

## Supplementary material

### Cytotoxic activity (screening)

**Table S1.** Cytotoxic activity of the *A. amadelpa* extract and compounds **1-3** and **5**

Sample	Cytotoxic activity				
	MCF-7	DU-145	HeLa	Panc-1	Skov-3
	% Viability (10 $\mu$ M)	% Viability (10 $\mu$ M)	% Viability (10 $\mu$ M)	% Viability (10 $\mu$ M)	% Viability (10 $\mu$ M)
Extract*	28.53	26.91	10.41	50.14	81.57
<b>1</b>	58.89	40.17	40.92	97.16	81.24
<b>2</b>	36.88	35.73	46.38	100.08	73.31
<b>3</b>	78.96	38.26	37.31	98.20	69.87
<b>5</b>	96.50	33.10	32.42	95.56	60.30

\* The viability% of the extract was measured at 100  $\mu$ g/mL.

**Table S2.** 1D-NMR spectral data of compounds **3 – 6** in  $CD_3OD$

C/H	<b>3</b>			<b>4*</b>			<b>5</b>			<b>6</b>		
	$^{13}C$	$^1H$	$J_{Hz}$	$^{13}C$	$^1H$	$J_{Hz}$	$^{13}C$	$^1H$	$J_{Hz}$	$^{13}C$	$^1H$	$J_{Hz}$
1	129.3			129.8			130.5			129.6		
2	132.5	7.74, d, 8.5		130.6	7.75, dd, 1.8, 8.4		131.4	7.79, dd, 1.8, 8.4		128.7	7.79, dd, 1.6, 8.4	
3	116.5	6.88, d, 8.5		115.9	7.03, d, 8.4		114.3	6.97, d, 8.4		114.7	6.88, d, 8.4	
4	164.1			160.4			162.6			156.4		
5	116.5	6.88, d, 8.5		110.4			83.7			108.6		
6	132.5	7.74, d, 8.5		134.7	8.04, d, 1.8		141.3	8.26, d, 1.8		134.3	8.10, d, 1.6	
7	191.2	9.75, s		190.1	9.75, s		190.0	9.73, s		172.1		

\* NMR spectral data of compound **4** in DMSO

## **Spectral data**

**Figure S1:**  $^1\text{H}$ -NMR spectrum of compound **1** in  $\text{CD}_3\text{OD}$

**Figure S2:** HH-COSY NMR spectrum of compound **1** in  $\text{CD}_3\text{OD}$

**Figure S3:**  $^{13}\text{C}$ -NMR spectrum of compound **1** in  $\text{CD}_3\text{OD}$

**Figure S4:**  $^{13}\text{C}$ -DEPT-135 NMR spectrum of compound **1** in  $\text{CD}_3\text{OD}$

**Figure S5:** HSQC NMR spectrum of compound **1** in  $\text{CD}_3\text{OD}$

**Figure S6:** HMBC NMR spectrum of compound **1** in  $\text{CD}_3\text{OD}$

**Figure S7:** HMBC NMR spectrum ( $\delta_{\text{H}}$  9.7-6.5 and  $\delta_{\text{C}}$  80-200) of compound **1** in  $\text{CD}_3\text{OD}$

**Figure S8:** (-) ESI-MS spectrum of compound **1**

**Figure S9:**  $^1\text{H}$ -NMR spectrum of compound **2** in  $\text{CD}_3\text{OD}$

**Figure S10:**  $^{13}\text{C}$ -NMR spectrum of compound **2** in  $\text{CD}_3\text{OD}$

**Figure S11:** HSQC NMR spectrum of compound **2** in  $\text{CD}_3\text{OD}$

**Figure S12:** HMBC NMR spectrum of compound **2** in  $\text{CD}_3\text{OD}$

**Figure S13:** EI-MS spectrum of compound **2**

**Figure S14:**  $^1\text{H}$ -NMR spectrum of compound **3** in  $\text{CD}_3\text{OD}$

**Figure S15:** HH-COSY NMR spectrum of compound **3** in  $\text{CD}_3\text{OD}$

**Figure S16:**  $^{13}\text{C}$ -NMR spectrum of compound **3** in  $\text{CD}_3\text{OD}$

**Figure S17:**  $^{13}\text{C}$ -DEPT-135 NMR spectrum of compound **3** in  $\text{CD}_3\text{OD}$

**Figure S18:** HSQC NMR spectrum of compound **3** in  $\text{CD}_3\text{OD}$

**Figure S19:** HMBC NMR spectrum of compound **3** in  $\text{CD}_3\text{OD}$

**Figure S20:** EI-MS spectrum of compound **3**

## Compound 1

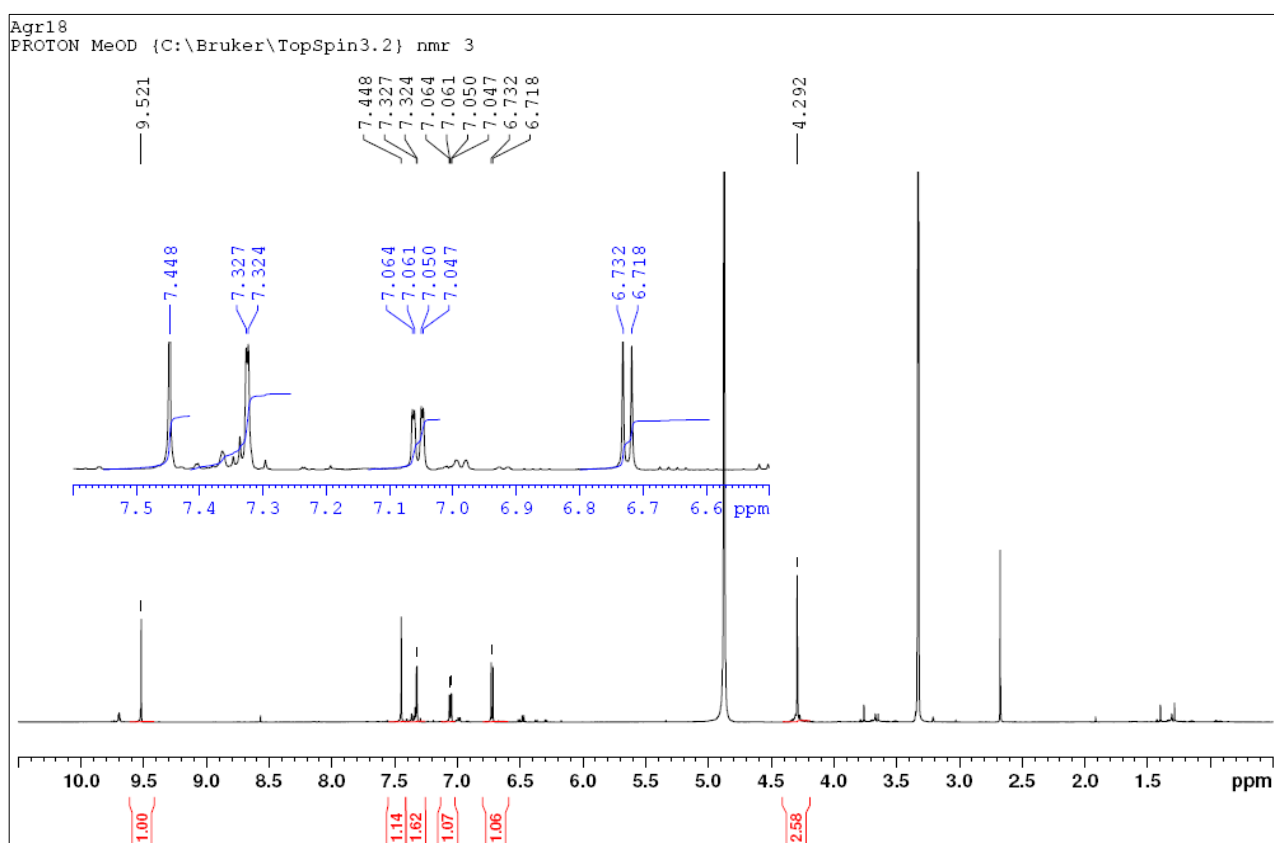


Fig. S1:  $^1\text{H}$ -NMR spectrum of compound **1** in  $\text{CD}_3\text{OD}$

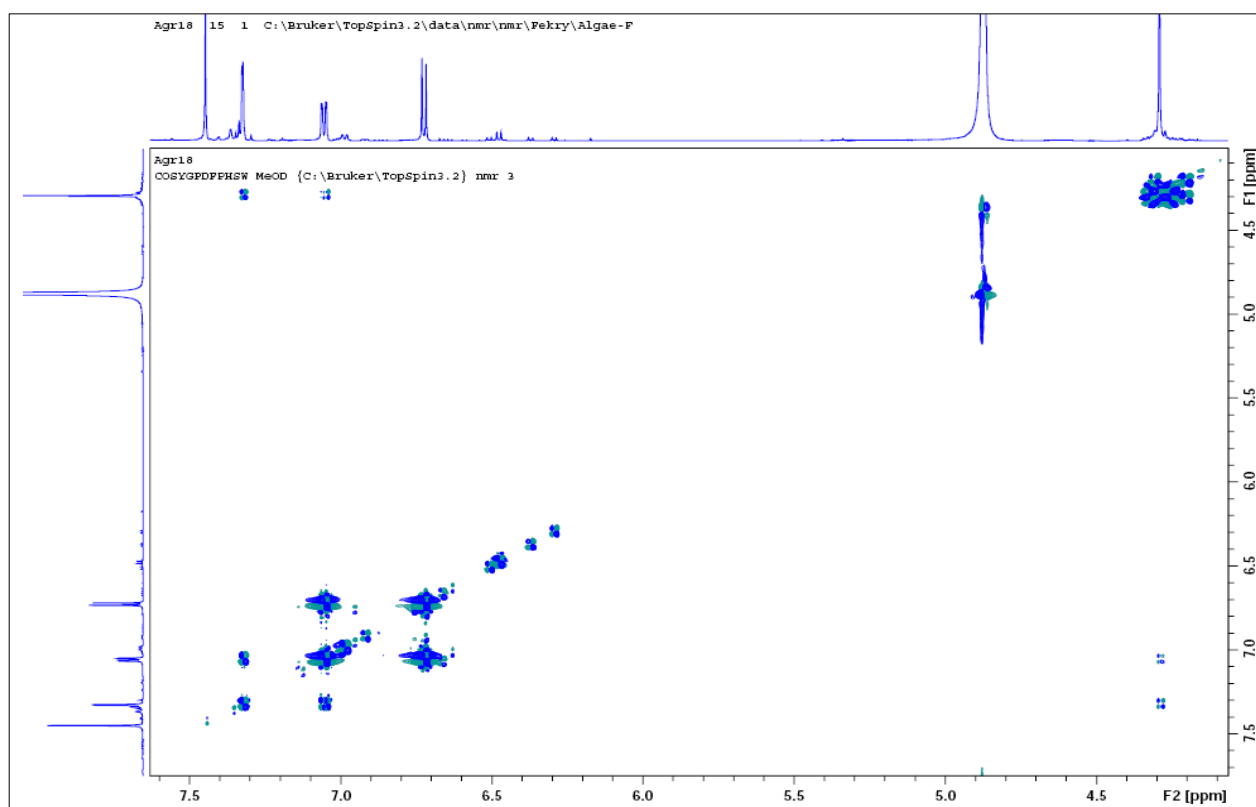
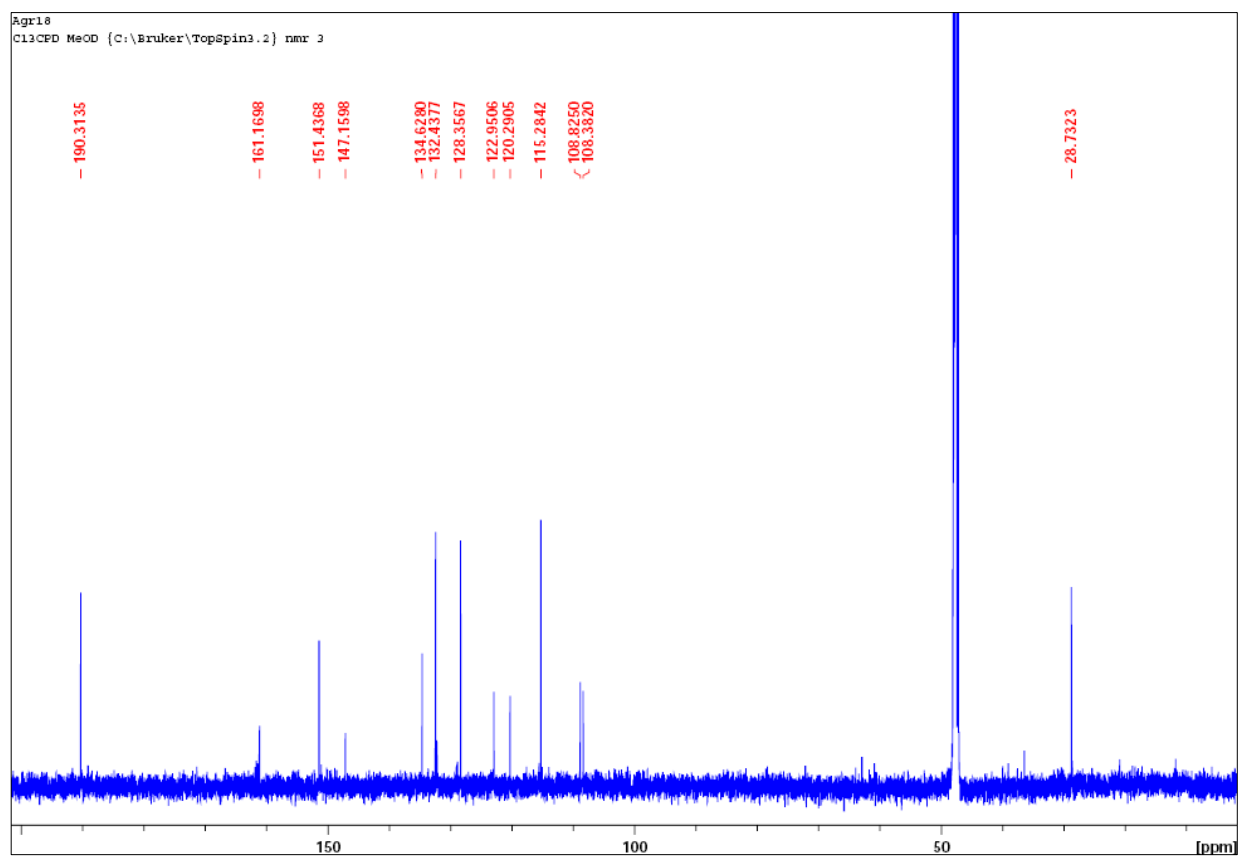
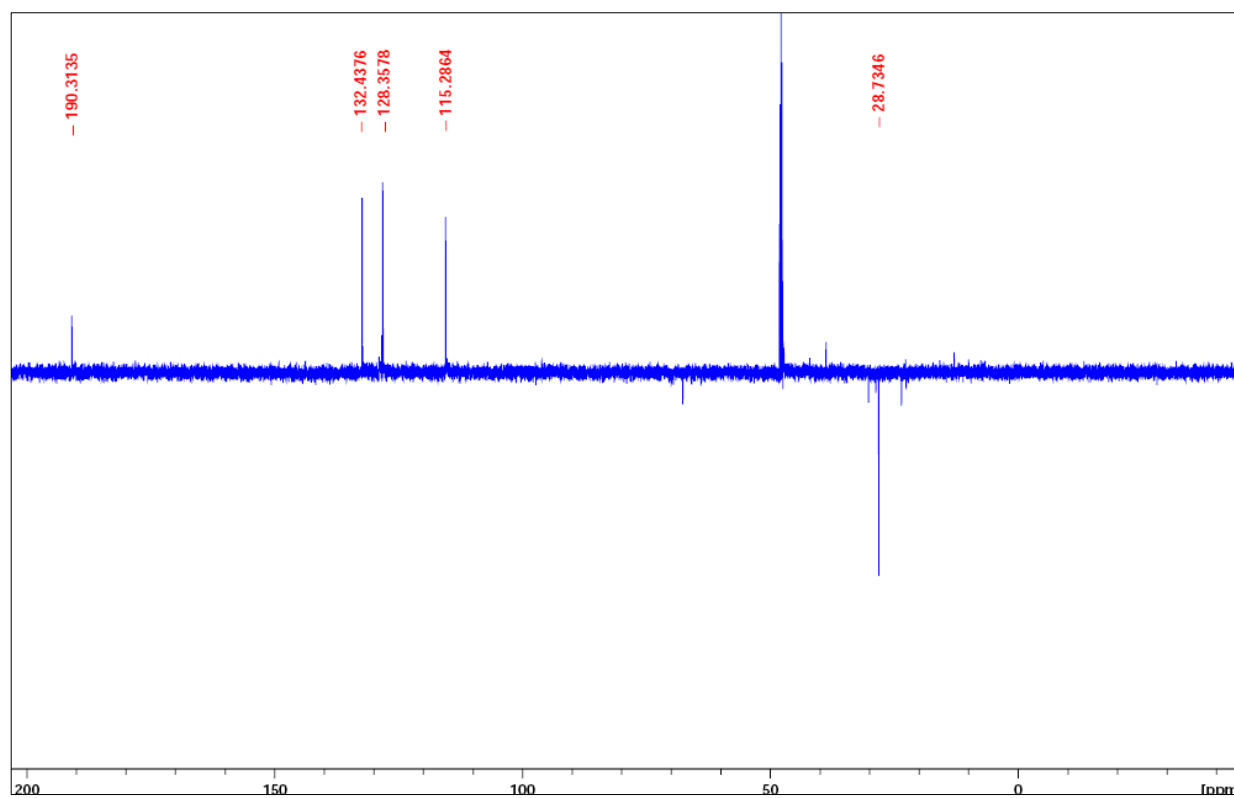


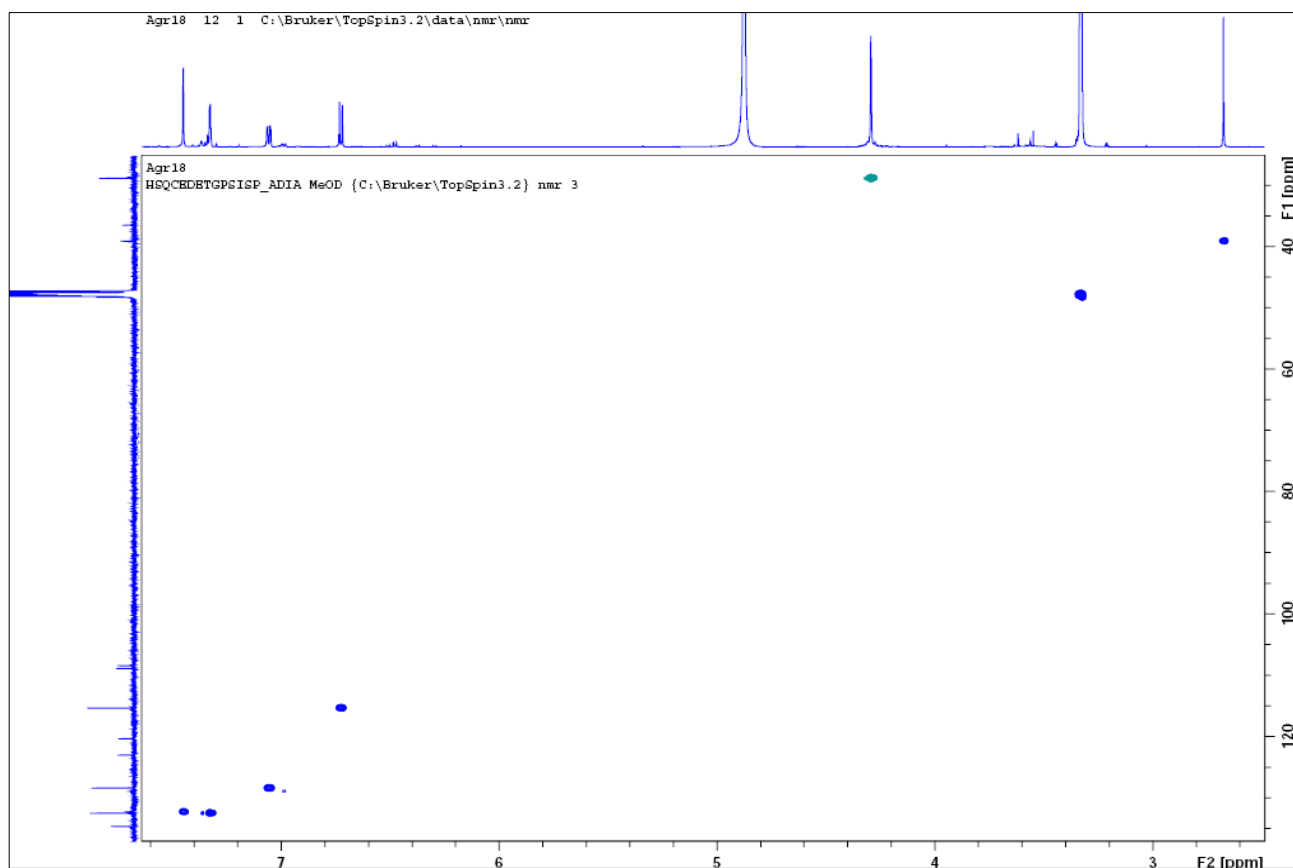
Fig. S2: HH-COSY NMR spectrum of compound **1** in  $\text{CD}_3\text{OD}$



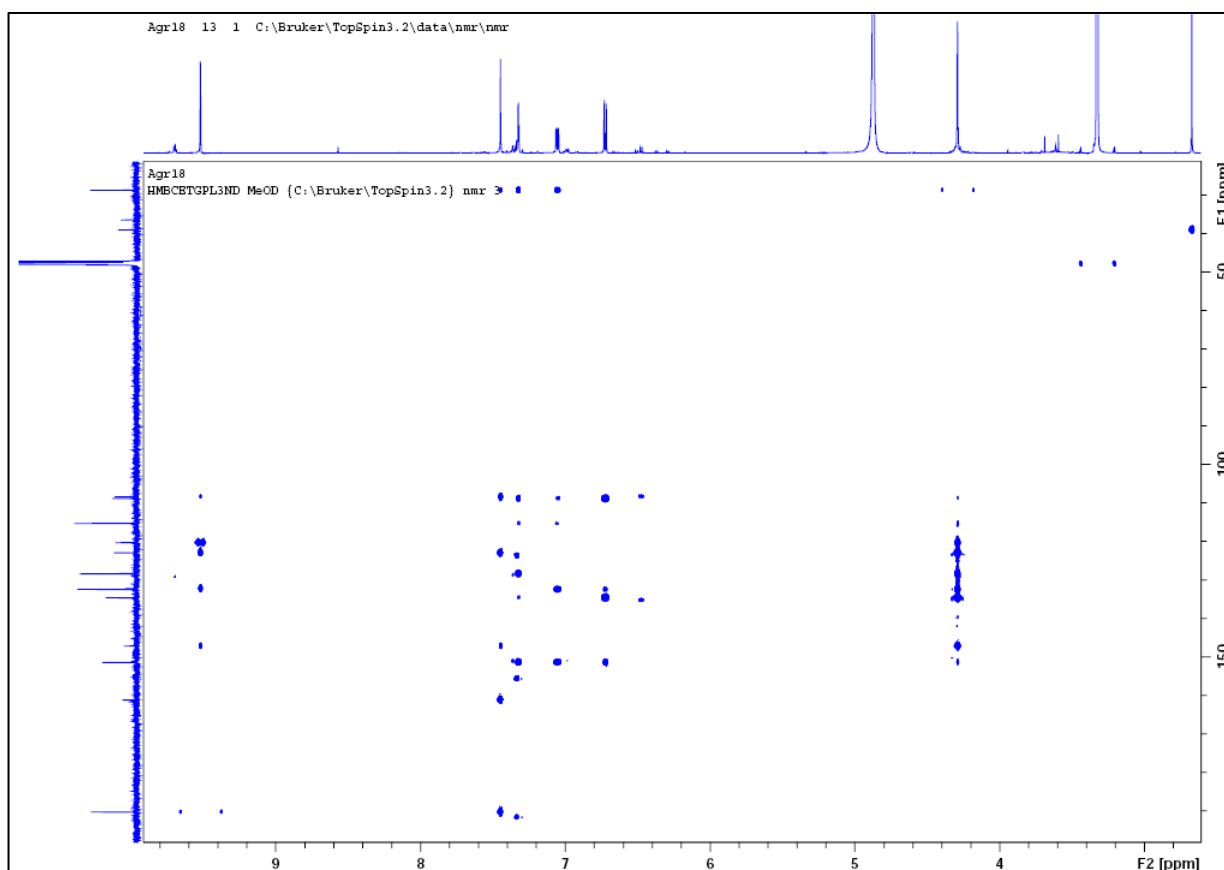
**Fig. S3:**  $^{13}\text{C}$ -NMR spectrum of compound **1** in  $\text{CD}_3\text{OD}$



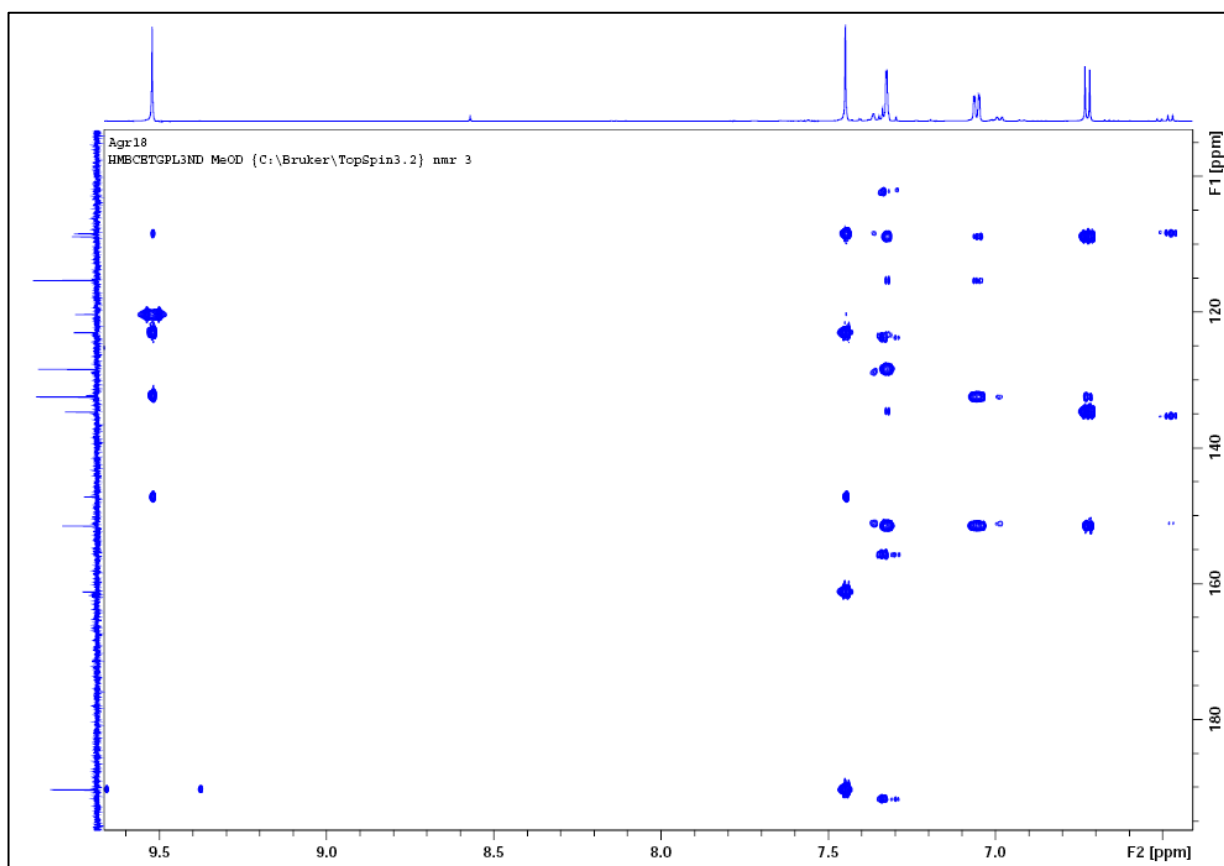
**Fig. S4:**  $^{13}\text{C}$ -DEPT135 NMR spectrum of compound **1** in  $\text{CD}_3\text{OD}$



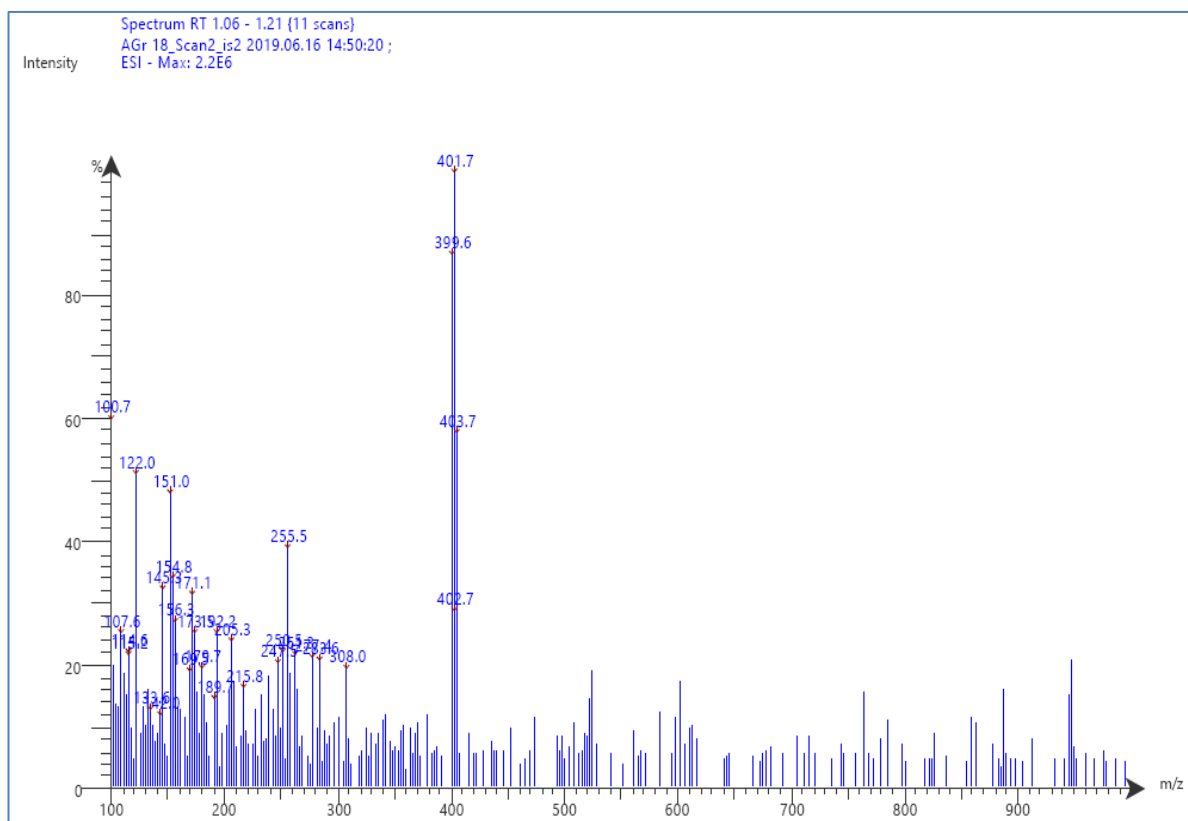
**Fig. S5:** HSQC NMR spectrum of compound **1** in CD<sub>3</sub>OD



**Fig. S6:** HMBC NMR spectrum of compound **1** in CD<sub>3</sub>OD



**Fig. S7:** HMBC NMR spectrum ( $\delta_{\text{H}}$  9.7-6.5 and  $\delta_{\text{C}}$  80-200) of compound **1** in CD<sub>3</sub>OD



**Figure S8:** (-) ESI-MS spectrum of compound **1**

## Compound 2

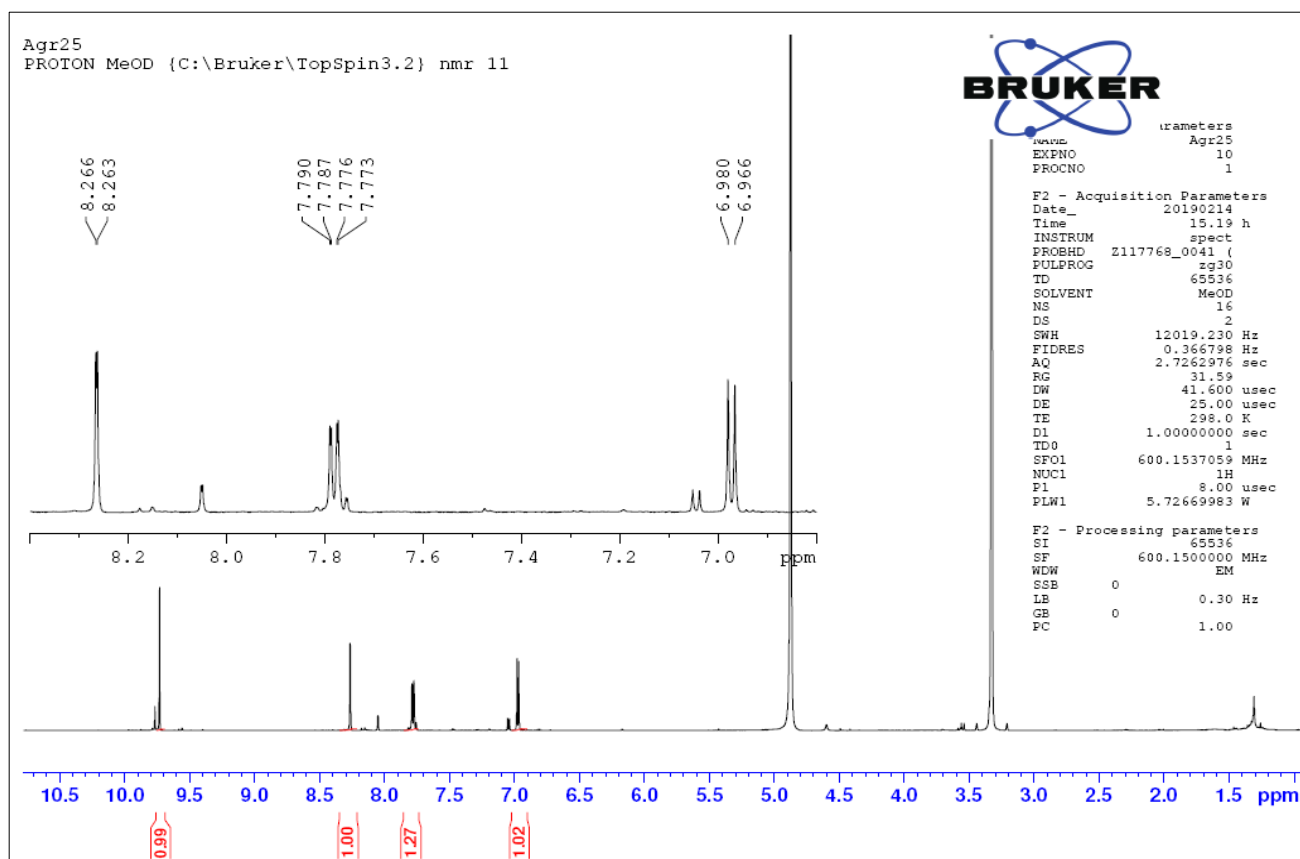


Fig. S9:  $^1\text{H}$ -NMR spectrum of compound 2 in  $\text{CD}_3\text{OD}$

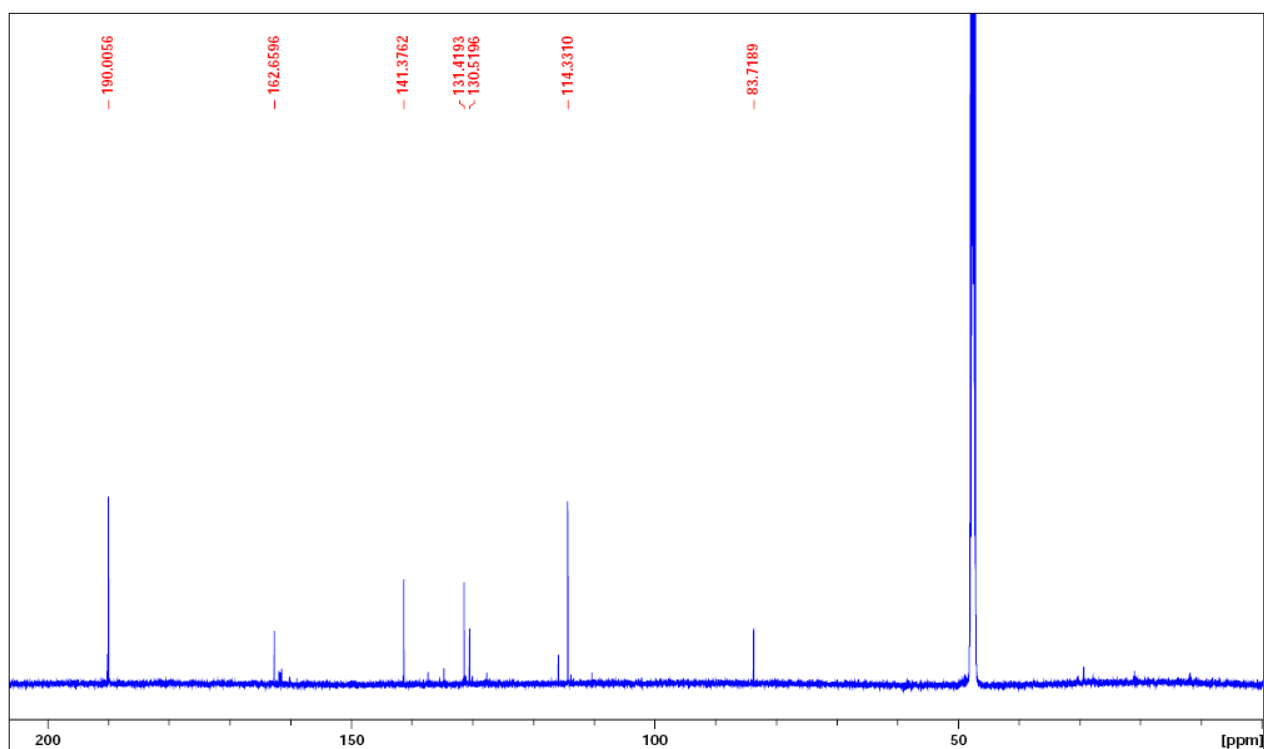


Fig. S10:  $^{13}\text{C}$ -NMR spectrum of compound 2 in  $\text{CD}_3\text{OD}$

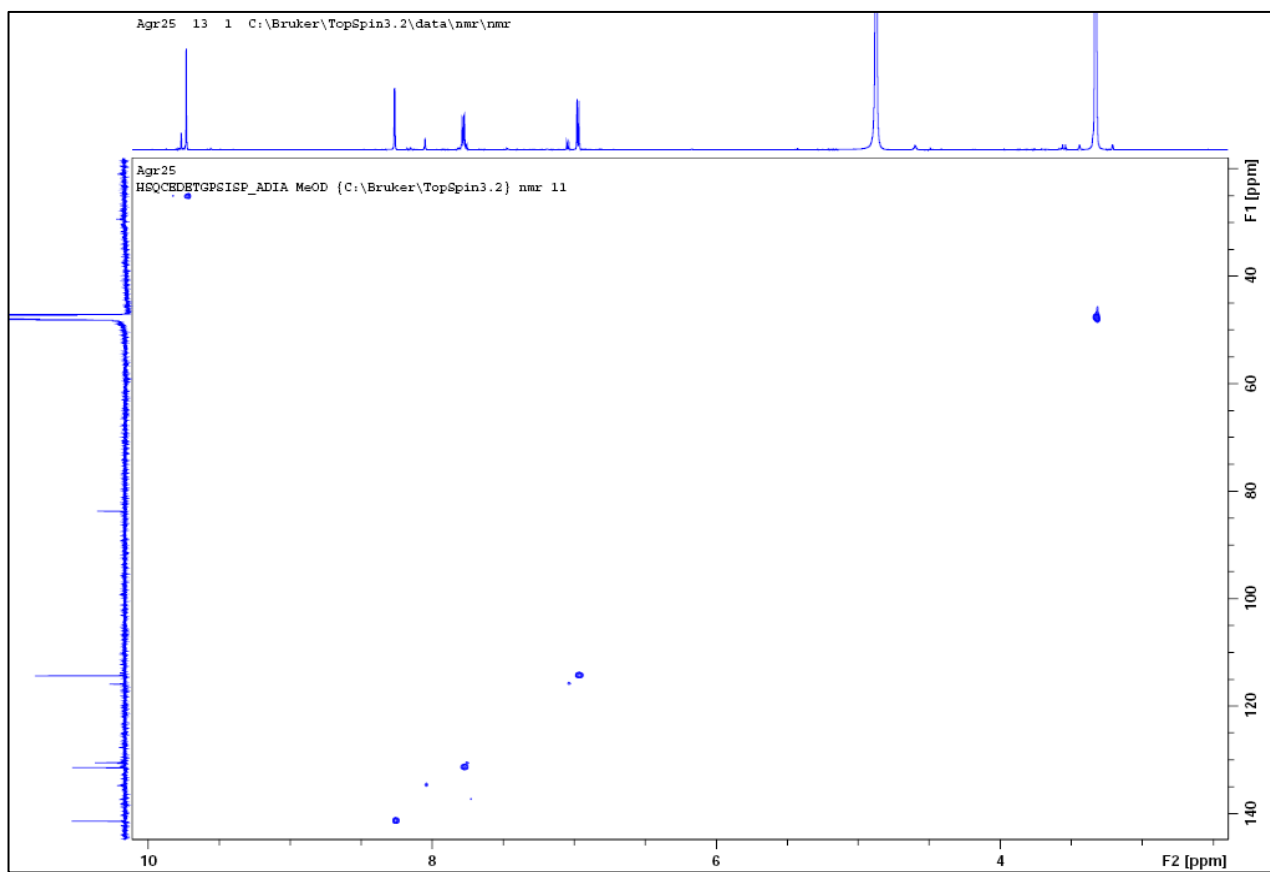


Fig. S11: HSQC NMR spectrum of compound **2** in CD<sub>3</sub>OD

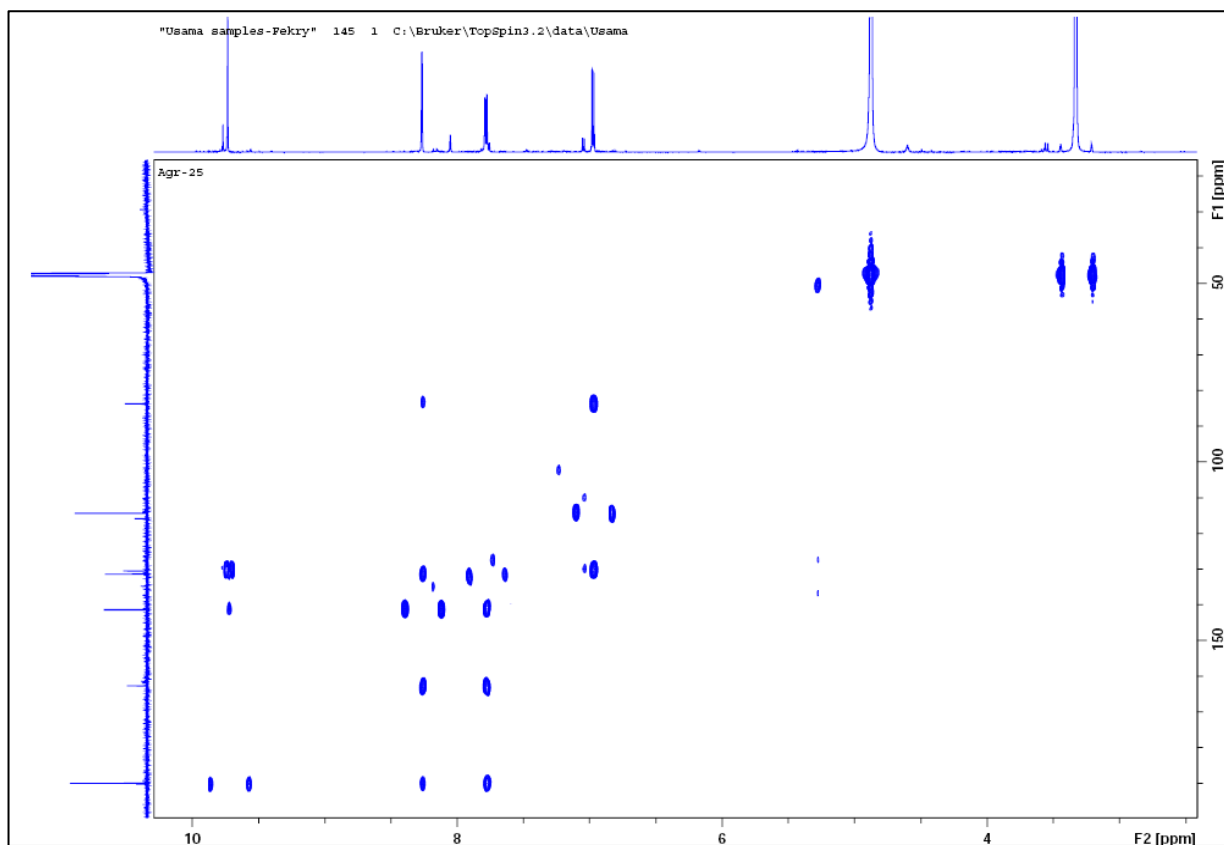
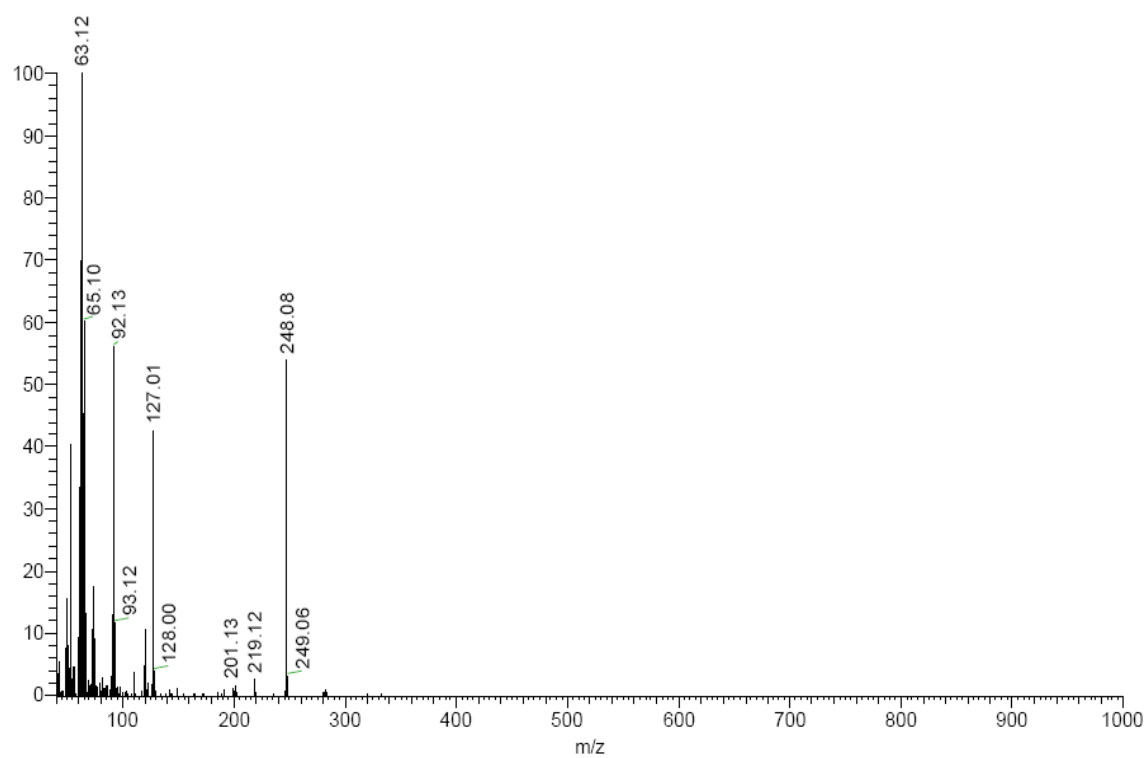


Fig. S12: HMBC NMR spectrum of compound **2** in CD<sub>3</sub>OD



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T: {0,0} + c EI Full ms [40.00-1000.00]



**Fig. S13:** EI-MS spectrum of compound **2**

### Compound 3

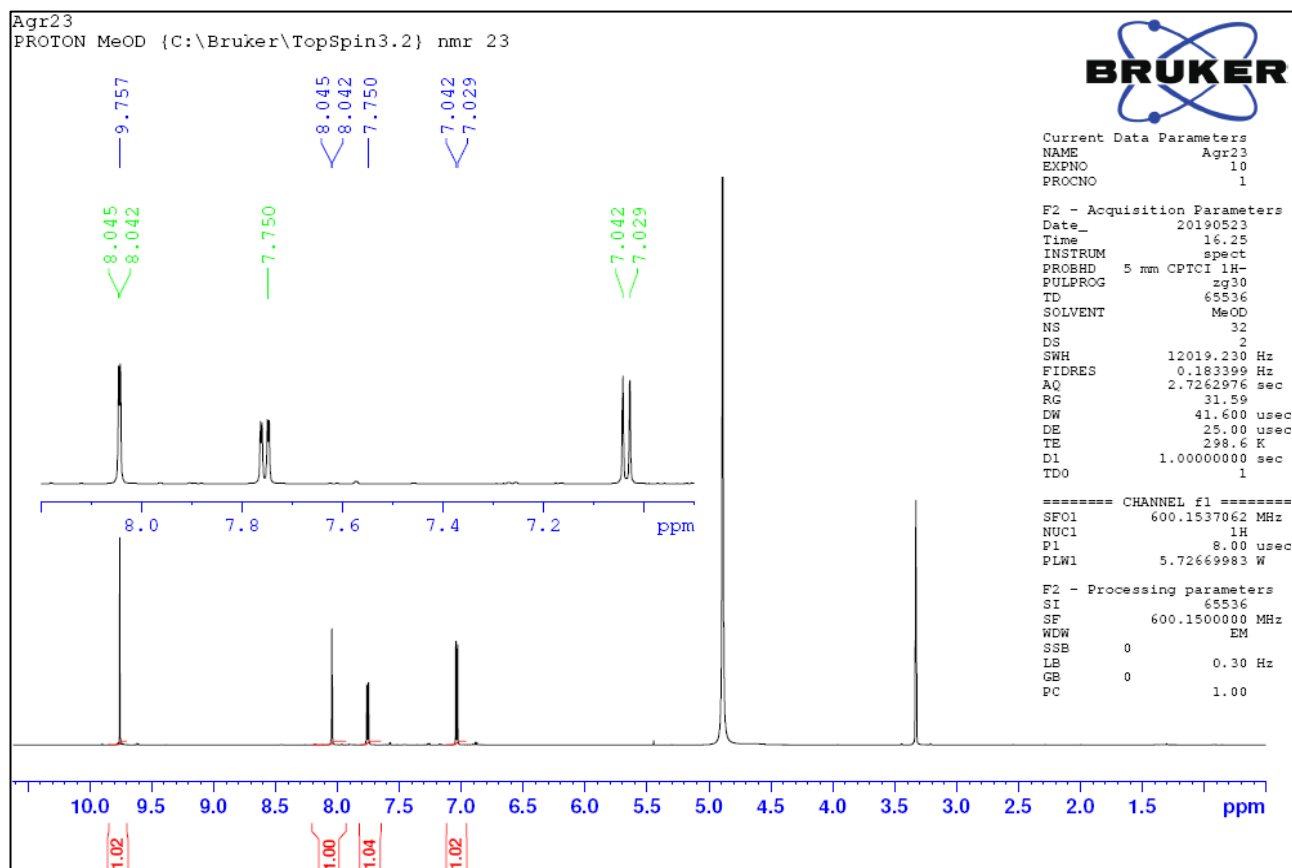


Fig. S14:  $^1\text{H}$  NMR spectrum of compound 3 in  $\text{CD}_3\text{OD}$

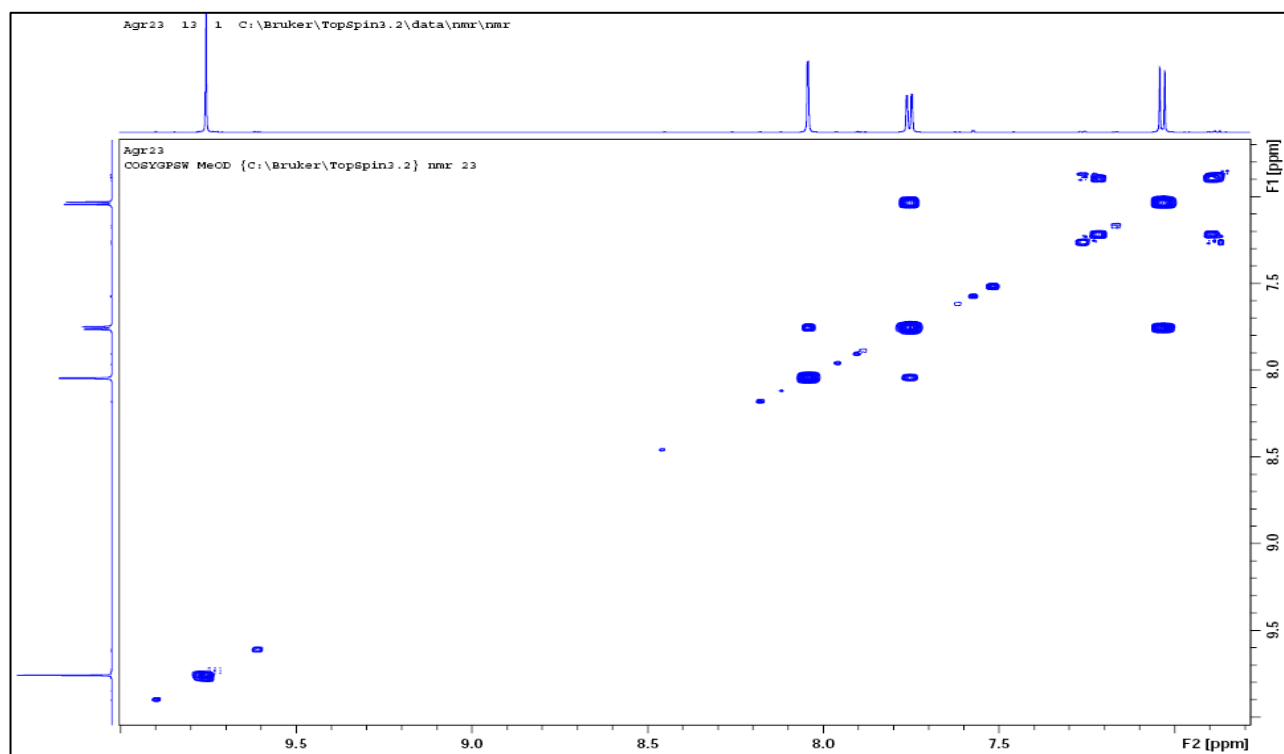


Fig. S15: HH-COSY NMR spectrum of compound 3 in  $\text{CD}_3\text{OD}$

