

Pyrrole Alkaloids from the Fruiting Bodies of the Edible

Mushroom *Lentinula edodes*

Zhen-Zhu Zhao, Fei Zhang, Bao-Yu Ji, Ning Zhou, Hui Chen, Yan-Jun Sun, Wei-Sheng Feng*,
Xiao-Ke Zheng*

School of Pharmacy, Henan University of Chinese Medicine, Zhengzhou 450046, China

Corresponding Authors

fwsh@hactcm.edu.cn (W.-S. Feng); zhengxk.2006@163.com (X.-K. Zheng)

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1. Spectroscopic data

Figure S1. ¹H NMR spectrum of 1 (600 MHz, CD₃OD)

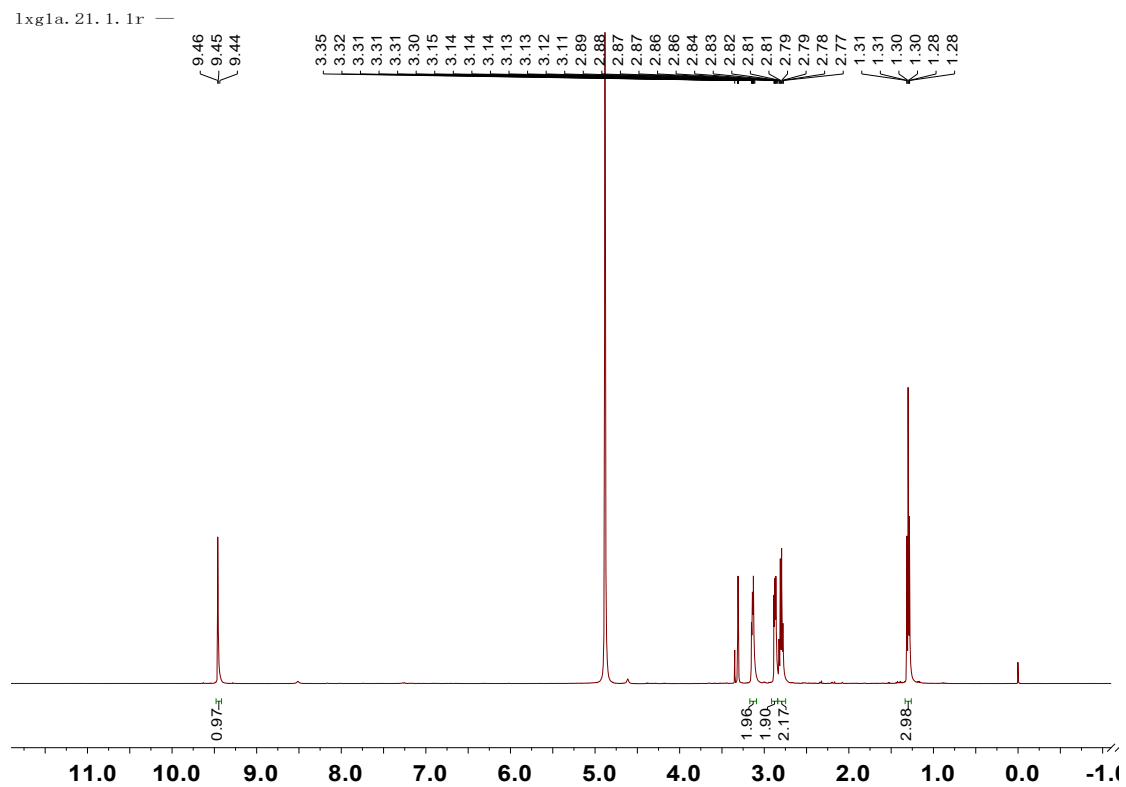


Figure S2. ¹³C and DEPT NMR spectra of 1 (150 MHz, CD₃OD)

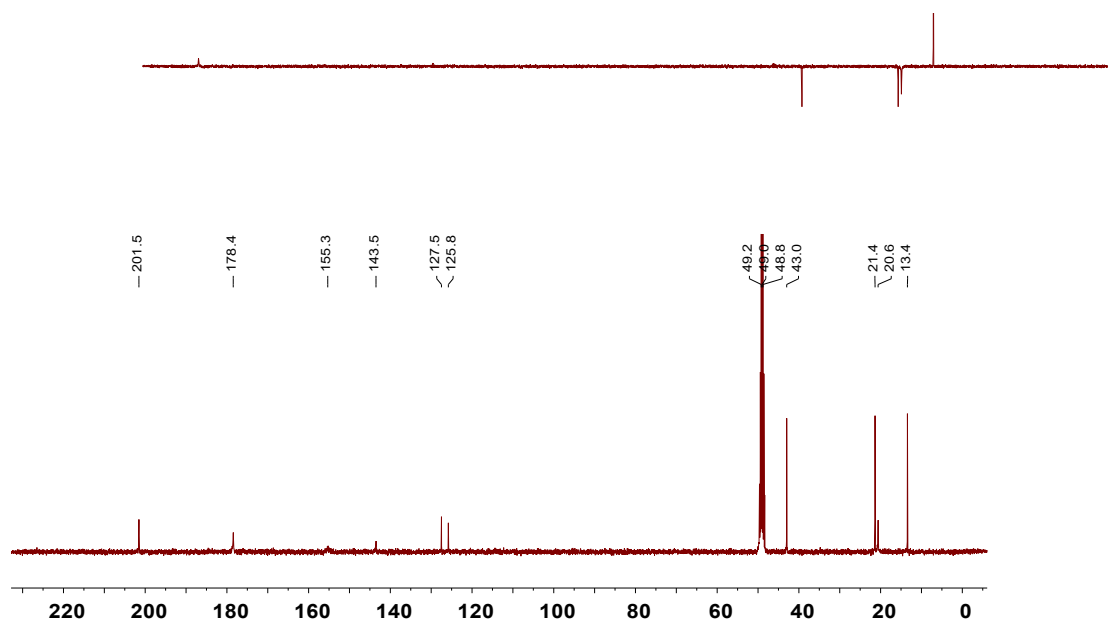


Figure S3. HMBC spectrum of 1

1xg1a.27.1.2rr — 1xg1a hmhc

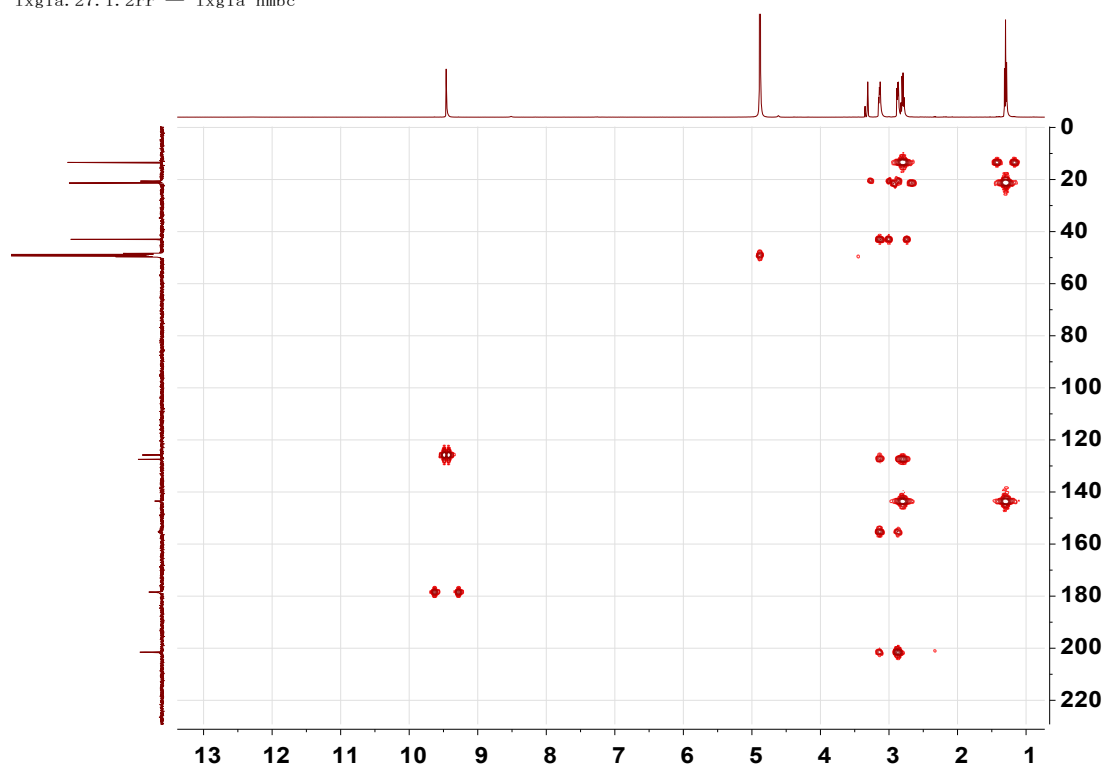


Figure S4. HRESIMS report of 1

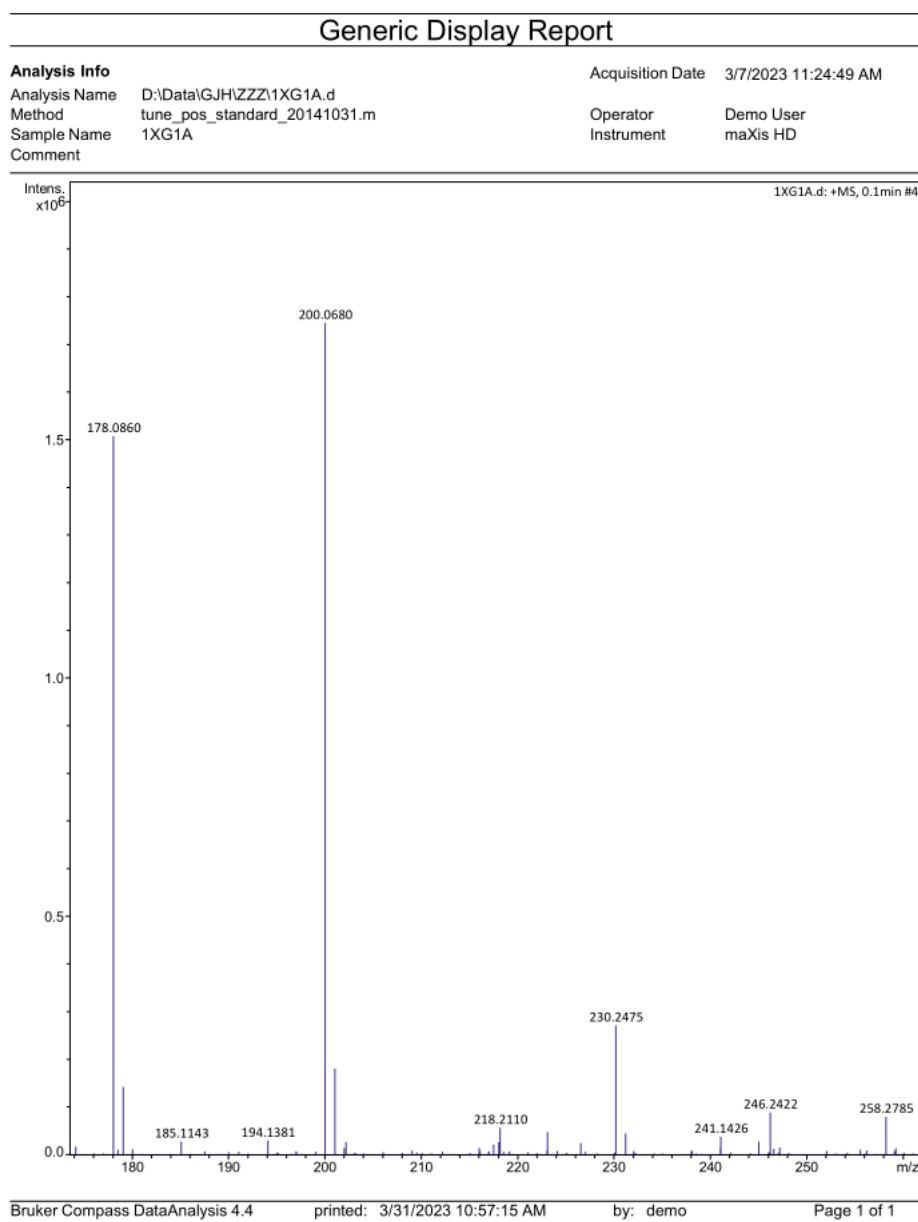


Figure S5. IR report of 1

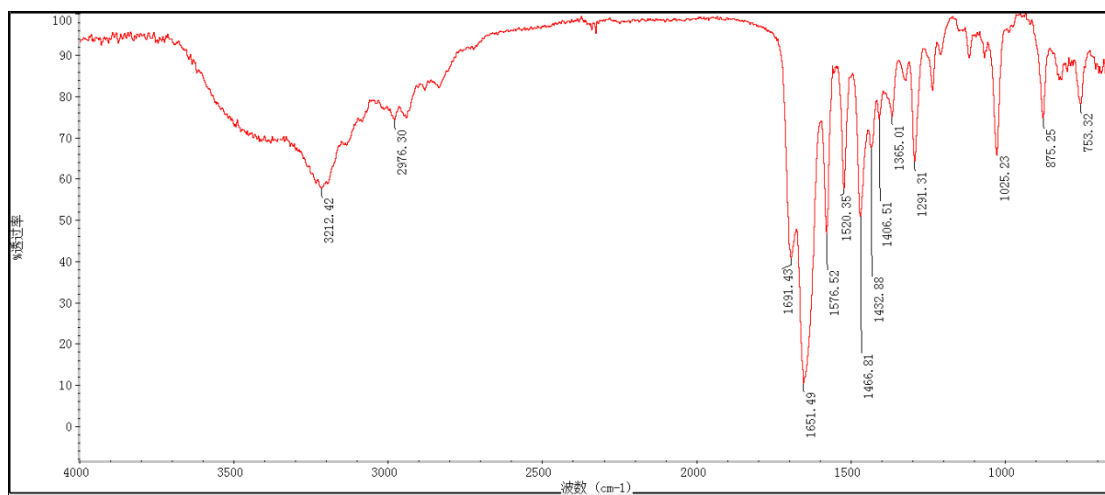


Figure S6. ^1H NMR spectrum of **2** (600 MHz, CD_3OD)

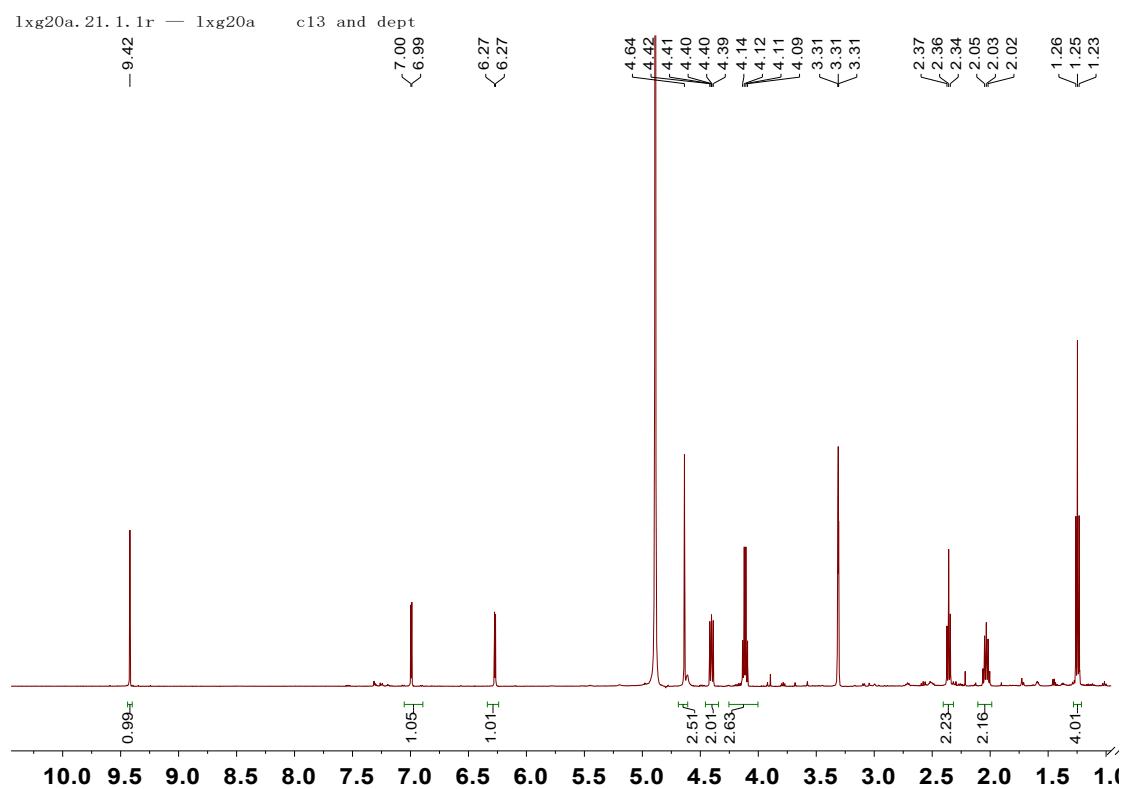


Figure S7. ^{13}C and DEPT NMR spectra of **2** (150 MHz, CD_3OD)

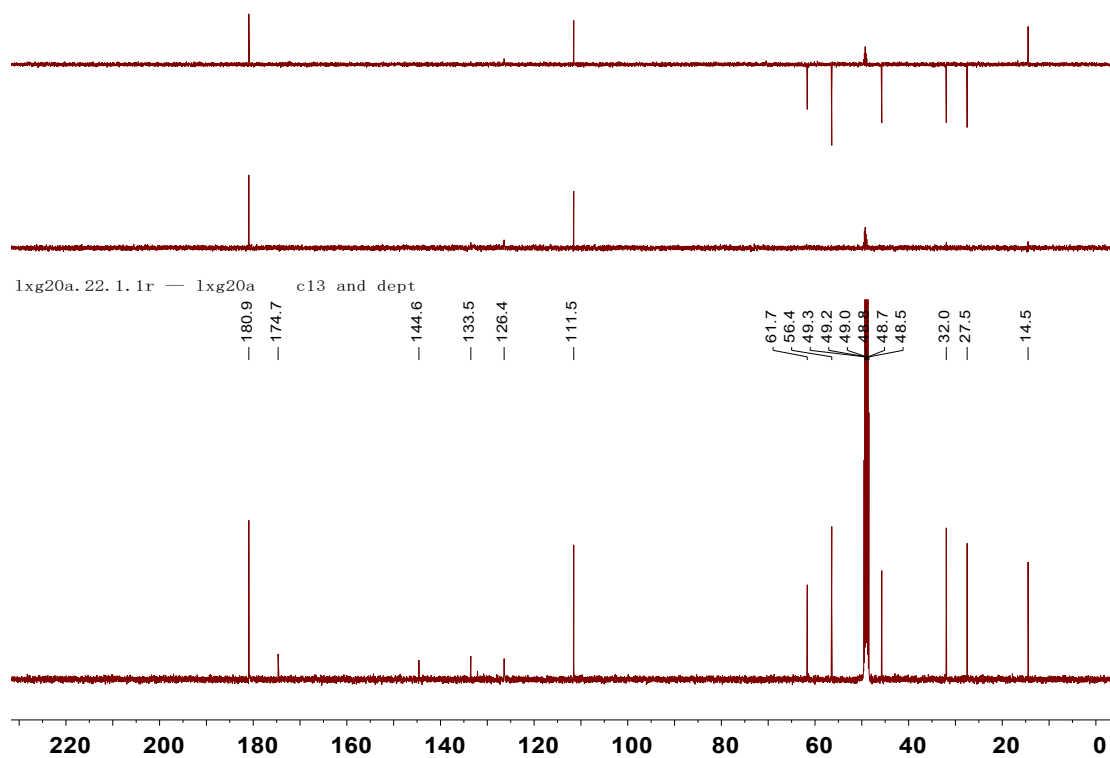


Figure S8. HSQC spectrum of 2

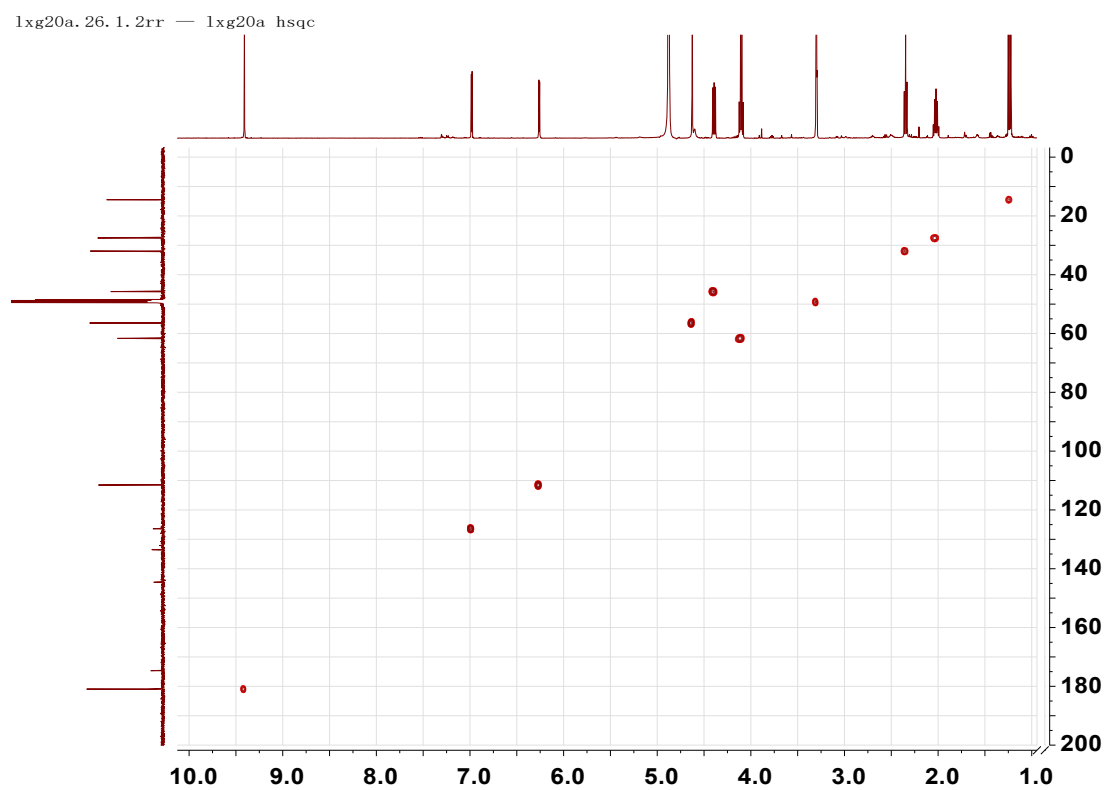


Figure S9. HMBC spectrum of 2

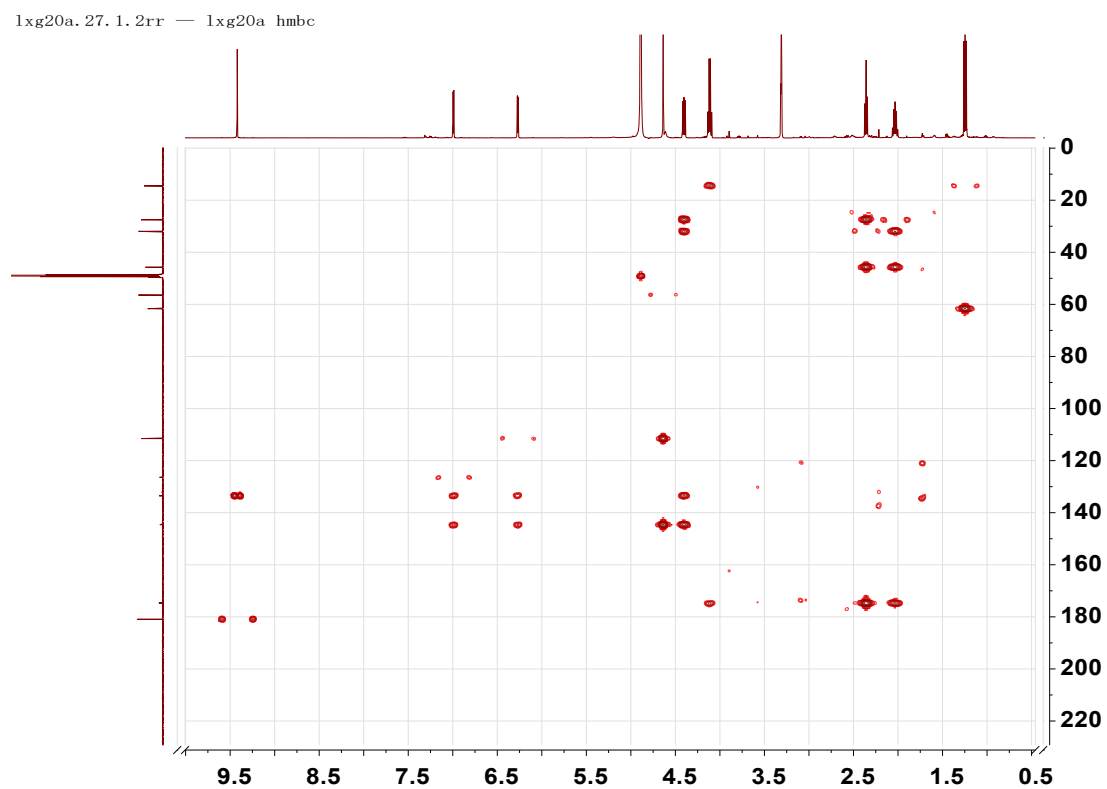


Figure S10. HRESIMS report of 2

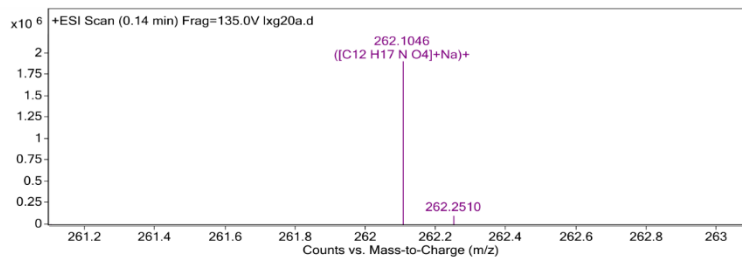
Qualitative Analysis Report

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Sample Type	Sample	Position	P1-A4
Instrument Name	Instrument 1	User Name	
Acq Method	s.m	Acquired Time	4/13/2018 2:13:55 PM
IRM Calibration Status	Success	DA Method	Default.m
Comment			

Sample Group Info.
Acquisition SW 6200 series TOF/6500 series
Version Q-TOF B.05.01 (B5125.2)

User Spectra

Fragmentor Voltage 135 **Collision Energy** 0 **Ionization Mode** ESI



Peak List

m/z	z	Abund	Formula	Ion
102.1269	1	513321.69		
200.1268	1	393223.44		
222.111	1	1169930.88		
262.1046	1	1912241.25	C12 H17 N O4	(M+Na)+
278.0785	1	541678.94		
461.2267	1	366489.53		
501.2225	1	1421629.38		
502.2253	1	391769.81		

Formula Calculator Element Limits

Element	Min	Max
C	3	60
H	0	120
O	0	30
N	0	3

Formula Calculator Results

Formula	CalculatedMass	CalculatedMz	Mz	Diff. (mDa)	Diff. (ppm)	DBE
C12 H17 N O4	239.1158	262.1050	262.1046	0.40	1.53	5.0000

--- End Of Report ---

Figure S11. IR report of 2

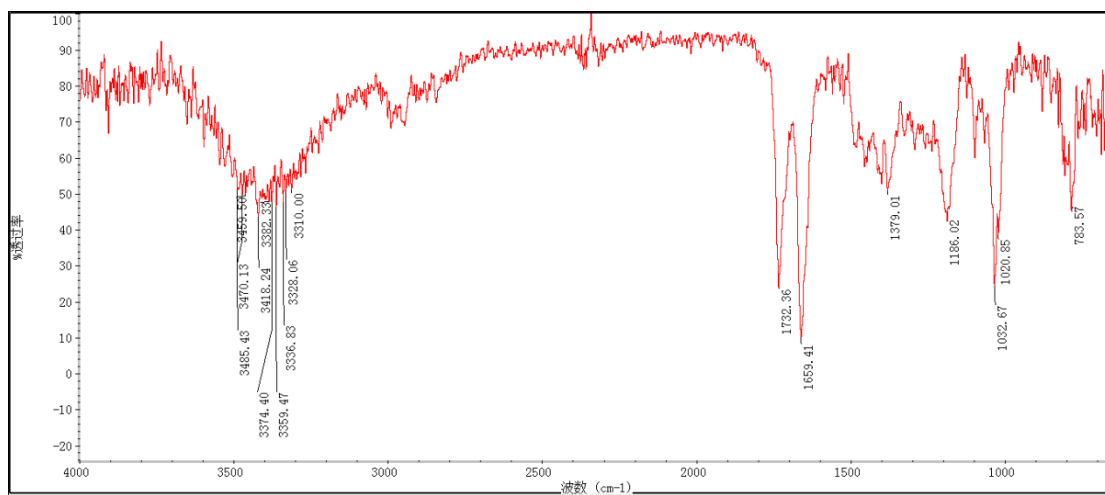


Figure S12. ¹H NMR spectrum of 3 (600 MHz, CD₃OD)

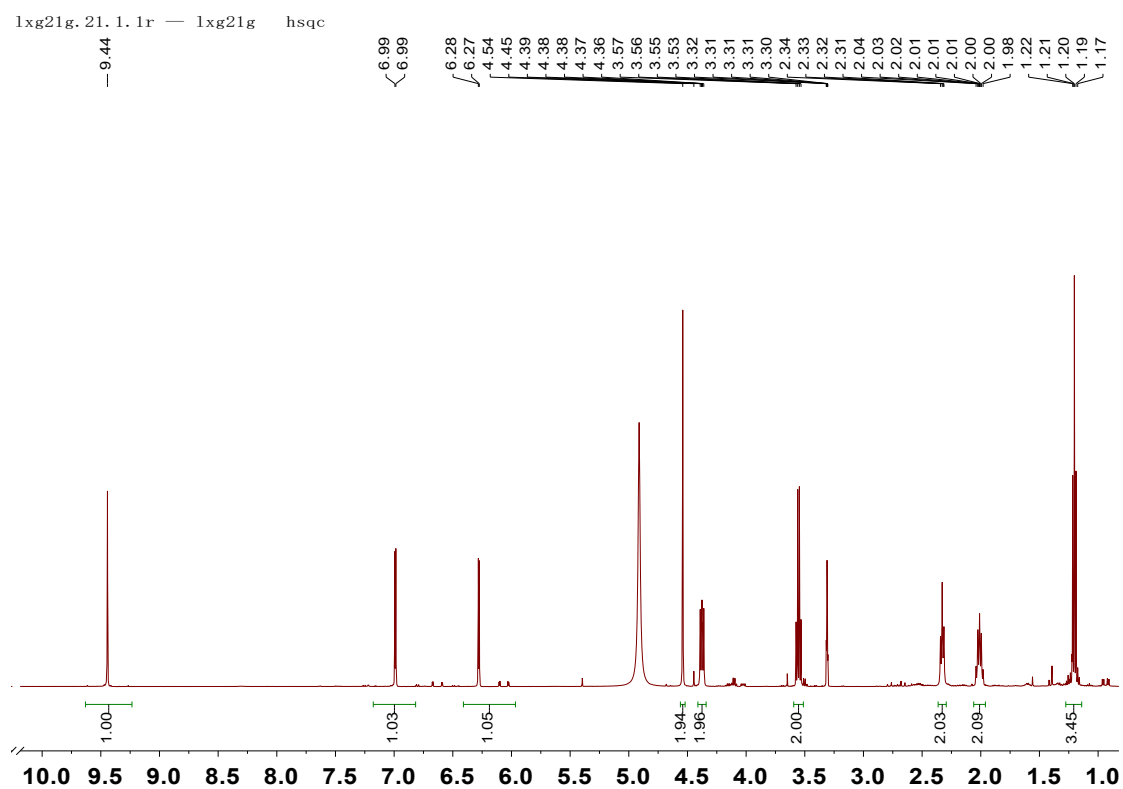


Figure S13. ¹³C and DEPT NMR spectra of 3 (150 MHz, CD₃OD)

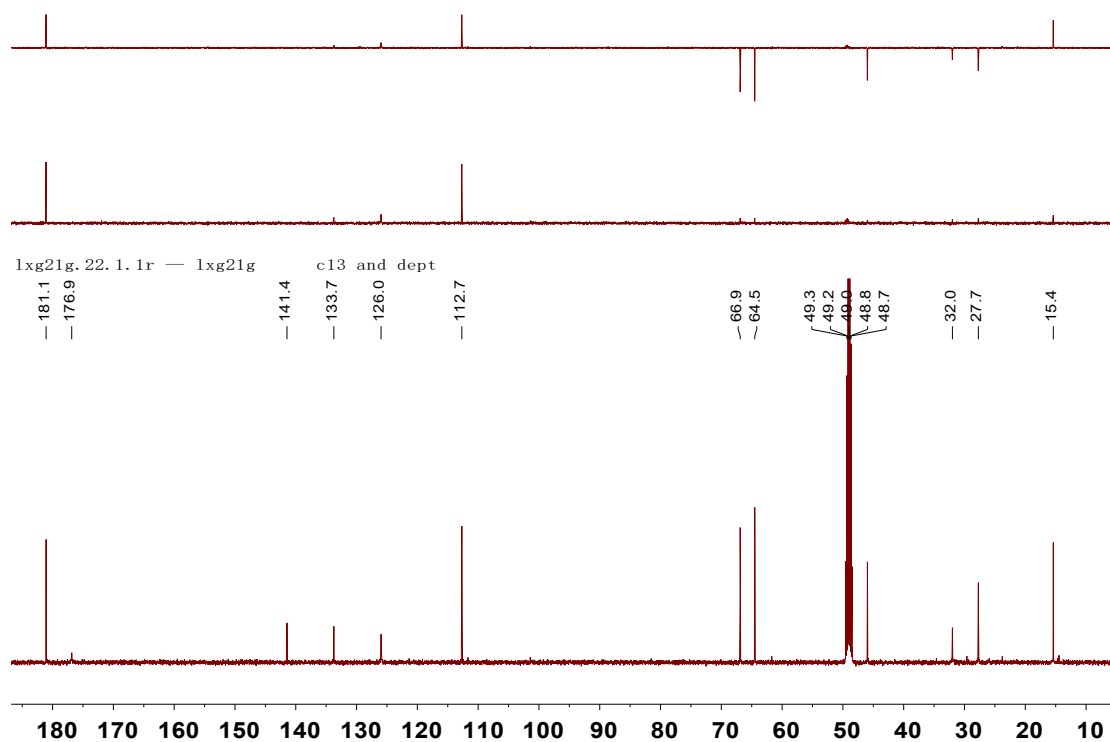


Figure S14. HSQC spectrum of 3

1xg21g.26.1.2rr — 1xg21g hsqc

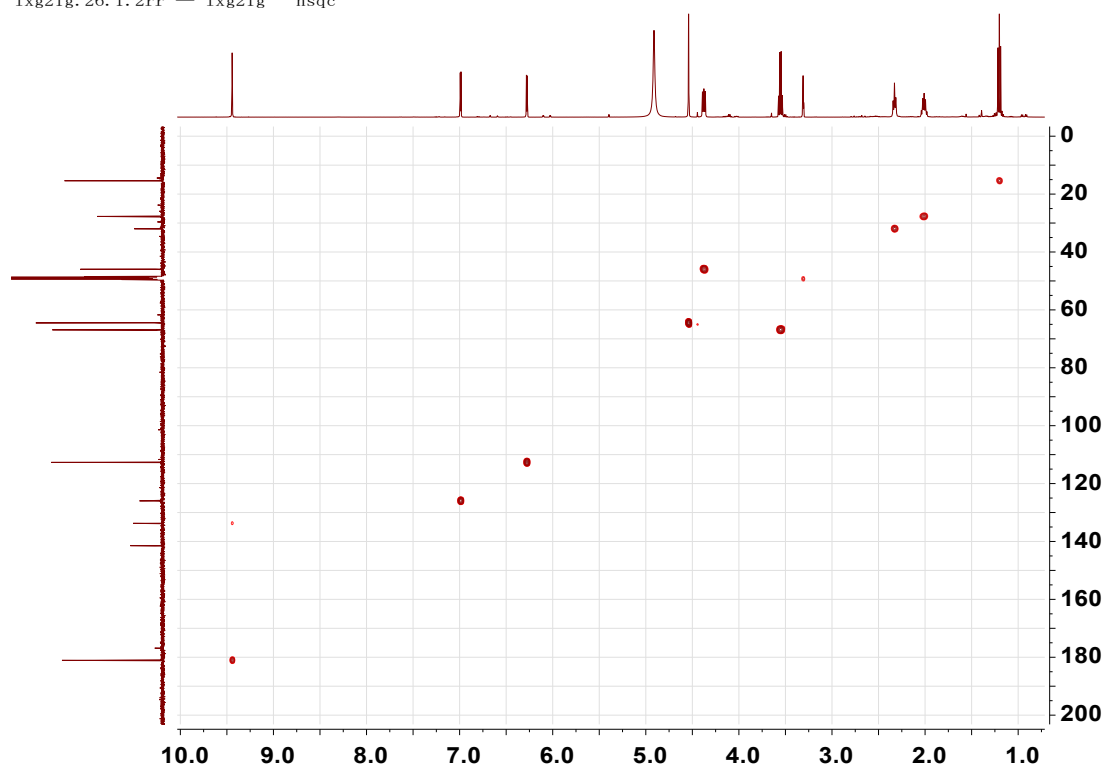


Figure S15. HMBC spectrum of 3

1xg21g.27.1.2rr — 1xg21g hmbc

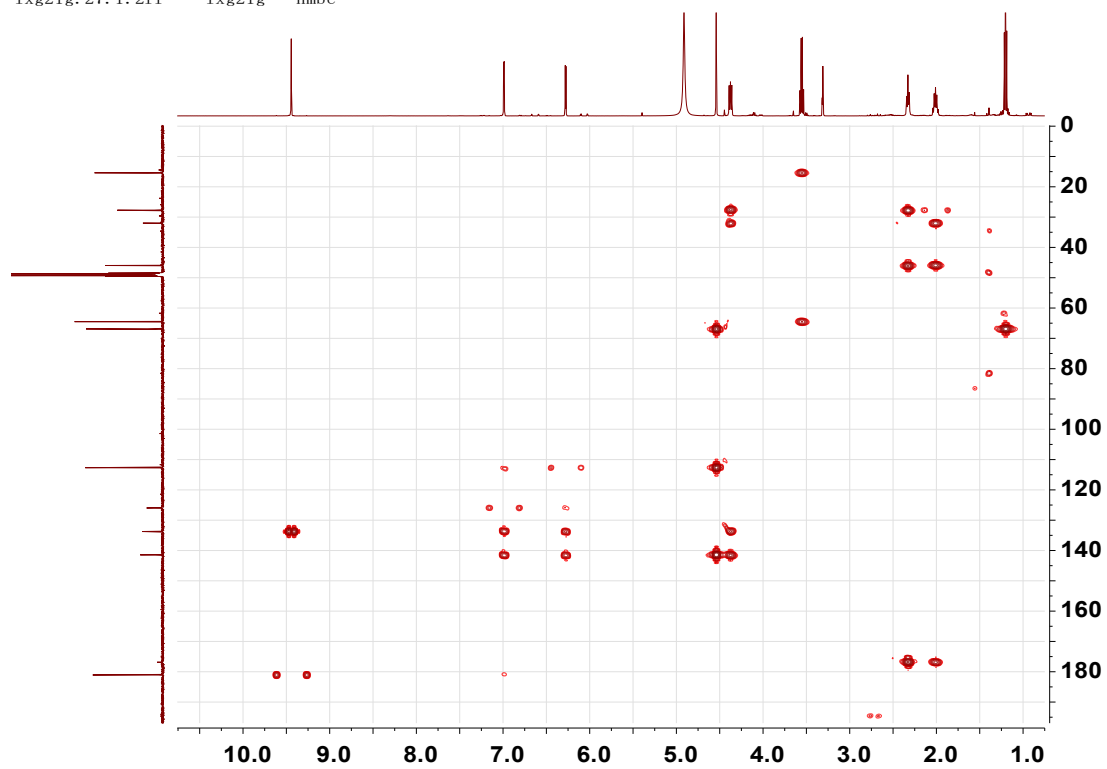


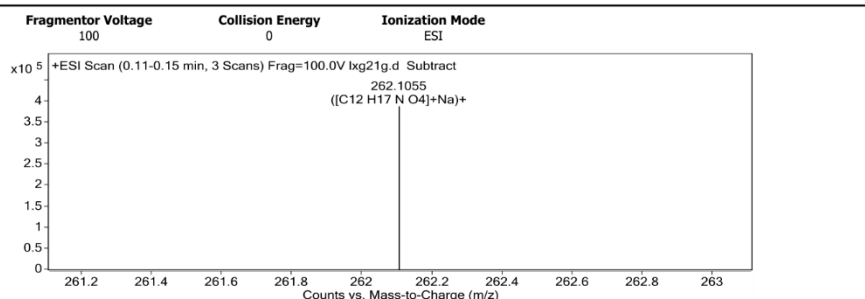
Figure S16. HRESIMS report of 3

Qualitative Analysis Report

Data Filename lkg21g.d **Sample Name** lkg21g
Sample Type Sample **Position** P1-A5
Instrument Name Instrument 1 **User Name**
Acq Method s.m **Acquired Time** 5/3/2018 10:10:32 AM
IRM Calibration Status Success **DA Method** Default.m
Comment

Sample Group **Info.**
Acquisition SW 6200 series TOF/6500 series
Version Q-TOF B.05.01 (B5125.2)

User Spectra



Peak List

m/z	z	Abund	Formula	Ion
194.081	1	35750.83		
262.1055	1	389479.88	C12 H17 N O4	(M+Na)+
263.1085	1	49929	C12 H17 N O4	(M+Na)+
278.0791	1	127673.75		
501.2211	1	110860.15		
502.2235	1	29897.03		
523.2029	1	27776.94		
540.2571	1	29902.53		

Formula Calculator Element Limits

Element	Min	Max
C	3	60
H	0	120
O	0	30
N	0	3

Formula Calculator Results

Formula	CalculatedMass	CalculatedMz	Mz	Diff. (mDa)	Diff. (ppm)	DBE
C12 H17 N O4	239.1158	262.1050	262.1055	-0.50	-1.91	5.0000

--- End Of Report ---

Figure S17. IR report of 3

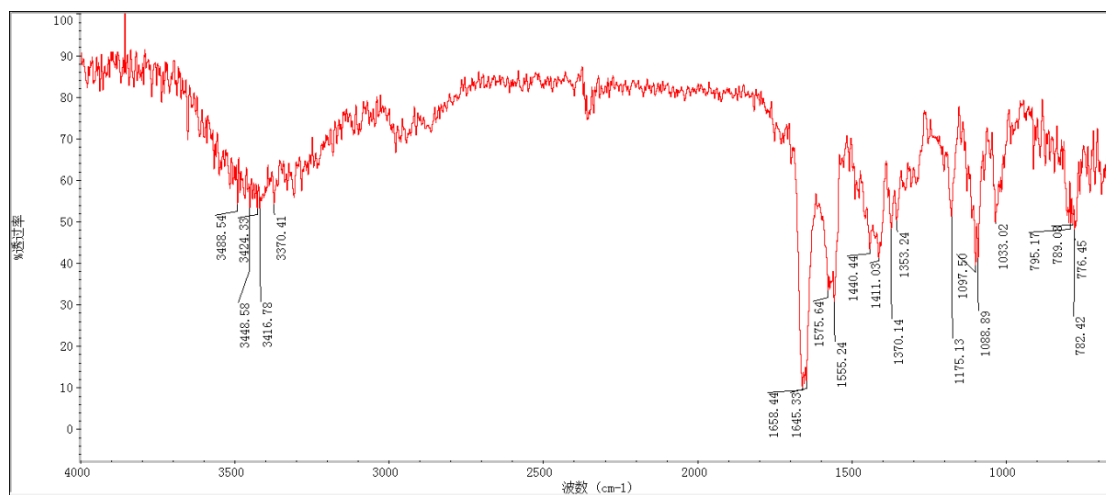


Figure S18. ¹H NMR spectrum of 4 (600 MHz, CD₃OD)

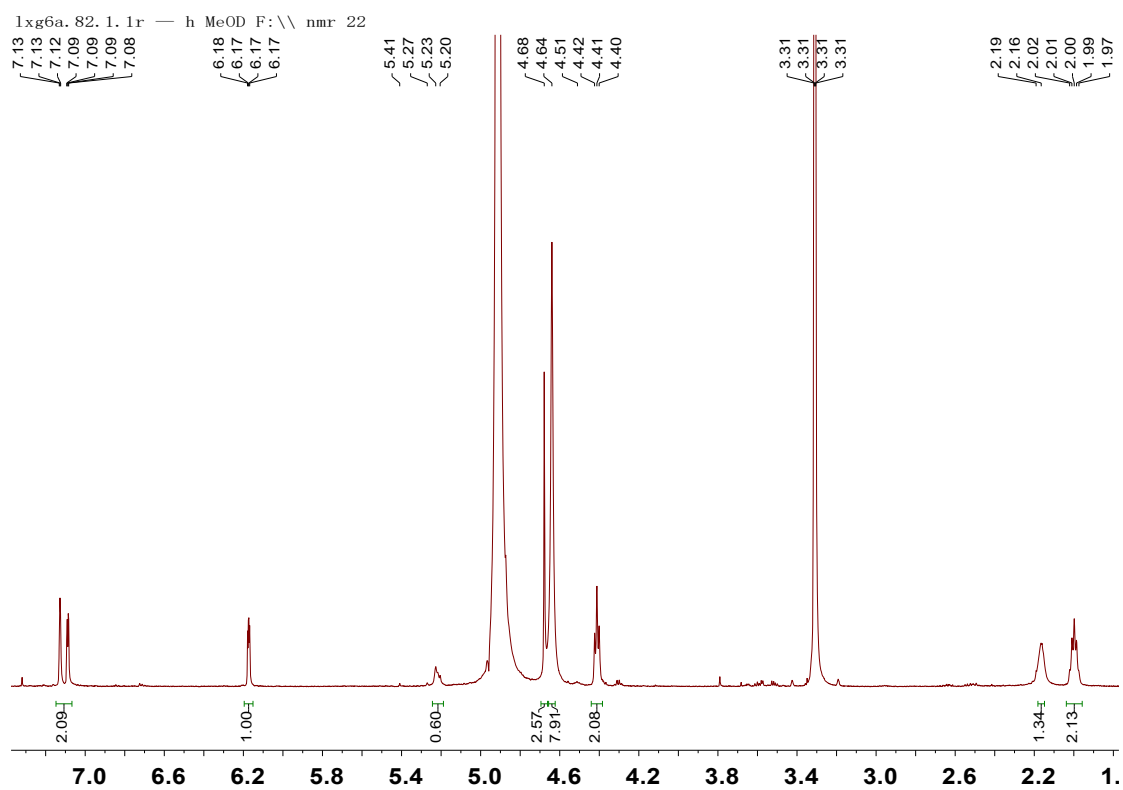


Figure S19. ¹³C and DEPT NMR spectra of 4 (150 MHz, CD₃OD)

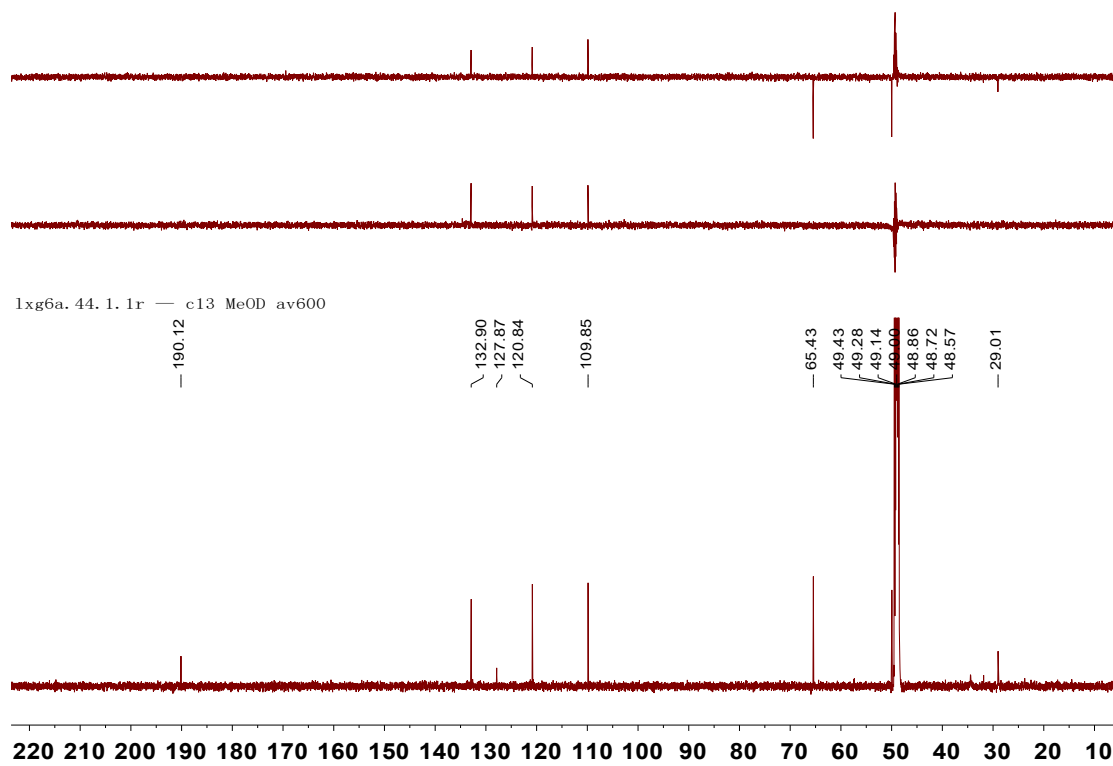


Figure S20. HSQC spectrum of 4

1xg6a. 84. 1. 2rr — hsqc MeOD av600

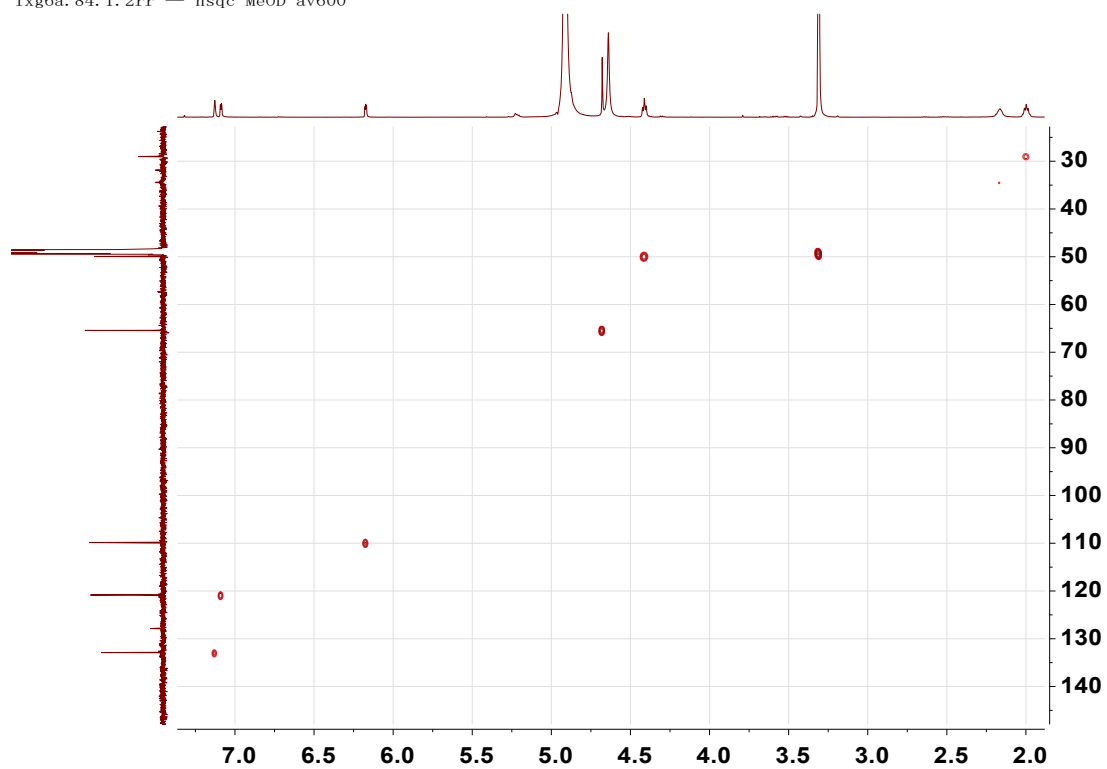


Figure S21. ^1H - ^1H COSY spectrum of 4

1xg6a. 86. 1. 2rr — cosy MeOD av600

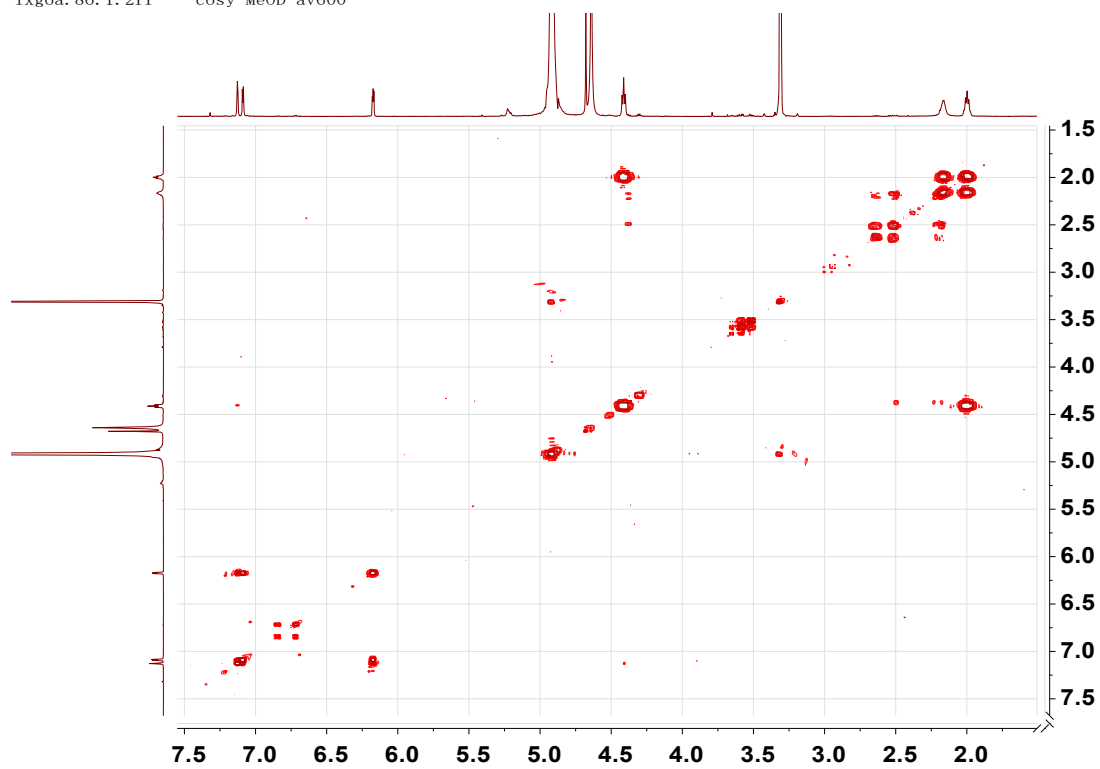


Figure S22. HMBC spectrum of 4

1xg6a.83.1.2rr — hmbc MeOD av600

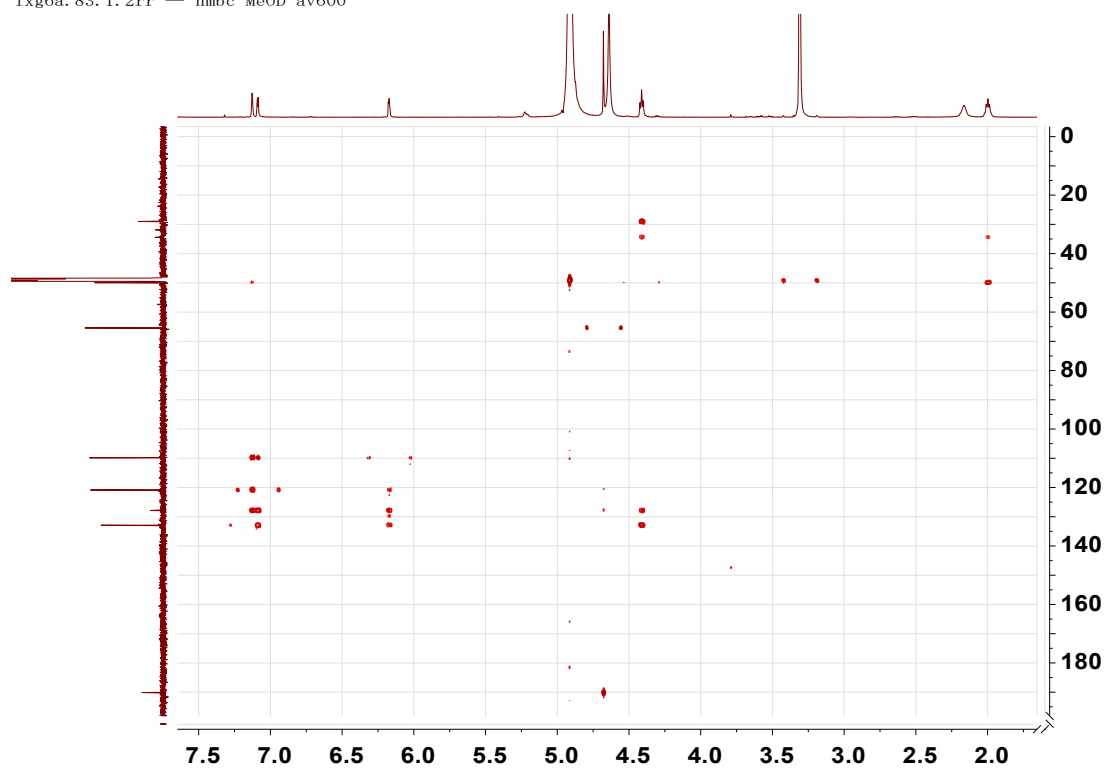


Figure S23. HRESIMS report of 4

Formula Predictor Report - lxg6a.lcd

Page 1 of 1

Data File: E:\DATA\2018\0128\lxg6a.lcd

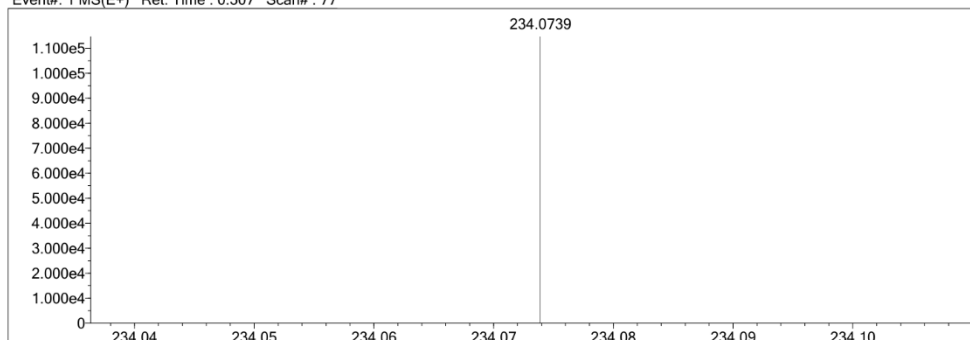
Elmt	Val.	Min	Max	Elmt	Val.	Min	Max	Elmt	Val.	Min	Max	Elmt	Val.	Min	Max	Use Adduct
H	1	0	100	O	2	0	50	Si	4	0	0	Br	1	0	0	Na
C	4	0	100	F	1	0	0	S	2	0	0	I	3	0	0	
N	3	0	10	Na	1	0	0	Cl	1	0	0					

Error Margin (ppm): 5
 HC Ratio: unlimited
 Max Isotopes: all
 MSn Iso RI (%): 75.00

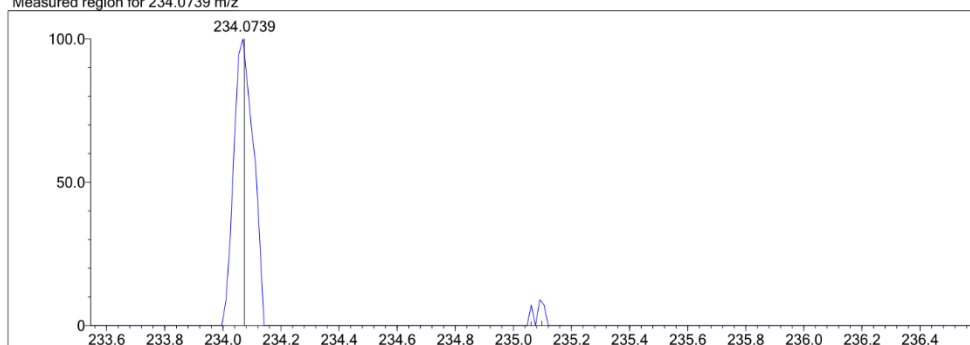
DBE Range: -2.0 - 100.0
 Apply N Rule: yes
 Isotope RI (%): 1.00
 MSn Logic Mode: AND

Electron Ions: both
 Use MSn Info: yes
 Isotope Res: 10000
 Max Results: 10

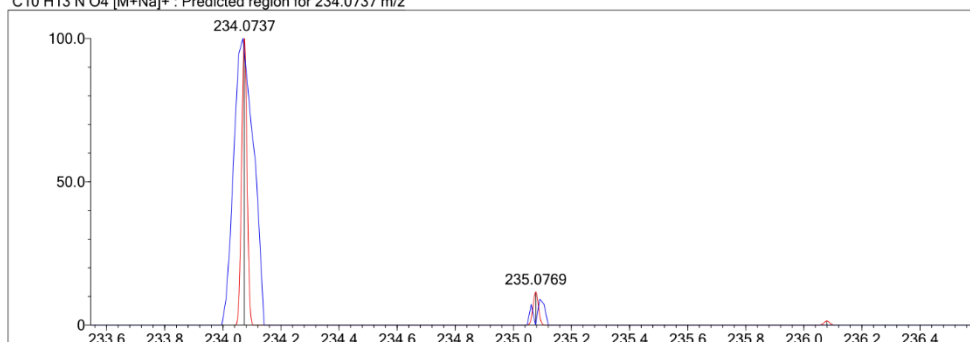
Event#: 1 MS(E+) Ret. Time : 0.507 Scan# : 77



Measured region for 234.0739 m/z



C10 H13 N O4 [M+Na]+ : Predicted region for 234.0737 m/z



Formula (M)	Ion	Meas. m/z	Pred. m/z	Df. (mDa)	Df. (ppm)	DBE
C10 H13 N O4	[M+Na]+	234.0739	234.0737	0.2	0.85	5.0

Figure S24. IR report of 4

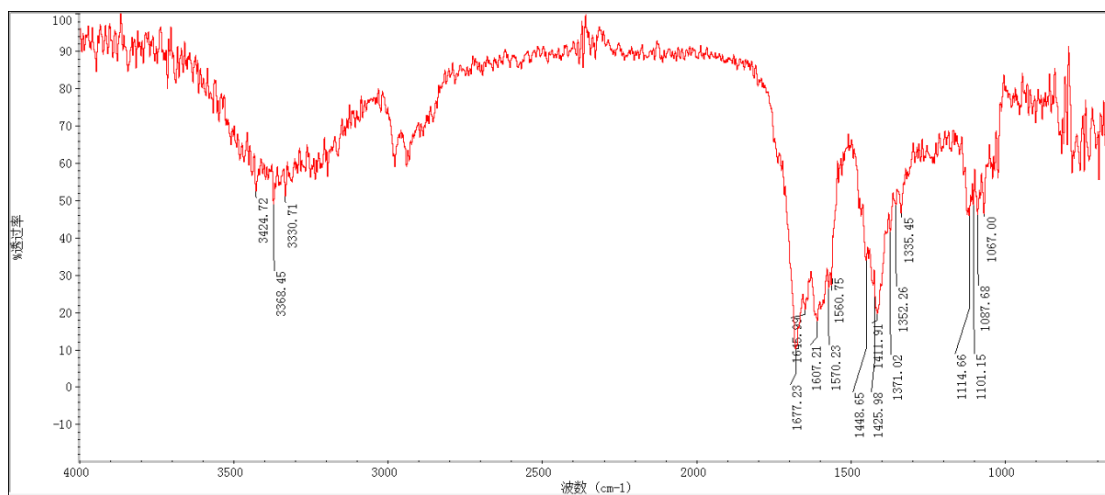


Figure S25. ¹H NMR spectrum of 5 (600 MHz, CD₃OD)

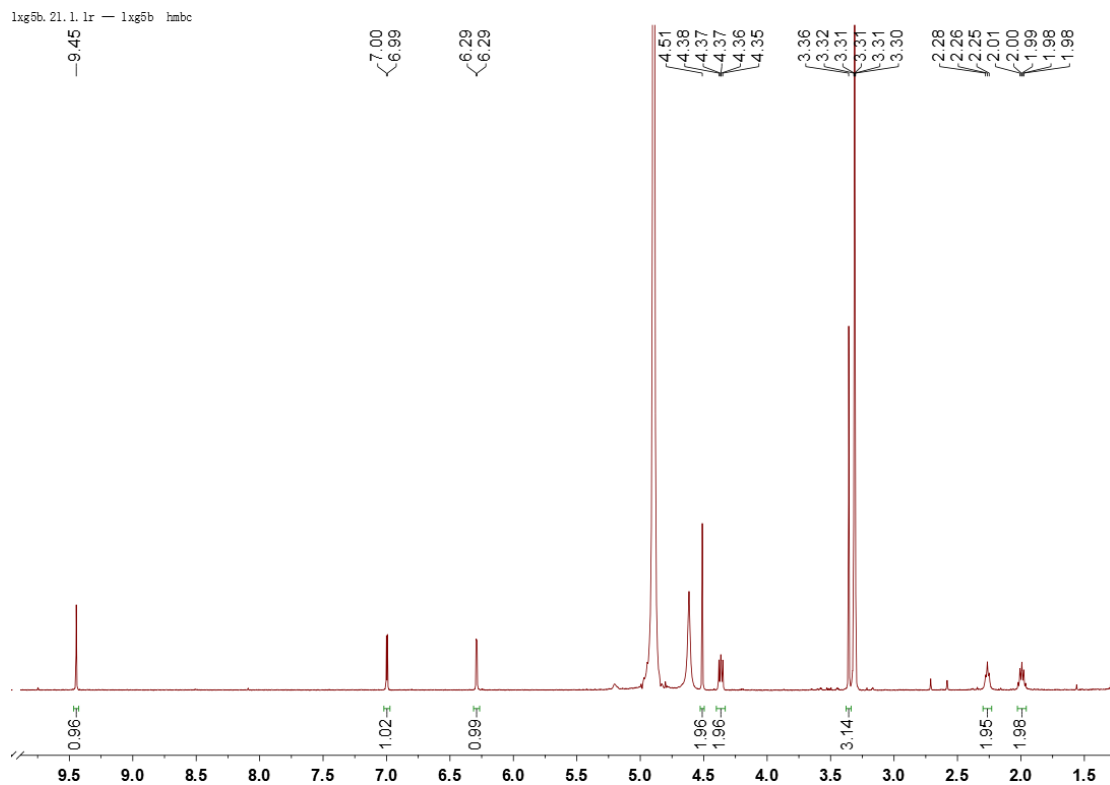


Figure S26. ¹³C and DEPT NMR spectra of 5 (150 MHz, CD₃OD)

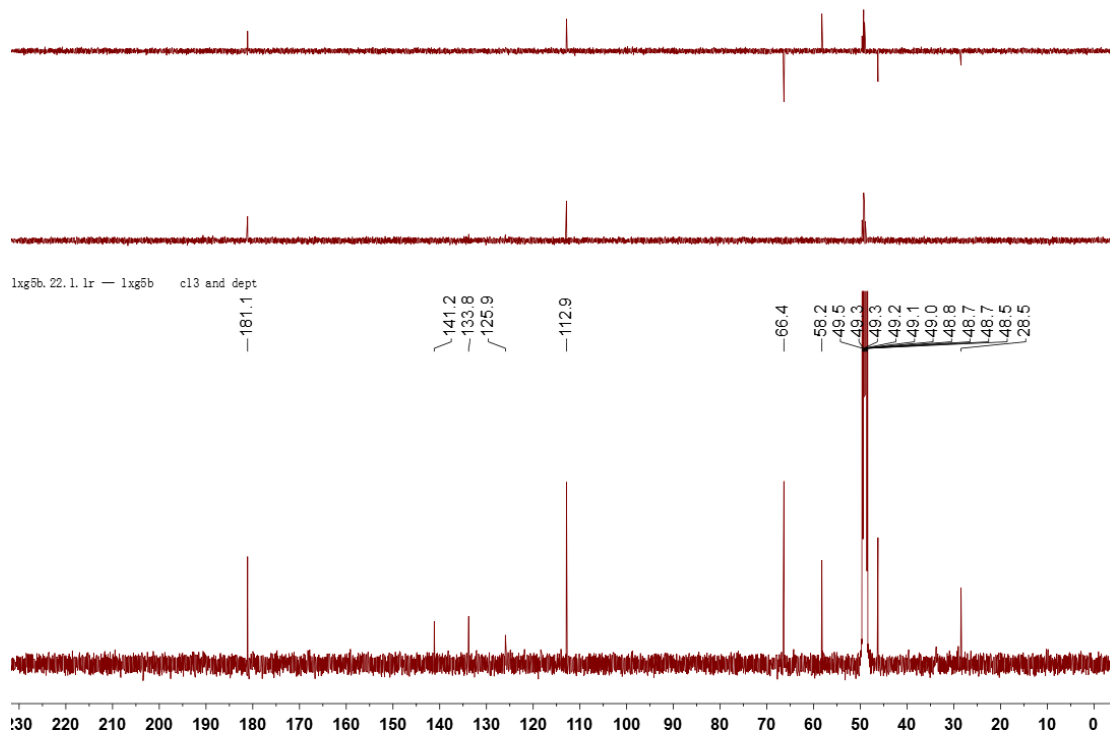


Figure S27. ¹H NMR spectrum of 6 (600 MHz, CD₃OD)

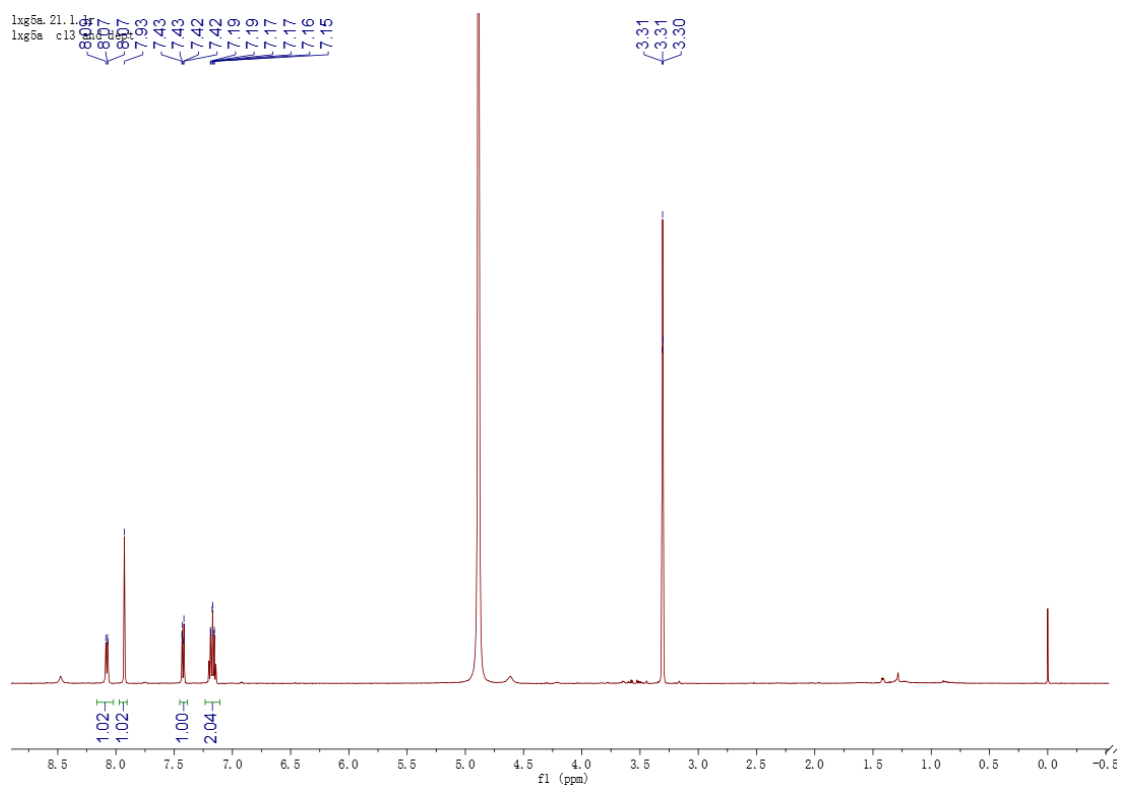


Figure S28. ¹³C and DEPT NMR spectra of 6 (150 MHz, CD₃OD)

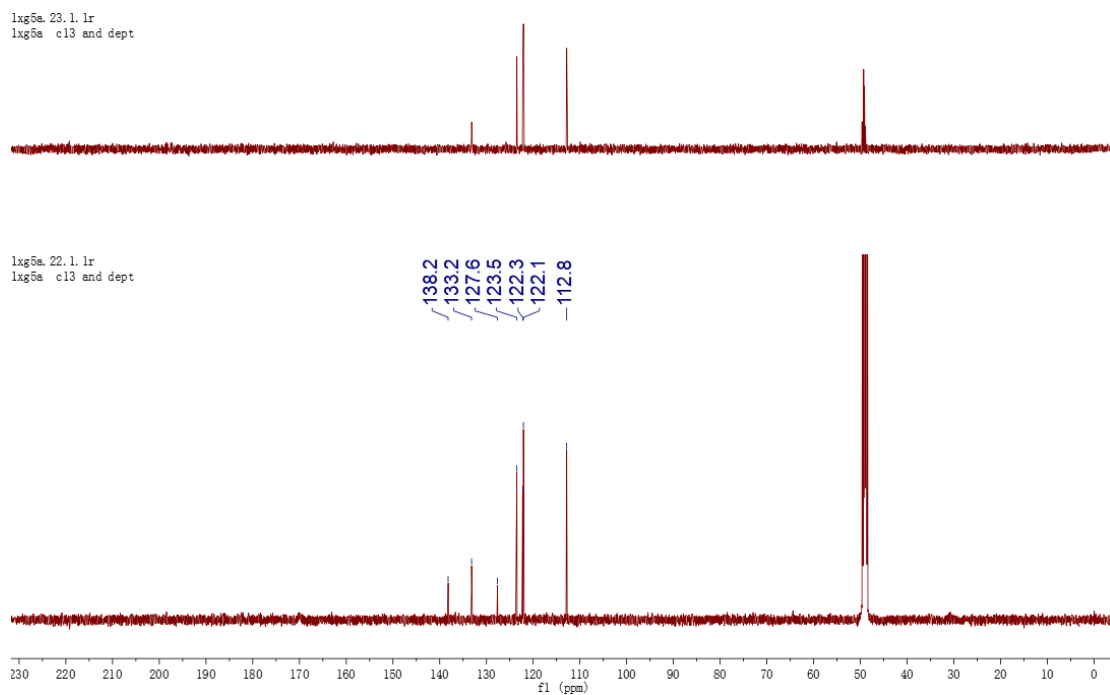


Figure S29. ¹H NMR spectrum of 7 (600 MHz, CD₃OD)

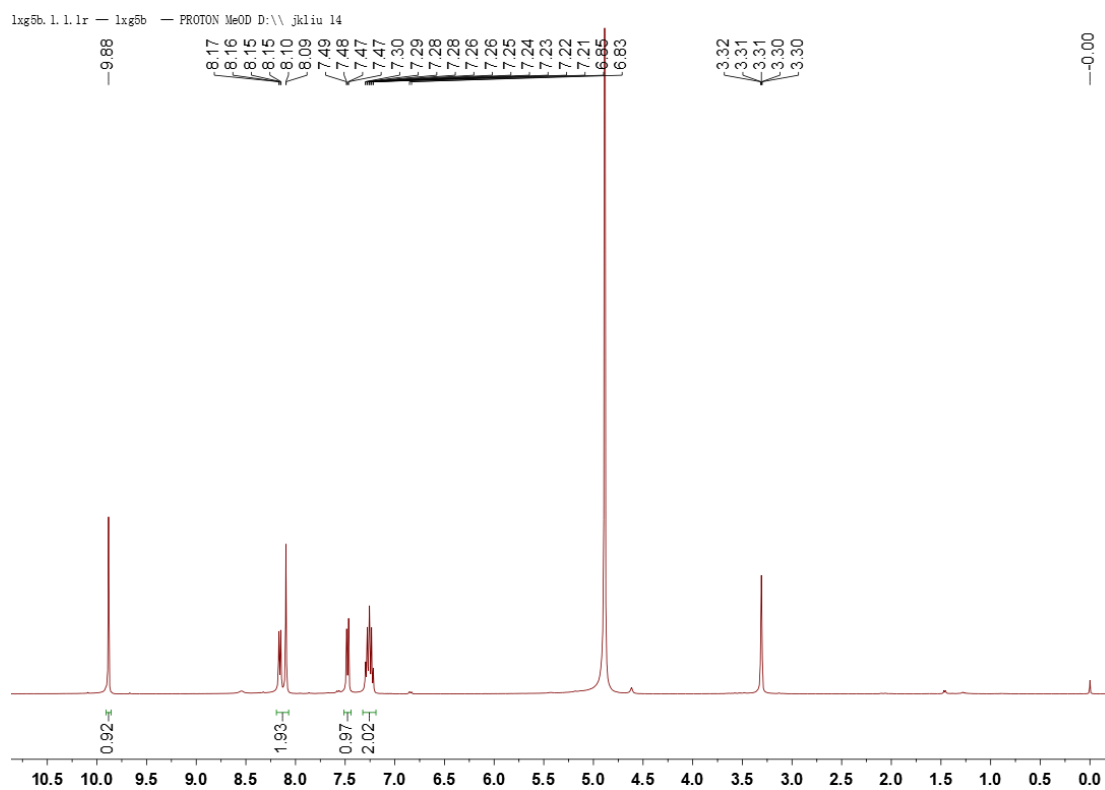


Figure S30. ¹³C and DEPT NMR spectra of 7 (150 MHz, CD₃OD)

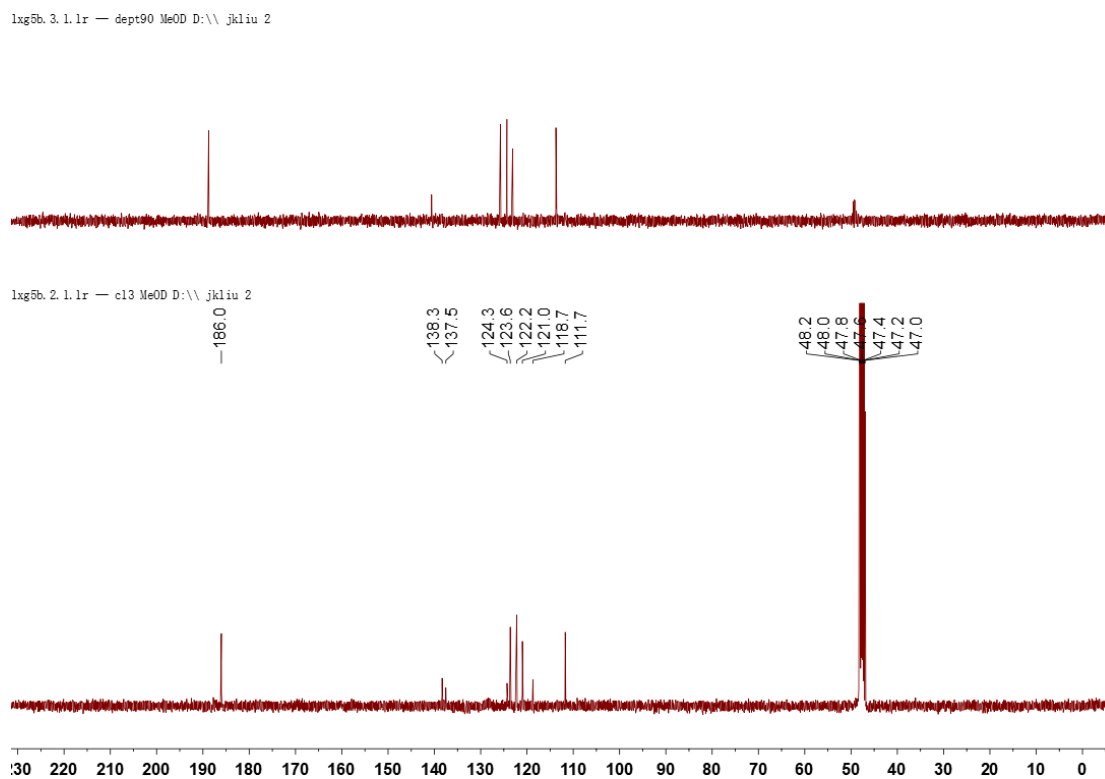


Figure S31. ¹H NMR spectrum of 8 (600 MHz, CD₃OD)

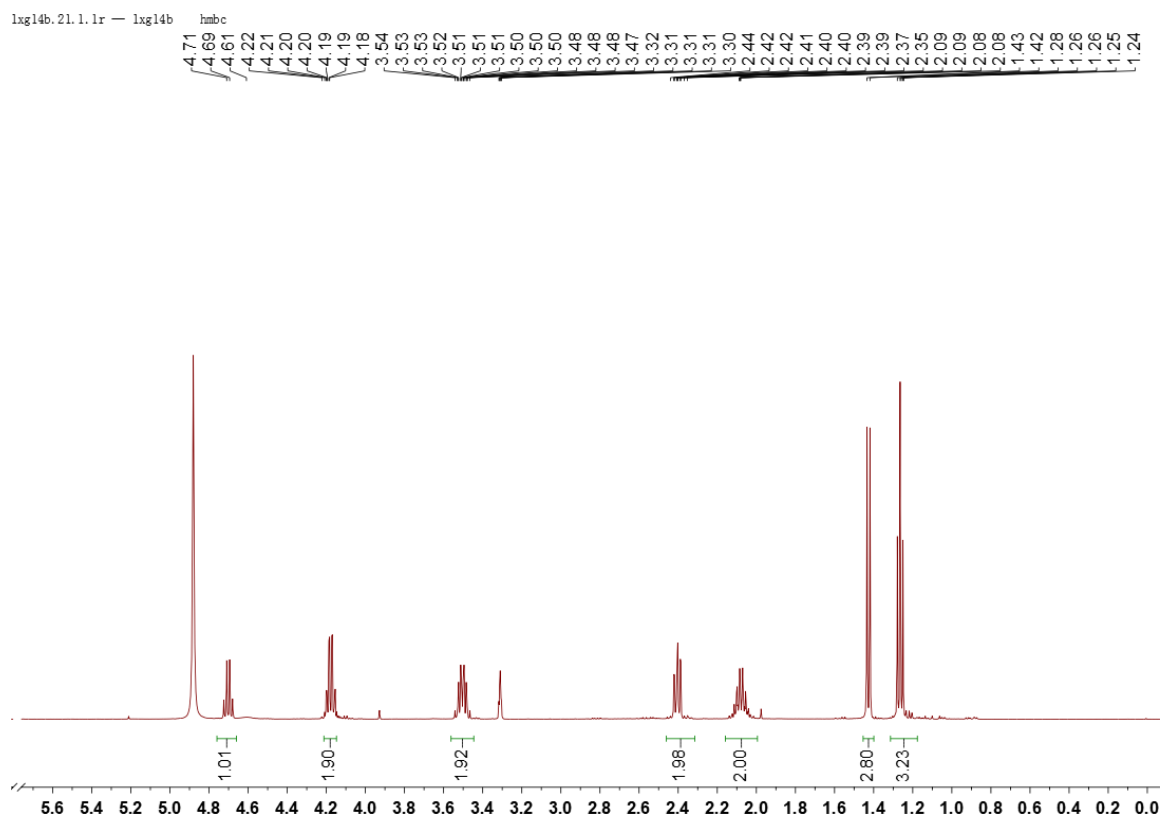


Figure S32. ¹³C and DEPT NMR spectra of 8 (150 MHz, CD₃OD)

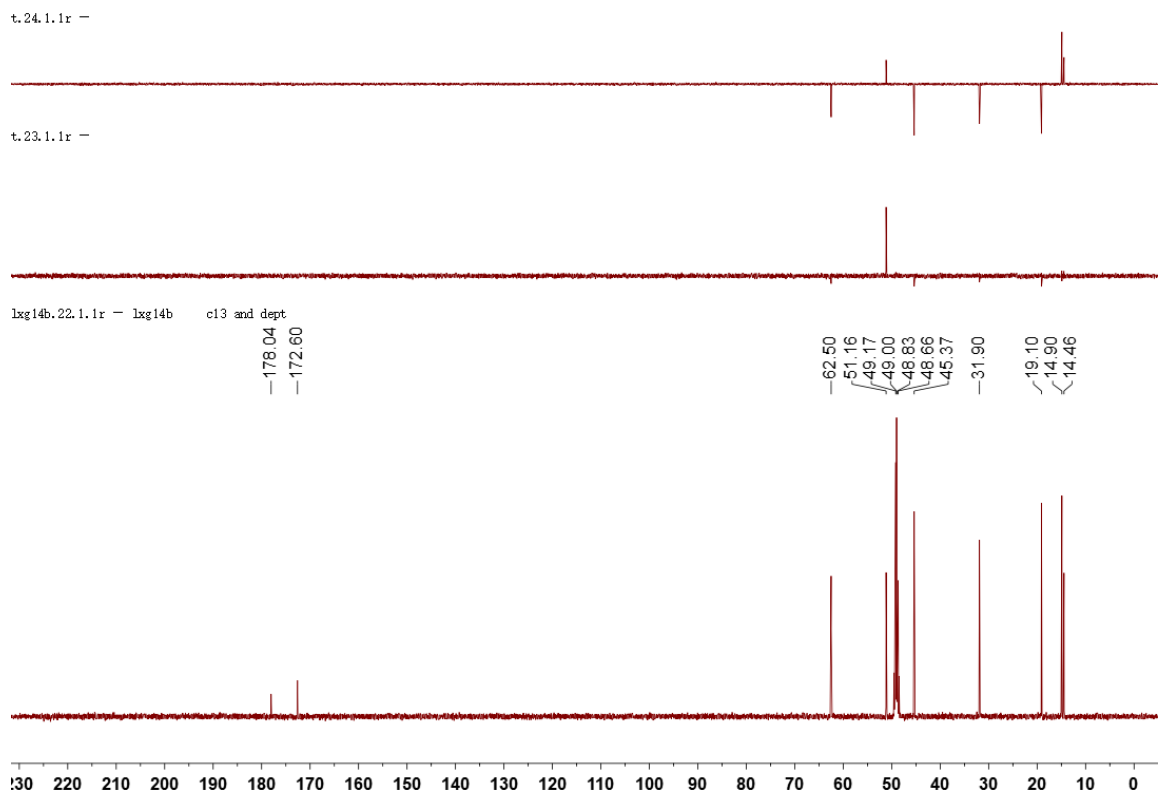


Figure S33. HSQC spectrum of 8

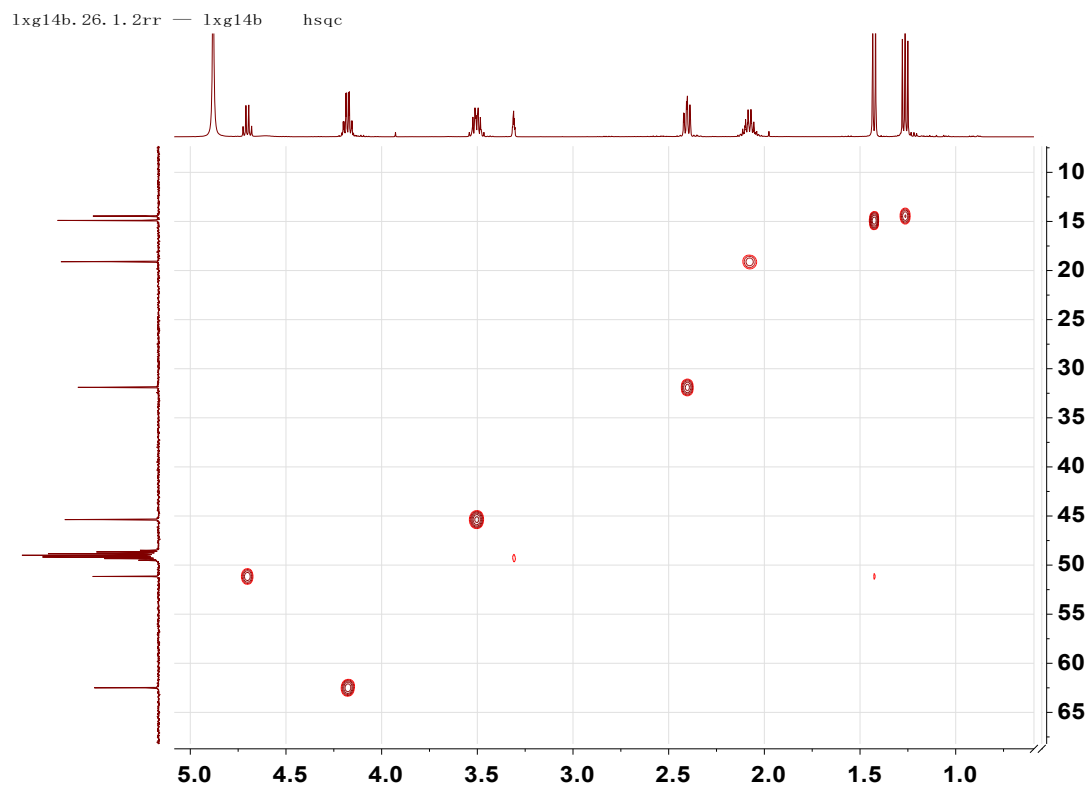


Figure S34. HMBC spectrum of 8

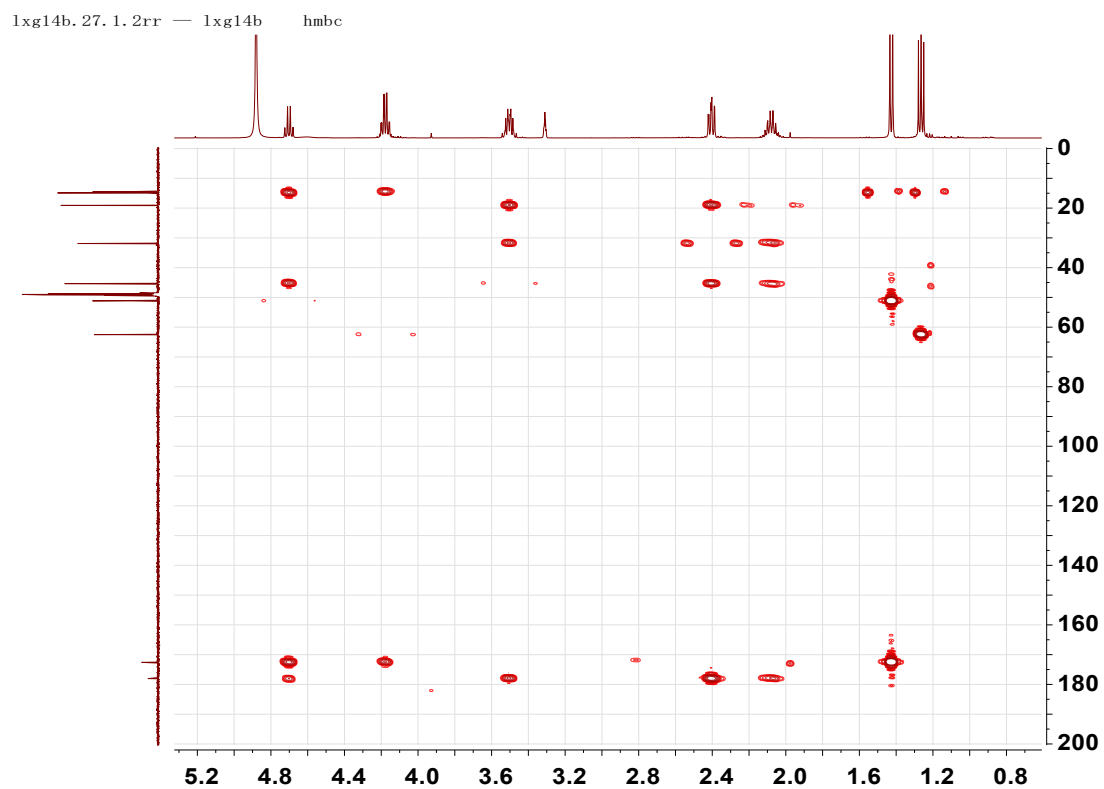


Figure S35. ¹H NMR spectrum of 9 (600 MHz, CD₃OD)

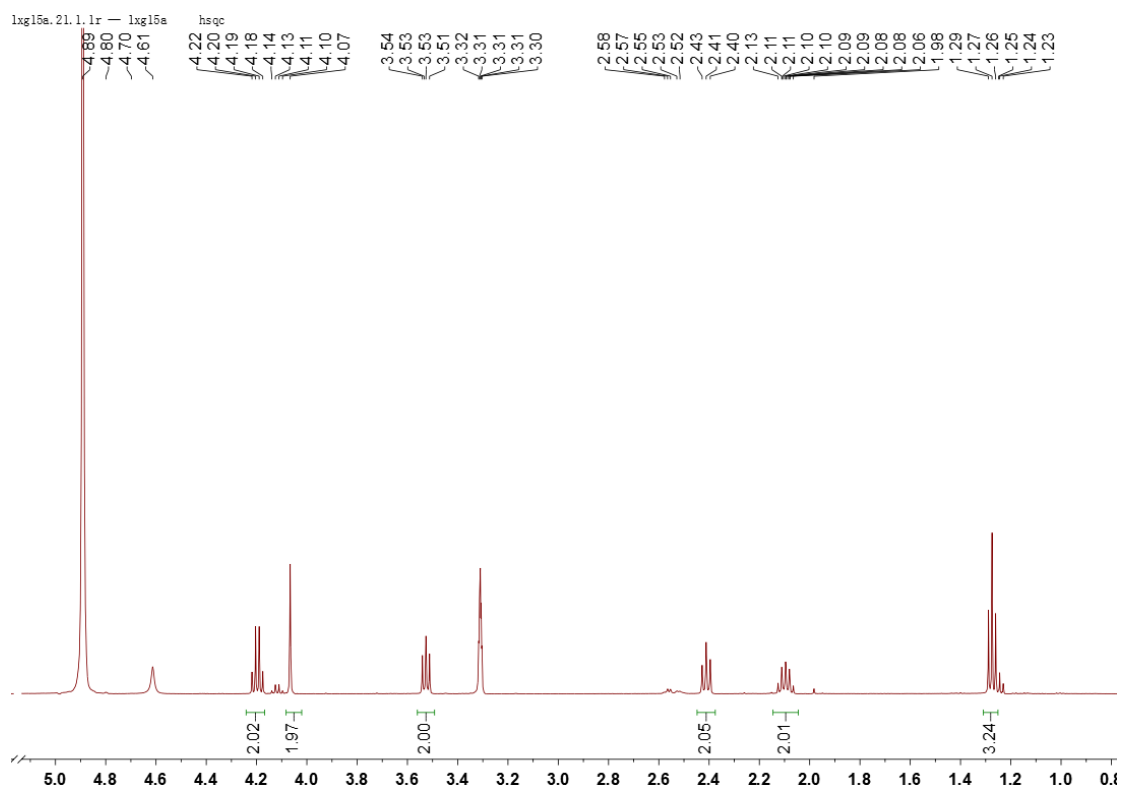


Figure S36. ¹³C and DEPT NMR spectra of 9 (150 MHz, CD₃OD)

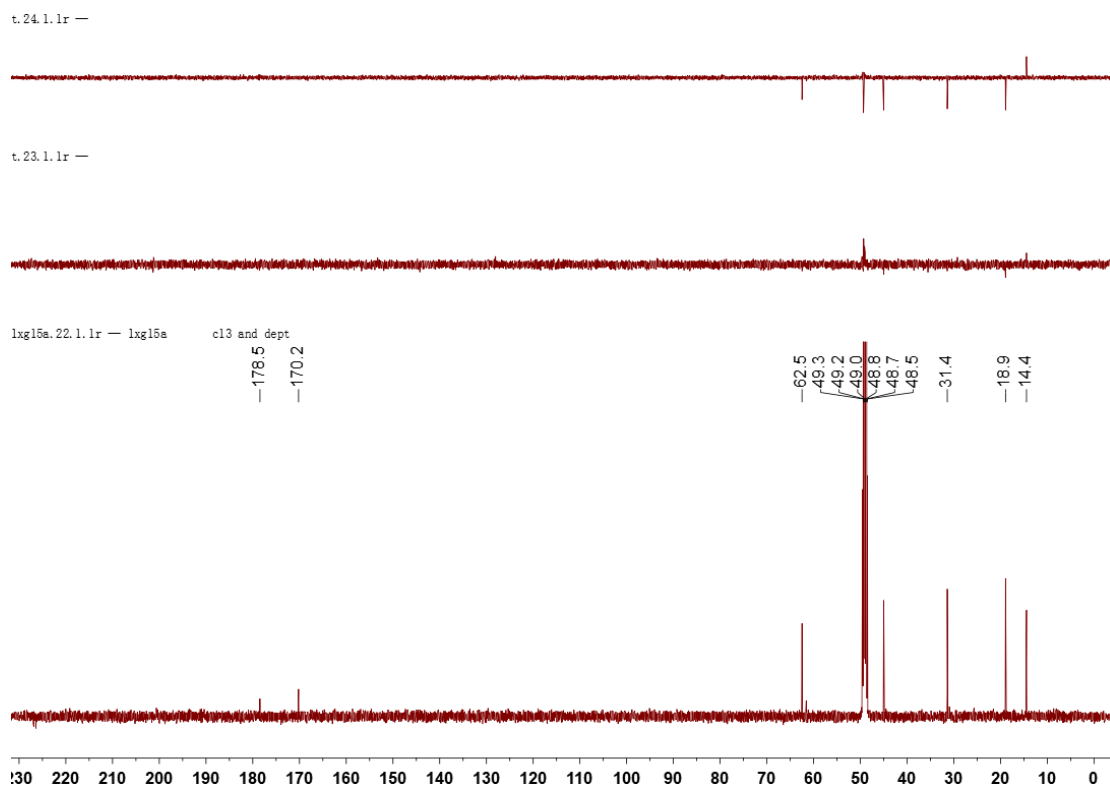


Figure S37. HSQC spectrum of 9

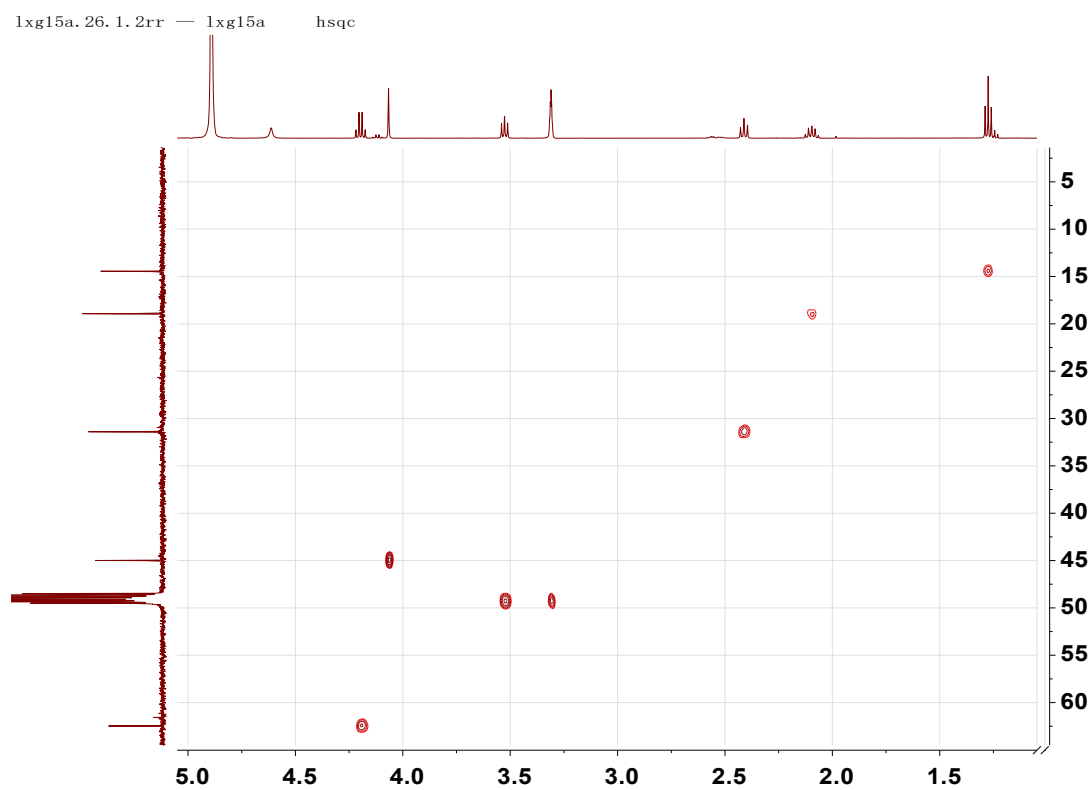


Figure S38. HMBC spectrum of 9

