: NOESY spectrum of compound **1**.



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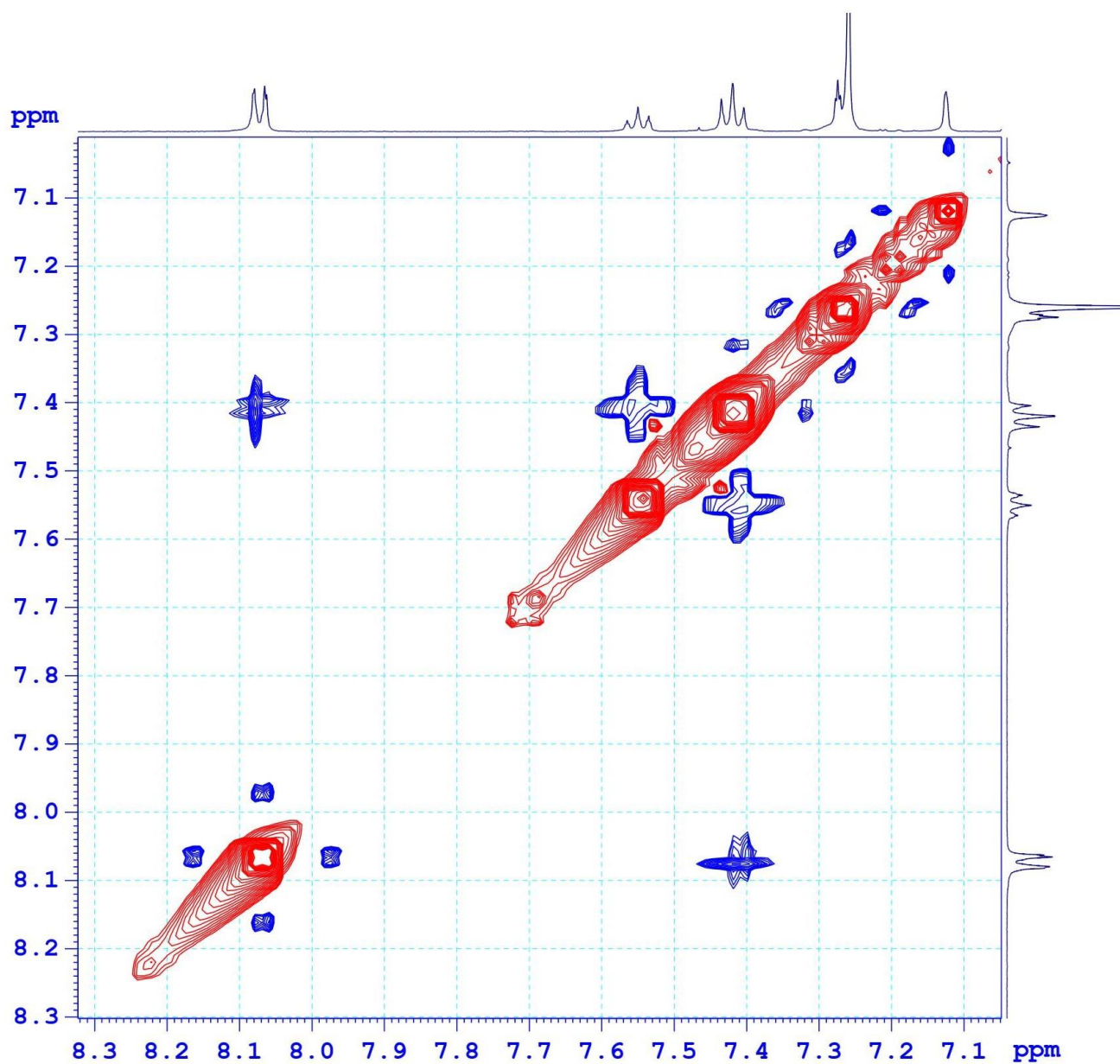


Figure S14: NOESY spectrum of compound **1**.

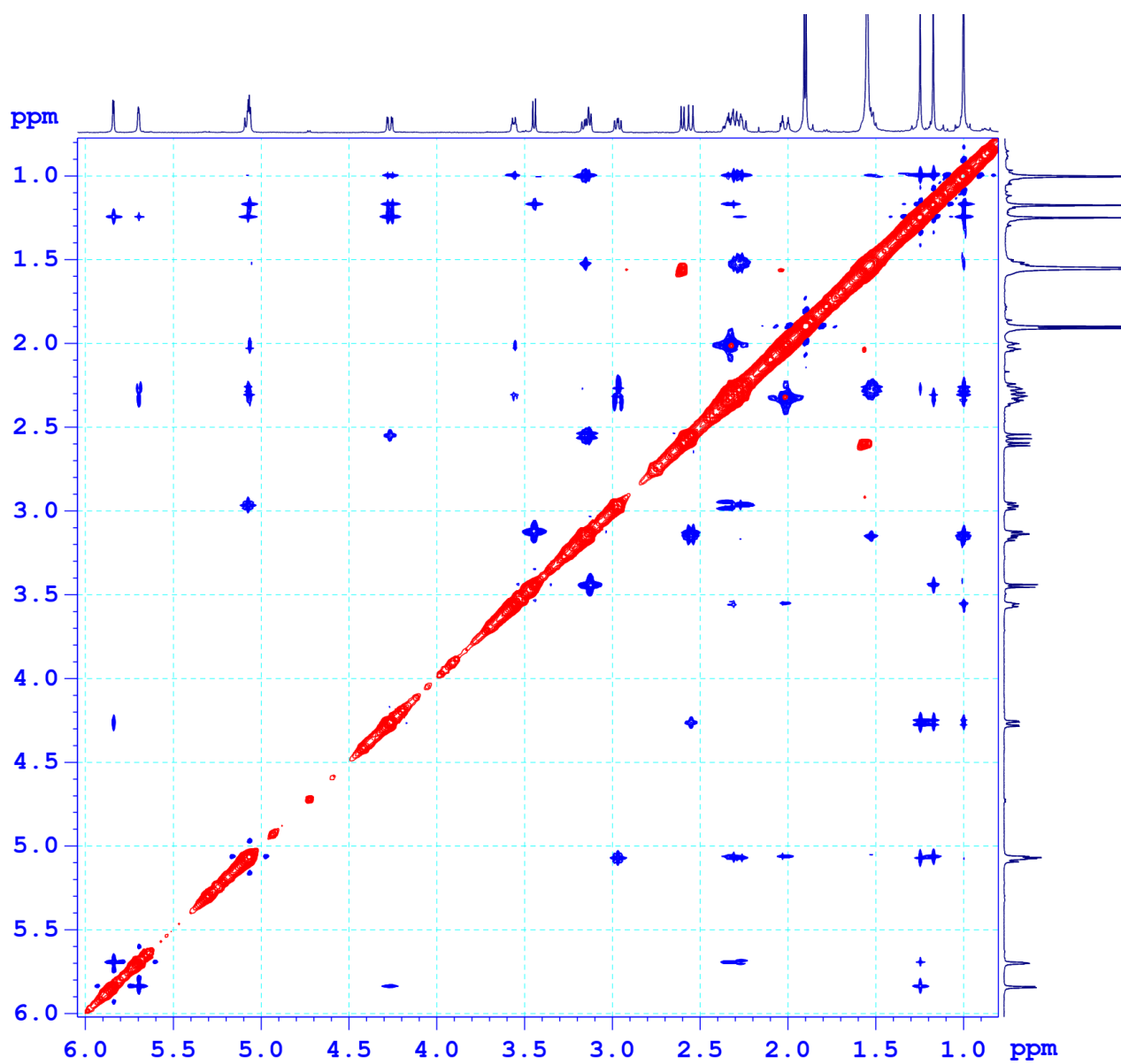


Figure S15: NOESY spectrum of compound **1**.

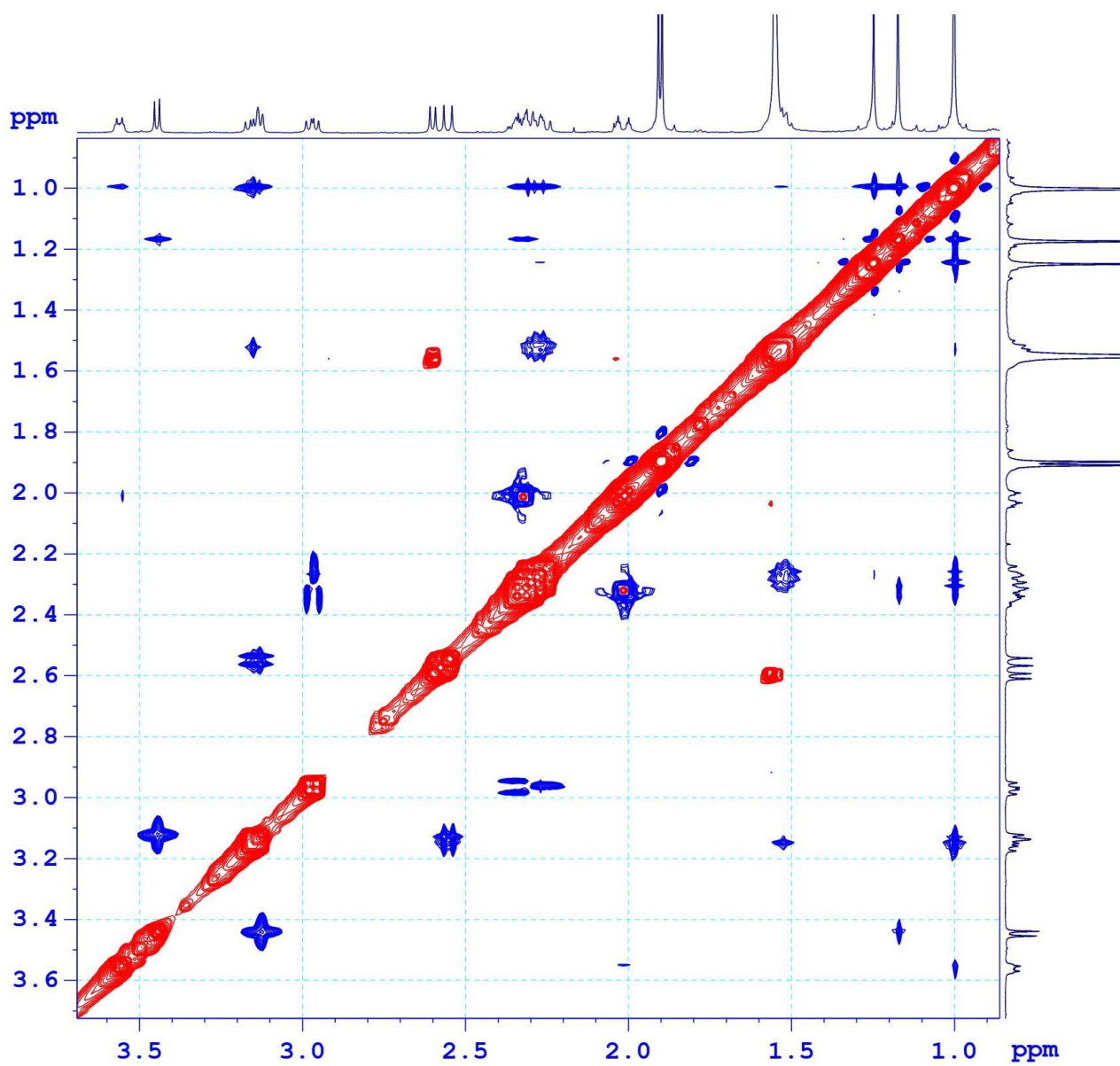


Figure S16: NOESY spectrum of compound **1**.

AZE33-CDC13-HSQC

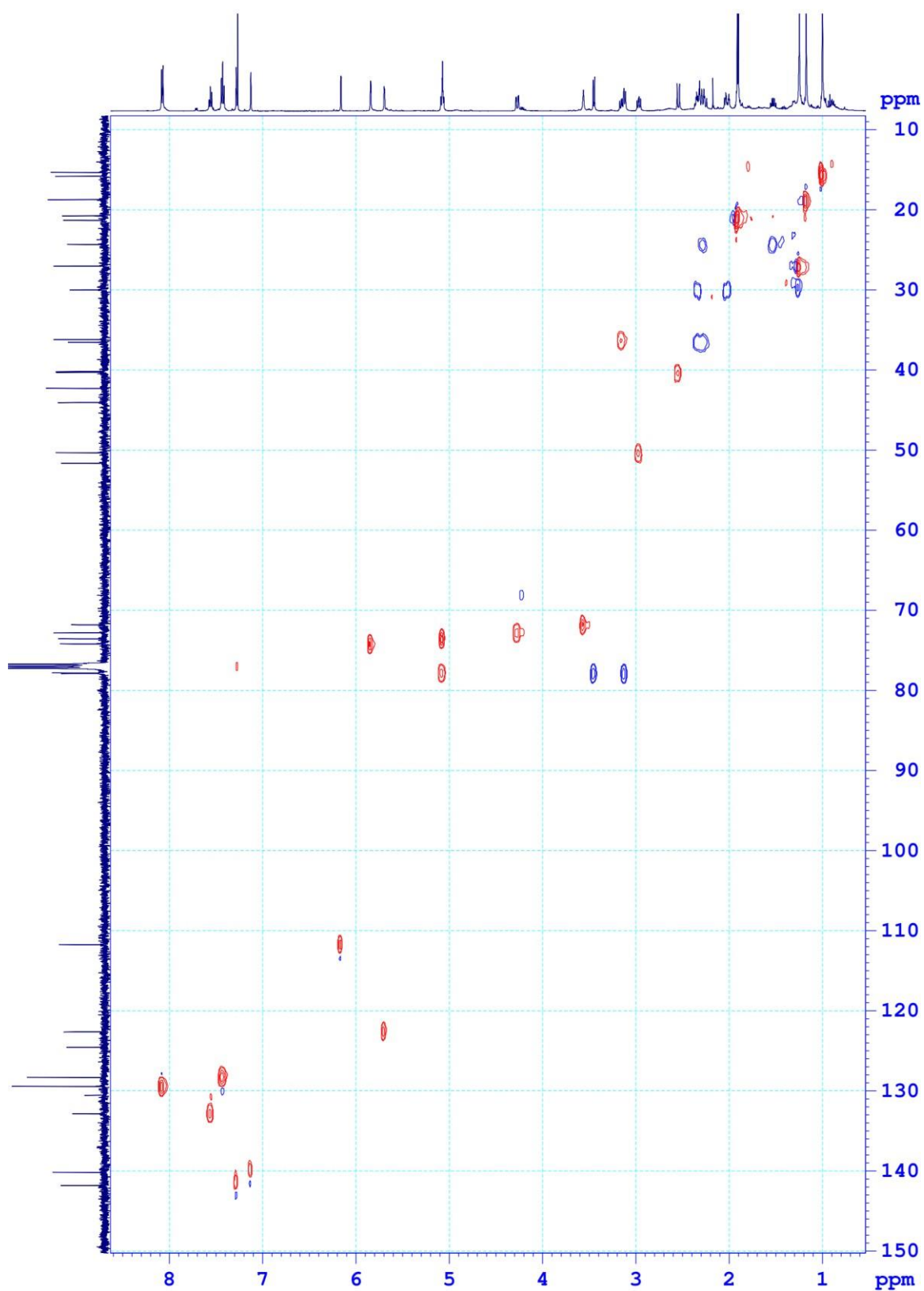


Figure S17: HSQC spectrum of compound 1.

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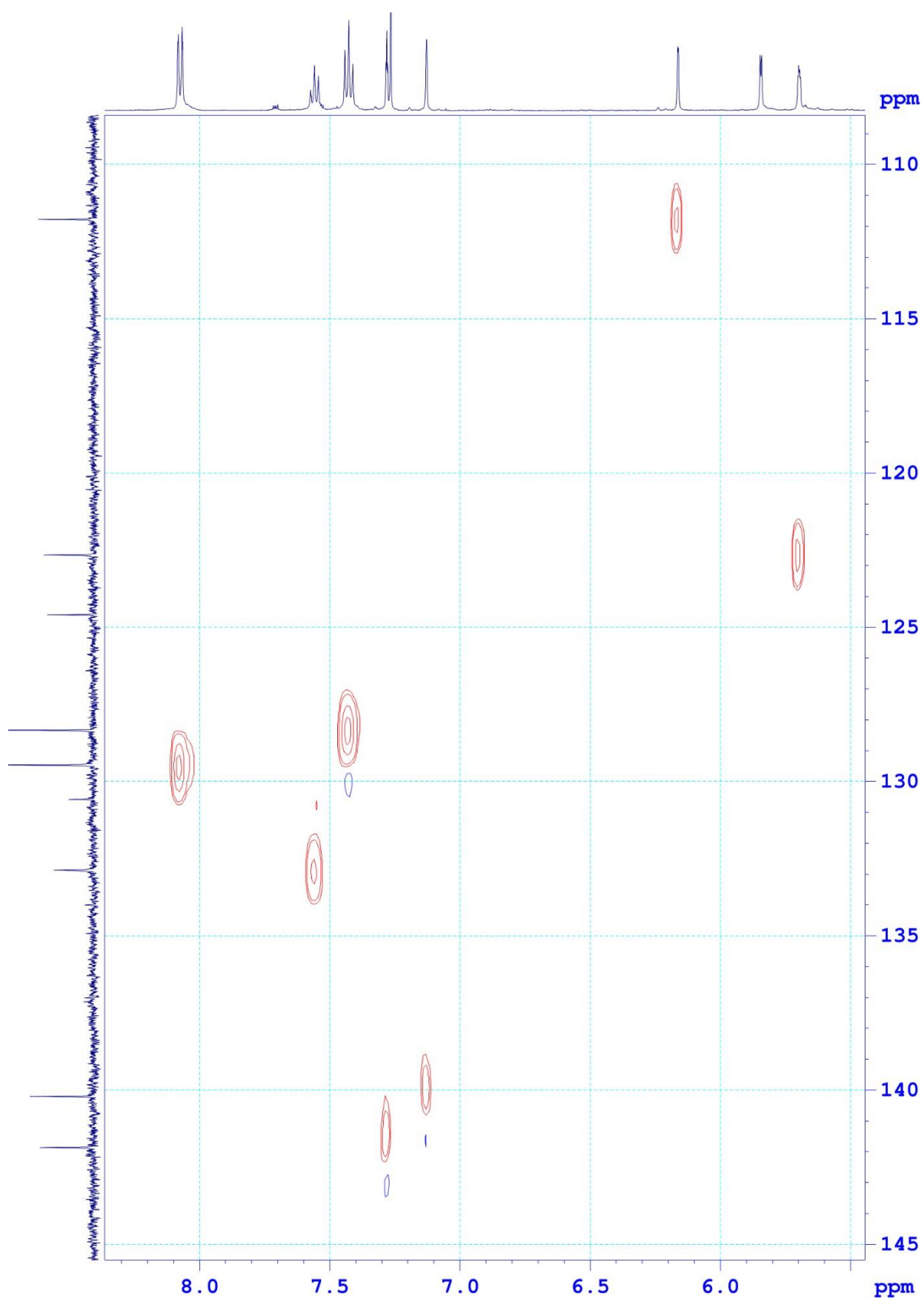


Figure S18: HSQC spectrum of compound **1**.

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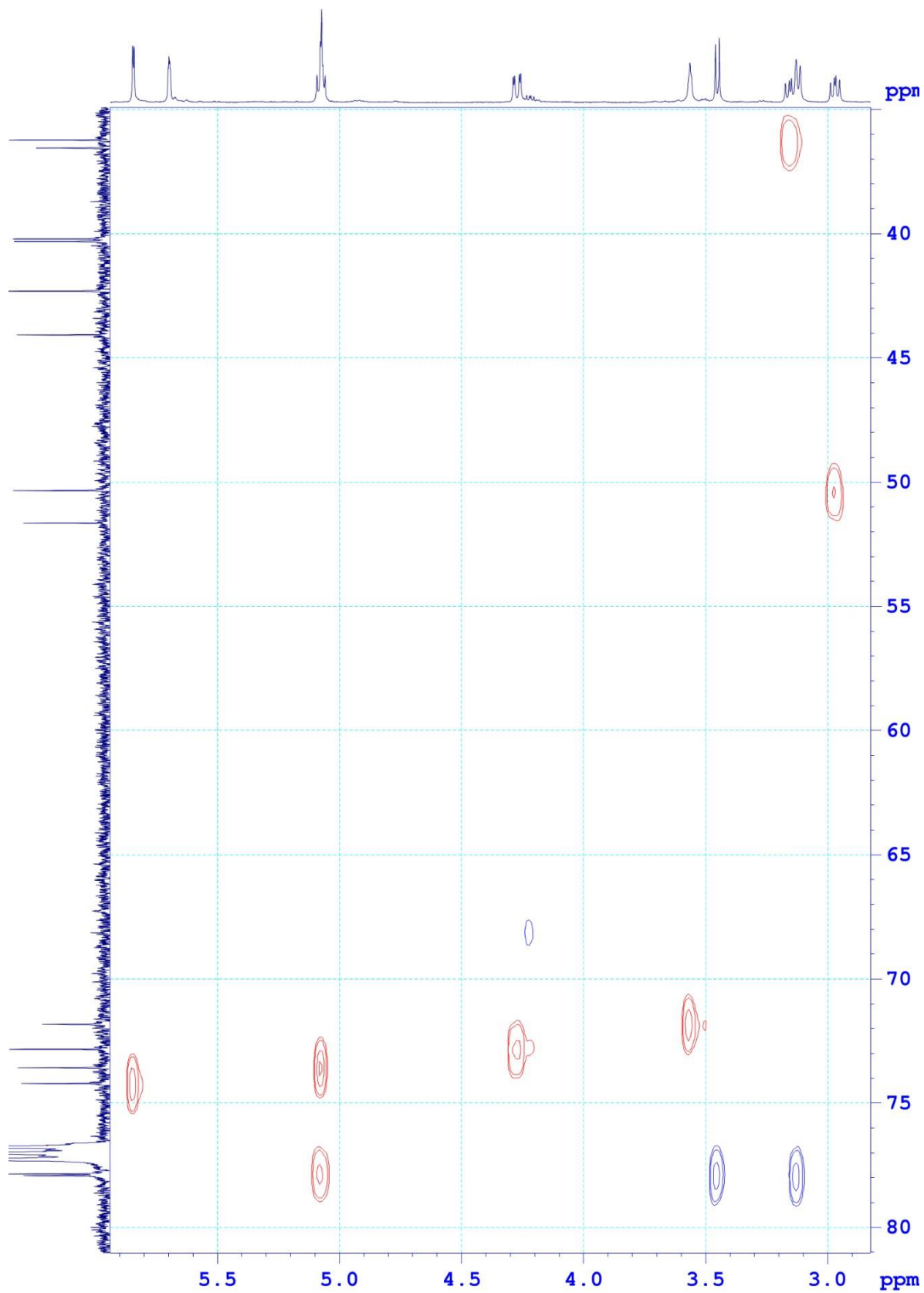


Figure S19: HSQC spectrum of compound **1**.

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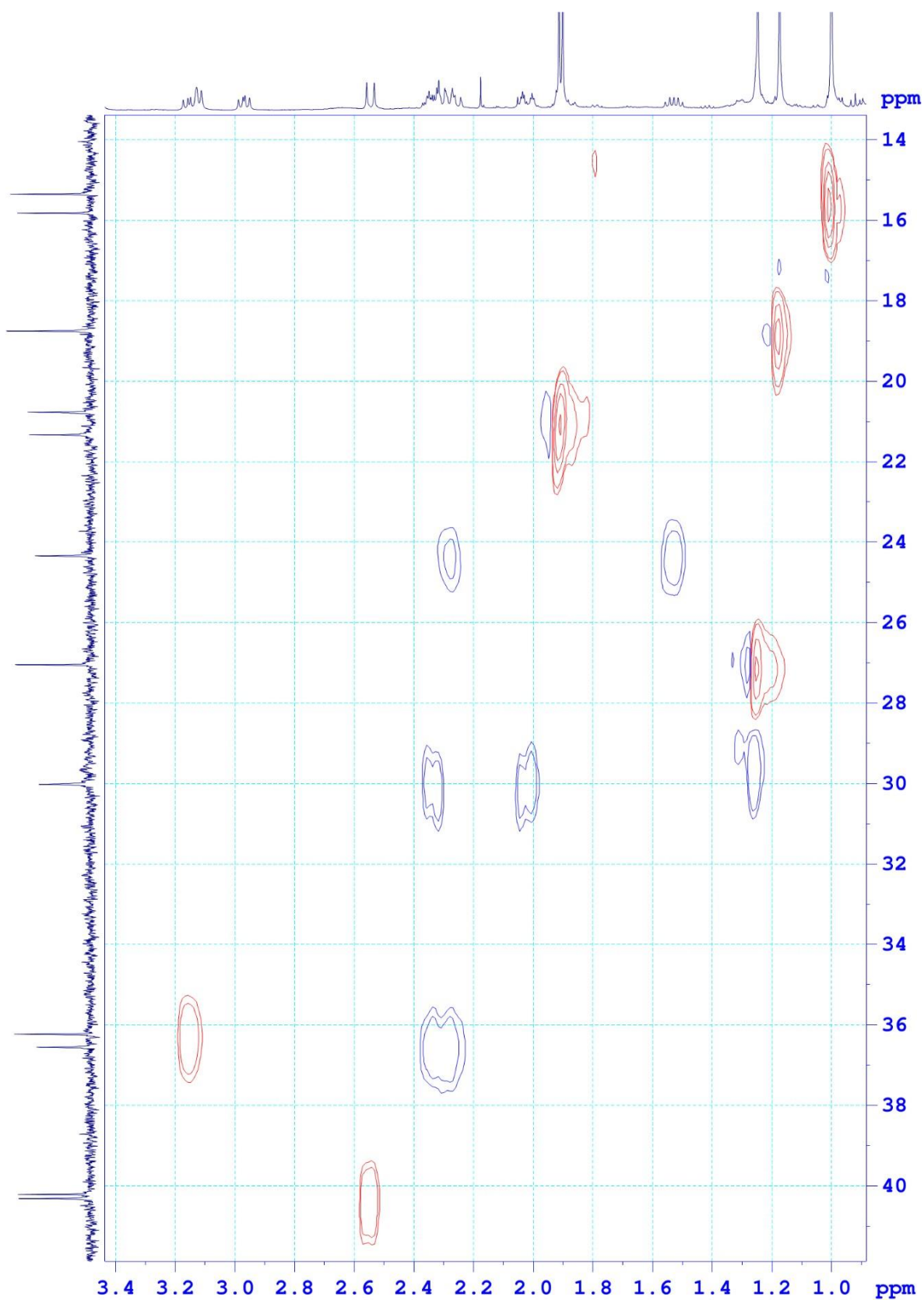


Figure S20: HSQC spectrum of compound **1**.

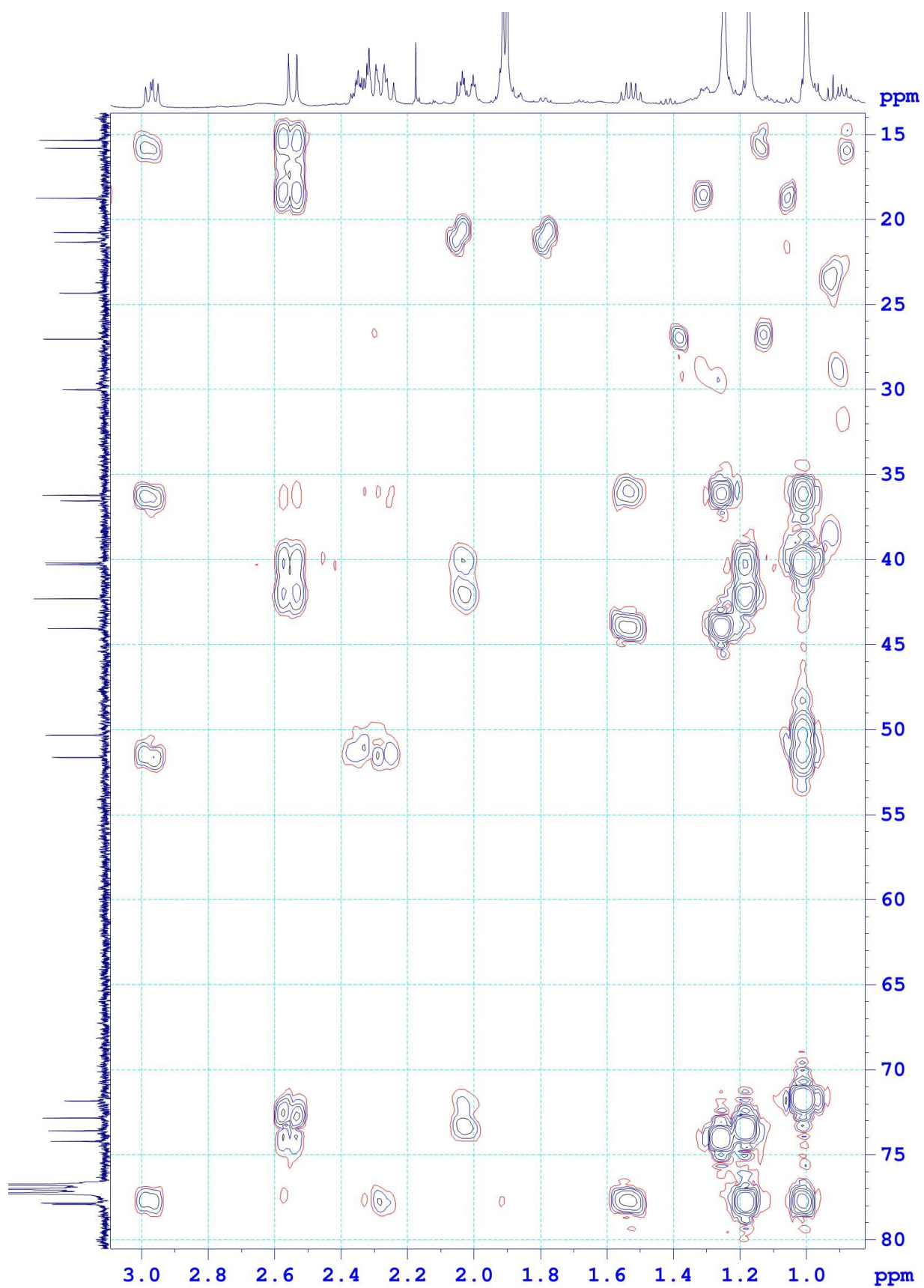


Figure S21: HSQC spectrum of compound **1**.

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AZE33-CDC13-HMBC

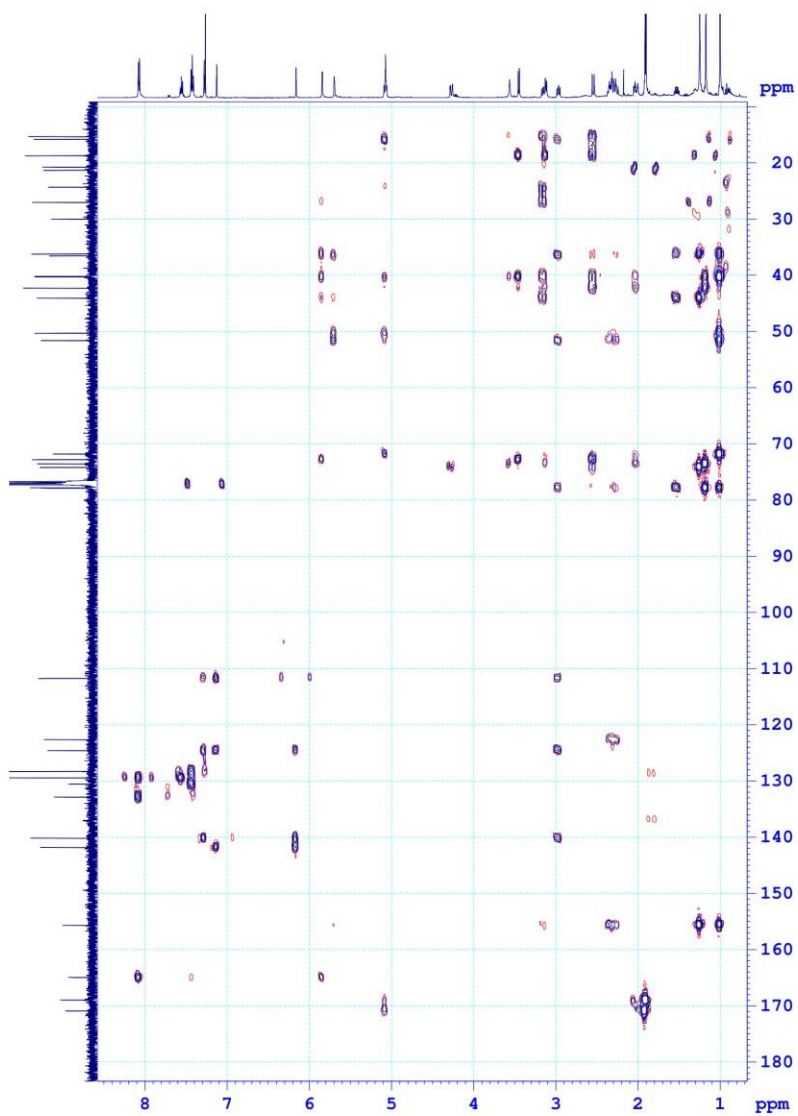
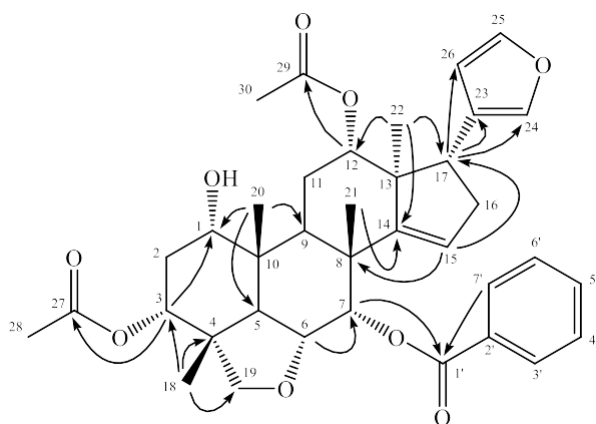


Figure S22: HMBC spectrum of compound 1.



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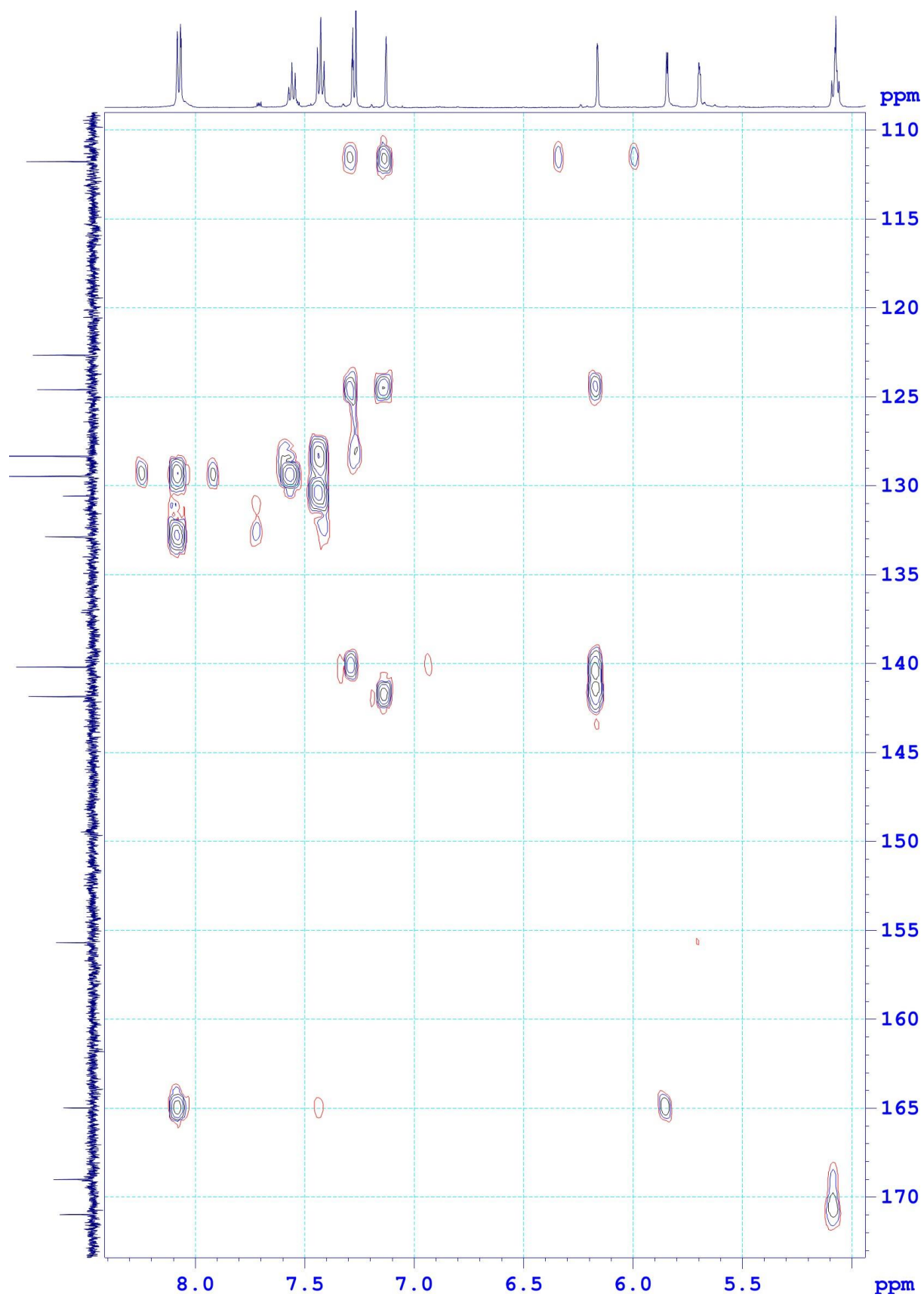


Figure S23: HMBC spectrum of compound **1**.

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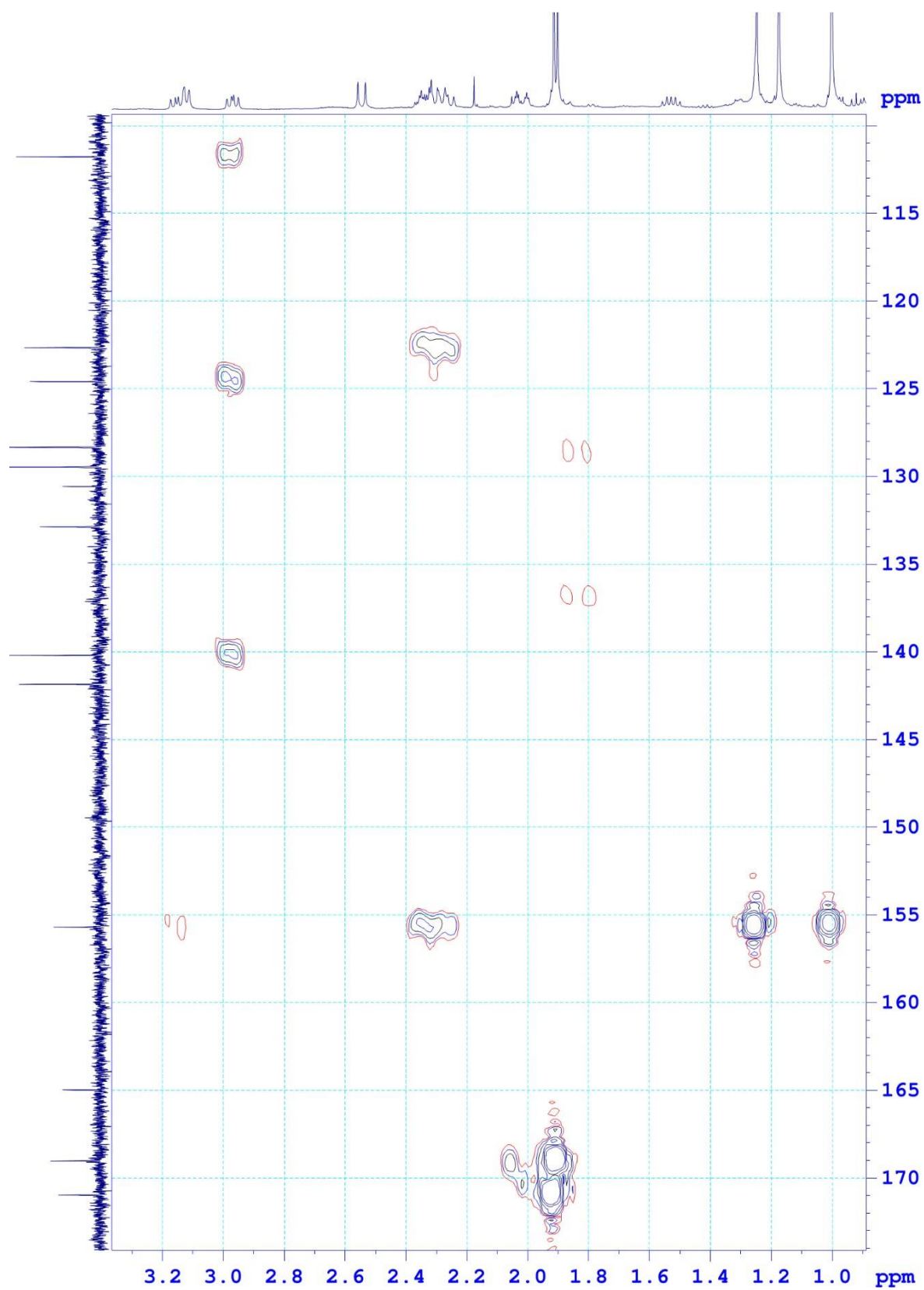


Figure S24: HMBC spectrum of compound **1**.

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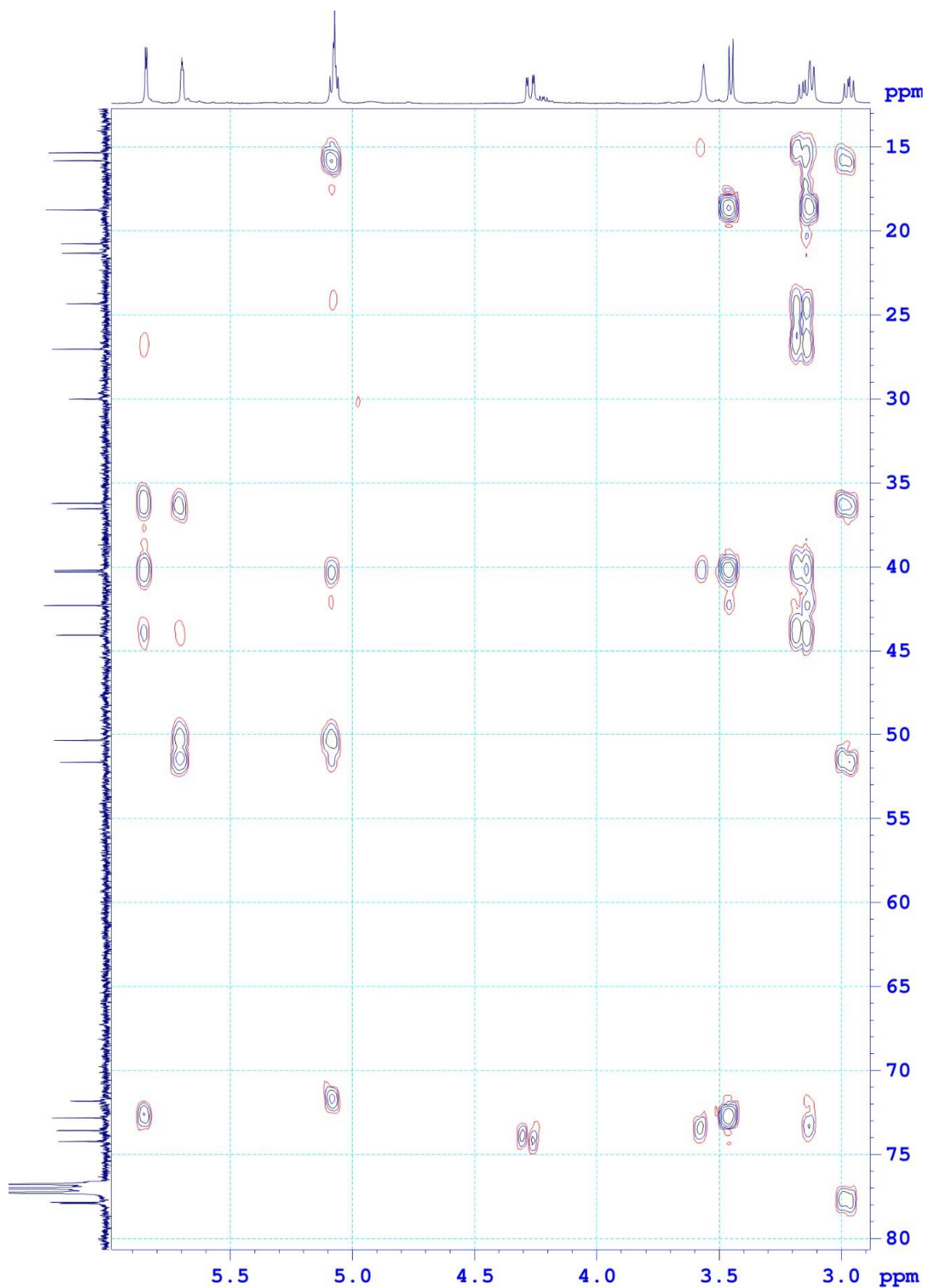


Figure S25: HMBC spectrum of compound 1.

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FT-MS

Analysis Info

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Method broadband first signal
Sample Name kuo-AZE-3X1-2-1-2
Comment ESI Positive

10/13/2017 2:40:04 PM

Instrument: FT-MS solariX

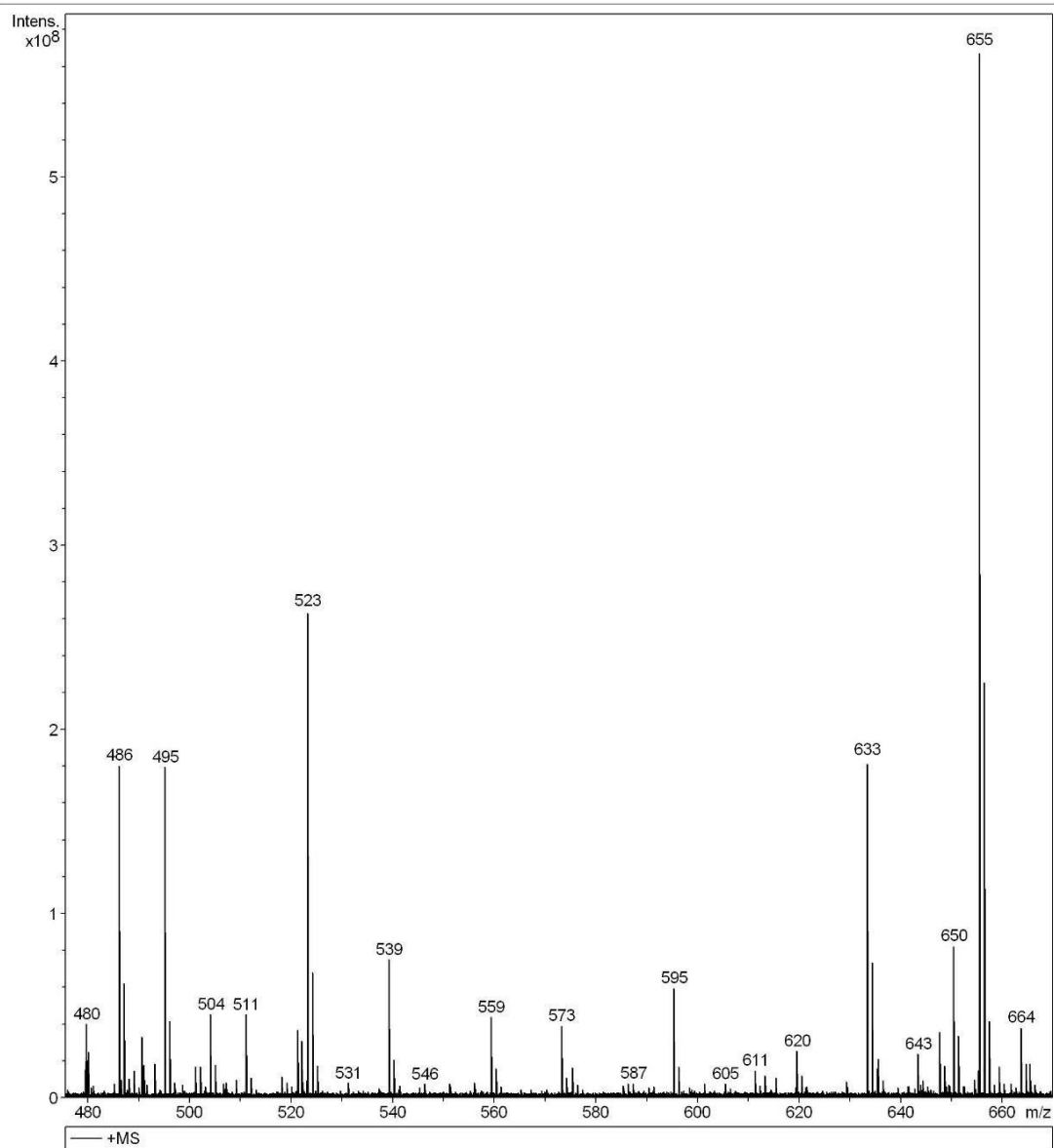


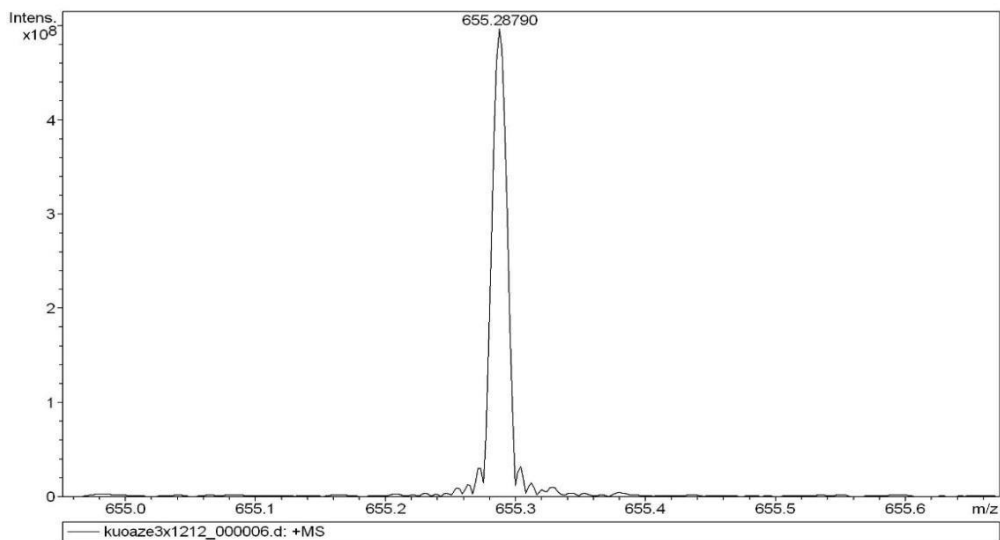
Figure S26: MS spectrum of compound 1.

Mass Spectrum SmartFormula Report

Analysis Info

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Method broadband first signal
Sample Name kuo-AZE-3X1-2-1-2
Comment ESI Positive

10/13/2017 2:38:19 PM
Operator: YU HSIAO-CHING
Instrument: BRUKER FT-MS solariX



Meas. m/z	#	Formula	Score	m/z	err [mDa]	err [ppm]	mSigma	rdb	e ⁻ Conf	N-Rule
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Figure S27: HRMS spectrum of compound **1**.

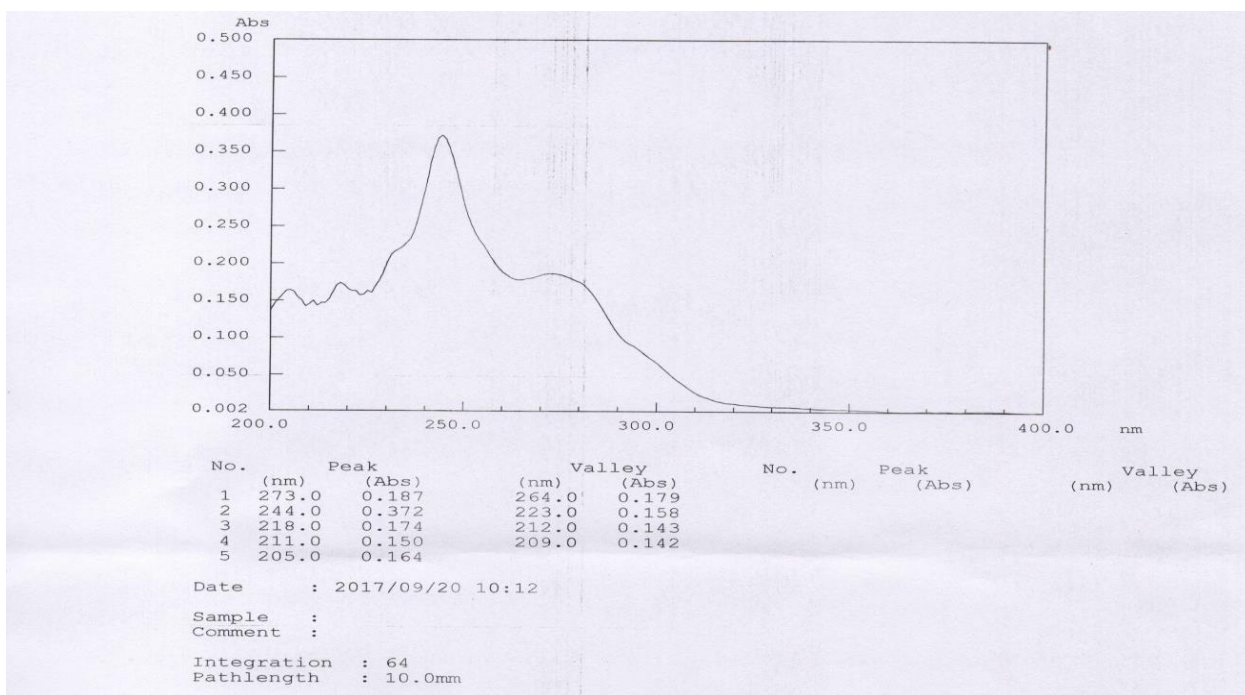


Figure S28: UV spectrum of compound 1.

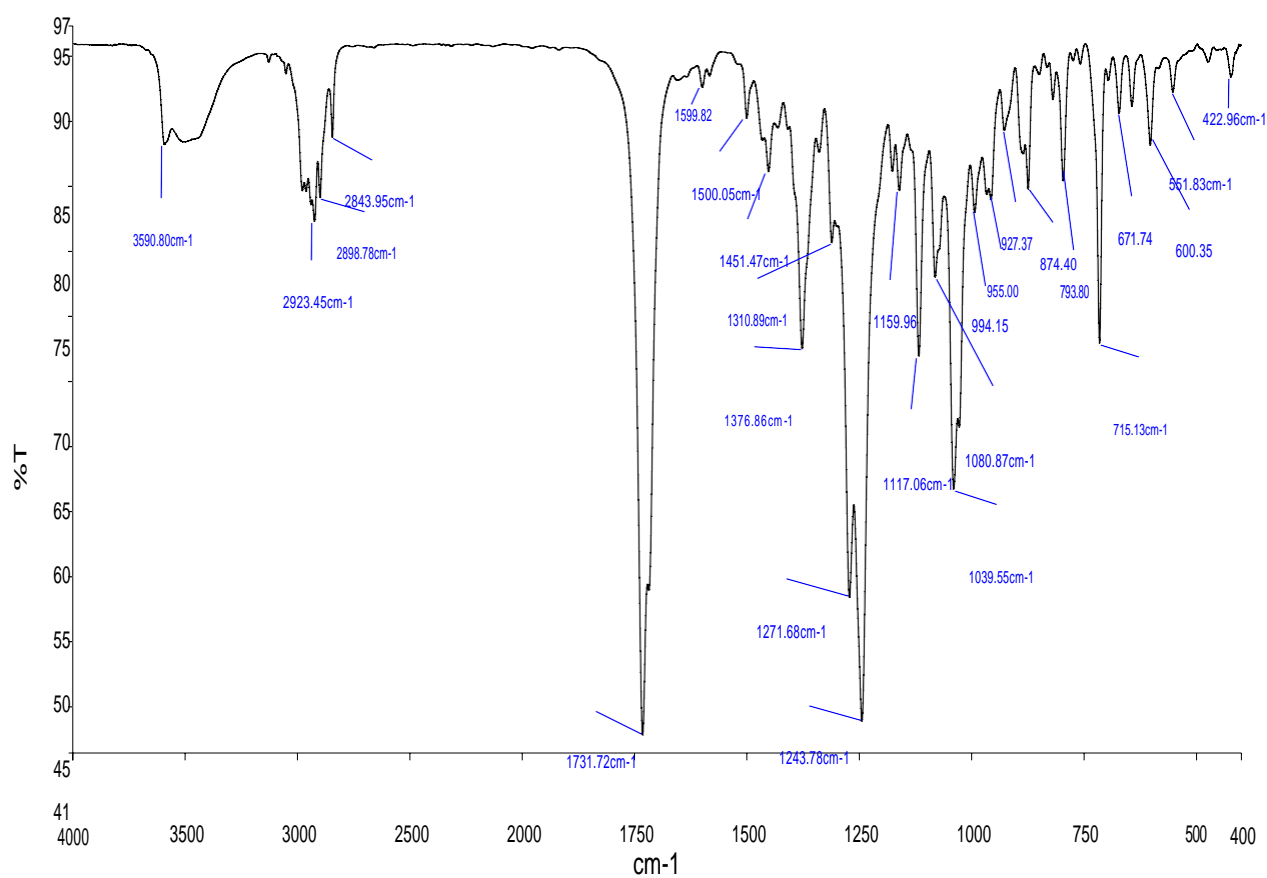


Figure S29: IR spectrum of compound 1.

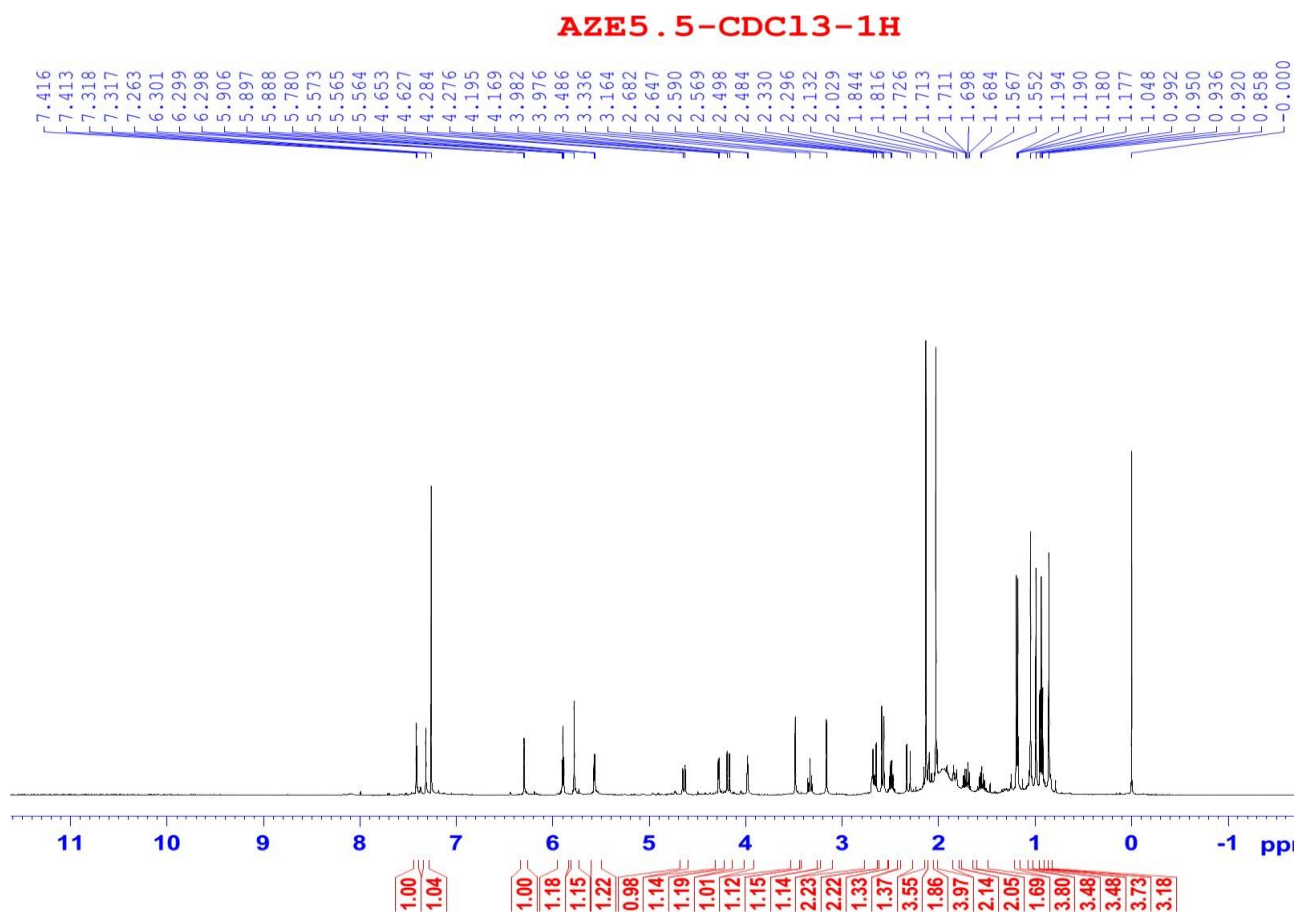


Figure S30: ^1H -NMR spectrum of compound **2**.

AZE5.5-CDC13-C13CPD

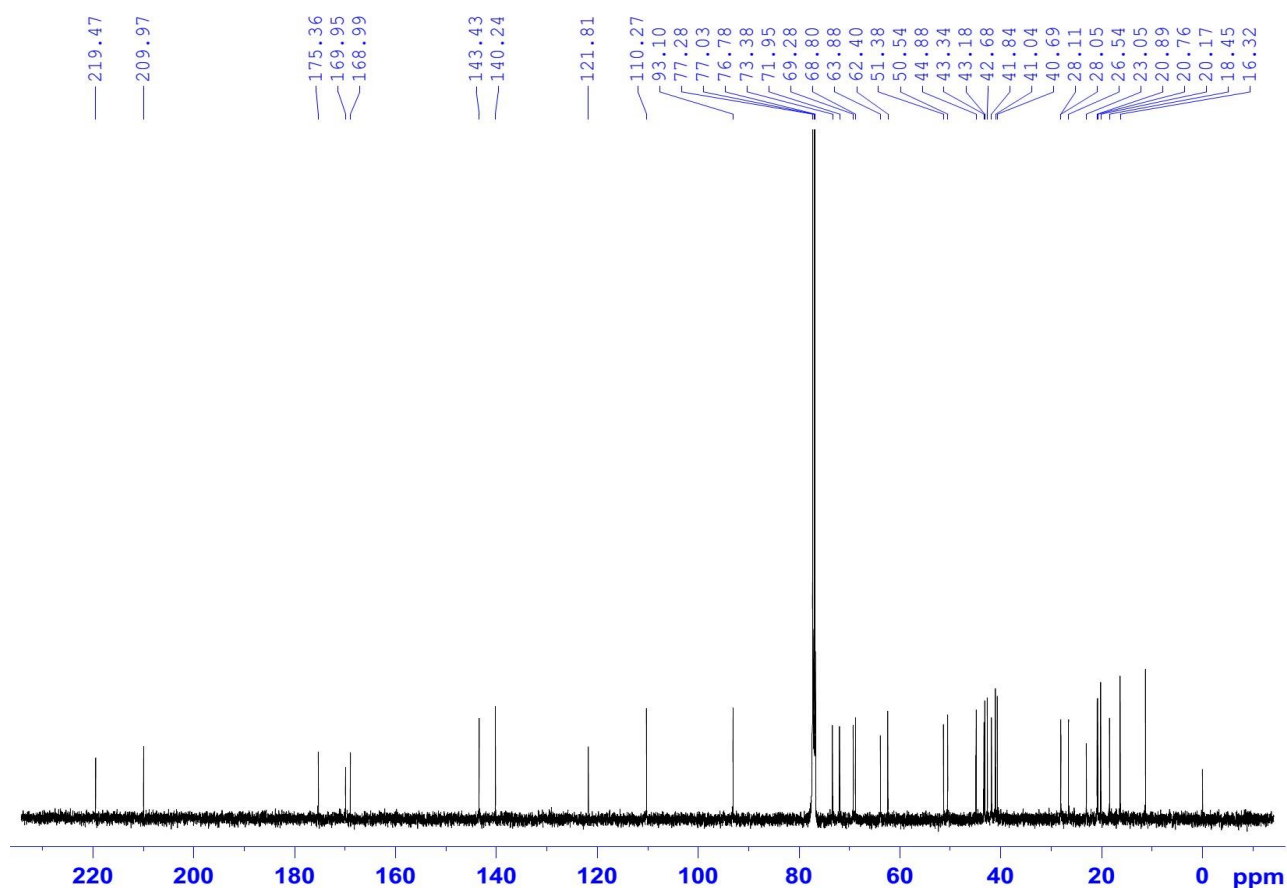
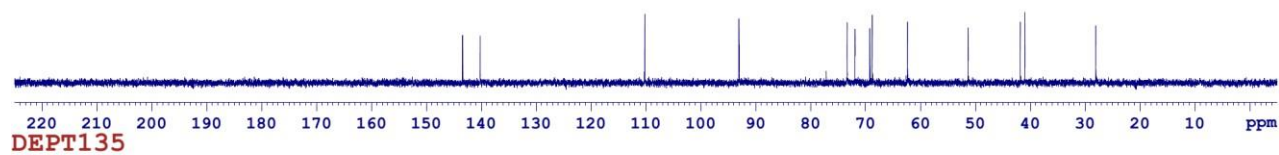


Figure S31: ^{13}C -NMR spectrum of compound **2**.

AZE5.5-CDCl3-C13CPD & DEPT

DEPT90



CH&CH3

CH2

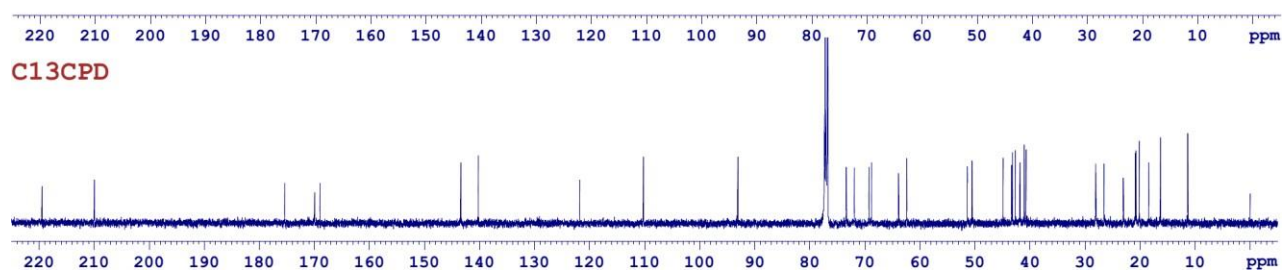


Figure S32: DEPT spectrum of compound 2.

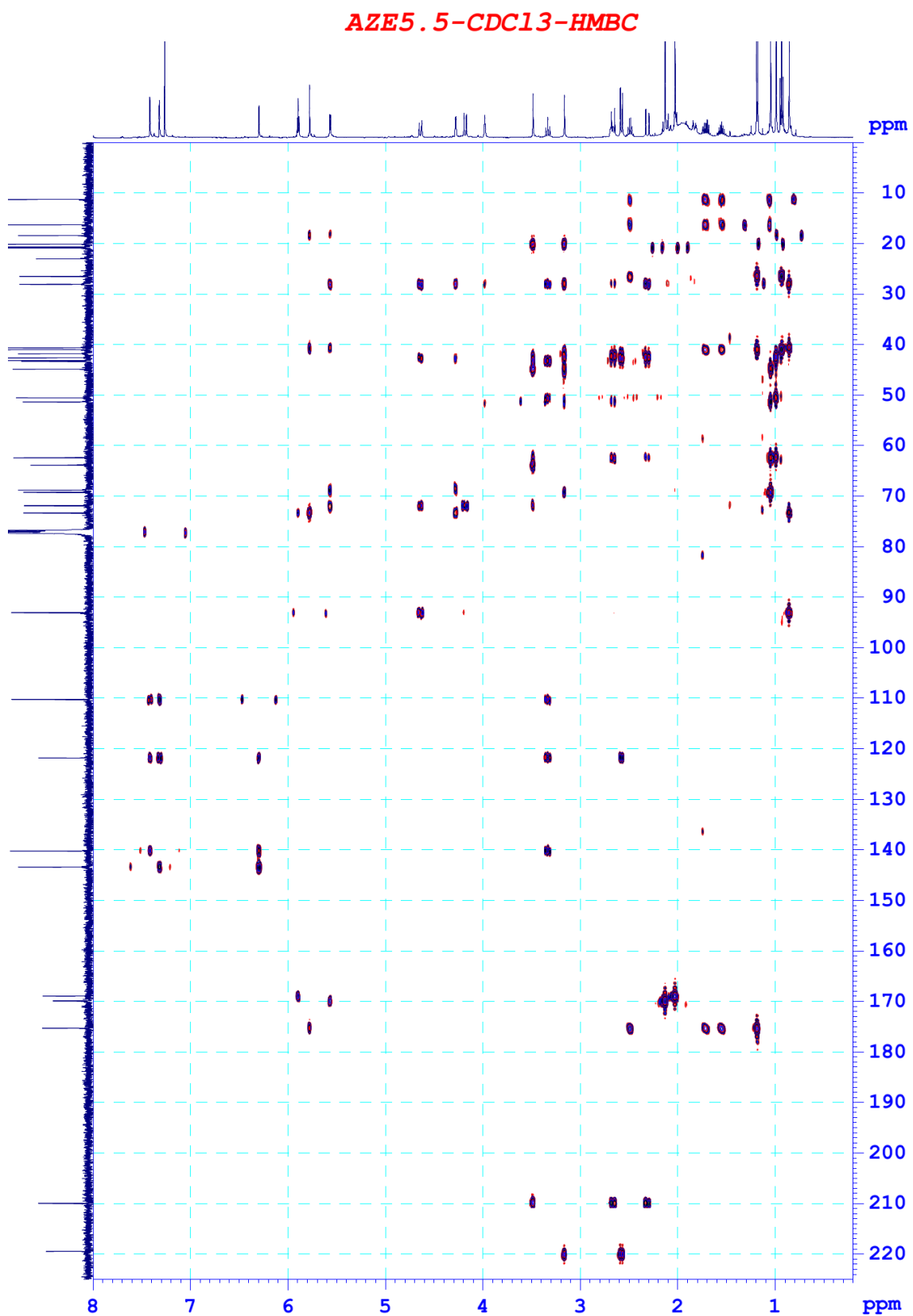


Figure S33: HMBC spectrum of compound **2**.

AZE5.5-CDC13-NOESY

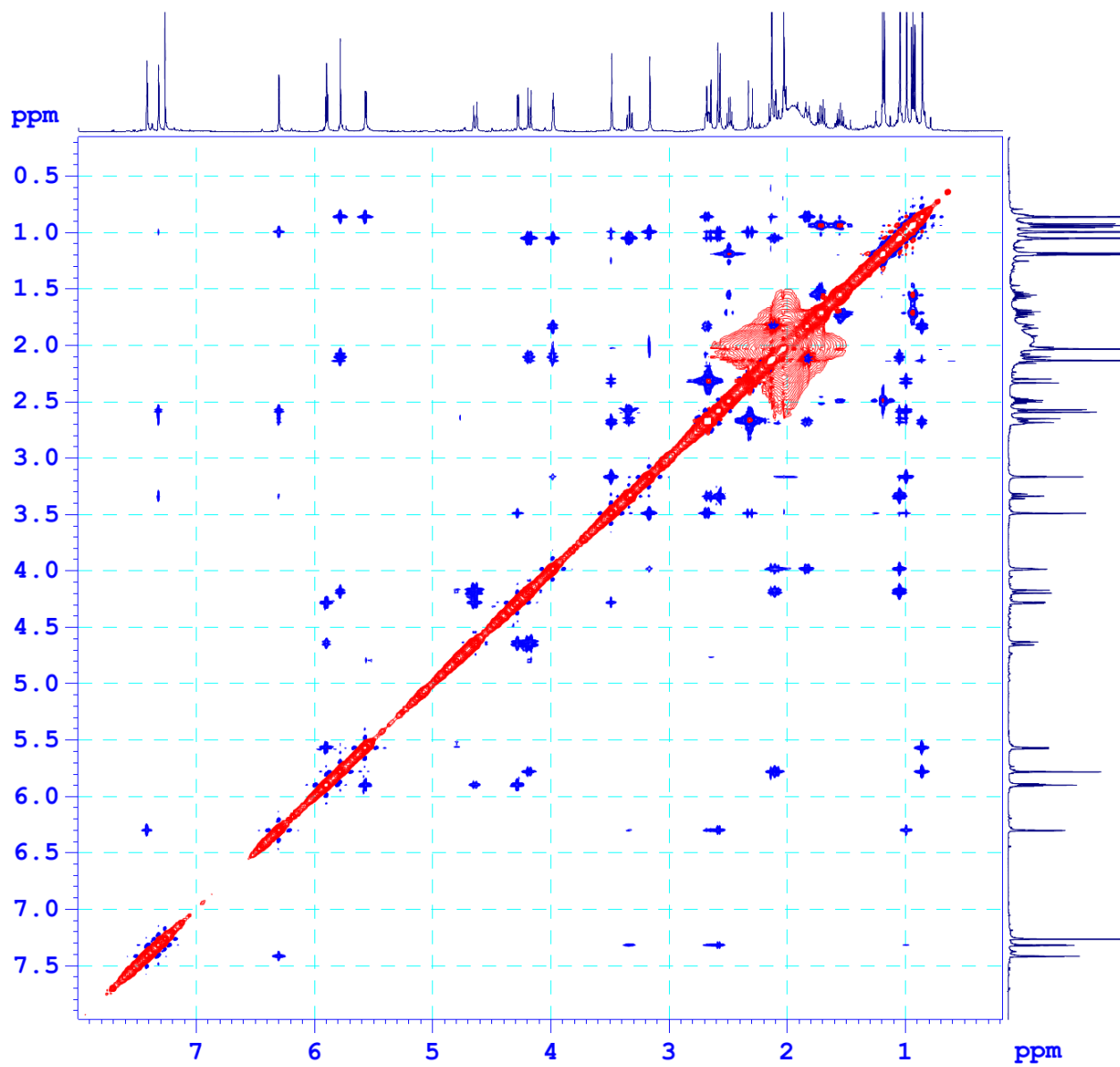


Figure S34: NOESY spectrum of compound 2.

AZE5.5-CDC13-COSYGP

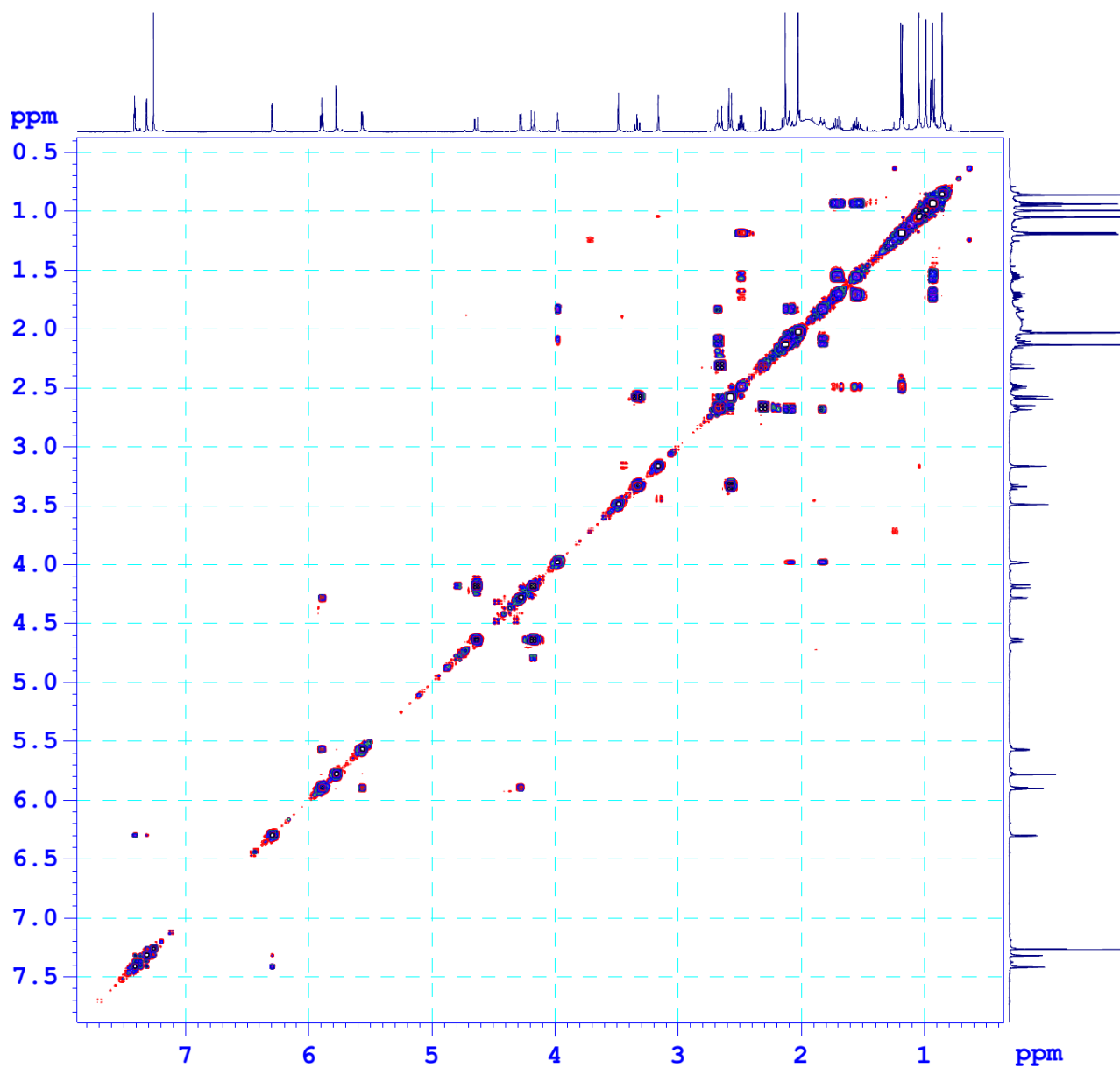


Figure S35: COSY spectrum of compound **2**.

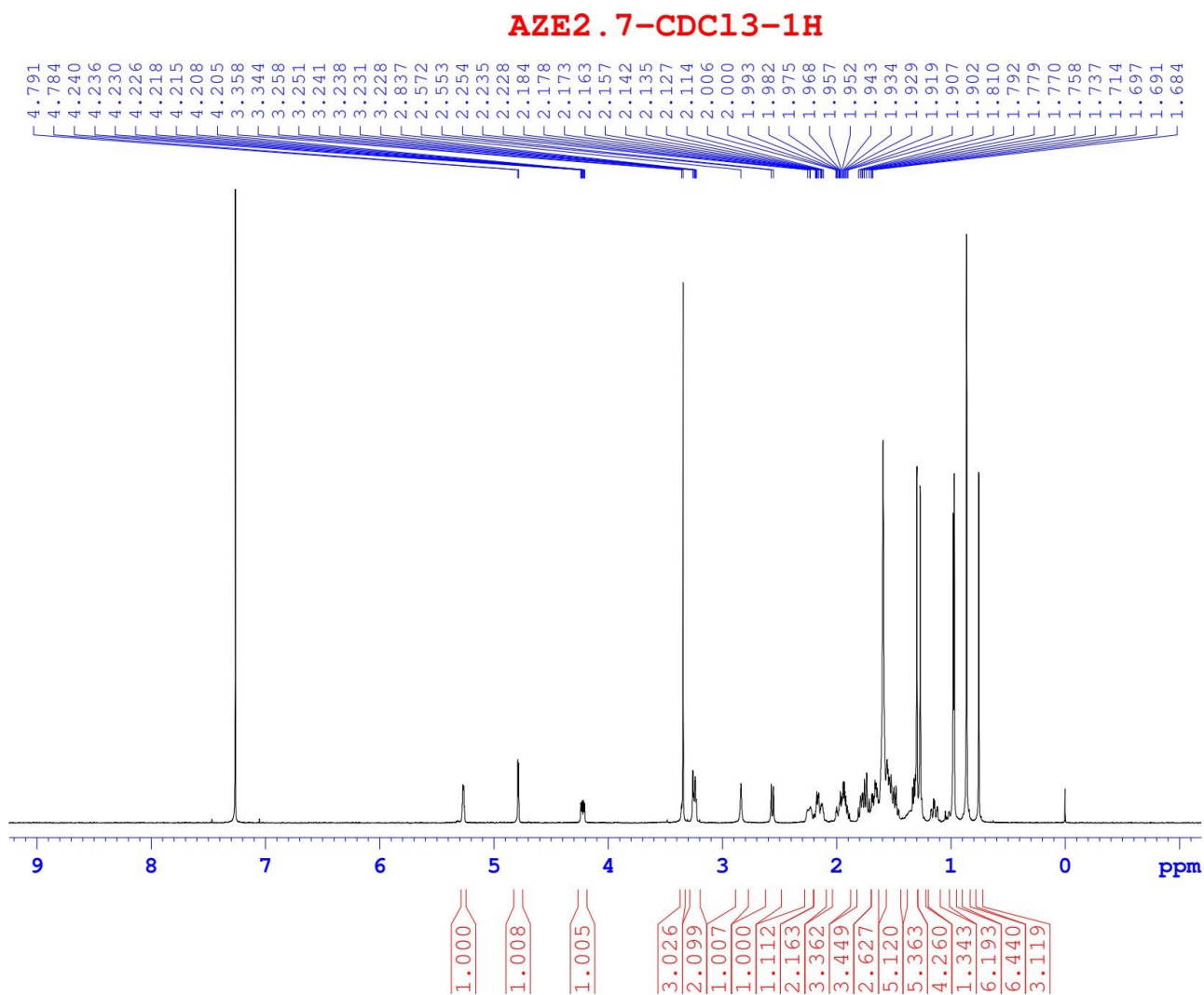


Figure S36: ^1H -NMR spectrum of compound **3**.

AZE2.7-CDC13-C13CPD

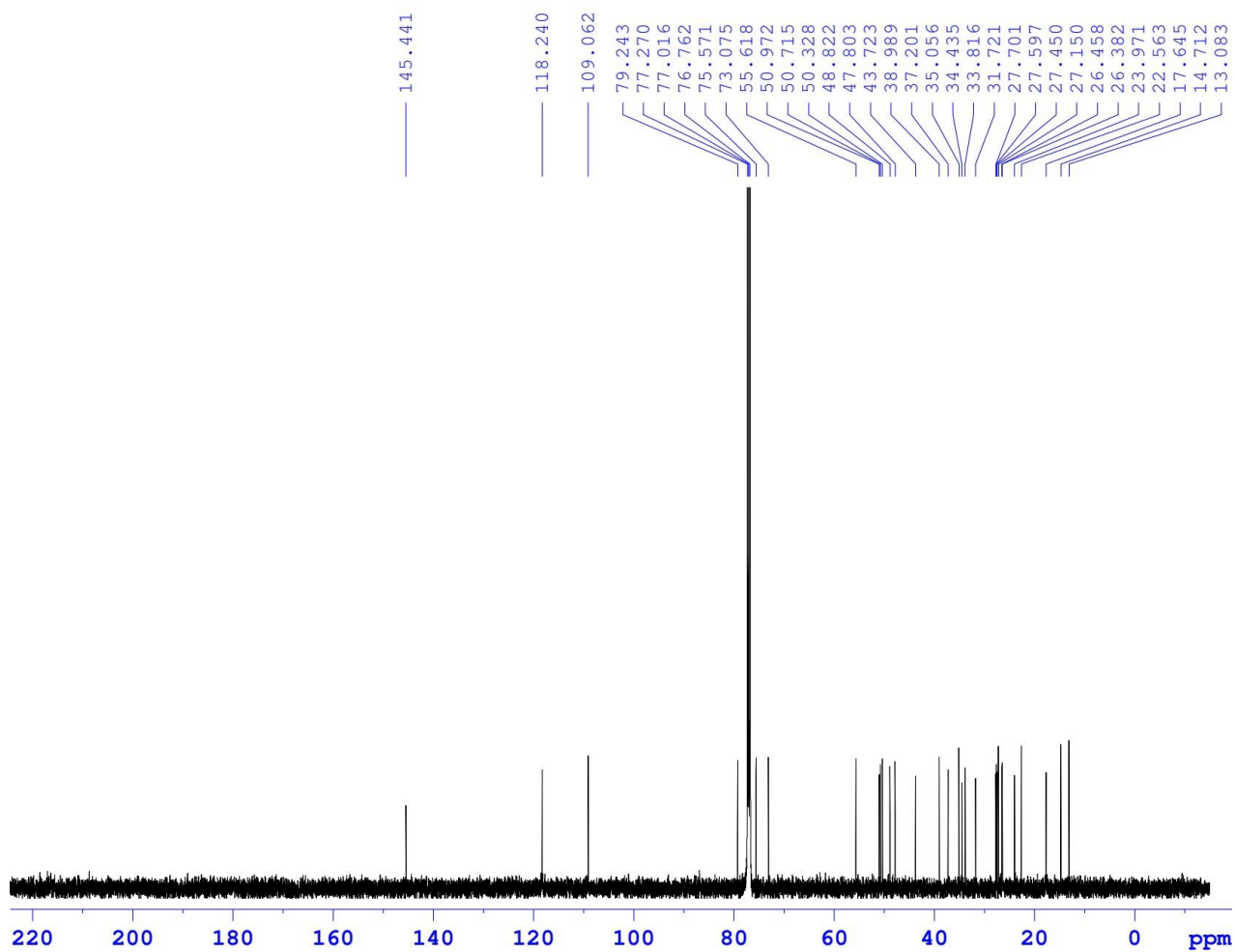
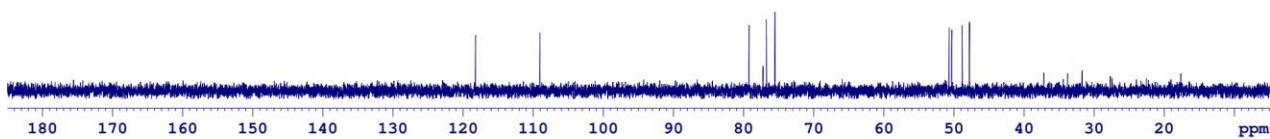


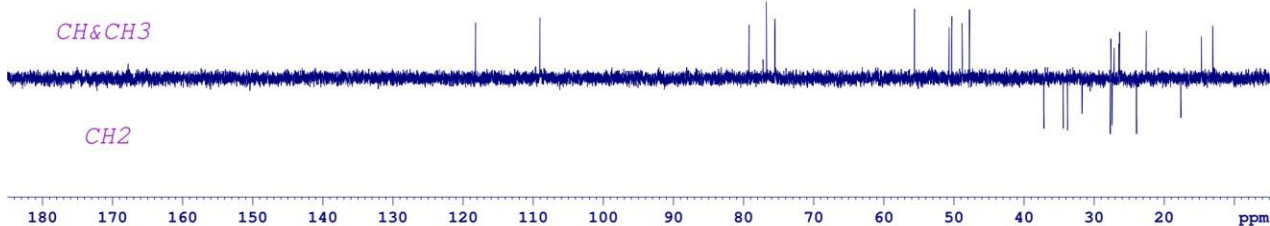
Figure S37: ^{13}C -NMR spectrum of compound **3**.

AZE2.7-CDC13-C13CPD&DEPT

DEPT90



DEPT135



C13CPD

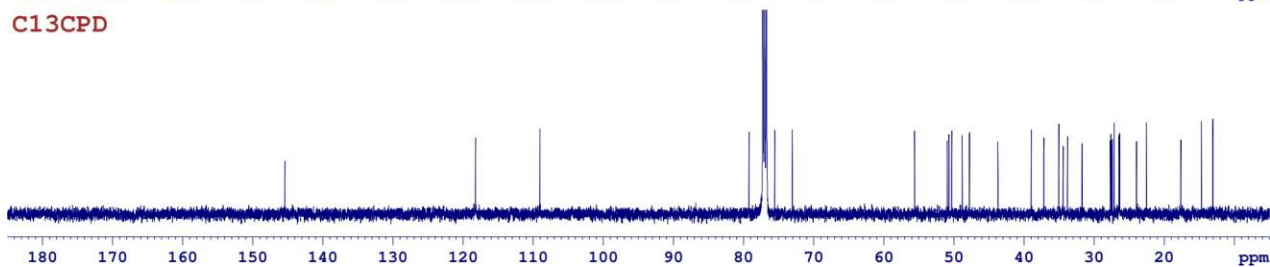


Figure S38: DEPT spectrum of compound 3.

AZE2.7-CDC13-HMBC

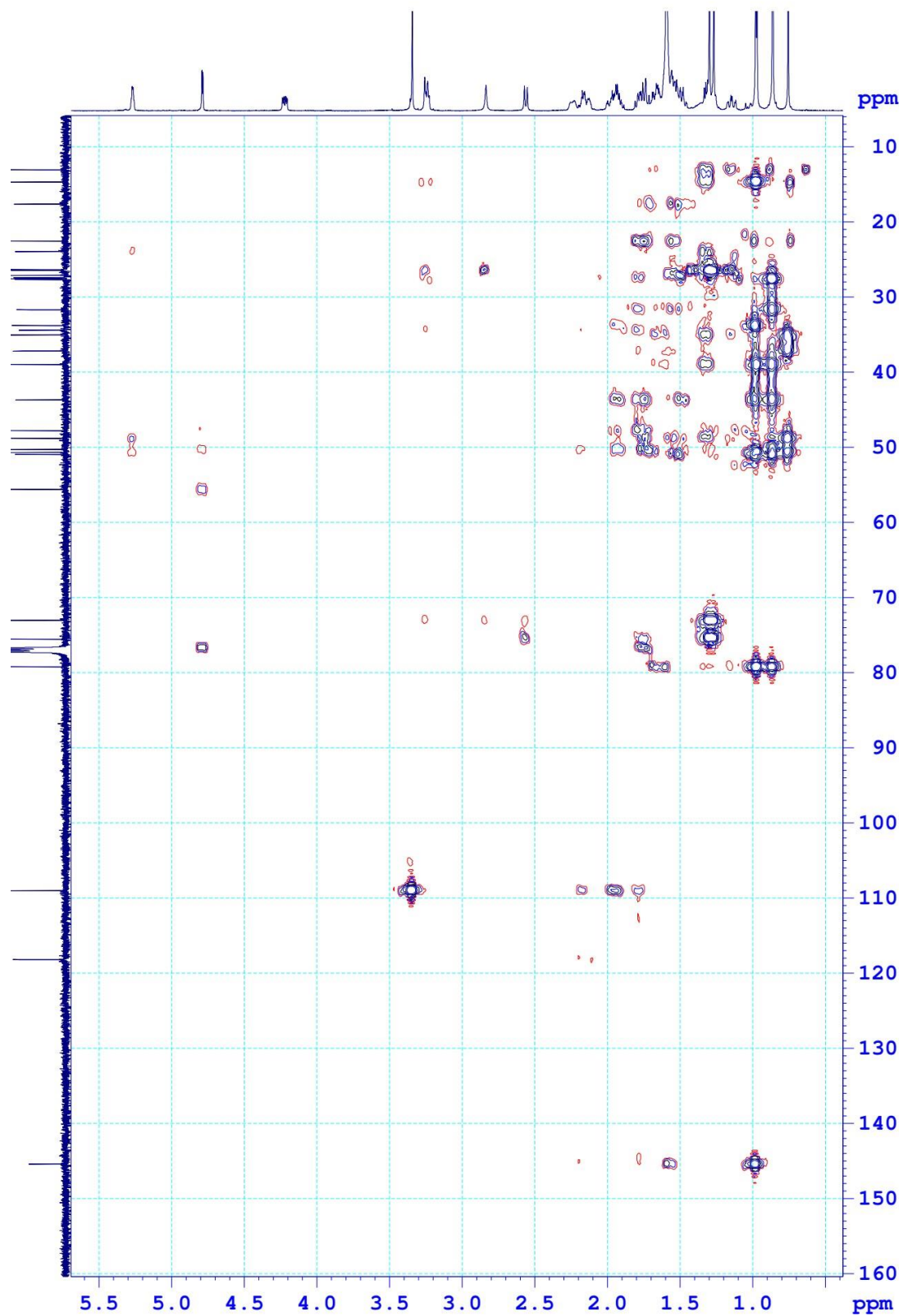


Figure S39: HMBC spectrum of compound **3**.

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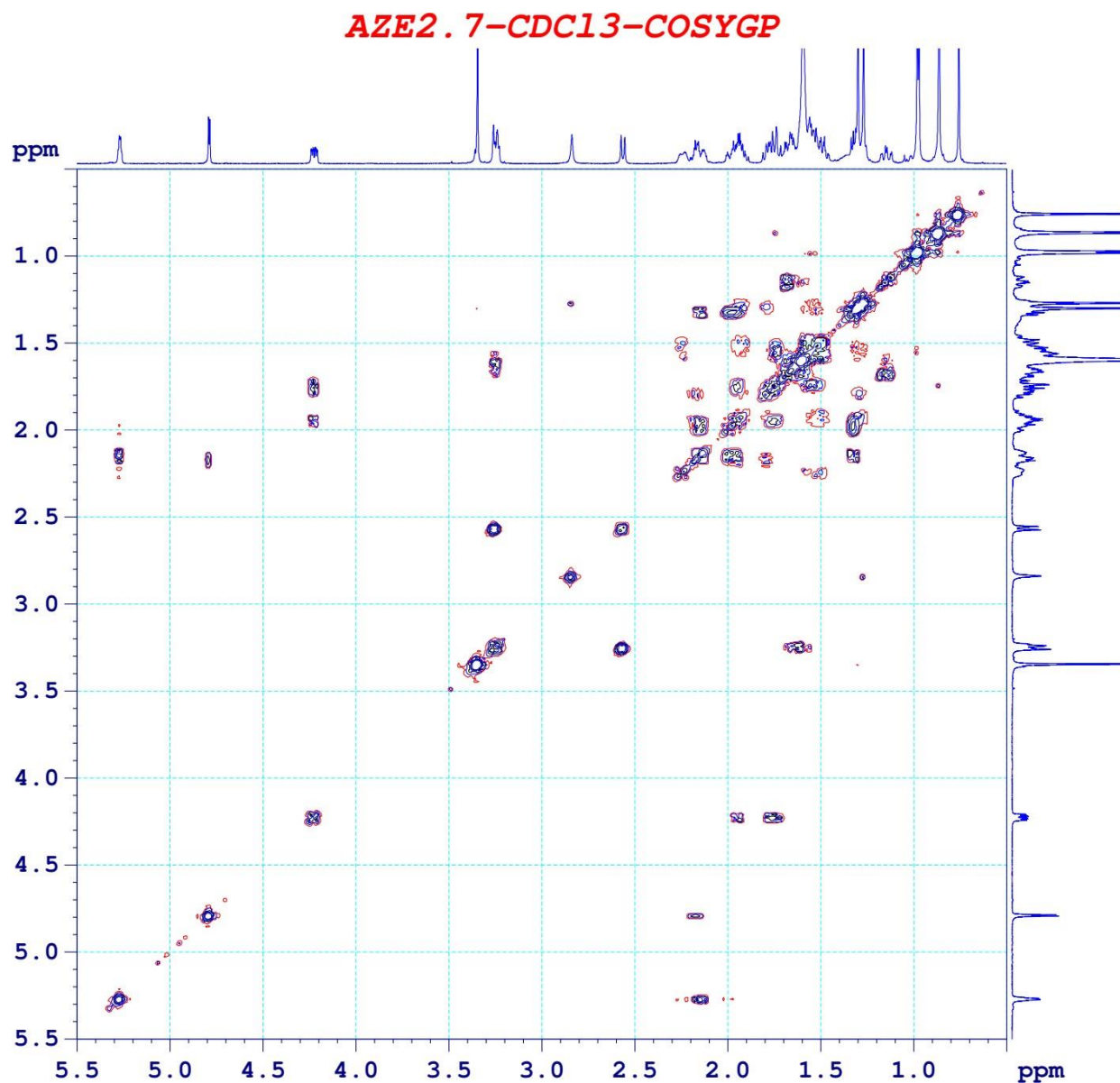


Figure S40: COSY spectrum of compound **3**.

AZE10.3.1-CDC13-1H

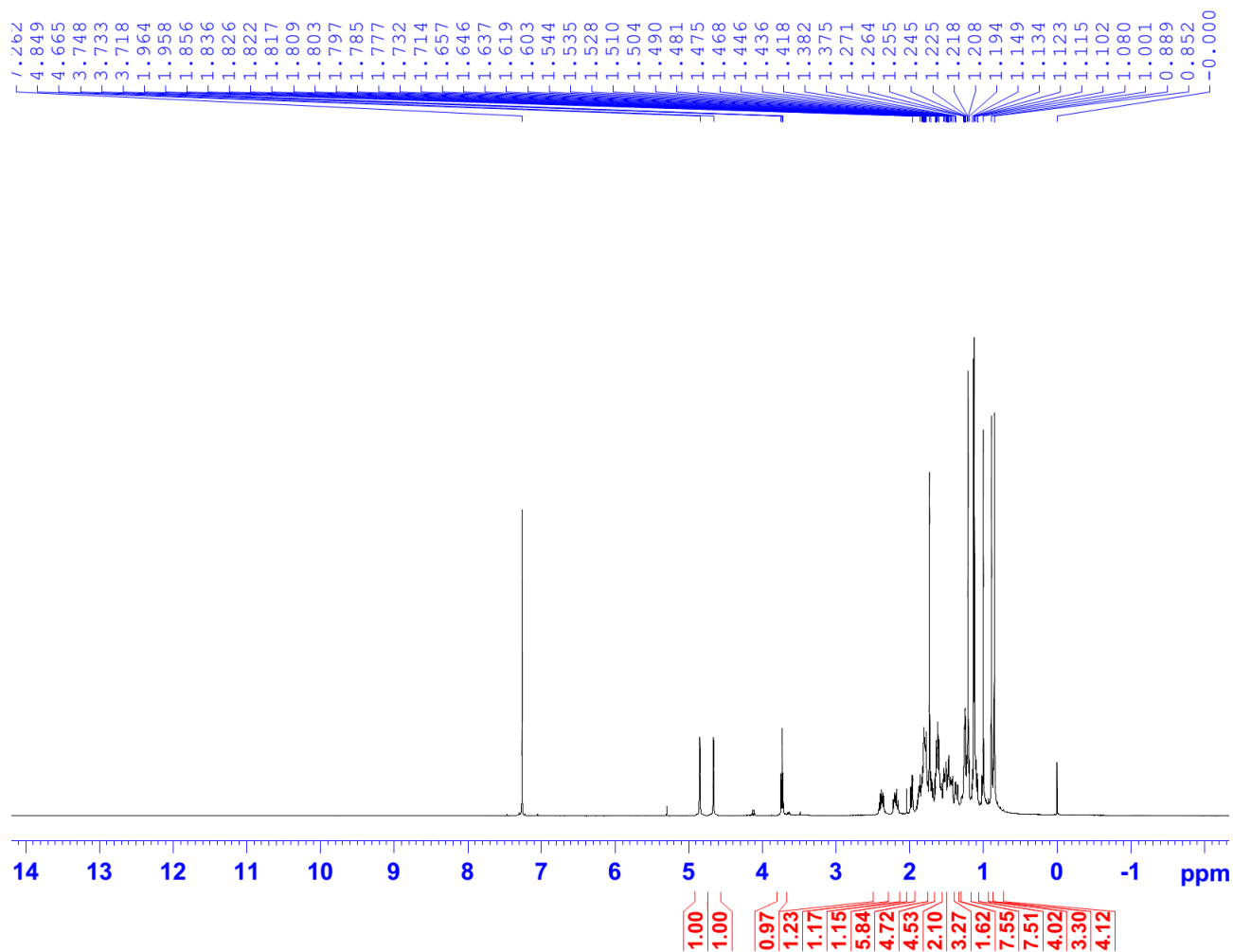


Figure S41: ^1H -NMR spectrum of compound **4**.

AZE10.3.1-CDC13-C13CPD

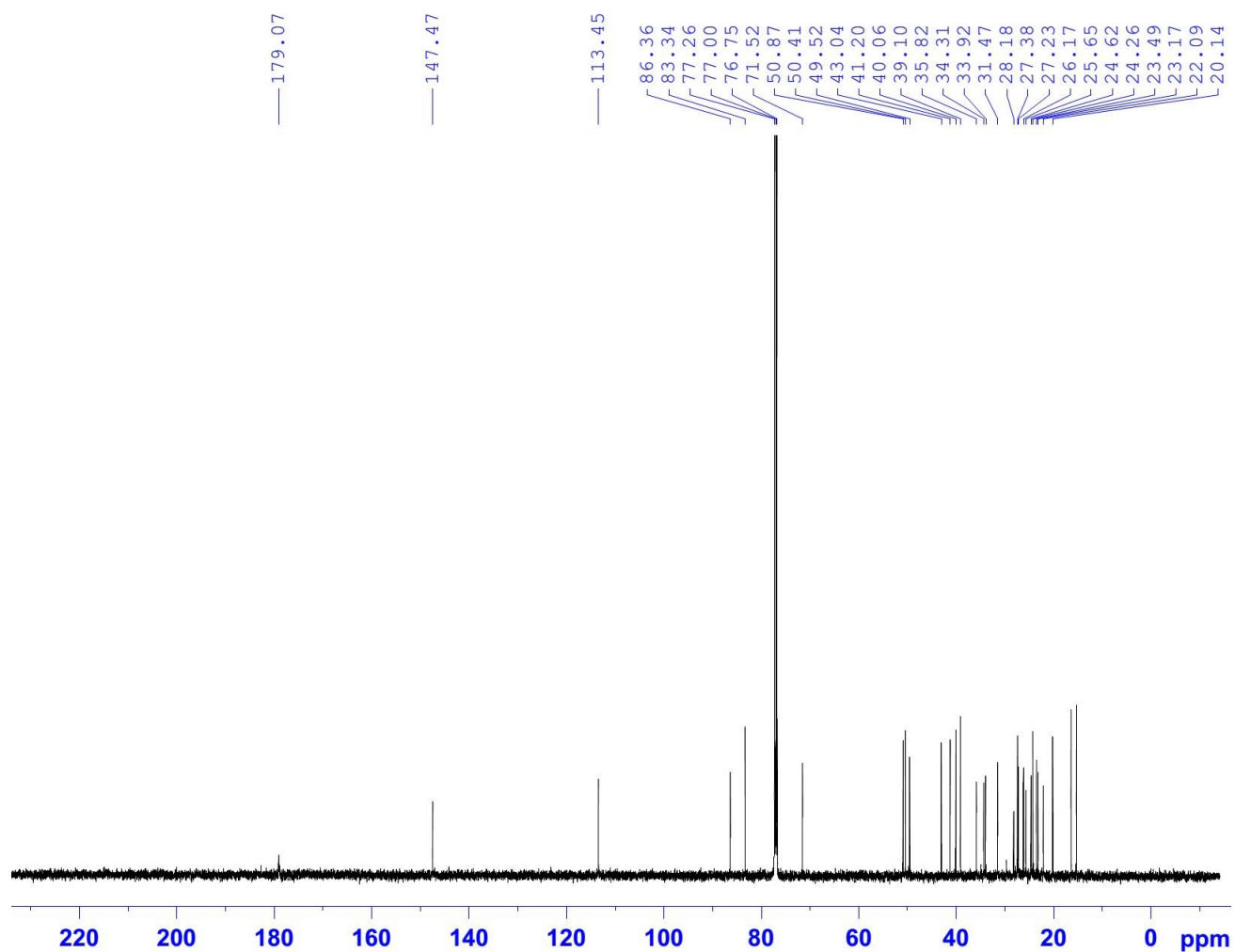
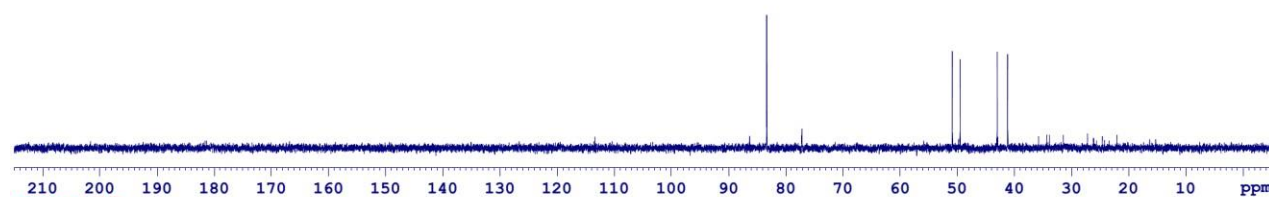


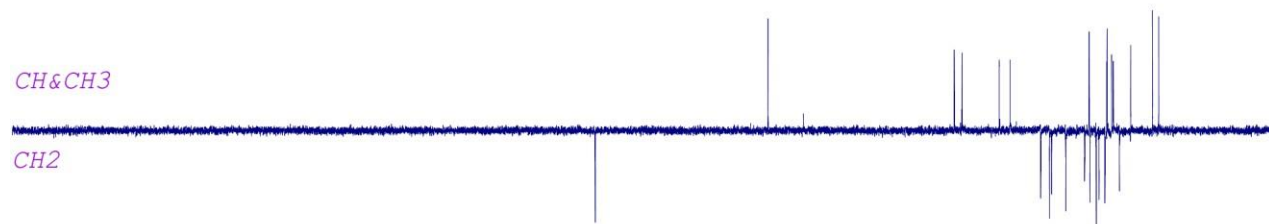
Figure S42: ^{13}C -NMR spectrum of compound **4**.

AZE10.3.1-CDC13-C13CPD&DEPT

DEPT90



DEPT135



CH&CH3

CH2



C13CPD

Figure S43: DEPT spectrum of compound 4.

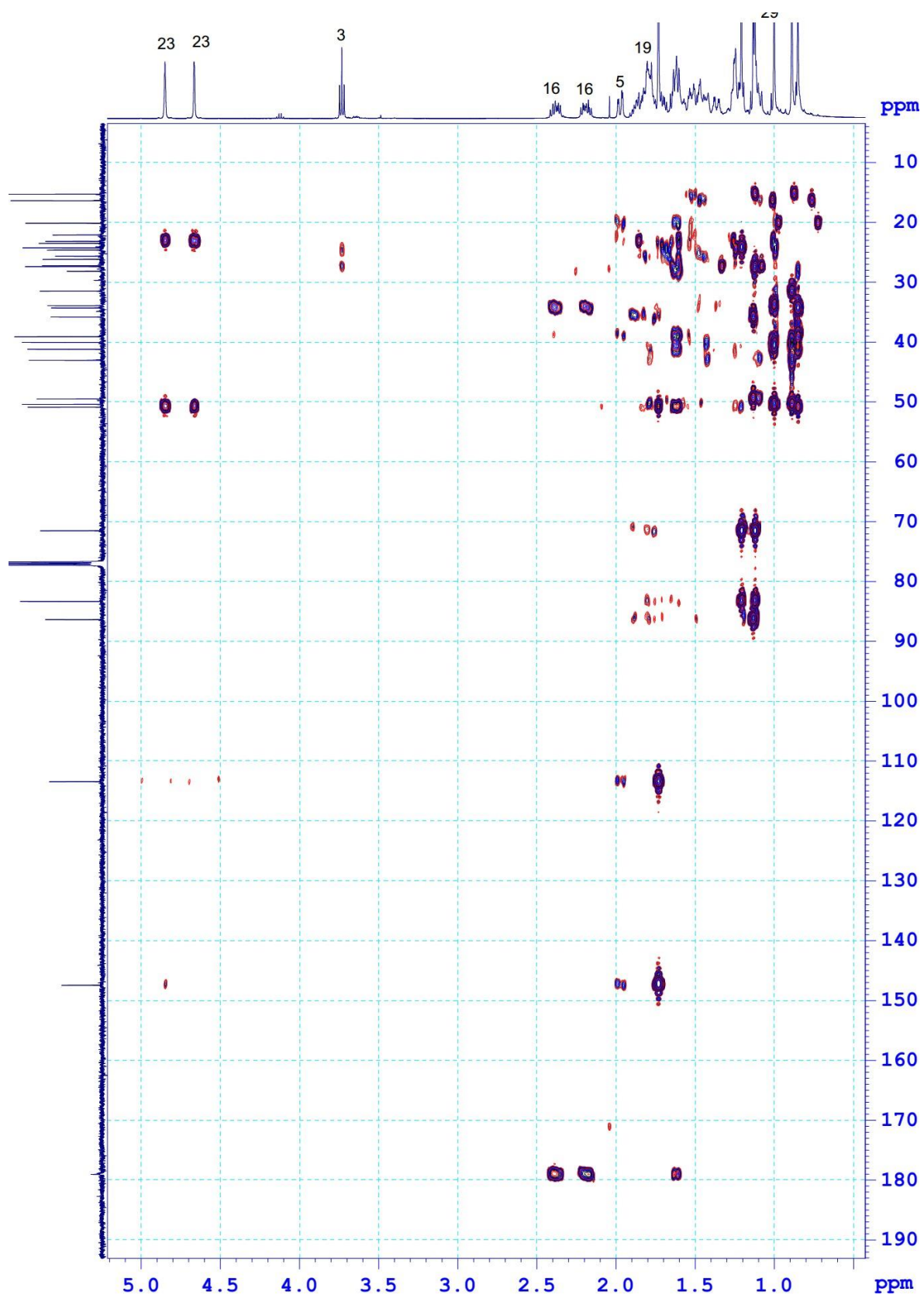


Figure S44: HMBC spectrum of compound **4**.

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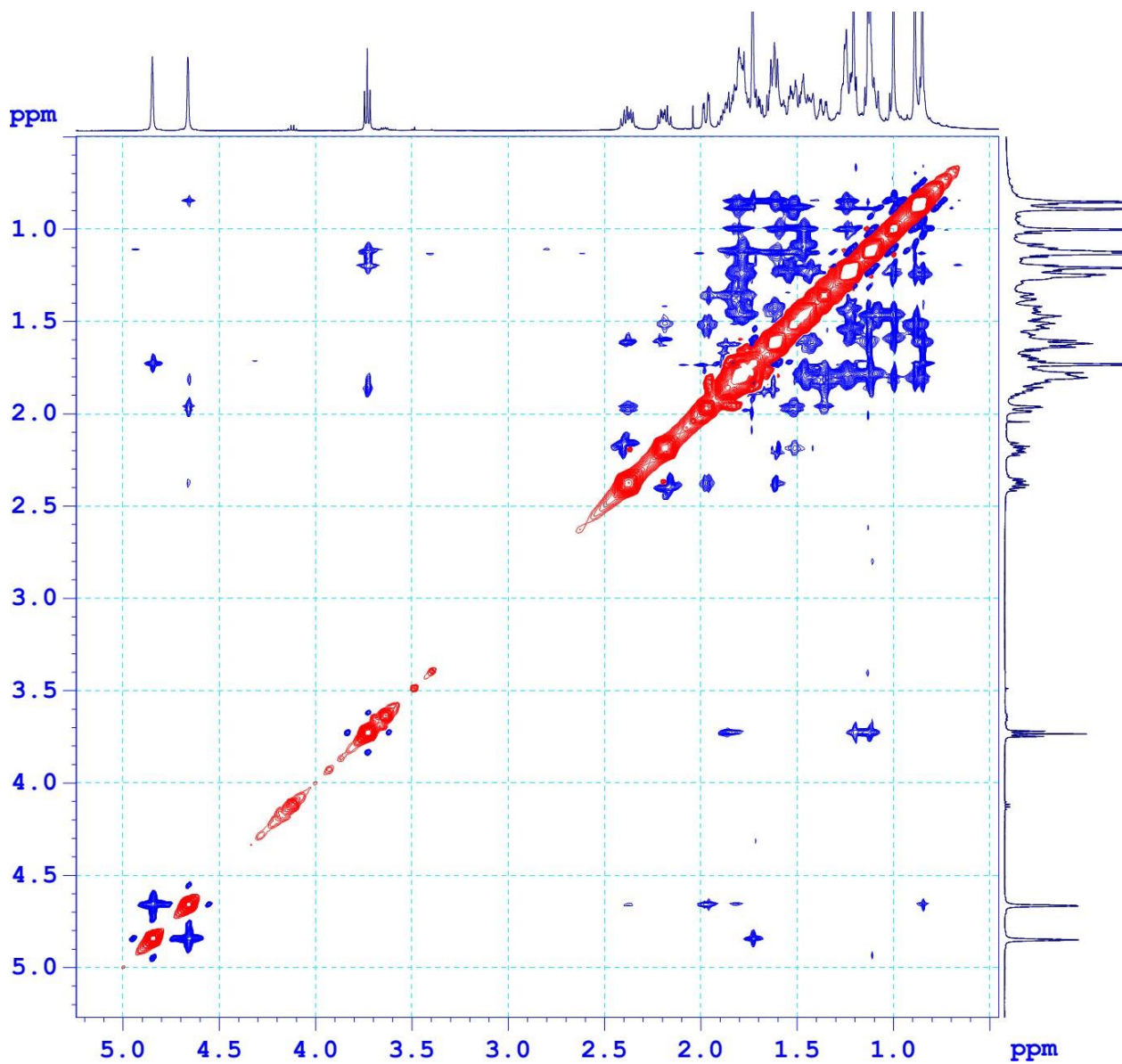


Figure S45: NOESY spectrum of compound 4.

AZE10.3.1-CDC13-COSYGP

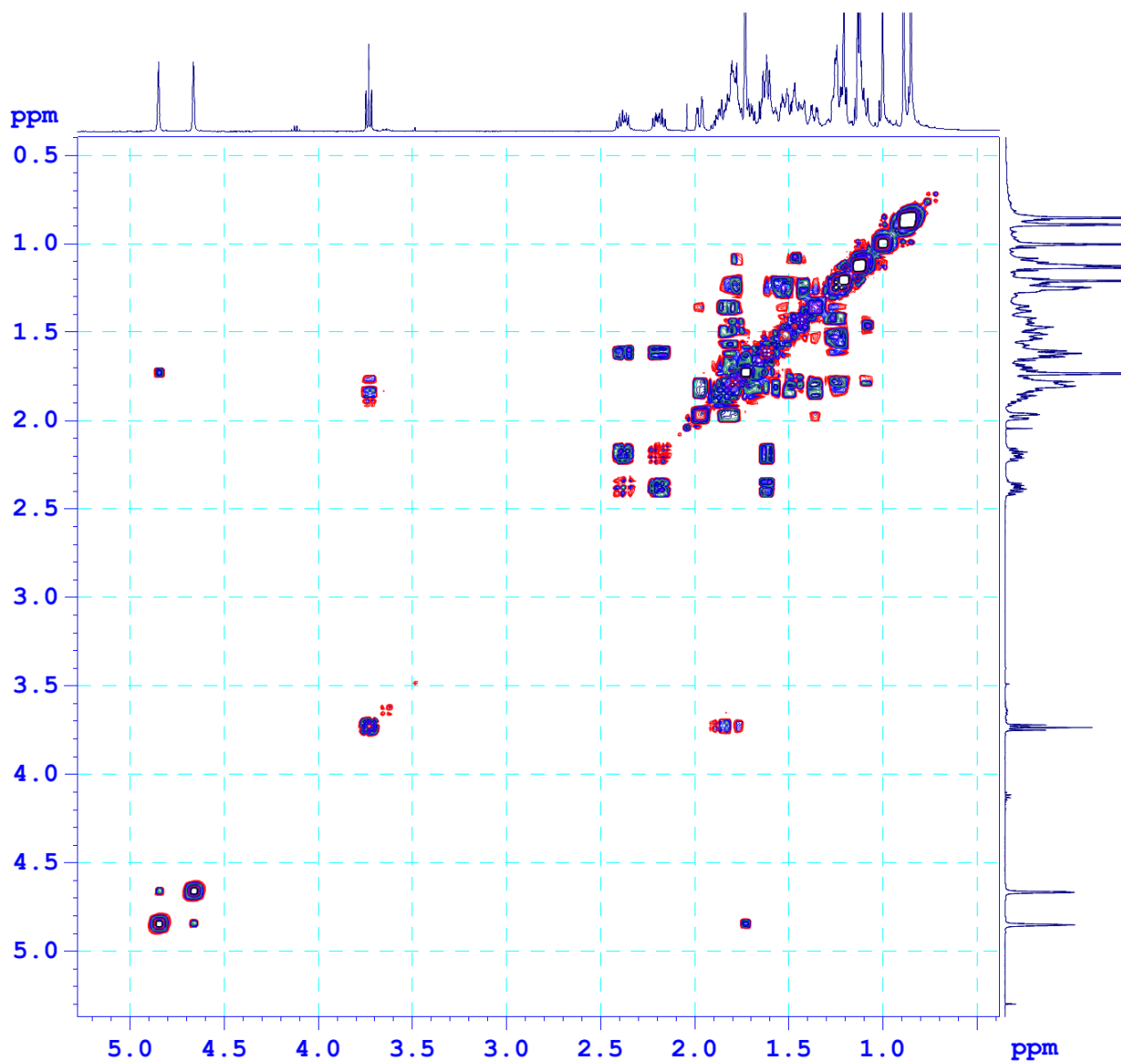


Figure S46: COSY spectrum of compound 4.

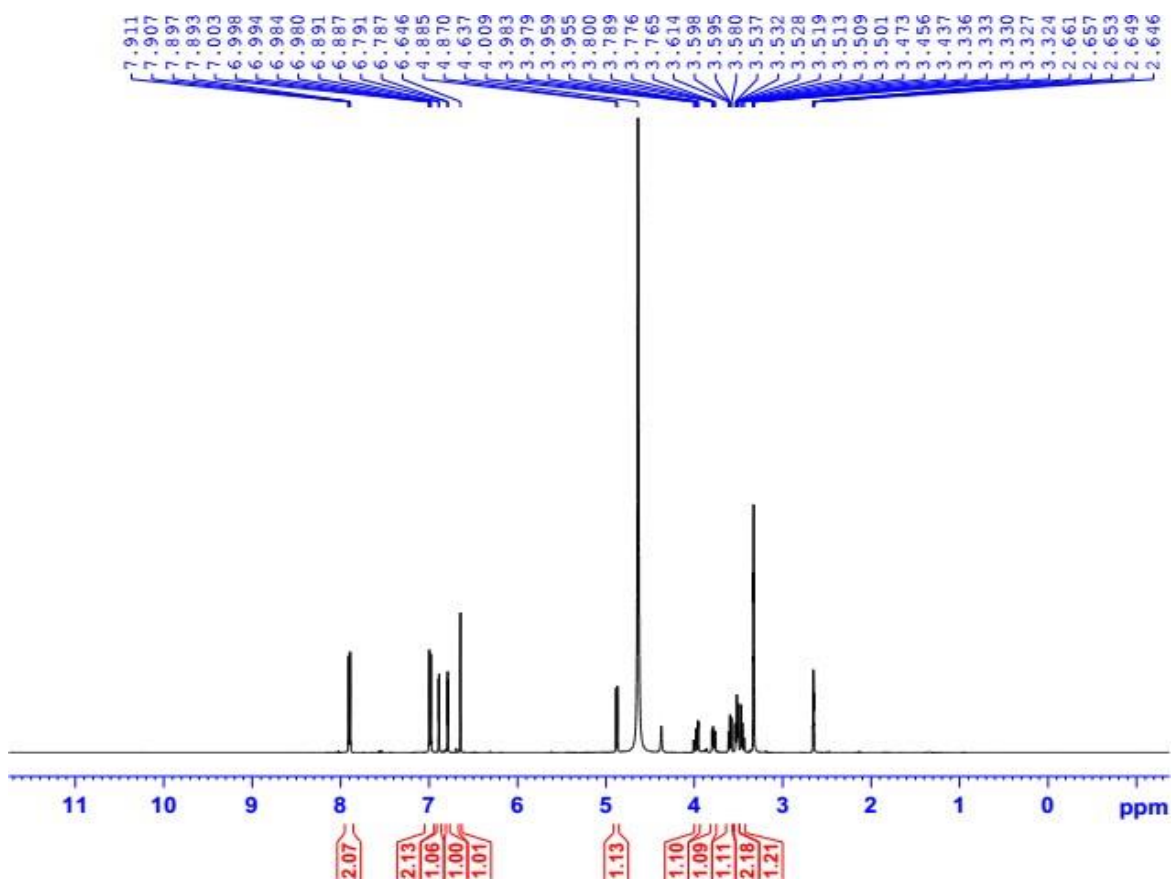


Figure S47: $^1\text{H-NMR}$ spectrum of compound 5.

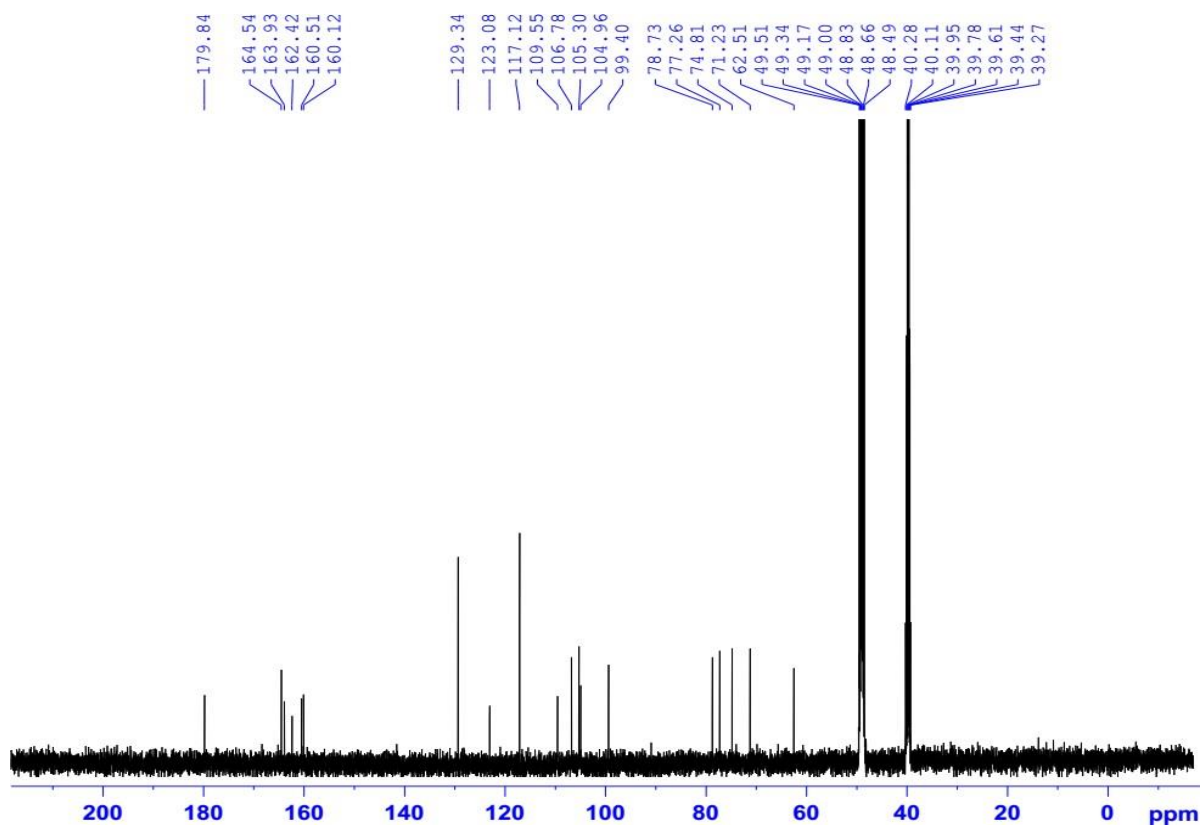


Figure S48: ^{13}C -NMR spectrum of compound 5.

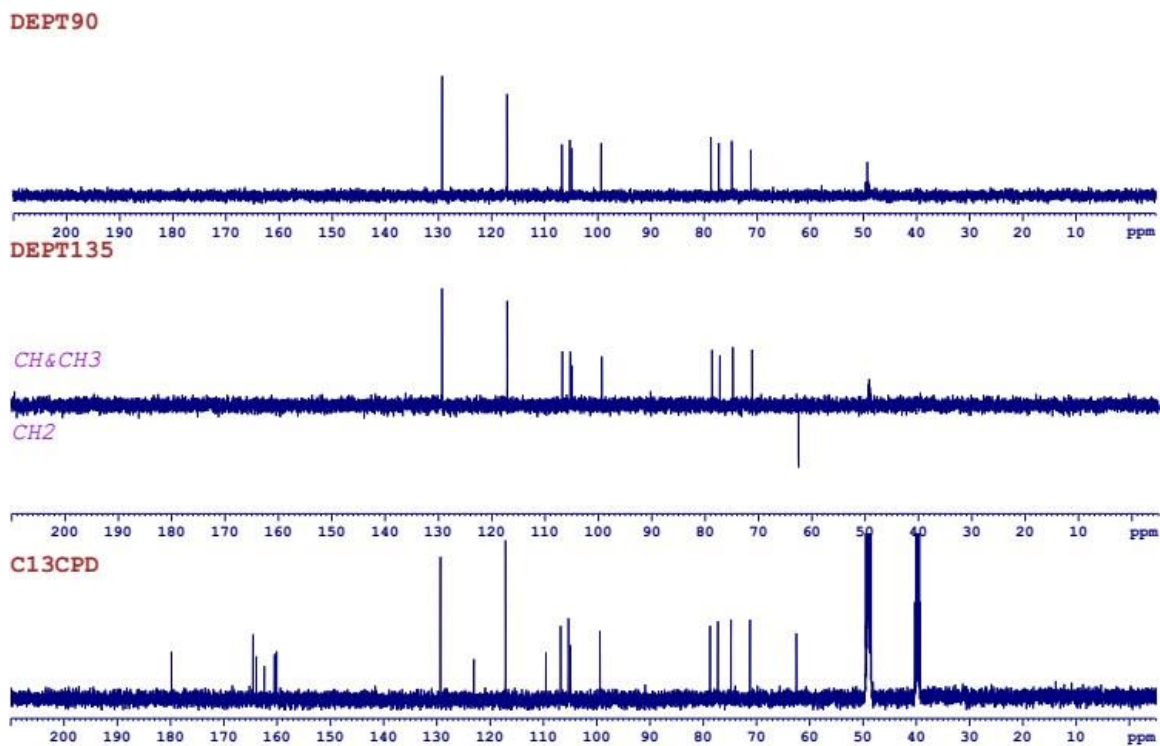


Figure S49: DEPT spectrum of compound 5.

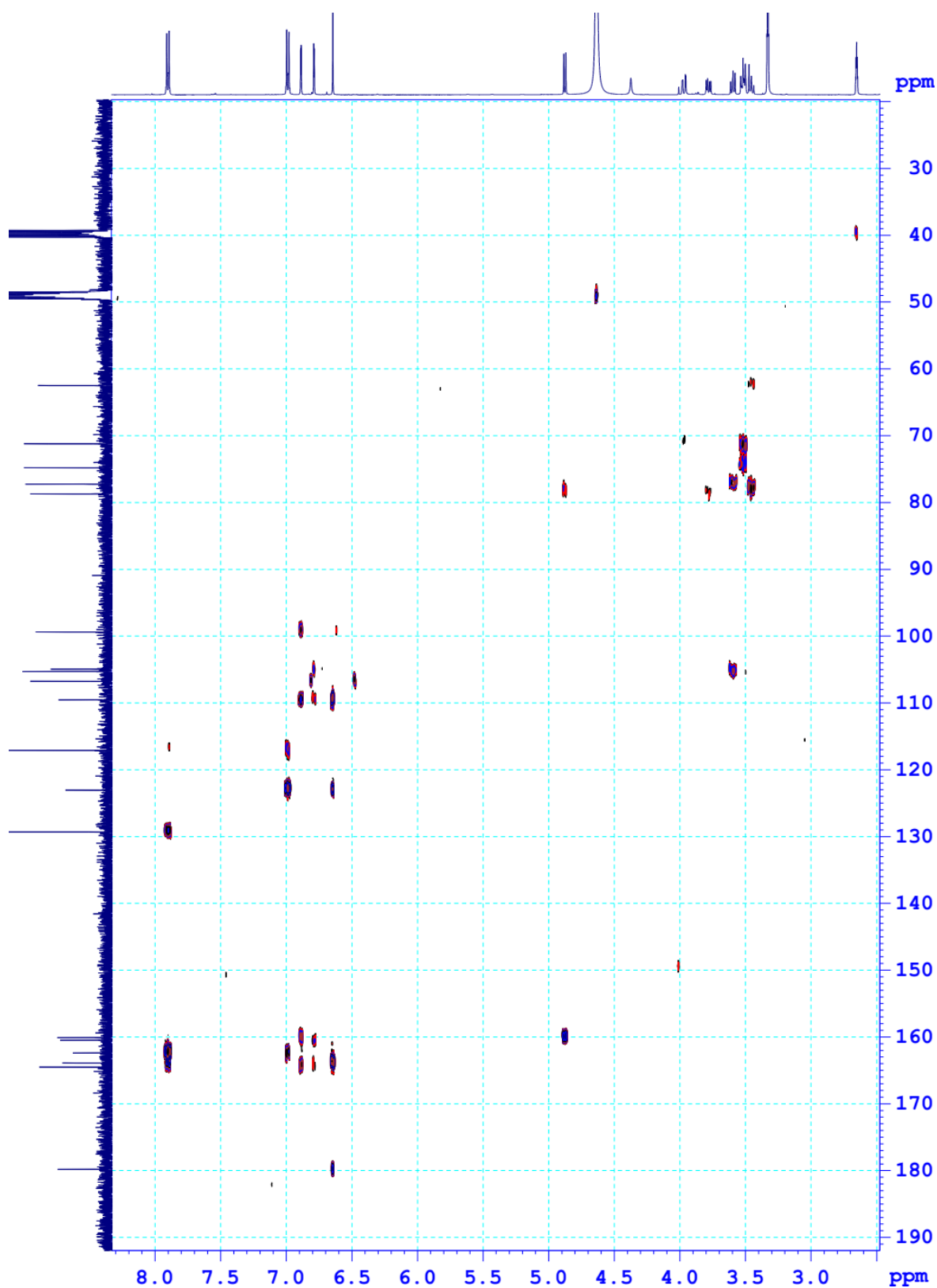


Figure S50: HMBC spectrum of compound **5**.

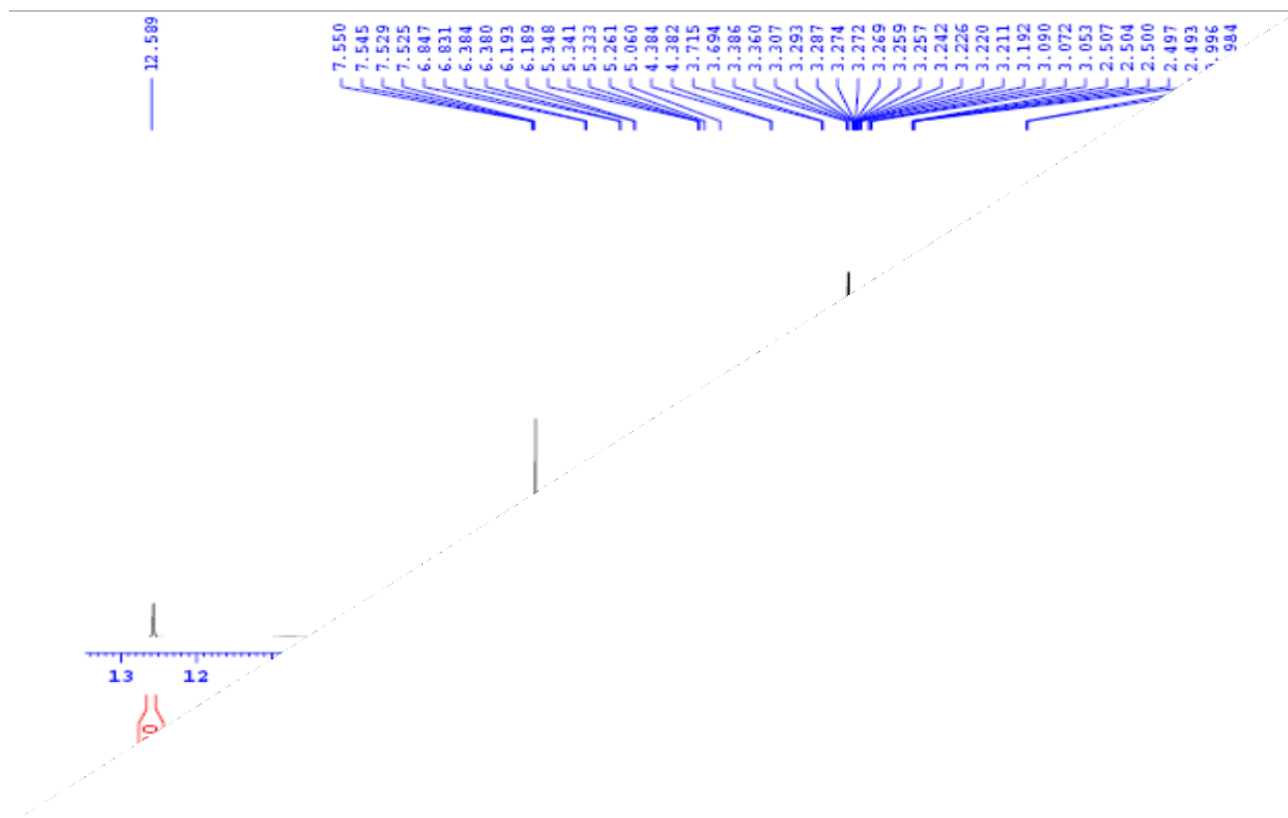


Figure S51: $^1\text{H-NMR}$ spectrum of compound **6**.

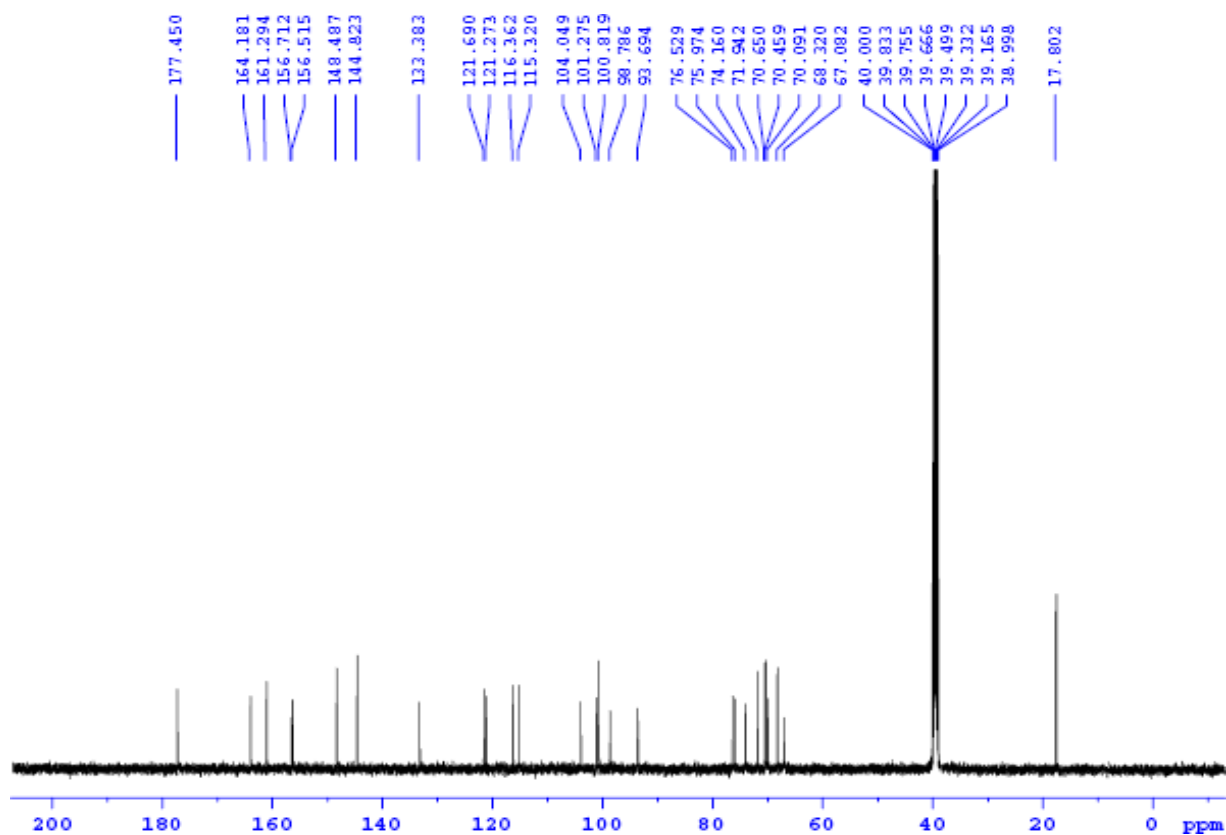


Figure S52: ^{13}C -NMR spectrum of compound 6.

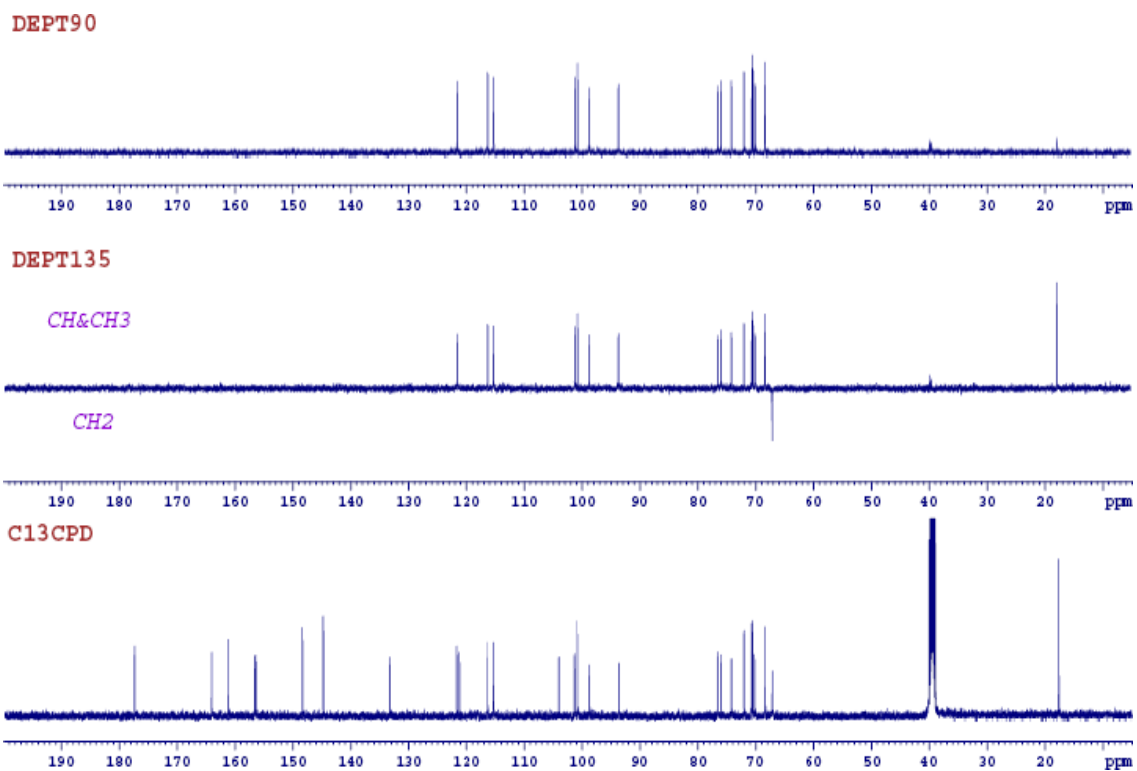


Figure S53: DEPT spectrum of compound 6.

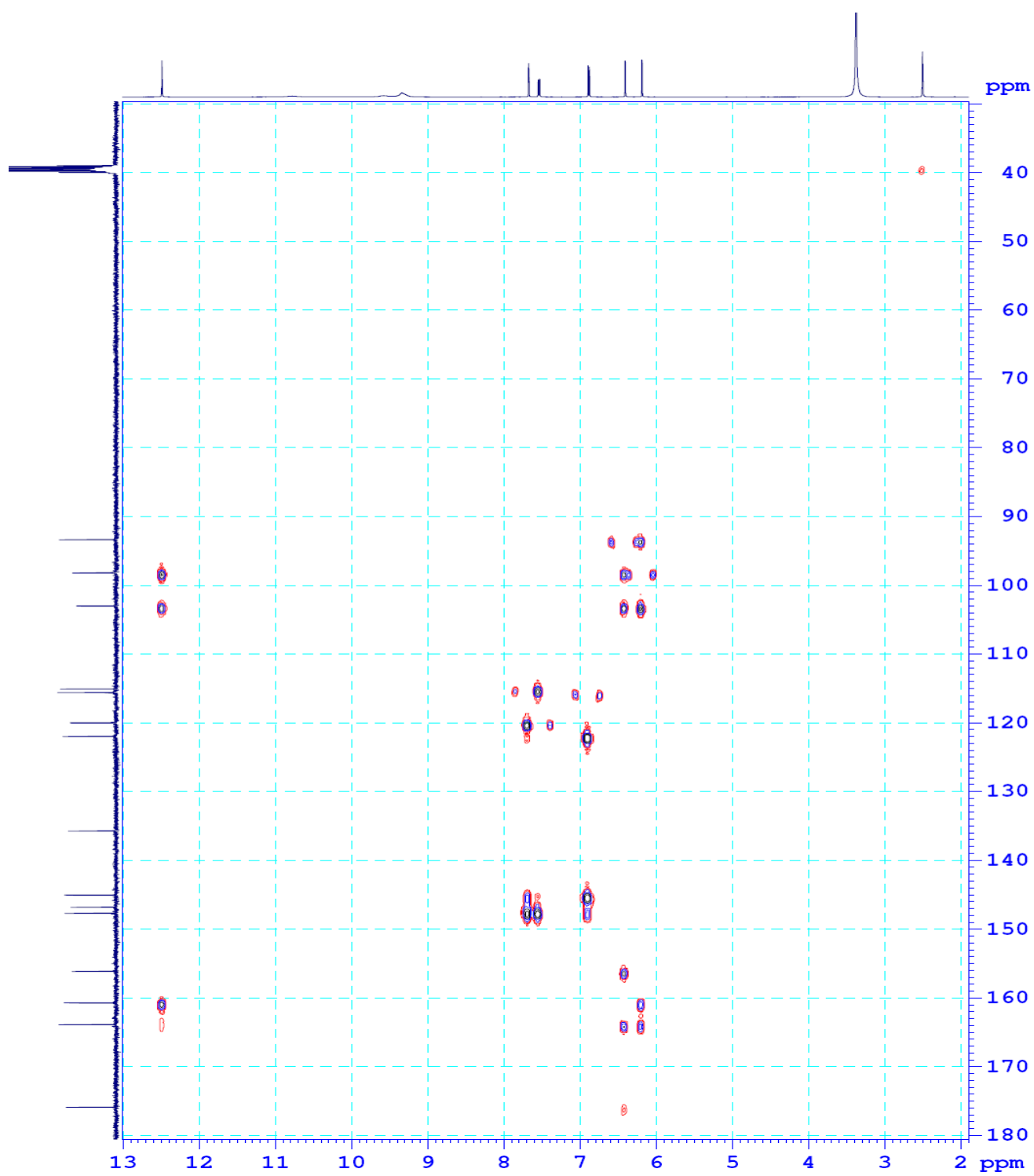


Figure S54: HMBC spectrum of compound **6**.

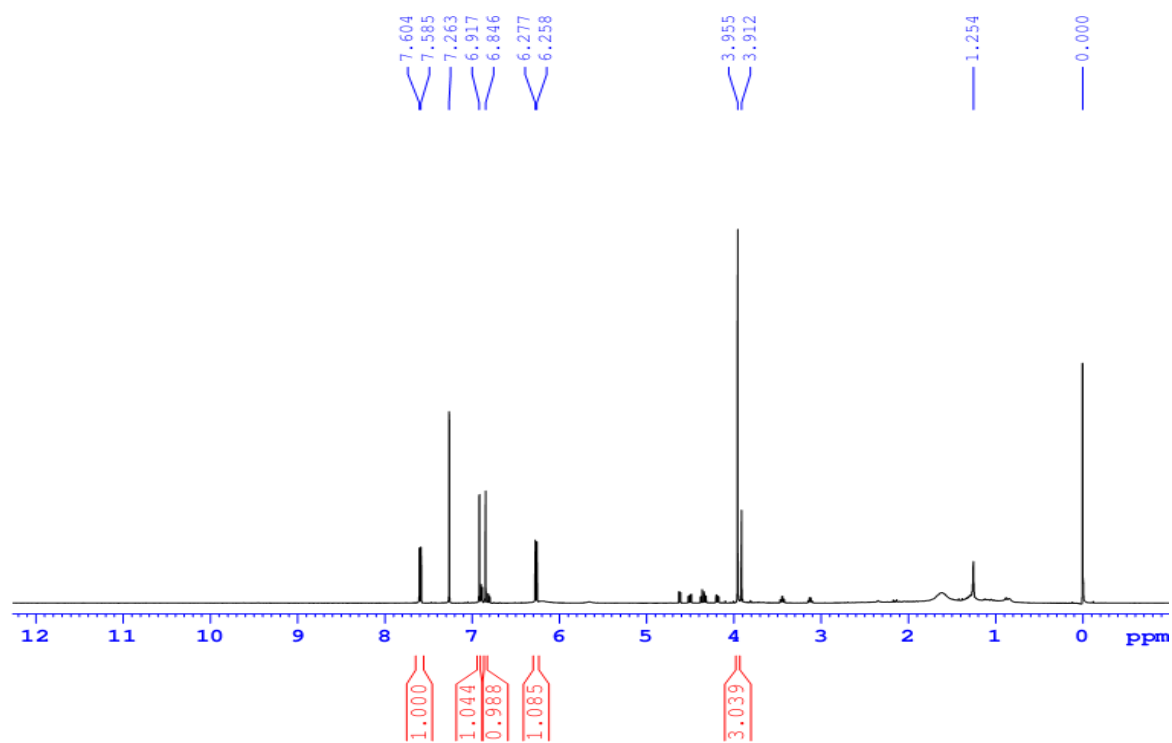


Figure S55: ¹H-NMR spectrum of compound 7.

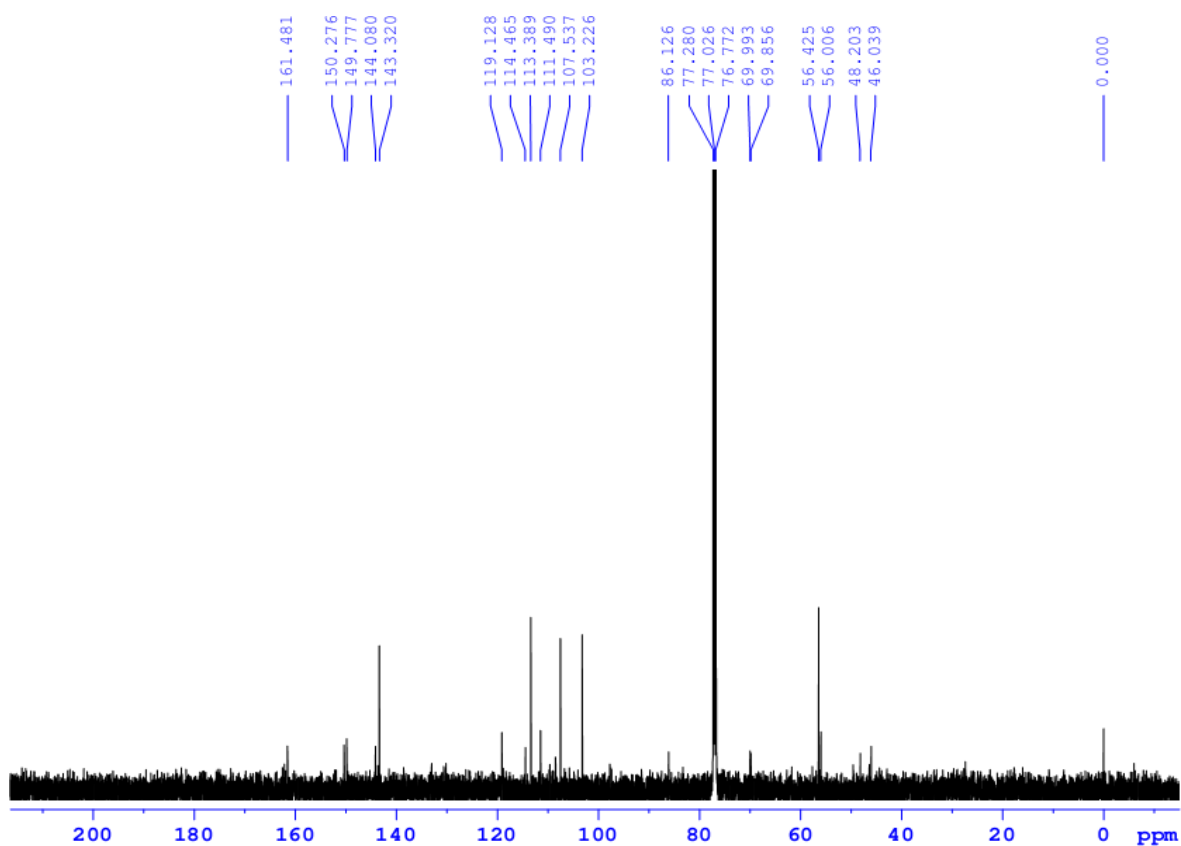


Figure S56: ^{13}C -NMR spectrum of compound 7.

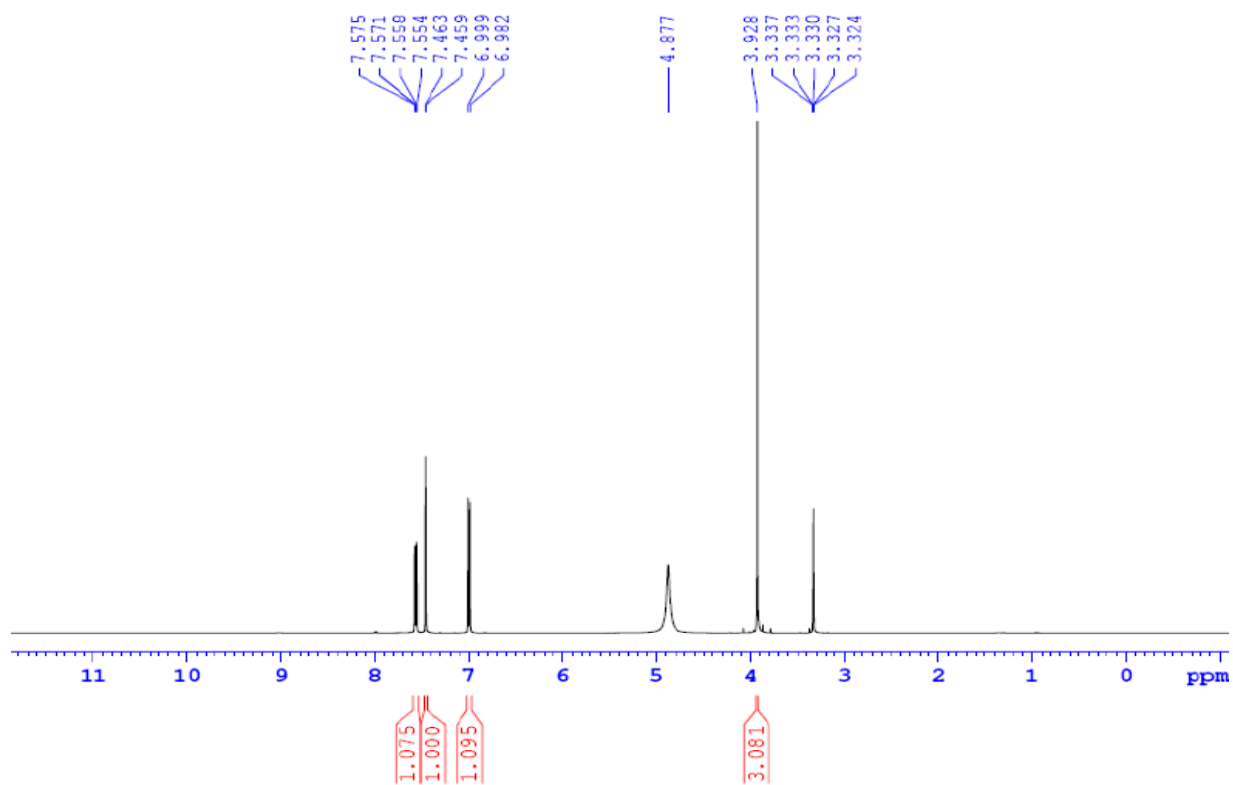


Figure S57: ^1H -NMR spectrum of compound **8**.

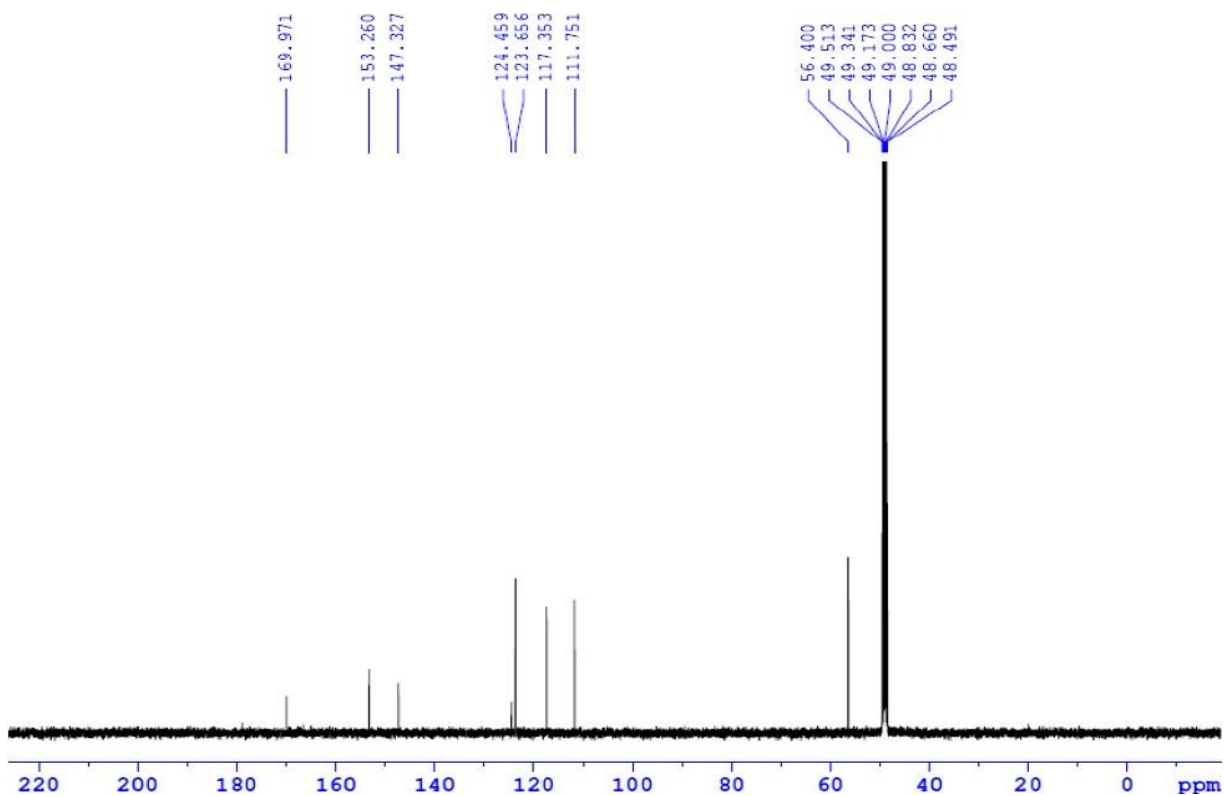


Figure S58: ¹³C-NMR spectrum of compound **8**.

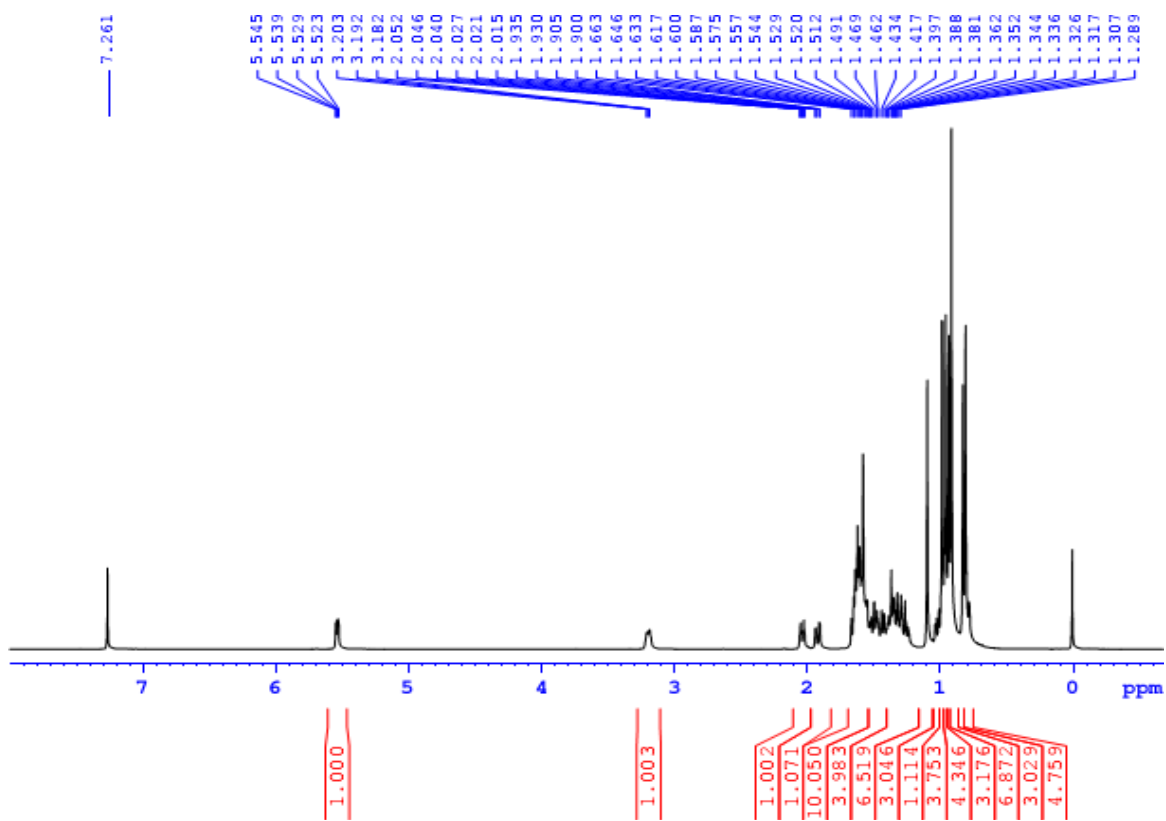


Figure S59: ^1H -NMR spectrum of compound **9**.

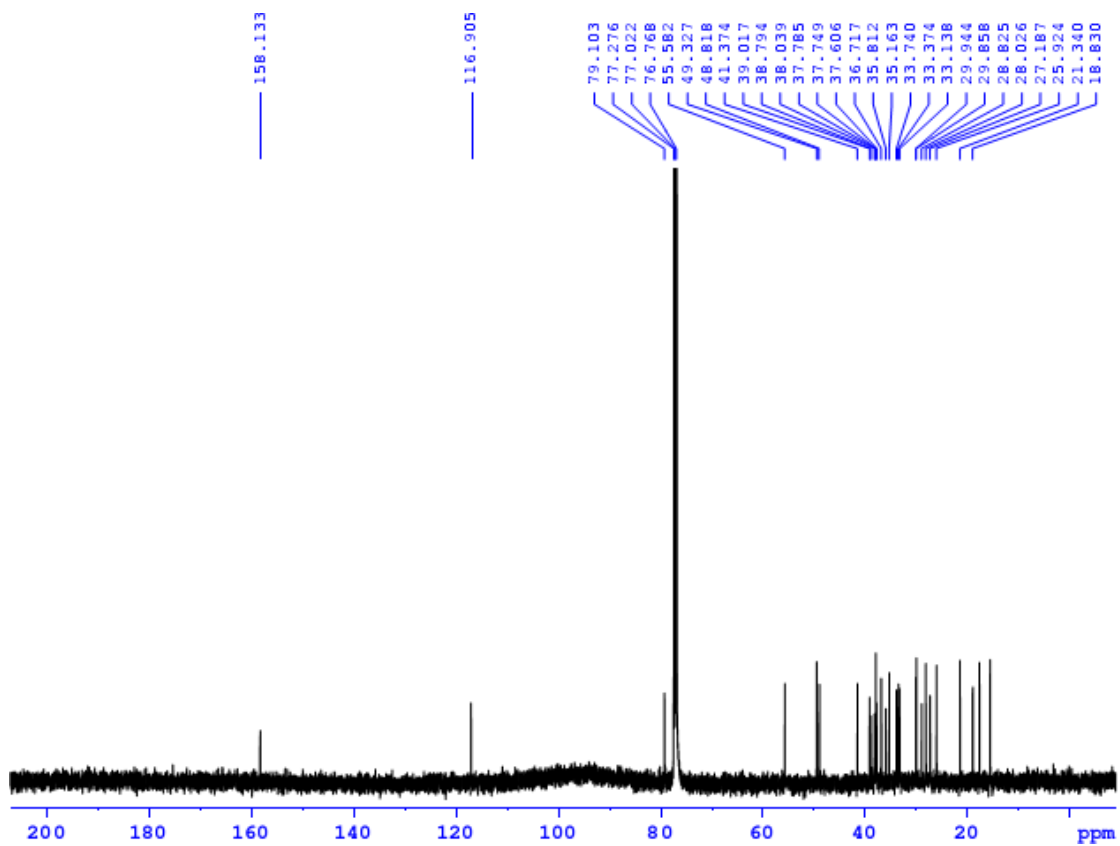


Figure S60: ^{13}C -NMR spectrum of compound **9**.

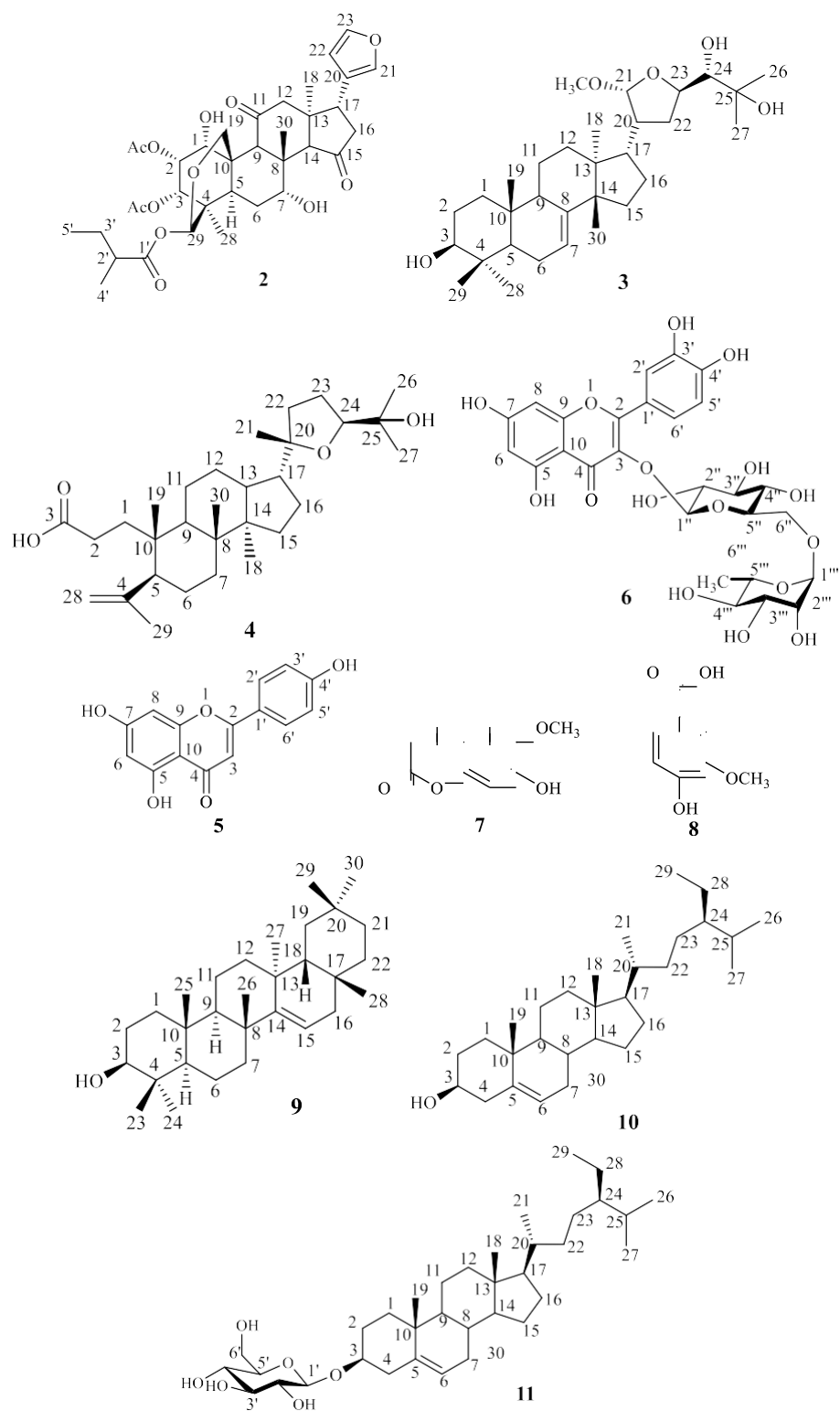


Figure S61: The structure of compounds **2-11**

meliatoxin B1 (**2**), meliasenin S (**3**), eichlerianic acid (**4**), apigenin (**5**), quercetin 3-*O*-[α -L-rhamnopyranosyl-(1 \rightarrow 6)]- β -D- glucopyranoside (rutin) (**6**), scopoletin (**7**), vanillic acid (**8**), taraxerol (**9**), β -sitosterol (**10**), and β -sitosterol-3-*O*- β -D-glucopyranoside (**11**)

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