Electronic Supplementary Material (ESI) for RSC Advances.

Penchinones A–D, two pairs of *cis*-*trans* isomers with rearranged neolignane carbon skeletons from *Penthorum chinense*

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Supplementary Information

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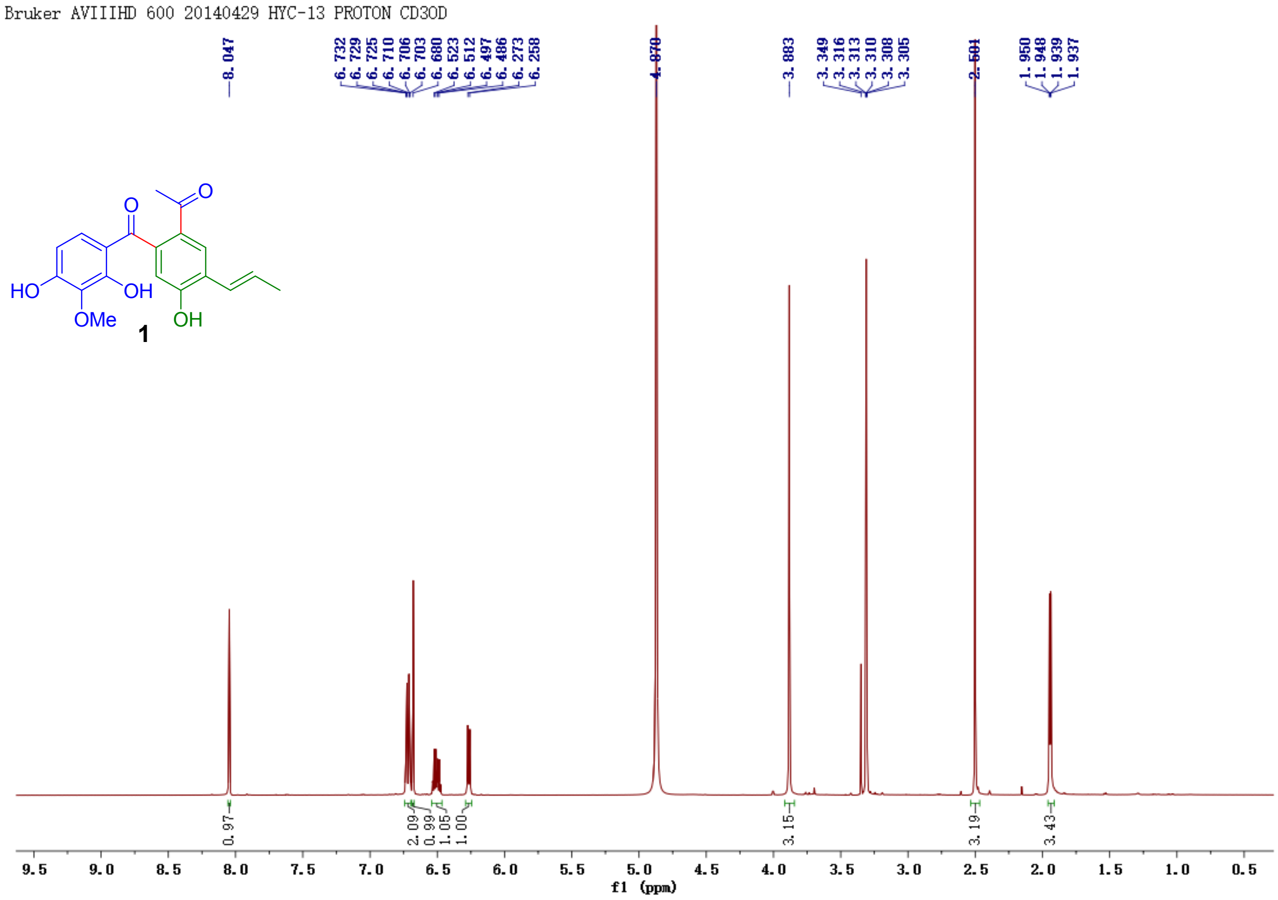


Figure S1. The ^{1}H NMR Spectrum of Compound **1** in CD_3OD (600 MHz)

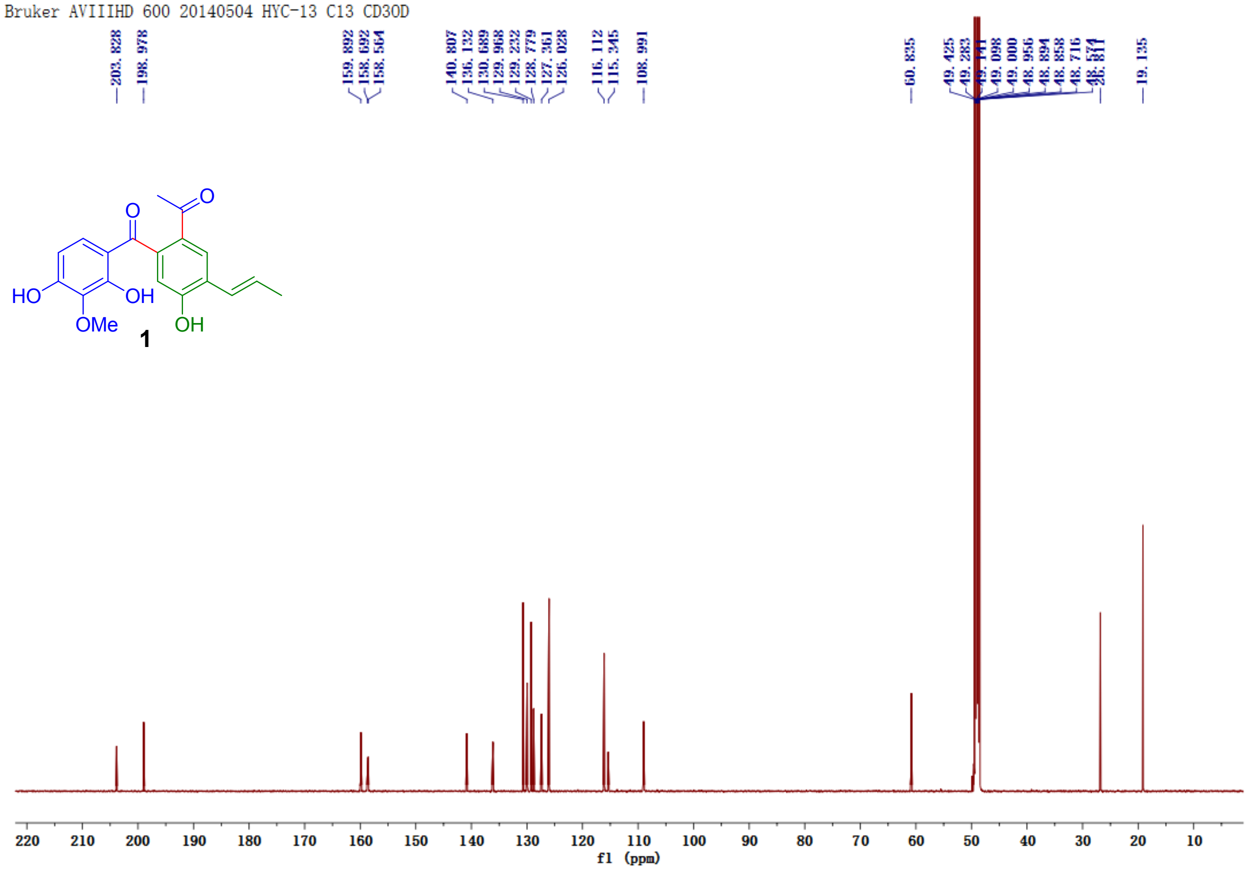


Figure S2. The ^{13}C NMR Spectrum of Compound **1** in CD_3OD (150 MHz)

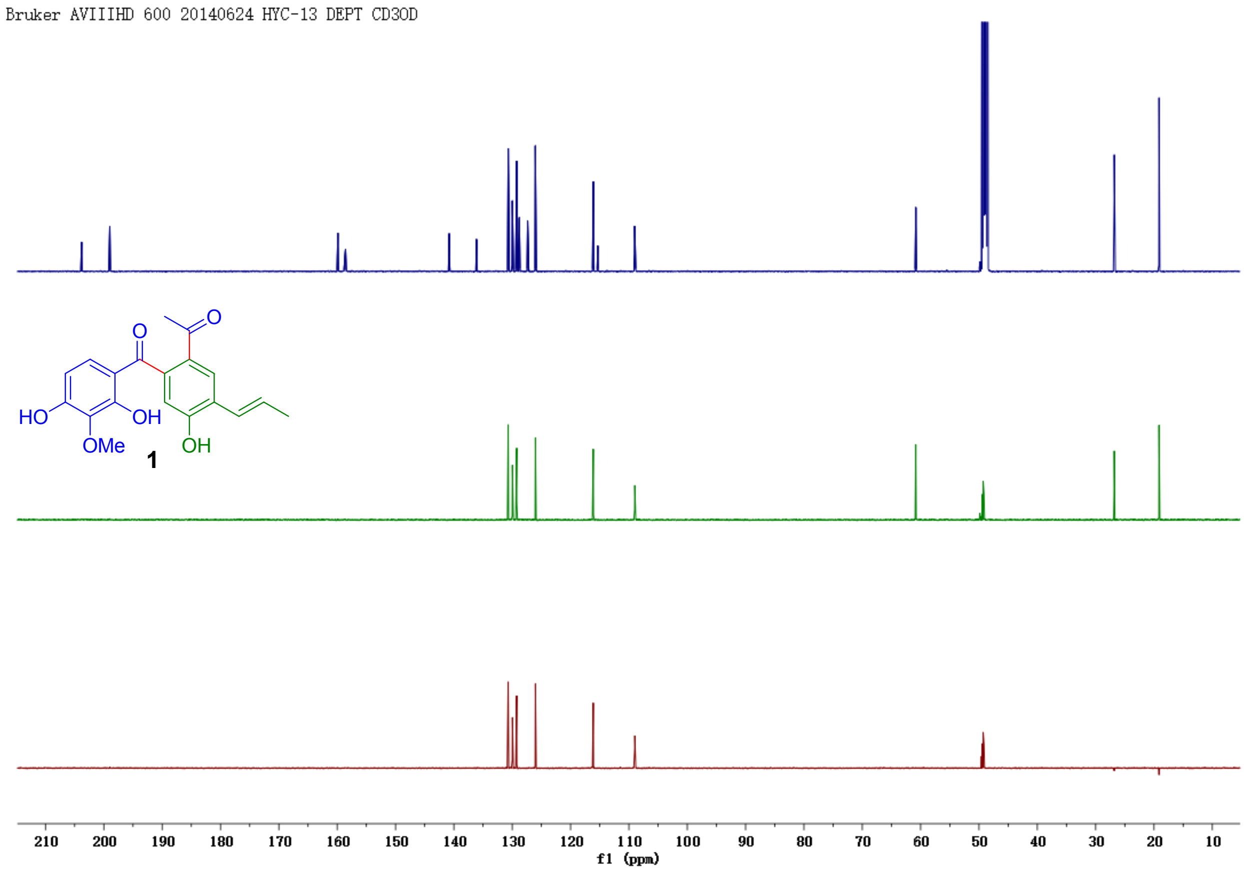


Figure S3. The DEPT Spectrum of Compound **1** in CD_3OD

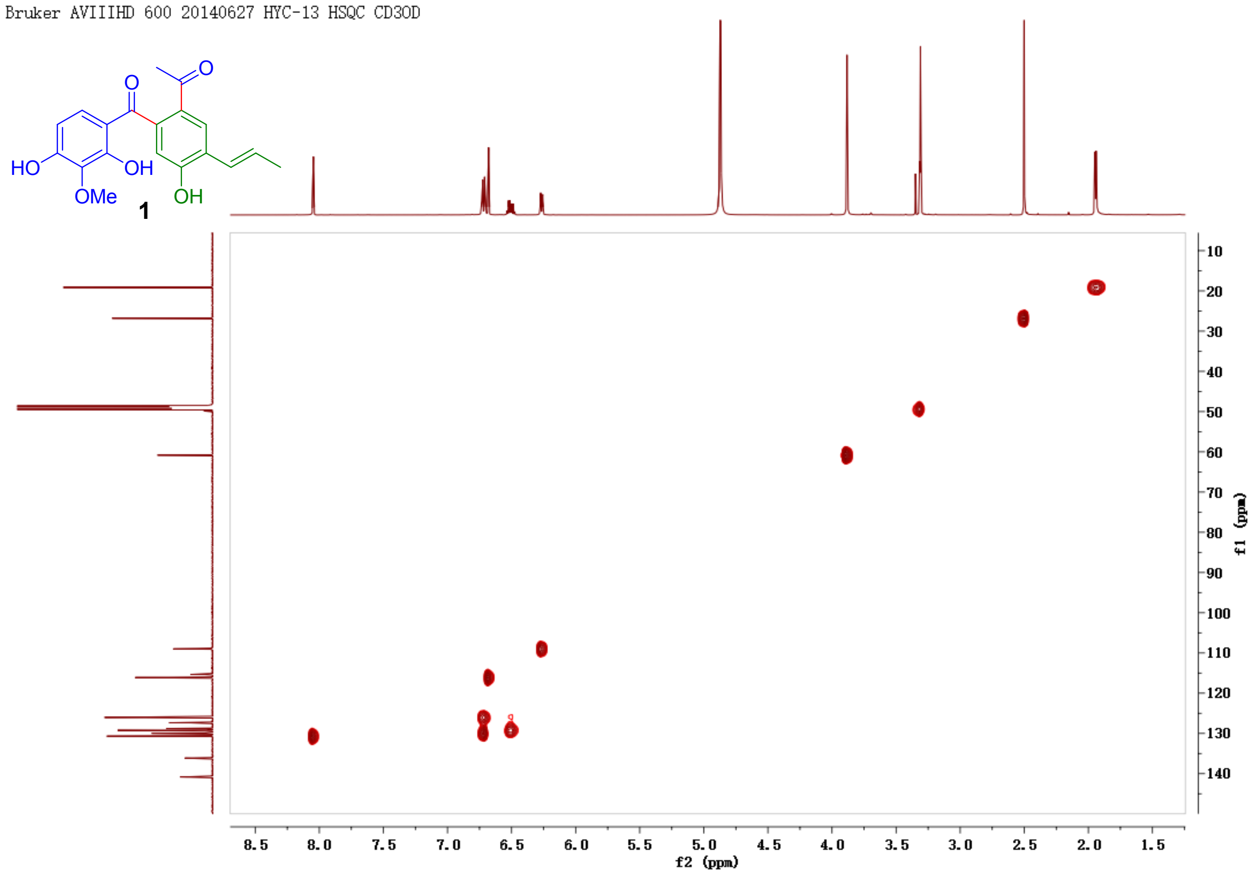


Figure S4. The HSQC Spectrum of Compound **1** in CD_3OD

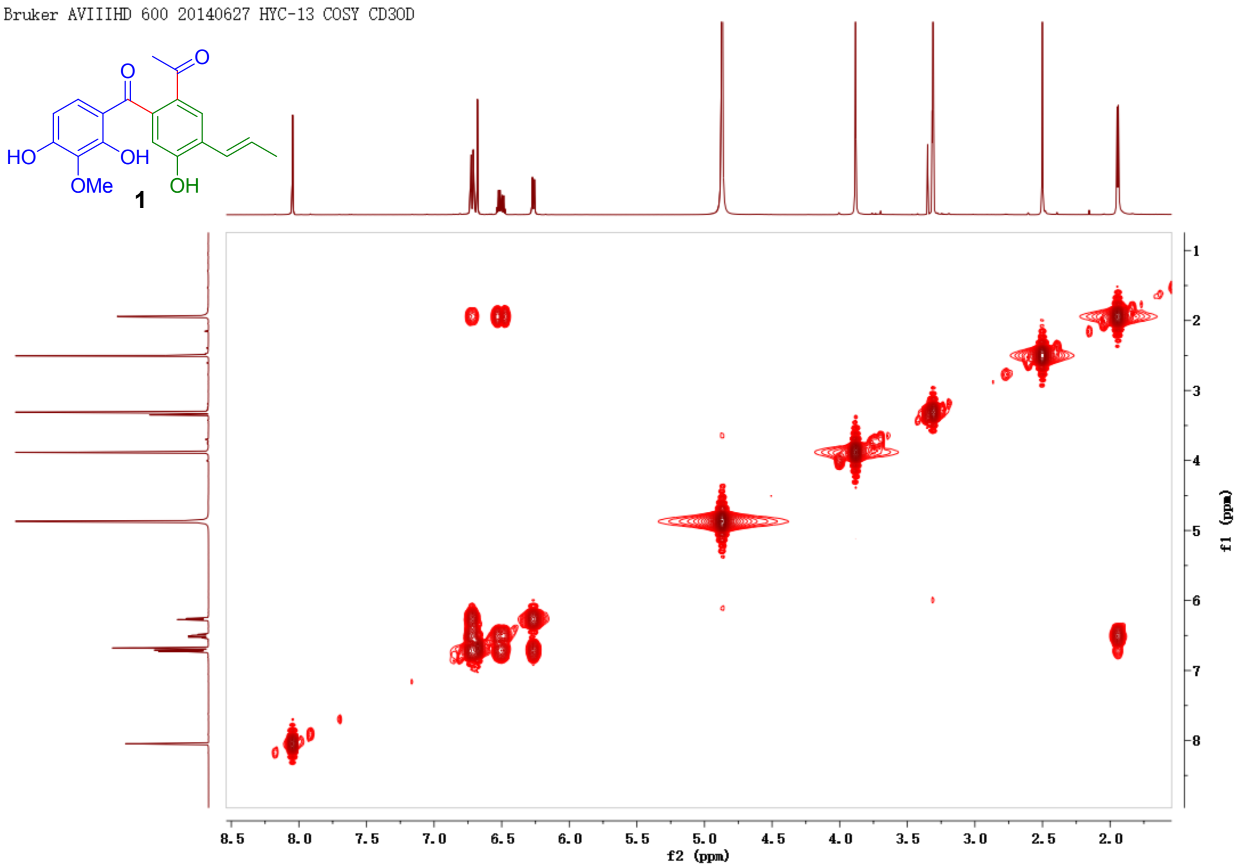


Figure S5. The ^{1}H-^{1}H gCOSY Spectrum of Compound **1** in CD_3OD

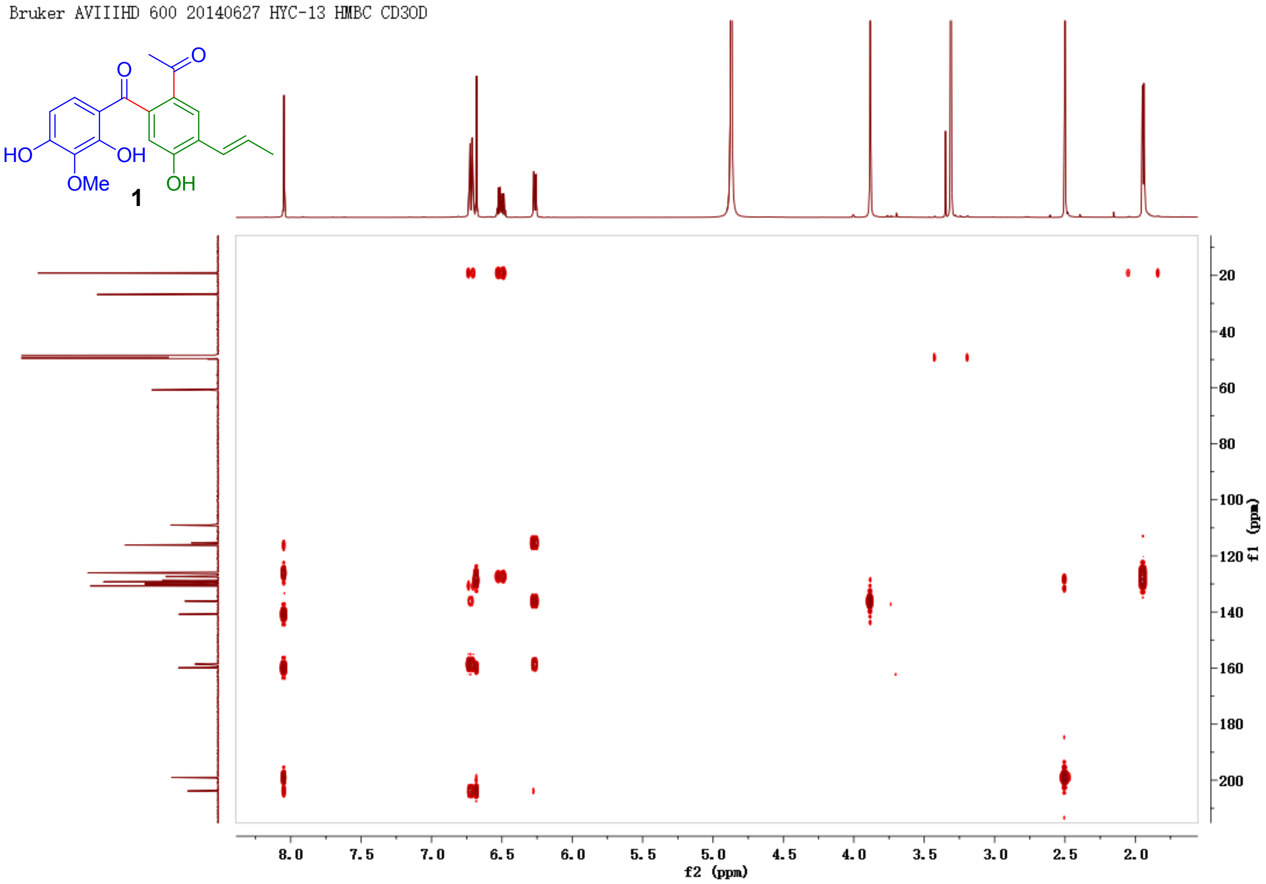


Figure S6. The HMBC Spectrum of Compound **1** in CD_3OD

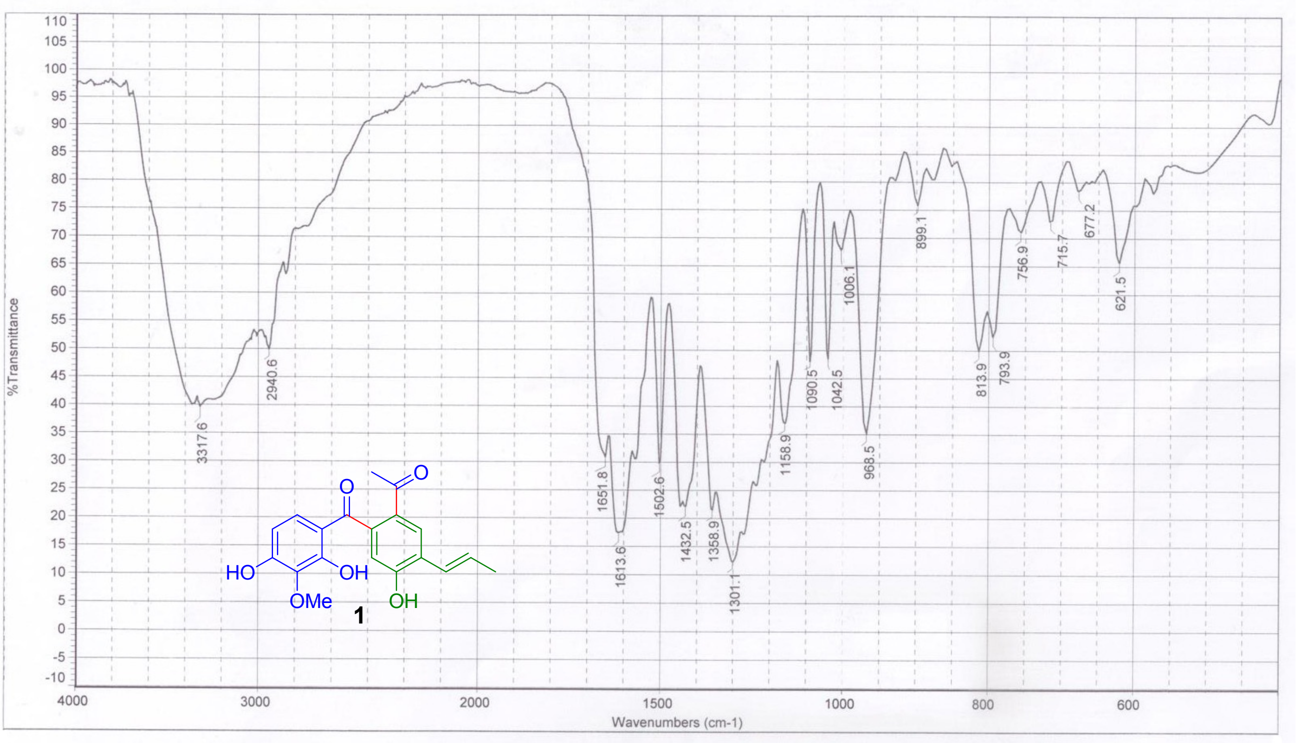
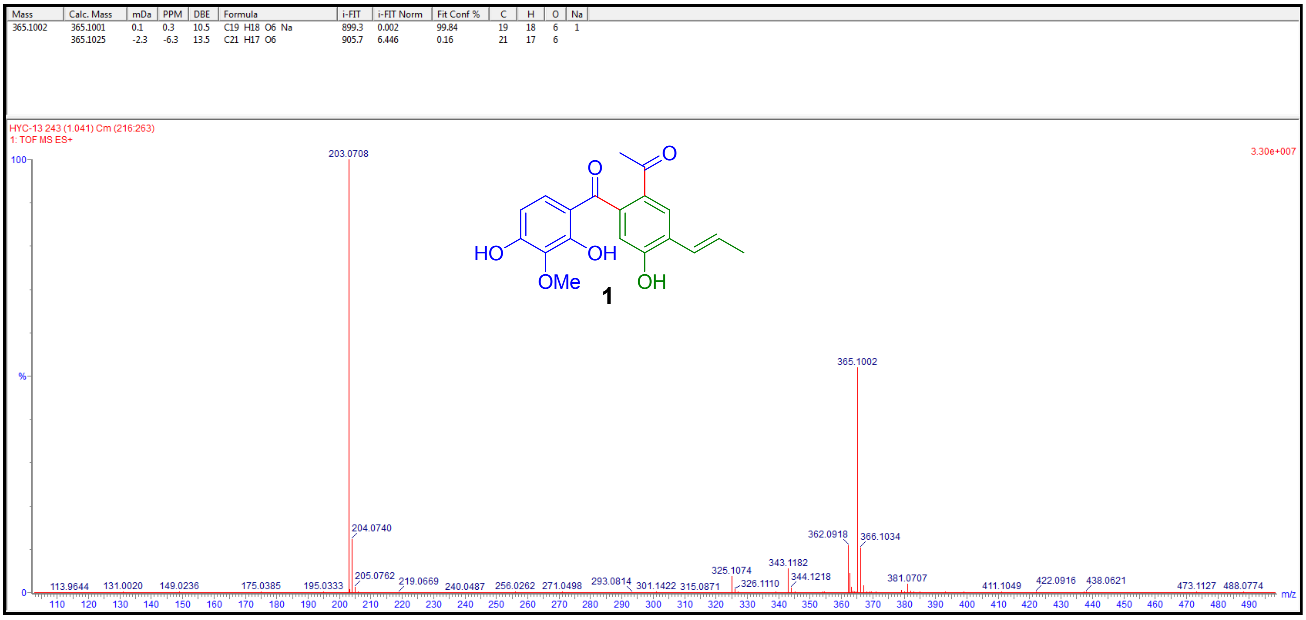


Figure S7. The IR Spectrum of Compound **1**



Mass	Calc. Mass	mDa	PPM	DBE	Formula	i-FIT	i-FIT Norm	Fit Conf %	C	H	O	Na
365.1002	365.1001	0.1	0.3	10.5	C19 H18 O6 Na	899.3	0.002	99.84	19	18	6	1
	365.1025	-2.3	-6.3	13.5	C21 H17 O6	905.7	6.446	0.16	21	17	6	

HYC-13 243 (1.041) Cm (216:263)
1: TOF MS ES+

Figure S8. The (+)-HRESIMS Spectroscopic Data of Compound **1**

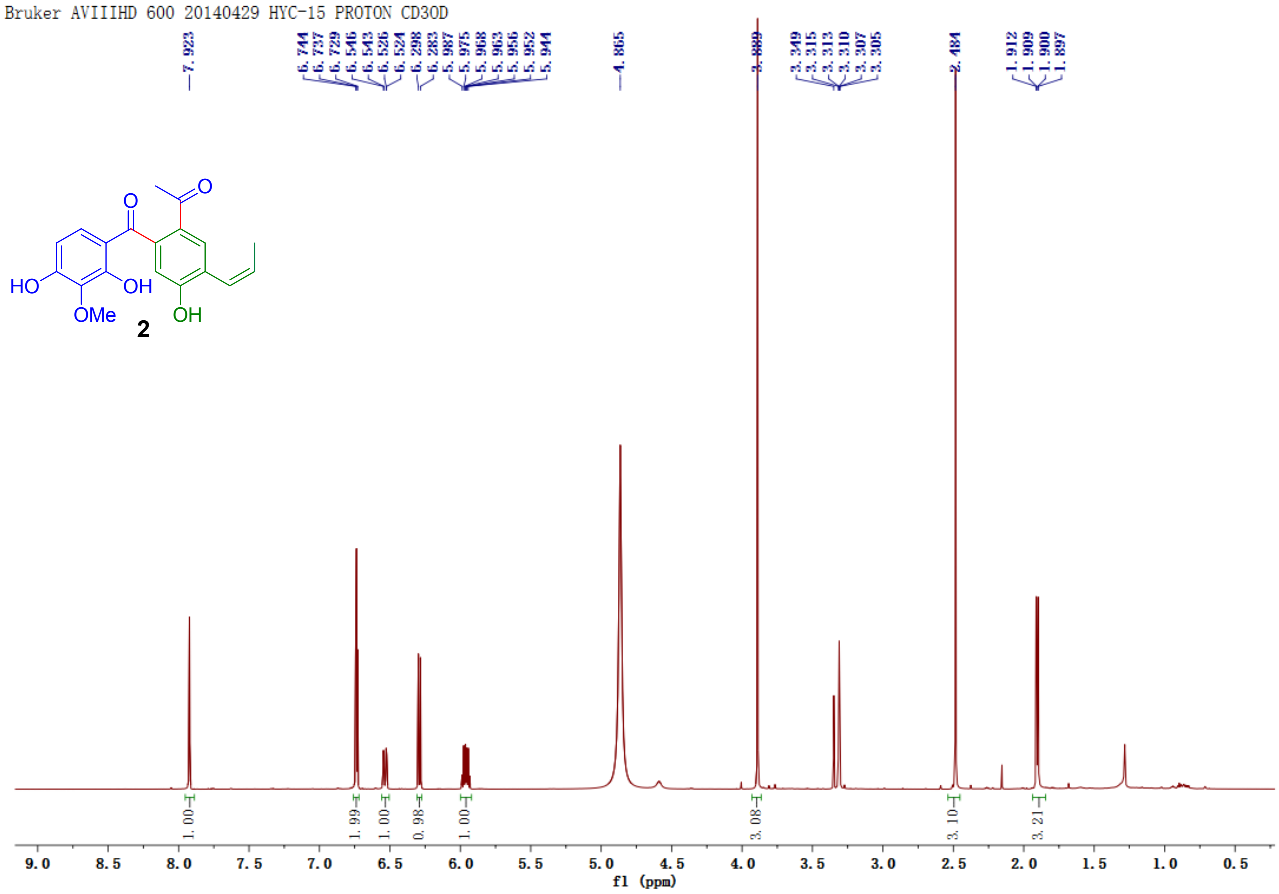


Figure S9. The ^{1}H NMR Spectrum of Compound **2** in CD_3OD (600 MHz)

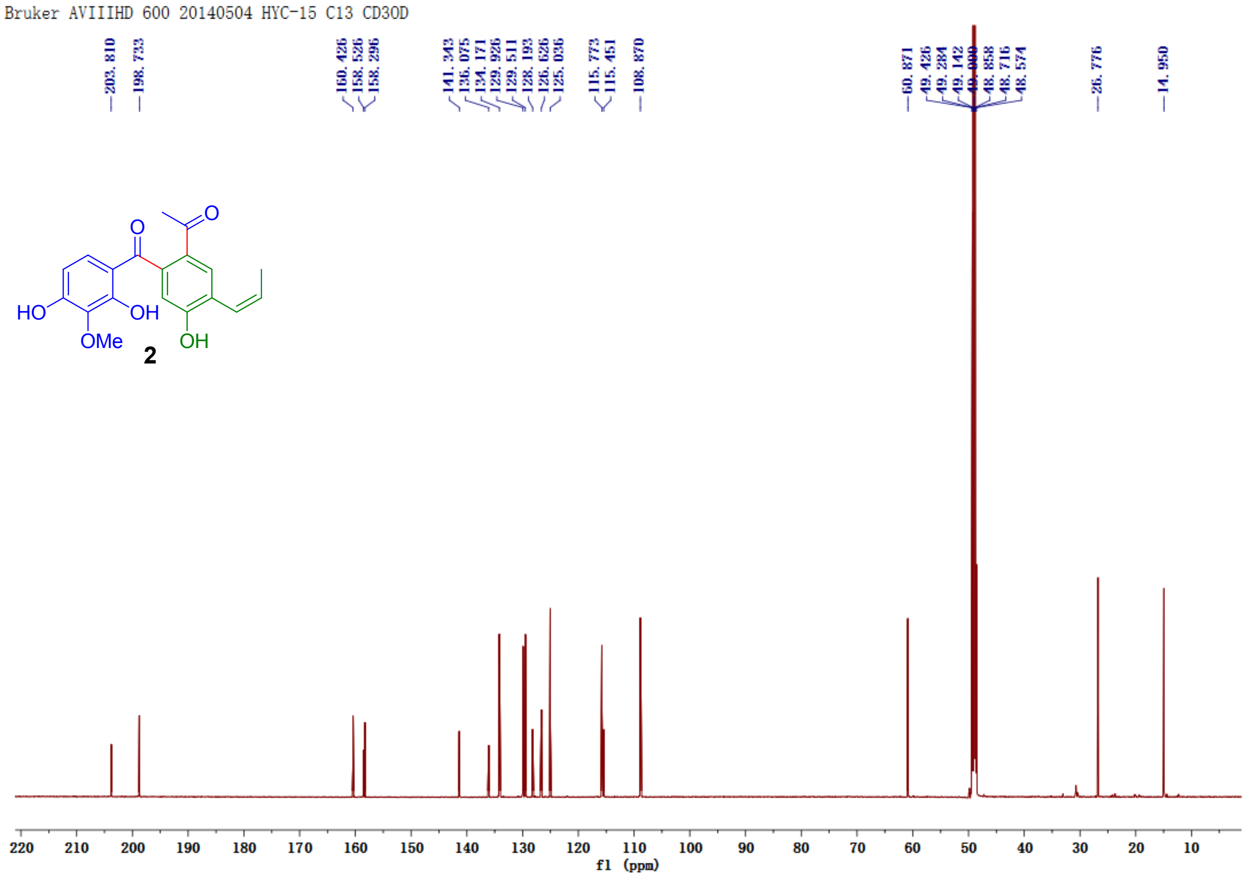


Figure S10. The ^{13}C NMR Spectrum of Compound **2** in CD_3OD (150 MHz)

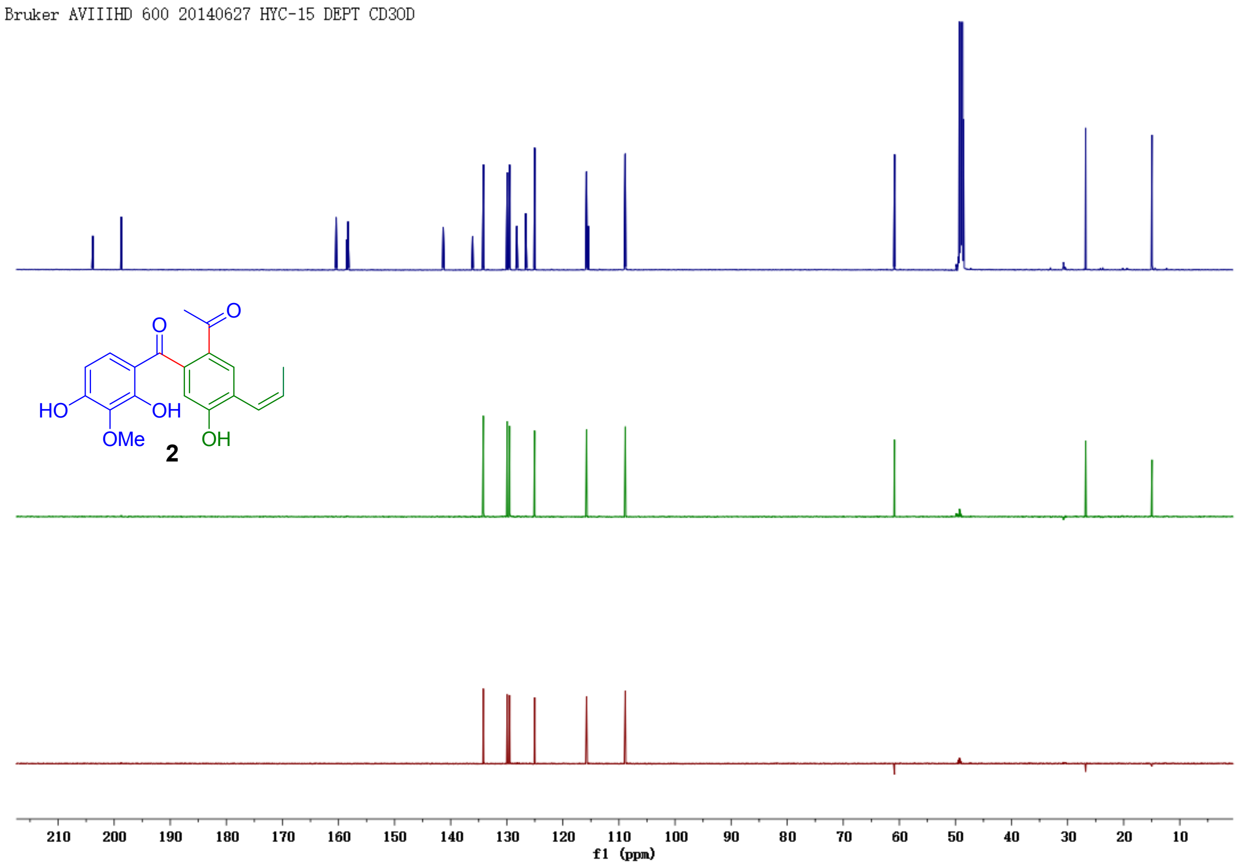


Figure S11. The DEPT Spectrum of Compound **2** in CD_3OD

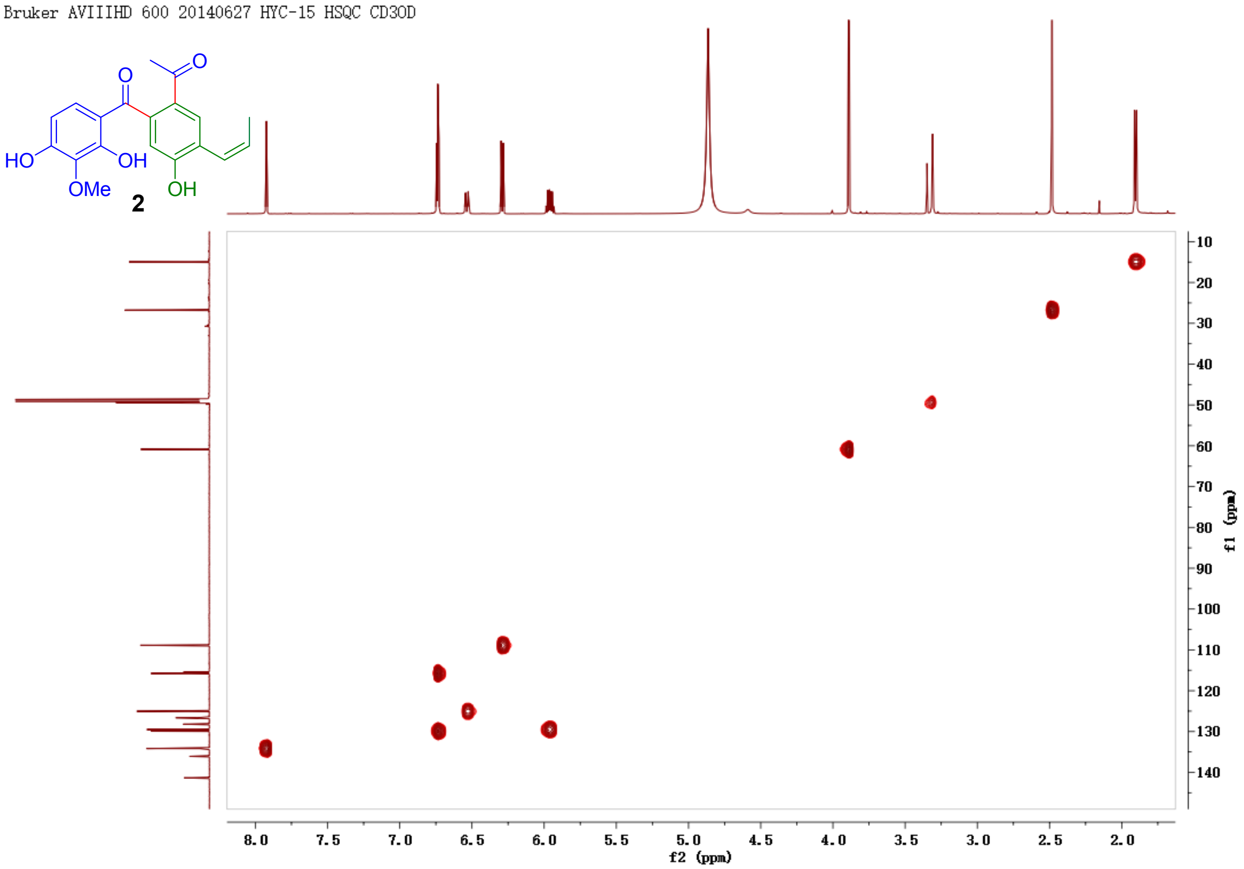


Figure S12. The HSQC Spectrum of Compound **2** in CD_3OD

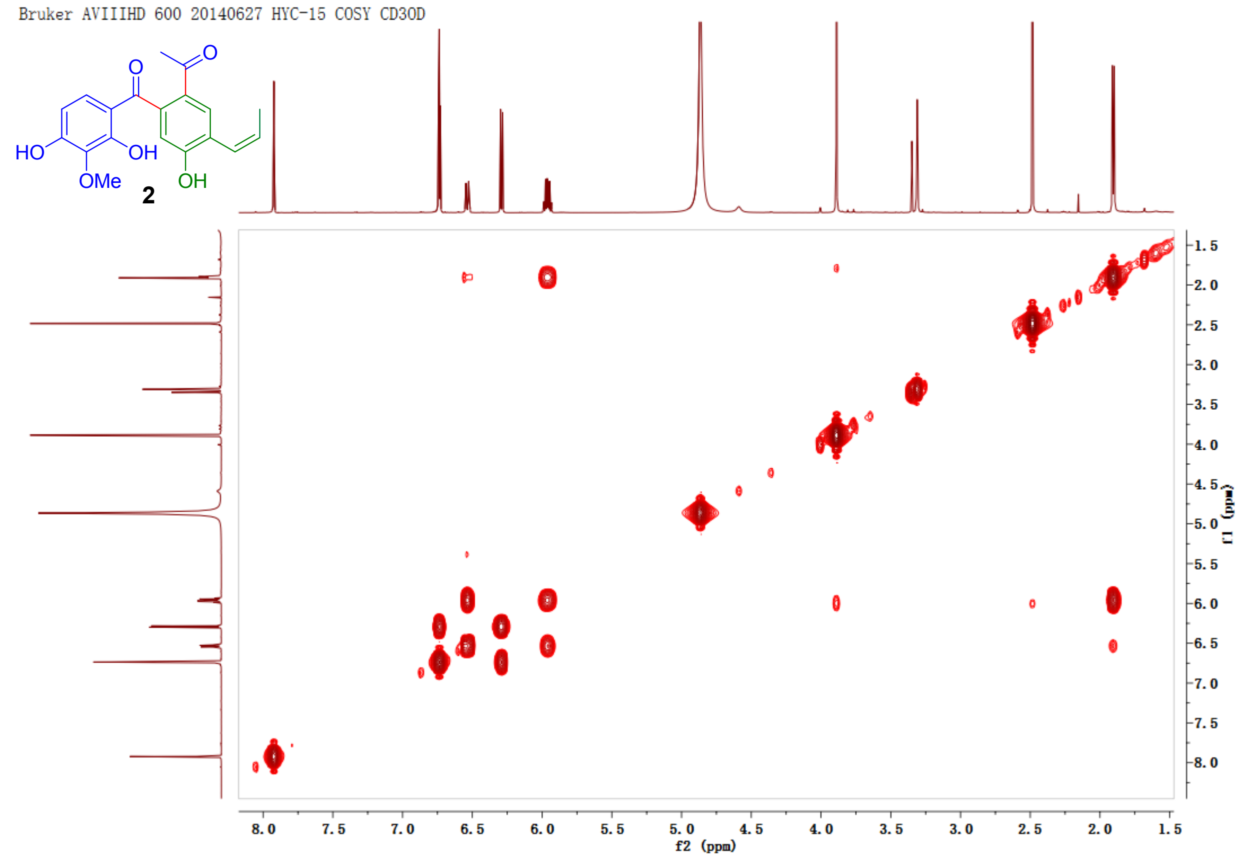


Figure S13. The ^{1}H-^{1}H gCOSY Spectrum of Compound **2** in CD$_3$OD

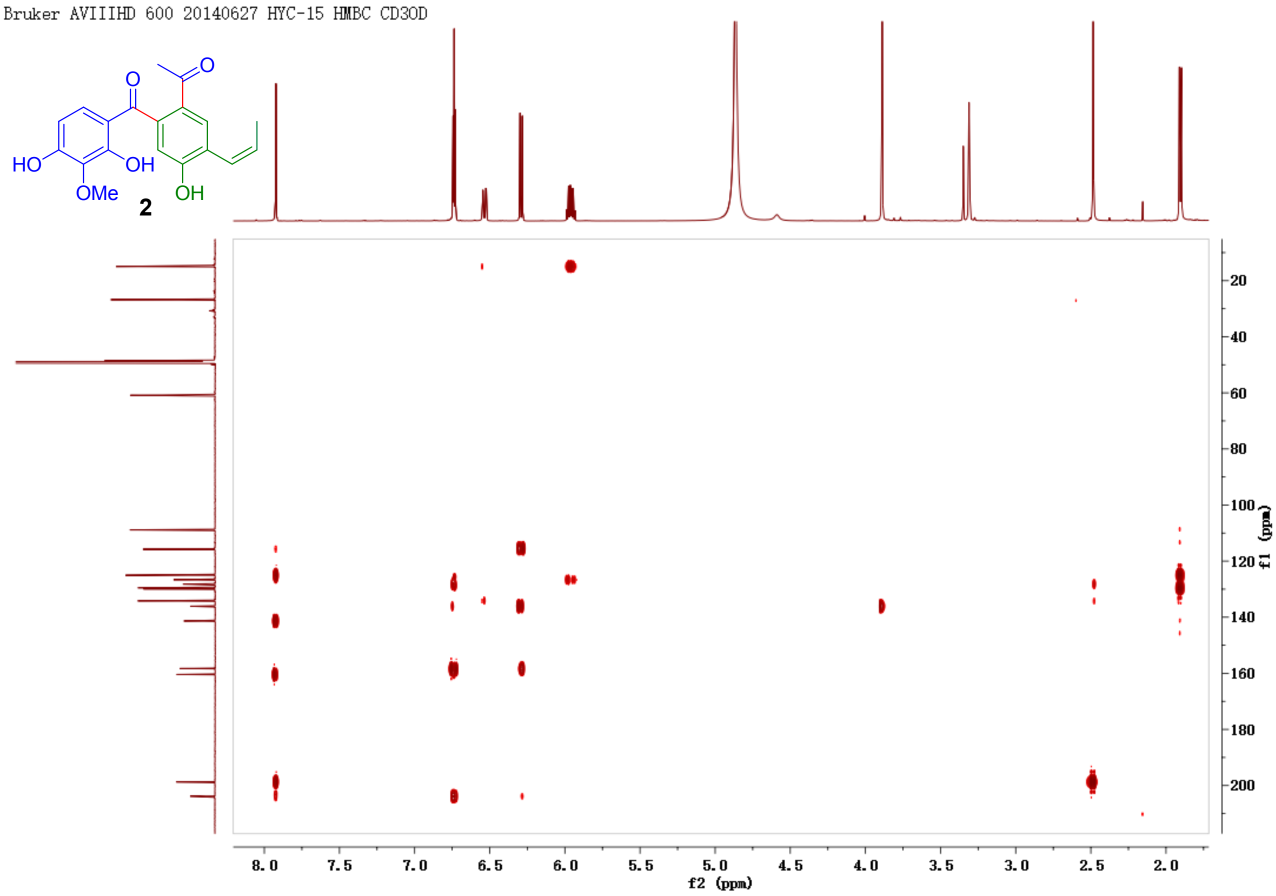


Figure S14. The HMBC Spectrum of Compound **2** in CD$_3$OD

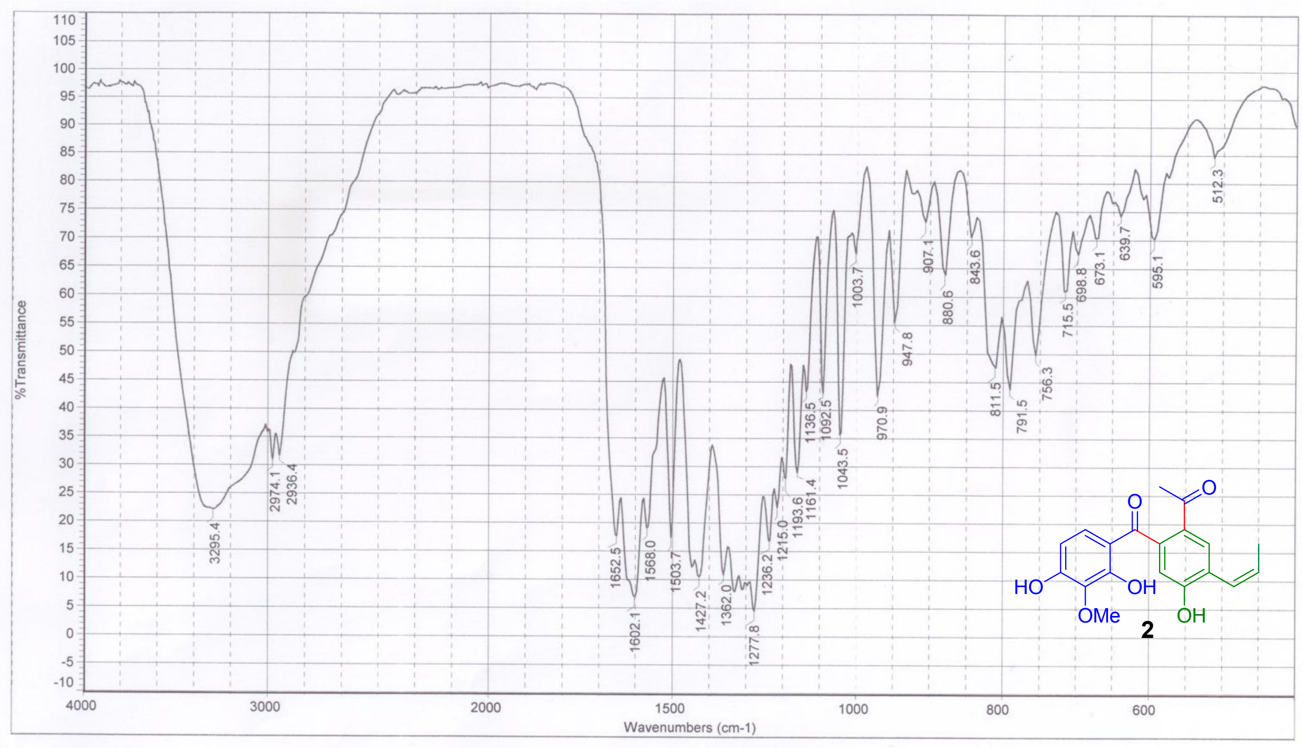
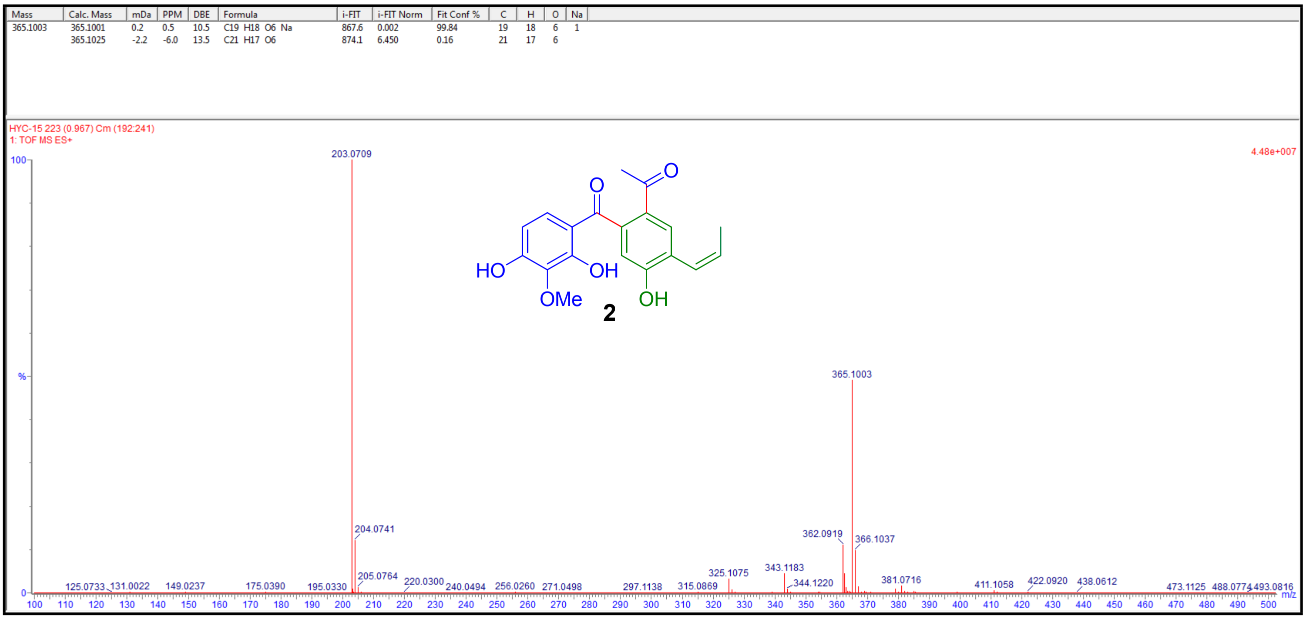


Figure S15. The IR Spectrum of Compound **2**



Mass	Calc. Mass	mDa	PPM	DBE	Formula	i-FIT	i-FIT Norm	Fit Conf %	C	H	O	Na
365.1003	365.1001	0.2	0.5	10.5	C19 H18 O6 Na	867.6	0.002	99.84	19	18	6	1
	365.1025	-2.2	-6.0	13.5	C21 H17 O6	874.1	6.450	0.16	21	17	6	

Figure S16. The (+)-HRESIMS Spectroscopic Data of Compound **2**

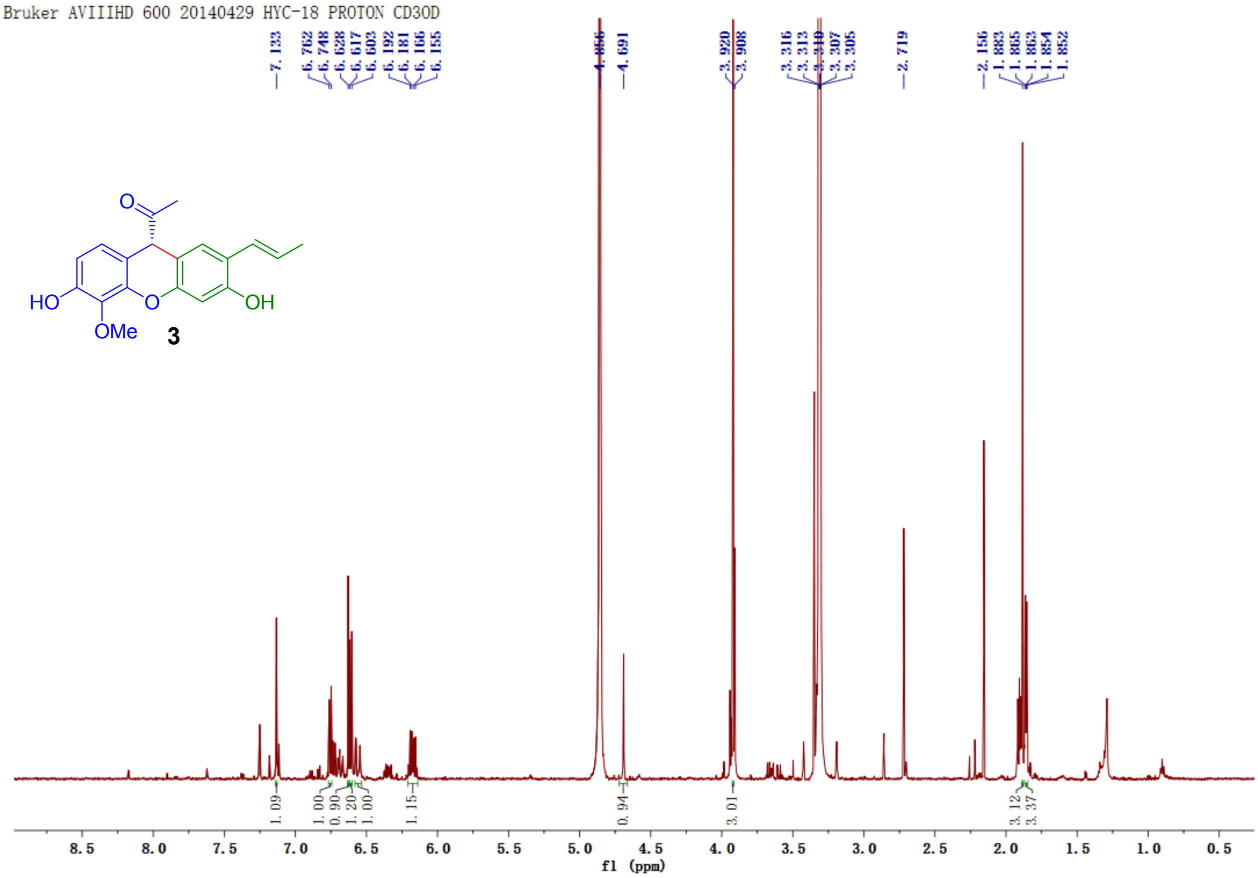


Figure S17. The ^{1}H NMR Spectrum of Compound **3** in CD_3OD (600 MHz)

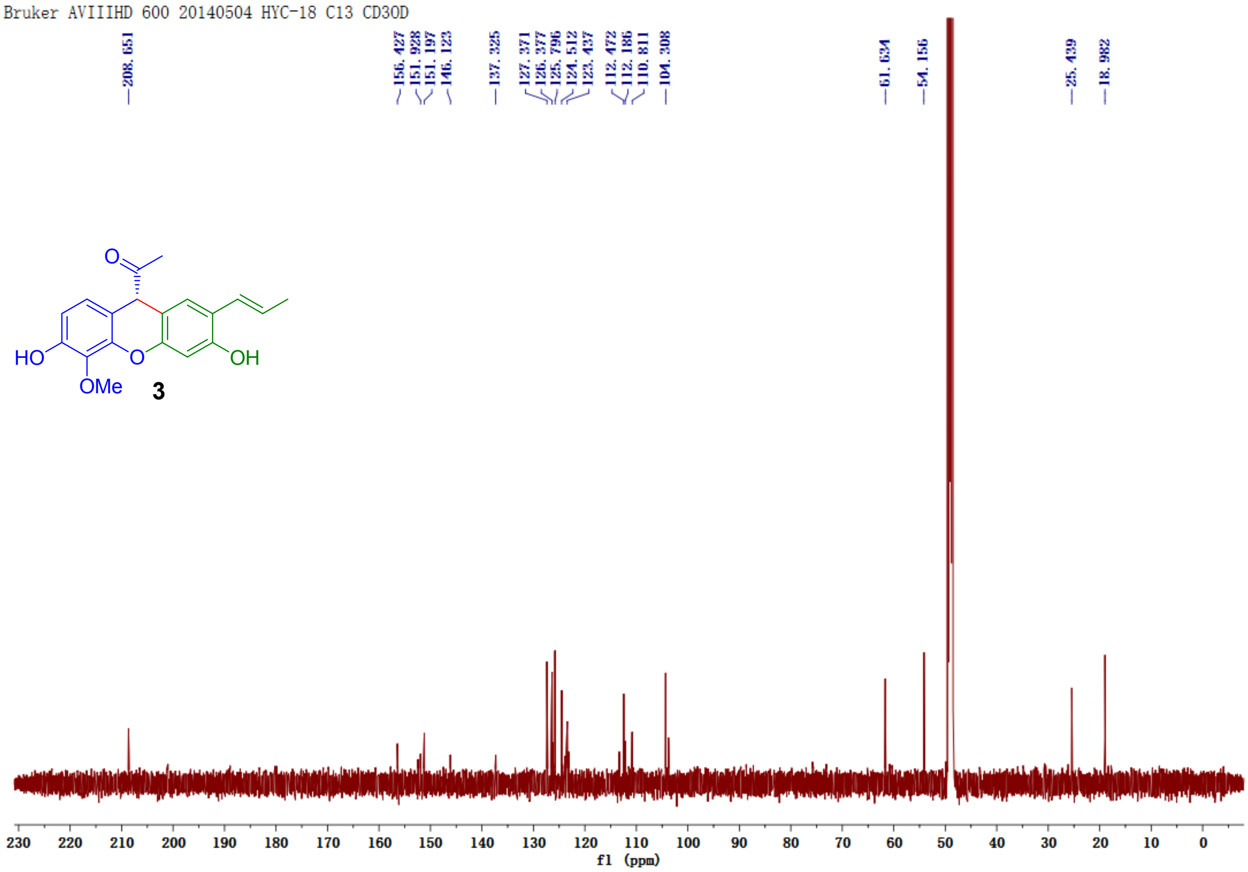


Figure S18. The ^{13}C NMR Spectrum of Compound **3** in CD_3OD (150 MHz)

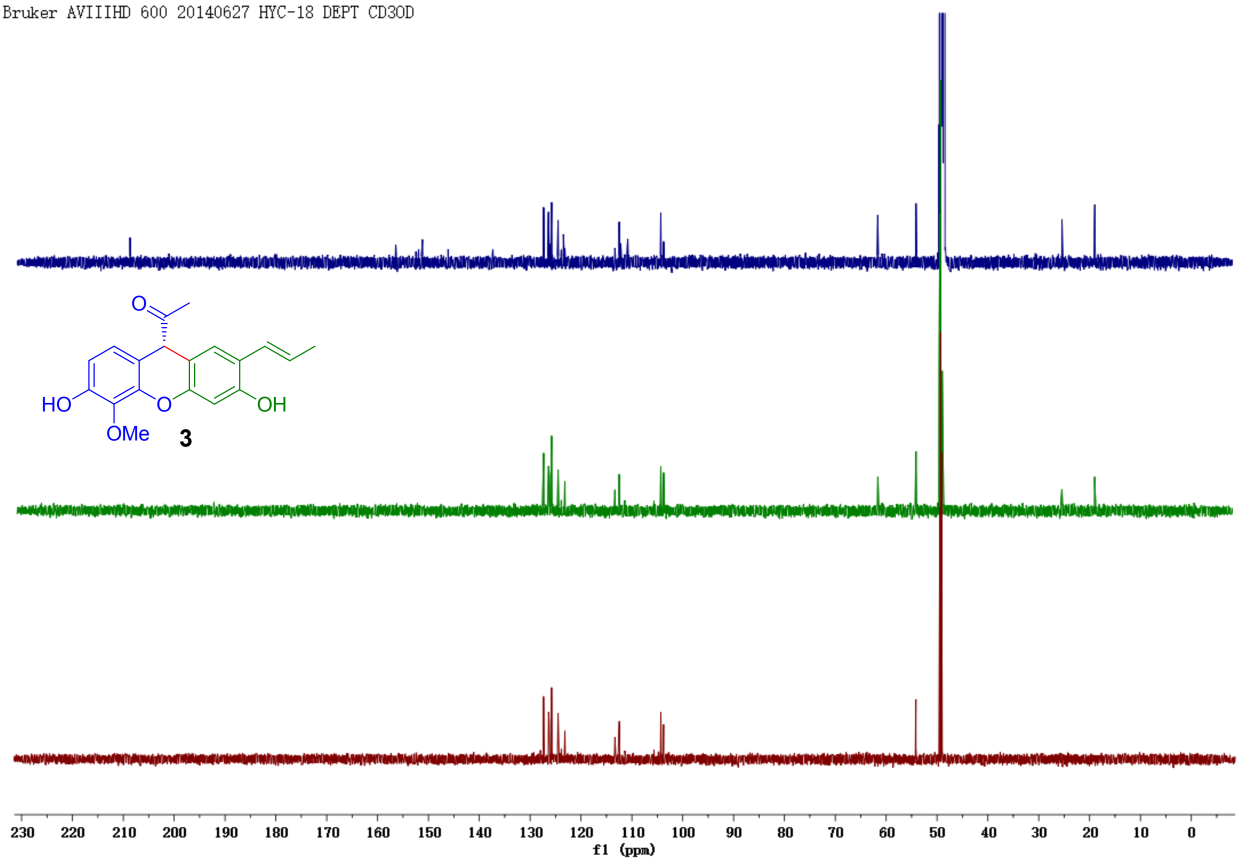


Figure S19. The DEPT Spectrum of Compound **3** in CD_3OD

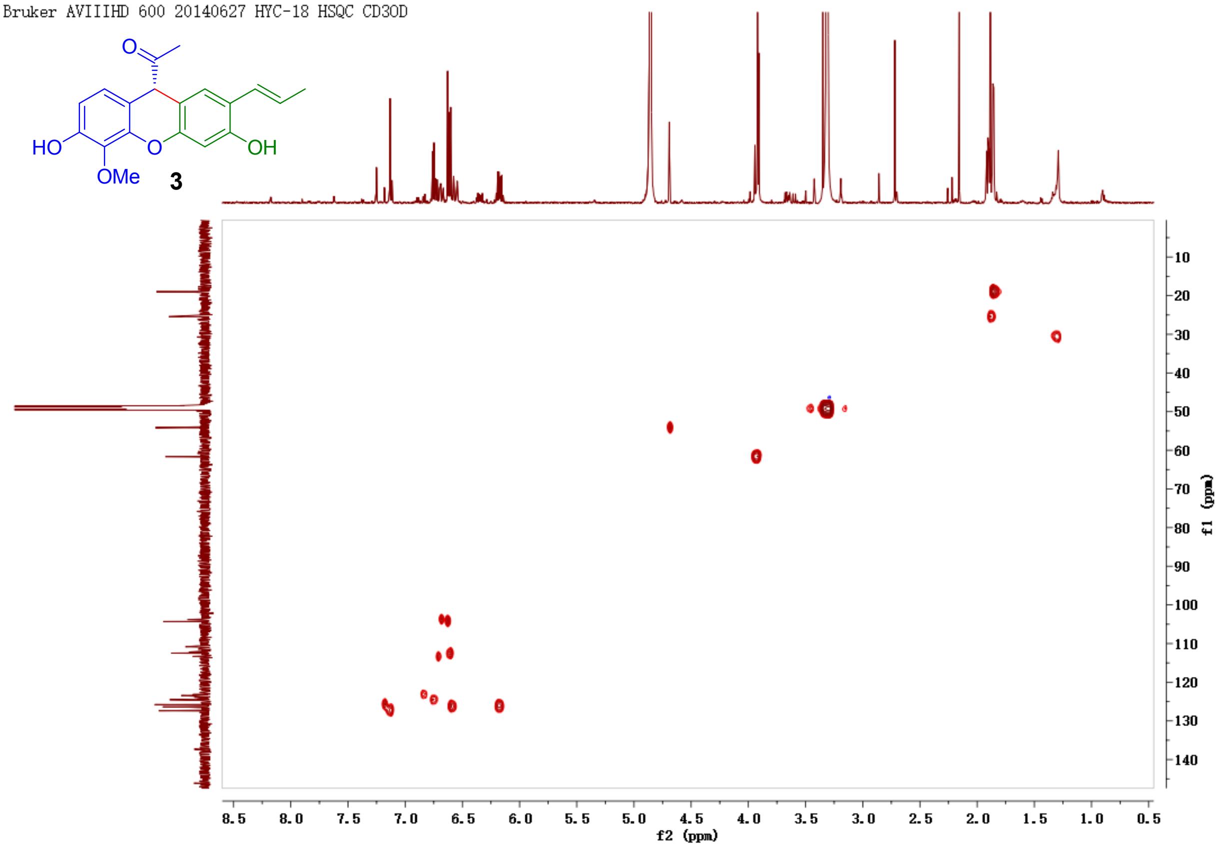


Figure S20. The HSQC Spectrum of Compound **3** in CD_3OD

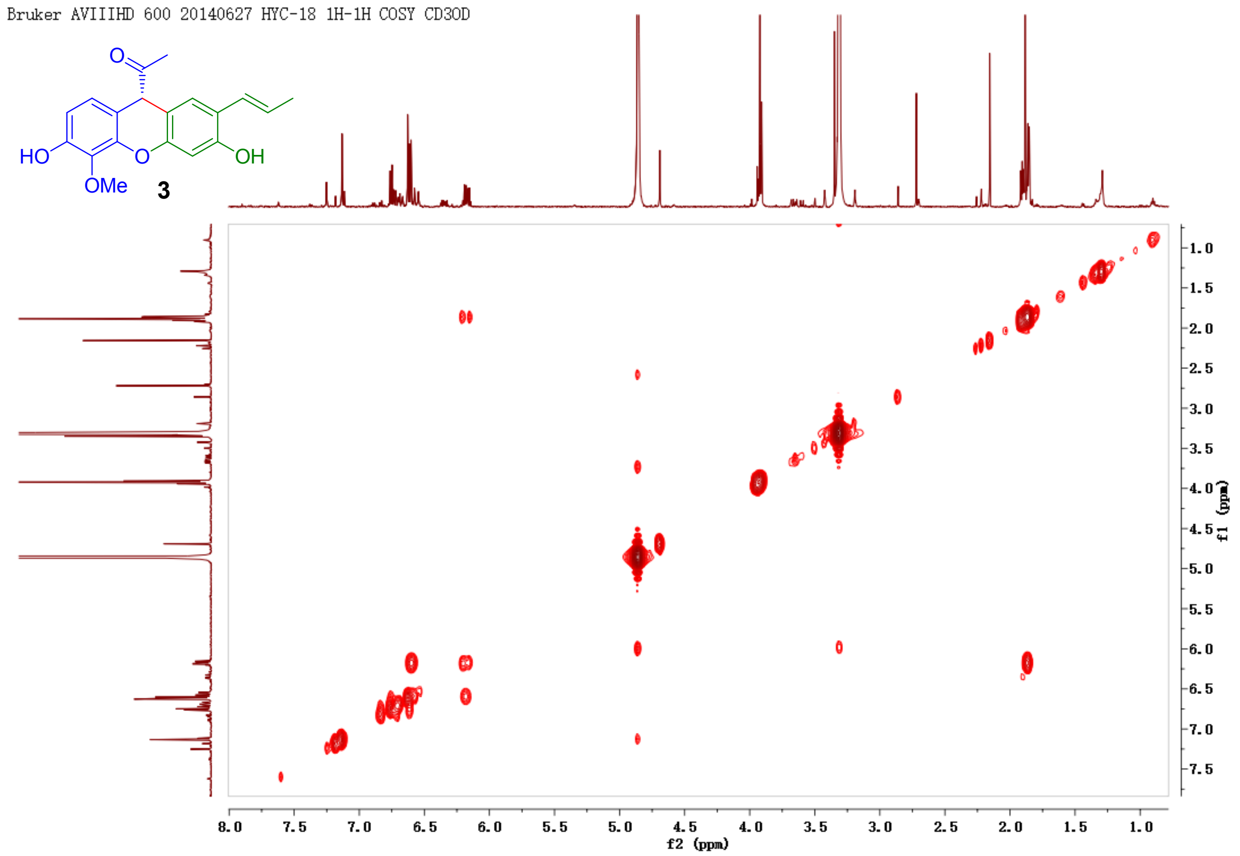


Figure S21. The ^{1}H-^{1}H gCOSY Spectrum of Compound **3** in CD_3OD

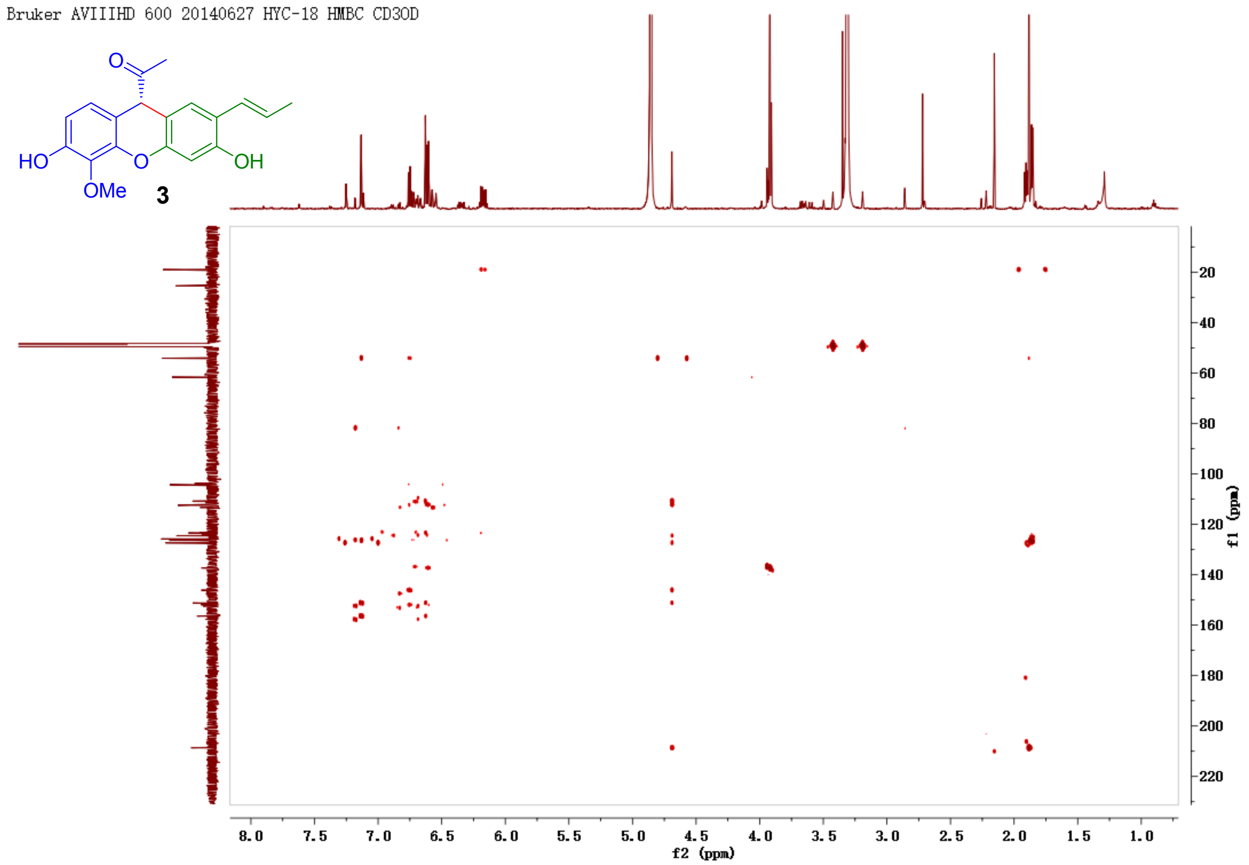


Figure S22. The HMBC Spectrum of Compound **3** in CD_3OD

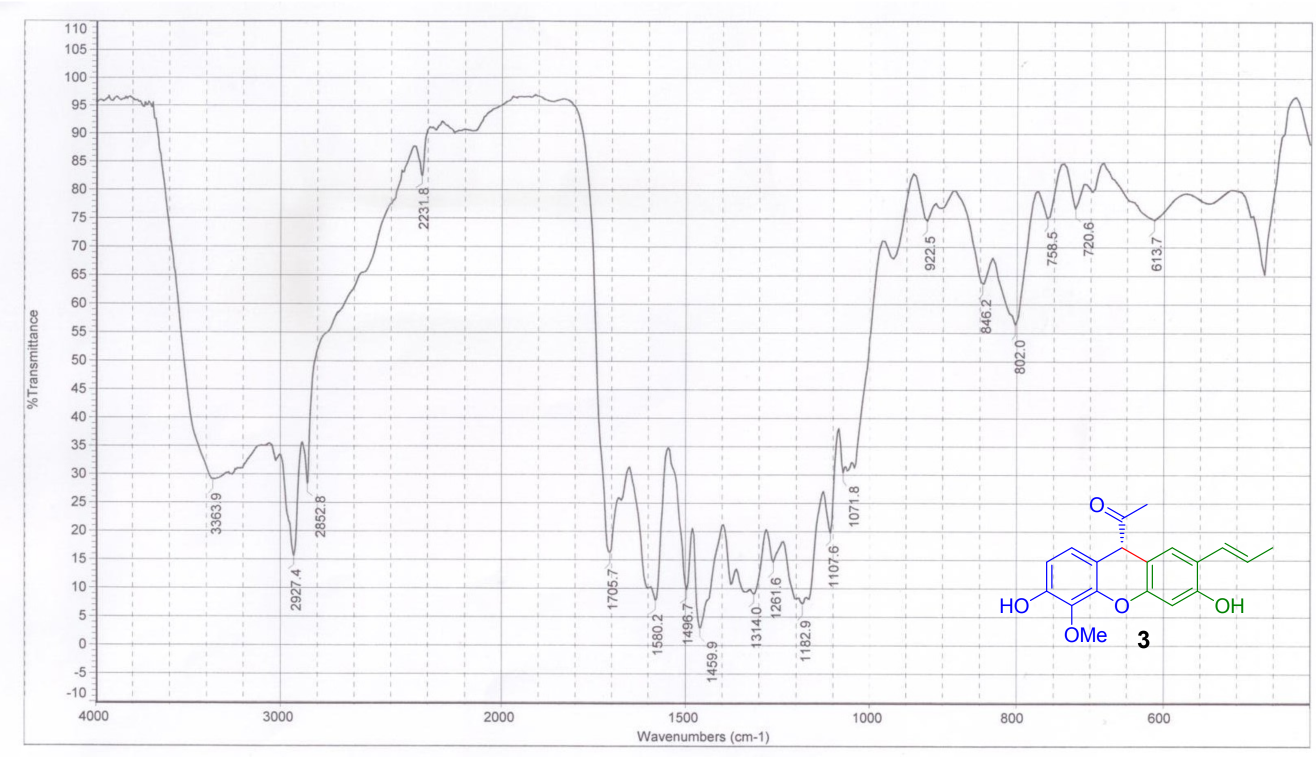
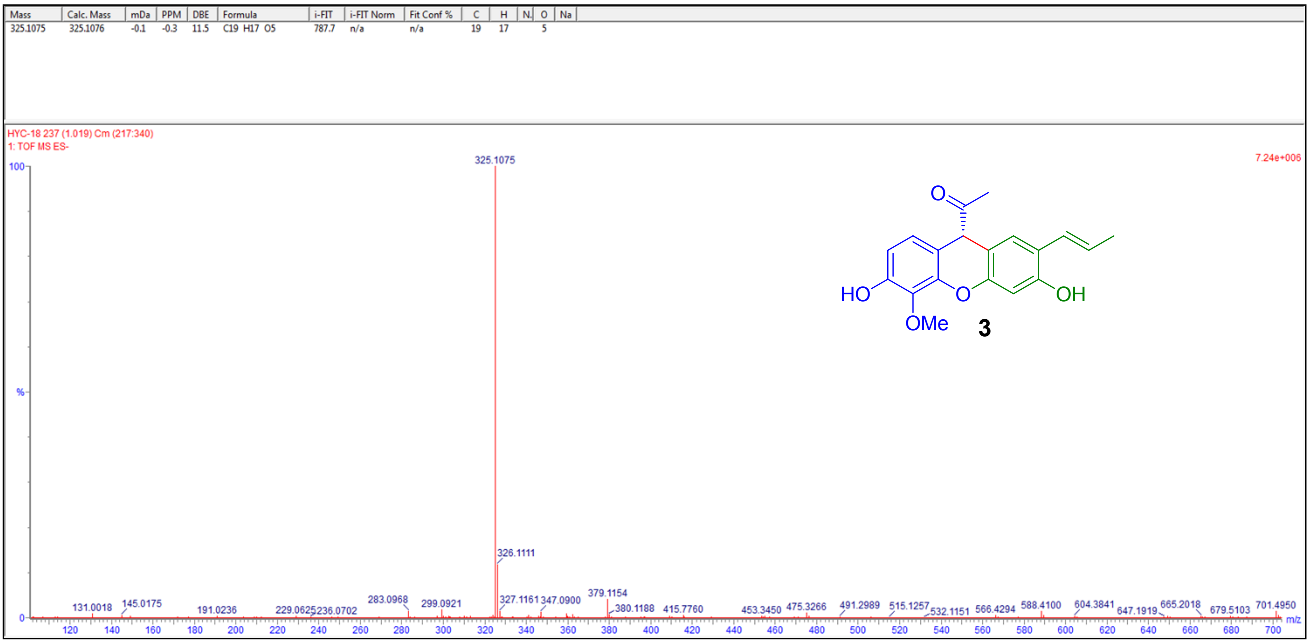


Figure S23. The IR Spectrum of Compound **3**



Mass	Calc. Mass	mDa	PPM	DBE	Formula	i-FIT	i-FIT Norm	Fit Conf %	C	H	N	O	Na
325.1075	325.1076	-0.1	-0.3	11.5	C19 H17 O5	787.7	n/a	n/a	19	17		5	

Figure S24. The (–)-HRESIMS Spectroscopic Data of Compound **3**

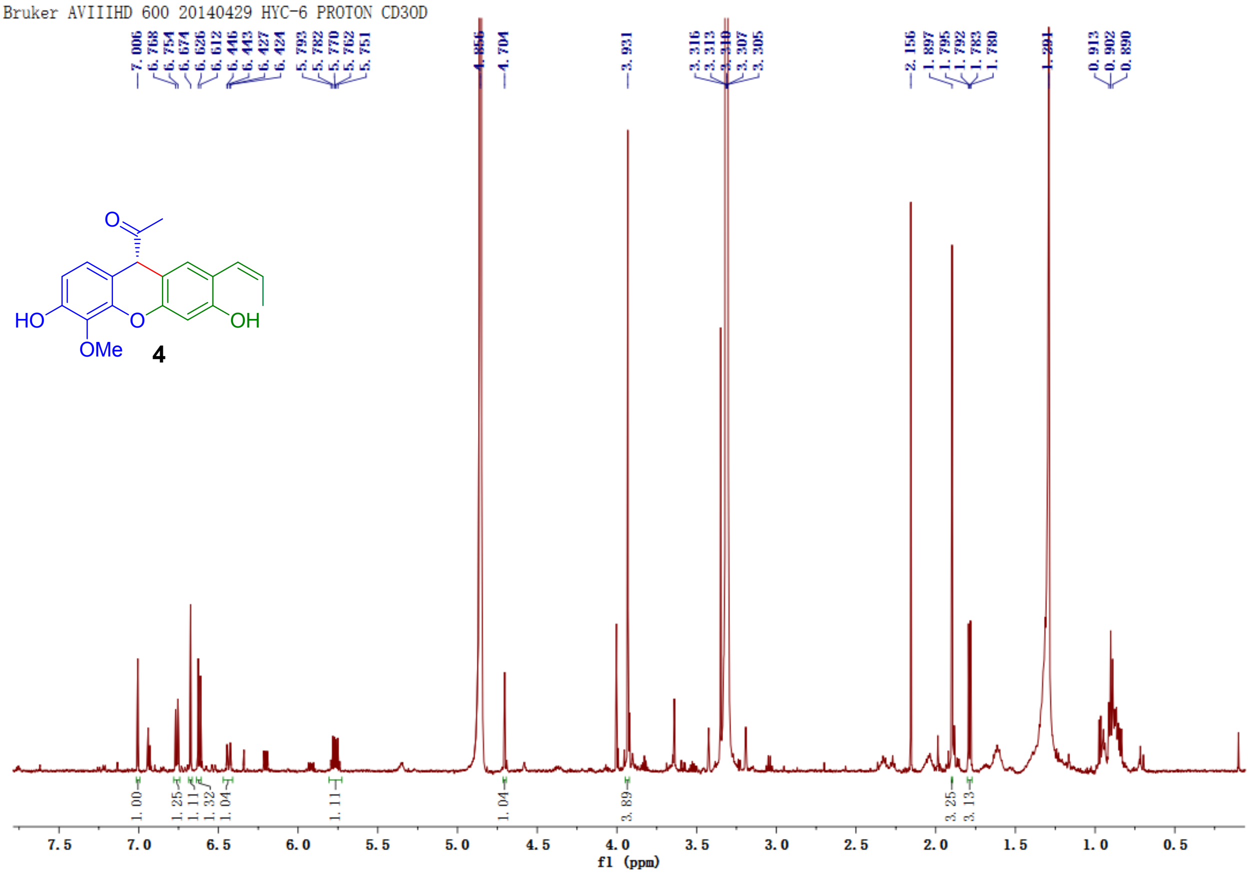


Figure S25. The ^{1}H NMR Spectrum of Compound **4** in CD_3OD (600 MHz)

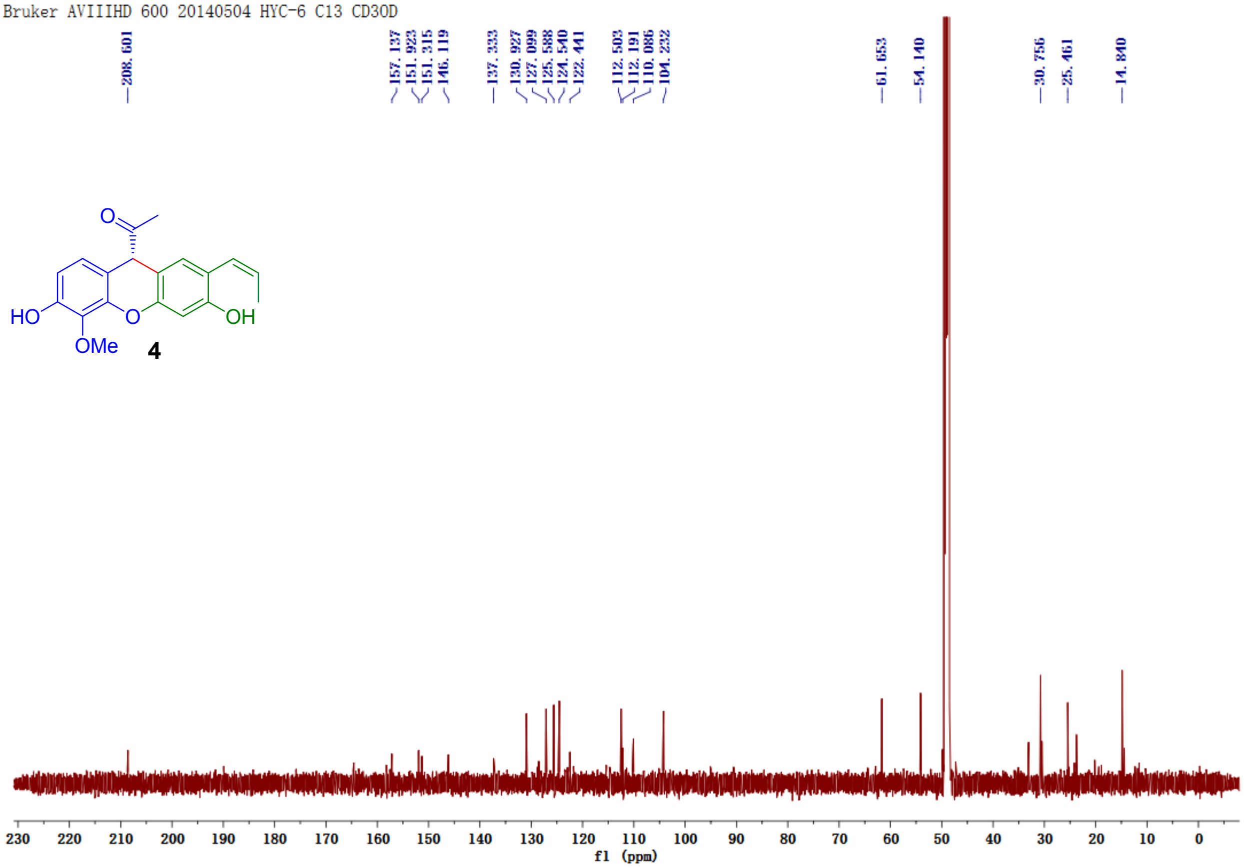


Figure S26. The ^{13}C NMR Spectrum of Compound **4** in CD_3OD (150 MHz)

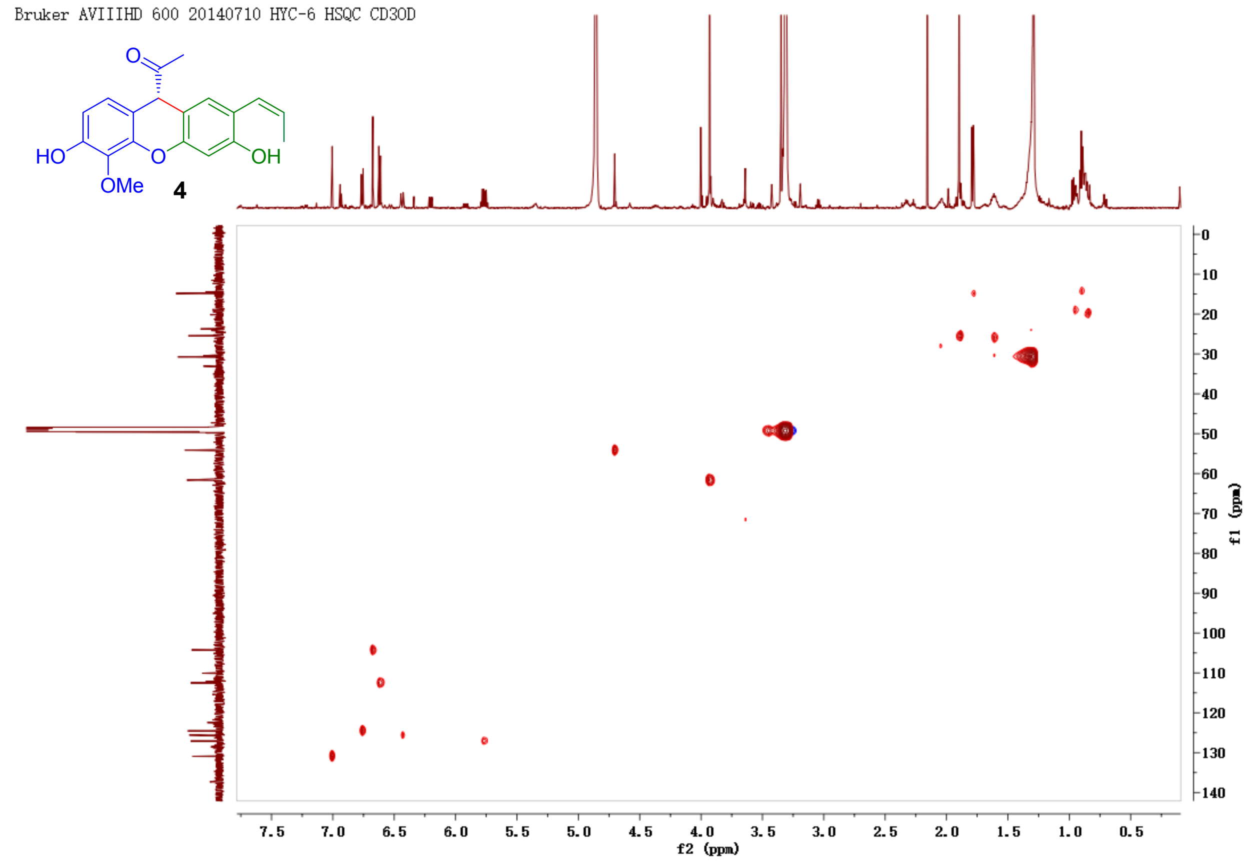


Figure S27. The HSQC Spectrum of Compound **4** in CD_3OD

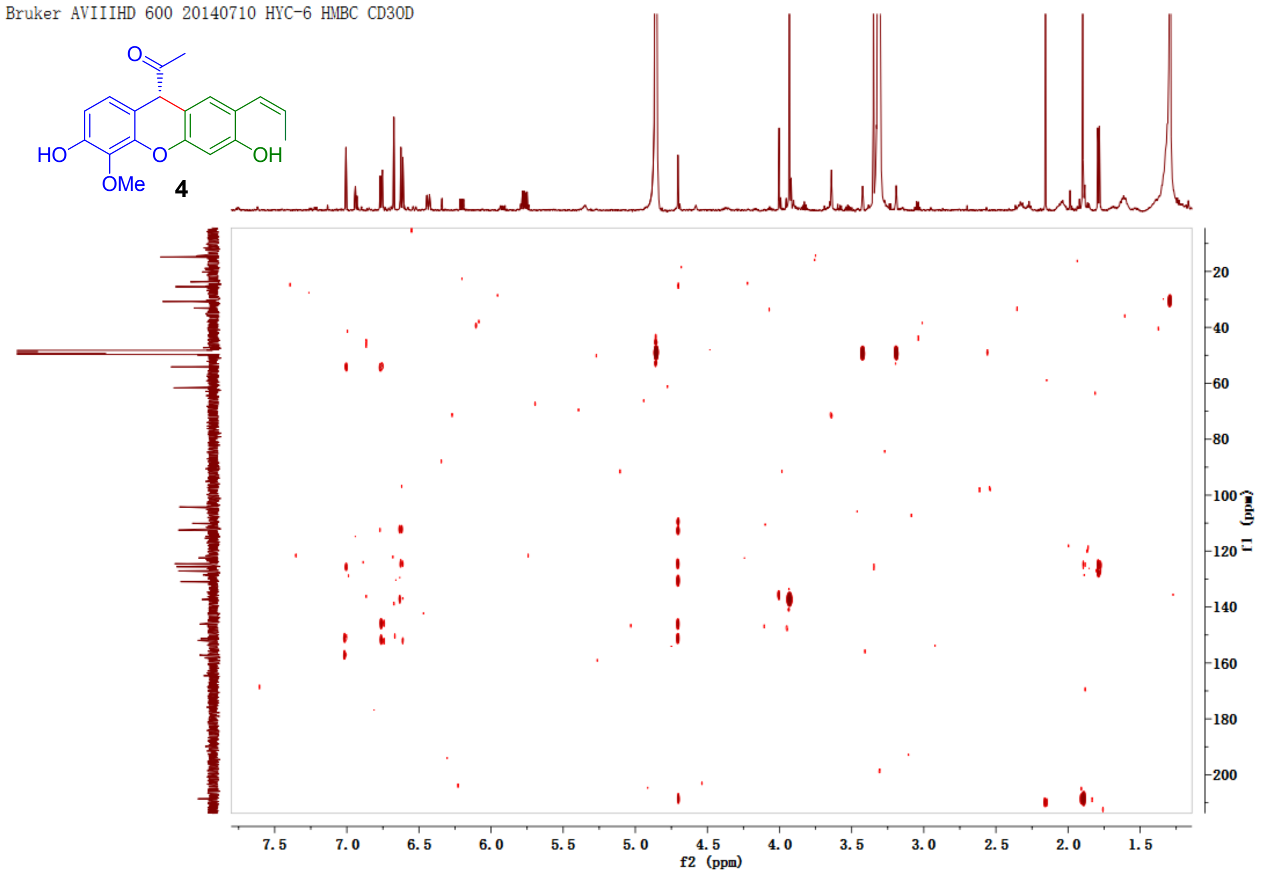
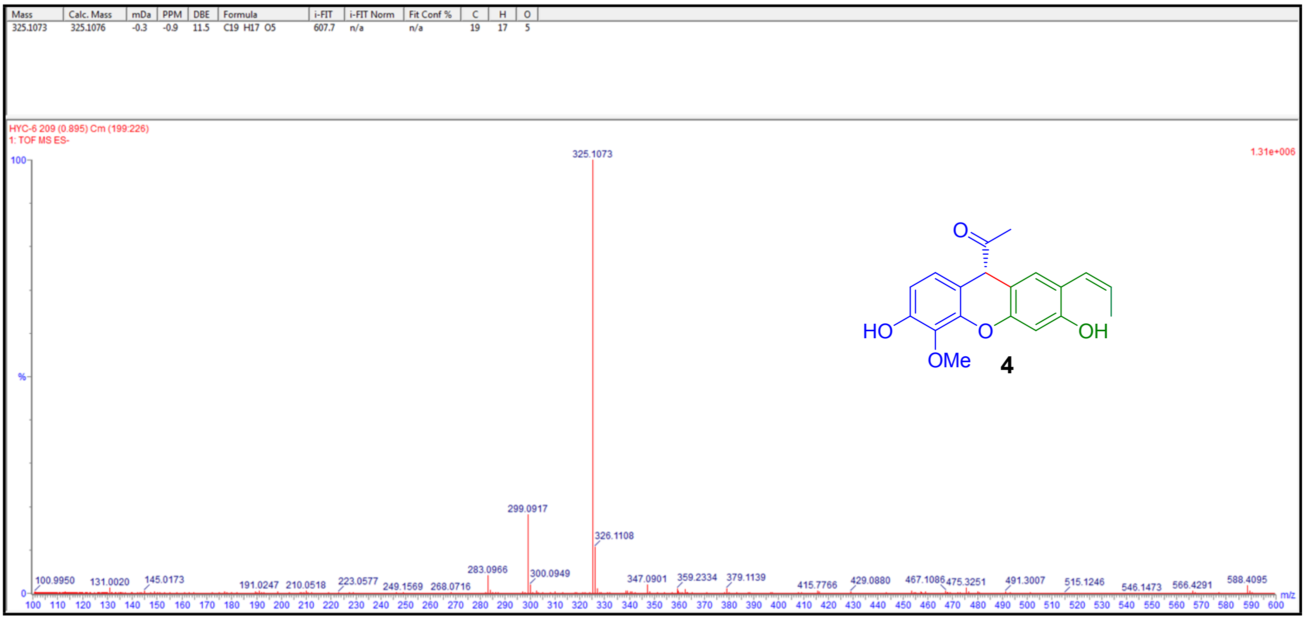


Figure S28. The HMBC Spectrum of Compound **4** in CD_3OD



Mass	Calc. Mass	mDa	PPM	DBE	Formula	i-FIT	i-FIT Norm	Fit Conf %	C	H	O
325.1073	325.1076	-0.3	-0.9	11.5	C19 H17 O5	607.7	n/a	n/a	19	17	5

HYC-6 209 (0.895) Cm (199:226)
1: TOF MS ES-

Figure S29. The (–)-HRESIMS Spectroscopic Data of Compound **4**

Table S1. Atomic Coordinates (× 10^4) and Equivalent Isotropic Displacement Parameters (Å^2 × 10^3) for Compound **2**

	x	y	z	U(eq)
O(3)	7095(1)	-972(1)	4971(1)	22(1)
O(1S)	3697(1)	1244(1)	6695(1)	18(1)
O(4)	7859(1)	-187(1)	3849(1)	22(1)
O(2)	7460(1)	-432(1)	6271(1)	22(1)
O(7)	8323(1)	603(1)	7025(1)	19(1)
O(6')	12409(1)	2476(1)	6799(1)	23(1)
O(8)	6313(1)	1629(1)	6425(1)	21(1)
C(10)	5658(2)	-997(1)	5049(1)	28(1)
C(3)	7628(1)	-311(1)	5068(1)	17(1)
C(2)	7836(1)	-36(1)	5727(1)	16(1)
C(1)	8407(1)	639(1)	5807(1)	16(1)
C(7)	8550(1)	943(1)	6490(1)	16(1)
C(4')	9103(1)	1677(1)	6556(1)	15(1)
C(3')	8299(1)	2282(1)	6517(1)	16(1)
C(2')	8916(1)	2939(1)	6582(1)	16(1)
C(1')	10293(1)	3010(1)	6683(1)	16(1)
C(7')	10963(1)	3702(1)	6728(1)	18(1)
C(8')	10599(1)	4248(1)	7111(1)	20(1)
C(9')	9483(1)	4293(1)	7625(1)	23(1)
C(4)	8036(1)	70(1)	4492(1)	18(1)
C(6)	8814(1)	1006(1)	5212(1)	18(1)
C(5)	8650(1)	726(1)	4566(1)	20(1)
C(5')	10475(1)	1736(1)	6655(1)	18(1)
C(6')	11074(1)	2397(1)	6710(1)	17(1)
C(8)	6828(1)	2213(1)	6429(1)	18(1)
C(9)	5990(1)	2865(1)	6355(1)	29(1)

Table S2. Anisotropic Displacement Parameters for Compound **2**

	U11	**U22**	**U33**	**U23**	**U13**	**U12**
O(3)	27(1)	13(1)	25(1)	-2(1)	-1(1)	-5(1)
O(1S)	15(1)	19(1)	20(1)	2(1)	0(1)	-2(1)
O(4)	26(1)	20(1)	18(1)	-3(1)	0(1)	-7(1)
O(2)	34(1)	15(1)	18(1)	1(1)	-1(1)	-7(1)
O(7)	25(1)	14(1)	19(1)	1(1)	-1(1)	-2(1)
O(6')	14(1)	16(1)	38(1)	-2(1)	-3(1)	0(1)
O(8)	16(1)	16(1)	31(1)	-2(1)	1(1)	-2(1)
C(10)	29(1)	28(1)	28(1)	-2(1)	0(1)	-14(1)
C(3)	16(1)	12(1)	23(1)	-1(1)	-1(1)	0(1)
C(2)	16(1)	13(1)	21(1)	3(1)	0(1)	1(1)
C(1)	14(1)	13(1)	21(1)	0(1)	-1(1)	1(1)
C(7)	12(1)	13(1)	21(1)	1(1)	0(1)	2(1)
C(4')	18(1)	14(1)	13(1)	0(1)	0(1)	-1(1)
C(3')	17(1)	14(1)	16(1)	0(1)	0(1)	1(1)
C(2')	18(1)	13(1)	19(1)	0(1)	0(1)	2(1)
C(1')	19(1)	14(1)	16(1)	-1(1)	1(1)	-1(1)
C(7')	17(1)	16(1)	22(1)	1(1)	0(1)	-2(1)
C(8')	20(1)	14(1)	24(1)	0(1)	-3(1)	-3(1)
C(9')	23(1)	20(1)	24(1)	-4(1)	-1(1)	1(1)
C(4)	16(1)	18(1)	19(1)	-2(1)	-1(1)	2(1)
C(6)	18(1)	14(1)	23(1)	0(1)	1(1)	-3(1)
C(5)	23(1)	19(1)	19(1)	2(1)	1(1)	-4(1)
C(5')	17(1)	13(1)	22(1)	0(1)	0(1)	3(1)
C(6')	15(1)	18(1)	18(1)	-1(1)	-1(1)	-1(1)
C(8)	18(1)	16(1)	19(1)	-1(1)	1(1)	0(1)
C(9)	16(1)	19(1)	52(1)	0(1)	-3(1)	2(1)

Table S3. Bond Lengths for Compound **2**

Bond	Length
O(3)-C(3)	1.3791(15)
O(3)-C(10)	1.4389(18)
O(1S)-H(1SB)	0.821(9)
O(1S)-H(1SA)	0.823(9)
O(4)-C(4)	1.3477(16)
O(4)-H(4)	0.8400
O(2)-C(2)	1.3475(16)
O(2)-H(2)	0.8400
O(7)-C(7)	1.2432(16)
O(6')-C(6')	1.3471(16)
O(6')-H(6')	0.8400
O(8)-C(8)	1.2238(16)
C(10)-H(10A)	0.9800
C(10)-H(10B)	0.9800
C(10)-H(10C)	0.9800
C(3)-C(4)	1.3908(19)
C(3)-C(2)	1.3939(18)
C(2)-C(1)	1.4133(17)
C(1)-C(6)	1.4065(18)
C(1)-C(7)	1.4493(18)
C(7)-C(4')	1.5062(17)
C(4')-C(5')	1.3828(18)
C(4')-C(3')	1.4053(17)
C(3')-C(2')	1.3972(17)
C(3')-C(8)	1.4789(18)
C(2')-C(1')	1.3904(18)
C(2')-H(2')	0.9500
C(1')-C(6')	1.4039(18)
C(1')-C(7')	1.4773(17)
C(7')-C(8')	1.3272(19)
C(7')-H(7')	0.9500
C(8')-C(9')	1.4950(19)
C(8')-H(8')	0.9500
C(9')-H(9'1)	0.9800
C(9')-H(9'2)	0.9800
C(9')-H(9'3)	0.9800
C(4)-C(5)	1.3987(18)
C(6)-C(5)	1.3689(19)
C(6)-H(6)	0.9500
C(5)-H(5)	0.9500
C(5')-C(6')	1.3961(18)
C(5')-H(5')	0.9500
C(8)-C(9)	1.5011(18)
C(9)-H(9A)	0.9800
C(9)-H(9B)	0.9800
C(9)-H(9C)	0.9800

Table S4. Bond Angles for Compound **2**

Bond	**Angle**
C(3)-O(3)-C(10)	113.42(10)
H(1SB)-O(1S)-H(1SA)	105.7(14)
C(4)-O(4)-H(4)	109.5
C(2)-O(2)-H(2)	109.5
C(6')-O(6')-H(6')	109.5
O(3)-C(10)-H(10A)	109.5
O(3)-C(10)-H(10B)	109.5
H(10A)-C(10)-H(10B)	109.5
O(3)-C(10)-H(10C)	109.5
H(10A)-C(10)-H(10C)	109.5
H(10B)-C(10)-H(10C)	109.5
O(3)-C(3)-C(4)	118.49(11)
O(3)-C(3)-C(2)	121.62(11)
C(4)-C(3)-C(2)	119.78(12)
O(2)-C(2)-C(3)	117.68(11)
O(2)-C(2)-C(1)	122.28(12)
C(3)-C(2)-C(1)	120.03(12)
C(6)-C(1)-C(2)	118.47(12)
C(6)-C(1)-C(7)	121.41(11)
C(2)-C(1)-C(7)	120.12(11)
O(7)-C(7)-C(1)	122.42(11)
O(7)-C(7)-C(4')	118.52(11)
C(1)-C(7)-C(4')	118.87(11)
C(5')-C(4')-C(3')	120.17(12)
C(5')-C(4')-C(7)	116.59(11)
C(3')-C(4')-C(7)	123.23(11)
C(2')-C(3')-C(4')	118.54(11)
C(2')-C(3')-C(8)	121.66(11)
C(4')-C(3')-C(8)	119.78(11)
C(1')-C(2')-C(3')	122.23(12)
C(1')-C(2')-H(2')	118.9
C(3')-C(2')-H(2')	118.9
C(2')-C(1')-C(6')	118.03(11)
C(2')-C(1')-C(7')	122.69(12)
C(6')-C(1')-C(7')	119.21(11)
C(8')-C(7')-C(1')	127.40(12)
C(8')-C(7')-H(7')	116.3
C(1')-C(7')-H(7')	116.3
C(7')-C(8')-C(9')	128.28(12)
C(7')-C(8')-H(8')	115.9
C(9')-C(8')-H(8')	115.9
C(8')-C(9')-H(9'1)	109.5
C(8')-C(9')-H(9'2)	109.5
H(9'1)-C(9')-H(9'2)	109.5
C(8')-C(9')-H(9'3)	109.5
H(9'1)-C(9')-H(9'3)	109.5
H(9'2)-C(9')-H(9'3)	109.5
O(4)-C(4)-C(3)	121.00(12)
O(4)-C(4)-C(5)	118.37(12)
C(3)-C(4)-C(5)	120.63(12)

C(5)-C(6)-C(1)	121.46(12)
C(5)-C(6)-H(6)	119.3
C(1)-C(6)-H(6)	119.3
C(6)-C(5)-C(4)	119.54(12)
C(6)-C(5)-H(5)	120.2
C(4)-C(5)-H(5)	120.2
C(4')-C(5')-C(6')	120.41(12)
C(4')-C(5')-H(5')	119.8
C(6')-C(5')-H(5')	119.8
O(6')-C(6')-C(5')	122.16(12)
O(6')-C(6')-C(1')	117.24(11)
C(5')-C(6')-C(1')	120.59(12)
O(8)-C(8)-C(3')	119.75(12)
O(8)-C(8)-C(9)	121.06(12)
C(3')-C(8)-C(9)	119.18(11)
C(8)-C(9)-H(9A)	109.5
C(8)-C(9)-H(9B)	109.5
H(9A)-C(9)-H(9B)	109.5
C(8)-C(9)-H(9C)	109.5
H(9A)-C(9)-H(9C)	109.5
H(9B)-C(9)-H(9C)	109.5

Table S5. Hydrogen Coordinates ($\times 10^4$) and Isotropic Displacement Parameters ($\text{Å}^2 \times 10^3$) for Compound **2**

	x	**y**	**z**	**U(eq)**
H(1SB)	4485(10)	1349(9)	6624(8)	27
H(1SA)	3686(17)	1054(8)	7077(6)	27
H(4)	7404	-558	3869	32
H(2)	7638	-218	6639	33
H(6')	12790	2085	6755	34
H(10A)	5412	-830	5511	43
H(10B)	5345	-1481	4989	43
H(10C)	5237	-695	4700	43
H(2')	8377	3350	6555	20
H(7')	11742	3762	6451	22
H(8')	11115	4664	7050	23
H(9'1)	9003	3843	7641	34
H(9'2)	8859	4667	7490	34
H(9'3)	9854	4397	8083	34
H(6)	9213	1457	5260	22
H(5)	8951	977	4171	25
H(5')	11012	1324	6686	21
H(9A)	6306	3138	5958	43
H(9B)	6067	3149	6775	43
H(9C)	5048	2733	6284	43

Table S6. Hydrogen Bonds for Compound **2**

D-H...A	**d(D-H)**	**d(H...A)**	**d(D...A)**	**<(DHA)**
O(1S)-H(1SB)...O(8)	0.821(9)	1.934(9)	2.7539(13)	177.2(17)
O(1S)-H(1SA)...O(7)#1	0.823(9)	1.973(9)	2.7877(13)	170.2(16)
O(4)-H(4)...O(1S)#2	0.84	2.02	2.7490(13)	144.2
O(4)-H(4)...O(3)	0.84	2.30	2.7441(13)	113.7
O(2)-H(2)...O(7)	0.84	1.86	2.5984(13)	145.6
O(6')-H(6')...O(1S)#3	0.84	1.84	2.6794(13)	176.8

Table S7. Torsion Angles for Compound **2**

	Torsion Angle
C(10)-O(3)-C(3)-C(4)	-104.45(14)
C(10)-O(3)-C(3)-C(2)	79.30(15)
O(3)-C(3)-C(2)-O(2)	-1.92(18)
C(4)-C(3)-C(2)-O(2)	-178.11(12)
O(3)-C(3)-C(2)-C(1)	178.85(11)
C(4)-C(3)-C(2)-C(1)	2.65(19)
O(2)-C(2)-C(1)-C(6)	177.74(12)
C(3)-C(2)-C(1)-C(6)	-3.06(18)
O(2)-C(2)-C(1)-C(7)	-2.82(18)
C(3)-C(2)-C(1)-C(7)	176.38(12)
C(6)-C(1)-C(7)-O(7)	-172.67(12)
C(2)-C(1)-C(7)-O(7)	7.91(19)
C(6)-C(1)-C(7)-C(4')	2.25(18)
C(2)-C(1)-C(7)-C(4')	-177.18(11)
O(7)-C(7)-C(4')-C(5')	82.13(15)
C(1)-C(7)-C(4')-C(5')	-92.98(14)
O(7)-C(7)-C(4')-C(3')	-98.19(15)
C(1)-C(7)-C(4')-C(3')	86.70(15)
C(5')-C(4')-C(3')-C(2')	0.02(18)
C(7)-C(4')-C(3')-C(2')	-179.65(11)
C(5')-C(4')-C(3')-C(8)	-178.45(12)
C(7)-C(4')-C(3')-C(8)	1.88(18)
C(4')-C(3')-C(2')-C(1')	-0.13(19)
C(8)-C(3')-C(2')-C(1')	178.31(12)
C(3')-C(2')-C(1')-C(6')	0.90(19)
C(3')-C(2')-C(1')-C(7')	177.87(12)
C(2')-C(1')-C(7')-C(8')	48.7(2)
C(6')-C(1')-C(7')-C(8')	-134.32(15)
C(1')-C(7')-C(8')-C(9')	4.3(2)
O(3)-C(3)-C(4)-O(4)	3.07(19)
C(2)-C(3)-C(4)-O(4)	179.38(12)
O(3)-C(3)-C(4)-C(5)	-176.47(11)
C(2)-C(3)-C(4)-C(5)	-0.15(19)
C(2)-C(1)-C(6)-C(5)	0.99(19)
C(7)-C(1)-C(6)-C(5)	-178.44(12)
C(1)-C(6)-C(5)-C(4)	1.5(2)

O(4)-C(4)-C(5)-C(6)	178.54(12)
C(3)-C(4)-C(5)-C(6)	-1.9(2)
C(3')-C(4')-C(5')-C(6')	-0.71(19)
C(7)-C(4')-C(5')-C(6')	178.98(11)
C(4')-C(5')-C(6')-O(6')	-179.16(12)
C(4')-C(5')-C(6')-C(1')	1.51(19)
C(2')-C(1')-C(6')-O(6')	179.05(11)
C(7')-C(1')-C(6')-O(6')	1.97(18)
C(2')-C(1')-C(6')-C(5')	-1.58(18)
C(7')-C(1')-C(6')-C(5')	-178.66(11)
C(2')-C(3')-C(8)-O(8)	-174.68(12)
C(4')-C(3')-C(8)-O(8)	3.74(18)
C(2')-C(3')-C(8)-C(9)	4.46(19)
C(4')-C(3')-C(8)-C(9)	-177.12(12)

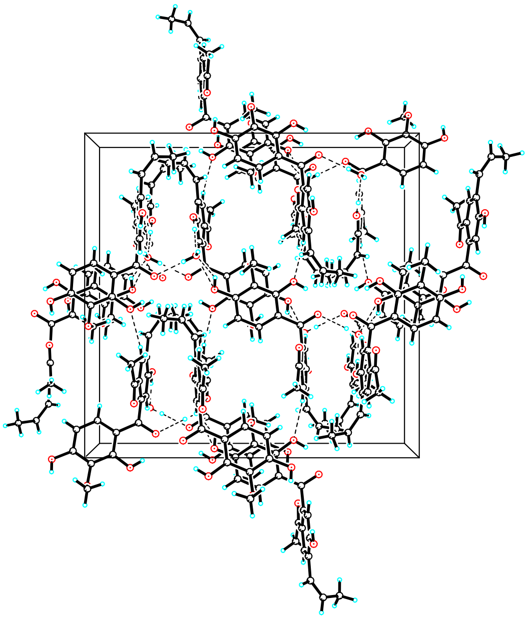


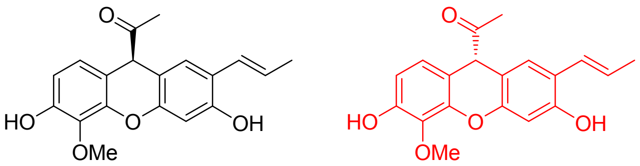
Figure S30. Crystal Cell Diagram for Compound **2**

ECD calculation details for 3

The calculations were performed on the enantiomers (*S*)-**3** and (*R*)-**3** (Figure S31). Conformational analysis was carried out via Monte Carlo searching with the MMFF94 molecular mechanics force field using the Spartan 10 software.[29]

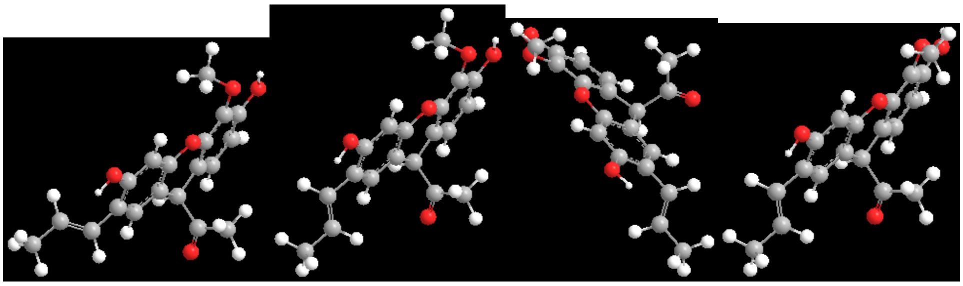
Conformational analyses of (*S*)-**3** showed 4 lowest energy conformers (**3**C1–**3**C4) (Figure S32) having relative energy within 2 kcal/mol (Table S8). Subsequently, the conformers were re-optimized using DFT at the B3LYP/6-31+G (d, p) level in vacuum with the Gaussian 09 program.[30] The B3LYP/6-31G+(d, p) harmonic vibrational frequencies were further calculated to confirm their stability. The energies, oscillator strengths, and rotational strengths of the first 40 electronic excitations were calculated using the TDDFT methodology at the B3LYP/6-311++G (2d, 2p) level in vacuum. The ECD spectra were simulated by the Gausssum 2.25 program[31] (σ= 0.3 eV). To get the final spectra of (*S*)-**3**, the simulated spectra of the 4 lowest energy conformations were averaged according to the Boltzmann distribution theory and their relative Gibbs free energy (ΔG). The corresponding theoretical ECD spectrum of (*R*)-**3** was depicted by inverting that of (*S*)-**3**.

All quantum computations were performed using Gaussian 09 program package, on an IBM cluster machine located at the High Performance Computing Center of Peking Union Medical College. In the region of 200-400 nm, the theoretically calculated ECD spectra of (*R*)-**3** were in agreement with the experimental ECD spectra of **3**. This allowed the assignment of 7*R* configuration for **3**.



(*S*)-**3** (*R*)-**3**

Figure S31. The pair of enantiomers [(*S*)-**3** and (*R*)-**3**] in the ECD calculation.



3C1 (0.000 Kcal/mol) **3C2** (0.003 Kcal/mol) **3C3** (0.077 Kcal/mol) **3C4** (0.393 Kcal/mol)

Figure S32. B3LYP/6-31+G (d, p) optimized four lowest energy 3D conformers of (*S*)-**3** and their relative Gibbs free energies (ΔG < 2 Kcal/mol).

Table S8. Energy Analysis of Conformers of (*S*)-**3**

Conf.	MMFF energy		B3LYP/6-31+G (d, p) Gibbs free energy (298.15 K)		
	ΔE (Kcal/mol)	Boltzmann Distribution	G (Hartree)	ΔG (Kcal/mol)	Boltzmann Distribution
3C1	0.00	0.351	-1110.743868	0.000	0.295
3C2	0.23	0.239	-1110.743864	0.003	0.294
3C3	0.23	0.238	-1110.743745	0.077	0.259
3C4	0.47	0.160	-1110.743241	0.393	0.152

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