

Supporting Information

Rec. Nat. Prod. 15:1 (2021) 1-9

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

Fenqin Zhao, Yahui Yan, Jiawei Li, Yizhu Dong, Jin Xie,

Ruyue Chen and Hui Yang *

*Institute of Pharmacy, School of Pharmacy, Henan University, Kaifeng 475004,
People's Republic of China*

Table of Contents	Page
Figure S1: ¹ H NMR spectrum of 1 in CD ₃ OD (400 MHz)	3
Figure S2: ¹³ C NMR spectrum of 1 in CD ₃ OD (100 MHz)	3
Figure S3: ¹³ C NMR spectrum of 1 in Acetone- <i>d</i> ₄ (400 MHz)	4
Figure S4: HSQC spectrum of 1 in CD ₃ OD	4
Figure S5: Selected HSQC spectrum of 1 in CD ₃ OD	5
Figure S6: HMBC spectrum of 1 in CD ₃ OD	5
Figure S7: Selected HMBC spectrum of 1 in CD ₃ OD	6
Figure S8: ¹ H- ¹ H COSY spectrum of 1 in CD ₃ OD	6
Figure S9: NOE spectrum of 1 in CD ₃ OD	7
Figure S10: HRMS spectrum of 1 (POS)	8
Figure S11: HRMS spectrum of 1 (NEG)	8
Figure S12: ¹ H NMR spectrum of 2 in CD ₃ OD (400 MHz)	9
Figure S13: ¹³ C NMR spectrum of 2 in CD ₃ OD (100 MHz)	9
Figure S14: ¹ H NMR spectrum of 3 in CD ₃ OD (400 MHz)	10
Figure S15: ¹³ C NMR spectrum of 3 in CD ₃ OD (100 MHz)	10
Figure S16: HSQC spectrum of 3 in CD ₃ OD	11
Figure S17: Selected HSQC spectrum of 3 in CD ₃ OD (1)	11
Figure S18: Selected HSQC spectrum of 3 in CD ₃ OD (2)	12
Figure S19: HMBC spectrum of 3 in CD ₃ OD	12

* Corresponding author: E-Mail: yanghui_wg@henu.edu.cn.

Figure S20: Selected HMBC spectrum of 3 in CD ₃ OD	13
Figure S21: NOE spectrum of 3 in CD ₃ OD	13
Figure S22: HRMS spectrum of 3	14
Figure S23: ¹ H NMR spectrum of 4 in CD ₃ OD (400 MHz)	15
Figure S24: ¹³ C NMR spectrum of 4 in CD ₃ OD (100 MHz)	15
Figure S25: MS spectrum of 4	16
Figure S26: ¹ H NMR spectrum of 5 in CD ₃ OD (400 MHz)	17
Figure S27: ¹³ C NMR spectrum of 5 in CD ₃ OD (100 MHz)	17
Figure S28: MS spectrum of 5	18
Figure S29: ¹ H NMR spectrum of 6 in CD ₃ OD (400 MHz)	19
Figure S30: ¹³ C NMR spectrum of 6 in CD ₃ OD (100 MHz)	19
Figure S31: ¹ H NMR spectrum of 7 in CD ₃ OD (400 MHz)	20
Figure S32: ¹³ C NMR spectrum of 7 in CD ₃ OD (100 MHz)	20
Figure S33: ¹ H NMR spectrum of 8 in CD ₃ OD (400 MHz)	21
Figure S34: ¹³ C NMR spectrum of 8 in CD ₃ OD (100 MHz)	21
Figure S35: HRMS spectrum of 8	22
Figure S36: ¹ H NMR spectrum of 9 in CD ₃ OD (400 MHz)	23
Figure S37: ¹³ C NMR spectrum of 9 in CD ₃ OD (100 MHz)	23
Figure S38: ¹ H NMR spectrum of 10 in CD ₃ OD (400 MHz)	24
Figure S39: ¹³ C NMR spectrum of 10 in CD ₃ OD (100 MHz)	24
Figure S40: MS spectrum of 10	25
Figure S41: ¹ H NMR spectrum of 11 in CD ₃ OD (400 MHz)	26
Figure S42: ¹³ C NMR spectrum of 11 in CD ₃ OD (100 MHz)	26
Figure S43: MS spectrum of 11	27
Figure S44: ¹ H NMR spectrum of 12 in CDCl ₃ (400 MHz)	28
Figure S45: Selected ¹ H NMR spectrum of 12 in CDCl ₃	28
Figure S46: ¹³ C NMR spectrum of 12 in CDCl ₃ (100 MHz)	29
Figure S47: Selected ¹³ C NMR spectrum of 12 in CDCl ₃	29
Figure S48: ¹ H NMR spectrum of 13 in CD ₃ OD (400 MHz)	30
Figure S49: ¹³ C NMR spectrum of 13 in CD ₃ OD (100 MHz)	30
Figure S50: Selected ¹³ C NMR spectrum of 13 in CD ₃ OD	31
Figure S51: Selected ¹³ C NMR spectrum of 13 in CD ₃ OD	31
Figure S52: ¹ H NMR spectrum of 14 in CD ₃ OD (400 MHz)	32
Figure S53: ¹³ C NMR spectrum of 14 in CD ₃ OD (100 MHz)	32
Figure S54: Selected ¹³ C NMR spectrum of 14 in CD ₃ OD (1)	33
Figure S55: Selected ¹³ C NMR spectrum of 14 in CD ₃ OD (2)	33

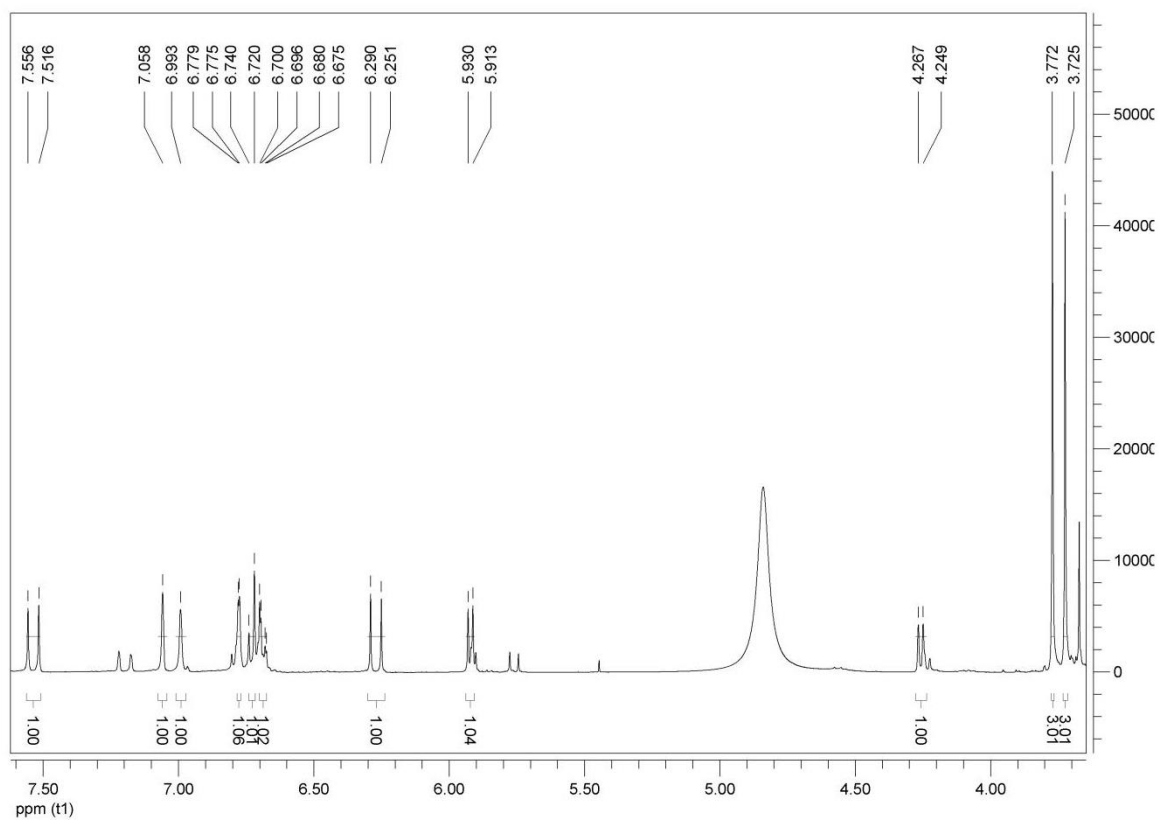


Figure S1: ^1H NMR spectrum of **1** in CD_3OD (400 MHz)

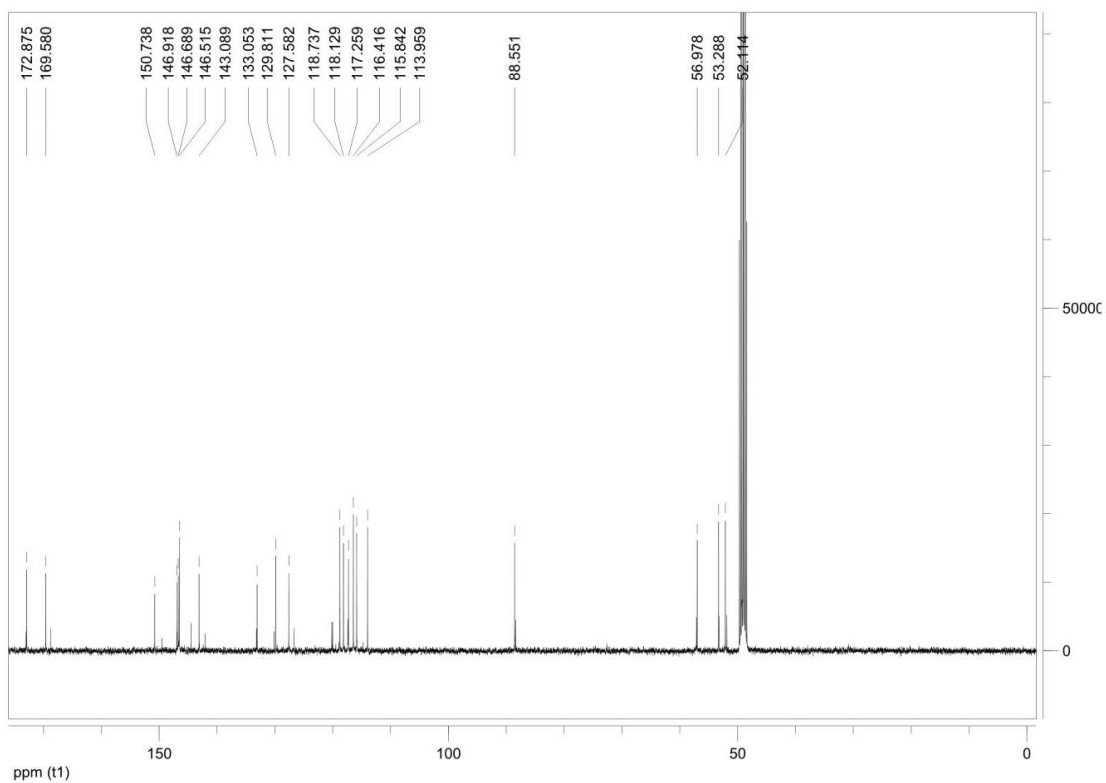


Figure S2: ^{13}C NMR spectrum of **1** in CD_3OD (100 MHz)

© 2020 ACG Publications. All rights reserved

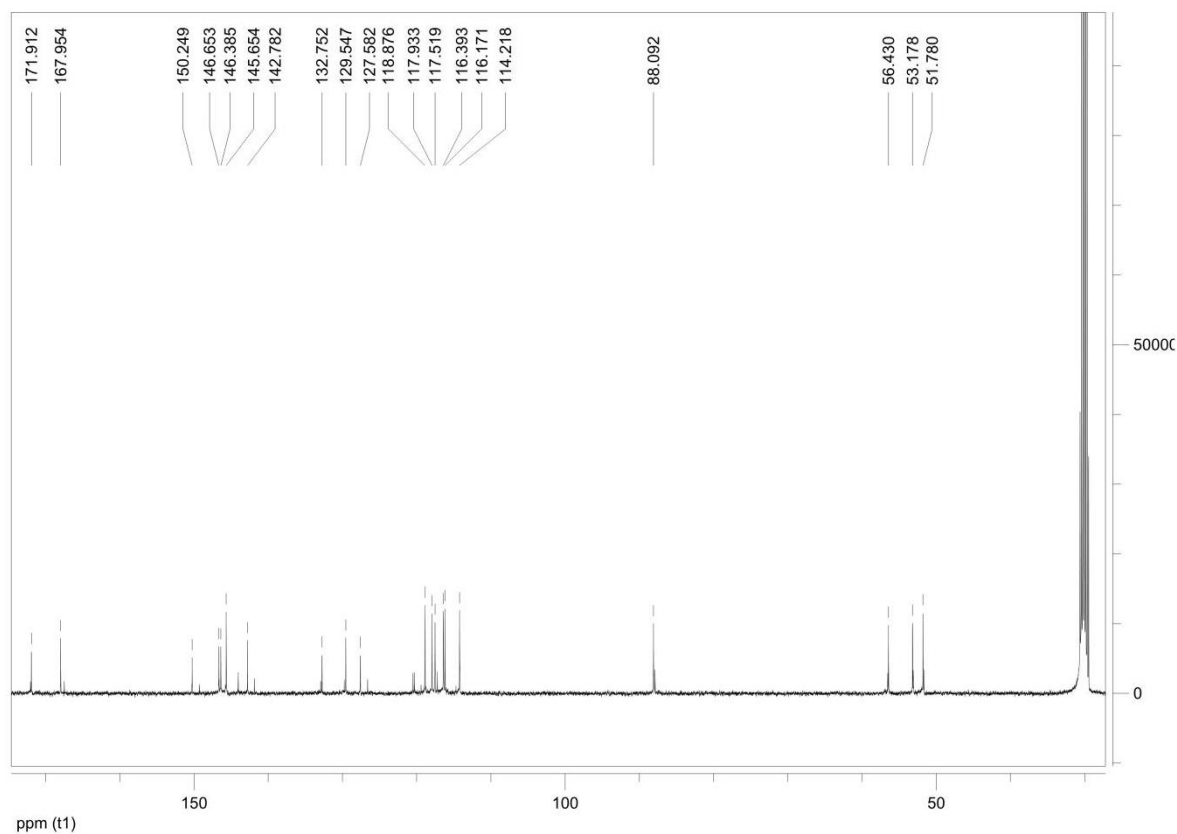


Figure S3: ^{13}C NMR spectrum of **1** in Acetone- d_4 (100 MHz)

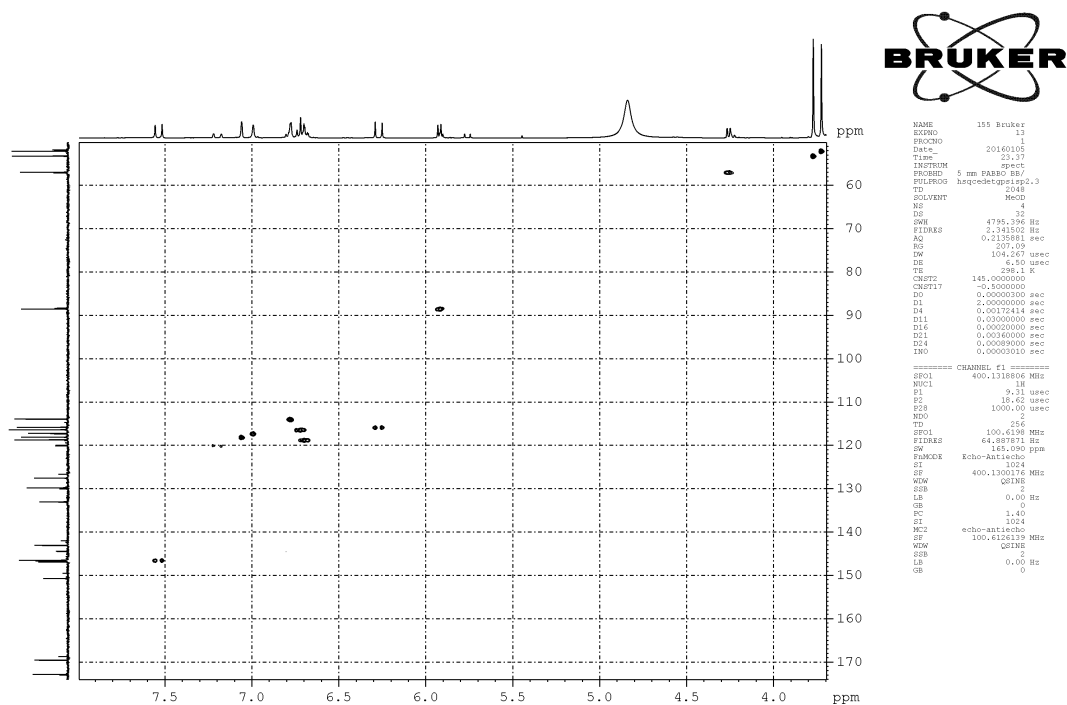


Figure S4: HSQC spectrum of **1** in CD_3OD

© 2020 ACG Publications. All rights reserved

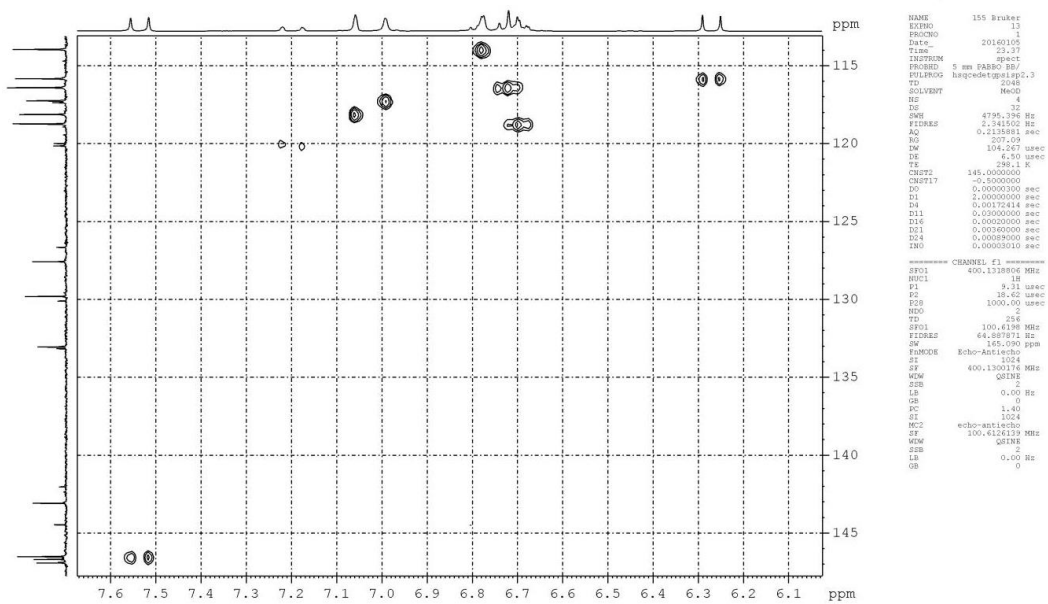


Figure S5: Selected HSQC spectrum of **1** in CD₃OD

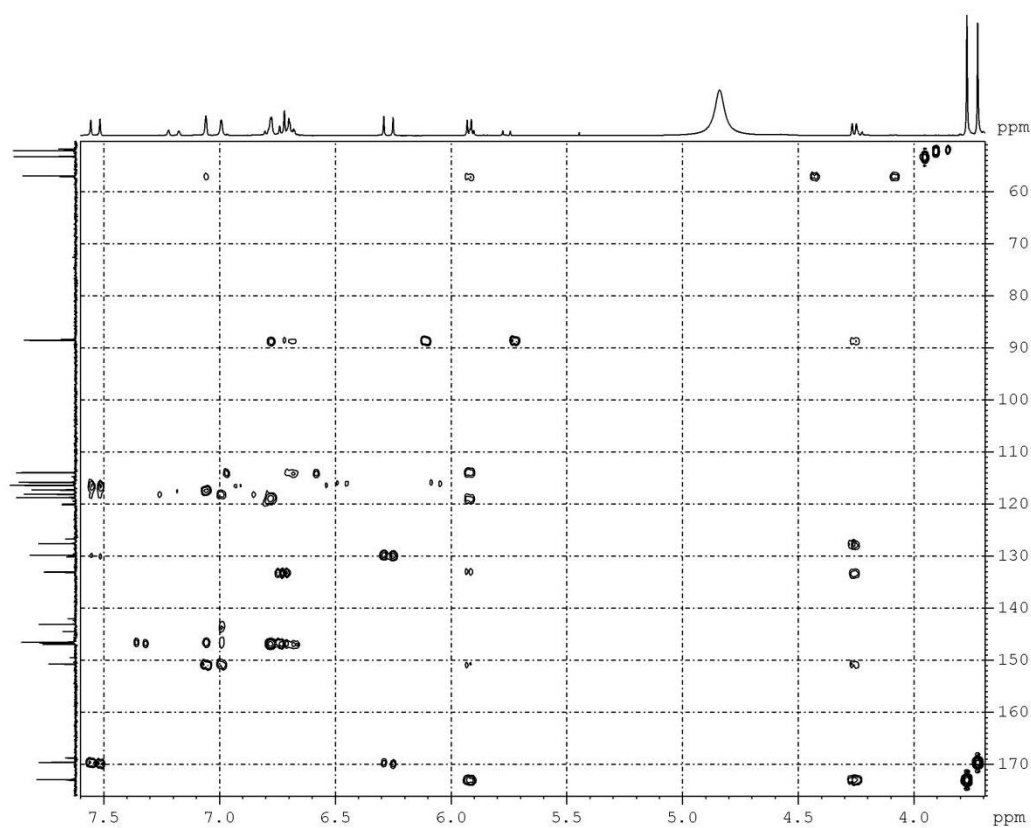


Figure S6: HMBC spectrum of **1** in CD₃OD

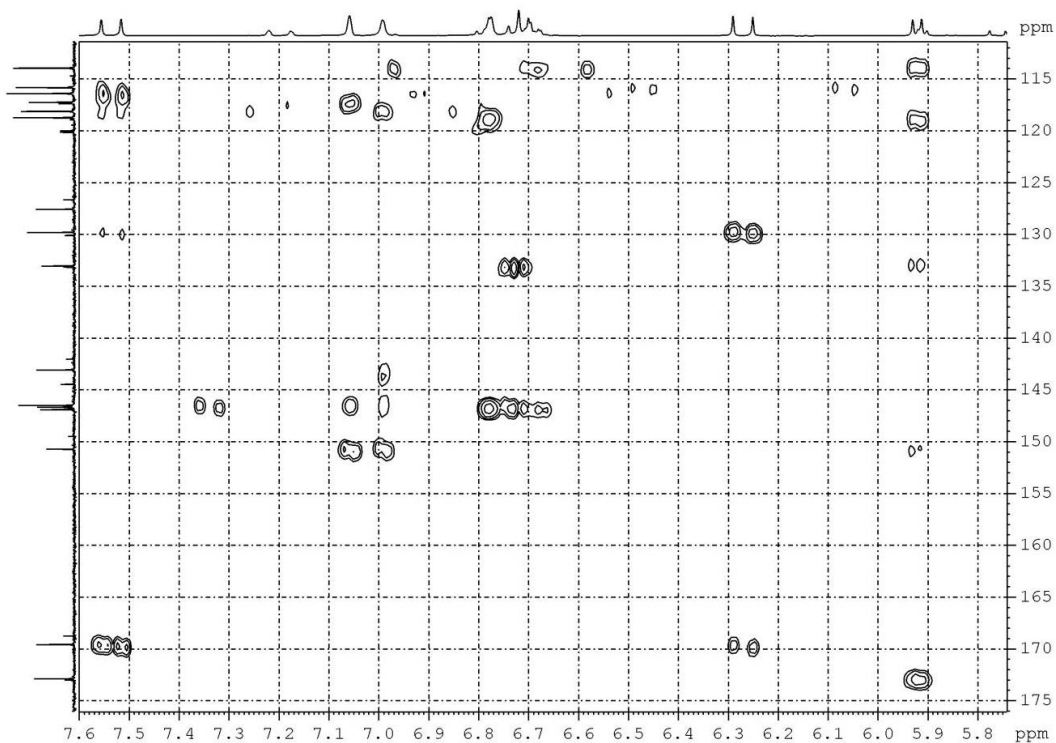


Figure S7: Selected HMBC spectrum of **1** in CD₃OD

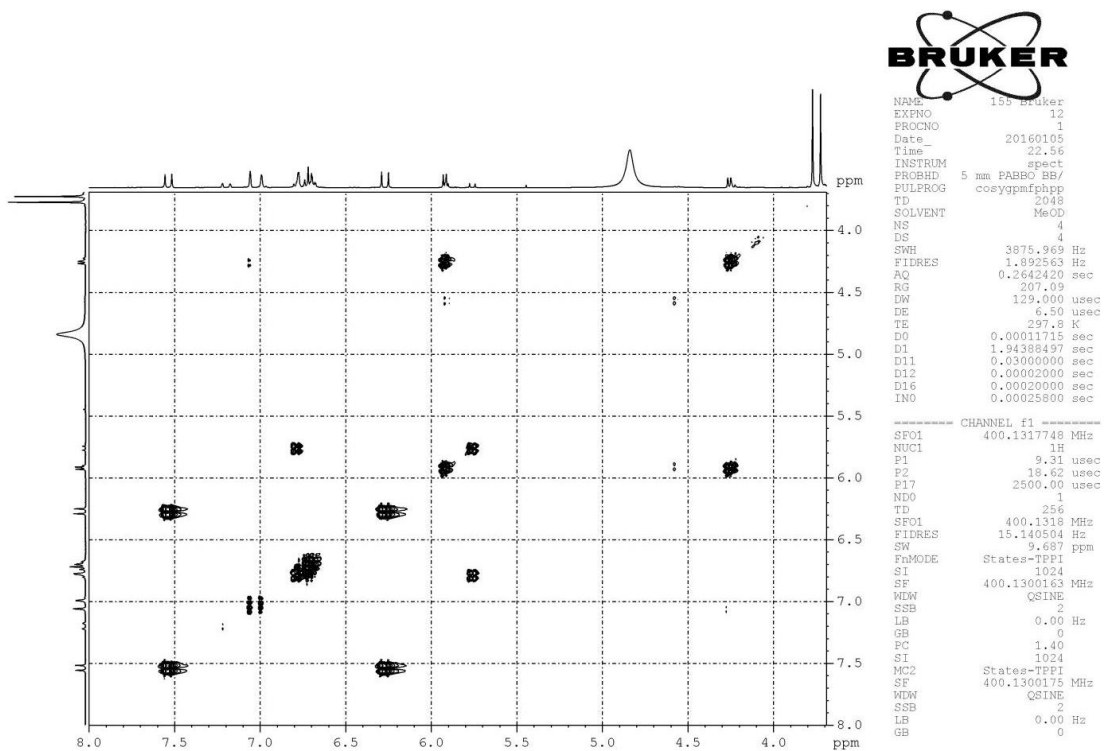


Figure S8: ¹H-¹H COSY spectrum of **1** in CD₃OD

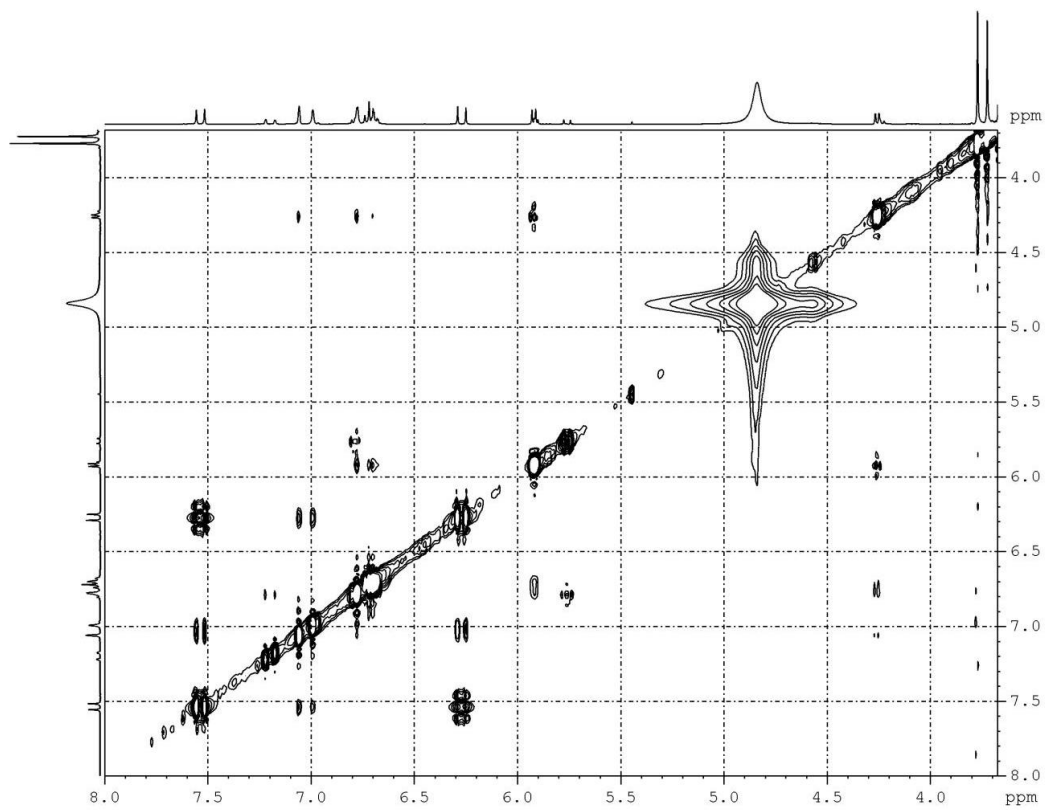


Figure S9: NOE spectrum of **1** in CD₃OD

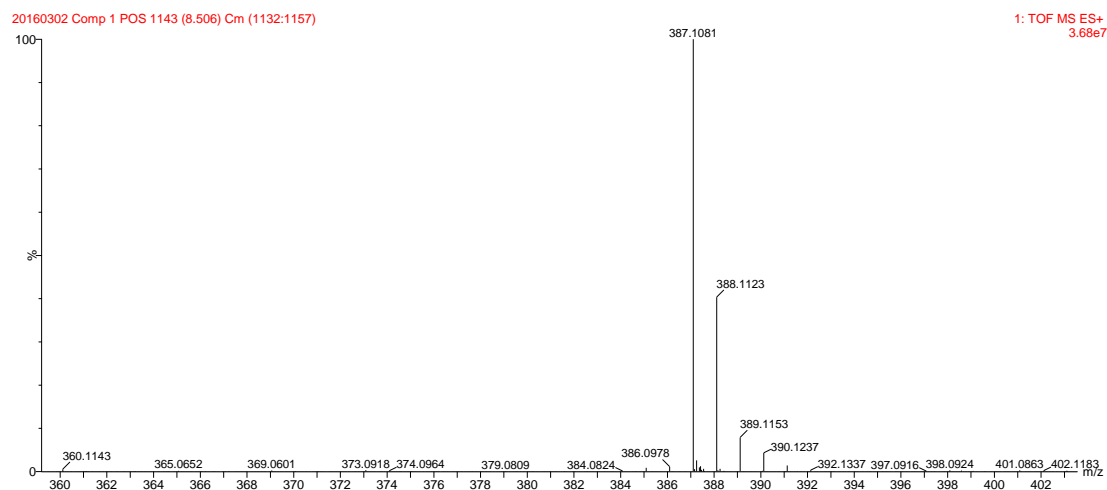


Figure S10: HRMS spectrum of 1 (POS)

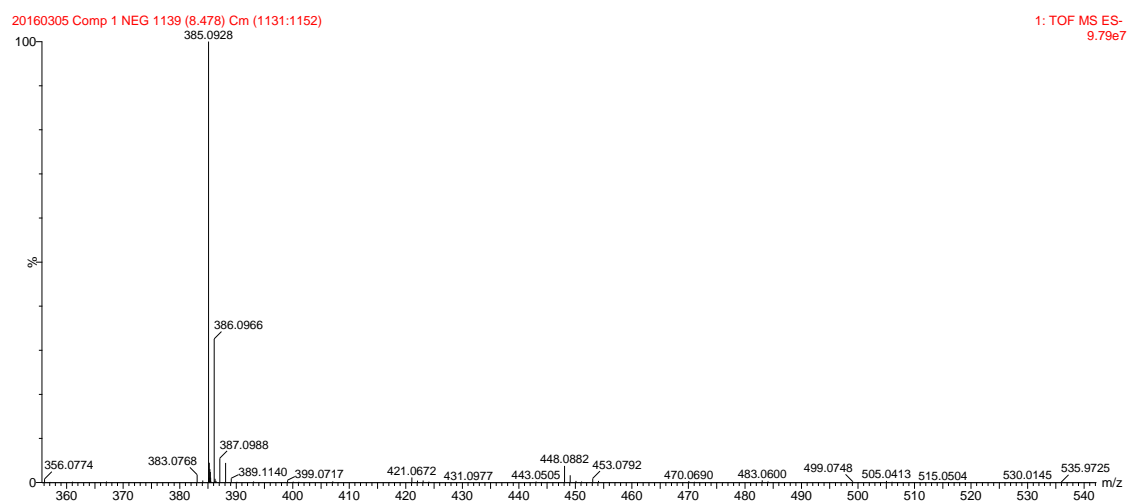


Figure S11: HRMS spectrum of 1 (NEG)

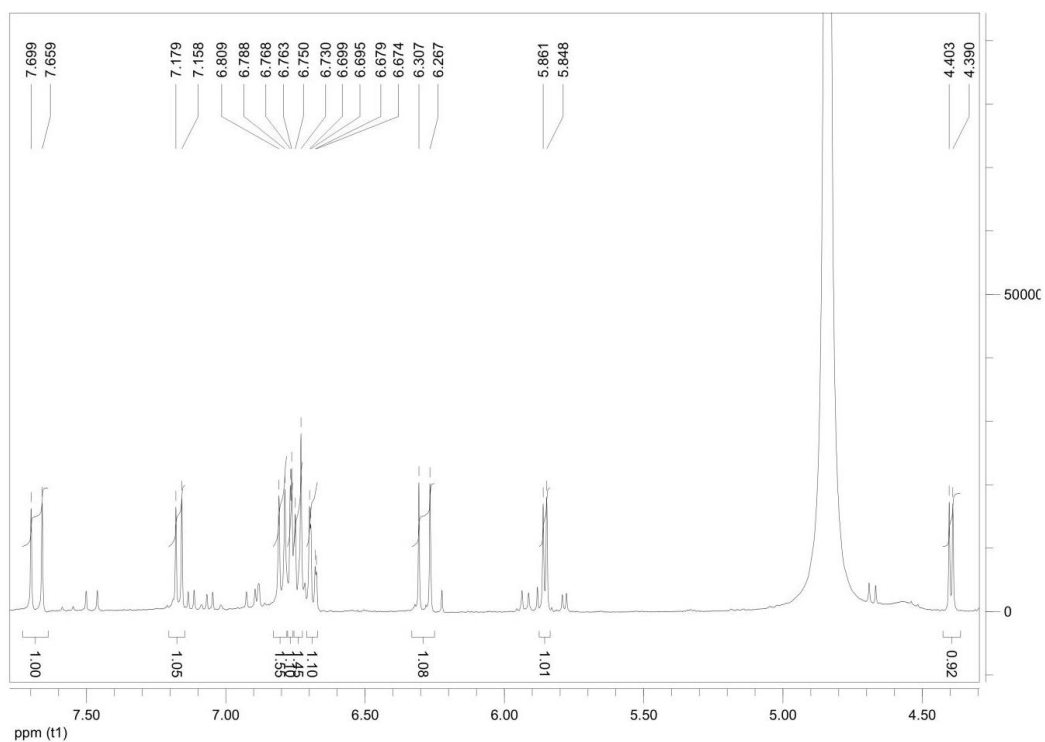


Figure S12: ^1H NMR spectrum of **2** in CD_3OD (400 MHz)

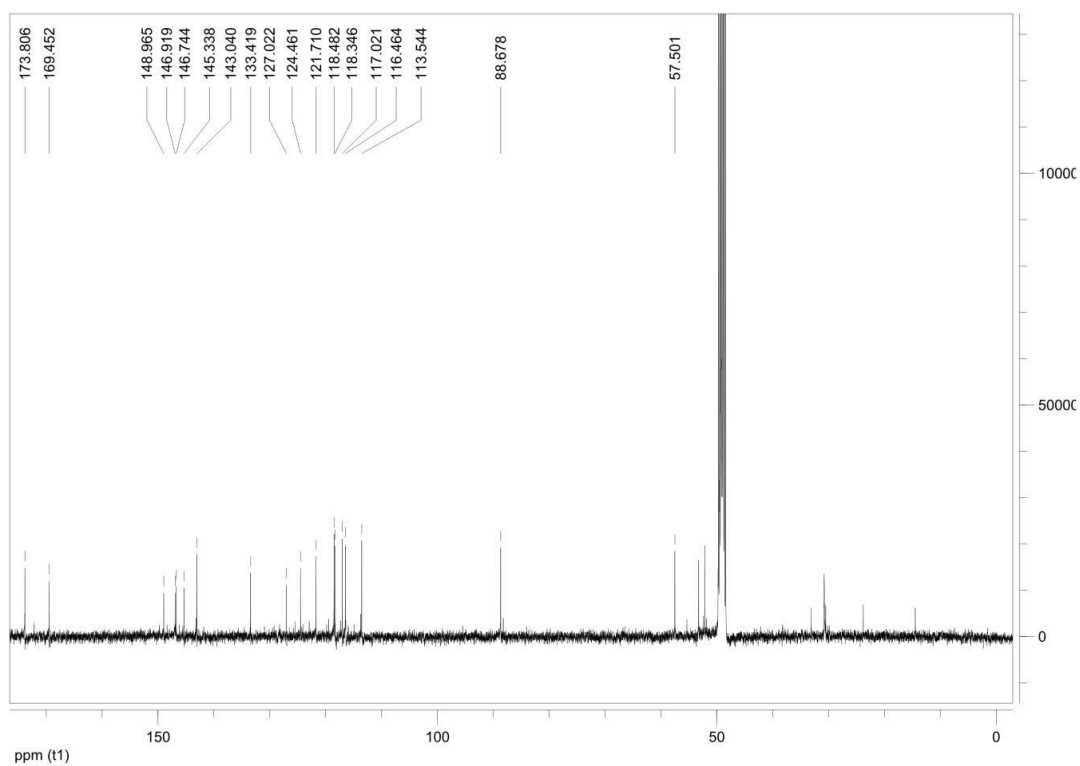


Figure S13: ^{13}C NMR spectrum of **2** in CD_3OD (100 MHz)

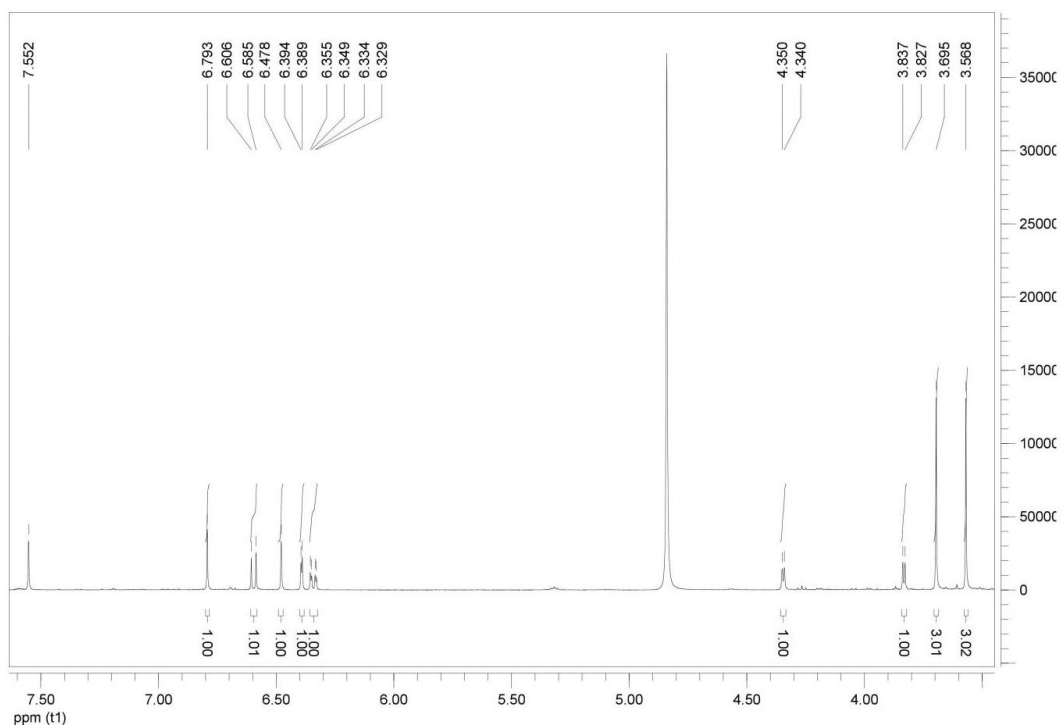


Figure S14: ^1H NMR spectrum of **3** in CD_3OD (400 MHz)

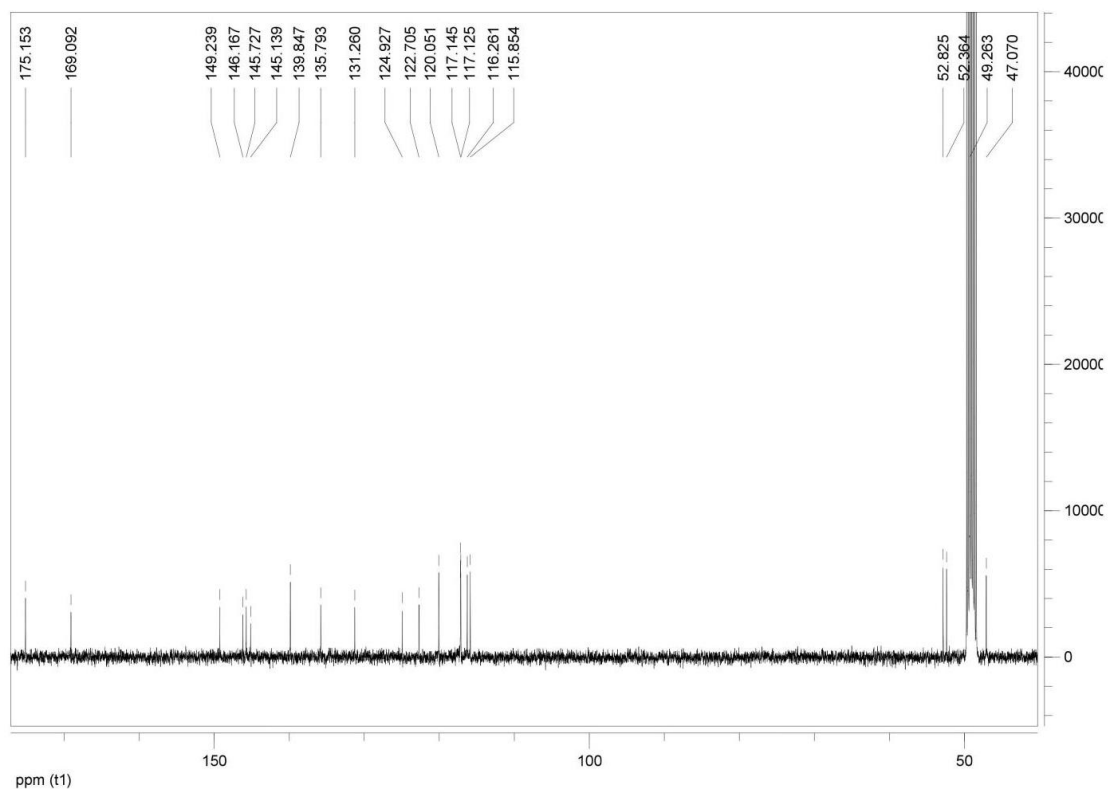


Figure S15: ^{13}C NMR spectrum of **3** in CD_3OD (100 MHz)

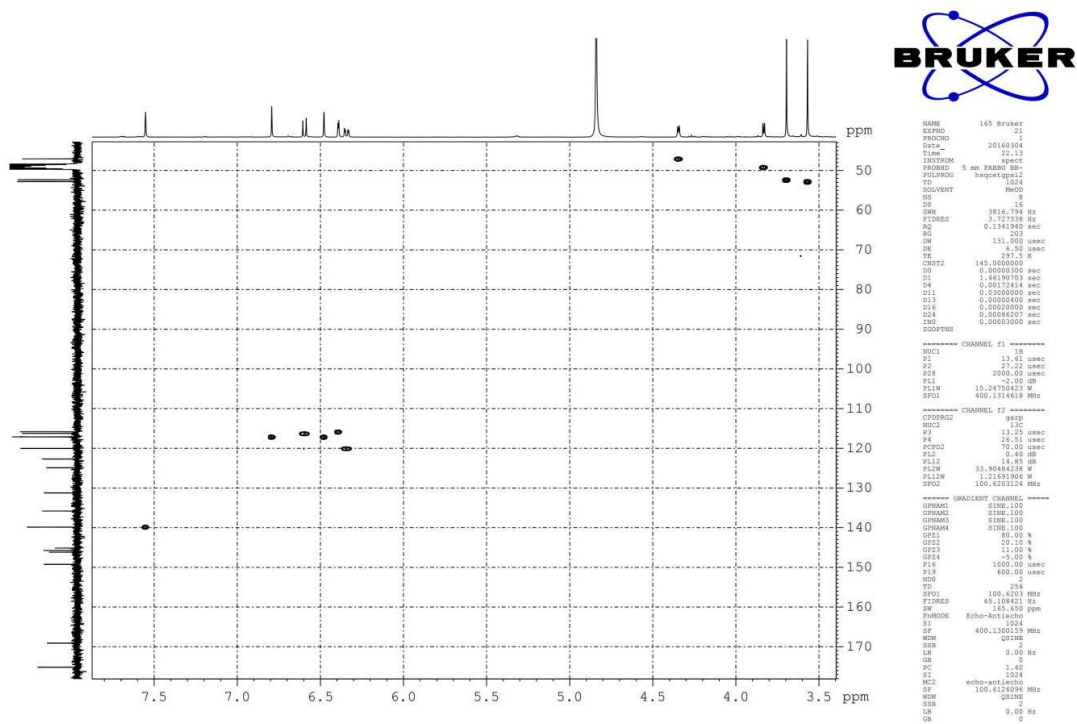


Figure S16: HSQC spectrum of **3** in CD₃OD

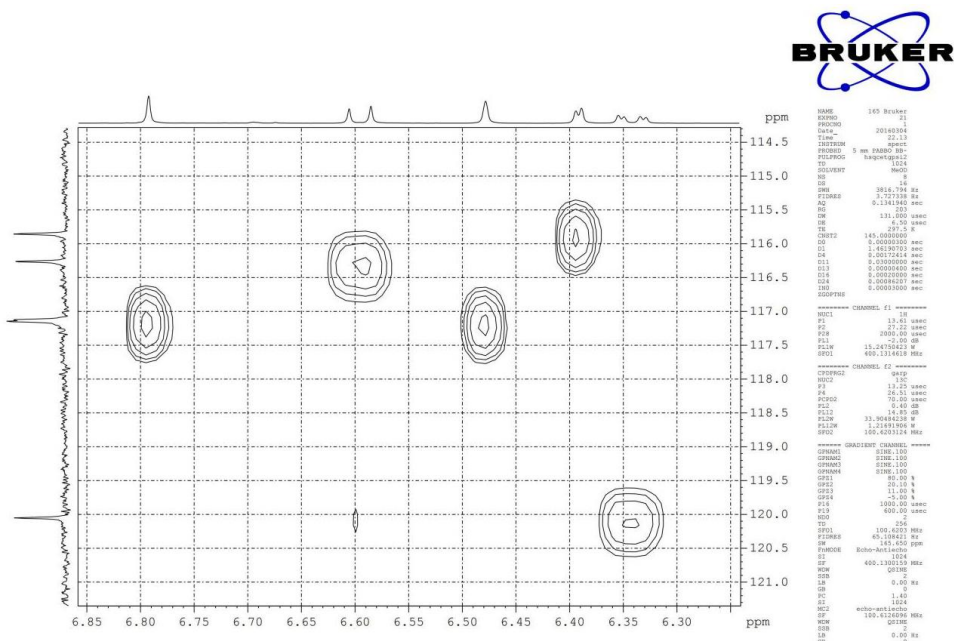


Figure S17: Selected HSQC spectrum of **3** in CD₃OD (1)

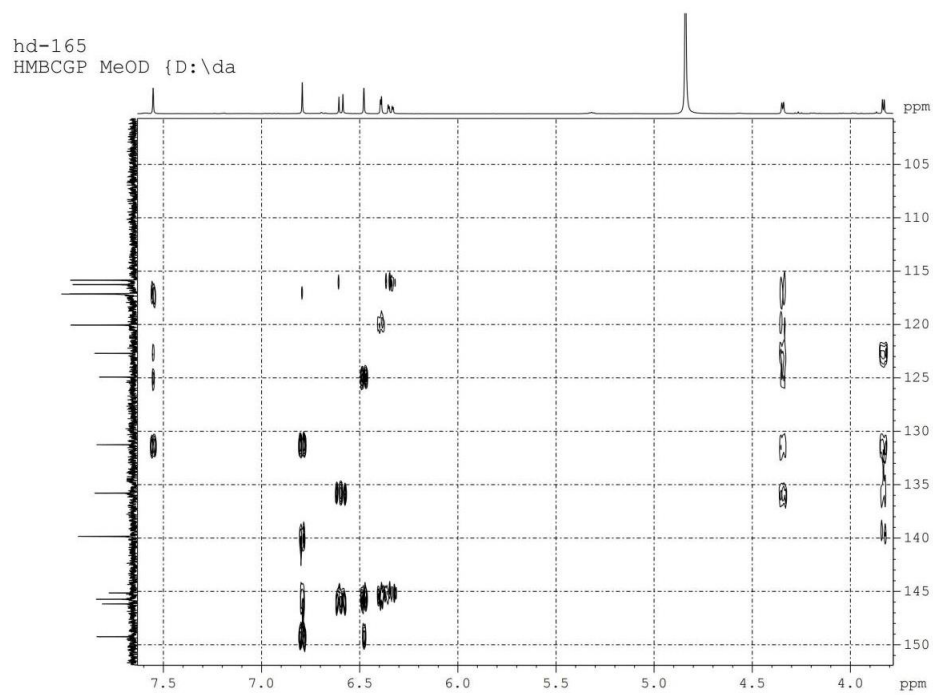


Figure S20: Selected HMBC spectrum of **3** in CD₃OD

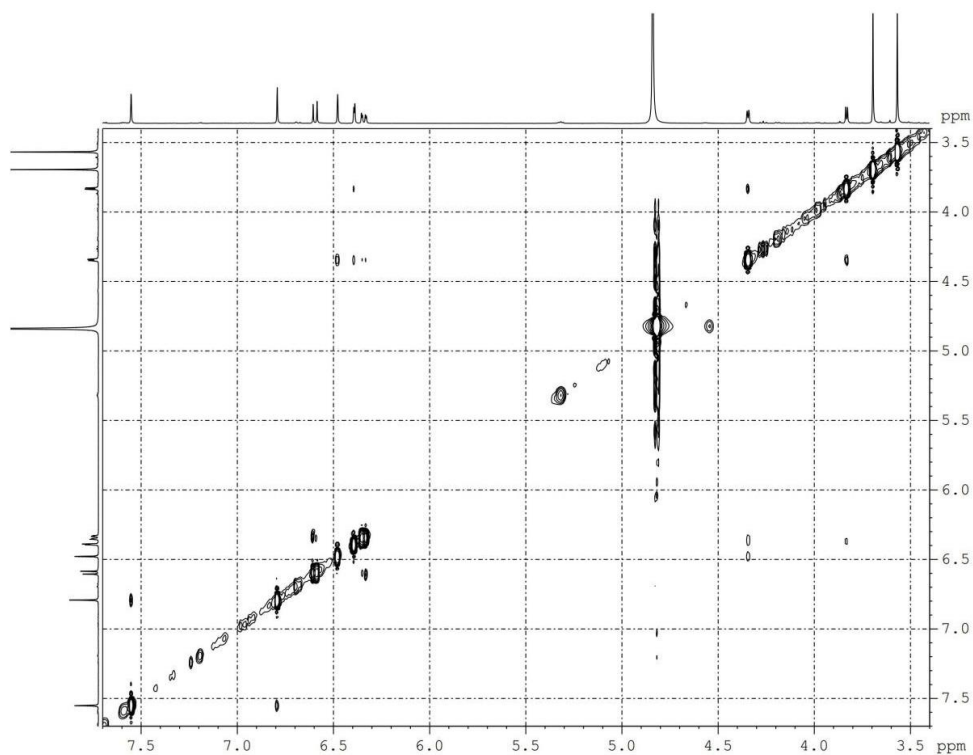


Figure S21: NOE spectrum of **3** in CD₃OD

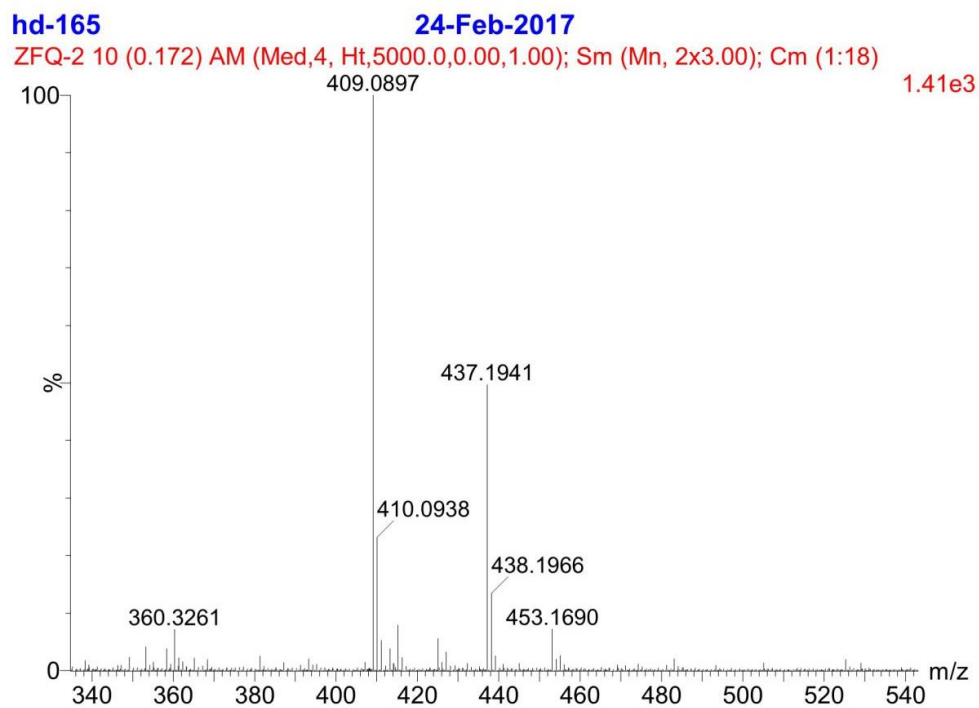


Figure S22: HRMS spectrum of **3**

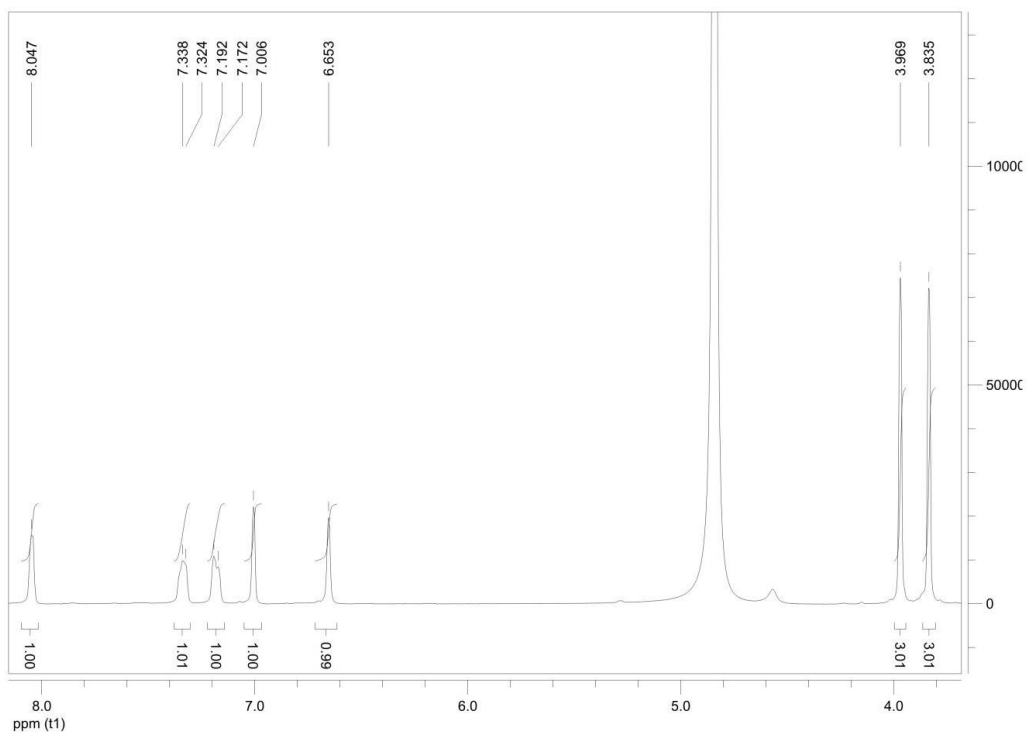


Figure S23: ^1H NMR spectrum of **4** in CD_3OD (100 MHz)

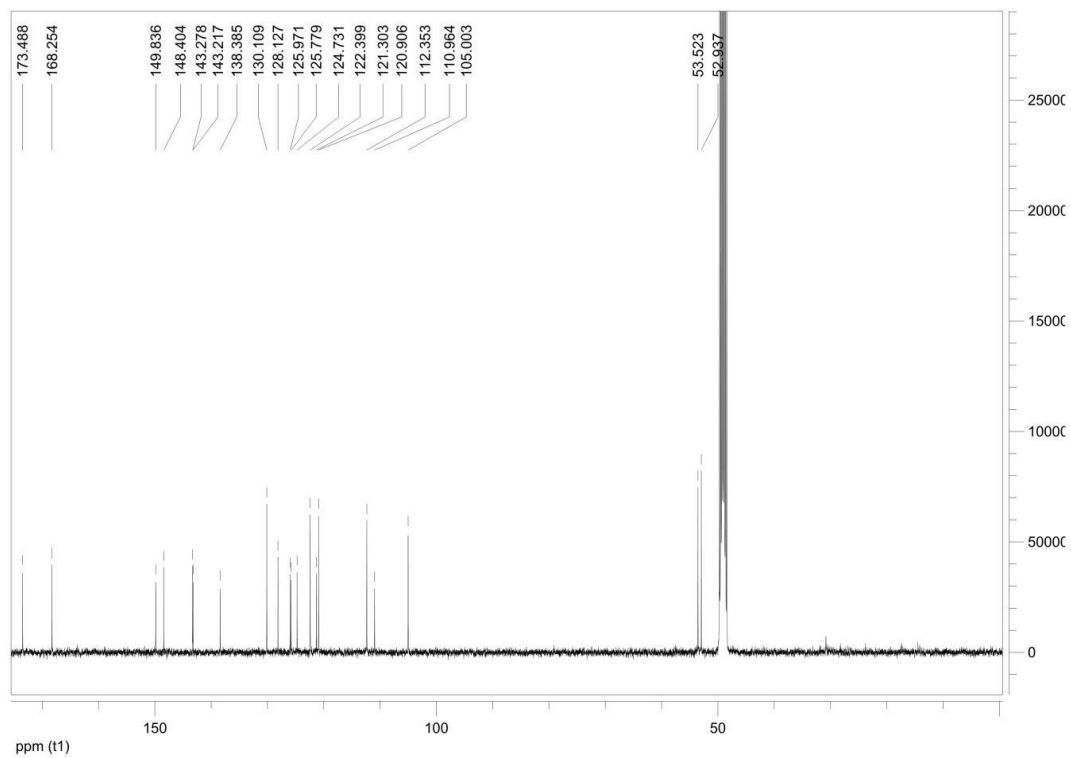


Figure S24: ^{13}C NMR spectrum of **4** in CD_3OD (100 MHz)

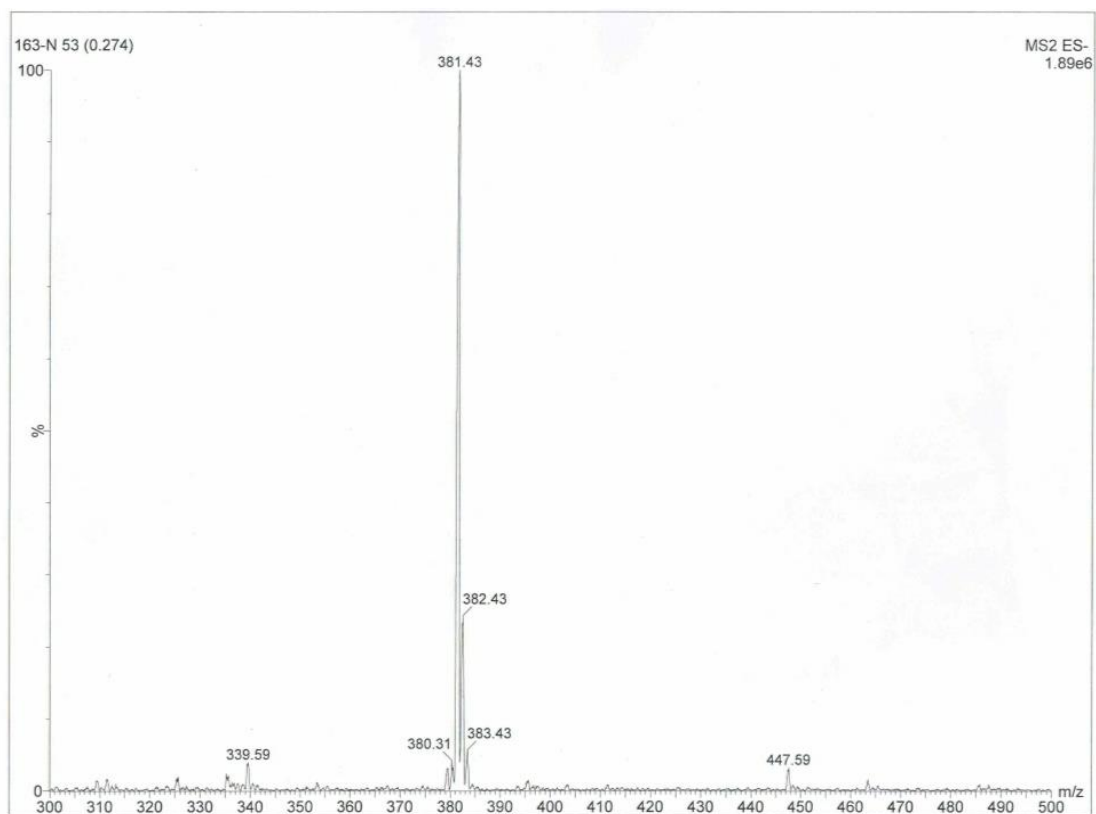


Figure S25: MS spectrum of **4**

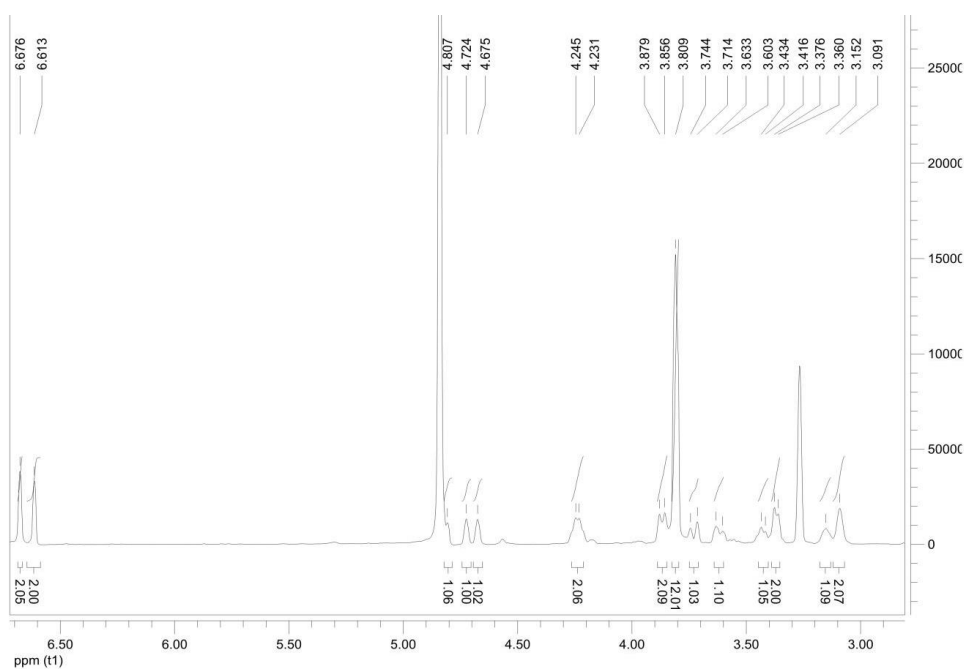


Figure S26: ^1H NMR spectrum of **5** in CD_3OD (400 MHz)

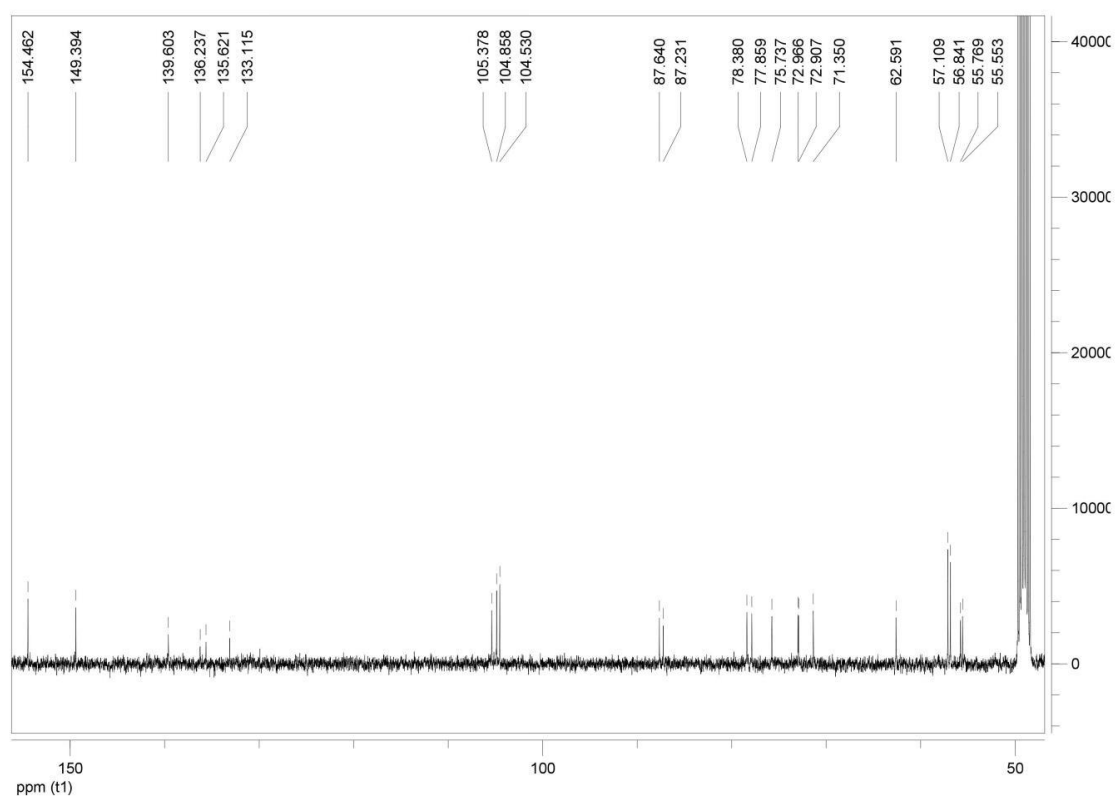


Figure S27: ^{13}C NMR spectrum of **5** in CD_3OD (100 MHz)

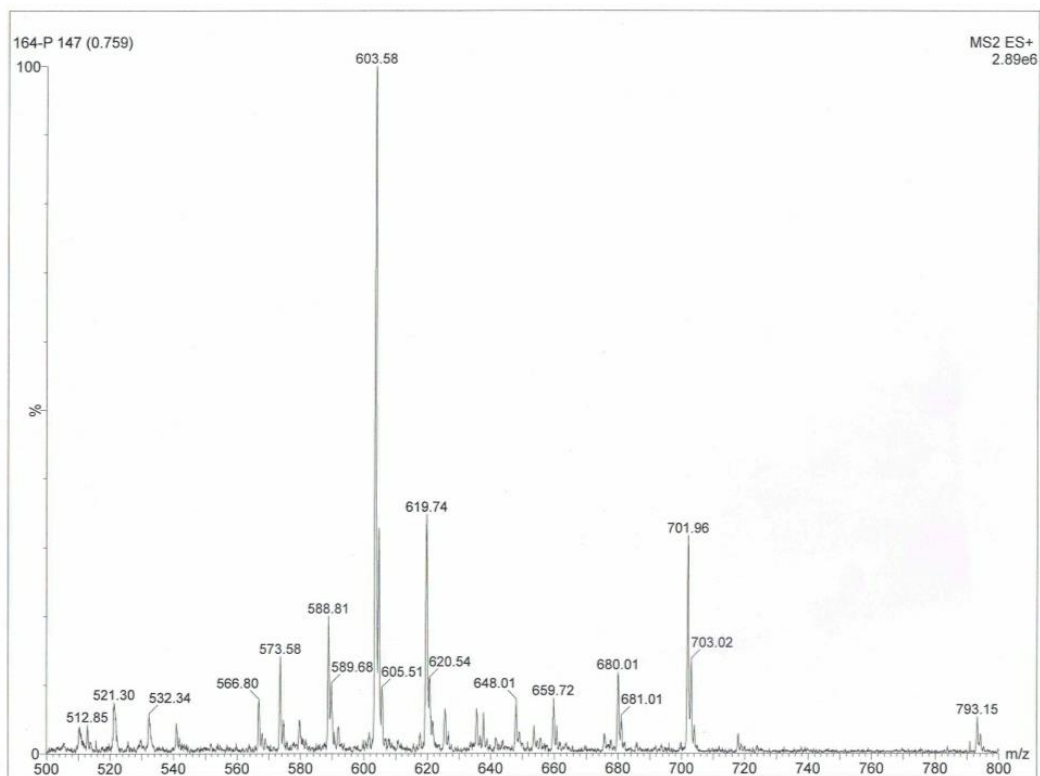


Figure S28: MS spectrum of **5**

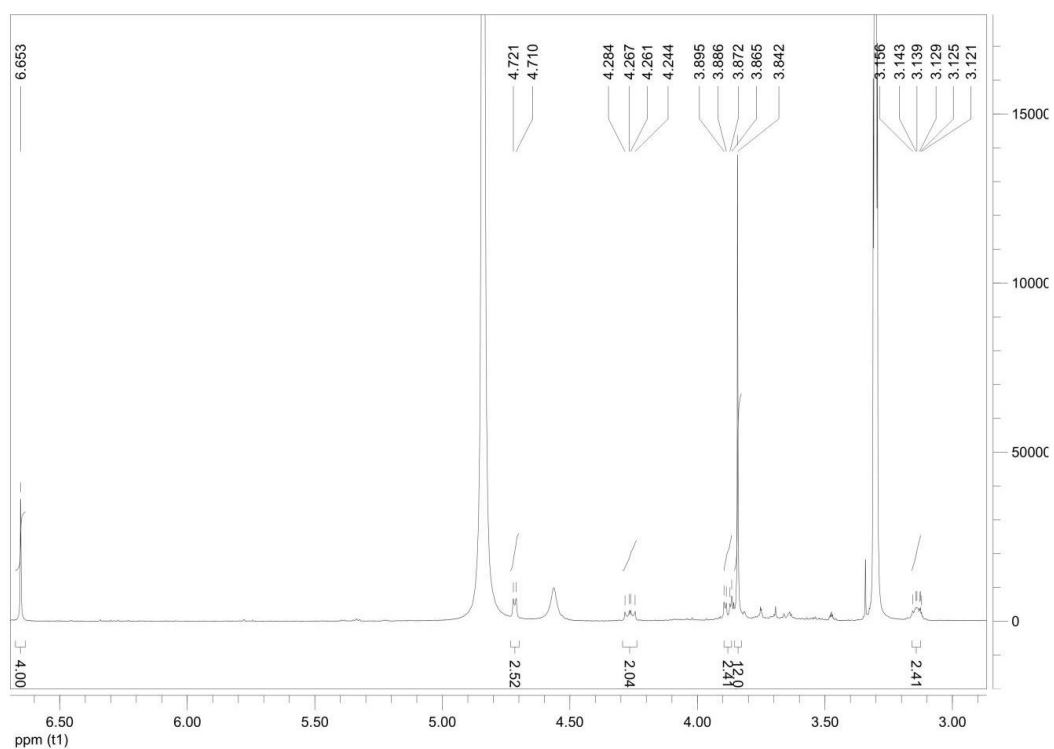


Figure S29: ^1H NMR spectrum of **6** in CD_3OD (400 MHz)

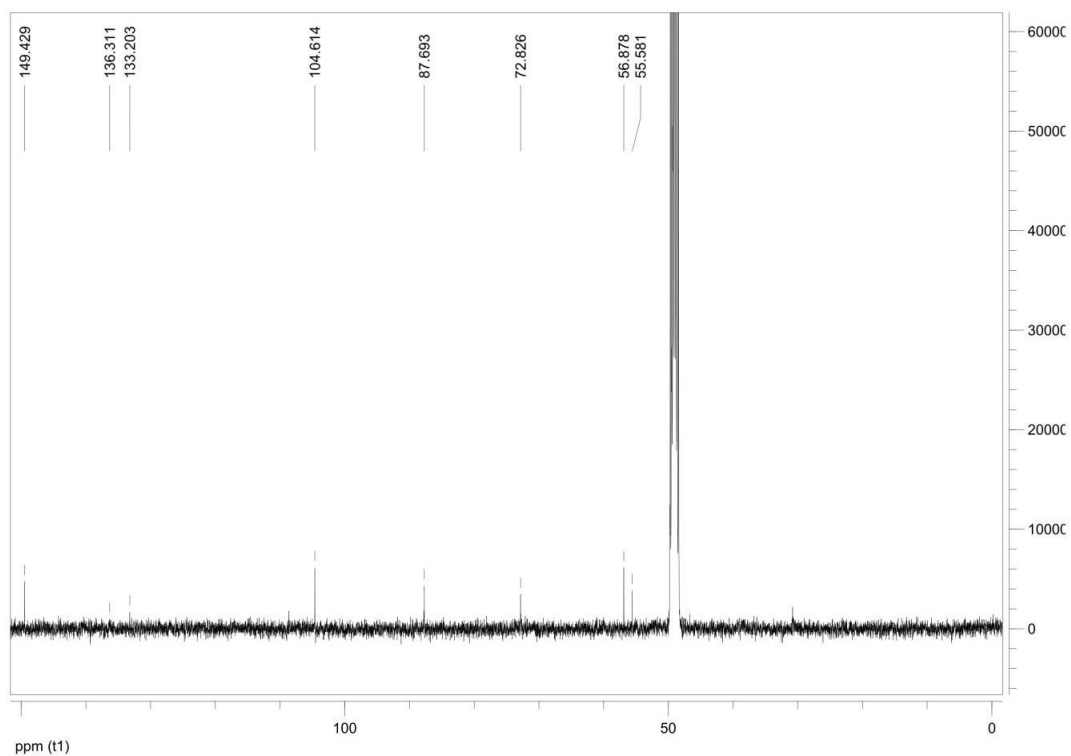


Figure S30: ^{13}C NMR spectrum of **6** in CD_3OD (100 MHz)

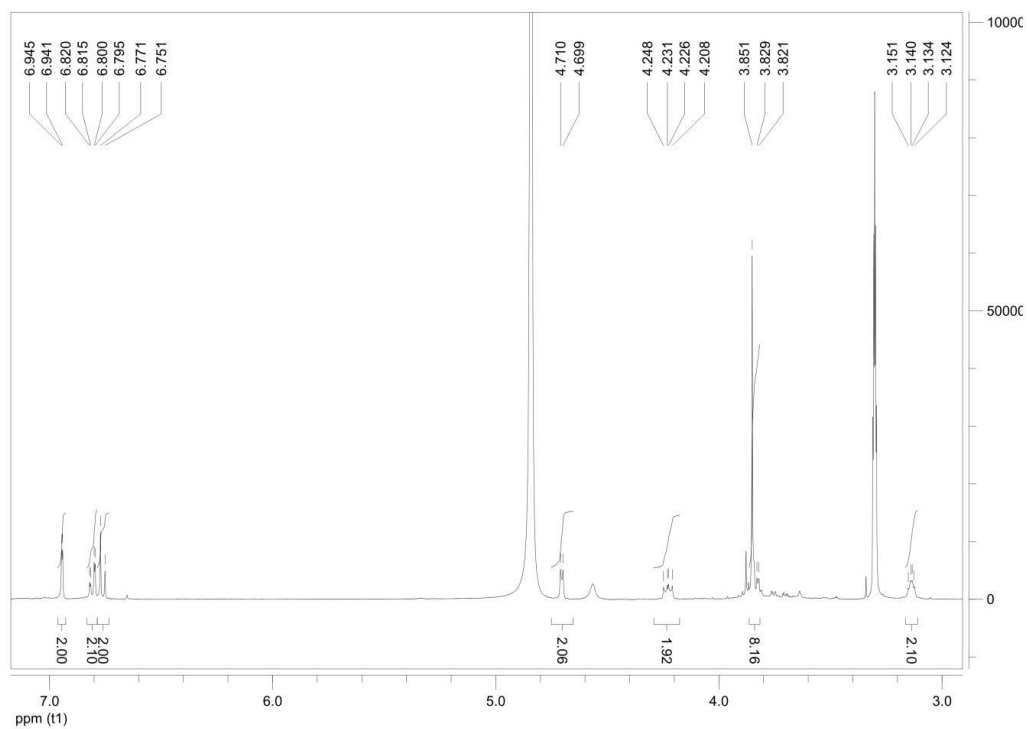


Figure S31: ^1H NMR spectrum of **7** in CD_3OD (400 MHz)

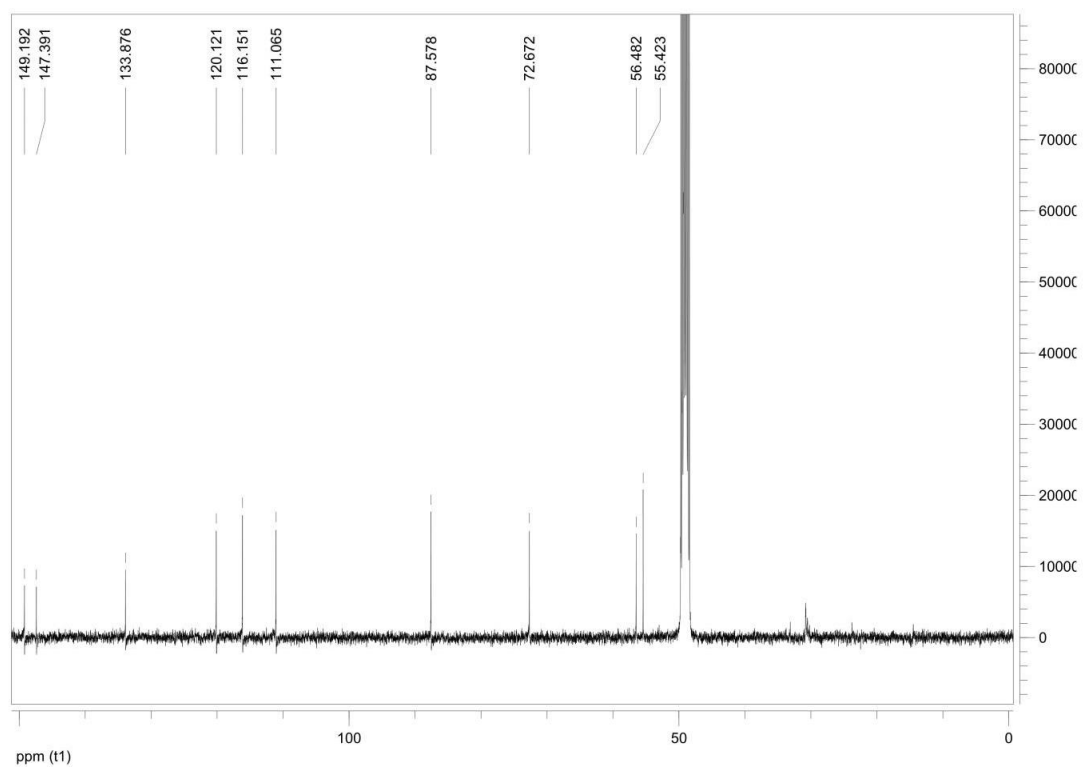


Figure S32: ^{13}C NMR spectrum of **7** in CD_3OD (100 MHz)

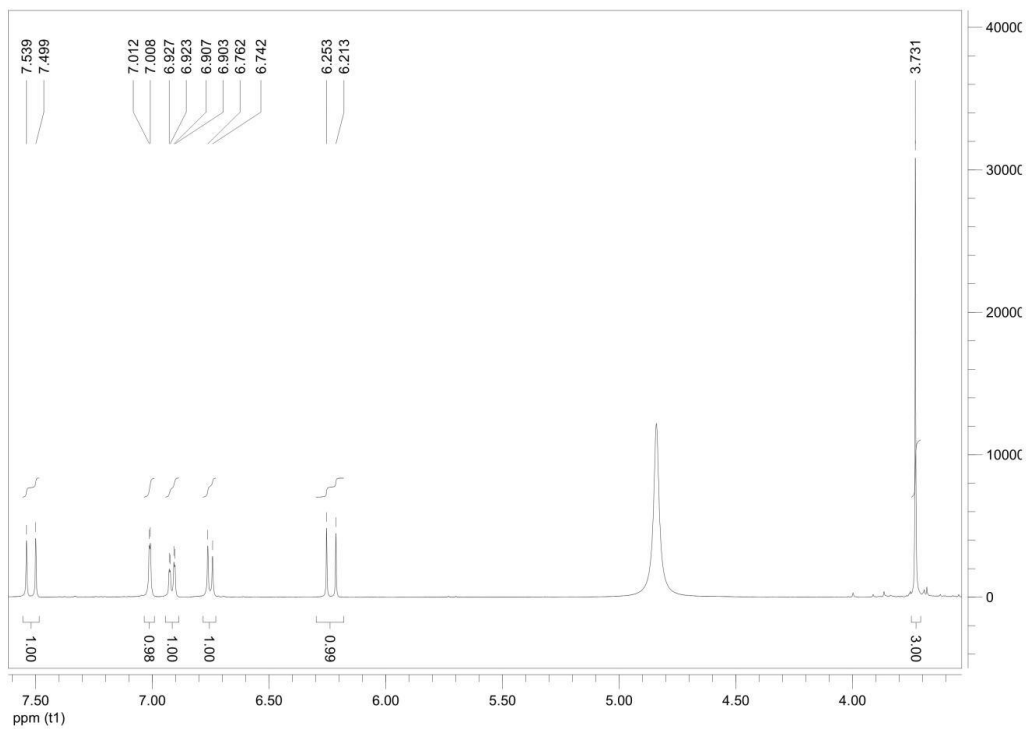


Figure S33: ^1H NMR spectrum of **8** in CD_3OD (400 MHz)

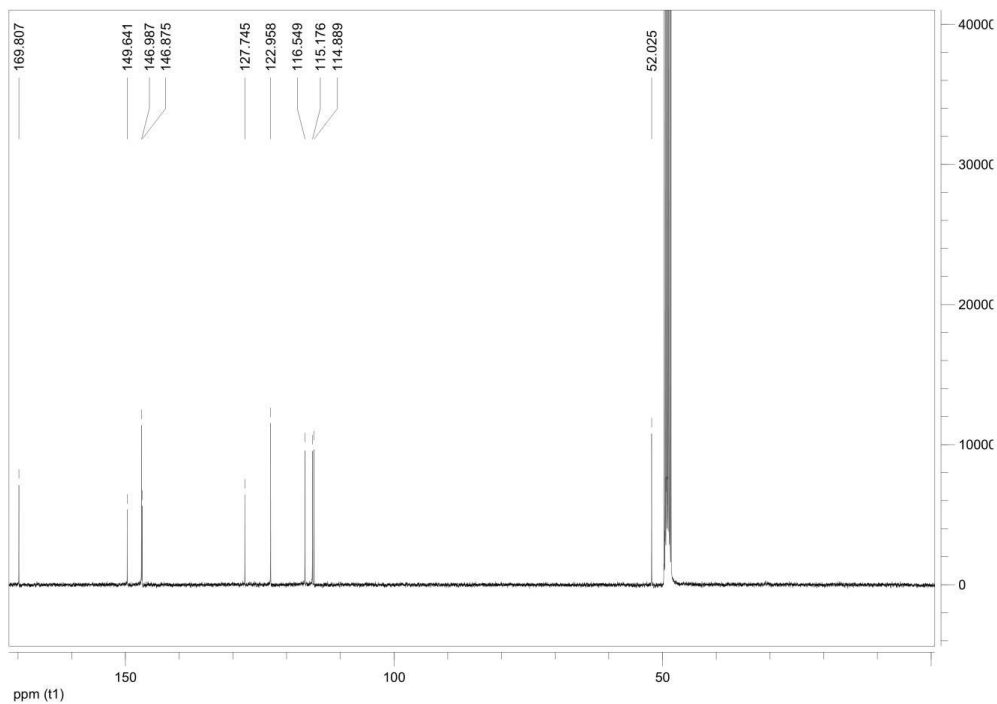


Figure S34: ^{13}C NMR spectrum of **8** in CD_3OD (100 MHz)

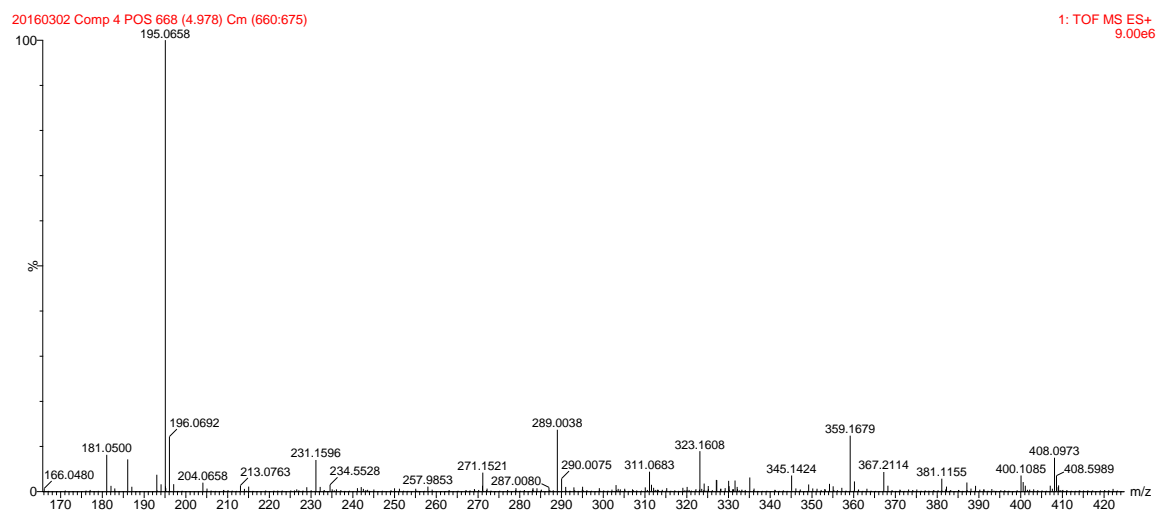


Figure S35: HRMS spectrum of **8**

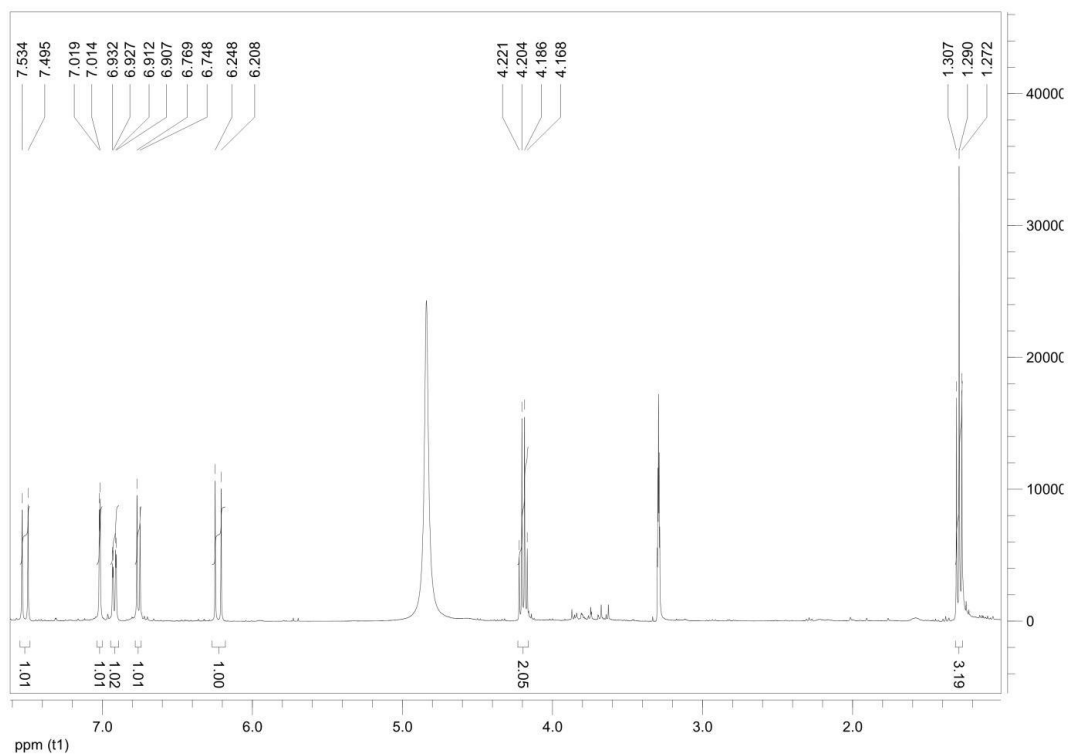


Figure S36: ^1H NMR spectrum of **9** in CD_3OD (400 MHz)

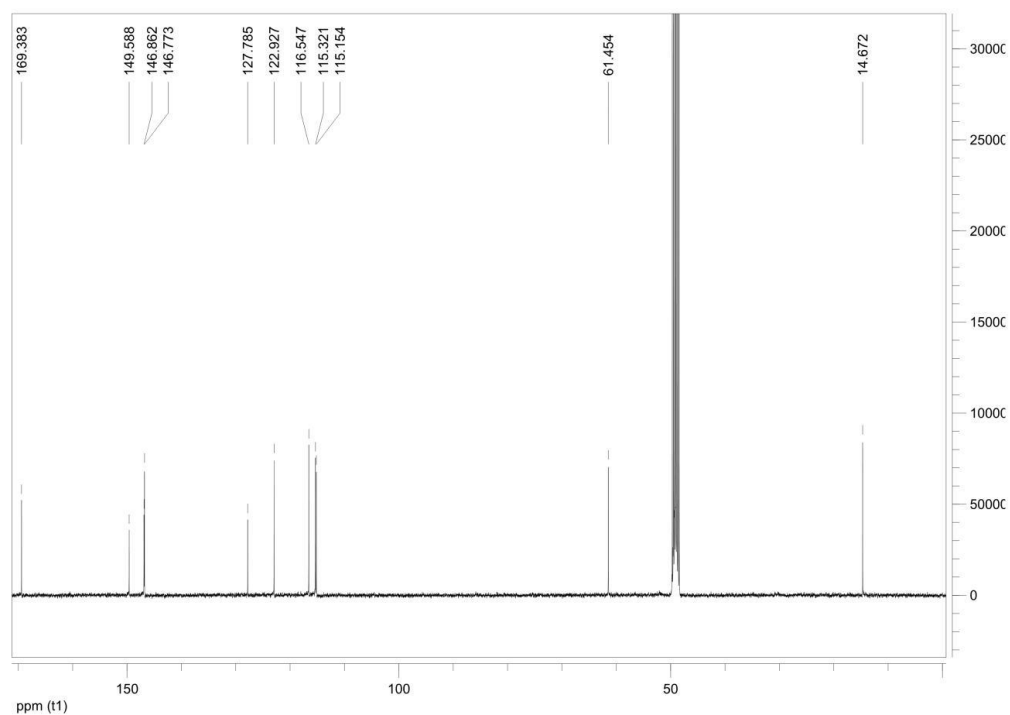


Figure S37: ^{13}C NMR spectrum of **9** in CD_3OD (100 MHz)

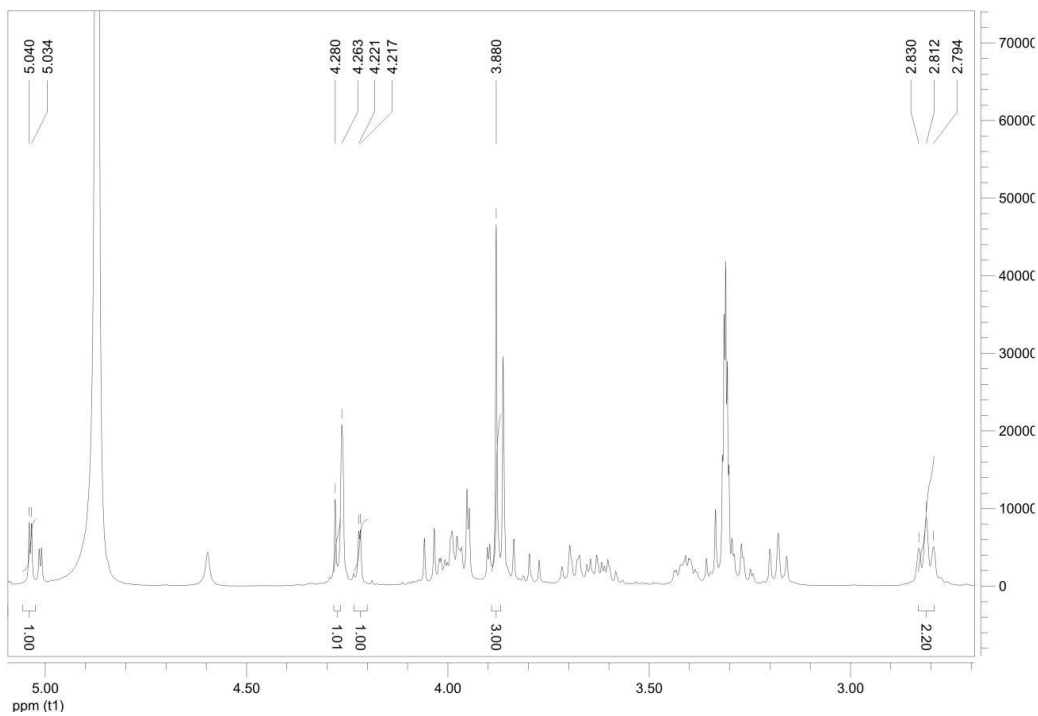


Figure S38: ^1H NMR spectrum of **10** in CD_3OD (400 MHz)

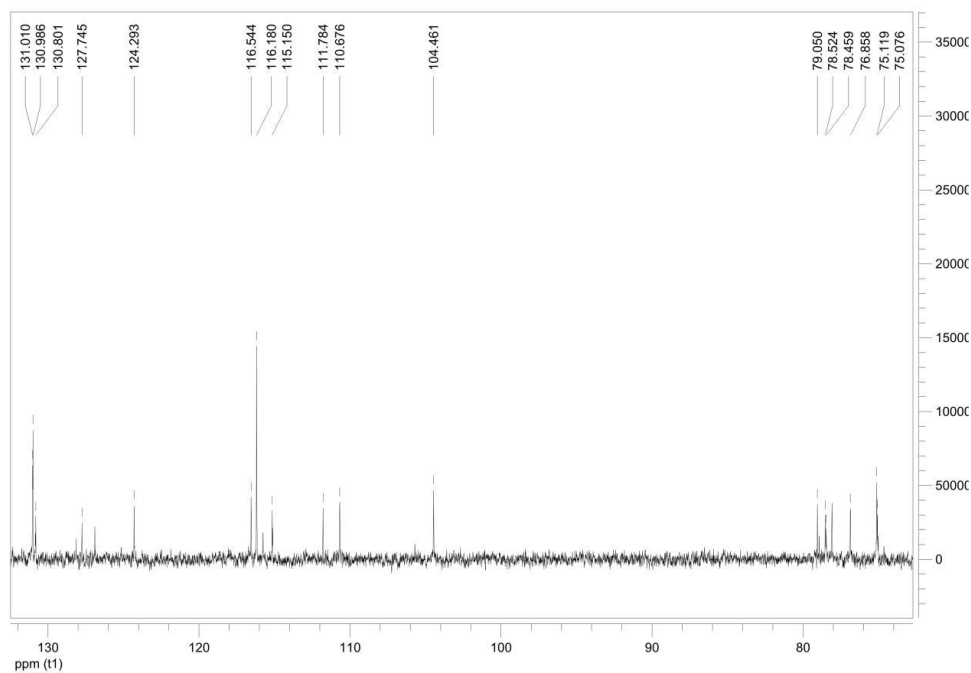


Figure S39: ^{13}C NMR spectrum of **10** in CD_3OD (100 MHz)

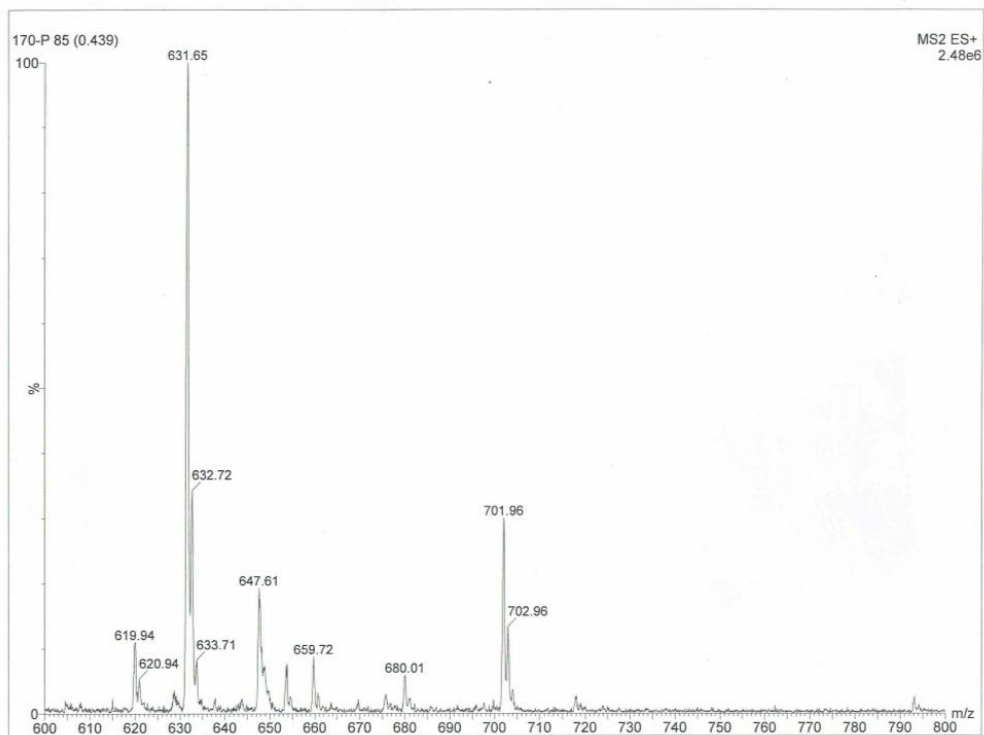


Figure S40: MS spectrum of **10**

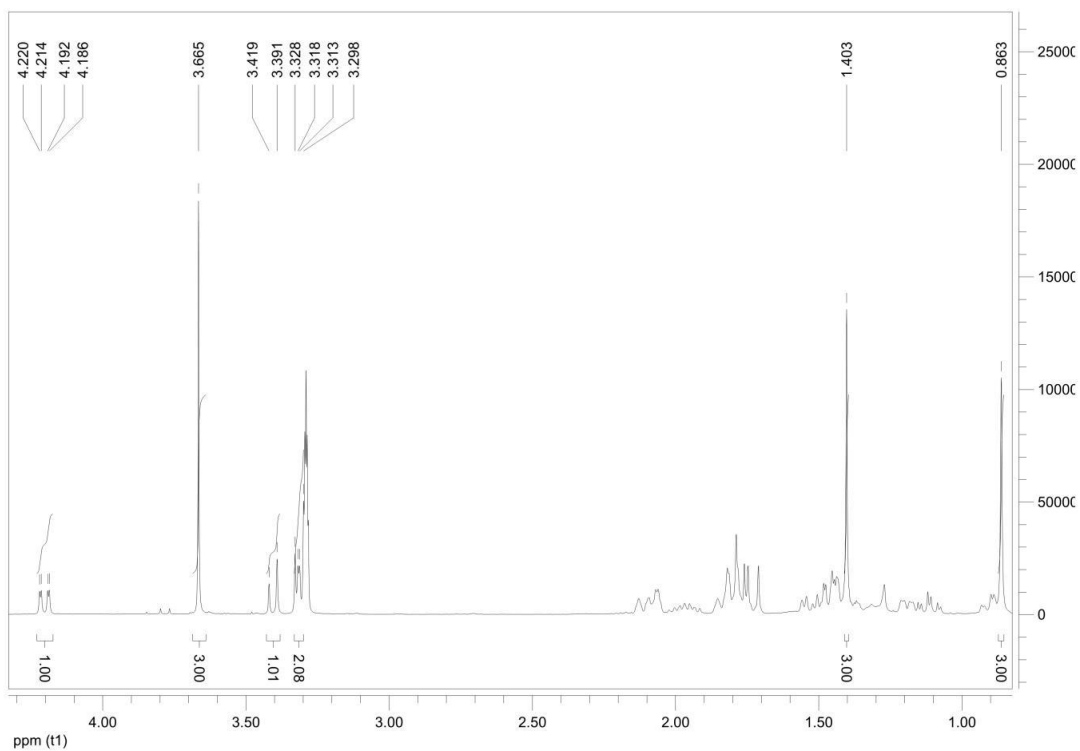


Figure S41: ^1H NMR spectrum of **11** in CD_3OD (400 MHz)

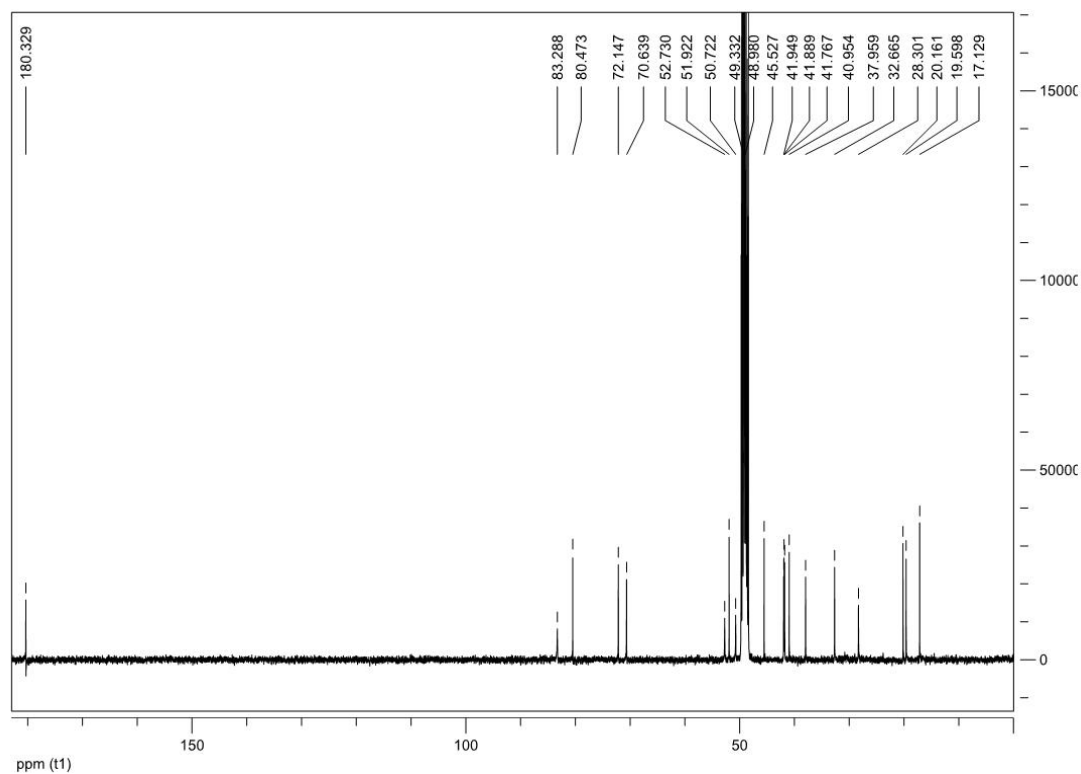


Figure S42: ^{13}C NMR spectrum of **11** in CD_3OD (100 MHz)

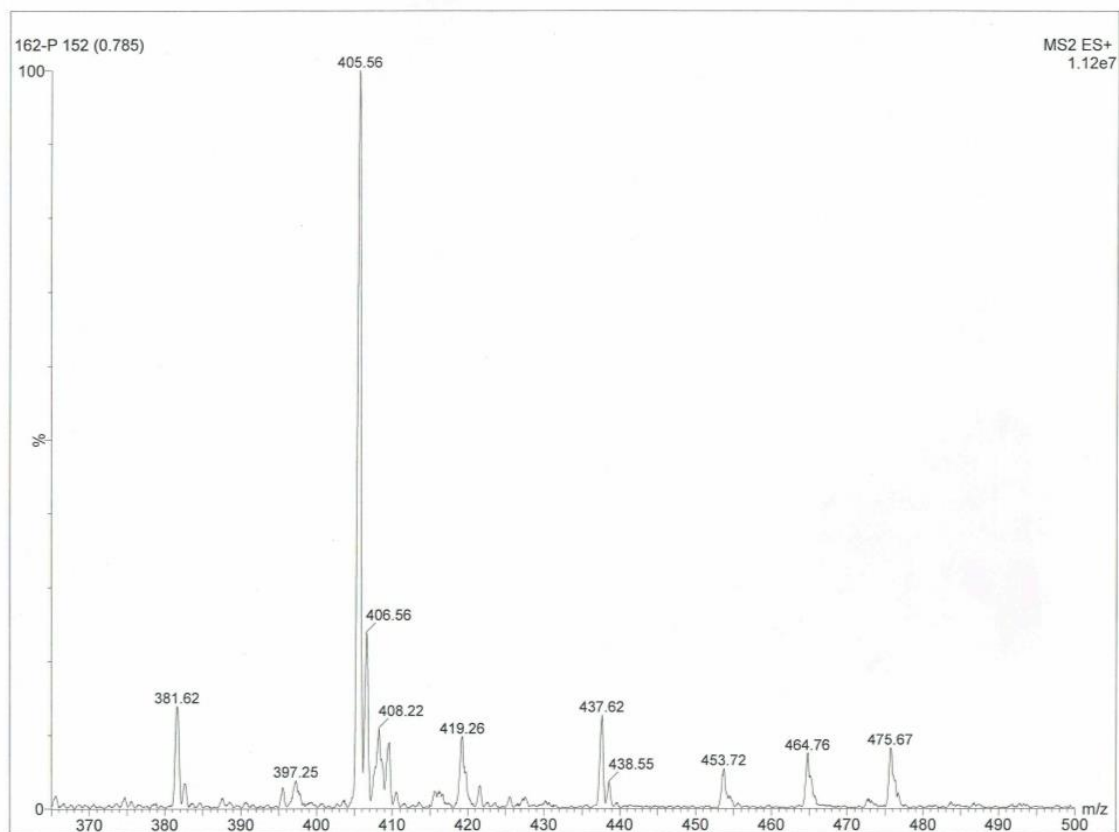


Figure S43: MS spectrum of **11**

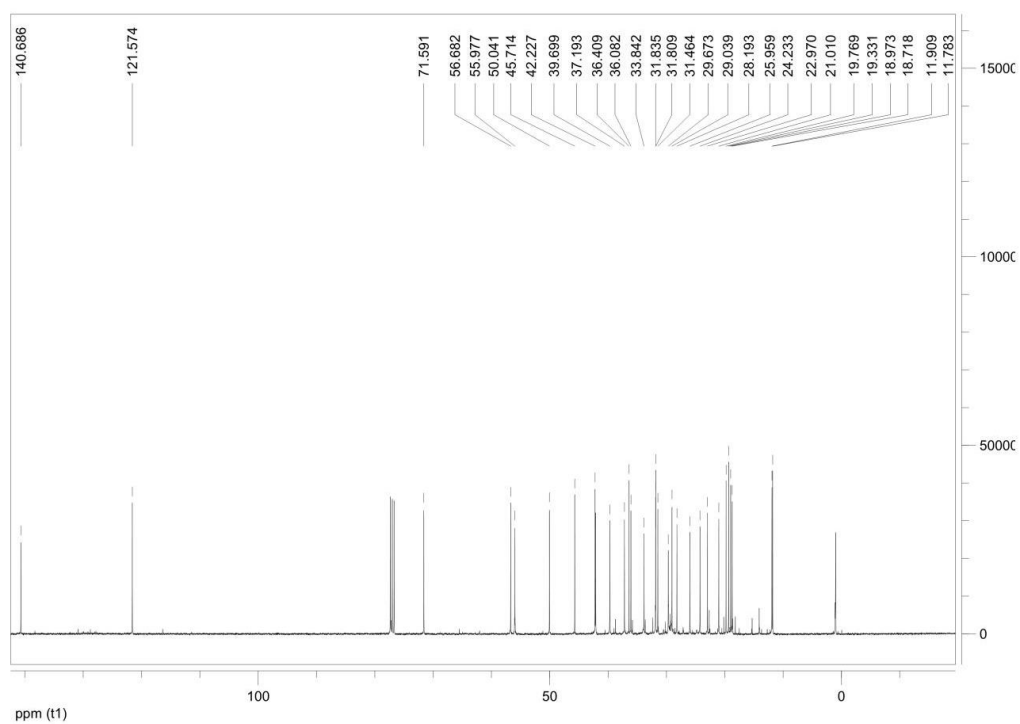


Figure S46: ^{13}C NMR spectrum of **12** in CDCl_3 (100 MHz)

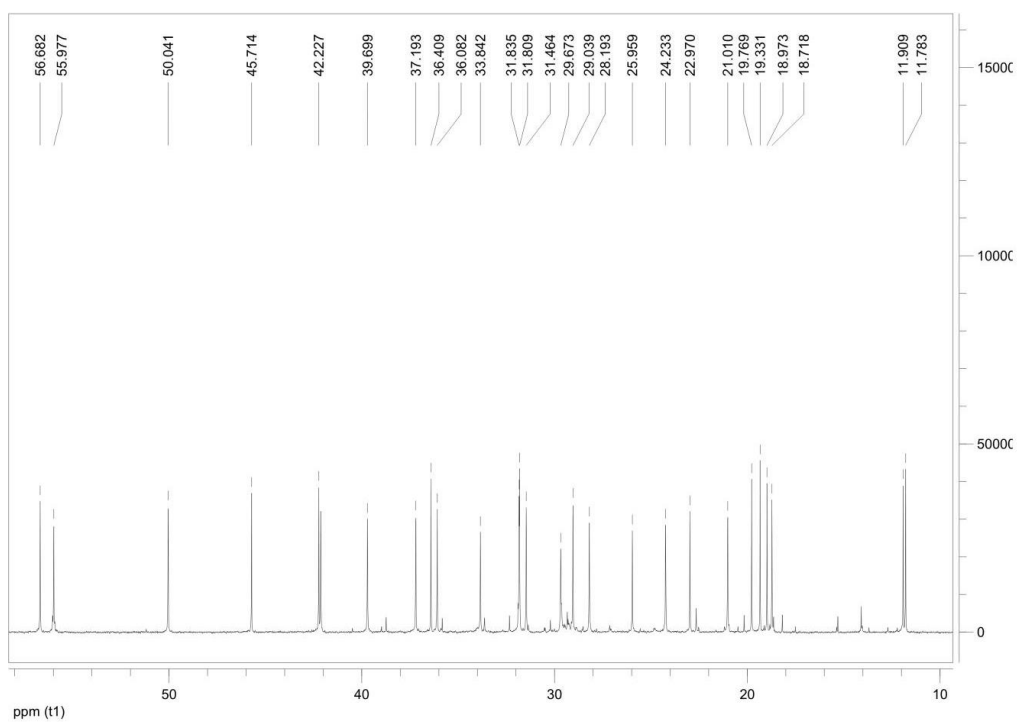


Figure S47: Selected ^{13}C NMR spectrum of **12** in CDCl_3

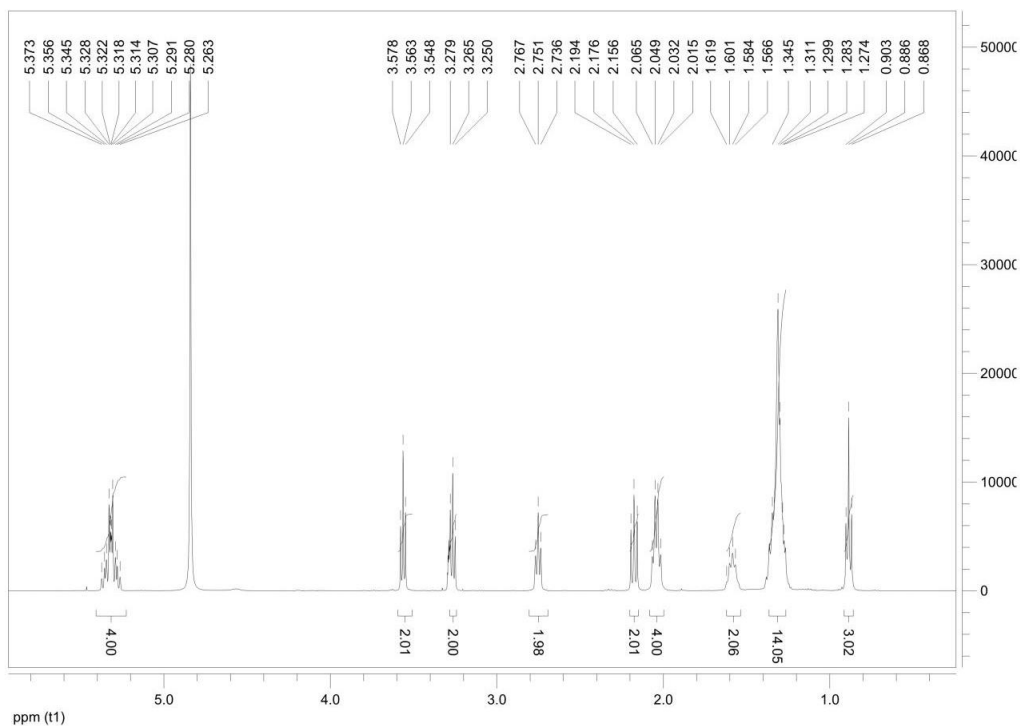


Figure S48: ^1H NMR spectrum of **13** in CD_3OD (400 MHz)

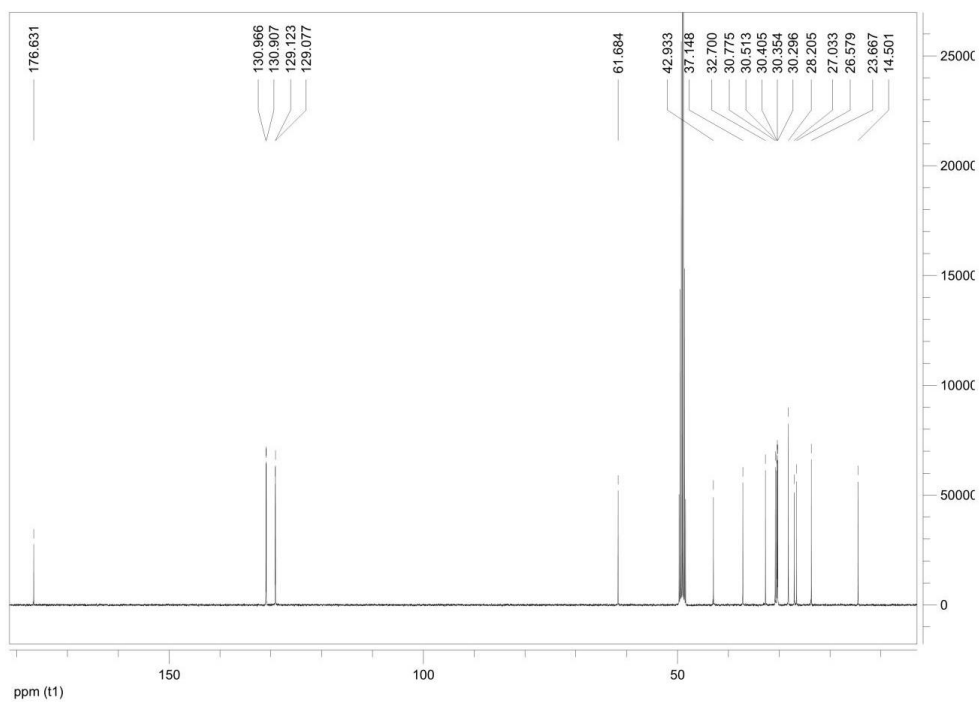


Figure S49: ^{13}C NMR spectrum of **13** in CD_3OD (100 MHz)

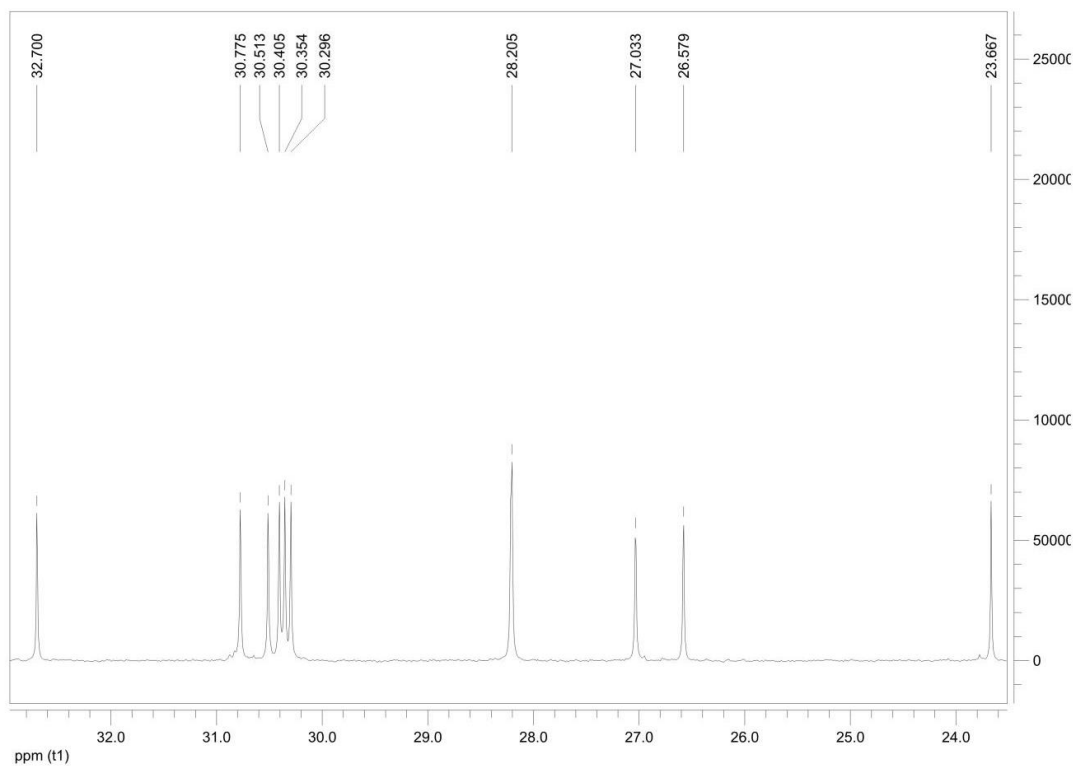


Figure S50: Selected ^{13}C NMR spectrum of **13** in CD_3OD (1)

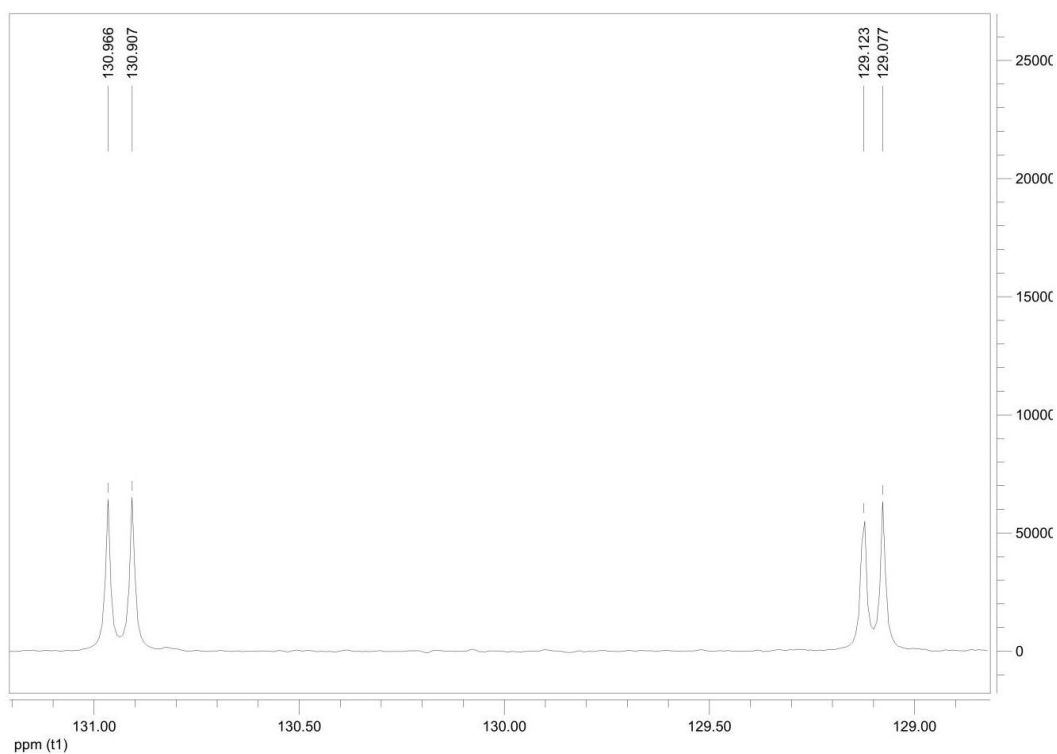


Figure S51: Selected ^{13}C NMR spectrum of **13** in CD_3OD (2)

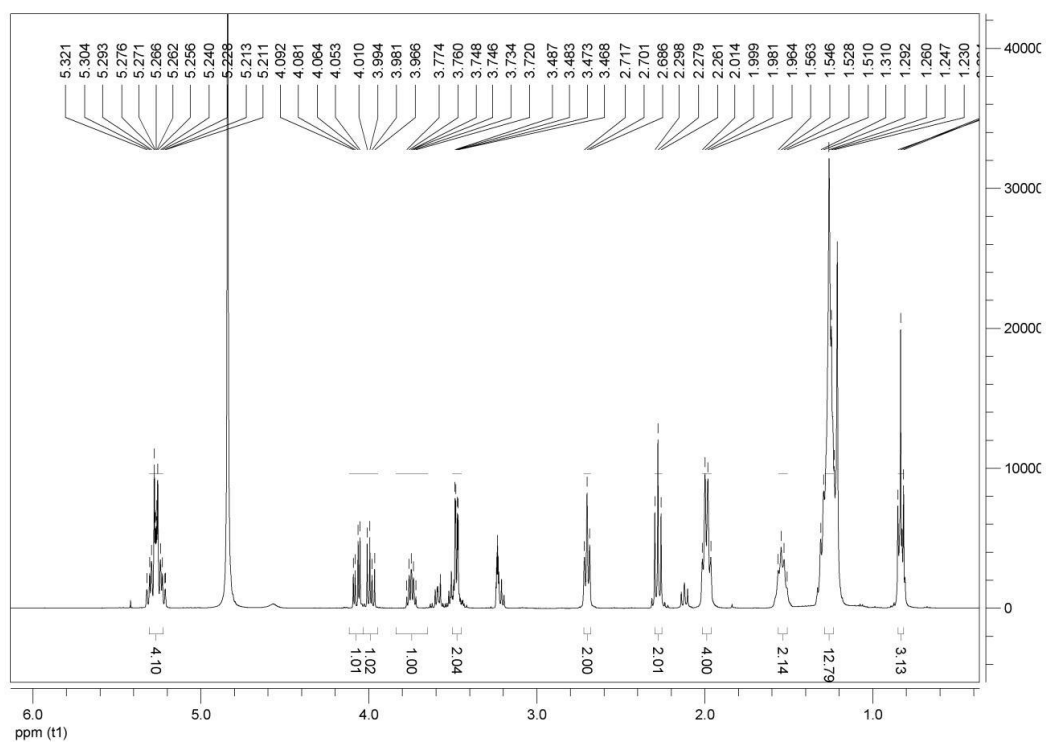
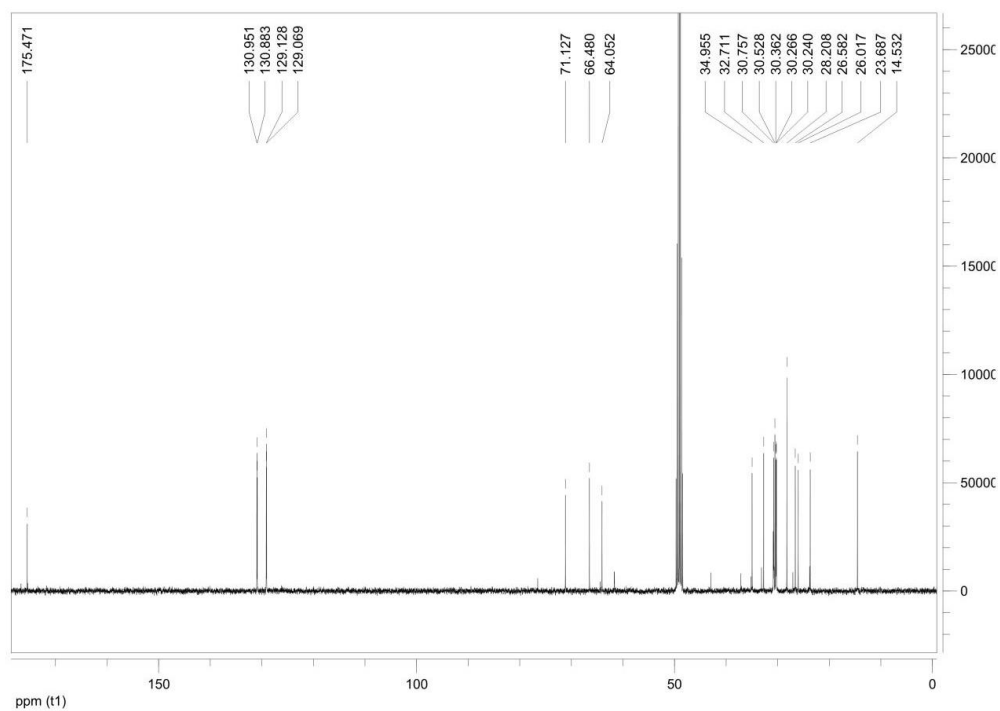


Figure S52: ^1H NMR spectrum of **14** in CD_3OD (400 MHz)



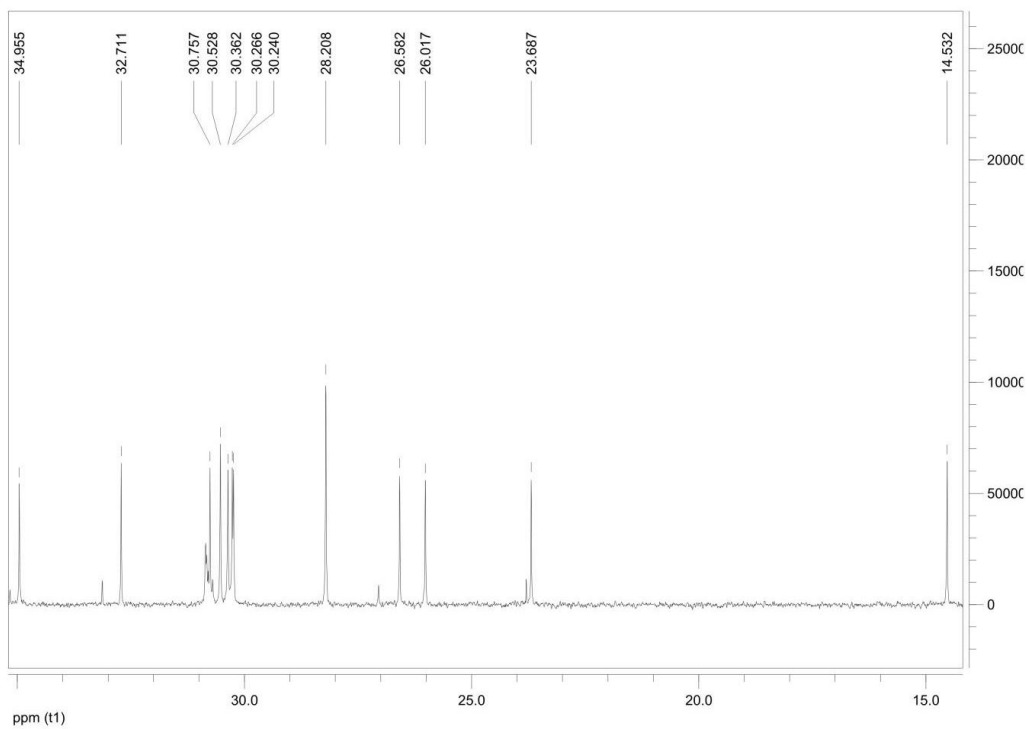


Figure S54: Selected ^{13}C NMR spectrum of **14** in CD_3OD (1)

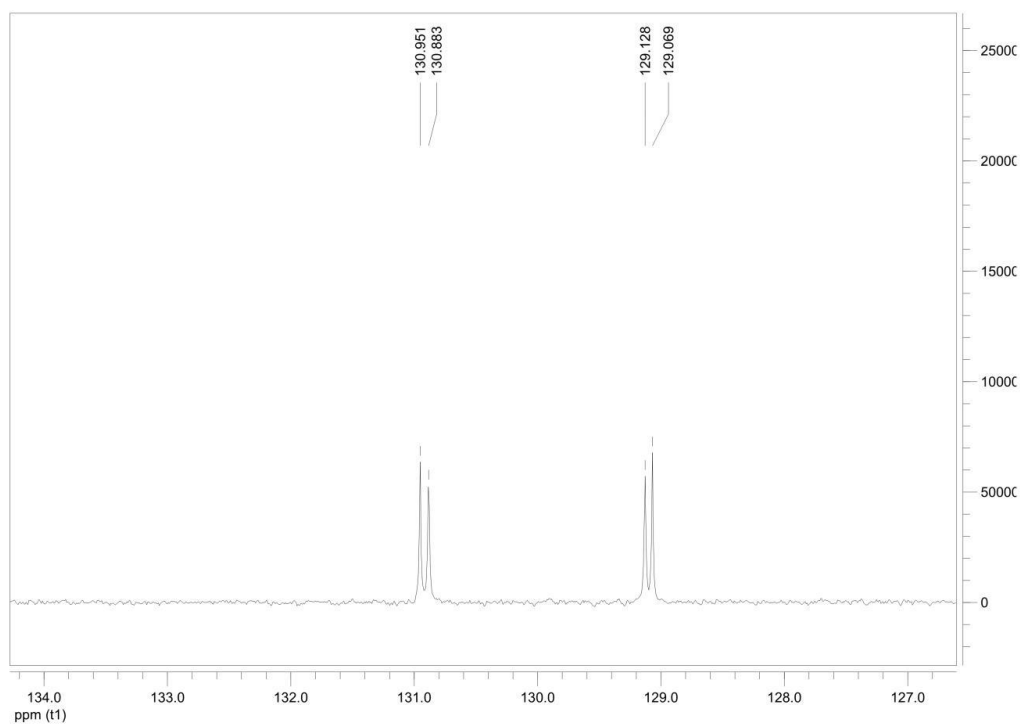


Figure S55: Selected ^{13}C NMR spectrum of **14** in CD_3OD (2)