

## Supporting information

### **FOUR NEW NORLIGNANS FROM *POUZOLZIA ZEYLANICA* (L.) BENN. VAR. *MICROPHYLLA***

**Chu-Qian Zhong, Shu-Hong Tao, Zhi-Bo Yi, Li-Bing Guo,\* Yu-Feng Xie,  
and Yan-Fen Chen**

**Abstract** – Four new norlignans, pouzolignan D (1), pouzolignan K-M (2-4), together with four known flavonoids, rhamnocitrin (5), rhamnetin (6), isorhamnetin (7) and quercetin(8), were isolated from the aerial parts of *Pouzolzia zeylanica* (L.) Benn. var. *microphylla* (Wedd.) W. T. Wang. Their structures were elucidated by spectroscopic methods, including UV, IR, HR-ESI-TOF-MS, 1D and 2D NMR experiments.

**Index for compound 1:**

Figure S1.  $^1\text{H}$  NMR spectrum (500 MHz,  $\text{CD}_3\text{COCD}_3$ ) of compound **1**

Figure S2.  $^{13}\text{C}$  NMR spectrum (125 MHz,  $\text{CD}_3\text{COCD}_3$ ) of compound **1**

Figure S3. DEPT spectrum (125 MHz,  $\text{CD}_3\text{COCD}_3$ ) of compound **1**

Figure S4. HMBC spectrum ( $\text{CD}_3\text{COCD}_3$ ) of compound **1**

Figure S5. 2D NOESY spectrum ( $\text{CD}_3\text{OD}$ ) of compound **1**

Figure S6. HR-ESI-TOF-MS spectrum of compound **1**

**Index for compound 2:**

Figure S7.  $^1\text{H}$  NMR spectrum (500 MHz,  $\text{CD}_3\text{OD}$ ) of compound **2**

Figure S8.  $^{13}\text{C}$  NMR spectrum (125 MHz,  $\text{CD}_3\text{OD}$ ) of compound **2**

Figure S9. DEPT spectrum (125 MHz,  $\text{CD}_3\text{OD}$ ) of compound **2**

Figure S10. HSQC spectrum ( $\text{CD}_3\text{OD}$ ) of compound **2**

Figure S11. HMBC spectrum ( $\text{CD}_3\text{OD}$ ) of compound **2**

Figure S12a. 1D NOESY spectrum ( $\text{CD}_3\text{OD}$ ) of compound **2**

Figure S12b. 1D NOESY spectrum ( $\text{CD}_3\text{OD}$ ) of compound **2**

Figure S13. 2D NOESY spectrum ( $\text{CD}_3\text{OD}$ ) of compound **2**

Figure S14a. HR-ESI-TOF-MS spectrum of compound **2**

Figure S14b. HR-ESI-TOF-MS spectrum of compound **2**

**Index for compound 3:**

Figure S15.  $^1\text{H}$  NMR spectrum (500 MHz,  $\text{CD}_3\text{OD}$ ) of compound **3**

Figure S16.  $^{13}\text{C}$  NMR spectrum (125 MHz,  $\text{CD}_3\text{OD}$ ) of compound **3**

Figure S17. DEPT spectrum (125 MHz,  $\text{CD}_3\text{OD}$ ) of compound **3**

Figure S18. HSQC spectrum ( $\text{CD}_3\text{OD}$ ) of compound **3**

Figure S19. HMBC spectrum ( $\text{CD}_3\text{OD}$ ) of compound **3**

Figure S20. HR-ESI-TOF-MS spectrum of compound **3**

**Index for compound 4:**

Figure S21.  $^1\text{H}$  NMR spectrum (500 MHz,  $\text{CD}_3\text{OD}$ ) of compound **4**

Figure S22.  $^{13}\text{C}$  NMR spectrum (125 MHz,  $\text{CD}_3\text{OD}$ ) of compound **4**

Figure S23. DEPT spectrum (125 MHz,  $\text{CD}_3\text{OD}$ ) of compound **4**

Figure S24. HSQC spectrum ( $\text{CD}_3\text{OD}$ ) of compound **4**

Figure S25. HMBC spectrum ( $\text{CD}_3\text{OD}$ ) of compound **4**

Figure S26. HR-ESI-TOF-MS spectrum of compound **4**

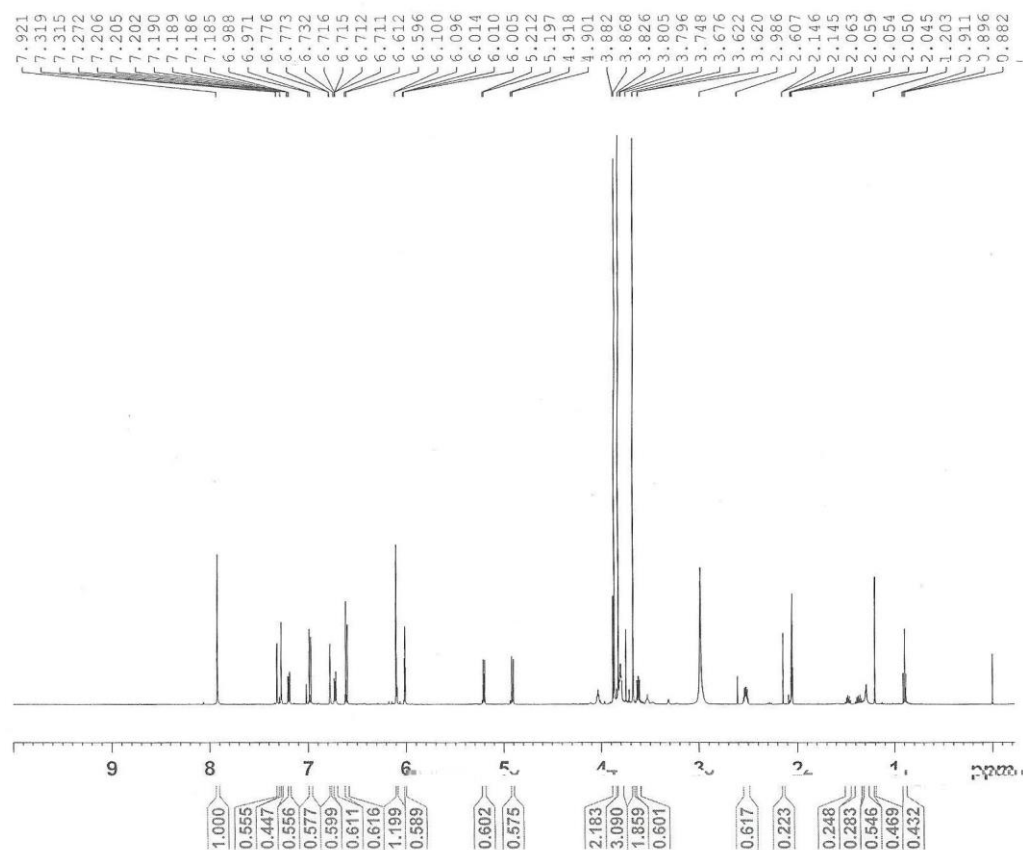


Figure S1.  $^1\text{H}$  NMR spectrum (500 MHz,  $\text{CD}_3\text{COCD}_3$ ) of compound **1**

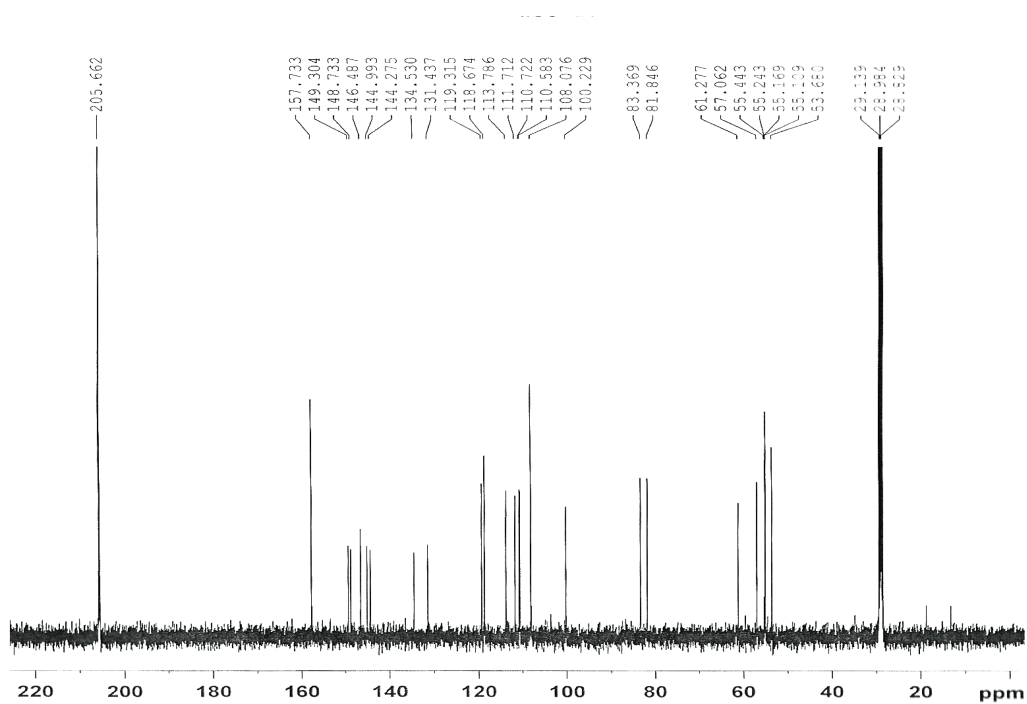


Figure S2.  $^{13}\text{C}$  NMR spectrum (125 MHz,  $\text{CD}_3\text{COCD}_3$ ) of compound **1**



Figure S3. DEPT spectrum (125 MHz,  $\text{CD}_3\text{COCD}_3$ ) of compound **1**

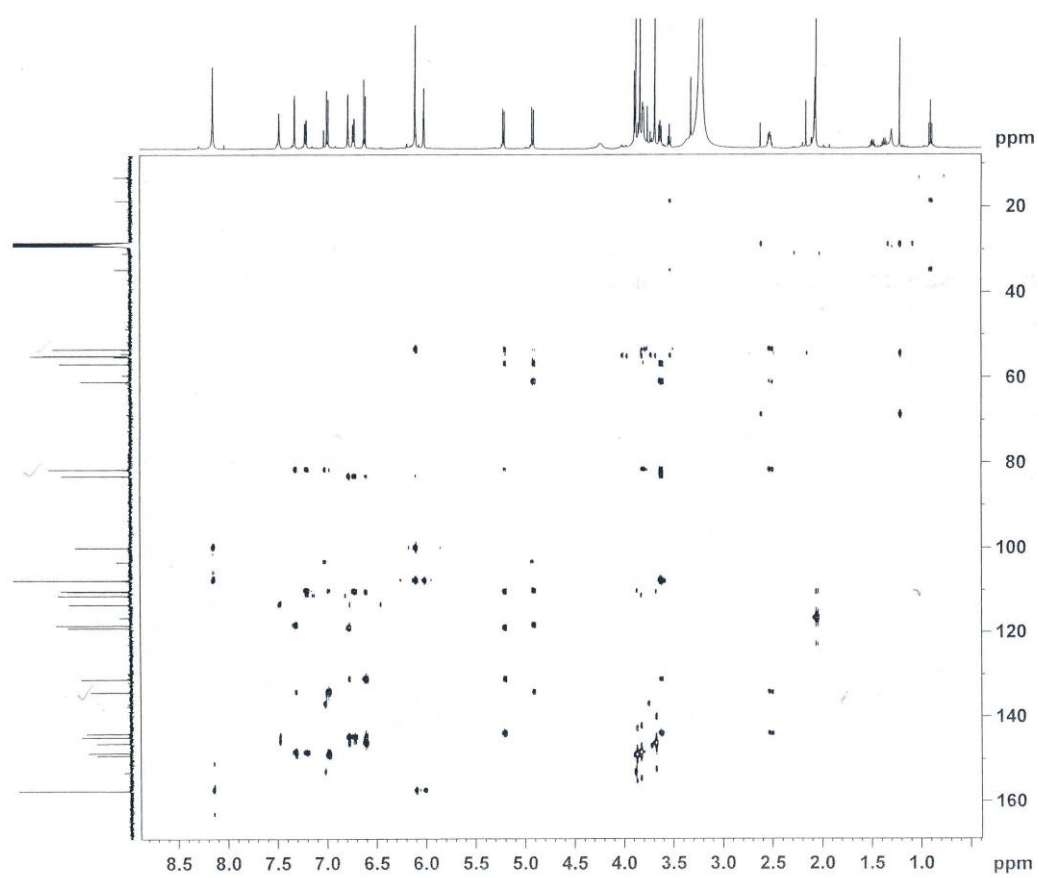


Figure S4. HMBC spectrum ( $\text{CD}_3\text{COCD}_3$ ) of compound **1**

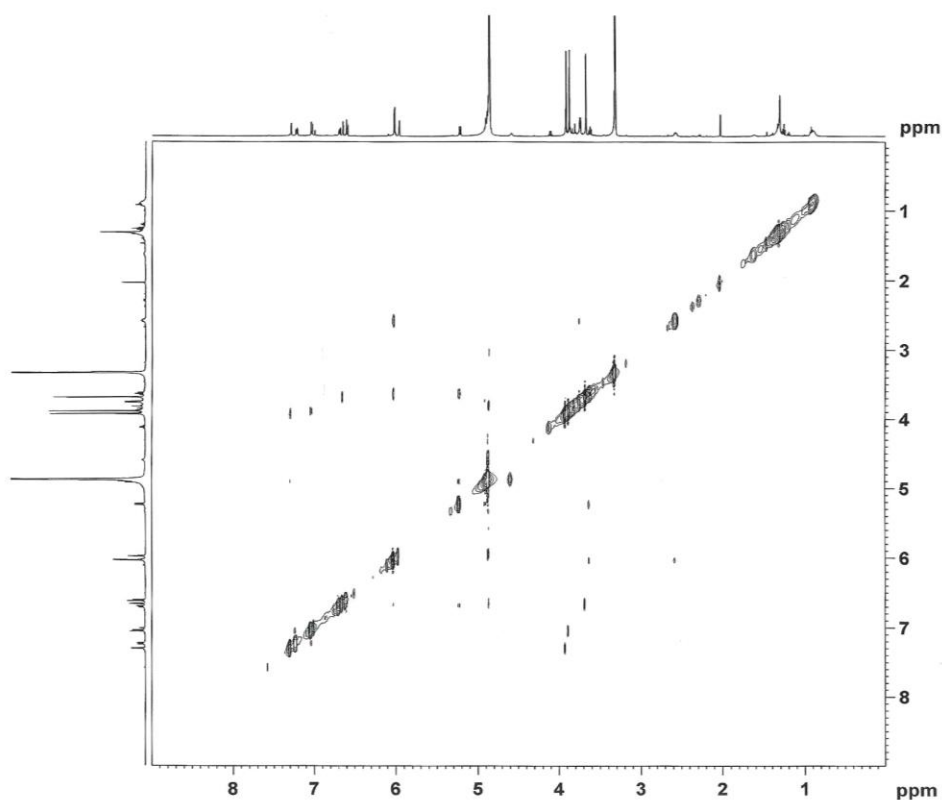


Figure S5. 2D NOESY spectrum (CD<sub>3</sub>OD) of compound 1

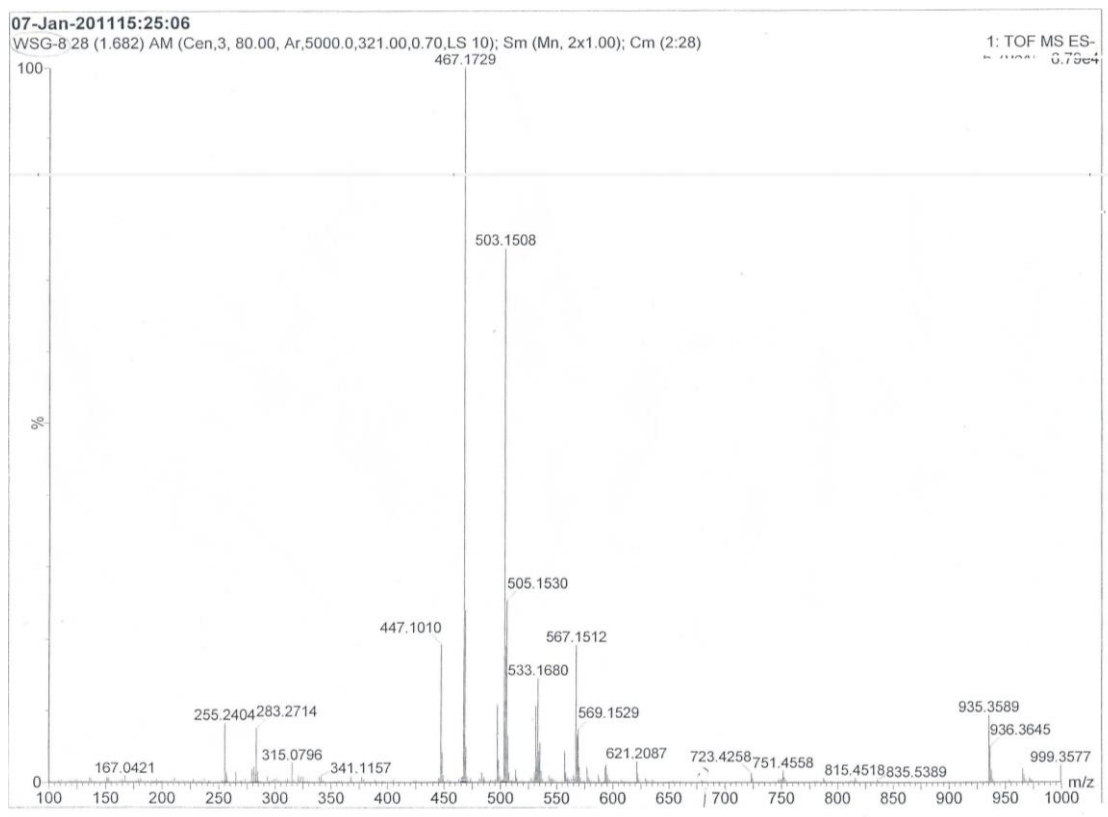


Figure S6. HR-ESI-TOF-MS spectrum of compound 1

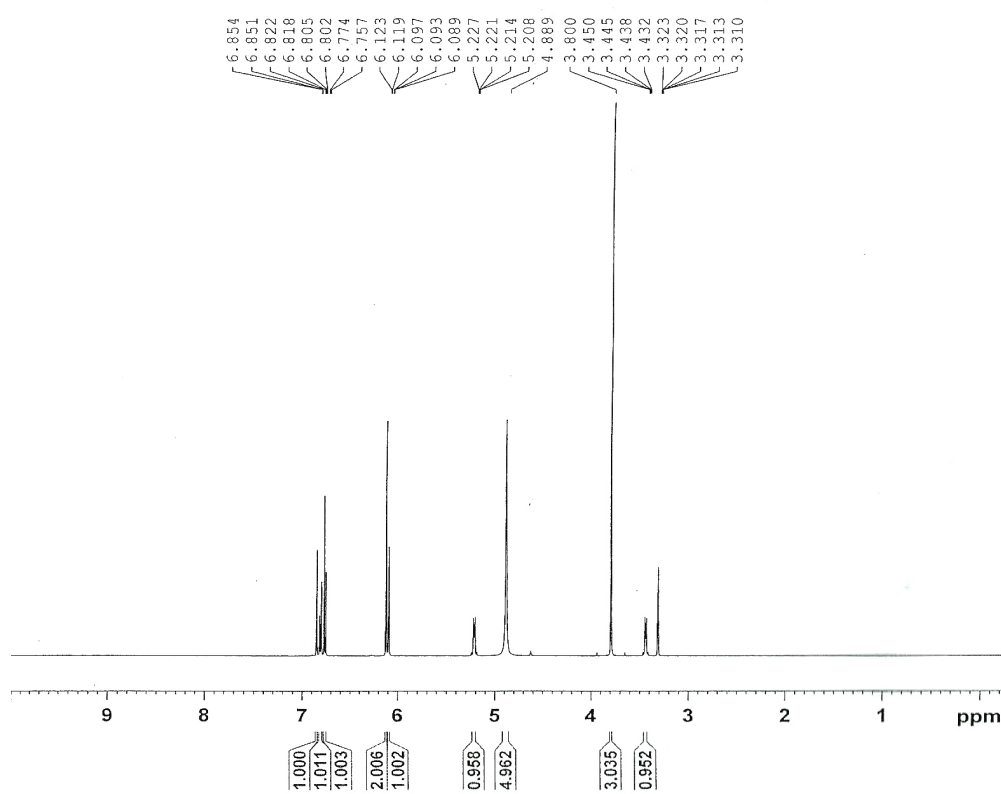


Figure S7.  $^1\text{H}$  NMR spectrum (500 MHz,  $\text{CD}_3\text{OD}$ ) of compound **2**

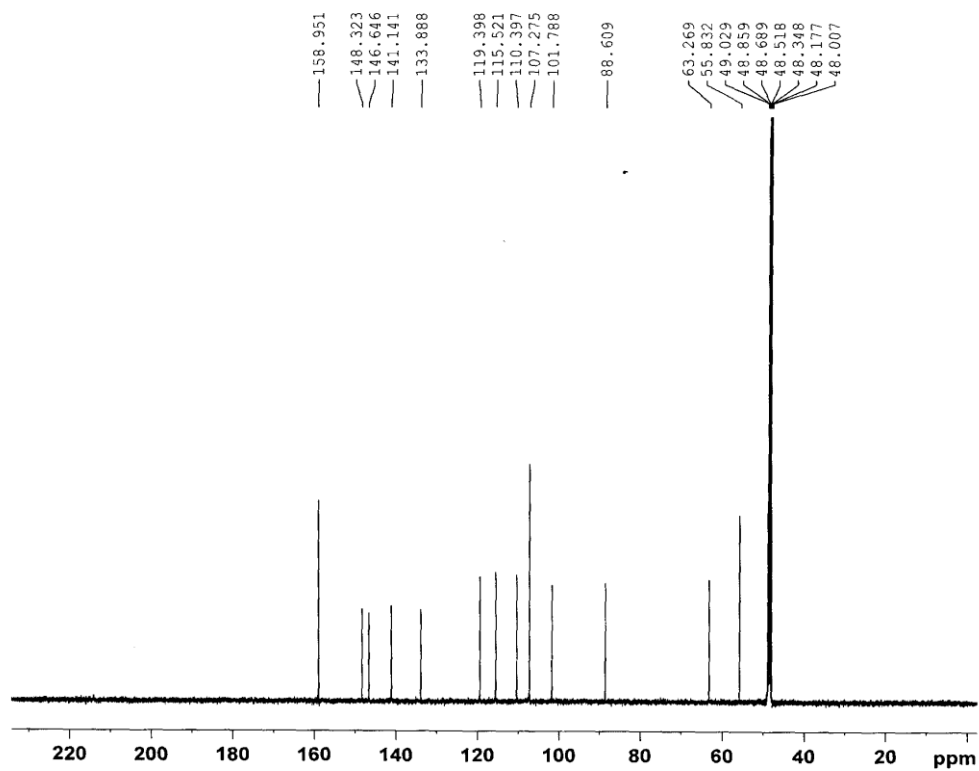


Figure S8.  $^{13}\text{C}$  NMR spectrum (125 MHz,  $\text{CD}_3\text{OD}$ ) of compound **2**

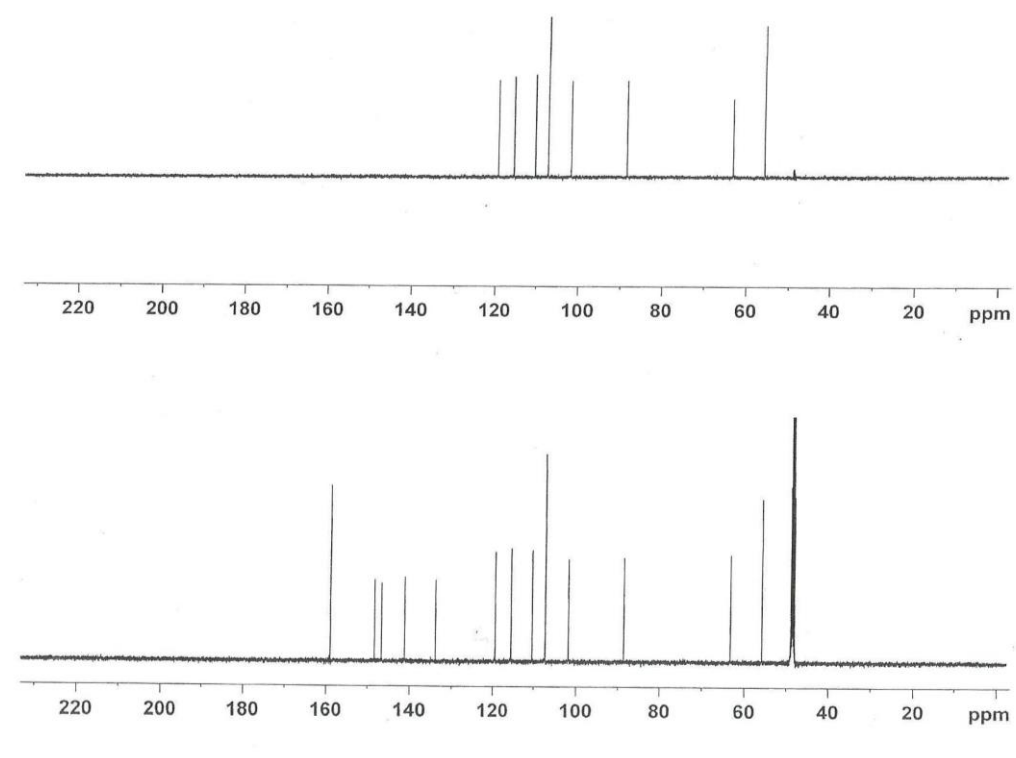


Figure S9. DEPT spectrum (125 MHz, CD<sub>3</sub>OD) of compound **2**

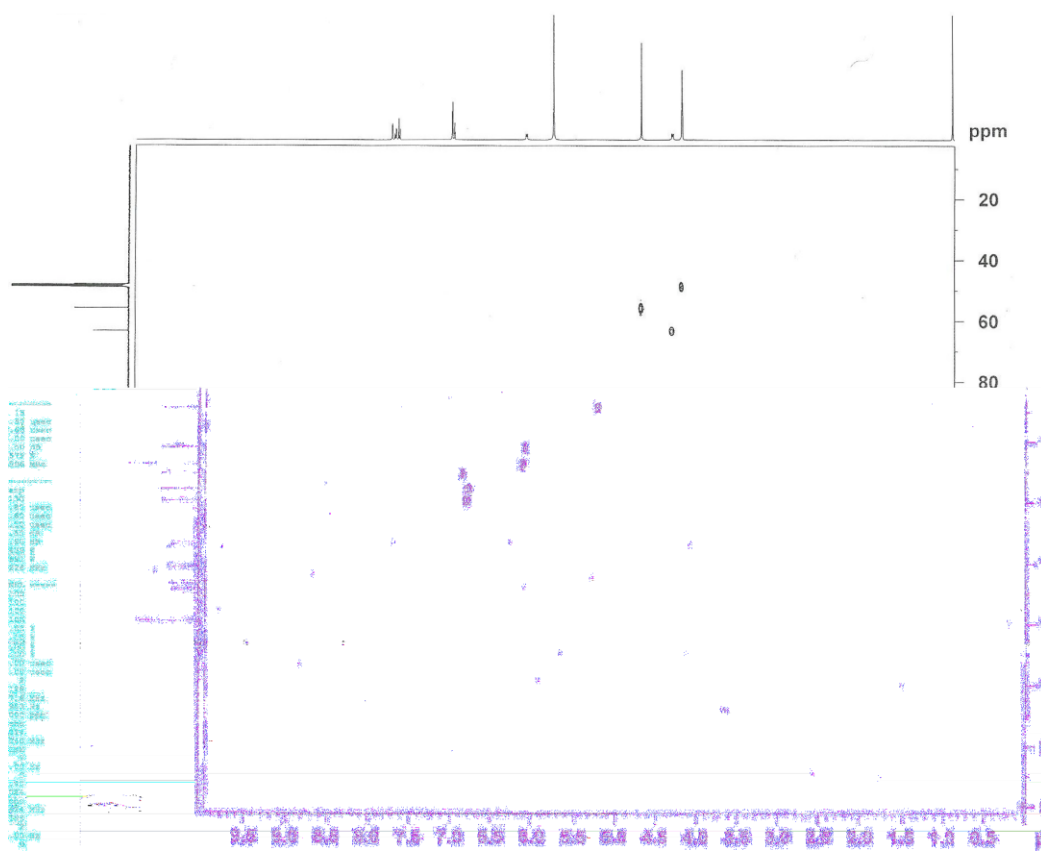


Figure S10. HSQC spectrum (CD<sub>3</sub>OD) of compound **2**

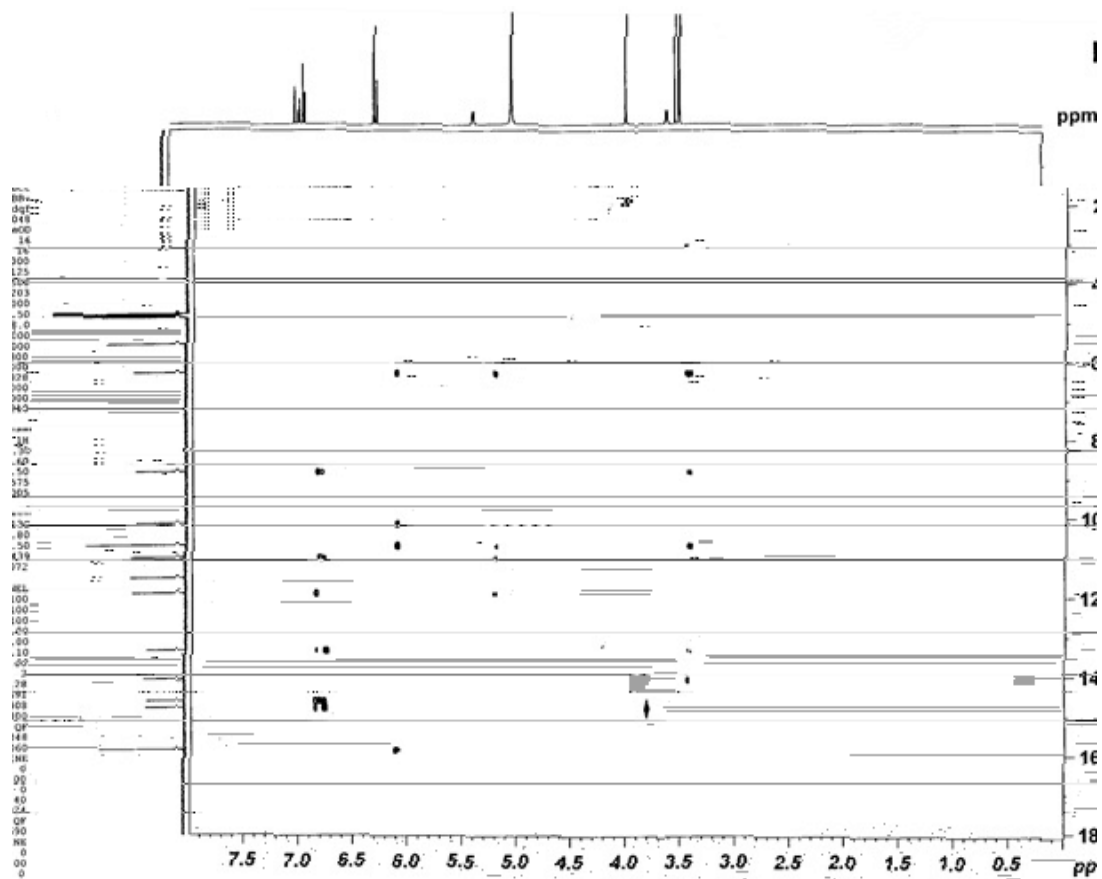


Figure S11. HMBC spectrum (CD<sub>3</sub>OD) of compound 2

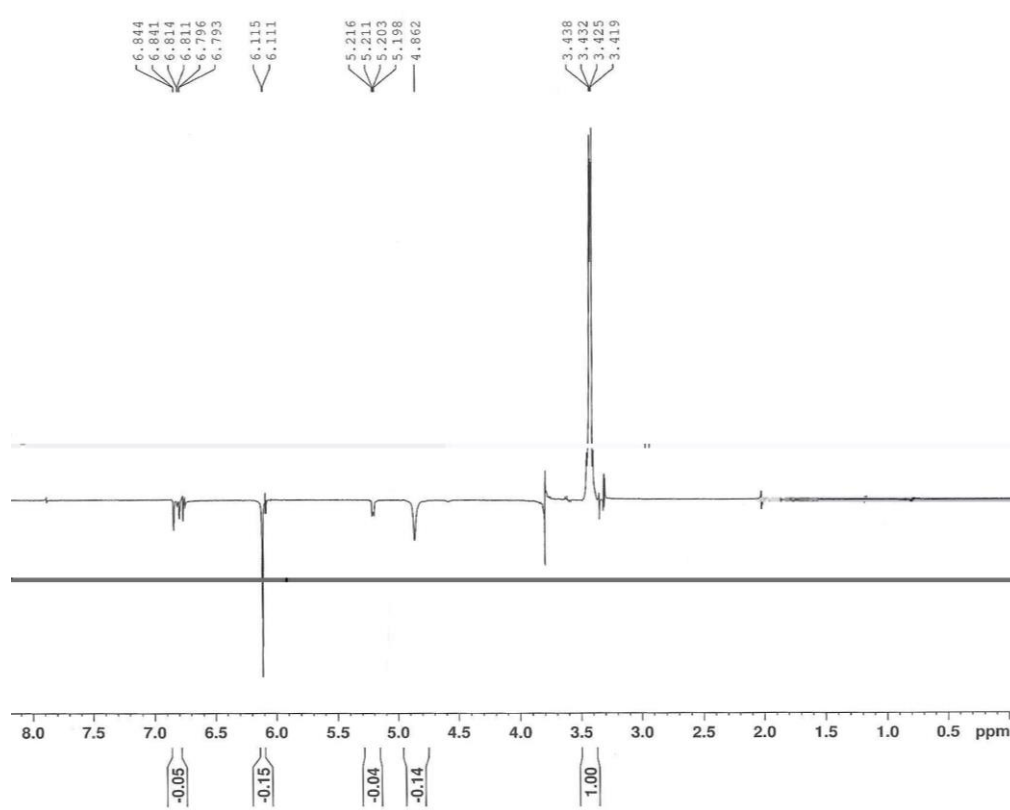


Figure S12a. 1D NOESY spectrum (CD<sub>3</sub>OD) of compound 2

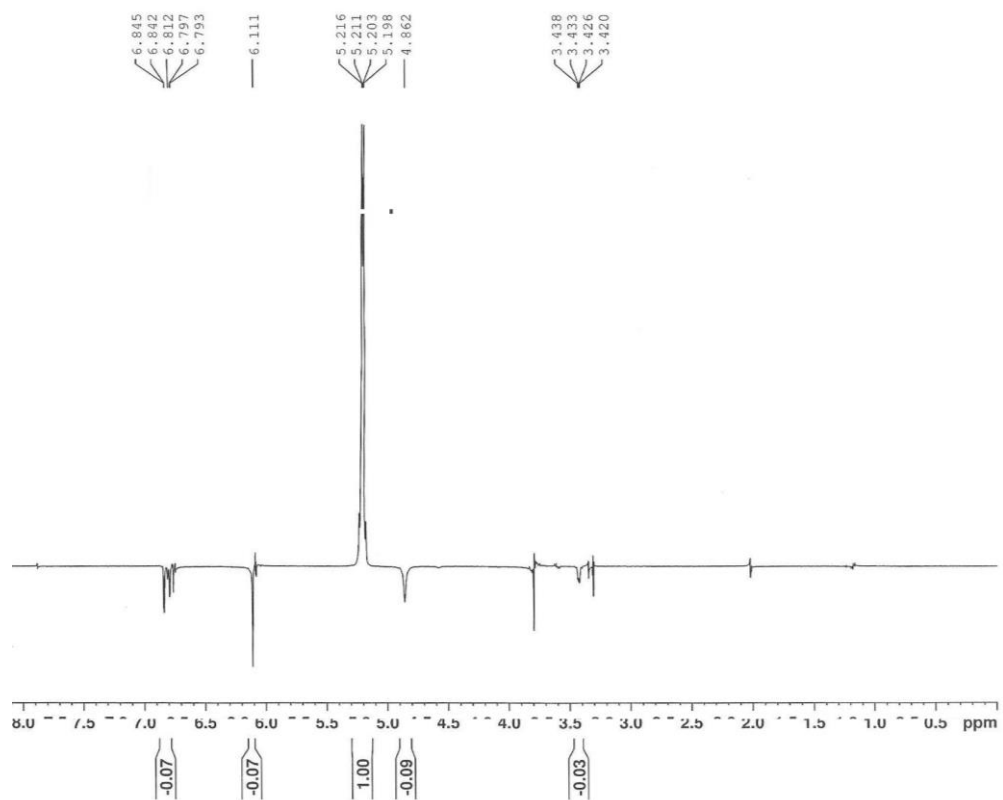


Figure S12b. 1D NOESY spectrum (CD<sub>3</sub>OD) of compound 2

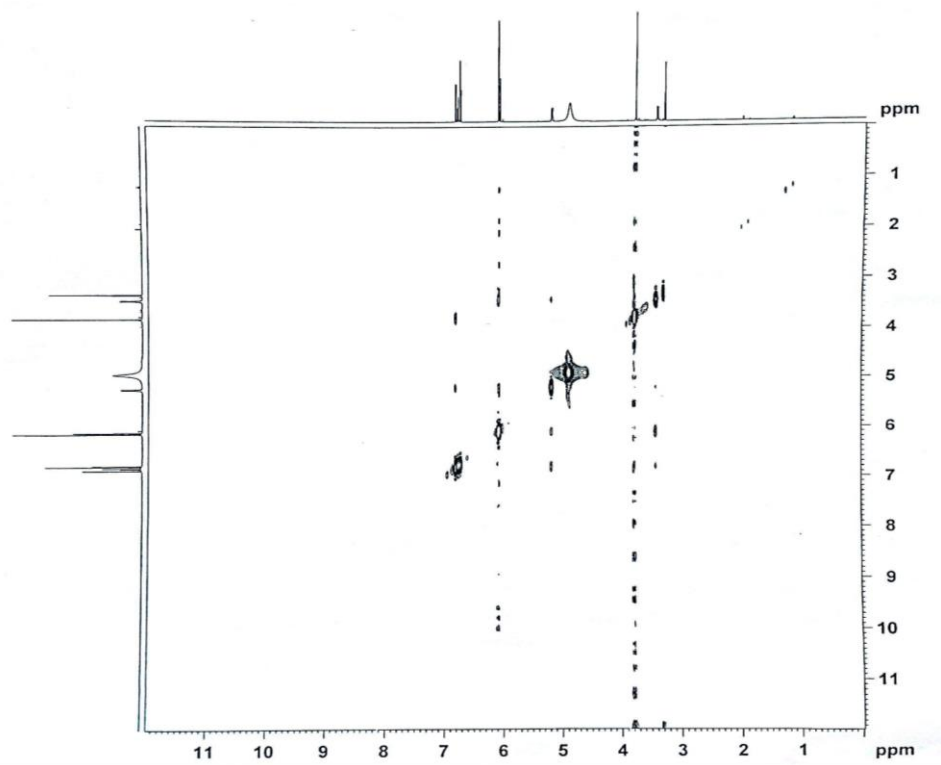


Figure S13. 2D NOESY spectrum (CD<sub>3</sub>OD) of compound 2

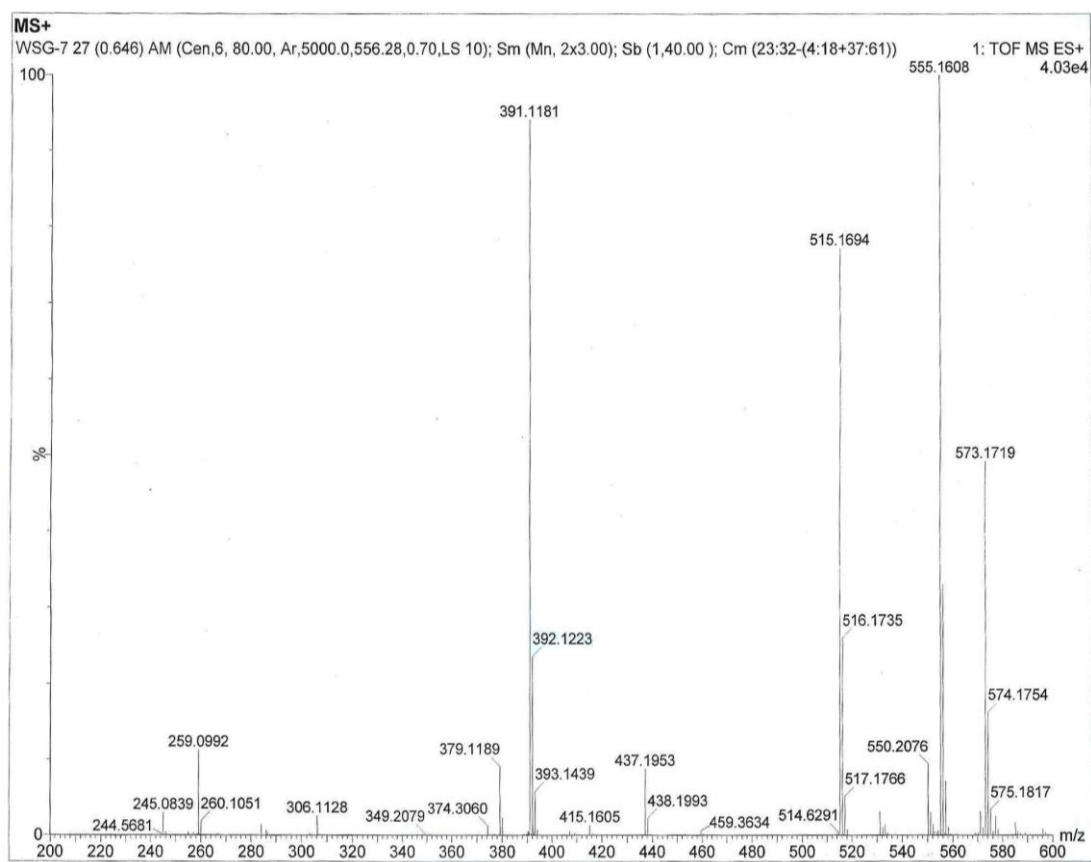


Figure S14a. HR-ESI-TOF-MS spectrum of compound 2

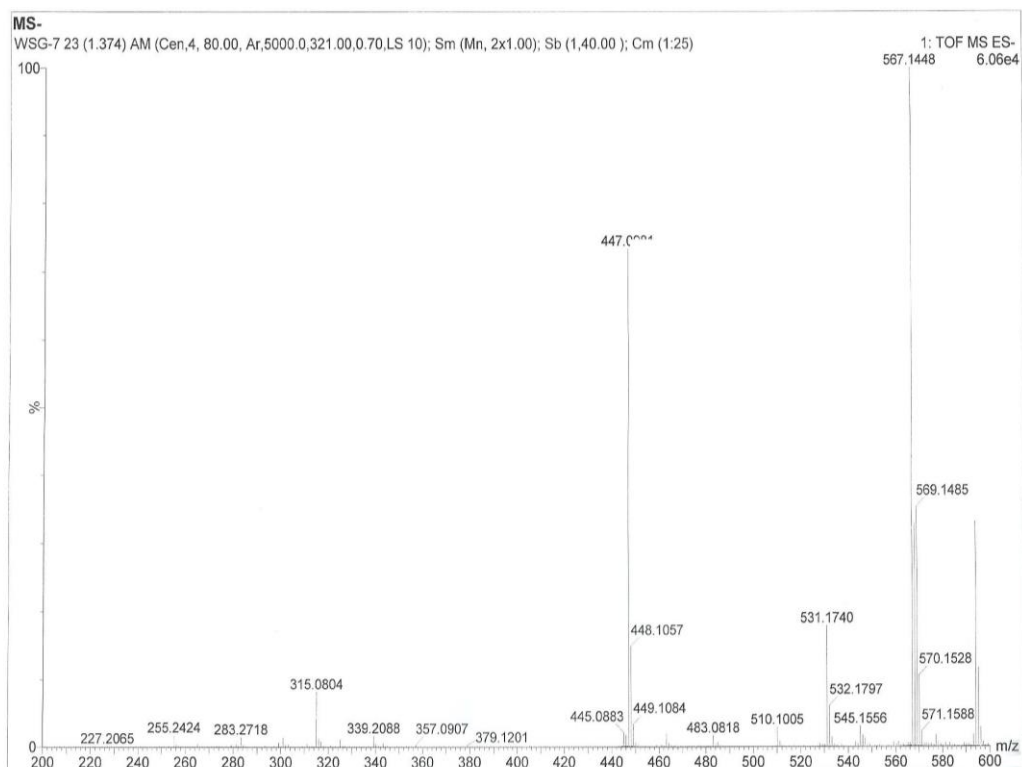


Figure S14b. HR-ESI-TOF-MS spectrum of compound 2

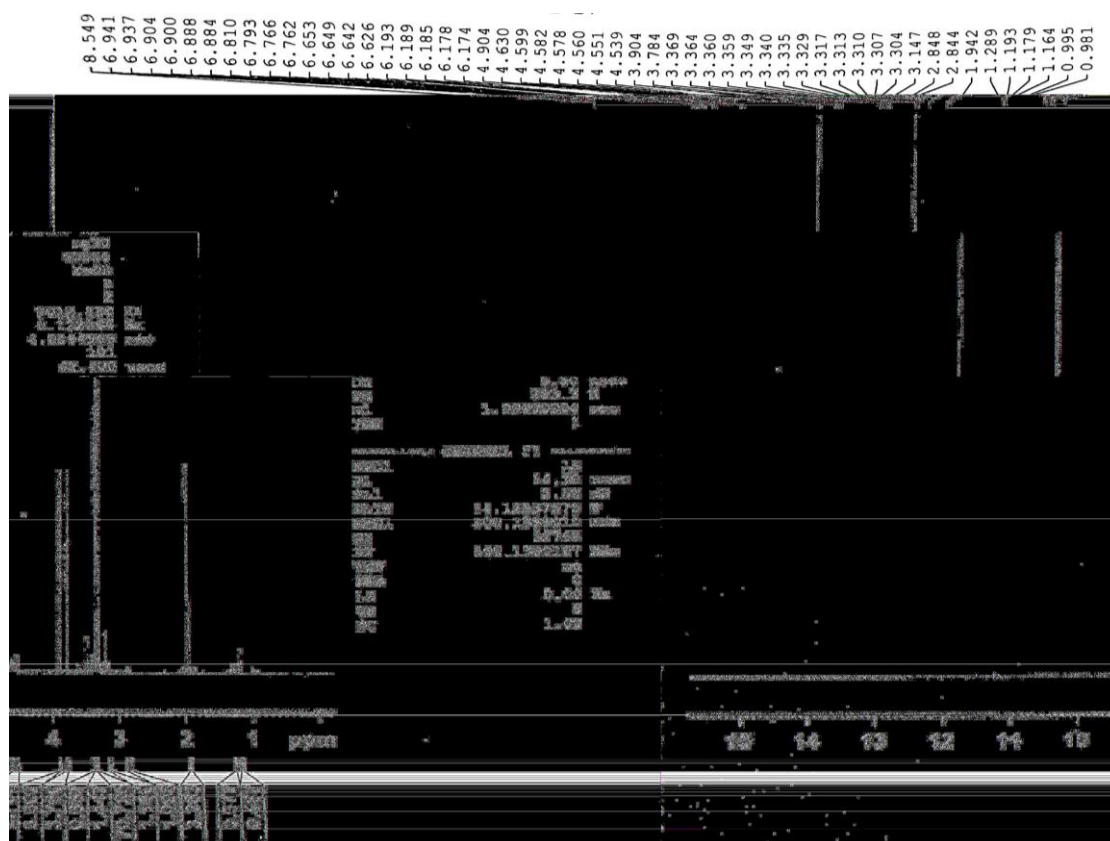


Figure S15.  $^1\text{H}$  NMR spectrum (500 MHz,  $\text{CD}_3\text{OD}$ ) of compound 3

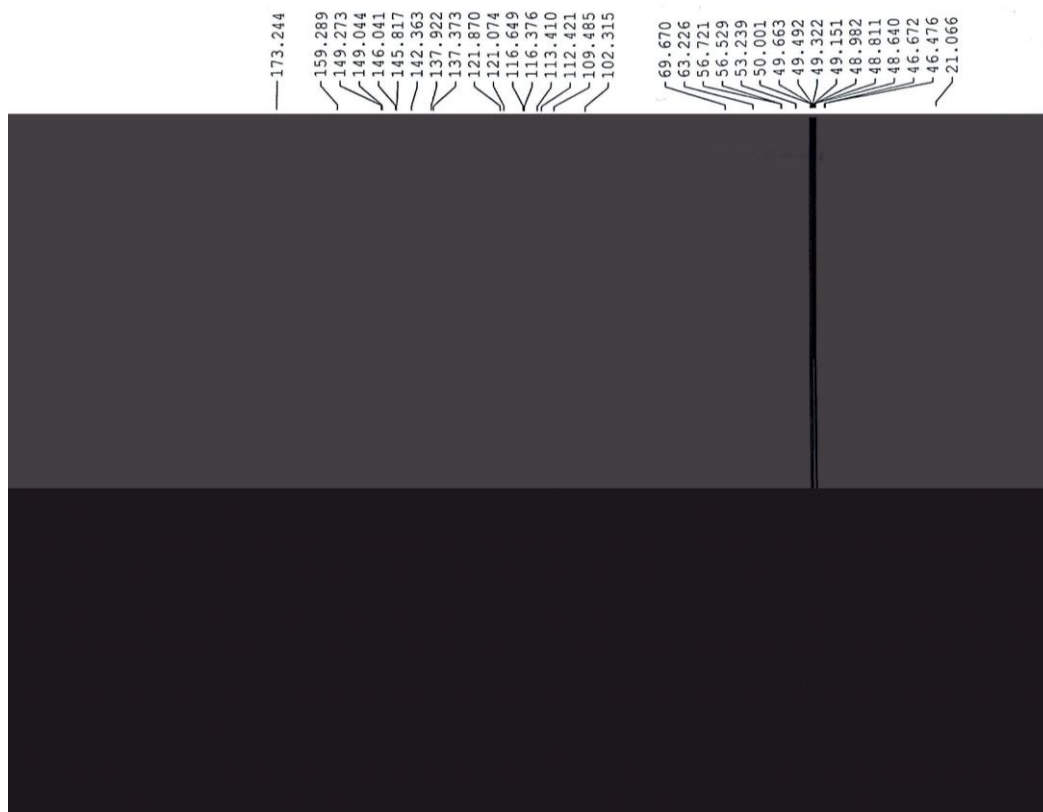


Figure S16.  $^{13}\text{C}$  NMR spectrum (125 MHz,  $\text{CD}_3\text{OD}$ ) of compound **3**

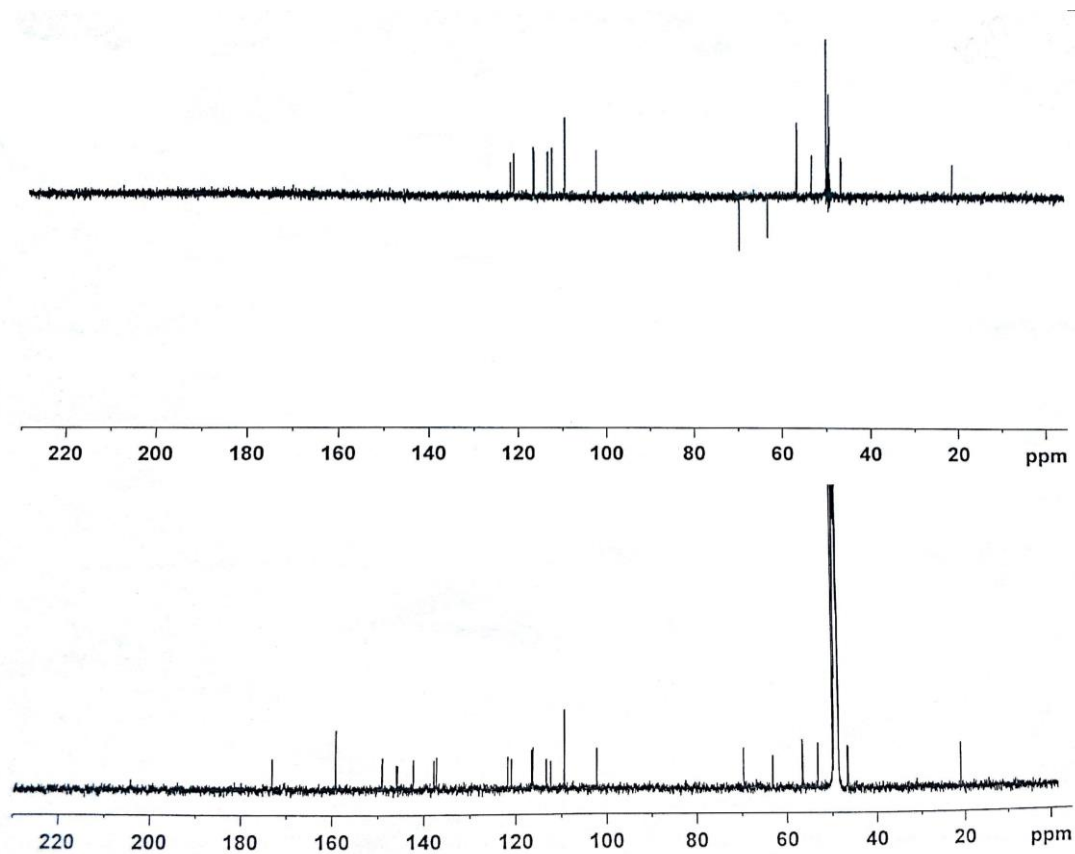


Figure S17. DEPT spectrum (125 MHz,  $\text{CD}_3\text{OD}$ ) of compound **3**

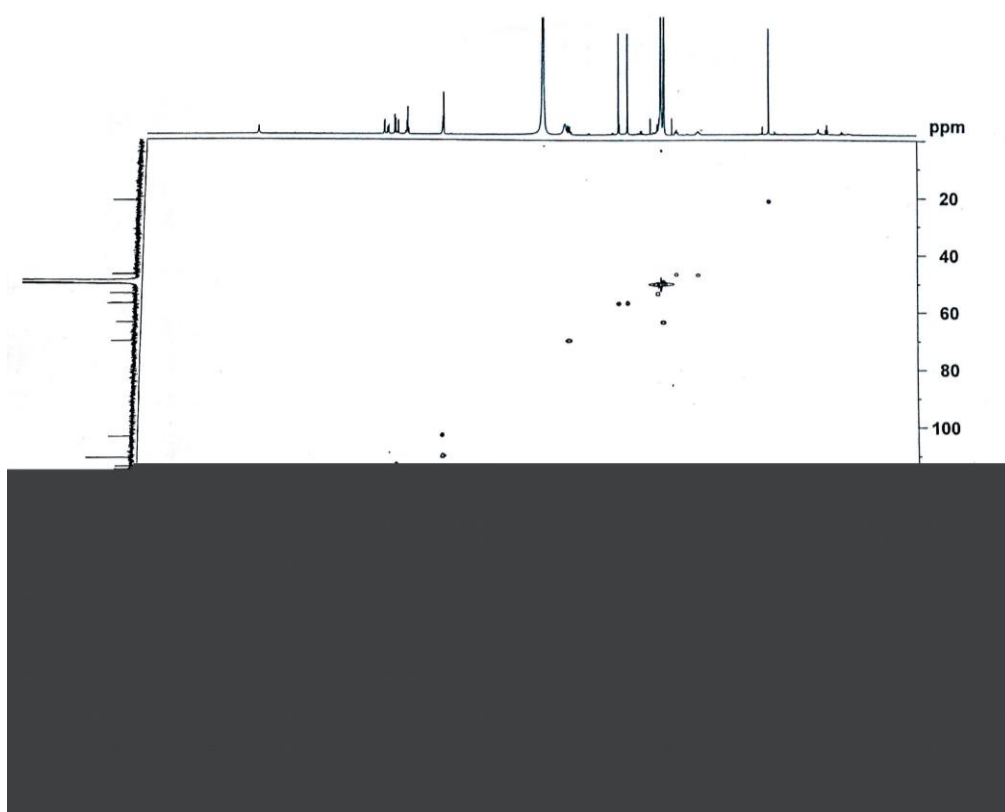


Figure S18. HSQC spectrum (CD<sub>3</sub>OD) of compound **3**

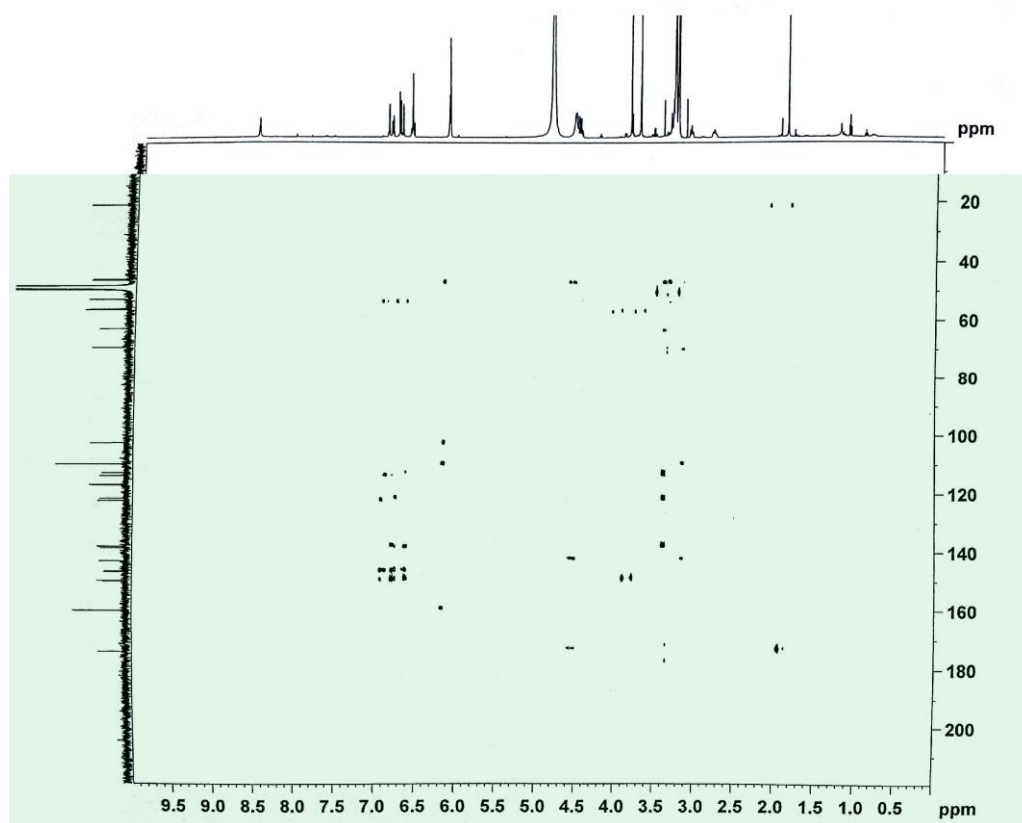


Figure S19. HMBC spectrum (CD<sub>3</sub>OD) of compound **3**

## Elemental Composition Report

Page 1

### Single Mass Analysis

Tolerance = 5.0 mDa / DBE: min = -1.5, max = 50.0

Selected filters: None

Monoisotopic Mass, Even Electron Ions

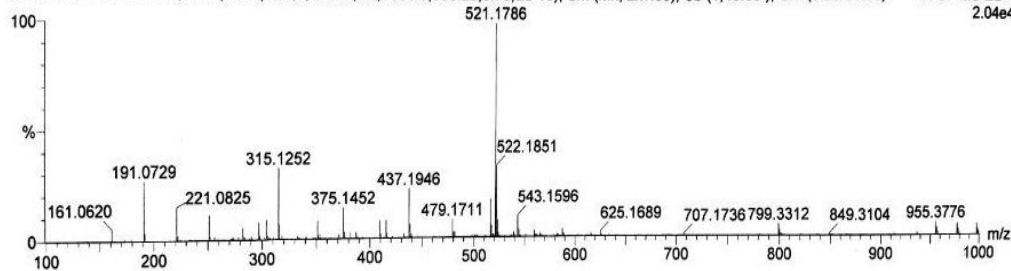
211 formula(e) evaluated with 3 results within limits (up to 50 closest results for each mass)

Elements Used:

C: 0-50 H: 0-100 O: 0-20 Na: 0-1

MS+06-Jun-201513:13:55

Y150223-WSG-E-27 14 (0.217) AM (Cen,6, 80.00, Ar,5000.0,556.28,0.70,LS 10); Sm (Mn, 2x1.00); Sb (1,40.00); Cm (8:23-56:88) 1: TOF MS ES+ 2.04e4



Mass	Calc. Mass	mDa	PPM	DBE	i-FIT	Formula
521.1786	521.1788	-0.2	-0.4	12.5	45.9	C27 H30 O9 Na
	521.1812	-2.6	-5.0	15.5	12.0	C29 H29 O9
	521.1753	3.3	6.3	24.5	106.5	C36 H25 O4

Figure S20. HR-ESI-TOF-MS spectrum of compound 3

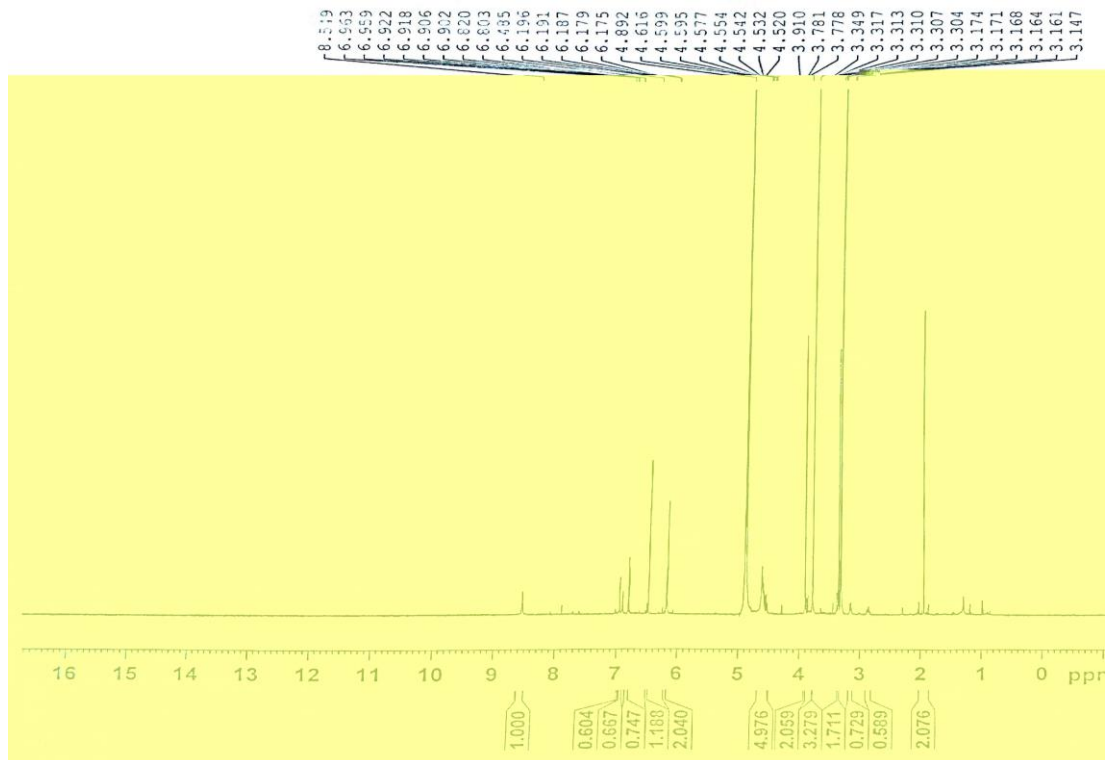


Figure S21. <sup>1</sup>H NMR spectrum (500 MHz, CD<sub>3</sub>OD) of compound 4

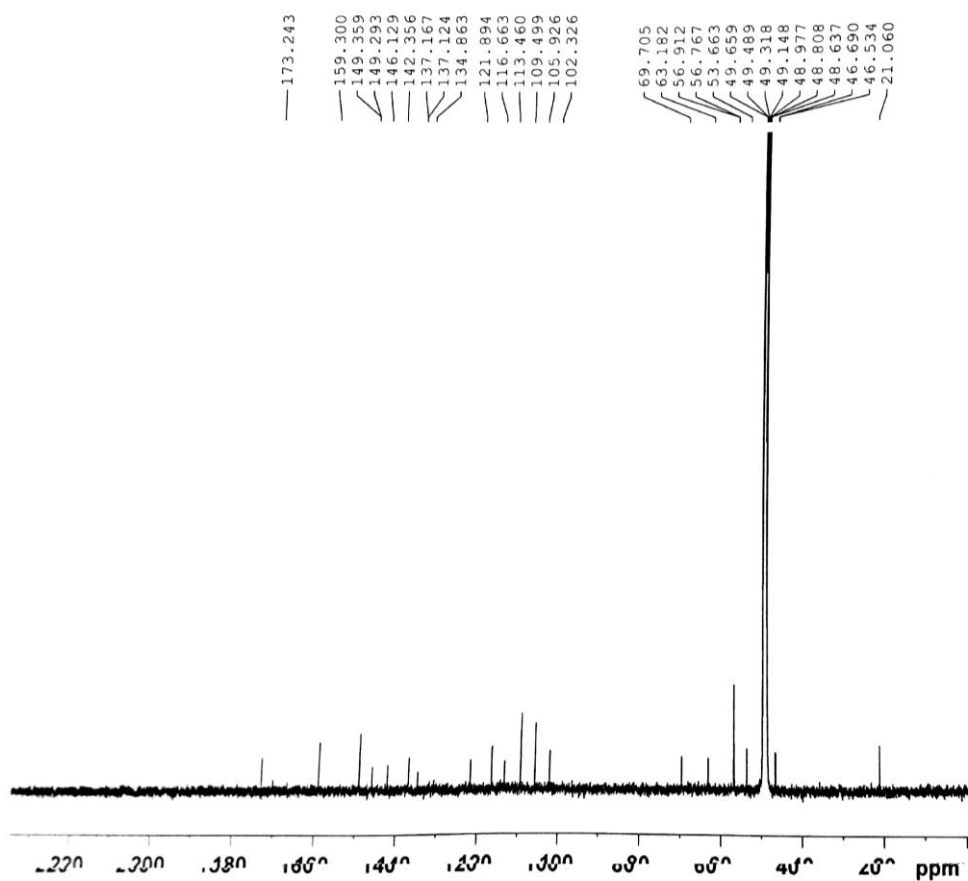


Figure S22.  $^{13}\text{C}$  NMR spectrum (125 MHz,  $\text{CD}_3\text{OD}$ ) of compound 4

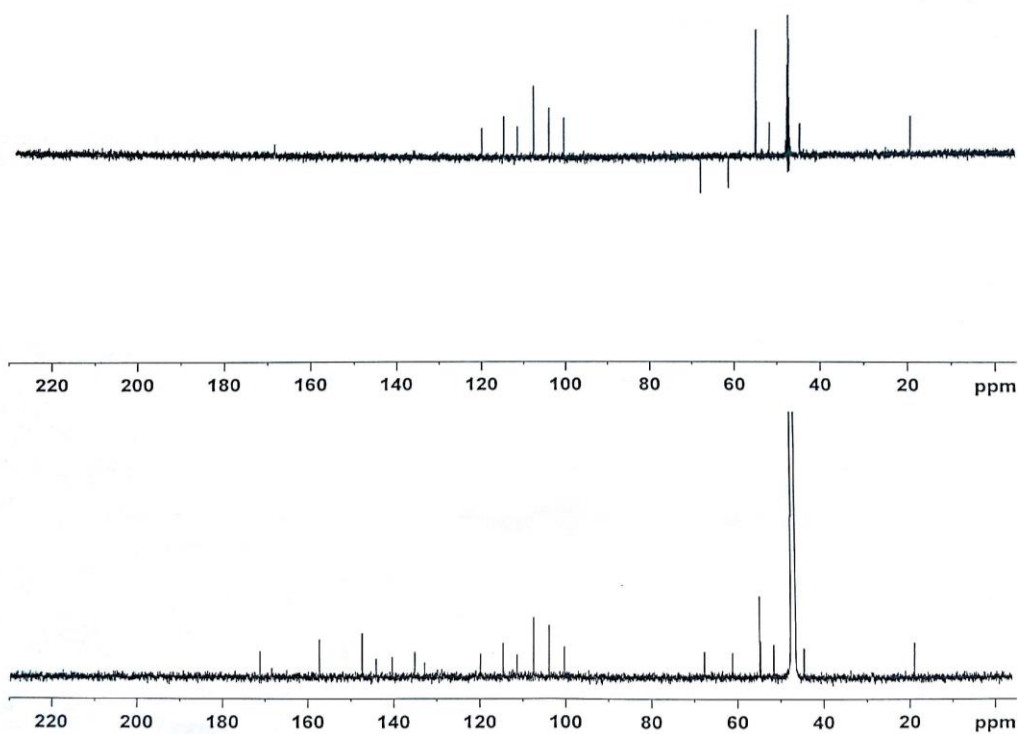


Figure S23. DEPT spectrum (125 MHz,  $\text{CD}_3\text{OD}$ ) of compound 4

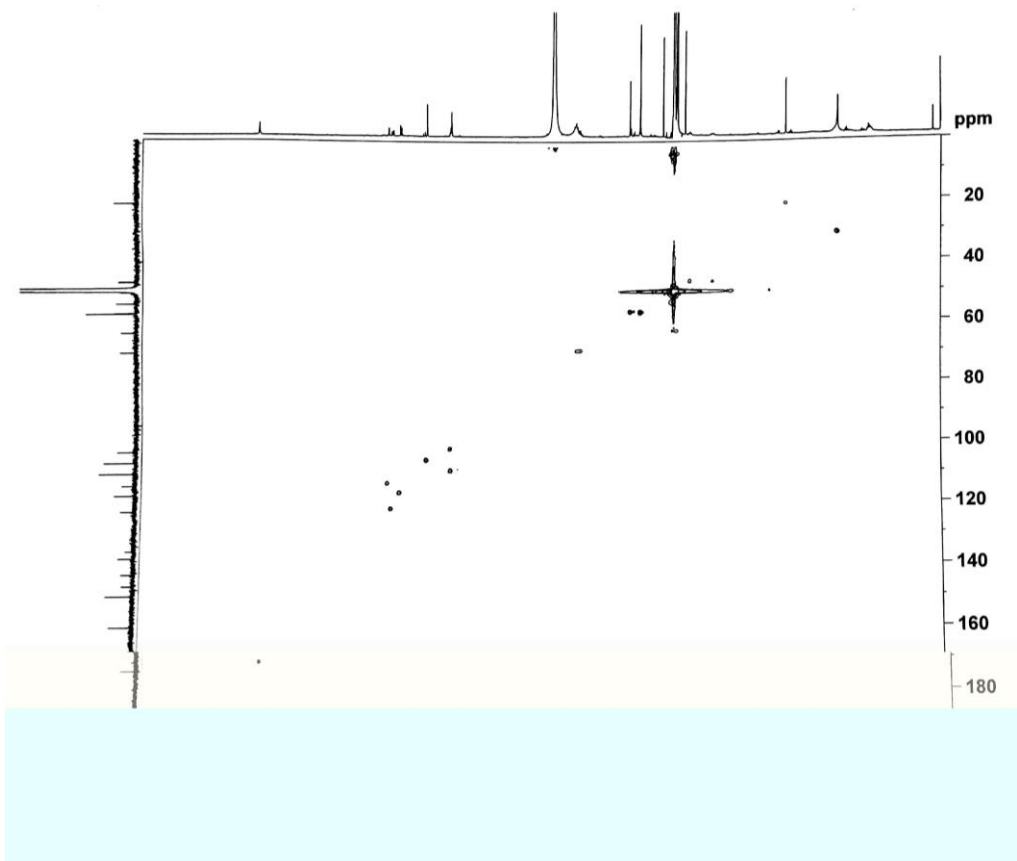


Figure S24. HSQC spectrum (CD<sub>3</sub>OD) of compound 4

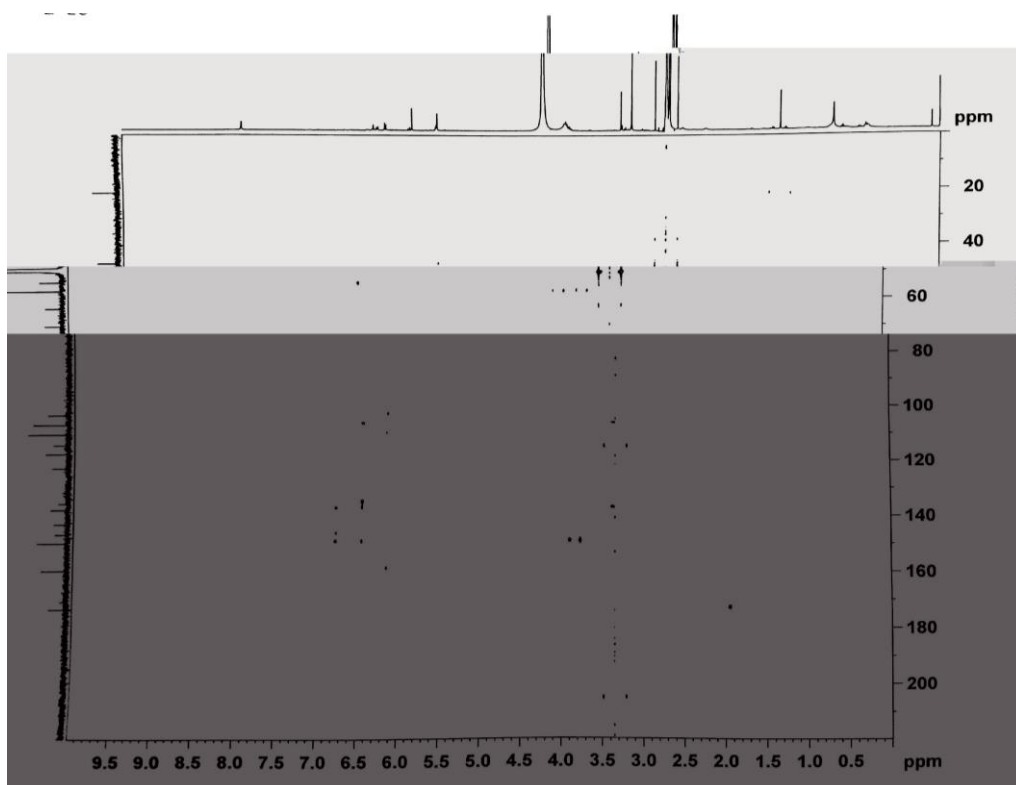


Figure S25. HMBC spectrum (CD<sub>3</sub>OD) of compound 4

Single Mass Analysis

Tolerance = 5.0 mDa / DBE: min = -1.5, max = 50.0

Selected filters: None

Monoisotopic Mass, Even Electron Ions

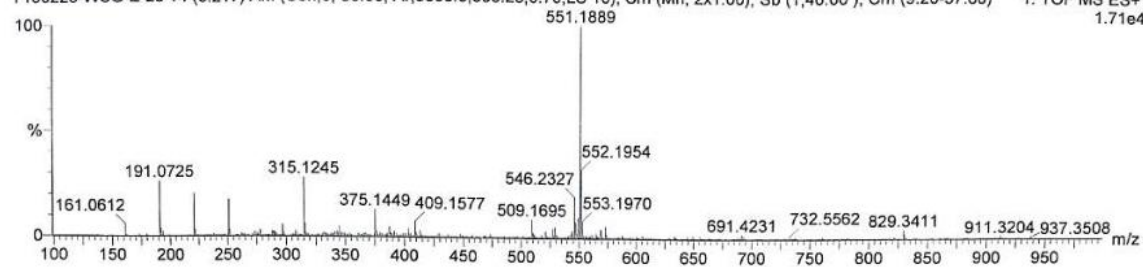
233 formula(e) evaluated with 3 results within limits (up to 50 closest results for each mass)

Elements Used:

C: 0-50 H: 0-100 O: 0-20 Na: 0-1

MS+06-Jun-201513:08:14

Y150223-WSG-E-25 14 (0.217) AM (Cen,6, 80.00, Ar,5000.0,556.28,0.70,LS 10); Sm (Mn, 2x1.00); Sb (1,40.00); Cm (9:20-37:60) 1: TOF MS ES+ 1.71e4



Minimum: -1.5  
Maximum: 5.0 50.0 50.0

Mass	Calc. Mass	mDa	PPM	DBE	i-FIT	Formula
551.1889	551.1893	-0.4	-0.7	12.5	18.1	C28 H32 O10 Na
	551.1917	-2.8	-5.1	15.5	11.1	C30 H31 O10
	551.1858	3.1	5.6	24.5	148.8	C37 H27 O5

Figure S26. HR-ESI-TOF-MS spectrum of compound 4