

## Supporting Information

*Rec. Nat. Prod.* X:X (202X) XX-XX

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

Nguyen Ngoc Tuan<sup>1,†</sup>, Ping-Chung Kuo<sup>2,†</sup>, Vu Dinh Hoang<sup>3</sup>,  
Vu Thi Hien<sup>4,5</sup>, Le Dang Quang<sup>6</sup>, Tran Trung Hieu<sup>4</sup>, Yue-Chiun Li<sup>2</sup>,  
Nguyen Tan Thanh<sup>7</sup>, Tian-Shung Wu<sup>2,8,\*</sup> and Tran Dinh Thang<sup>1,\*</sup>

<sup>1</sup> *Institute of Biotechnology and Food Technology, Industrial University of Ho Chi Minh City, Ho Chi Minh City, Vietnam*

<sup>2</sup> *School of Pharmacy, College of Medicine, National Cheng Kung University, Tainan, Taiwan*

<sup>3</sup> *The School of Chemical Engineering, Hanoi University of Science and Technology, Hanoi, Vietnam*

<sup>4</sup> *School of Natural Sciences Education, Vinh University, Vinh City, Vietnam*

<sup>5</sup> *Faculty of Hydrometeorology, Ho Chi Minh City University of Natural Resources and Environment, Ho Chi Minh City, Vietnam*

<sup>6</sup> *R&D Center of Bioactive Compounds, Vietnam Institute of Industrial Chemistry, Hanoi, Vietnam*

<sup>7</sup> *School of Chemistry, Biology and Environment, Vinh University, Vinh City, Vietnam*

<sup>8</sup> *Department of Pharmacy, College of Pharmacy and Health Care, Tajen University, Pingtung, Taiwan*

Table of Contents	Page
<b>Table S1:</b> Comparison table of the NMR data of Trichllins G and E	4
<b>Figure S1:</b> <sup>1</sup> H NMR spectrum of compound 1.	5
<b>Figure S2:</b> <sup>1</sup> H NMR spectrum of compound 1.	6
<b>Figure S3:</b> <sup>1</sup> H NMR spectrum of compound 1.	6
<b>Figure S4:</b> <sup>13</sup> C NMR spectrum of compound 1.	7
<b>Figure S5:</b> <sup>13</sup> C NMR spectrum of compound 1.	7
<b>Figure S6:</b> <sup>13</sup> C NMR spectrum of compound 1.	8

\*Corresponding author: E-Mail: tswu@mail.ncku.edu.tw; Phone/Fax: 886-6-2747538

\*Corresponding author: E-Mail: thangtd@iuh.edu.vn; Phone:084-0913049689 Fax:084-0913049689

---

<b>Figure S7:</b> $^{13}\text{C}$ NMR spectrum of compound <b>1</b> .	8
<b>Figure S8:</b> DEPT spectrum of compound <b>1</b> .	9
<b>Figure S9:</b> DEPT spectrum of compound <b>1</b> .	9
<b>Figure S10:</b> COSY spectrum of compound <b>1</b> .	10
<b>Figure S11:</b> COSY spectrum of compound <b>1</b> .	11
<b>Figure S12:</b> COSY spectrum of compound <b>1</b> .	12
<b>Figure S13:</b> NOESY spectrum of compound <b>1</b> .	13
<b>Figure S14:</b> NOESY spectrum of compound <b>1</b> .	14
<b>Figure S15:</b> NOESY spectrum of compound <b>1</b> .	15
<b>Figure S16:</b> NOESY spectrum of compound <b>1</b> .	16
<b>Figure S17:</b> HSQC spectrum of compound <b>1</b> .	17
<b>Figure S18:</b> HSQC spectrum of compound <b>1</b> .	18
<b>Figure S19:</b> HSQC spectrum of compound <b>1</b> .	19
<b>Figure S20:</b> HSQC spectrum of compound <b>1</b> .	20
<b>Figure S21:</b> HSQC spectrum of compound <b>1</b> .	21
<b>Figure S22:</b> HMBC spectrum of compound <b>1</b> .	22
<b>Figure S23:</b> HMBC spectrum of compound <b>1</b> .	23
<b>Figure S24:</b> HMBC spectrum of compound <b>1</b> .	24
<b>Figure S25:</b> HMBC spectrum of compound <b>1</b> .	25
<b>Figure S26:</b> MS spectrum of compound <b>1</b> .	26
<b>Figure S27:</b> HRMS spectrum of compound <b>1</b> .	27
<b>Figure S28:</b> UV spectrum of compound <b>1</b> .	28
<b>Figure S29:</b> IR spectrum of compound <b>1</b> .	28
<b>Figure S30:</b> $^1\text{H}$ NMR spectrum of compound <b>2</b> .	29
<b>Figure S31:</b> $^{13}\text{C}$ NMR spectrum of compound <b>2</b> .	30
<b>Figure S32:</b> DEPT spectrum of compound <b>2</b> .	31
<b>Figure S33:</b> HMBC spectrum of compound <b>2</b> .	32
<b>Figure S34:</b> NOESY spectrum of compound <b>2</b> .	33
<b>Figure S35:</b> COSY spectrum of compound <b>2</b> .	34
<b>Figure S36:</b> $^1\text{H}$ NMR spectrum of compound <b>3</b> .	35
<b>Figure S37:</b> $^{13}\text{C}$ NMR spectrum of compound <b>3</b> .	36
<b>Figure S38:</b> DEPT spectrum of compound <b>3</b> .	37
<b>Figure S39:</b> HMBC spectrum of compound <b>3</b> .	38
<b>Figure S40:</b> COSY spectrum of compound <b>3</b> .	39
<b>Figure S41:</b> $^1\text{H}$ NMR spectrum of compound <b>4</b> .	40

---

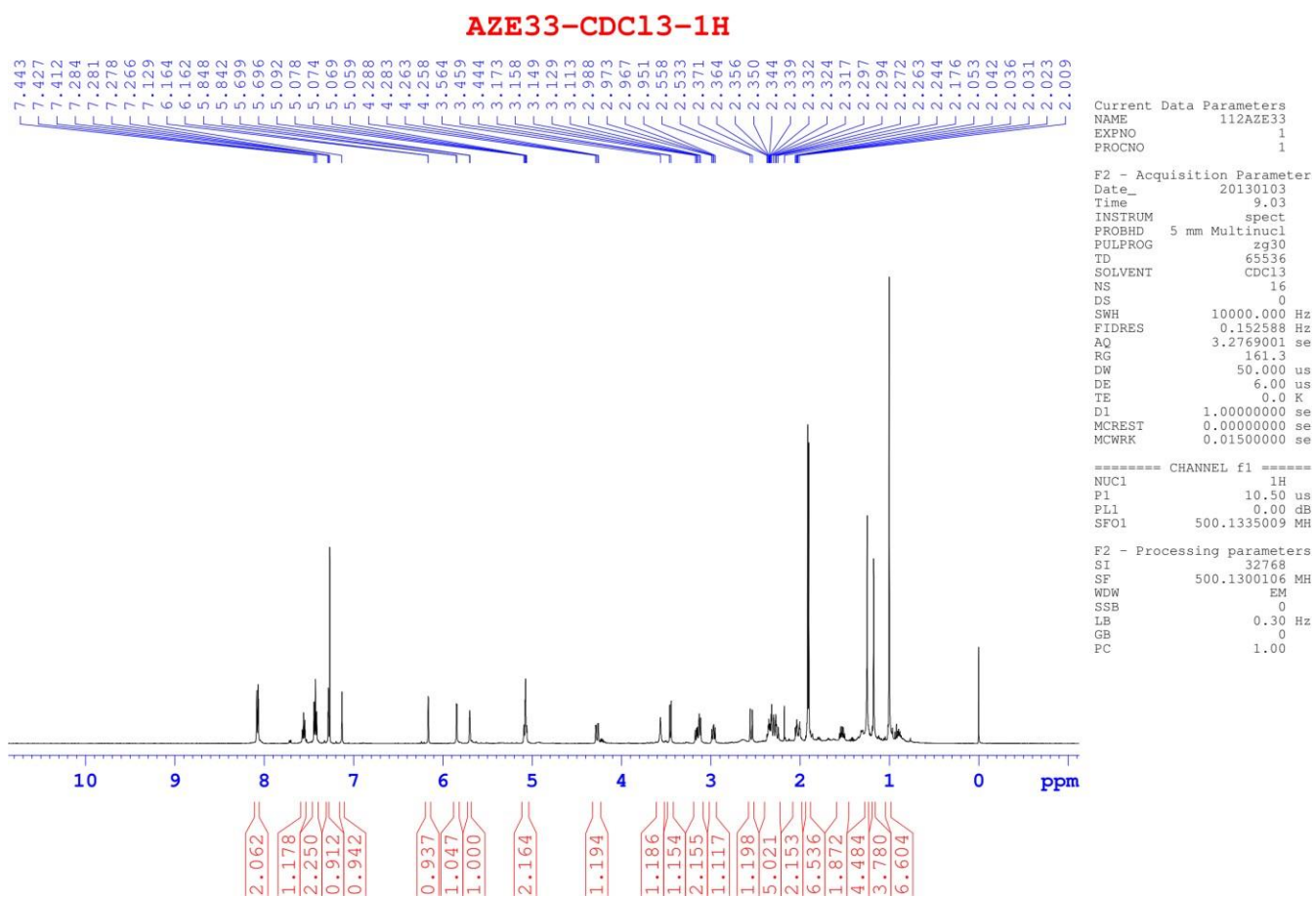
---

<b>Figure S42:</b> $^{13}\text{C}$ NMR spectrum of compound <b>4</b> .	41
<b>Figure S43:</b> DEPT spectrum of compound <b>4</b> .	42
<b>Figure S44:</b> HMBC spectrum of compound <b>4</b> .	43
<b>Figure S45:</b> NOESY spectrum of compound <b>4</b> .	44
<b>Figure S46:</b> COSY spectrum of compound <b>4</b> .	45
<b>Figure S47:</b> $^1\text{H}$ -NMR spectrum of compound <b>5</b> .	46
<b>Figure S48:</b> $^{13}\text{C}$ -NMR spectrum of compound <b>5</b> .	47
<b>Figure S49:</b> DEPT spectrum of compound <b>5</b> .	48
<b>Figure S50:</b> HMBC spectrum of compound <b>5</b> .	49
<b>Figure S51:</b> $^1\text{H}$ -NMR spectrum of compound <b>6</b> .	50
<b>Figure S52:</b> $^{13}\text{C}$ -NMR spectrum of compound <b>6</b> .	51
<b>Figure S53:</b> DEPT spectrum of compound <b>6</b> .	52
<b>Figure S54:</b> HMBC spectrum of compound <b>6</b> .	53
<b>Figure S55:</b> $^1\text{H}$ -NMR spectrum of compound <b>7</b> .	54
<b>Figure S56:</b> $^{13}\text{C}$ -NMR spectrum of compound <b>7</b> .	55
<b>Figure S57:</b> $^1\text{H}$ -NMR spectrum of compound <b>8</b> .	56
<b>Figure S58:</b> $^{13}\text{C}$ -NMR spectrum of compound <b>8</b> .	57
<b>Figure S59:</b> $^1\text{H}$ -NMR spectrum of compound <b>9</b> .	58
<b>Figure S60:</b> $^{13}\text{C}$ -NMR spectrum of compound <b>9</b> .	59
<b>Figure S61:</b> The structure of compounds <b>2-11</b>	60

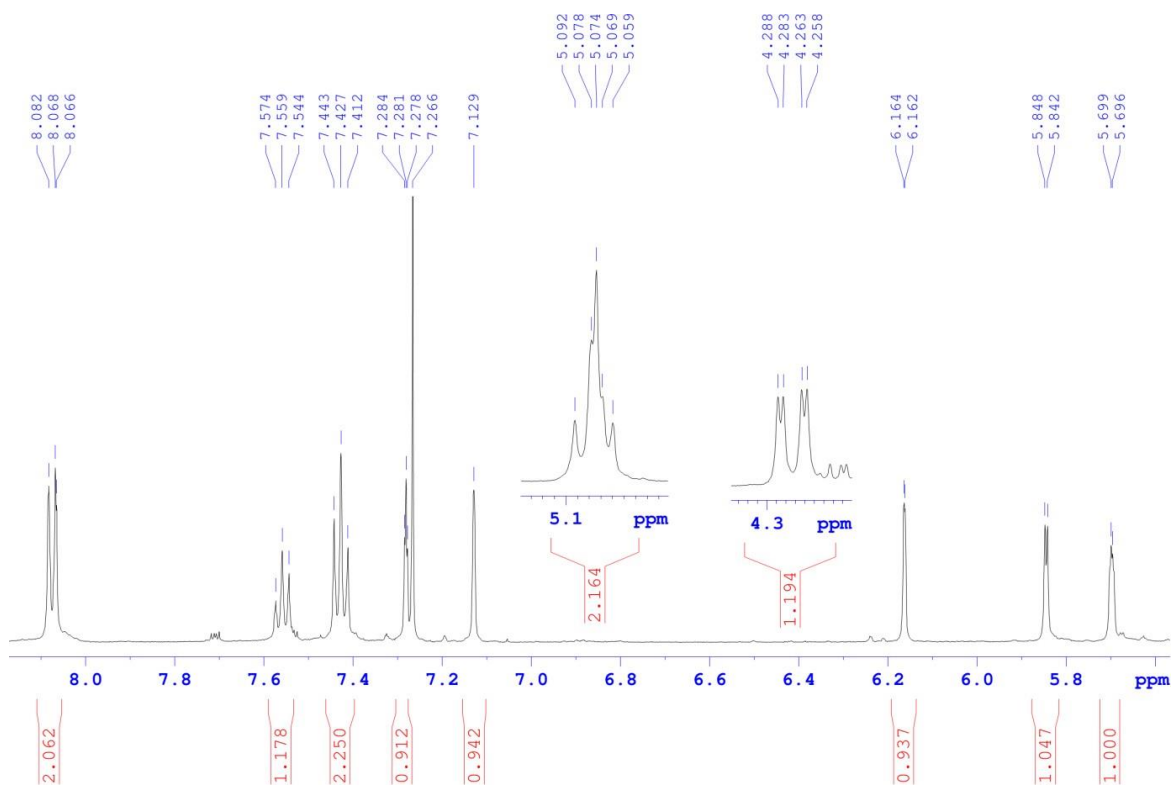
---

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

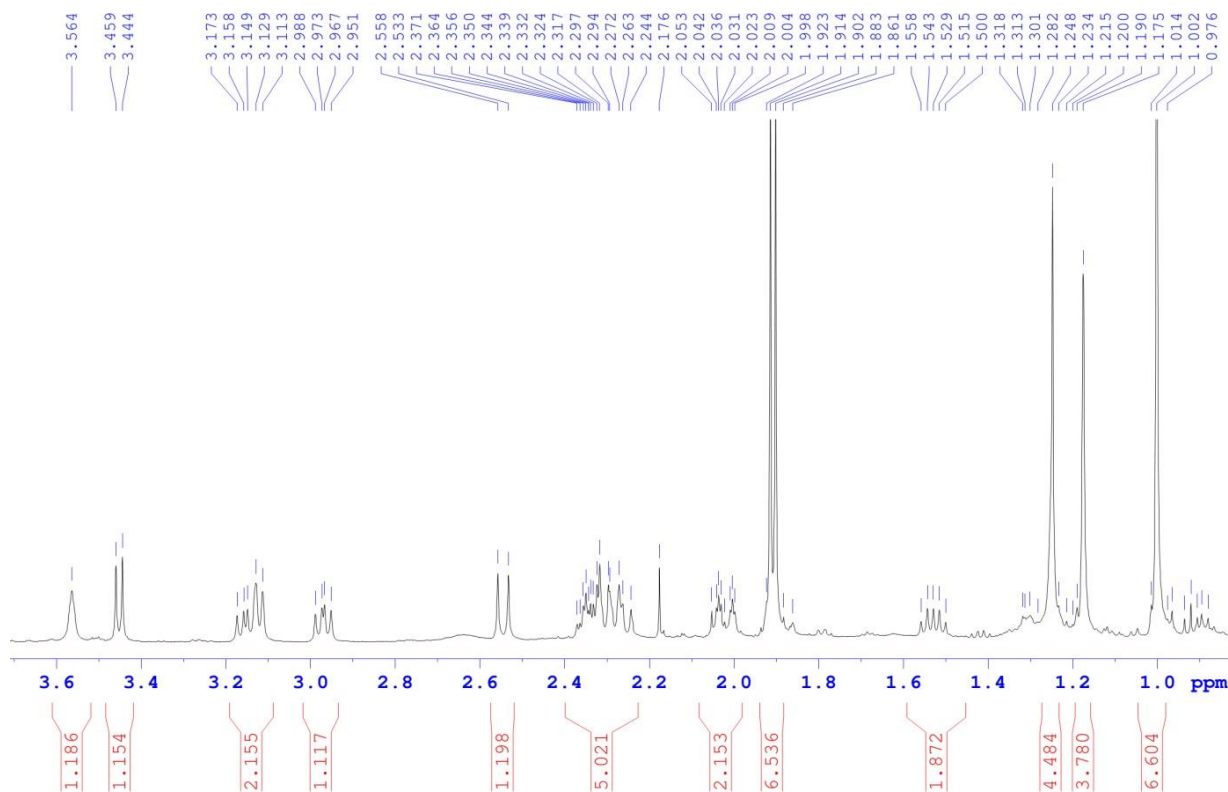
Position	trichilin G		trichilin E	
	$\delta_{\text{H}}$ (ppm, multi., $J$ in Hz)	$\delta_{\text{C}}$ (ppm)	$\delta_{\text{H}}$ (ppm, multi., $J$ in Hz)	$\delta_{\text{C}}$ (ppm)
1	3.56 (br s)	71.8	5.06 (br t, 2.9)	71.1
2	1.53 (m), 2.27 (m)	24.3	2.22 (dt, 16.3, 2.6), 2.34 (dt, 6.3, 3.1)	30.5
3	3.56 (br 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



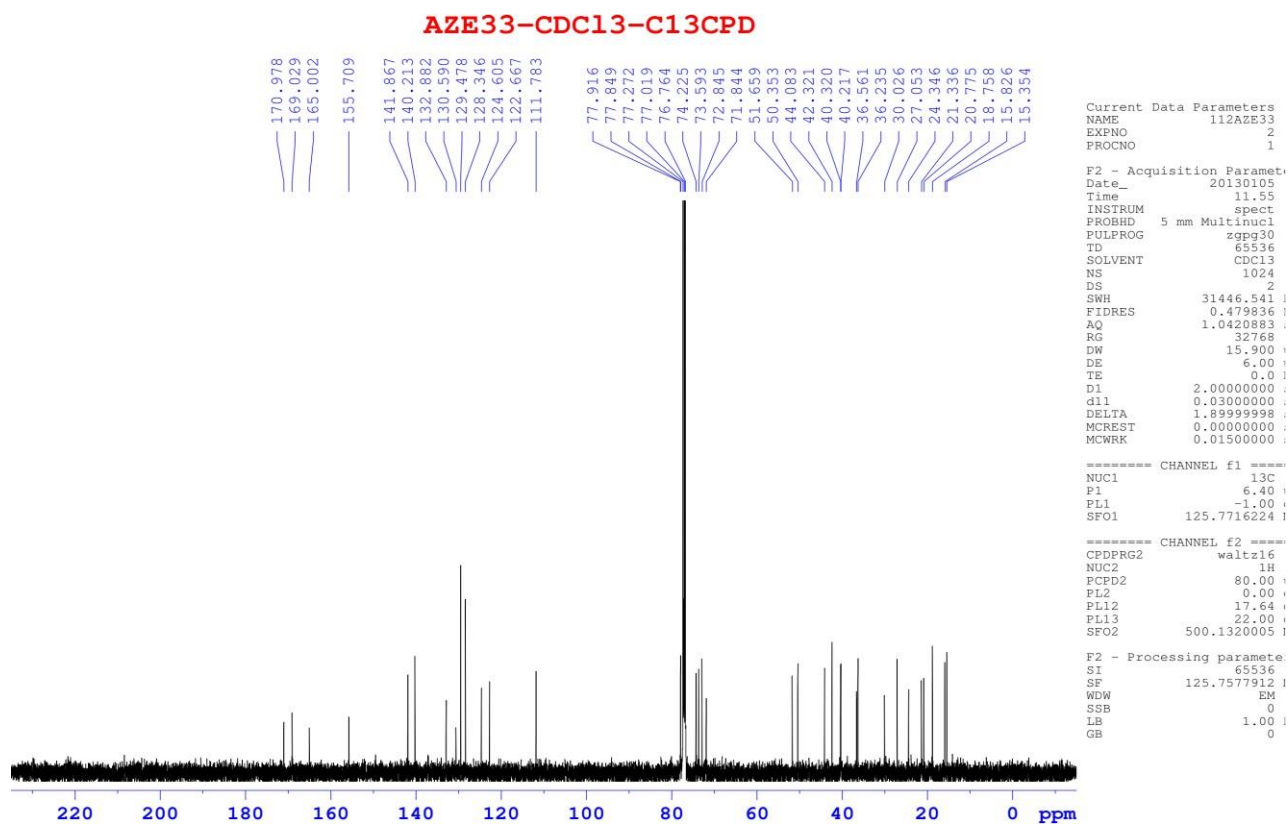
**Figure S1:**  $^1\text{H}$  NMR spectrum of compound **1**.



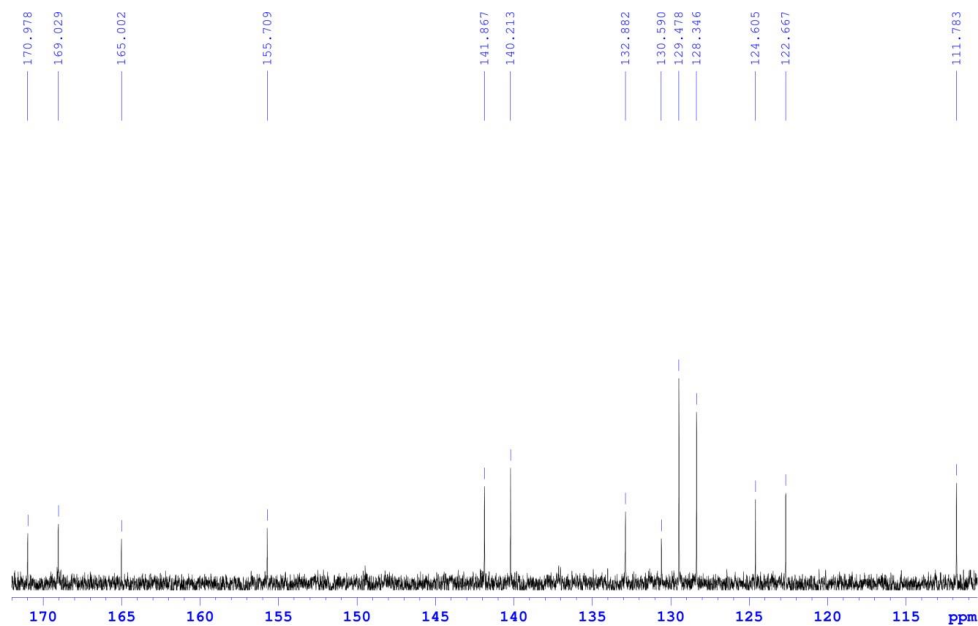
**Figure S2:**  $^1\text{H}$  NMR spectrum of compound **1**.



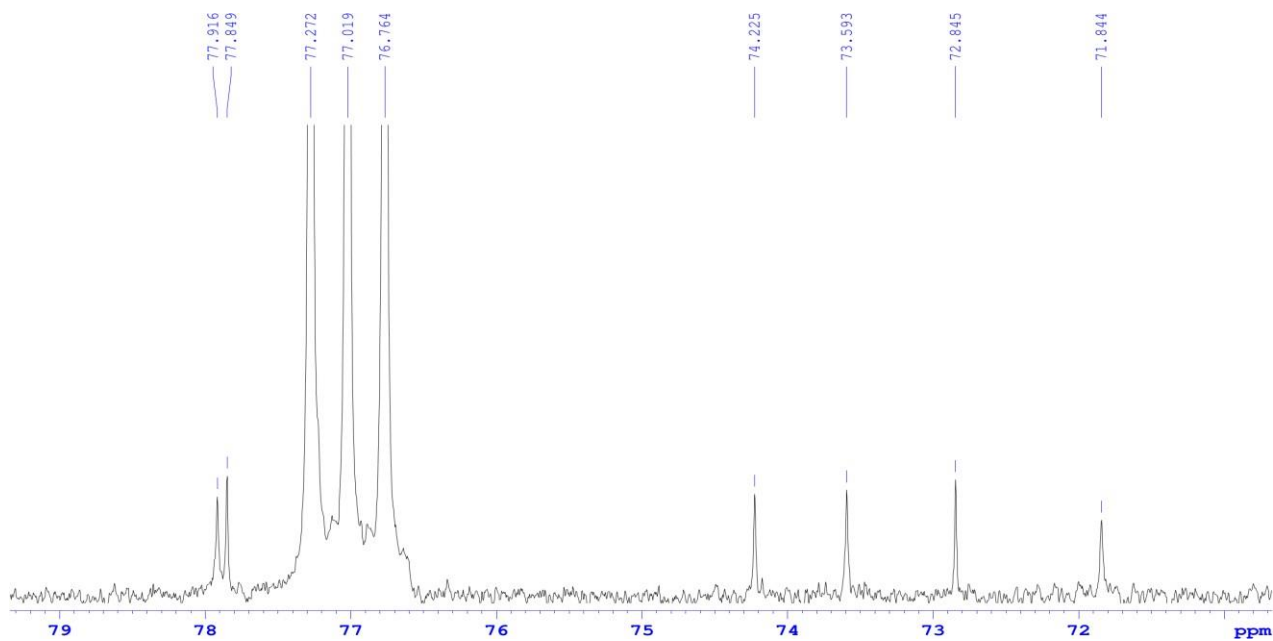
**Figure S3:**  $^1\text{H}$  NMR spectrum of compound **1**.



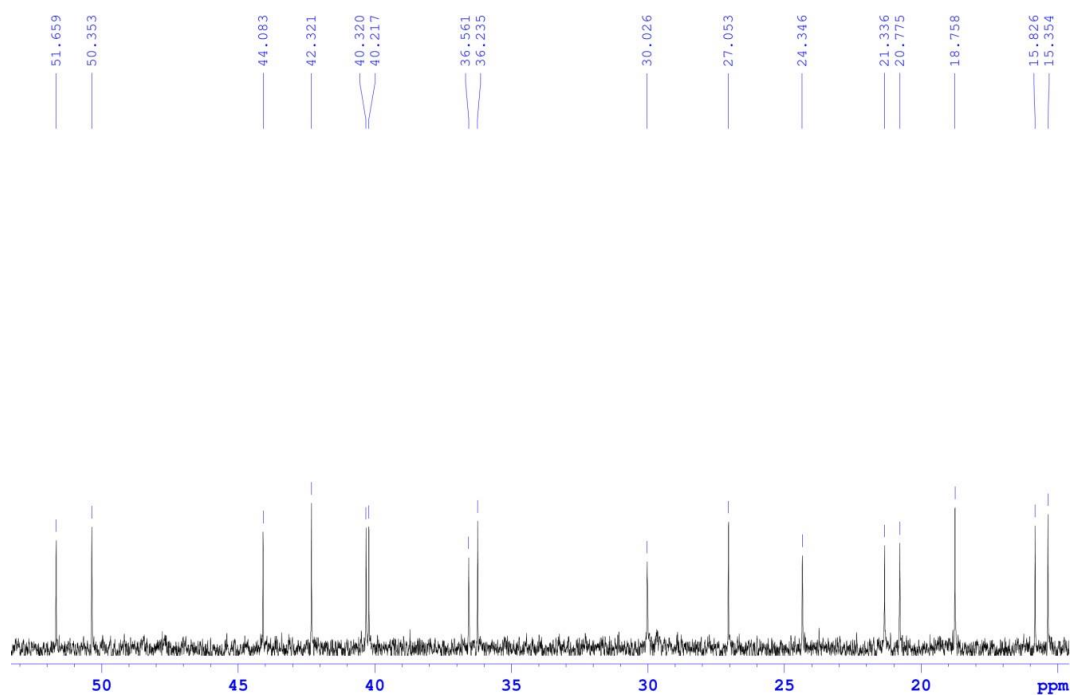
**Figure S4:**  $^{13}\text{C}$  NMR spectrum of compound **1**.



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



**Figure S6:**  $^{13}\text{C}$  NMR spectrum of compound 1.

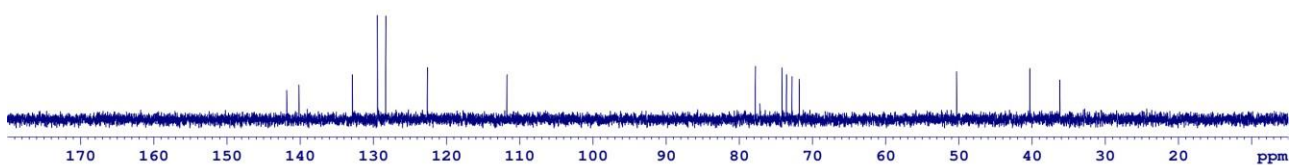


**Figure S7:**  $^{13}\text{C}$  NMR spectrum of compound 1.



AZE33-CDC13-C13CPD&DEPT

DEPT90



DEPT135

*CH&CH3*

*CH2*



C13CPD

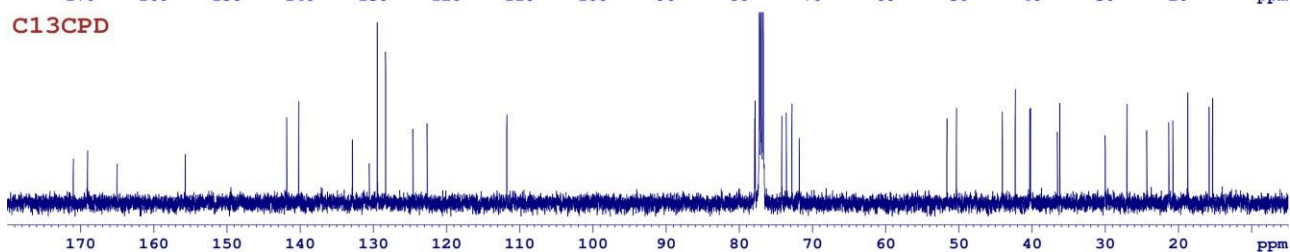
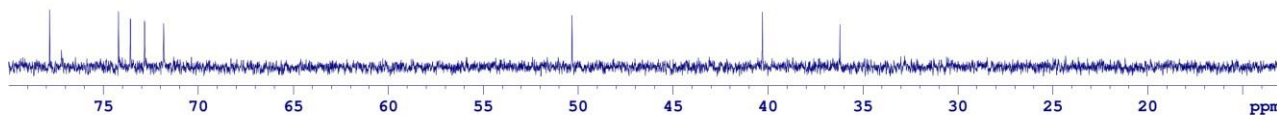


Figure S8: DEPT spectrum of compound 1.

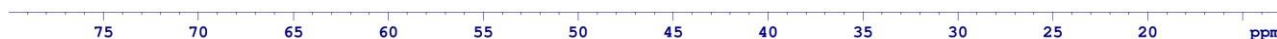
DEPT90



DEPT135

*CH&CH3*

*CH2*



C13CPD

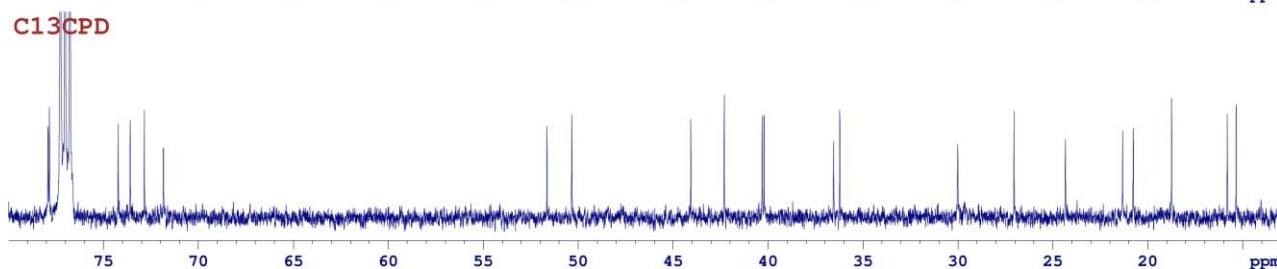
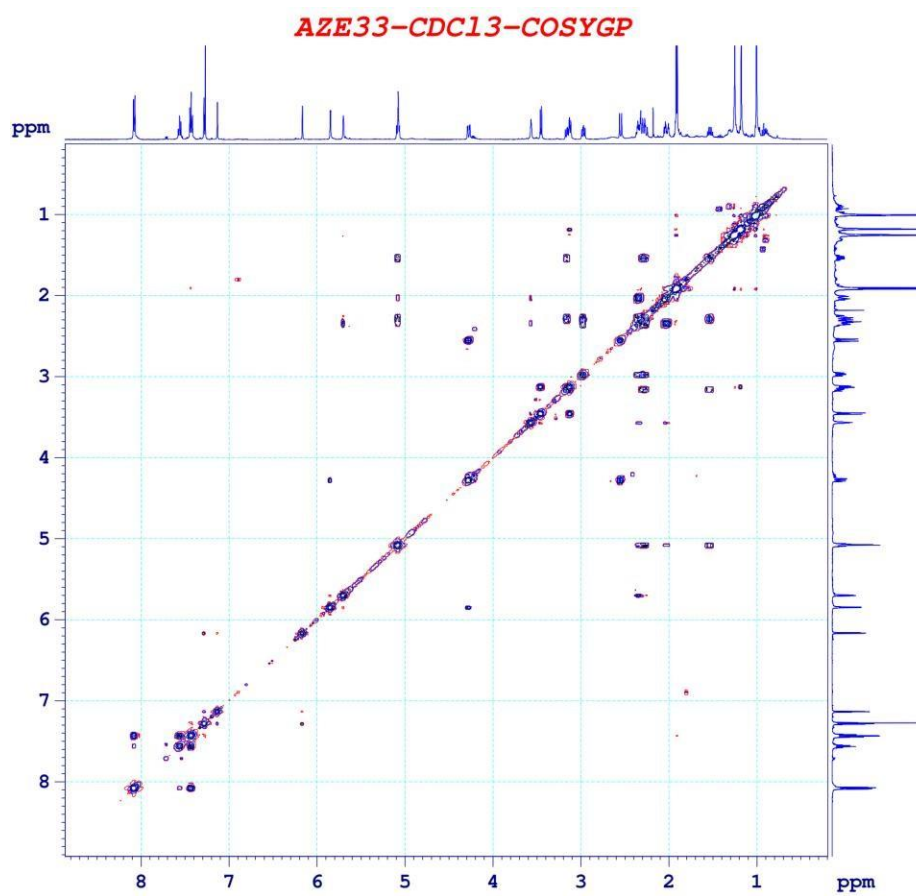
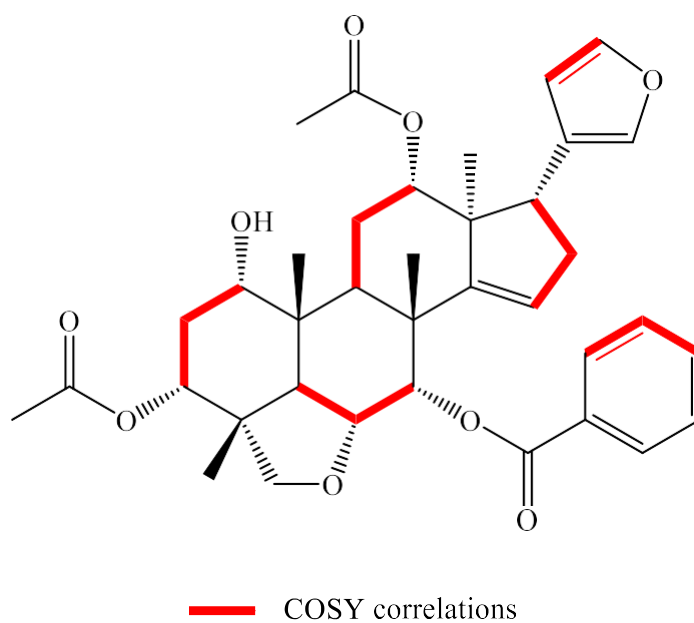
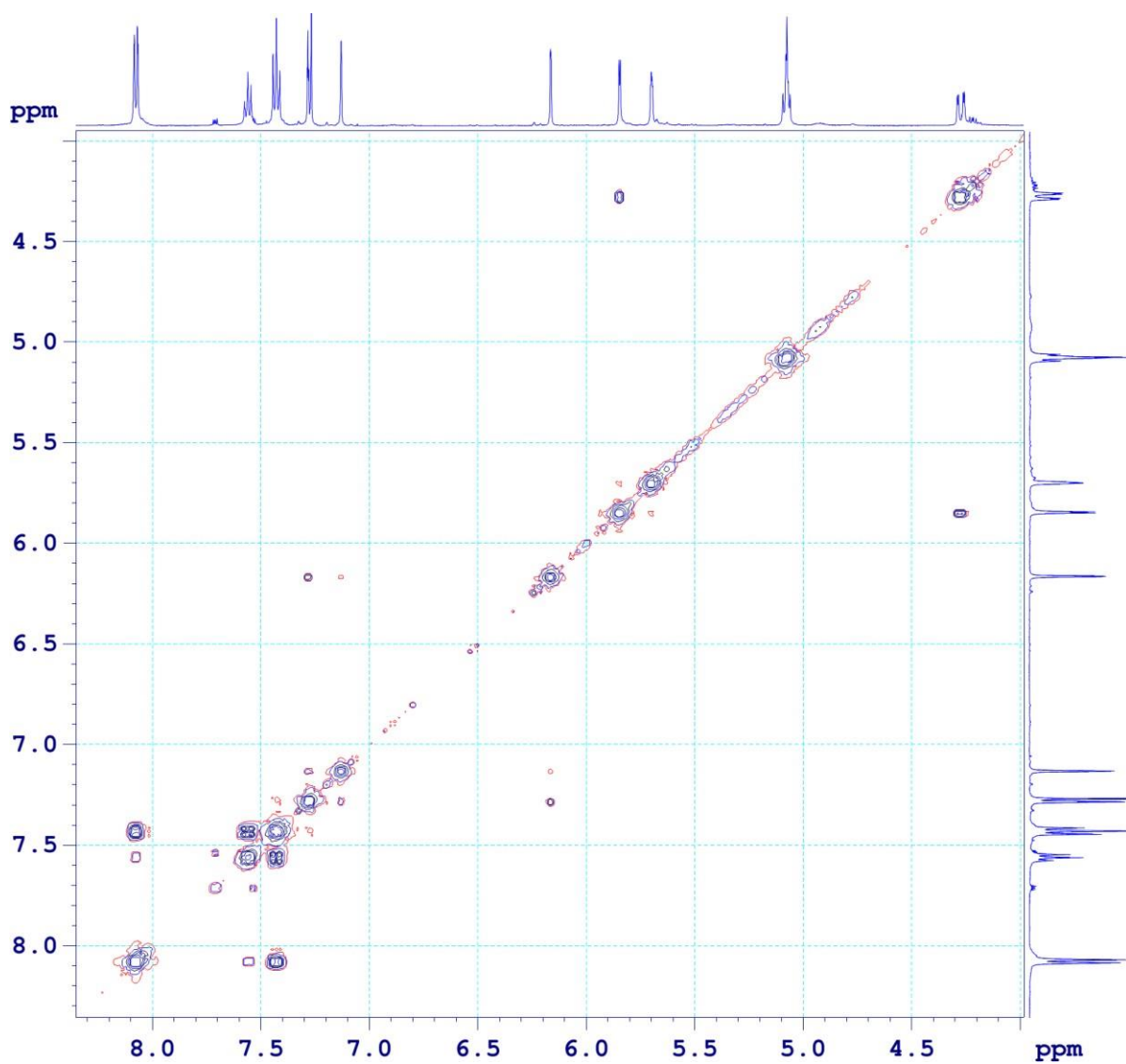


Figure S9: DEPT spectrum of compound 1.

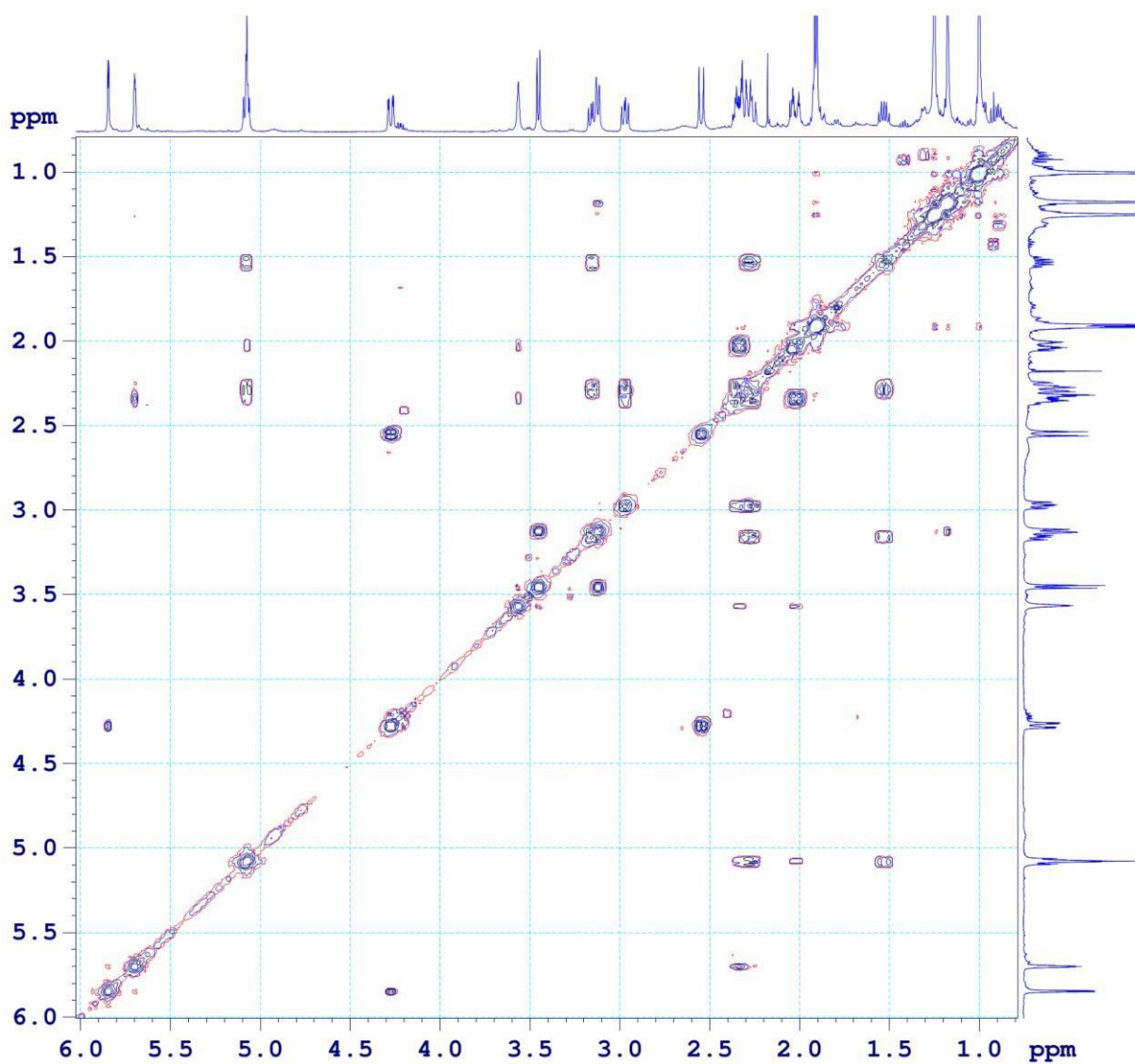


**Figure S10: COSY spectrum of compound 1.**

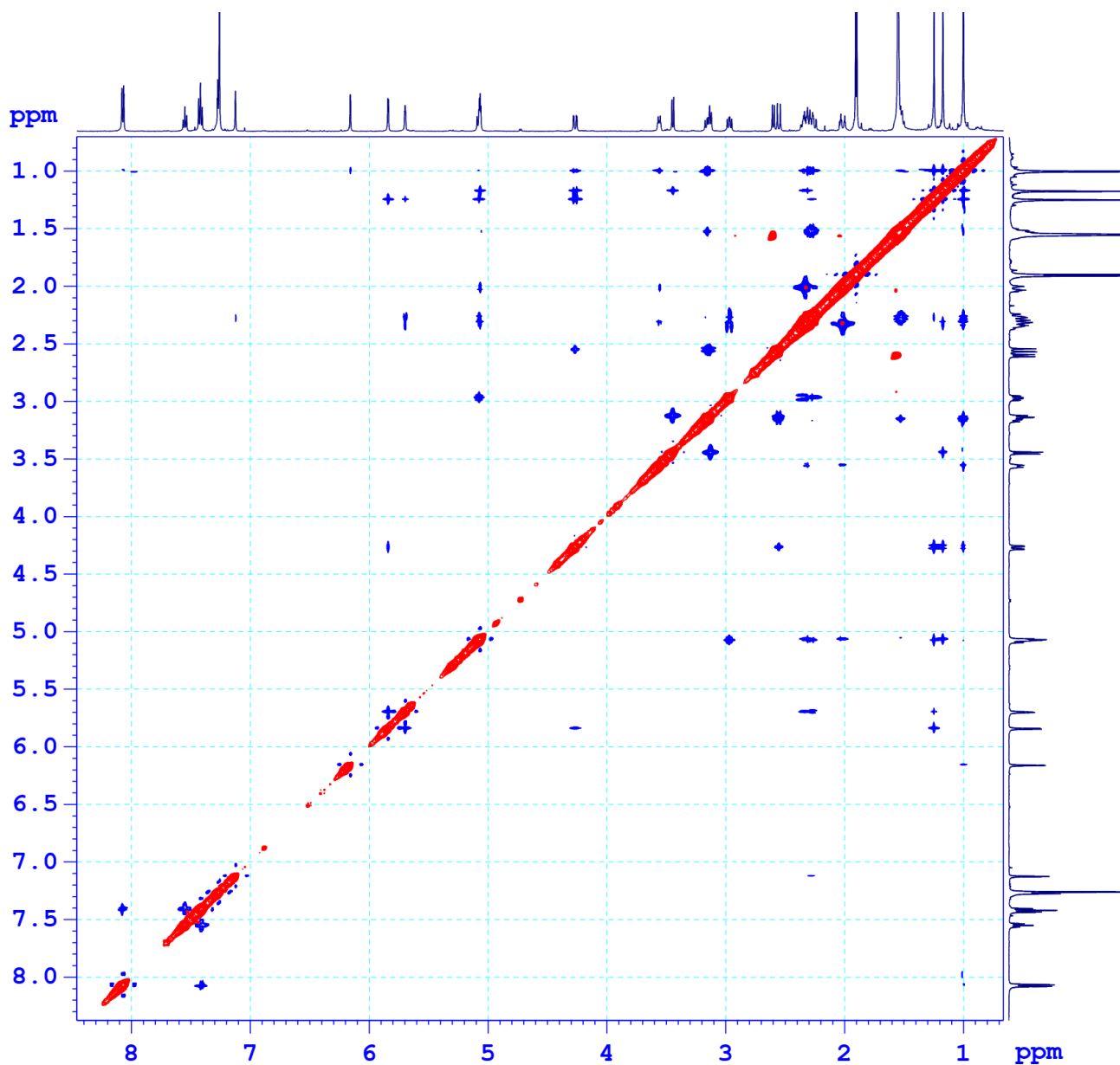




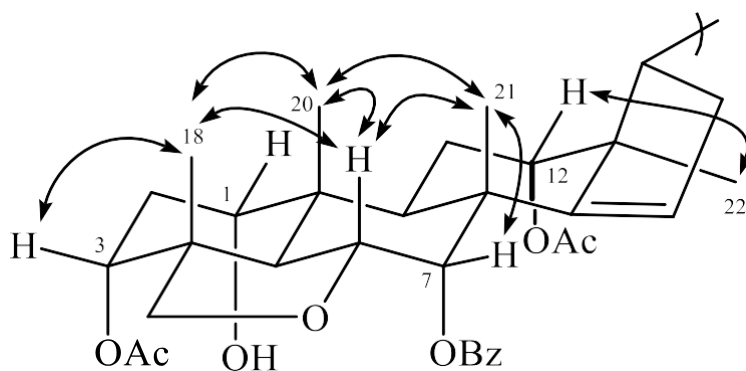
**Figure S11:** COSY spectrum of compound **1**.



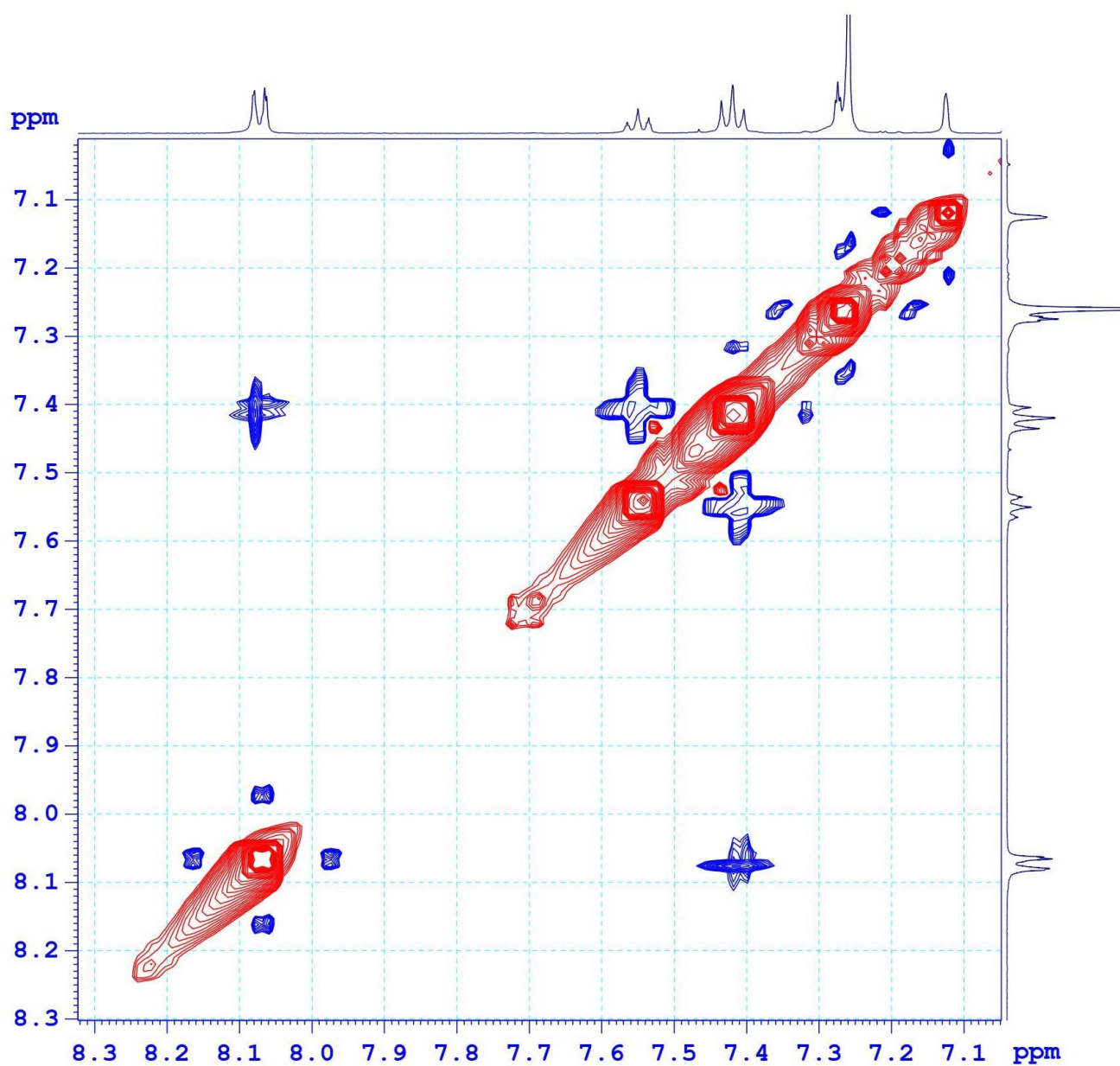
**Figure S12:** COSY spectrum of compound **1**.



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



© 2021 ACG Publications. All rights reserved.



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

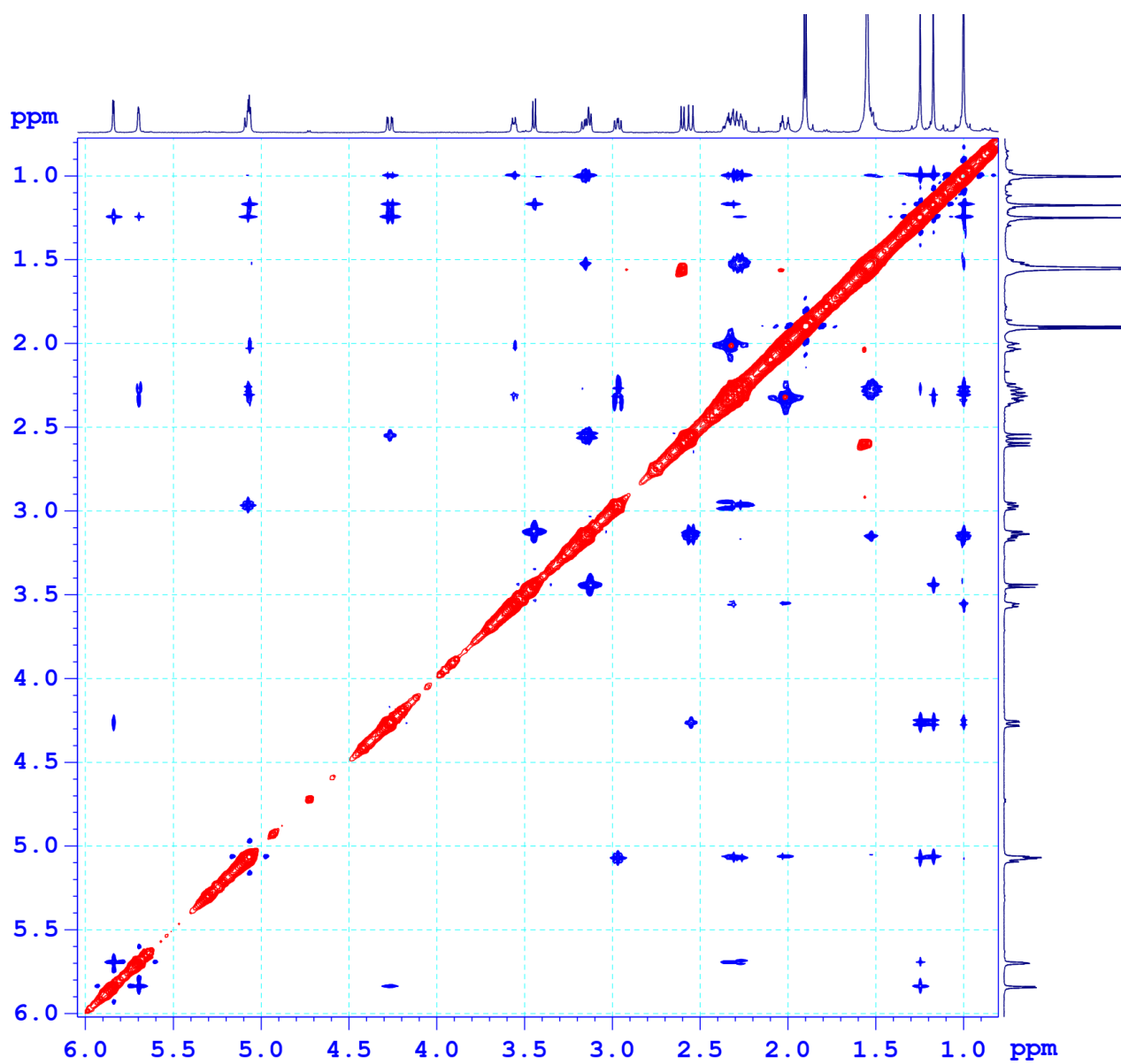
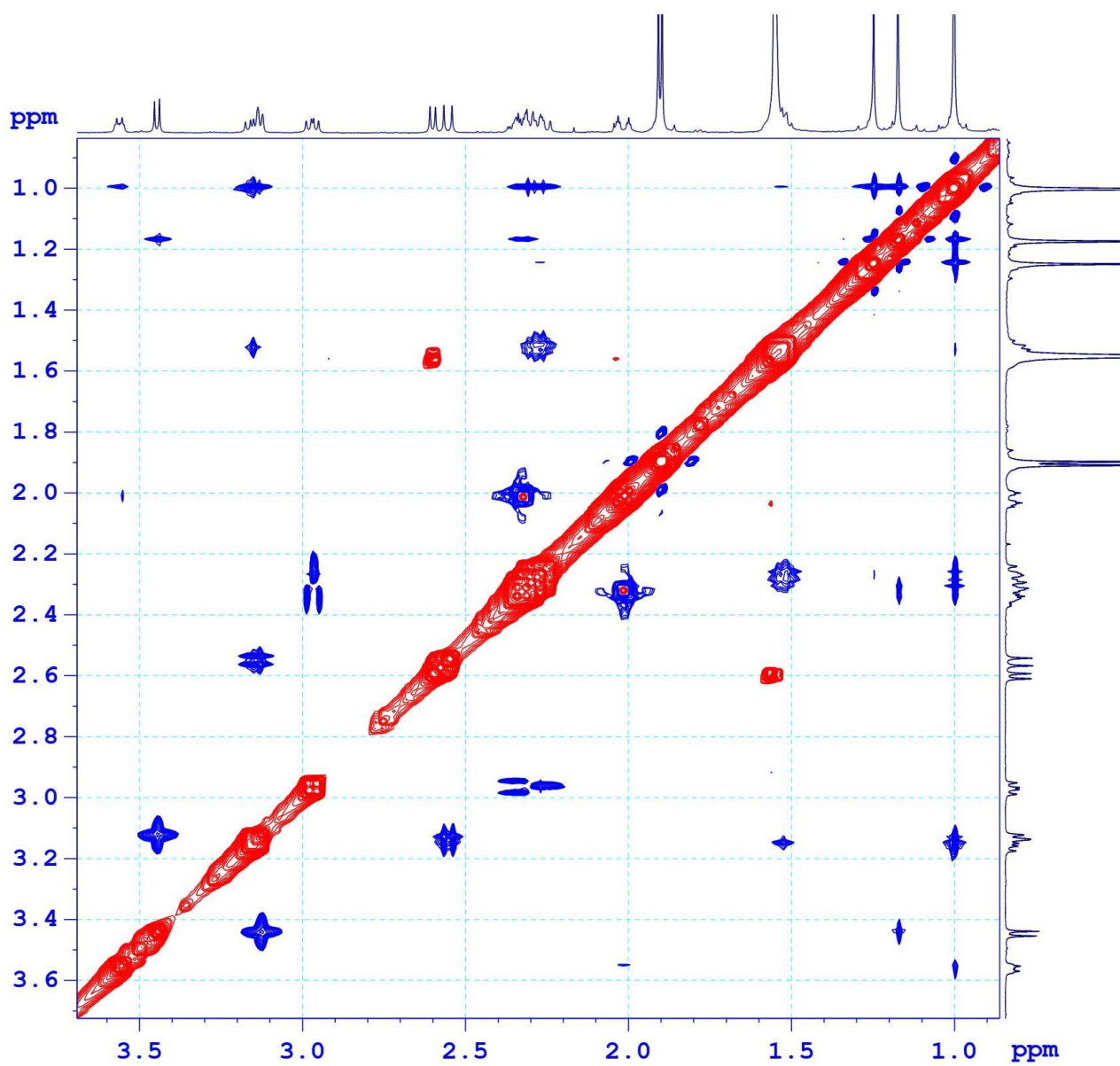


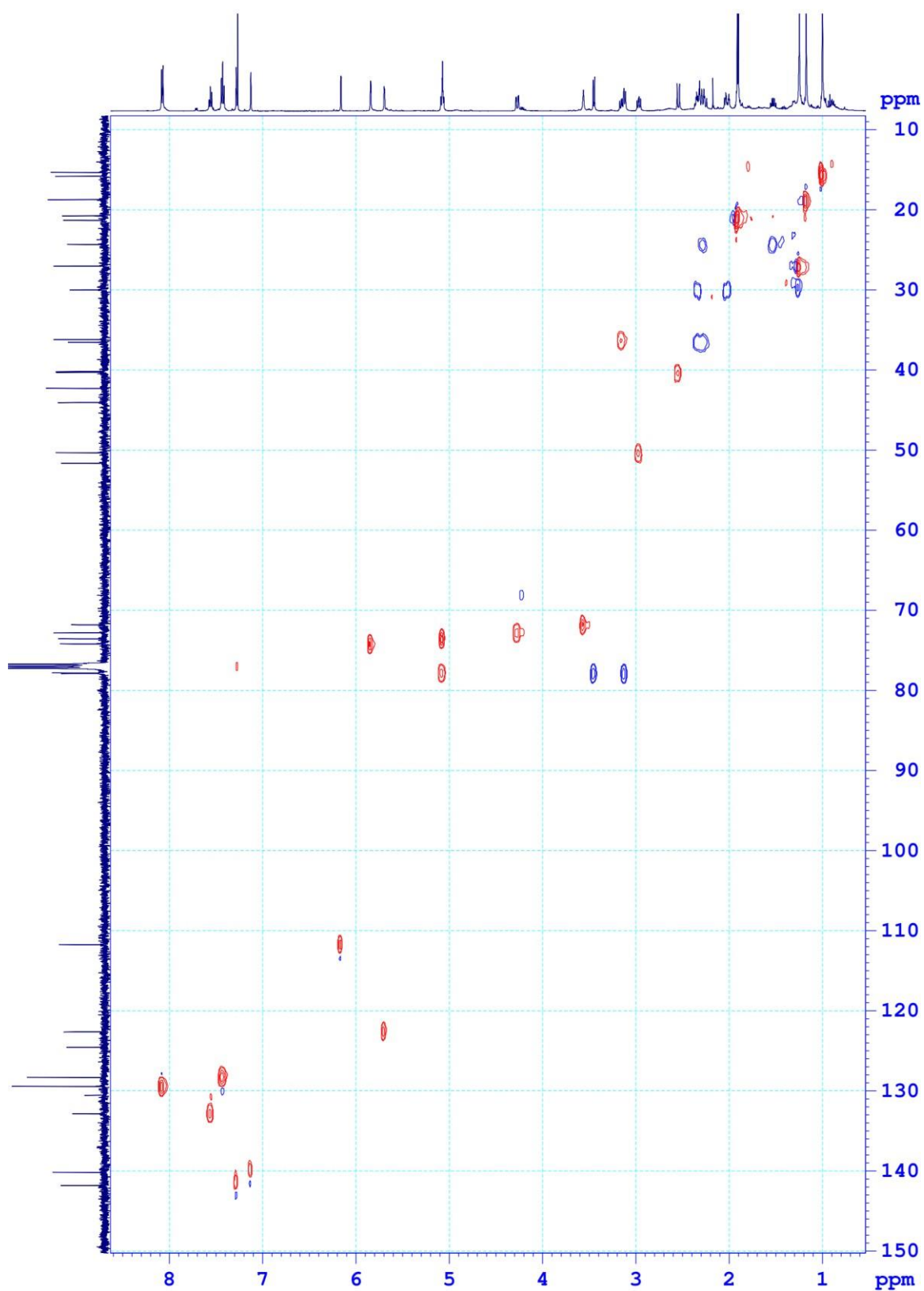
Figure S15: NOESY spectrum of compound 1.



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

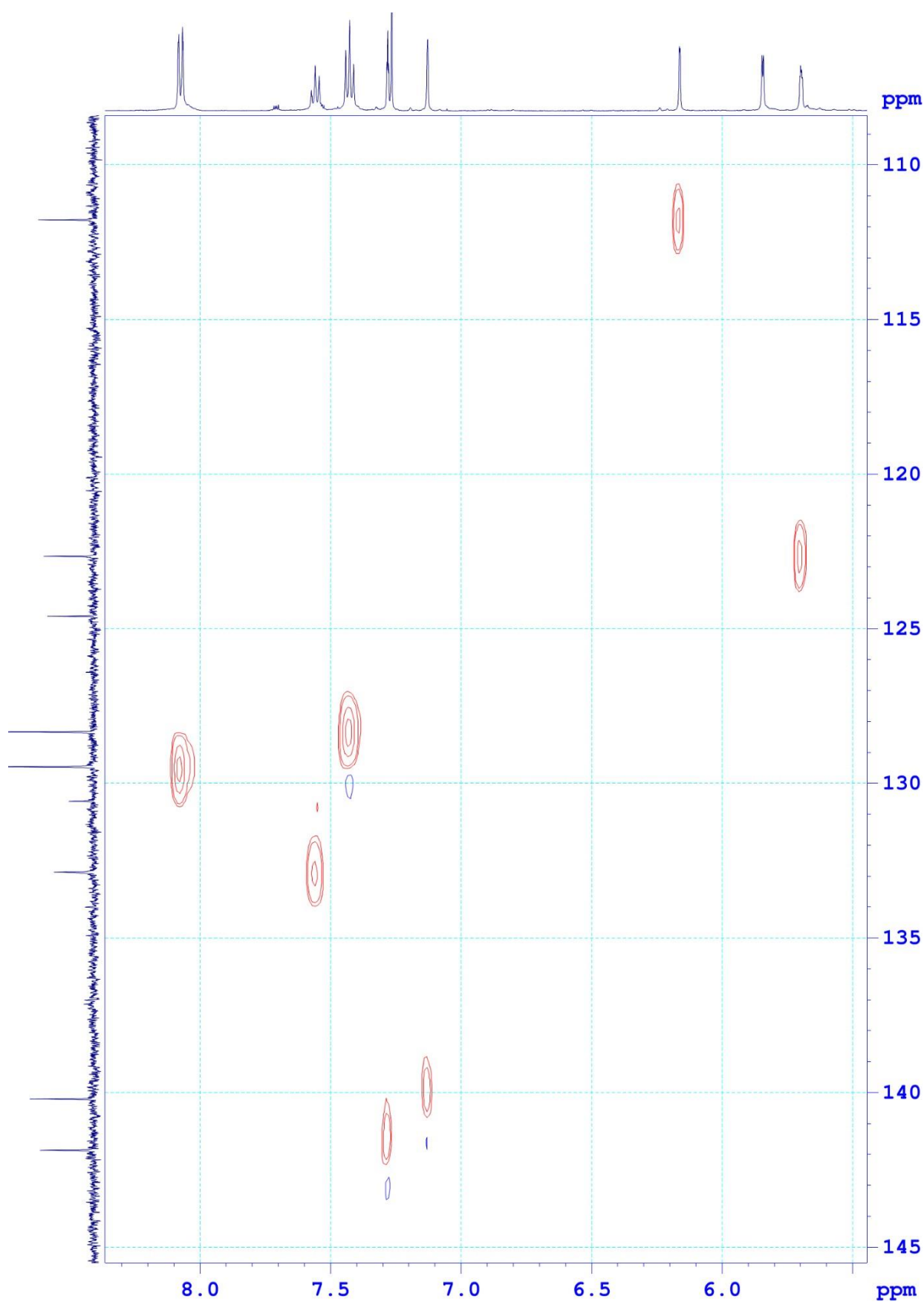


**AZE33-CDC13-HSQC**



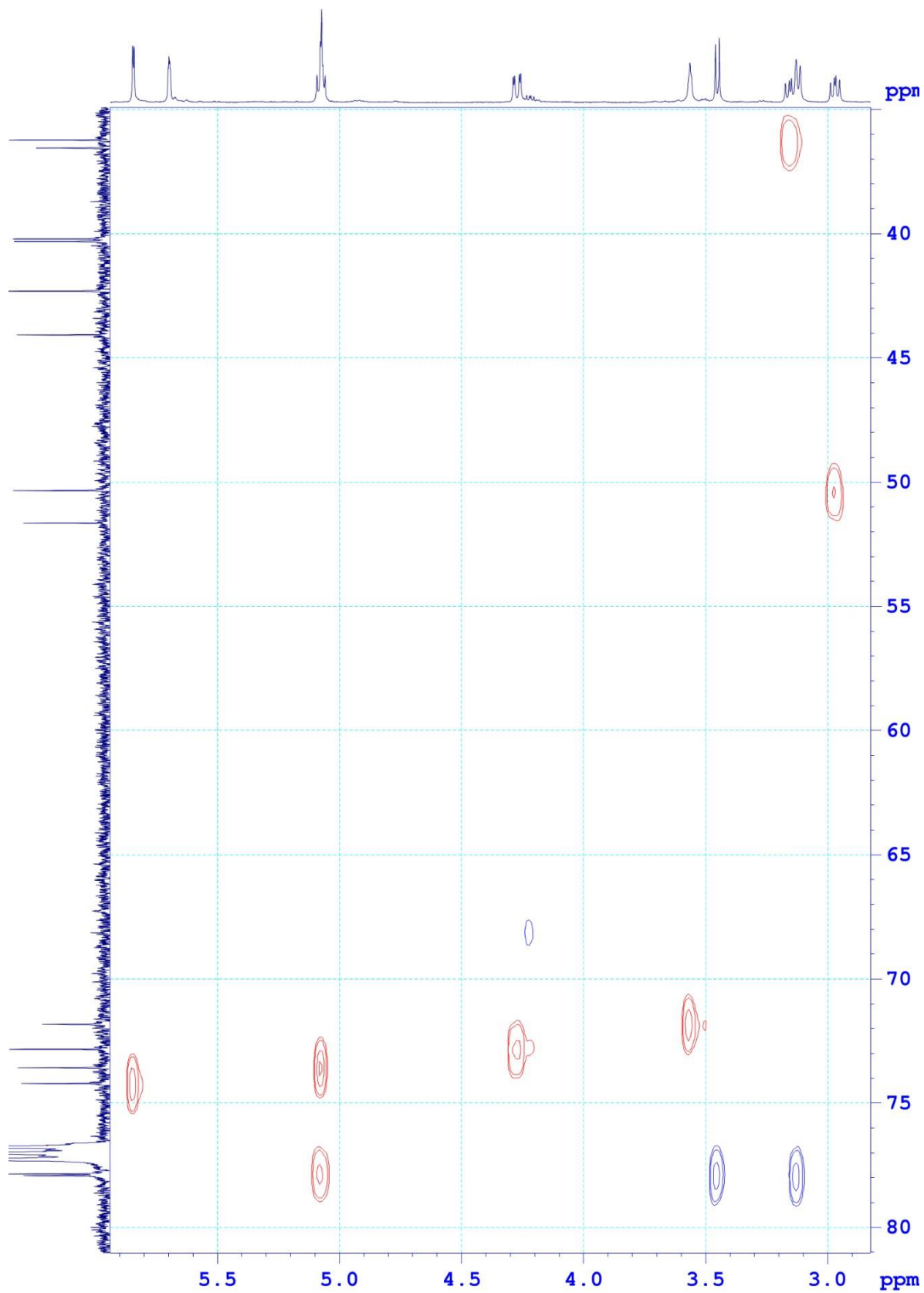
**Figure S17:** HSQC spectrum of compound **1**.

© 2021 ACG Publications. All rights reserved.



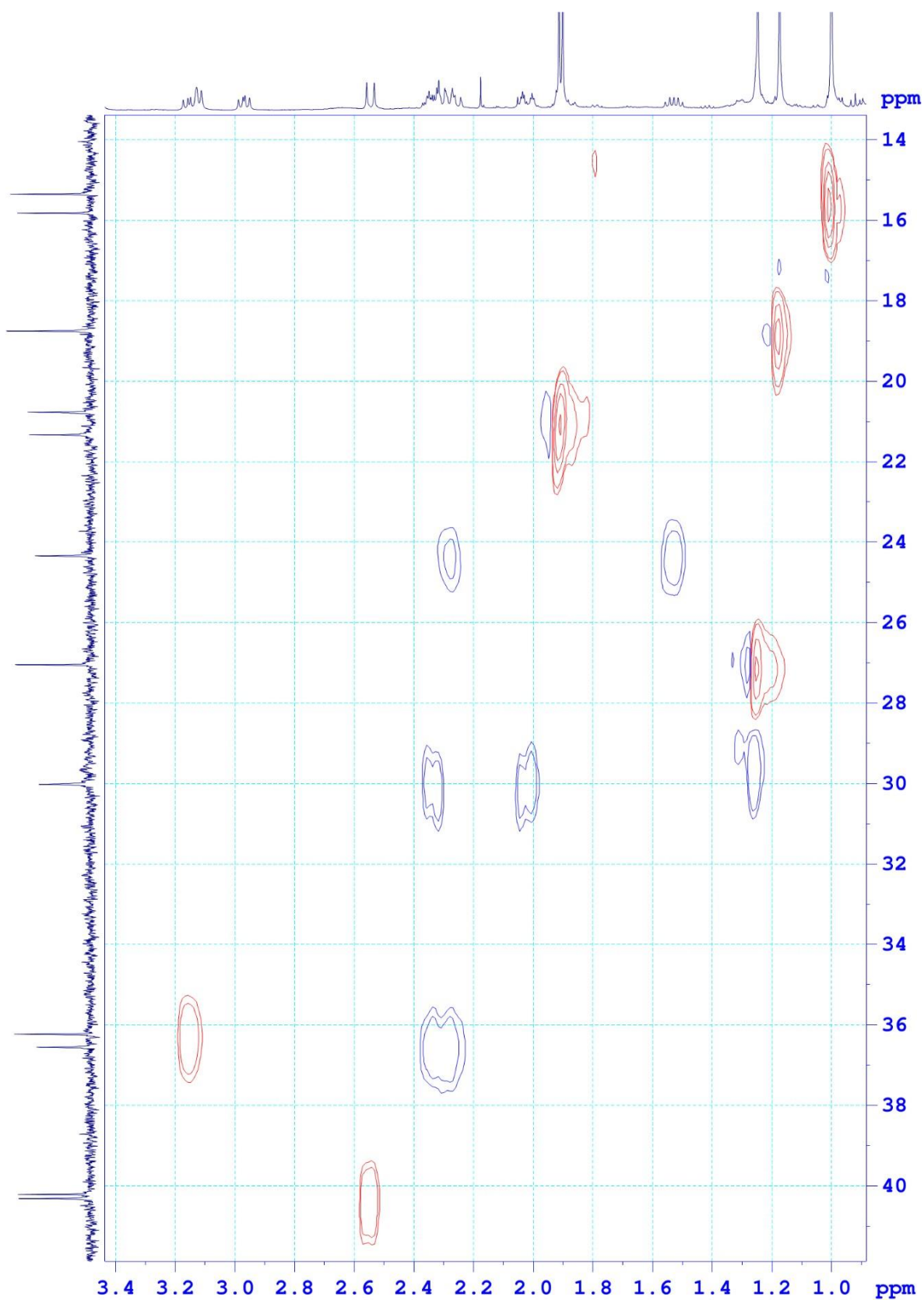
**Figure S18:** HSQC spectrum of compound **1**.

© 2021 ACG Publications. All rights reserved.

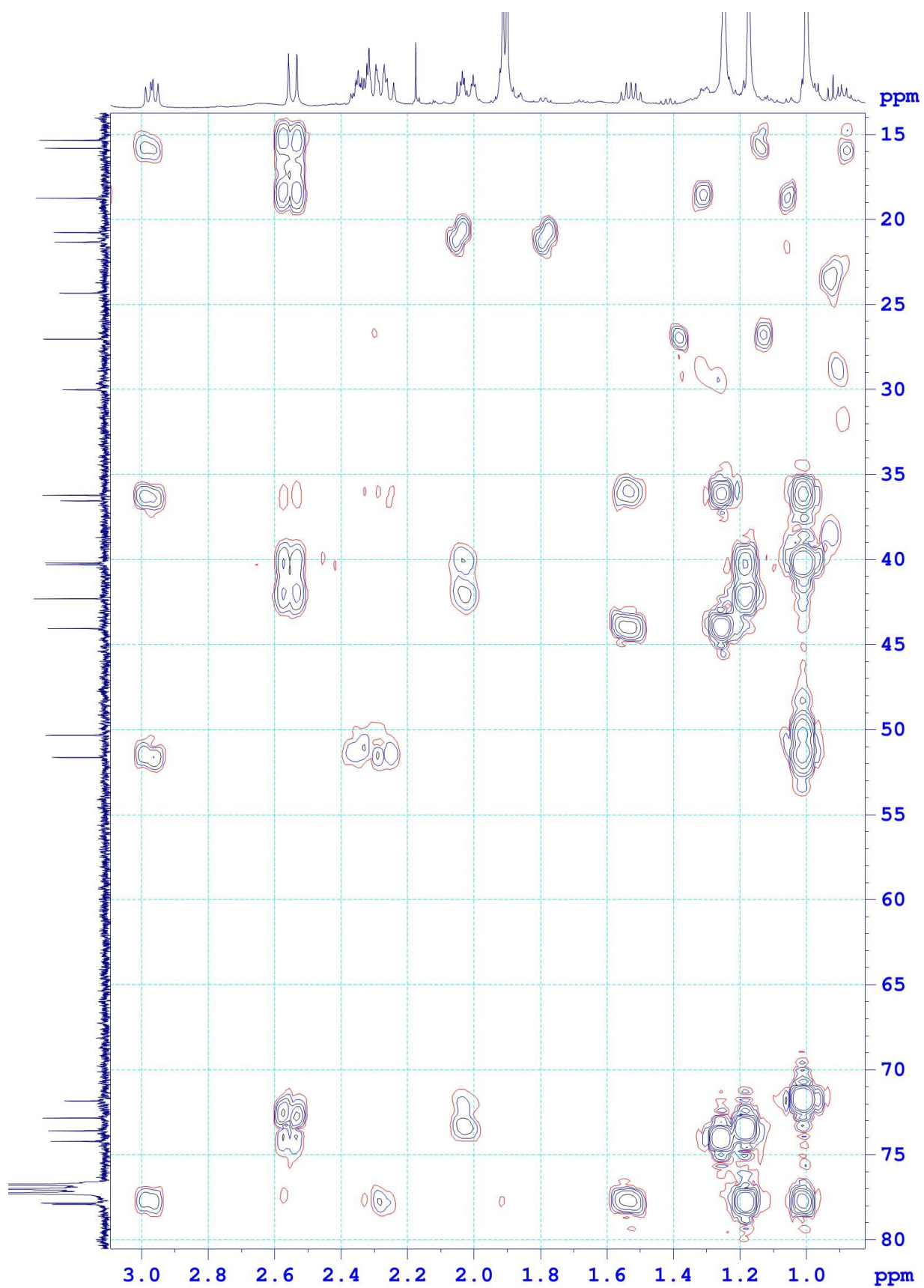


**Figure S19:** HSQC spectrum of compound **1**.

© 2021 ACG Publications. All rights reserved.



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



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

© 2021 ACG Publications. All rights reserved.

AZE33-CDC13-HMBC

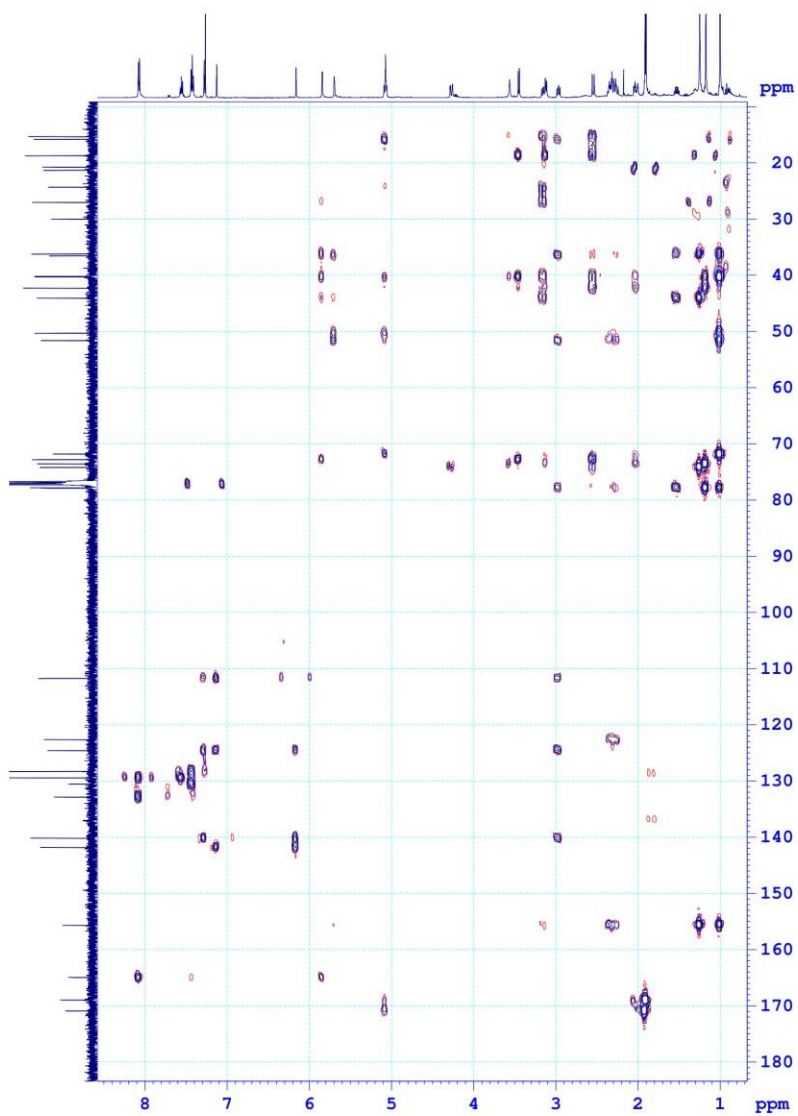
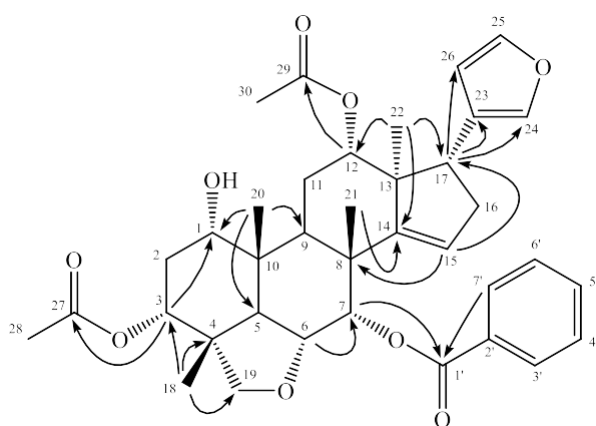
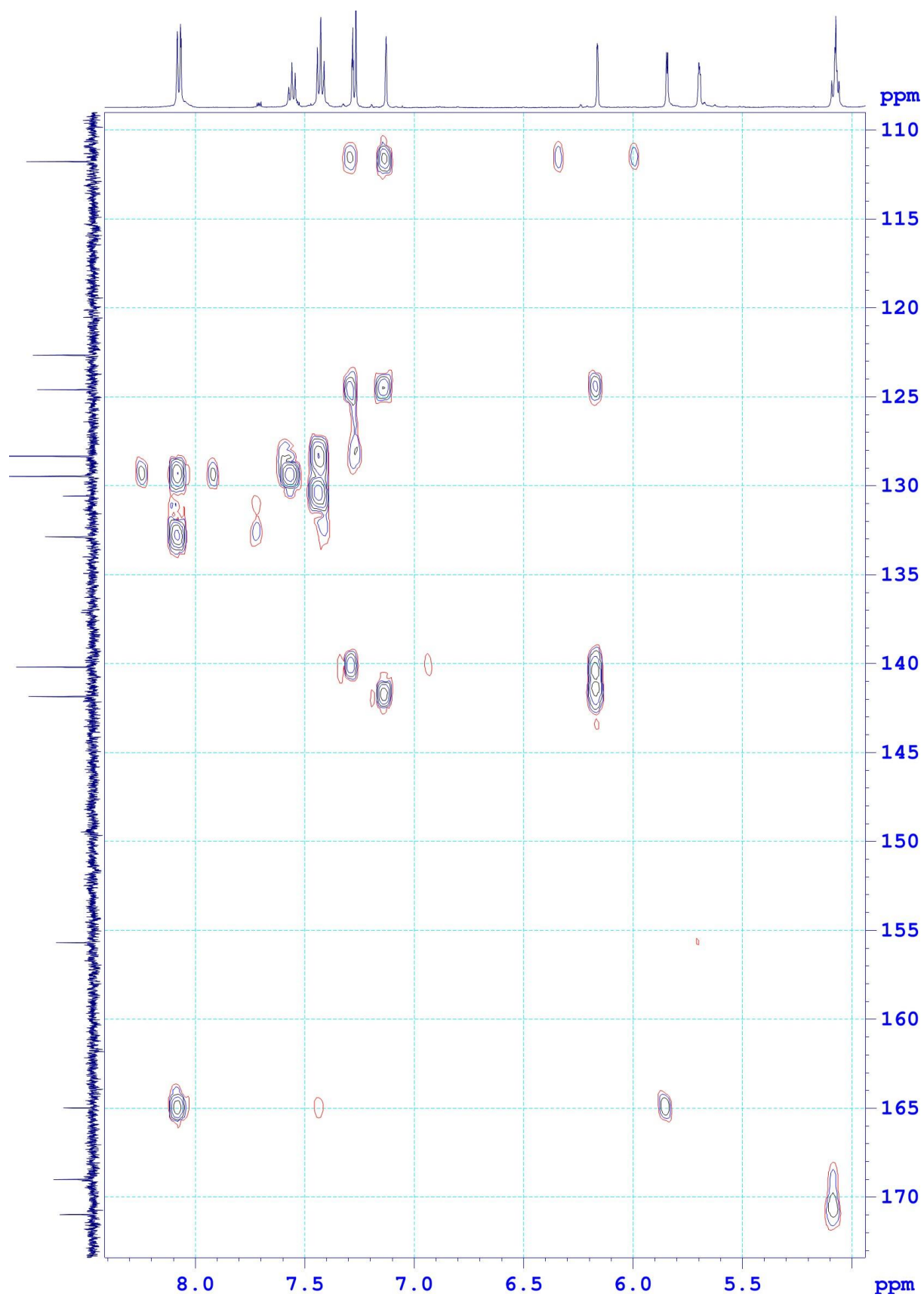


Figure S22: HMBC spectrum of compound 1.

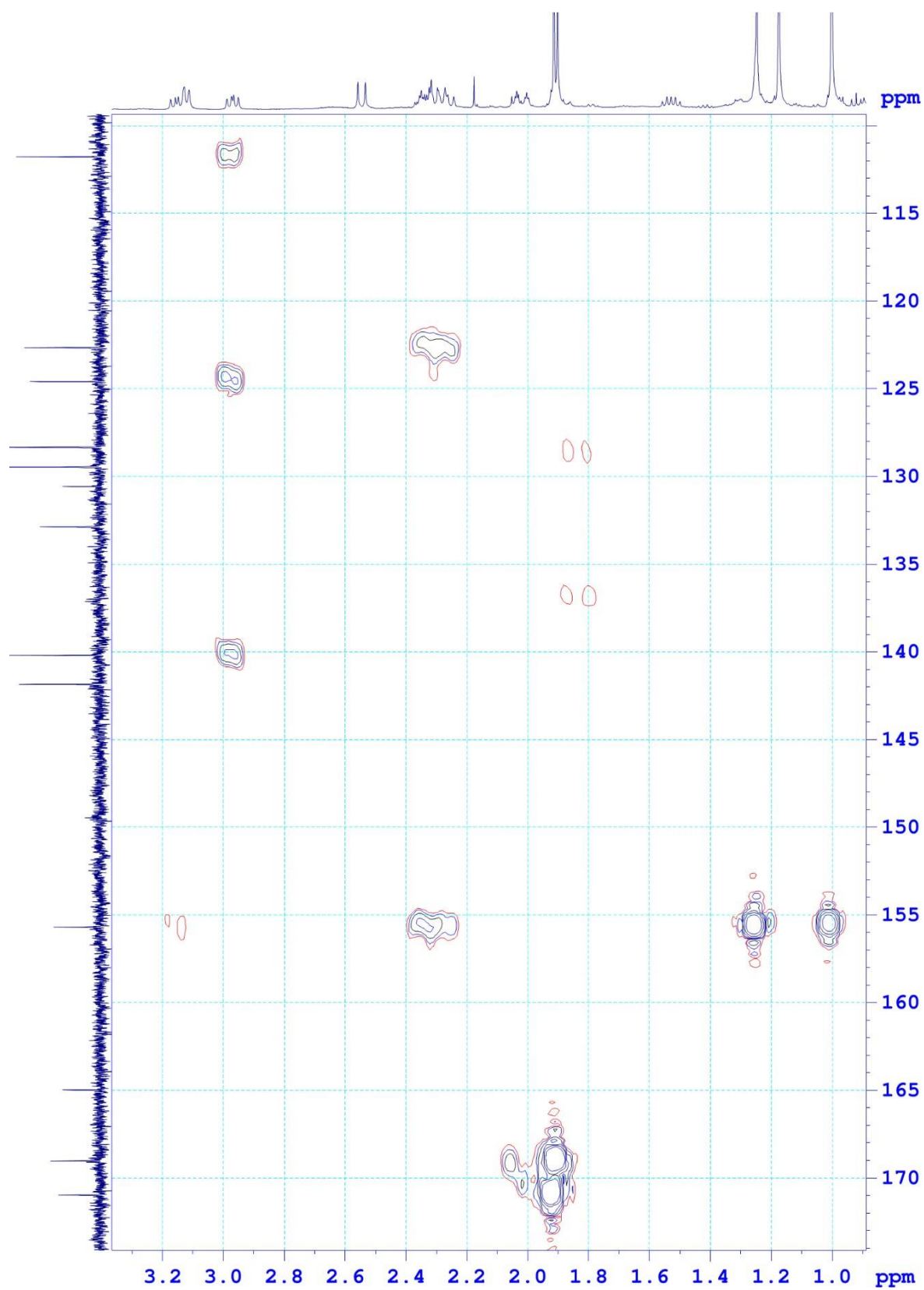


© 2021 ACG Publications. All rights reserved.



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

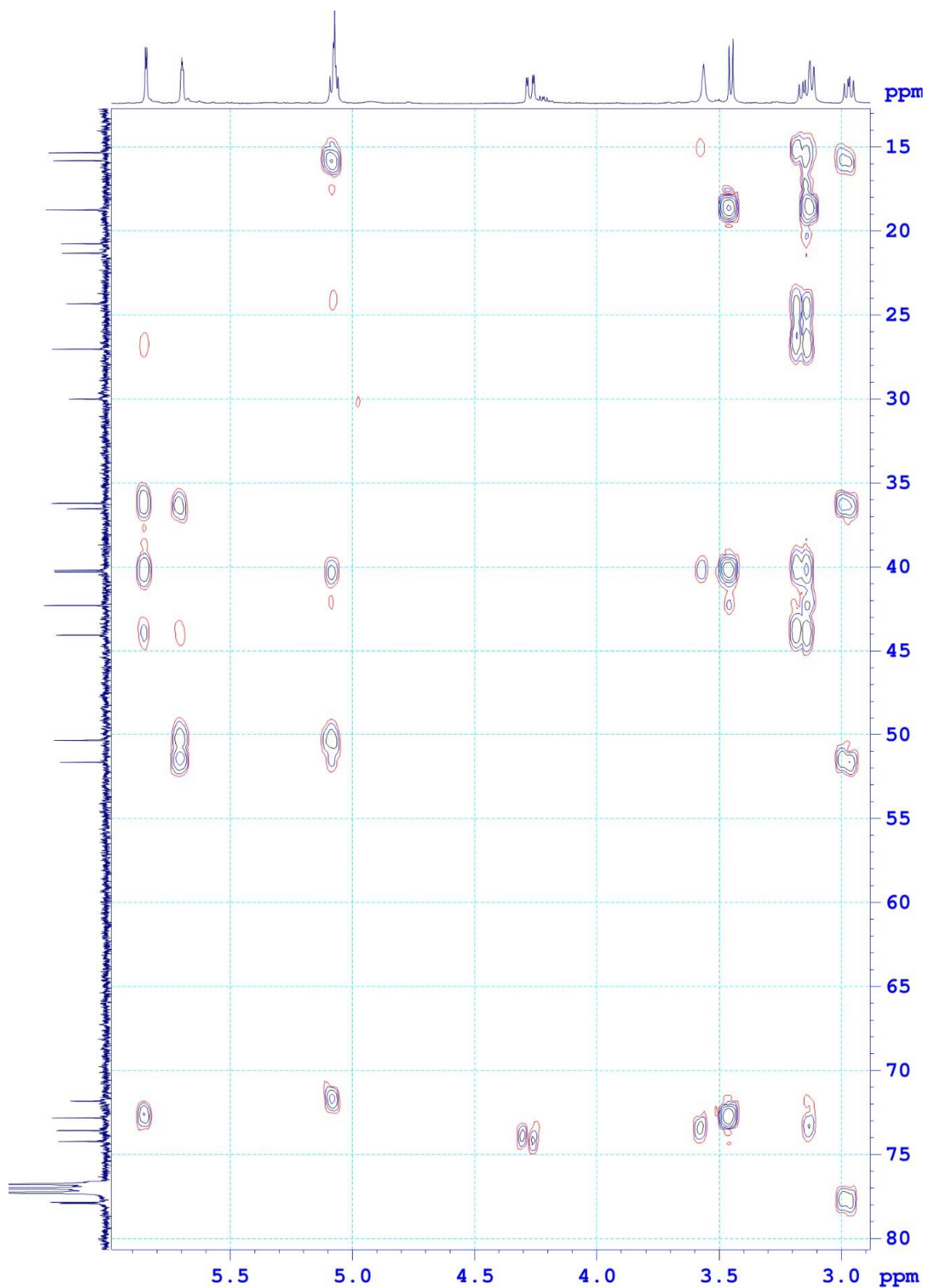
© 2021 ACG Publications. All rights reserved.



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

© 2021 ACG Publications. All rights reserved.





**Figure S25:** HMBC spectrum of compound 1.

© 2021 ACG Publications. All rights reserved.

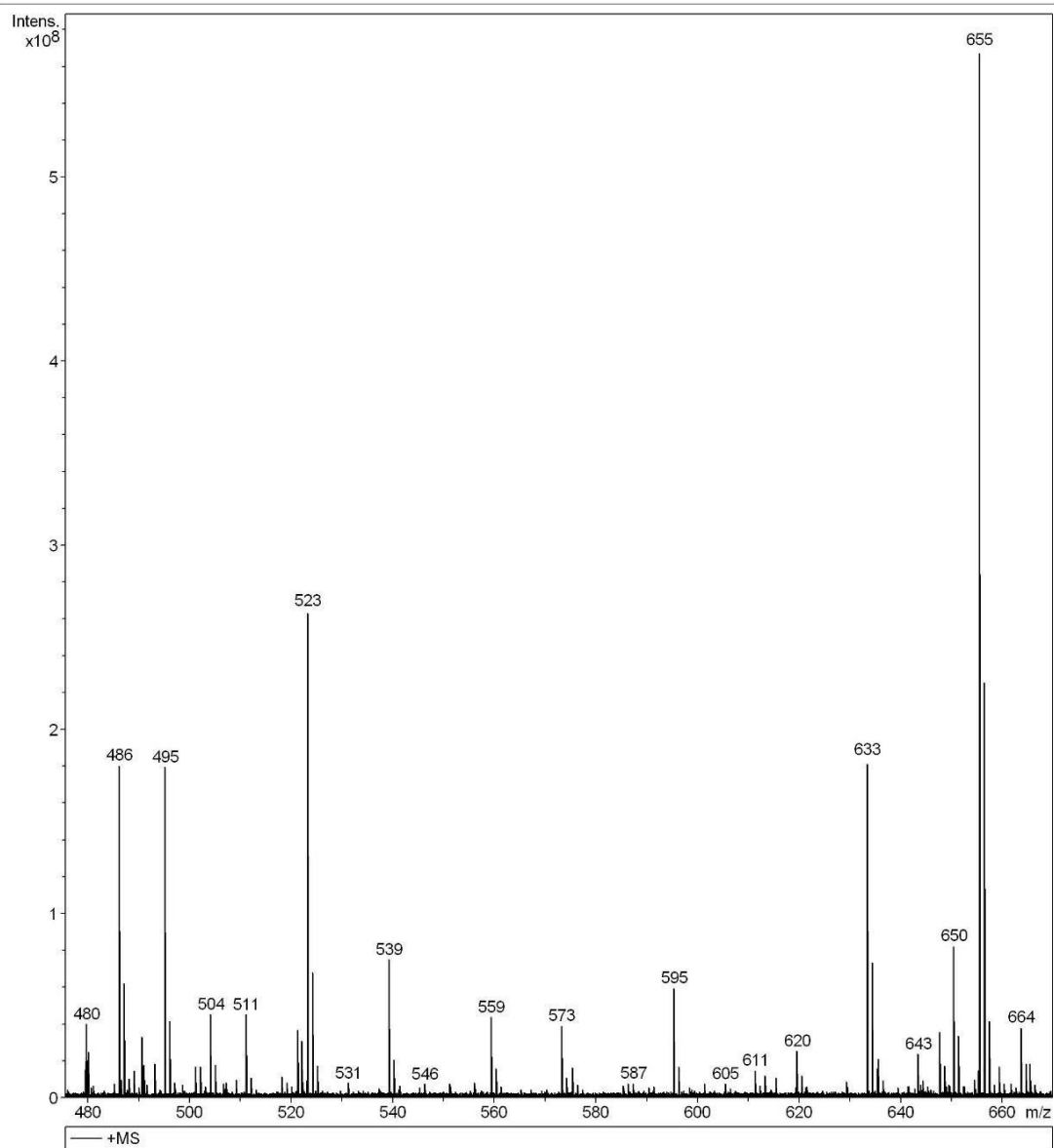
## FT-MS

### Analysis Info

Analysis Name D:\Data\g9\kuoaze3x1212\_000005.d  
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



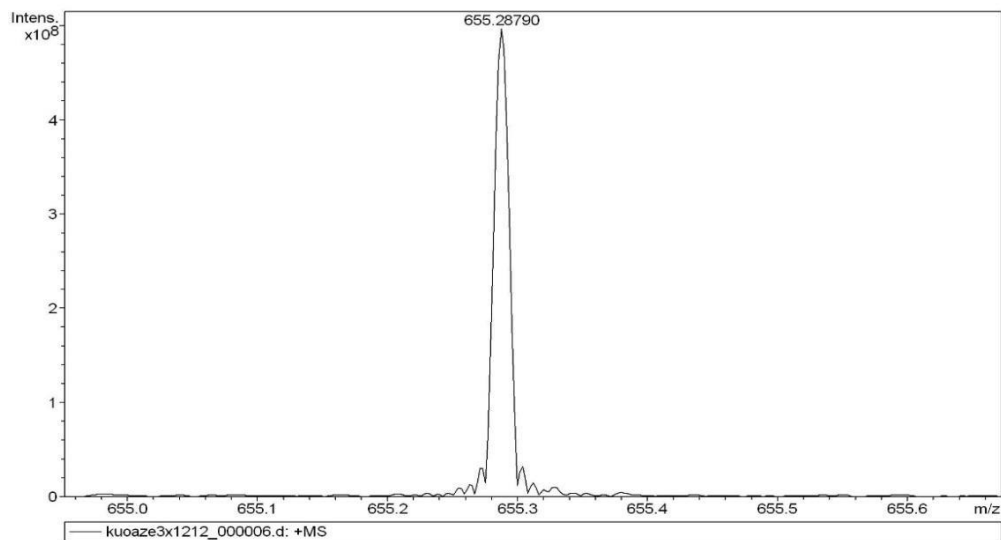
**Figure S26:** MS spectrum of compound 1.

## Mass Spectrum SmartFormula Report

### Analysis Info

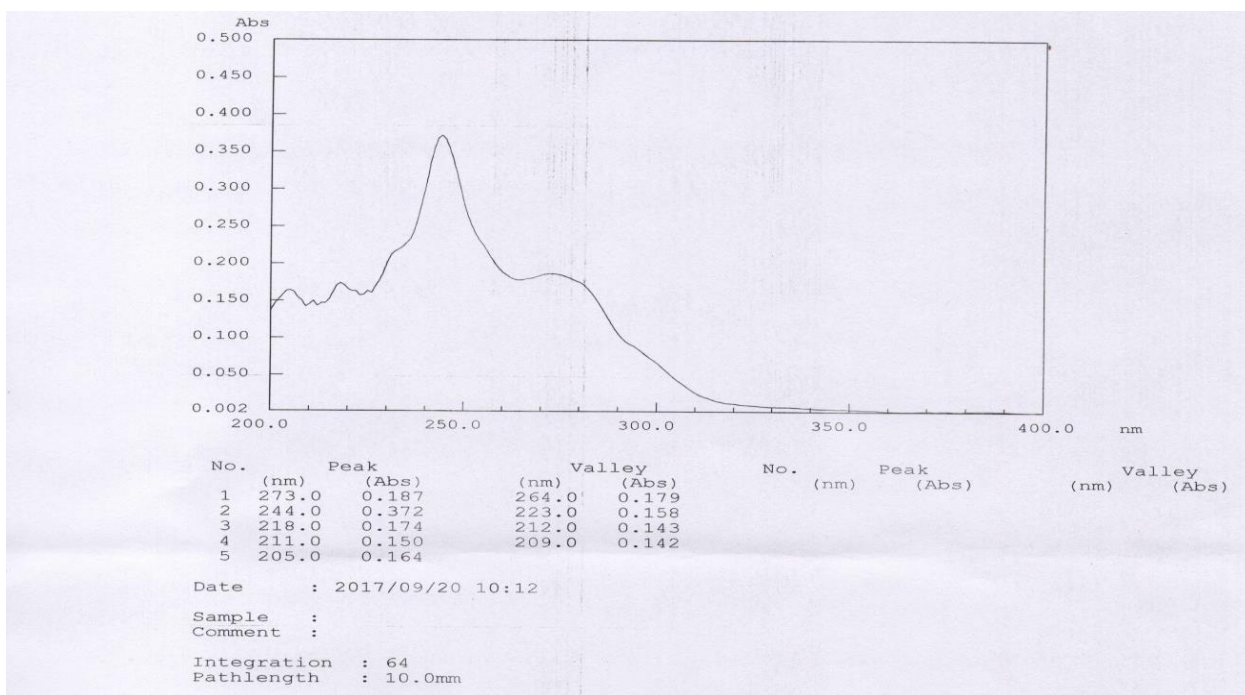
Analysis Name D:\Data\g9\kuoaze3x1212\_000006.d  
Method broadband first signal  
Sample Name kuo-AZE-3X1-2-1-2  
Comment ESI Positive

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

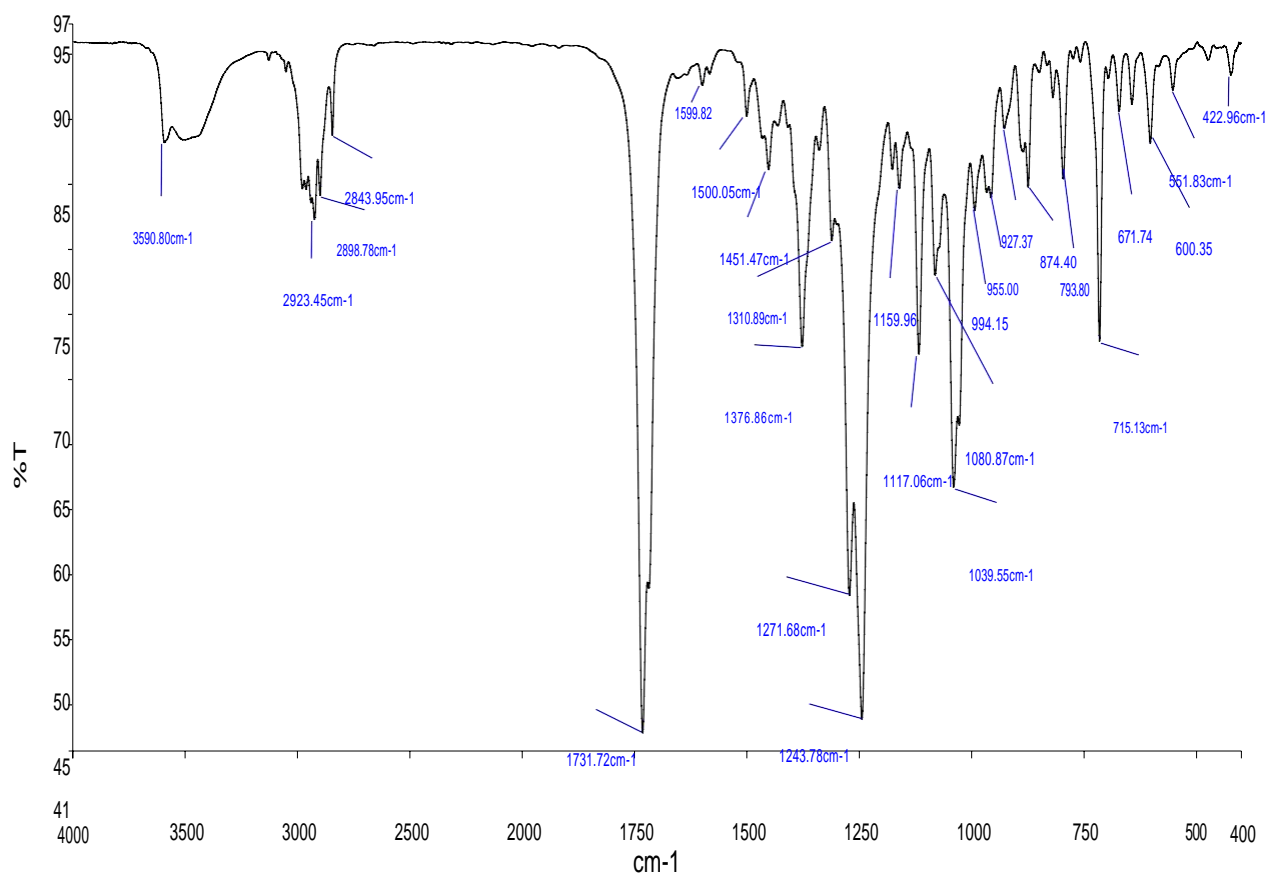


Meas. m/z	#	Formula	Score	m/z	err [mDa]	err [ppm]	mSigma	rdb	e <sup>-</sup> Conf	N-Rule
655.28790	1	C <sub>37</sub> H <sub>44</sub> NaO <sub>9</sub>	100.00	655.28775	-0.15	-0.22	4.2	15.5	even	ok

**Figure S27:** HRMS spectrum of compound **1**.



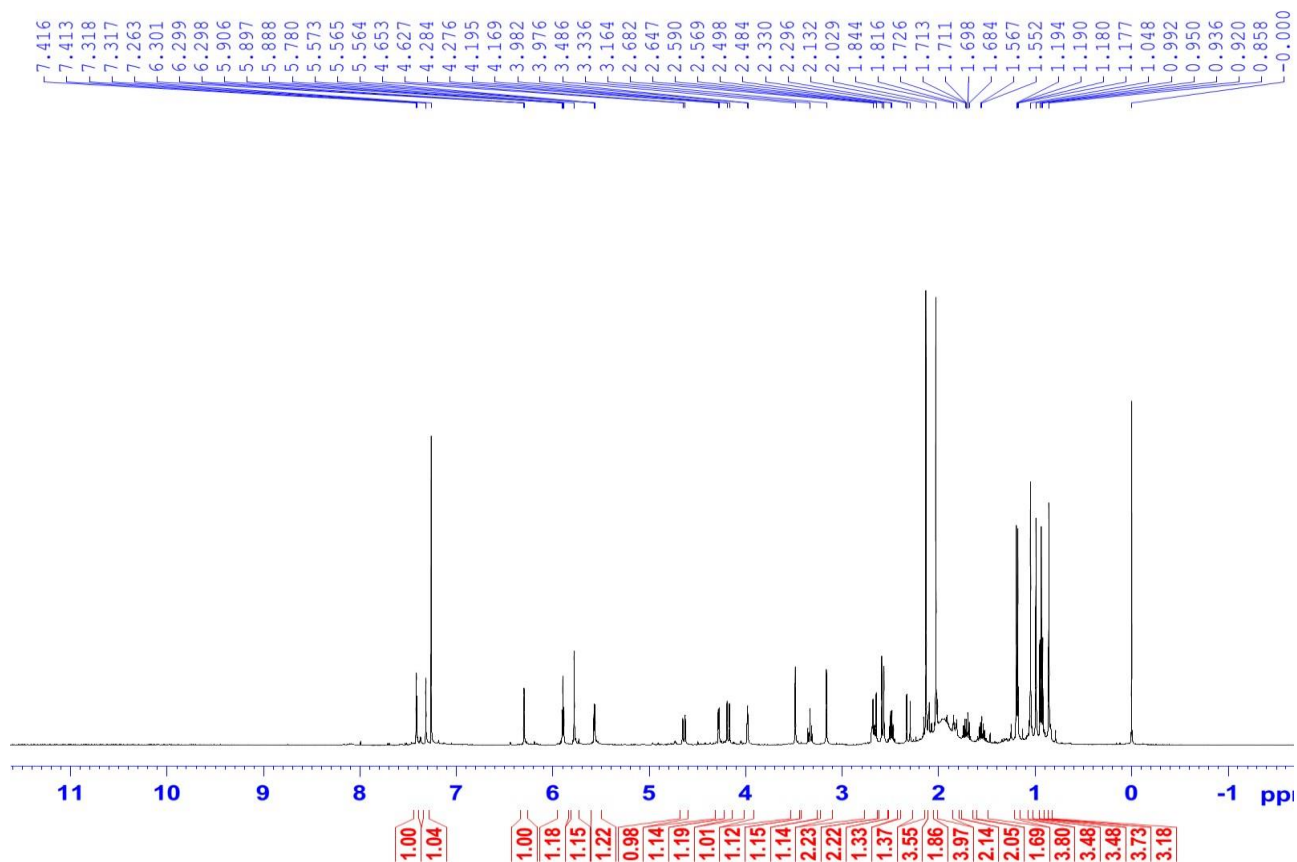
**Figure S28: UV spectrum of compound 1.**



**Figure S29: IR spectrum of compound 1.**

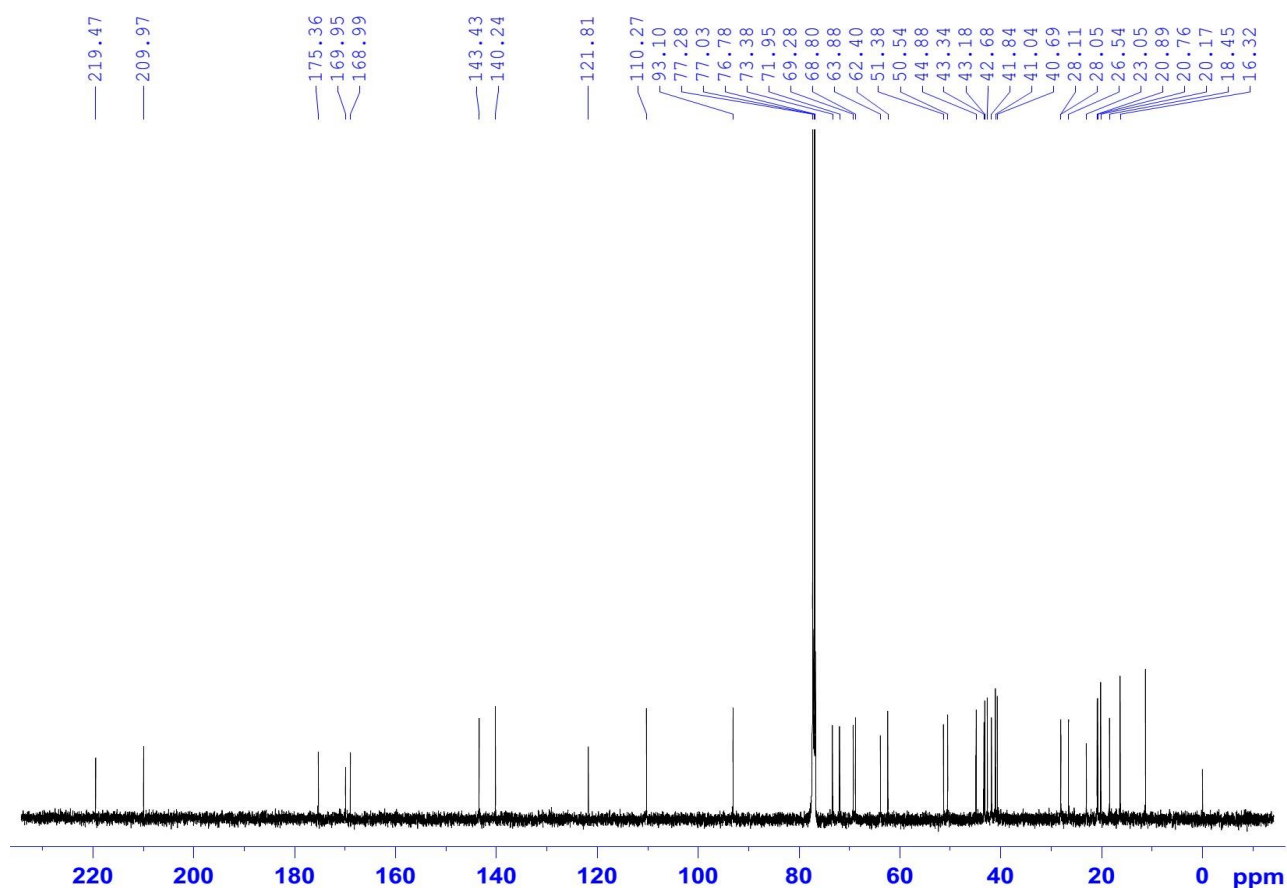
© 2021 ACG Publications. All rights reserved.

**AZE5.5-CDC13-1H**



**Figure S30:**  $^1\text{H}$ -NMR spectrum of compound **2**.

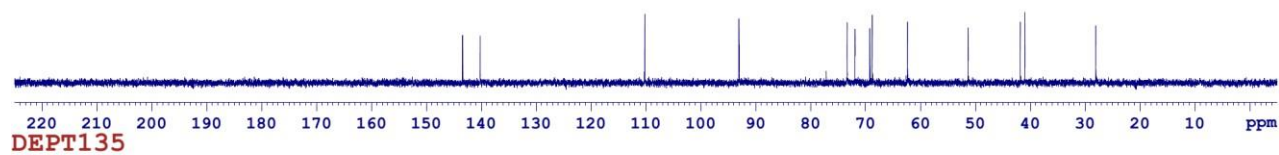
**AZE5.5-CDC13-C13CPD**



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

AZE5.5-CDCl3-C13CPD &DEPT

DEPT90



CH&CH3

CH2



C13CPD

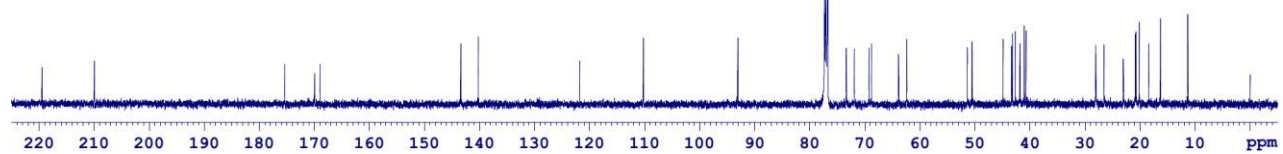
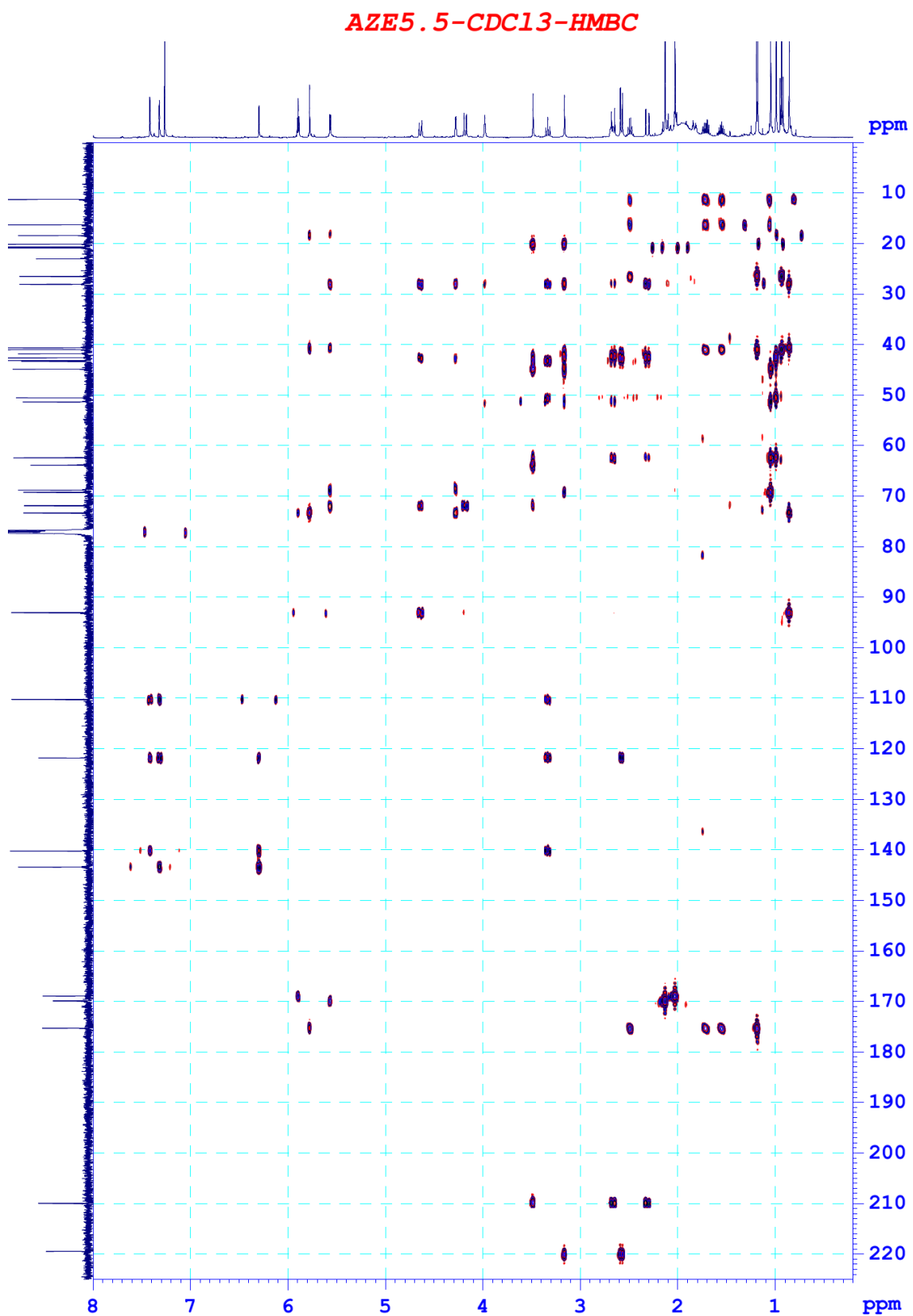


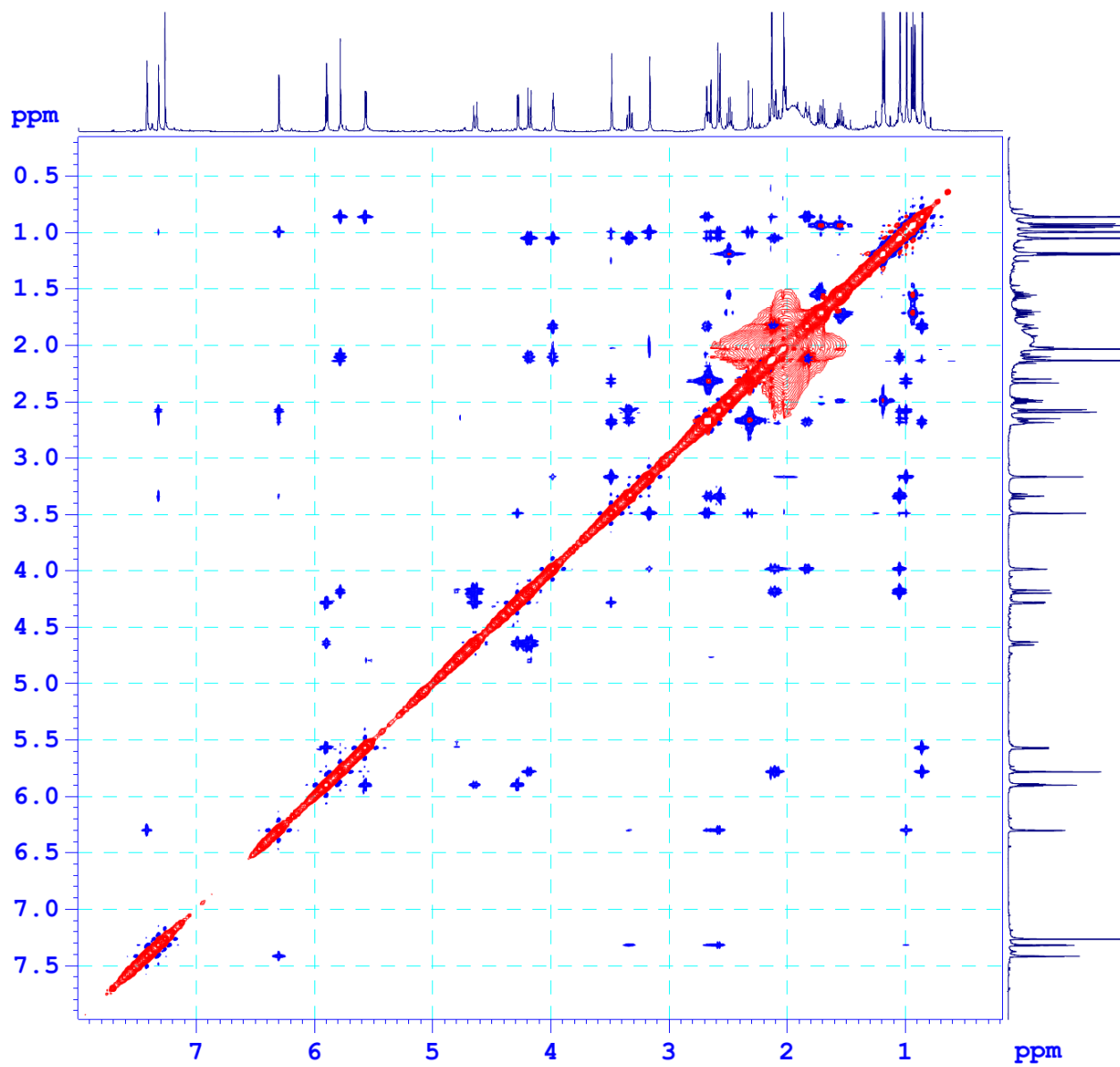
Figure S32: DEPT spectrum of compound 2.



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

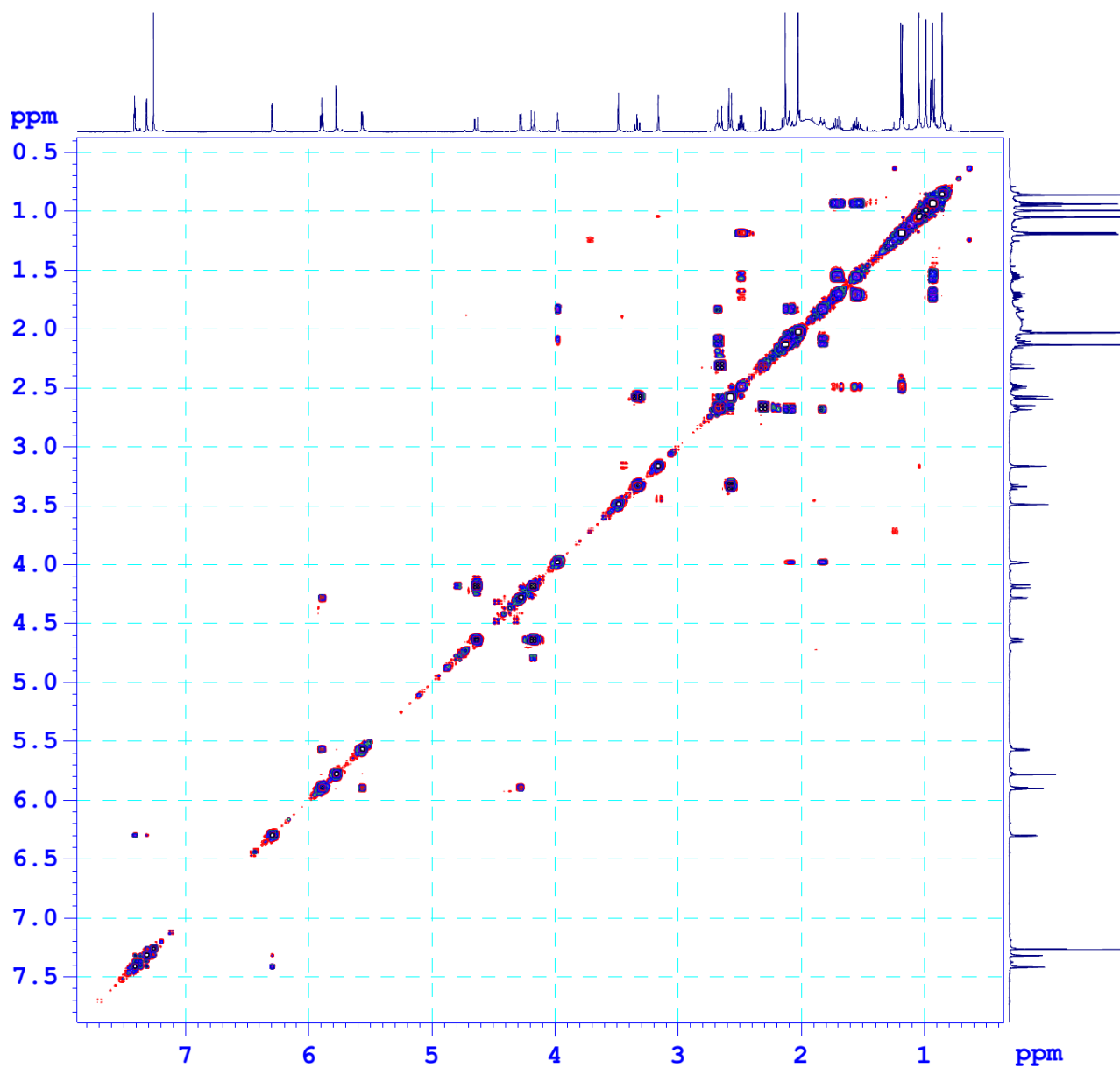


*AZE5.5-CDC13-NOESY*

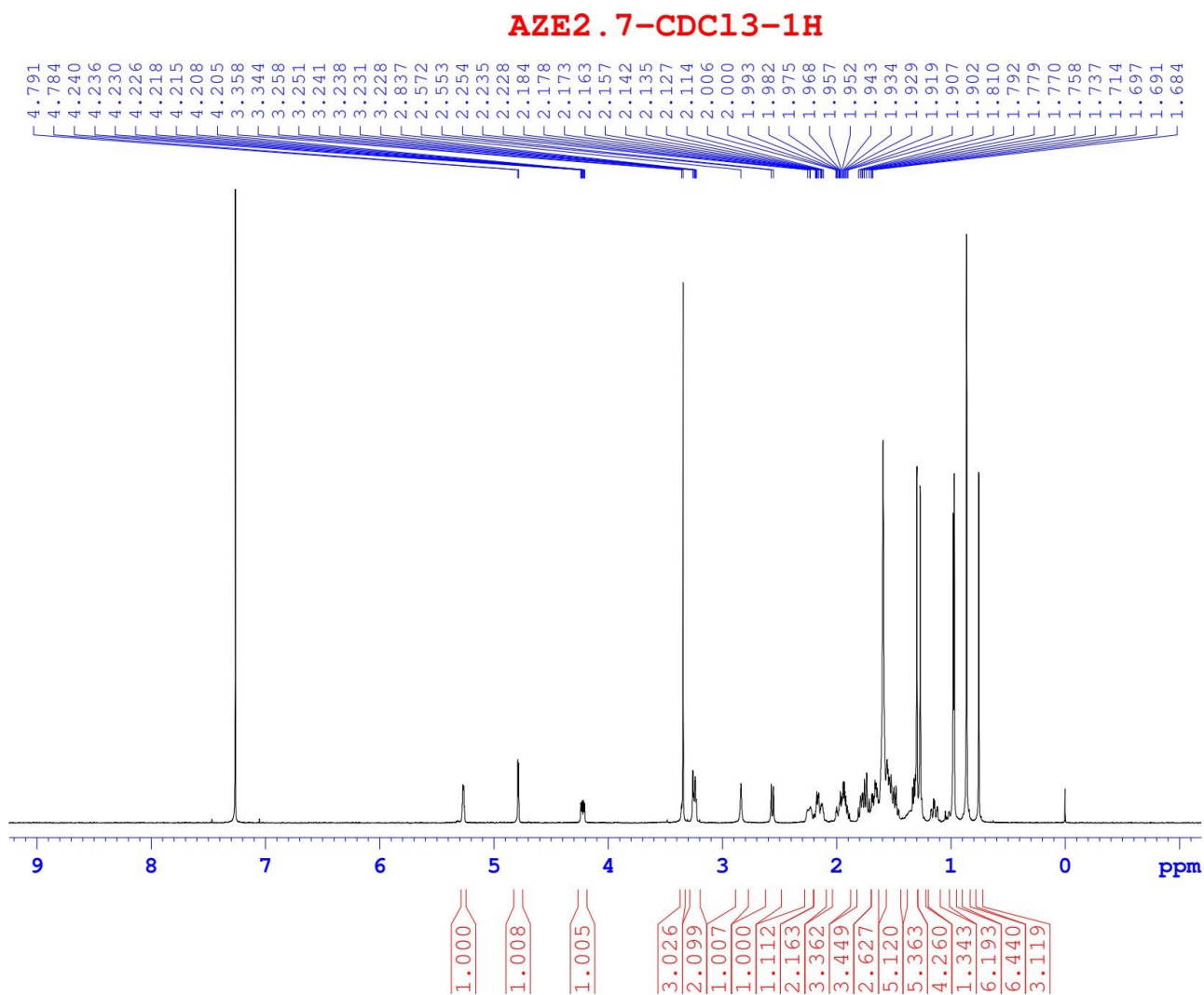


**Figure S34:** NOESY spectrum of compound 2.

*AZE5.5-CDC13-COSYGP*

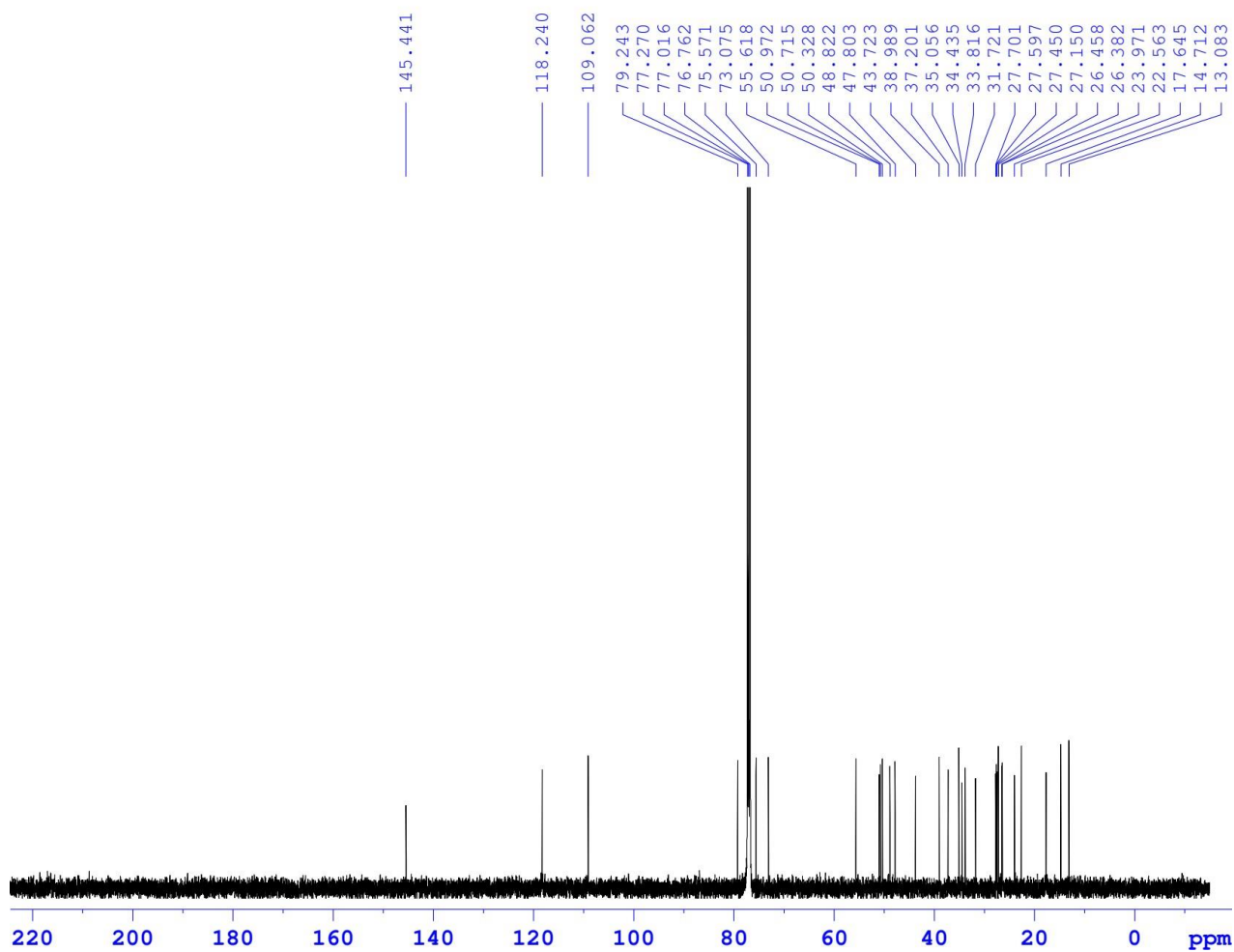


**Figure S35:** COSY spectrum of compound **2**.



**Figure S36:**  $^1\text{H}$ -NMR spectrum of compound **3**.

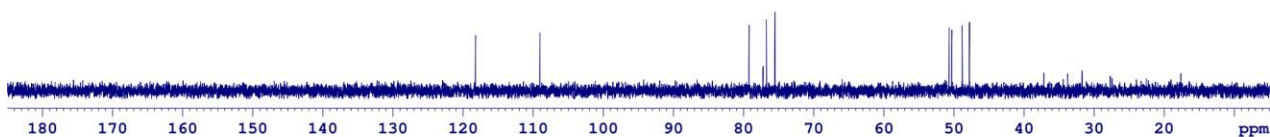
**AZE2.7-CDC13-C13CPD**



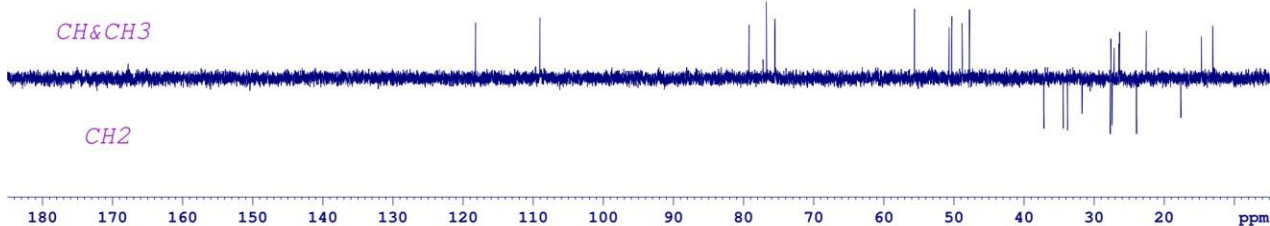
**Figure S37:**  $^{13}\text{C}$ -NMR spectrum of compound **3**.

AZE2.7-CDC13-C13CPD&DEPT

DEPT90



DEPT135



C13CPD

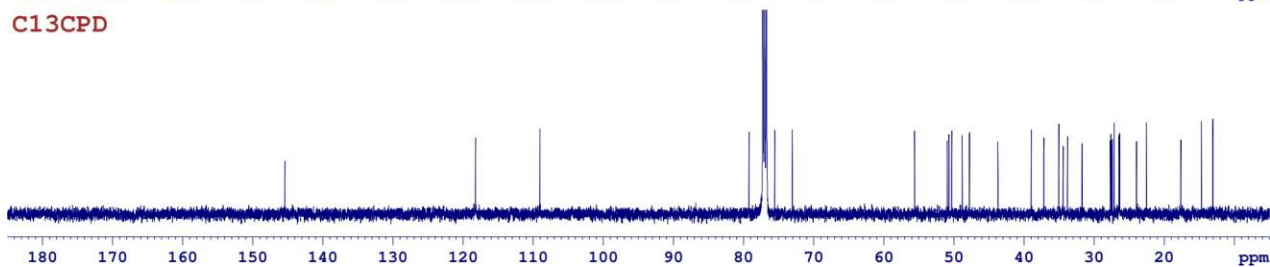
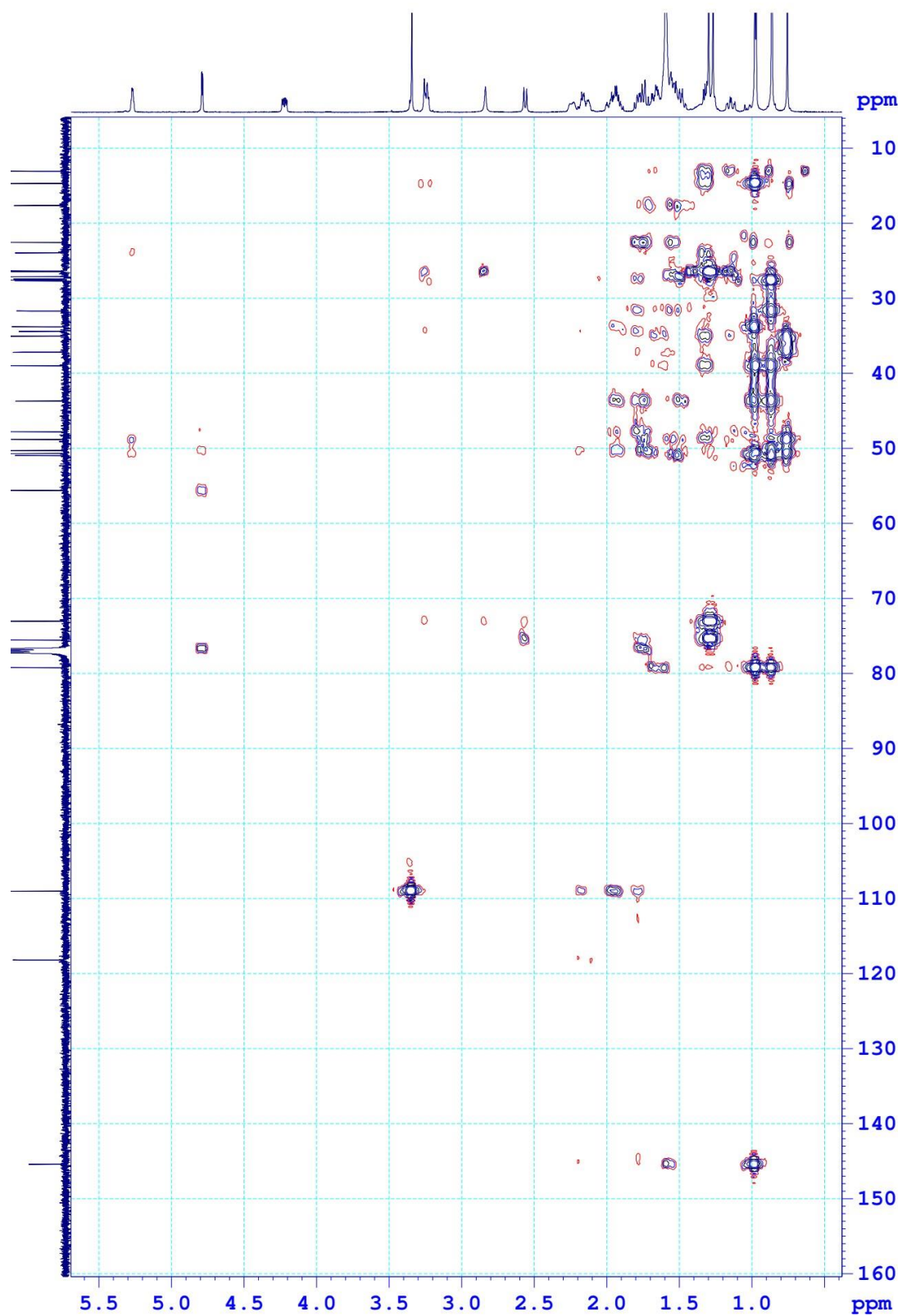


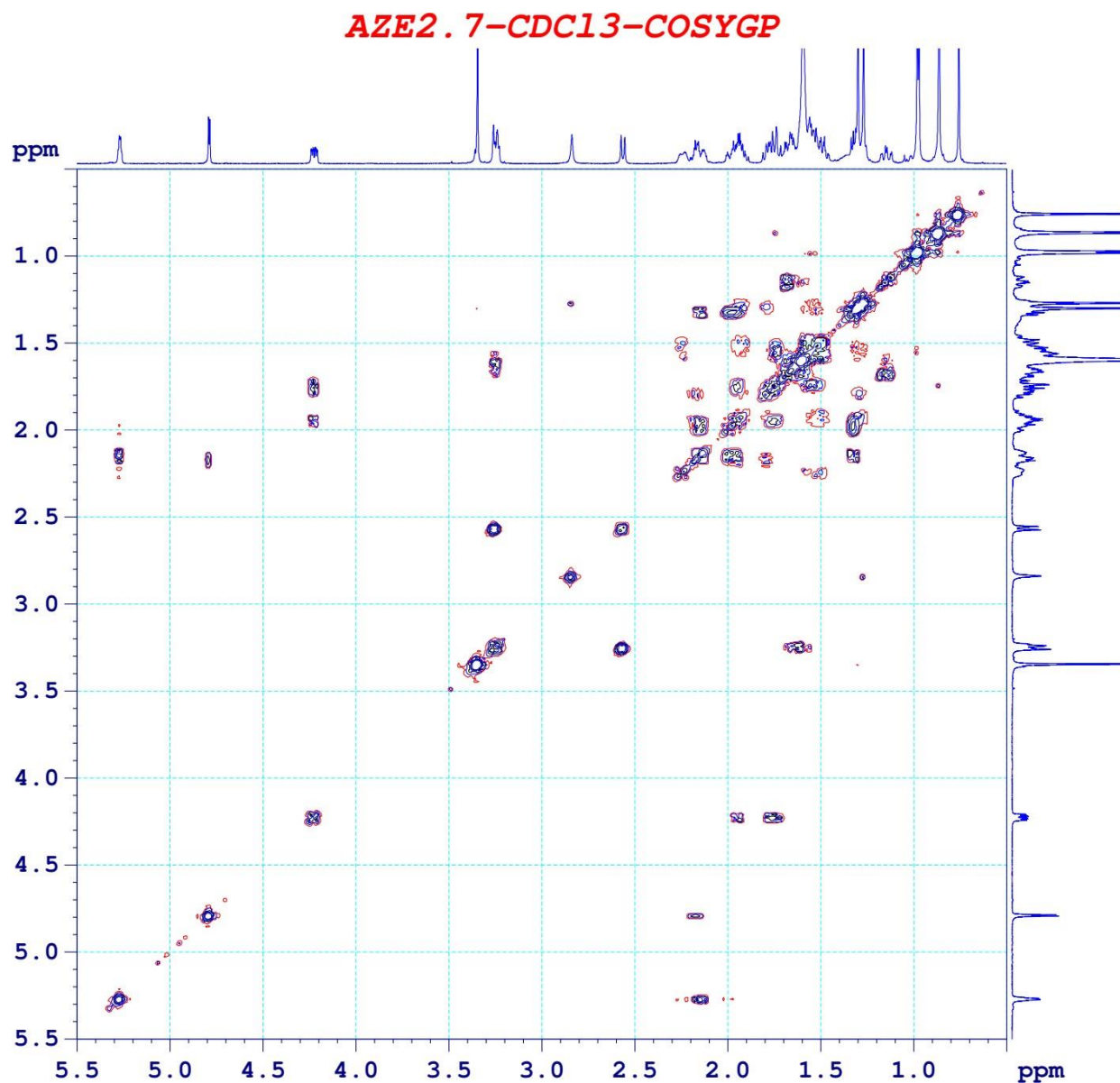
Figure S38: DEPT spectrum of compound 3.

**AZE2.7-CDC13-HMBC**



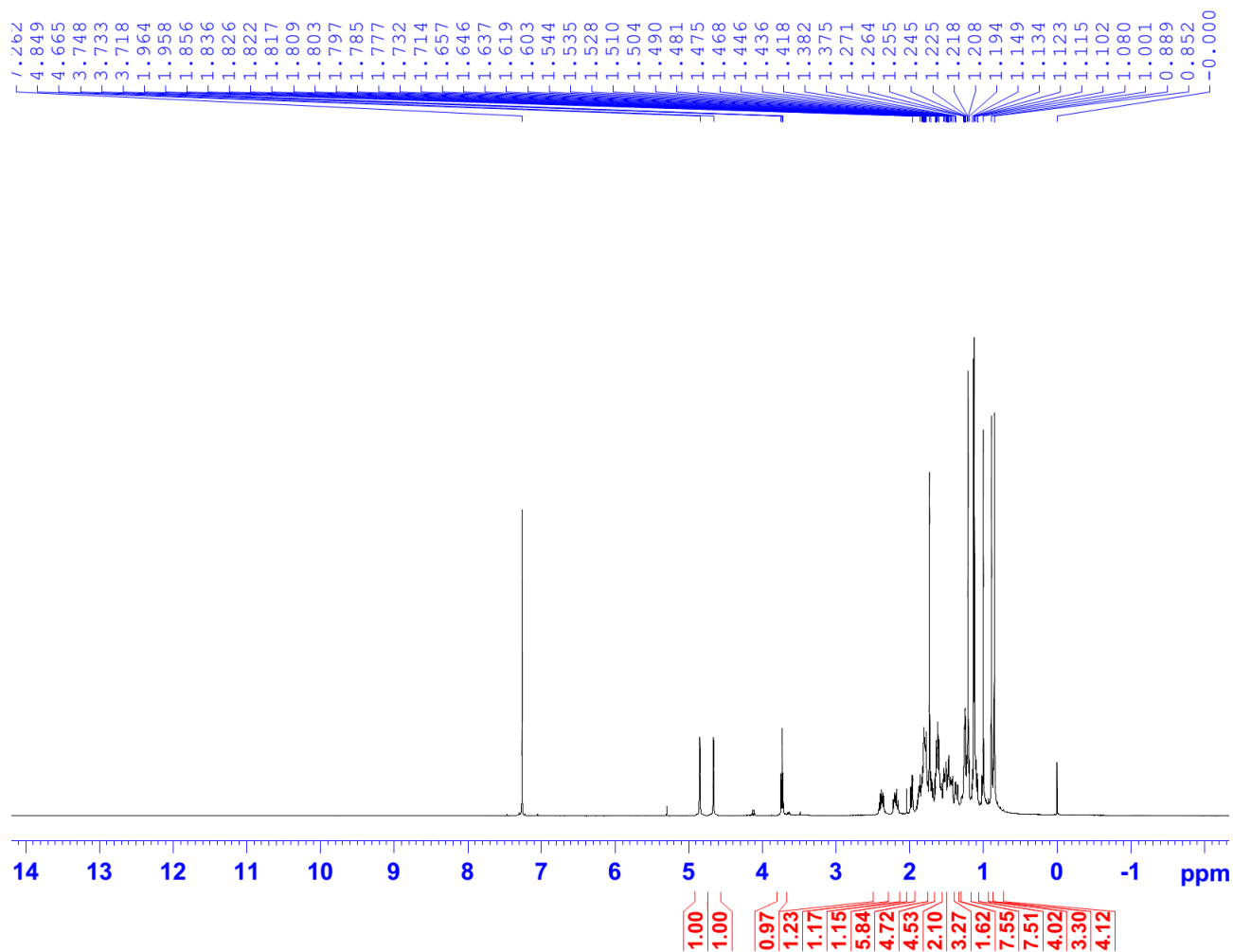
**Figure S39:** HMBC spectrum of compound **3**.

© 2021 ACG Publications. All rights reserved.



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

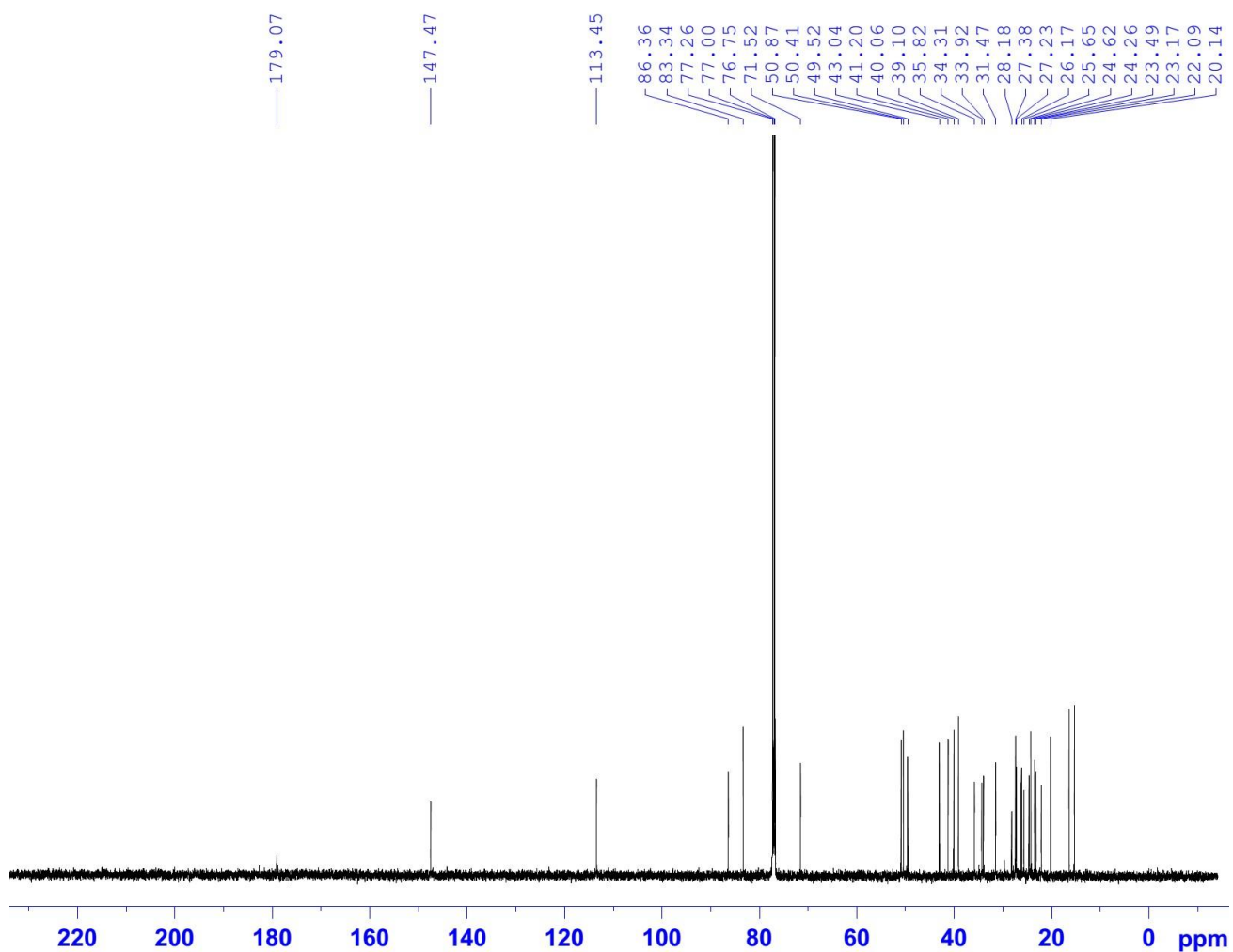
**AZE10.3.1-CDC13-1H**



**Figure S41:** <sup>1</sup>H-NMR spectrum of compound **4**.



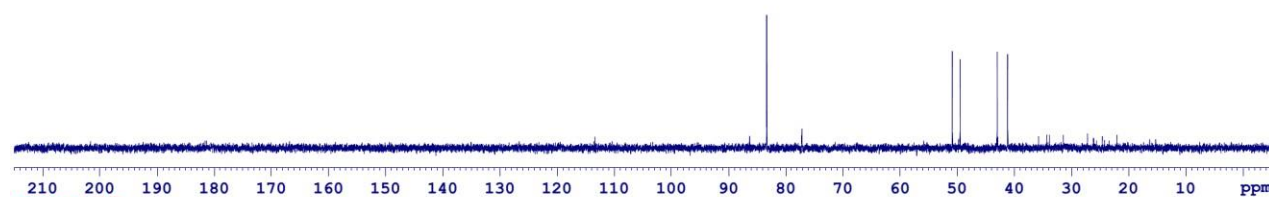
**AZE10.3.1-CDC13-C13CPD**



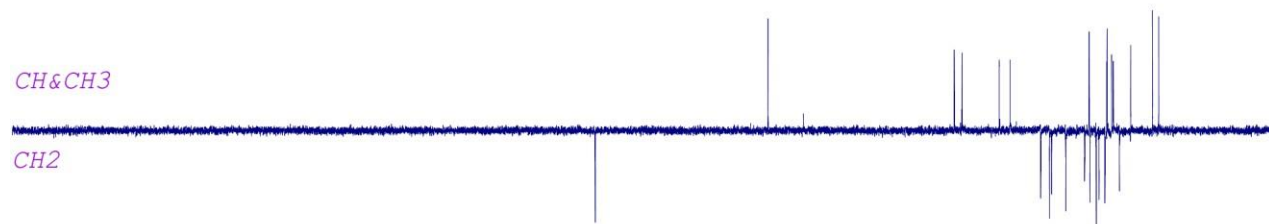
**Figure S42:**  $^{13}\text{C}$ -NMR spectrum of compound **4**.

AZE10.3.1-CDC13-C13CPD&DEPT

DEPT90



DEPT135



CH&CH3

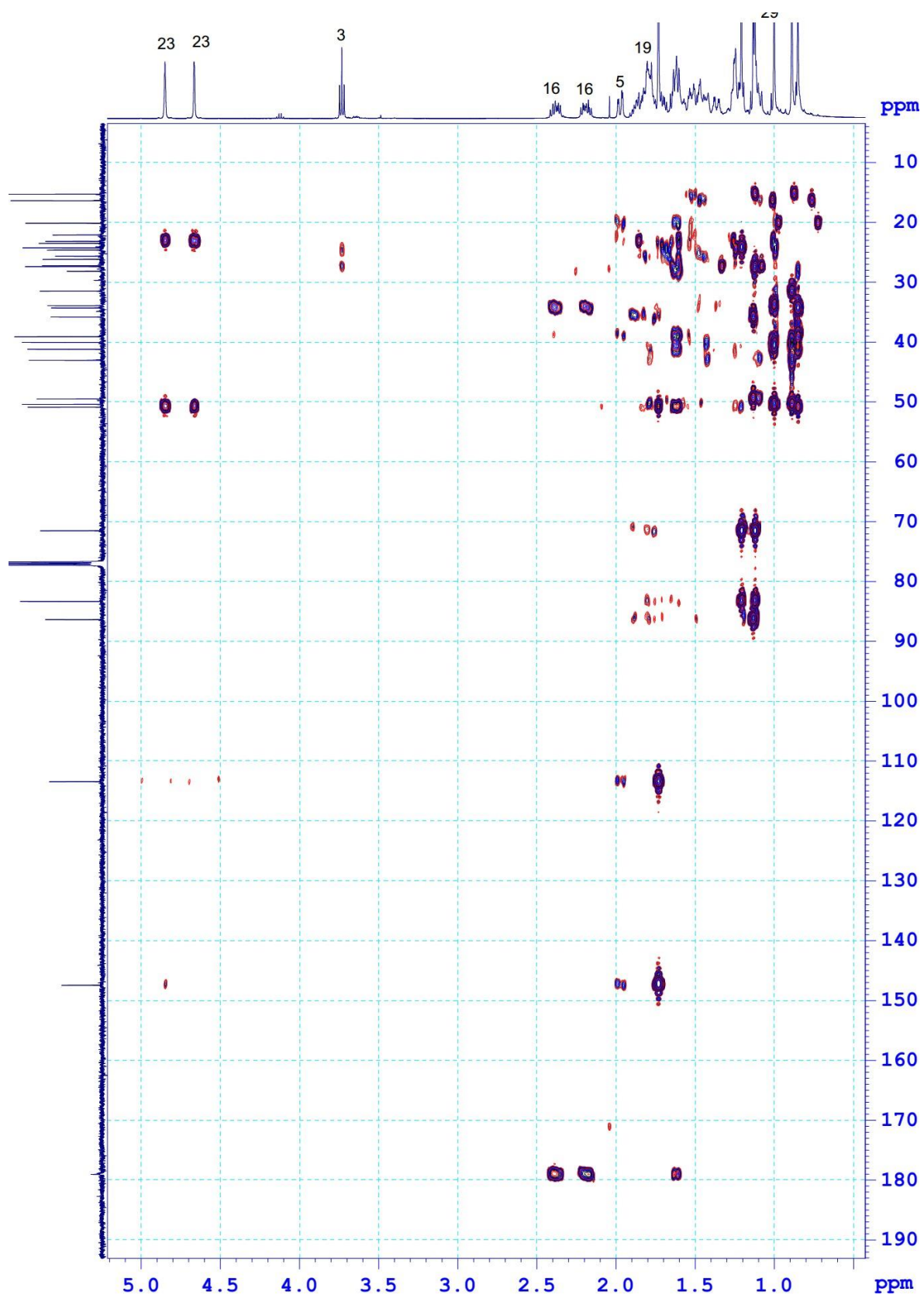
CH2



C13CPD



Figure S43: DEPT spectrum of compound 4.



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

© 2021 ACG Publications. All rights reserved.

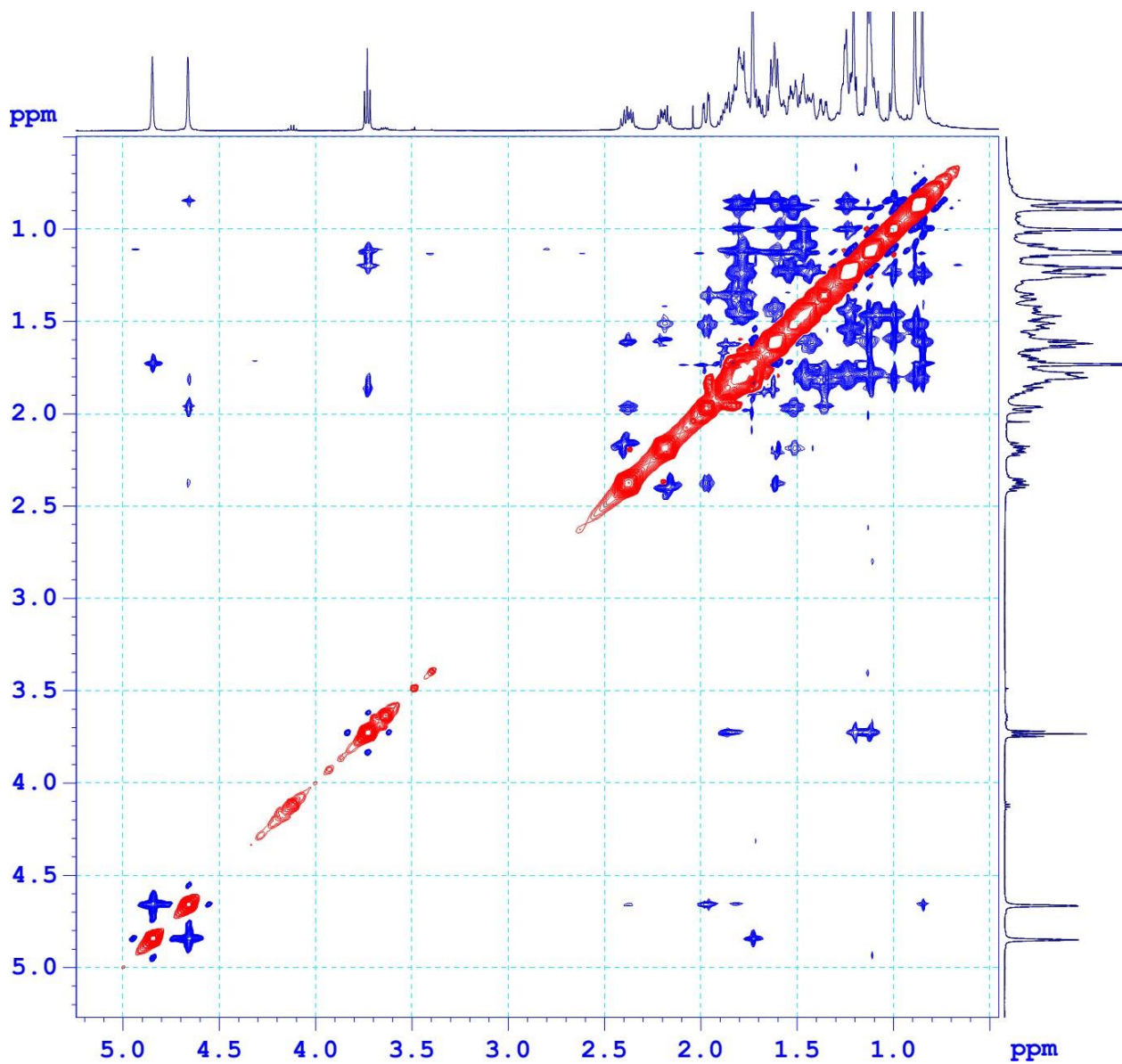
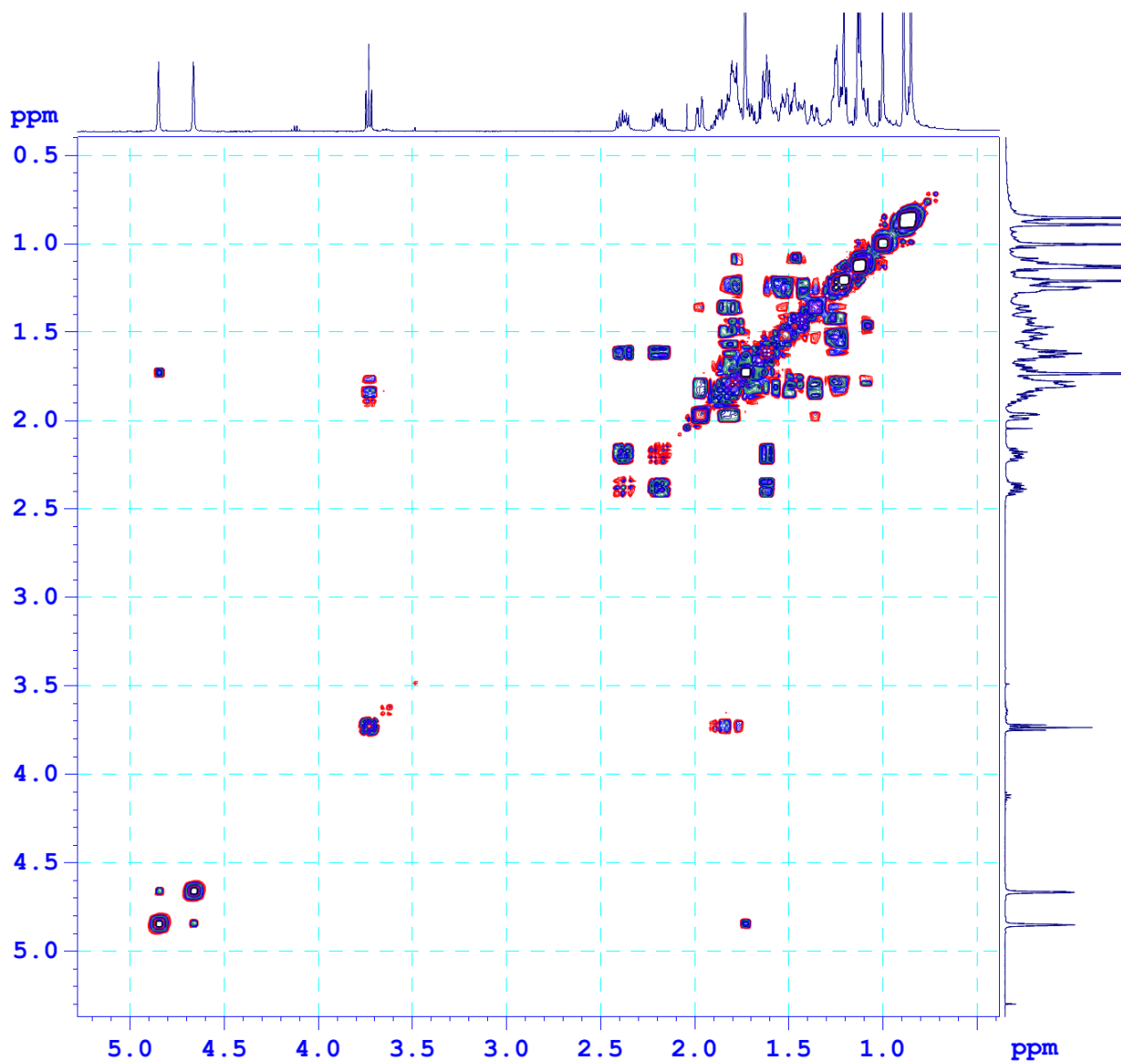
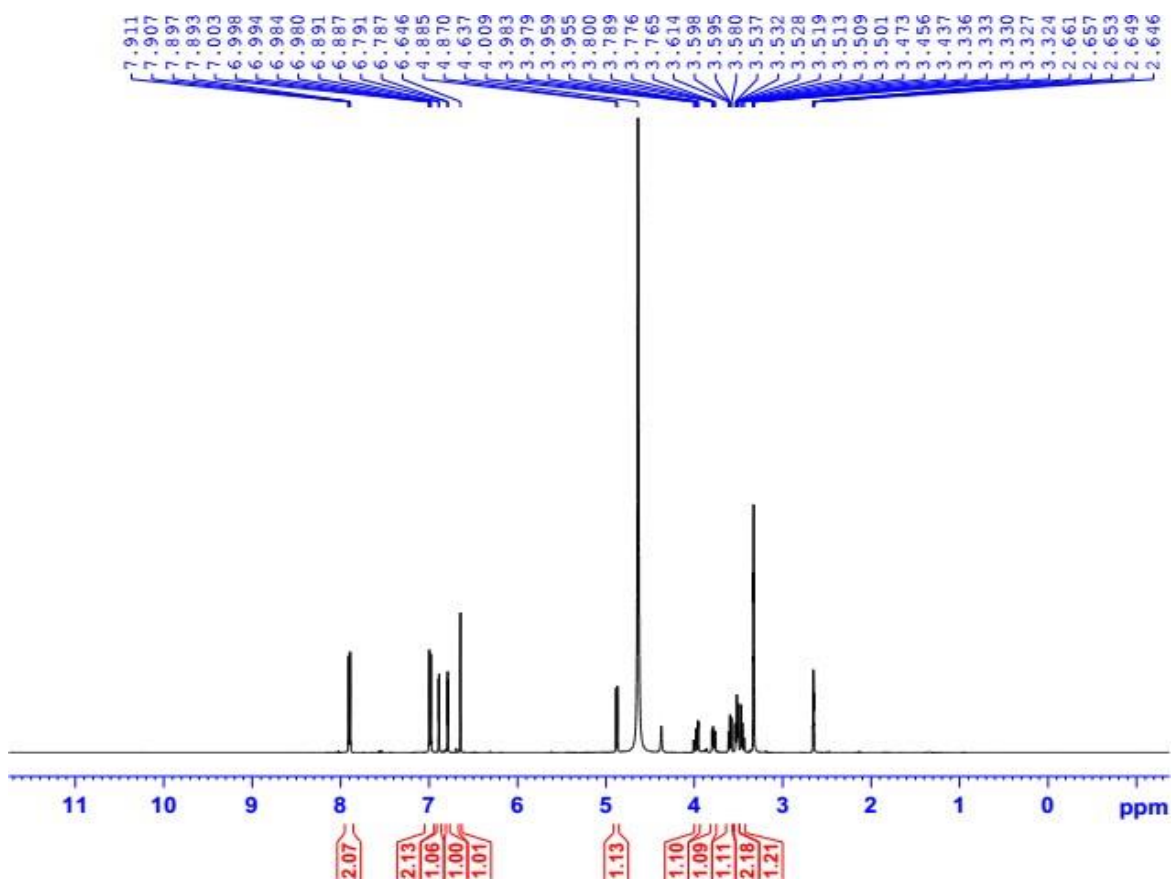


Figure S45: NOESY spectrum of compound 4.

*AZE10.3.1-CDC13-COSYGP*



**Figure S46:** COSY spectrum of compound 4.



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

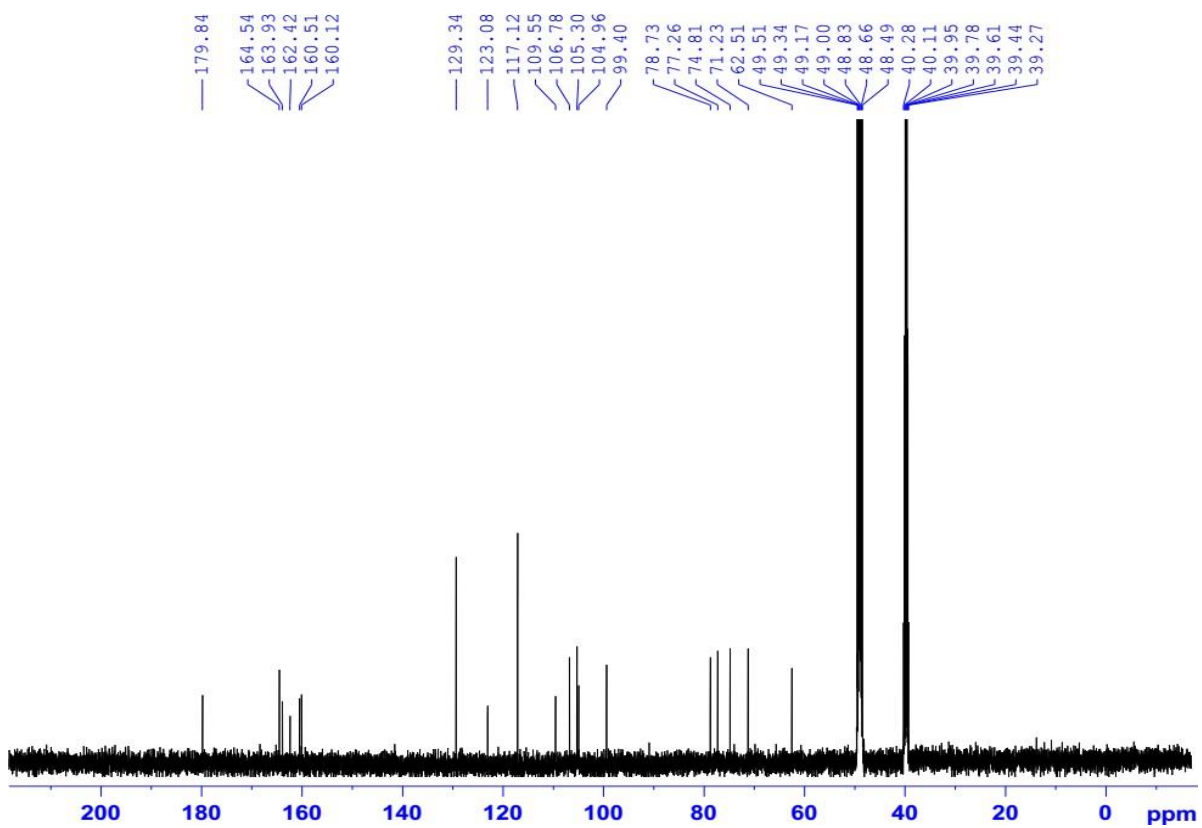


Figure S48:  $^{13}\text{C}$ -NMR spectrum of compound 5.

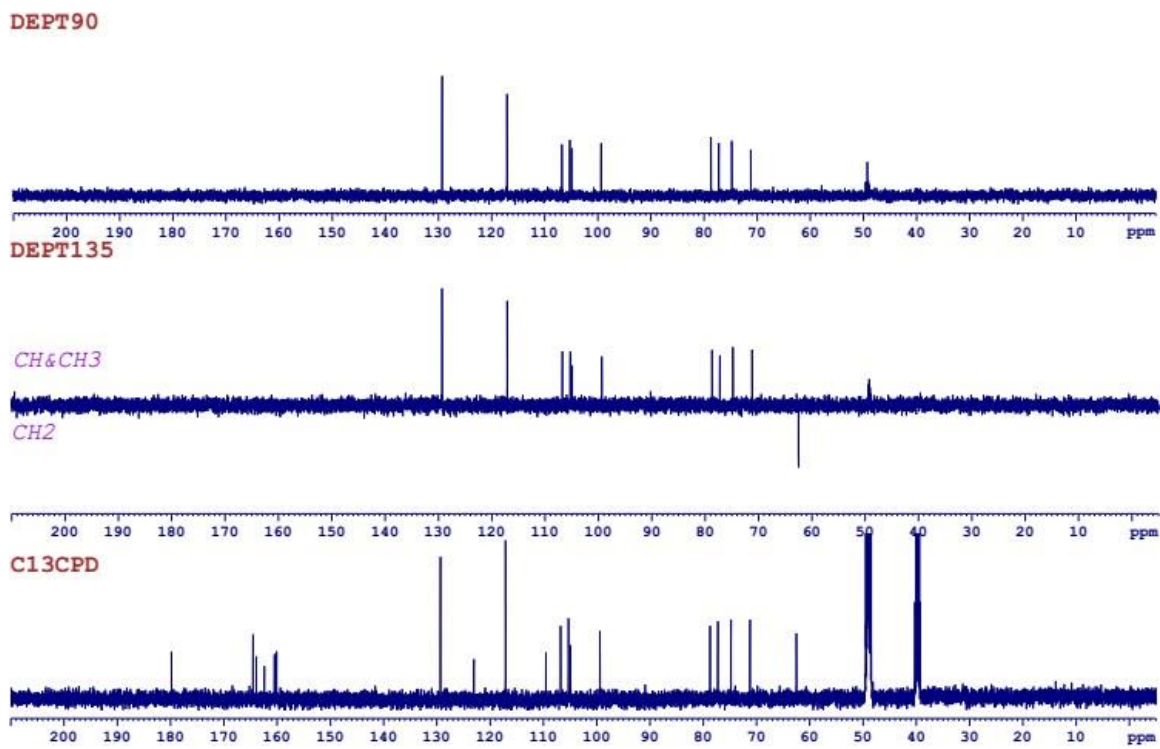
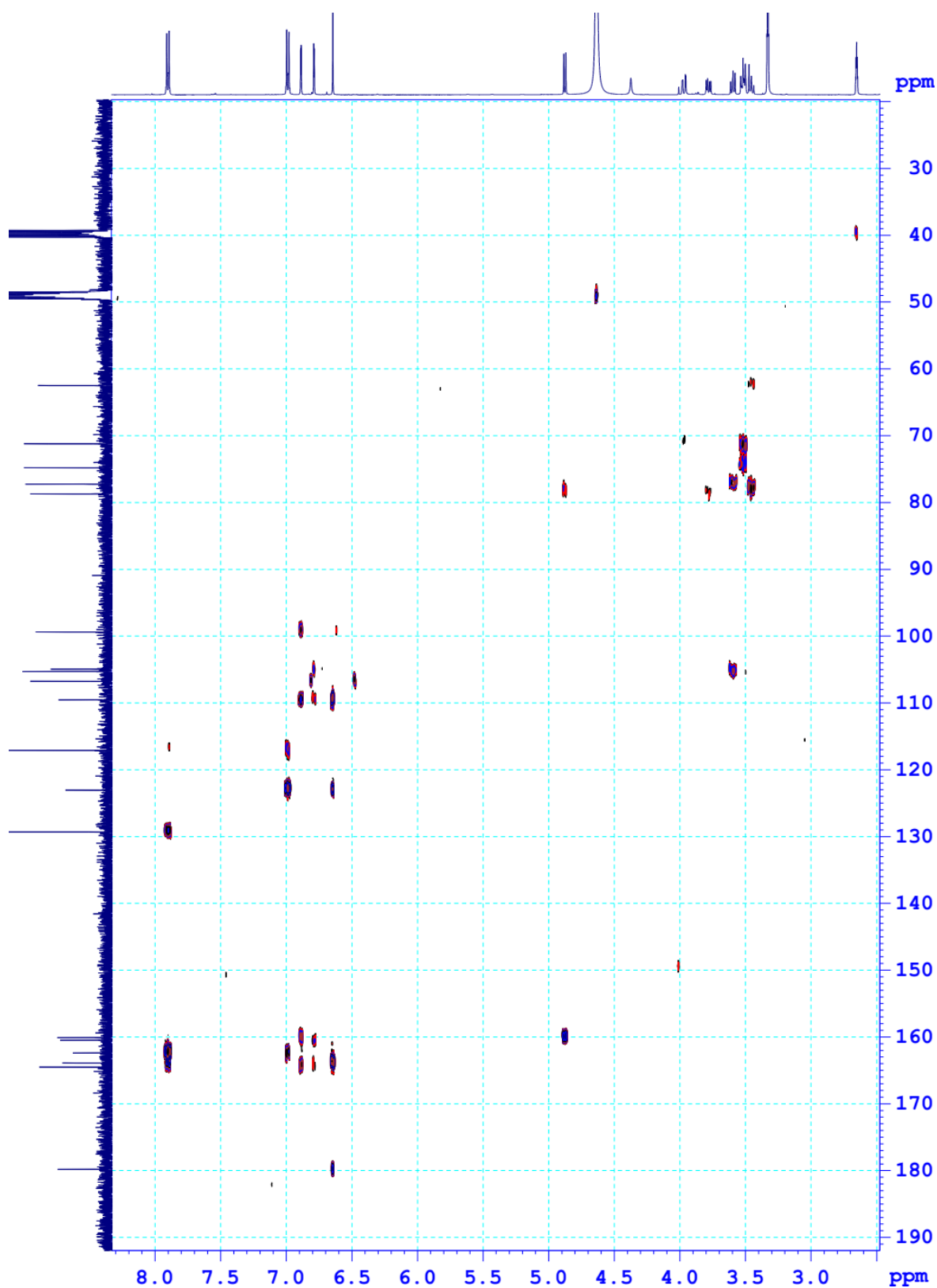
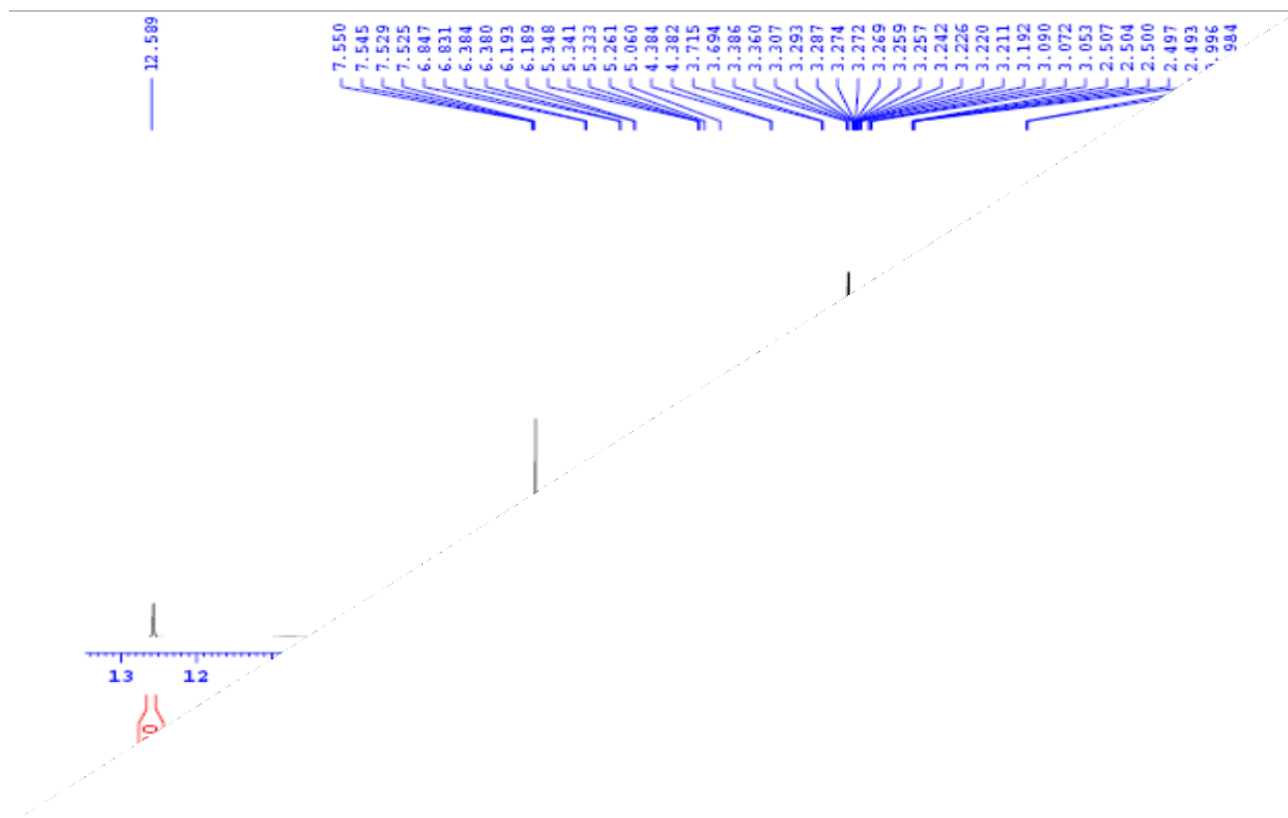


Figure S49: DEPT spectrum of compound 5.

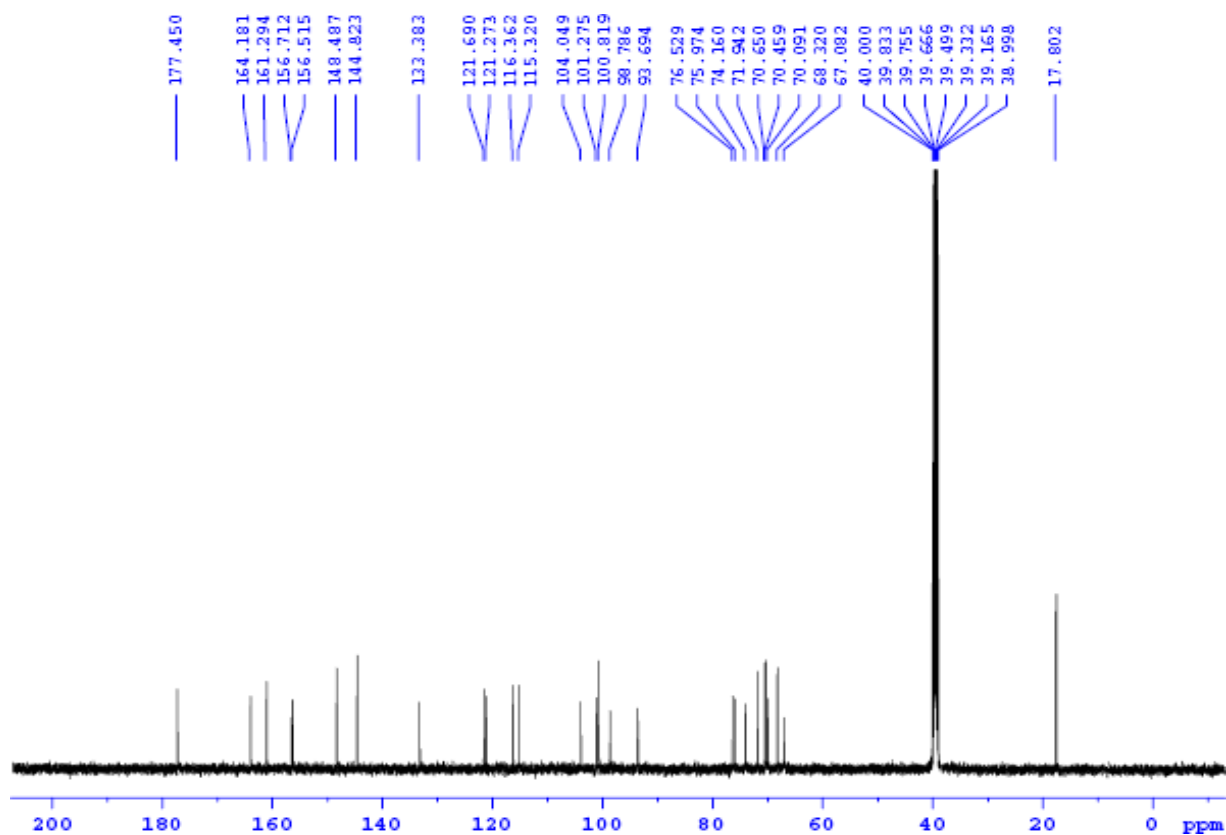




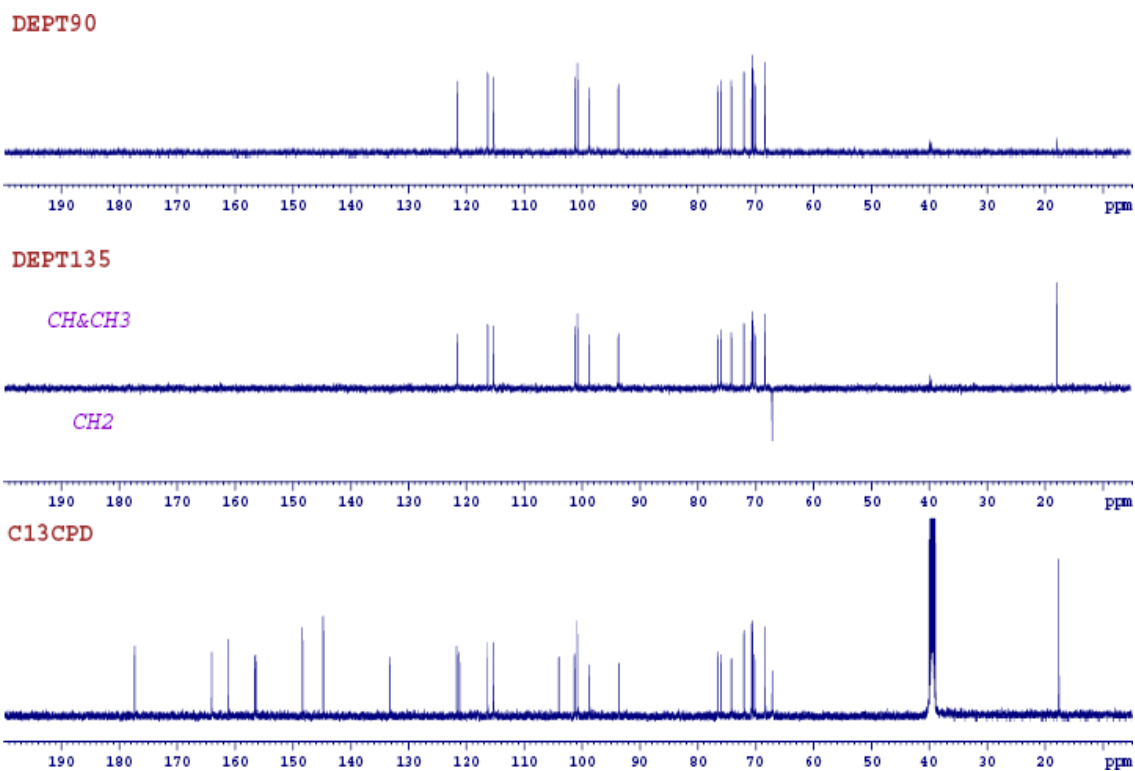
**Figure S50:** HMBC spectrum of compound **5**.



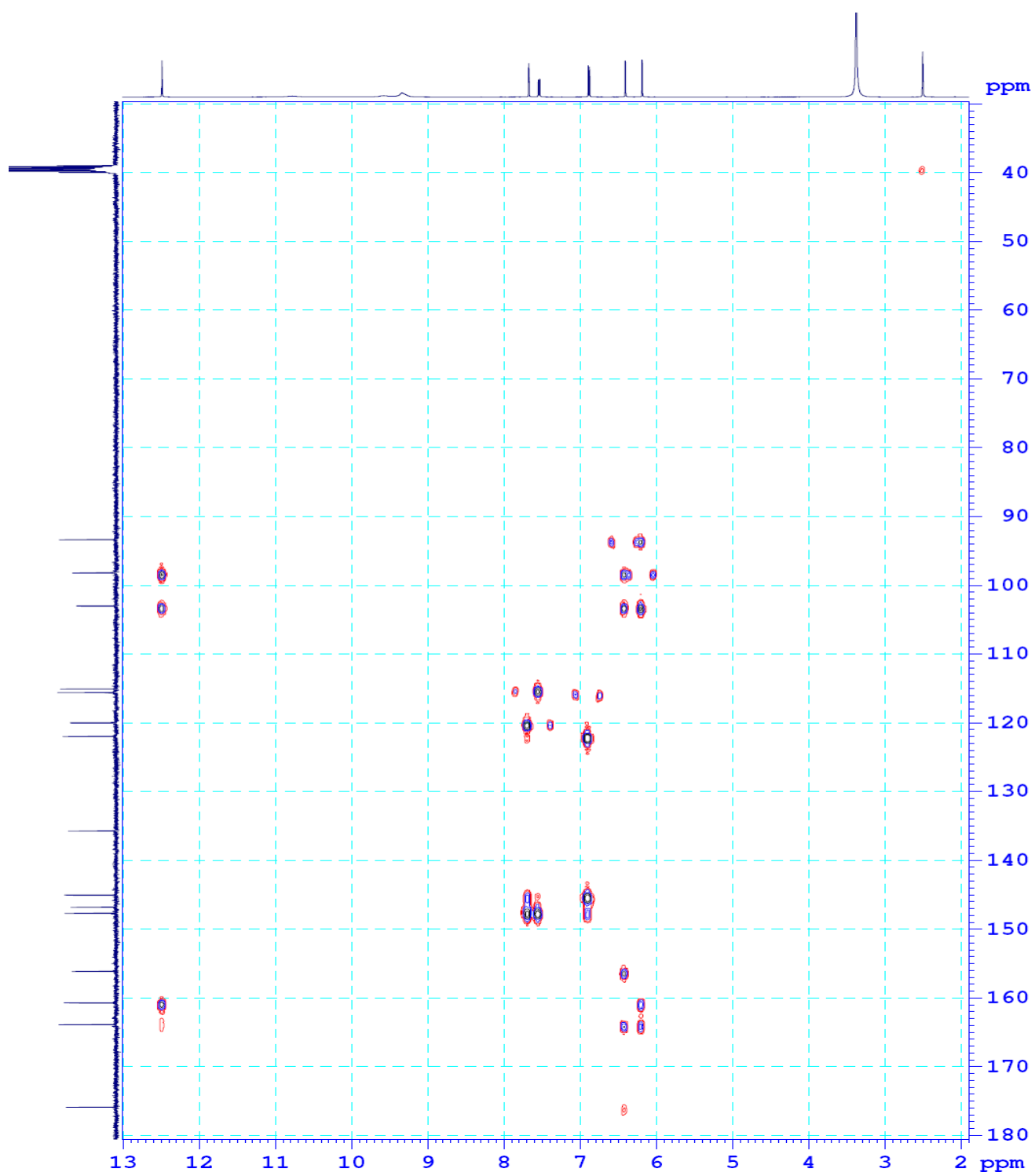
**Figure S51:**  $^1\text{H}$ -NMR spectrum of compound **6**.



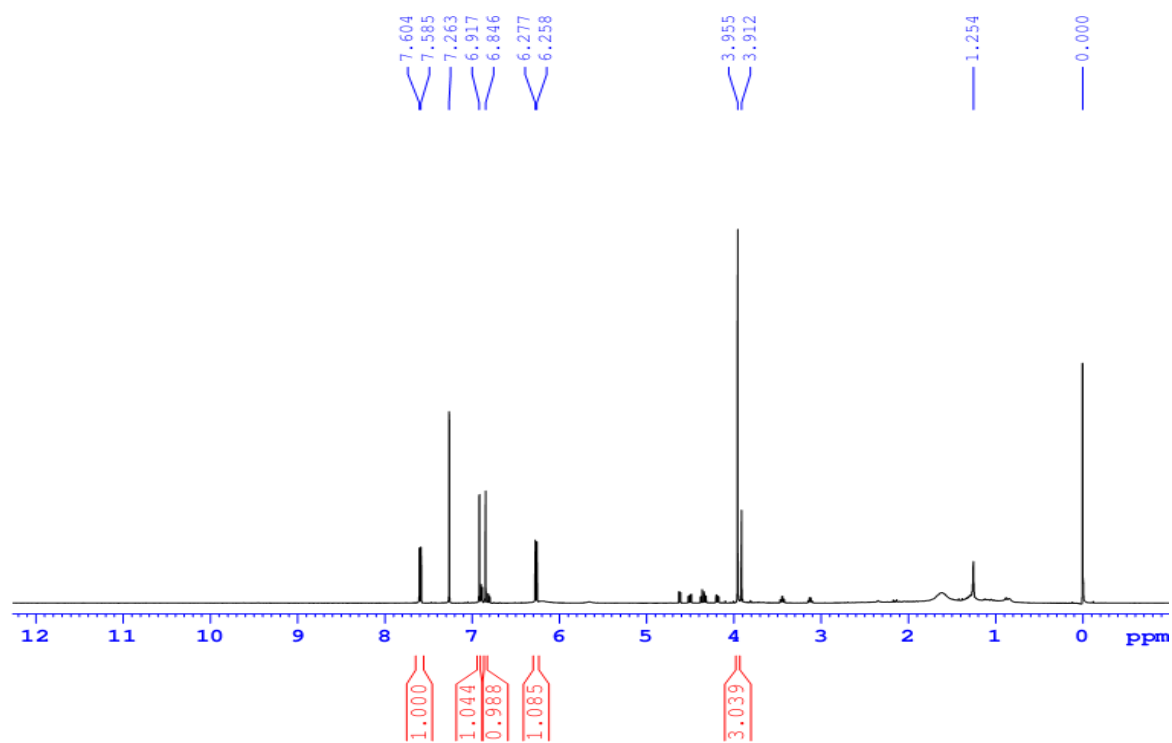
**Figure S52:**  $^{13}\text{C}$ -NMR spectrum of compound **6**.



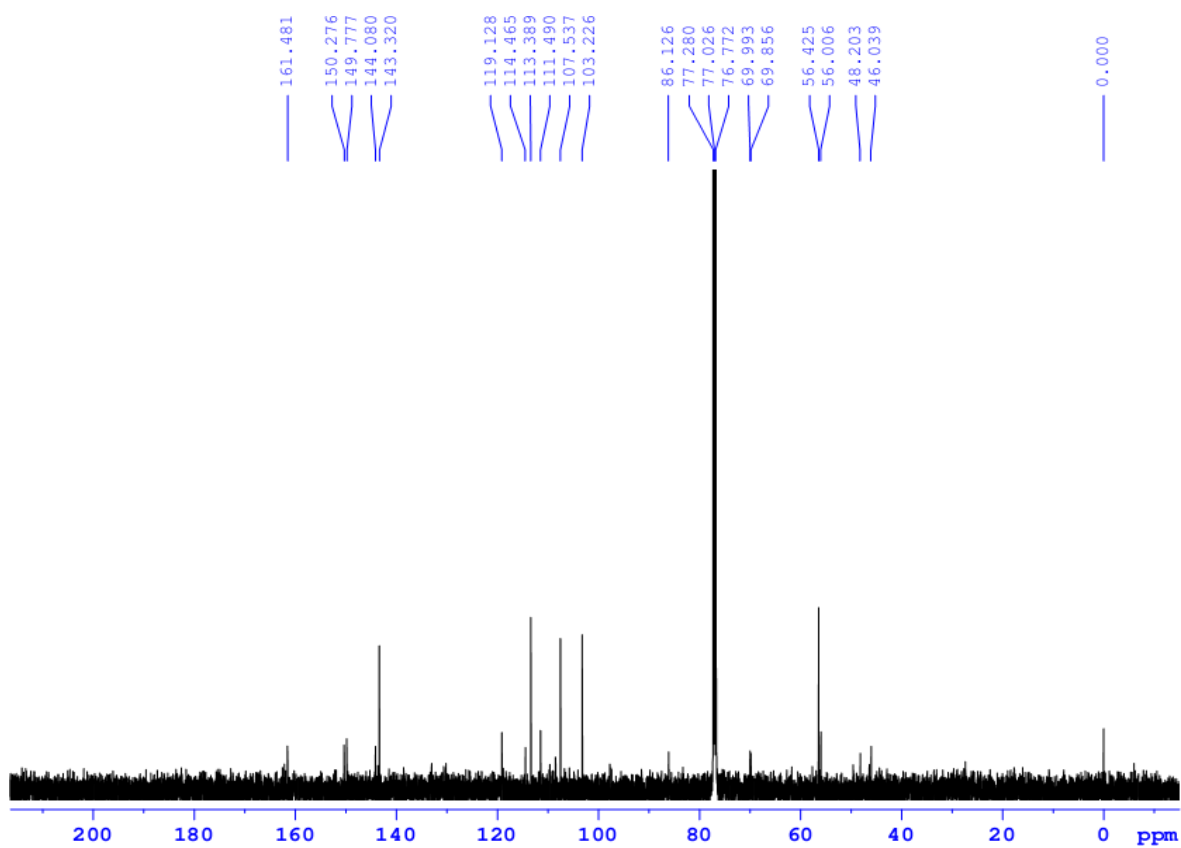
**Figure S53:** DEPT spectrum of compound 6.



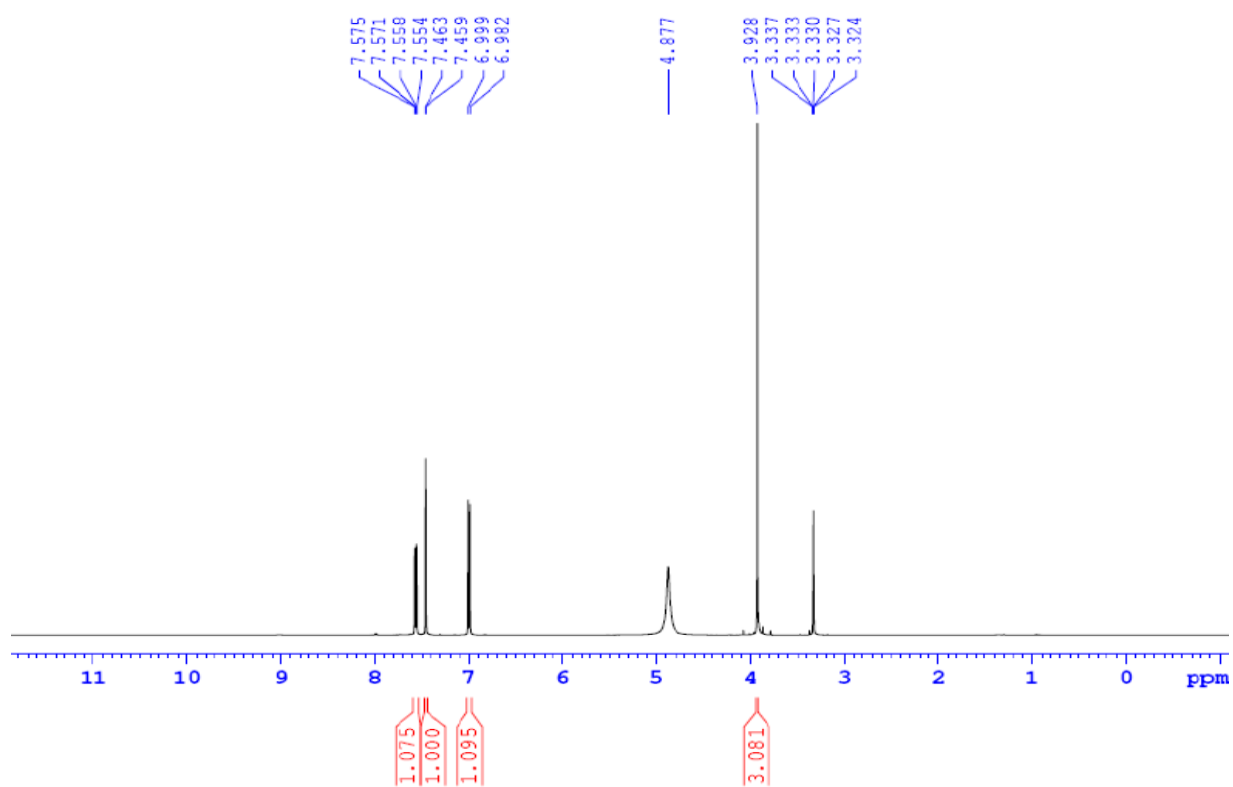
**Figure S54:** HMBC spectrum of compound **6**.



**Figure S55:**  $^1\text{H-NMR}$  spectrum of compound 7.

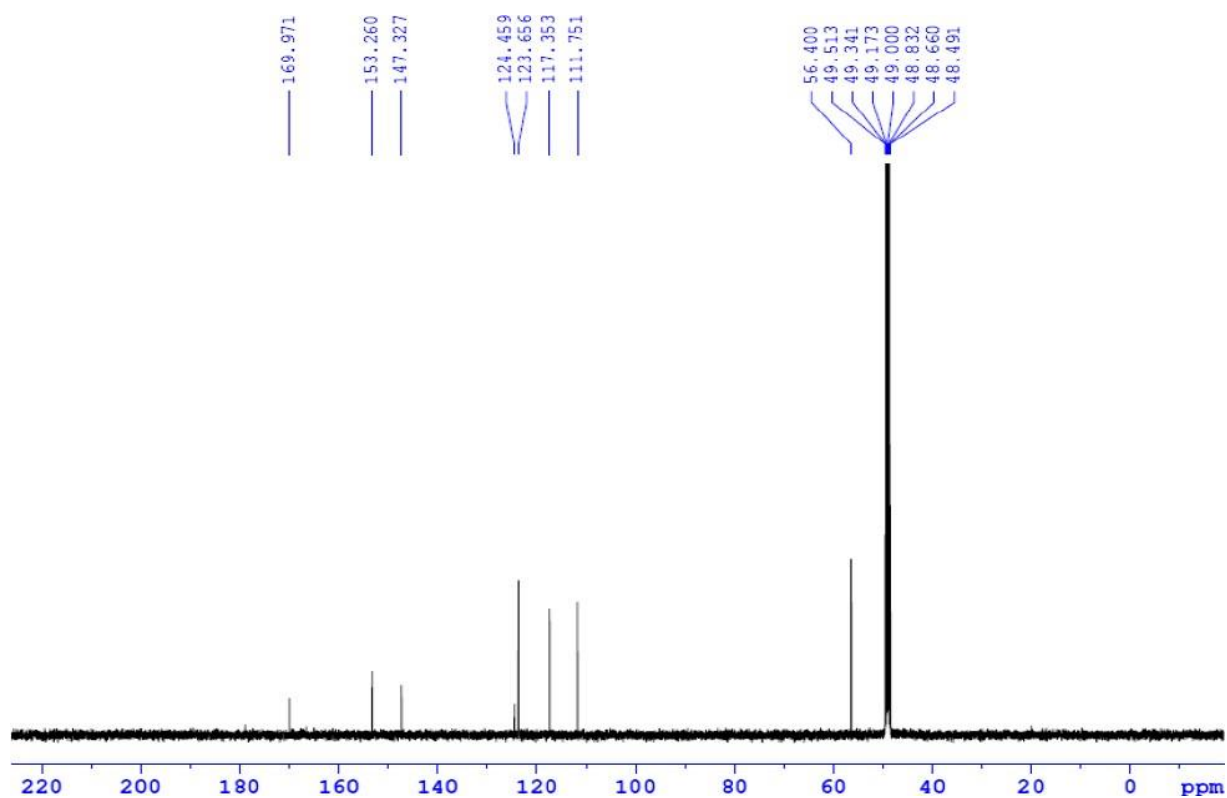


**Figure S56:**  $^{13}\text{C}$ -NMR spectrum of compound **7**.

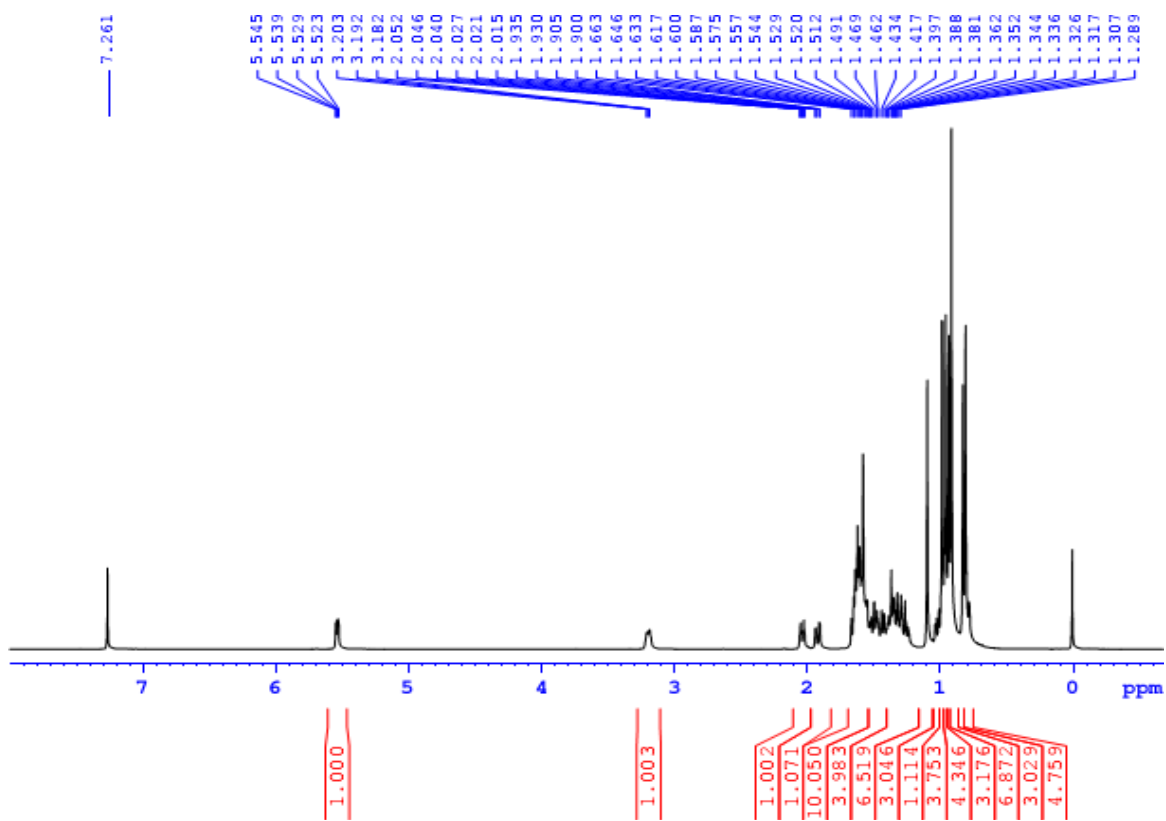


**Figure S57:**  $^1\text{H-NMR}$  spectrum of compound **8**.

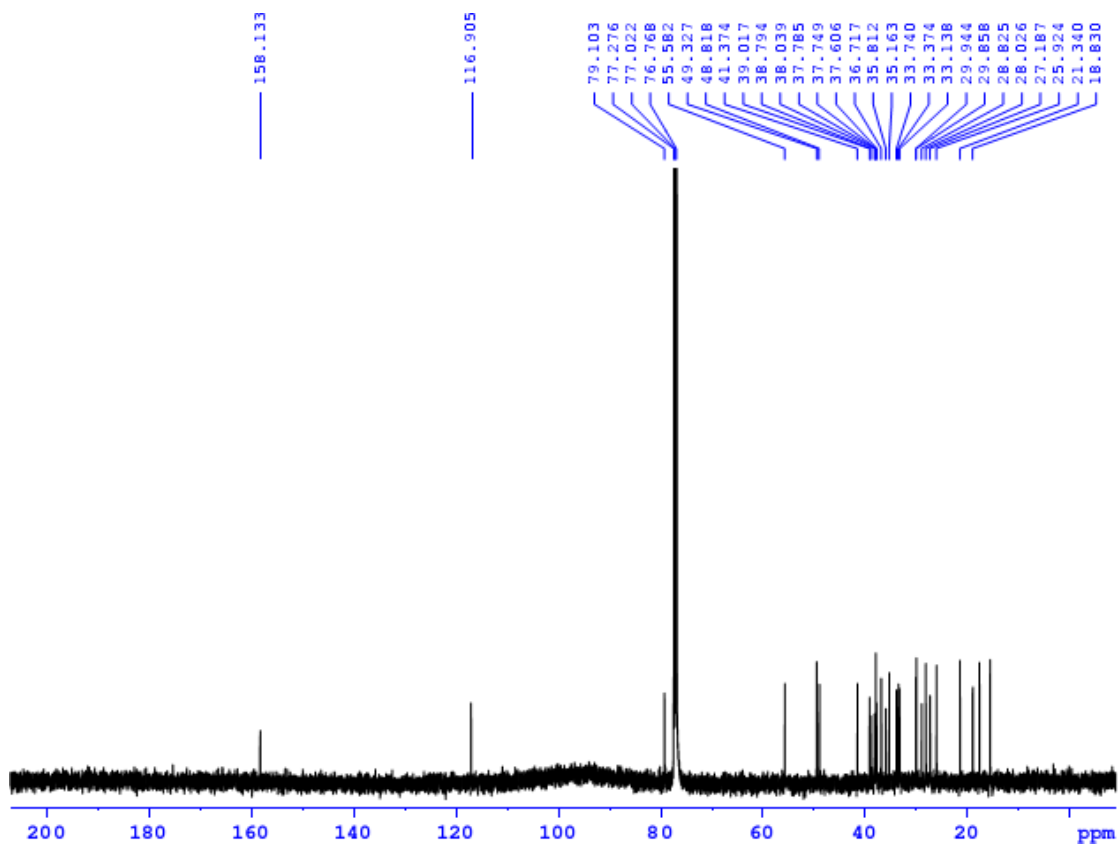




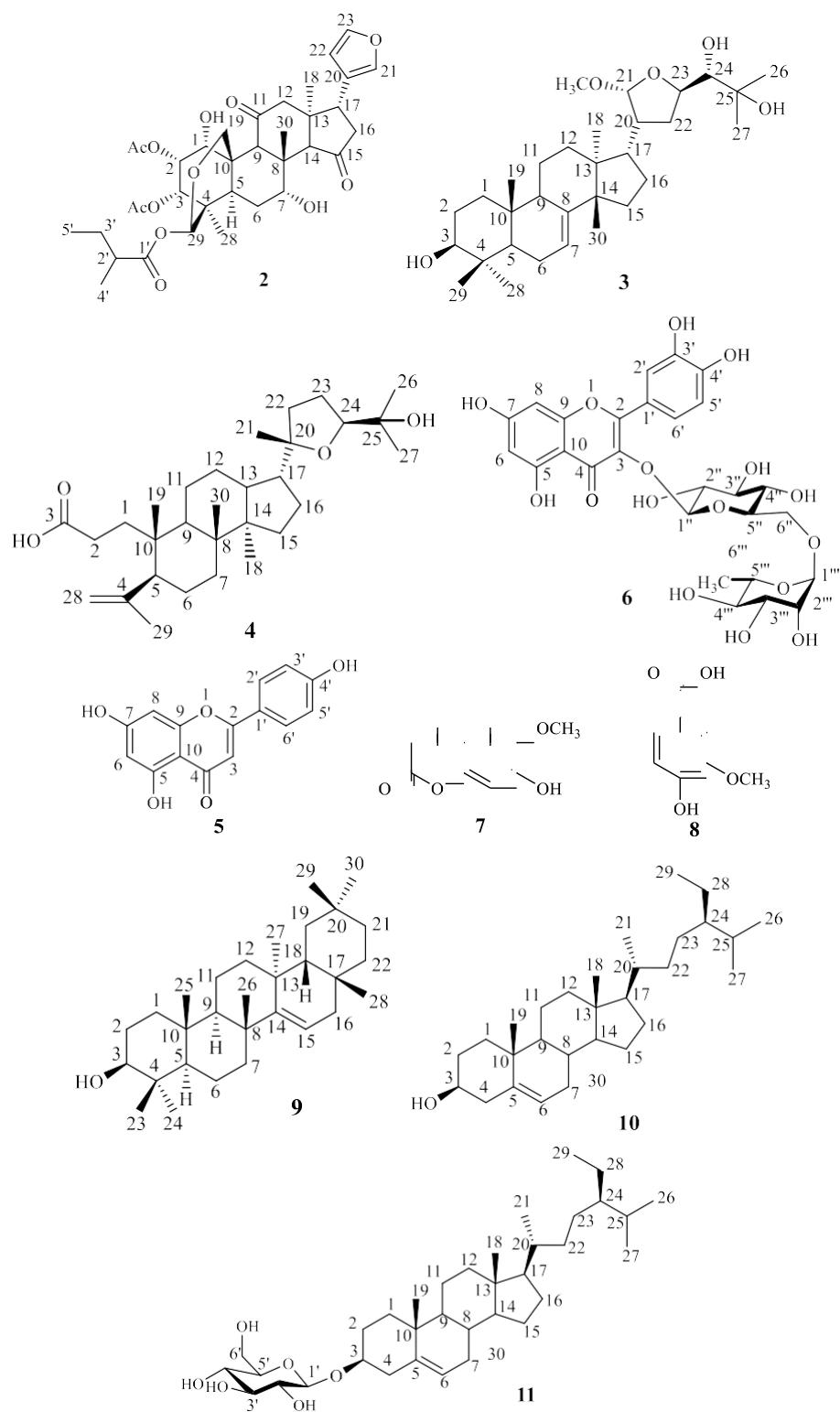
**Figure S58:**  $^{13}\text{C}$ -NMR spectrum of compound **8**.



**Figure S59:**  $^1\text{H-NMR}$  spectrum of compound **9**.



**Figure S60:**  $^{13}\text{C}$ -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*-[ $\alpha$ -L-rhamnopyranosyl-(1 $\rightarrow$ 6)]- $\beta$ -D- glucopyranoside (rutin) (**6**), scopoletin (**7**), vanillic acid (**8**), taraxerol (**9**),  $\beta$ -sitosterol (**10**), and  $\beta$ -sitosterol-3-*O*- $\beta$ -D-glucopyranoside (**11**)

© 2021 ACG Publications. All rights reserved.