

## Supporting Information

*Rec. Nat. Prod.* X:X (2020) XX-XX

### Chemical Constituents of the Seeds of *Pharbitis purpurea* and Laxative Effect of Methyl Caffate in Rats

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Ruyue Chen and Hui Yang \*

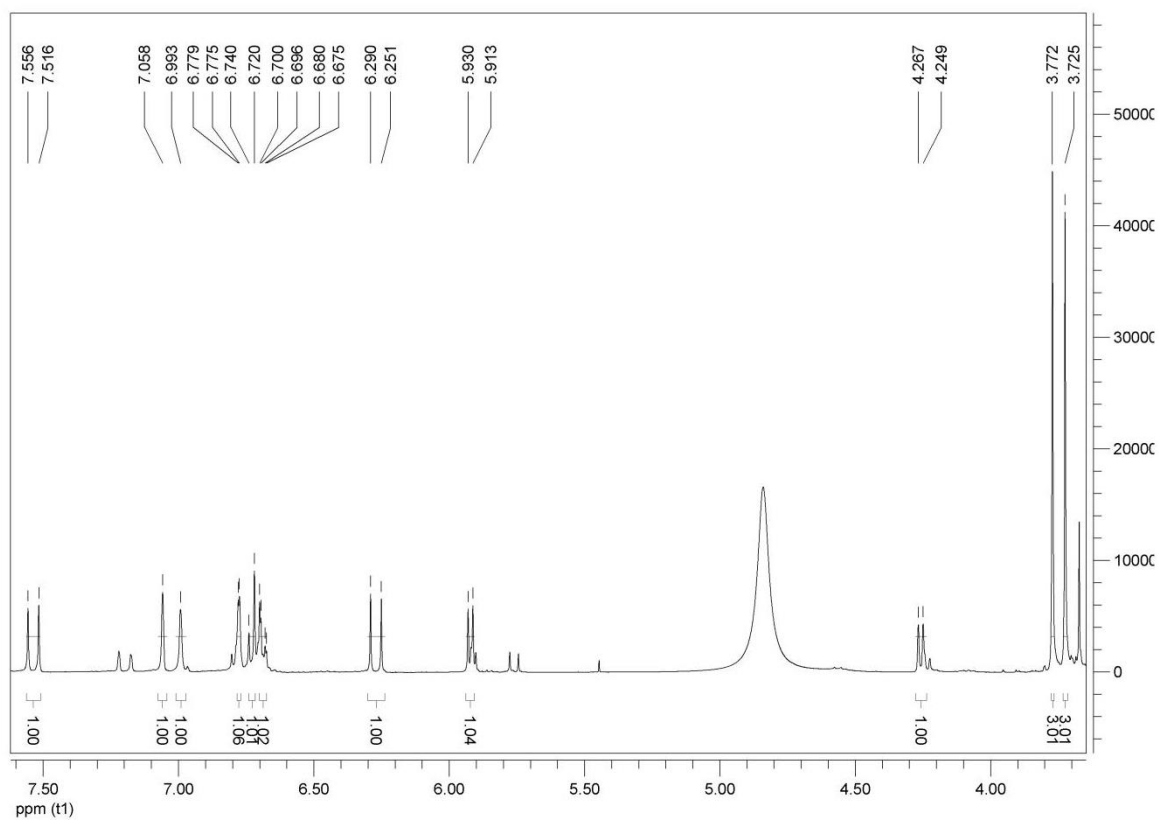
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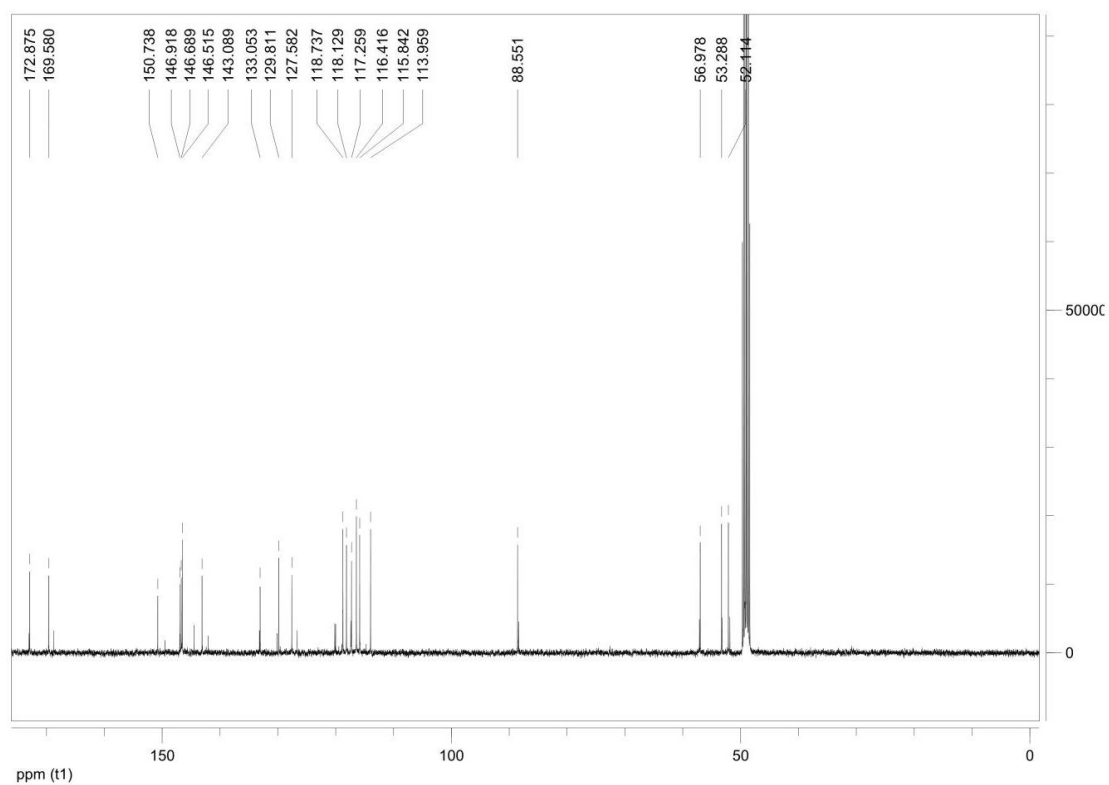
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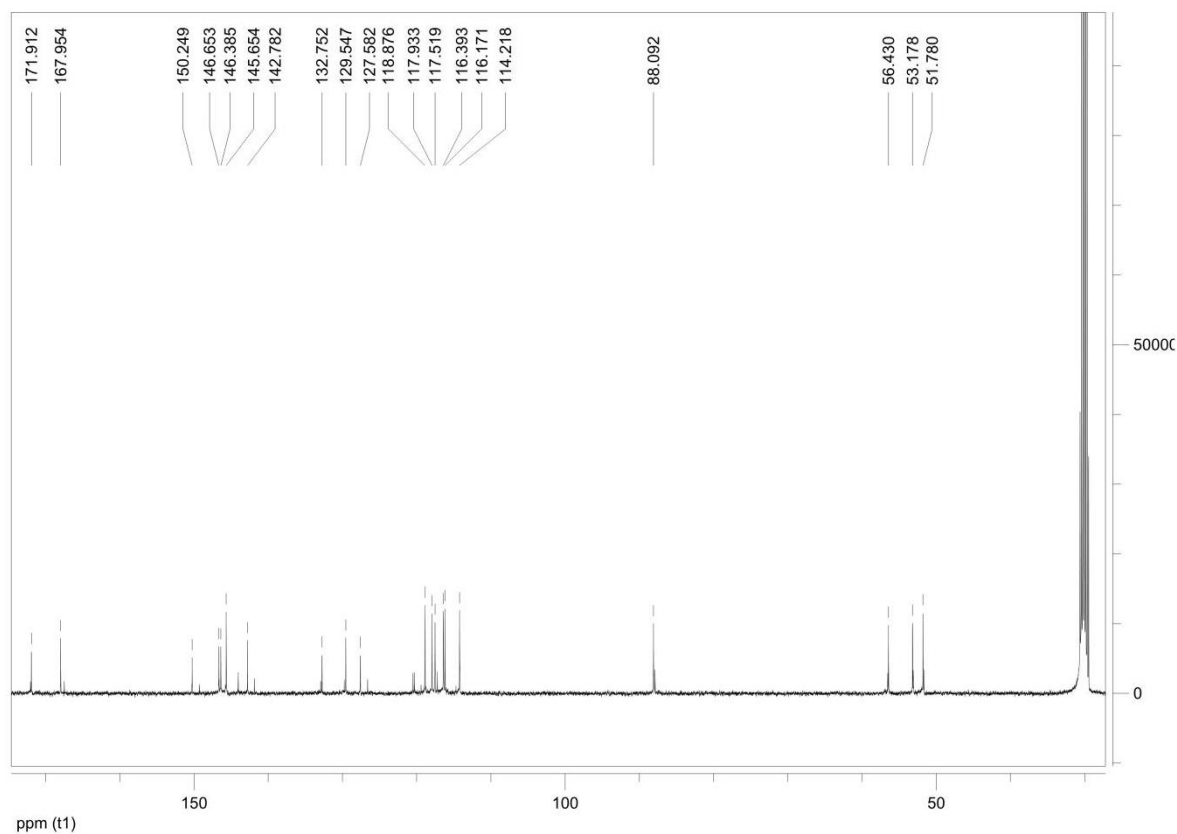


**Figure S1:**  $^1\text{H}$  NMR spectrum of **1** in  $\text{CD}_3\text{OD}$  (400 MHz)

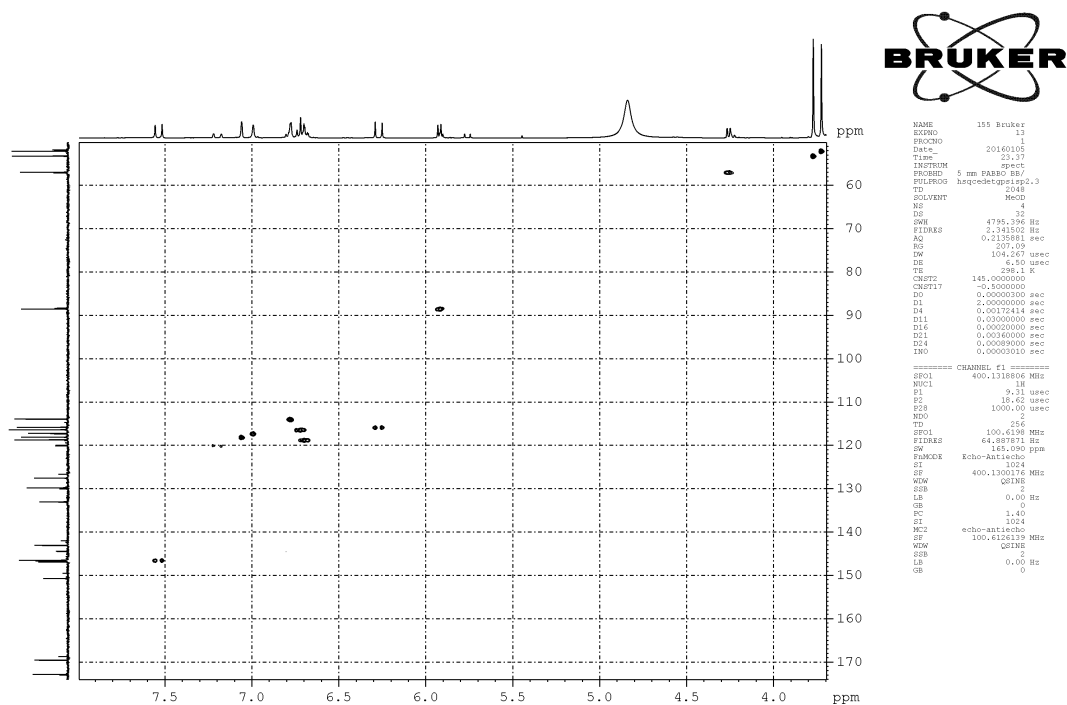


**Figure S2:**  $^{13}\text{C}$  NMR spectrum of **1** in  $\text{CD}_3\text{OD}$  (100 MHz)

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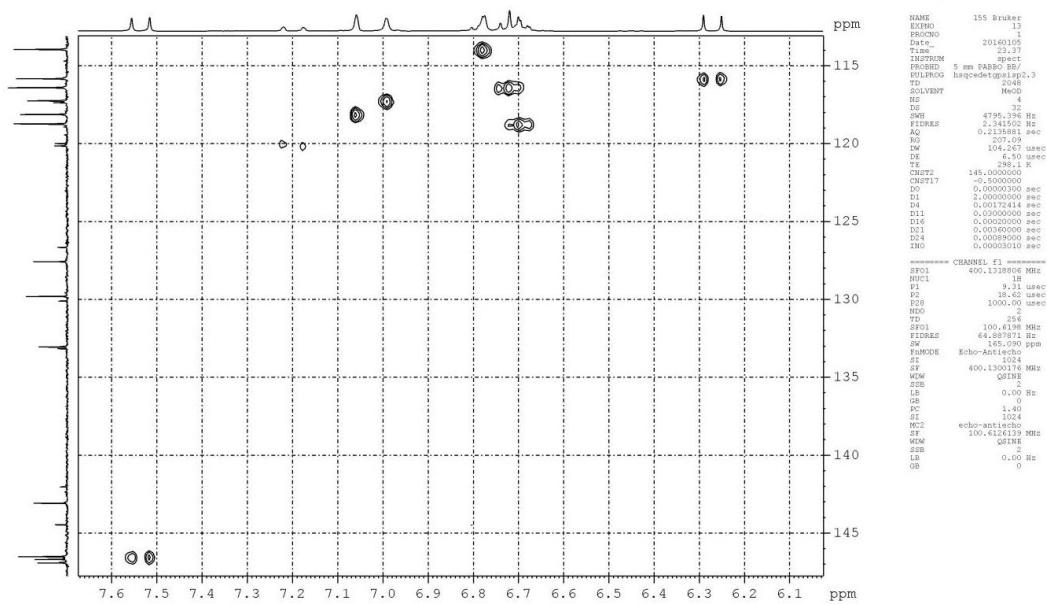


**Figure S3:**  $^{13}\text{C}$  NMR spectrum of **1** in Acetone- $d_4$  (100 MHz)

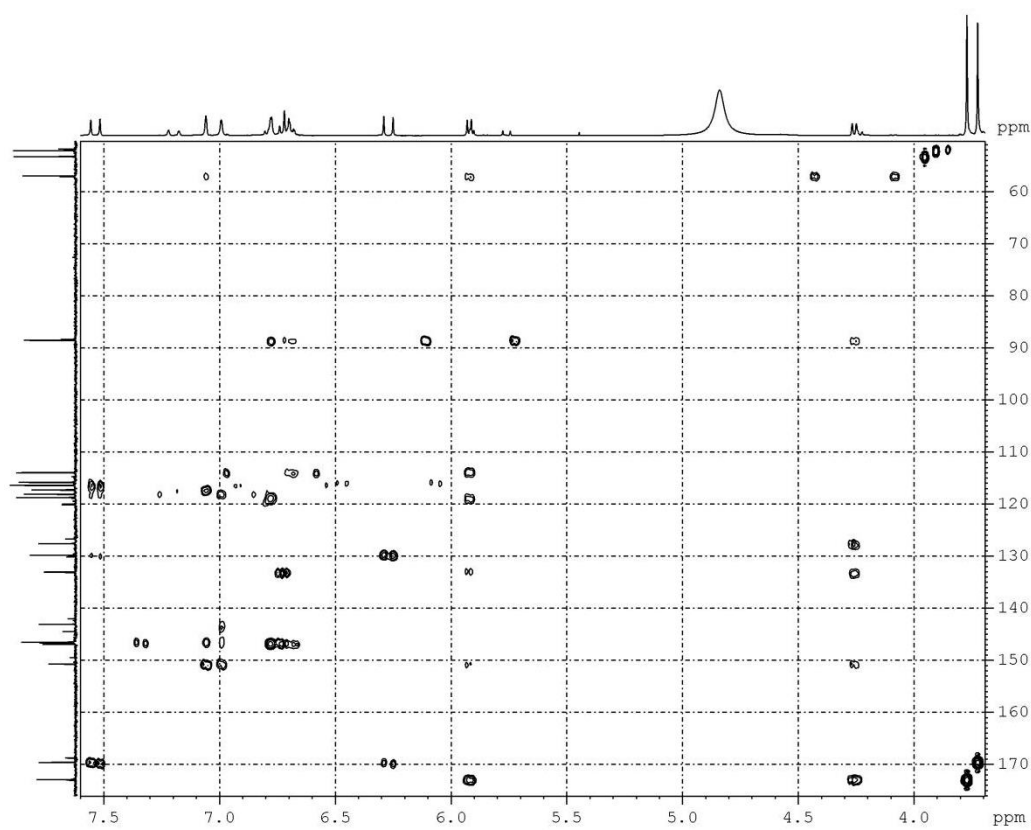


**Figure S4:** HSQC spectrum of **1** in  $\text{CD}_3\text{OD}$

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**Figure S5:** Selected HSQC spectrum of **1** in CD<sub>3</sub>OD



**Figure S6:** HMBC spectrum of **1** in CD<sub>3</sub>OD

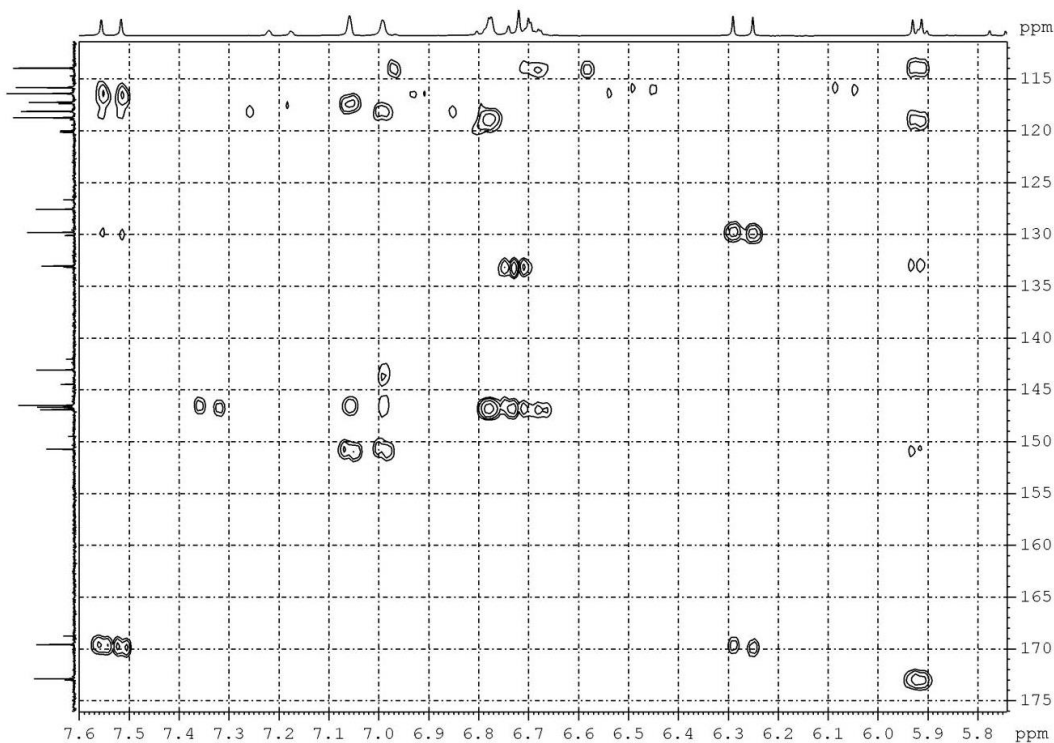


Figure S7: Selected HMBC spectrum of **1** in CD<sub>3</sub>OD

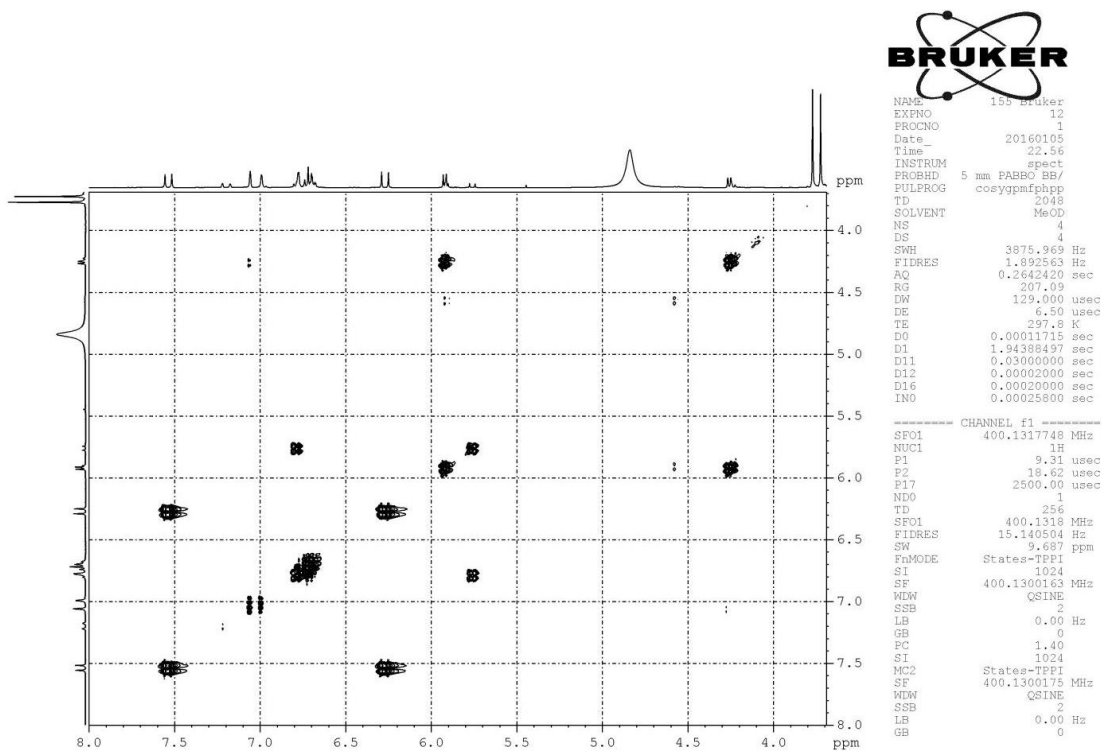
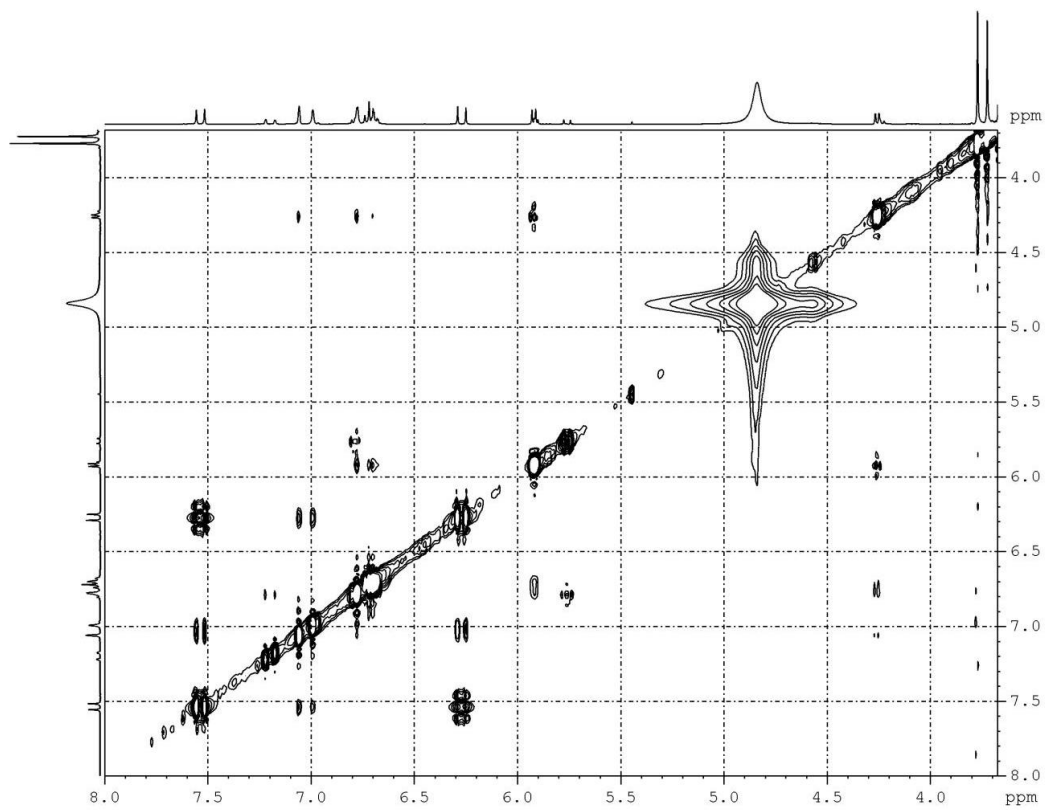
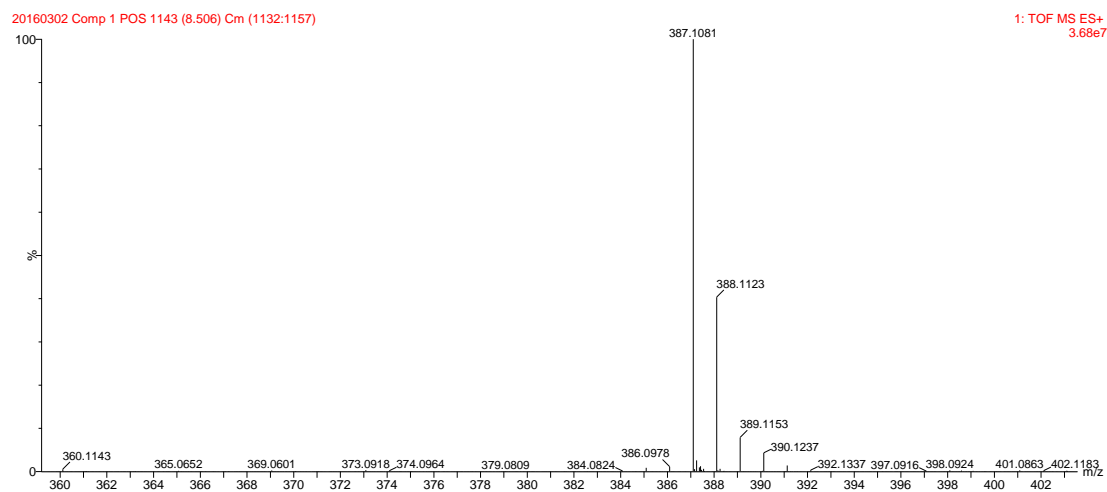


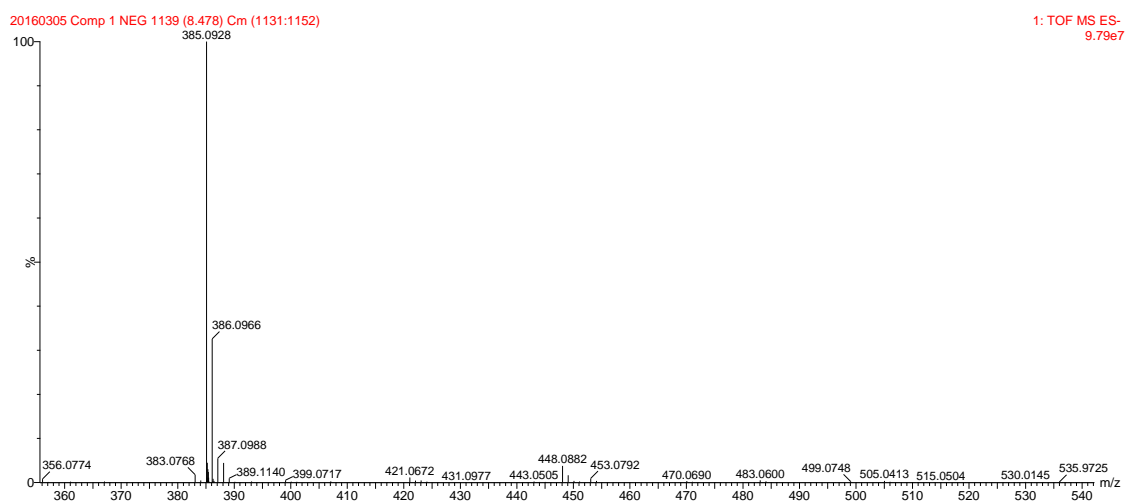
Figure S8: <sup>1</sup>H-<sup>1</sup>H COSY spectrum of **1** in CD<sub>3</sub>OD



**Figure S9:** NOE spectrum of **1** in CD<sub>3</sub>OD

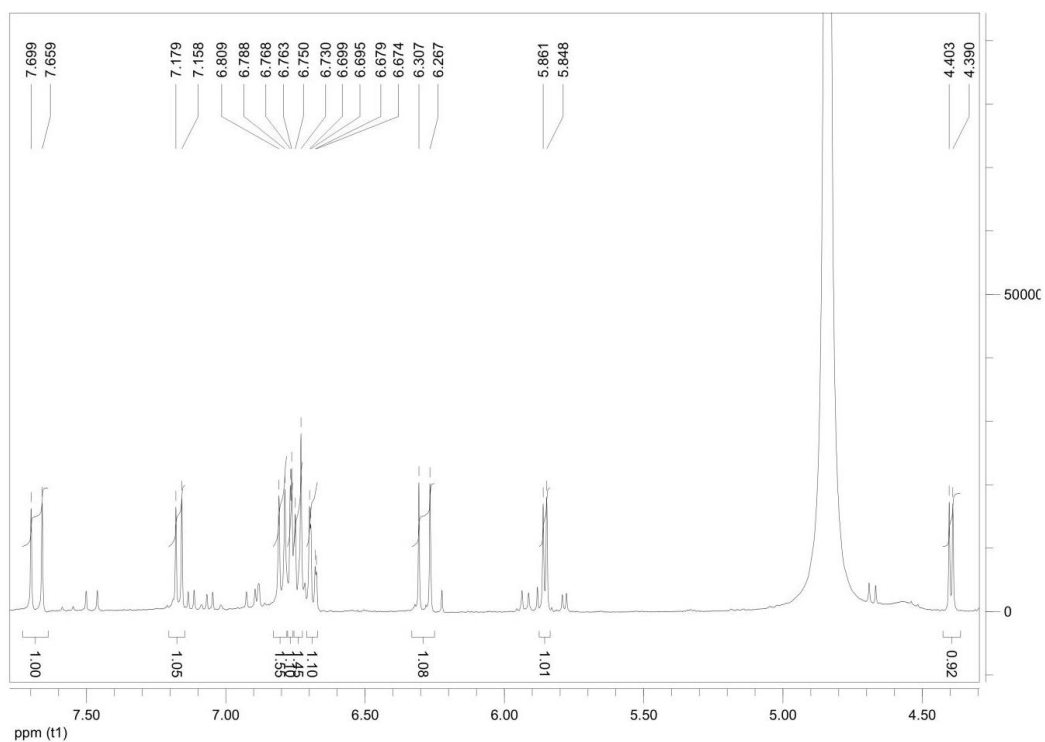


**Figure S10: HRMS spectrum of 1 (POS)**

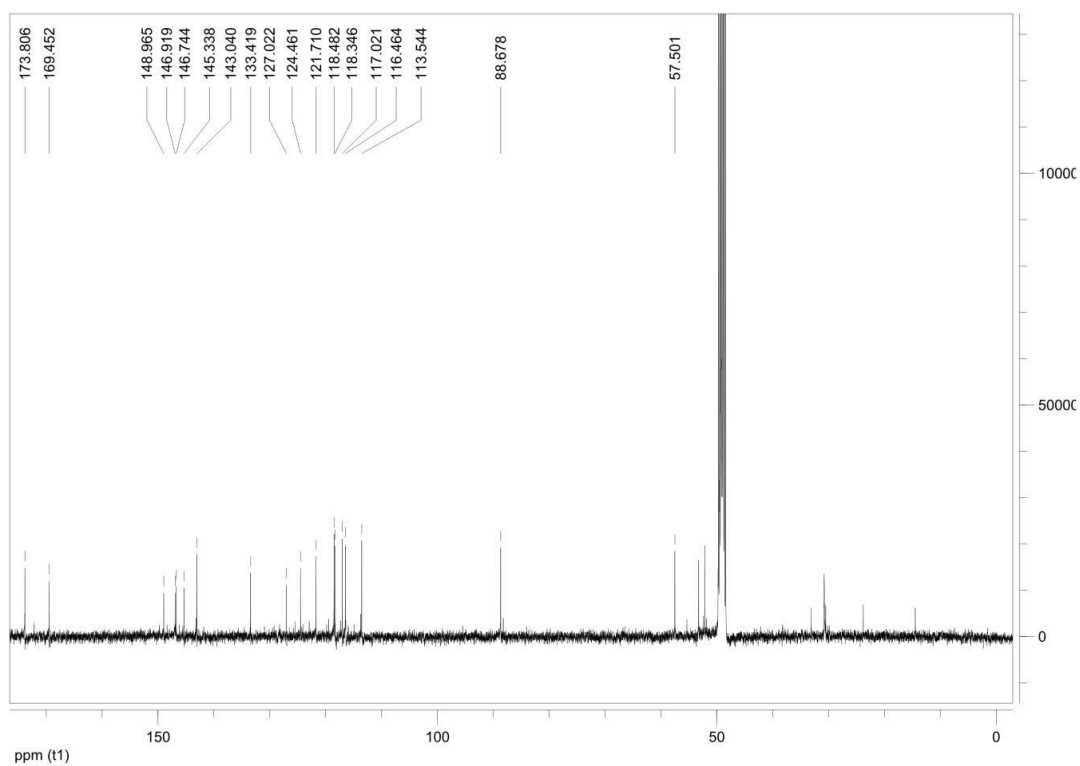


**Figure S11: HRMS spectrum of 1 (NEG)**

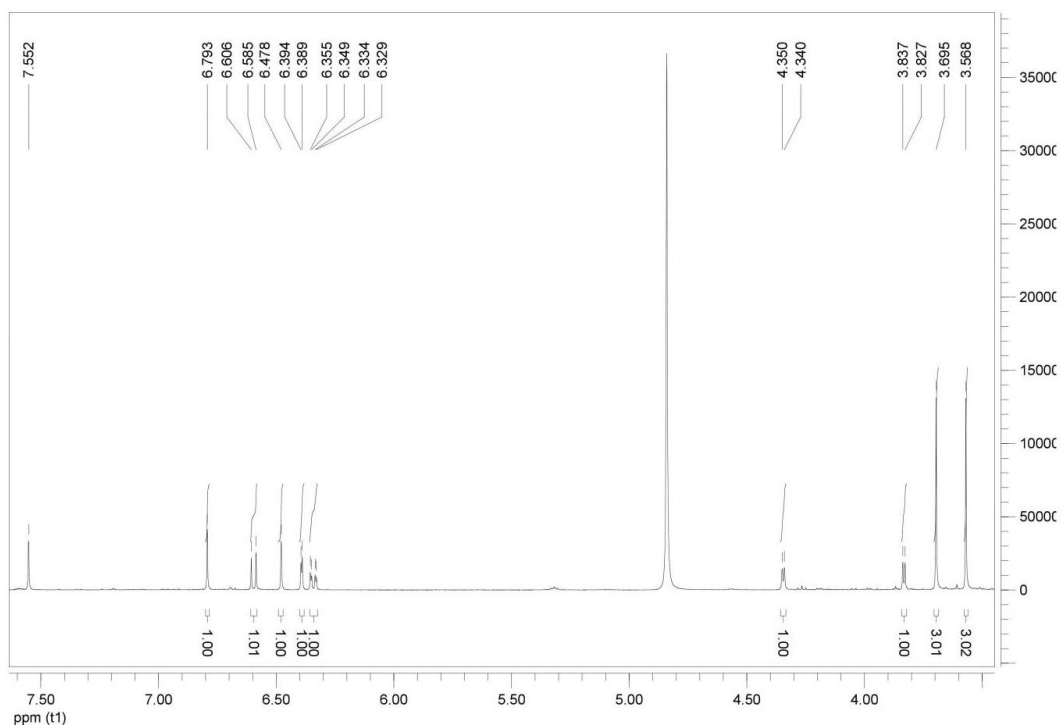




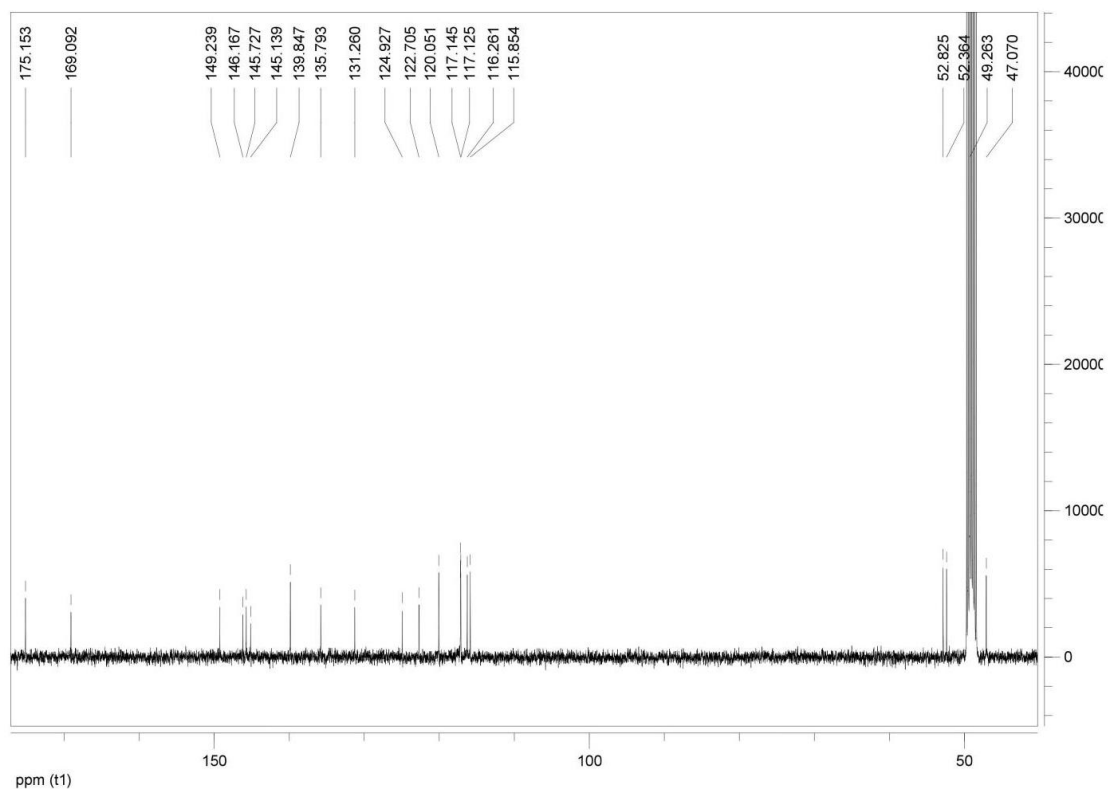
**Figure S12:**  $^1\text{H}$  NMR spectrum of **2** in  $\text{CD}_3\text{OD}$  (400 MHz)



**Figure S13:**  $^{13}\text{C}$  NMR spectrum of **2** in  $\text{CD}_3\text{OD}$  (100 MHz)



**Figure S14:**  $^1\text{H}$  NMR spectrum of **3** in  $\text{CD}_3\text{OD}$  (400 MHz)



**Figure S15:**  $^{13}\text{C}$  NMR spectrum of **3** in  $\text{CD}_3\text{OD}$  (100 MHz)

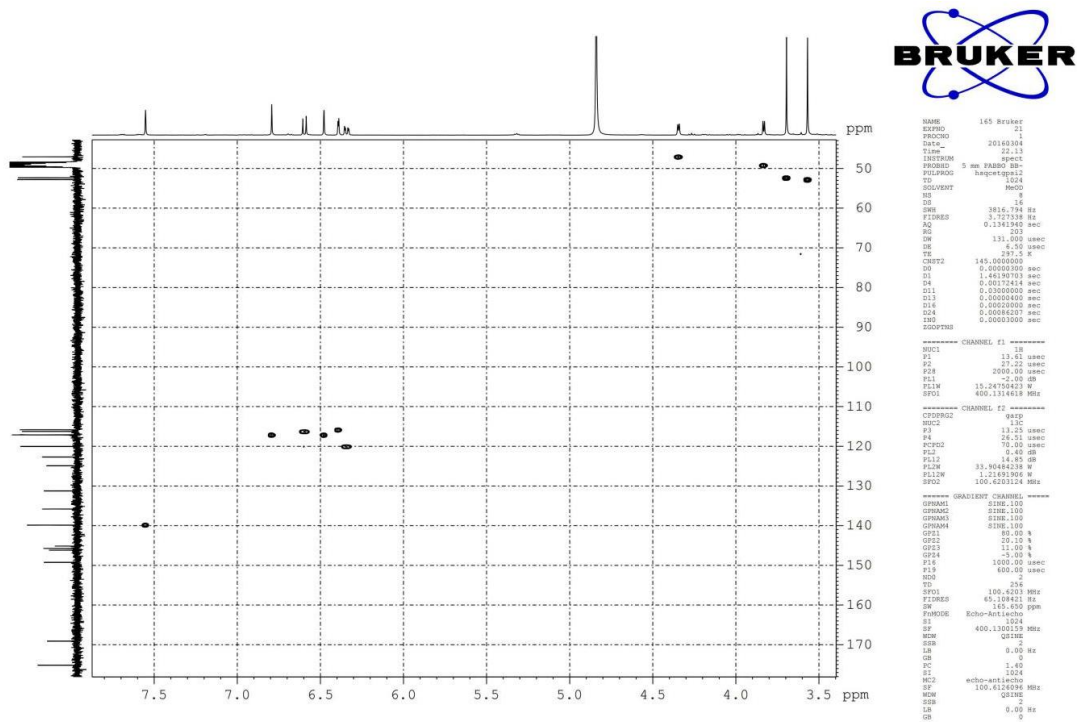


Figure S16: HSQC spectrum of **3** in CD<sub>3</sub>OD

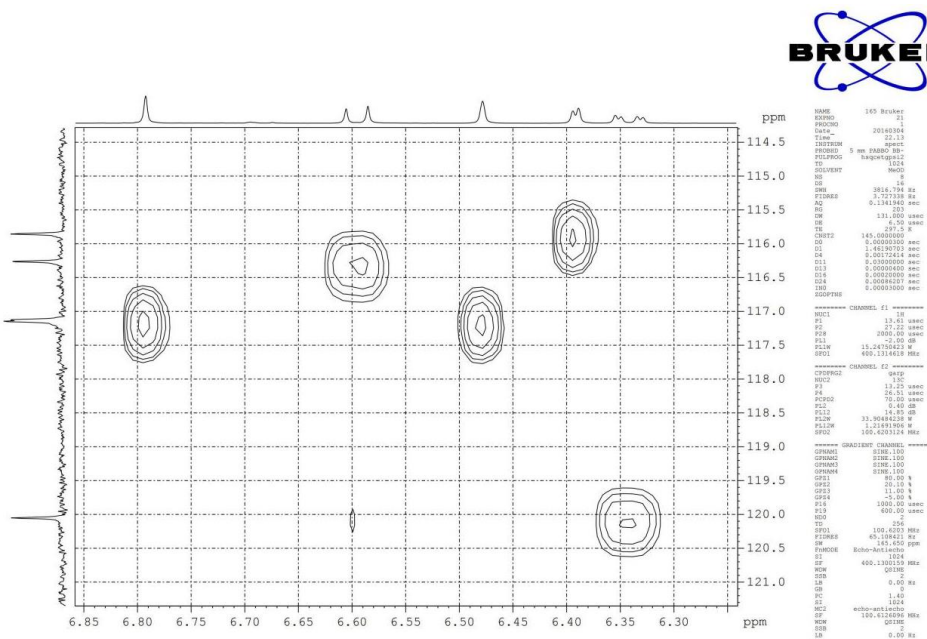
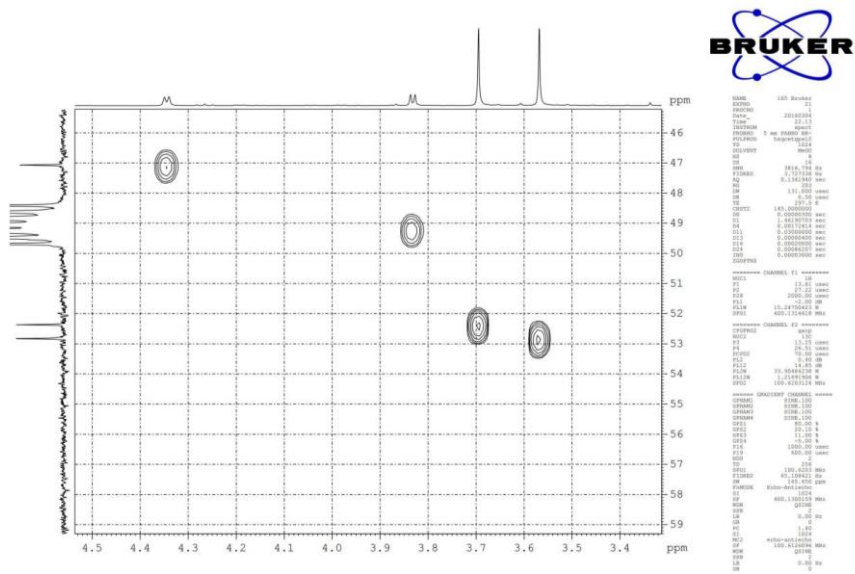
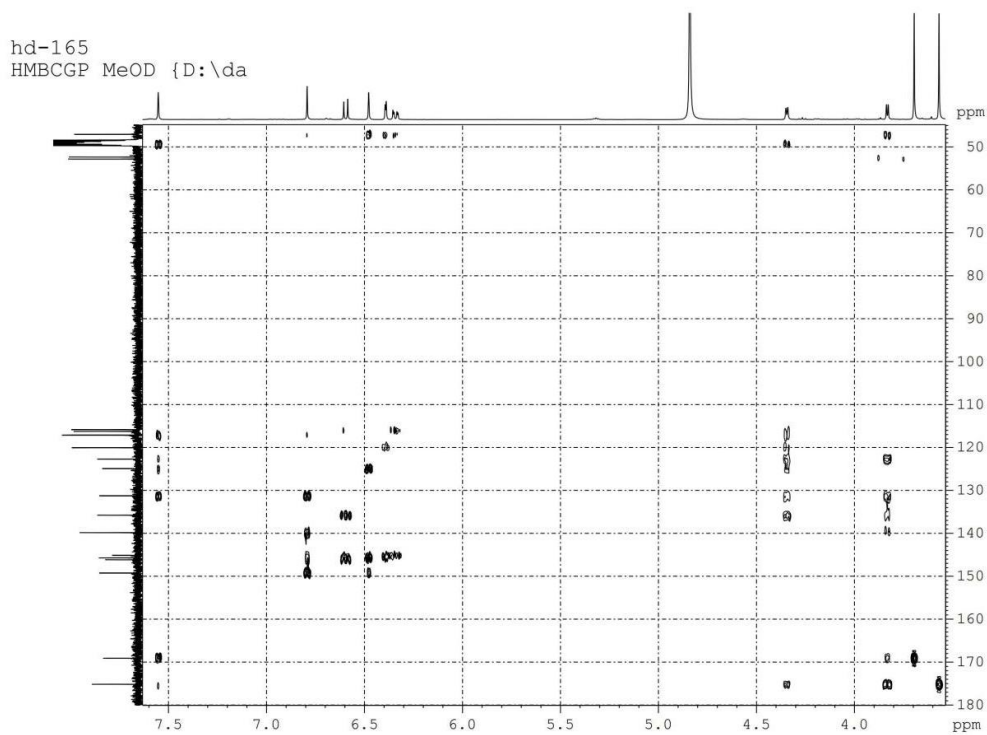


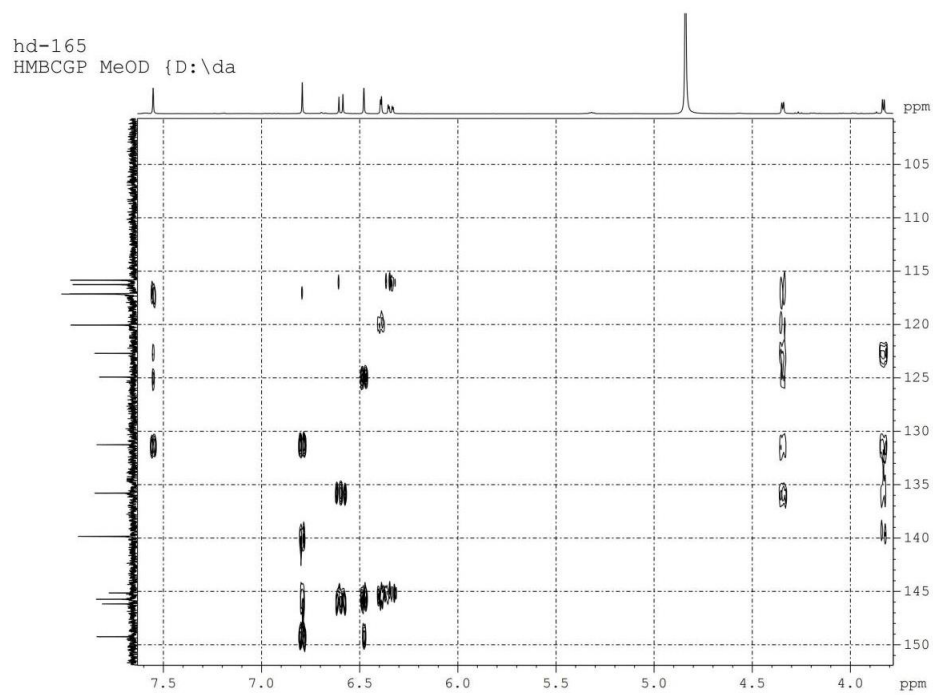
Figure S17: Selected HSQC spectrum of **3** in CD<sub>3</sub>OD (1)



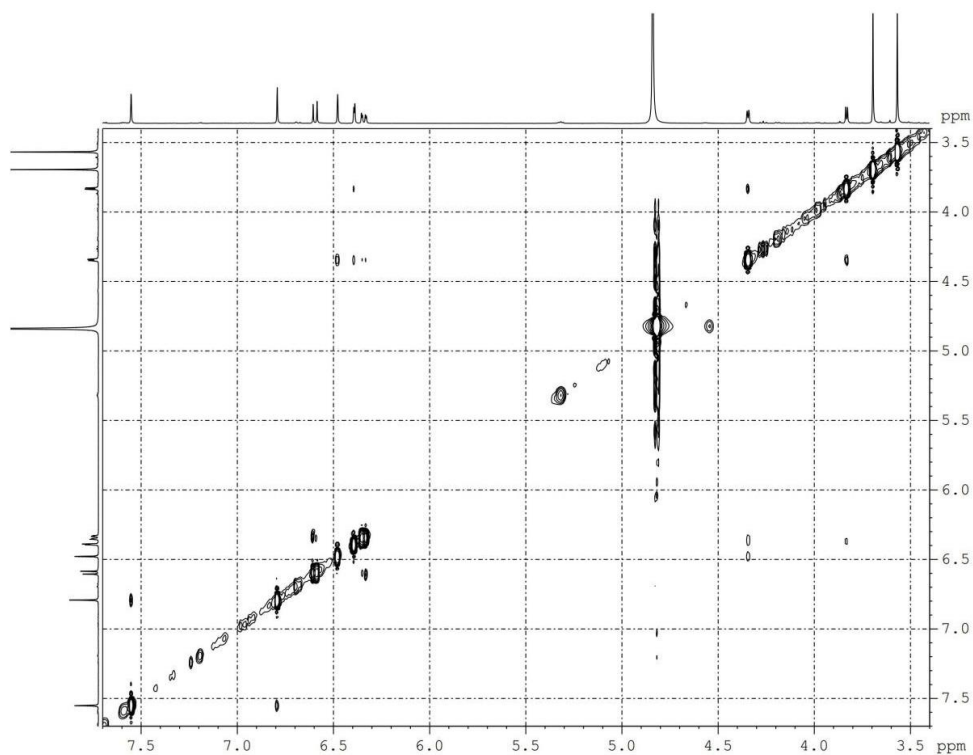
**Figure S18:** Selected HSQC spectrum of **3** in CD<sub>3</sub>OD (2)



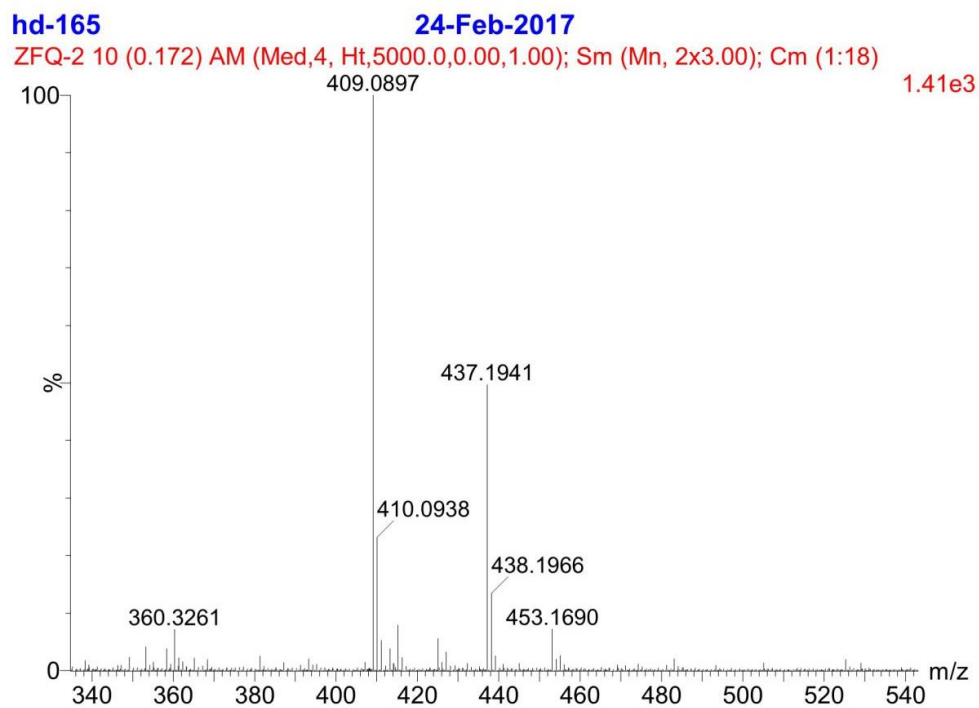
**Figure S19:** HMBC spectrum of **3** in CD<sub>3</sub>OD



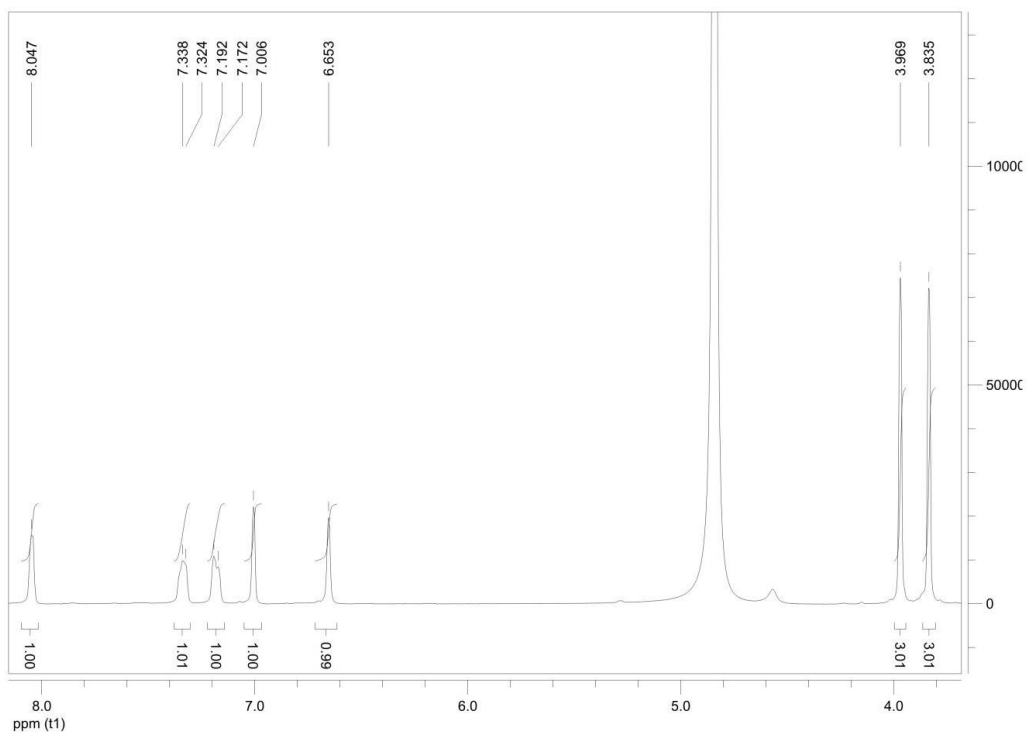
**Figure S20:** Selected HMBC spectrum of **3** in CD<sub>3</sub>OD



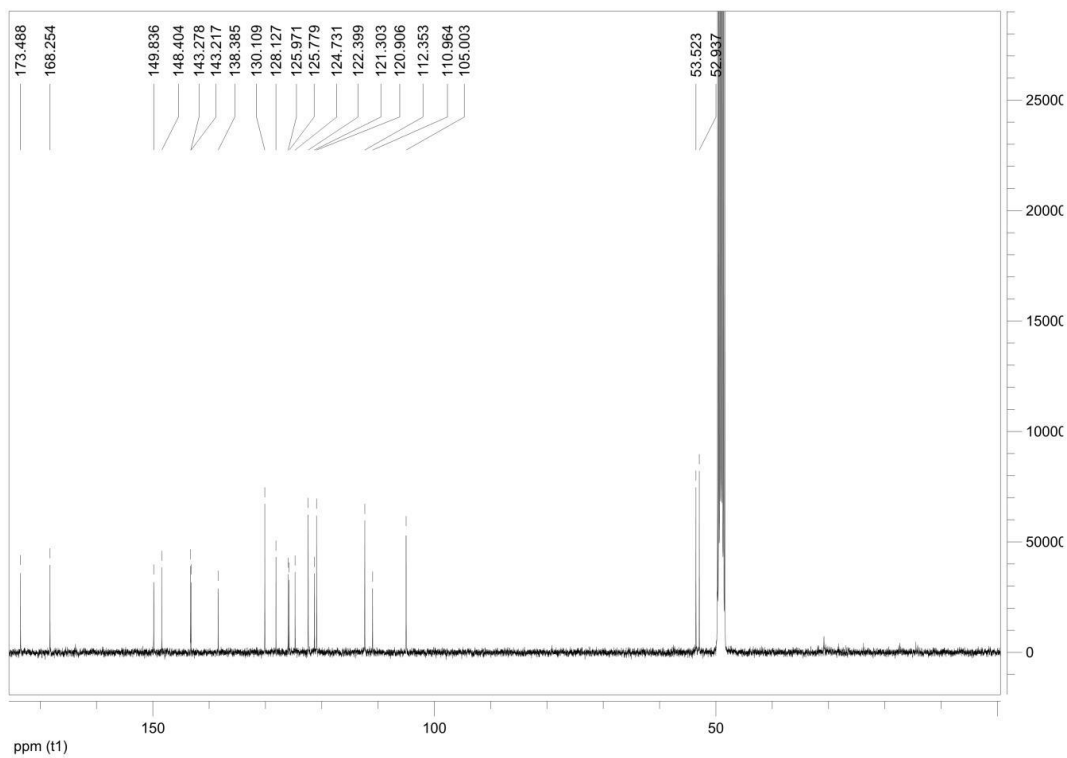
**Figure S21:** NOE spectrum of **3** in CD<sub>3</sub>OD



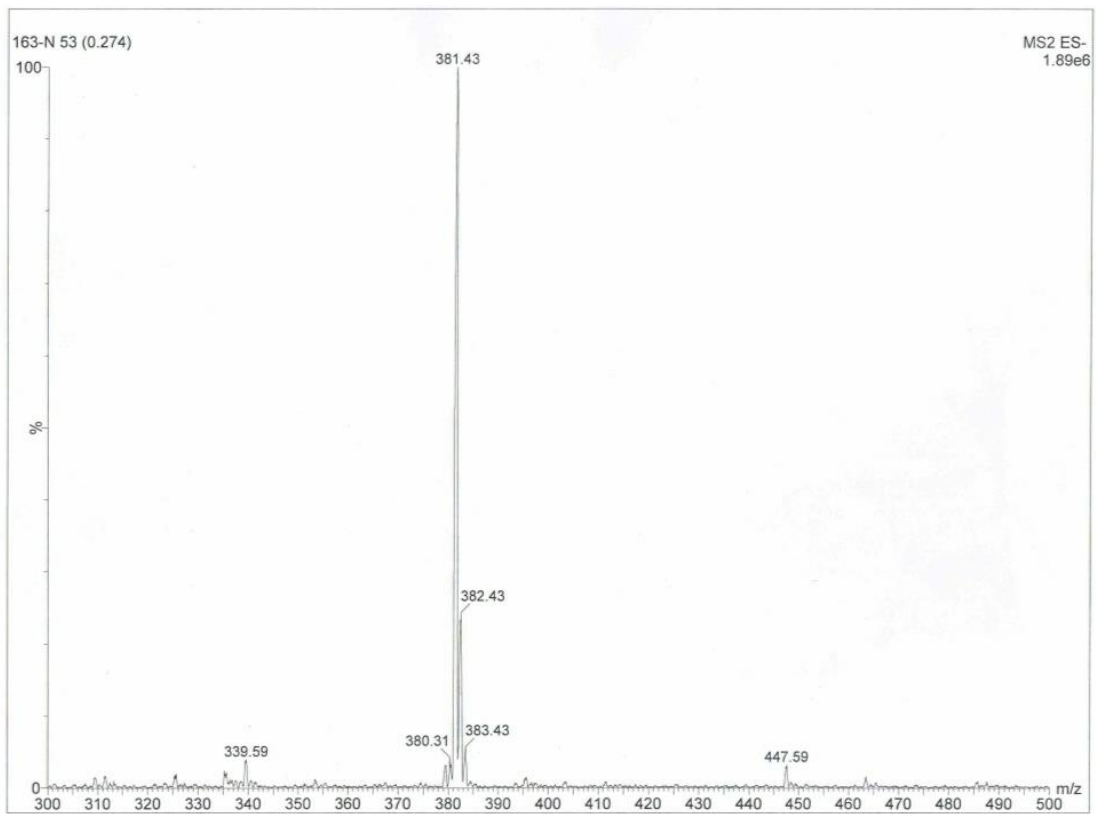
**Figure S22:** HRMS spectrum of **3**



**Figure S23:**  $^1\text{H}$  NMR spectrum of **4** in  $\text{CD}_3\text{OD}$  (100 MHz)

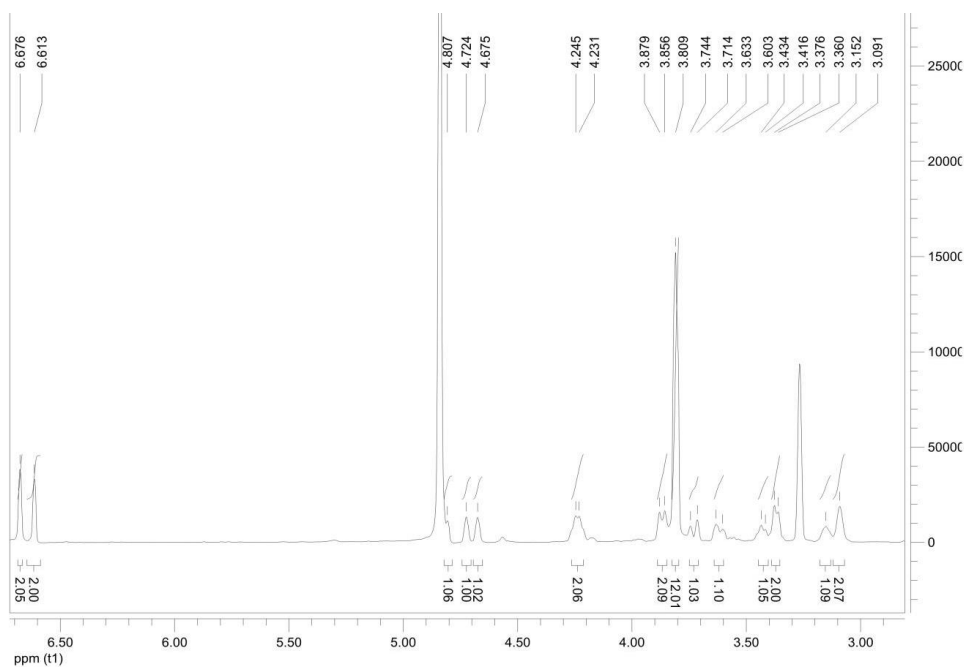


**Figure S24:**  $^{13}\text{C}$  NMR spectrum of **4** in  $\text{CD}_3\text{OD}$  (100 MHz)

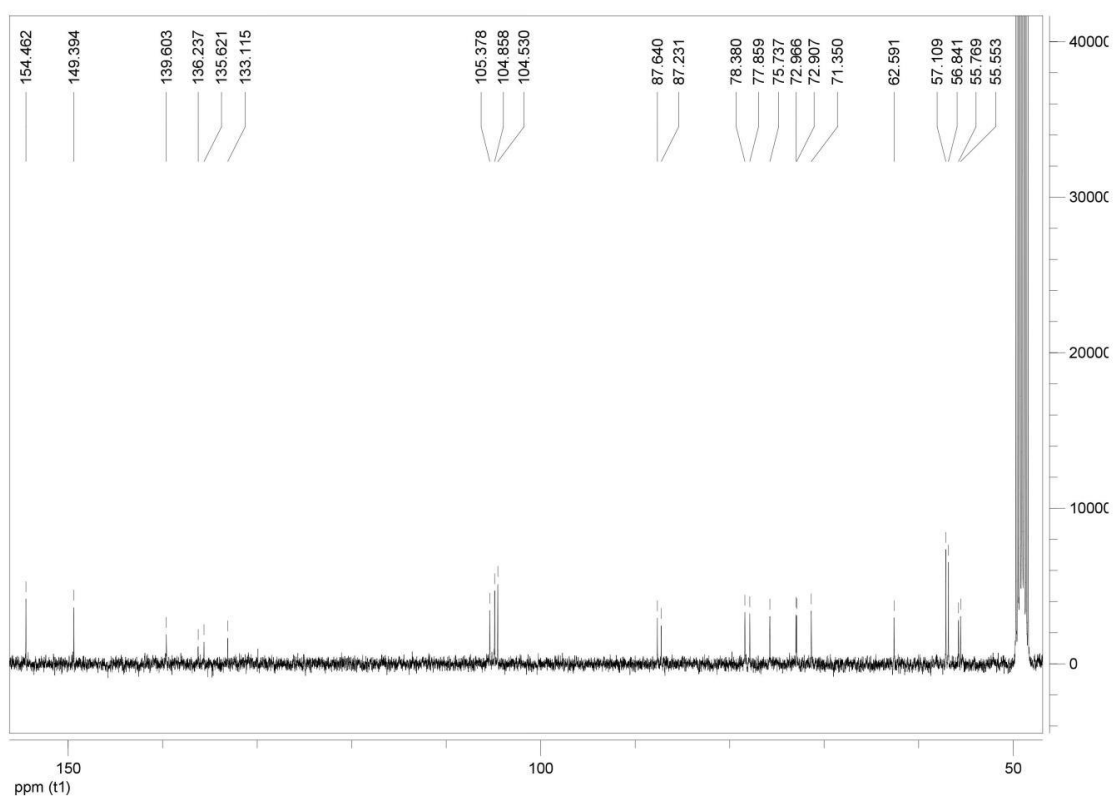


**Figure S25:** MS spectrum of **4**

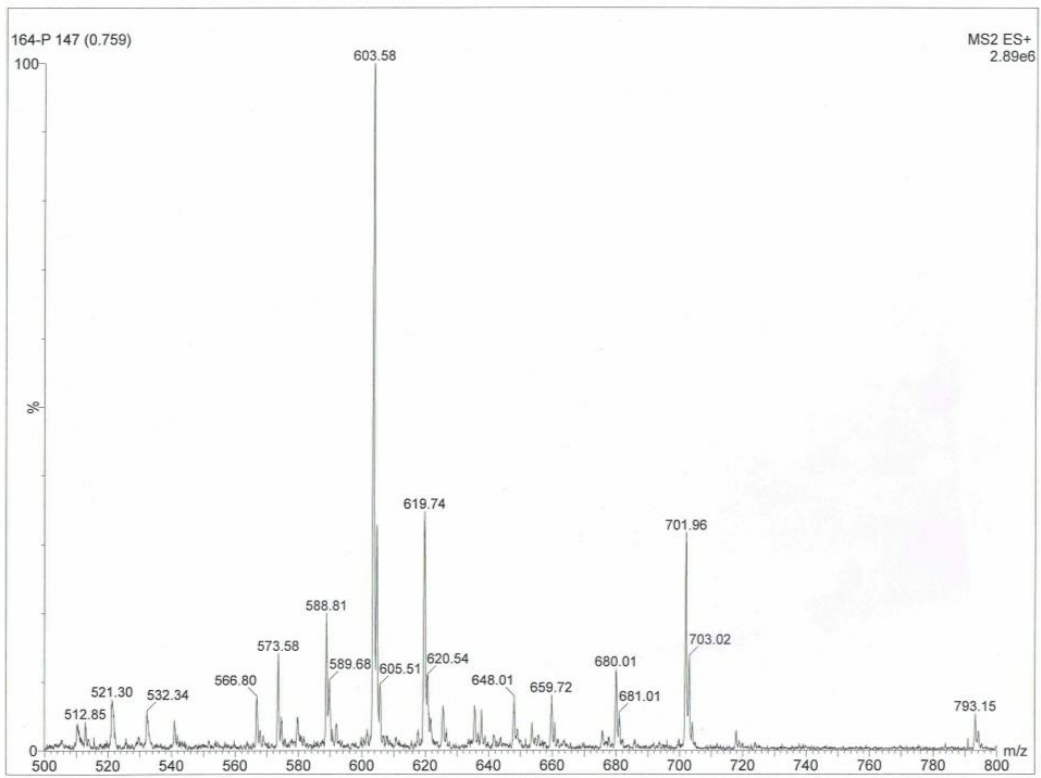




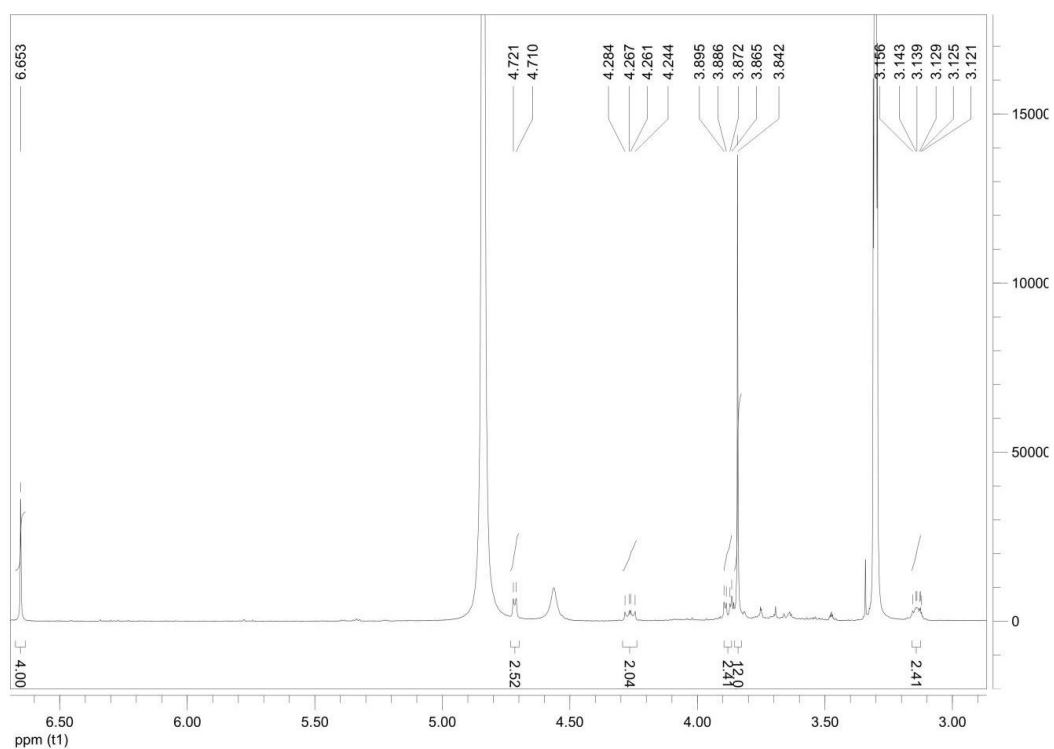
**Figure S26:**  $^1\text{H}$  NMR spectrum of **5** in  $\text{CD}_3\text{OD}$  (400 MHz)



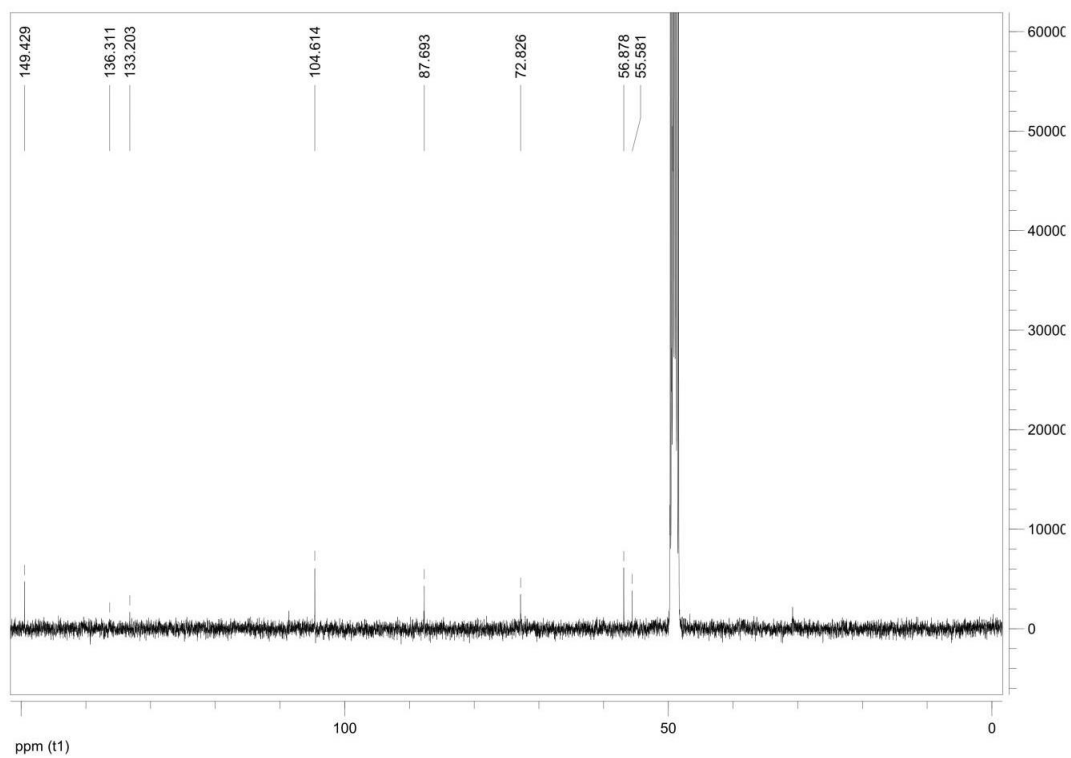
**Figure S27:**  $^{13}\text{C}$  NMR spectrum of **5** in  $\text{CD}_3\text{OD}$  (100 MHz)



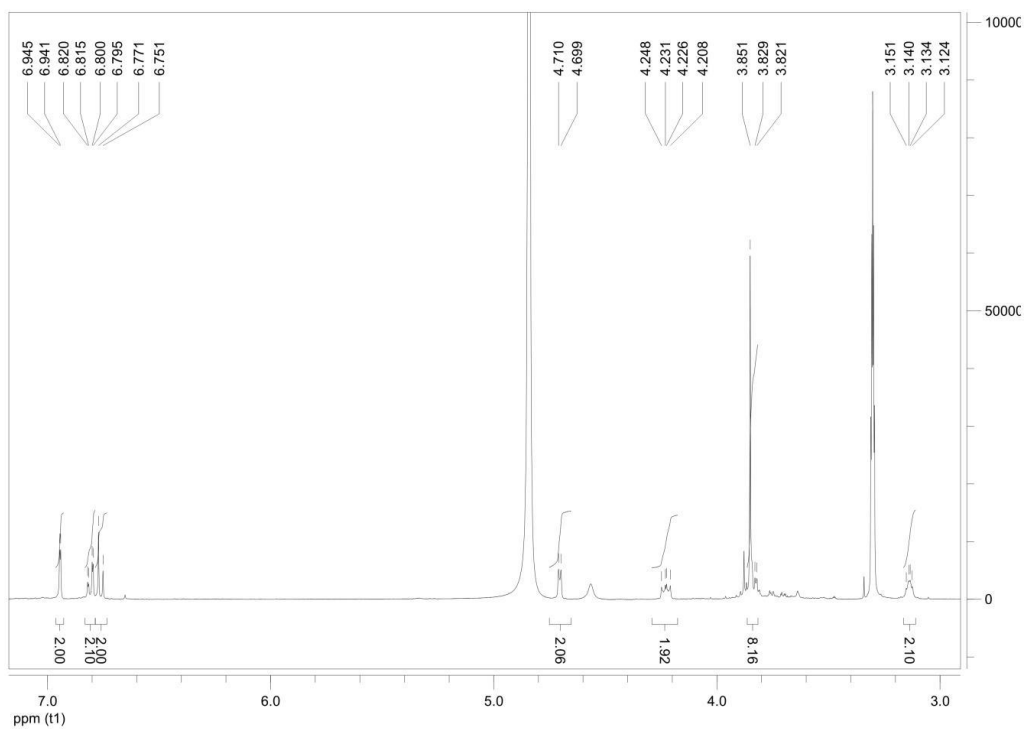
**Figure S28:** MS spectrum of **5**



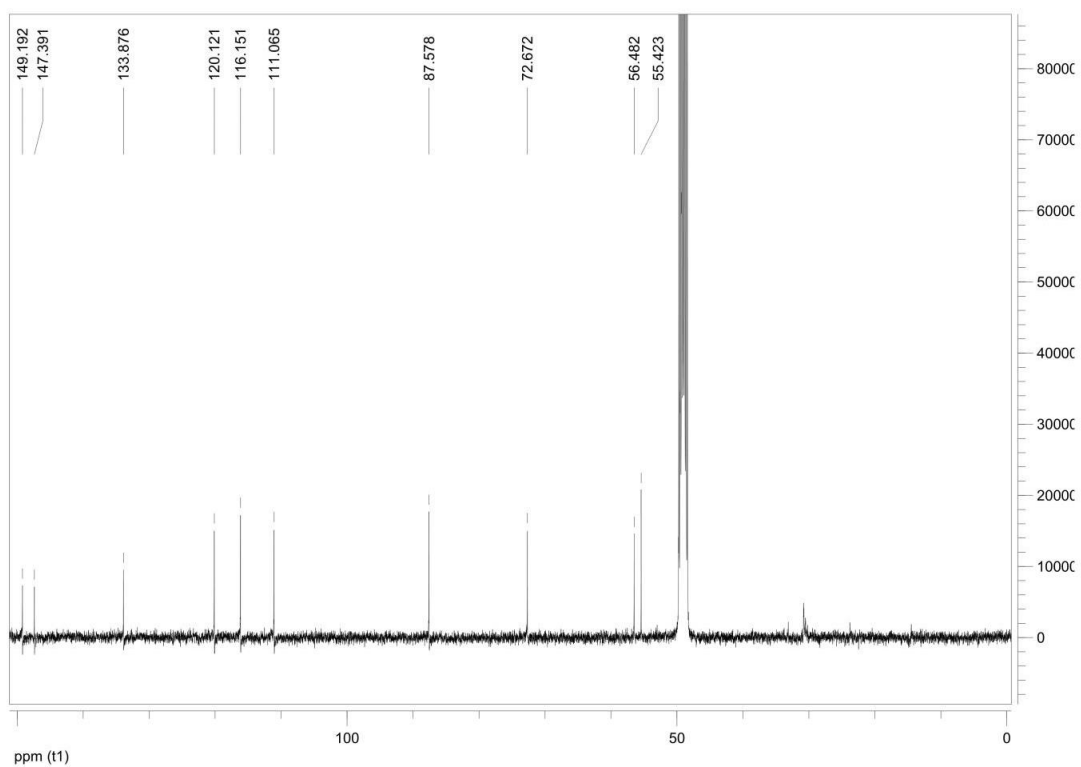
**Figure S29:**  $^1\text{H}$  NMR spectrum of **6** in  $\text{CD}_3\text{OD}$  (400 MHz)



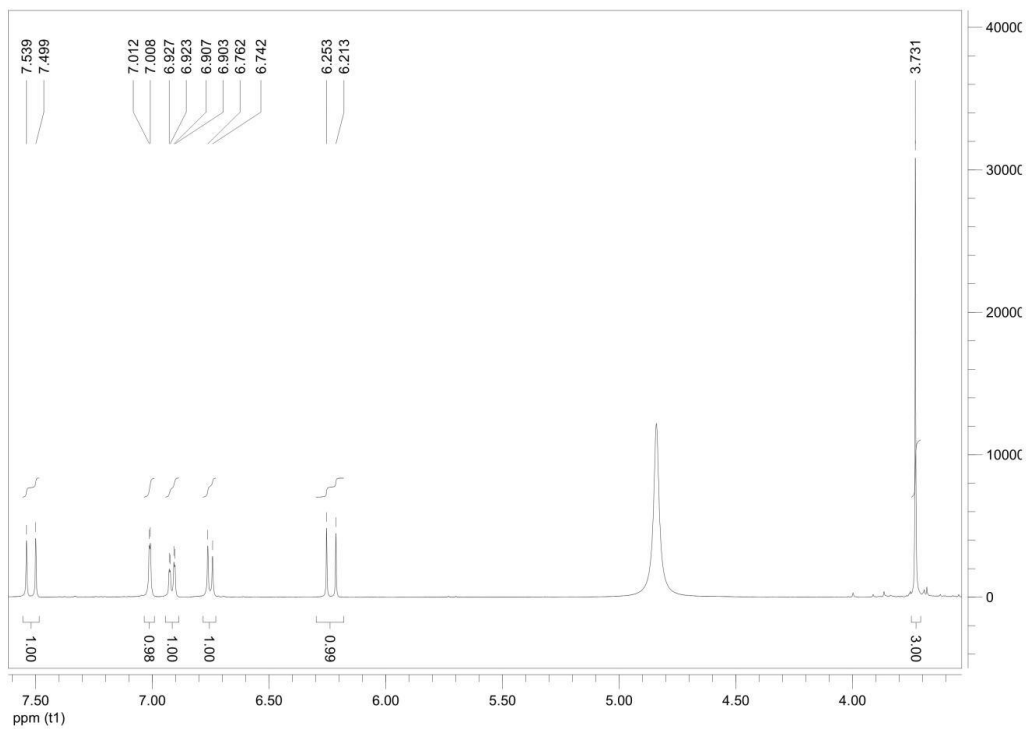
**Figure S30:**  $^{13}\text{C}$  NMR spectrum of **6** in  $\text{CD}_3\text{OD}$  (100 MHz)



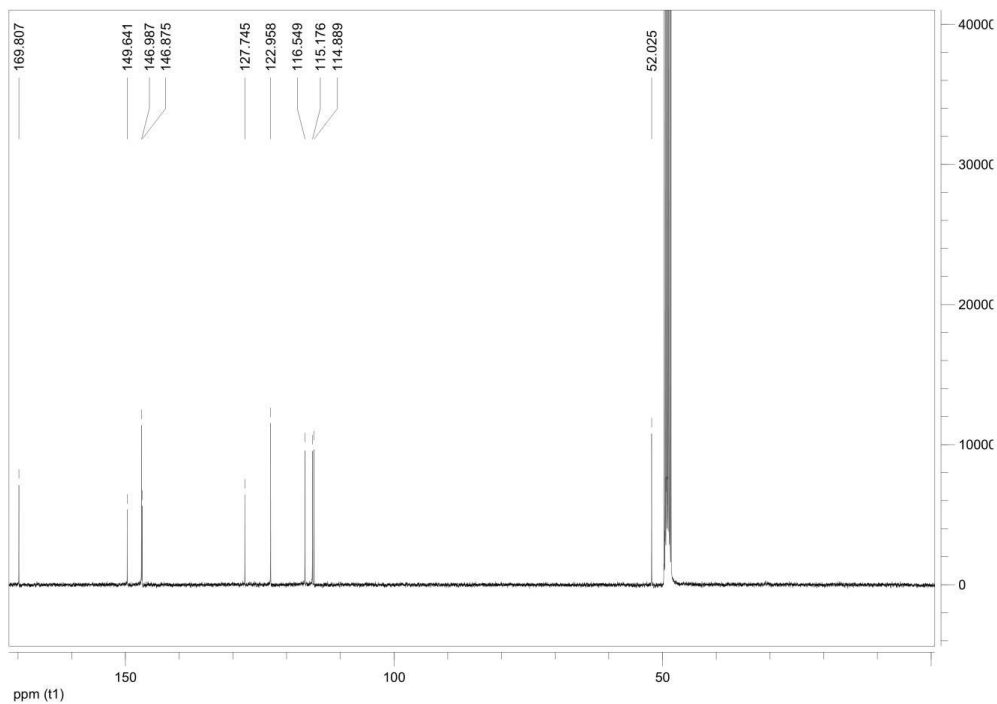
**Figure S31:**  $^1\text{H}$  NMR spectrum of **7** in  $\text{CD}_3\text{OD}$  (400 MHz)



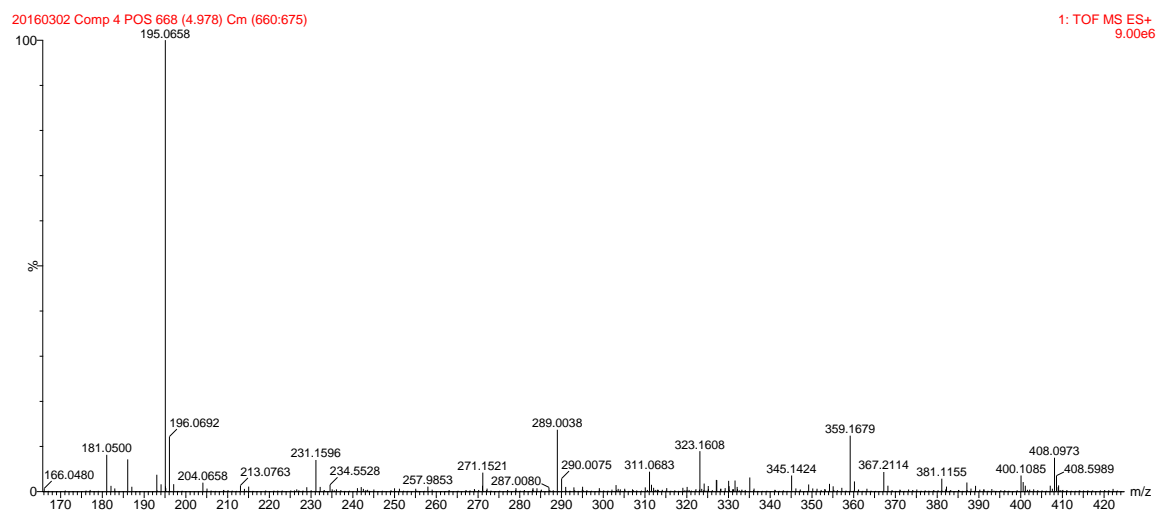
**Figure S32:**  $^{13}\text{C}$  NMR spectrum of **7** in  $\text{CD}_3\text{OD}$  (100 MHz)



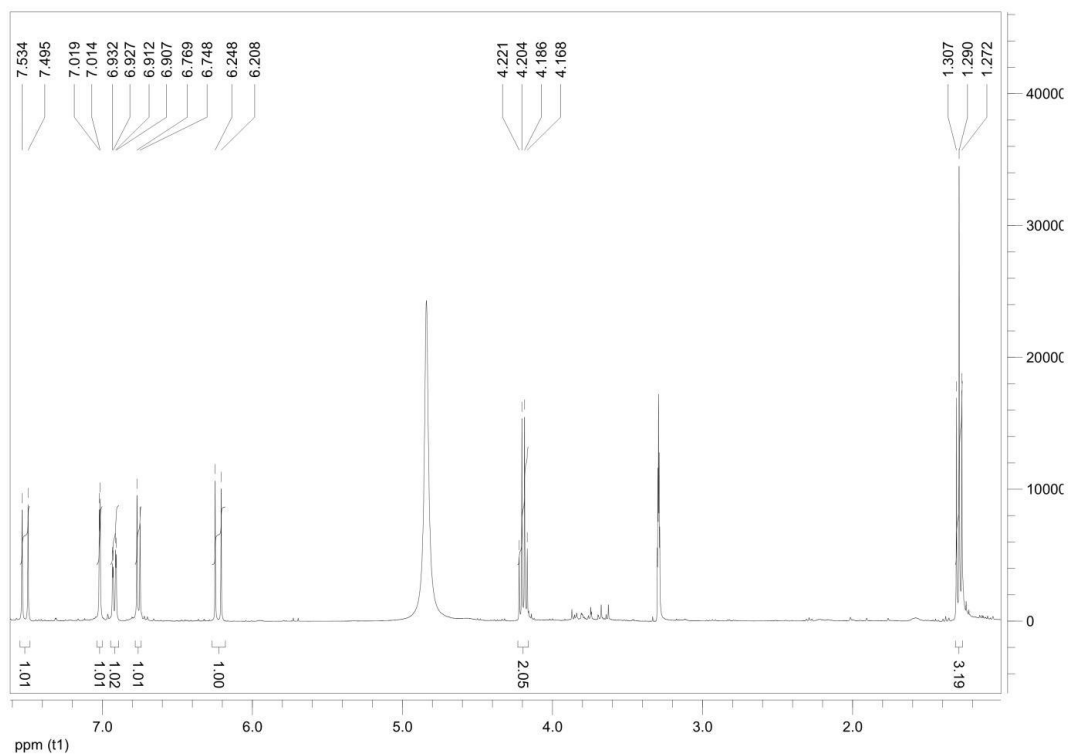
**Figure S33:**  $^1\text{H}$  NMR spectrum of **8** in  $\text{CD}_3\text{OD}$  (400 MHz)



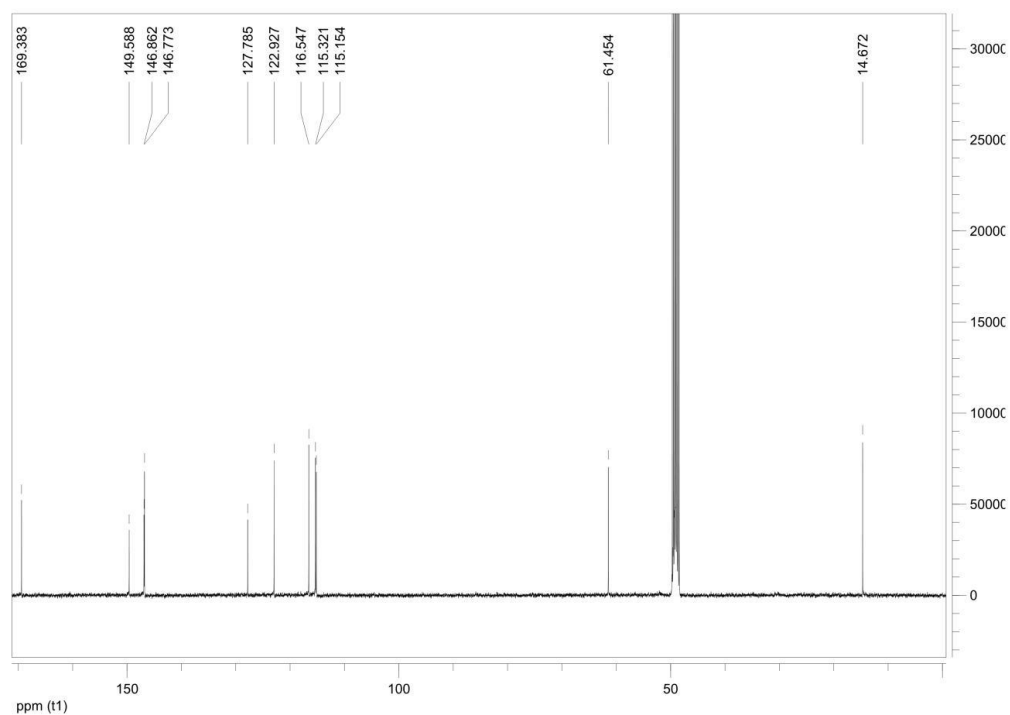
**Figure S34:**  $^{13}\text{C}$  NMR spectrum of **8** in  $\text{CD}_3\text{OD}$  (100 MHz)



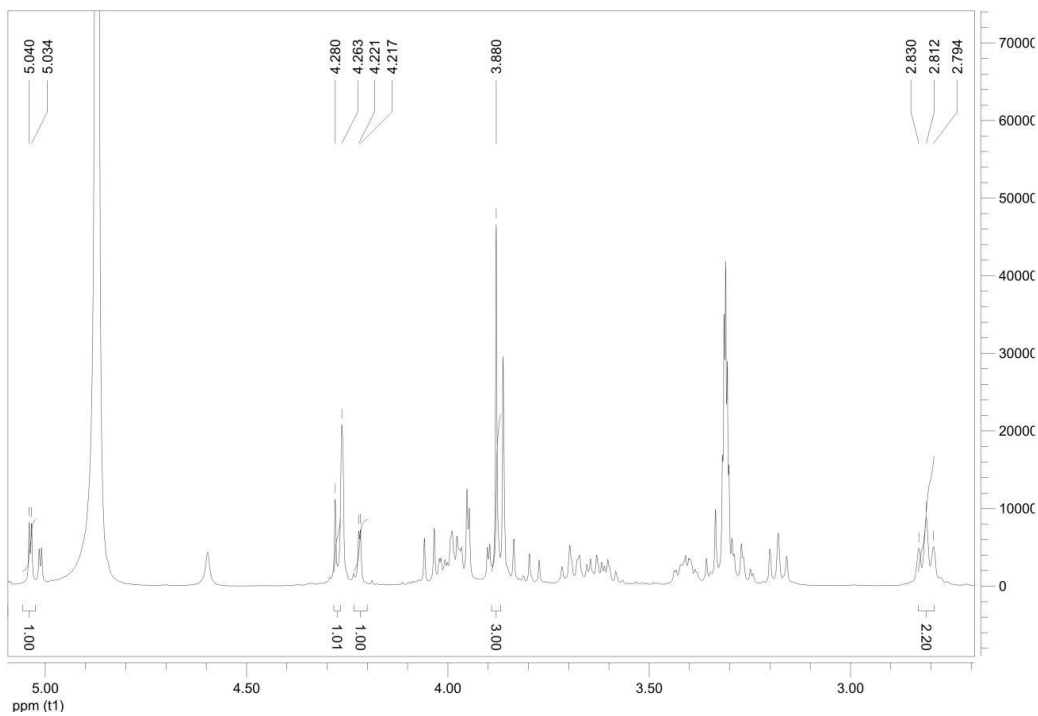
**Figure S35:** HRMS spectrum of **8**



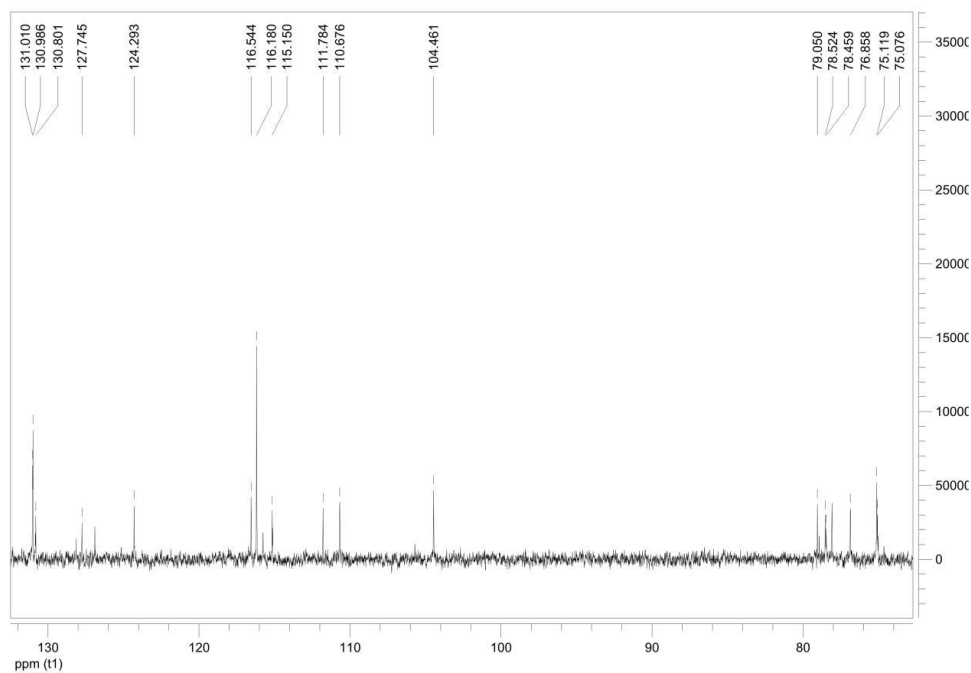
**Figure S36:**  $^1\text{H}$  NMR spectrum of **9** in  $\text{CD}_3\text{OD}$  (400 MHz)



**Figure S37:**  $^{13}\text{C}$  NMR spectrum of **9** in  $\text{CD}_3\text{OD}$  (100 MHz)

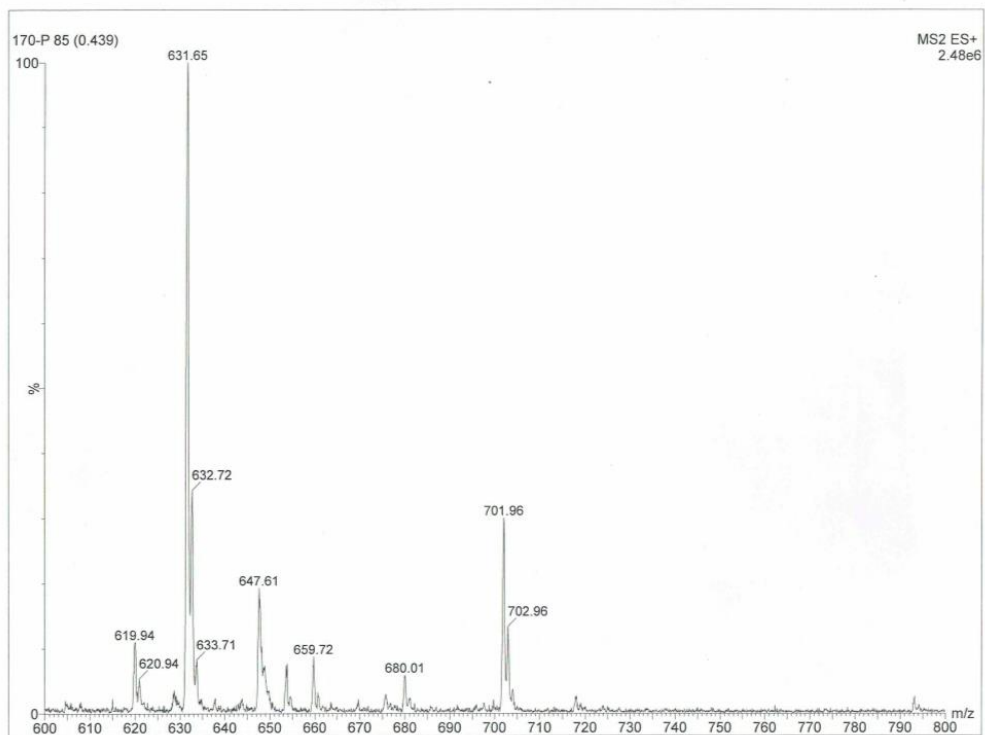


**Figure S38:**  $^1\text{H}$  NMR spectrum of **10** in  $\text{CD}_3\text{OD}$  (400 MHz)

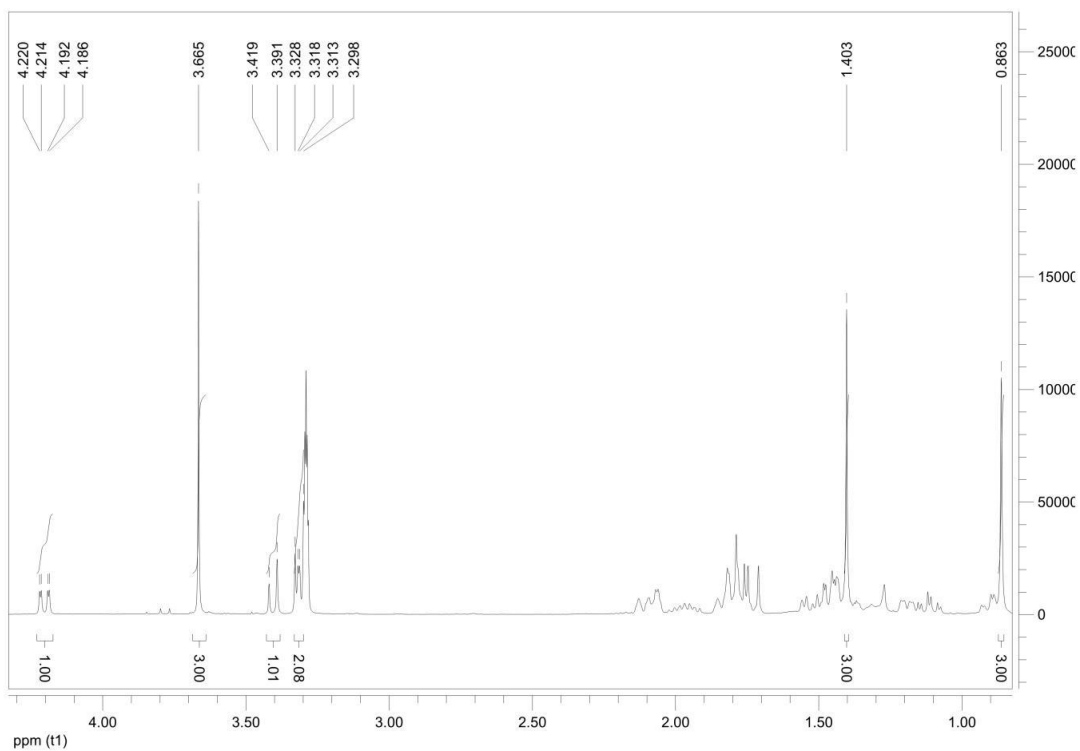


**Figure S39:**  $^{13}\text{C}$  NMR spectrum of **10** in  $\text{CD}_3\text{OD}$  (100 MHz)

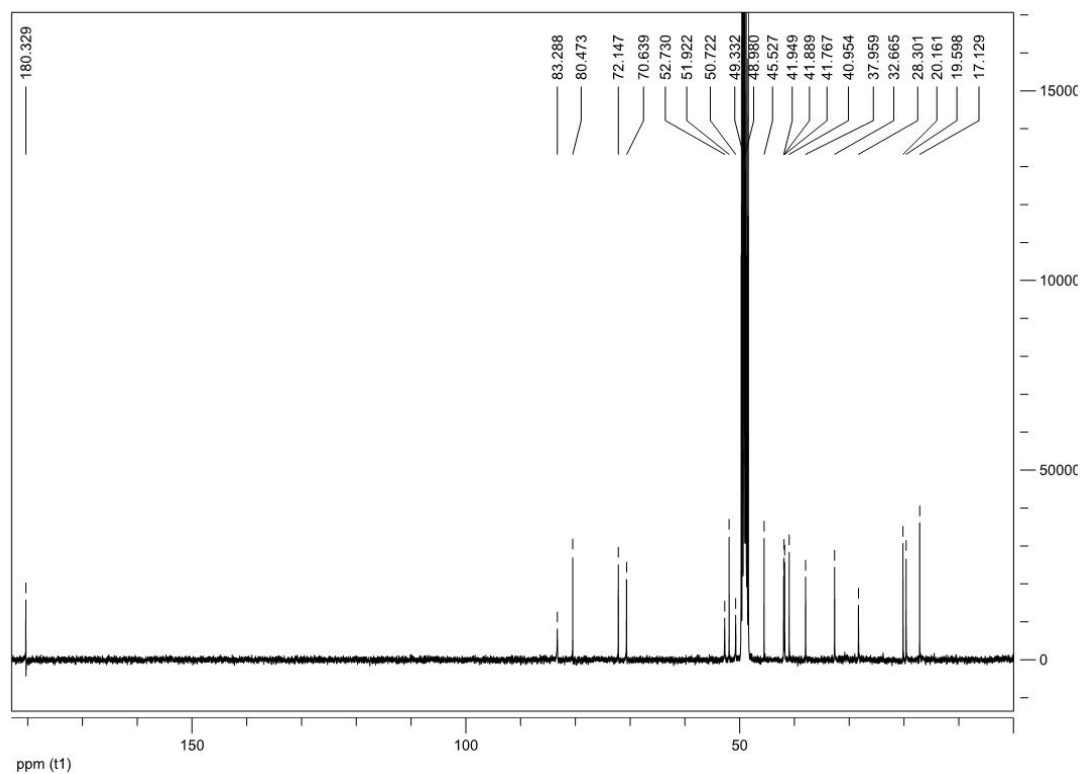




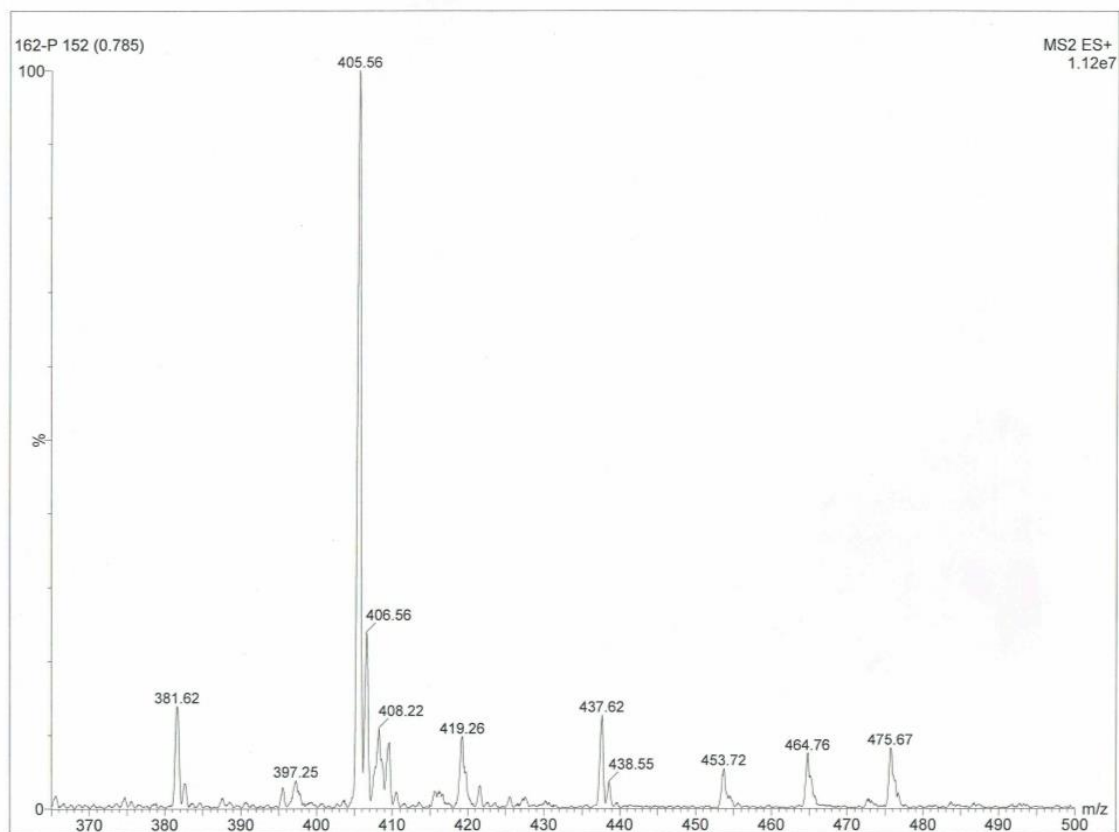
**Figure S40:** MS spectrum of **10**



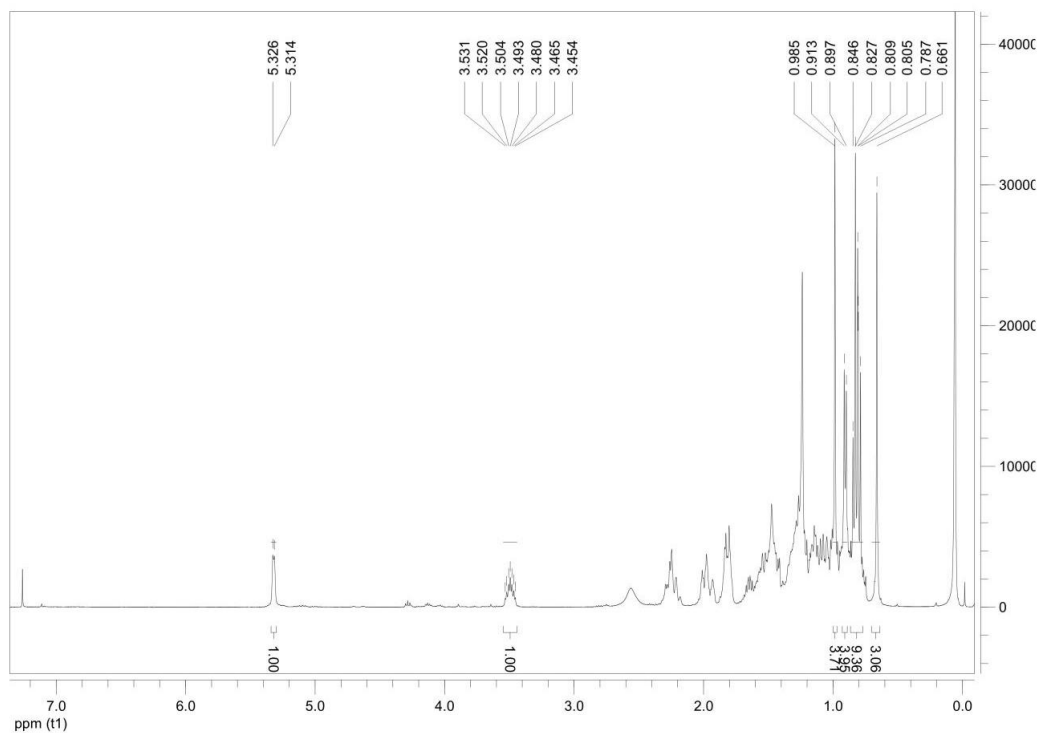
**Figure S41:**  $^1\text{H}$  NMR spectrum of **11** in  $\text{CD}_3\text{OD}$  (400 MHz)



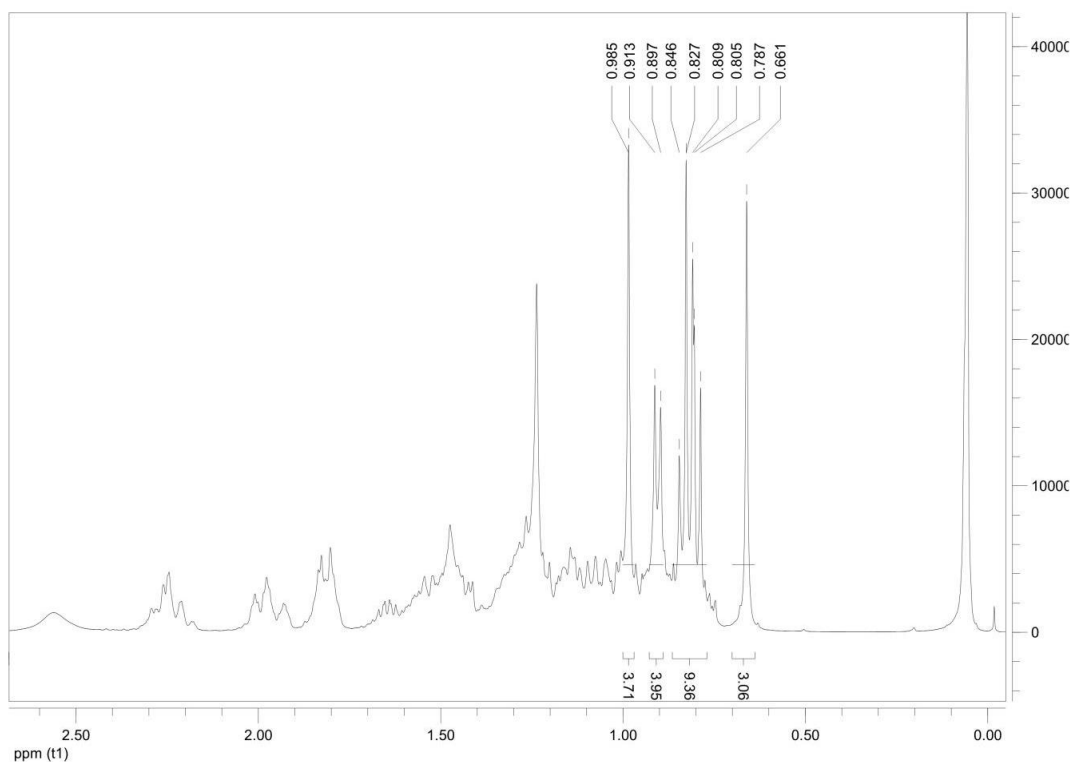
**Figure S42:**  $^{13}\text{C}$  NMR spectrum of **11** in  $\text{CD}_3\text{OD}$  (100 MHz)



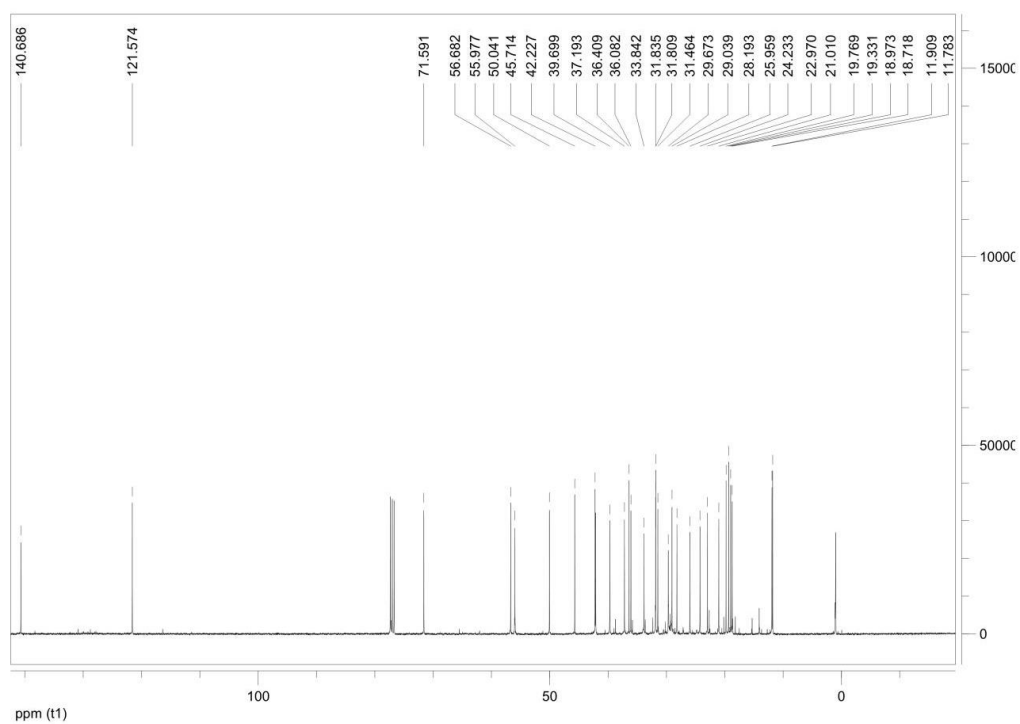
**Figure S43:** MS spectrum of **11**



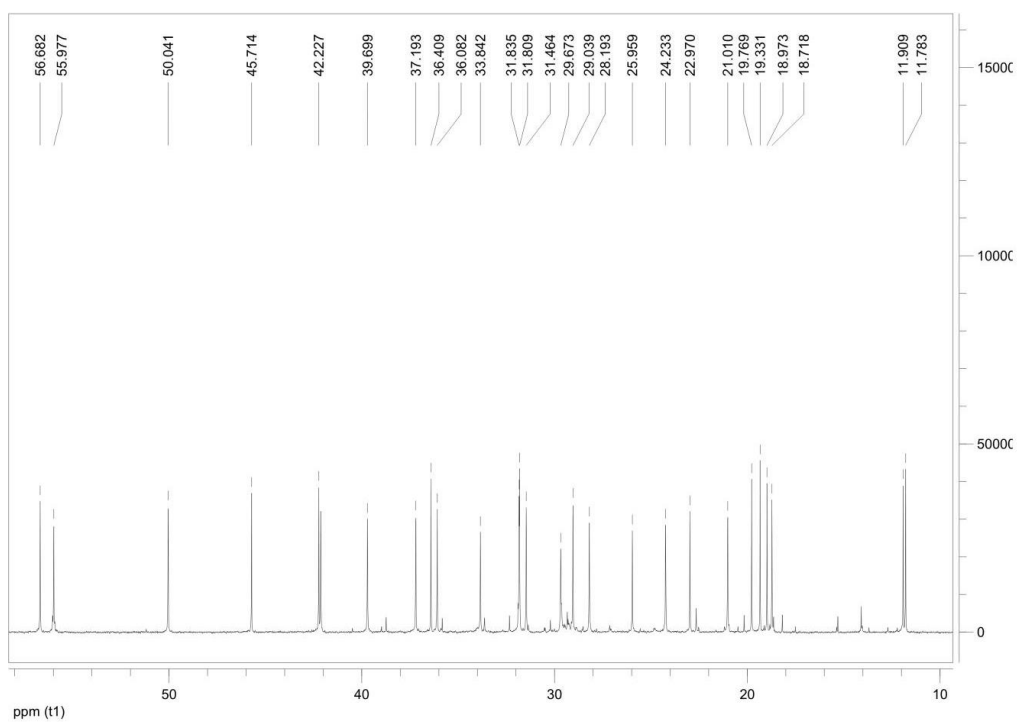
**Figure S44:**  $^1\text{H}$  NMR spectrum of **12** in  $\text{CDCl}_3$  (400 MHz)



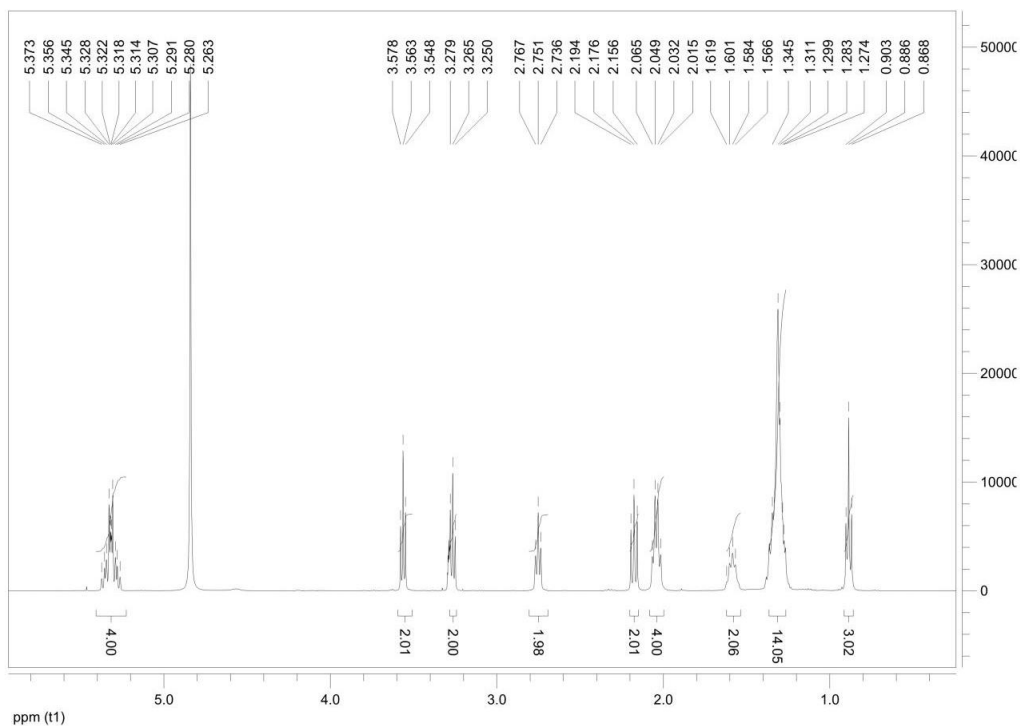
**Figure S45:** Selected  $^1\text{H}$  NMR spectrum of **12** in  $\text{CDCl}_3$



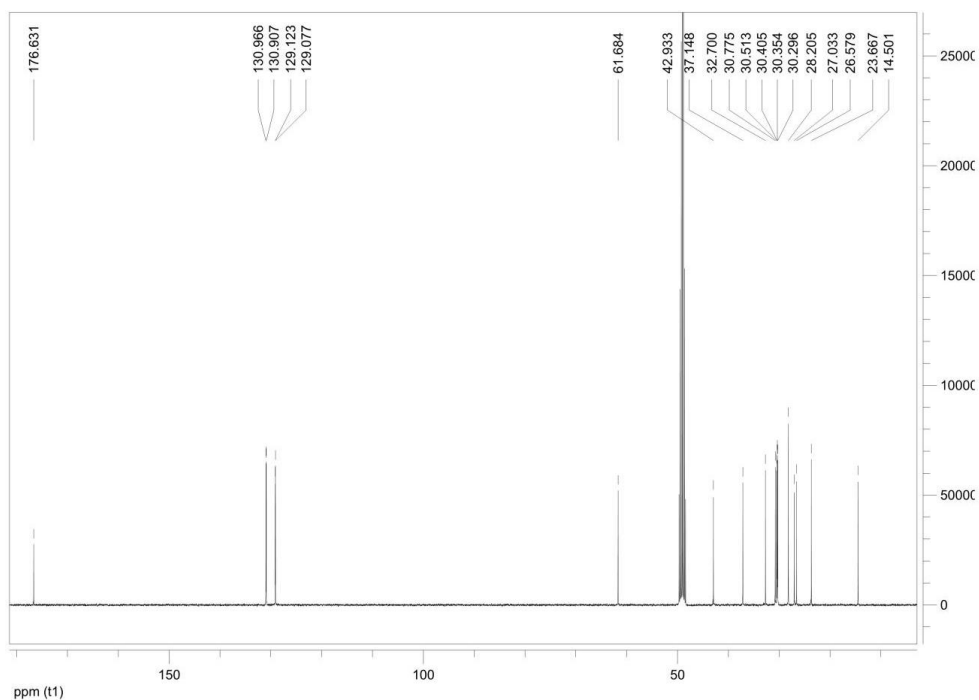
**Figure S46:**  $^{13}\text{C}$  NMR spectrum of **12** in  $\text{CDCl}_3$  (100 MHz)



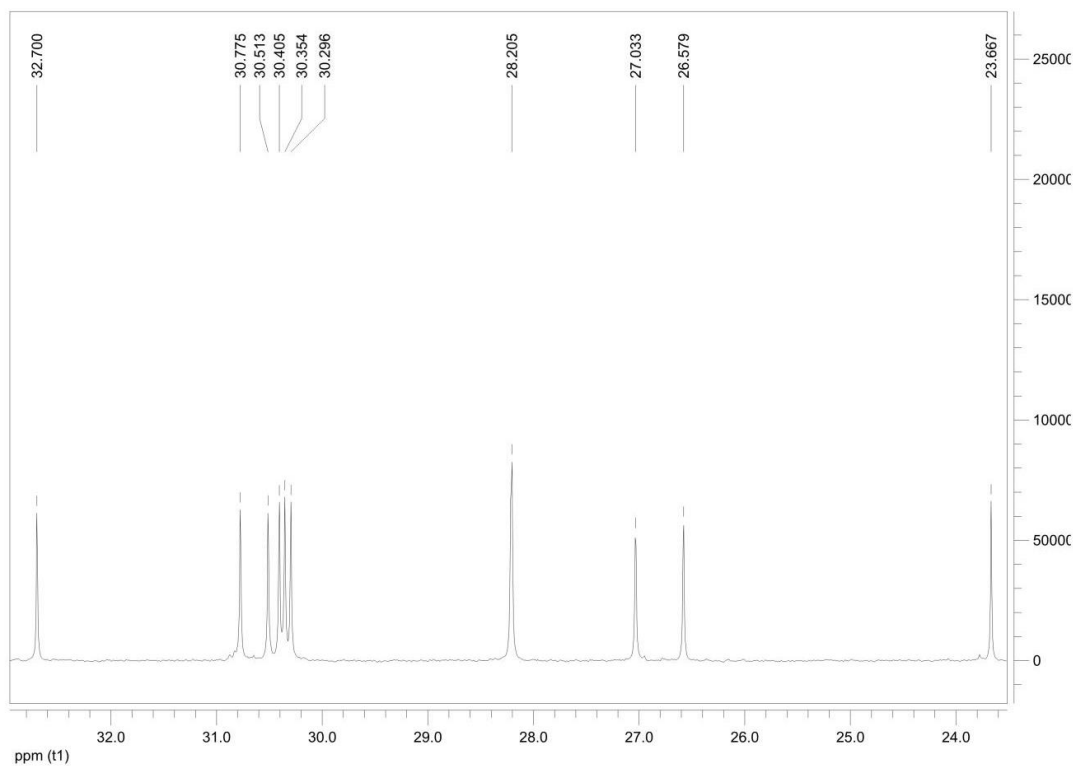
**Figure S47:** Selected  $^{13}\text{C}$  NMR spectrum of **12** in  $\text{CDCl}_3$



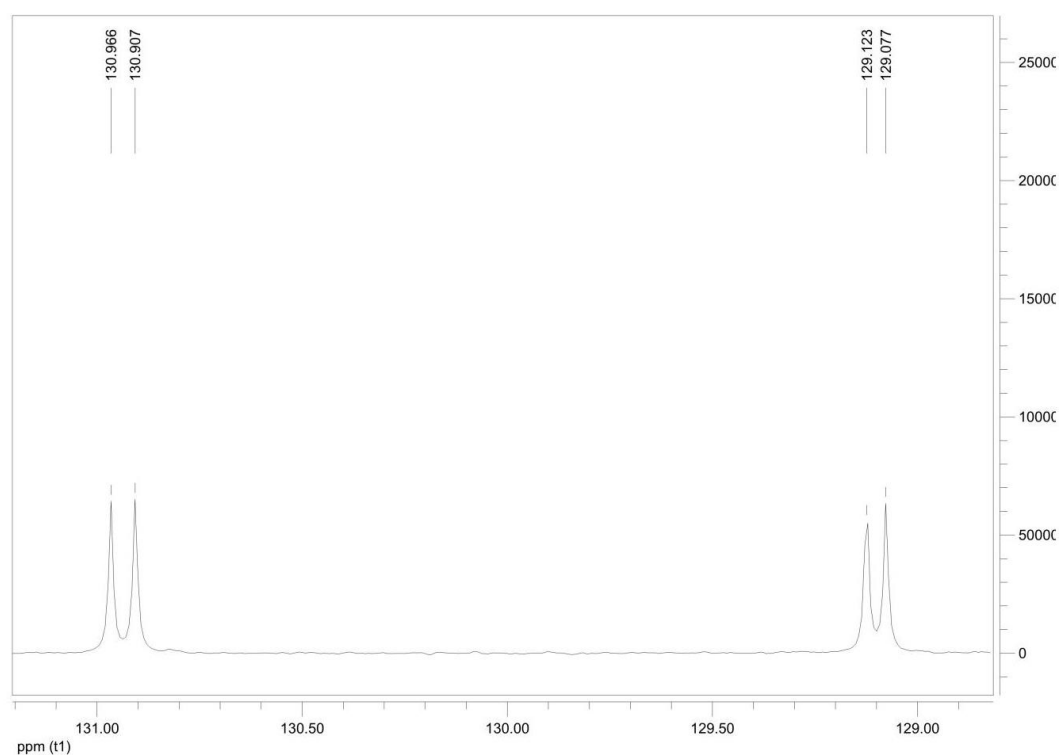
**Figure S48:**  $^1\text{H}$  NMR spectrum of **13** in  $\text{CD}_3\text{OD}$  (400 MHz)



**Figure S49:**  $^{13}\text{C}$  NMR spectrum of **13** in  $\text{CD}_3\text{OD}$  (100 MHz)



**Figure S50:** Selected  $^{13}\text{C}$  NMR spectrum of **13** in  $\text{CD}_3\text{OD}$  (1)



**Figure S51:** Selected  $^{13}\text{C}$  NMR spectrum of **13** in  $\text{CD}_3\text{OD}$  (2)

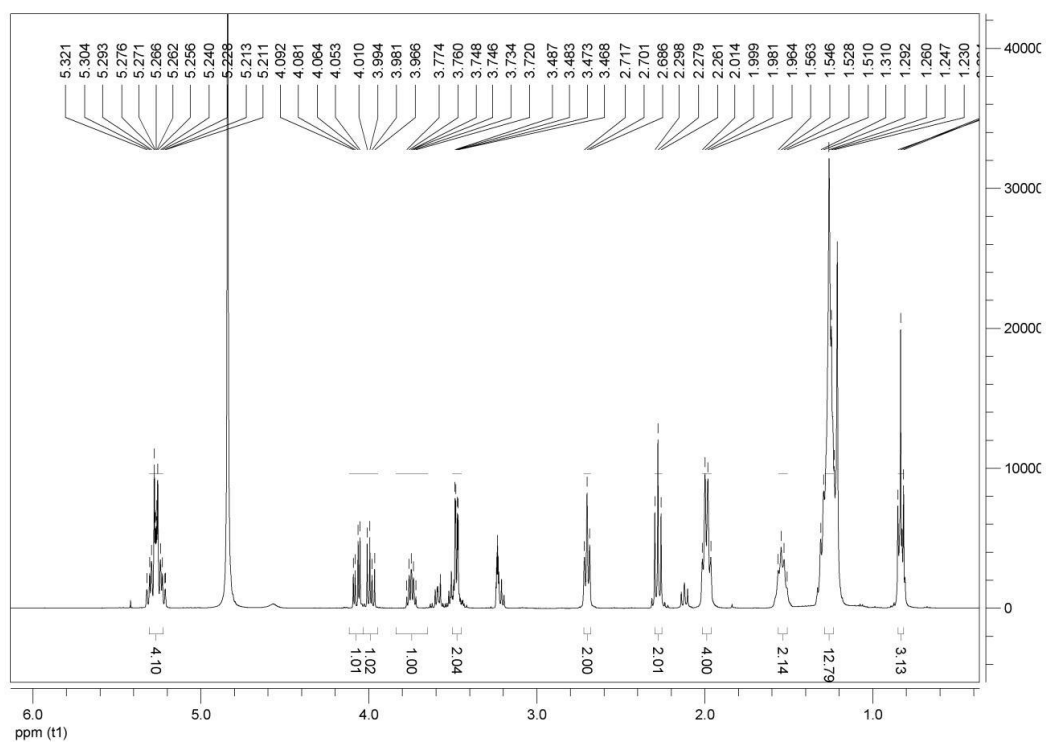


Figure S52:  $^1\text{H}$  NMR spectrum of **14** in  $\text{CD}_3\text{OD}$  (400 MHz)

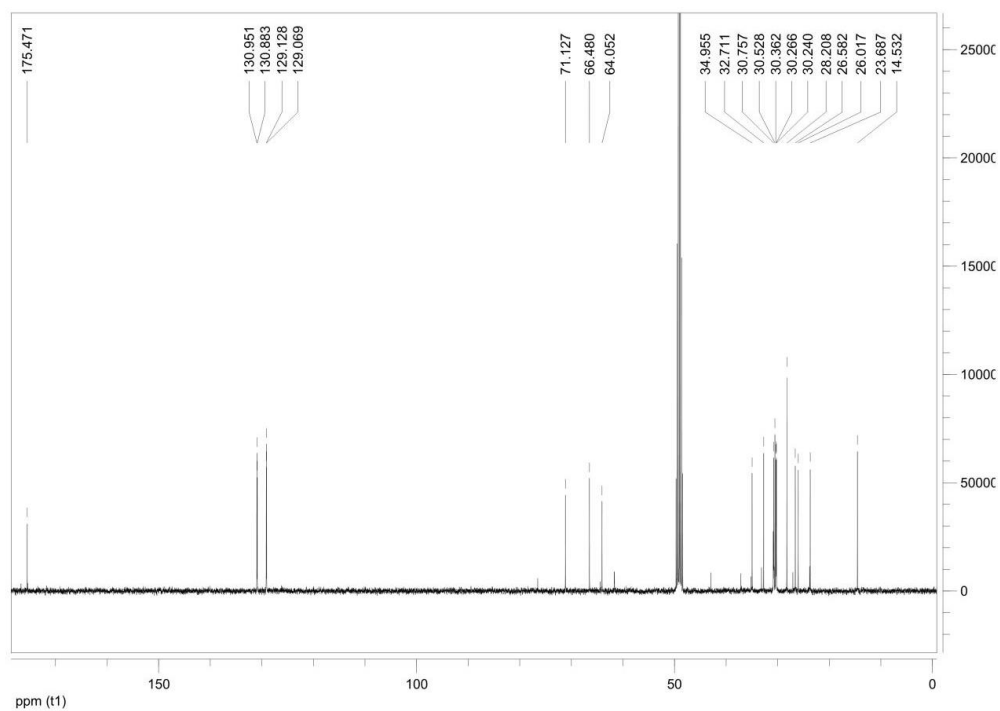
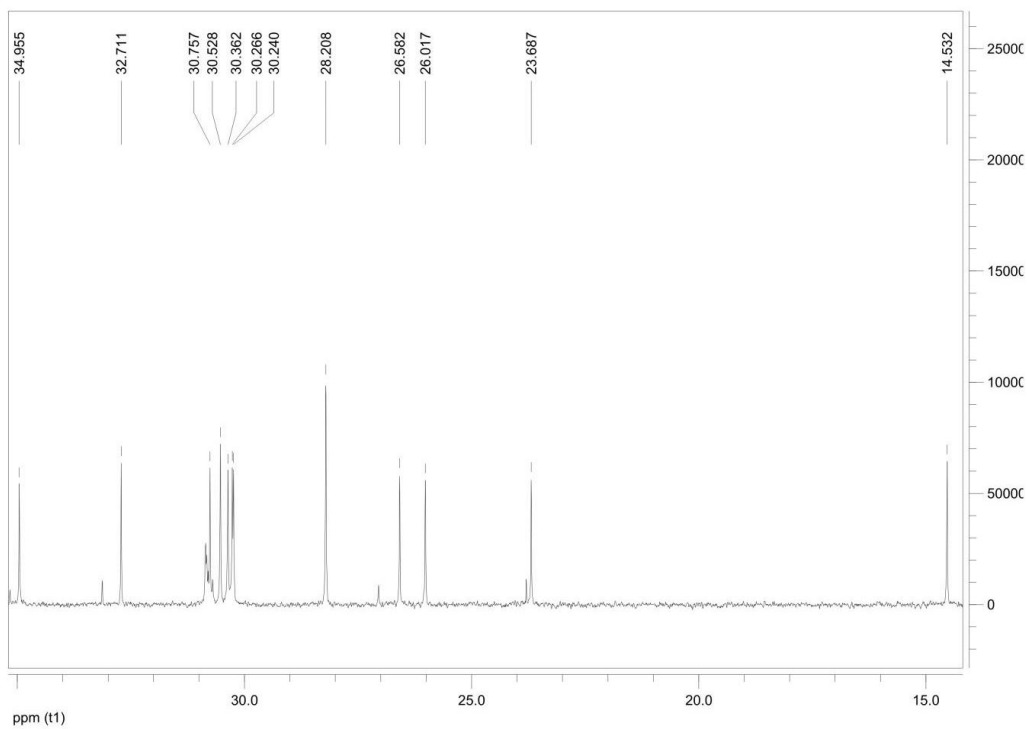
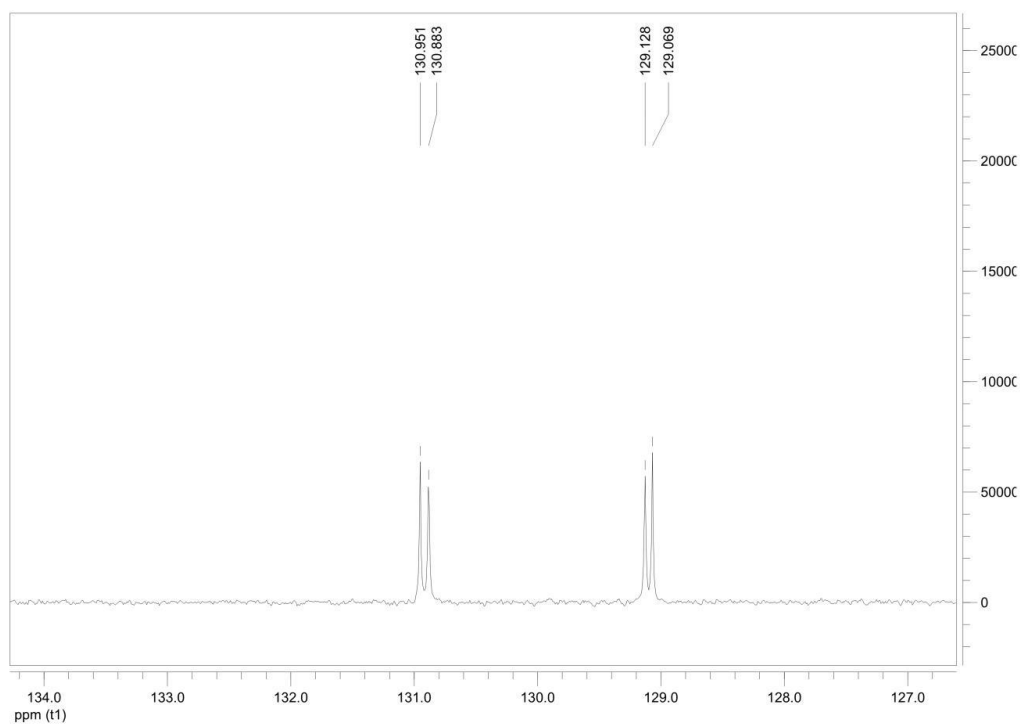


Figure S53:  $^{13}\text{C}$  NMR spectrum of **14** in  $\text{CD}_3\text{OD}$  (100 MHz)





**Figure S54:** Selected  $^{13}\text{C}$  NMR spectrum of **14** in  $\text{CD}_3\text{OD}$  (1)



**Figure S55:** Selected  $^{13}\text{C}$  NMR spectrum of **14** in  $\text{CD}_3\text{OD}$  (2)