

Supporting Information

Concise Total Syntheses of Two Flavans and Structure Revision Assisted by Quantum NMR Calculations

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1. Experimental Procedures

1.1 General experimental procedures

All air and moisture sensitive reactions were carried out under a nitrogen atmosphere with dry solvents under anhydrous conditions. All solvents were reagent grade, and used without further purification. Thin layer chromatography (TLC) analysis was performed on a 0.25 mm Qingdao silica gel plate (60 F-254) with ultraviolet irradiation (254 nm) and stained with vanillin. Silica gel (ZCX-II) (200-300 mesh) flash column chromatography using Qingdao Ocean Chemical Co., Ltd., China products. ^1H and ^{13}C NMR spectra were recorded on a Bruker Advance 500 MHz spectrometer. (^1H : 500 MHz, ^{13}C : 125 MHz). All NMR chemical shifts were referenced to residual solvent peaks as an internal standard and recorded in ppm.

1.1.1 Spectra recorded in different deuterium solvents:

CDCl_3 (^1H NMR: 7.28 ppm, ^{13}C NMR: 77.0 ppm);

CD_3OD (^1H NMR: 3.33 ppm, ^{13}C NMR: 47.6 ppm);

CD_3COCD_3 (^1H NMR: 2.05 ppm, ^{13}C NMR: 30.0, 206.3 ppm);

$\text{DMSO-}d_6$ (^1H NMR: 2.50 ppm, ^{13}C NMR: 39.5 ppm).

1.1.2 The following is an explanation of the abbreviations:

Multiplicity: s = singlet, d = doublet, t = triplet, q = quartet, m = multiplet. EA = ethyl acetate. ACN = acetonitrile. PTSA = *p*-toluenesulfonic acid. PPTS = pyridinium 4-toluenesulfonate. DMSO = dimethyl sulfoxide. DHP = 3,4-dihydro-2H-pyran. EDDA = ethylenediamine diacetate.

All coupling constants *J* are quoted in Hz. High resolution mass spectra (HRMS) were obtained on an IonSpec QFT mass spectrometer with ESI ionization. Heating mantle was used as the heat source, when reactions required heating.

1.1 X-ray crystallographic data of flavan 1

The single crystal X-ray diffraction data of flavan 1 was collected by the method of CuK α radiation using XtaLAB AFC12 (RINC): Kappa single crystal diffractometer. The crystal was kept at 99.99(10) K during data collection.

1.2 X-ray crystallographic analysis of flavan 1.

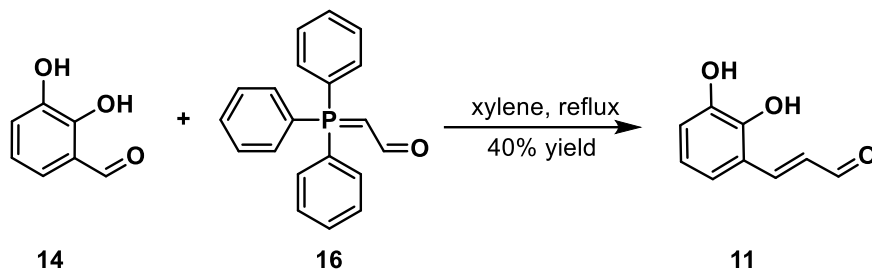
Table 1 Crystal data and structure refinement for flavan 1

Identification code	Flavan 1_collect
Empirical formula	C ₃₄ H ₃₂ O ₁₀
Formula weight	600.59
Temperature/K	99.99(10)
Crystal system	monoclinic
Space group	I2/a
<i>a</i> /Å	15.5676(5)
<i>b</i> /Å	13.8531(3)
<i>c</i> /Å	26.8877(10)
α /°	90
β /°	99.841(3)
γ /°	90
Volume/Å ³	5713.3(3)
<i>Z</i>	8
ρ_{calc} /cm ³	1.396
μ /mm ⁻¹	0.857
F(000)	2528.0
Crystal size/mm ³	0.3 × 0.05 × 0.05
Radiation	CuK α (λ = 1.54184)

2 Θ range for data collection/ $^{\circ}$	6.674 to 148.608
Index ranges	$-16 \leq h \leq 19$, $-17 \leq k \leq 13$, $-33 \leq l \leq 31$
Reflections collected	15091
Independent reflections	5654 [$R_{\text{int}}^{\circ} = 0.0335$, $R_{\text{sigma}}^{\circ} = 0.0411$]
Data/restraints/parameters	5654/0/469
Goodness-of-fit on F^2	1.057
Final R indexes [$I \geq 2\sigma(I)$]	$R_1^{\circ} = 0.0610$, $wR_2^{\circ} = 0.1490$
Final R indexes [all data]	$R_1^{\circ} = 0.0845$, $wR_2^{\circ} = 0.1618$
Largest diff. peak/hole/ $e\text{\AA}^{-3}$	0.20/-0.29

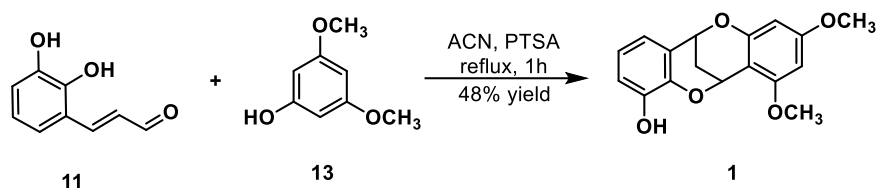
1.3 The synthetic procedures

1.3.1 The synthesis of 2,3-dihydroxycinnamaldehyde **11**



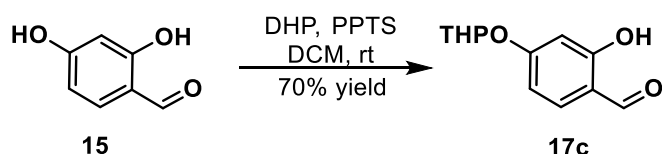
2,3-Dihydroxybenzaldehyde **14** (500 mg, 3.62 mmol) and formylmethylene triphenylphosphorane **16** (1.32 g, 4.35 mmol) were dissolved in xylene (20 mL). The resulting mixture was heated to 100 $^{\circ}\text{C}$ in an oil bath and stirred for 6 h at that temperature under nitrogen atmosphere. After cooling to room temperature, the reaction mixture was directly purified by 15 cm flash column chromatography (silica gel, hexane:EtOAc = 5:1 to 3:1) to provide the product **11** (237 mg, 40% yield) as a yellow solid powder. ^1H NMR (500 MHz, CD_3OD): δ 9.60 (d, $J = 7.9$ Hz, 1H), 7.92 (d, $J = 15.9$ Hz, 1H), 7.05 (d, $J = 8.9$ Hz, 1H), 6.90-6.79 (m, 2H), 6.72 (s, 1H). ^{13}C NMR (125 MHz, CD_3OD): δ 195.5, 150.2, 146.1, 145.4, 128.0, 121.2, 119.4, 119.1, 117.1. HRMS (ESI) m/z : $[\text{M} + \text{H}]^+$ calcd for $\text{C}_9\text{H}_9\text{O}_3$, 165.0546, found 165.0546.

1.3.2 The synthesis of flavan **1**



2,3-Dihydroxycinnamaldehyde **11** (72 mg, 0.44 mmol) and phloroglucinol **13** (68 mg, 0.44 mmol) were dissolved in ACN (3 mL), and PTSA (7.6 mg, 0.04 mmol) were then added. The resulting mixture was heated to 80 °C in an oil bath and stirred for 1 h at that temperature. After most of the starting material was consumed, the mixture was cooled to room temperature, extracted with EtOAc (3 × 25 mL), washed with brine, and concentrated in vacuum. The crude product was purified by flash column chromatography (silica gel, hexane:CH₂Cl₂ = 3:1) to afford **1** (63 mg, 48% yield) as a white solid powder. ¹H NMR (500 MHz, DMSO-*d*₆): δ 9.00 (s, 1H), 6.80 (d, *J* = 7.1 Hz, 1H), 6.69 (t, *J* = 8.3 Hz, 2H), 6.11 (s, 1H), 5.97 (s, 1H), 5.62 (s, 1H), 5.34 (s, 1H), 3.80 (s, 3H), 3.67 (s, 3H), 2.16 (d, *J* = 14.1 Hz, 1H), 2.09 (d, *J* = 14.1 Hz, 1H). ¹³C NMR (125 MHz, DMSO): δ 161.9, 159.3, 155.0, 146.3, 142.3, 122.5, 121.4, 120.1, 116.6, 103.6, 93.4, 91.9, 67.2, 61.5, 56.2, 55.6, 26.5. HRMS (ESI) *m/z*: [M + H]⁺ calcd for C₁₇H₁₇O₅, 301.1071, found 301.1083.

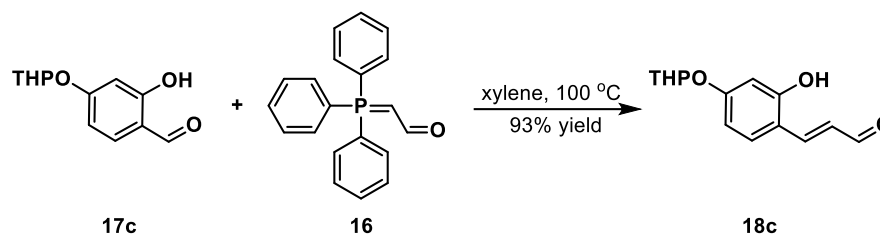
1.3.3 The synthesis of cinnamaldehyde **17c**



2,4-Dihydroxybenzaldehyde **15** (500 mg, 3.6 mmol) and PPTS (90 mg, 0.36 mmol) were dissolved in anhydrous CH₂Cl₂ (15 mL). Then, DHP (365 mg, 4.3 mmol) was added. The reaction mixture was stirred at room temperature until most of the ingredients were consumed. The mixture was then extracted with CH₂Cl₂ (3 × 25 mL), washed with brine, and concentrated in vacuum. The crude product was purified by flash column chromatography (silica gel, hexane:CH₂Cl₂ = 1:2) to afford **17c** (557 mg, 70% yield) as a colorless liquid. ¹H NMR (500 MHz, CDCl₃): δ 11.38 (s, 1H), 9.74 (s, 1H), 7.45 (d, *J* = 8.6 Hz, 1H), 6.75-6.48 (m, 2H), 5.52 (s, 1H), 3.98-3.76 (m, 1H), 3.64

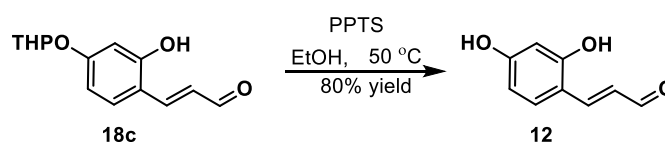
(d, $J = 10.6$ Hz, 1H), 1.86 (t, $J = 68.5$ Hz, 6H). ^{13}C NMR (125 MHz, CDCl_3): δ 194.6, 164.3, 164.1, 135.3, 115.7, 109.4, 103.6, 96.2, 62.2, 29.9, 25.0, 18.4. HRMS (ESI) m/z : $[\text{M} + \text{H}]^+$ calcd for $\text{C}_{12}\text{H}_{15}\text{O}_4$, 223.0965, found 223.0979.

1.3.4 The synthesis of cinnamaldehyde 18c



THP-ether aldehyde **17c** (557 mg, 2.5 mmol) and formylmethylene triphenylphosphorane **16** (912 mg, 3.0 mmol) were dissolved in xylene (15 mL). The resulting mixture was heated to 100 °C in an oil bath and stirred for 6 h at that temperature under nitrogen atmosphere. After cooling to room temperature, the reaction mixture was directly purified by 15 cm long flash column chromatography (silica gel, hexane:EtOAc = 10:1 to 5:1) to afford the product **18c** (580 mg, 93% yield) as a palm red solid powder. ^1H NMR (500 MHz, CDCl_3): δ 9.64 (d, $J = 8.0$ Hz, 1H), 7.73 (d, $J = 15.9$ Hz, 1H), 7.45 (d, $J = 8.7$ Hz, 1H), 7.00-6.81 (m, 1H), 6.70-6.58 (m, 2H), 5.48 (s, 1H), 3.88 (t, $J = 10.8$ Hz, 1H), 3.65 (d, $J = 11.7$ Hz, 1H), 1.87 (t, $J = 73.9$ Hz, 4H). ^{13}C NMR (125 MHz, CD_3OD): δ 195.6, 161.3, 158.9, 150.5, 130.5, 125.8, 115.1, 108.3, 103.0, 96.1, 61.8, 29.9, 24.8, 18.4. HRMS (ESI) m/z : $[\text{M} + \text{Na}]^+$ calcd for $\text{C}_{14}\text{H}_{16}\text{O}_4\text{Na}$, 271.0941, found 271.0940.

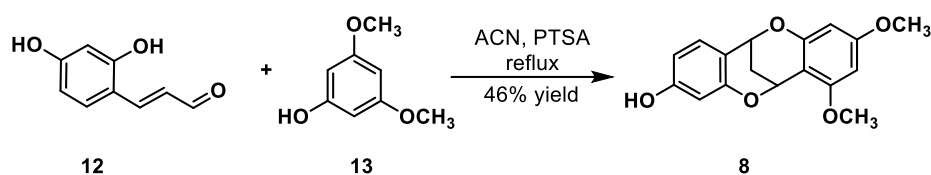
1.3.5 The synthesis of cinnamaldehyde 12



Cinnamaldehyde **18c** (580 mg, 2.34 mmol) and PPTS (59 mg, 0.23 mmol) were dissolved in EtOH (15 mL). The reaction mixture was stirred at room temperature until most of the starting materials are consumed. The mixture was then extracted with EA (3 \times 25 mL), washed with brine, and concentrated in vacuum. The crude product was

purified by flash column chromatography (silica gel, hexane:EtOAc = 3:1 to 1:1) to afford **12** (305 mg, 80% yield) as a yellow powder. ^1H NMR (500 MHz, CD_3OD): δ 9.48 (s, 1H), 7.81 (d, $J = 15.7$ Hz, 1H), 7.39 (d, $J = 8.3$ Hz, 2H), 6.72 (d, $J = 7.6$ Hz, 1H), 6.35 (s, 3H). ^{13}C NMR (125 MHz, CD_3OD): δ 195.9, 162.4, 159.5, 151.5, 131.0, 124.6, 113.5, 107.9, 102.1. HRMS (ESI) m/z : $[\text{M} + \text{H}]^+$ calcd for $\text{C}_9\text{H}_9\text{O}_3$, 165.0546, found 165.0547.

1.3.6 The synthesis of flavan **8**



2,4-Dihydroxycinnamaldehyde **12** (126 mg, 0.77 mmol) and phloroglucinol **13** (118 mg, 0.77 mmol) were dissolved in ACN (10 mL), PTSA (15.2 mg, 0.08 mmol) was then added. The resulting mixture was heated to 80 °C in an oil bath and stirred for 4 h at that temperature. After most of the starting material was consumed, the mixture was cooled to room temperature and extracted with EtOAc (3×25 mL), washed with brine, and concentrated in vacuum. The crude product was purified by flash column chromatography (silica gel, hexane:EtOAc = 6:1 to 3:1) to afford **8** (106 mg, 46% yield) as a brown solid powder. ^1H NMR (500 MHz, CDCl_3): δ 7.21 (d, $J = 8.3$ Hz, 1H), 6.40 (d, $J = 5.8$ Hz, 1H), 6.36 (d, $J = 2.4$ Hz, 1H), 6.03 (s, 1H), 5.98 (s, 1H), 5.66 (s, 1H), 5.27 (s, 1H), 3.86 (s, 3H), 3.73 (s, 3H), 2.29 (d, $J = 13.8$ Hz, 1H), 2.18 (d, $J = 13.7$ Hz, 1H). ^{13}C NMR (125 MHz, CDCl_3): δ 161.8, 159.1, 157.9, 154.9, 131.7, 113.8, 108.4, 103.5, 93.0, 91.6, 67.5, 62.0, 55.9, 55.3, 26.8. HRMS (ESI) m/z : $[\text{M} + \text{H}]^+$ calcd for $\text{C}_{17}\text{H}_{17}\text{O}_5$, 301.1071, found 301.1076.

2. The Comparison of ^1H and ^{13}C NMR Data of Natural and Synthetic Flavan 1 in $\text{DMSO-}d_6$

Position	Nature sample 1 (500 MHz) ^a		Synthetic sample 1 (500 MHz) ^b		$\Delta\delta_{\text{H}}$ /ppm	$\Delta\delta_{\text{C}}$ /ppm
	δ_{H} (mult, J in Hz)	δ_{C}	δ_{H} (mult, J in Hz)	δ_{C}		
2	5.34 (1H, s)	67.2	5.34 (1H, s)	67.2	0.00	0.0
3a	2.08 (1H, dt, 2.5, 14.0)	26.5	2.09 (1H, dt, 2.5, 14.0)	26.5	+0.01	0.0
3b	2.16 (1H, s)		2.16 (1H, s)		0.00	
4	5.62 (1H, s)	61.5	5.62 (1H, s)	61.5	0.00	0.0
5	—	159.3	—	159.3	—	0.0
6	6.11 (1H, d, 2.3)	91.8	6.11 (1H, d, 2.3)	91.9	0.00	+0.1
7	—	161.9	—	161.9	—	0.0
8	5.97 (1H, d, 2.3)	93.4	5.97 (1H, d, 2.3)	93.4	0.00	0.0
9	—	155.0	—	155.0	—	0.0
10	—	103.5	—	103.6	—	+0.1
1'	—	122.5	—	122.5	—	0.0
2'	—	146.1	—	146.3	—	+0.2
3'	—	142.2	—	142.3	—	+0.1
4'	6.70 (1H, d, 1.6)	116.5	6.70 (1H, d, 1.6)	116.6	0.00	+0.1
5'	6.68 (1H, d, 7.4)	120.1	6.69 (1H, d, 7.4)	120.1	+0.01	0.0
6'	6.80 (1H, dd, 1.5, 7.2)	121.4	6.80 (1H, dd, 1.5, 7.2)	121.4	0.00	0.0
5-OCH ₃	3.67 (3H, s)	56.1	3.67 (3H, s)	56.2	0.00	+0.1
7-OCH ₃	3.80 (3H, s)	55.6	3.80 (3H, s)	55.6	0.00	0.0

^aThe ^1H and ^{13}C NMR data were recorded on a Bruker Avance 500 spectrometer in $\text{DMSO-}d_6$ and referenced against residual DMSO in $\text{DMSO-}d_6$ as $\delta_{\text{H}} = 2.51$ ppm, $\delta_{\text{C}} = 39.5$ ppm.

^bThe ^1H and ^{13}C NMR data were recorded on a Bruker Avance 500 spectrometer in $\text{DMSO-}d_6$ and referenced against residual DMSO in $\text{DMSO-}d_6$ as $\delta_{\text{H}} = 2.51$ ppm, $\delta_{\text{C}} = 39.5$ ppm.

^c $\Delta\delta$ /ppm refers the relative difference of each signal between the synthetic and natural samples.

3. The Comparison of ^1H and ^{13}C NMR Data of Flavan **9** and Synthetic Flavan **8** in CDCl_3

Position	Nature sample Flavan 9 (500 MHz) ^a		Synthetic sample Flavan 8 (500 MHz) ^b		$\Delta\delta_{\text{H}}$ /ppm ^c	$\Delta\delta_{\text{C}}$ /ppm ^d
	δ_{H} (mult, J in Hz)	δ_{C}	δ_{H} (mult, J in Hz)	δ_{C}		
2	5.28 (1H, dd, 1.6, 5.4)	67.4	5.27 (1H, dd, 1.6, 5.4)	67.5	-0.01	+0.1
3a	2.18 (1H, m)	26.7	2.18 (1H, m)	26.8	0.00	+0.1
3b	2.29 (1H, m)		2.29 (1H, m)		0.00	0.0
4	5.67 (1H, dd, 4.4, 2.8)	62.1	5.66 (1H, dd, 4.4, 2.8)	62.0	-0.01	-0.1
5	—	159.1	—	159.1	—	0.0
6	6.04 (1H, d, 2.4)	91.6	6.03 (1H, d, 2.4)	91.6	-0.01	0.0
7	—	161.9	—	161.8	—	-0.1
8	5.99 (1H, d, 2.4)	92.9	5.98 (1H, d, 2.4)	93.0	-0.01	+0.1
9	—	154.8	—	154.9	—	+0.1
10	—	103.3	—	103.5	—	+0.2
1'	—	114.1	—	113.8	—	-0.3
2'	—	154.7	—	154.9	—	+0.2
3'	—	103.4	—	103.5	—	+0.1
4'	6.36 (1H, d, 2.4)	157.4	6.36 (1H, d, 2.4)	157.9	0.00	+0.5
5'	6.40 (1H, dd, 8.4, 2.4)	108.2	6.40 (1H, dd, 8.4, 2.4)	108.4	0.00	+0.2
6'	7.22 (1H, d, 8.4)	131.8	7.21 (1H, d, 8.4)	131.7	-0.01	-0.1
5-OCH ₃	3.87 (3H, s)	55.9	3.86 (3H, s)	55.9	-0.01	0.0
7-OCH ₃	3.73 (3H, s)	55.3	3.73 (3H, s)	55.3	0.00	0.0

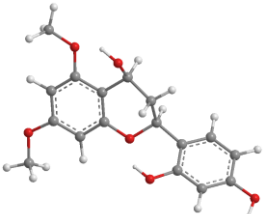
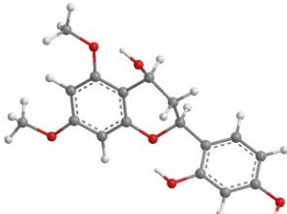
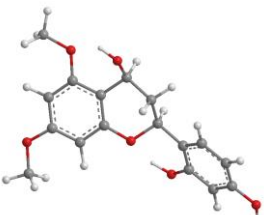
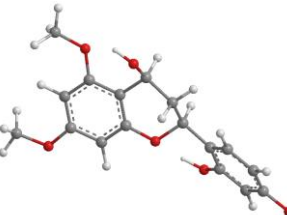
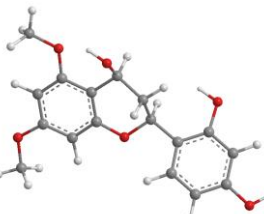
^aThe ^1H NMR data was recorded on a Bruker Avance 400 spectrometer in CDCl_3 , the ^{13}C NMR data was recorded on a Bruker Avance 100 spectrometer in CDCl_3 , both of them were referenced against residual CHCl_3 in CDCl_3 .

^bThe ^1H NMR data and ^{13}C NMR data were recorded on a Bruker Avance 500 spectrometer in CDCl_3 and referenced against residual CHCl_3 in CDCl_3 as $\delta_{\text{H}} = 7.28$ ppm, $\delta_{\text{C}} = 77.0$ ppm.

^c $\Delta\delta/\text{ppm}$ refers the relative difference of each signal between the synthetic and natural samples.

4. (GIAO) DFT ^{13}C NMR Calculations of Flavans **9** and **8**

Table 1. Relative energies (kcal/mol) and conformational population (%) for the most stable conformers of **9** and **8** optimized on B3LYP-D3(BJ)/TZVP (IEF-PCM) level of theory

Compound	Conformer	ΔG (kcal/mol)	Population (%)
9	 9-C1	0	58.54
	 9-C2	0.422941336	28.65
	 9-C3	1.089356318	9.29
	 9-C4	1.706825568	3.27
	 9-C5	3.463224379	0.17

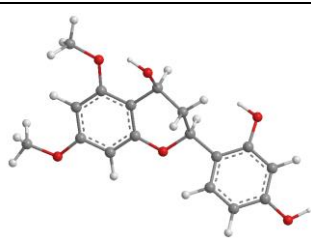
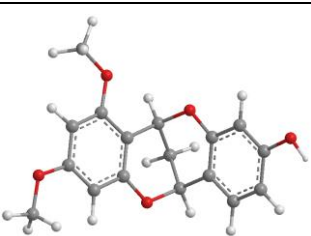
	 <p style="text-align: center;">9-C6</p>	3.850397678	0.09
8		0	100

Table 2. Experimental ^{13}C NMR data (δ_{C} in ppm) of **9** (proposed in the previous literature, *J. Asian Nat. Prod. Res.*, **2013**, *15*, 979-984) and shielding tensors (δ_{C} in ppm) of **9** and **8** calculated on $\omega\text{B97x-D}/6\text{-31G}^*/\text{B3LYP-D3(BJ)}/\text{TZVP}$ (IEF-PCM) level of theory

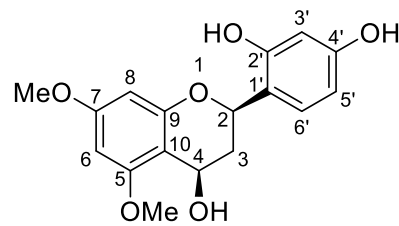
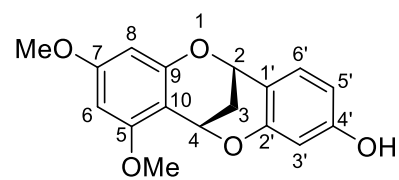
Compound	Nucleus	δ_{C} exp (CDCl_3)	Shielding tensor of 9	Shielding tensor of 8
 <p style="text-align: center;">9</p>	2	67.4	117.1556781	127.2923
	3	26.7	159.2900575	169.2824
	4	62.1	132.815813	132.5099
	5	159.1	41.67643849	41.8487
	6	91.6	106.3062955	106.9832
	7	161.9	40.87334304	39.4635
	8	92.9	104.5759509	107.5406
	9	154.8	45.18514977	44.2498
	10	103.3	91.38900668	96.4145
	 <p style="text-align: center;">8</p>	1'	114.1	83.8109682
2'		154.7	43.02193345	44.2371
3'		103.4	96.85620967	97.2474
4'		157.4	43.57126478	43.3194
5'		108.2	93.83536937	93.7141
6'		131.8	69.61627622	66.6211
5-OMe		55.9	141.1875069	141.3806
7-OMe		55.3	141.5587912	141.5492

Table 3. Experimental ^{13}C NMR data (δ_{C} in ppm) of **9** (proposed in the previous literature, *J. Asian Nat. Prod. Res.*, **2013**, *15*, 979-984) and calculated chemical shifts (δ_{C} in ppm) of **9** and **8** with STS strategy

No.	Exptl.	Cald. 9	dev	Cald. 8	dev
2	67.4	76.37	8.97	68.68	1.28
3	26.7	30.57	3.87	24.98	1.72
4	62.1	59.35	2.75	63.25	1.15
5	159.1	158.61	0.49	157.80	1.30
6	91.6	93.01	1.41	94.52	2.92
7	161.9	159.45	2.45	160.17	1.73
8	92.9	94.72	1.82	94.00	1.10
9	154.8	154.97	0.17	155.42	0.62
10	103.3	107.01	3.71	103.57	0.27
1'	114.1	114.87	0.77	114.33	0.23
2'	154.7	157.22	2.52	155.43	0.73
3'	103.4	102.33	1.07	103.72	0.32
4'	157.4	156.65	0.75	156.34	1.06
5'	108.2	105.31	2.89	107.06	1.14
6'	131.8	129.21	2.59	132.65	0.85
5-OMe	55.9	50.68	5.22	54.43	1.47
7-OMe	55.3	50.27	5.03	54.25	1.05
		MAE	2.73	MAE	1.11
		RMS	3.47	RMS	1.28
		P_{mean}	0.56%	P_{mean}	39.26%
		P_{rel}	0.00%	P_{rel}	100.00%

5. The Copies of the NMR Spectra

Figure 1. ^1H NMR Spectrum (500 MHz, $\text{DMSO-}d_6$) of Flavan 1

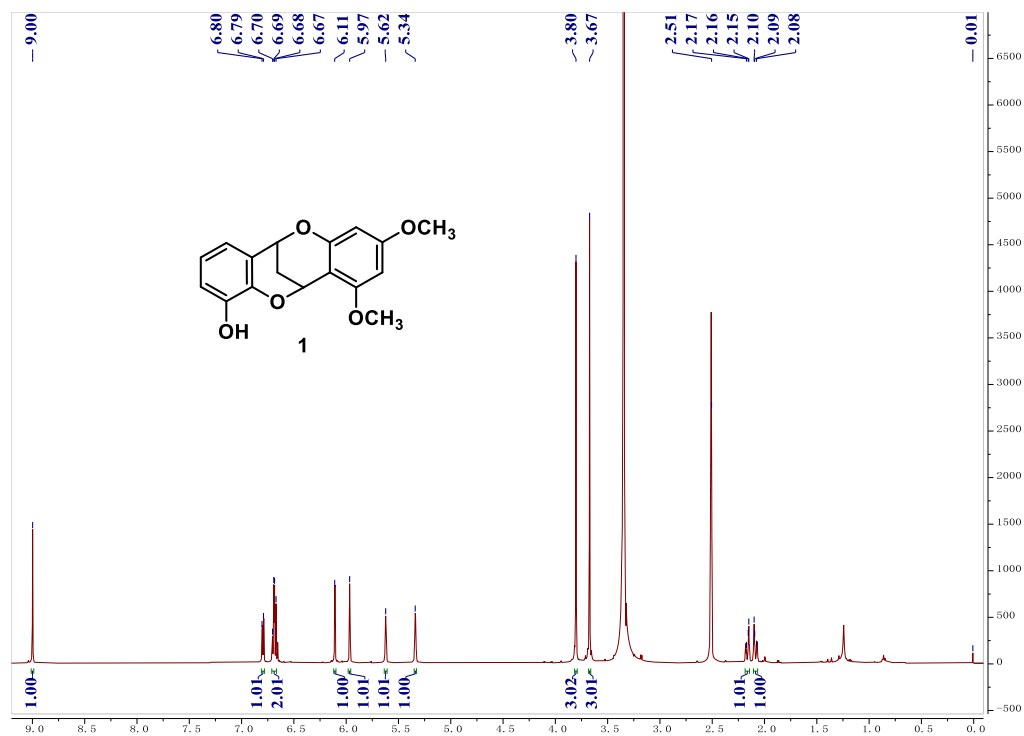


Figure 2. ^{13}C NMR Spectrum (125 MHz, $\text{DMSO-}d_6$) of Flavan 1

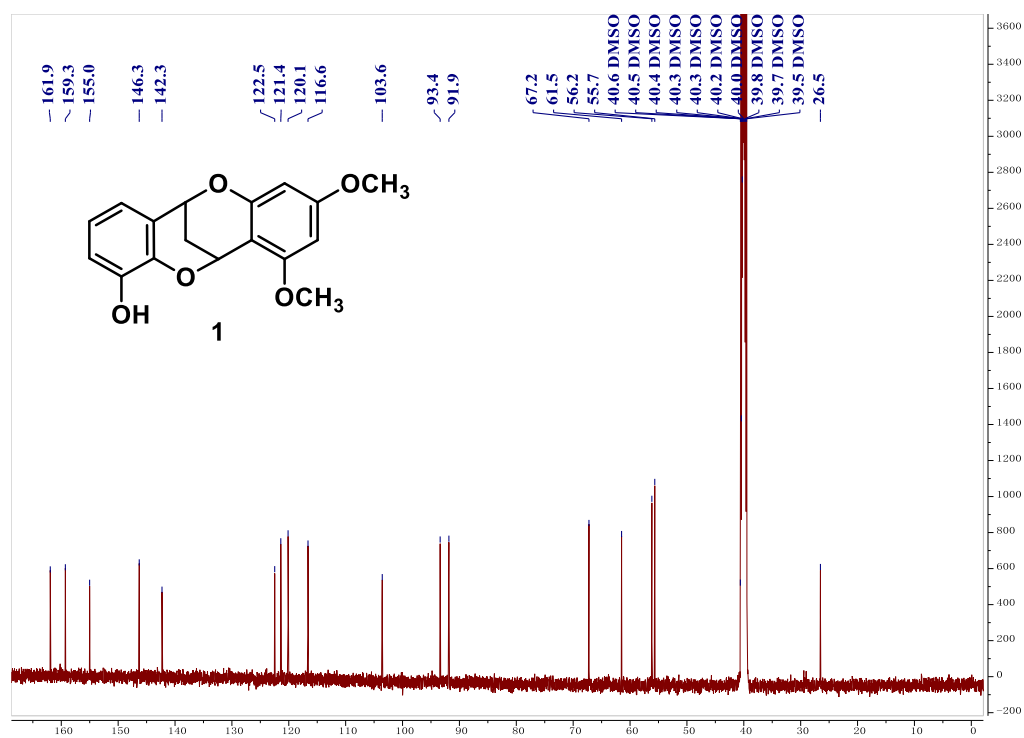


Figure 3. HSQC Spectrum of Flavan 1

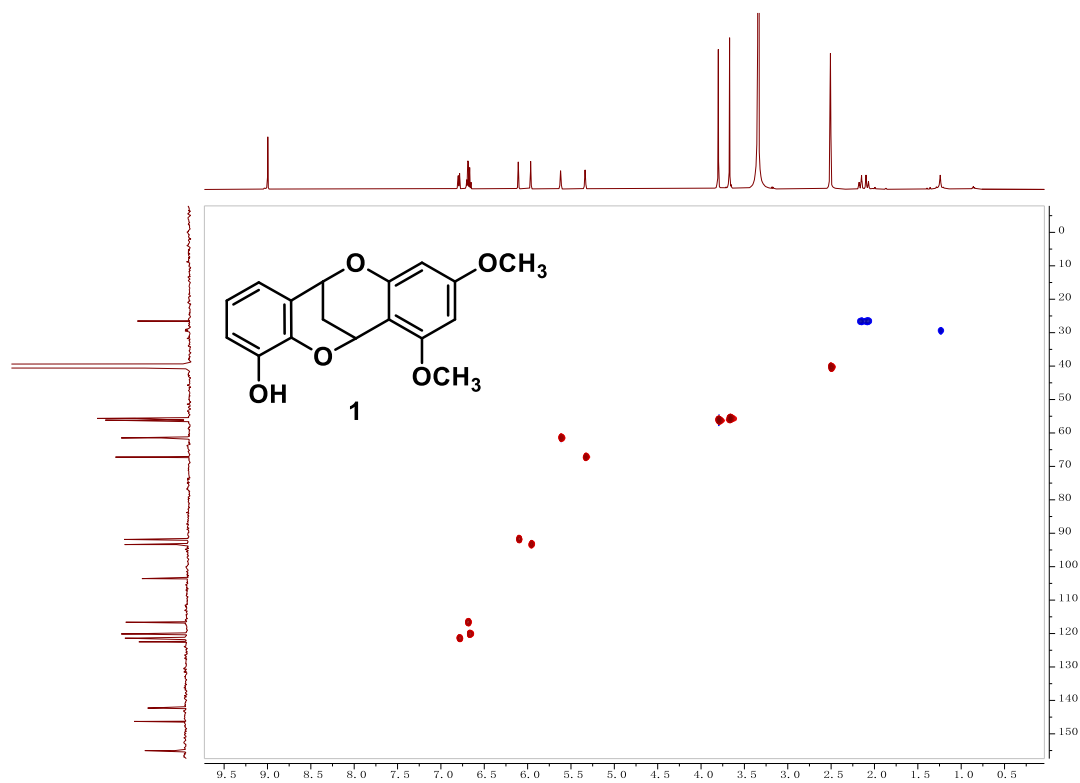


Figure 4. ^1H - ^1H COSY Spectrum of Flavan 1

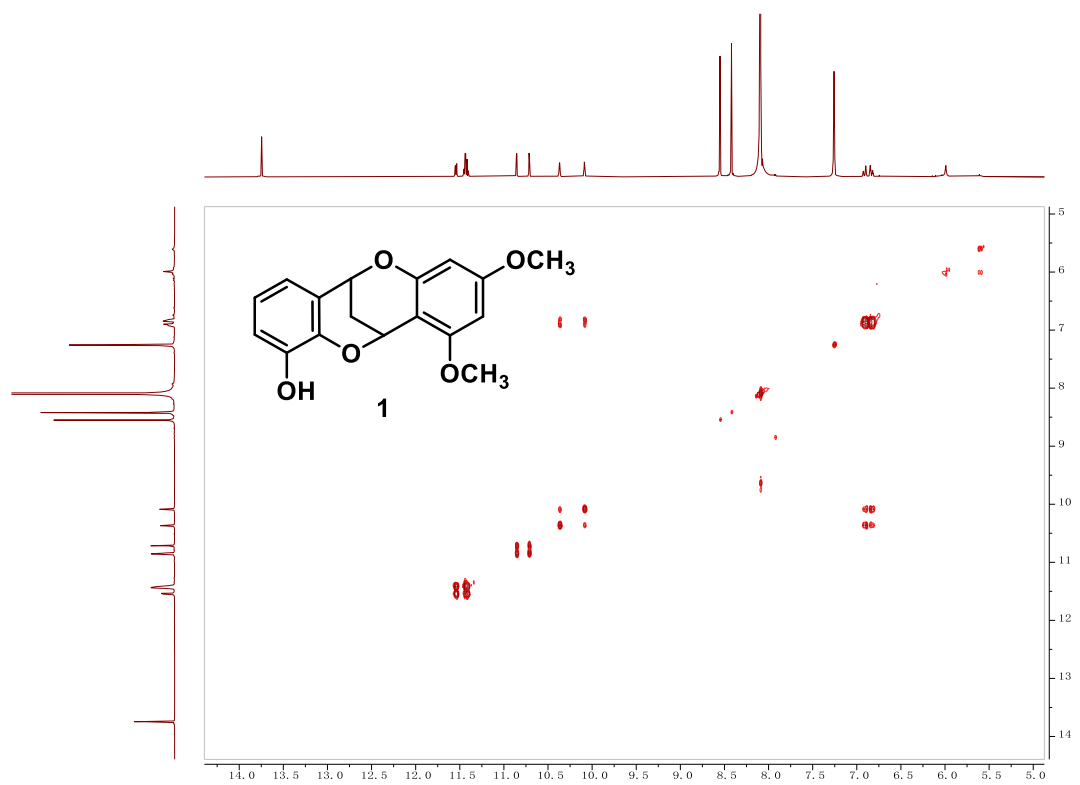


Figure 5. HMBC Spectrum of Flavan 1

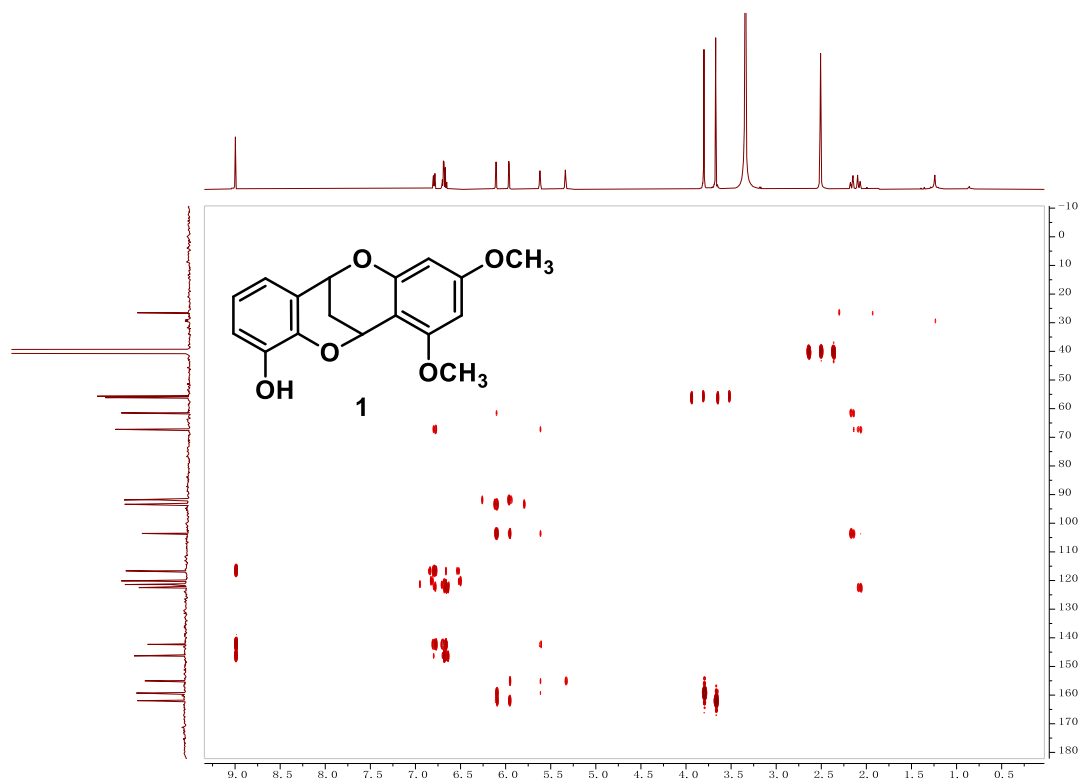


Figure 6. NOESY Spectrum of Flavan 1

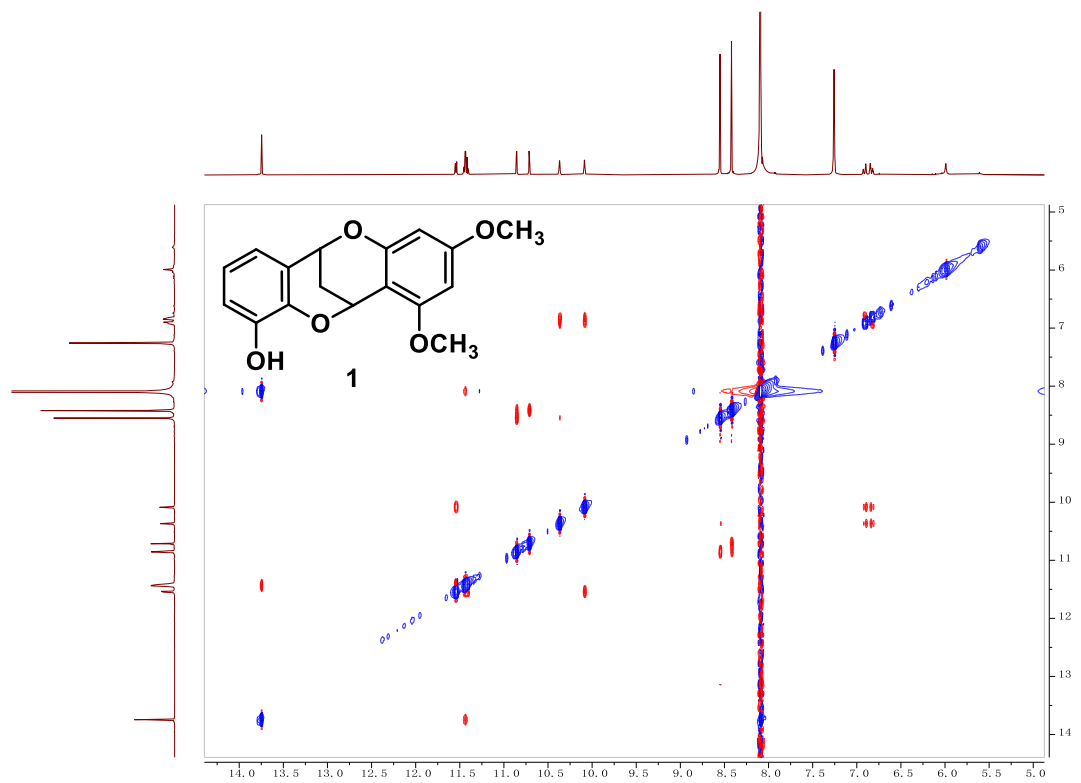


Figure 7. ¹H NMR Spectrum (500 MHz, CDCl₃) of Flavan 8

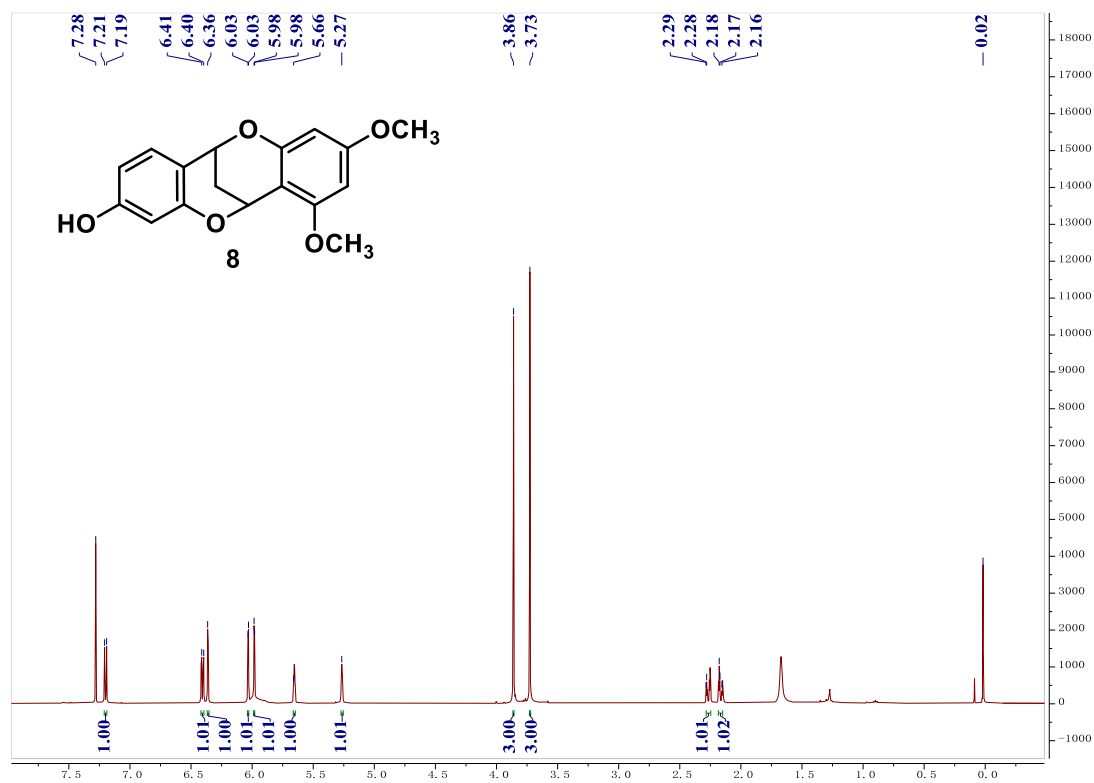


Figure 8. ¹³C NMR Spectrum (125 MHz, CDCl₃) of Flavan 8

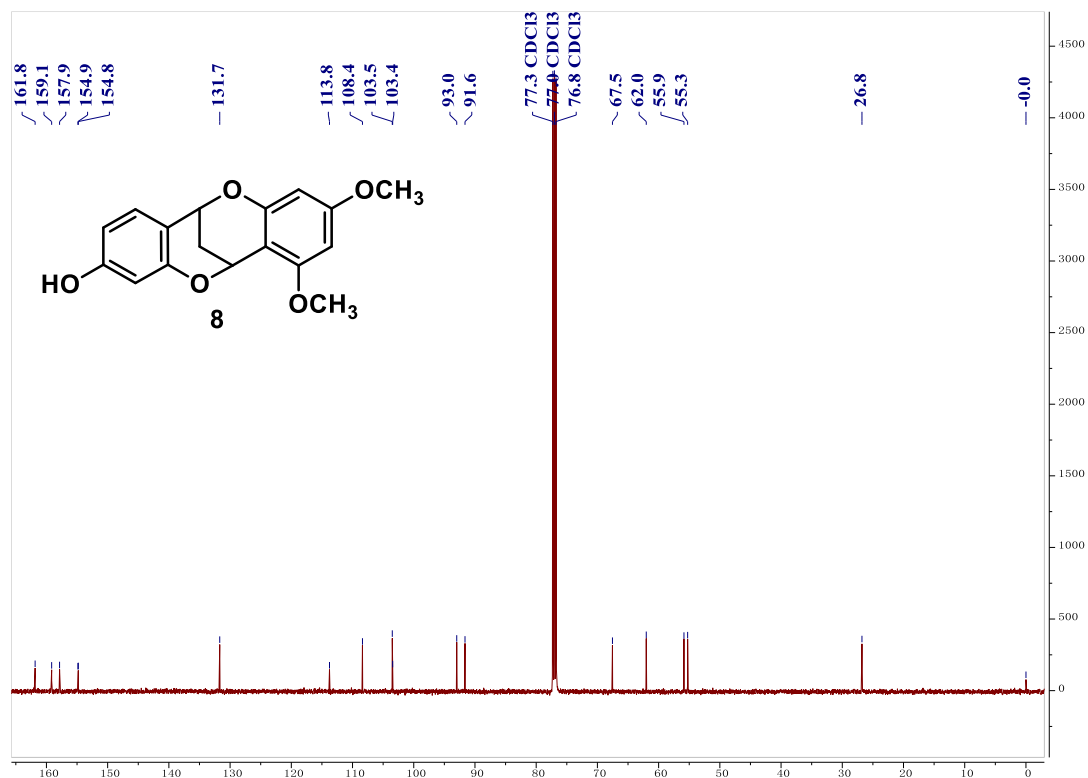


Figure 9. HSQC Spectrum of Flavan 8

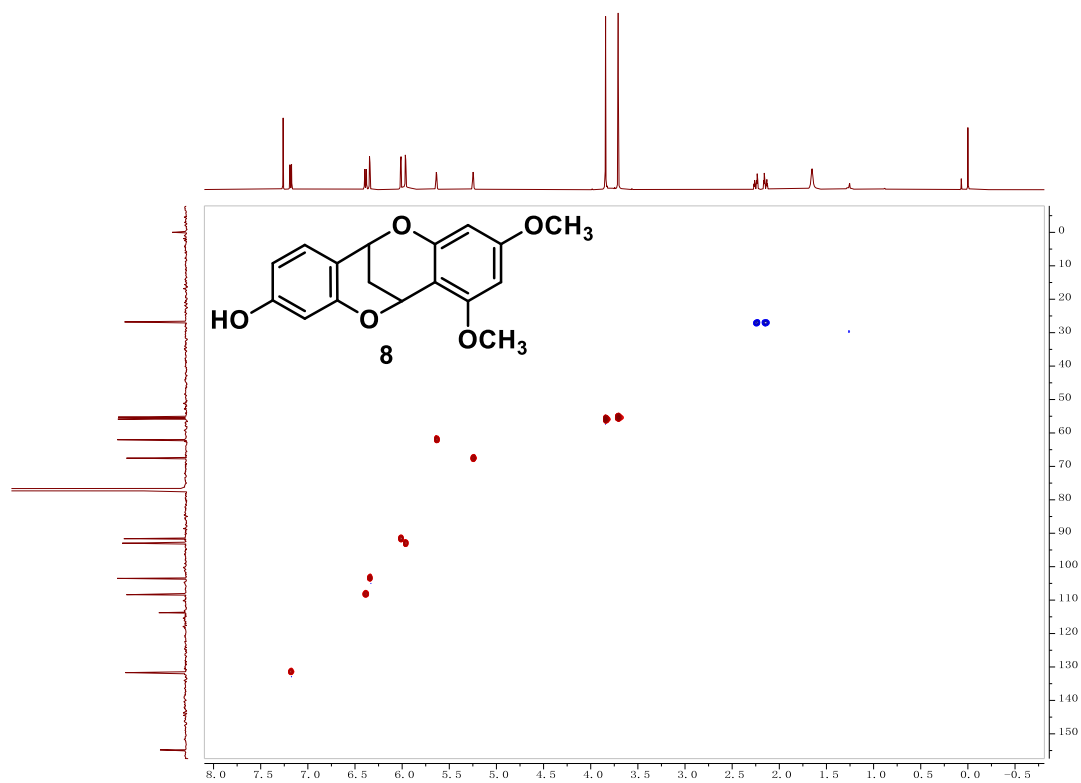


Figure 10. ^1H - ^1H COSY Spectrum of Flavan 8

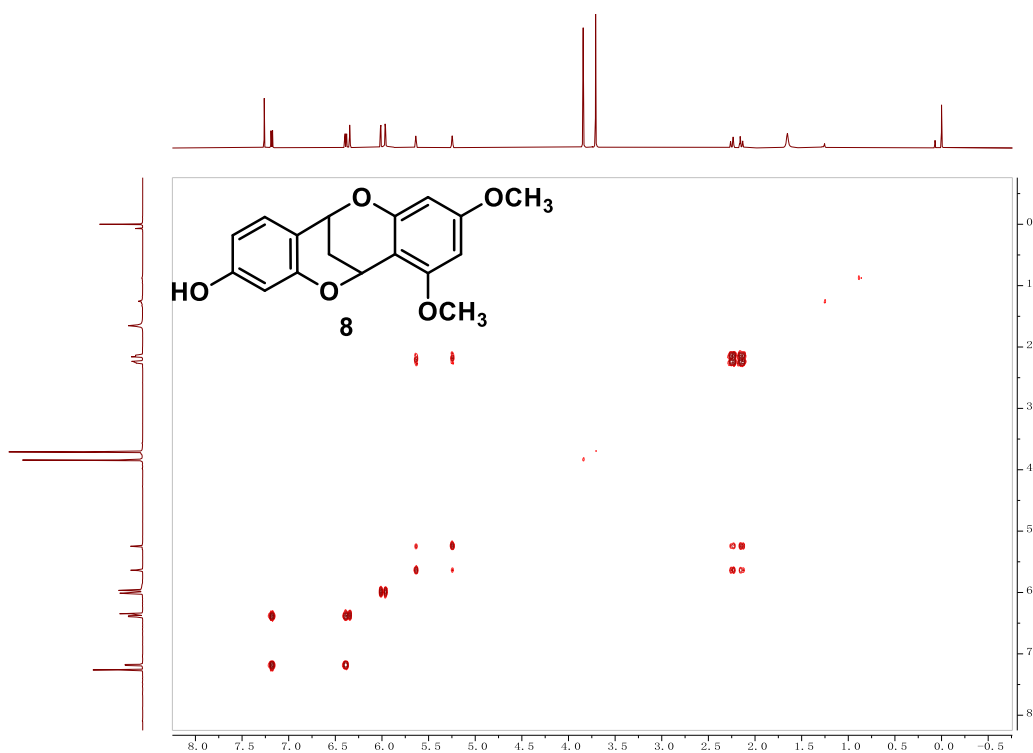


Figure 11. HMBC Spectrum of Flavan 8

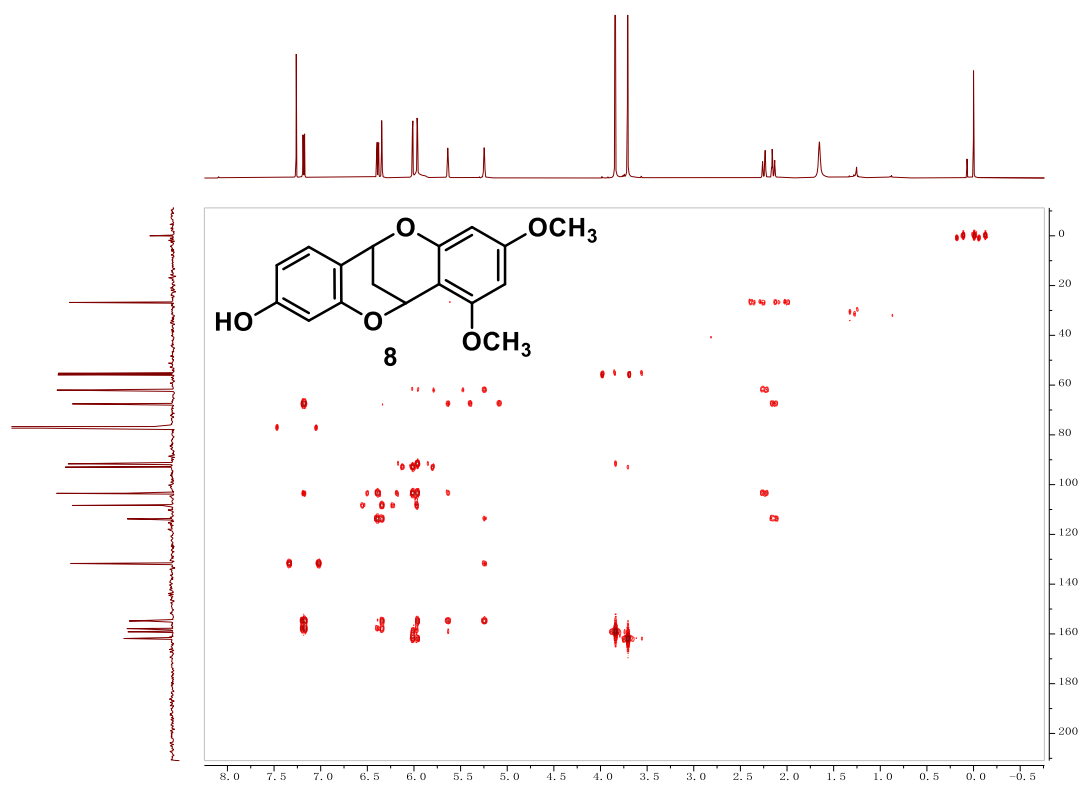


Figure 12. NOESY Spectrum of Flavan 8

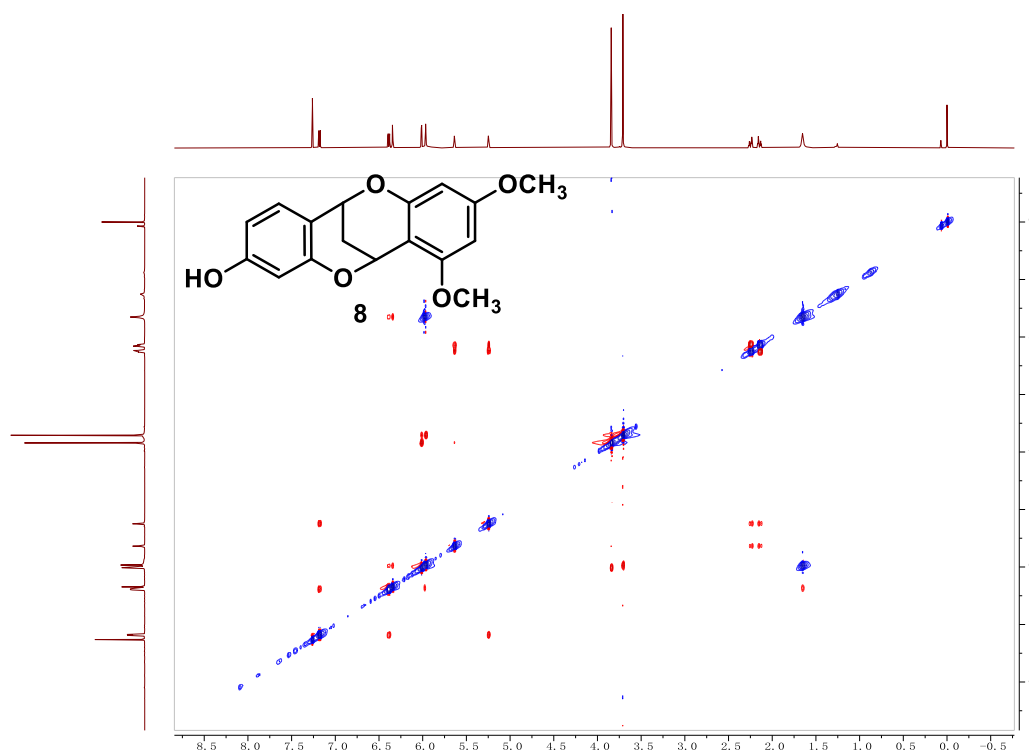


Figure 13. ^1H NMR Spectrum (500 MHz, CDCl_3) of Compound 17c

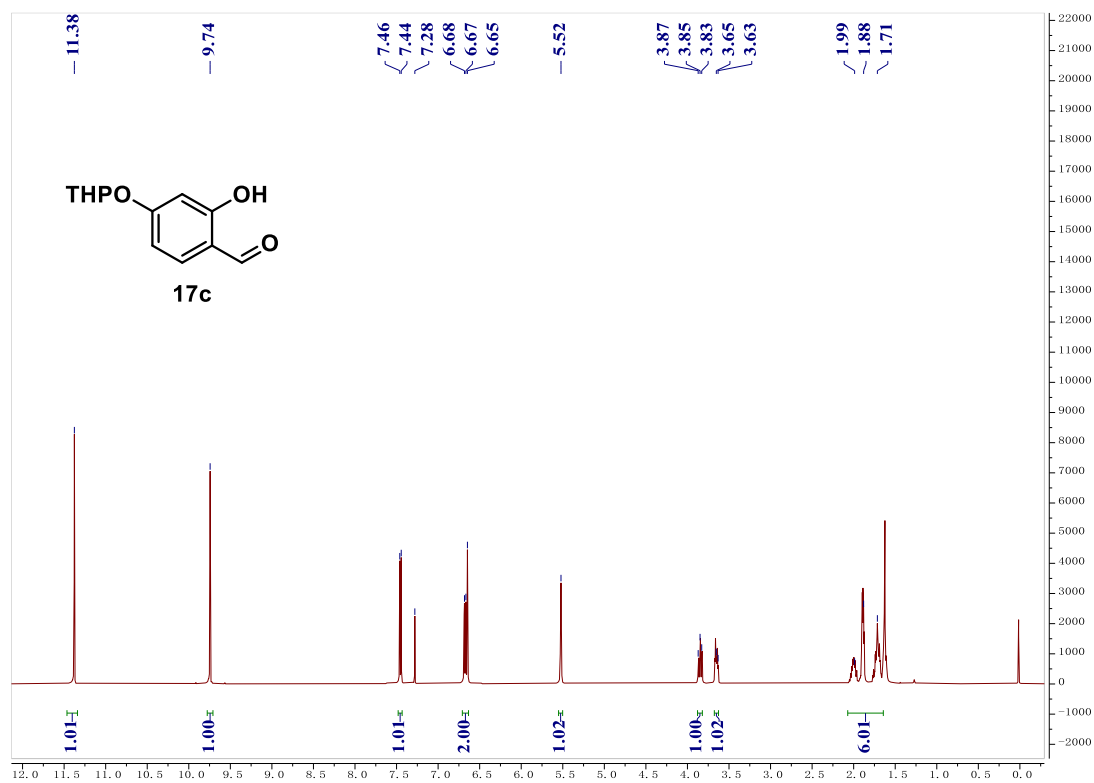


Figure 14. ^{13}C NMR Spectrum (125 MHz, CDCl_3) of Compound 17c

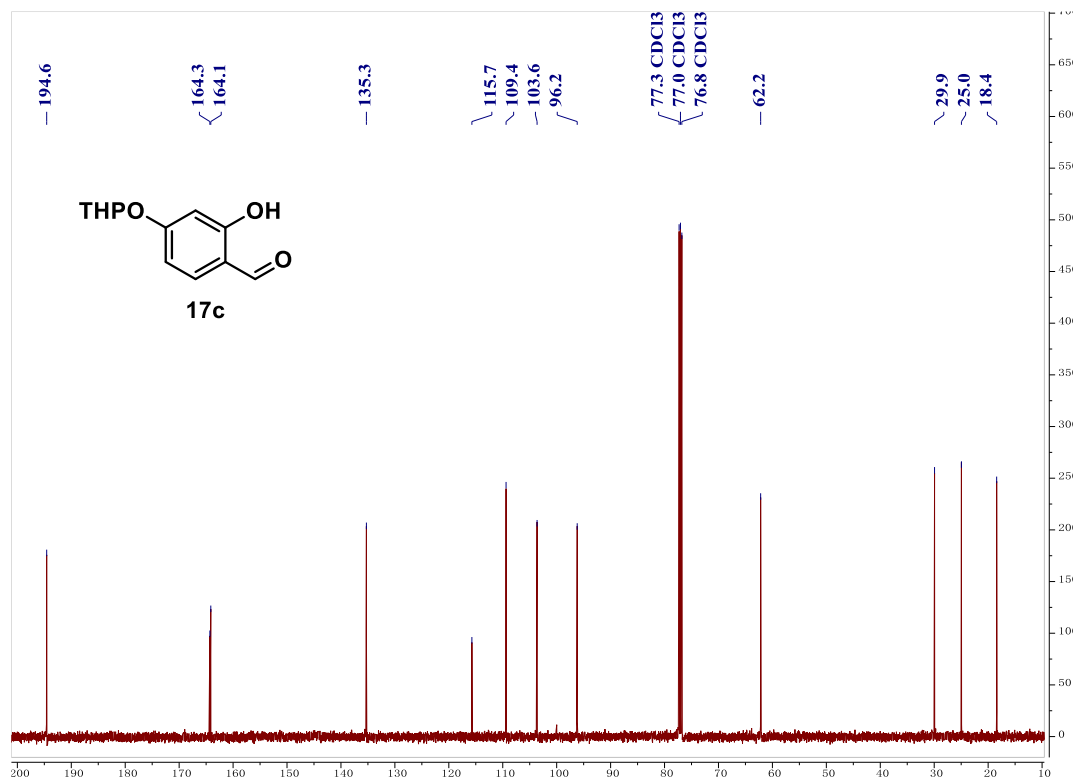


Figure 15. ^1H NMR Spectrum (500 MHz, CDCl_3) of Compound 18c

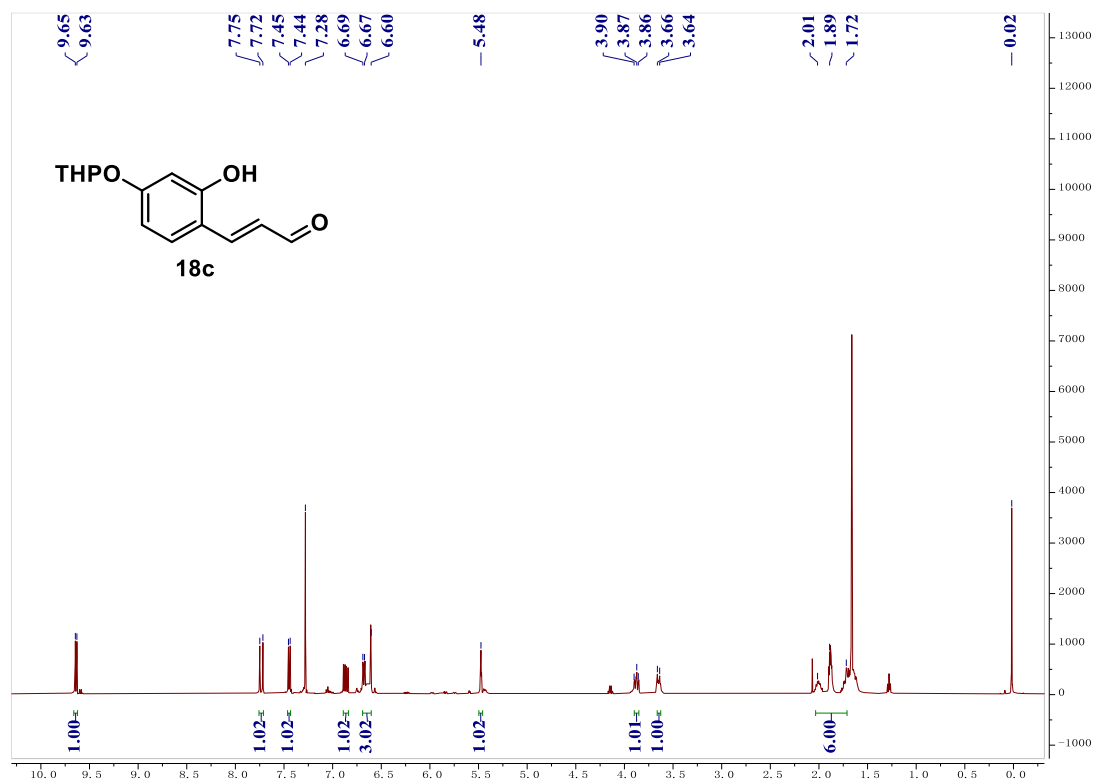


Figure 16. ^{13}C NMR Spectrum (125 MHz, CD_3OD) of Compound 18c

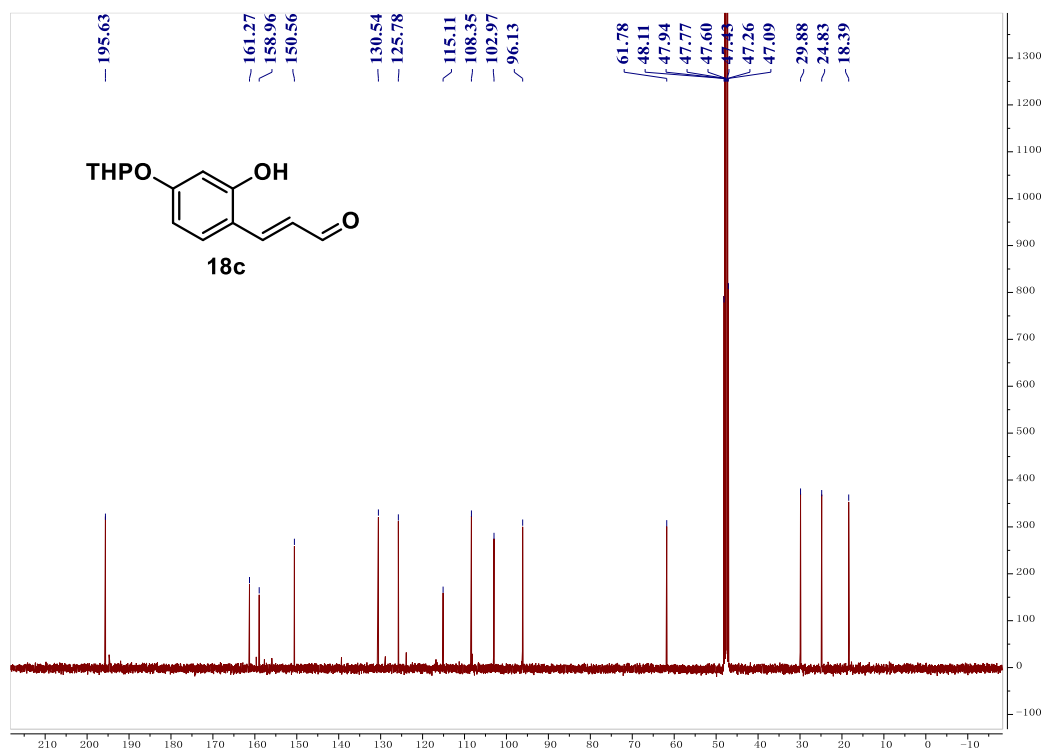


Figure 17. ^1H NMR Spectrum (500 MHz, CD_3OD) of Compound 12

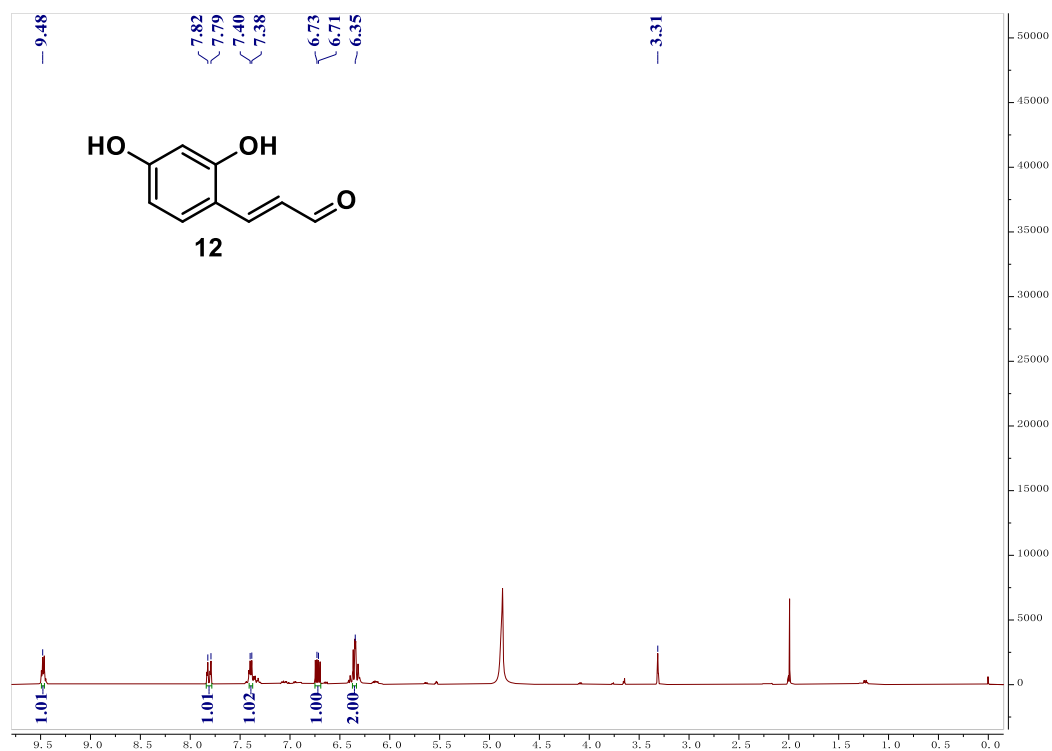


Figure 18. ^{13}C NMR Spectrum (125 MHz, CD_3OD) of Compound 12

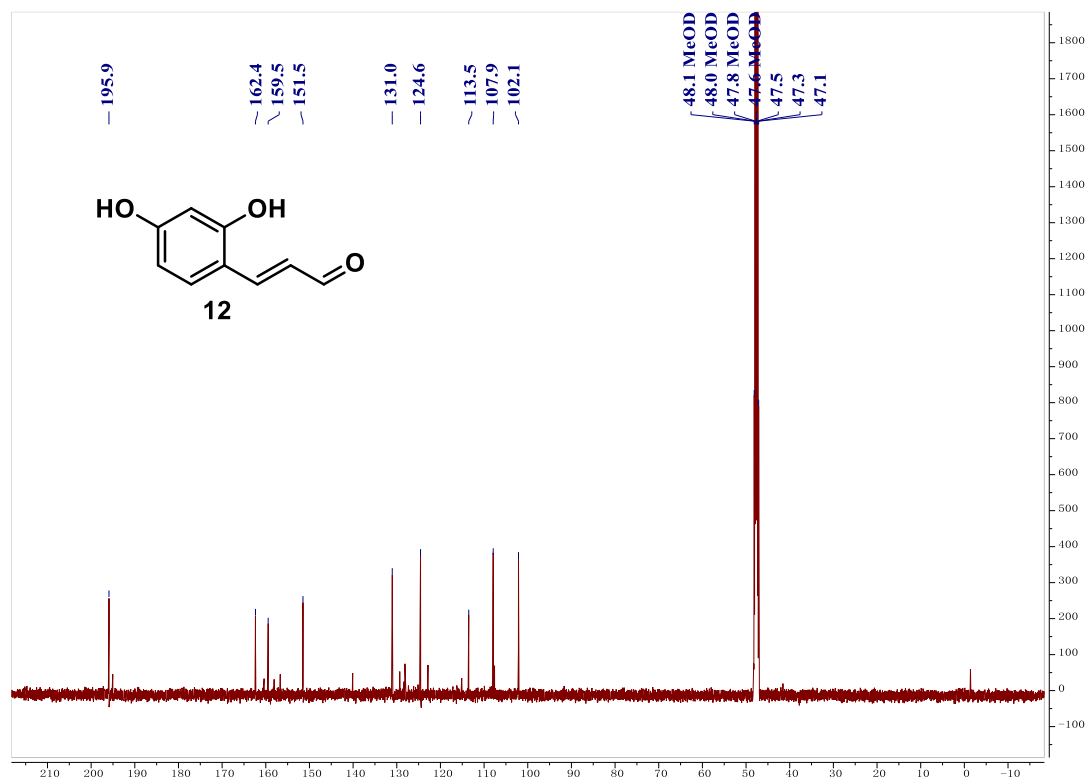


Figure 19. ^1H NMR Spectrum (500 MHz, CD_3OD) of Compound 11

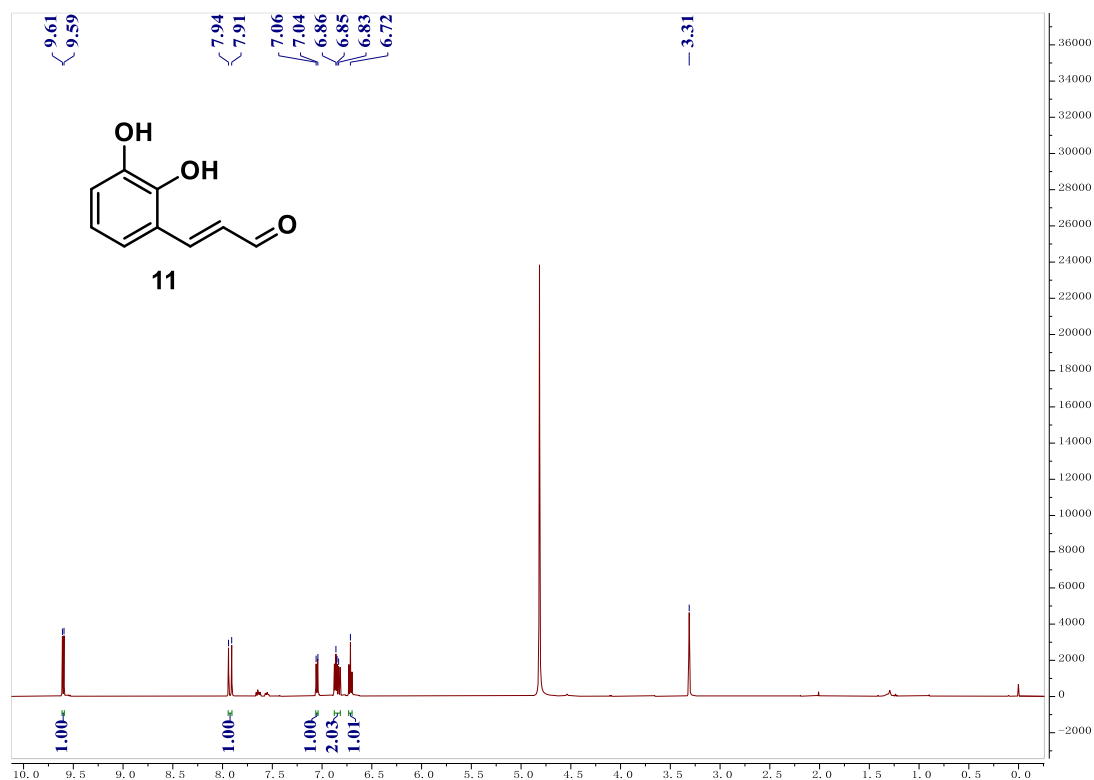


Figure 20. ^{13}C NMR Spectrum (125 MHz, CD_3OD) of Compound 11

