

Supporting Information

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Chemical Constituents from the Whole Plant of *Pachysandra terminalis*

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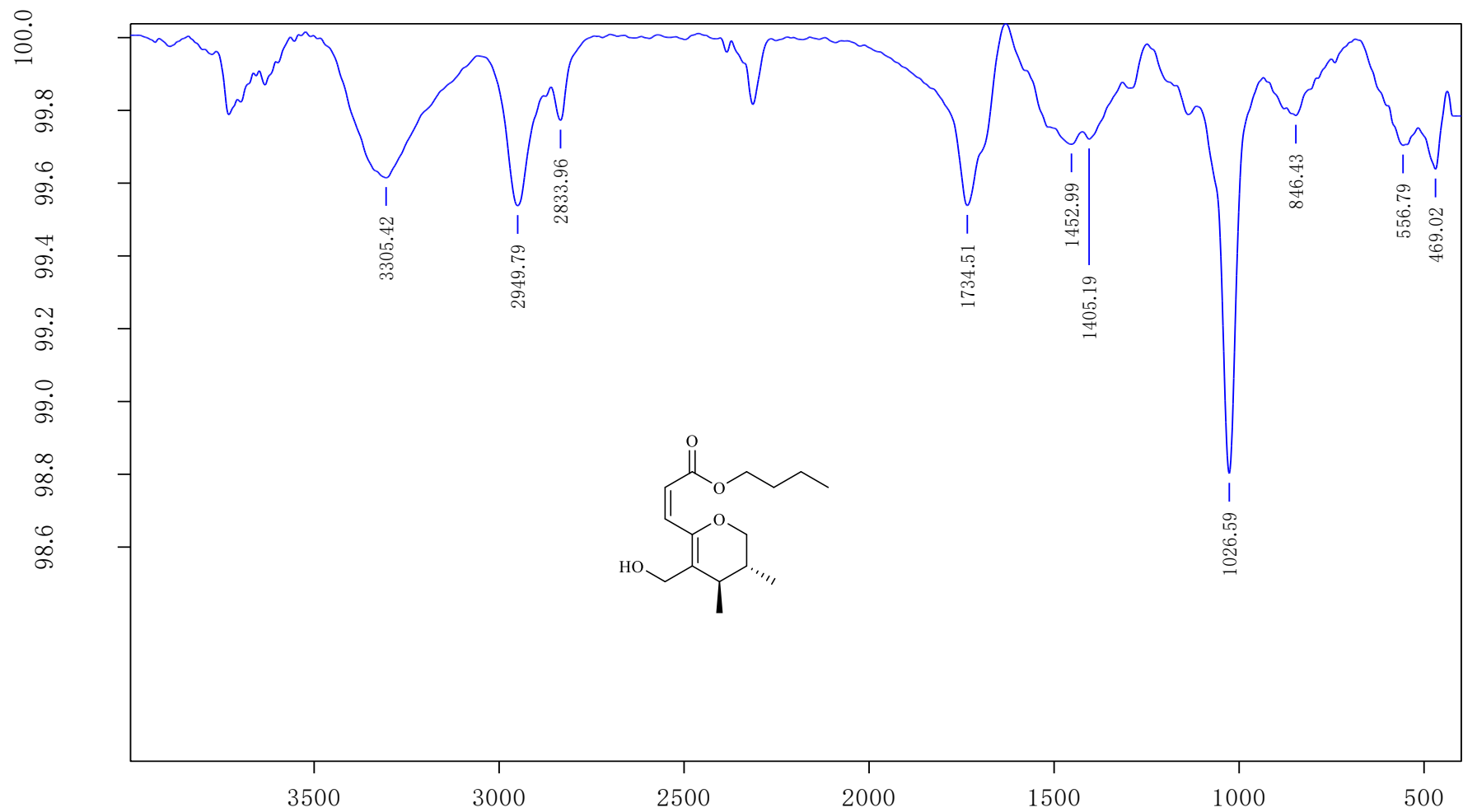
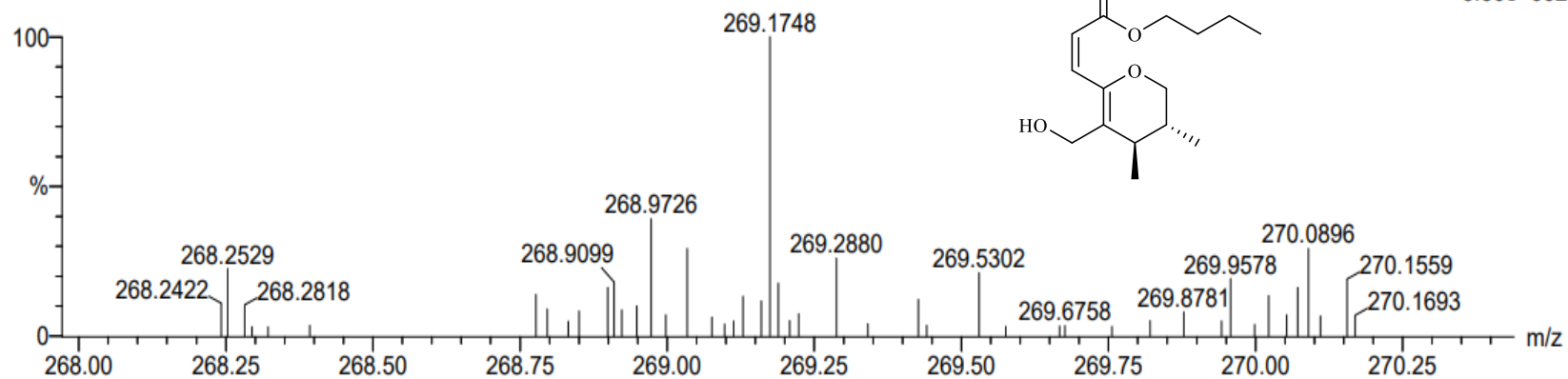


Figure S1: The IR spectrum of **1** (in KBr)

0503-6-PT37- 50 (0.295)

1: TOF MS ES+
6.50e+002



Minimum: -1.5
Maximum: 5.0 10.0 50.0

Mass	Calc. Mass	mDa	PPM	DBE	i-FIT	Norm	Conf (%)	Formula
269.1748	269.1753	-0.5	-1.9	3.5	202.6	n/a	n/a	C ₁₅ H ₂₅ O ₄

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

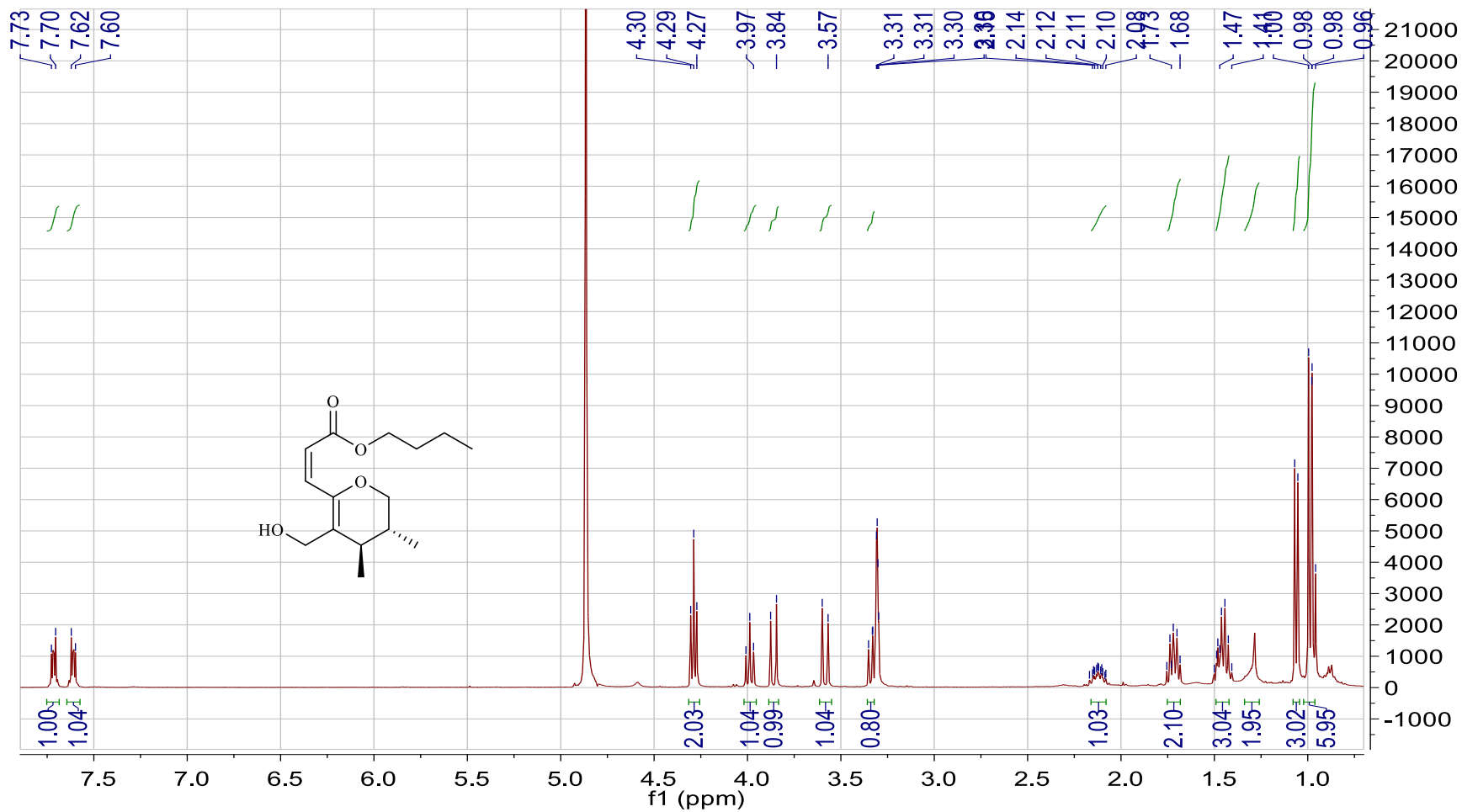


Figure S3: The ^1H NMR spectrum of **1** (in CD_3OD)

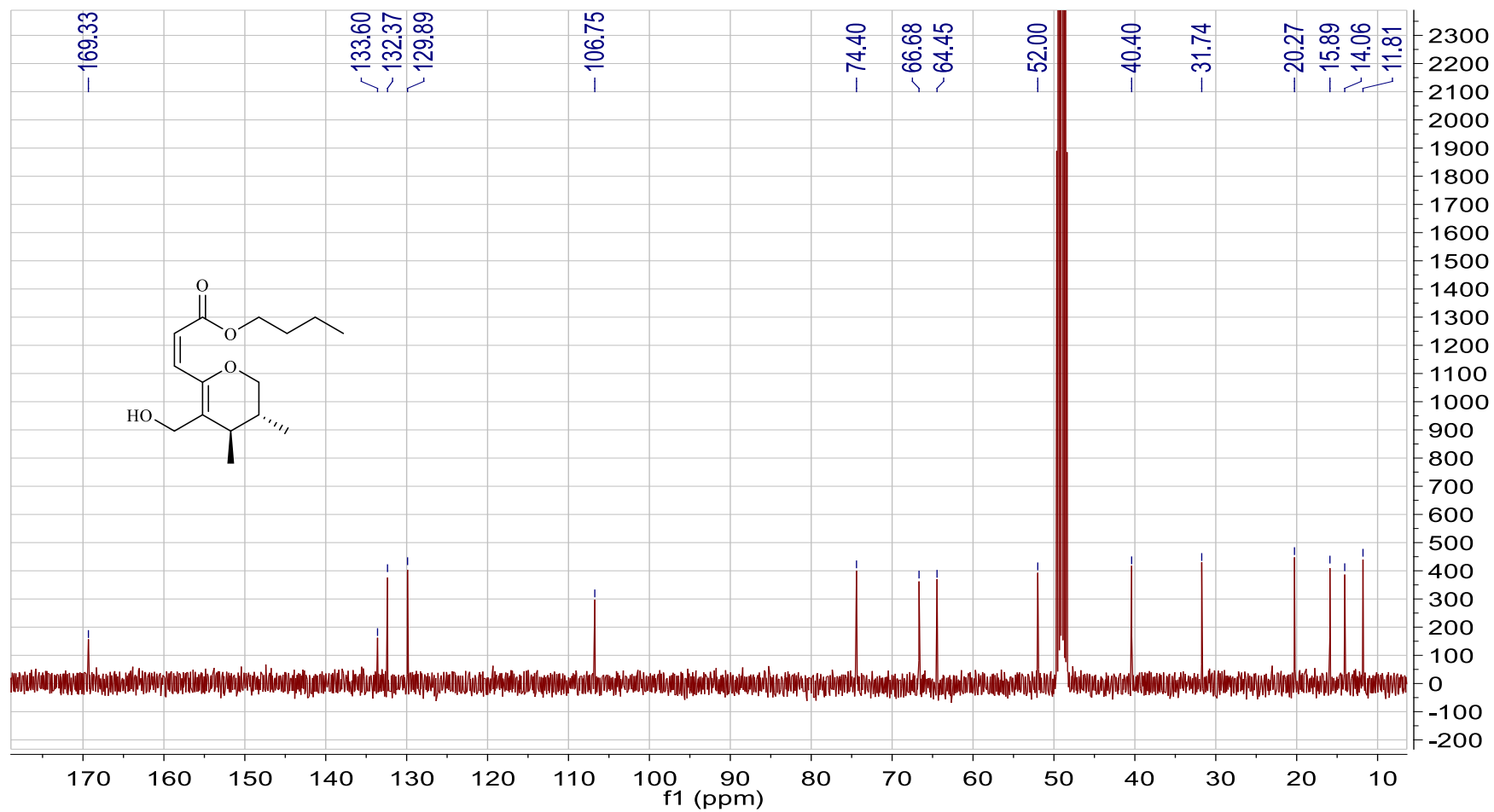


Figure S4: The ^{13}C NMR spectrum of **1** (in CD_3OD)

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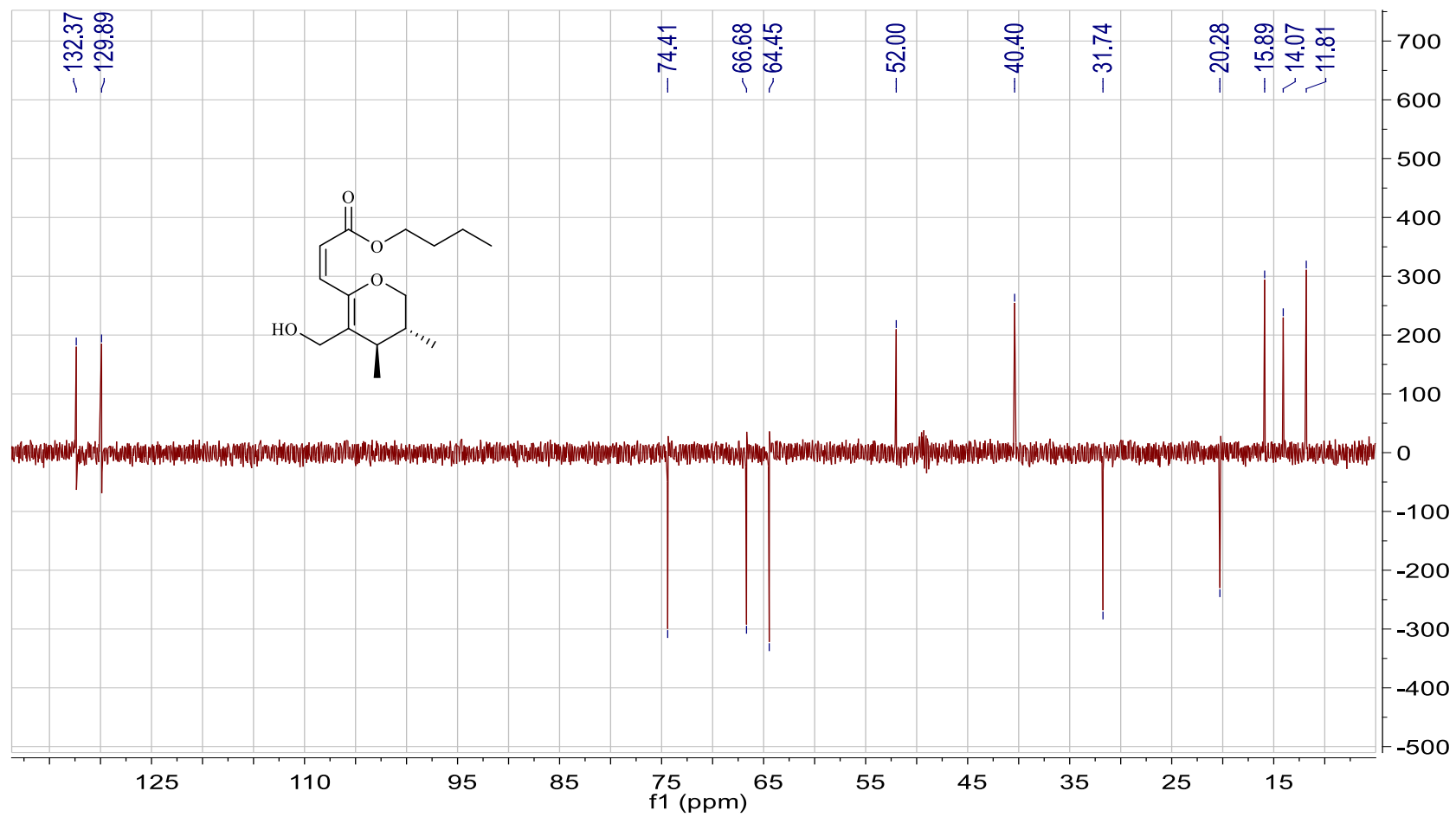


Figure S5: The DEPT spectrum of **1** (in CD₃OD)

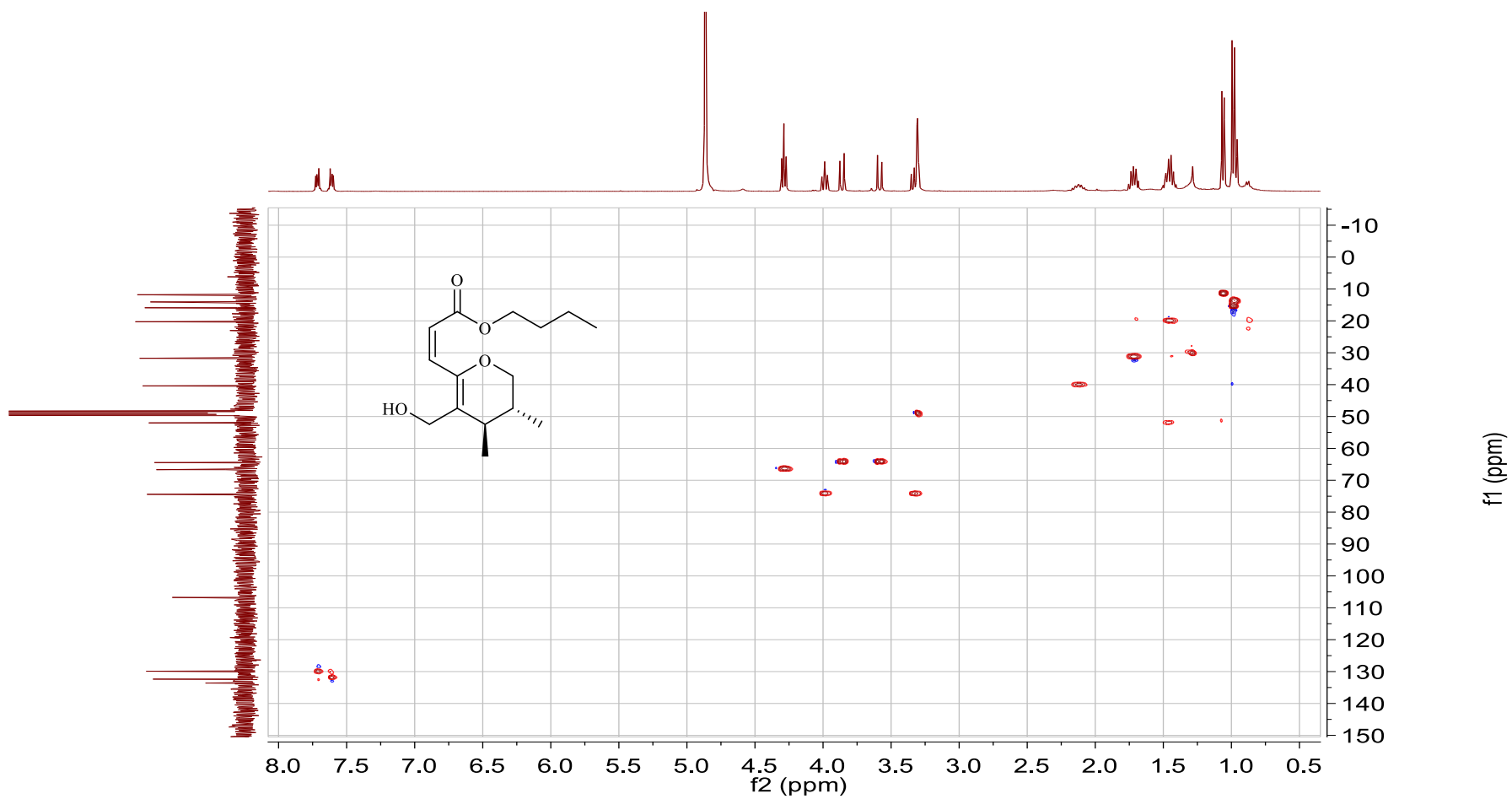


Figure S6: The HSQC spectrum of **1** (in CD₃OD)

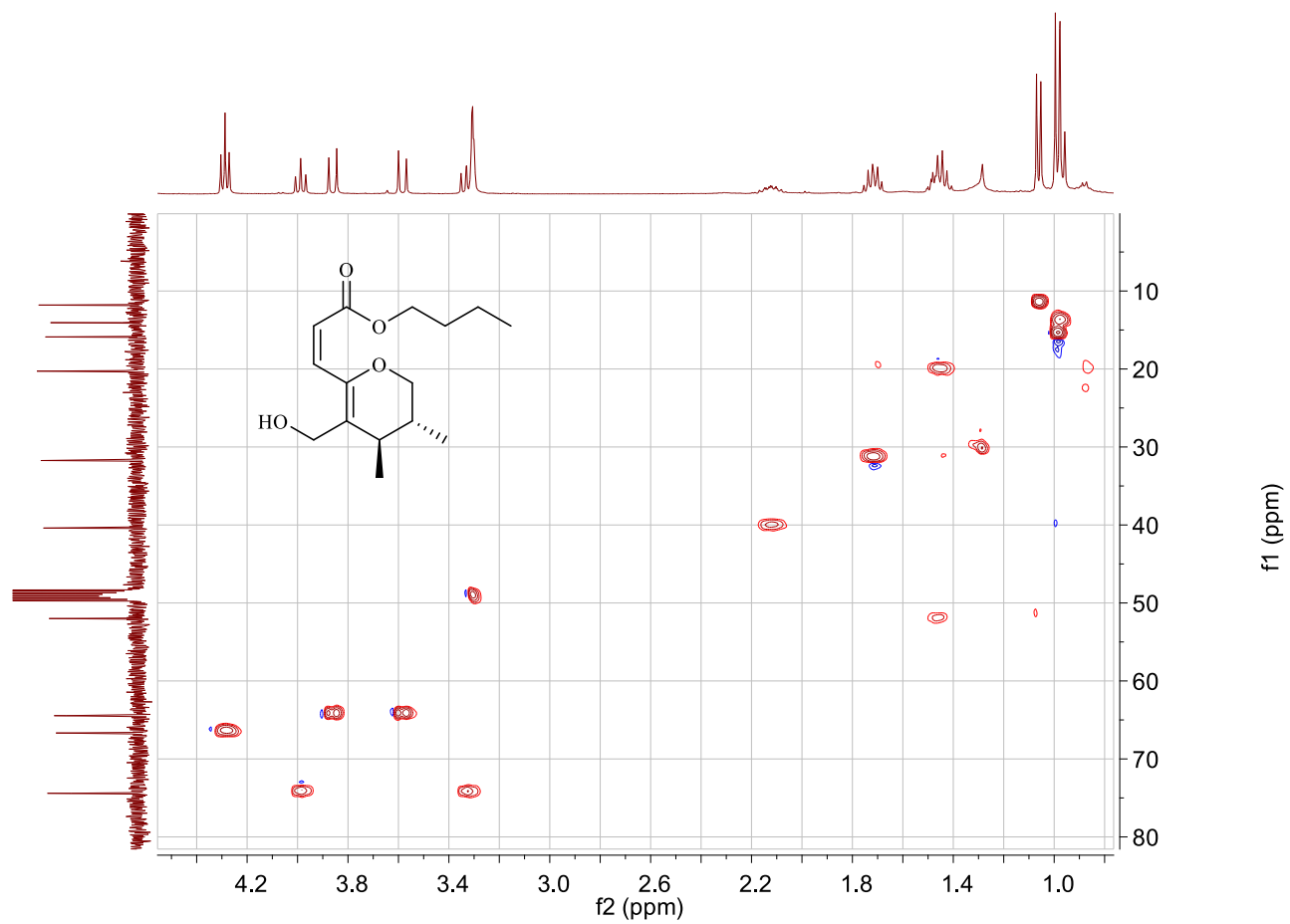


Figure S7: The HSQC spectrum of **1** (in CD_3OD) (From δc 0 ppm to δc 80 ppm)

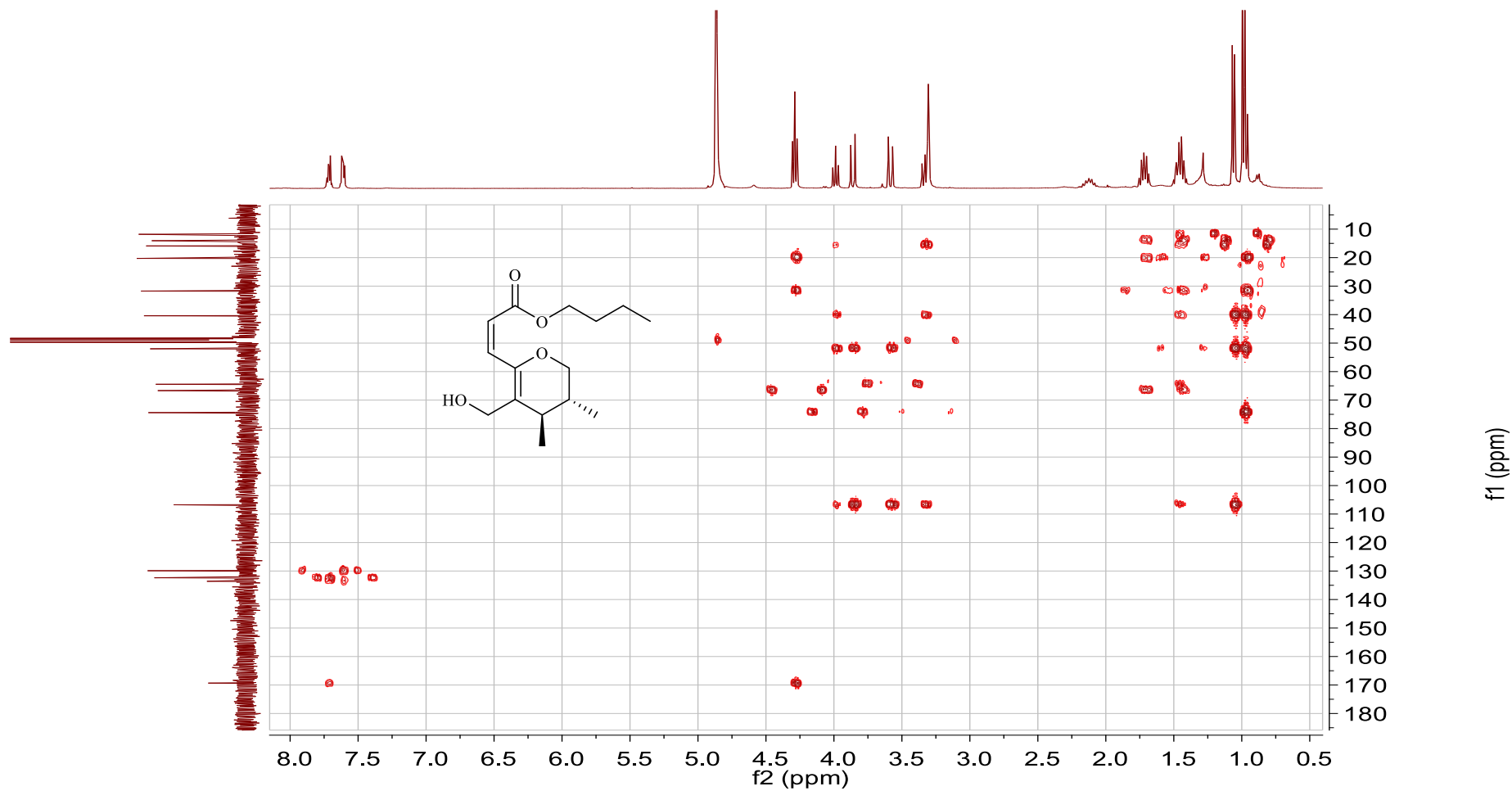


Figure S8: The HMBC spectrum of **1** (in CD_3OD)

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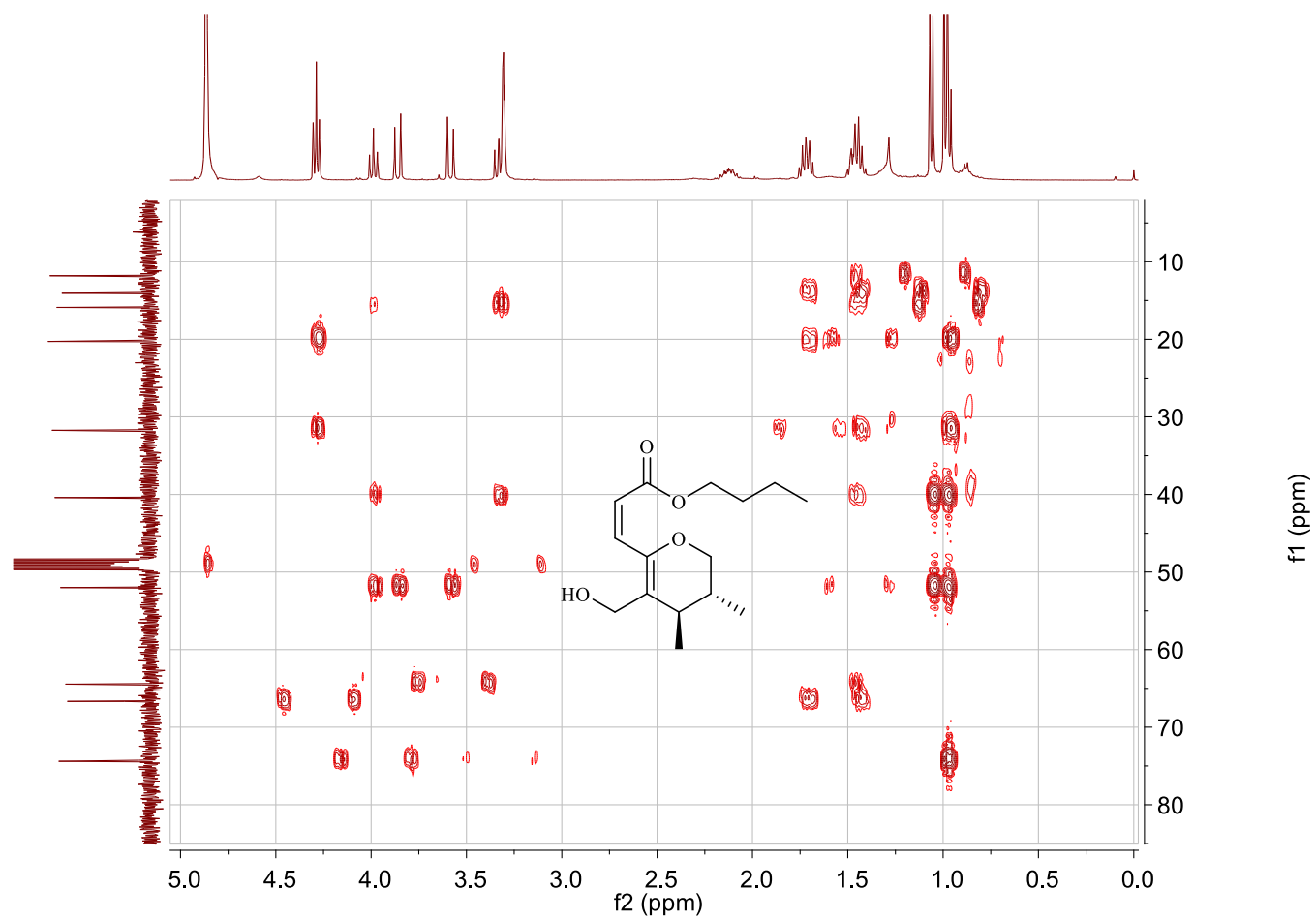


Figure S9: The HMBC spectrum of **1** (in CD₃OD) (From δ c 10 ppm to δ c 85 ppm)

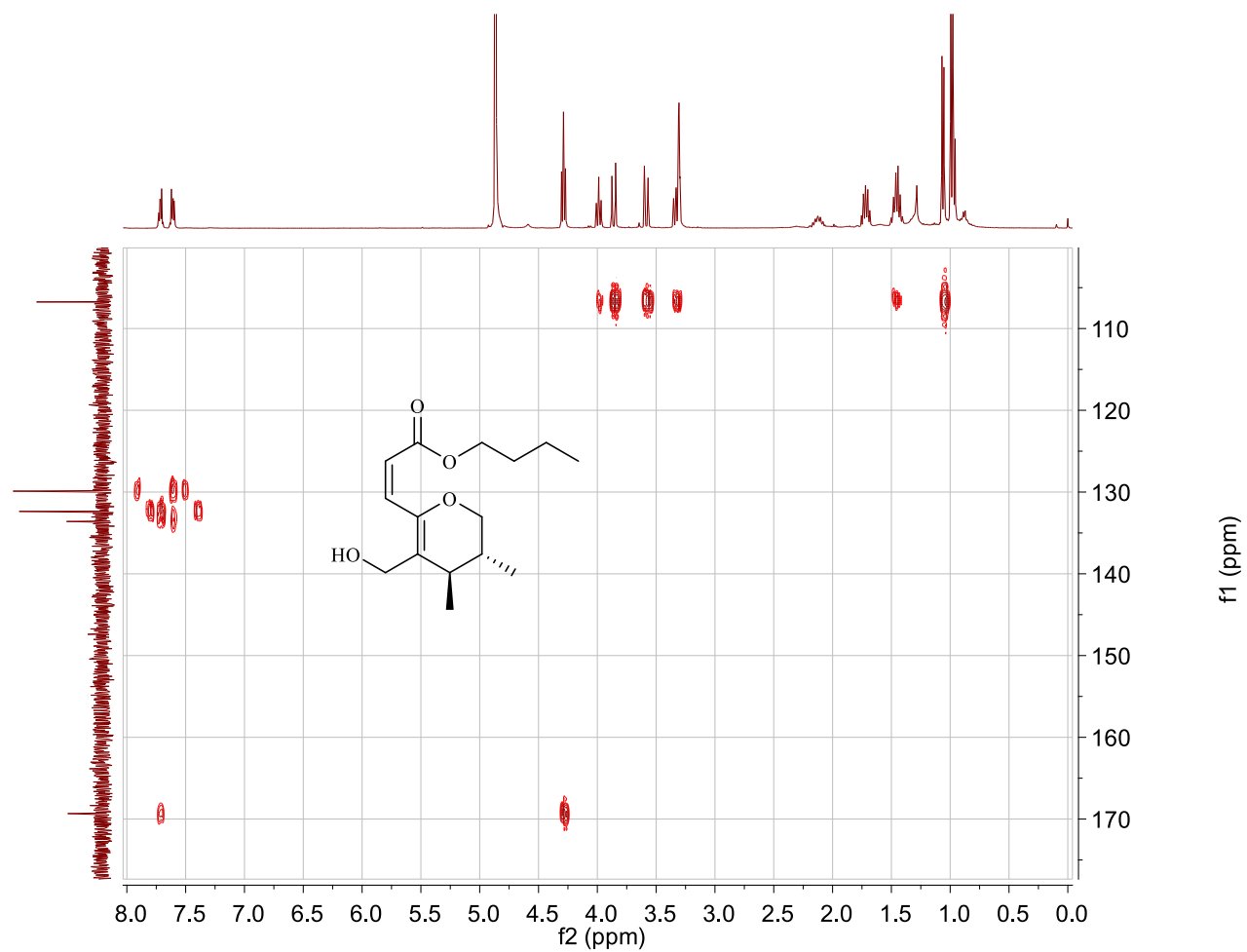


Figure S10: The HMBC spectrum of **1** (in CD₃OD) (From δ c 100 ppm to δ c 180 ppm)

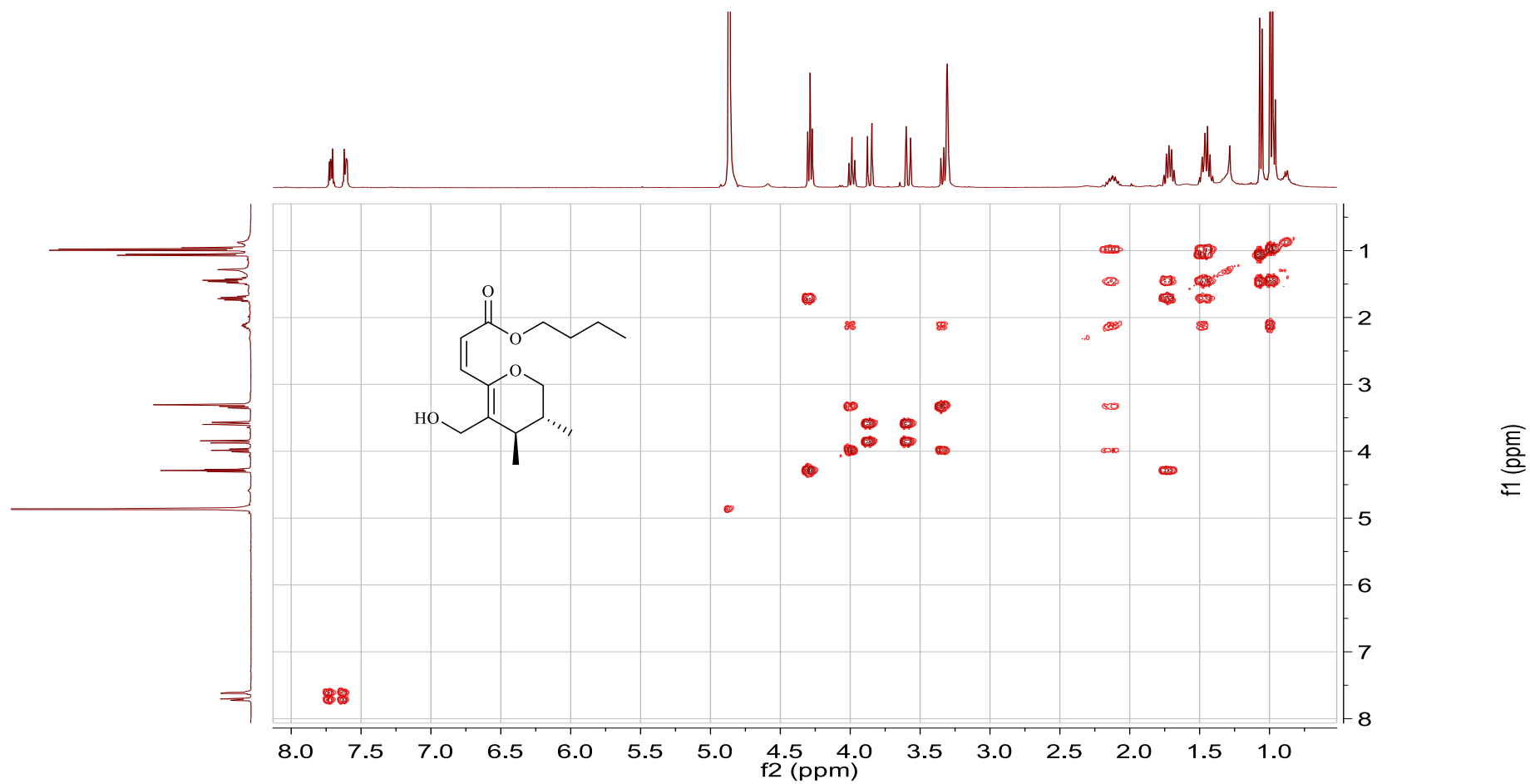


Figure S11: The ^1H - ^1H COSY spectrum of **1** (in CD_3OD)

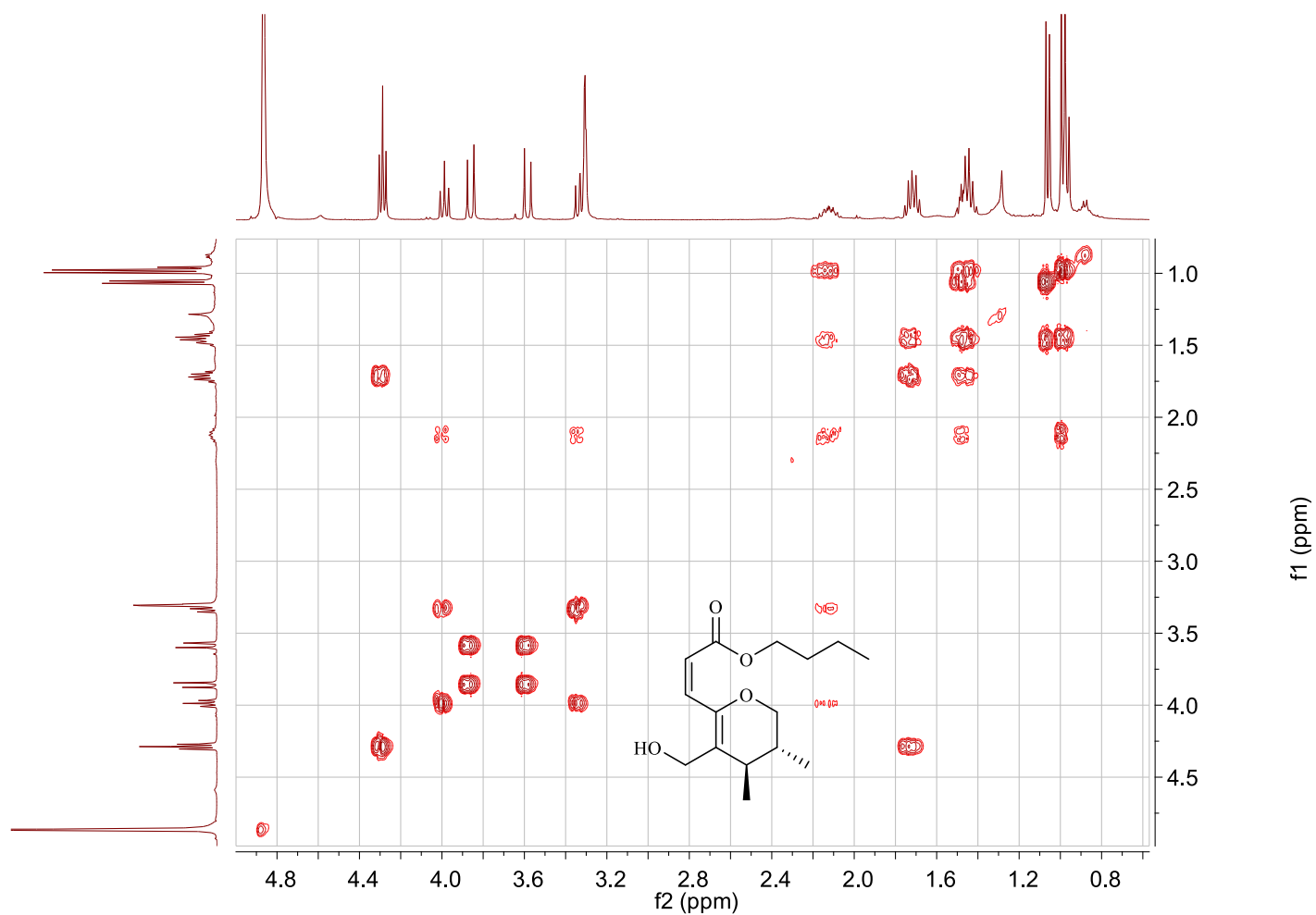


Figure S12. The ¹H-¹H COSY spectrum of **1** (in CD₃OD) (From δ_{H} 0.5 ppm to δ_{H} 5.0 ppm)

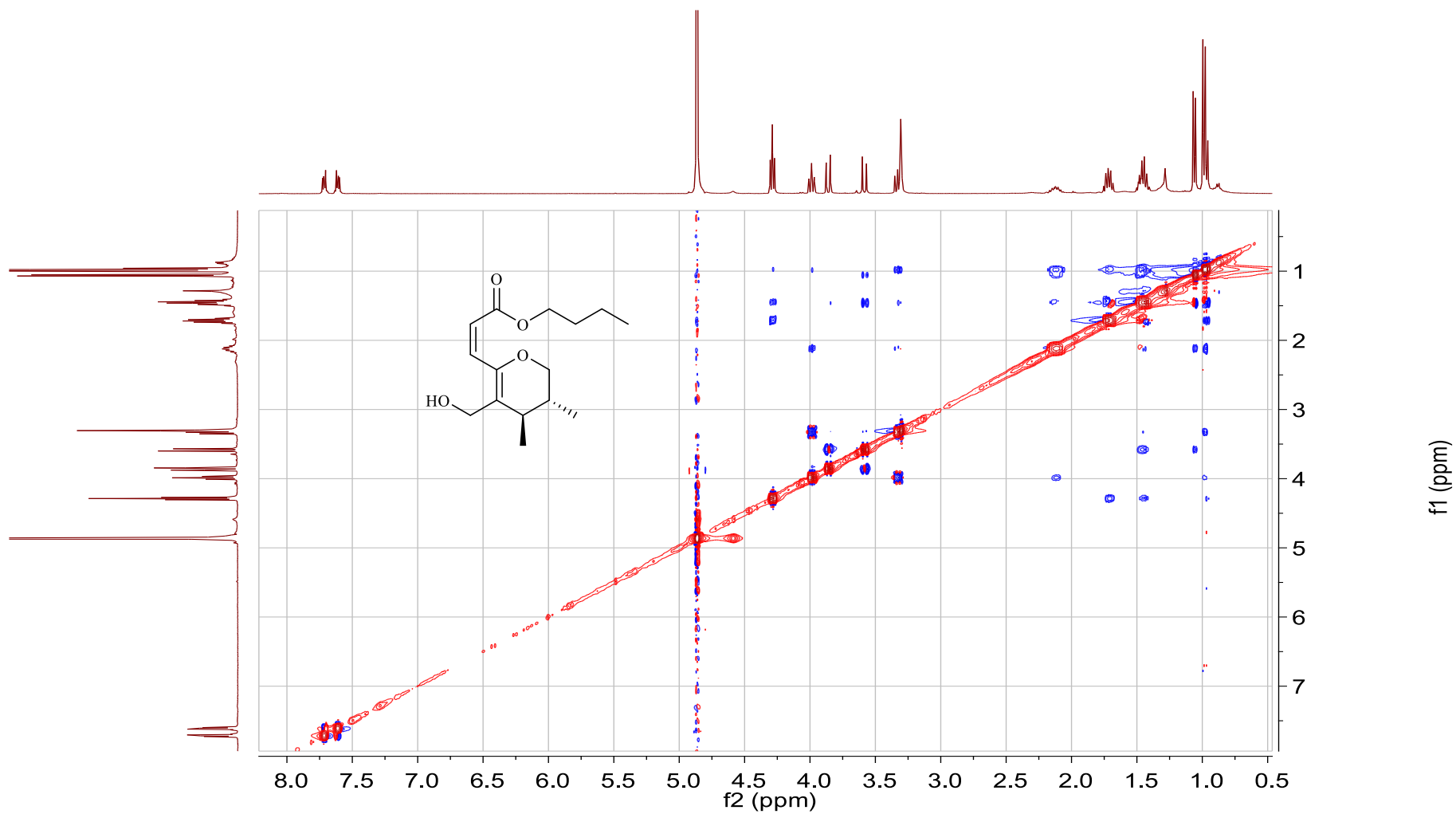


Figure S13: The NOESY spectrum of **1** (in CD₃OD)

Structure Match

As Drawn (0)

Substructure (0)

Similarity (26K)

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Similarity

85-89 (4)

80-84 (12)

75-79 (131)

70-74 (976)

65-69 (4,950)

60-64 (19K)

Reaction Role

Product (4)

Reactant (2)

Reference Role

Preparation (4)

Synthetic Preparation (4)

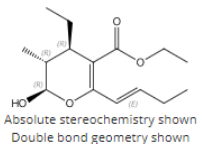
Filtering: Similarity: 85-89 X Number of Components: 1 X [Clear All Filters](#)

4 Results

Sort: Relevance View: Partial

1 86

2047814-51-5



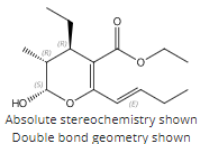
Absolute stereochemistry shown
Double bond geometry shown

C₁₅H₂₄O₄
Ethyl (2R,3R,4R)-6-(1E)-1-buten-1-yl-4-ethyl-3,4-dihydro-2-hydroxy-3-methyl-2H-pyran-2-ylideneacetate

1 Reference 2 Reactions 0 Suppliers

2 86

2047814-49-1



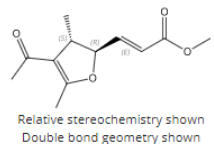
Absolute stereochemistry shown
Double bond geometry shown

C₁₅H₂₄O₄
Ethyl (2S,3R,4R)-6-(1E)-1-buten-1-yl-4-ethyl-3,4-dihydro-2-hydroxy-3-methyl-2H-pyran-2-ylideneacetate

1 Reference 2 Reactions 0 Suppliers

3 85

80486-00-6



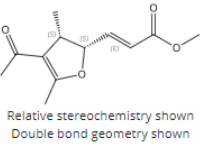
Relative stereochemistry shown
Double bond geometry shown

C₁₂H₁₆O₄
rel-Methyl (2E)-3-[(2R,3S)-4-acetyl-2,3-dihydro-3,5-dimethyl-2-furanyl]-2-propenoate

3 References 3 Reactions 0 Suppliers

4 85

80485-99-0



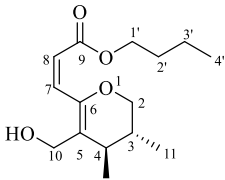
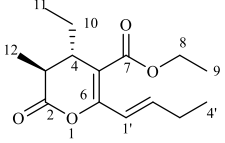
Relative stereochemistry shown
Double bond geometry shown

C₁₂H₁₆O₄
rel-Methyl (2E)-3-[(2R,3R)-4-acetyl-2,3-dihydro-3,5-dimethyl-2-furanyl]-2-propenoate

3 References 3 Reactions 0 Suppliers

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

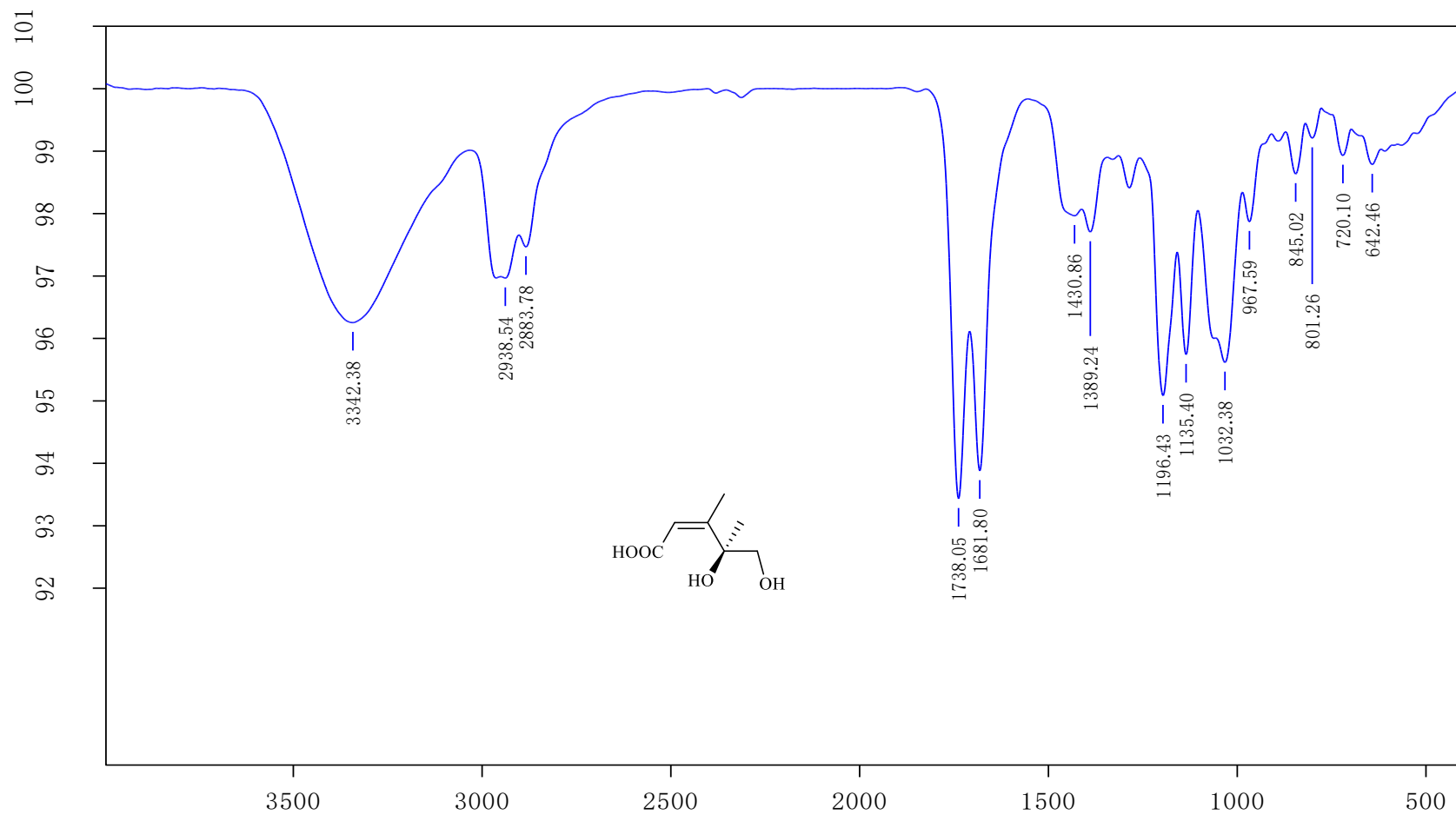
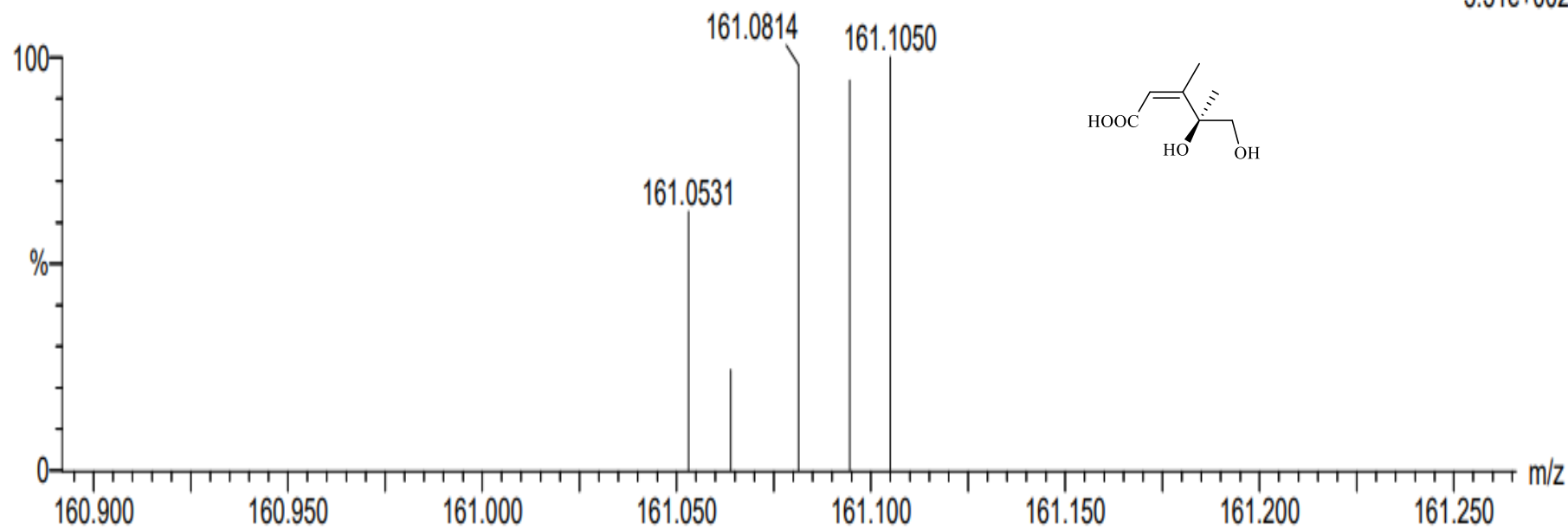


Figure S15: The IR spectrum of 2 (in KBr)

0503-6-D17- 25 (0.156)

1: TOF MS ES+
5.31e+002



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 O4

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

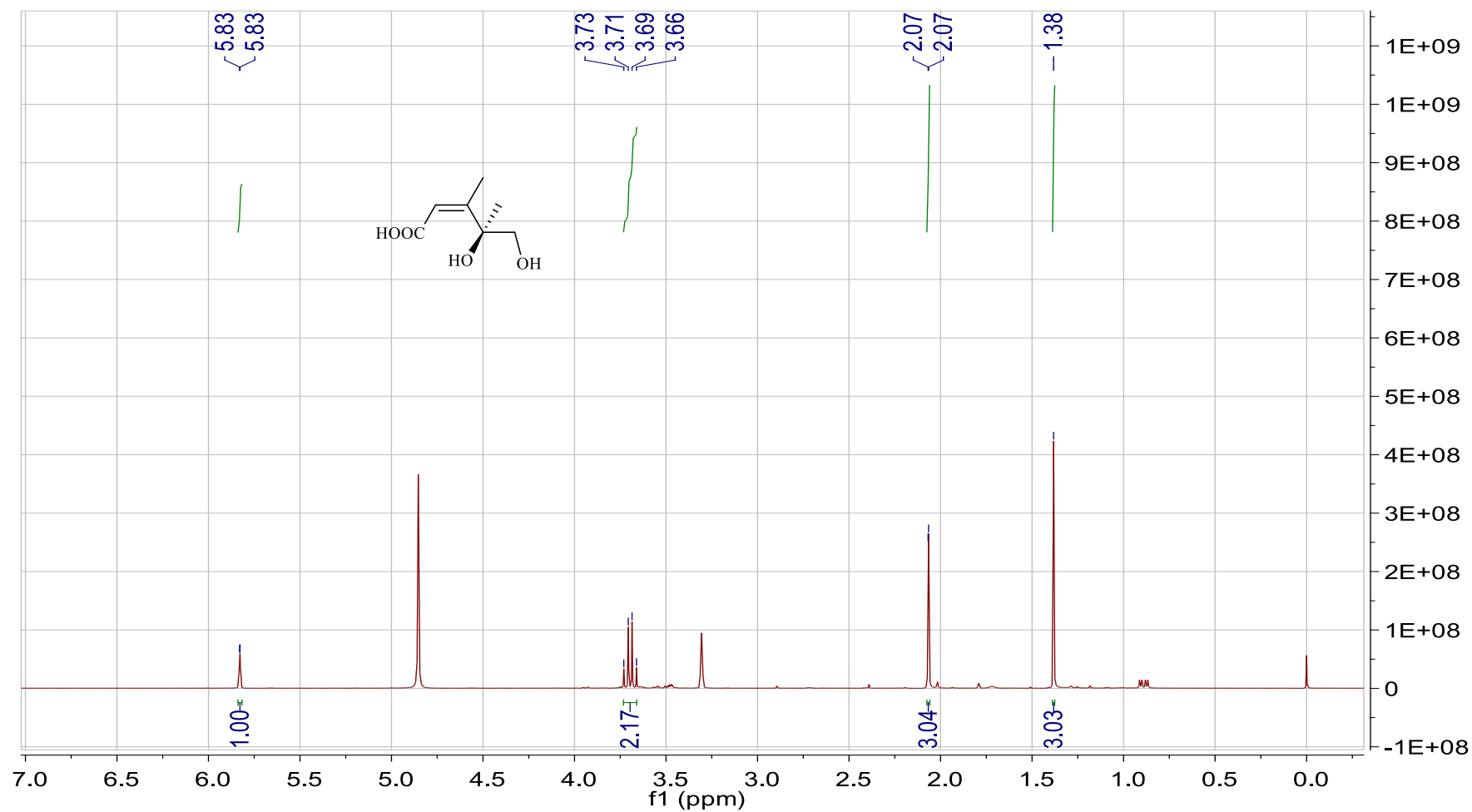


Figure S17: The ^1H NMR spectrum of **2** (in CD_3OD)

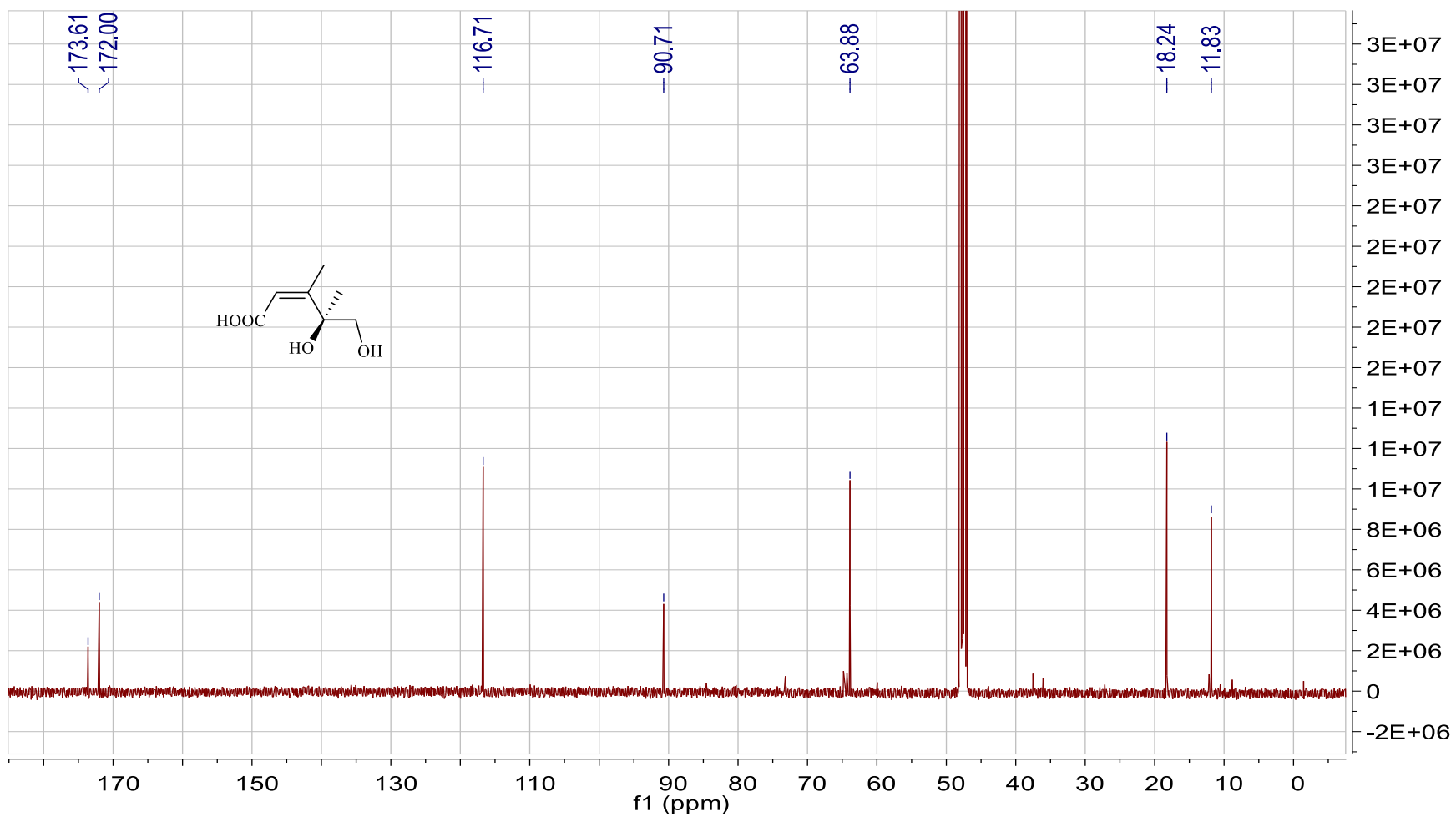


Figure S18: The ^{13}C NMR spectrum of **2** (in CD_3OD)

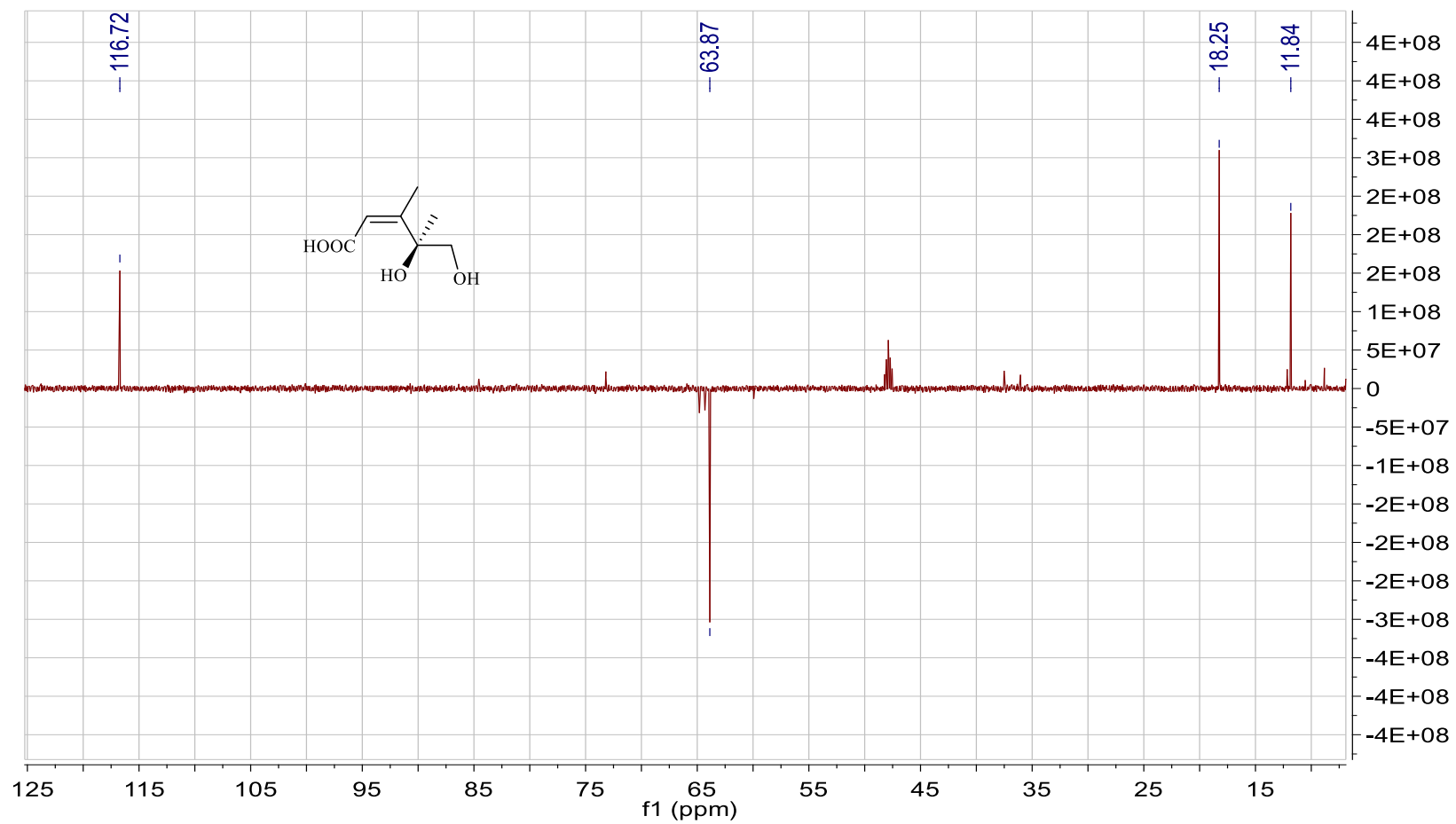


Figure S19: The DEPT 135 spectrum of **2** (in CD₃OD)

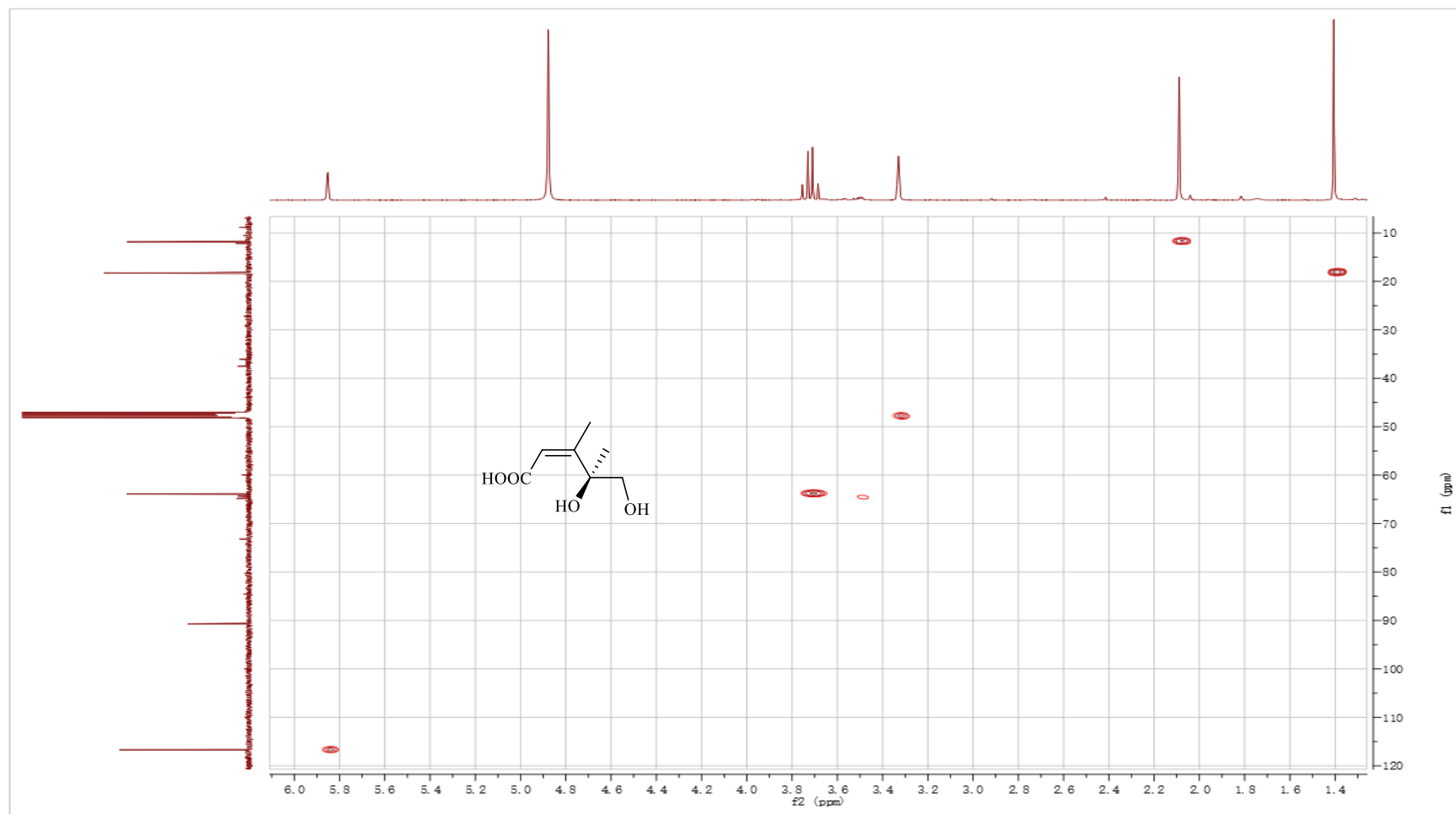


Figure S20: The HSQC spectrum of **2** (in CD_3OD)

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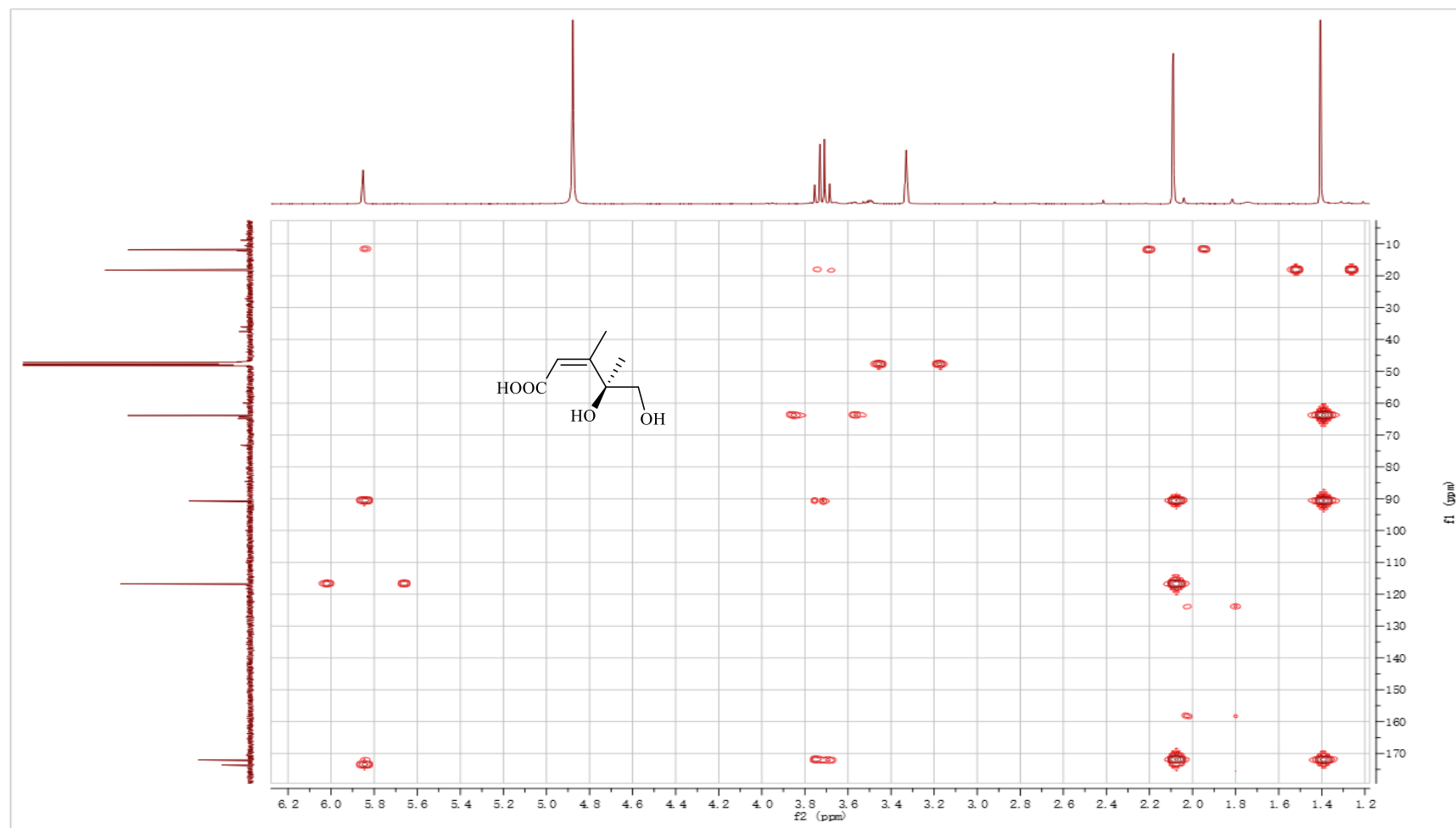


Figure S21: The HMBC spectrum of **2** (in CD₃OD)

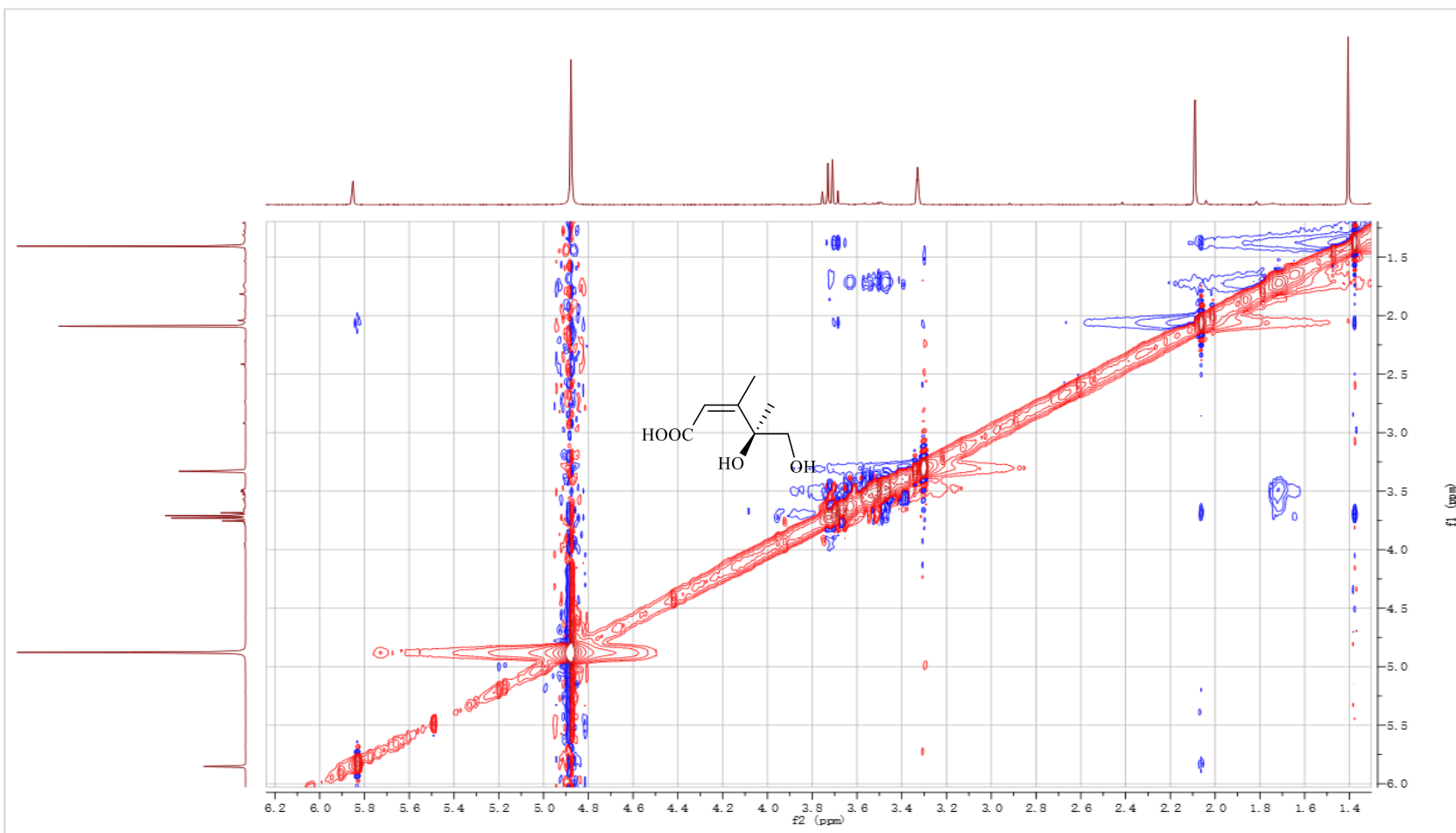


Figure S22: The NOESY spectrum of **2** (in CD₃OD)

Structure Match

As Drawn (0)

Substructure (2,139)

Similarity (45K)

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Filter by Exclude

Similarity

95-98 (2)

90-94 (15)

85-89 (92)

80-84 (267)

75-79 (1,115)

View All

Reaction Role

Product (5)

Reactant (1)

Reference Role

Preparation (10)

Synthetic Preparation (6)

Properties (3)

Reactant (2)

Reactant or Reagent (2)

View All

Commercial Availability

Filtering: Similarity: 2 Selected X

Clear All Filters

17 Results

Sort: Relevance View: Partial

1 96

99769-51-4

CC(C)C(C)C=C(O)C(=O)O

$C_8H_{14}O_3$
5-Hydroxy-3,5-dimethyl-2-hexenoic acid

2 References 0 Reactions 6 Suppliers

2 96

1195254-28-4

CC(C)C(C)C=C(O)C(=O)O

Double bond geometry shown

$C_8H_{14}O_3$
(2Z)-5-Hydroxy-3,5-dimethyl-2-hexenoic acid

1 Reference 0 Reactions 0 Suppliers

3 92

1704347-82-9

CC(C)C(C)C=C(O)C(=O)O

$C_8H_{14}O_3$
4-Methoxy-3,4-dimethyl-2-pentenoic acid

0 References 0 Reactions 4 Suppliers

4 92

77732-48-0

CC(C)C(C)C=C(O)C(=O)O

$C_8H_{14}O_3$
5-Hydroxy-2,5-dimethyl-2-hexenoic acid

2 References 2 Reactions 5 Suppliers

5 92

857545-20-1

CC(C)C(C)C=C(O)C(=O)O

$C_8H_{14}O_3$
4-Ethyl-4-hydroxy-2-hexenoic acid

1 Reference 0 Reactions 5 Suppliers

6 92

1379404-12-2

CC(C)C(C)C=C(O)C(=O)O

$C_8H_{14}O_3$
3-Ethyl-4-hydroxy-4-methyl-2-pentenoic acid

0 References 0 Reactions 6 Suppliers

7 92

1242567-04-9

CC(C)C(C)C=C(O)C(=O)O

$C_7H_{12}O_3$
5-Hydroxy-5-methyl-2-hexenoic acid

8 92

136429-17-9

CC(C)C(C)C=C(O)C(=O)O

Double bond geometry shown

$C_6H_{10}O_4$

9 92

98060-97-0

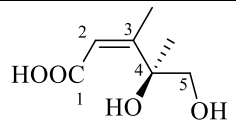
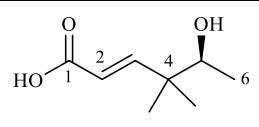
CC(C)C(C)C=C(O)C(=O)O

Double bond geometry shown

$C_7H_{12}O_3$

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-3 β -ol (3): Colorless crystal, ESI-MS m/z 417.4 ($[M+H]^+$). 1H -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 ($[M+H]^+$). 1H -NMR (400 MHz, $CDCl_3$) δ_H : 5.41 (1H, d, $J = 5.3$ Hz, 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, $J = 7.3$ Hz, CH_3 -21), 0.84 (3H, d, $J = 7.5$ Hz, 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 ($[M+H]^+$). 1H -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): C₁₀H₈O₅, light brown powder, ESI-MS *m/z* 209.0 ([M+H]⁺). ¹H-NMR (400 MHz, CDCl₃) δ_H: 3.89 (3H, s, -OCH₃), 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); ¹³C-NMR (100 MHz, CD₃OD) 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 (-OCH₃).

p-coumaric acid (7): C₉H₈O₃, white powder, ESI-MS *m/z* 165.0552 ([M+H]⁺). ¹H-NMR (400 MHz, CDCl₃) 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); ¹³C-NMR (100 MHz, CD₃OD) 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): C₉H₈O₃, white powder, ESI-MS *m/z* 165.1 ([M+H]⁺). ¹H-NMR (400 MHz, CDCl₃) 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); ¹³C-NMR (100 MHz, CD₃OD) 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): C₁₀H₁₀O₄, white powder, ESI-MS *m/z* 195.1 ([M+H]⁺). ¹H-NMR (400 MHz, CDCl₃) δ_H: 3.89 (3H, s, -OCH₃), 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); ¹³C-NMR (100 MHz, CD₃OD) 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 (-OCH₃).