

## Supporting Information

*Rec. Nat. Prod.* 18:5 (2024) 499-507

### Bronchodilator Monoterpenes from the Fruits of *Trachyspermum ammi* L.

Abdulaziz S. Saeedan <sup>1\*</sup>, Najeeb Ur Rehman <sup>1</sup>, Faisal K. Alkholifi <sup>1</sup>,  
Yousef A. Alanzi <sup>2</sup>, Anzarul Haque <sup>3</sup>, Omar K. M. Al-Rahimi <sup>2</sup>  
and Maged S. Abdel-Kader <sup>4,5\*</sup>

<sup>1</sup>Department of Pharmacology, College of Pharmacy, Prince Sattam Bin Abdulaziz University, P.O.  
Box 173, Al-Kharj 11942, Saudi Arabia

<sup>2</sup>College of Pharmacy, Prince Sattam Bin Abdulaziz University, P.O. Box 173, Al-Kharj 11942,  
Saudi Arabia

<sup>3</sup>Central Laboratories Unit, Qatar University, Doha 2713, Qatar

<sup>4</sup>Department of Pharmacognosy, College of Pharmacy, Prince Sattam Bin Abdulaziz University, P.O.  
Box 173, Al-Kharj 11942, Saudi Arabia

<sup>5</sup>Department of Pharmacology, Faculty of Pharmacy, Alexandria University, Alexandria 21215, Egypt

---

#### Table of contents

Title	Page
Figure S1: <sup>1</sup> HNMR spectrum of <b>1</b> .	3
Figure S2: <sup>1</sup> HNMR spectrum of <b>1</b> (Exp.).	3
Figure S3: <sup>1</sup> HNMR spectrum of <b>1</b> (Exp.).	4
Figure S4: <sup>13</sup> CNMR spectrum of <b>1</b> .	4
Figure S5: DEPT135 spectrum of <b>1</b> .	5
Figure S6: COSY spectrum of <b>1</b> .	5
Figure S7: HSQC spectrum of <b>1</b> .	6
Figure S8: HMBC spectrum of <b>1</b> .	6
Figure S9: <sup>1</sup> HNMR spectrum of <b>2</b> .	7
Figure S10: <sup>1</sup> HNMR spectrum of <b>2</b> (Exp.).	7
Figure S11: <sup>1</sup> HNMR spectrum of <b>2</b> (Exp.).	8
Figure S12: <sup>13</sup> CNMR spectrum of <b>2</b> .	8
Figure S13: DEPT135 spectrum of <b>2</b> .	9
Figure S14: COSY spectrum of <b>2</b> .	9

---

\* Corresponding author: [mp Pharm101@hotmail.com](mailto:mp Pharm101@hotmail.com) (M.S. Abdel Kader); [a.binsaeedan@psau.edu.sa](mailto:a.binsaeedan@psau.edu.sa) (A.S. Saeedan)

---

<b>Figure S15:</b> HSQC spectrum of <b>2</b> .	10
<b>Figure S16:</b> HMBC spectrum of <b>2</b> .	10
<b>Figure S17:</b> HRESIMS spectrum of <b>2</b> (Negative mode).	11
<b>Figure S18:</b> HRESIMS spectrum of <b>2</b> (Positive mode).	11
<b>Figure S19:</b> <sup>1</sup> HNMR spectrum of <b>2a</b> .	12
<b>Figure S20:</b> APT spectrum of <b>2a</b> .	12
<b>Figure S21:</b> APT spectrum of <b>2a</b> (Exp).	13
<b>Figure S22:</b> APT spectrum of <b>2a</b> (Exp).	13
<b>Figure S23:</b> COSY spectrum of <b>2a</b> .	14
<b>Figure S24:</b> COSY spectrum of <b>2a</b> (Exp).	14
<b>Figure S25:</b> HSQC spectrum <b>2a</b> (Exp).	15
<b>Figure S26:</b> HRESIMS spectrum of <b>2a</b> (Positive mode).	15
<b>Figure S27:</b> <sup>1</sup> HNMR spectrum of <b>3</b> .	16
<b>Figure S28:</b> <sup>1</sup> HNMR spectrum of <b>3</b> (Exp).	16
<b>Figure S29:</b> <sup>1</sup> HNMR spectrum of <b>3</b> (Exp).	17
<b>Figure S30:</b> <sup>13</sup> CNMR spectrum of <b>3</b> .	17
<b>Figure S31:</b> DEPT135 spectrum of <b>3</b> .	18
<b>Figure S32:</b> DEPT90 spectrum of <b>3</b> .	18
<b>Figure S33:</b> COSY spectrum of <b>3</b> .	19
<b>Figure S34:</b> COSY spectrum of <b>3</b> (Exp).	19
<b>Figure S35:</b> HSQC spectrum of <b>3</b> .	20
<b>Figure S36:</b> HSQC spectrum of <b>3</b> (Exp).	20
<b>Figure S37:</b> HSQC spectrum of <b>3</b> (Exp).	21
<b>Figure S38:</b> HMBC spectrum of <b>3</b> .	21
<b>Figure S39:</b> HMBC spectrum of <b>3</b> (Exp).	22
<b>Figure S40:</b> HMBC spectrum of <b>3</b> (Exp).	22
<b>Figure S41:</b> HRESIMS spectrum of <b>3</b> (Negative mode).	23
<b>Figure S42:</b> HRESIMS spectrum of <b>3</b> (Positive mode).	23
<b>Figure S43:</b> <sup>1</sup> HNMR spectrum of <b>3a</b> .	24
<b>Figure S44:</b> APT spectrum of <b>3a</b> (Exp).	24
<b>Figure S45:</b> APT spectrum of <b>3a</b> (Exp).	25
<b>Figure S46:</b> APT spectrum of <b>3a</b> (Exp).	25
<b>Figure S47:</b> HRESIMS spectrum of <b>3a</b> (Positive mode).	26
<b>Table S1:</b> NMR data of <b>1-3</b> in Pyridine <i>d</i> <sub>5</sub> and their acetyl derivatives (δ ppm, <i>J</i> in Hz)	27

---

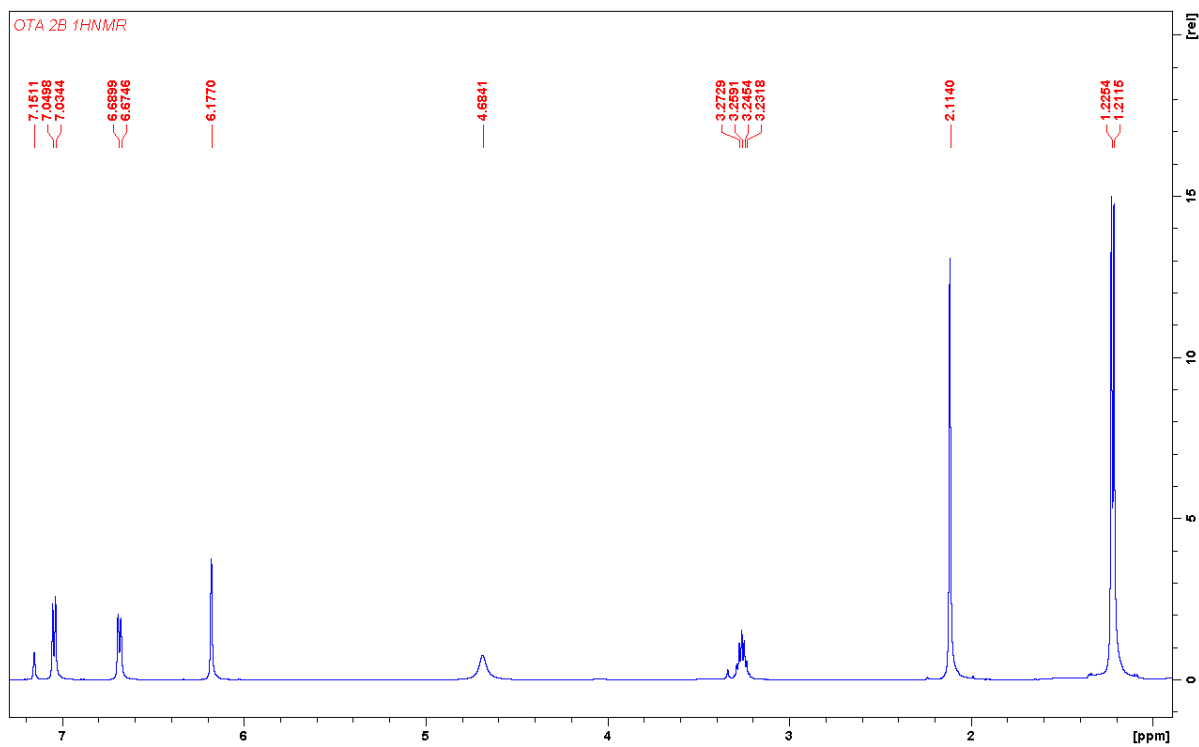


Figure S1: <sup>1</sup>H NMR spectrum of **1**.

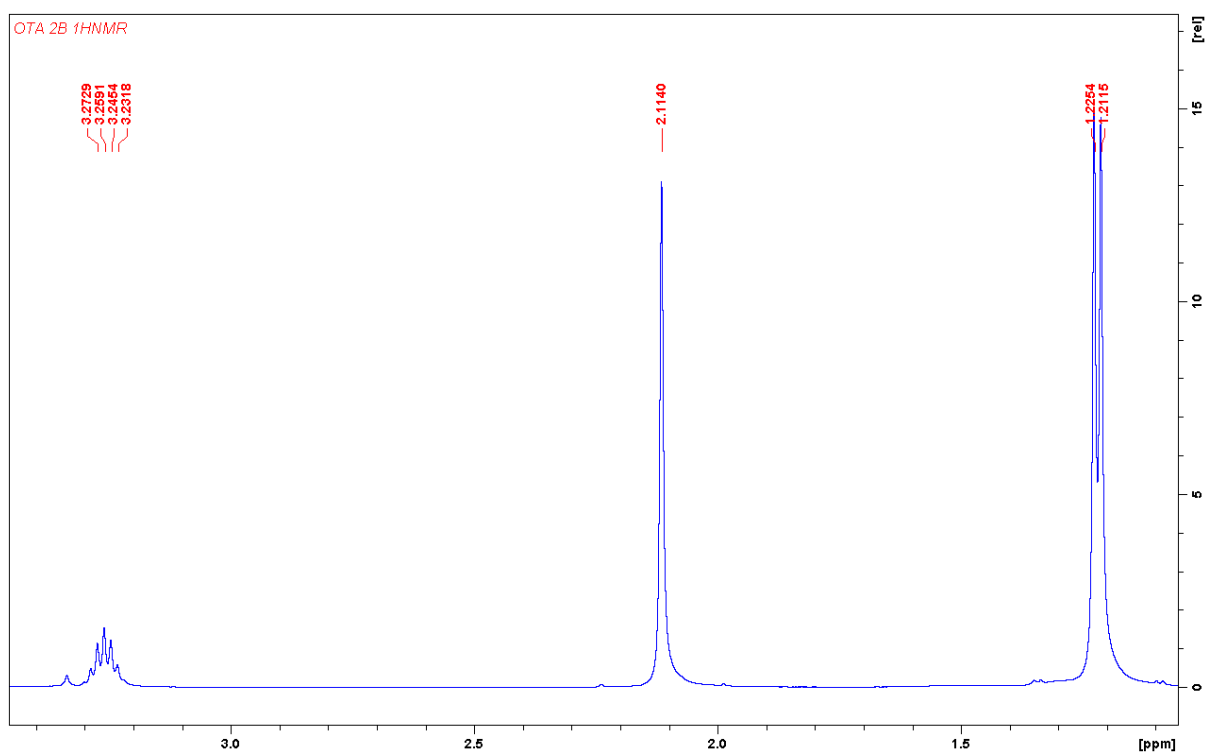


Figure S2: <sup>1</sup>H NMR spectrum of **1** (Exp.).

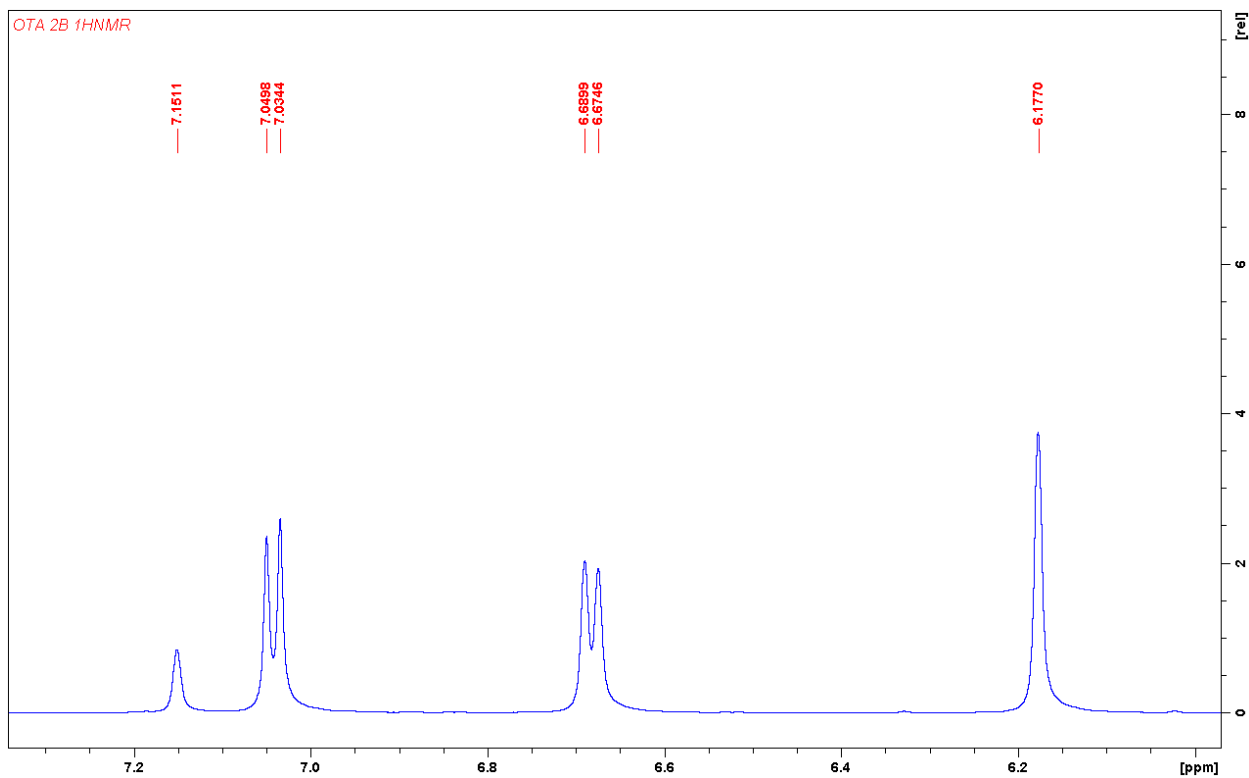


Figure S3:  $^1\text{H}$ NMR spectrum of **1** (Exp).

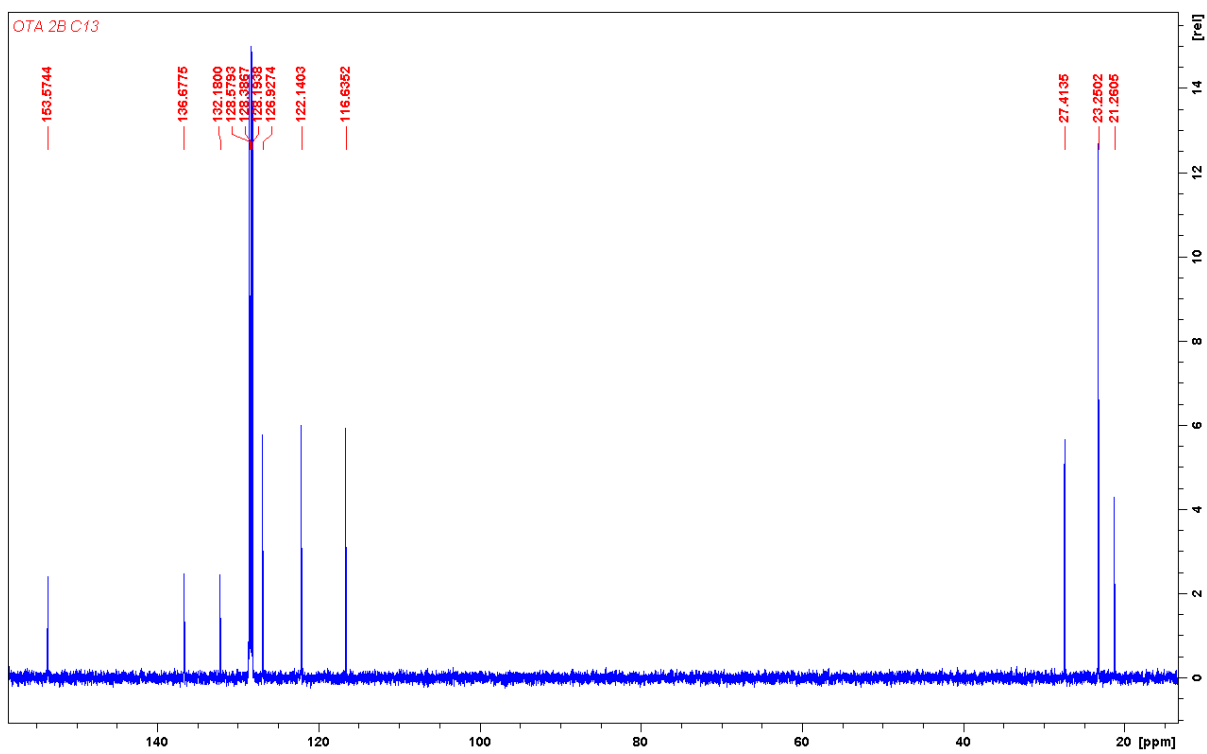


Figure S4:  $^{13}\text{C}$ NMR spectrum of **1**.

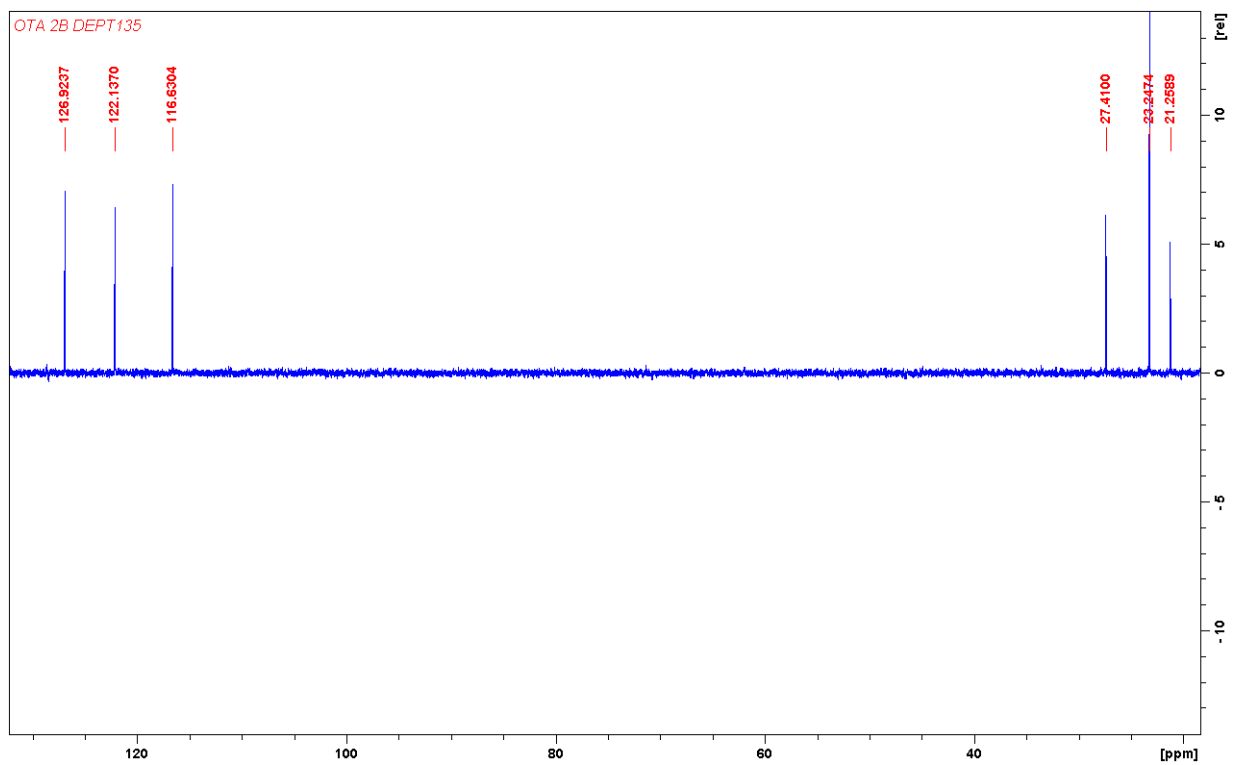


Figure S5: DEPT135 spectrum of 1.

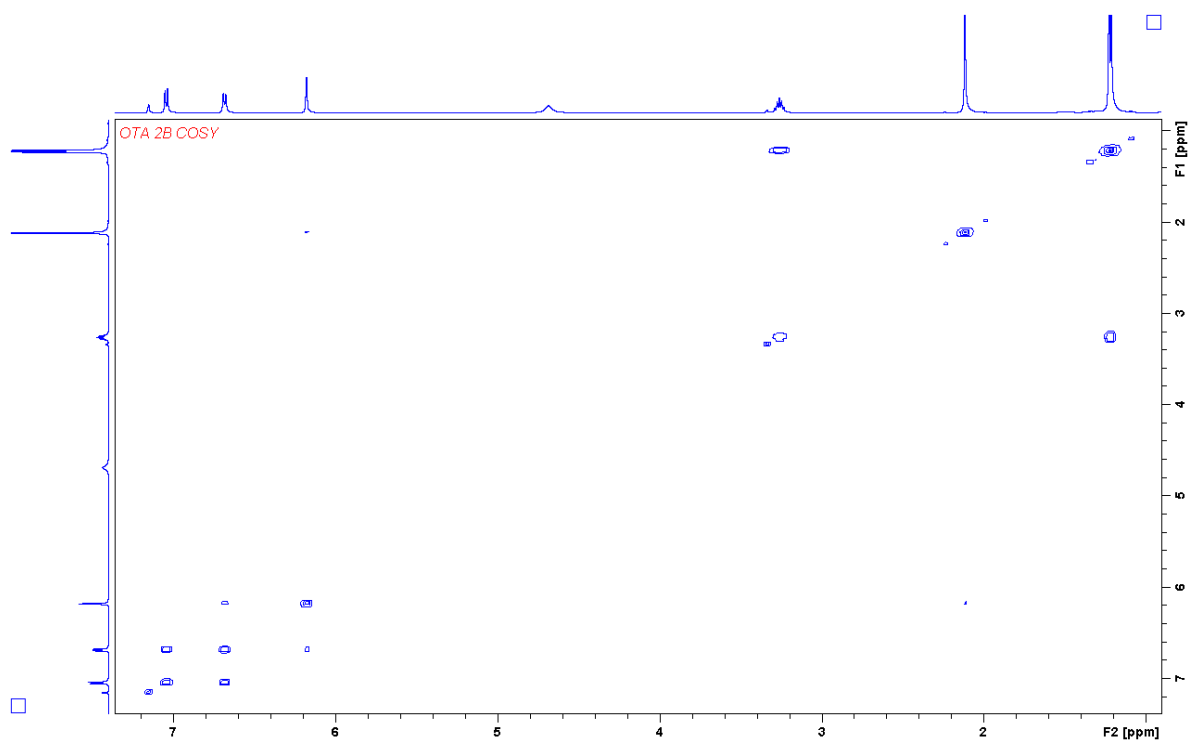


Figure S6: COSY spectrum of 1.

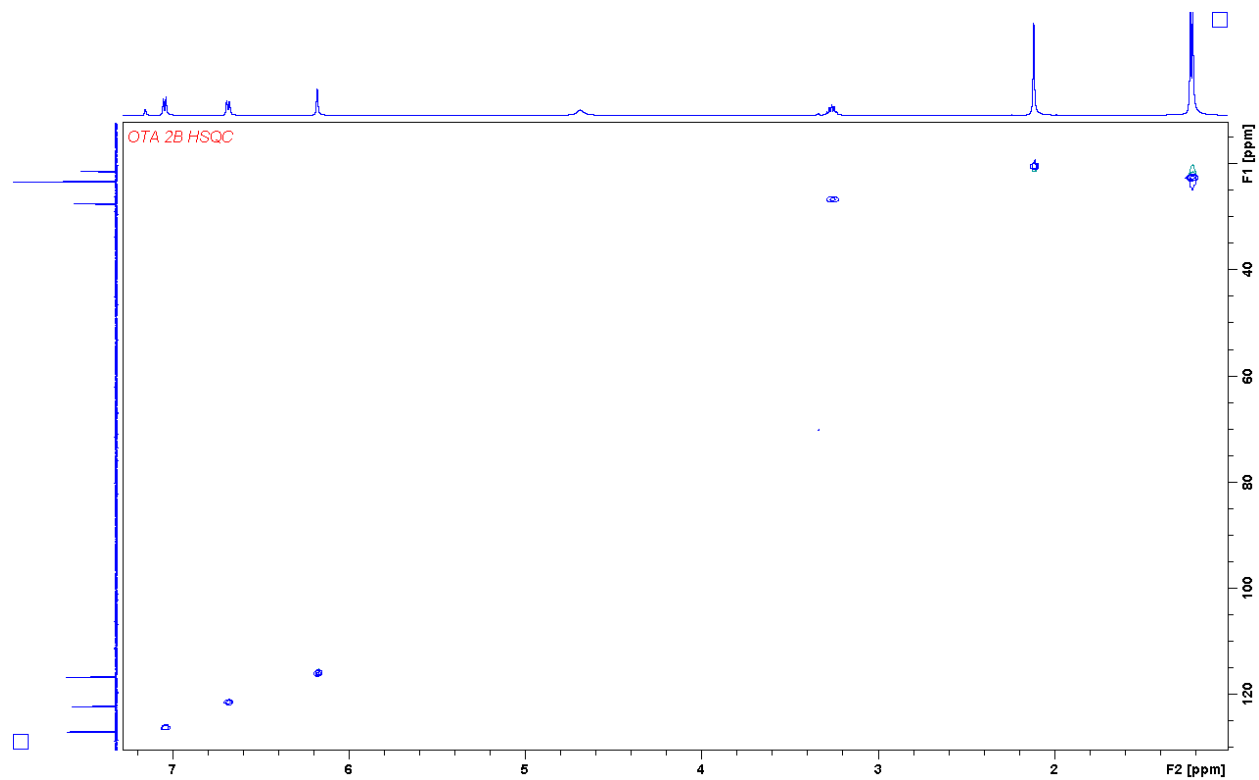


Figure S7: HSQC spectrum of **1**.

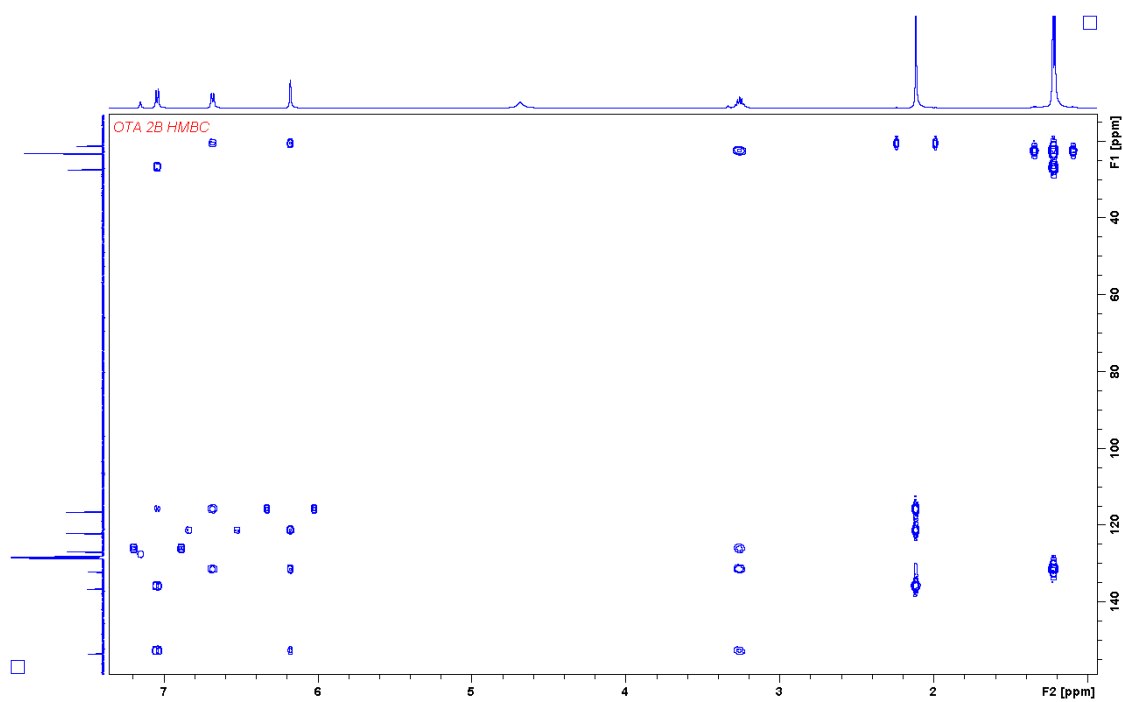


Figure S8: HMBC spectrum of **1**.

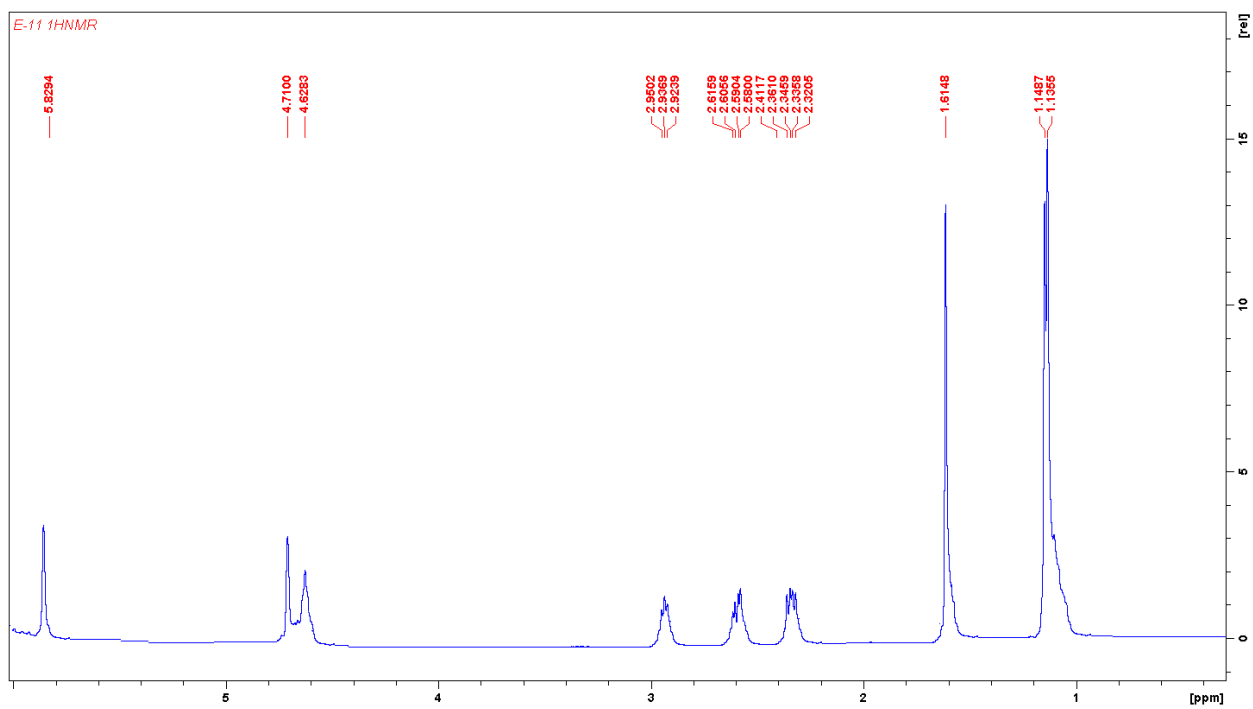


Figure S9: <sup>1</sup>H NMR spectrum of **2**.

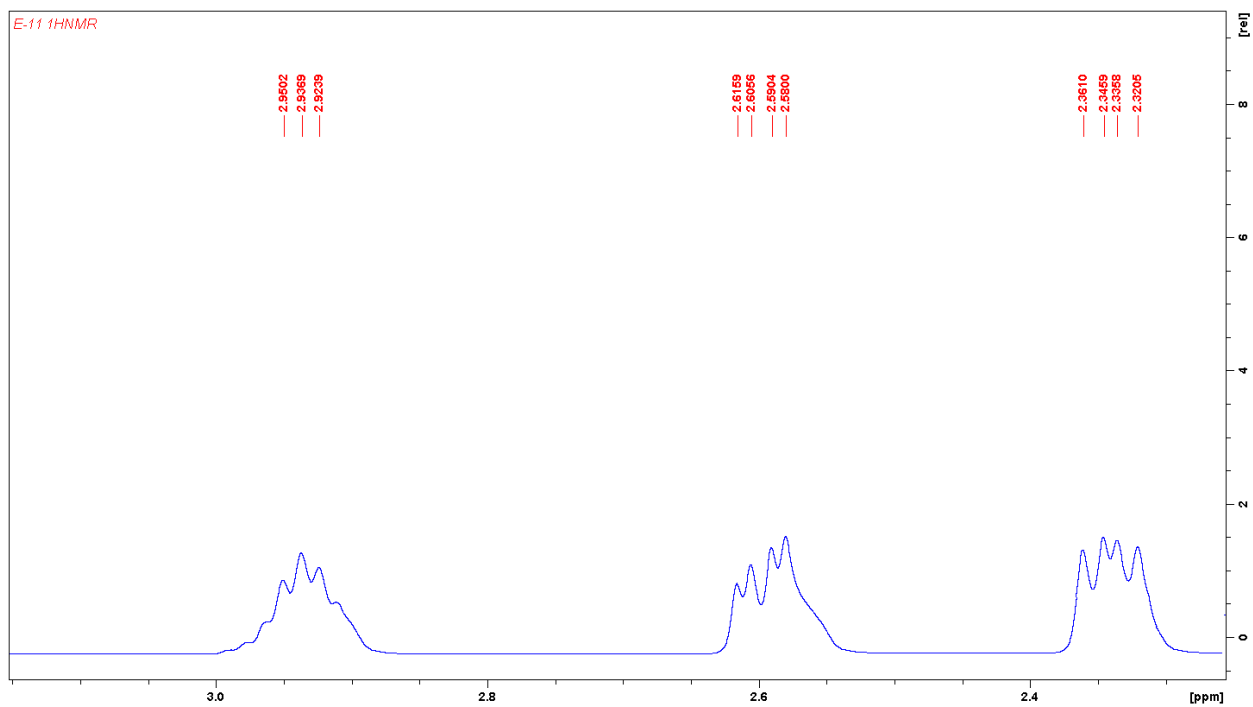


Figure S10: <sup>1</sup>H NMR spectrum of **2** (Exp).

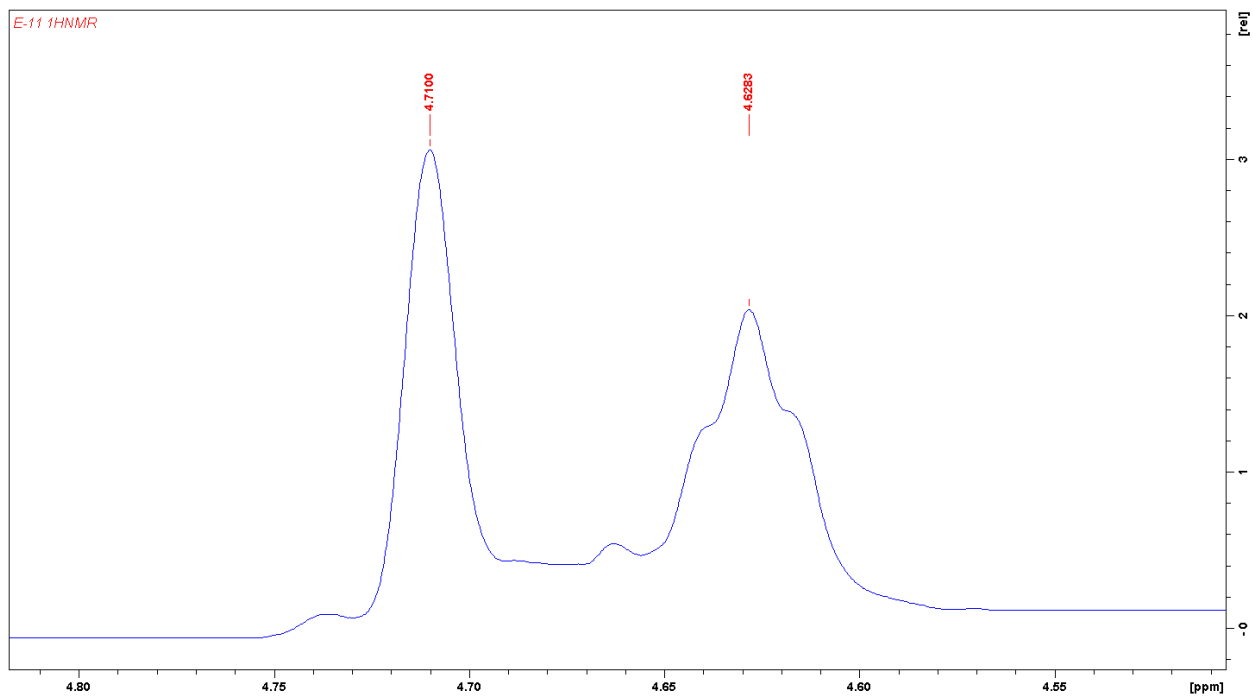


Figure S11: <sup>1</sup>H NMR spectrum of **2** (Exp).

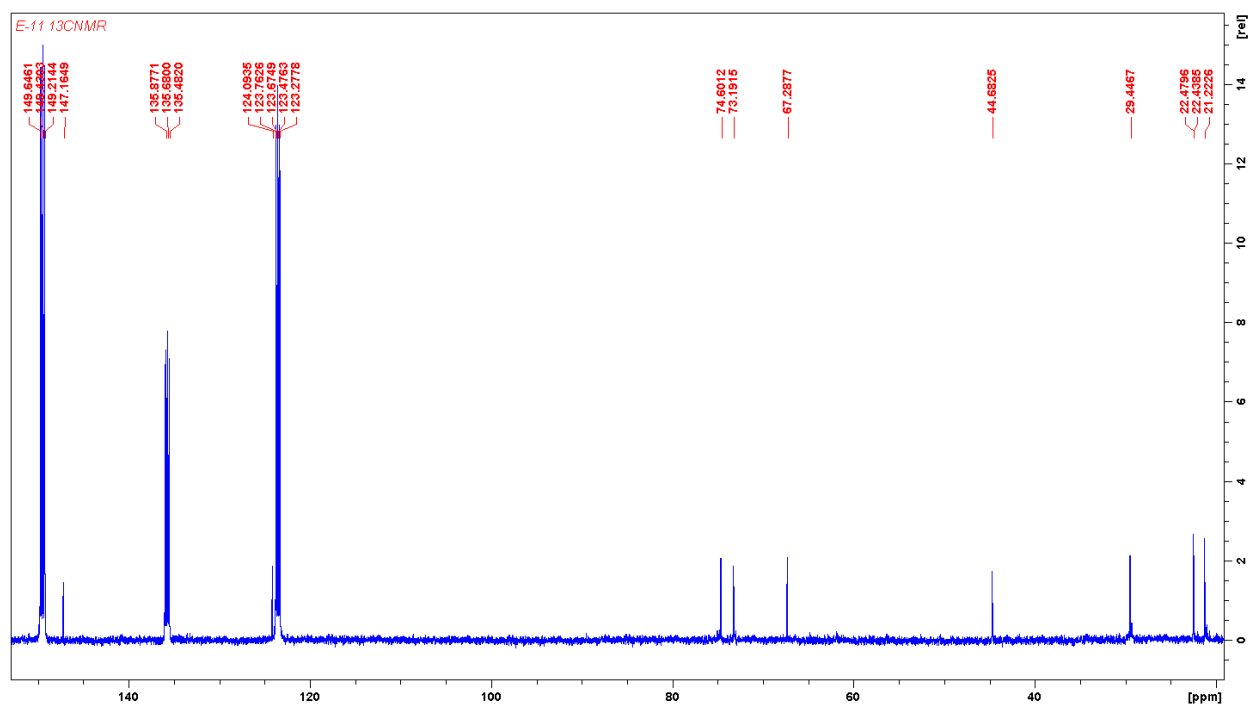


Figure S12: <sup>13</sup>C NMR spectrum of **2**.



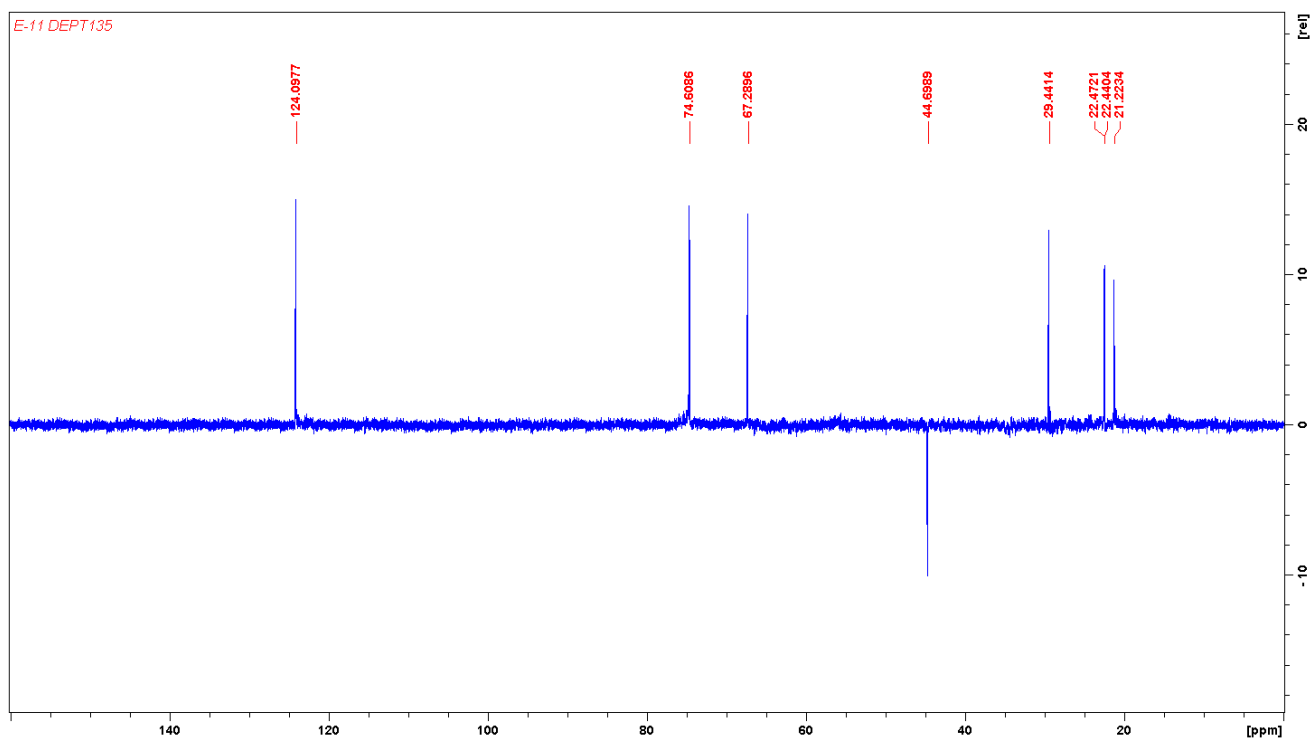


Figure S13: DEPT135 spectrum of **2**.

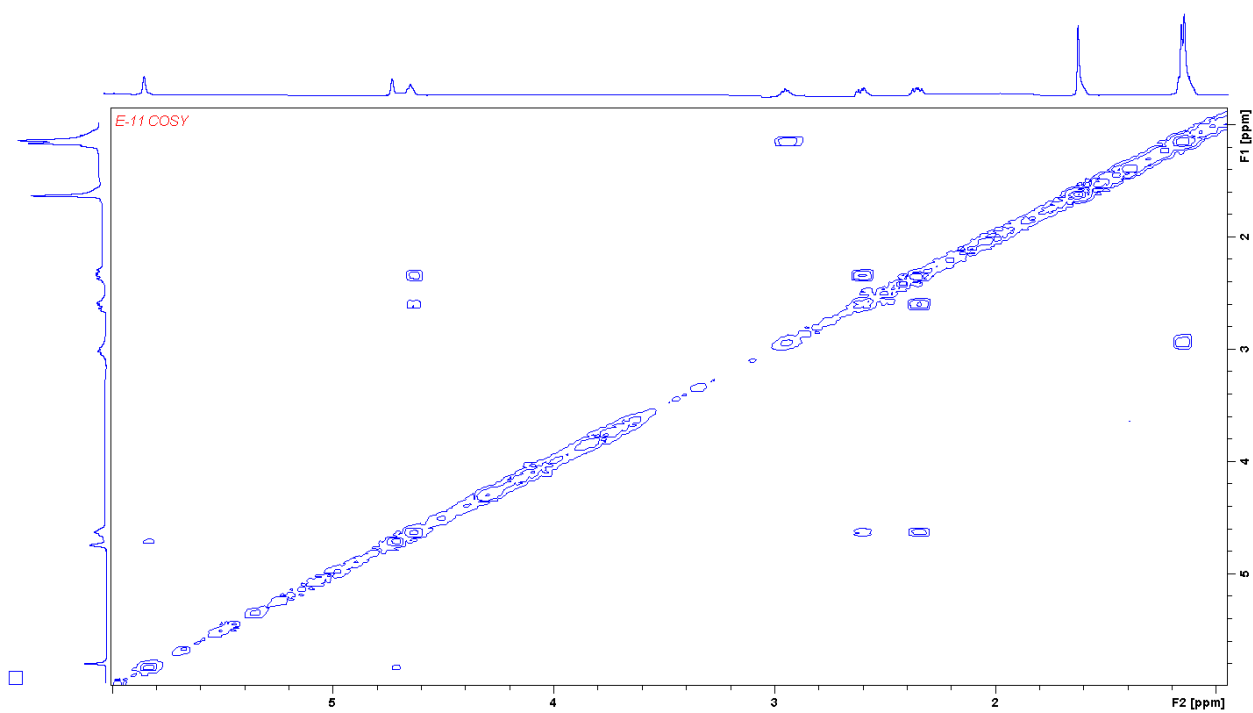


Figure S14: COSY spectrum of **2**.

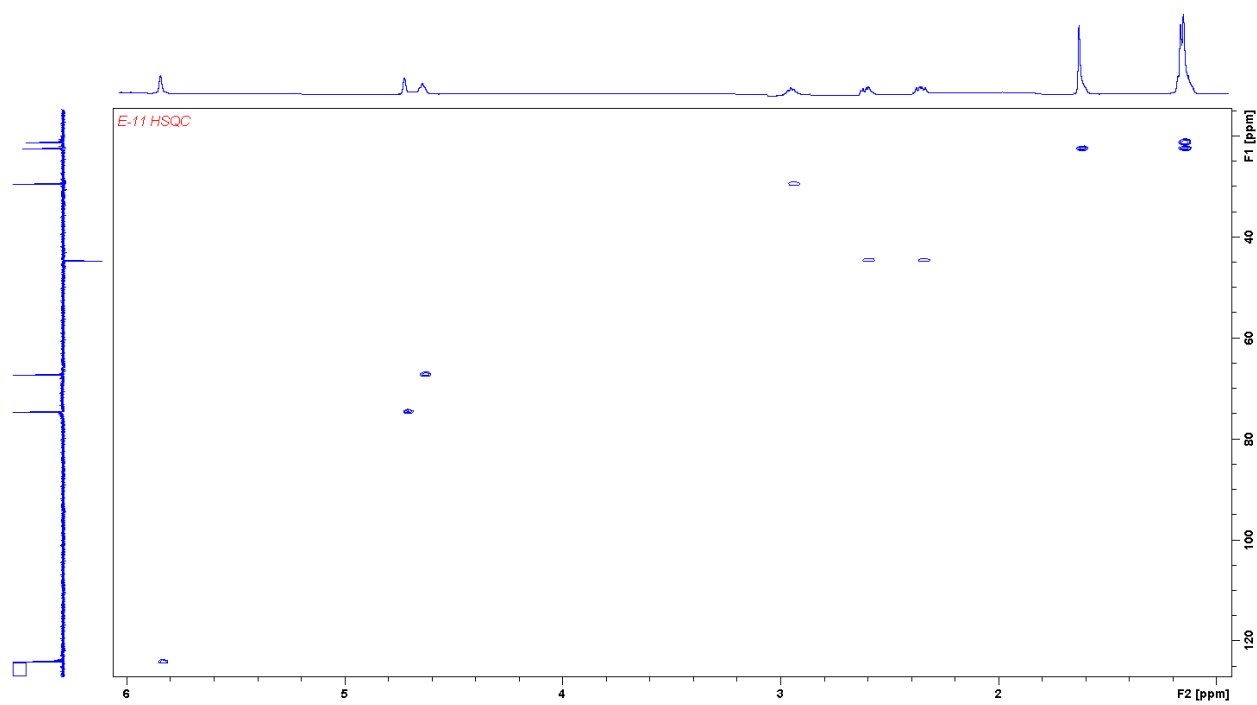


Figure S15: HSQC spectrum of **2**.

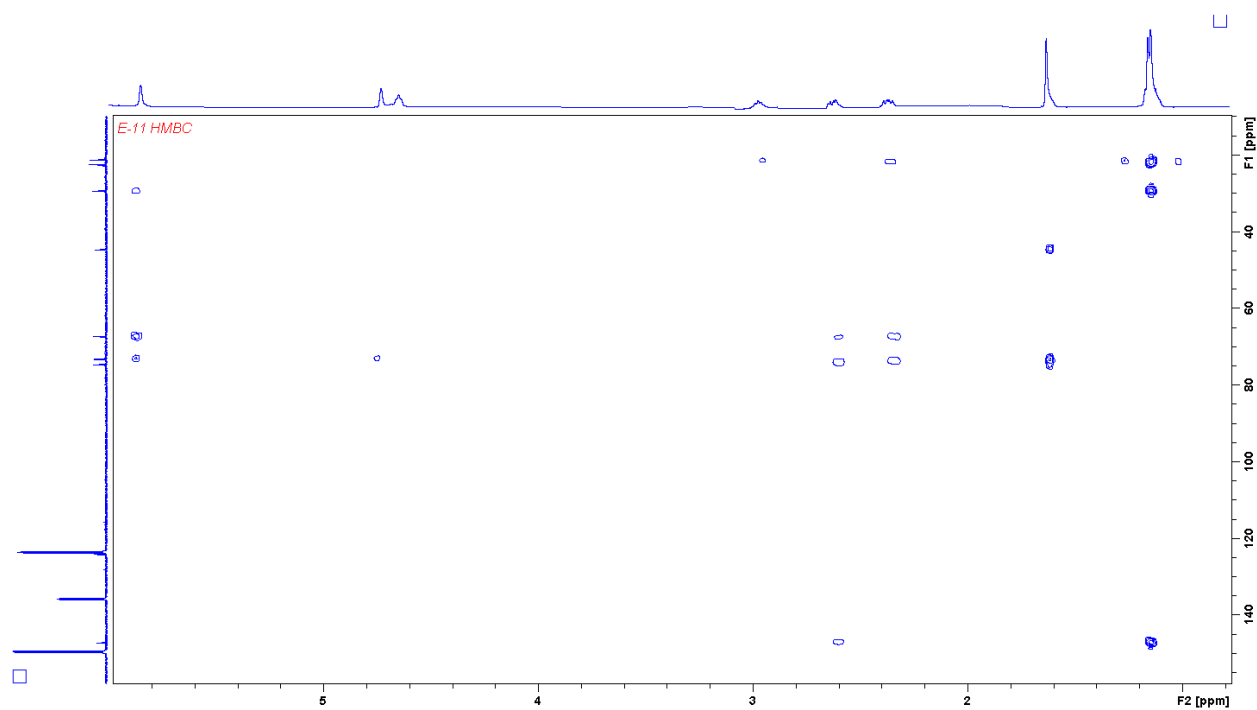
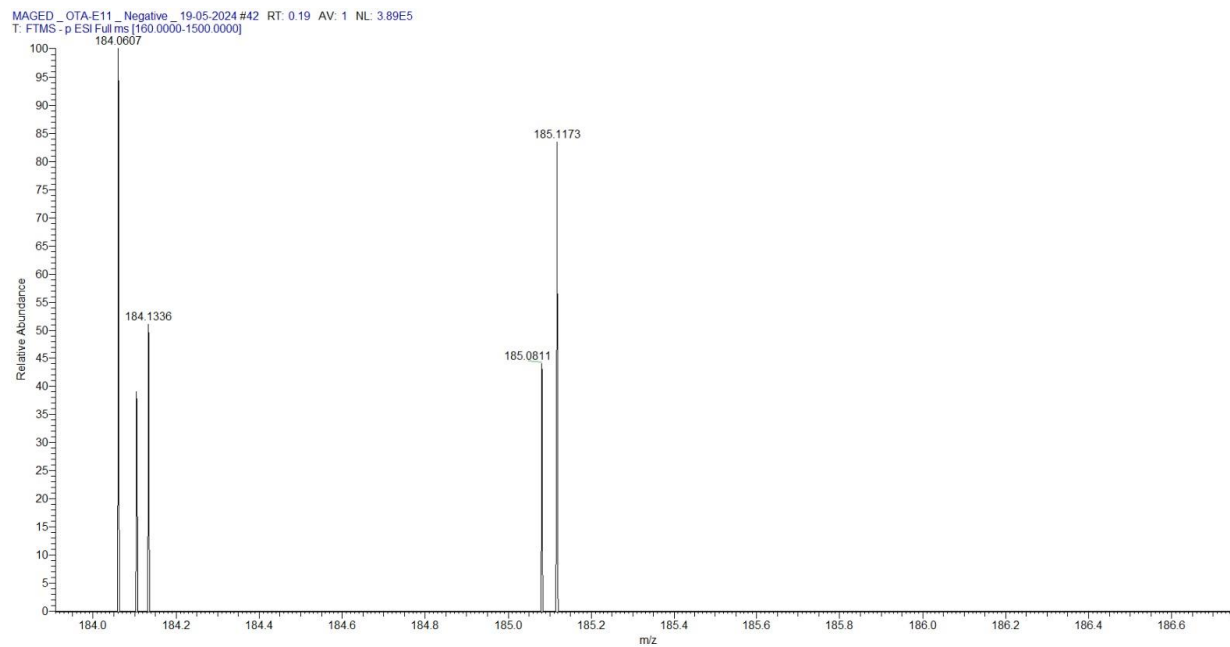
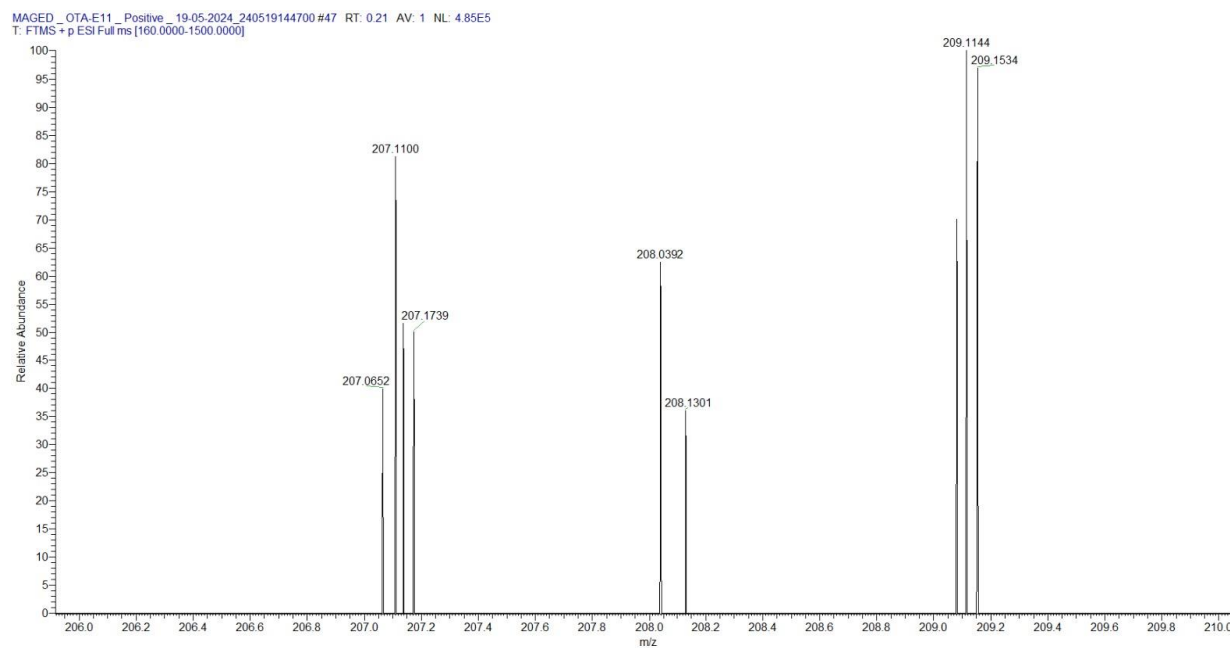


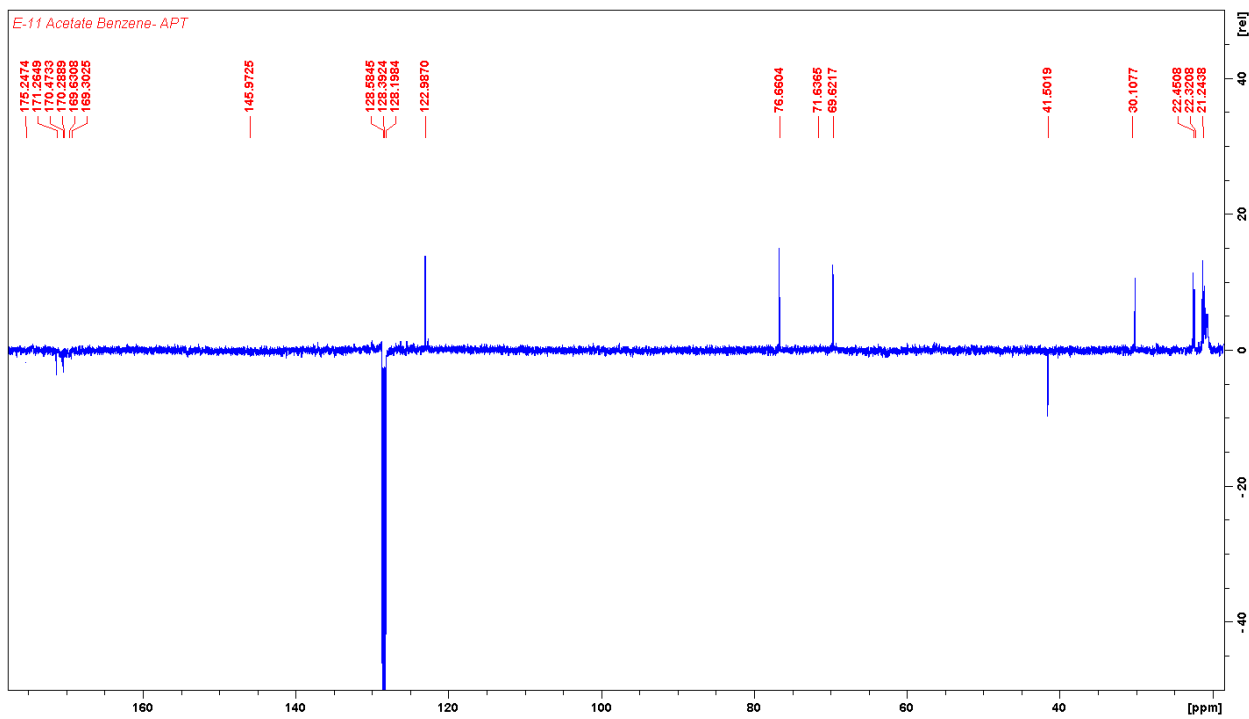
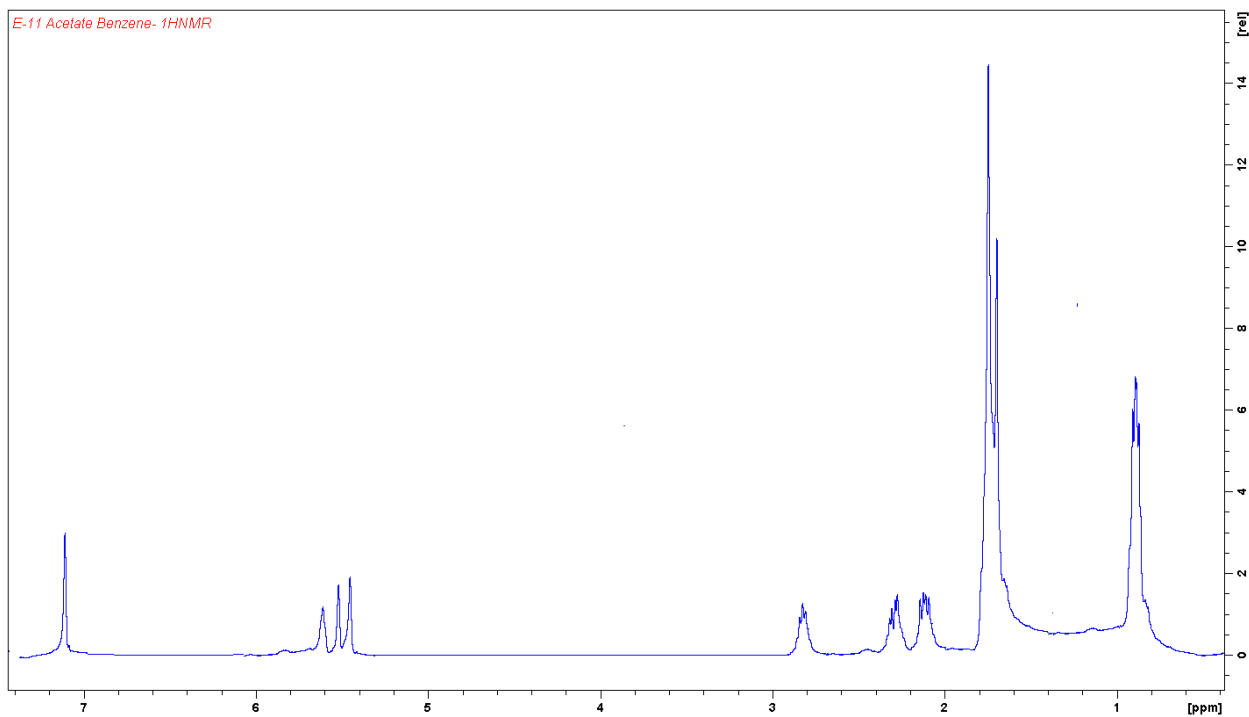
Figure S16: HMBC spectrum of **2**.



**Figure S17:** HRESIMS spectrum of **2** (Negative mode).



**Figure S18:** HRESIMS spectrum of **2** (Positive mode).



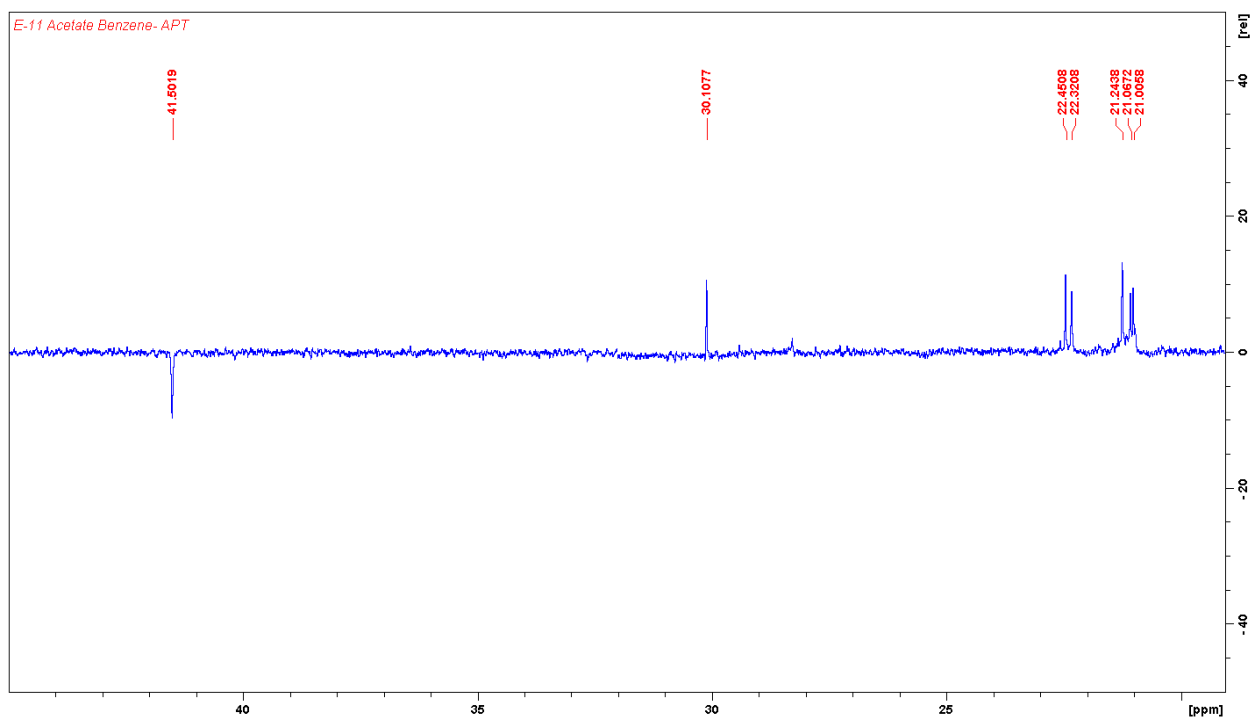


Figure S21: APT spectrum of 2a (Exp).

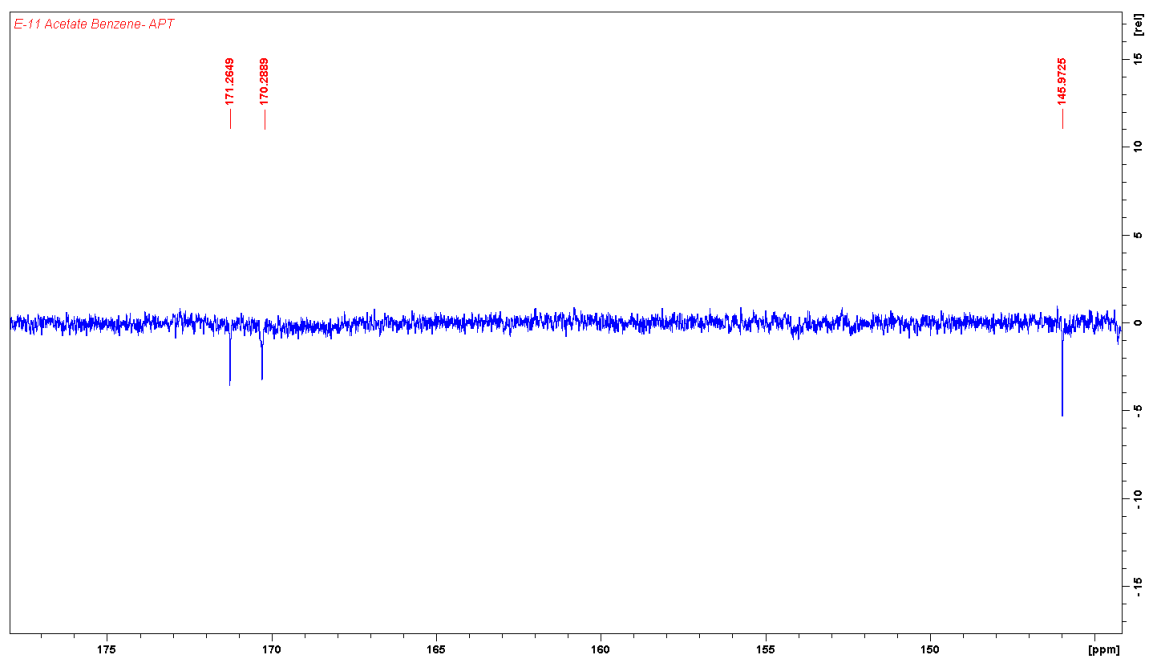


Figure S22: APT spectrum of 2a (Exp).

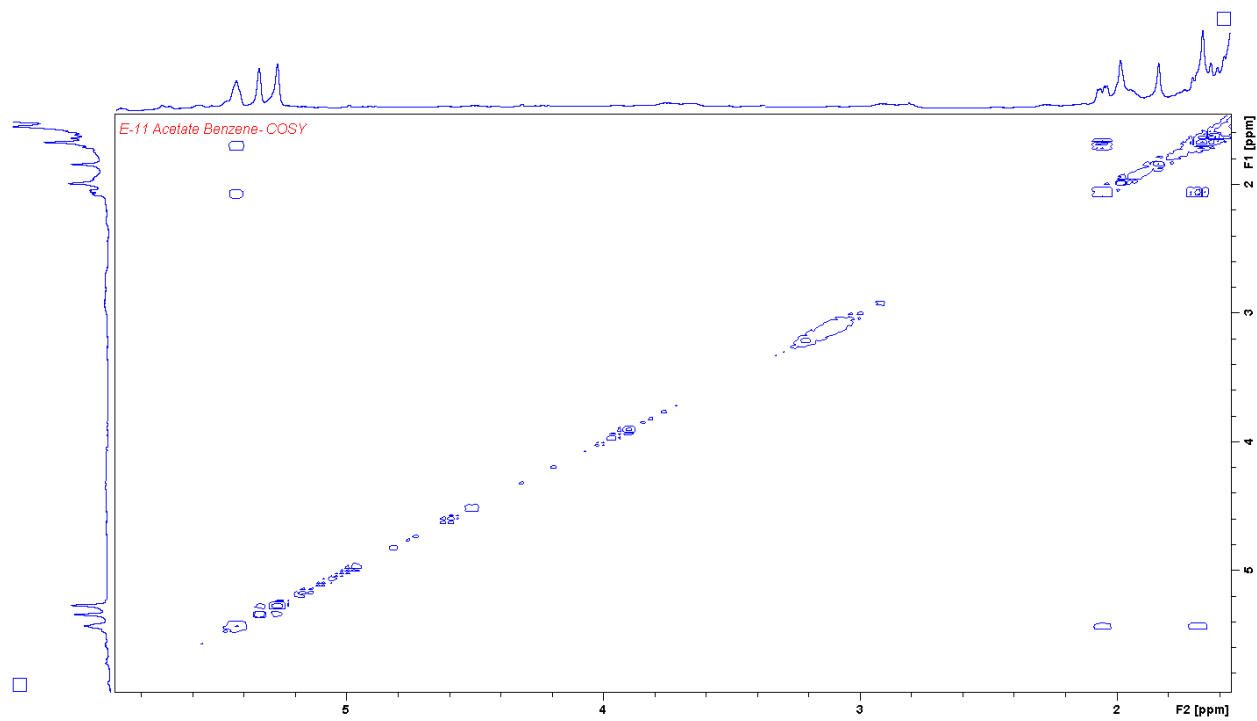


Figure S23: COSY spectrum of 2a.

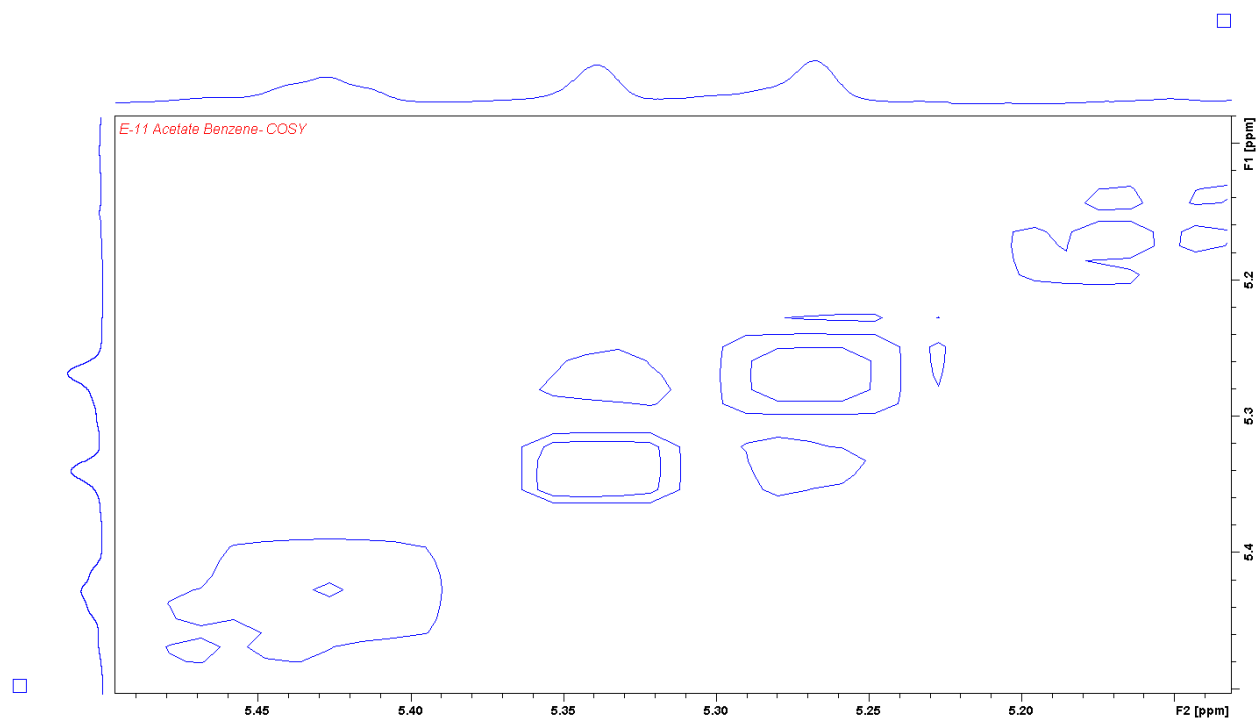


Figure S24: COSY spectrum of 2a (Exp).

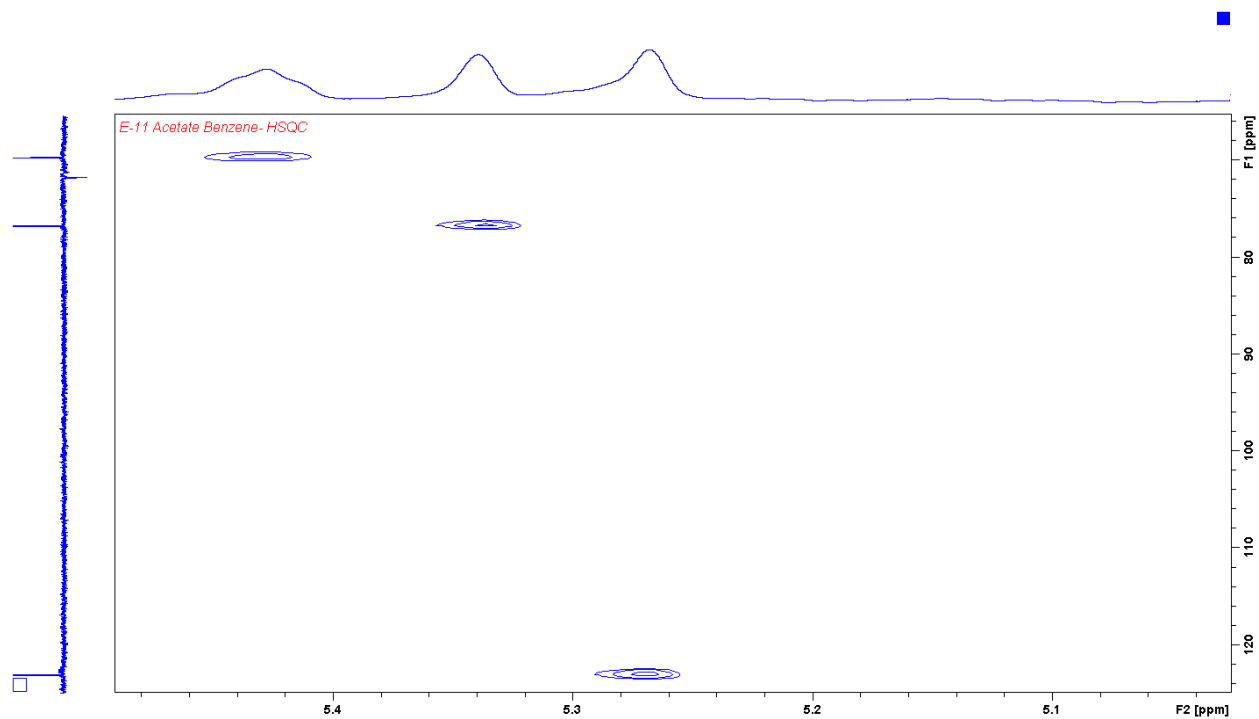


Figure S25: HSQC spectrum **2a** (Exp).

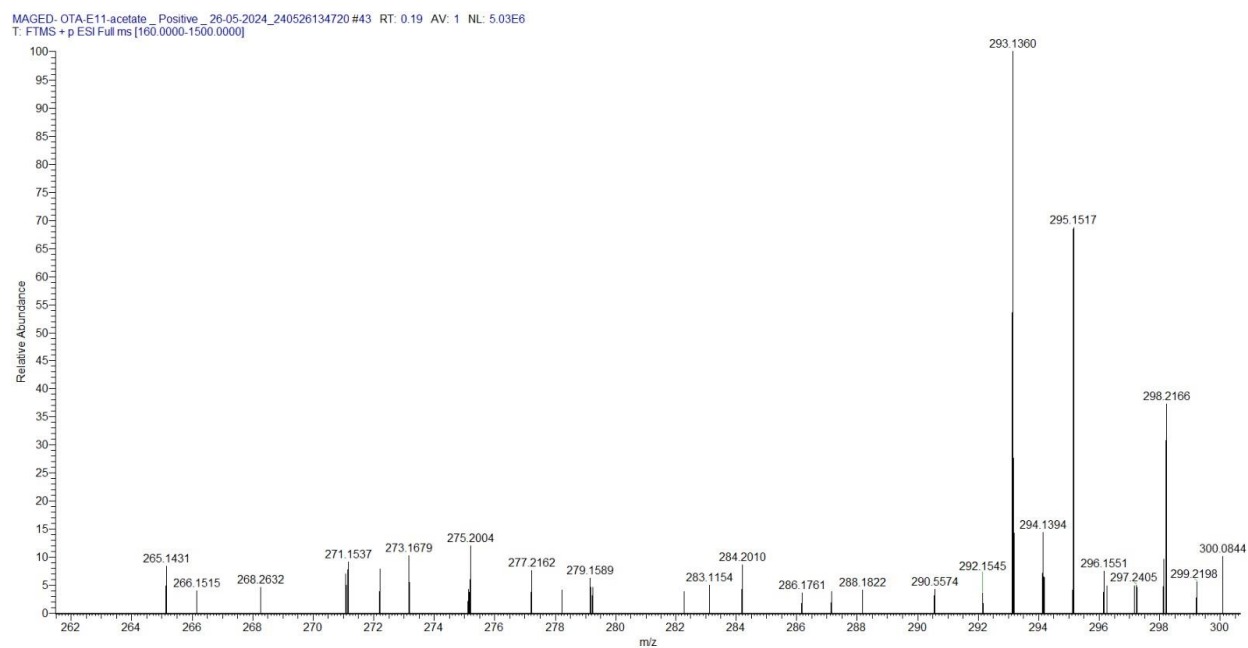


Figure S26: HRESIMS spectrum of **2a** (Positive mode).

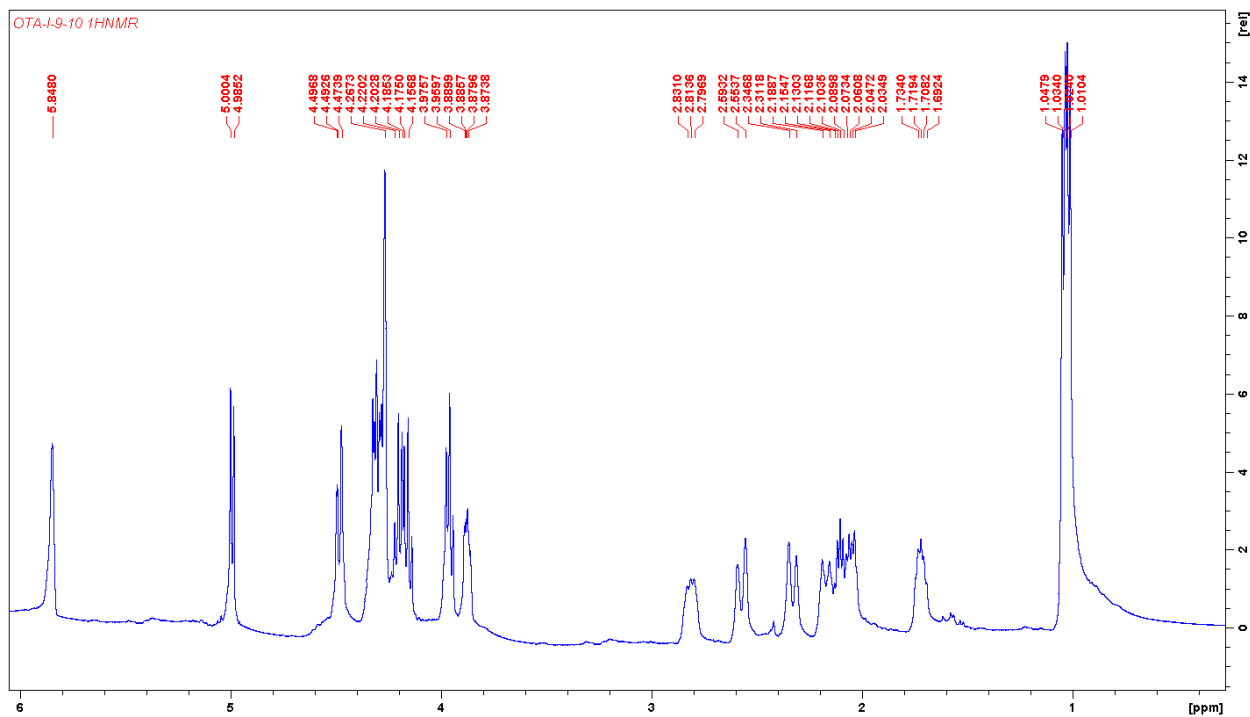


Figure S27: <sup>1</sup>HNMR spectrum of **3**.

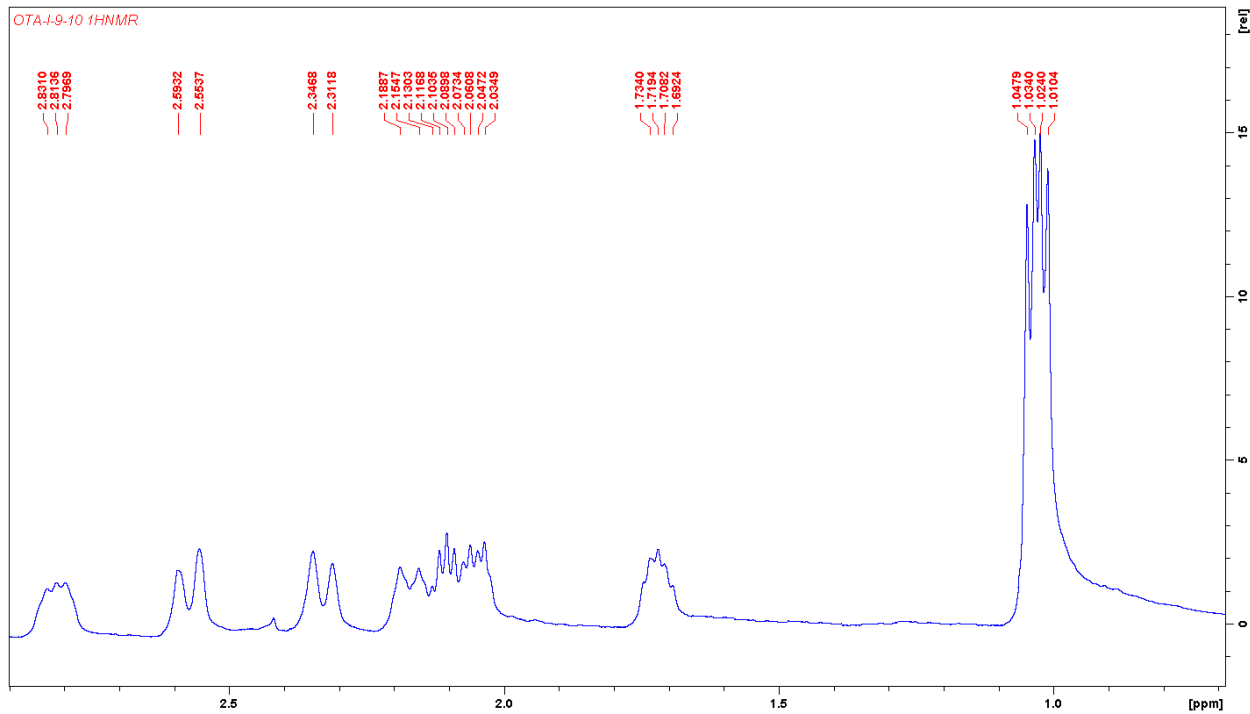


Figure S28: <sup>1</sup>HNMR spectrum of **3** (Exp.).



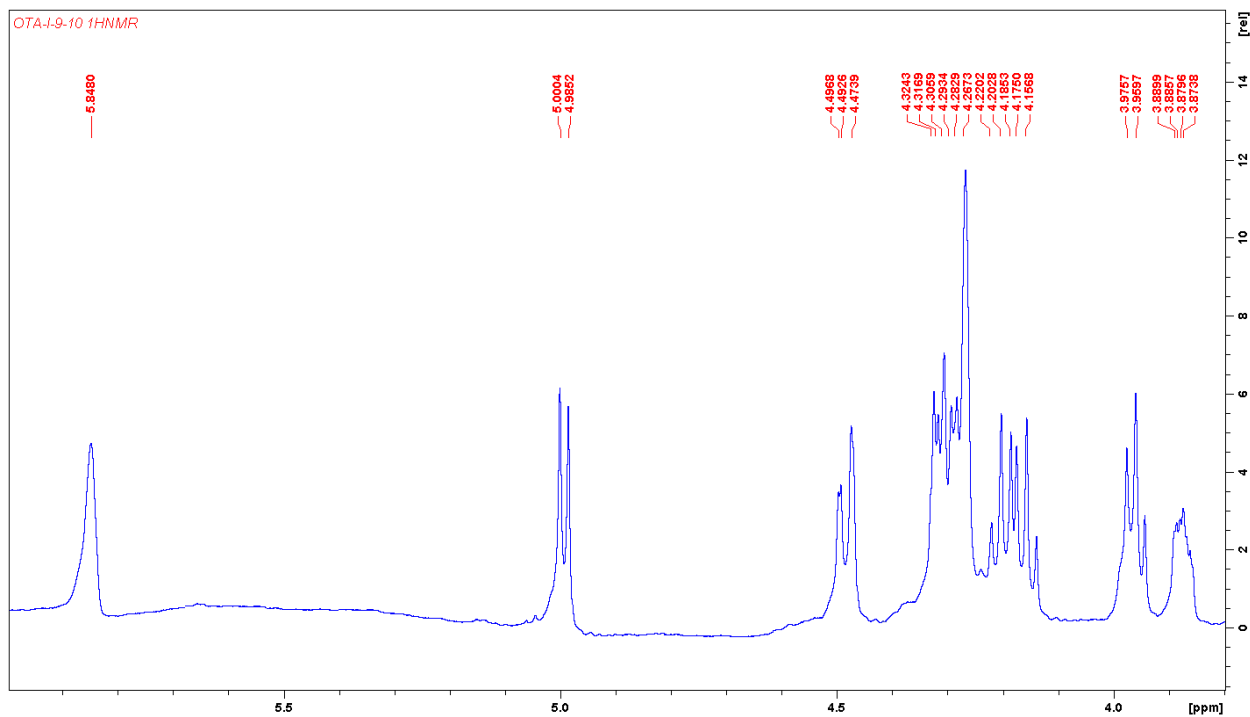


Figure S29: <sup>1</sup>H NMR spectrum of **3** (Exp.).

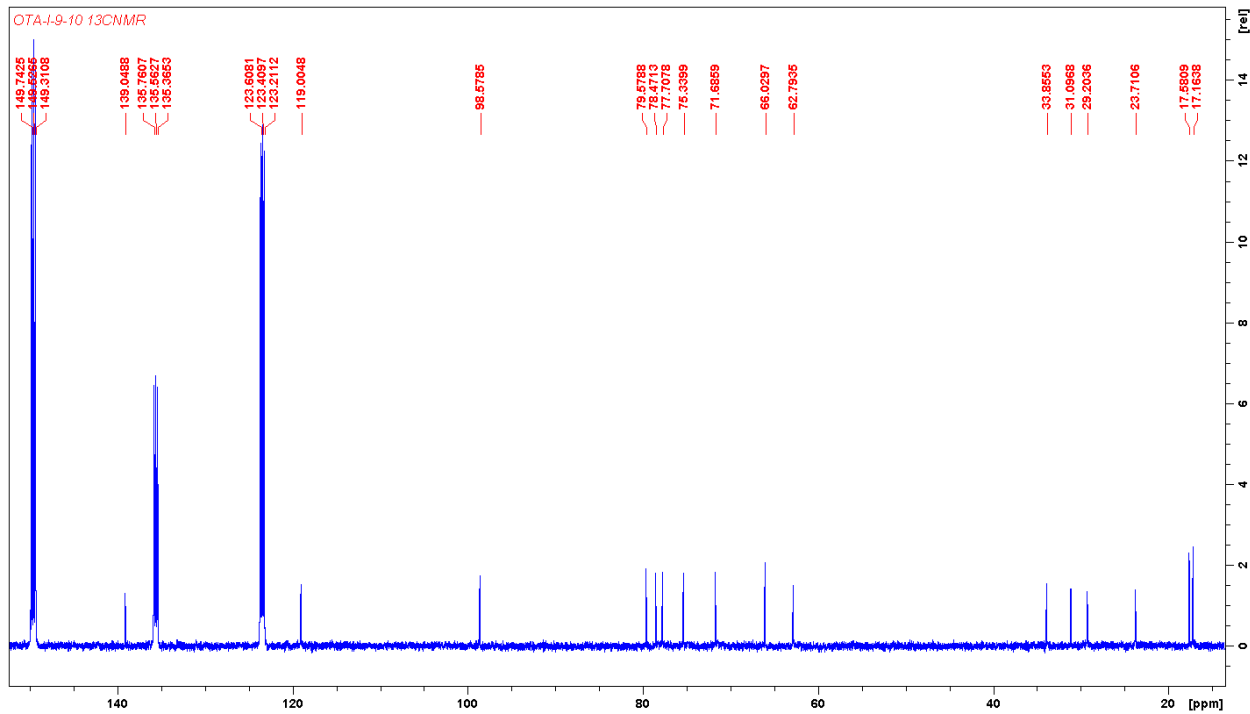


Figure S30: <sup>13</sup>C NMR spectrum of **3**.

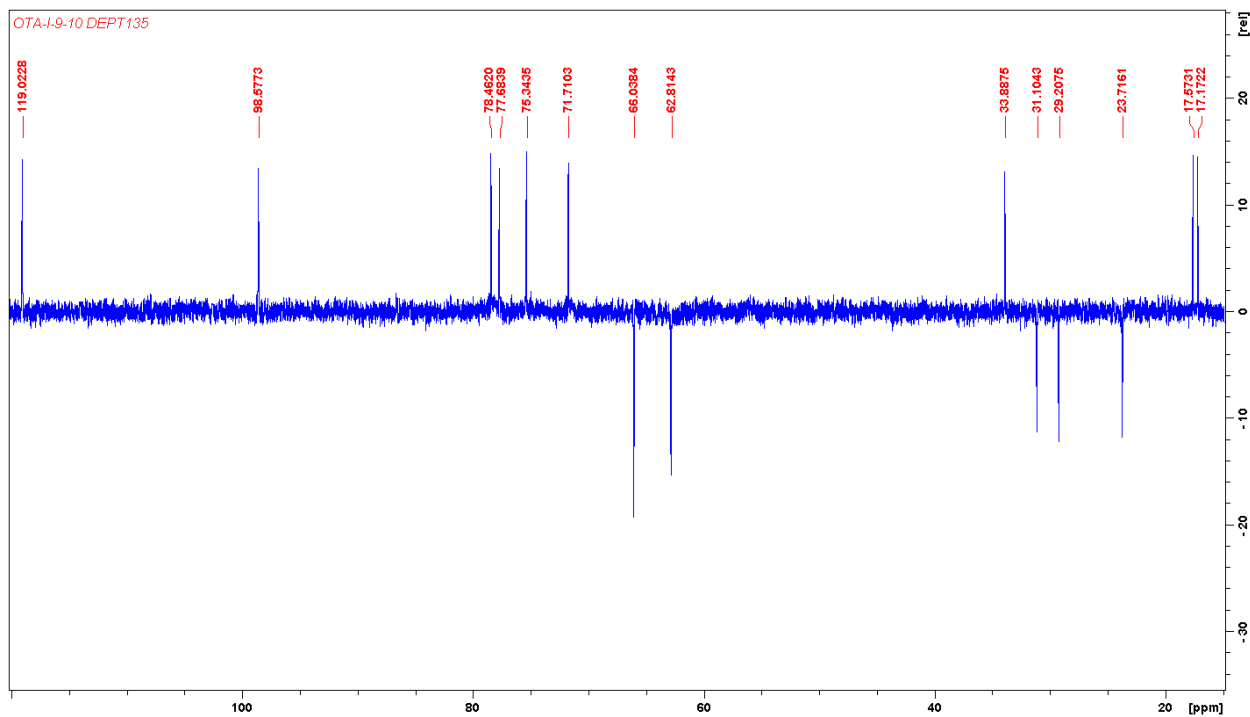


Figure S31: DEPT135 spectrum of **3**.

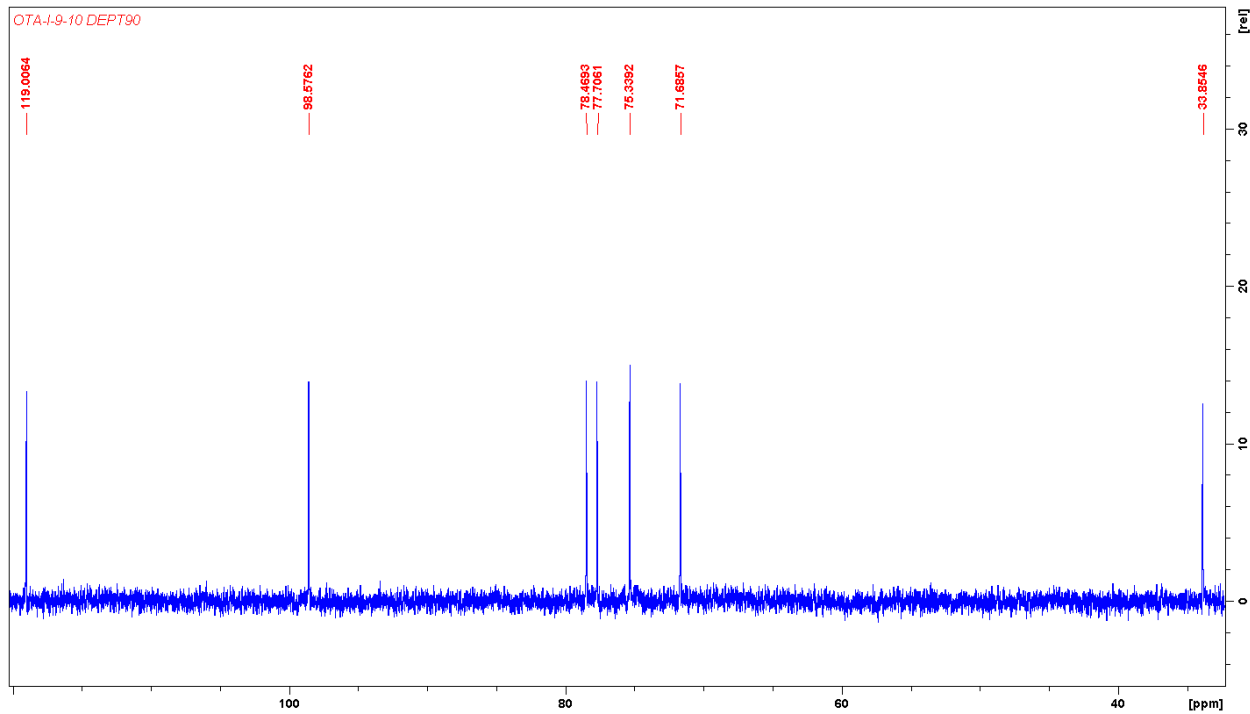


Figure S32: DEPT90 spectrum of **3**.

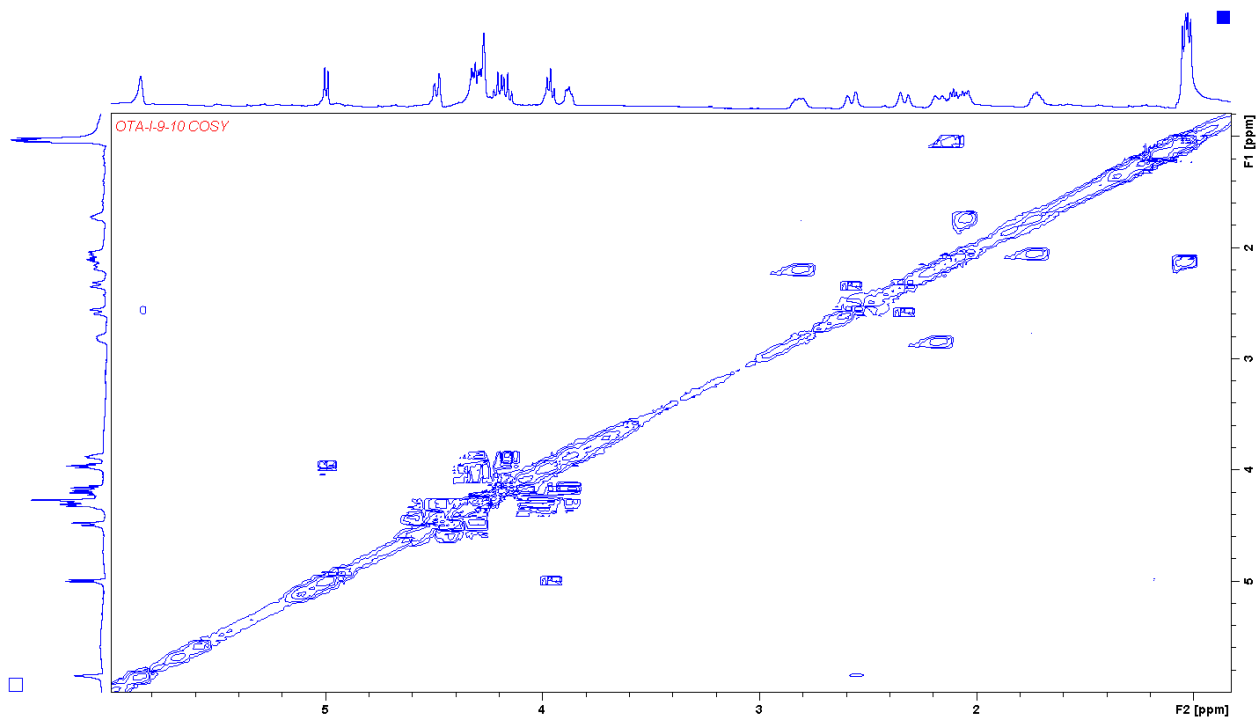


Figure S33: COSY spectrum of **3**.

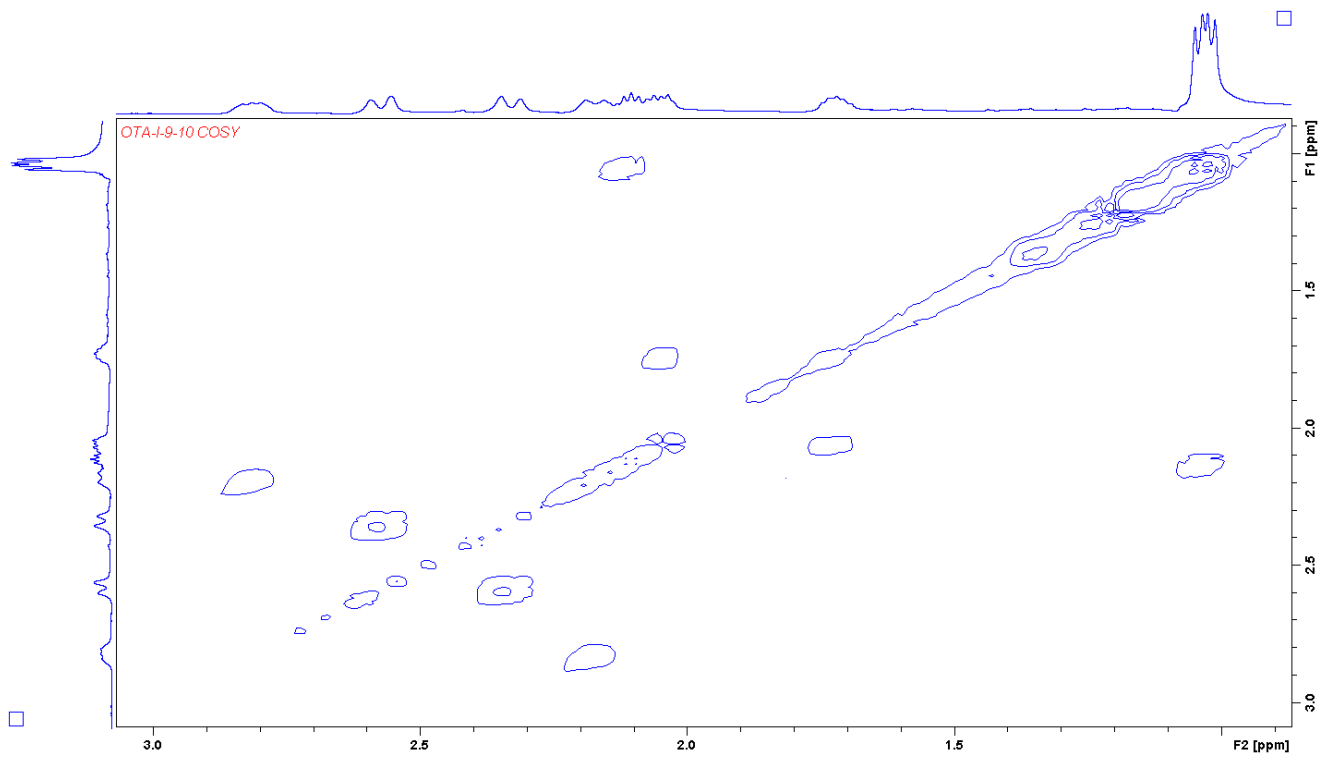


Figure S34: COSY spectrum of **3** (Exp).

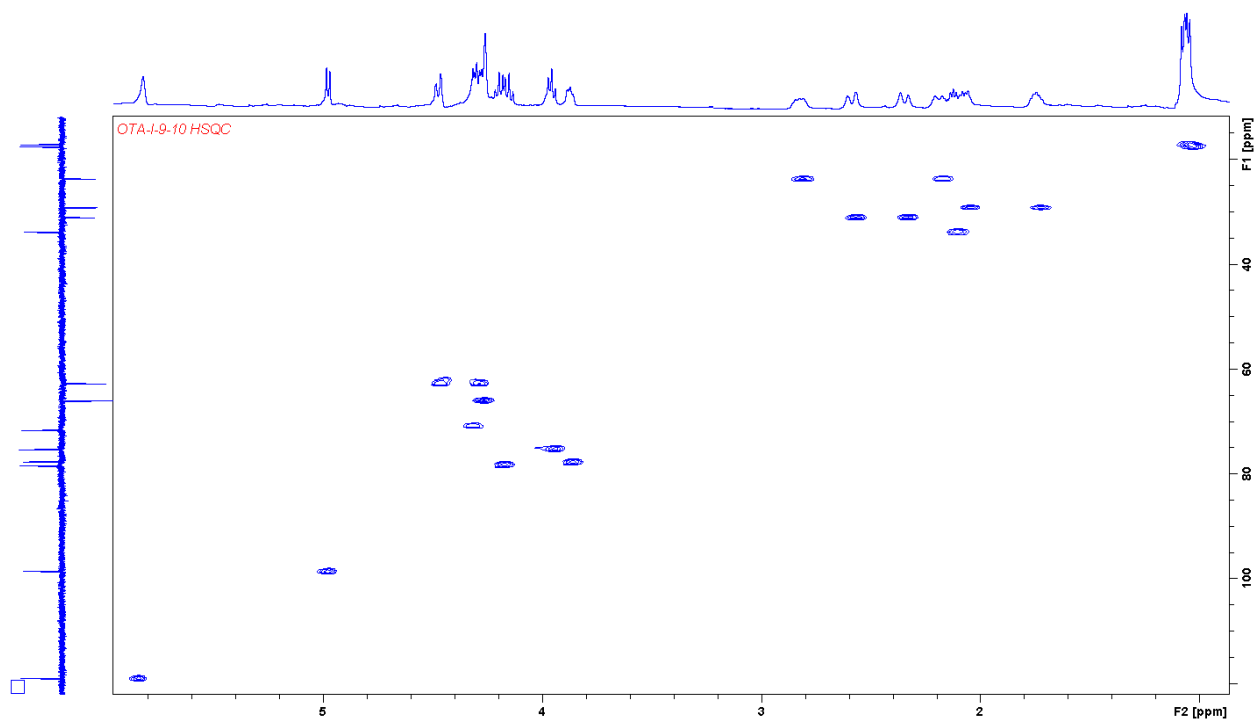


Figure S35: HSQC spectrum of **3**.

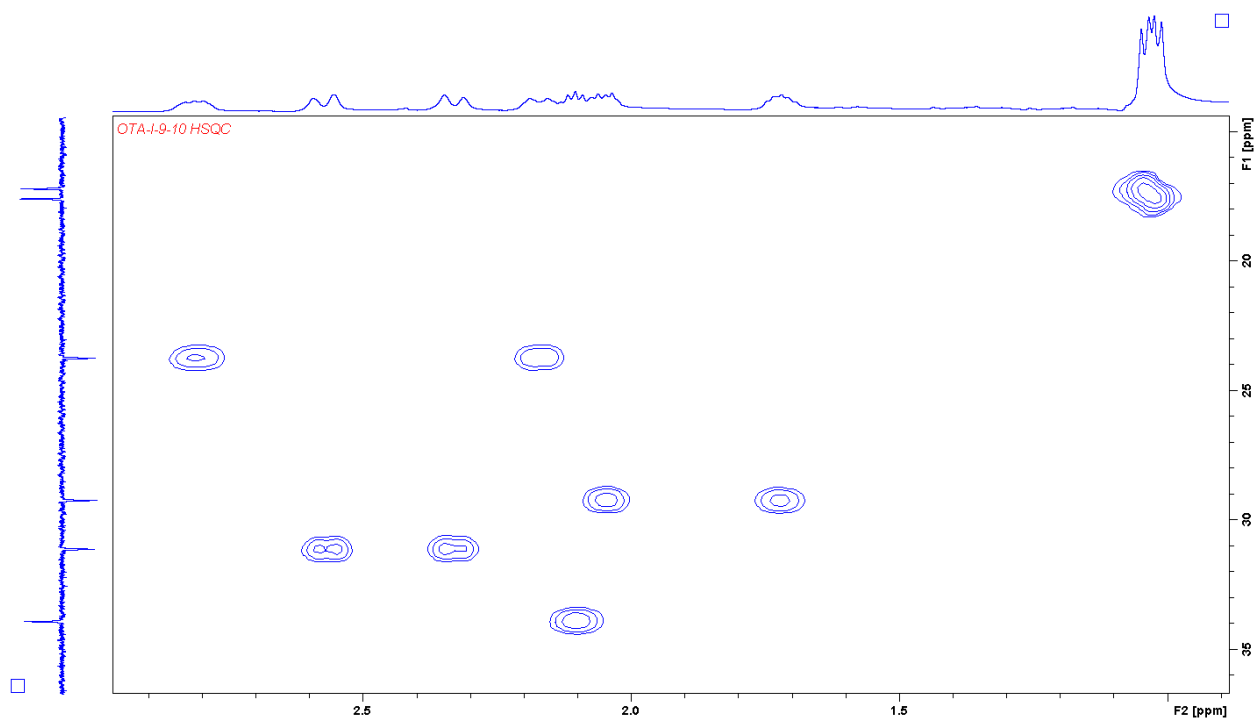


Figure S36: HSQC spectrum of **3** (Exp).

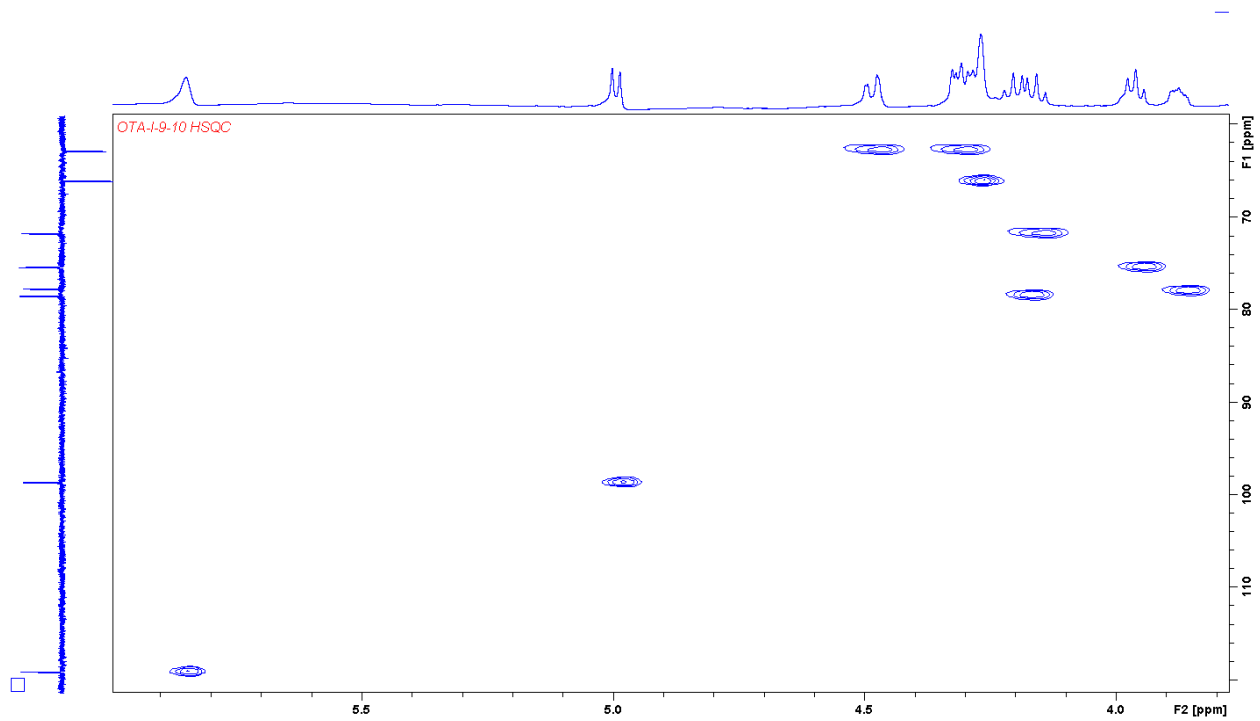


Figure S37: HSQC spectrum of **3** (Exp).

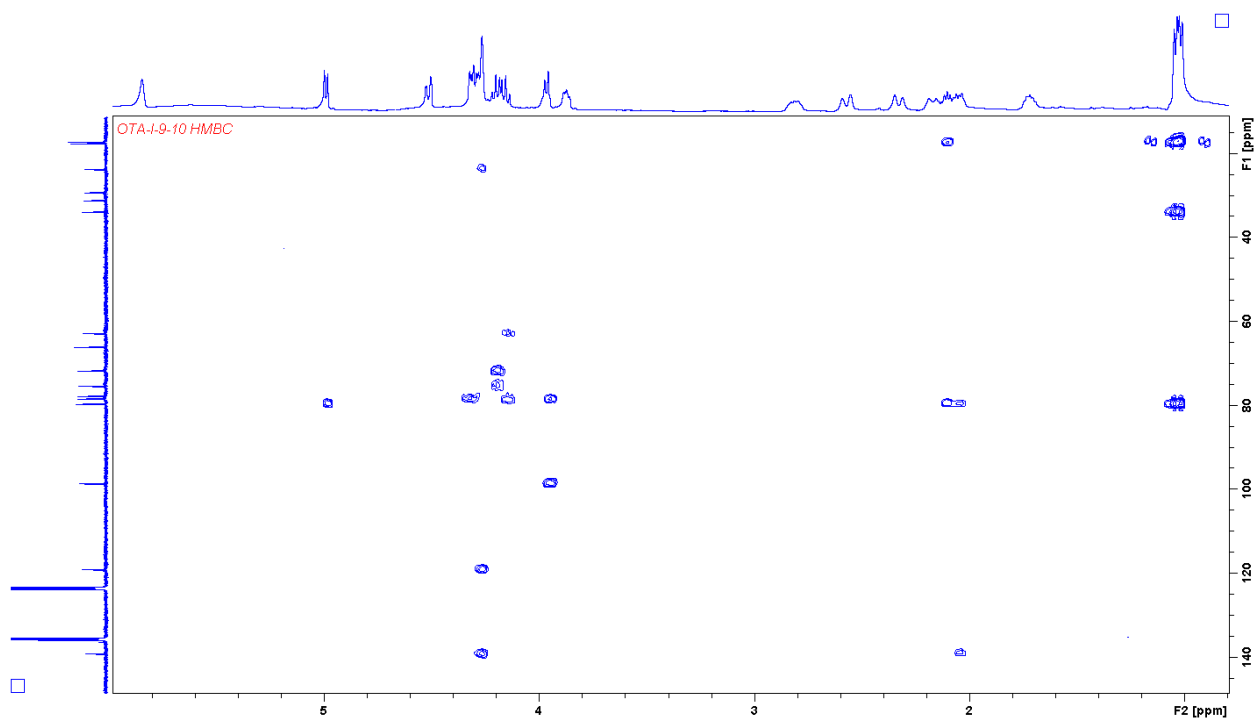


Figure S38: HMBC spectrum of **3**.

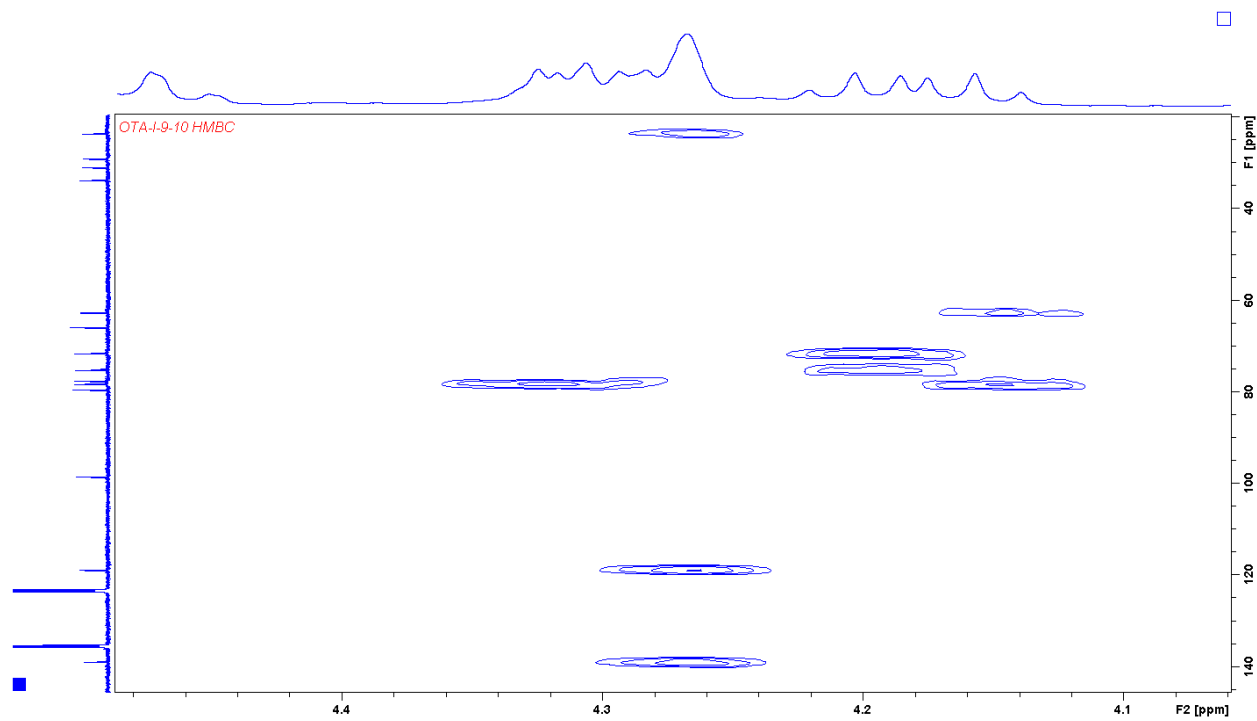


Figure S39: HMBC spectrum of **3** (Exp).

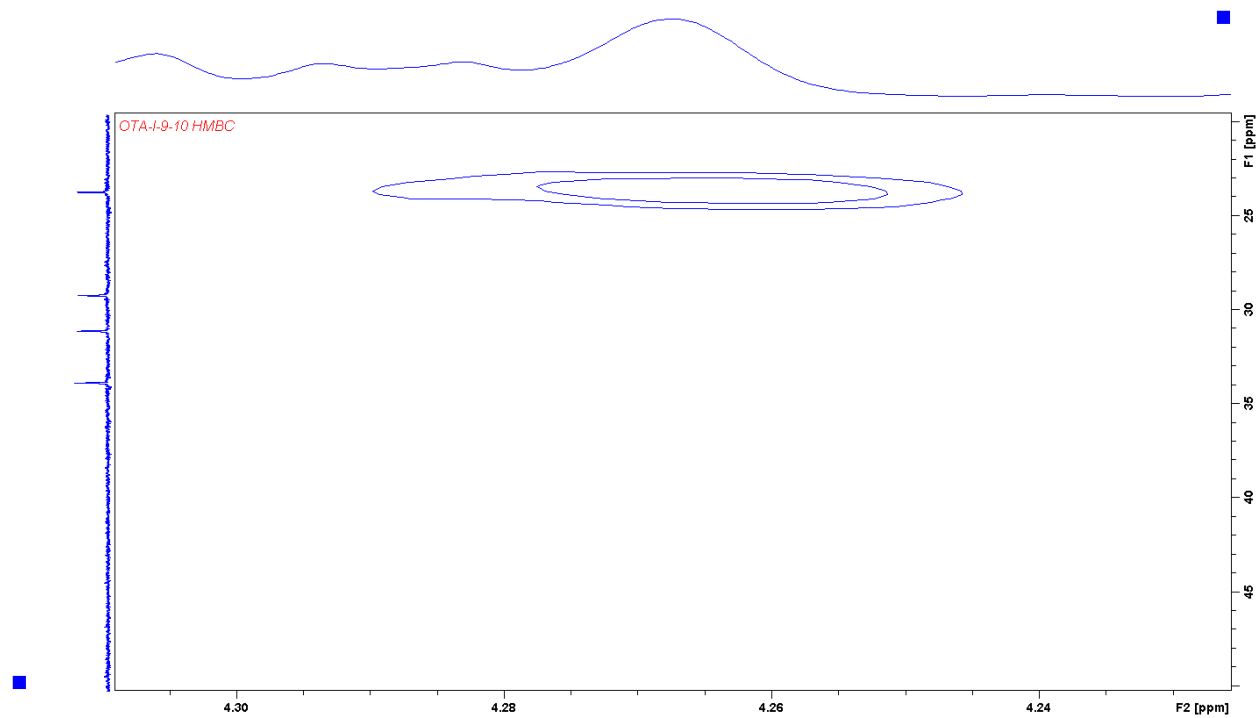


Figure S40: HMBC spectrum of **3** (Exp).

MAGED\_OTAI-9-10\_Negative\_19-05-2024\_#43 RT: 0.20 AV: 1 NL: 3.90E5  
T: FTMS - p ESI Full ms [160.0000-1500.0000]

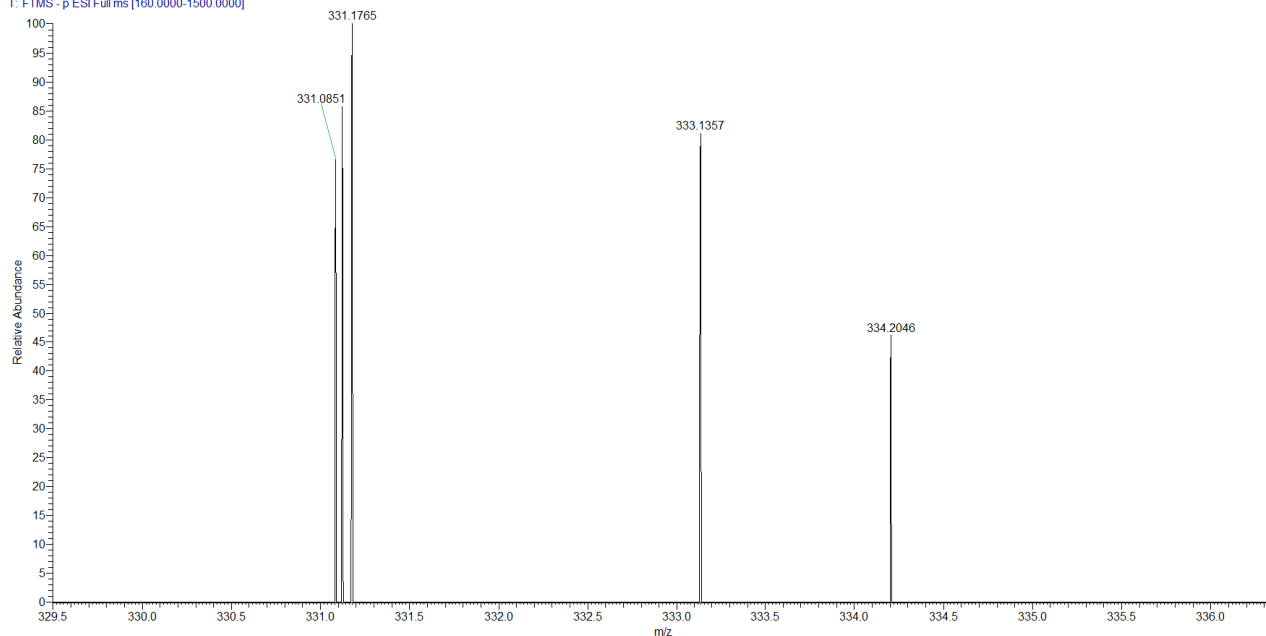


Figure S41: HRESIMS spectrum of **3** (Negative mode).

MAGED\_OTAI-9-10\_Positive\_19-05-2024\_240519145402\_#47 RT: 0.21 AV: 1 NL: 7.13E8  
T: FTMS + p ESI Full ms [160.0000-1500.0000]

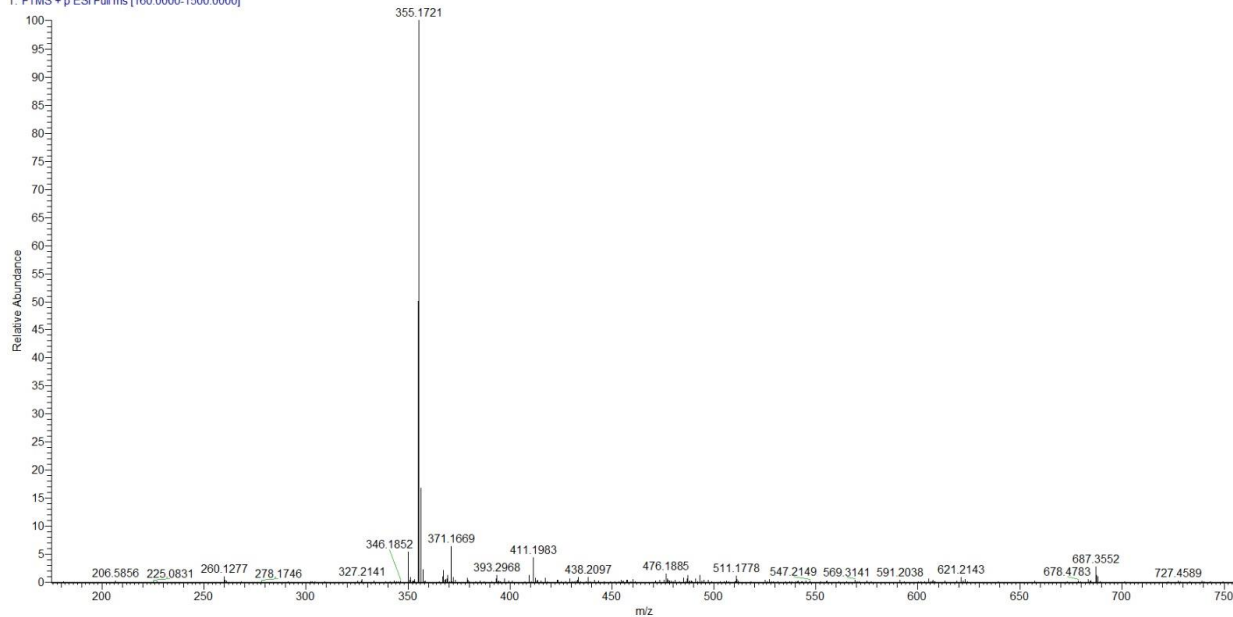


Figure S42: HRESIMS spectrum of **3** (Positive mode).

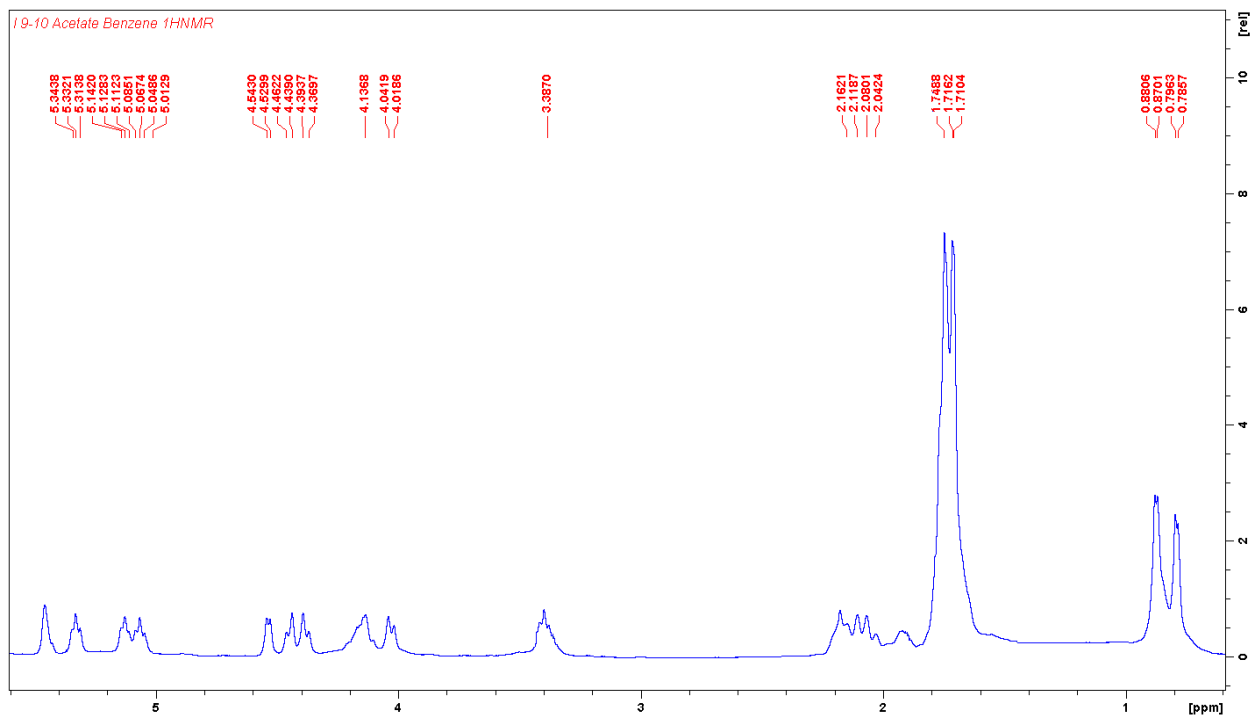


Figure S43: <sup>1</sup>H NMR spectrum of **3a**.

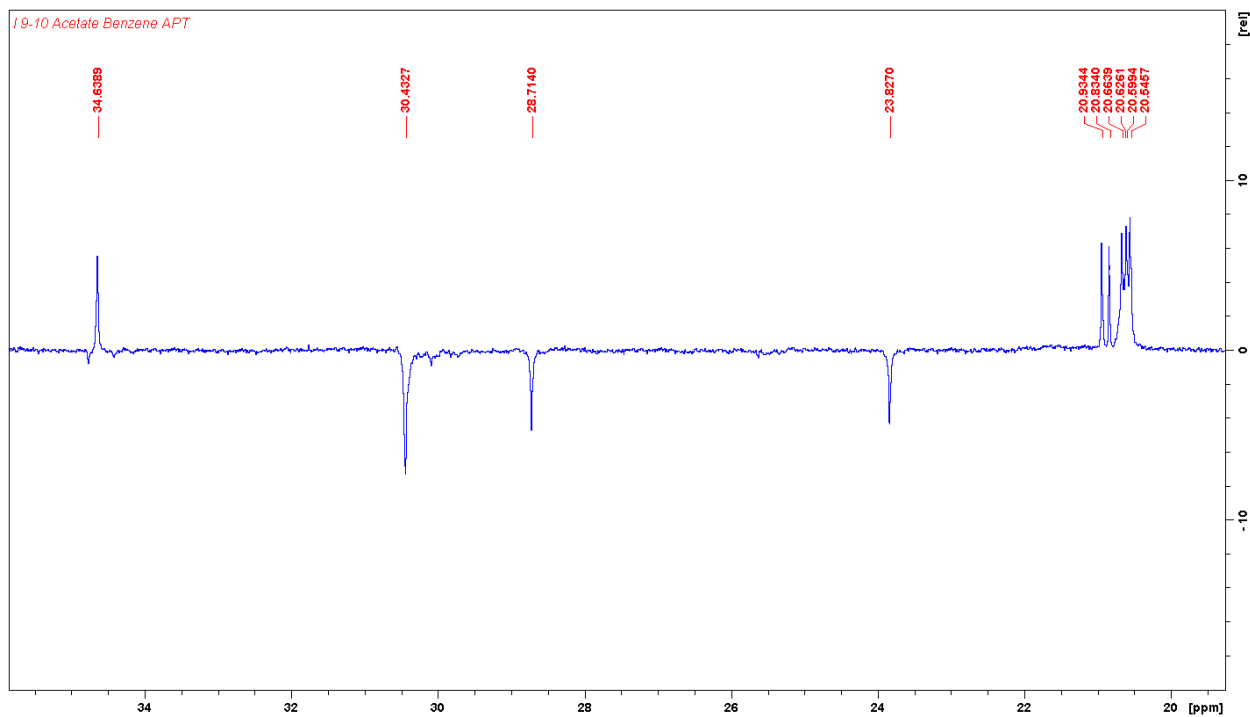


Figure S44: APT spectrum of **3a** (Exp).



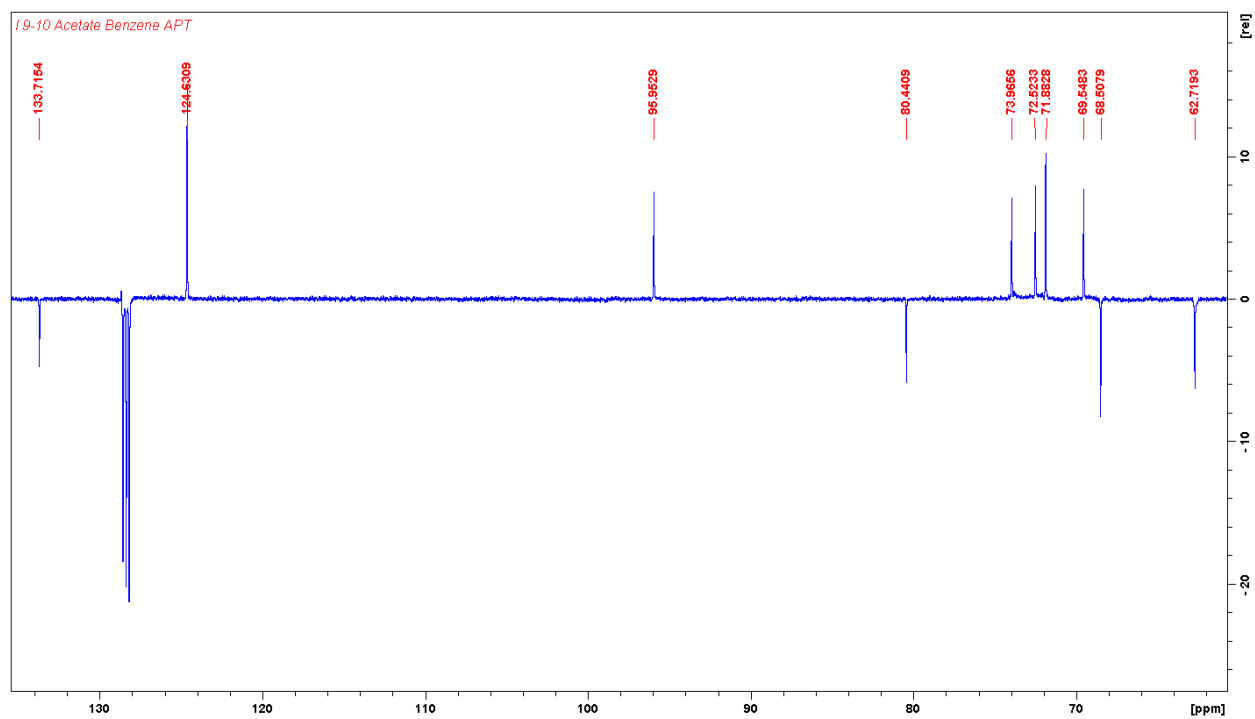


Figure S45: APT spectrum of **3a** (Exp).

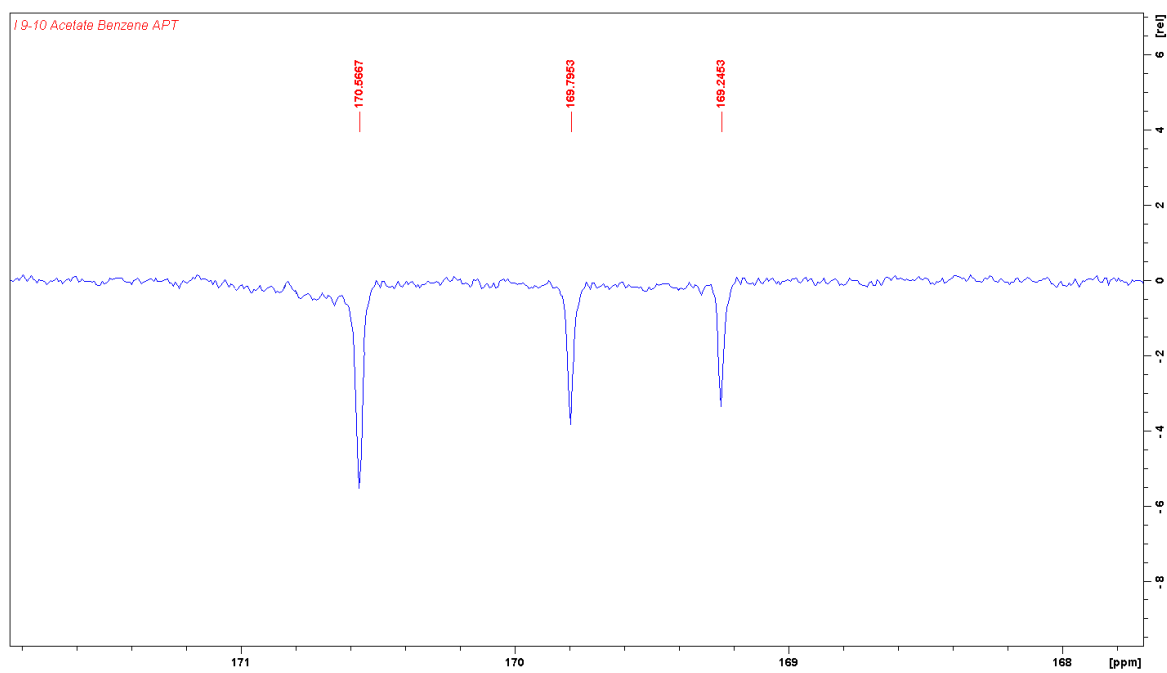
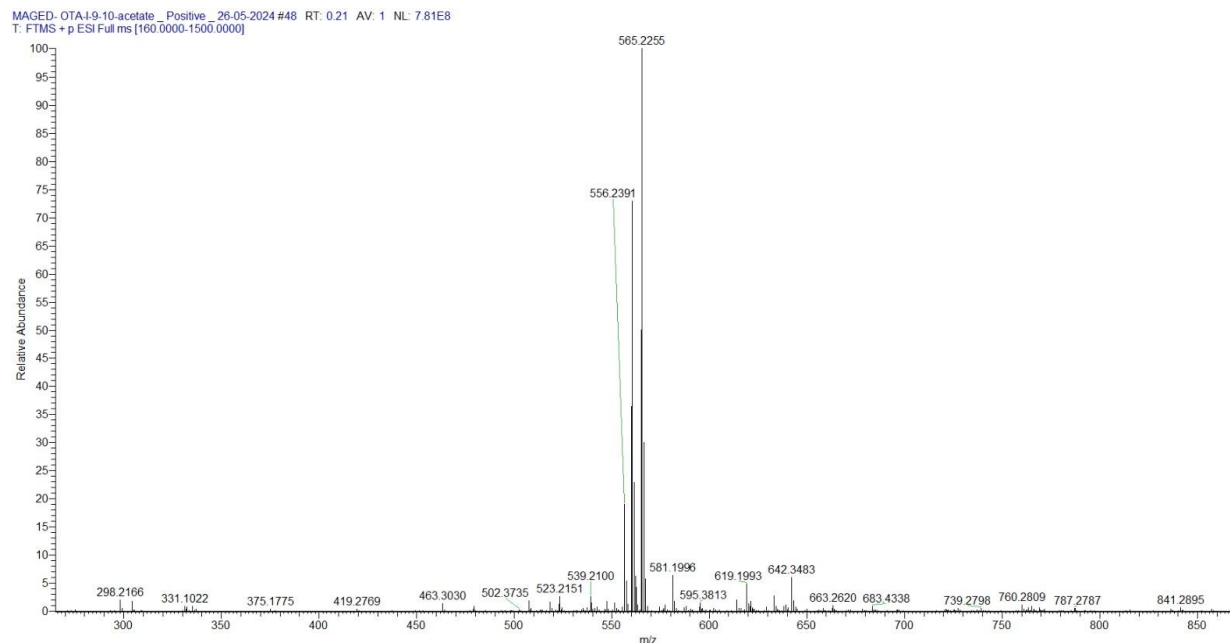


Figure S46: APT spectrum of **3a** (Exp).



**Figure S47:** HRESIMS spectrum of **3a** (Positive mode).

**Table S1:** NMR data of **1-3** in Pyridine *d*5 and their acetyl derivatives ( $\delta$  ppm, *J* in Hz)

	<b>1</b> *		<b>2</b>		<b>2a</b> *		<b>3</b>		<b>3a</b> **	
	<sup>1</sup> H	<sup>13</sup> C	<sup>1</sup> H	<sup>13</sup> C	<sup>1</sup> H	<sup>13</sup> C	<sup>1</sup> H	<sup>13</sup> C	<sup>1</sup> H	<sup>13</sup> C
1	-	136.68	-	73.19	-	71.64	-	139.05	-	133.72
2	6.18 bs	116.63	4.71 s	74.60	5.34 bs	76.66	5.85 bs	119.00	5.43 s	124.63
3	-	153.57	5.83 s	124.10	5.30 bs	122.99	2.33 bd <i>J</i> = 18.6 2.57 bd <i>J</i> = 18.6	31.10	1.95- 2.16 overlapped	30.43
4	-	132.18	-	147.16	-	146.00	-	79.58	-	80.44
5	7.04 bd <i>J</i> = 7.7	126.92	4.63 t <i>J</i> = 5.0	67.29	5.43 bs	69.62	1.71 m, 2.06 m	29.21	Obscured, 1.95- 2.16 overlapped	28.71
6	6.68 bd <i>J</i> = 7.7	122.14	2.34 dd <i>J</i> = 7.7, 12.7 2.60 dd <i>J</i> = 5.2, 7.7	44.68	2.15 dd <i>J</i> = 7.5, 12.2 2.34 dd <i>J</i> = 5.0, 7.5	41.50	2.18 bd <i>J</i> = 17.3 2.81 m	23.72	1.95- 2.16 overlapped	23.83
7	2.11 s	21.26	1.61 s	22.48	1.63 s	21.00	4.27 s	66.03	4.38 d <i>J</i> = 11.8, 4.45 d <i>J</i> = 11.8	68.51
8	3.25 m	27.41	2.94 sept <i>J</i> = 6.5	29.45	2.92 sept <i>J</i> = 6.5	30.11	2.10 m, overl.	33.86	1.95- 2.16 overlapped	34.64
9	1.22 d <i>J</i> = 7.0	23.25	1.14 d <i>J</i> = 6.6	21.22	0.93 d <i>J</i> = 6.0	21.07	1.04 d <i>J</i> = 6.8	17.59	0.88 d <i>J</i> = 5.3	20.83
10		23.25	1.14 d <i>J</i> = 6.6	22.44	0.89 d <i>J</i> = 6.0	21.24	1.02 d <i>J</i> = 6.8	17.64	0.79 d <i>J</i> = 5.3	20.93
1'							4.99 d <i>J</i> = 7.6	98.58	4.54 d <i>J</i> = 6.6	95.95
2'							3.96 t <i>J</i> = 8.0	75.34	5.13 t <i>J</i> = 6.7	72.52
3'							4.19 t <i>J</i> = 9.0	78.47	5.33 t <i>J</i> = 5.9	73.97
4'							4.14 t <i>J</i> = 9.0	71.69	5.06 t <i>J</i> = 9.4	69.55
5'							3.88 m	77.71	3.39 t <i>J</i> = 7.8	71.88
6'							4.30 dd <i>J</i> = 5.3, 10.4 4.48 dd <i>J</i> = 2.1, 10.4	62.80	4.03 bd <i>J</i> = 11.7 4.14 bd <i>J</i> = 5.8	62.72

\*Spectrum was measured in Benzene *d*6, Acetate:  $\delta_{\text{H}}$  1.66 s;  $\text{CH}_3$   $\delta_{\text{C}}$  22.32, 22.45, C=O  $\delta_{\text{C}}$  170.29, 171.26.

\*\*Spectrum was measured in Benzene *d*6, Acetate:  $\delta_{\text{H}}$  1.71- 1.74;  $\text{CH}_3$   $\delta_{\text{C}}$  20.55, 20.60, 20.63, C=O  $\delta_{\text{C}}$  169.25, 169.80, 170.57.