Supporting Information

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Chemical Constituents from the Whole Plant of *Pachysandra terminalis*

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Table of Contents **page**

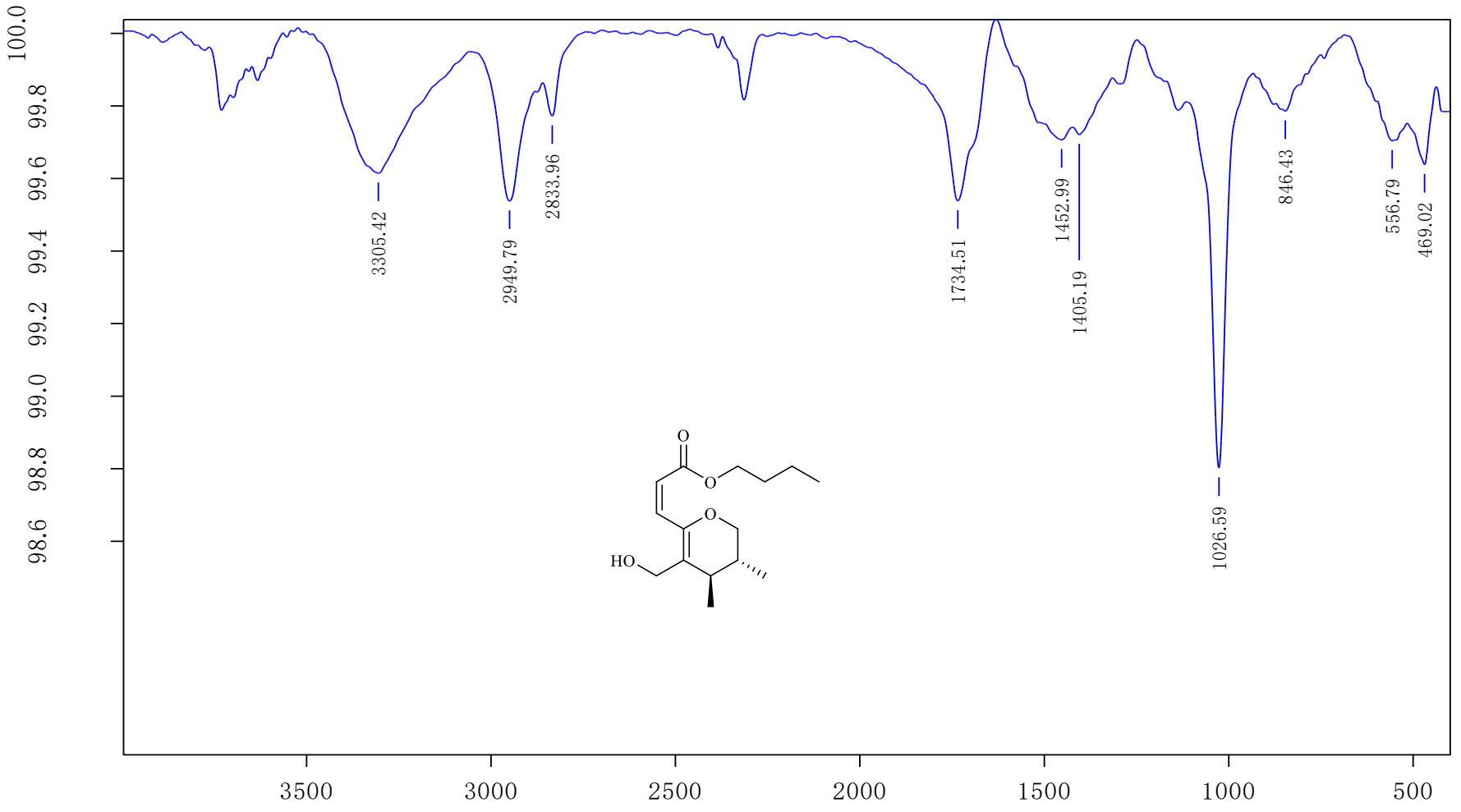
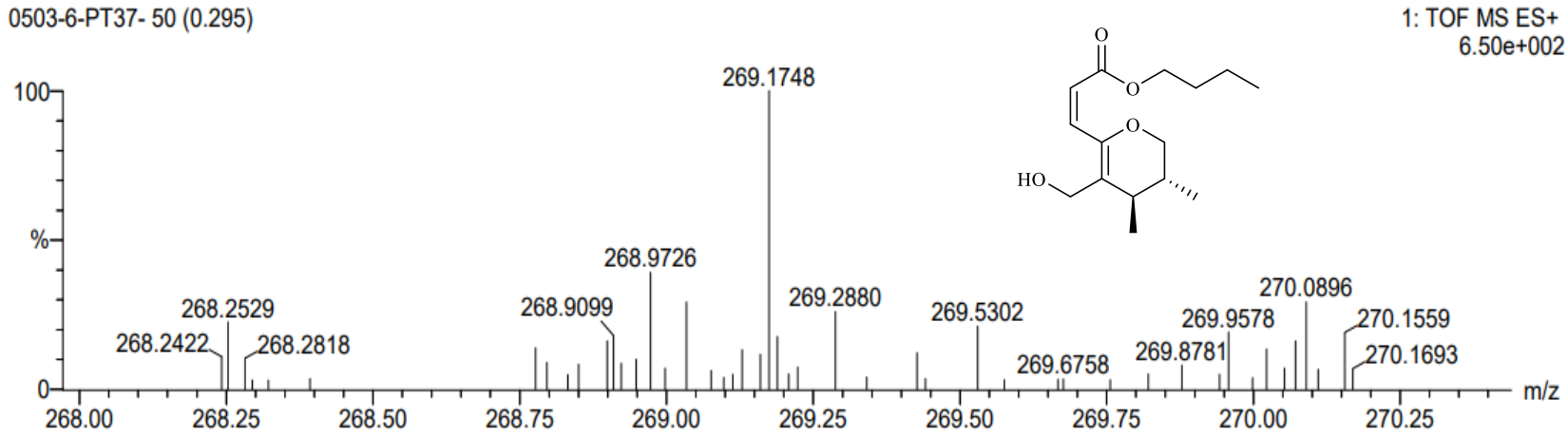


Figure S1: The IR spectrum of **1** (in KBr)



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269.1748	269.1753	-0.5	-1.9	3.5	202.6	n/a	n/a	C15 H25 O4

Figure S2: The HR-ESI-MS spectrum of **1** (in MeOH）

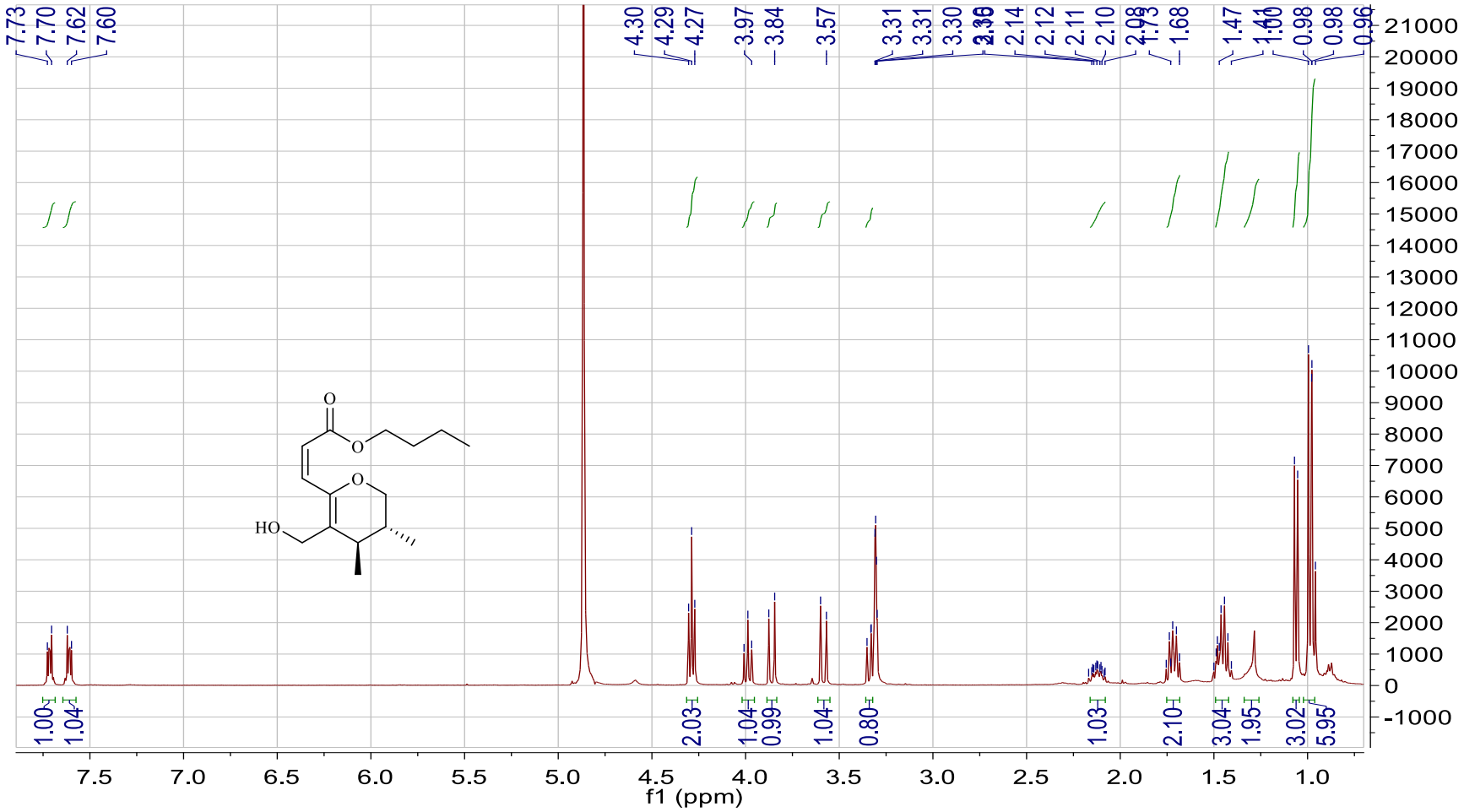


Figure S3: The ^{1}H NMR spectrum of **1** (in CD_3OD)

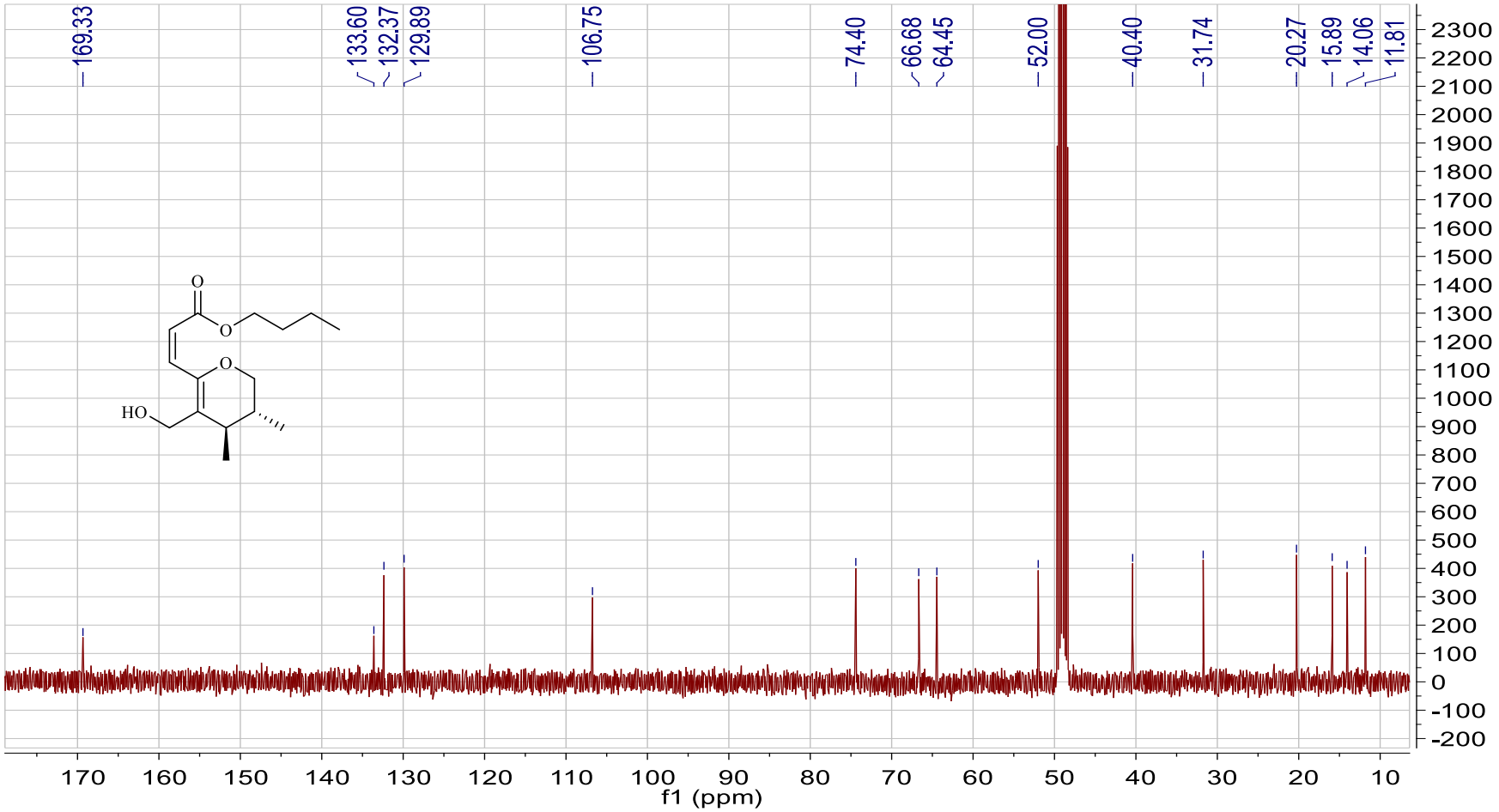


Figure S4: The ^{13}C NMR spectrum of **1** (in CD_3OD)

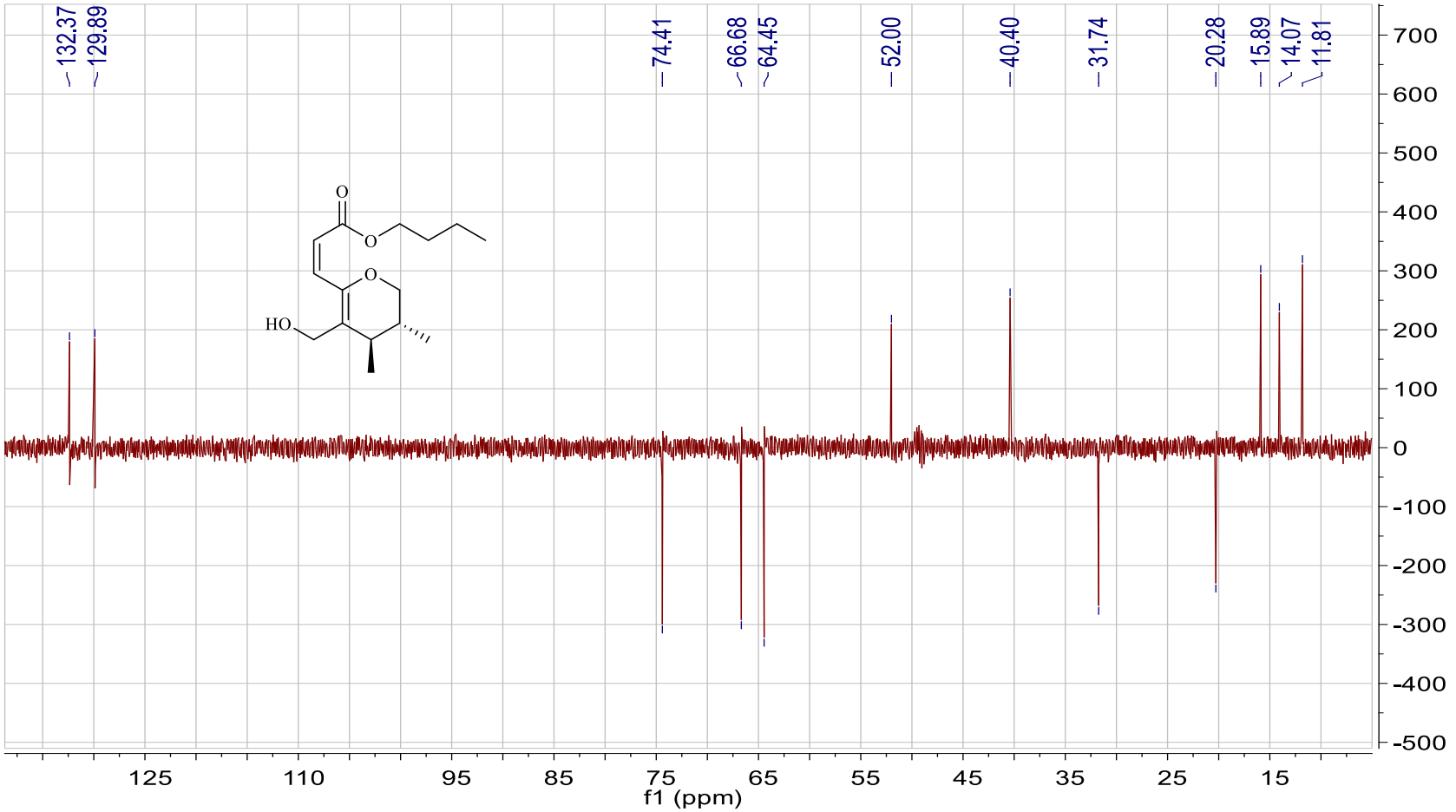


Figure S5: The DEPT spectrum of **1** (in CD_3OD)

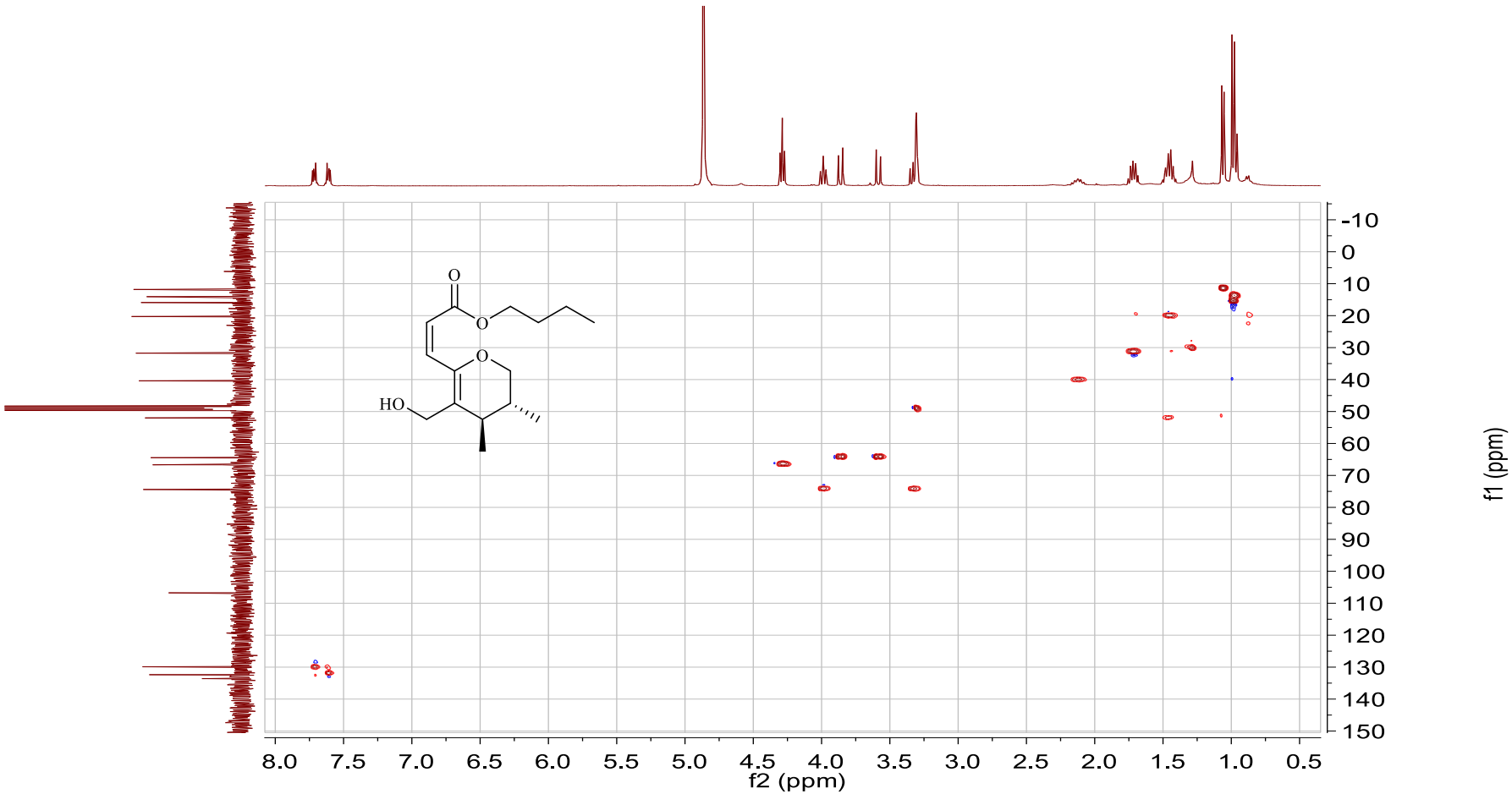


Figure S6: The HSQC spectrum of **1** (in CD_3OD)

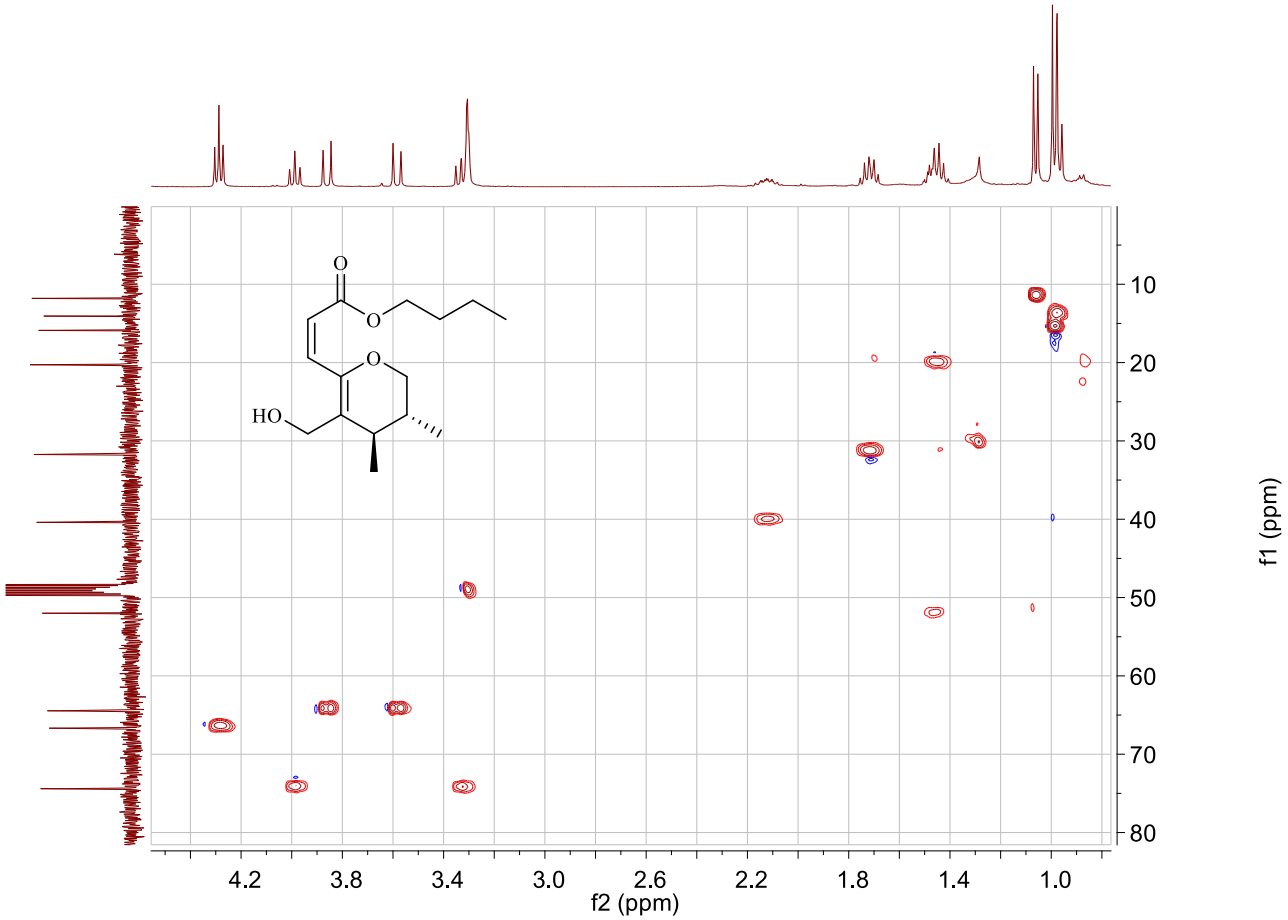


Figure S7: The HSQC spectrum of **1** (in CD_3OD) (From δc 0 ppm to δc 80 ppm)

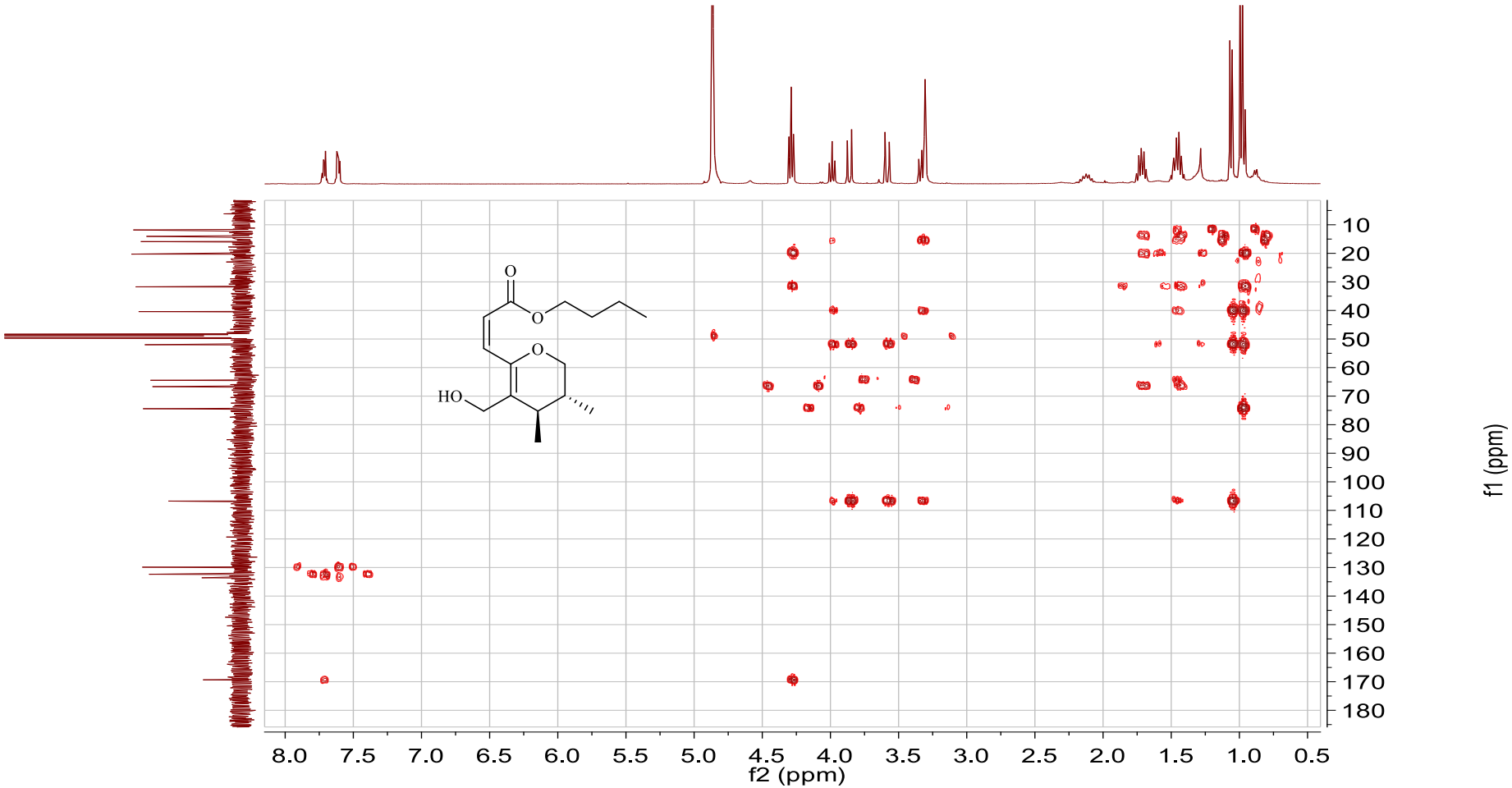


Figure S8: The HMBC spectrum of **1** (in CD_3OD)

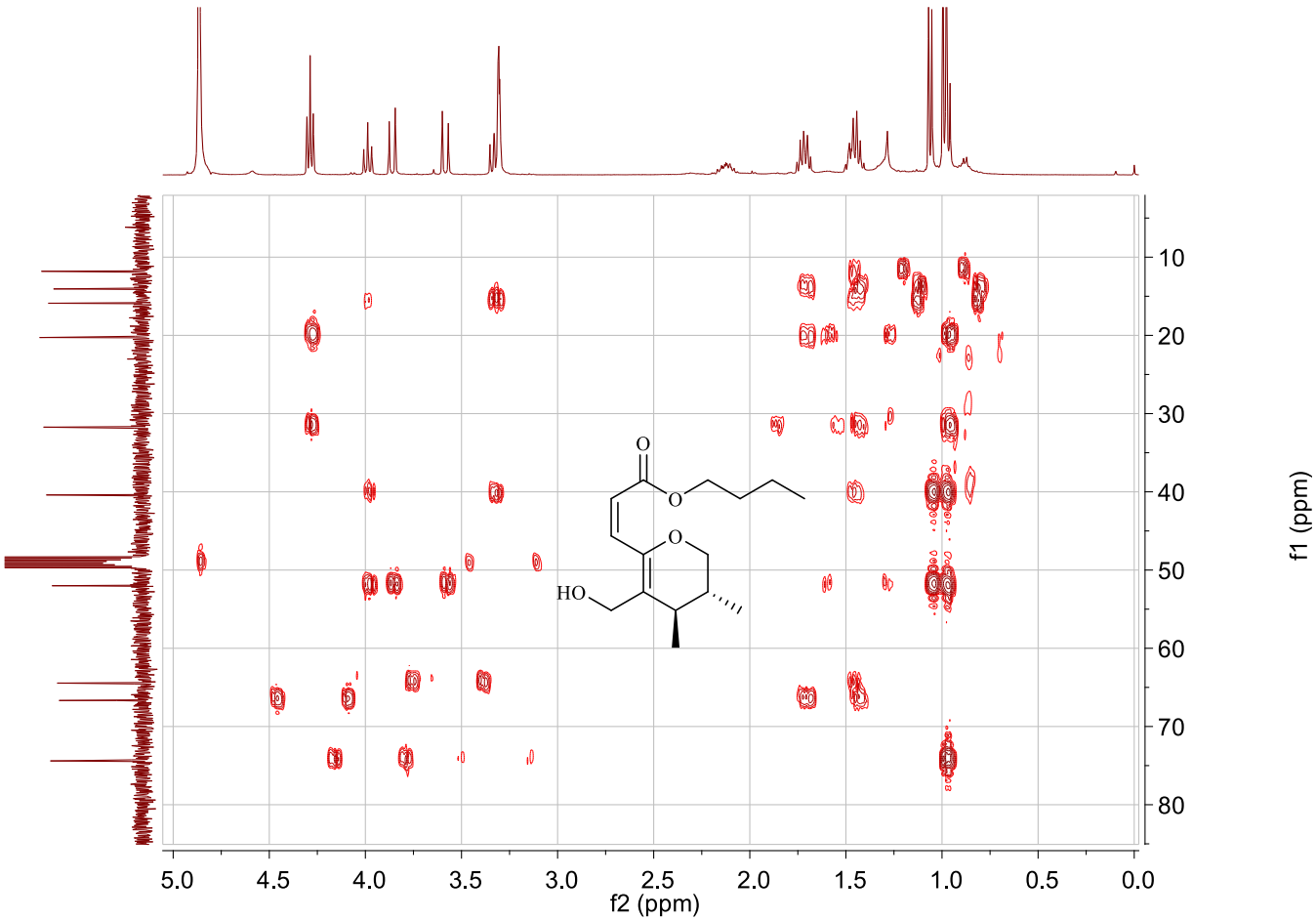


Figure S9: The HMBC spectrum of **1** (in CD_3OD) (From δc 10 ppm to δc 85 ppm)

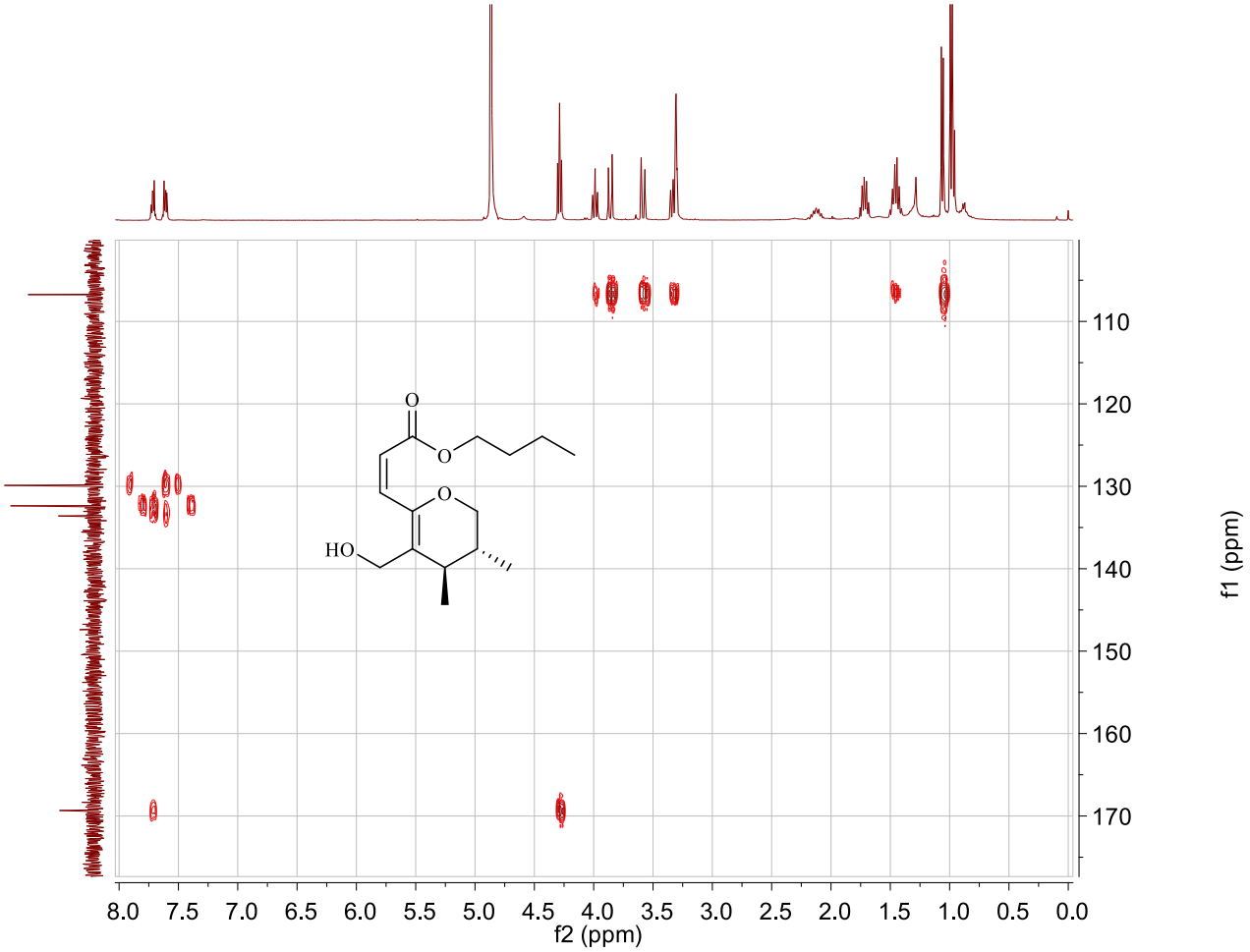


Figure S10: The HMBC spectrum of **1** (in CD_3OD) (From δc 100 ppm to δc 180 ppm)

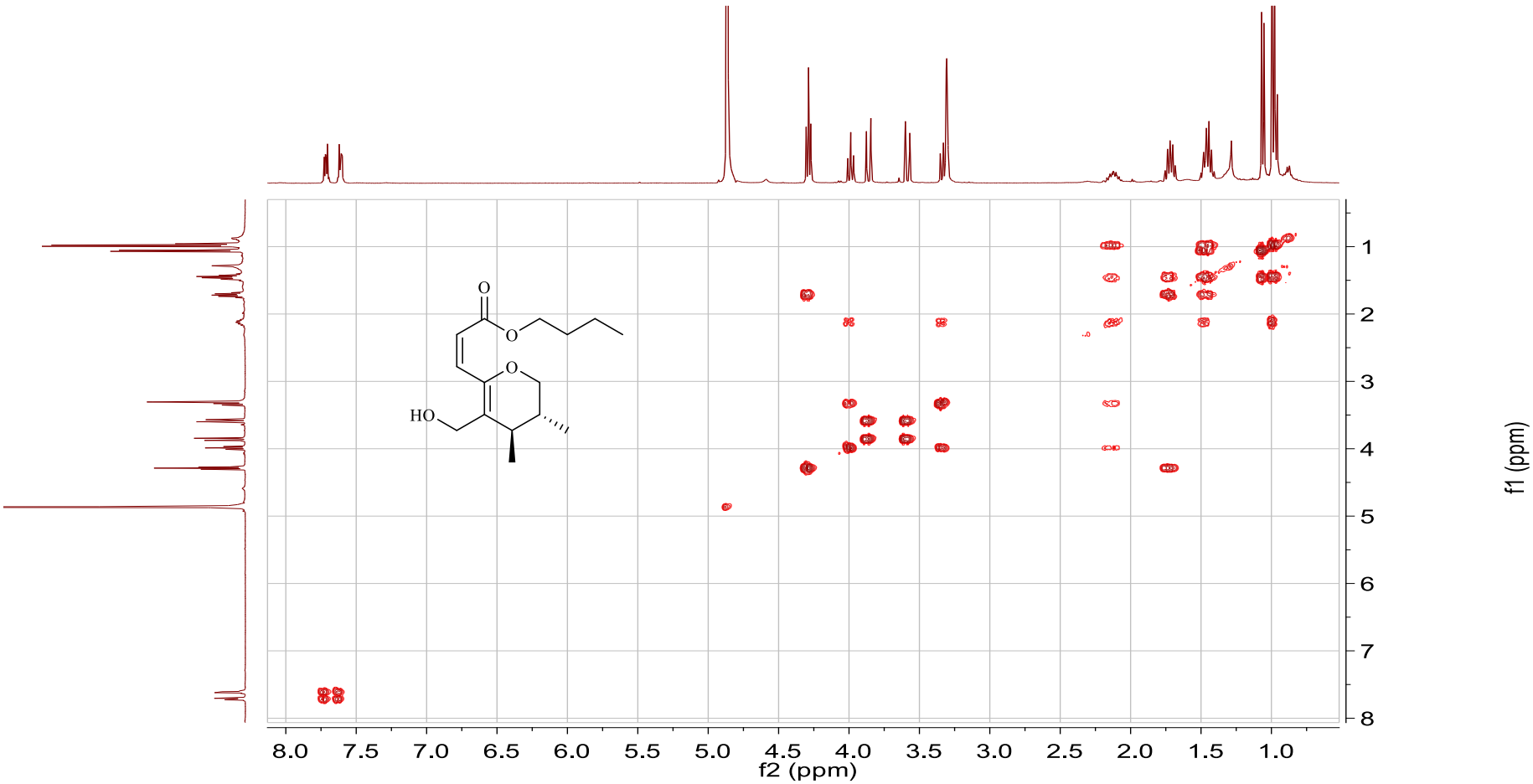


Figure S11: The ^{1}H-^{1}H COSY spectrum of **1** (in CD_3OD)

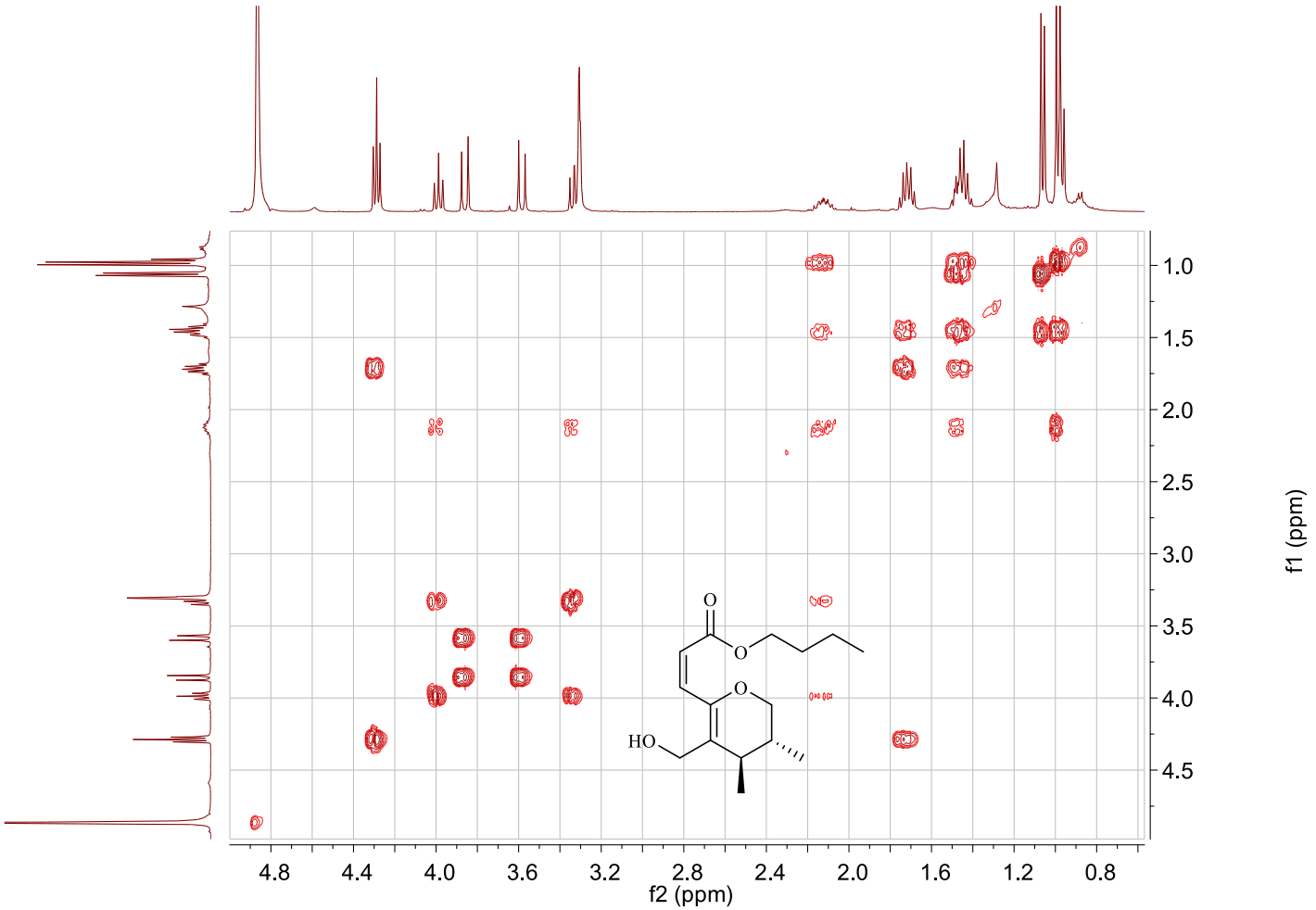


Figure S12. The ^{1}H-^{1}H COSY spectrum of **1** (in CD_3OD) (From δ_H 0.5 ppm to δ_H 5.0 ppm)

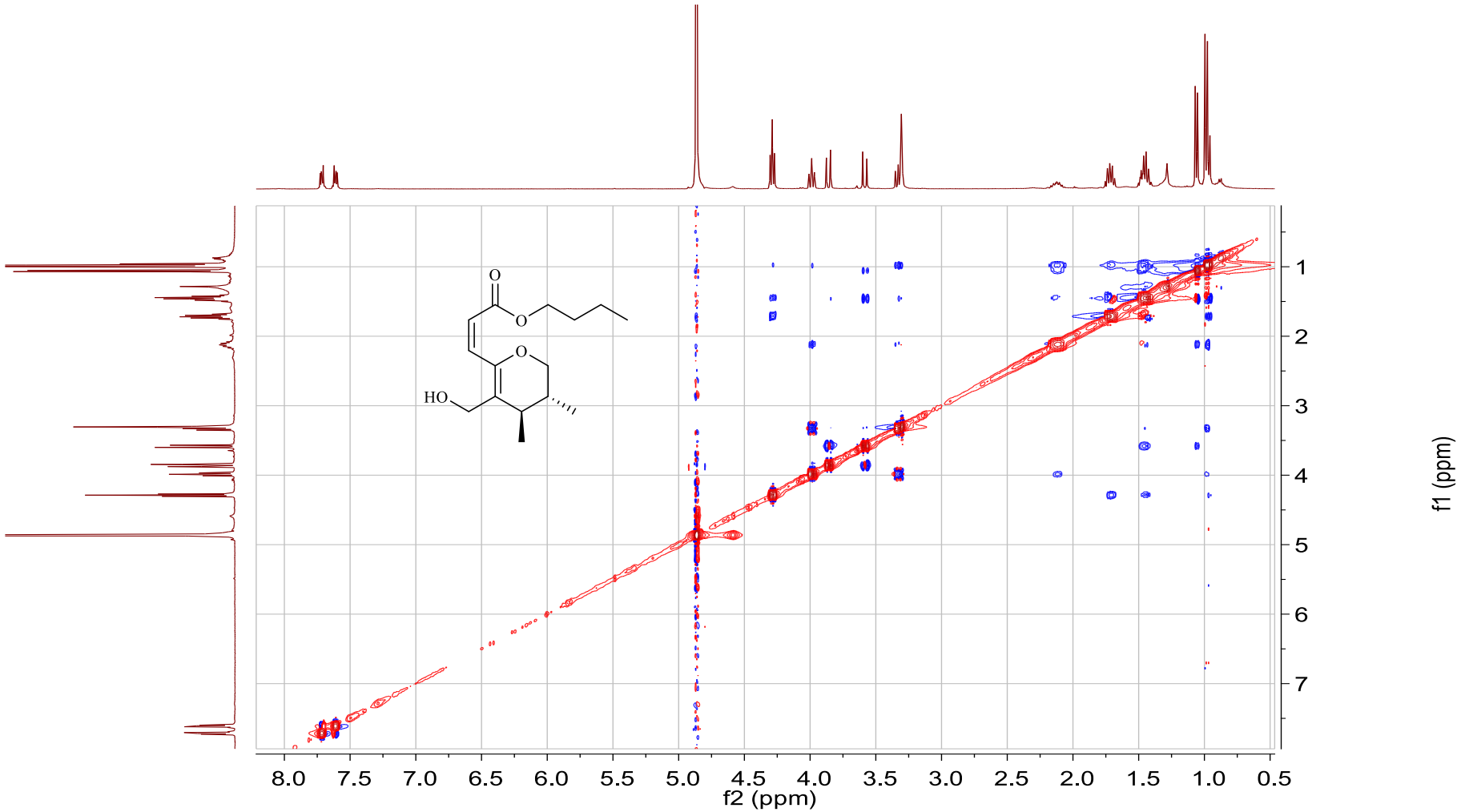


Figure S13: The NOESY spectrum of **1** (in CD_3OD)

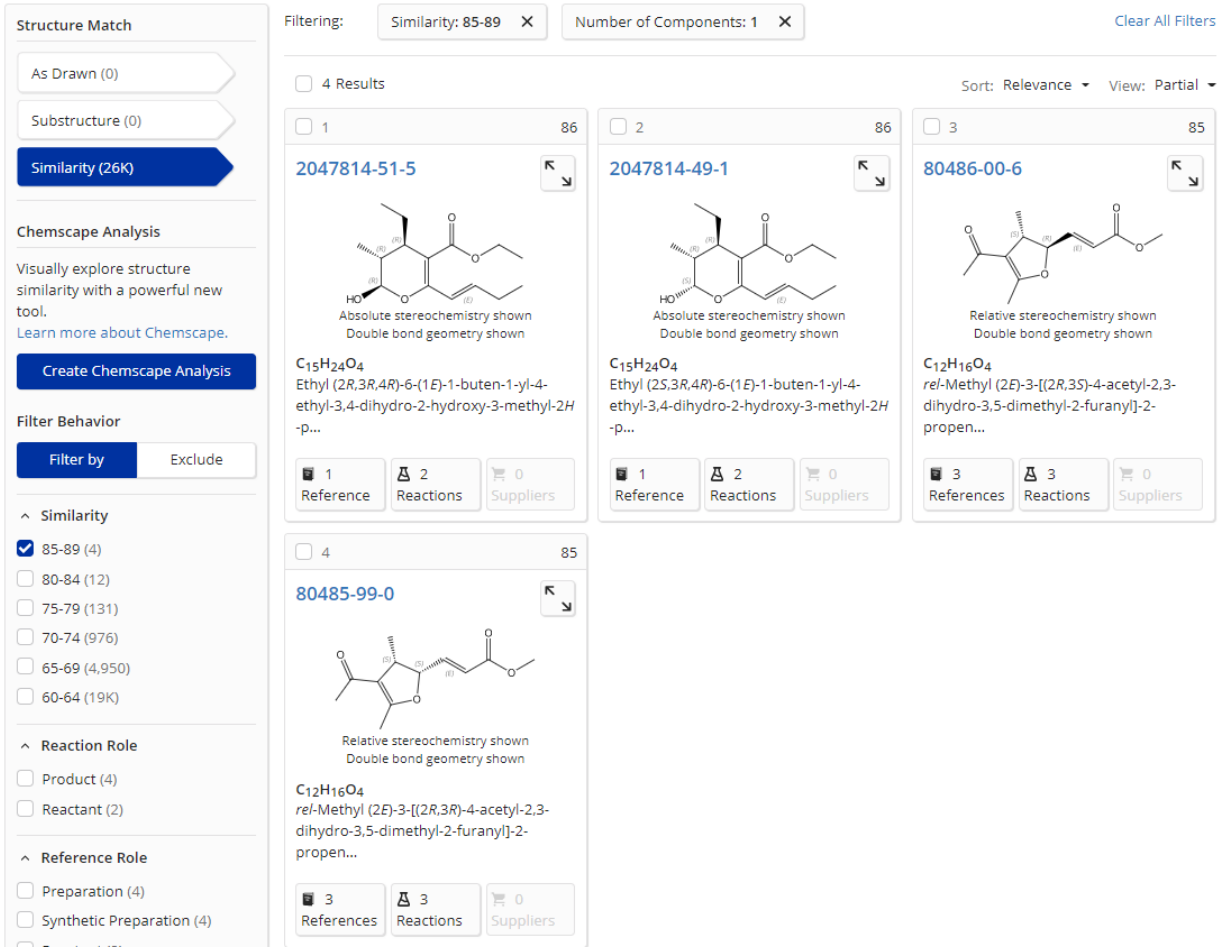
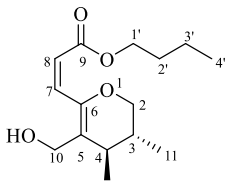
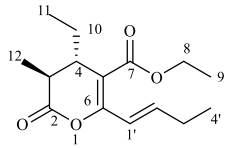


Figure S14: Search report of SciFinder of **1**

Table S1: Comparative ^{13}C NMR data of compound **1** with similar compound

Position	 Compound 1 δ_C	 Similar compound δ_C
2	74.4, CH_2	170.3, C
3	52.0, CH	41.7, CH
4	40.4, CH	37.6, CH
5	133.6, C	107.8, C
6	106.8, C	155.1, C
7	132.4, CH	166.7, C
8	129.9, CH	60.8, CH_2
9	169.3, C	26.1, CH_3
10	64.5, CH_2	16.2, CH_2
11	11.8, CH_3	12.7, CH_3
12	15.9, CH_3	11.1, CH_3
1′	66.7, CH_2	119.4, CH
2′	31.7, CH_2	141.7, CH
3′	20.3, CH_2	27.3, CH_2
4′	14.1, CH_3	14.2, CH_3

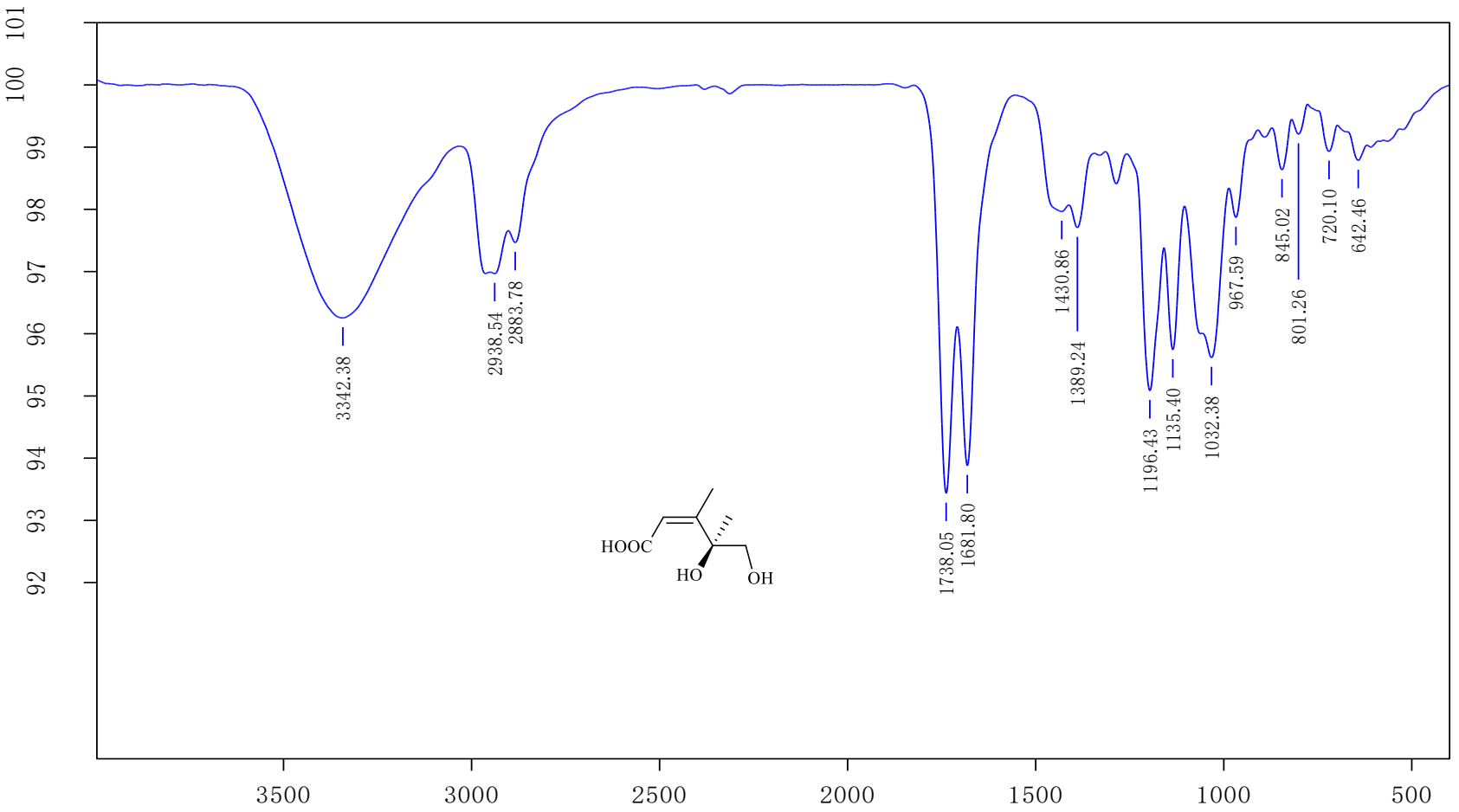
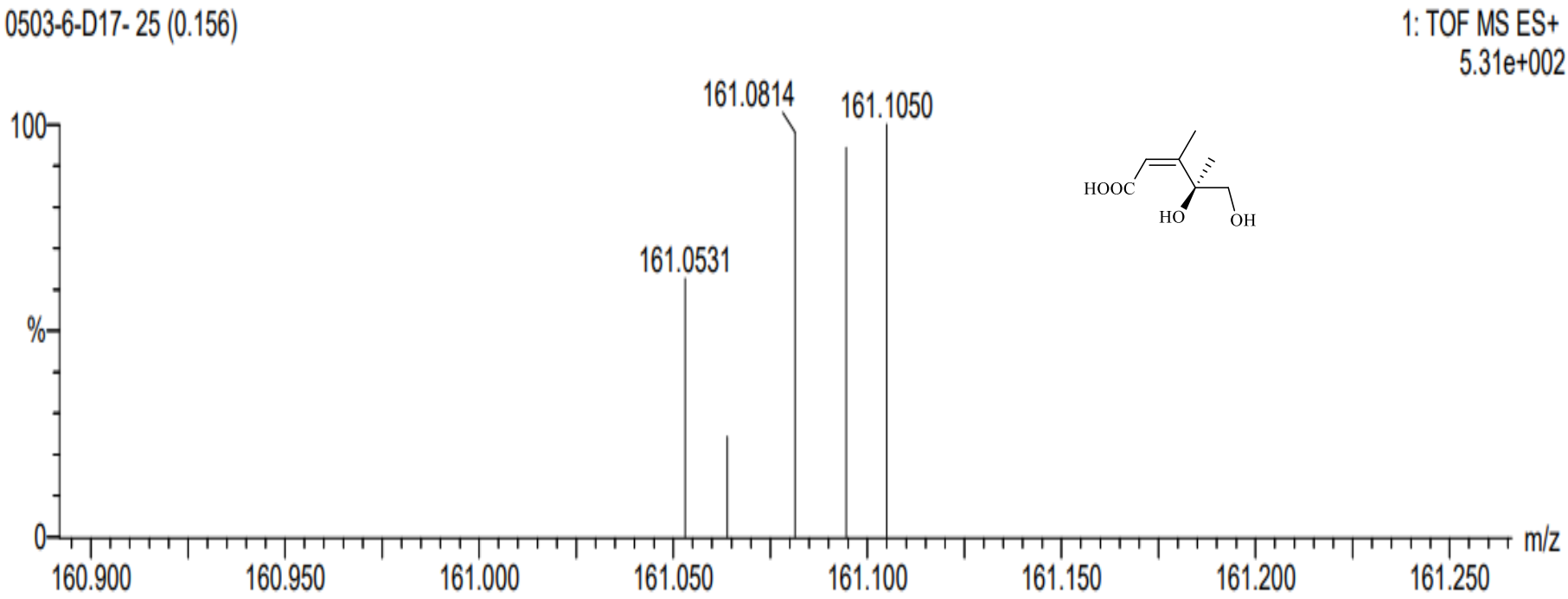


Figure S15: The IR spectrum of **2** (in KBr)



Minimum:				-1.5				
Maximum:		5.0	10.0	50.0				
Mass	Calc. Mass	mDa	PPM	DBE	i-FIT	Norm	Conf(%)	Formula
161.0814	161.0814	0.0	0.0	1.5	45.0	n/a	n/a	C7 H13 04

Figure S16: The HR-ESI-MS spectrum of **2** (in MeOH）

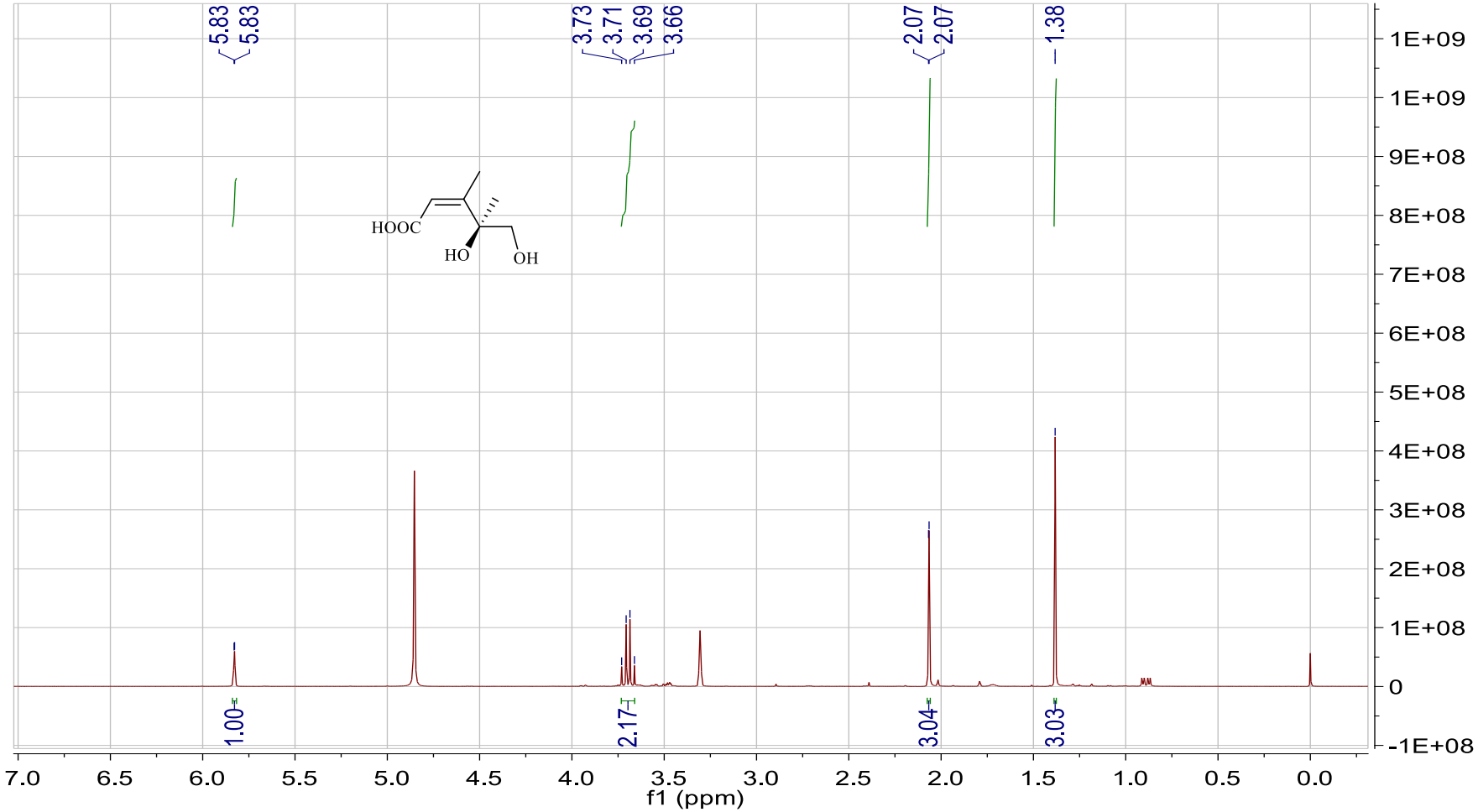


Figure S17: The ^{1}H NMR spectrum of **2** (in CD_3OD)

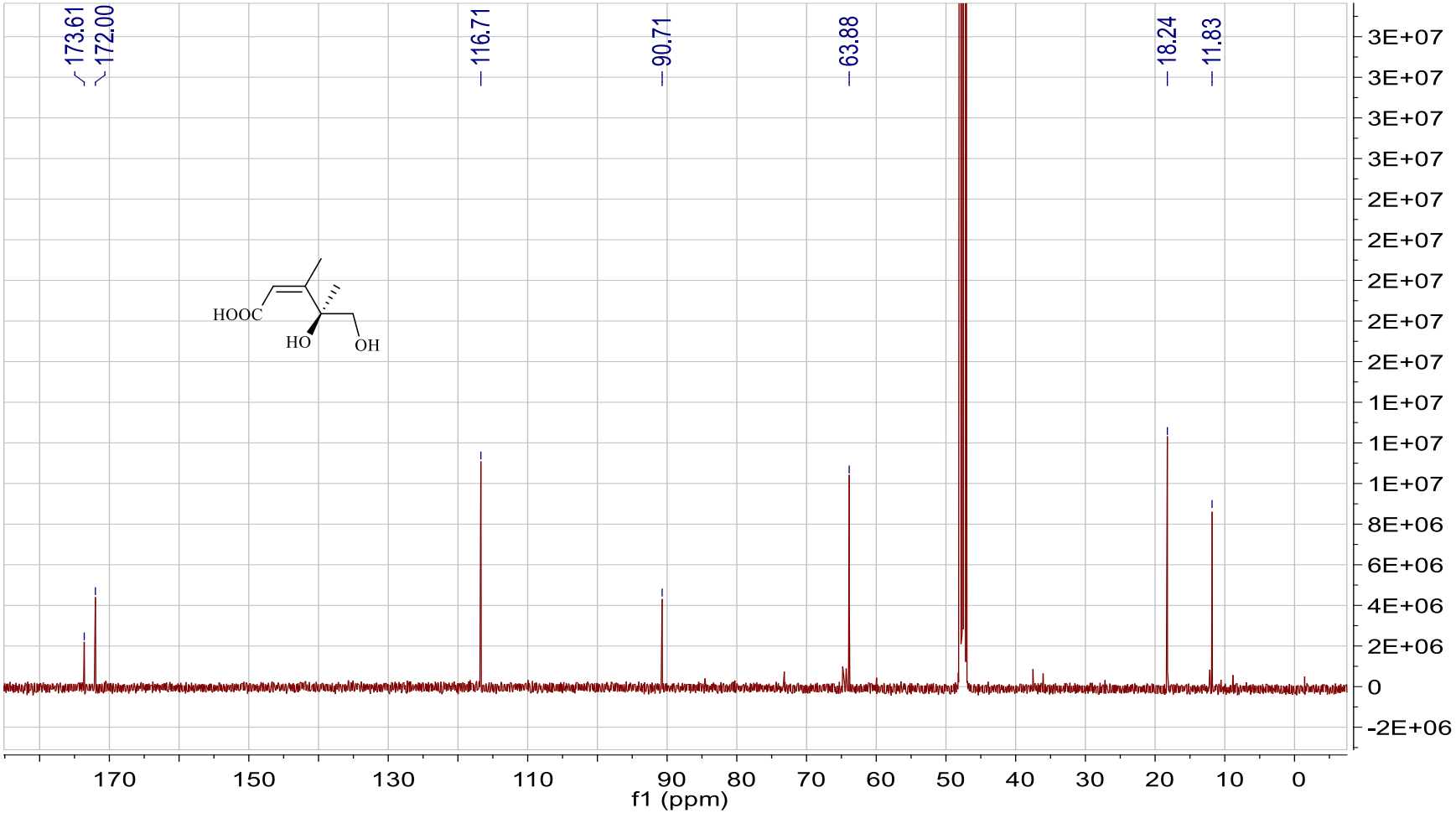


Figure S18: The ^{13}C NMR spectrum of **2** (in CD_3OD)

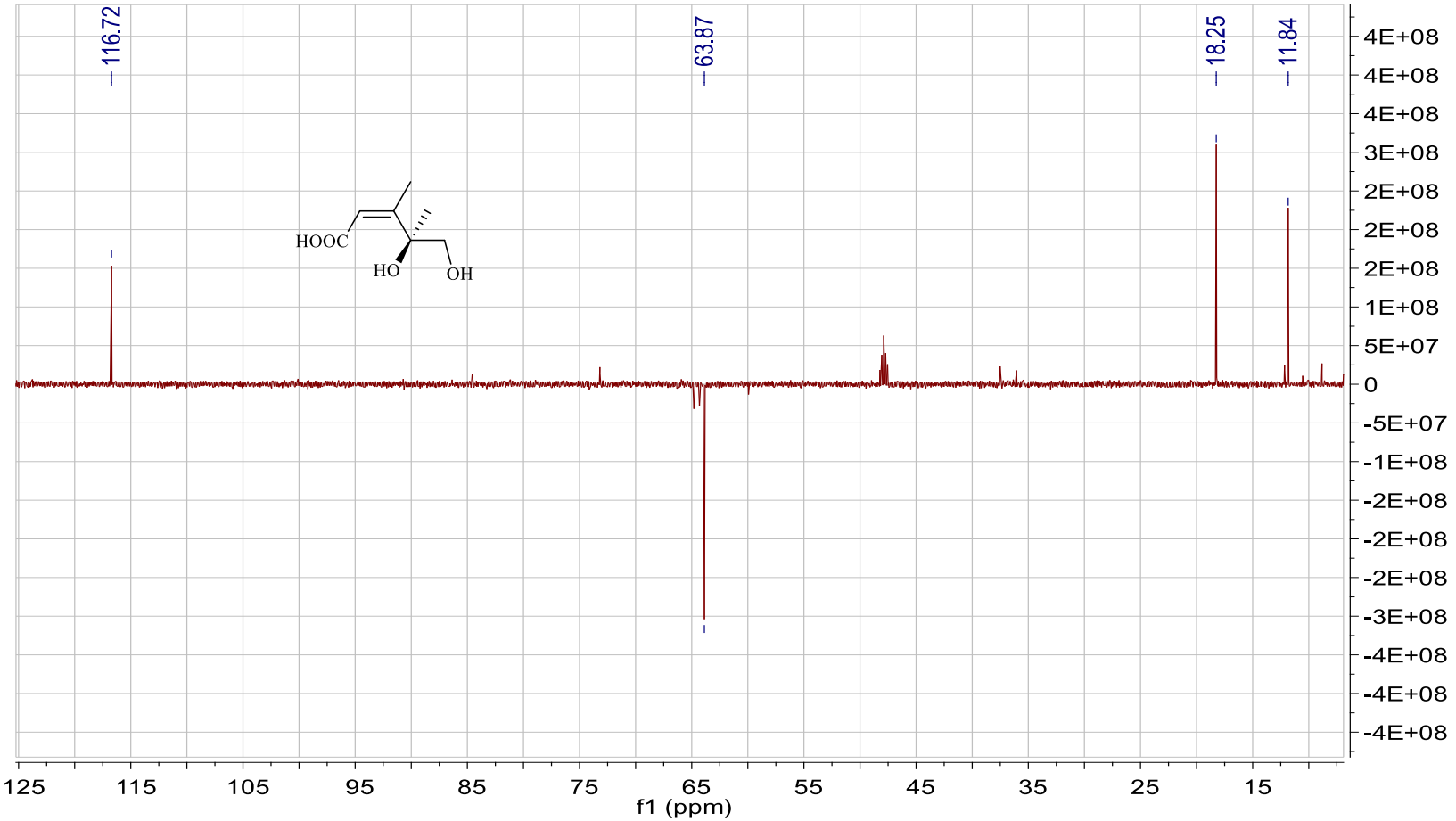


Figure S19: The DEPT 135 spectrum of **2** (in CD_3OD)

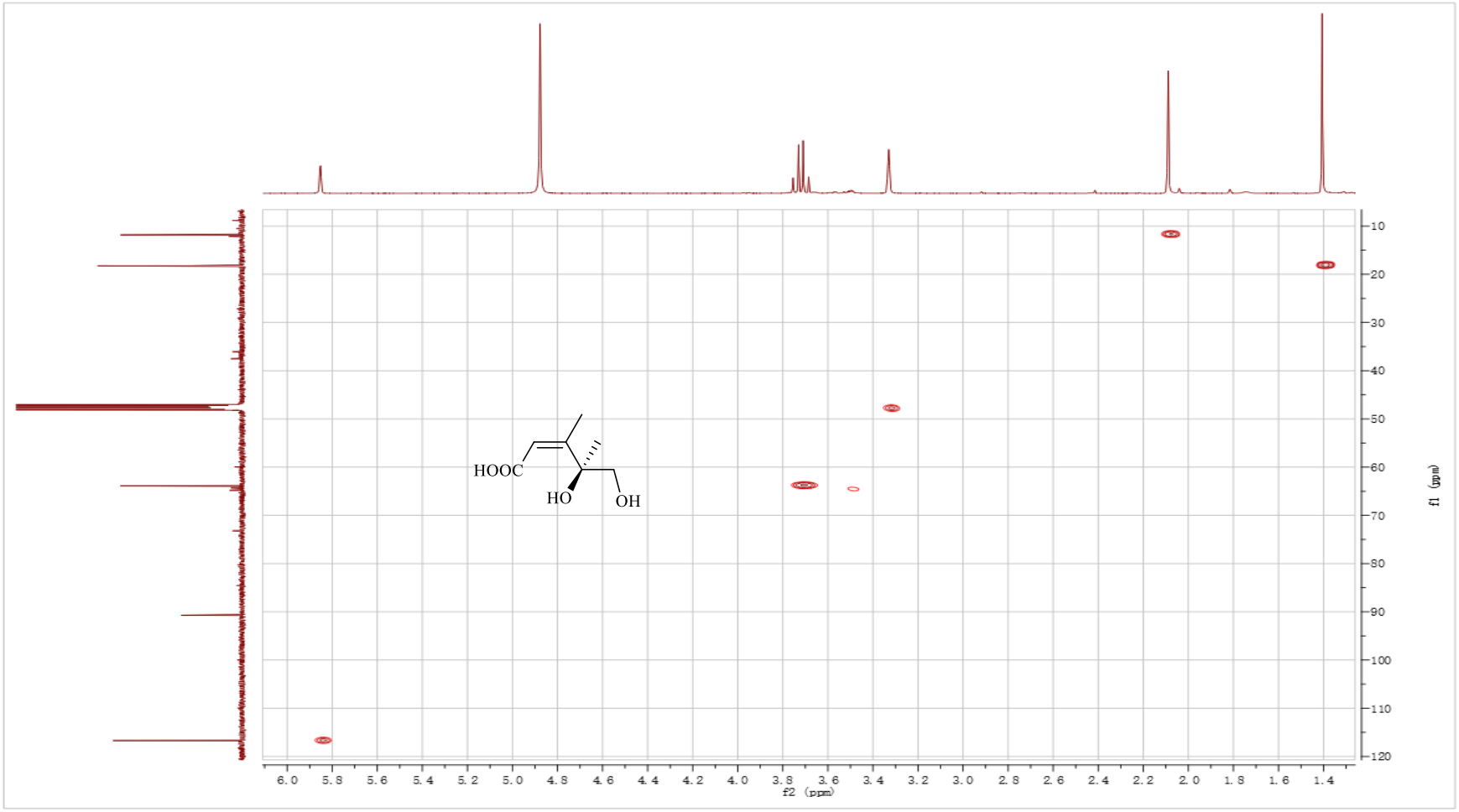


Figure S20: The HSQC spectrum of **2** (in CD_3OD)

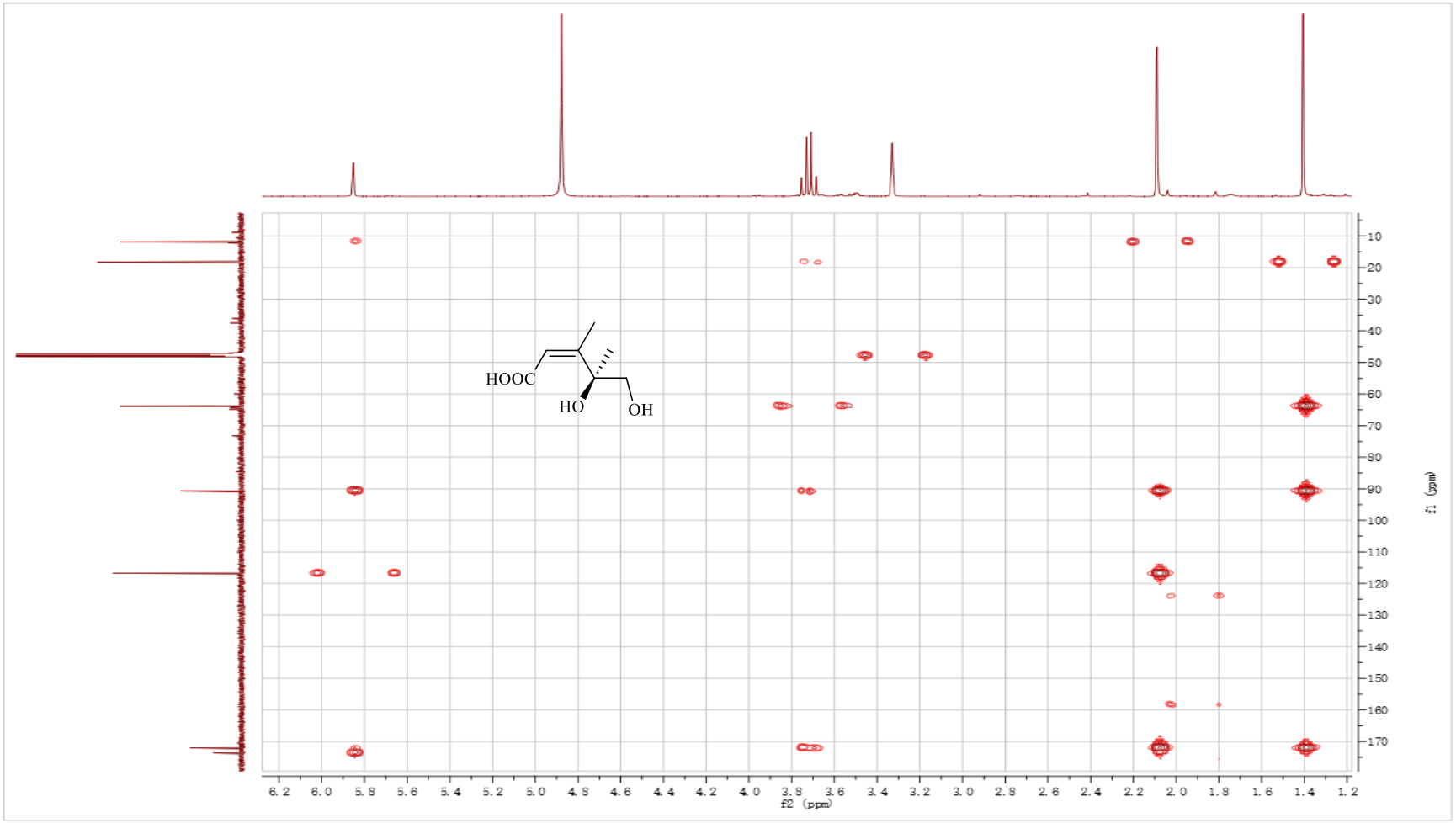


Figure S21: The HMBC spectrum of **2** (in CD_3OD)

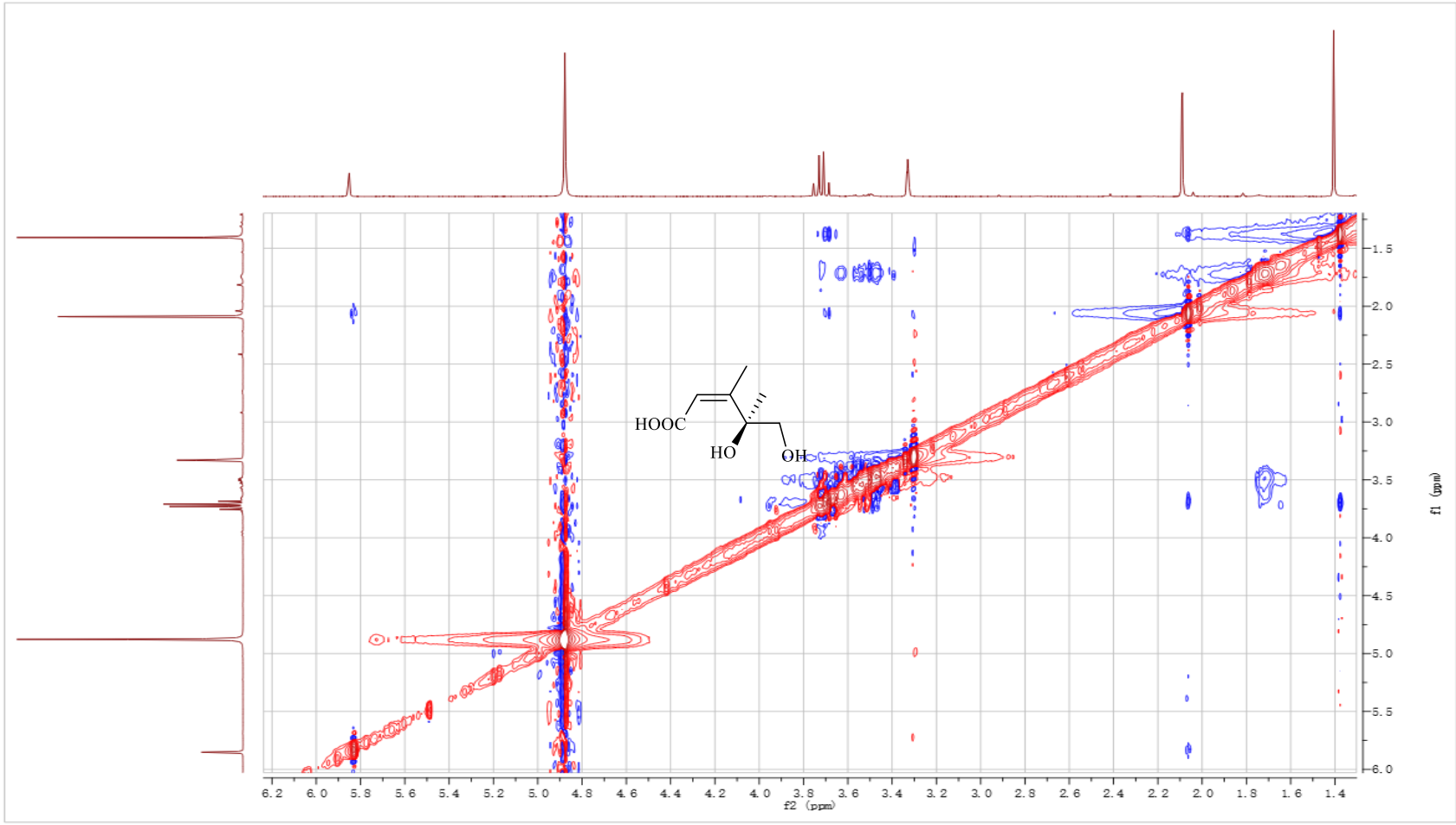


Figure S22: The NOESY spectrum of **2** (in CD_3OD)

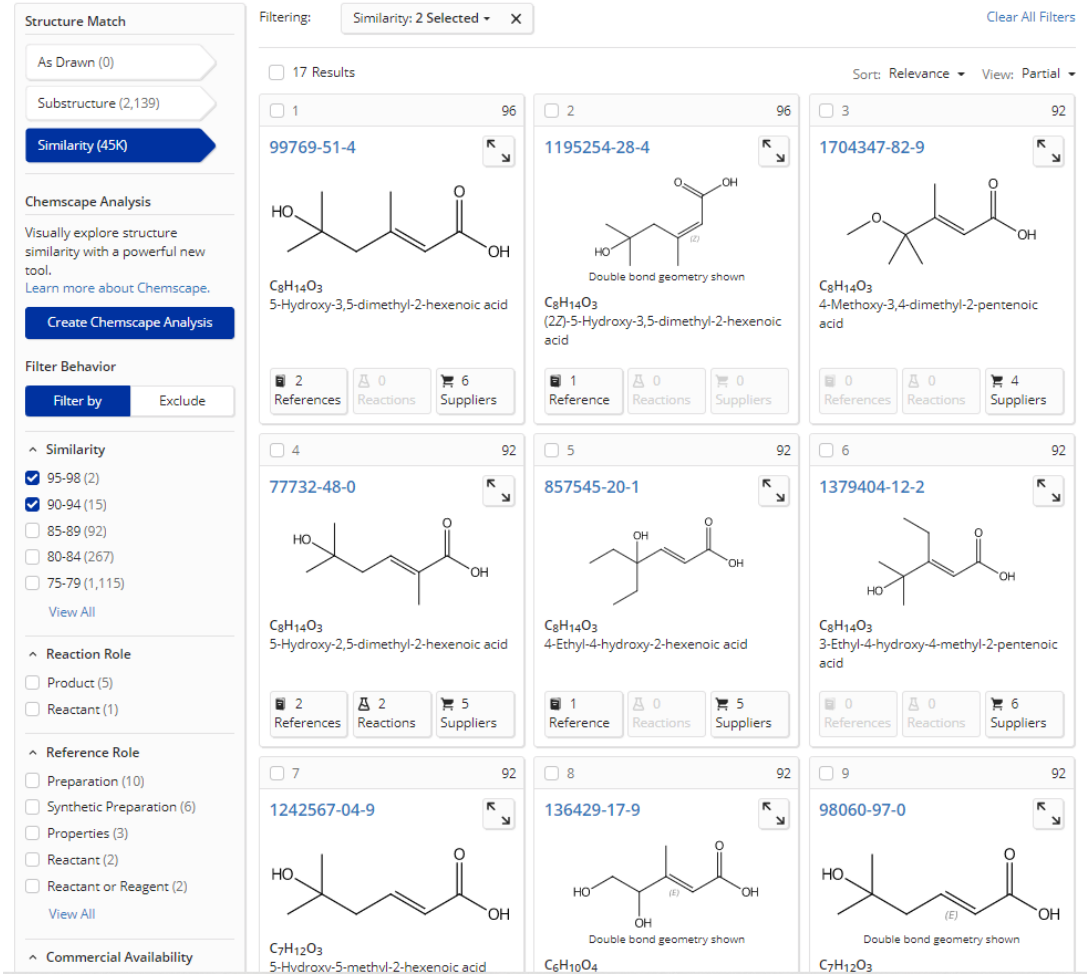
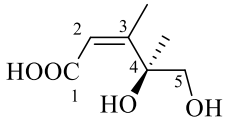
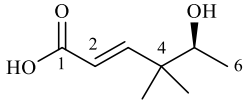


Figure S23: Search report of SciFinder of **2**

Table S2: Comparative ^{13}C NMR data of compound **2** with similar compound

Position		
	Compound 2 δ_C	**Similar compound δ_C**
1	173.6, C	170.5, C
2	116.7, CH	120.5, CH
3	172.0, C	157.3, CH
4	90.7, C	42.7, C
5	63.9, CH_2	74.8, CH
6	-	18.5, CH_3
CH_3-3	11.8, CH_3	-
CH_3-4	18.2, CH_3	22.9, CH_3 23.2, CH_3

*Stigmast-5,28(29)-dien-3β-ol (**3**):* Colorless crystal, ESI-MS *m/z* 417.4 ($[M+H]^+$). ^{1}H-NMR (400 MHz, $CDCl_3$) δ_H: 0.72 (3H, s, CH_3-18), 0.86 (6H, d, *J* = 6.6 Hz ,CH_3-26,27), 0.97 (3H, d, *J* = 8.0 Hz, CH_3-21), 1.02 (3H, s, CH_3-19), 3.39 (1H, m, H-3), 5.04 (1H, dd, *J* = 18.0 Hz, H-29), 5.18 (1H, tt, *J* = 11.7 Hz, H-29), 5.33 (1H, brd, *J* = 4.8 Hz, H-6), 5.75 (1H, dd, *J* = 11.7,18.0 Hz, H-28); In addition, there are 26 alkane hydrogen signals δ_H 1.2 ~ 2.3; ^{13}C-NMR (100 MHz, CD_3OD) δ_C: 37.7 (C-1), 32,3 (C-2), 72.5 (C-3), 43.1 (C-4), 142.3 (C-5), 122.5 (C-6), 33.3 (C-7), 30.1 (C-8), 51.8 (C-9), 37.4 (C- 10), 22.2 (C-11), 41.3 (C-12), 43.5 (C-13), 58.2 (C-14), 25.4 (C-15), 29.3 (C-16), 56.7 (C-17), 12.3 (C-18), 19.4 (C-19), 38.6 (C-20), 18.1 (C-21), 33.1 (C-22), 29.7 (C-23), 57.4 (C-24), 29.9 (C-25), 17.2 (C-26), 19.9 (C-27), 116.1 (C-28), 139.2 (C-29).

*β-sitosterol (**4**):* $C_{29}H_{50}O$, colorless crystal, ESI-MS *m/z* 415.4 ($[M+H]^+$). ^{1}H-NMR (400 MHz, $CDCl_3$) δ_H: 5.41 (1H, d, *J* = 5.3Hz, H-6), 3.58 (1H, m, H-3), 1.08 (3H, s, CH_3-19), 0.95 (3H, s, CH_3-18), 0.86 (3H, d *J* = 7.3Hz, CH_3-21), 0.84 (3H, d, *J* = 7.5Hz, CH_3-29), 0.79 (3H, s, CH_3-26), 0.73 (3H, s, CH_3-27); ^{13}C-NMR (100 MHz, $CDCl_3$) δ_C:37.5 (C-1), 31.7 (C-2), 72.3 (C-3), 42.6 (C-4), 141.3 (C-5), 121.3 (C-6), 31.5 (C-7), 31.6 (C-8), 50.5 (C-9), 36.8 (C-10), 22.5 (C-11), 39.3 (C-12), 42.7 (C-13), 56.7 (C-14), 23.9 (C-15), 27.8 (C-16), 56.5 (C-17), 12.4 (C-18), 19.1 (C-19), 36.3 (C-20), 19.2 (C-21), 33.7 (C-22), 26.4 (C-23), 45.5 (C-24), 29.1 (C-25), 19.9 (C-26), 19.3 (C-27), 23.3 (C-28), 12.1 (C-29).

*Carotene (**5**):* $C_{35}H_{60}O_6$, white powder, ESI-MS *m/z* 577.4 ($[M+H]^+$). ^{1}H-NMR (400 MHz, $CDCl_3$) δ_H: 5.32 (1H, br s, H-6), 5.12 (1H, d, *J* = 7.8 Hz, H-1'), 4.45 (1H, d, *J* = 11.4 Hz, H-6'), 4. 33 (1H, dd, *J* = 4.8, 11.4 Hz, H-6'), 4.29 (2H, m, H-3', 4'), 4.11 (1H, t, *J* = 7.8 Hz, H-2'), 4.08 (2H, m, H-3, 5'), 1.02 (3H, d, *J* = 6.0 Hz, H-21), 0.89 (3H, s, H-19), 0.81~0.93 (8H, m, H-9, 14, 26, 27), 0. 65 (3H, s, H-18); ^{13}C-NMR (100 MHz, CD_3OD) δ_C:37.2 (C-1), 28.4 (C-2), 79.2 (C-3), 39.8 (C-4), 140.3 (C-5), 121.7 (C-6), 32.6 (C-7), 32.9 (C-8), 51.1 (C-9), 37.0 (C-10), 21.2 (C-11), 40.2 (C-12), 42.4 (C-13), 56.8 (C-14), 25.1 (C-15), 30.4 (C-16), 56.9 (C-17), 12.3 (C-18), 20.0 (C-19), 37.2 (C-20), 19.7 (C-21), 34.1 (C-22), 27.3 (C-23), 46.9 (C-24), 30.2 (C-25), 19.9 (C-26), 19.1 (C-27), 24.4 (C-28), 12.8 (C-29), 102.3 (C-1'), 75.2 (C-2'), 79.3 (C-3'), 72.5 (C-4'), 78.2 (C-5'), 63. 4 (C-6').

*Fraxetin (**6**):* $C_{10}H_8O_5$, light brown powder, ESI-MS *m/z* 209.0 ($[M+H]^+$). ^{1}H-NMR (400 MHz, $CDCl_3$) δ_H: 3.89 (3H, s, -OCH_3), 6.19 (1H, d, *J* = 9.5 Hz, H-3), 6.68 (1H, s, H-5), 7.81 (1H, d, *J* = 9.5 Hz, H-4); ^{13}C-NMR (100 MHz, CD_3OD) δ_C: 162.3 (C-2), 111.2 (C-3), 145.3 (C-4), 99.6 (C-5), 145.7 (C-6), 139.3 (C-7), 132.6 (C-8), 139.2 (C-9), 110.7 (C-10),55.4 (-OCH_3).

*p-coumaric acid (**7**):* $C_9H_8O_3$, white powder, ESI-MS *m/z* 165.0552 ($[M+H]^+$). ^{1}H-NMR (400 MHz, $CDCl_3$) δ_H: 6.20 (1H, d, *J* = 15.8 Hz, H-8), 6.73 (2H, d, *J* = 8.7 Hz, H-2, 6), 7.54 (2H, d, *J* = 8.7 Hz, H-3, 5), 7.58 (1H, d, *J* = 15.8 Hz, H-7); ^{13}C-NMR (100 MHz, CD_3OD) δ_C: 159.8 (C-1), 115.4 (C-2), 132.1 (C-3), 126.3 (C-4), 132.1 (C-5), 115.4 (C-6), 145.3 (C-7), 114.2 (C-8), 169.6 (C-9).

*cis-p-hydroxycinnamic acid (**8**):* $C_9H_8O_3$, white powder, ESI-MS *m/z* 165.1 ($[M+H]^+$). ^{1}H-NMR (400 MHz, $CDCl_3$) δ_H: 5.74 (1H, d, *J* = 12.9 Hz, H-8), 6.71 (2H, d, *J* = 8.7 Hz, H-2, 6), 6.77 (1H, d, *J* = 12.9 Hz, H-7), 7.35 (2H, d, *J* = 8.7 Hz, H-3, 5); ^{13}C-NMR (100 MHz, CD_3OD) δ_C: 158.5 (C-1), 114.4 (C-2), 129.7 (C-3), 125.8 (C-4), 129.7 (C-5), 114.4 (C-6), 142.7 (C-7), 115.9 (C-8), 168.9 (C-9).

*Ferulic acid (**9**):* $C_{10}H_{10}O_4$, white powder, ESI-MS *m/z* 195.1 ($[M+H]^+$). ^{1}H-NMR (400 MHz, $CDCl_3$) δ_H: 3.89 (3H, s, -OCH_3), 7.60 (1H, d, *J* = 15.0 Hz, H-7), 7.18 (1H, d, *J* = 2.0 Hz, H-2), 7.06 (1H, dd, *J* = 8.0, 2.0 Hz, H-6), 6.81 (1H, d, *J* = 8.0 Hz, H-5), 6.31 (1H, d, *J* = 15 Hz, H-8); ^{13}C-NMR (100 MHz, CD_3OD) δ_C: 126.4 (C-1), 110.3 (C-2), 149.7 (C-3), 149.1 (C-4), 114.5 (C-5), 122.6 (C-6), 145.5 (C-7), 115.1 (C-8), 169.9 (C-9), 55.0 (-OCH_3).