

Supporting Information

Lorneic Acid Analogues from an Endophytic Actinomycete

Ruimin Yang,^{†, ‡, §, ⊥} Jing Yang,^{†, ‡, ⊥} Li Wang,^{†, §} Jian-Ping Huang,^{†, ‡} Zijun Xiong,^{†, §}

Jiaying Luo,[†] Mingming Yu,^{†, §} Yijun Yan,[†] and Sheng-Xiong Huang*,^{†, ‡}

[†]State Key Laboratory of Phytochemistry and Plant Resources in West China, Kunming Institute of Botany, Chinese Academy of Sciences, Kunming 650201, People's Republic of China

[‡]Yunnan Key Laboratory of Natural Medicinal Chemistry, Kunming Institute of Botany, Chinese Academy of Sciences, Kunming 650201, People's Republic of China

[§]University of the Chinese Academy of Sciences, Beijing 100049, People's Republic of China

[⊥]These authors contributed equally.

*Corresponding author: S.-X. Huang, email: sxhuang@mail.kib.ac.cn

Physical Chemical Data of Compounds 7 and 8

Lorneic acid K (7): colorless oil; $[\alpha]_{\text{D}}^{23.0}$ -8.4 (*c* 0.55, CH₃OH); ¹H NMR (600 MHz, CD₃OD): δ_{H} 7.27 (1H, d, *J* = 7.9 Hz, H-8), 7.24 (1H, s, H-11), 6.98 (1H, brd, *J* = 7.9 Hz, H-9), 6.69 (1H, brd, *J* = 15.6 Hz, H-6), 5.99 (1H, m, H-5), 4.93 (1H, m, H-13), 2.32 (2H, m, H-2), 2.29 (3H, s, H-17), 2.26 (2H, m, H-4), 1.78 (2H, m, H-3), 1.63 (2H, m, H-14), 1.42 (1H, m, H-15), 1.31 (1H, m, H-15), 0.90 (3H, t, *J* = 7.5 Hz, H-16); ¹³C NMR (150 MHz, CD₃OD): δ_{C} 178.2 (C-1), 143.1 (C-12), 137.8 (C-10), 134.0 (C-7), 132.2 (C-5), 129.3 (C-6), 128.7 (C-9), 127.2 (C-11), 127.0 (C-8), 70.8 (C-13), 42.0 (C-14), 34.5 (C-2), 33.6 (C-4), 25.9 (C-3), 21.3 (C-17), 20.2 (C-15), 14.4 (C-16); ESIMS *m/z* 299 [M + Na]⁺; HRESIMS *m/z* 299.1619 [M + Na]⁺ (calcd for C₁₇H₂₄O₃Na 299.1618).

Lorneic acids D (8): colorless oil; ESIMS: 255 [M + Na]⁺; ¹H NMR (600 MHz, CD₃OD) δ_{H} 7.24 (1H, s, H-9), 6.99 (1H, d, *J* = 7.9 Hz, H-6), 6.95 (1H, brd, *J* = 7.9 Hz, H-7), 6.58 (1H, brd, 15.6, H-11), 6.12 (1H, dt, *J* = 15.6, 6.5 Hz, H-12), 2.67 (2H, m, H-4), 2.35 (2H, m, H-2), 2.30 (3H, s, H-15), 2.23 (2H, m, H-13), 1.88 (2H, m, H-3), 1.09 (3H, t, *J* = 7.4 Hz, H-14); ¹³C NMR(150 MHz, CD₃OD) δ_{C} 178.6 (C-1), 136.4 (C-10), 135.7 (C-5), 135.1 (C-8), 134.1 (C-12), 129.4 (C-6), 127.6 (C-7), 126.5 (C-11), 126.1 (C-9), 33.3 (C-2), 32.0 (C-4), 26.3 (C-3), 25.8 (C-13), 21.0 (C-15), 13.7 (C-14).

Supplementary Figures

Figure S1. Proposed biosynthetic formation of **5** from *N*-acetylcystine and **2**.

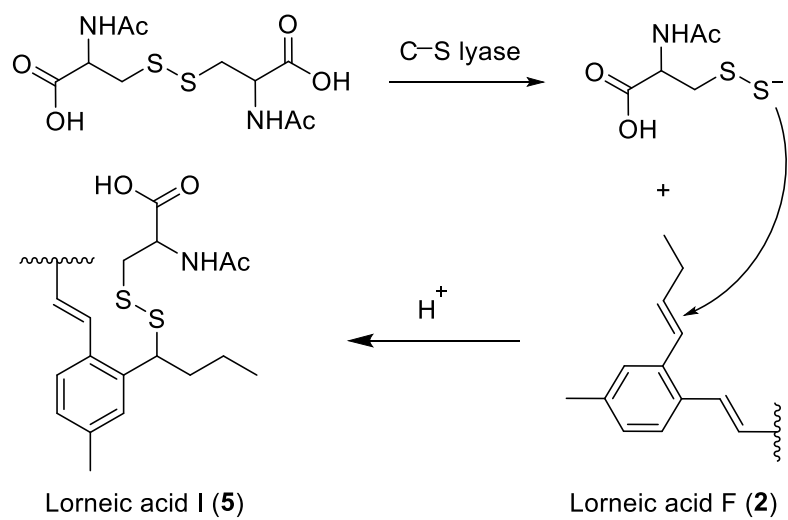


Figure S2. 1H NMR spectrum of **1** in CD_3OD (600 MHz).

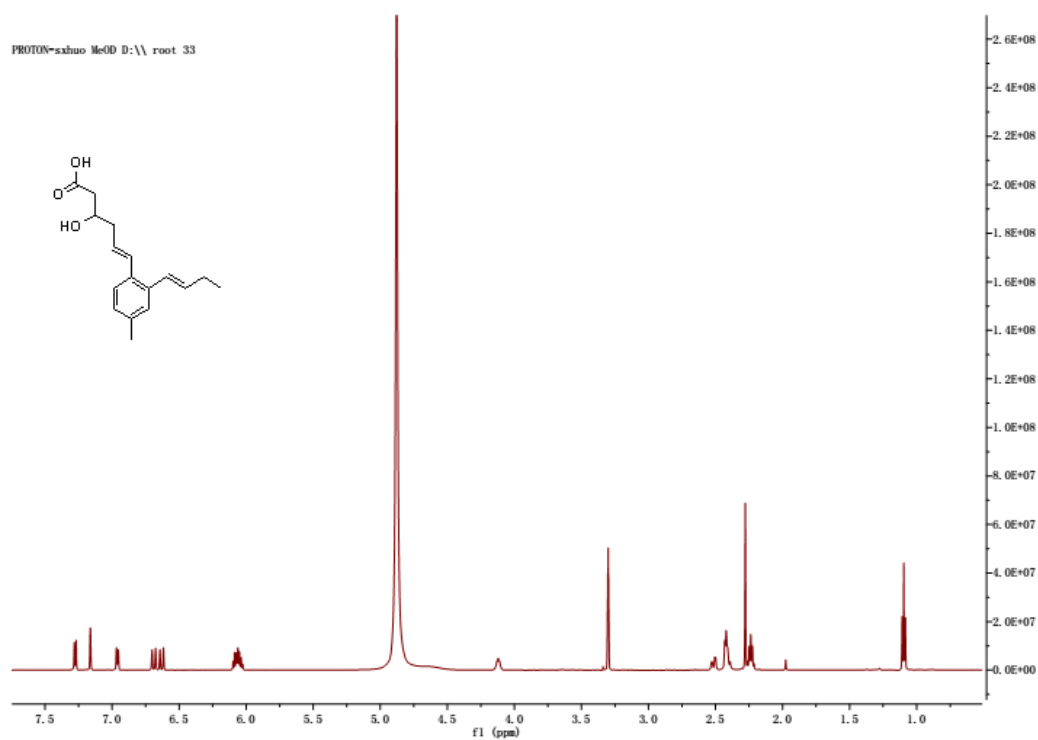


Figure S3. ^{13}C NMR spectrum of **1** in CD_3OD (150 MHz).

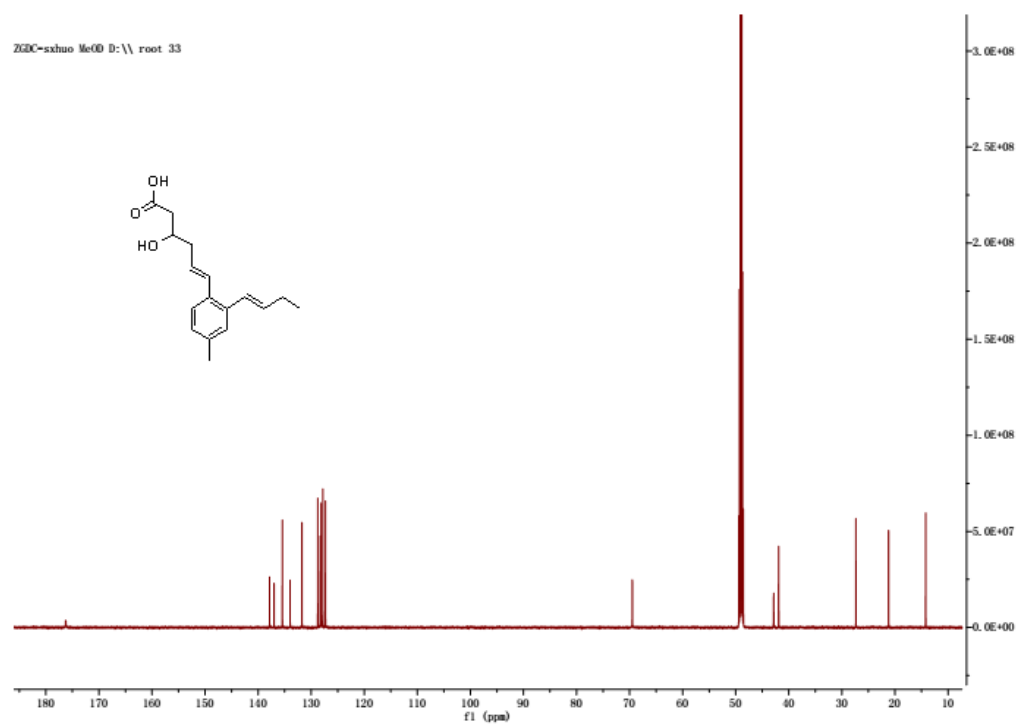


Figure S4. HSQC NMR spectrum of **1** in CD_3OD .

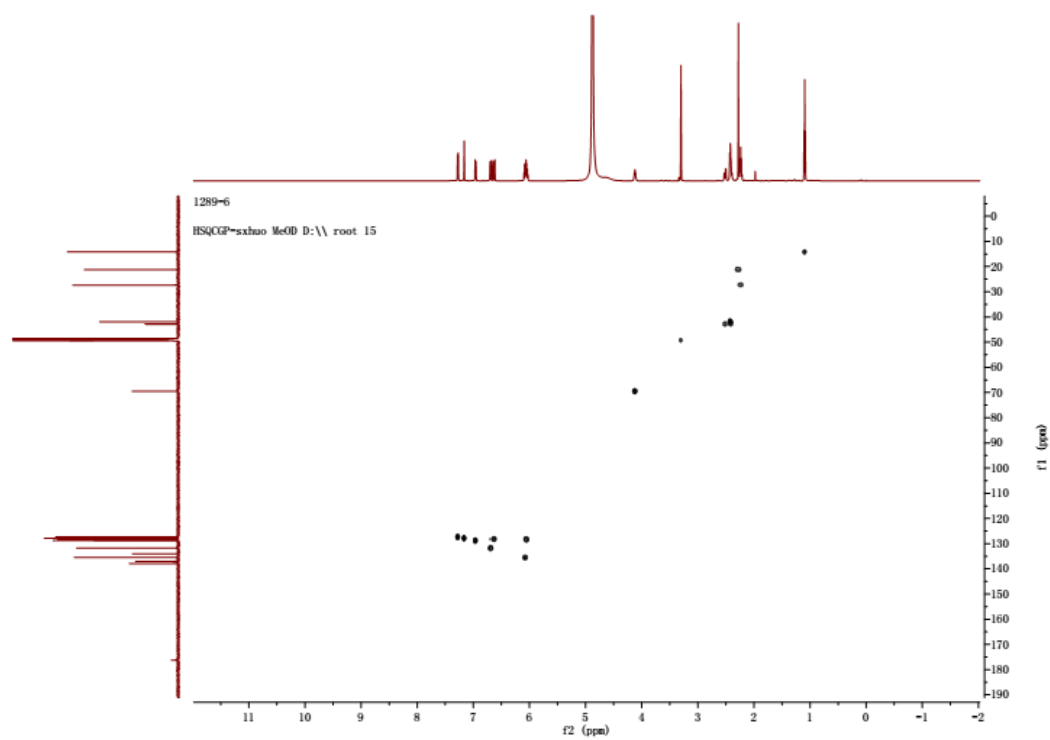


Figure S5. HMBC NMR spectrum of **1** in CD₃OD.

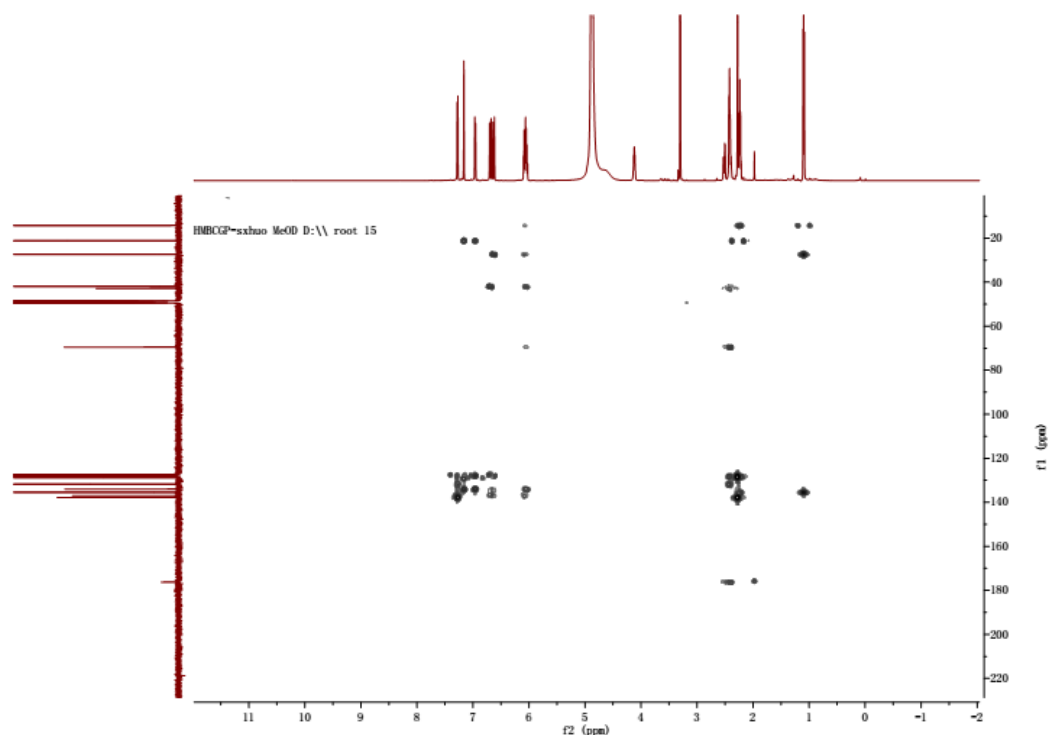
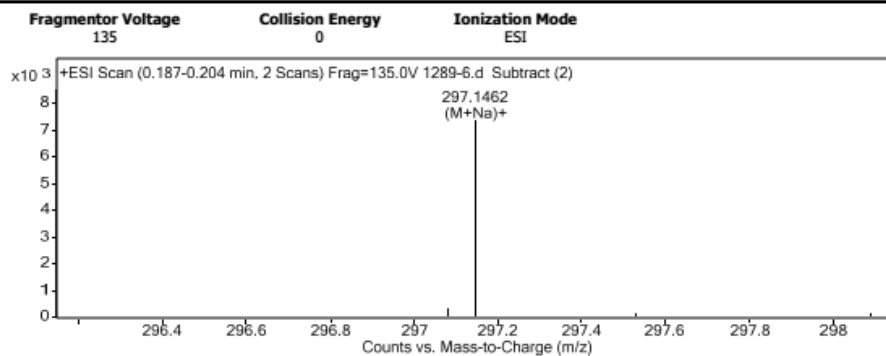


Figure S6. HRESIMS spectrum of **1**.

User Spectra



Peak List

m/z	z	Abund	Formula	Ion
274.274	1	6681.87		
297.1462	1	7349.21	C ₁₇ H ₂₂ O ₃	(M+Na)+
313.1157	1	5449.04		
318.3	1	7137.68		
354.1376	1	7126.06		
437.1939	1	6821.25		
453.1671	1	12701.51		
454.1706	1	3646.96		

Formula Calculator Element Limits

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

Formula Calculator Results

Formula	CalculatedMass	CalculatedMz	Mz	Diff. (mDa)	Diff. (ppm)	DBE
C ₁₇ H ₂₂ O ₃	274.1569	297.1461	297.1462	0.0	0.0	7.0000

Figure S7. ^1H NMR spectrum of **2** in CDCl_3 (600 MHz).

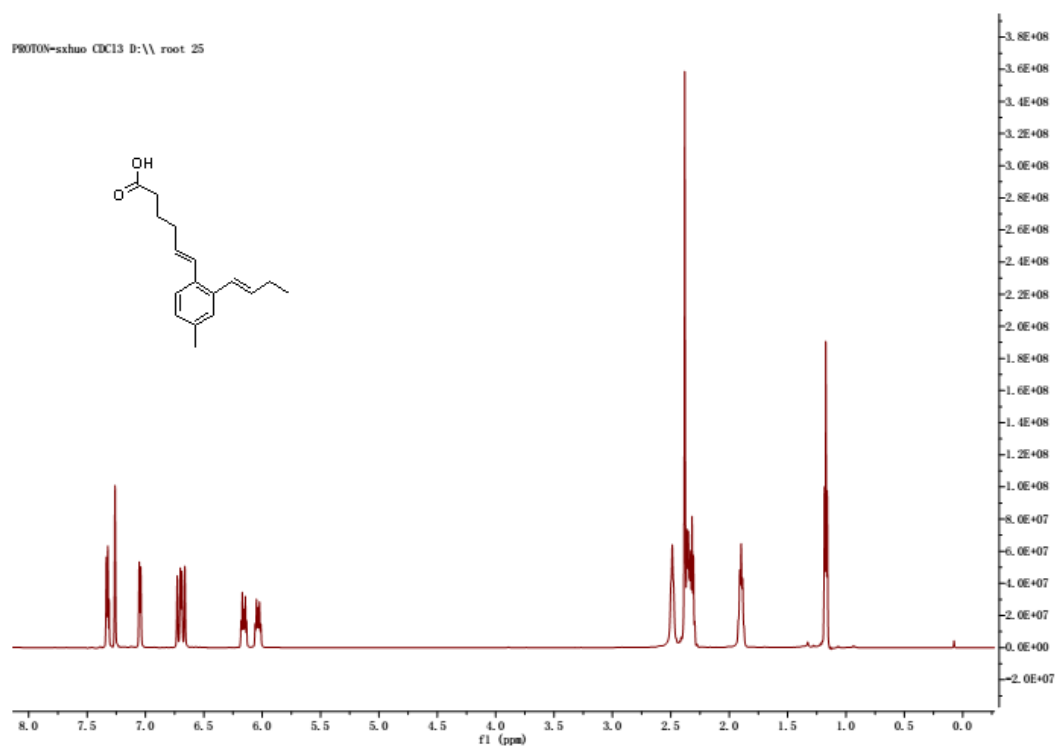


Figure S8. ^{13}C NMR spectrum of **2** in CDCl_3 (150 MHz).

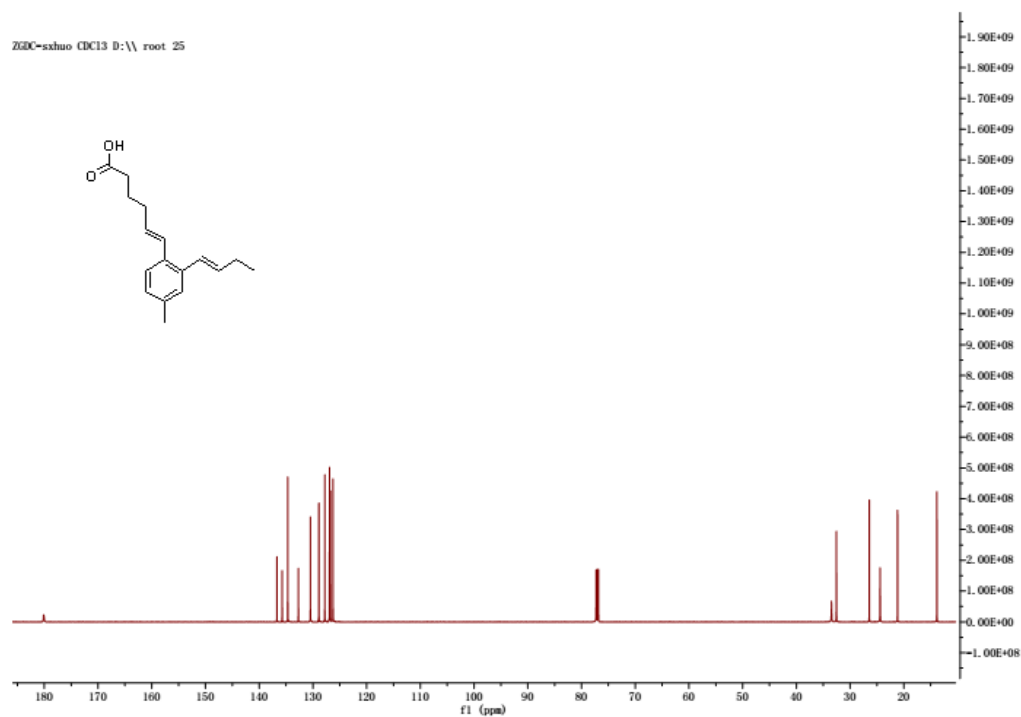


Figure S9. HSQC NMR spectrum of **2** in CDCl₃.

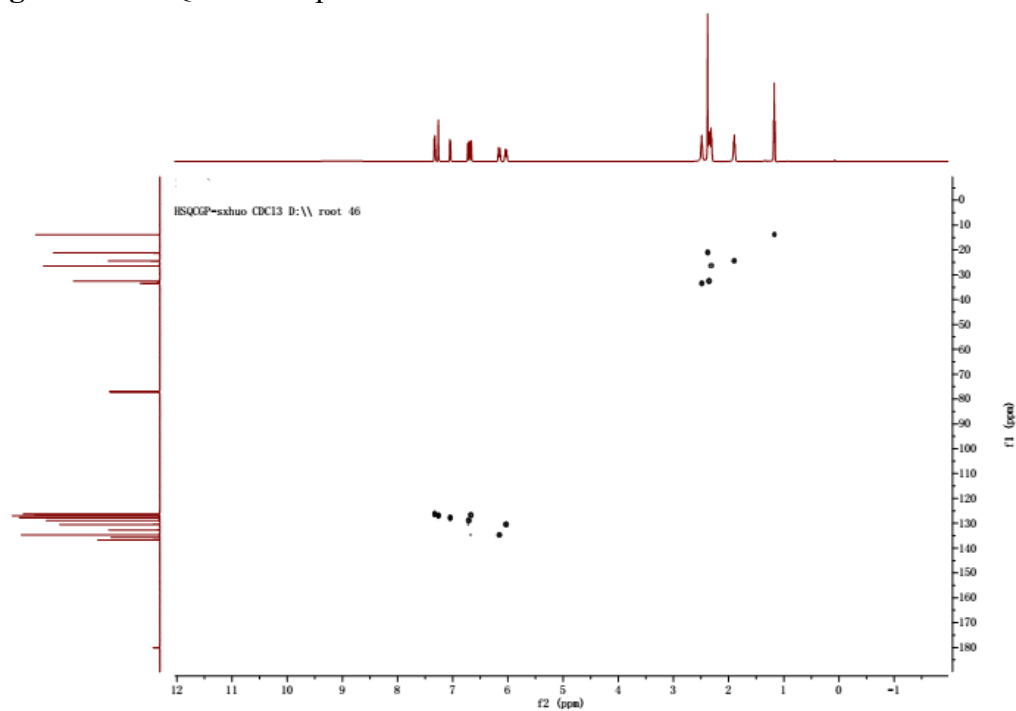


Figure S10. HMBC NMR spectrum of **2** in CDCl₃.

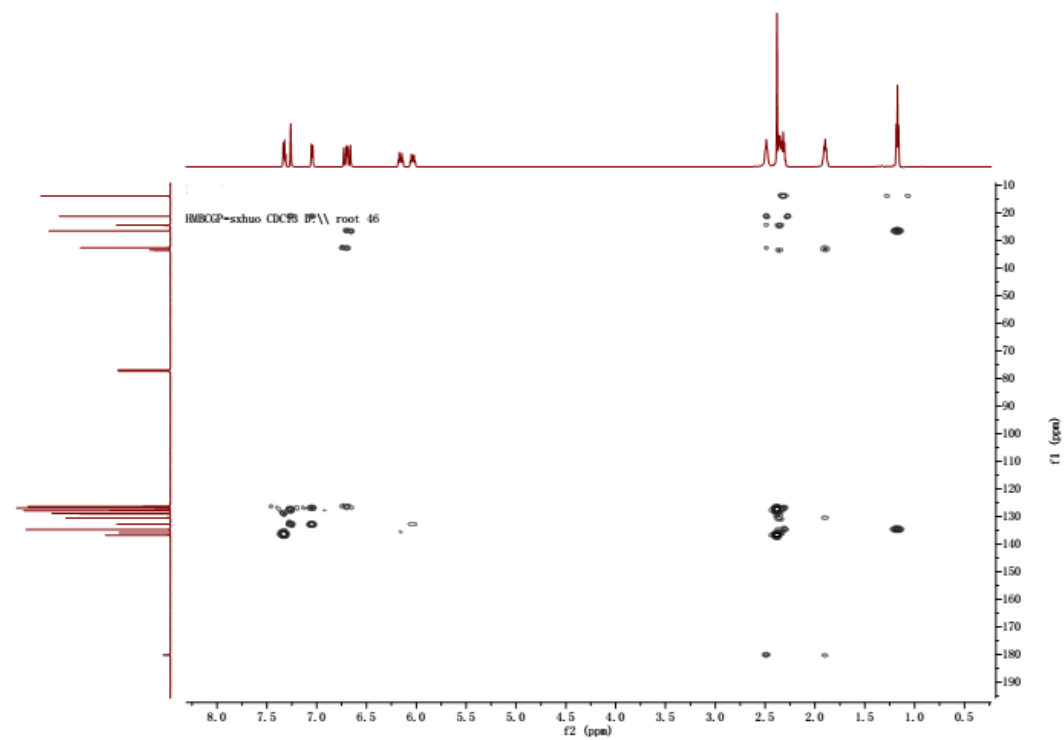


Figure S11. HRESIMS spectrum of **2**.

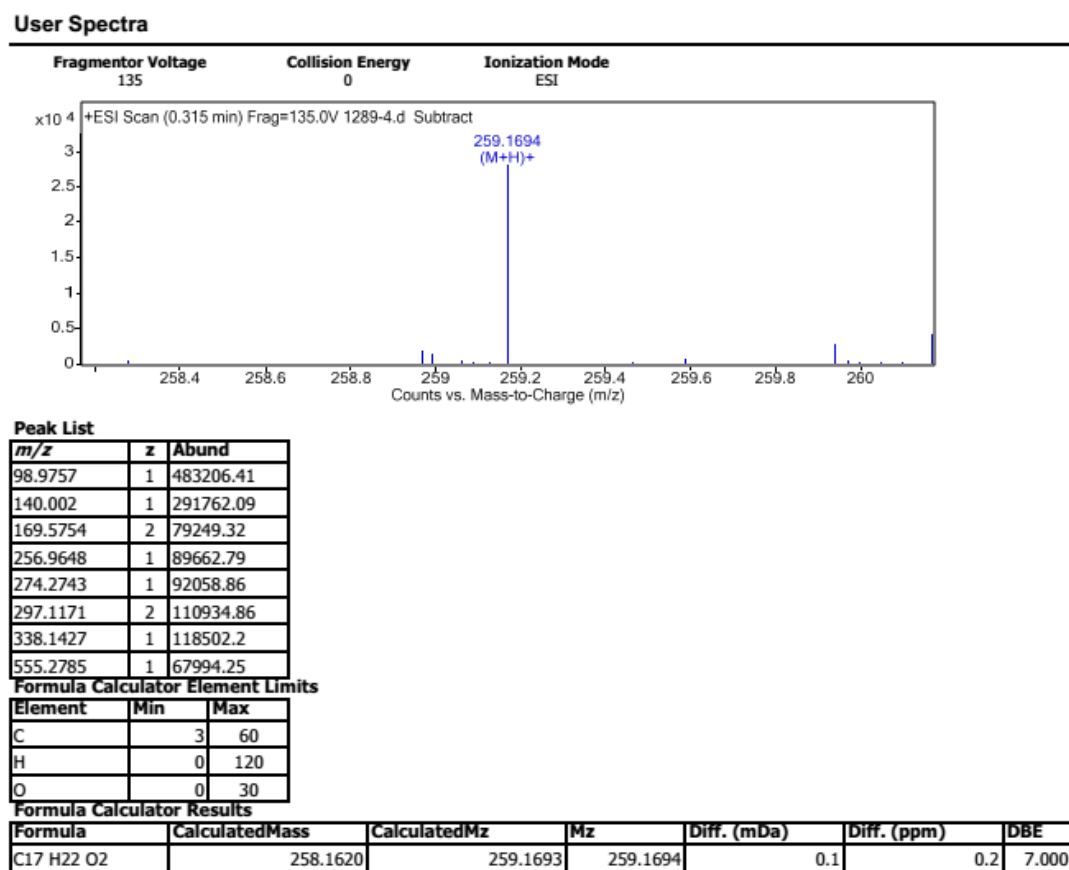


Figure S12. ^1H NMR spectrum of **3** in CD_3OD (600 MHz).

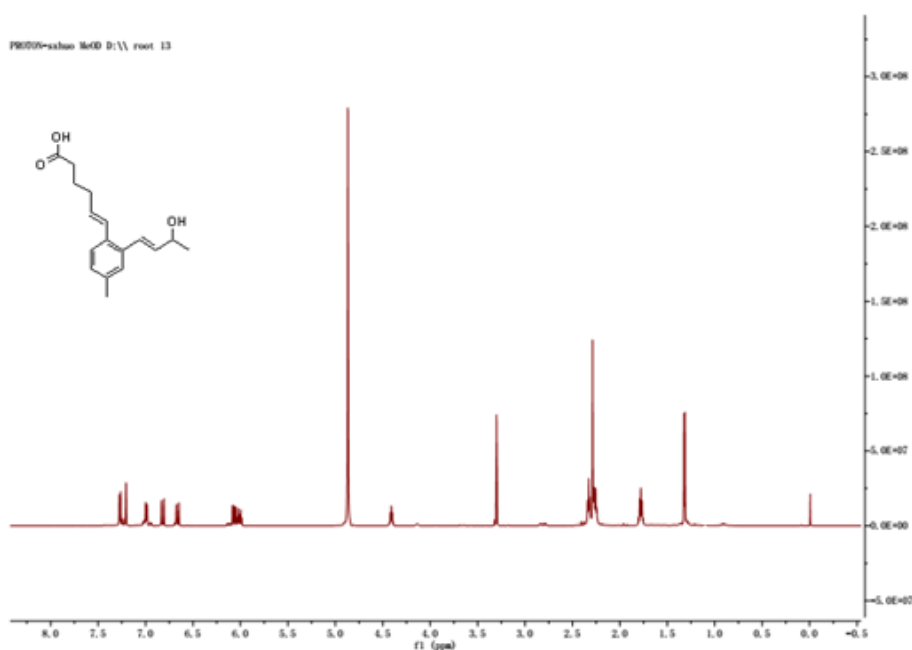


Figure S13. ^{13}C NMR spectrum of **3** in CD_3OD (150 MHz).

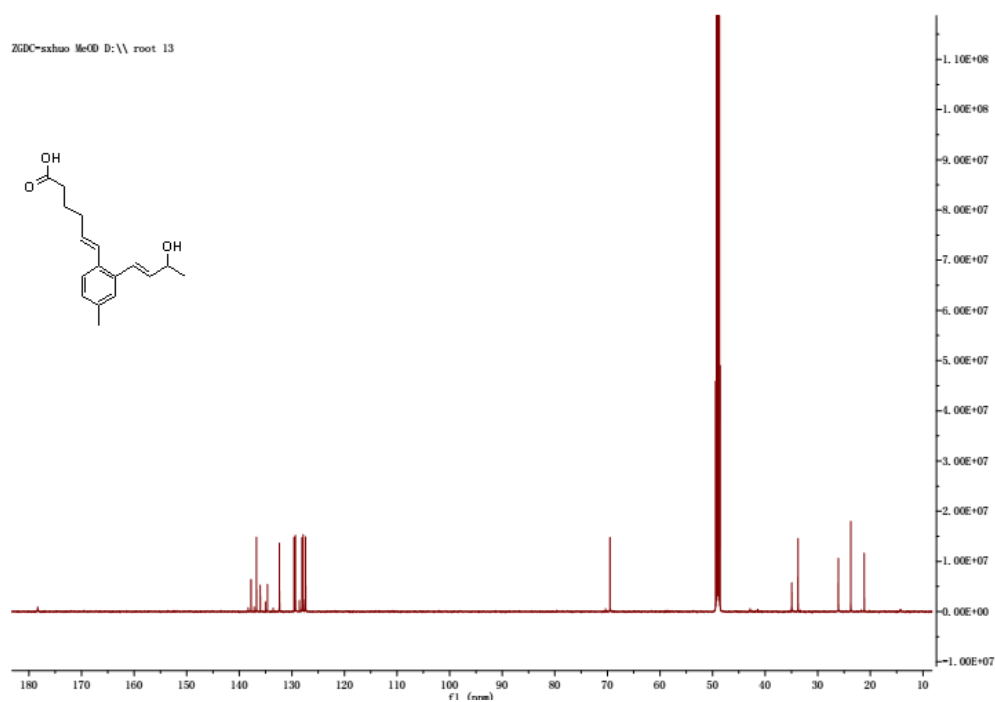


Figure S14. HSQC NMR spectrum of **3** in CD_3OD .

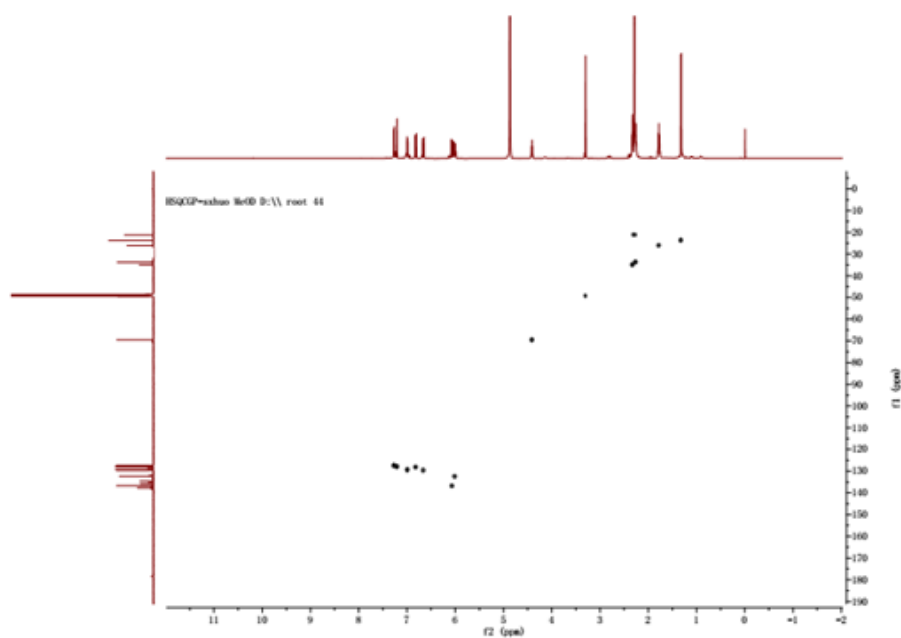


Figure S15. HMBC NMR spectrum of **3** in CD₃OD.

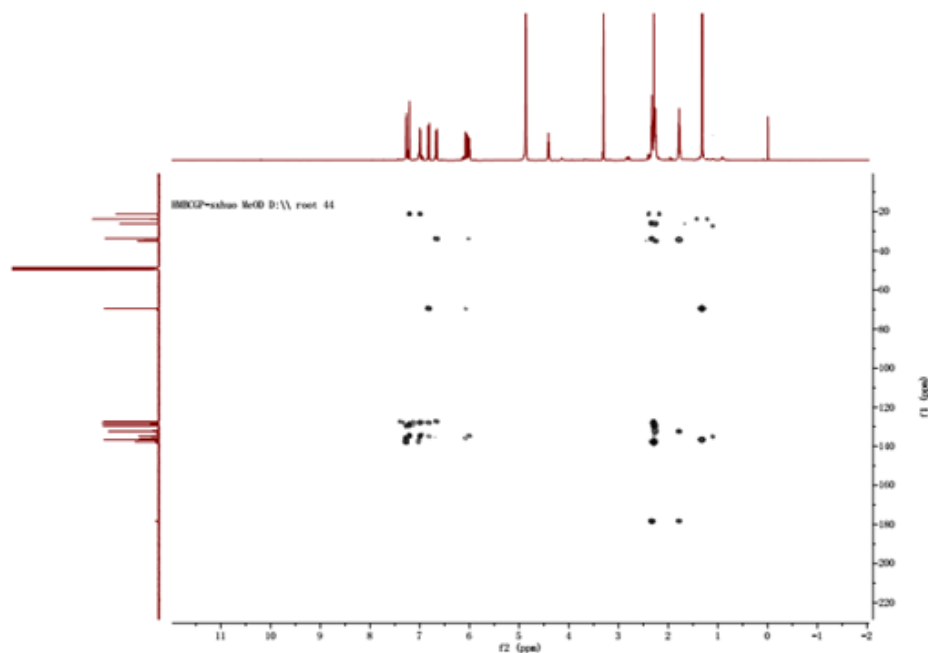
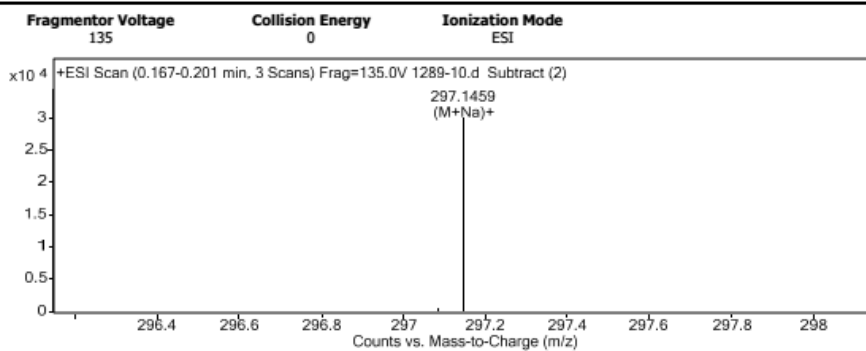


Figure S16. HRESIMS spectrum of **3**.

User Spectra



Peak List

m/z	z	Abund	Formula	Ion
257.1534	1	14962.57		
297.1459	1	29807.46	C17 H22 O3	(M+Na)+
298.149	1	5528.93	C17 H22 O3	(M+Na)+
313.1195	1	11939.65		
345.167	1	3549.97		
437.1929	1	4960.51		
453.1675	1	6465.17		
587.2979	1	3078.51		

Formula Calculator Element Limits

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

Formula Calculator Results

Formula	CalculatedMass	CalculatedMz	Mz	Diff. (mDa)	Diff. (ppm)	DBE
C17 H22 O3	274.1569	297.1461	297.1459	0.2	0.8	7.0000

Figure S17. ^1H NMR spectrum of **4** in CD_3OD (600 MHz).

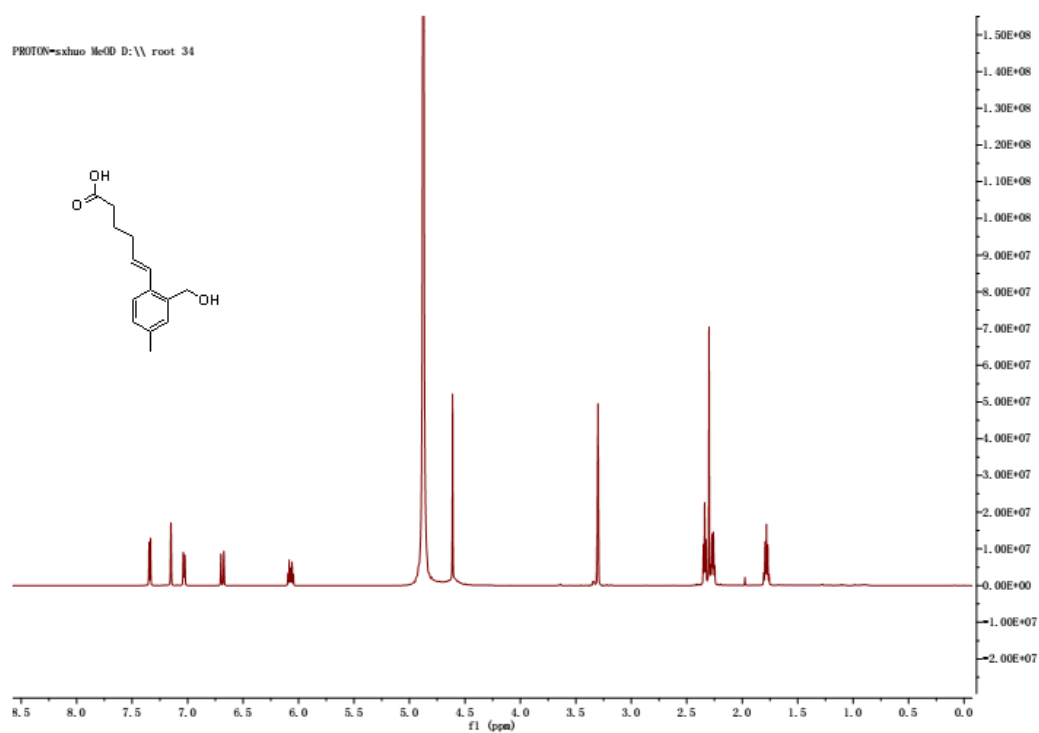


Figure S18. ^{13}C NMR spectrum of **4** in CD_3OD (150 MHz).

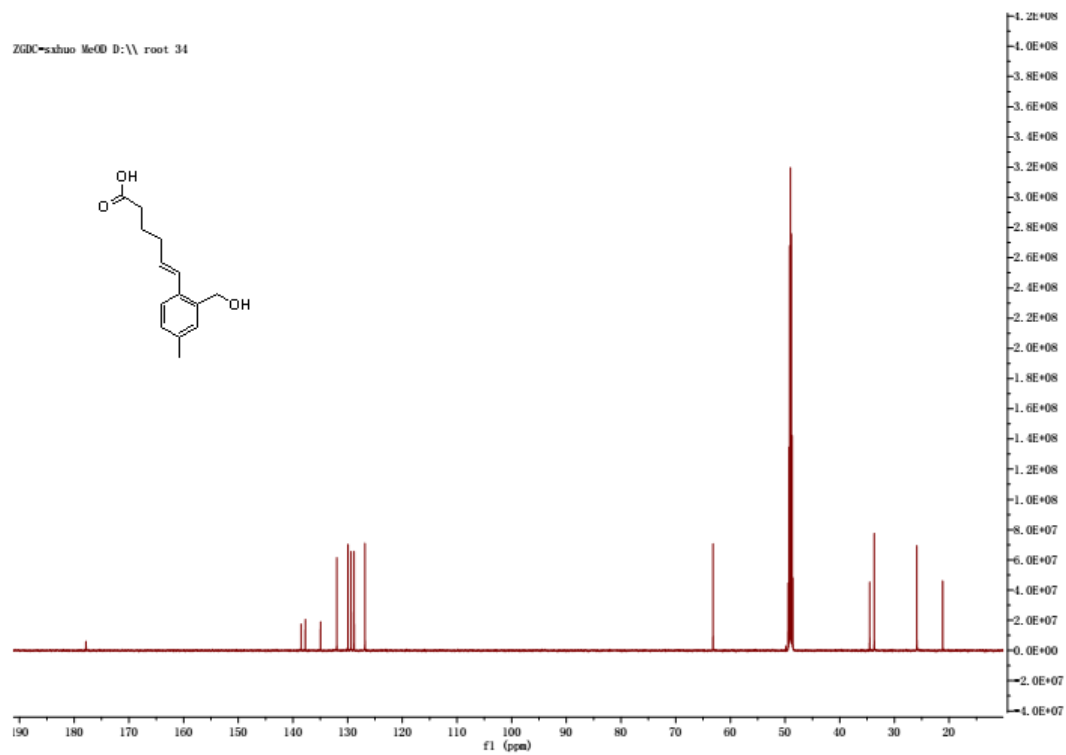


Figure S19. HSQC NMR spectrum of **4** in CD₃OD.

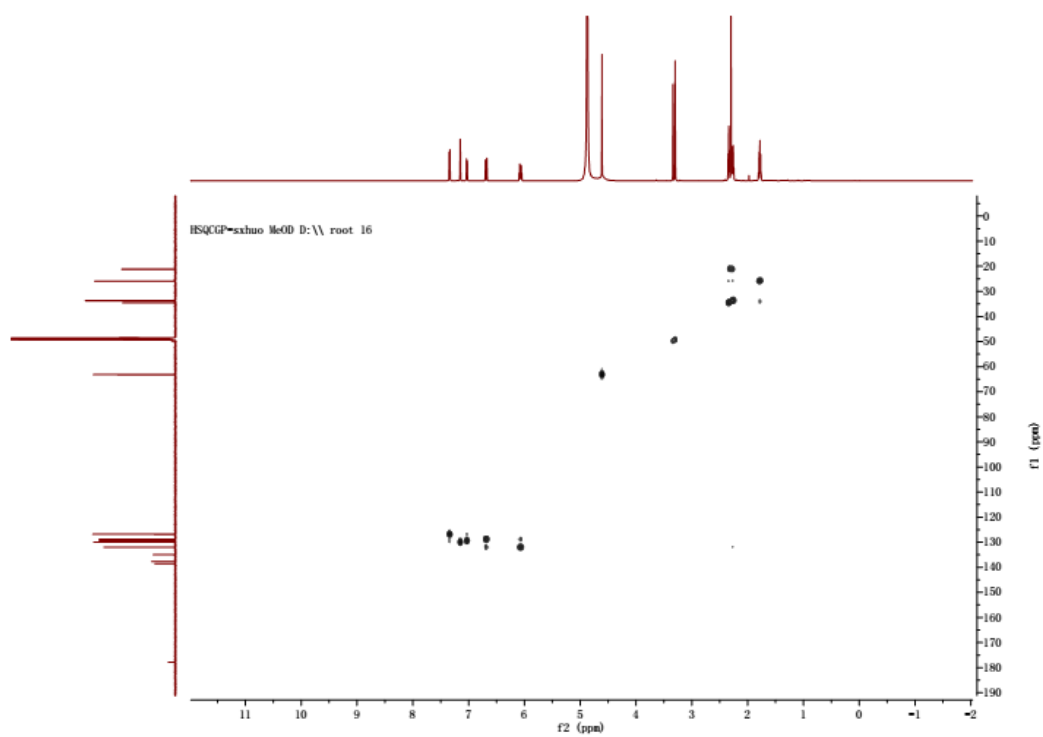


Figure S20. HMBC NMR spectrum of **4** in CD₃OD.

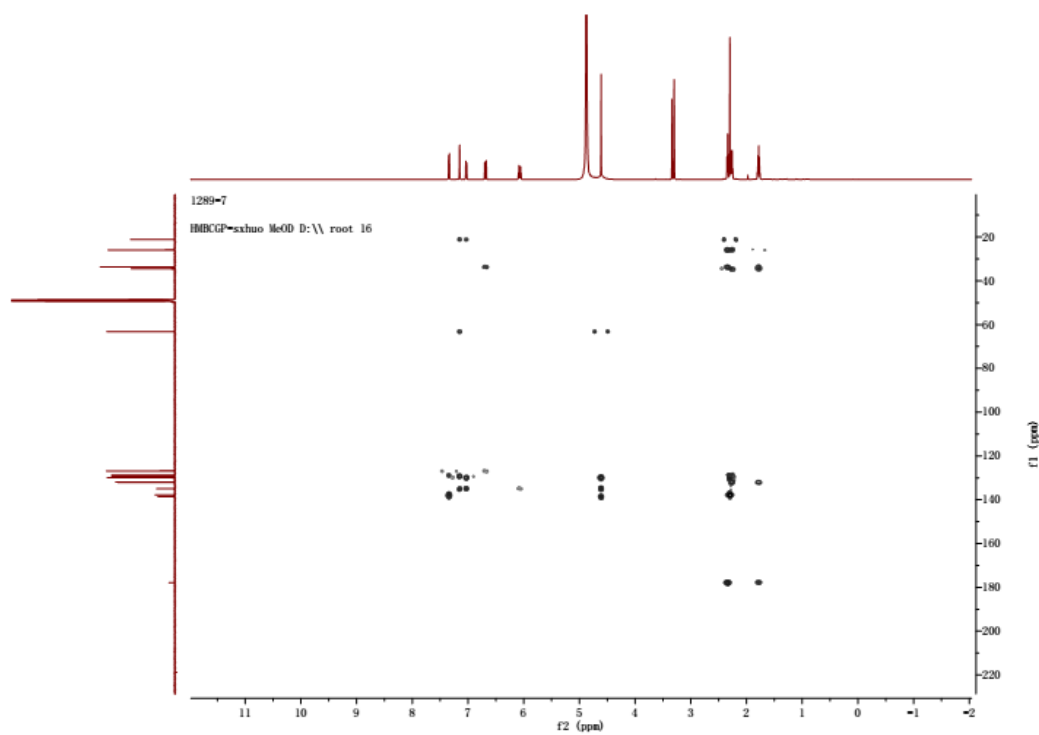


Figure S21. HRESIMS spectrum of **4**.

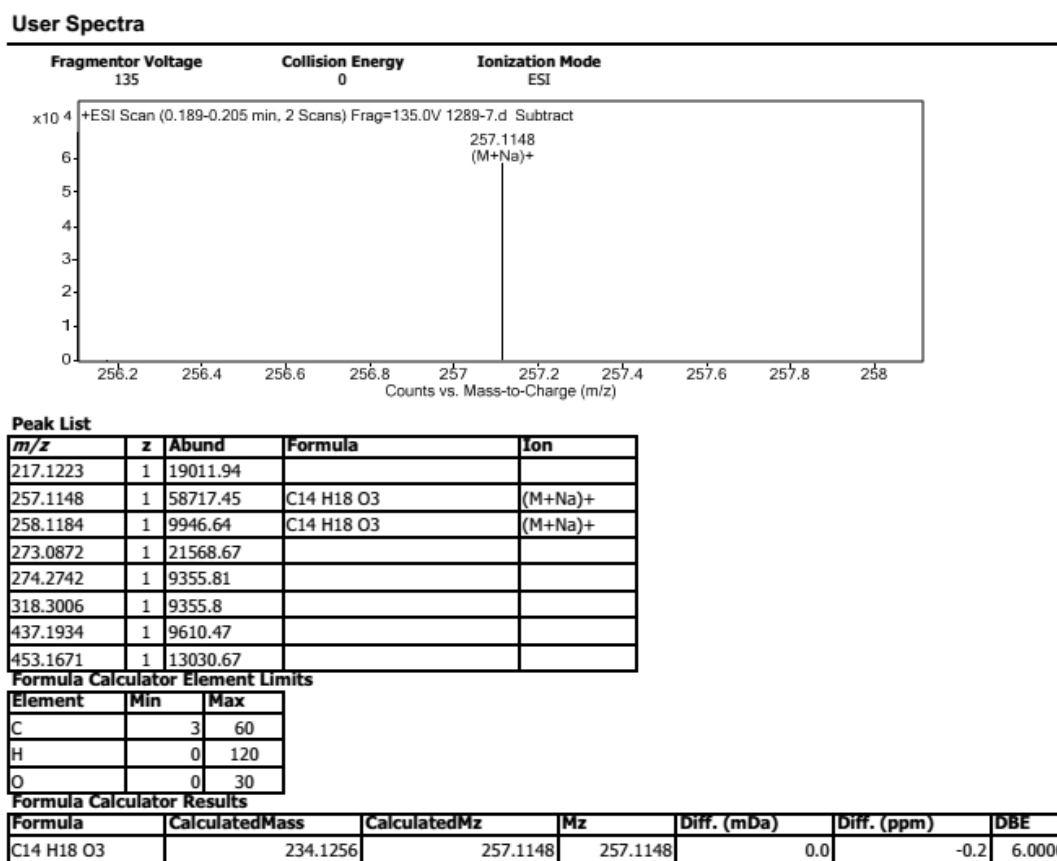


Figure S22. ¹H NMR spectrum of **5** in CD₃OD (600 MHz).

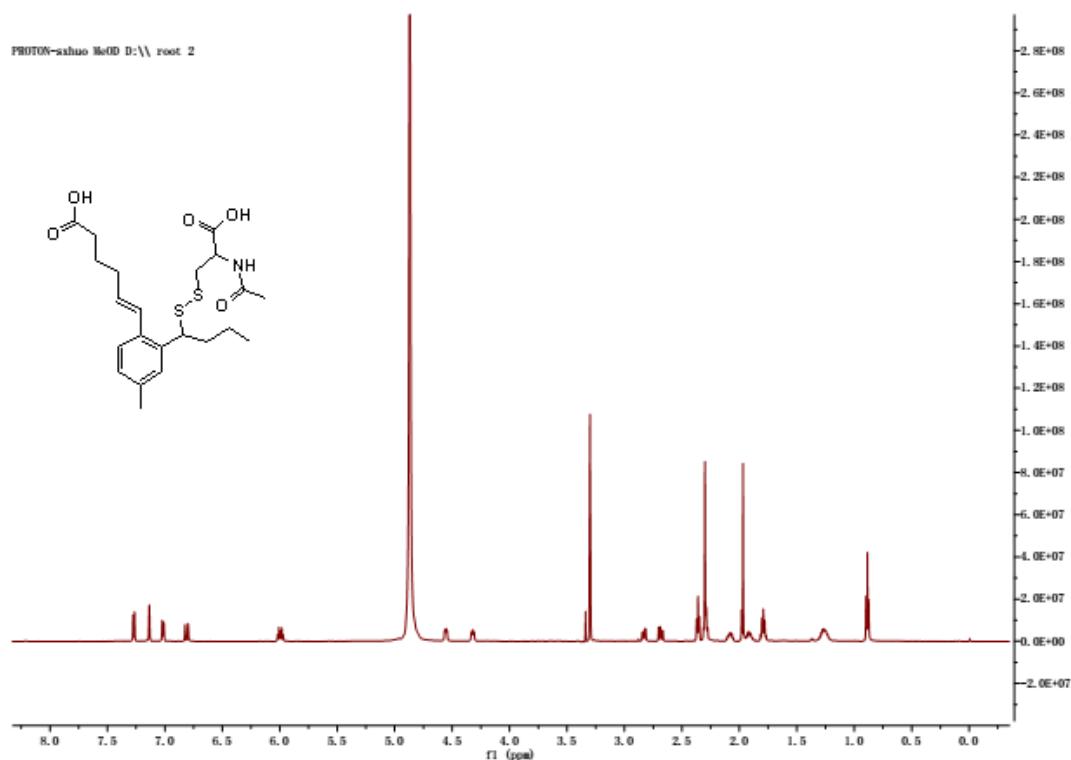


Figure S23. ^{13}C NMR spectrum of **5** in CD_3OD (150 MHz).

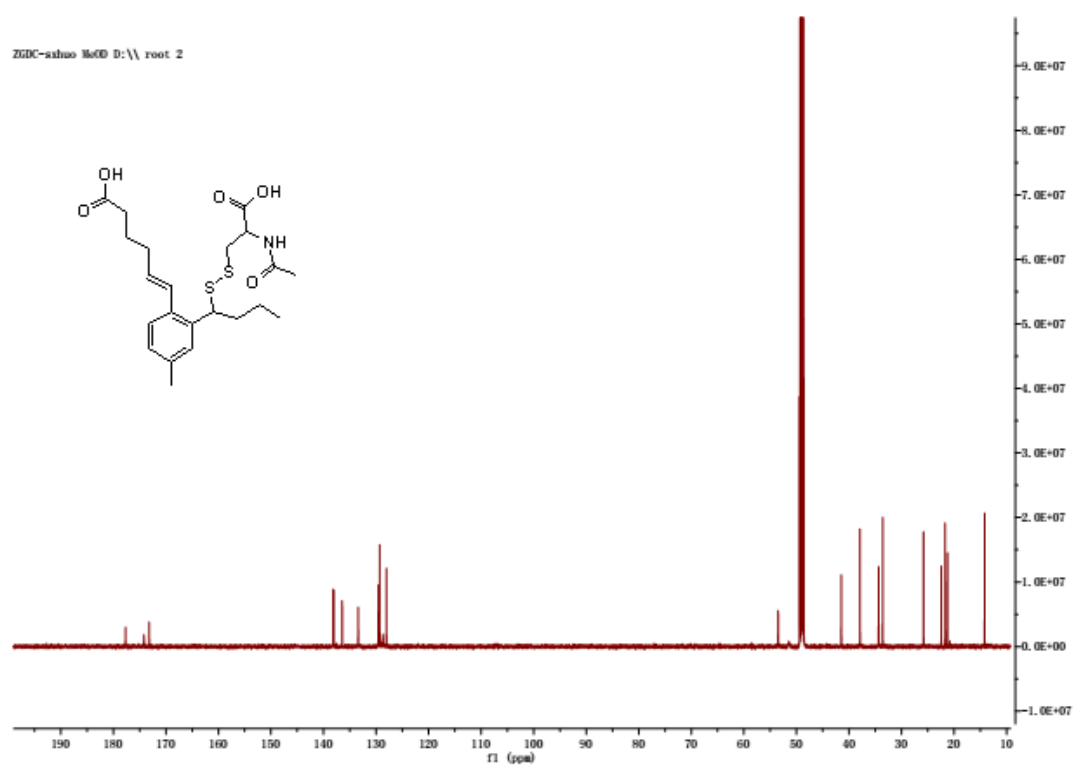


Figure S24. HSQC NMR spectrum of **5** in CD_3OD .

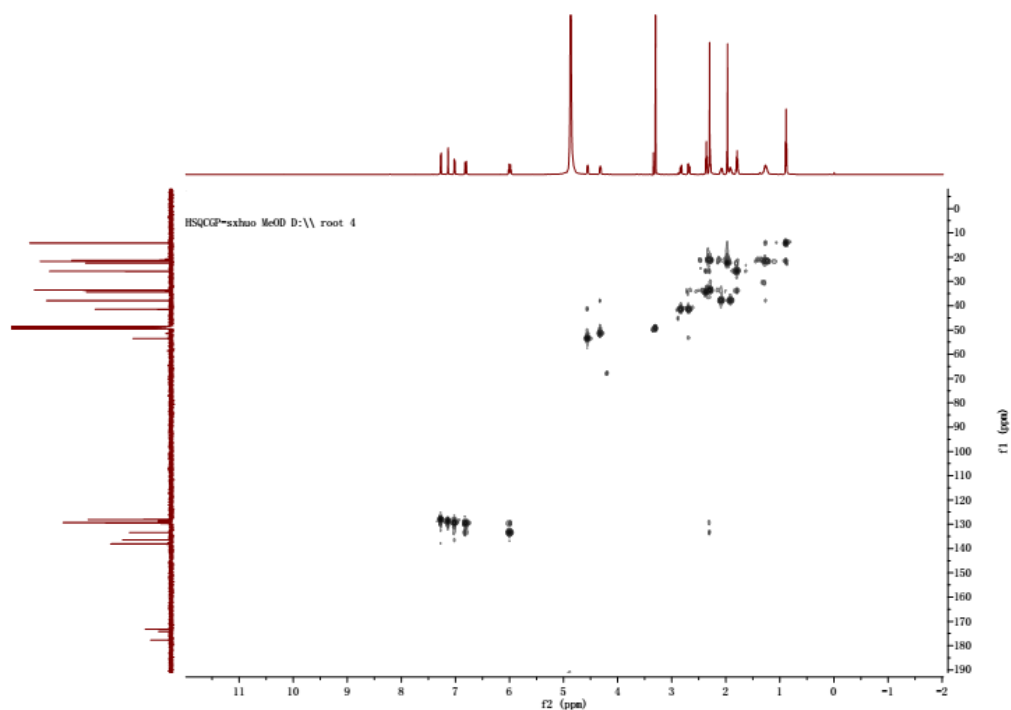


Figure S25. HMBC NMR spectrum of **5** in CD₃OD.

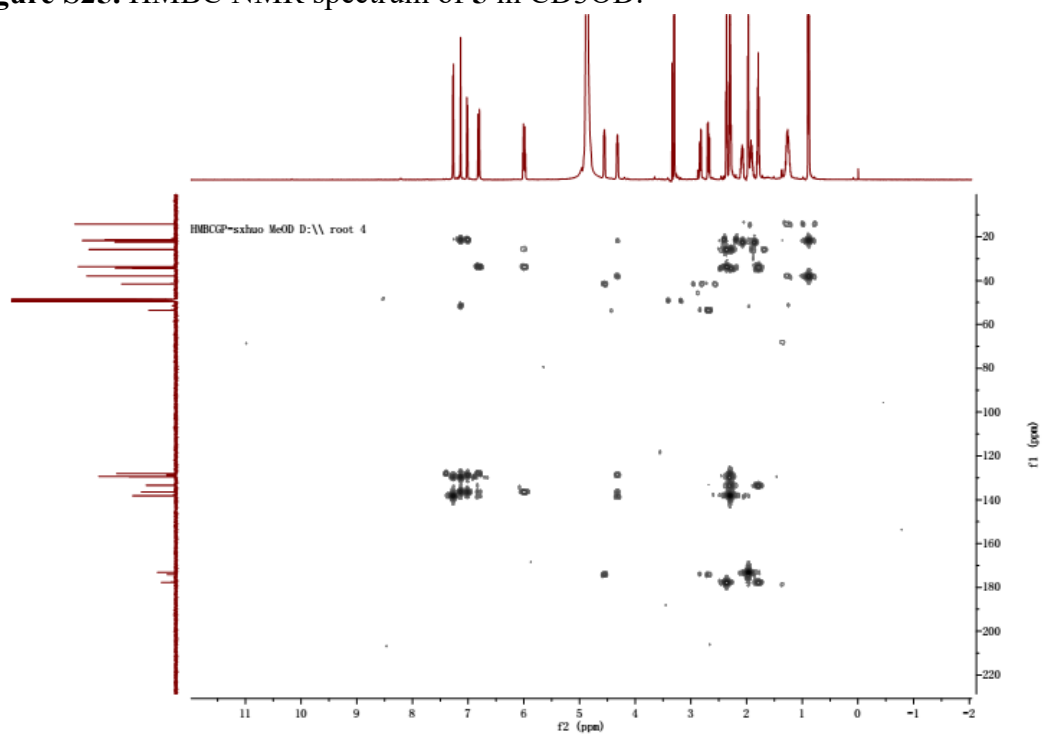


Figure S26. ¹H-¹H COSY NMR spectrum of **5** in CD₃OD.

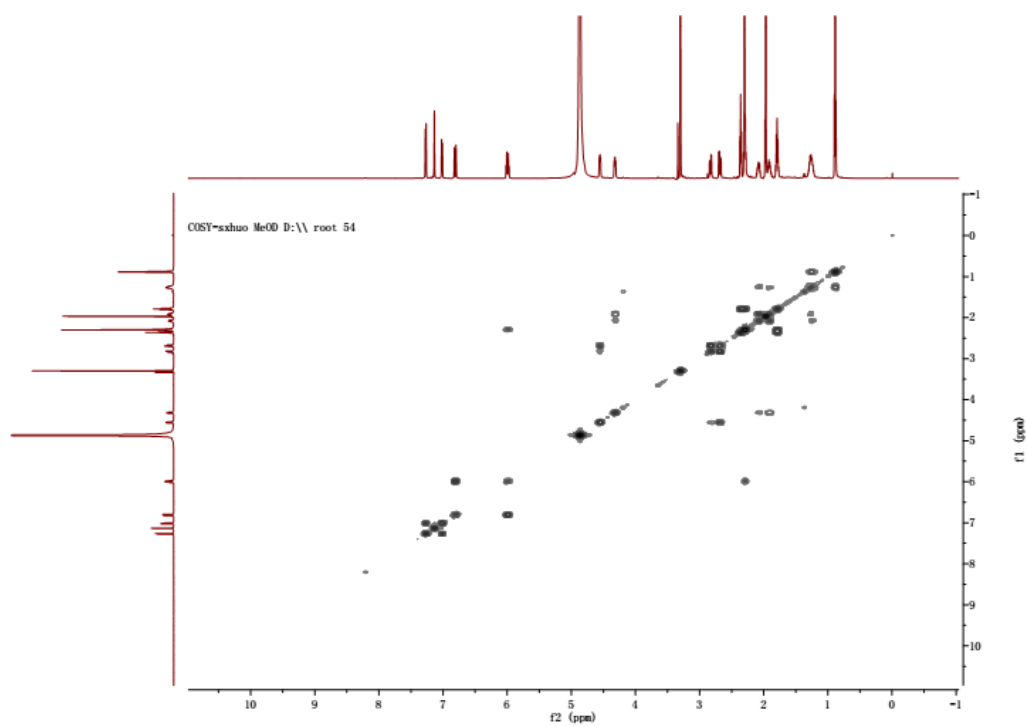


Figure S27. HRESIMS spectrum of **5**.

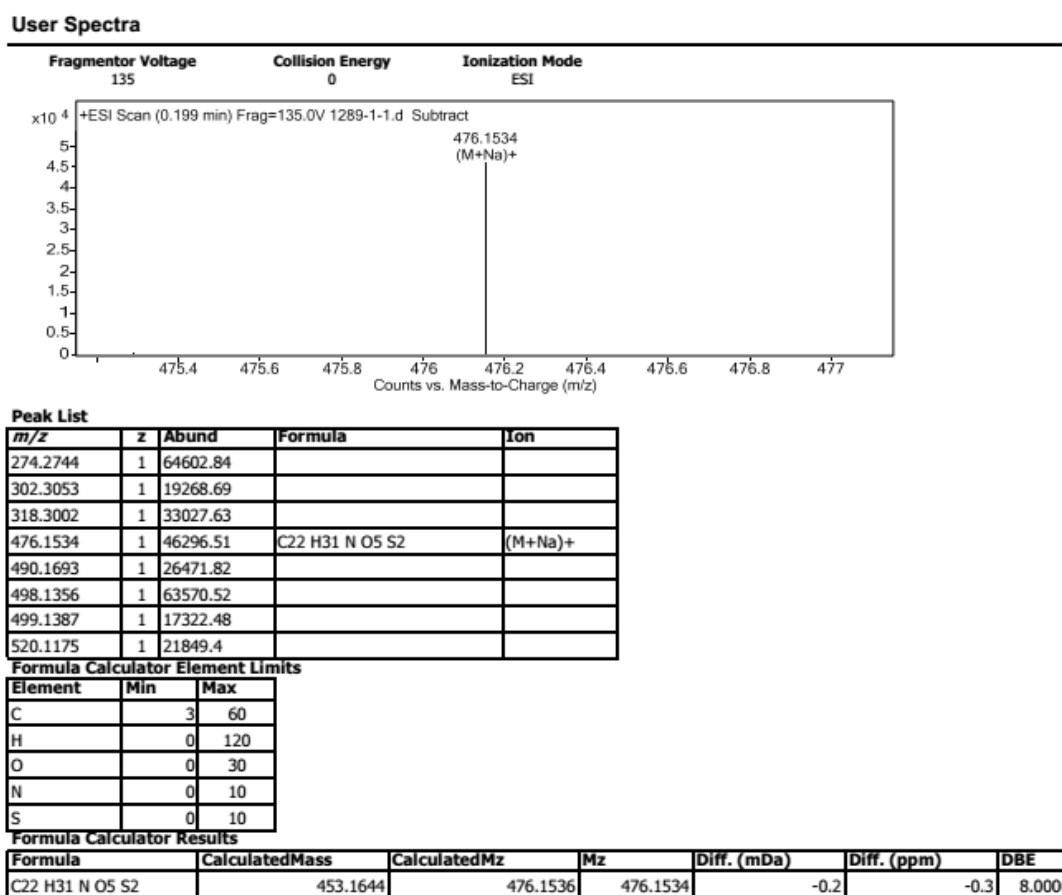


Figure S28. ¹H NMR spectrum of **6** in CD₃OD (600 MHz).

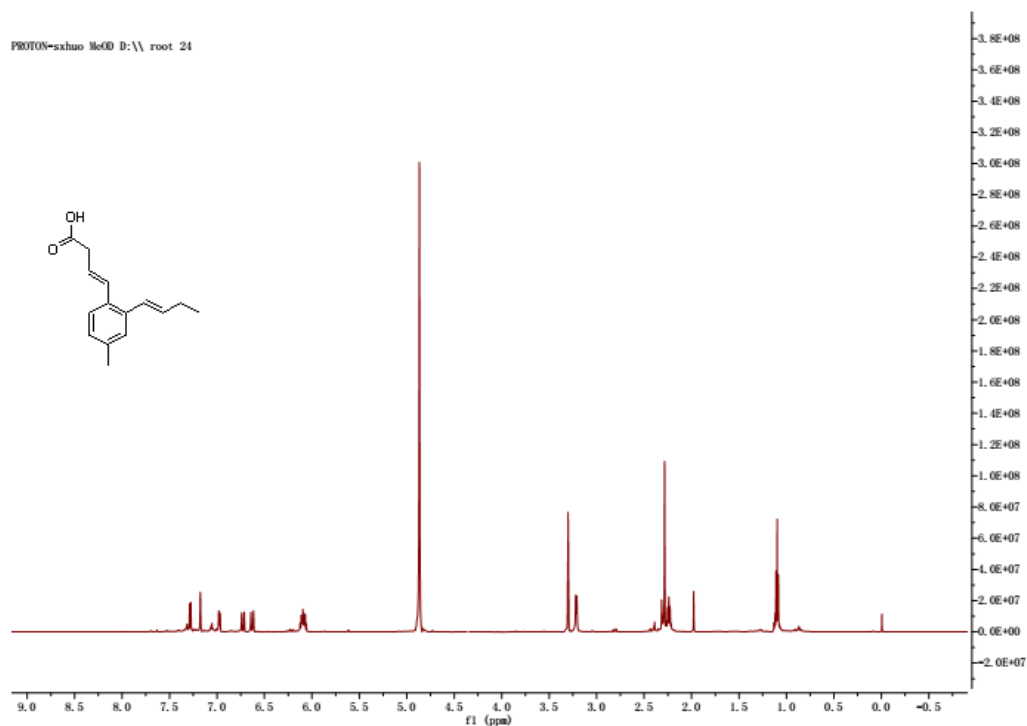


Figure S29. ^{13}C NMR spectrum of **6** in CD_3OD (150 MHz).

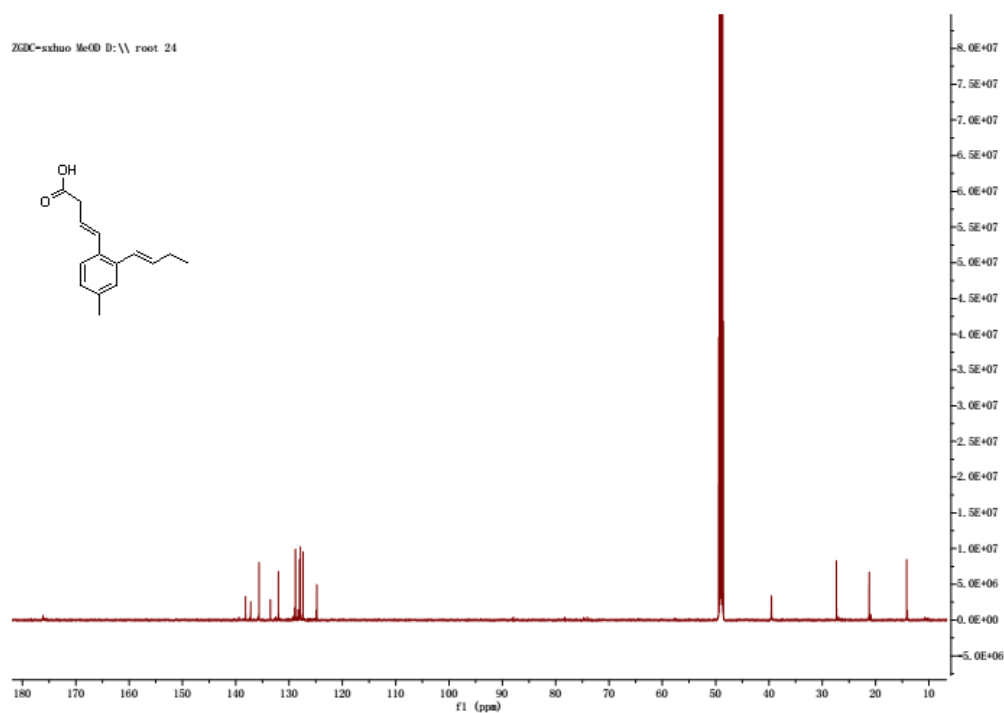


Figure S30. HSQC NMR spectrum of **6** in CD_3OD .

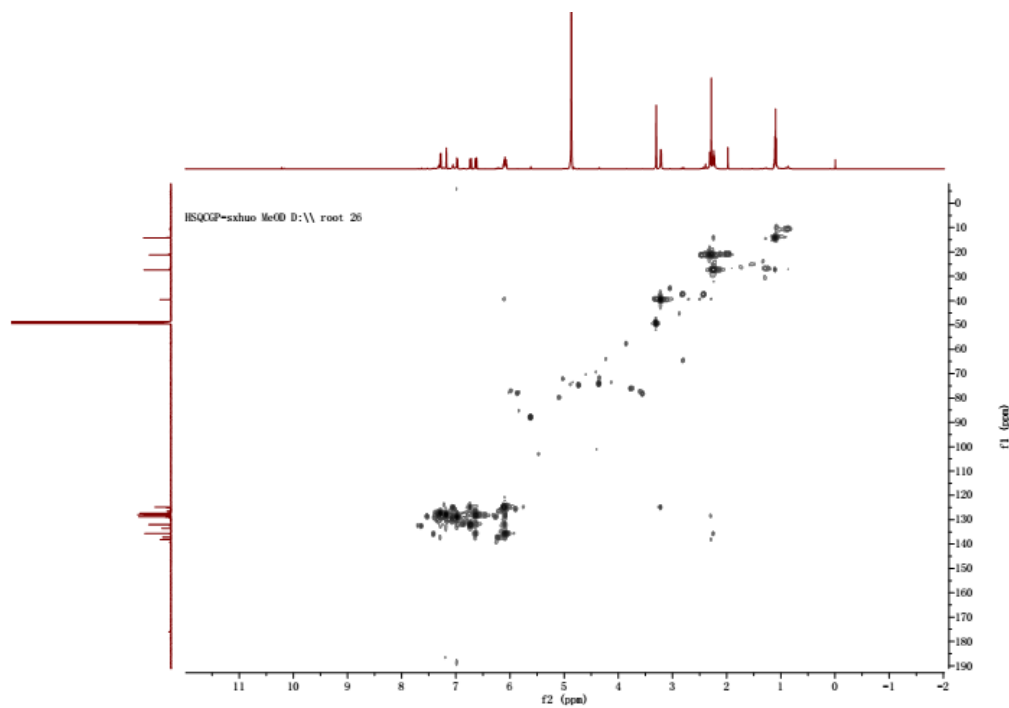


Figure S31. HMBC NMR spectrum of **6** in CD₃OD.

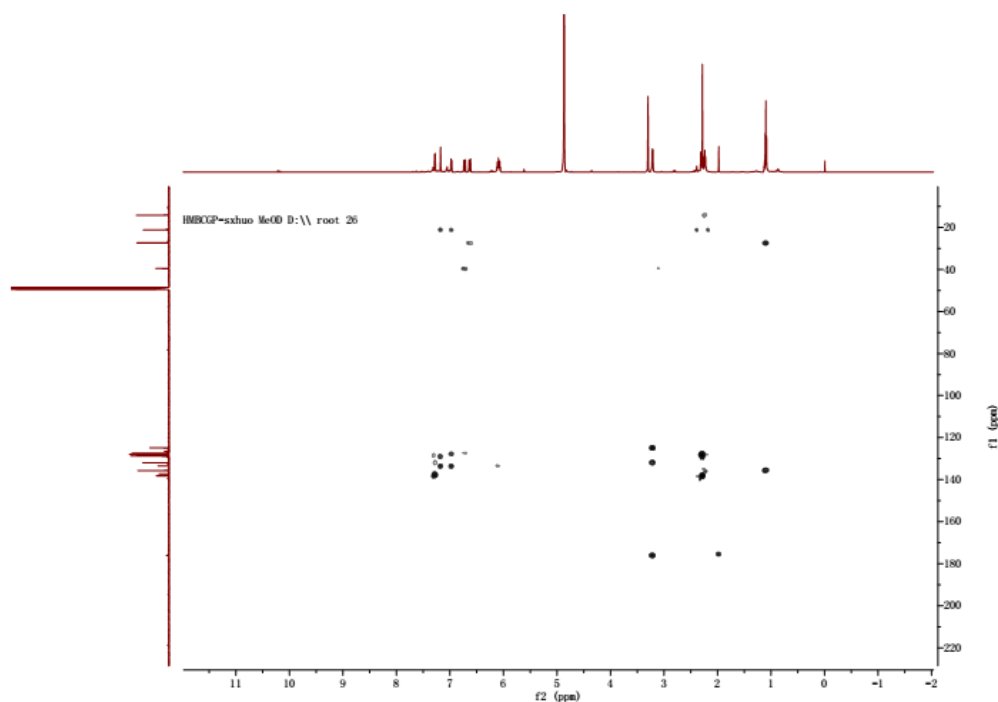
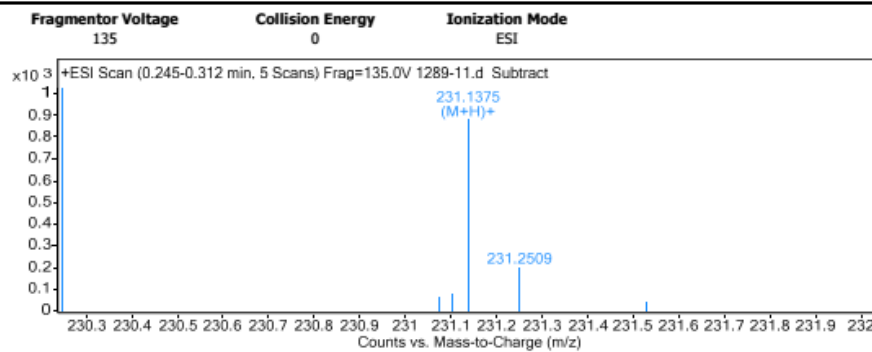


Figure S32. HRESIMS spectrum of **6**.

User Spectra



Peak List

m/z	z	Abund
150.1126	1	7343.22
269.1148	1	8740.27
274.2743	1	22745.83
301.1407	1	13787.54
318.3003	1	23937.56
437.1933	1	18520.69
453.1674	1	30024.55
454.1713	1	8355.63

Formula Calculator Element Limits

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

Formula Calculator Results

Formula	CalculatedMass	CalculatedMz	Mz	Diff. (mDa)	Diff. (ppm)	DBE
C15 H18 O2	230.1307	231.1380	231.1375	0.5	2.0	7.0000

Figure S33. ^1H NMR spectrum of **7** in CD_3OD (600 MHz).

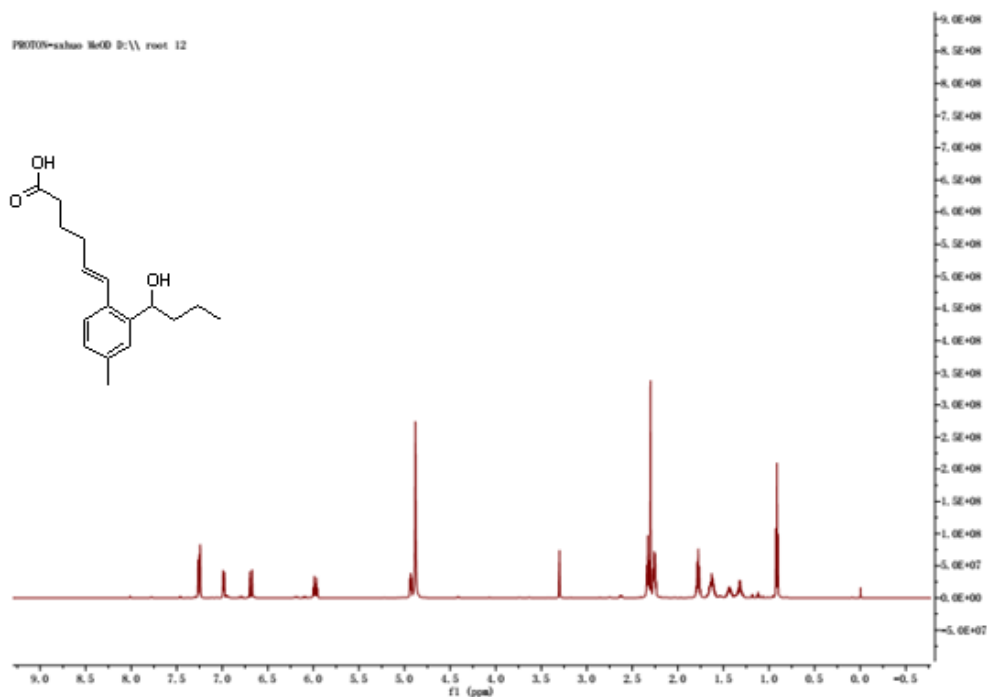


Figure S34. ^{13}C NMR spectrum of **7** in CD_3OD (150 MHz).

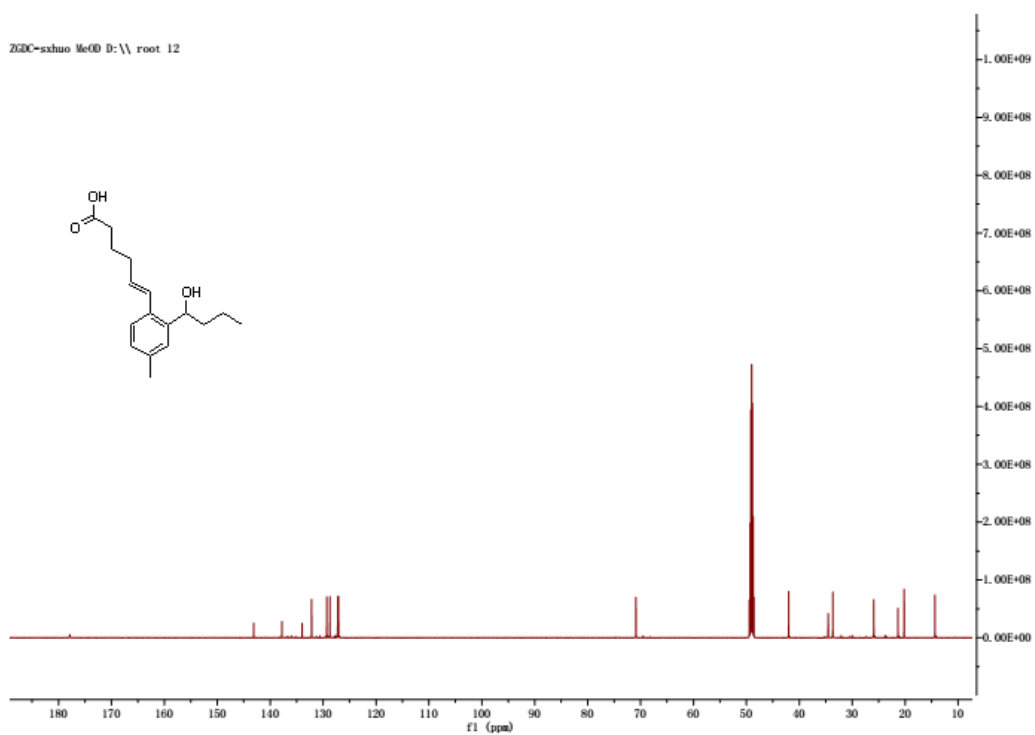


Figure S35. HSQC NMR spectrum of **7** in CD₃OD.

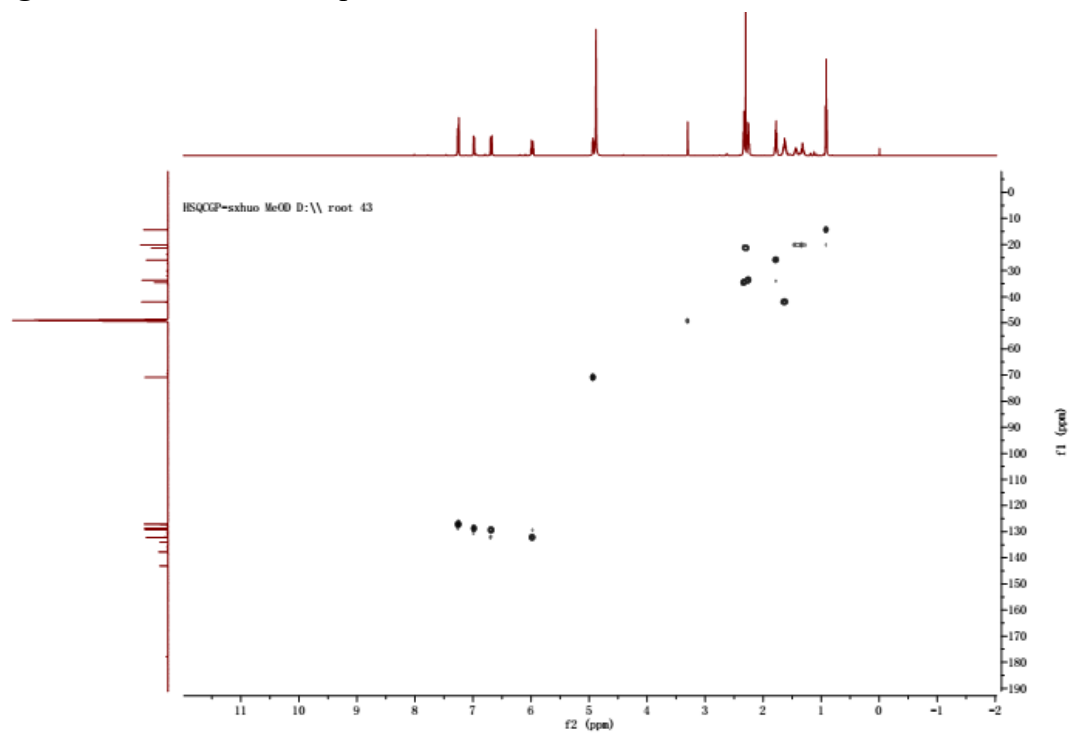


Figure S36. HMBC NMR spectrum of **7** in CD₃OD.

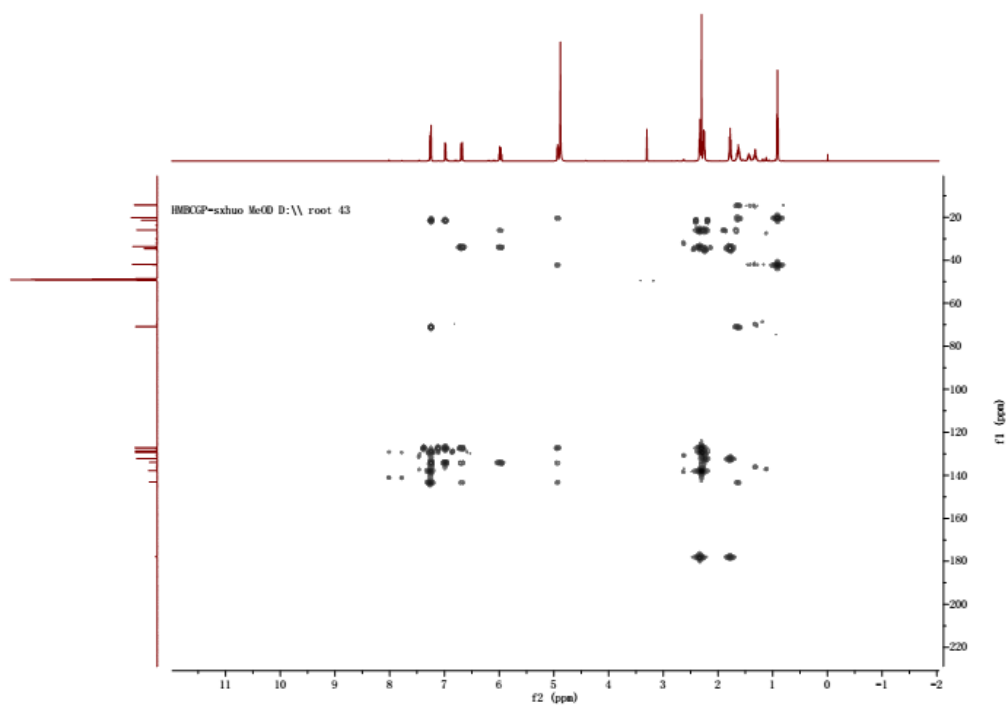


Figure S37. HRESIMS spectrum of 7.

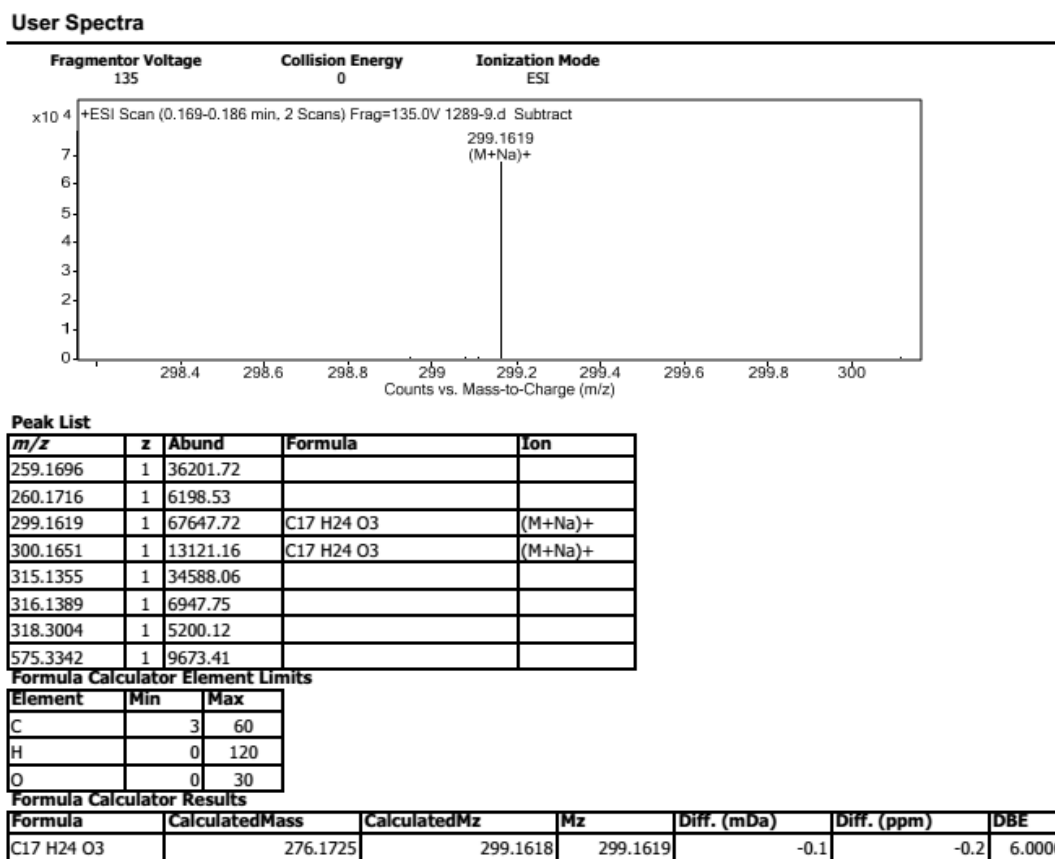


Figure S38. ^1H NMR spectrum of 8 in CDCl_3 (600 MHz).

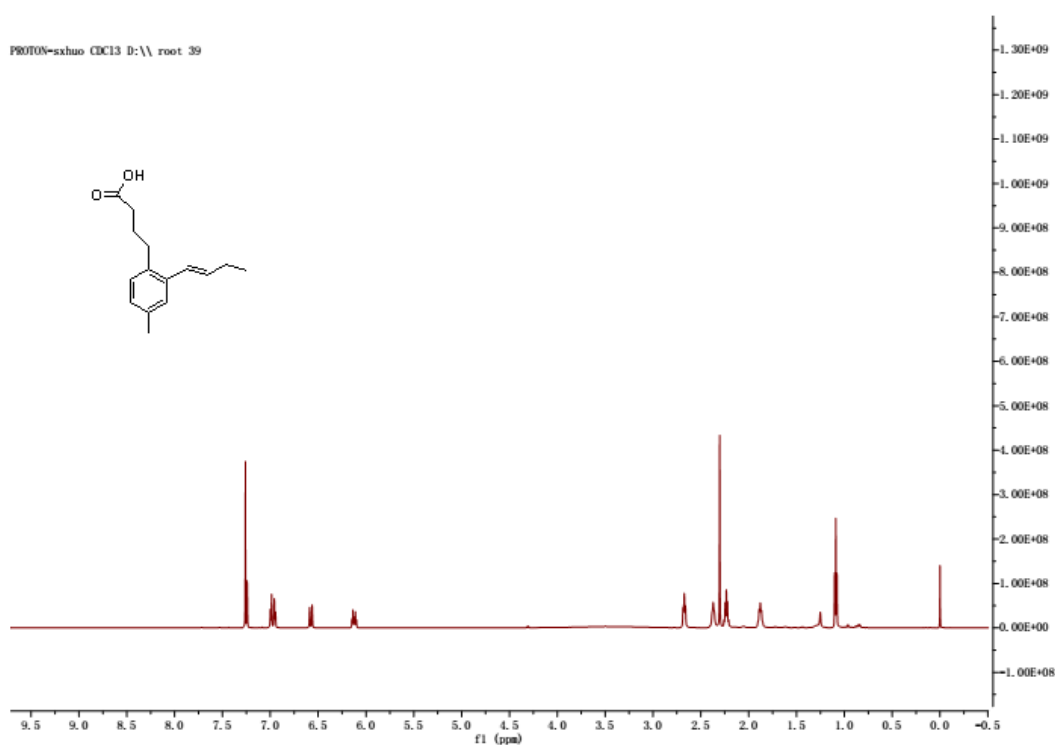


Figure S39. ^{13}C NMR spectrum of **8** in CDCl_3 (150 MHz).

