

Supplementary information

New Phenol and Chromone Derivatives from the Endolichenic Fungus *Daldinia* Species and Their Antiviral Activities

Dewu Zhang,^a Guowei Gu,^a Bingyuan Zhang,^{ab} Yujia Wang,^a Jinglin Bai,^a Yuang Fang,^a Tao Zhang,^a Shengjun Dai,^b Shan Cen^a and Liyan Yu^{*a}

^a *Division for Medicinal Microorganisms Related Strains CAMS Collection Center of Pathogenic Microorganisms, Institute of Medicinal Biotechnology, Chinese Academy of Medical Sciences and Peking Union Medical College, Beijing 100050, P. R. China*

^b *School of Pharmacy, Yantai University, Yantai 264005, P. R. China*

*To whom correspondence should be addressed.

E-mail: yly@cpcc.ac.cn

Contents

Table S1. Antiviral activities of 1–12	S4
Figure S1. ^1H NMR spectrum of 1	S5
Figure S2. ^{13}C NMR spectrum of 1	S6
Figure S3. DEPT spectrum of 1	S7
Figure S4. ^1H – ^1H COSY spectrum of 1	S8
Figure S5. HSQC spectrum of 1	S9
Figure S6. HMBC spectrum of 1	S10
Figure S7. HRESIMS spectrum of 1	S11
Figure S8. IR spectrum of 1	S12
Figure S9. UV spectrum of 1	S12
Figure S10. ^1H NMR spectrum of 2	S13
Figure S11. ^{13}C NMR spectrum of 2	S14
Figure S12. DEPT spectrum of 2	S15
Figure S13. ^1H – ^1H COSY spectrum of 2	S16
Figure S14. HSQC spectrum of 2	S17
Figure S15. HMBC spectrum of 2	S18
Figure S16. HRESIMS spectrum of 2	S19
Figure S17. IR spectrum of 2	S20
Figure S18. UV spectrum of 2	S20
Figure S19. ^1H NMR spectrum of 3	S21
Figure S20. ^{13}C NMR spectrum of 3	S22
Figure S21. DEPT spectrum of 3	S23
Figure S22. ^1H – ^1H COSY spectrum of 3	S24
Figure S23. HSQC spectrum of 3	S25
Figure S24. HMBC spectrum of 3	S26
Figure S25. HRESIMS spectrum of 3	S27
Figure S26. IR spectrum of 3	S28
Figure S27. UV spectrum of 3	S28
Figure S28. ^1H NMR spectrum of 9	S29
Figure S29. ^{13}C NMR spectrum of 9	S30
Figure S30. DEPT spectrum of 9	S31
Figure S31. ^1H – ^1H COSY spectrum of 9	S32

Figure S32. HSQC spectrum of 9	S33
Figure S33. HMBC spectrum of 9	S34
Figure S34. 1D NOE spectrum of 9	S35
Figure S35. HRESIMS spectrum of 9	S36
Figure S36. IR spectrum of 9	S37
Figure S37. UV spectrum of 9	S37
Figure S38. CD spectrum of 9	S38
Figure S39. ¹ H NMR spectrum of 10	S39
Figure S40. ¹³ C NMR spectrum of 10	S40
Figure S41. DEPT spectrum of 10	S41
Figure S42. ¹ H- ¹ H COSY spectrum of 10	S42
Figure S43. HSQC spectrum of 10	S43
Figure S44. HMBC spectrum of 10	S44
Figure S45. 1D NOE spectrum of 10	S45
Figure S46. HRESIMS spectrum of 10	S46
Figure S47. IR spectrum of 10	S47
Figure S48. UV spectrum of 10	S47
Figure S49. CD spectrum of 10	S48

Table S1 Antiviral activities of **1–12**.

compound	inhibition rate (%) in 10 μ M	
	IAV	ZIKV
1	39.46 \pm 6.33	19.6 \pm 7.04
2	0	0
3	58.13 \pm 1.12	0
4	40.95 \pm 2.68	17.10 \pm 3.88
5	10.03 \pm 0.99	0
6	0	30.61 \pm 2.74
7	6.77 \pm 1.72	28.66 \pm 1.28
8	0	42.70 \pm 0.81
9	35.72 \pm 2.20	28.33 \pm 3.96
10	0	14.48 \pm 1.80
11	43.08 \pm 4.94	17.31 \pm 1.12
12	18.75 \pm 0.90	12.23 \pm 8.98
Ribavirin	97.38 \pm 0.56 (50 μ M)	37.08 \pm 8.76

Figure S1. ¹H NMR spectrum of **1**

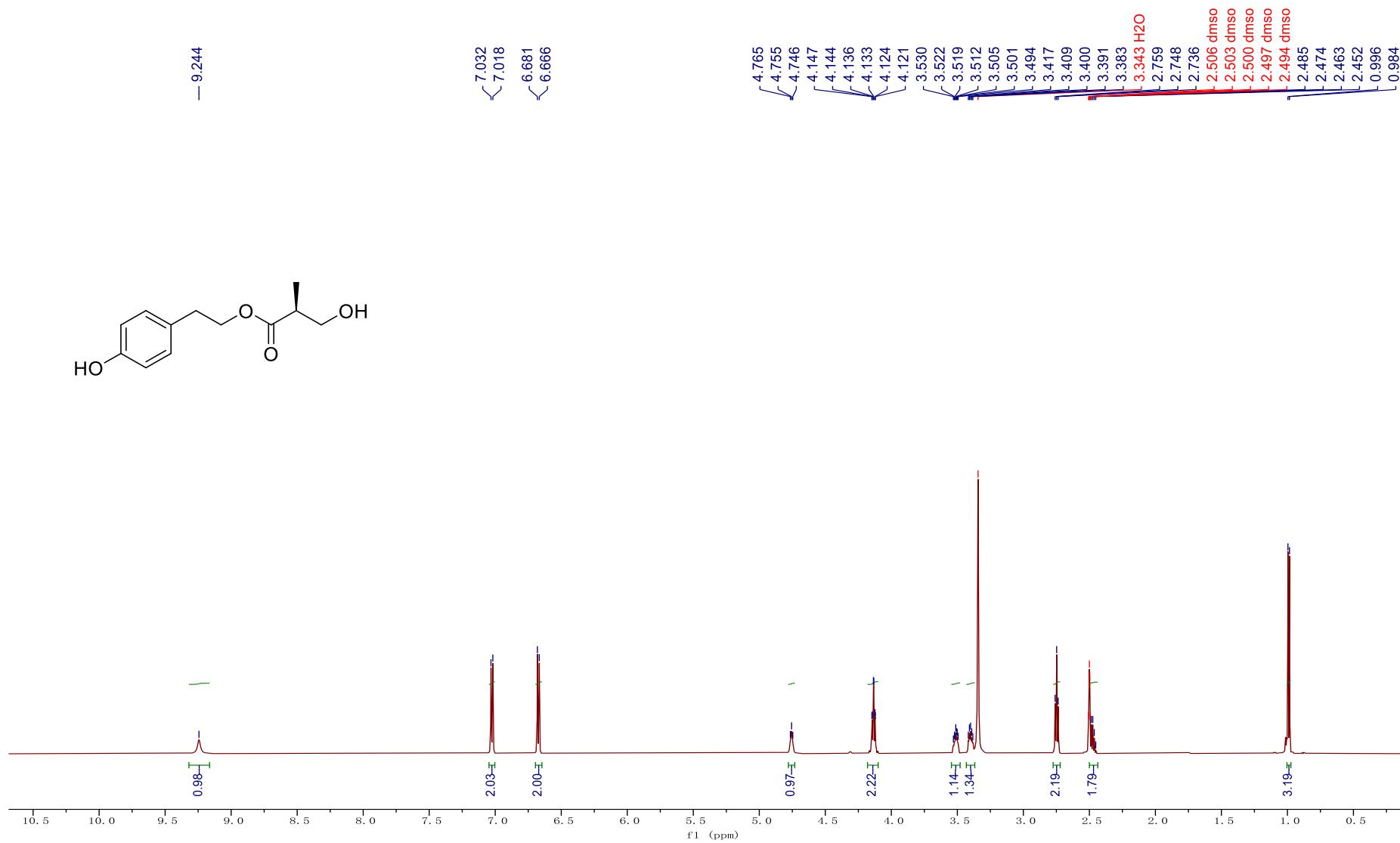


Figure S2. ^{13}C NMR spectrum of **1**

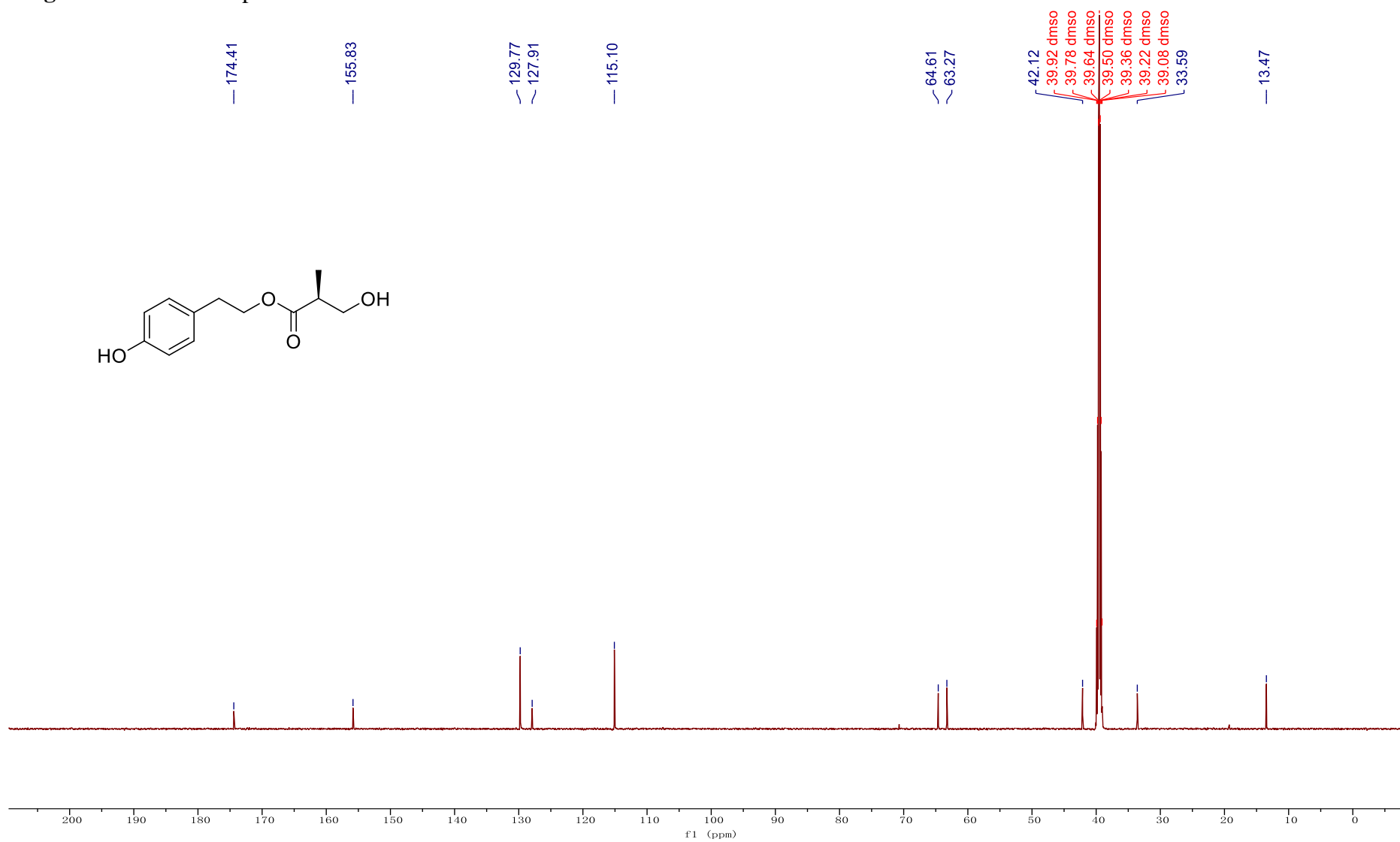
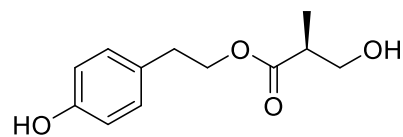


Figure S3. DEPT spectrum of **1**

DEPT_01
VNS-600 DEPT 770-35-5-2 IN dms0 Nov 3 2020
2



DEPT_01
VNS-600 DEPT 770-35-5-2 IN dms0 Nov 3 2020
1

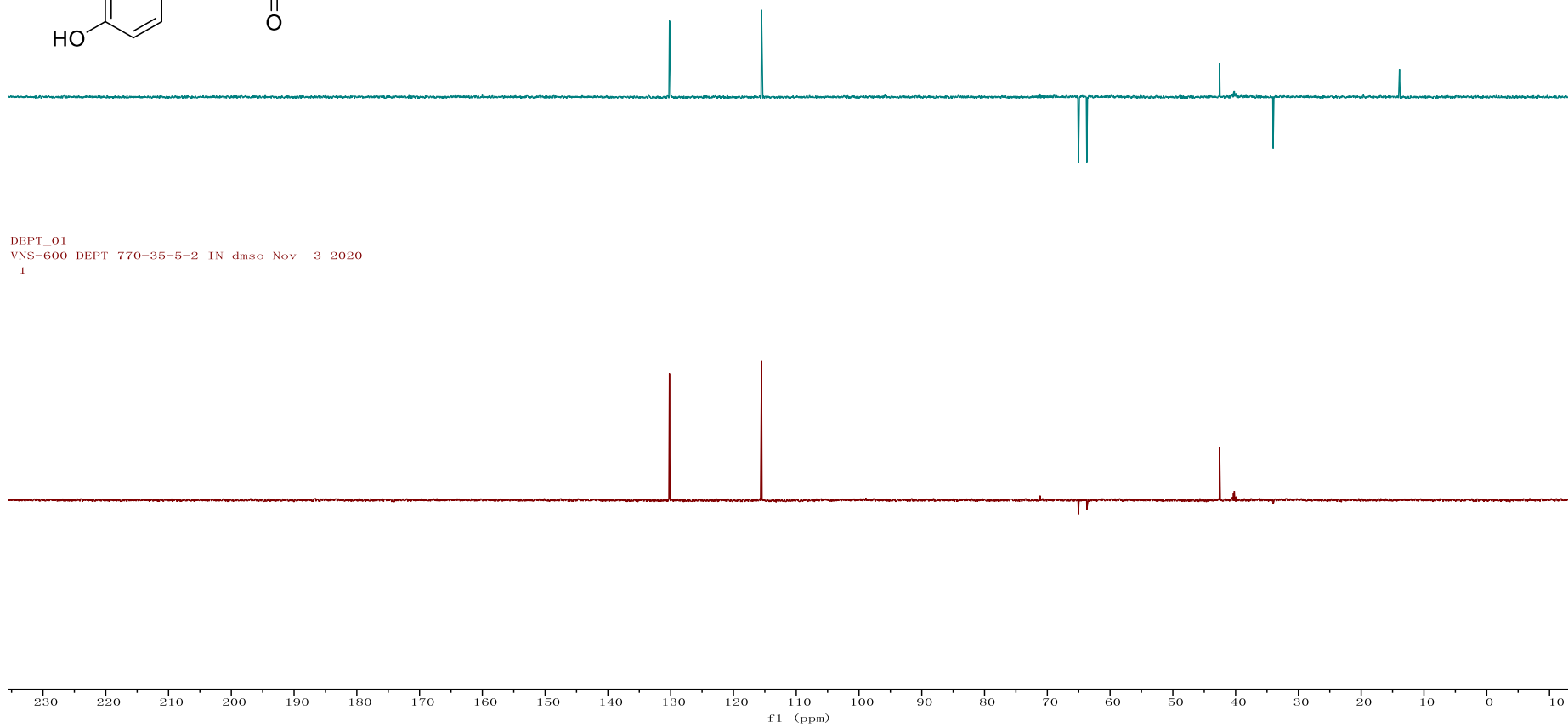


Figure S4. ^1H - ^1H COSY spectrum of **1**

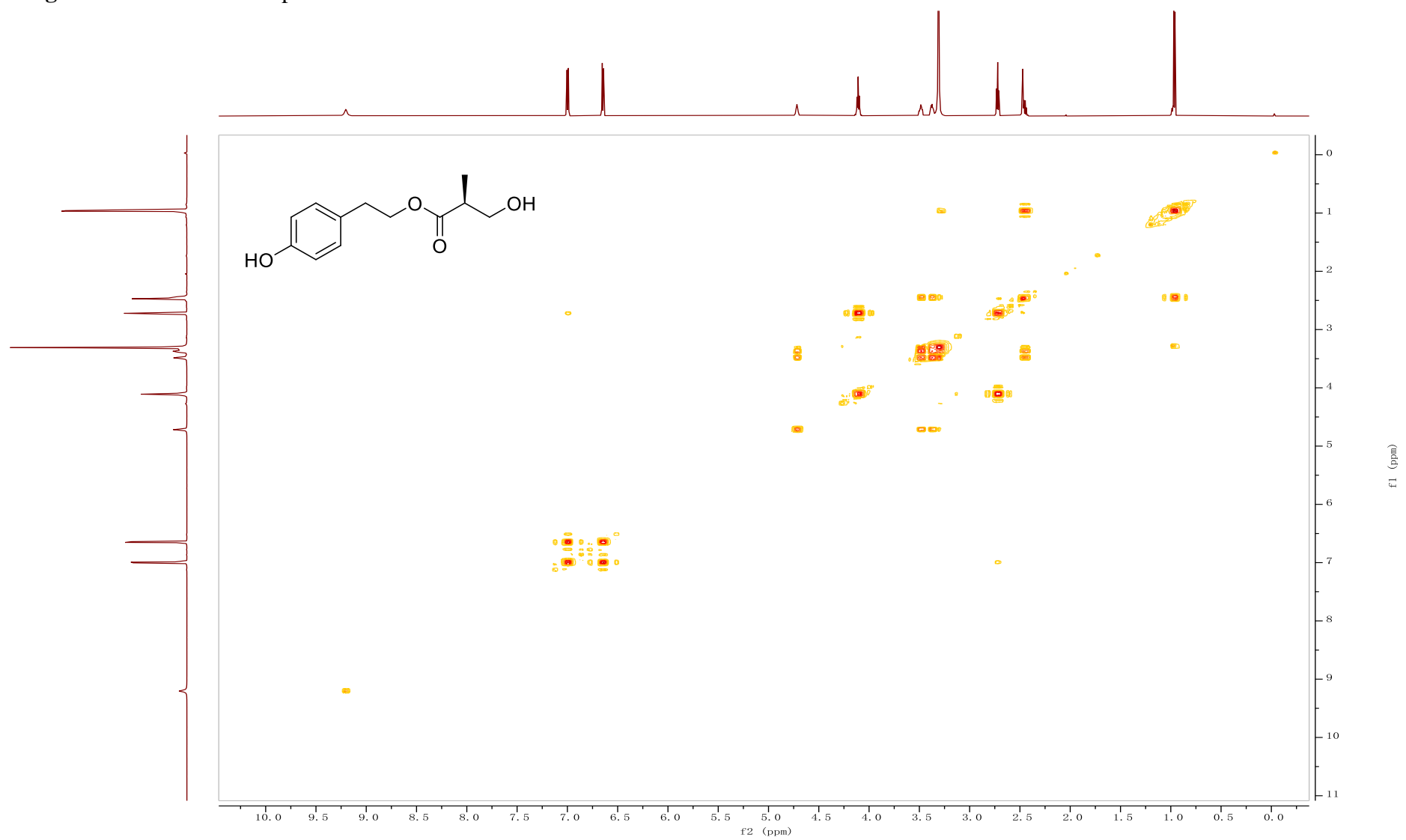


Figure S5. HSQC spectrum of **1**

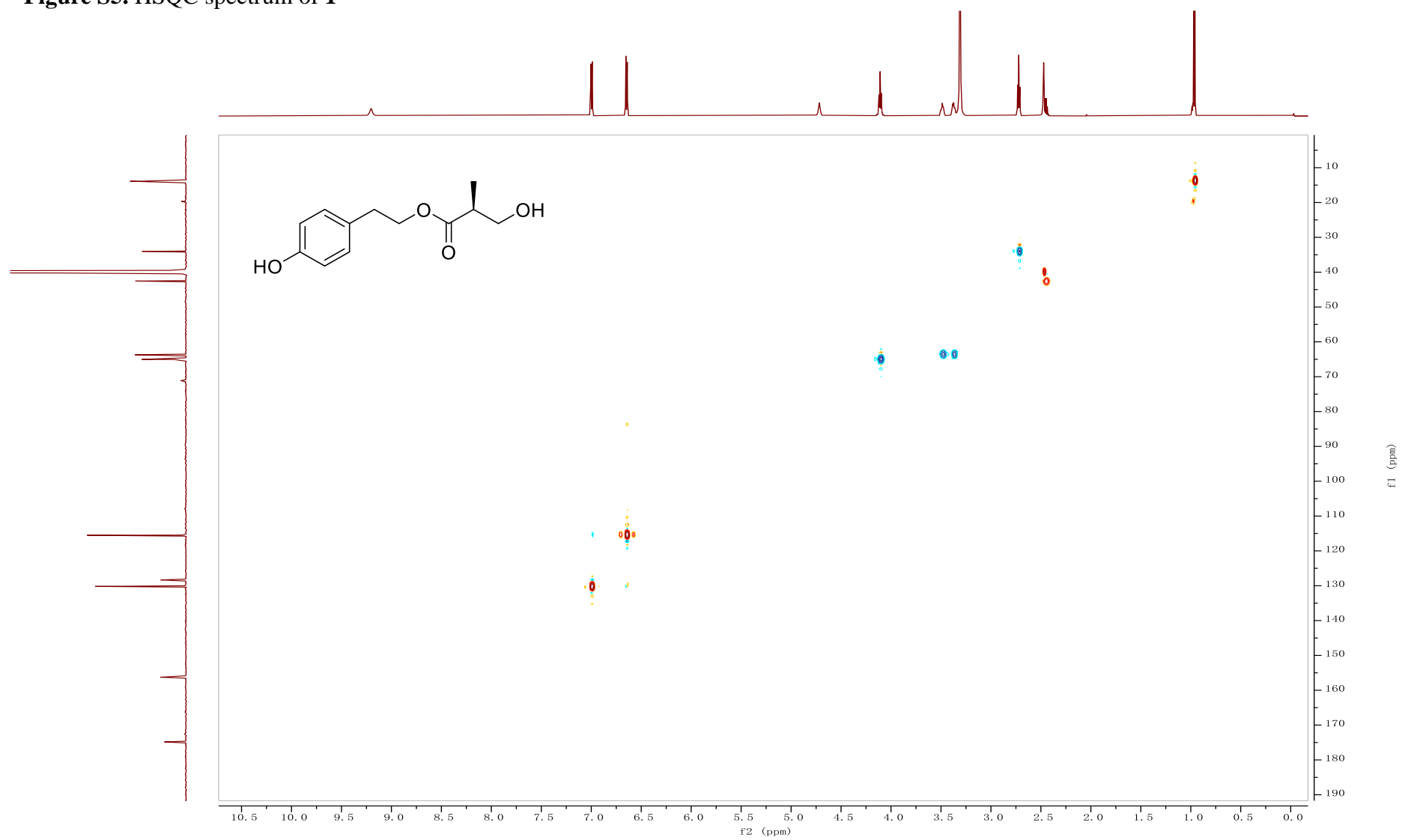


Figure S6. HMBC spectrum of **1**

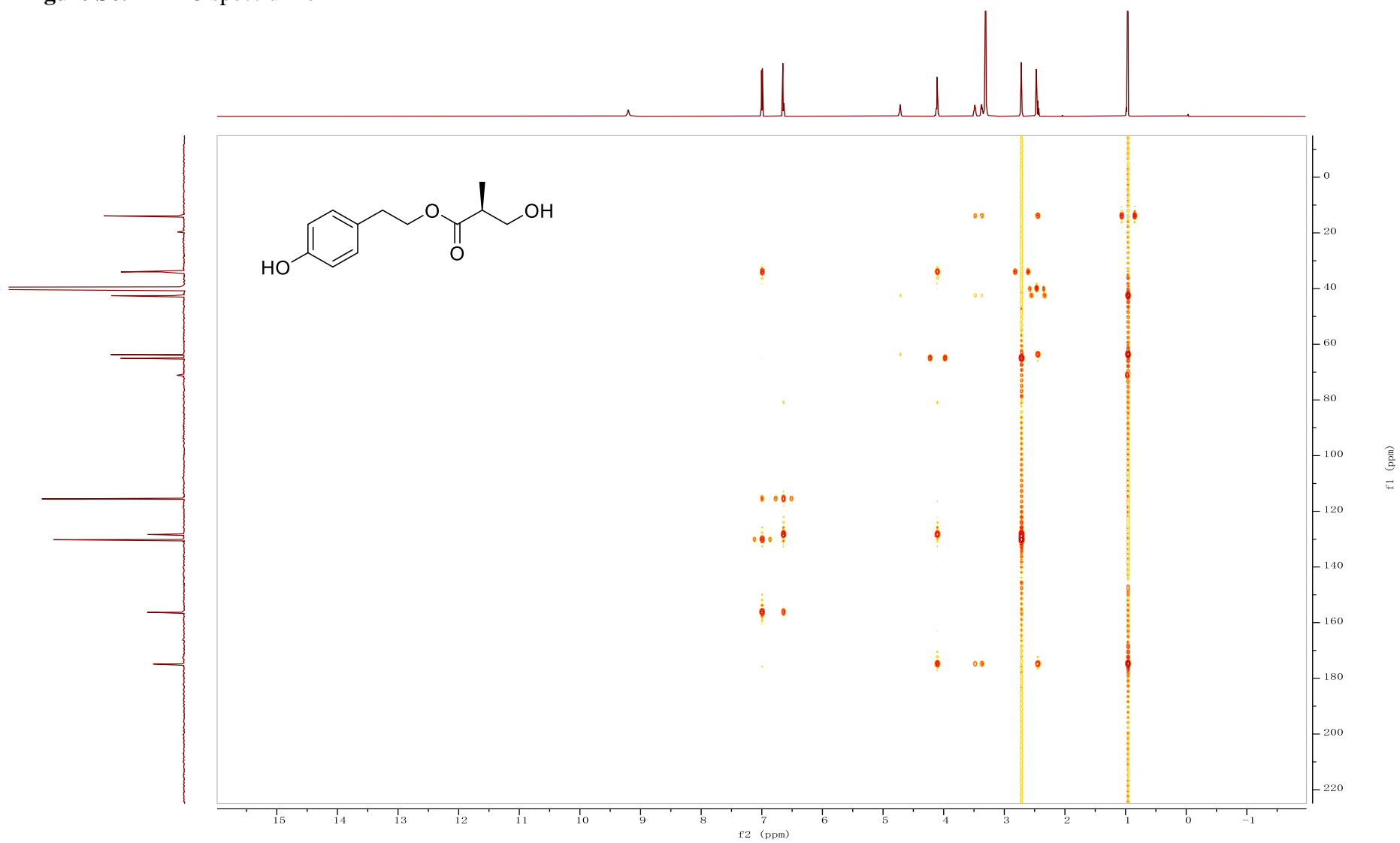


Figure S7. HRESIMS spectrum of **1**

/70-35-5-2 #61 RI: 0.48 AV: 1 NL: 5.55E/
T: FTMS + c ESI Full ms [50.00-700.00]

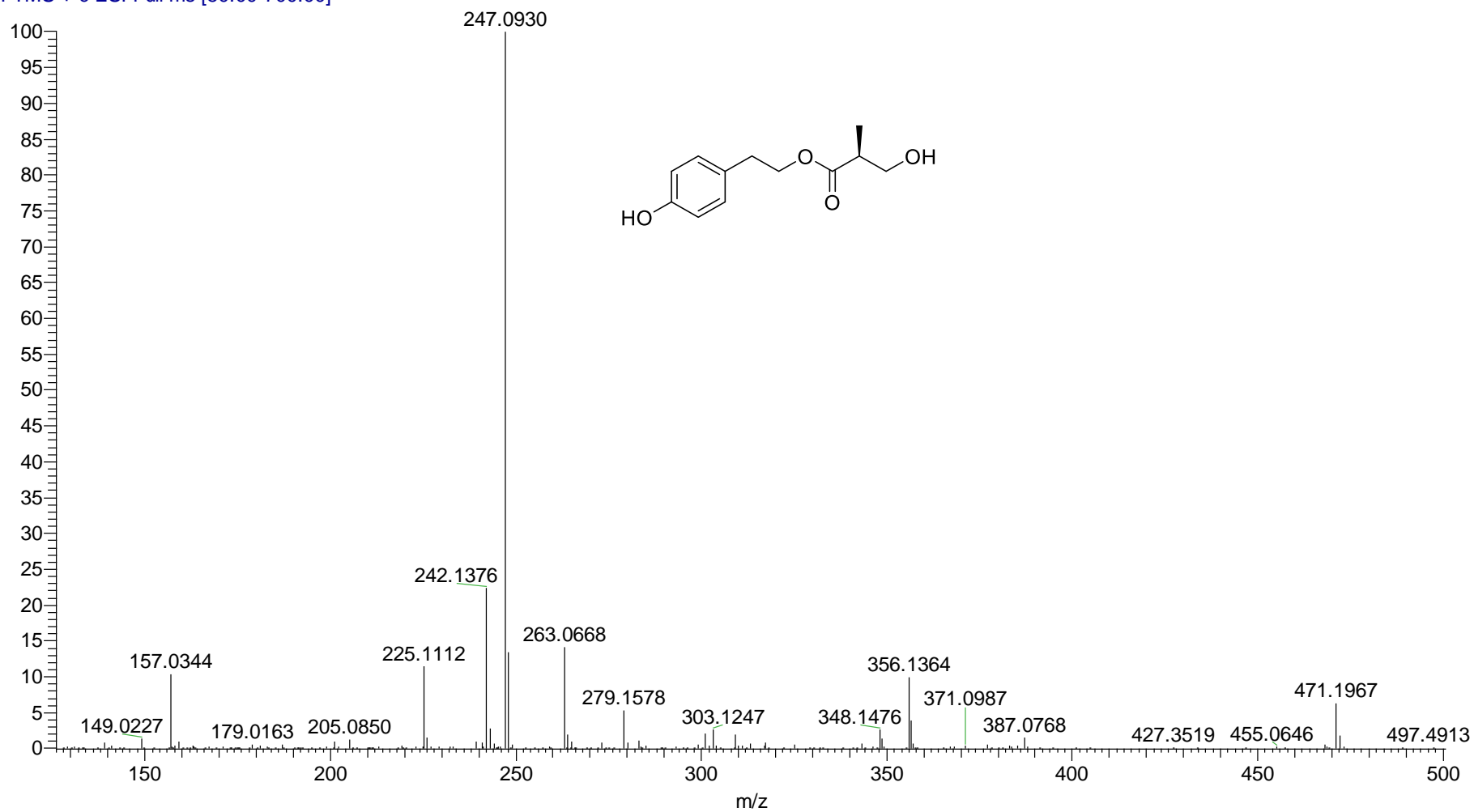


Figure S8. IR spectrum of **1**

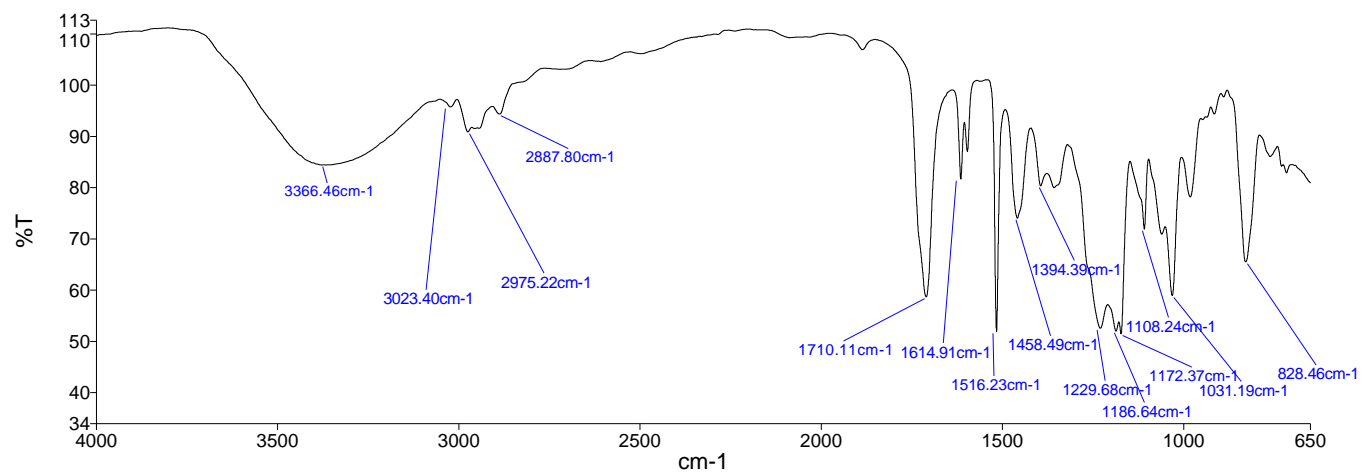


Figure S9. UV spectrum of **1**

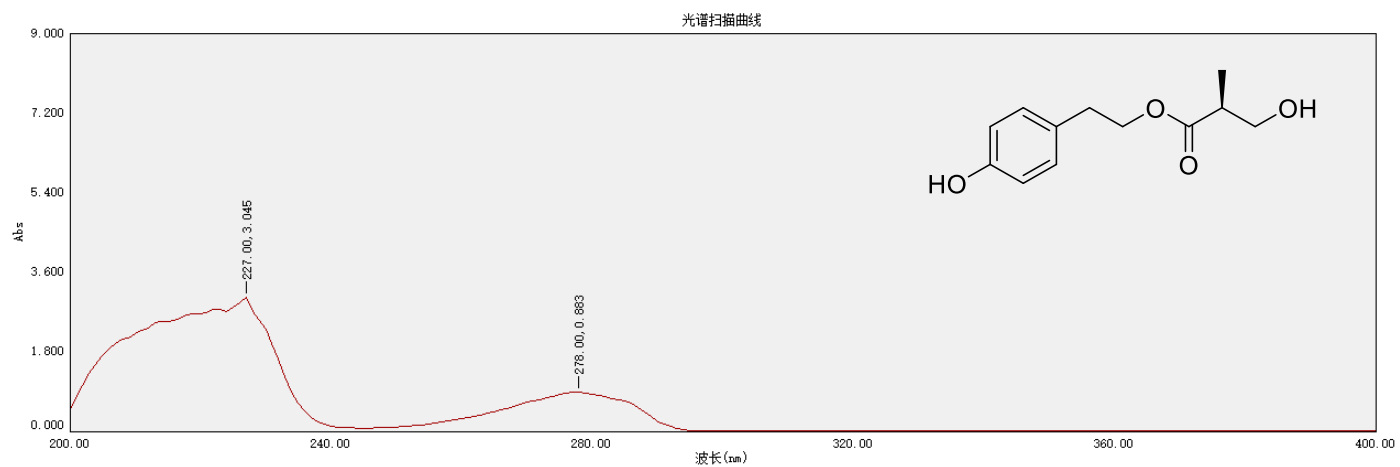


Figure S10. ¹H NMR spectrum of 2

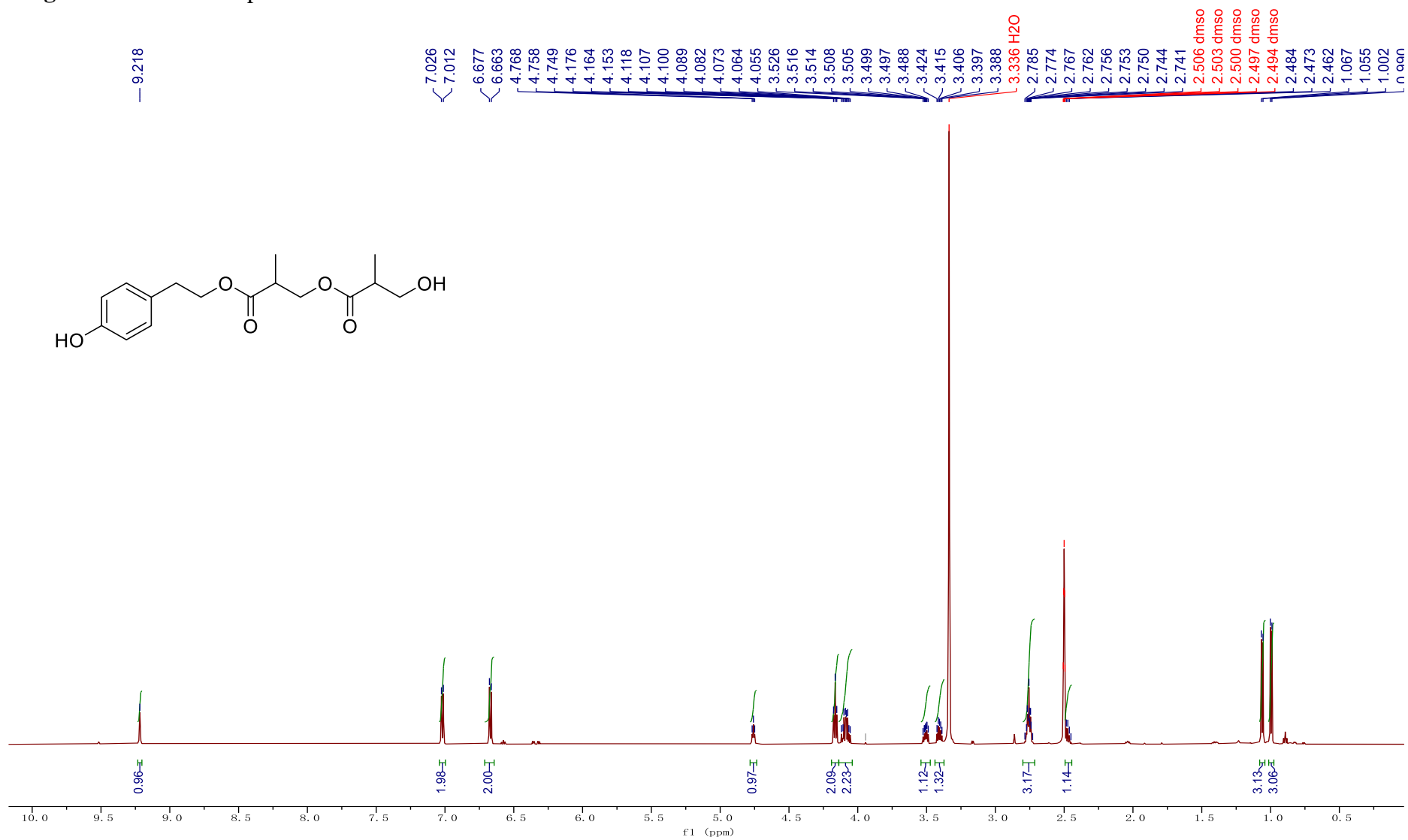


Figure S11. ¹³C NMR spectrum of 2

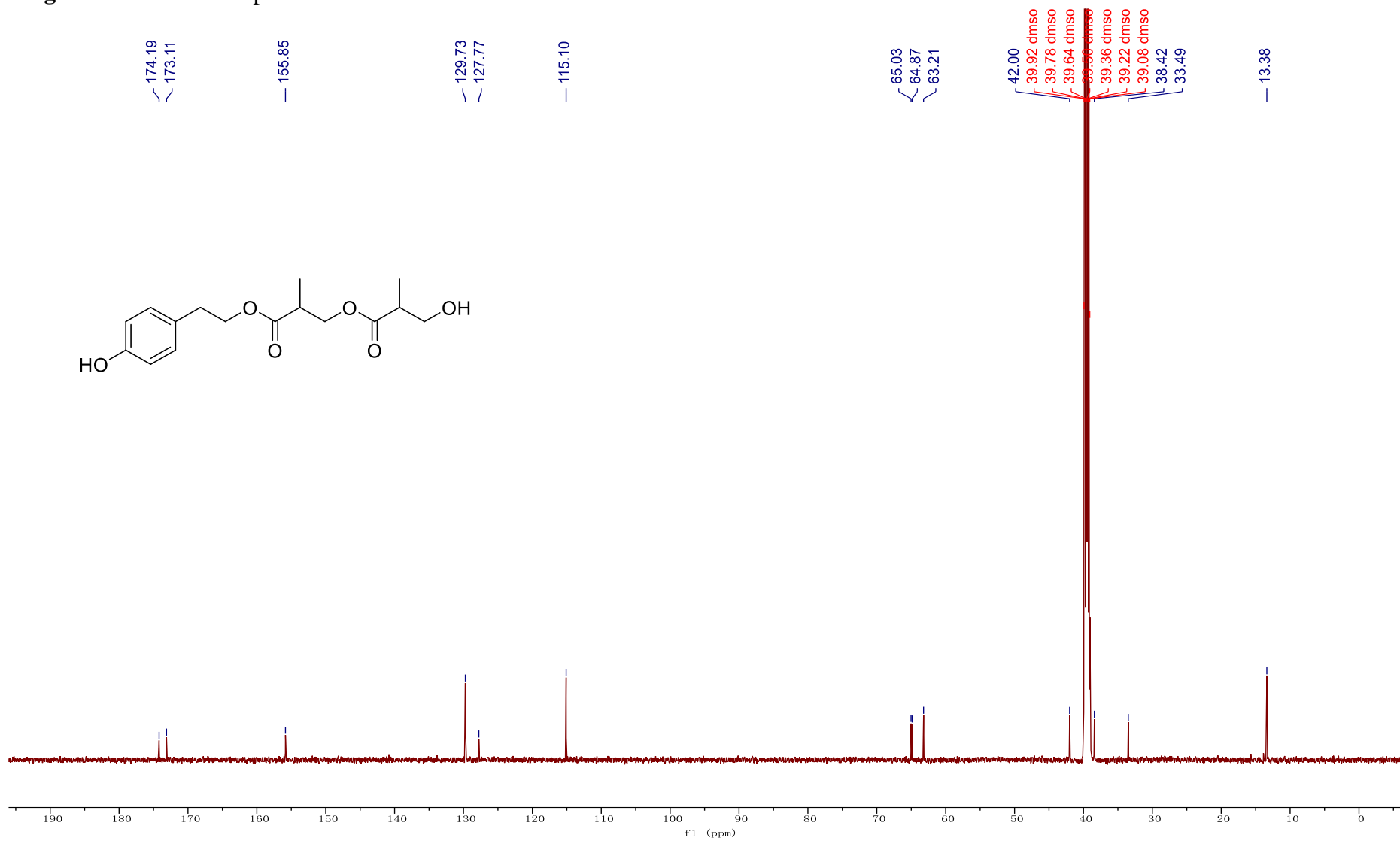


Figure S12. DEPT spectrum of **2**

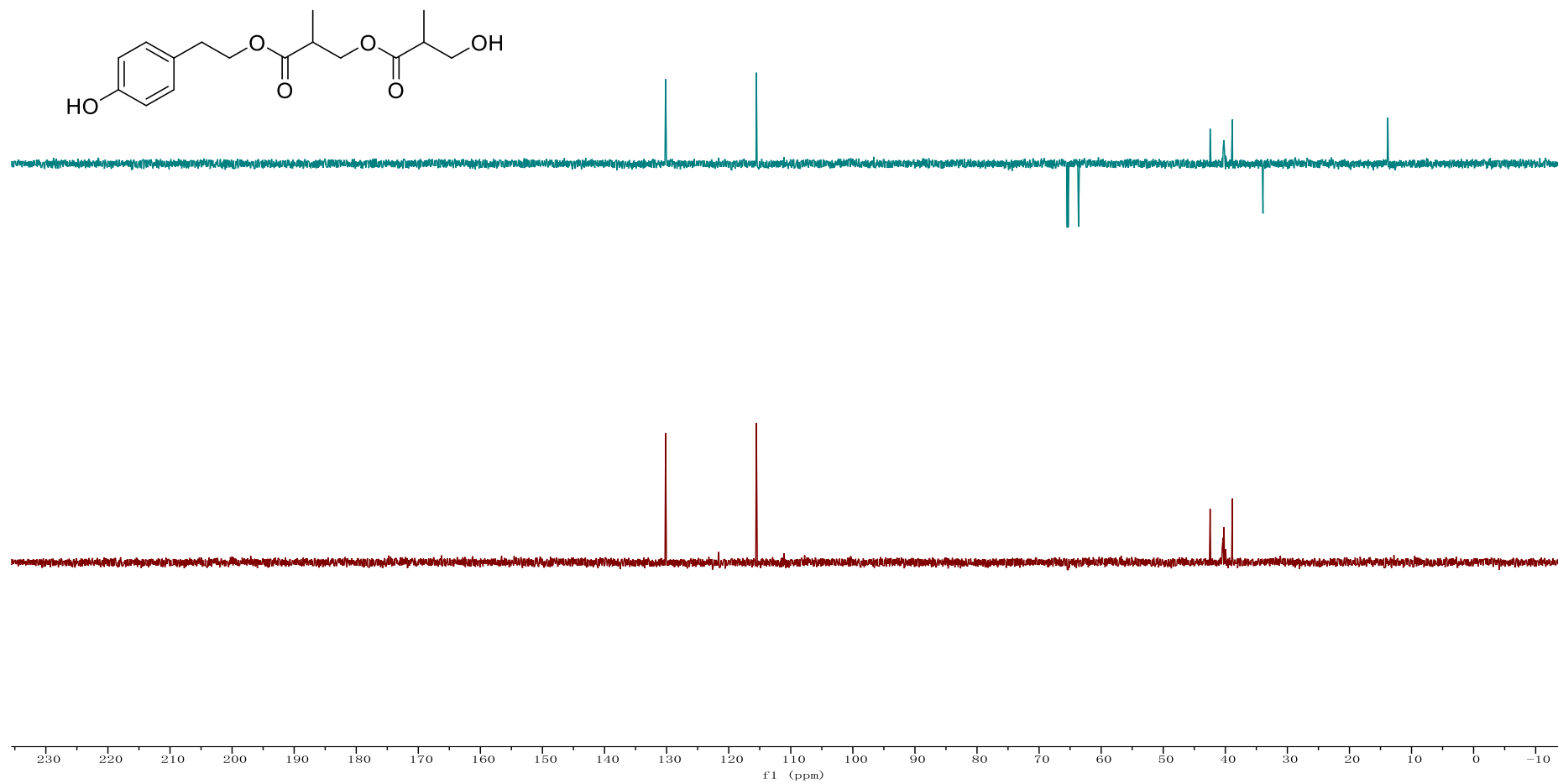


Figure S13. ^1H - ^1H COSY spectrum of **2**

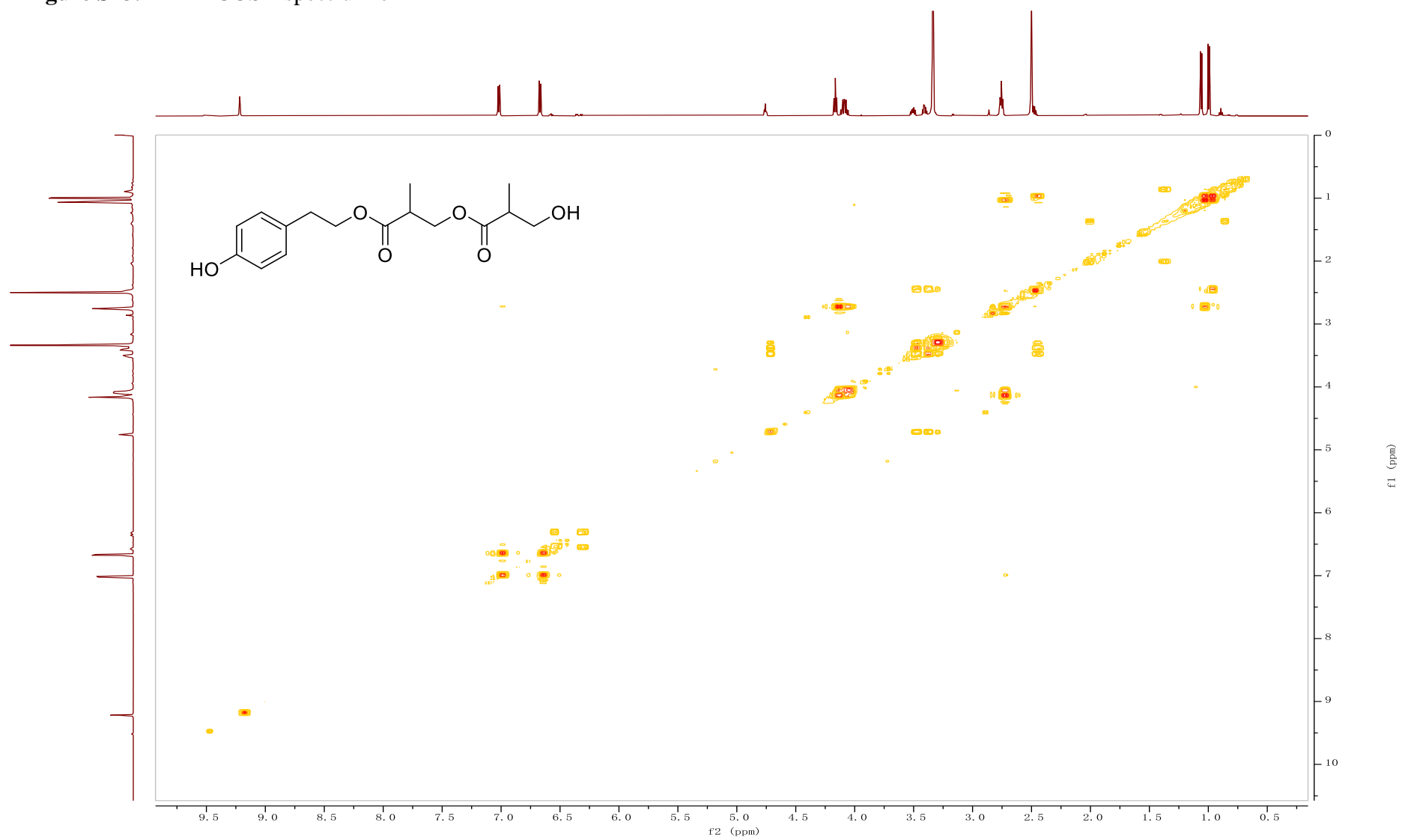


Figure S14. HSQC spectrum of **2**

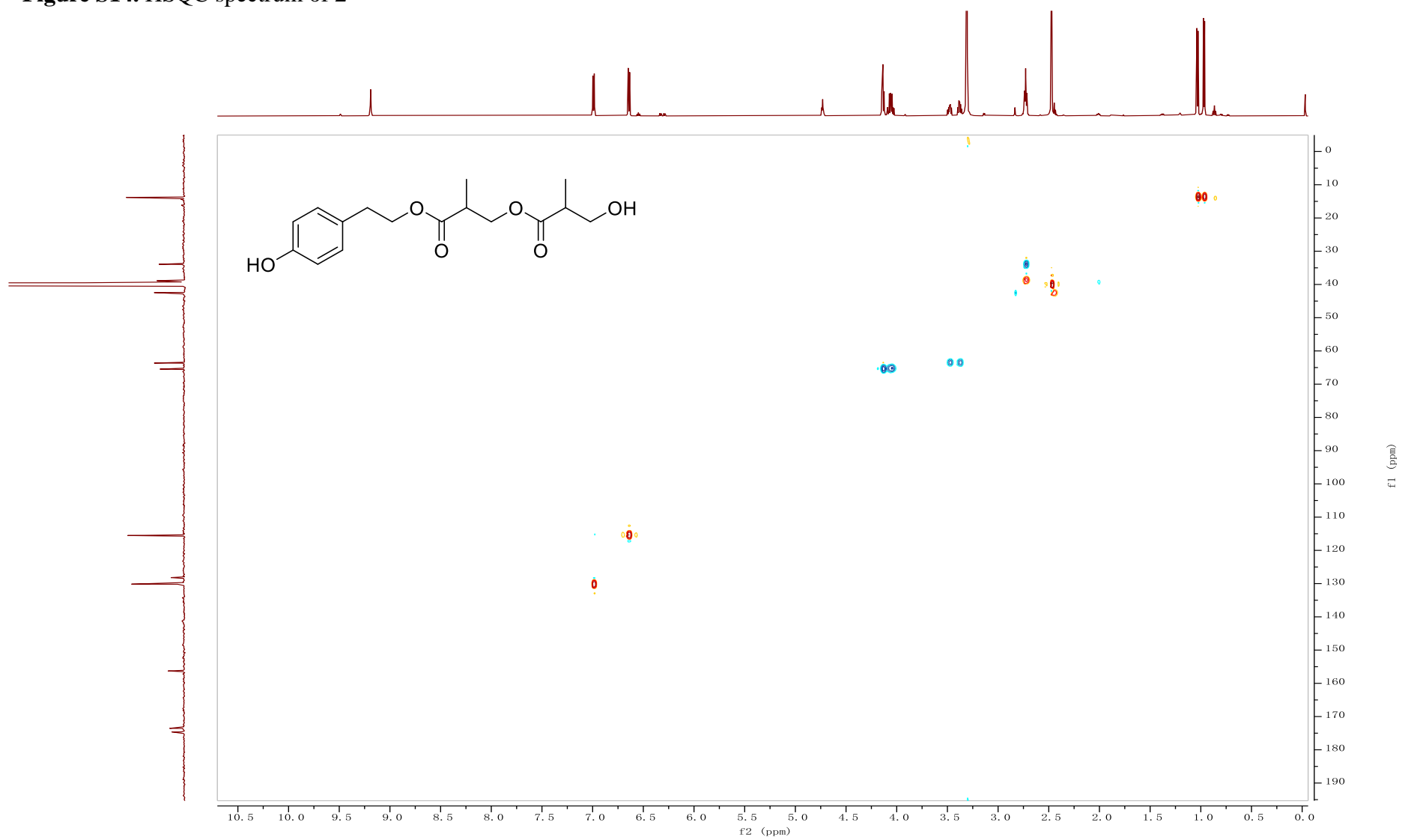


Figure S15. HMBC spectrum of **2**

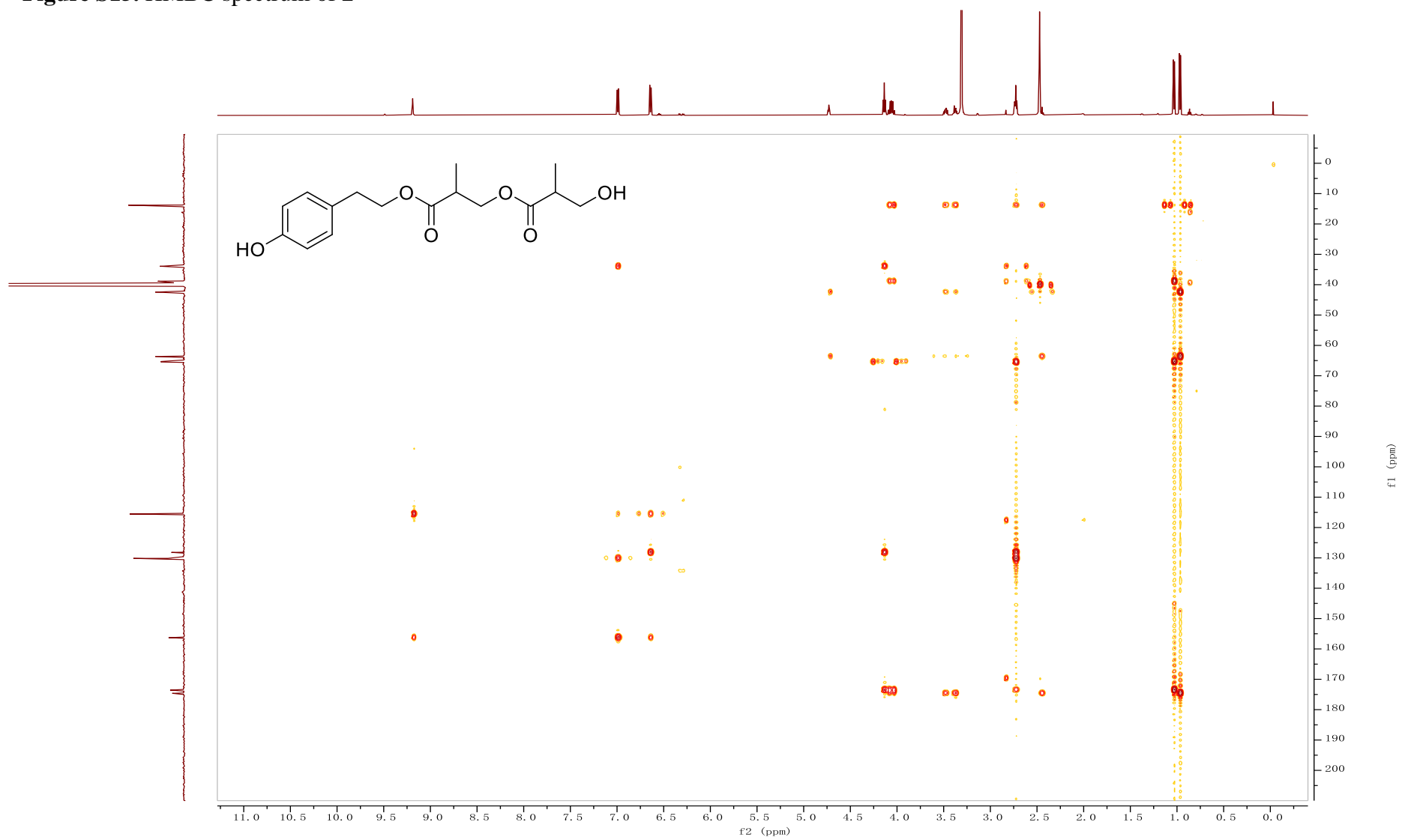


Figure S16. HRESIMS spectrum of **2**

770-35-6-3 #43 RT: 0.34 AV: 1 NL: 6.81E7
T: FTMS + c ESI Full ms [50.00-700.00]

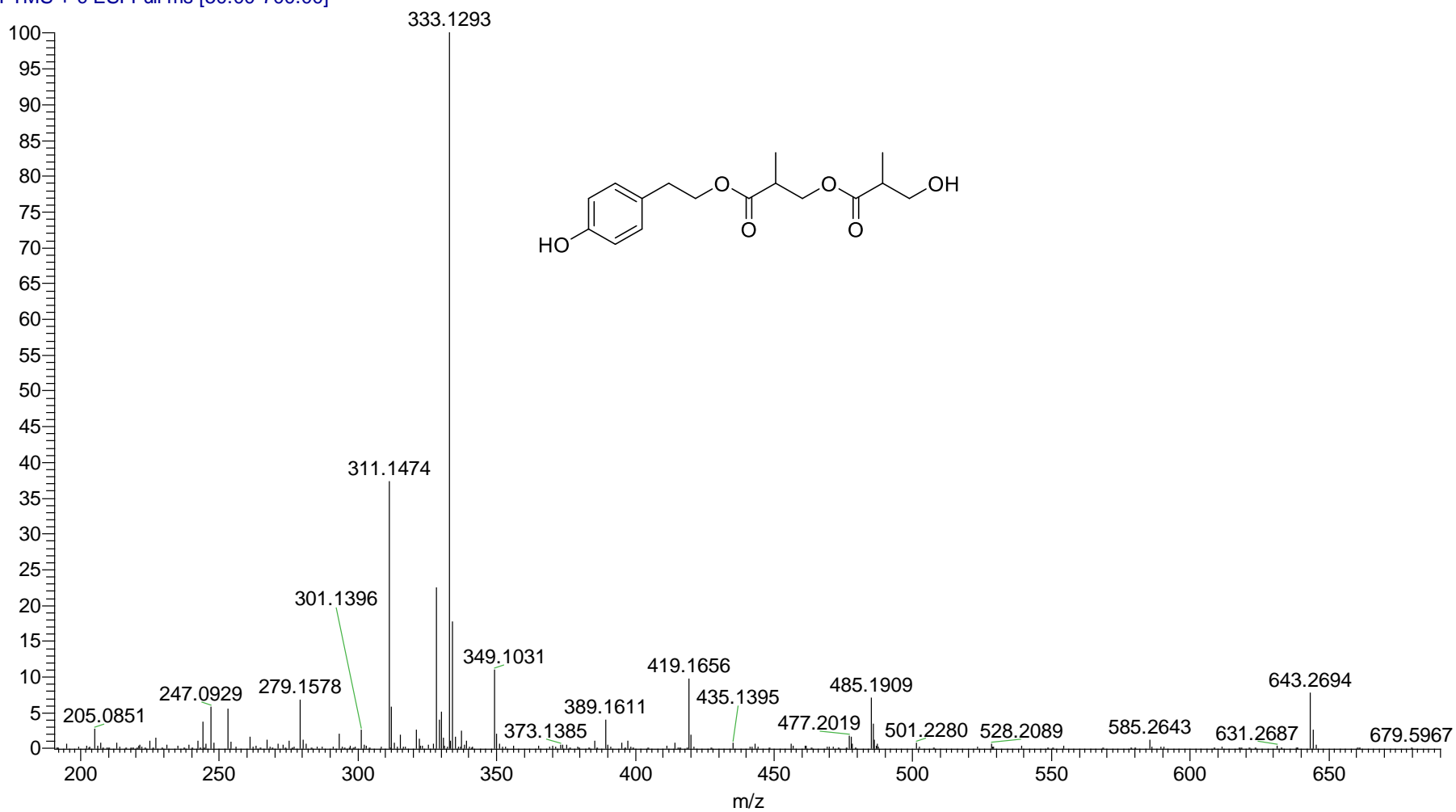


Figure S17. IR spectrum of **2**

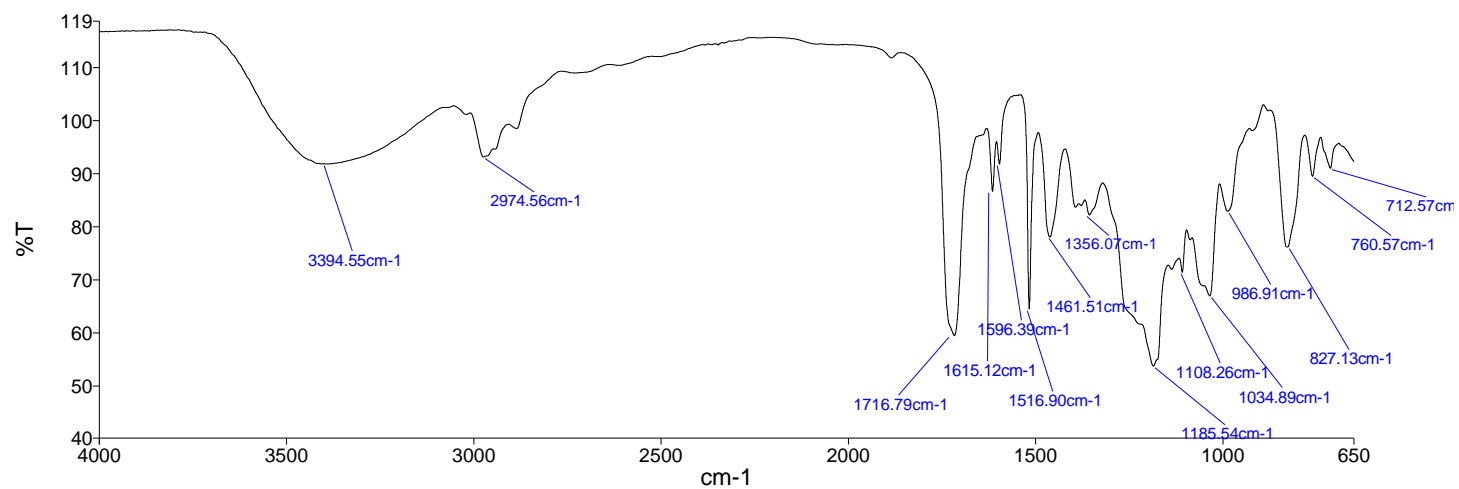


Figure S18. UV spectrum of **2**

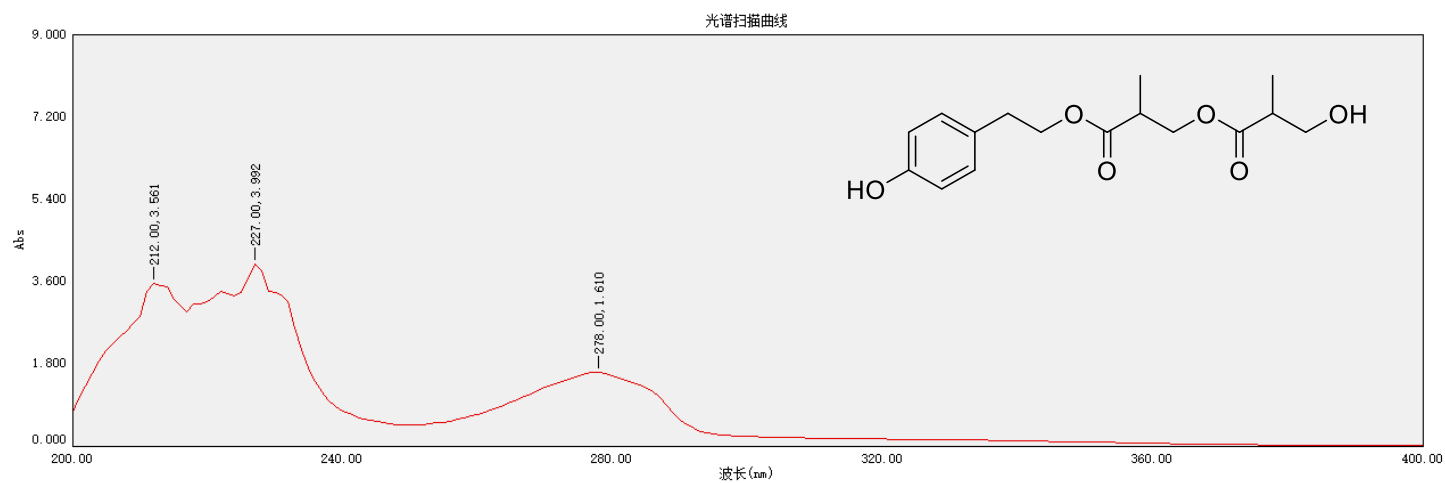


Figure S19. ¹H NMR spectrum of **3**

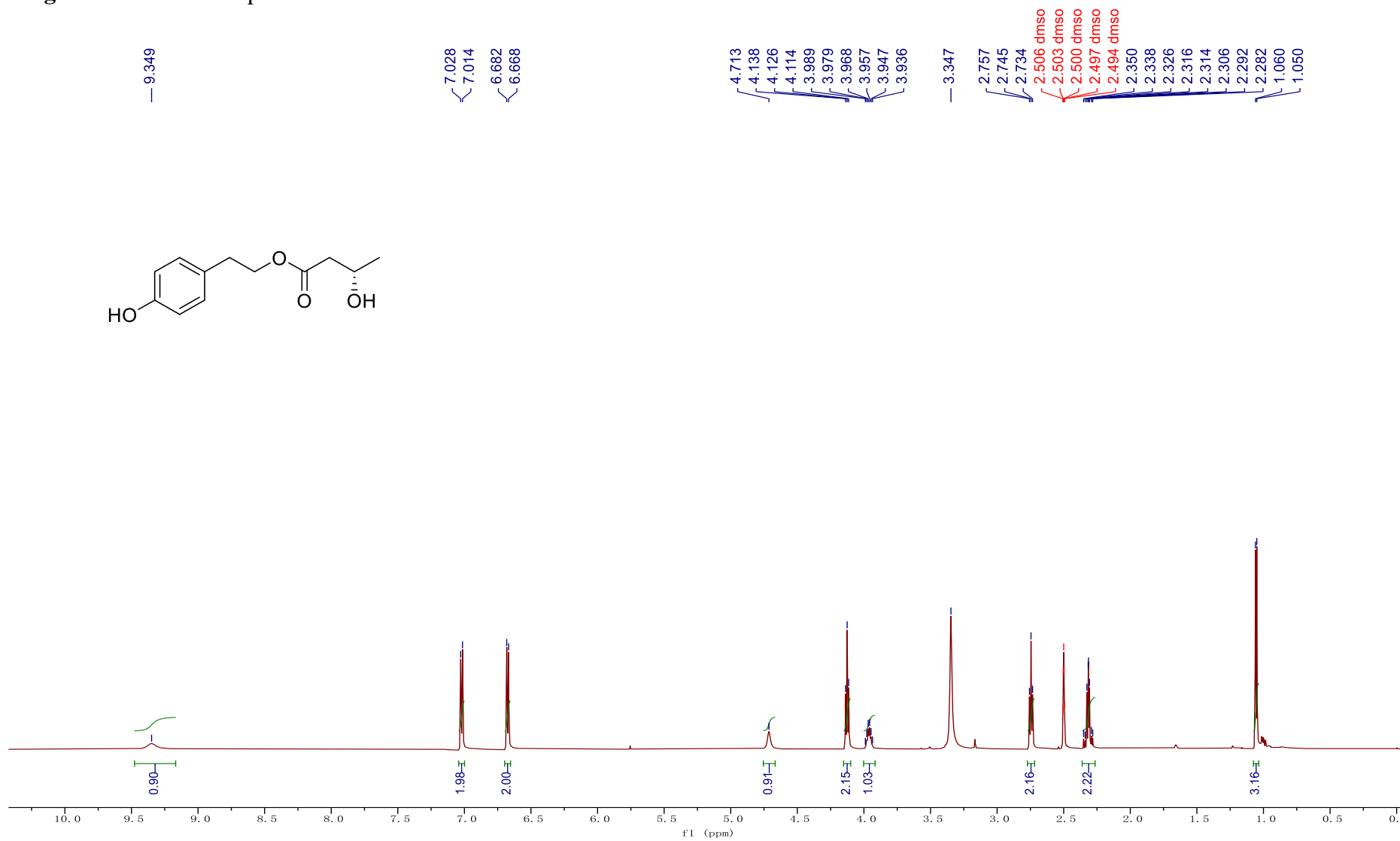


Figure S20. ^{13}C NMR spectrum of **3**

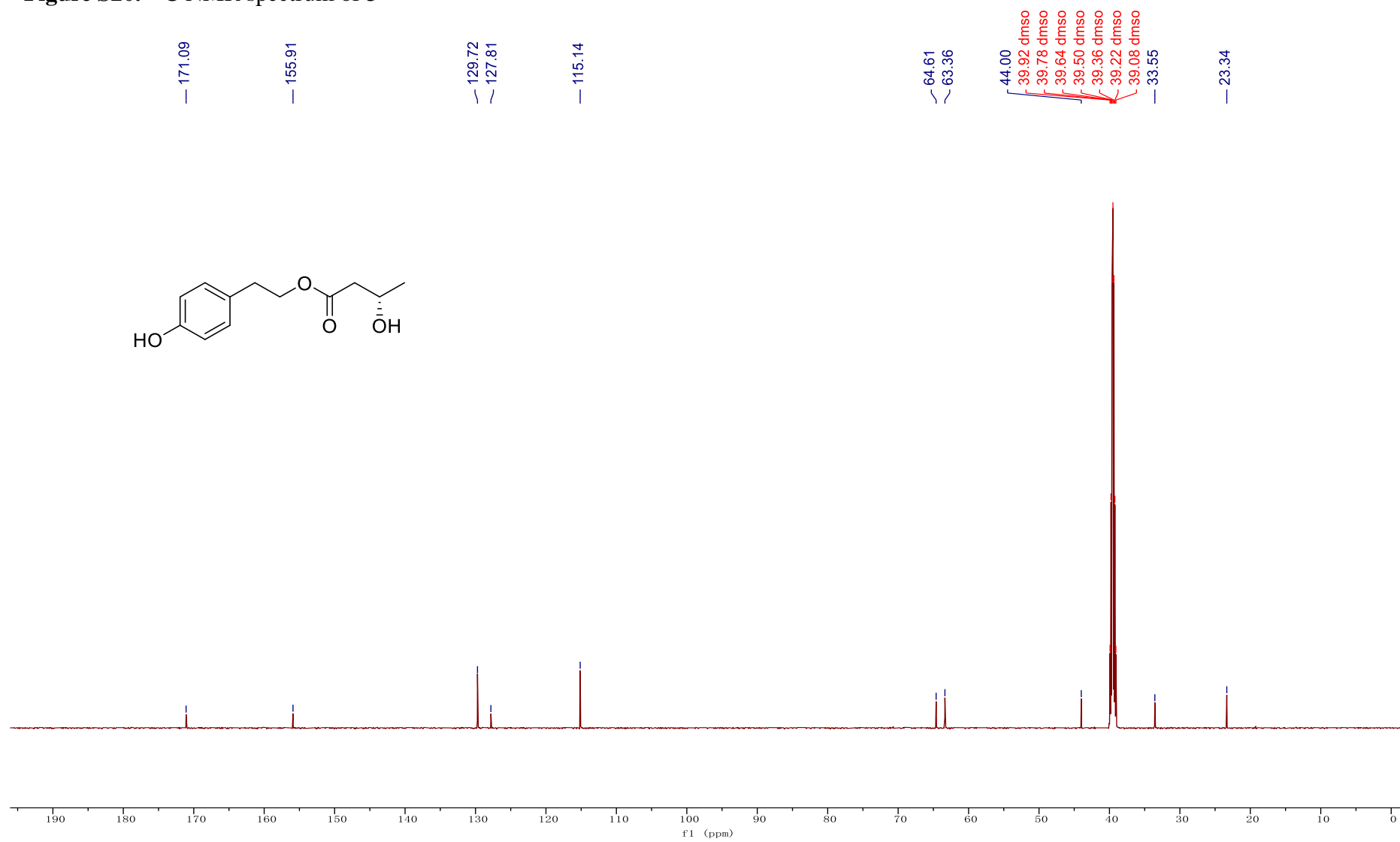


Figure S21. DEPT spectrum of **3**

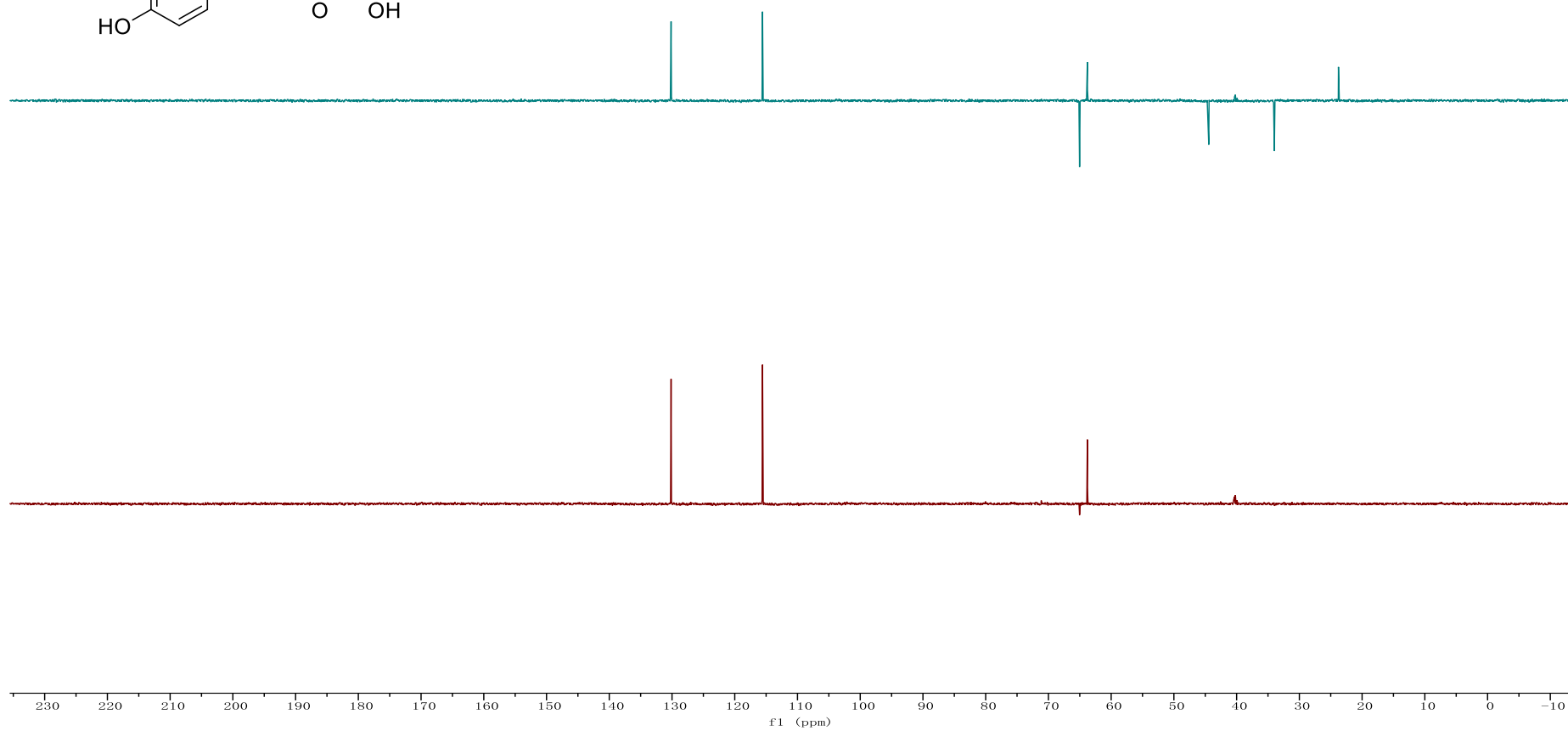
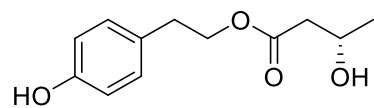


Figure S22. ^1H - ^1H COSY spectrum of **3**

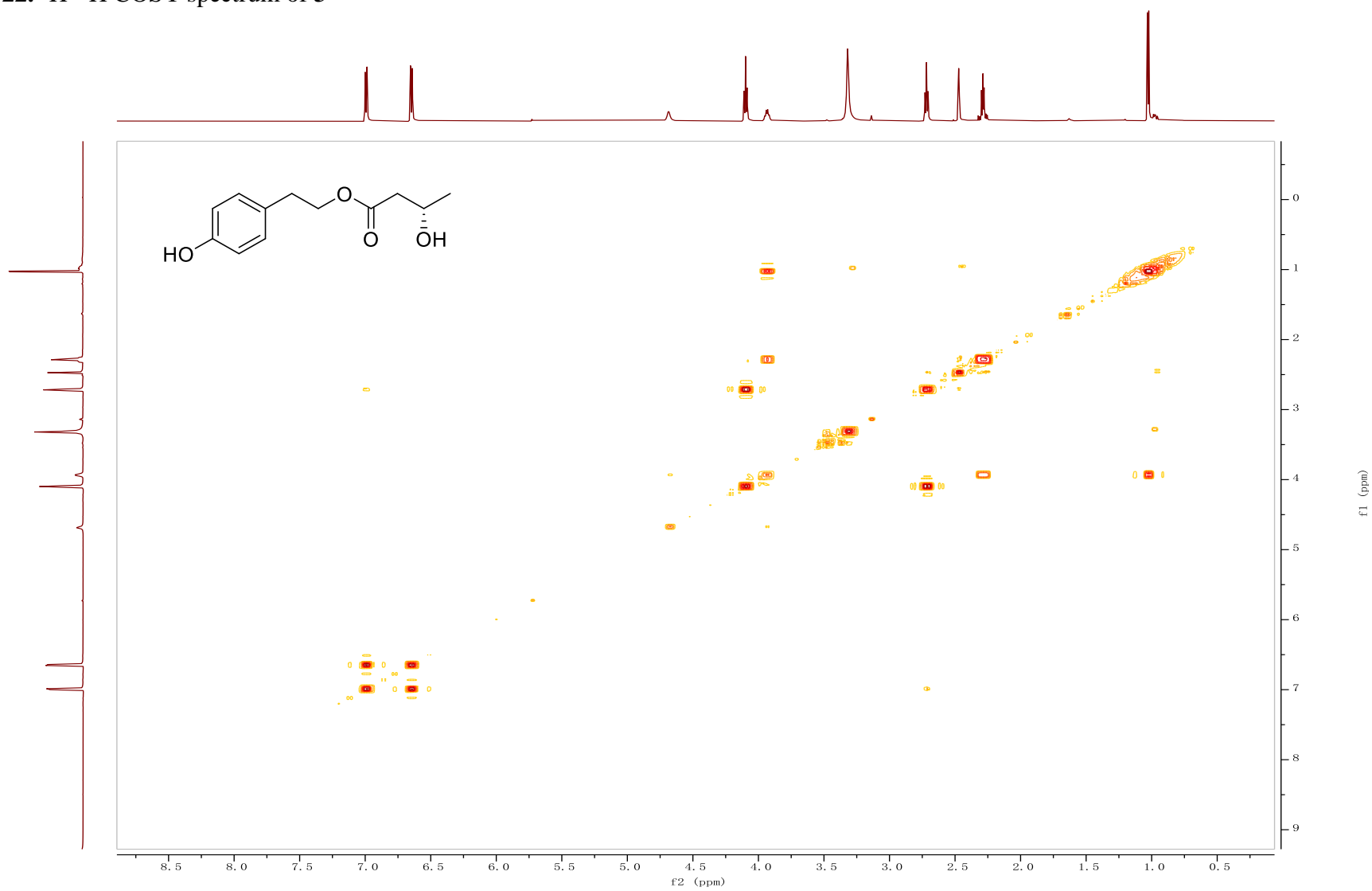


Figure S23. HSQC spectrum of **3**

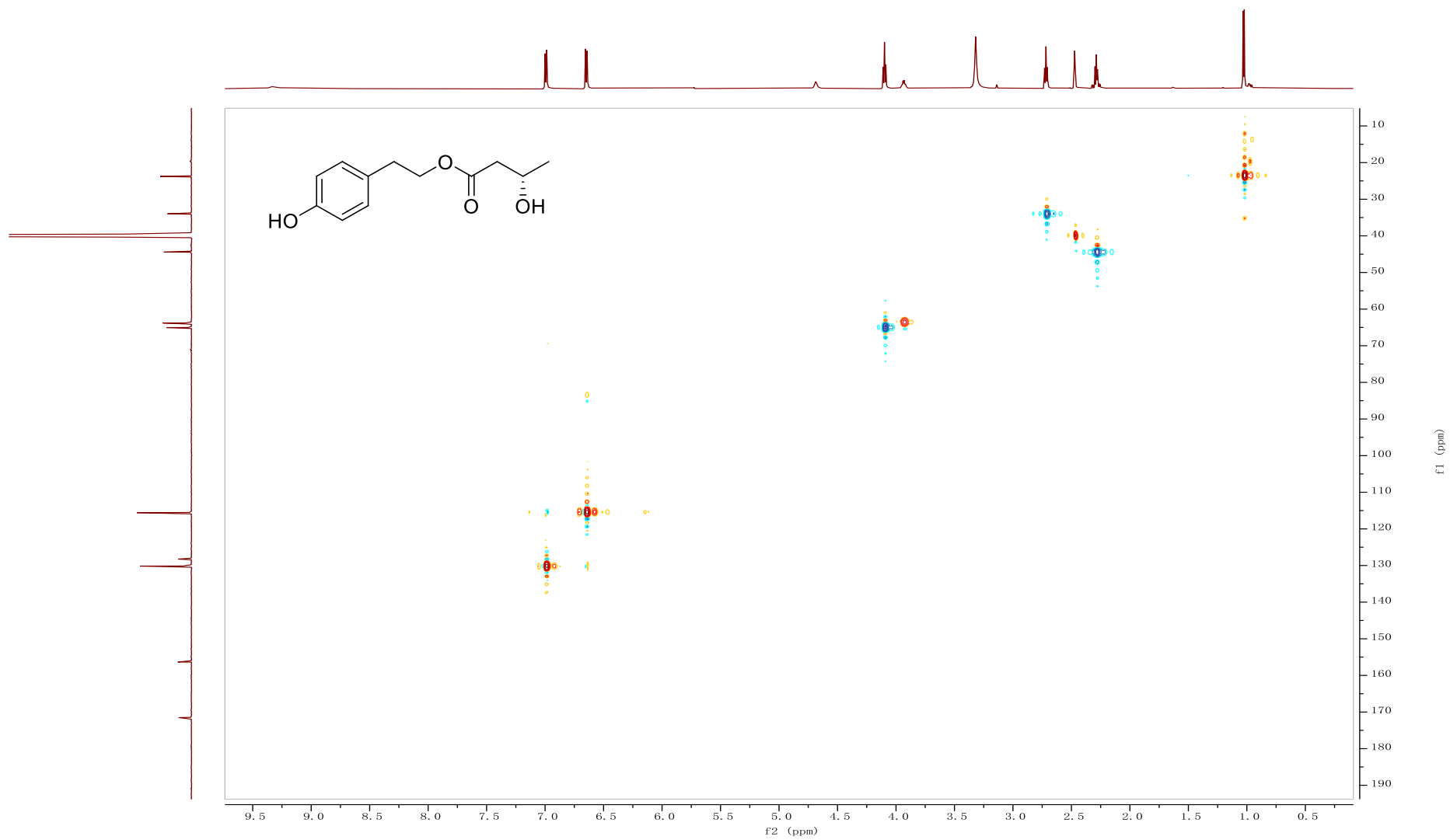


Figure S24. HMBC spectrum of **3**

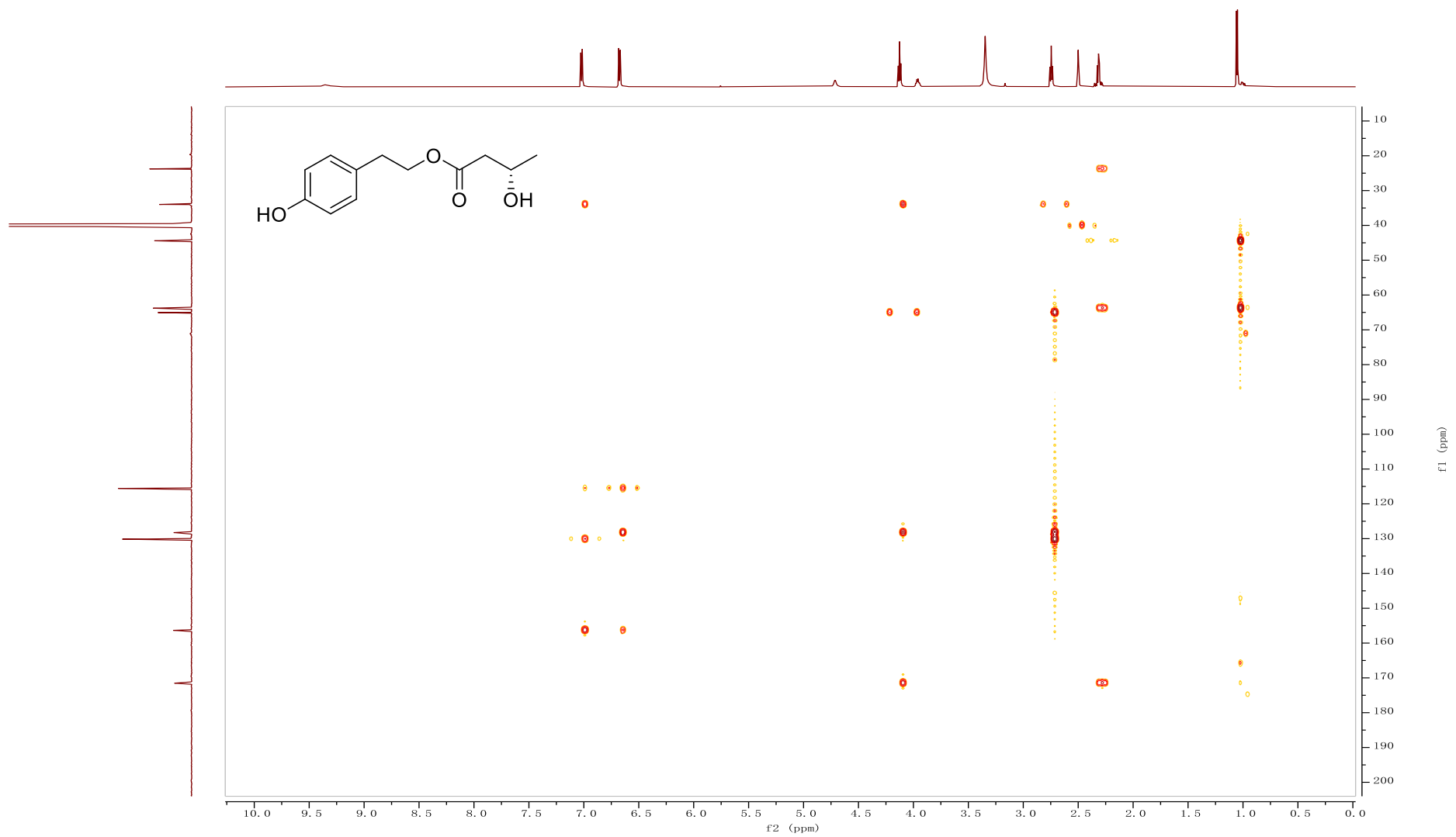


Figure S25. HRESIMS spectrum of **3**

/70-35-5-1 #64 RI: 0.50 AV: 1 NL: 7.6/E/
T: FTMS + c ESI Full ms [100.00-800.00]

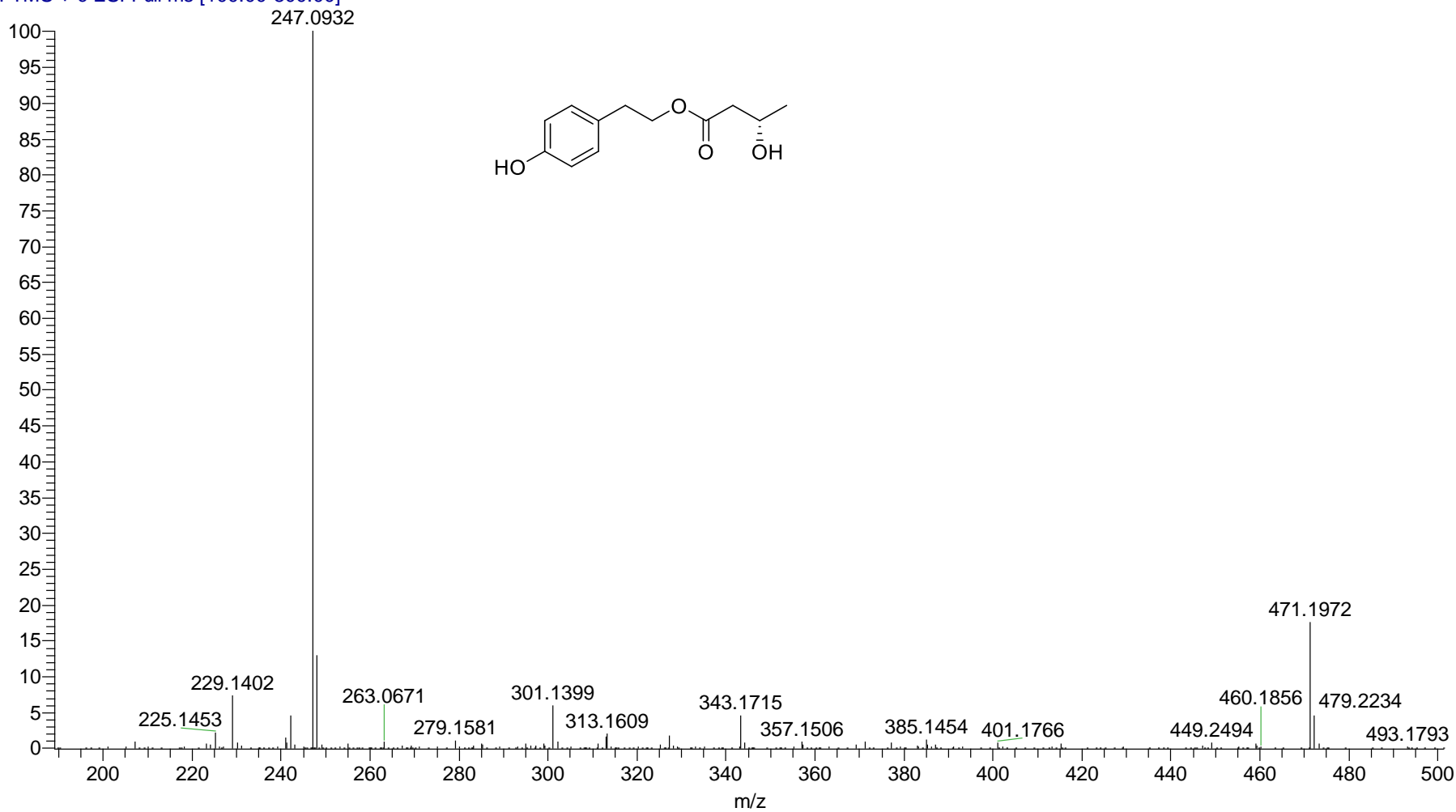


Figure S26. IR spectrum of **3**

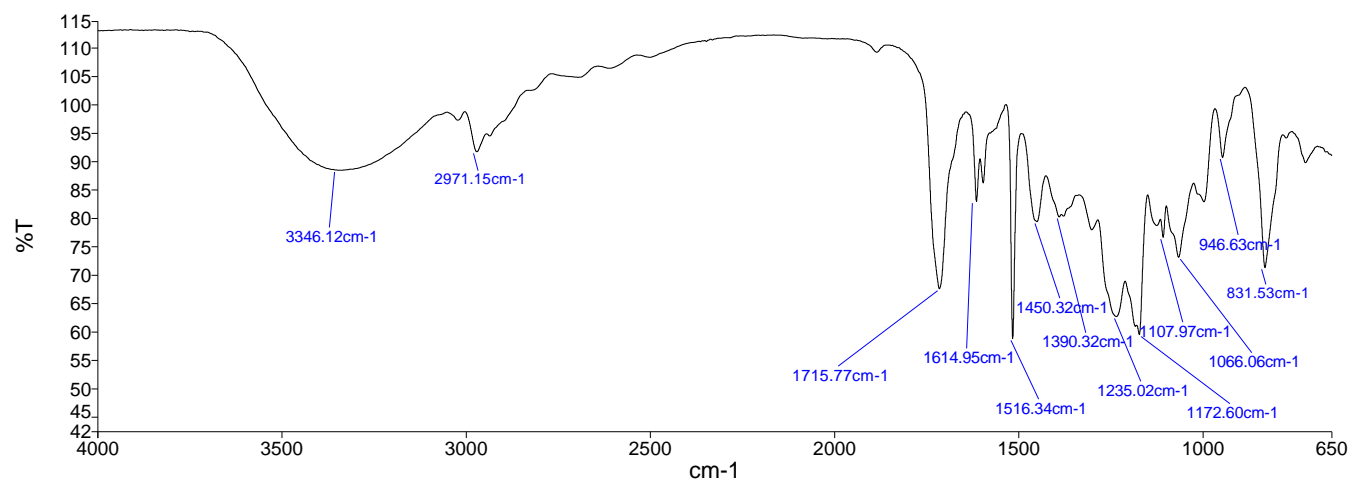


Figure S27. UV spectrum of **3**

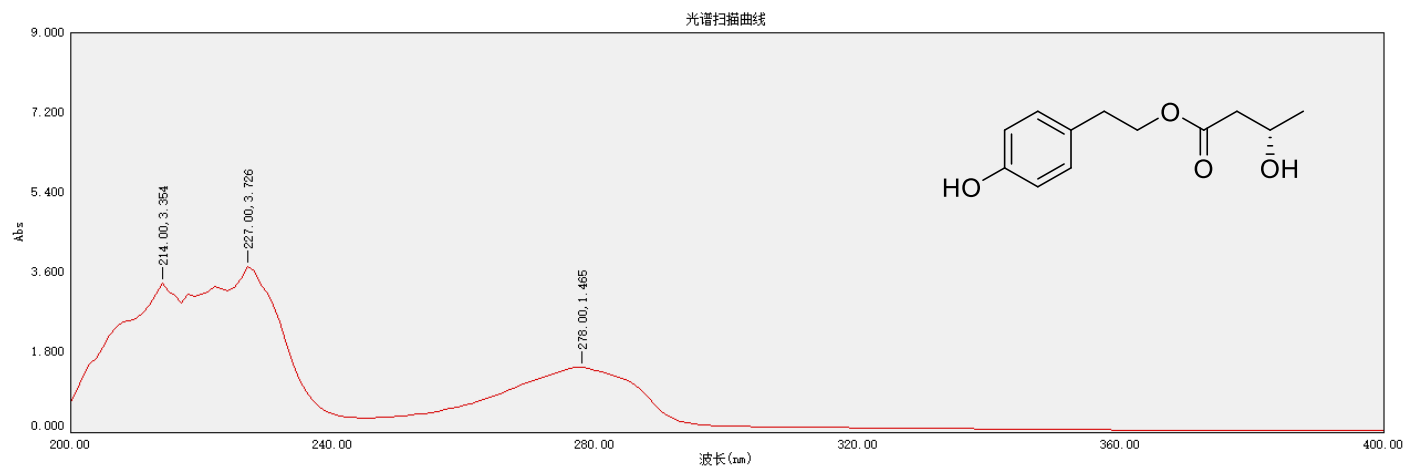


Figure S28. ¹H NMR spectrum of **9**

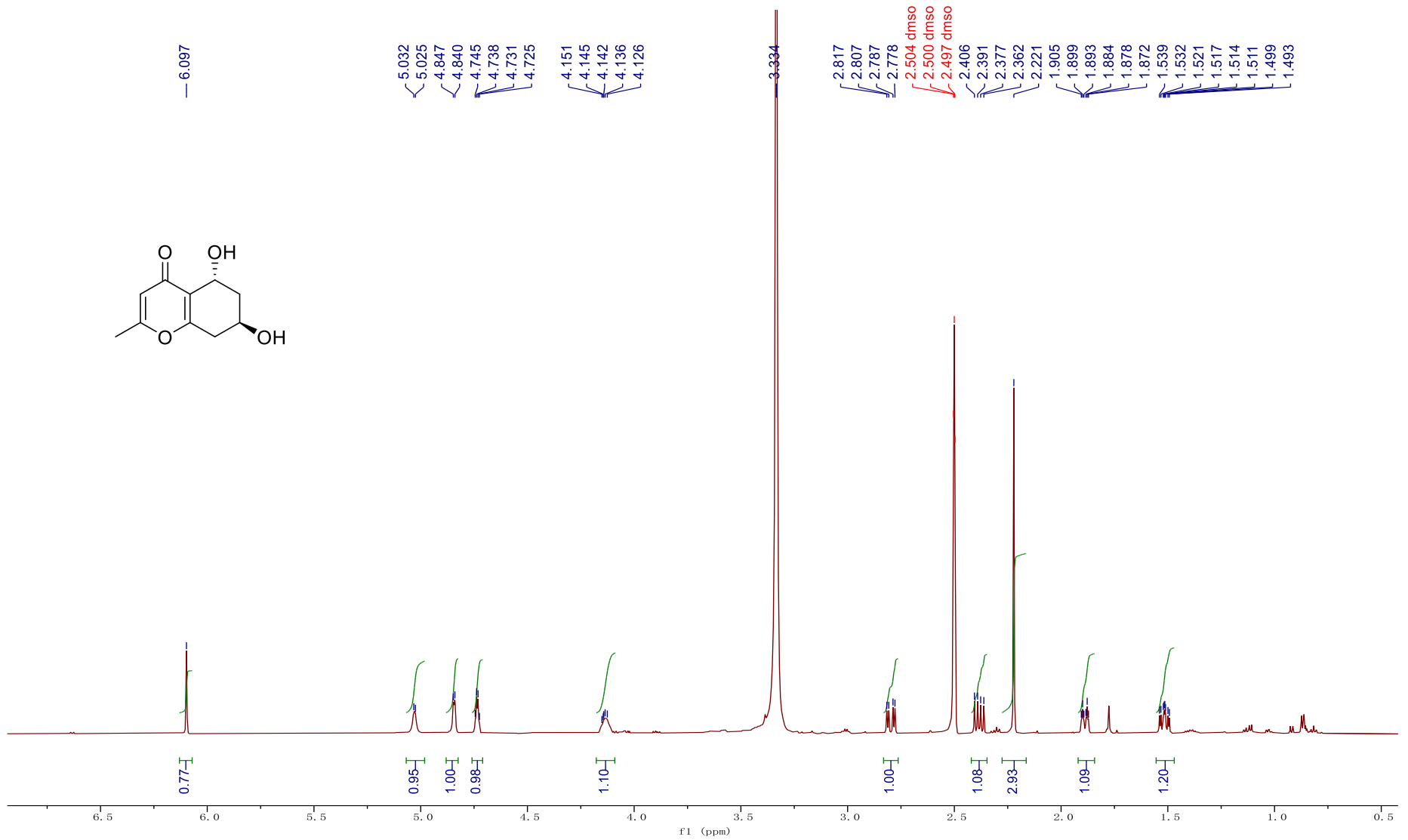


Figure S29. ^{13}C NMR spectrum of **9**

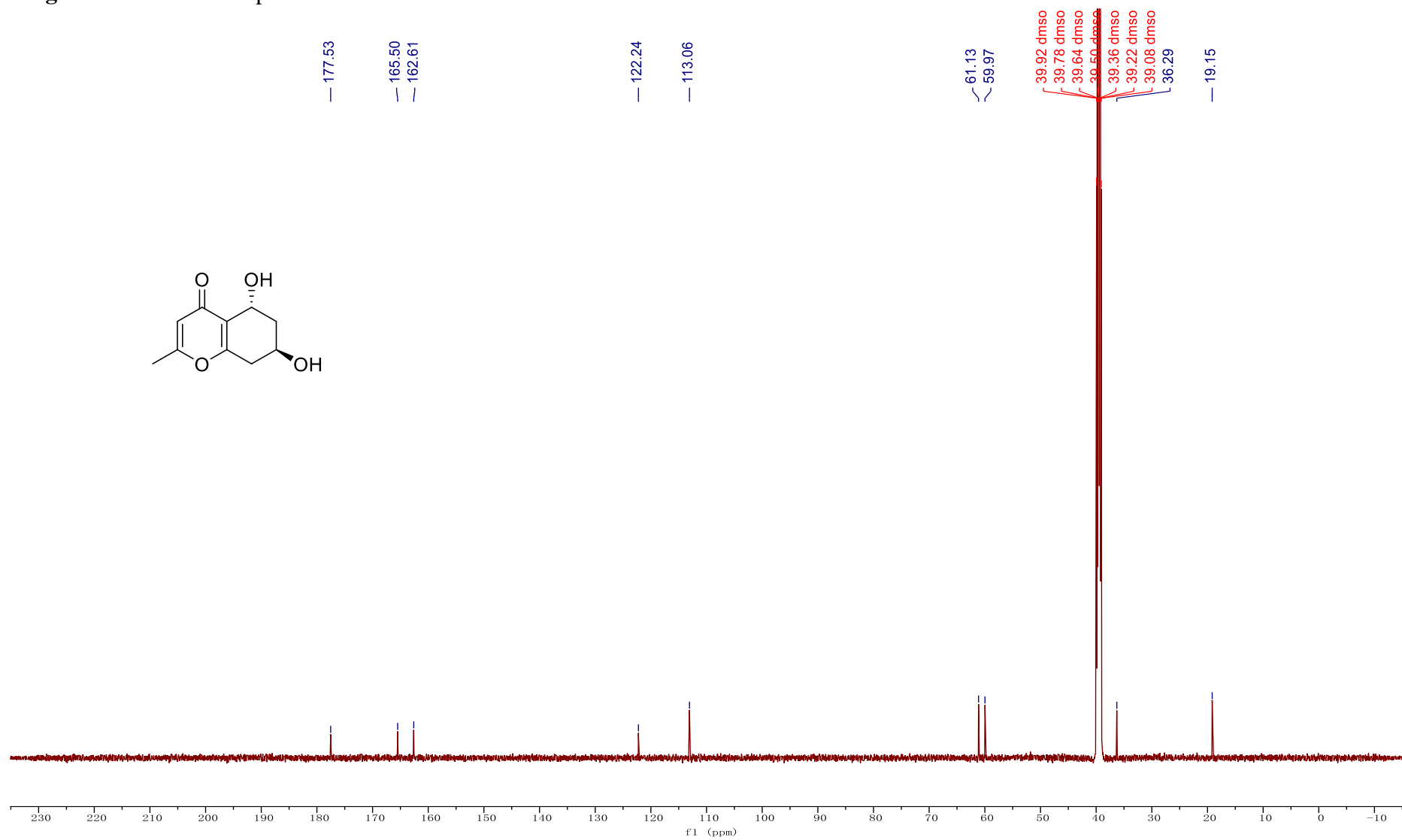


Figure S30. DEPT spectrum of **9**

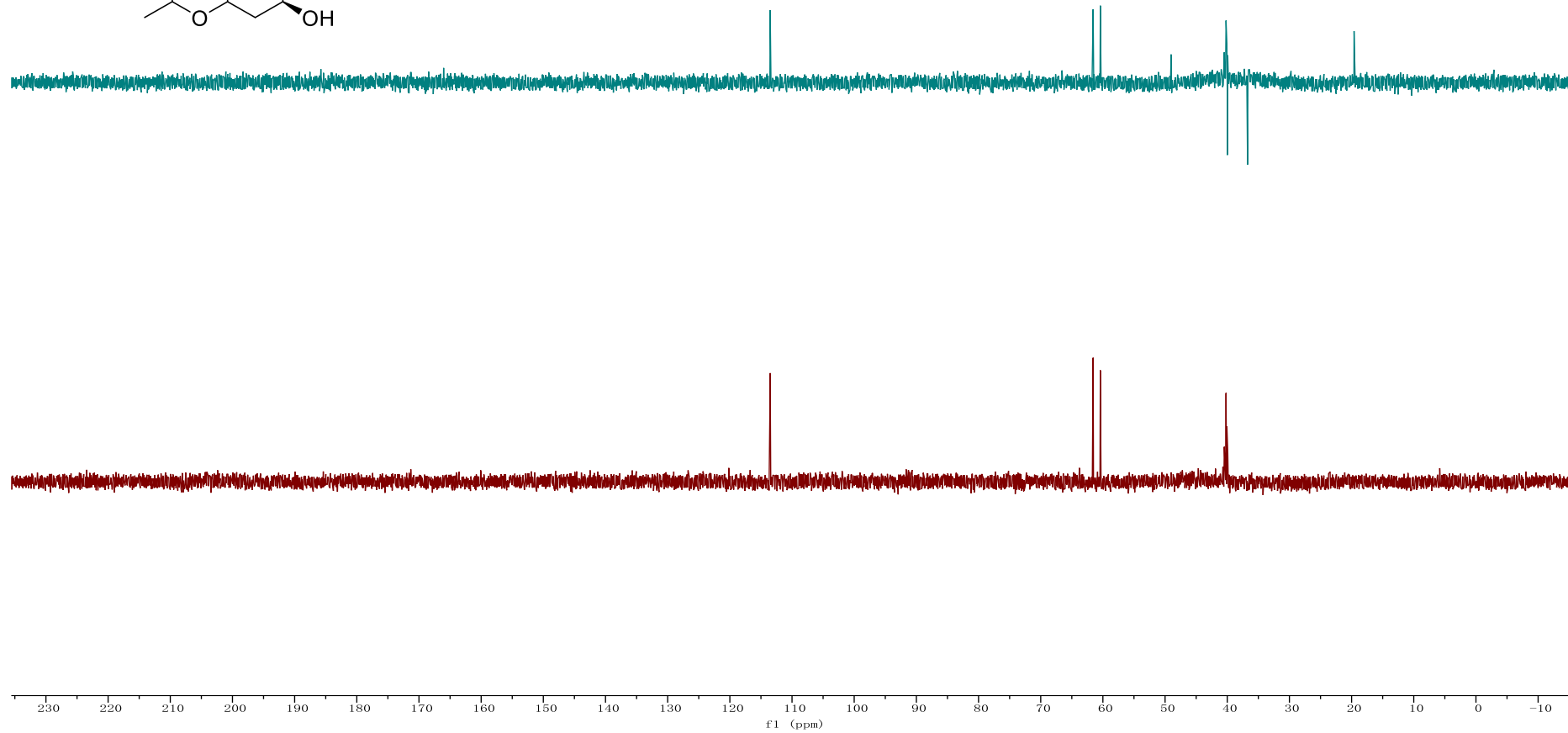
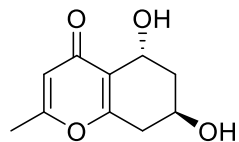


Figure S31. ^1H - ^1H COSY spectrum of **9**

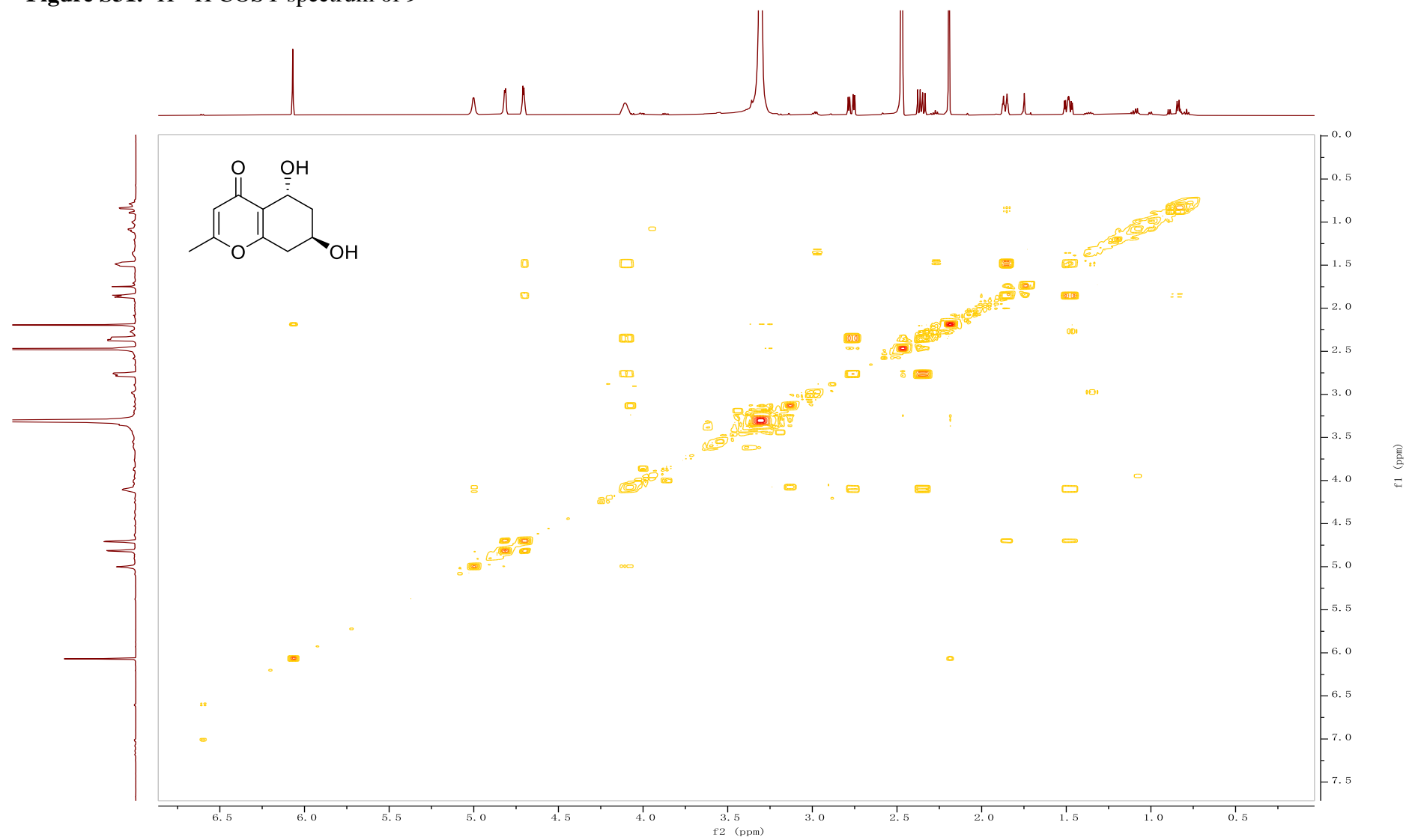


Figure S32. HSQC spectrum of **9**

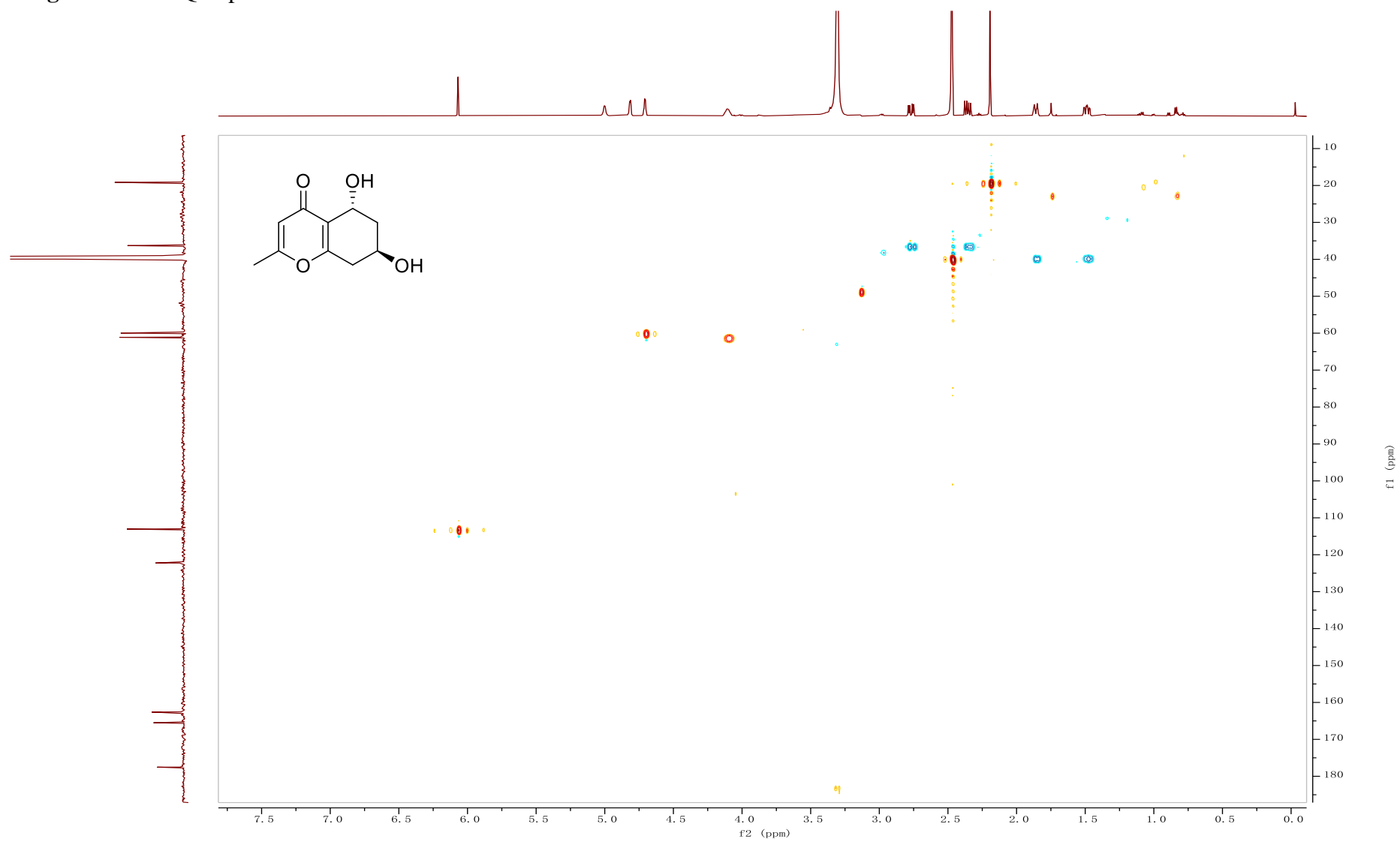


Figure S33. HMBC spectrum of **9**

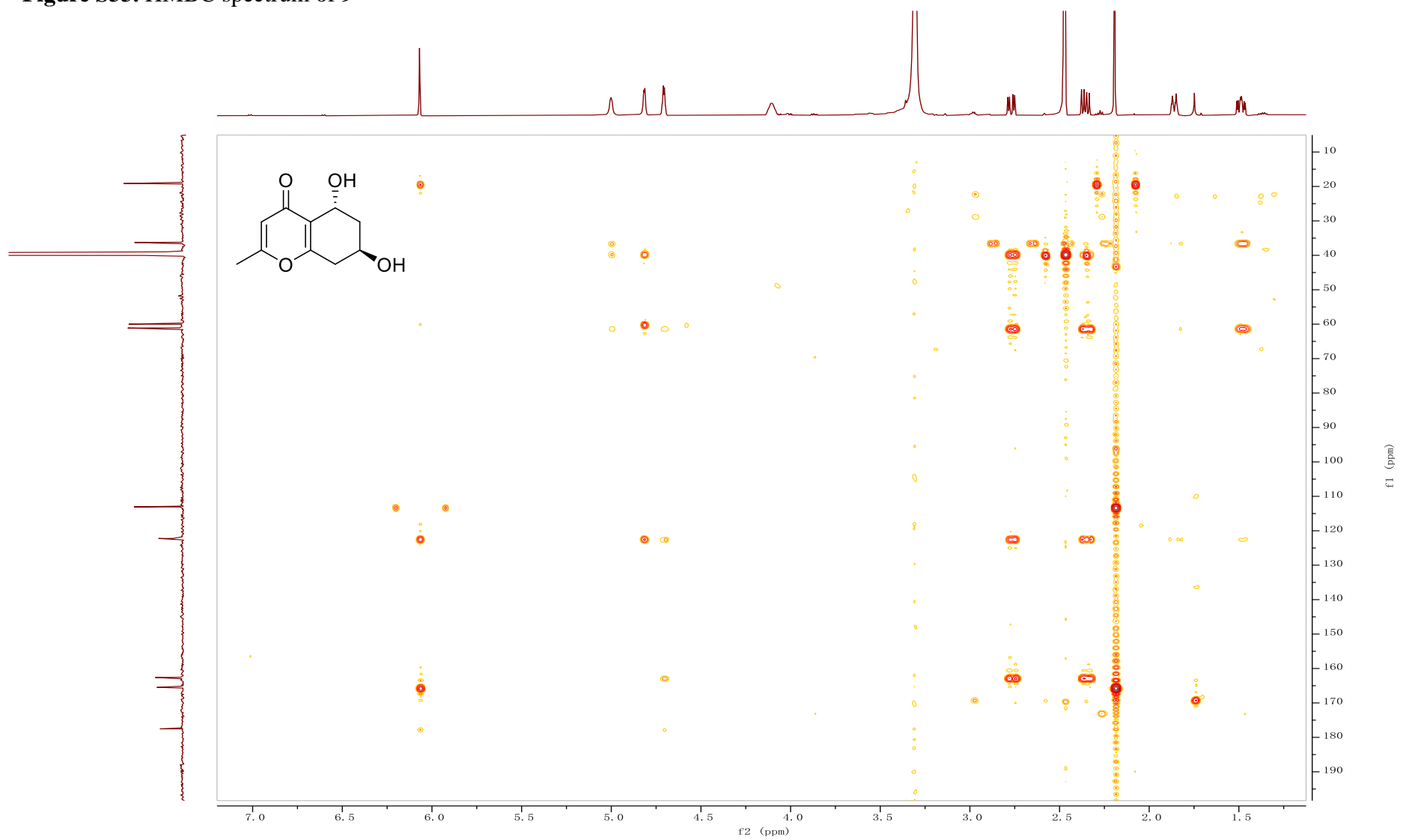


Figure S34. 1D NOE spectrum of **9**

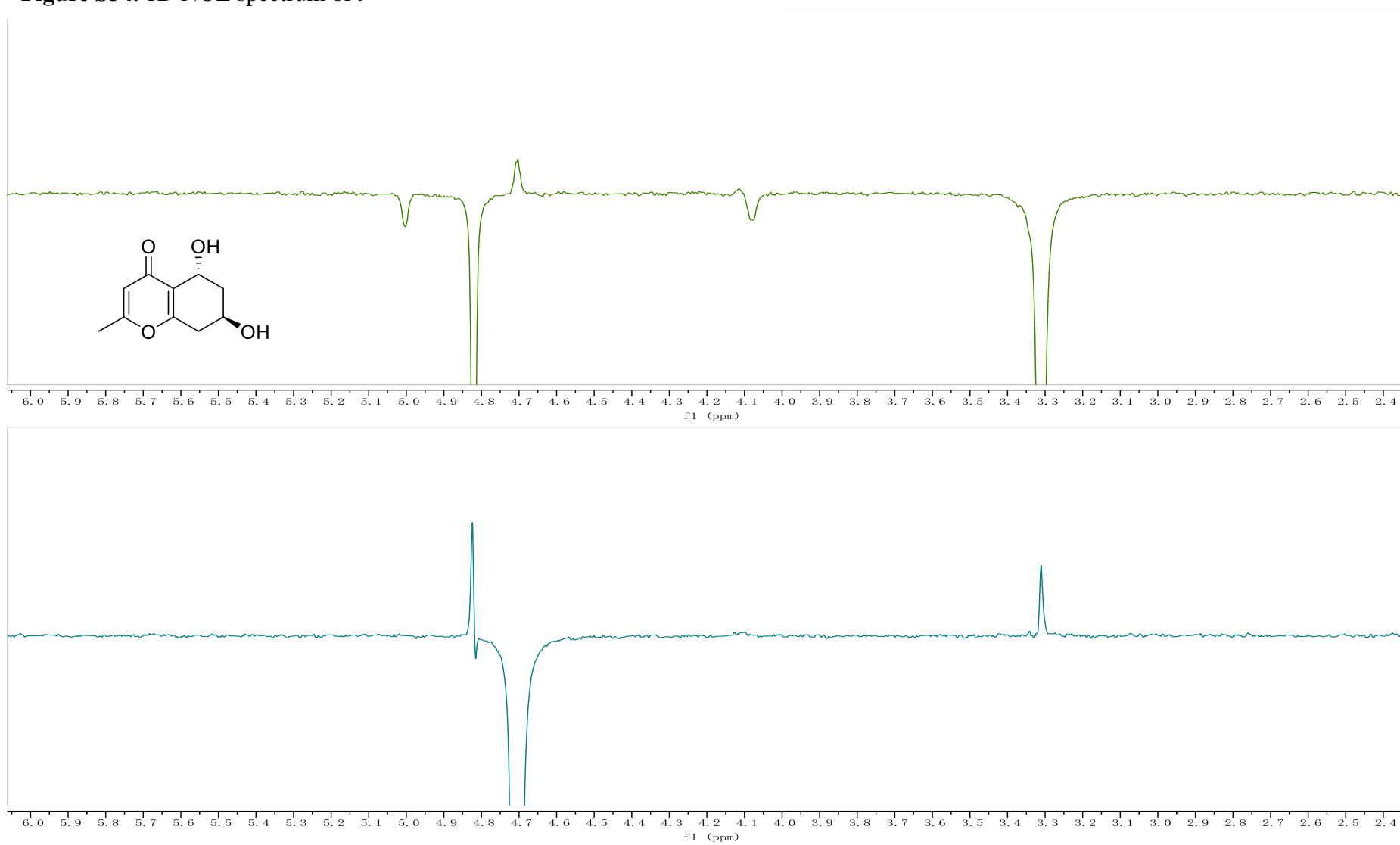


Figure S35. HRESIMS spectrum of **9**

/70-84-3 #51 R1: 0.40 AV: 1 NL: 7.63E7
T: FTMS + c ESI Full ms [50.00-700.00]

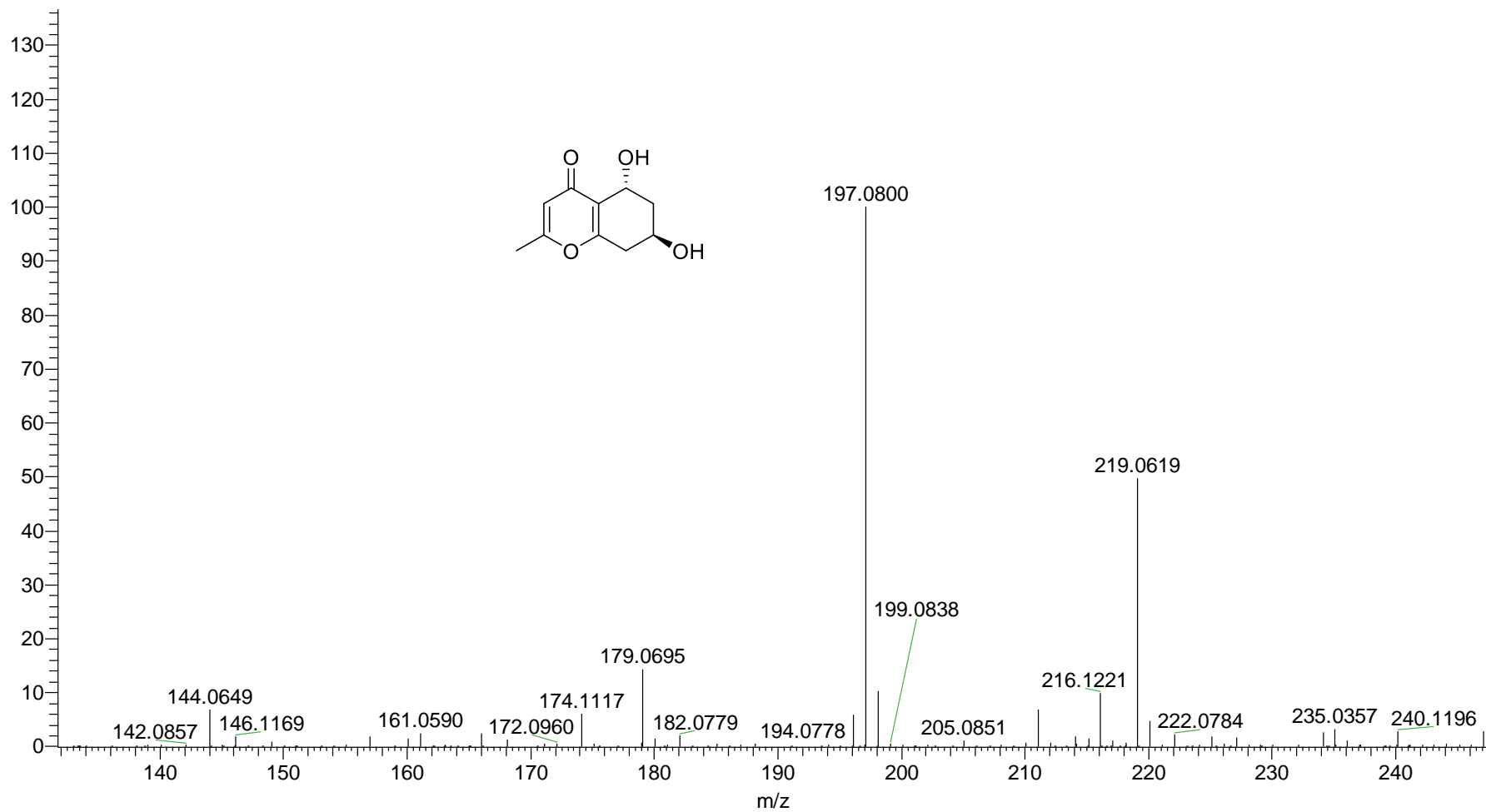


Figure S36. IR spectrum of 9

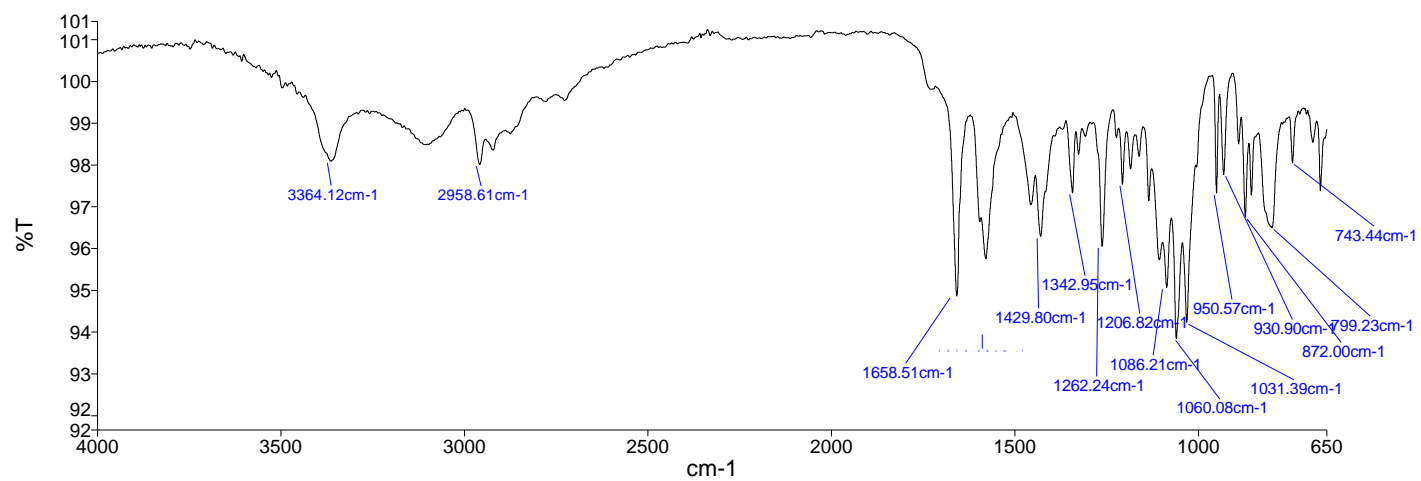


Figure S37. UV spectrum of 9

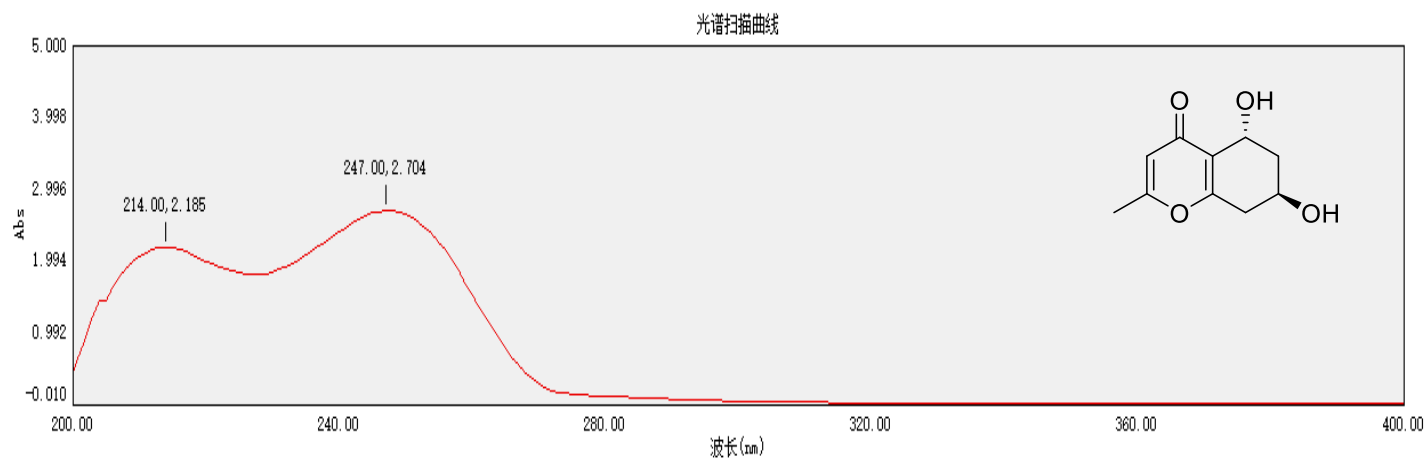
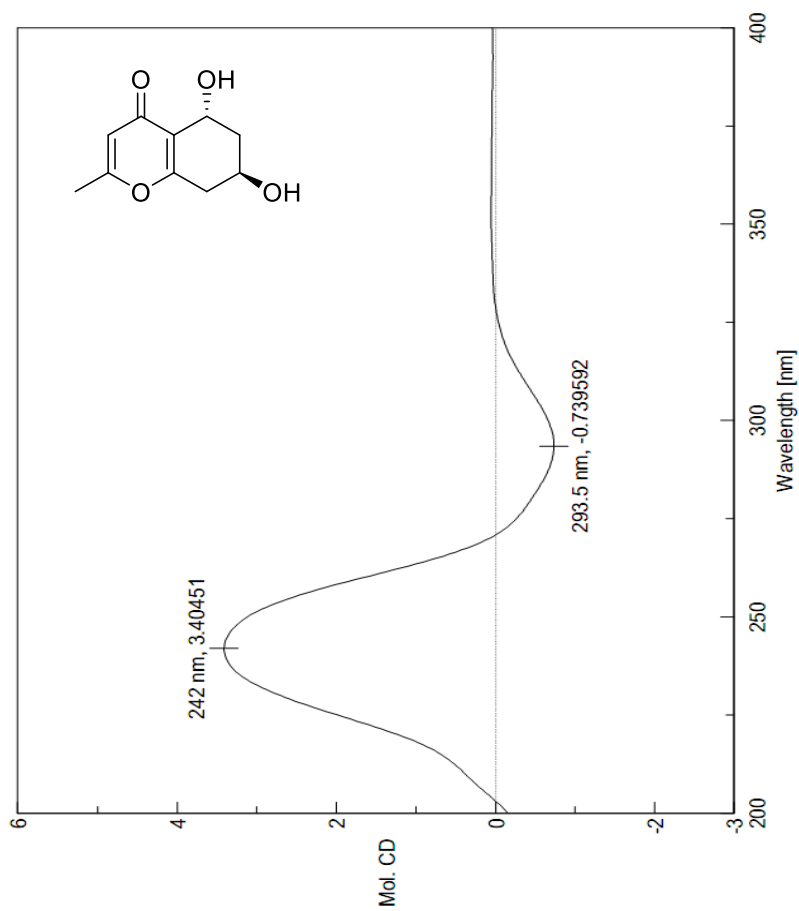


Figure S38. CD spectrum of **9**



[Comments]
 Sample name 770-84-3
 Comment

[Measurement Information]
 Division Name IMM-CD
 Sample Name JMM5
 Serial No. A024461168

Accessory Standard
 Accessory S/N A005461185
 Cell Length 1 mm

Measurement date 2021/1/29 15:51

Photometric Mode CD, HT, Abs
 Measure Range 400 - 200 nm
 Data pitch 0.5 nm
 Sensitivity Standard
 D.I.T. 1 sec
 Bandwidth 1.00 nm
 Start Mode Immediately
 Scanning Speed 100 nm/min
 Baseline Correction Baseline
 Shutter Control Auto
 CD Detector PMT
 PMT Voltage Auto
 Accumulations 2
 Solvent MEOH
 Concentration 0.4 (w/v)%

[Detailed Information] 2021/1/29 16:21
 Creation date 2021/1/29 16:21

Data array type Linear data array * 3
 Horizontal axis Wavelength [nm]
 Vertical axis(1) Mol. CD
 Vertical axis(2) HT [V]
 Vertical axis(3) Abs
 Start 400 nm
 End 200 nm
 Data interval 0.5 nm
 Data points 401

770-84-3-1-s-m.jws

Figure S39. ¹H NMR spectrum of **10**

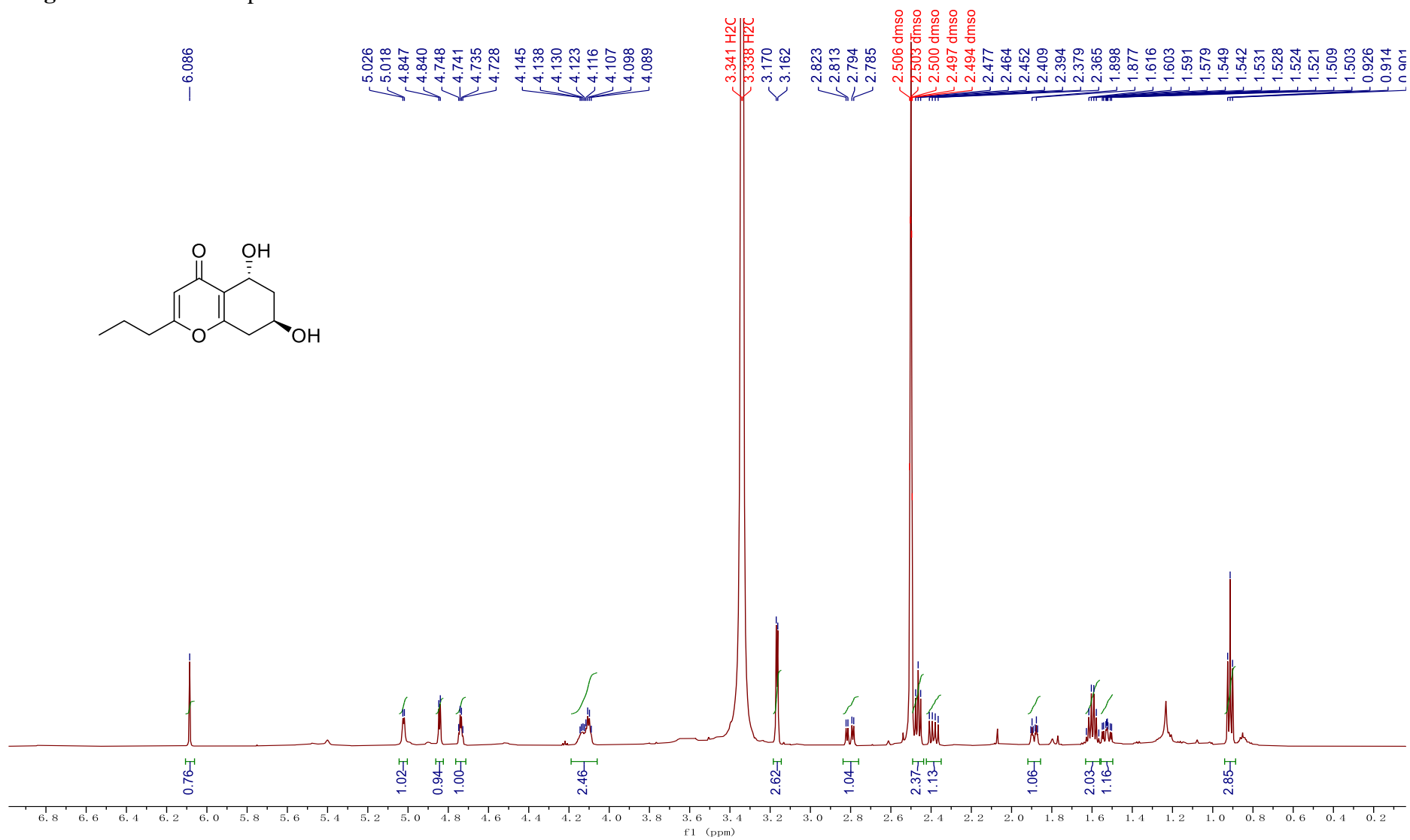


Figure S40. ^{13}C NMR spectrum of **10**

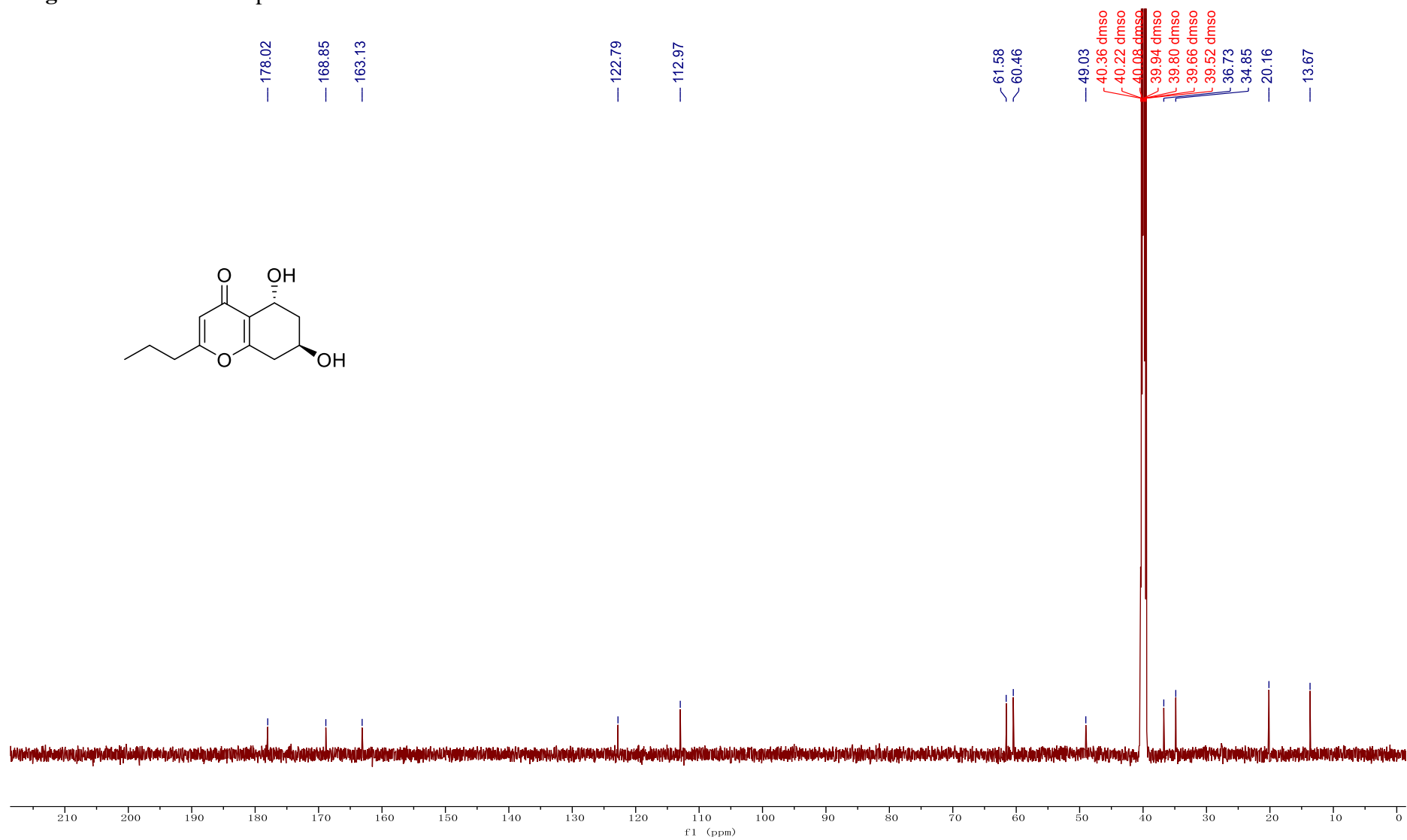


Figure S41. DEPT spectrum of **10**

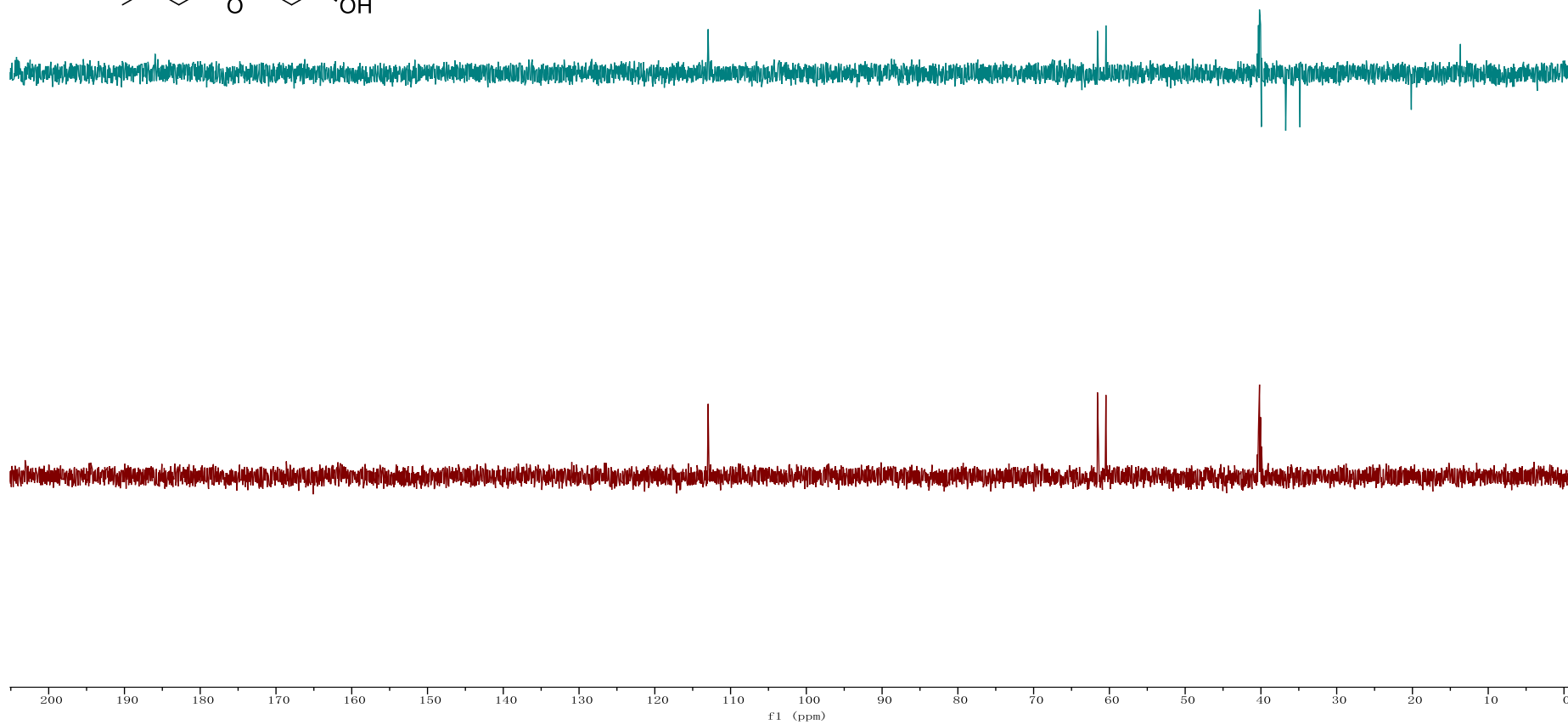
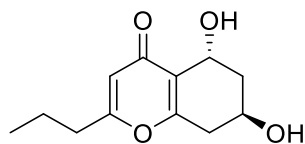


Figure S42. ^1H - ^1H COSY spectrum of **10**

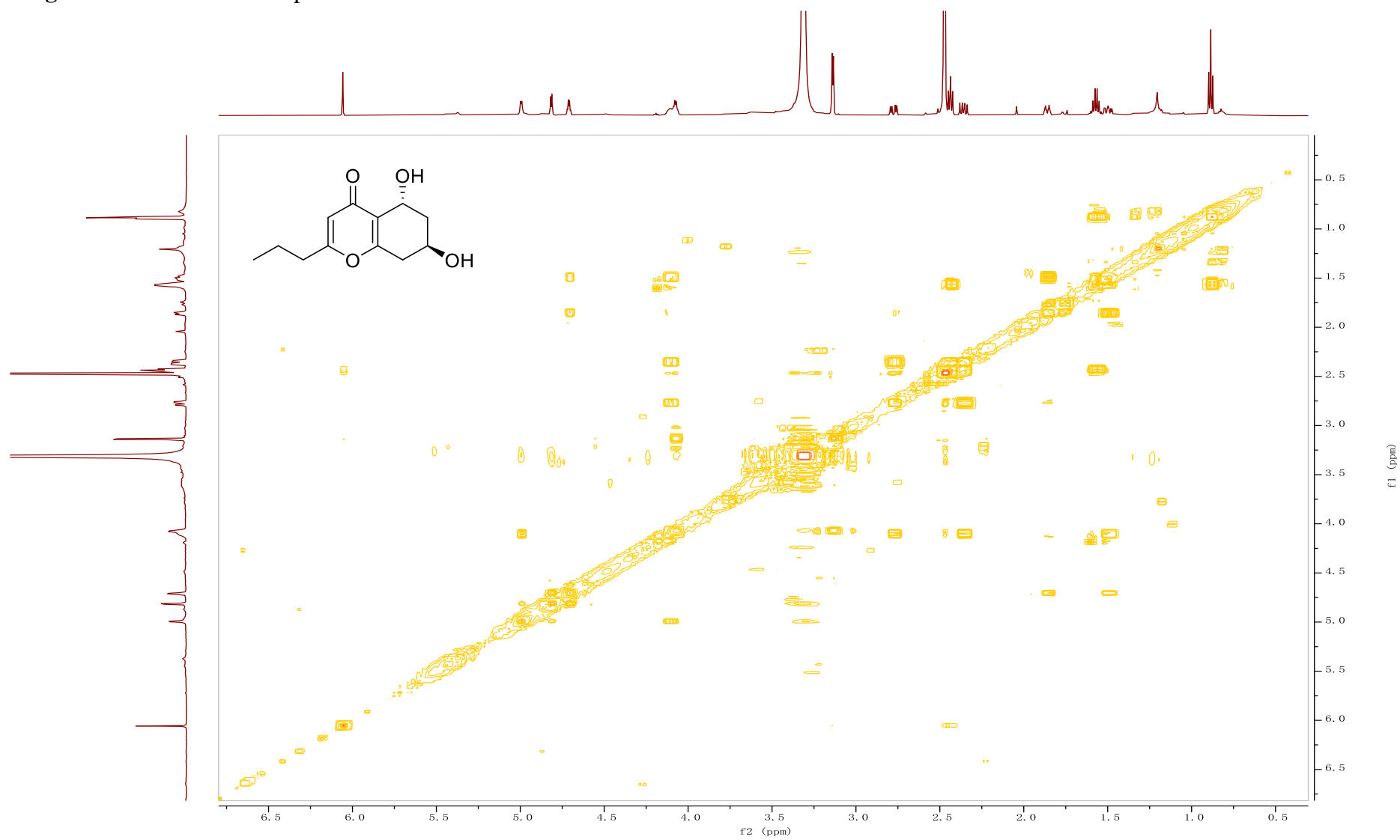


Figure S43. HSQC spectrum of **10**

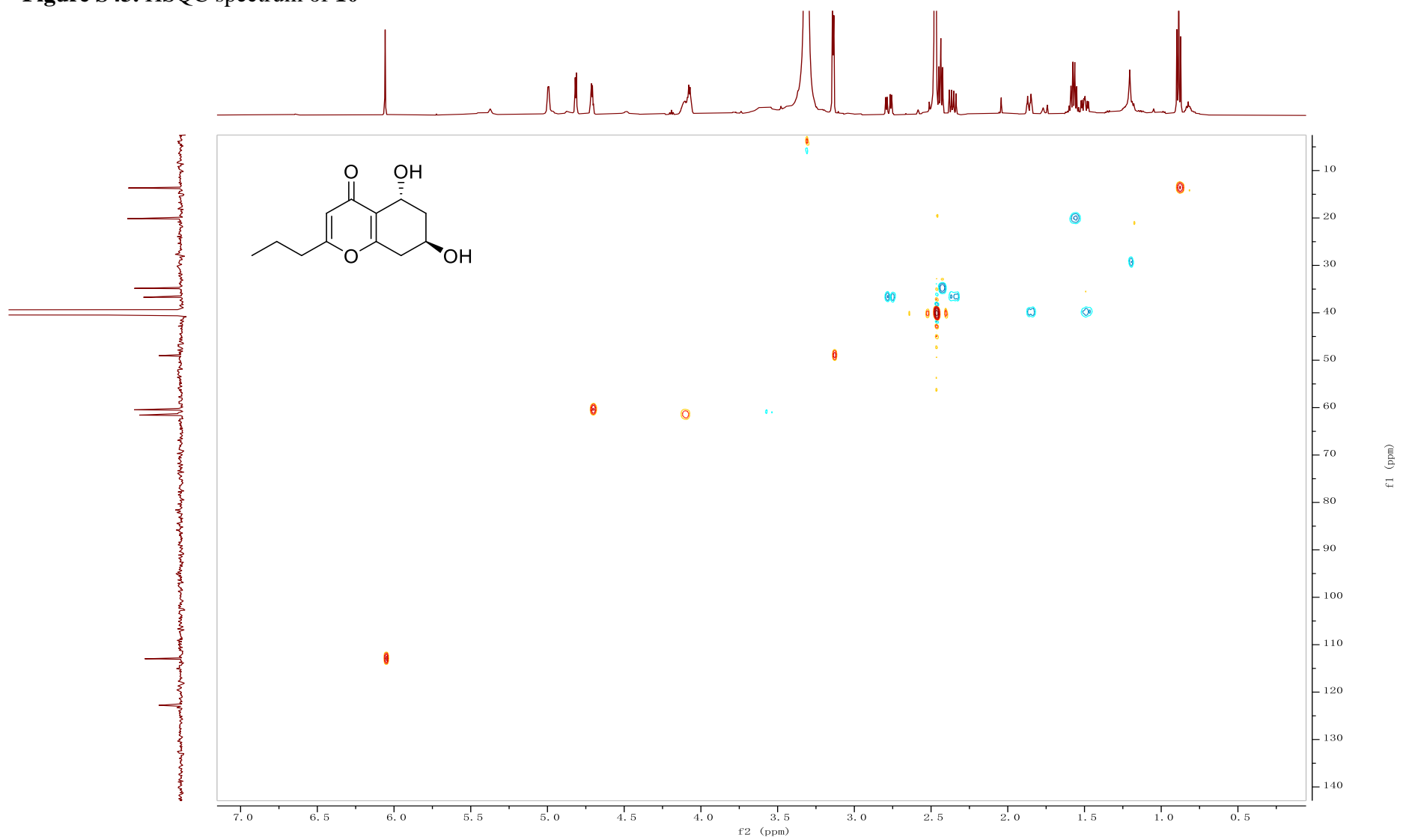


Figure S44. HMBC spectrum of **10**

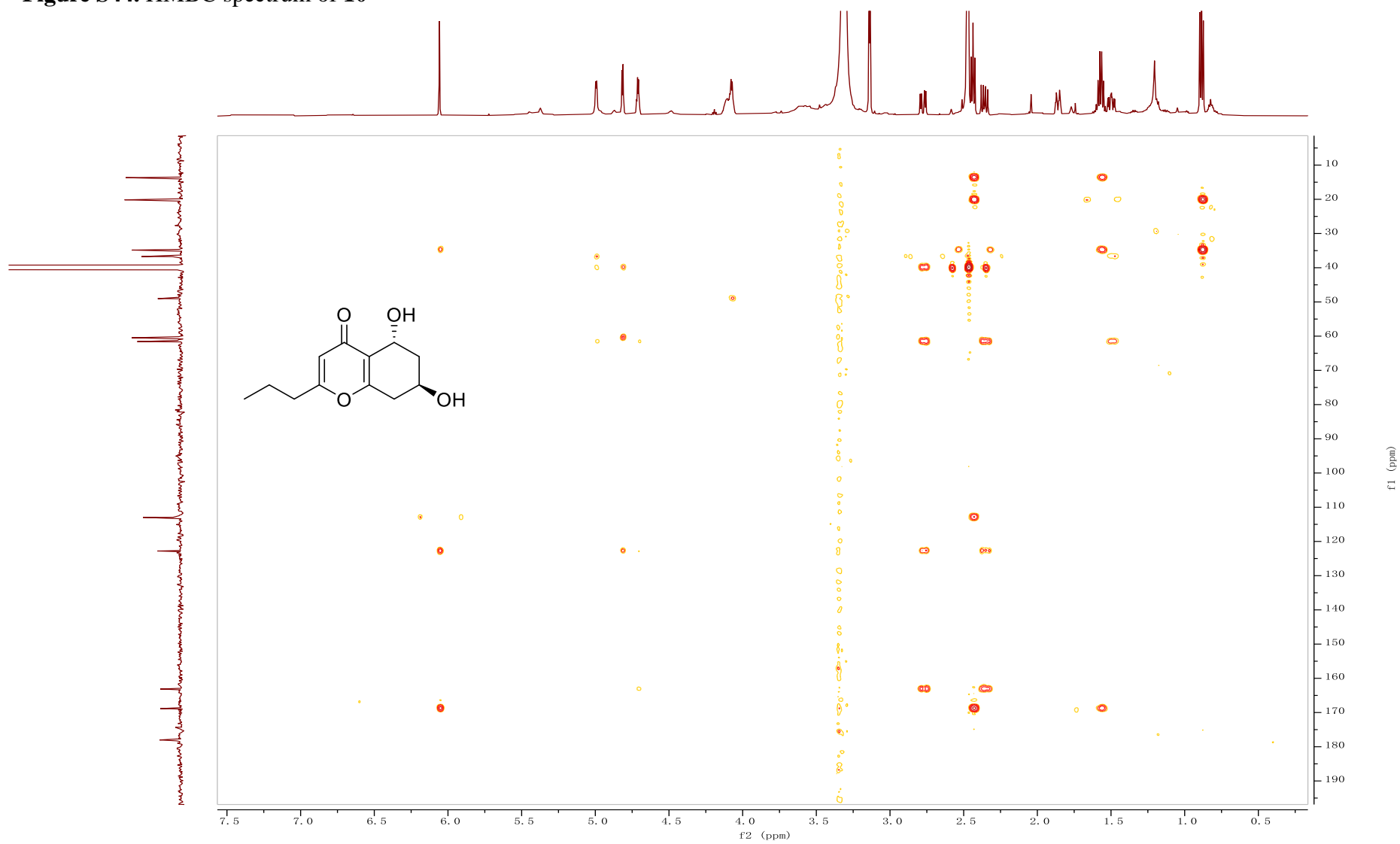


Figure S45. 1D NOE spectrum of 10

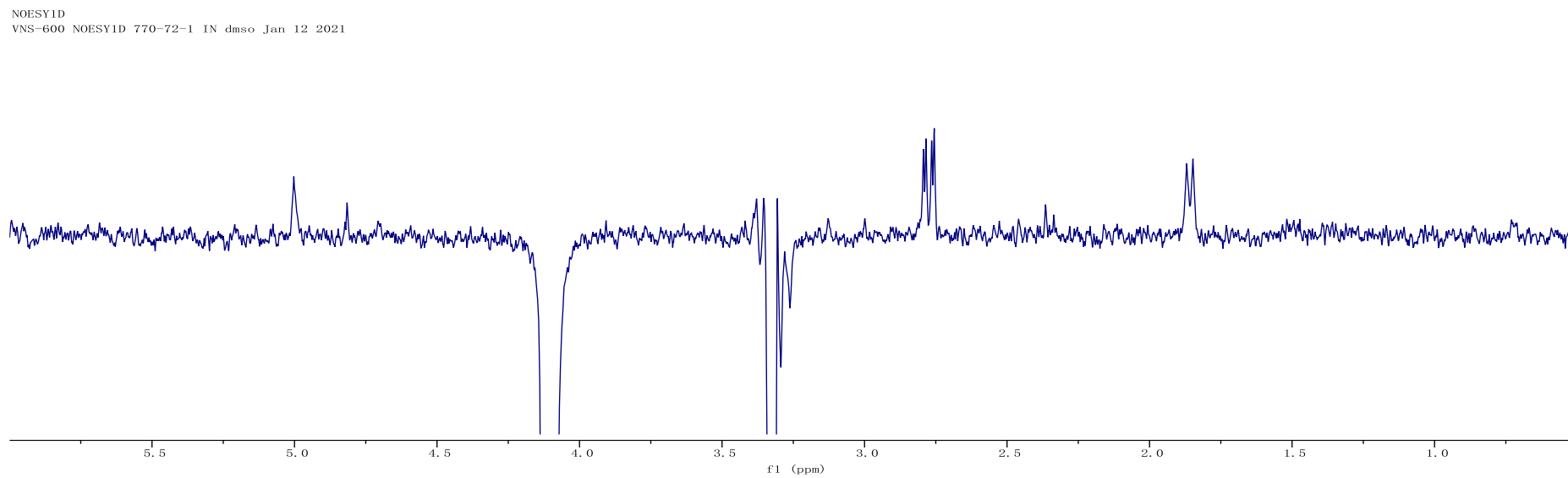
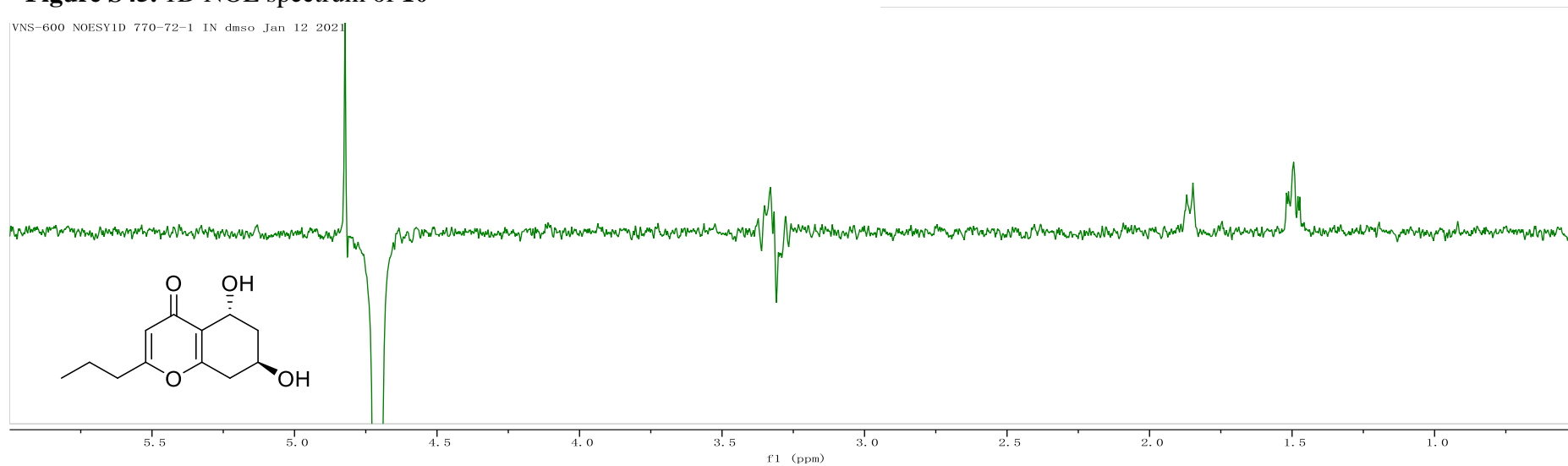


Figure S46. HRESIMS spectrum of **10**

110-12-1 #00 RT: 0.20 AV: 1 INL: 4.3/E/
T: FTMS + c ESI Full ms [50.00-700.00]

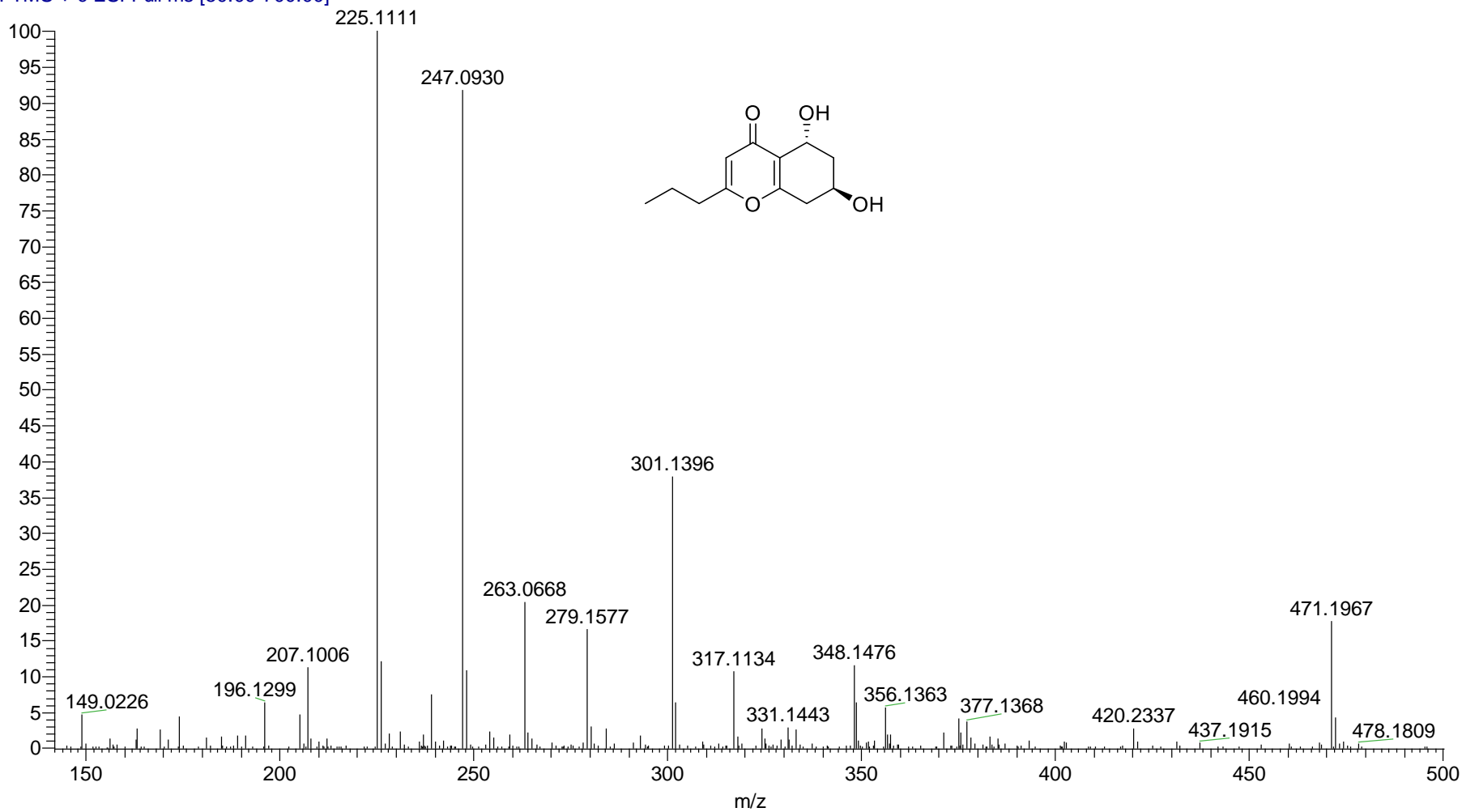


Figure S47. IR spectrum of 10

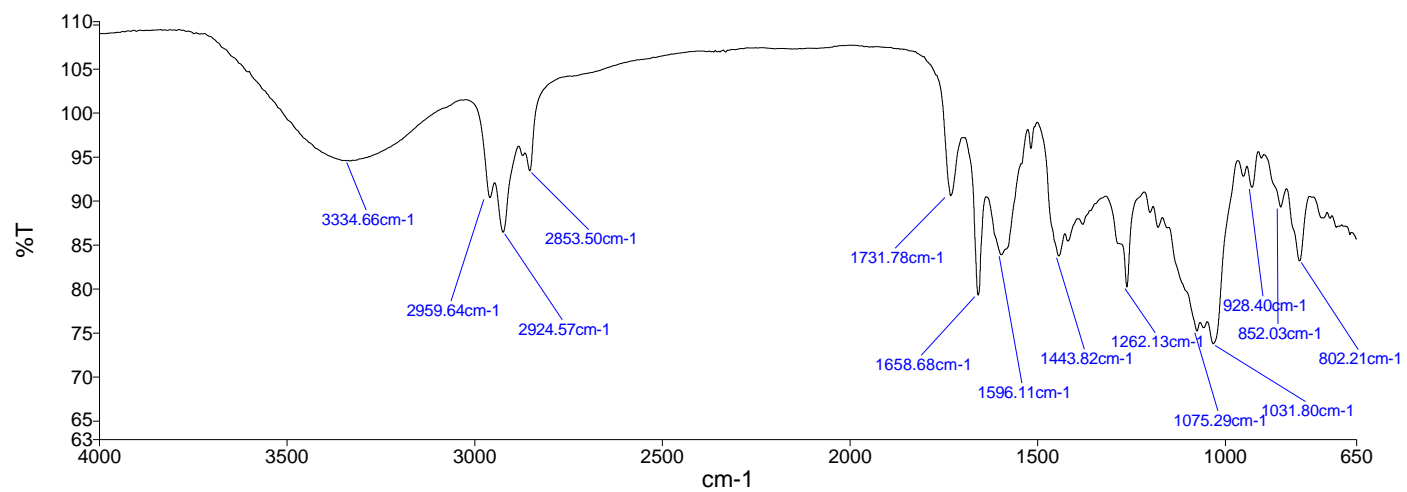


Figure S48. UV spectrum of 10

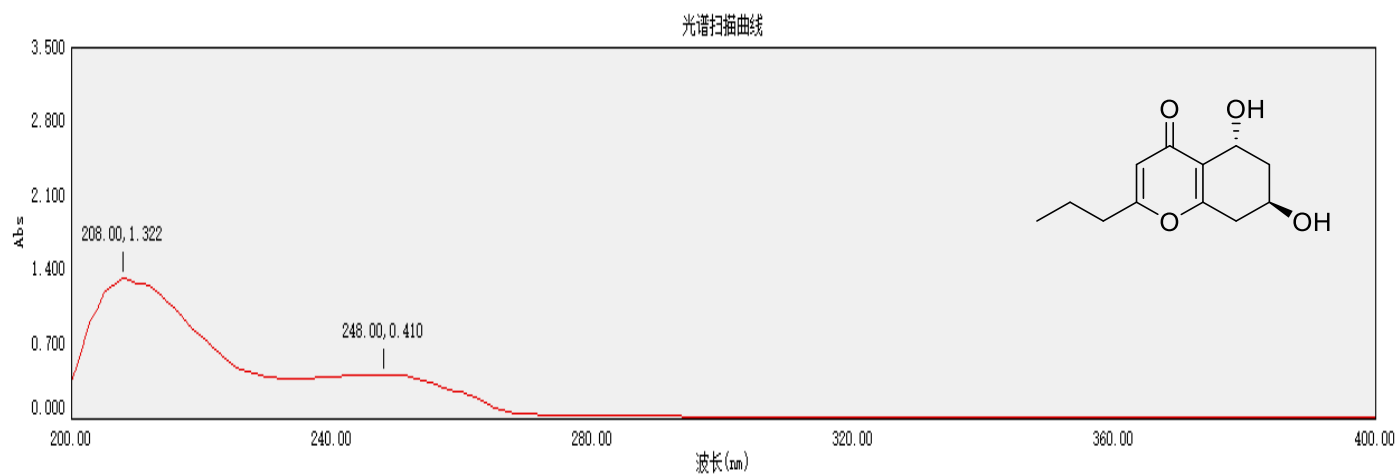
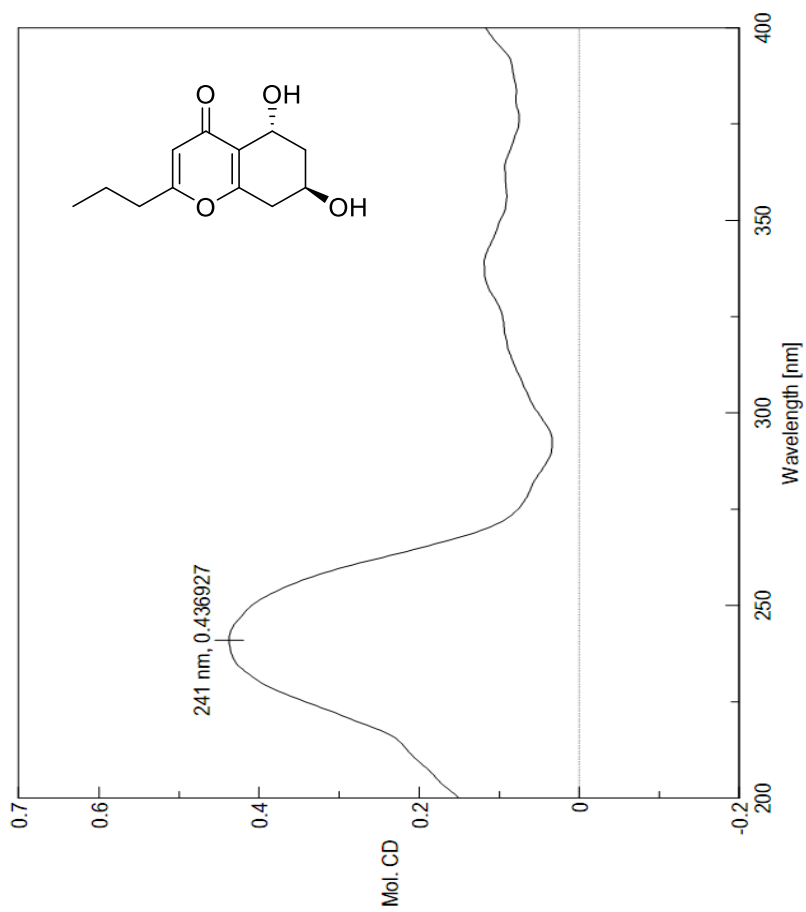


Figure S49. CD spectrum of **10**



[Comments]			
Sample name	770-72-1		
Comment			770-72-1-1-s-m.jws
[Measurement Information]			
Experiment Name	IMM-CD		
Compound Name	IMM5		
Serial No.	A024461168		
Accessory	Standard		
Accessory S/N	A005461185		
Cell Length	1 mm		
Measurement date	2021/11/29 15:43		
Photometric Mode	CD, HT, Abs		
Measure Range	400 - 200 nm		
Data pitch	0.5 nm		
Sensitivity	Standard		
D.I.T.	1 sec		
Bandwidth	1.00 nm		
Start Mode	Immediately		
Scanning Speed	100 nm/min		
Baseline Correction	Baseline		
Shutter Control	Auto		
CD Detector	PMT		
PMT Voltage	Auto		
Accumulations	2		
Solvent	MEOH		
Concentration	0.33 (w/v)%		
[Detailed Information]			
Creation date	2021/11/29 16:01		
Data array type	Linear data array * 3		
Horizontal axis	Wavelength [nm]		
Vertical axis(1)	Mol. CD		
Vertical axis(2)	HT [V]		
Vertical axis(3)	Abs		
Start	400 nm		
End	200 nm		
Data interval	0.5 nm		
Data points	401		