Supporting Information for

Lignans from the Fruit of *Schisandra glaucescens* with Antioxidant and Neuroprotective Properties

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[#]The authors contributed equally to this work.

Content

Figure S1. ^{1}H NMR (400 MHz, $CDCl_3$) spectrum of compound **1**

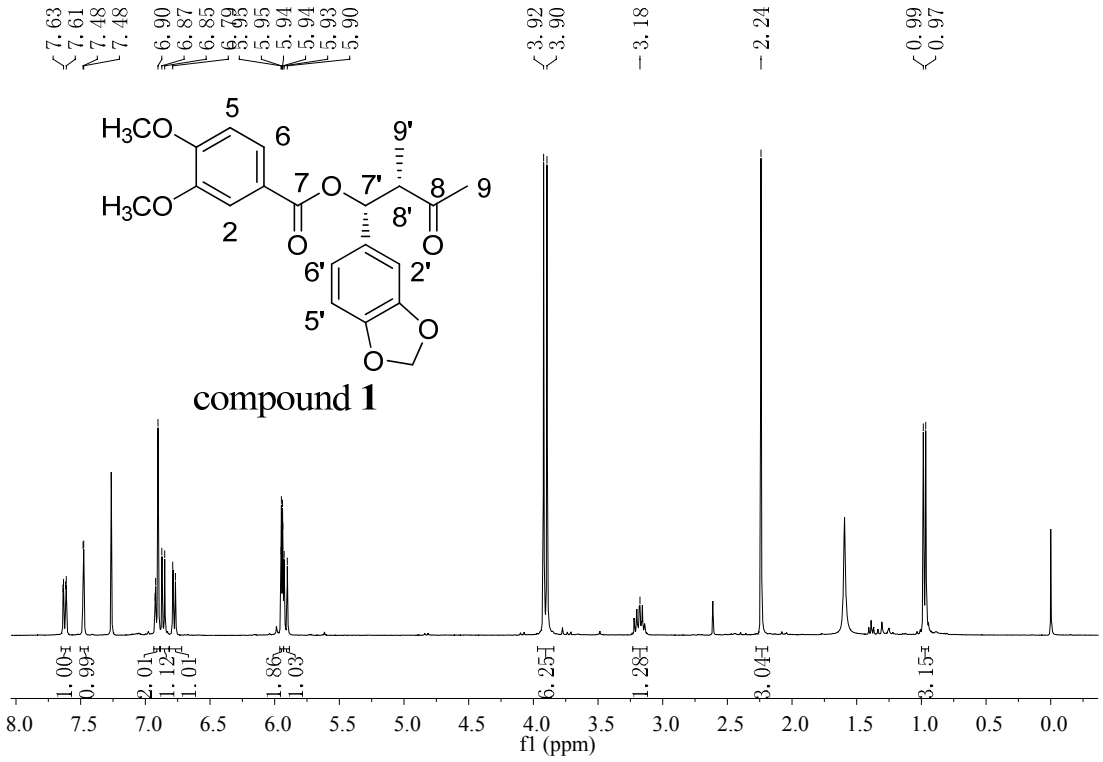


Figure S2. Partially intercepted ^{1}H NMR (400 MHz, $CDCl_3$) spectrum of compound **1**

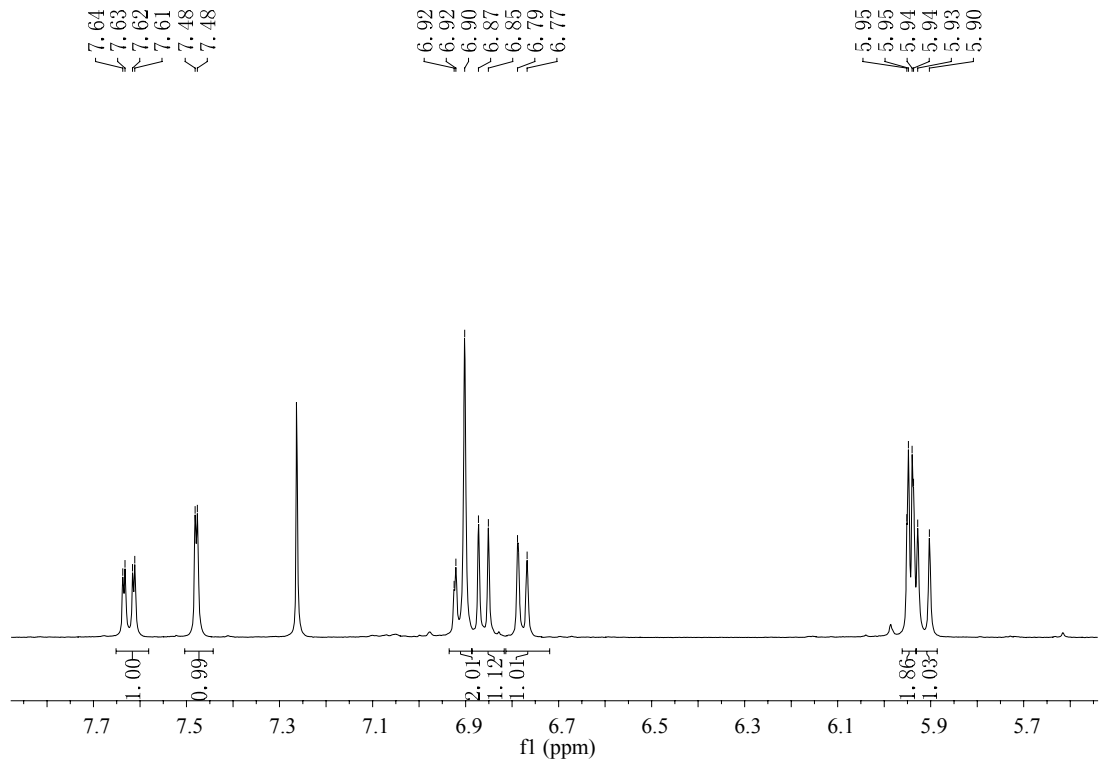


Figure S3. ^{13}C NMR (100 MHz, $CDCl_3$) spectrum of compound **1**

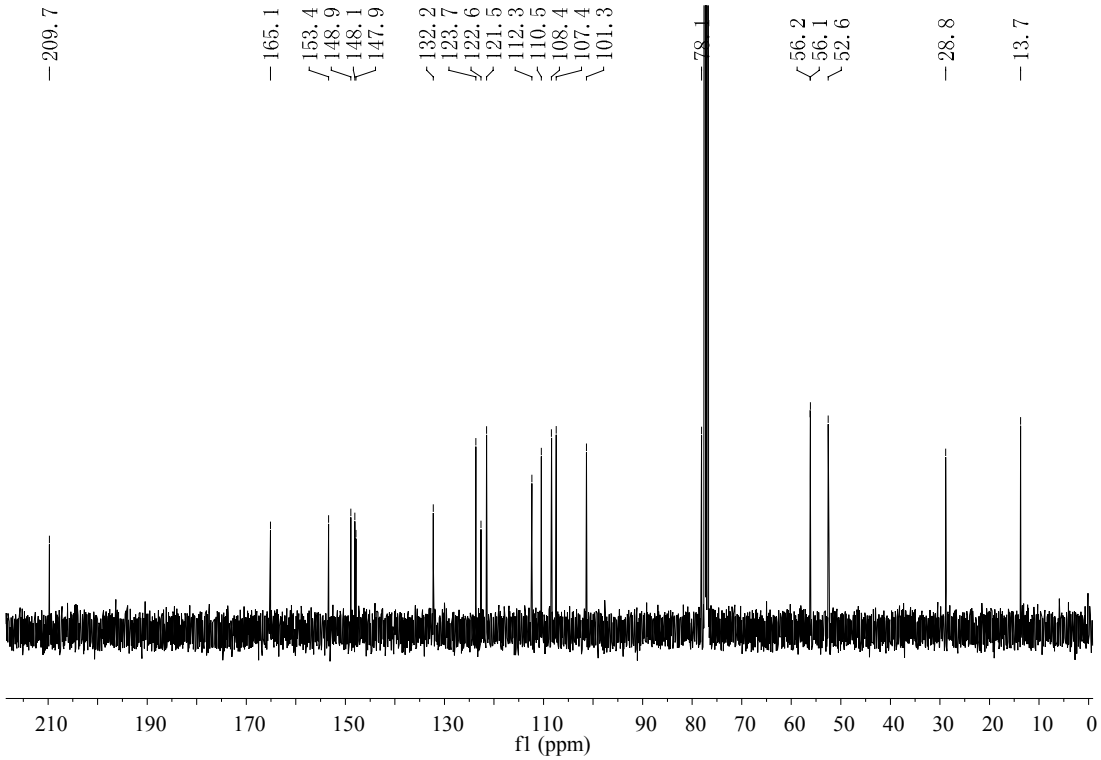


Figure S4. DEPT135 (100 MHz, $CDCl_3$) spectrum of compound **1**

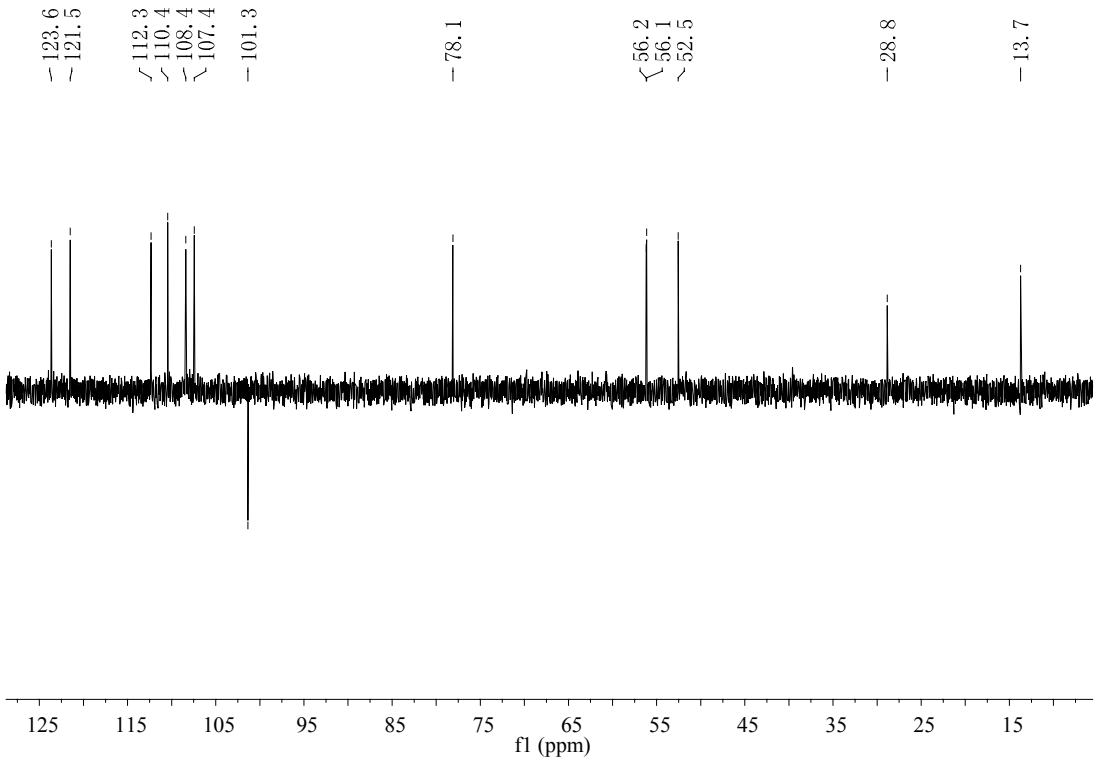


Figure S5. HSQC (400 MHz, $CDCl_3$) spectrum of compound **1**

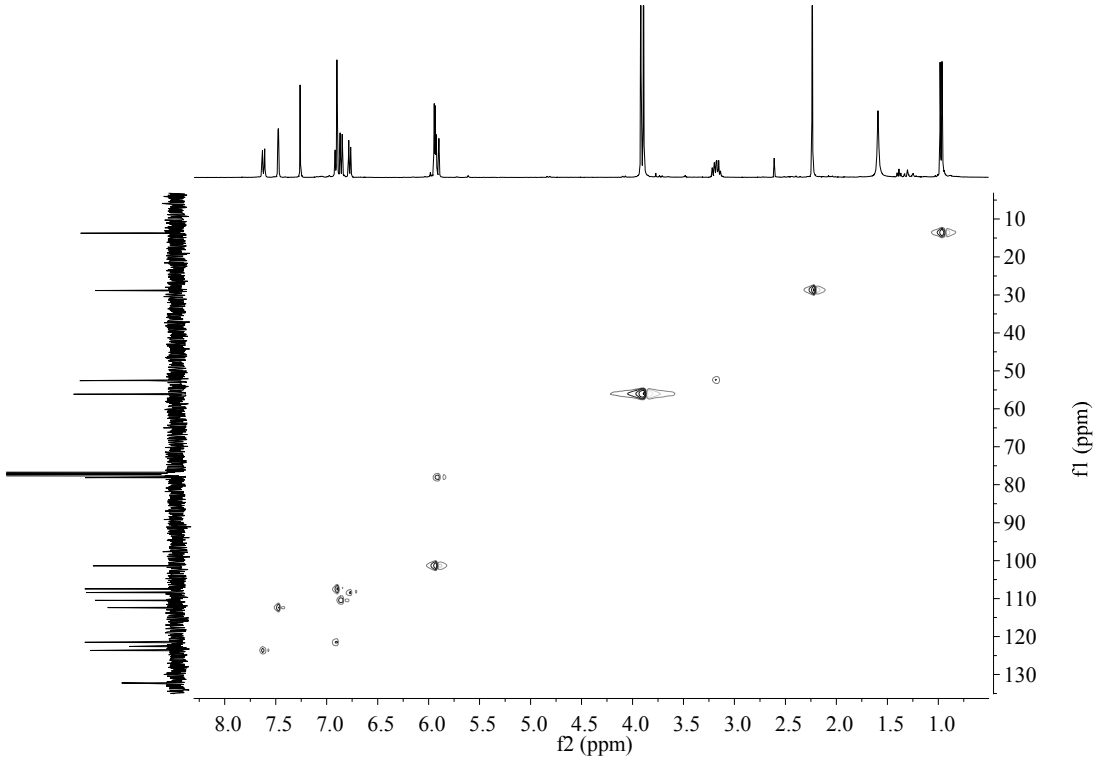


Figure S6. HMBC (400 MHz, $CDCl_3$) spectrum of compound **1**

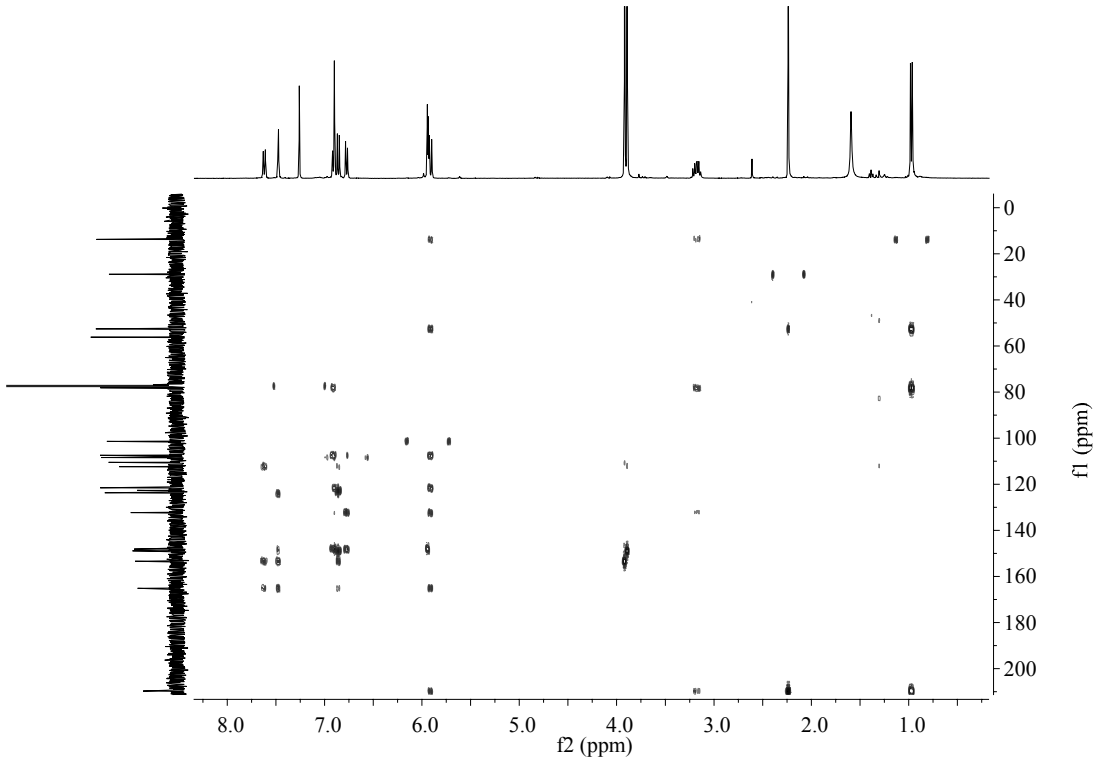


Figure S7. ^{1}H-^{1}H COSY (400 MHz, $CDCl_3$) spectrum of compound **1**

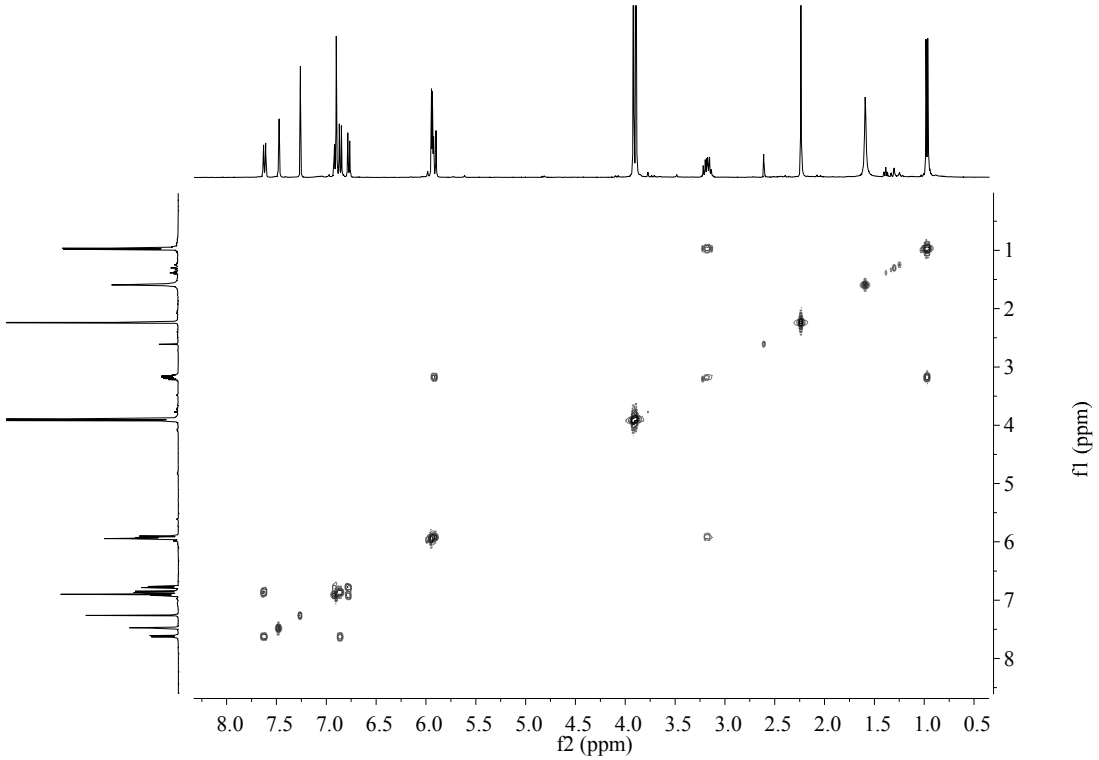


Figure S8. NOESY (400 MHz, $CDCl_3$) spectrum of compound **1**

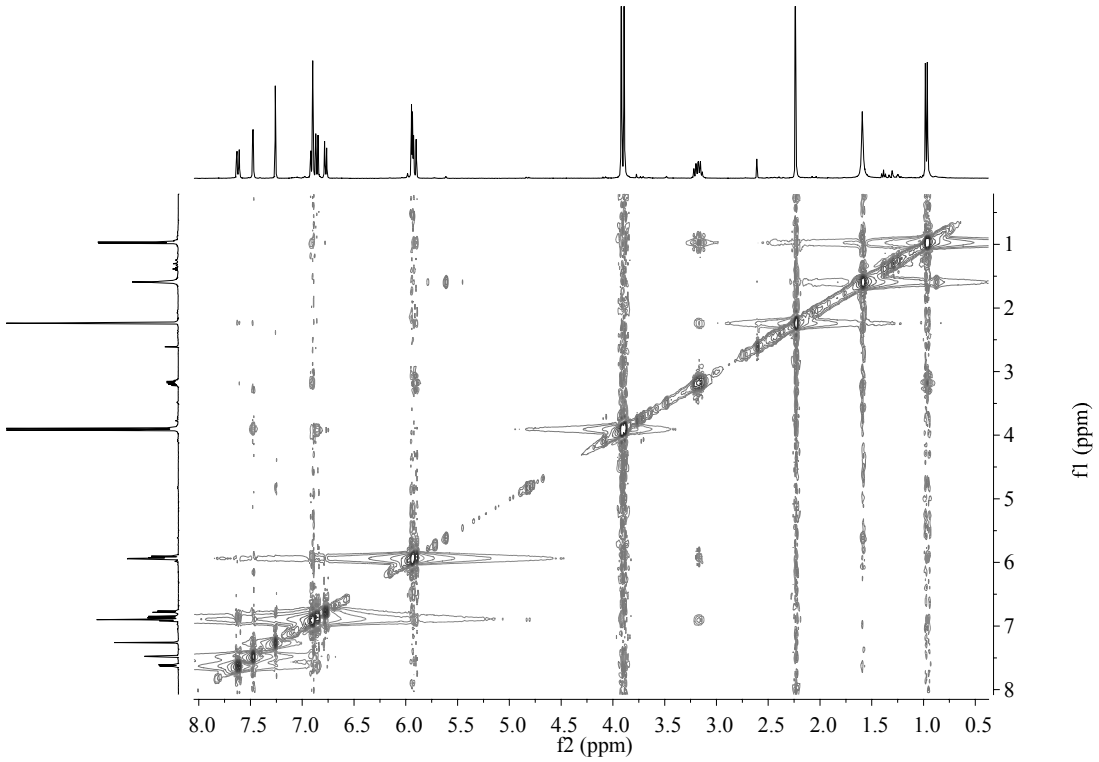


Figure S9. Partially intercepted NOESY (400 MHz, $CDCl_3$) spectrum of compound **1**

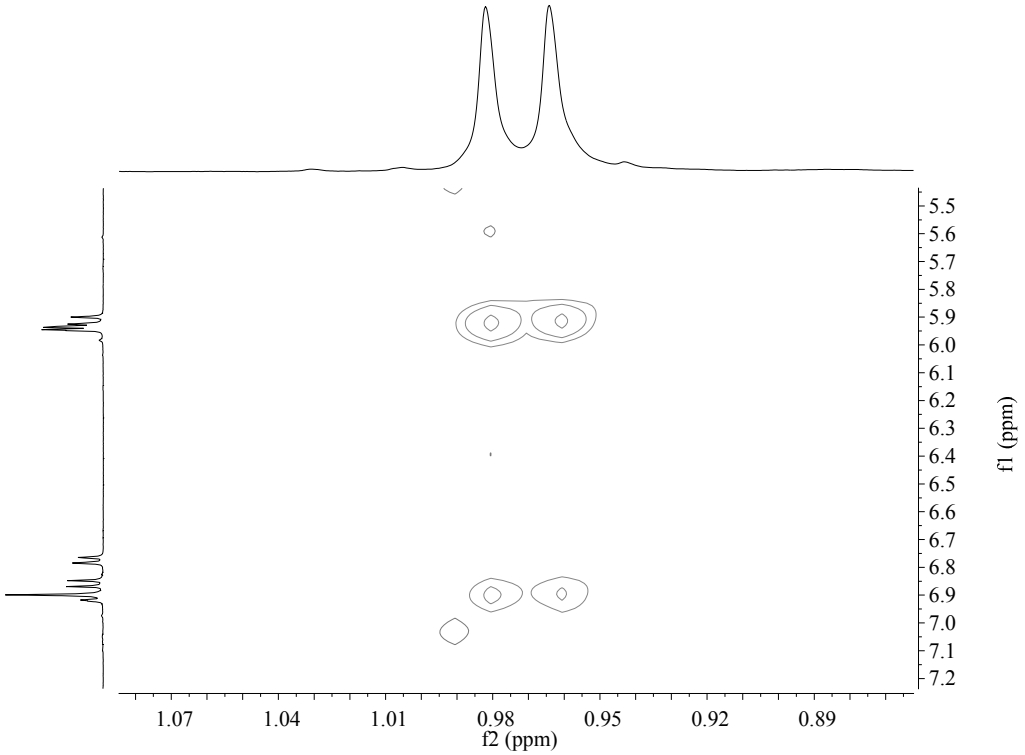
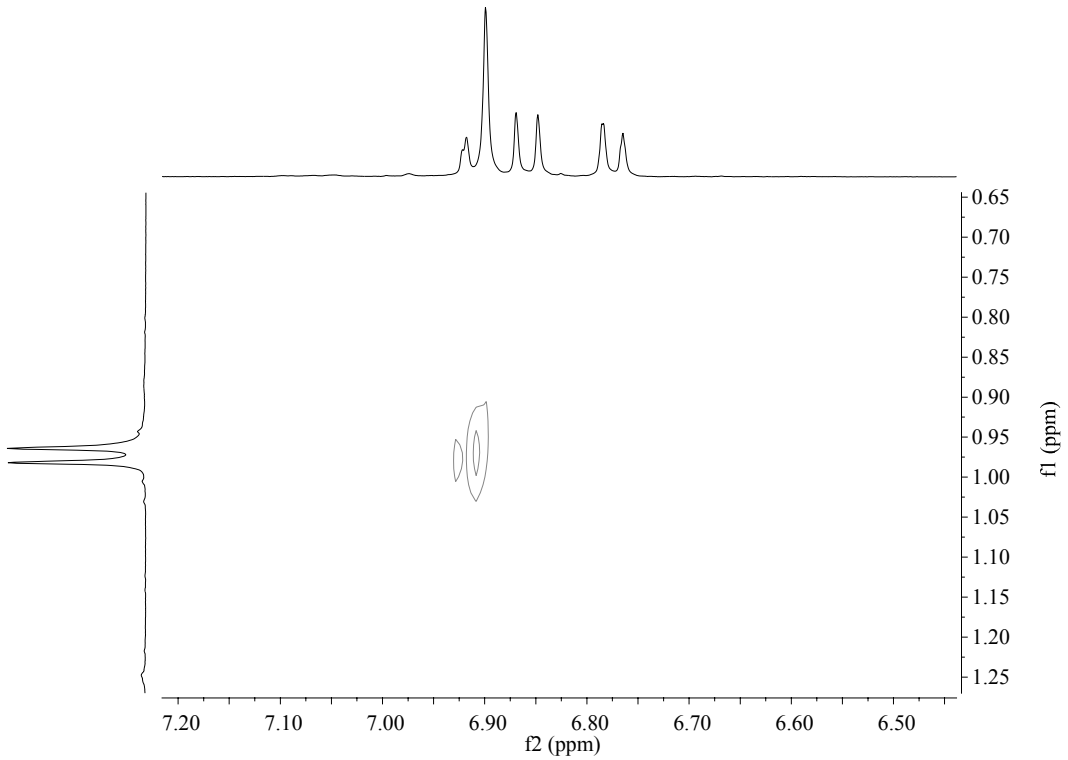


Figure S10. Partially intercepted NOESY (400 MHz, $CDCl_3$) spectrum of compound **1**



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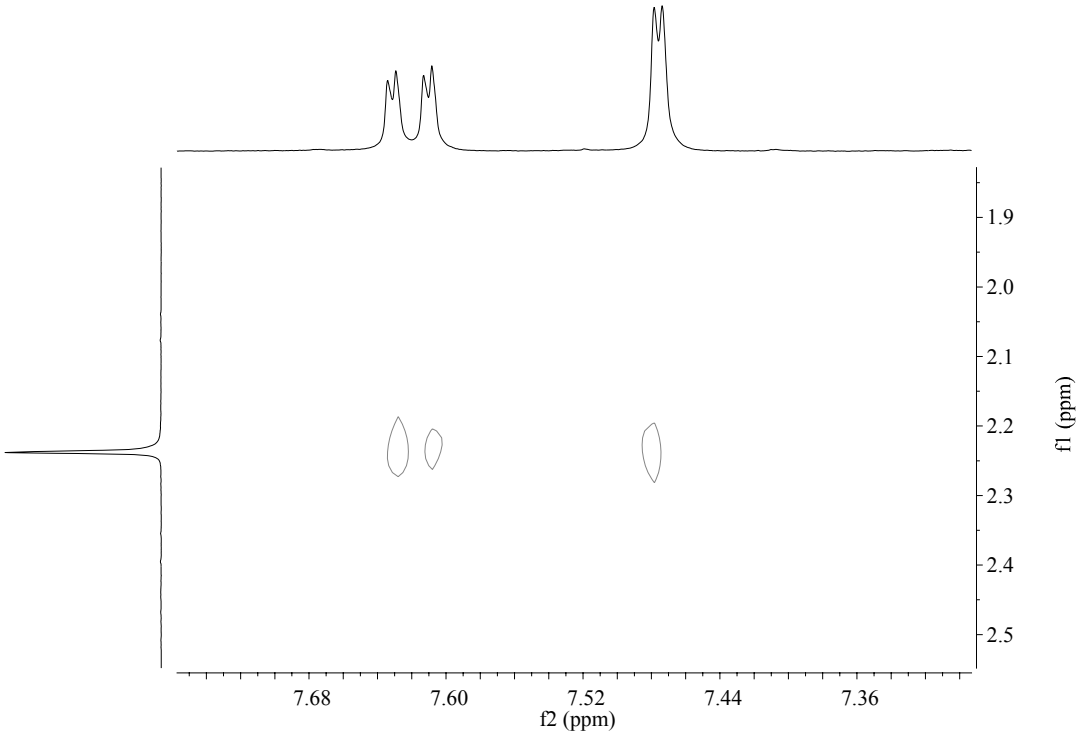


Figure S12. HRESIMS spectrum of compound **1**

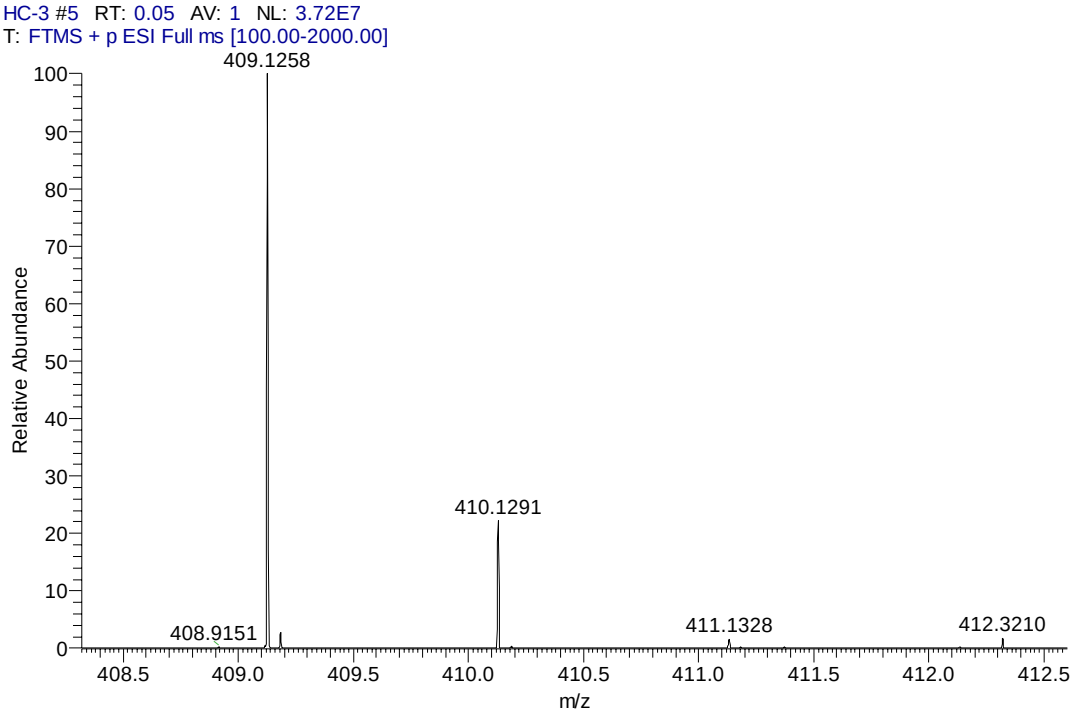


Figure S13. IR spectrum of compound **1**

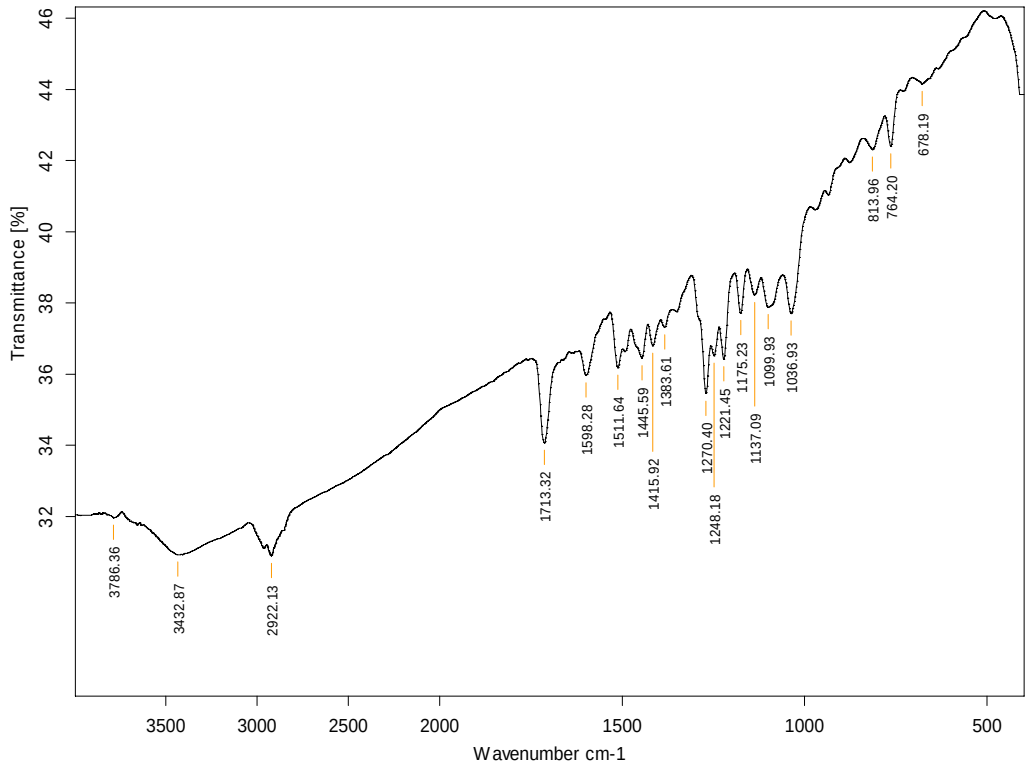


Figure S14. UV spectrum of compound **1**

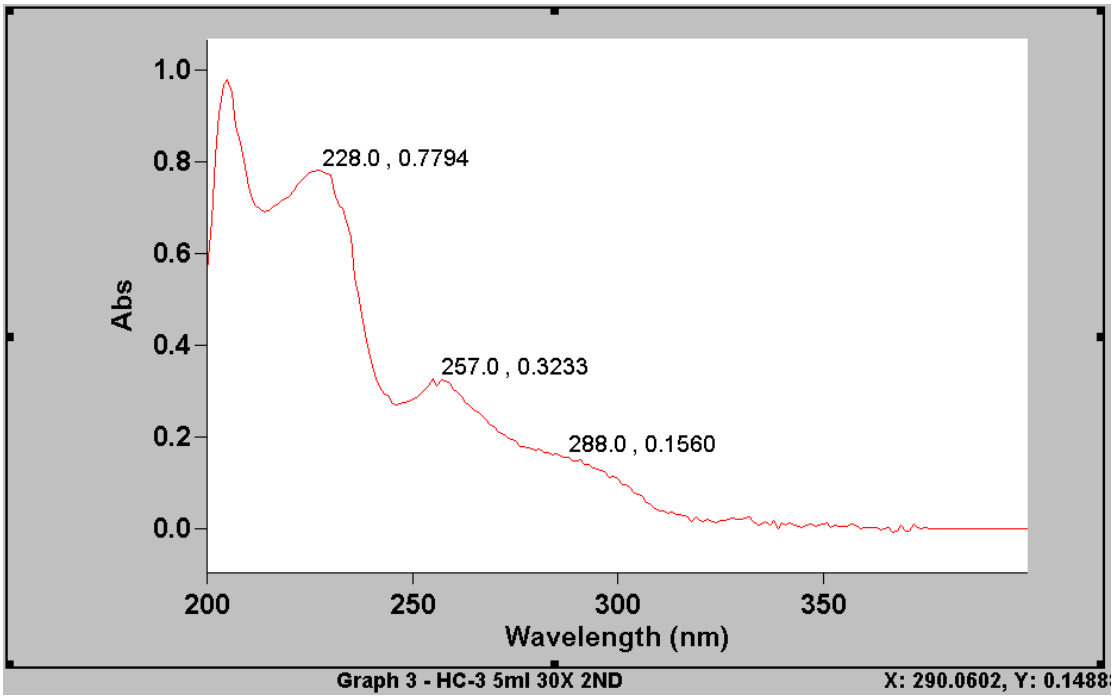


Figure S15. ECD spectrum of compound **1**

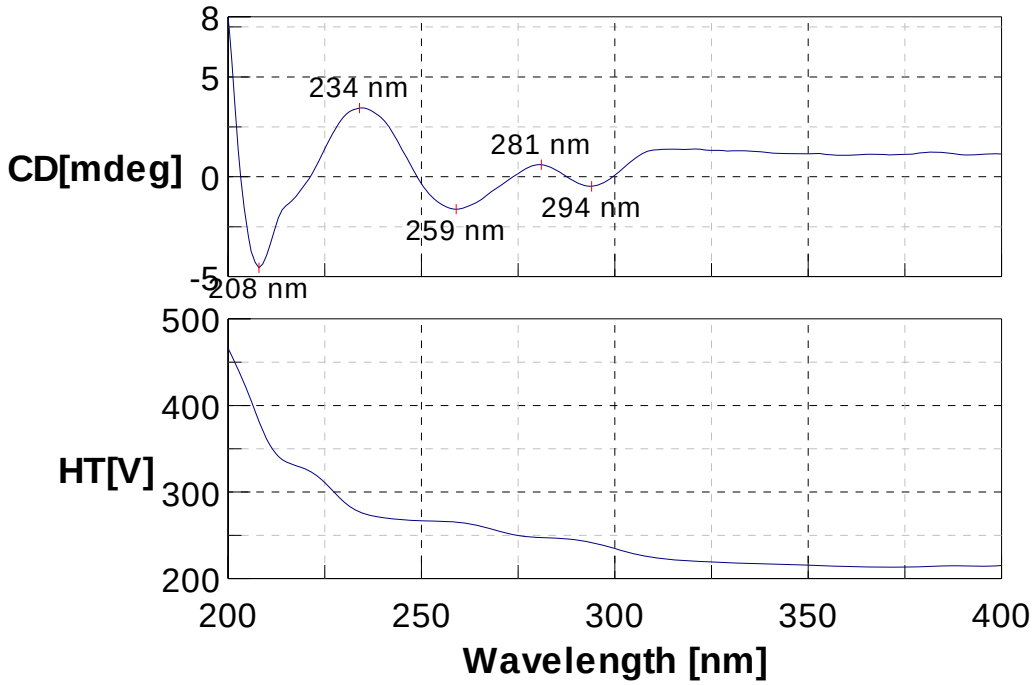


Figure S16. ^{1}H NMR (400 MHz, $CDCl_3$) spectrum of compound **2**

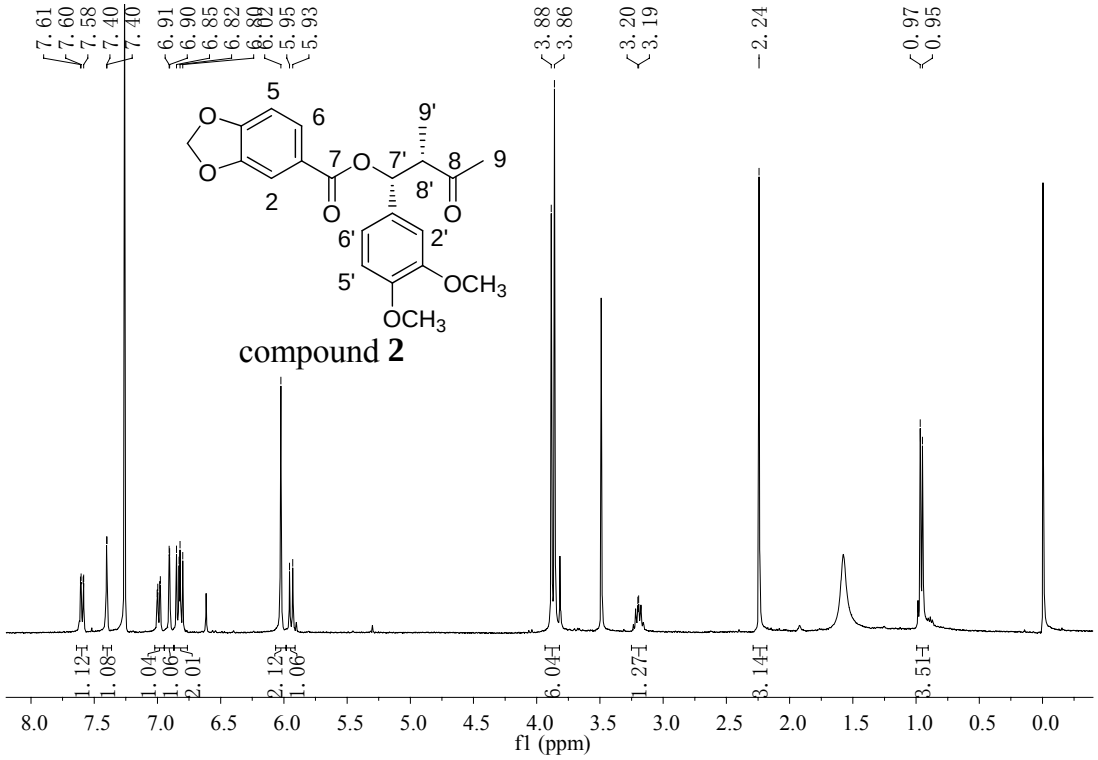
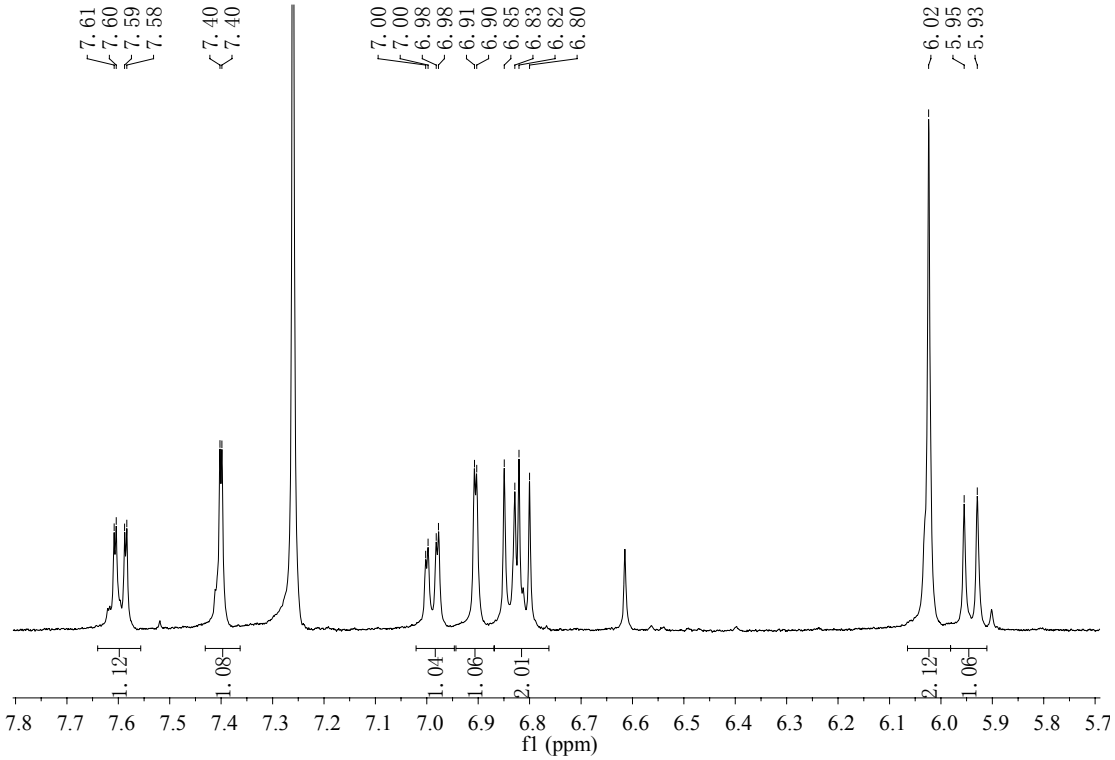


Figure S17. Partially intercepted ^{1}H NMR (400 MHz, $CDCl_3$) spectrum of compound **2**



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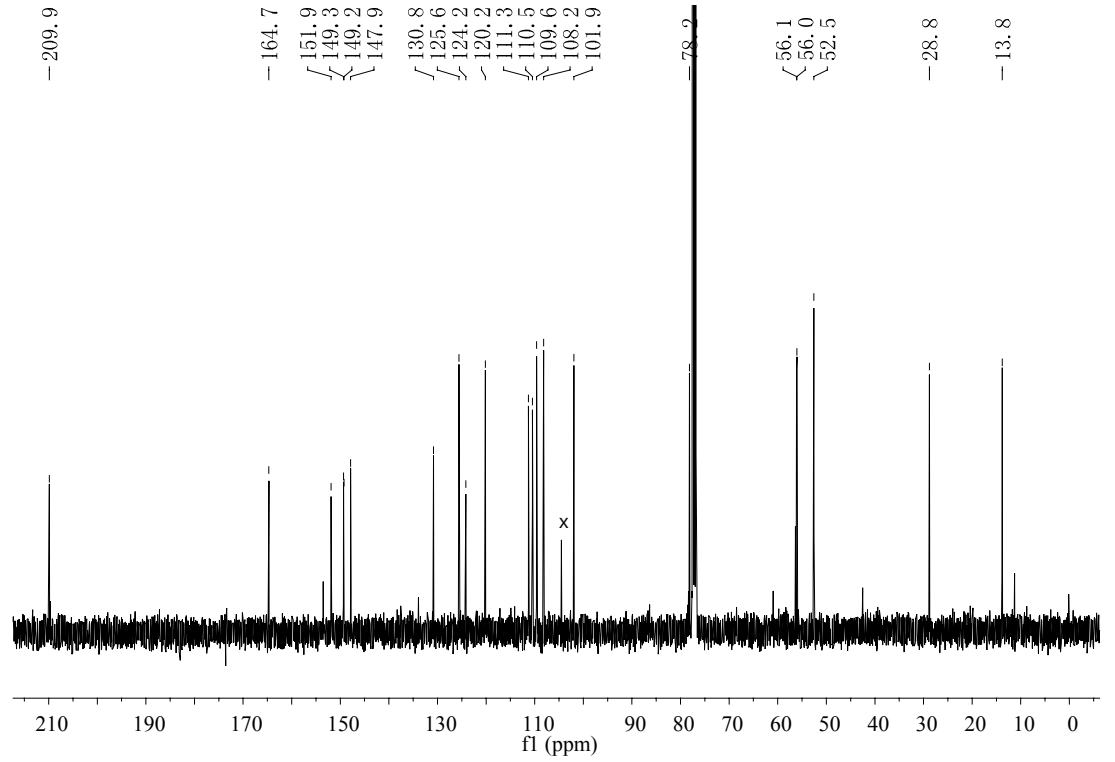

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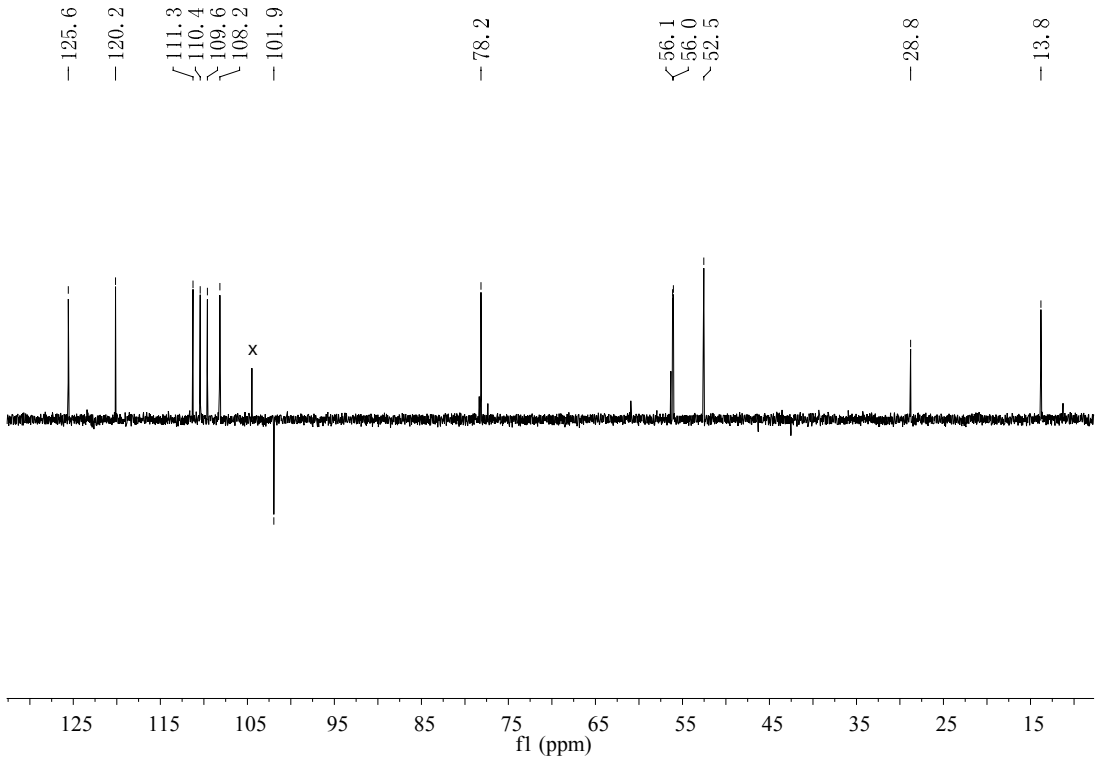

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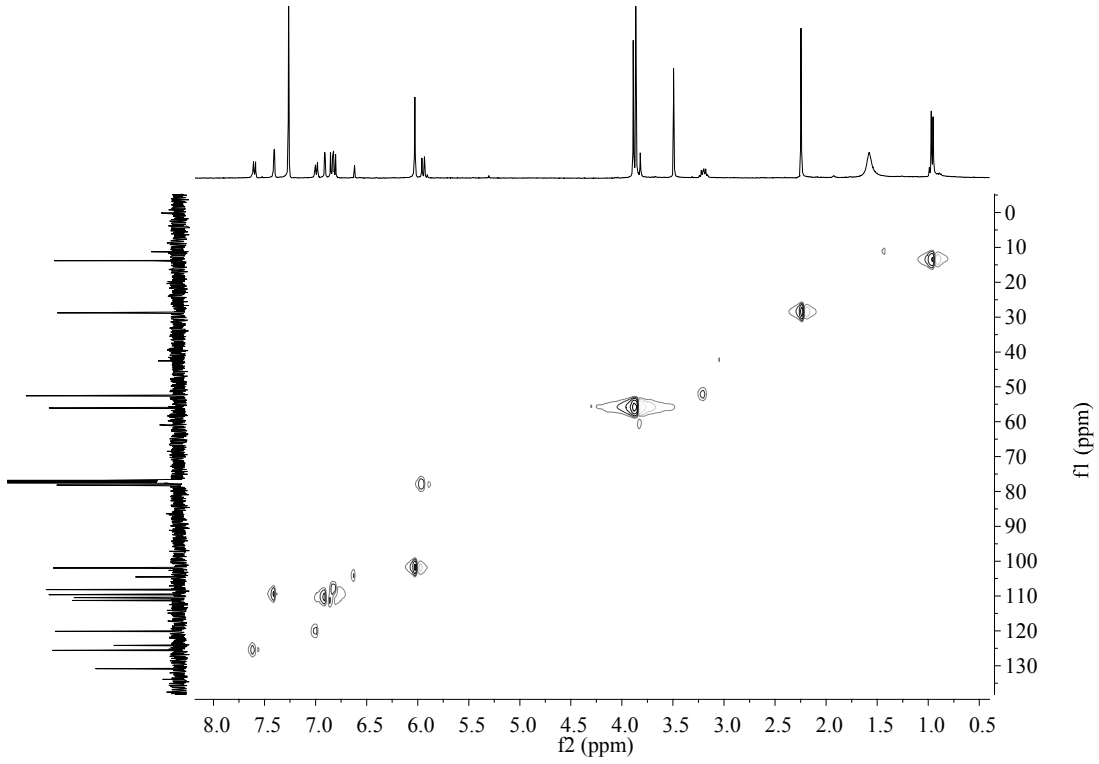

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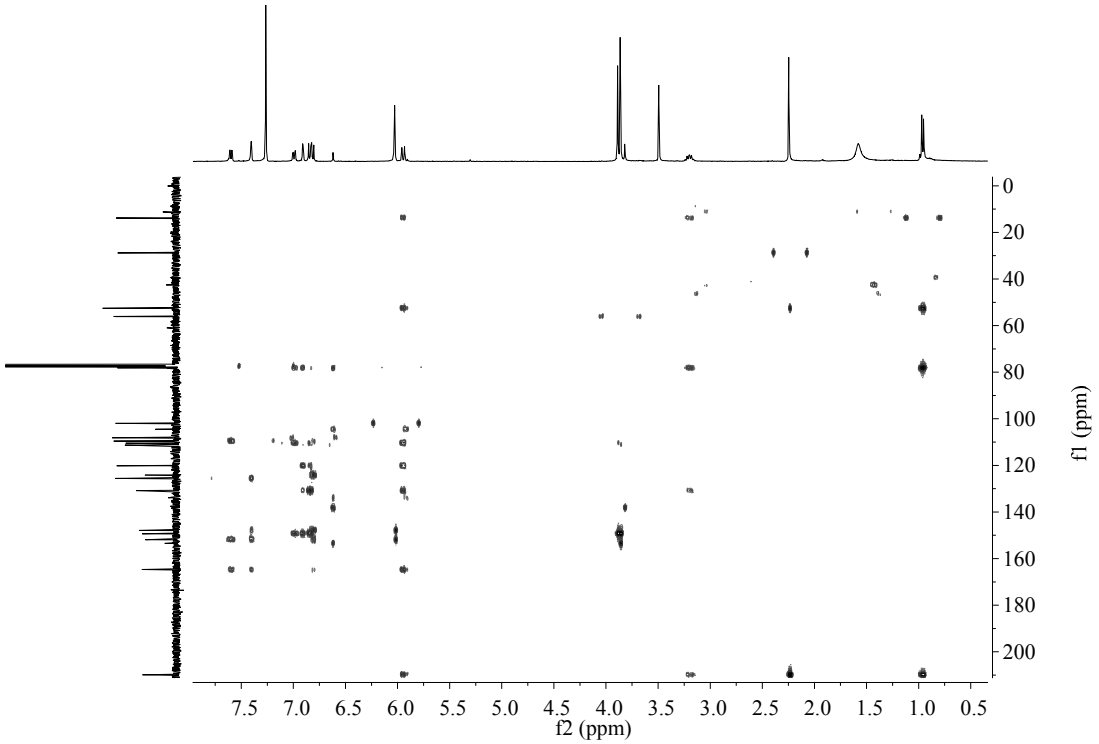


Figure S22. Partially intercepted HMBC (400 MHz, $CDCl_3$) spectrum of compound **2**

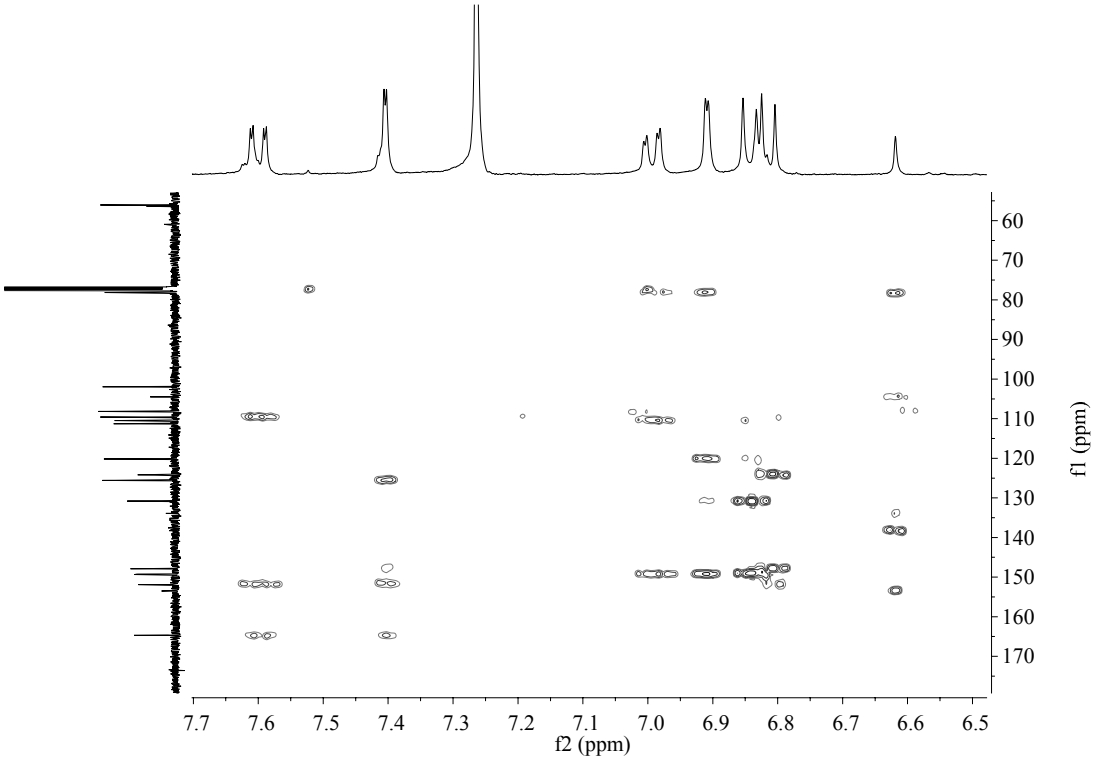


Figure S23. ^{1}H-^{1}H COSY (400 MHz, $CDCl_3$) spectrum of compound **2**

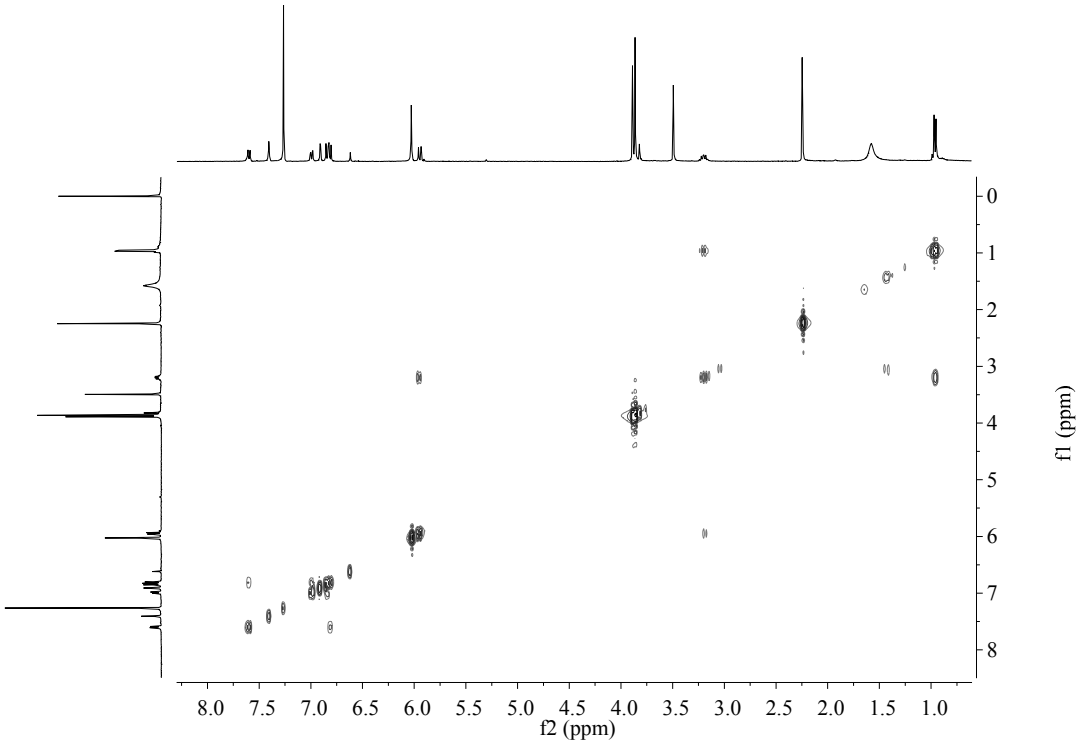
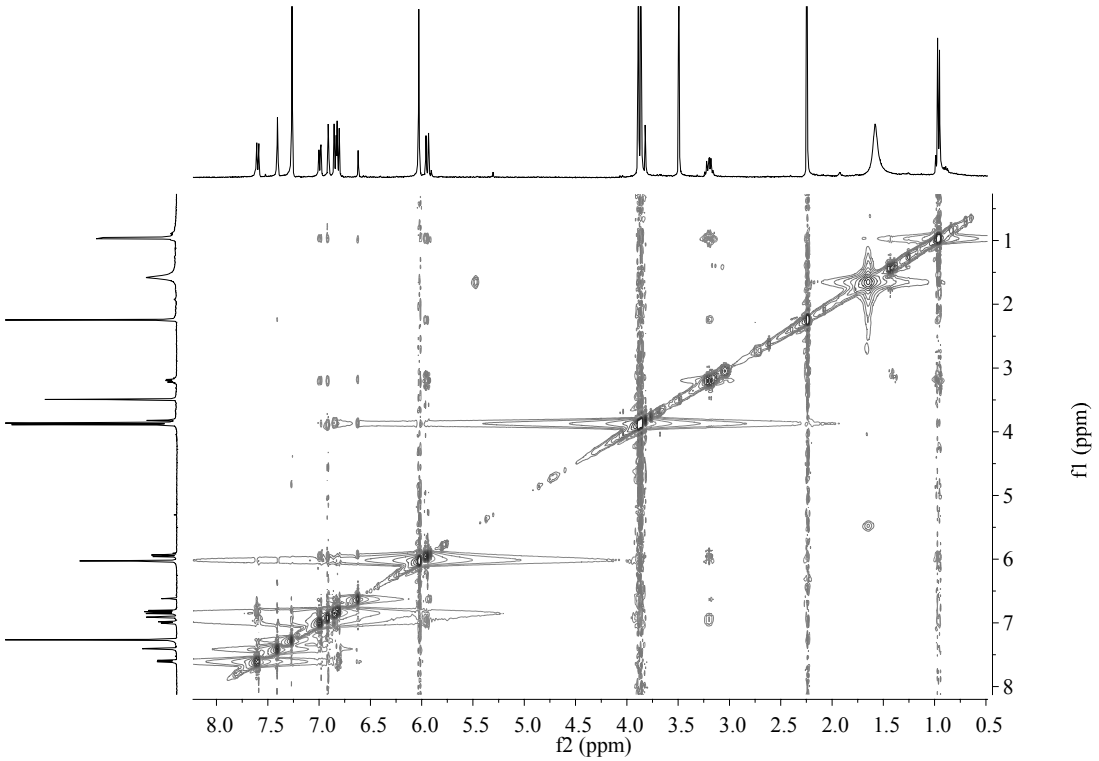


Figure S24. NOESY (400 MHz, $CDCl_3$) spectrum of compound **2**



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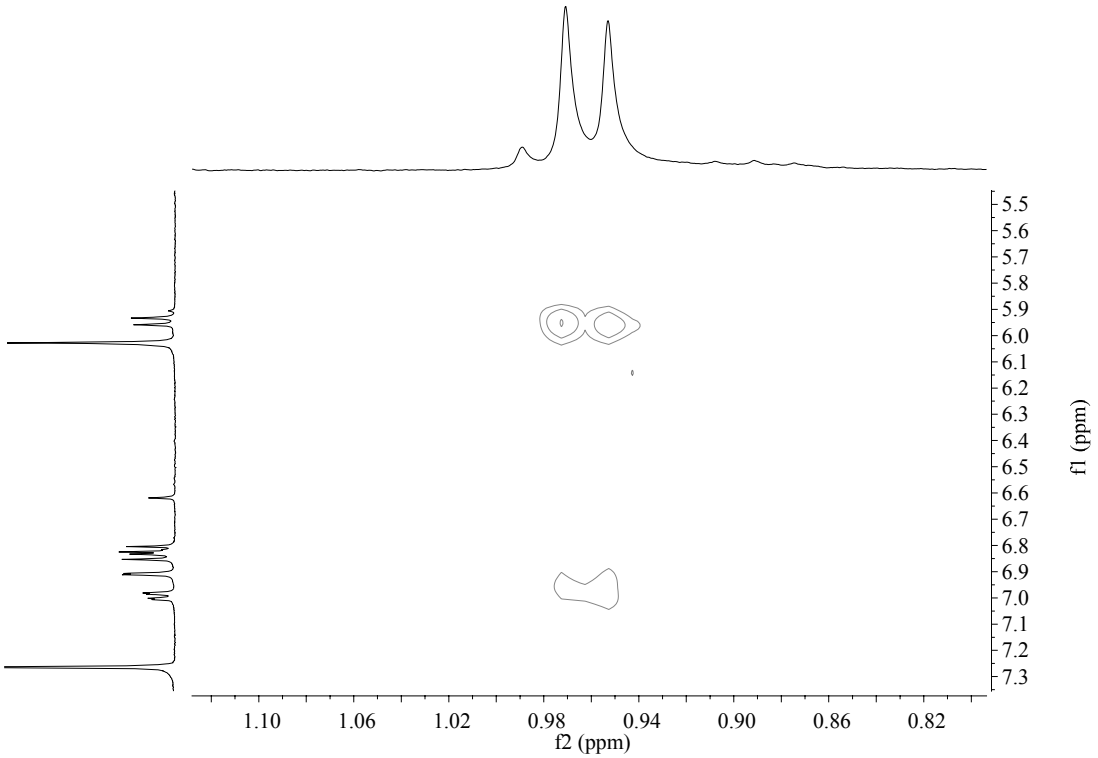
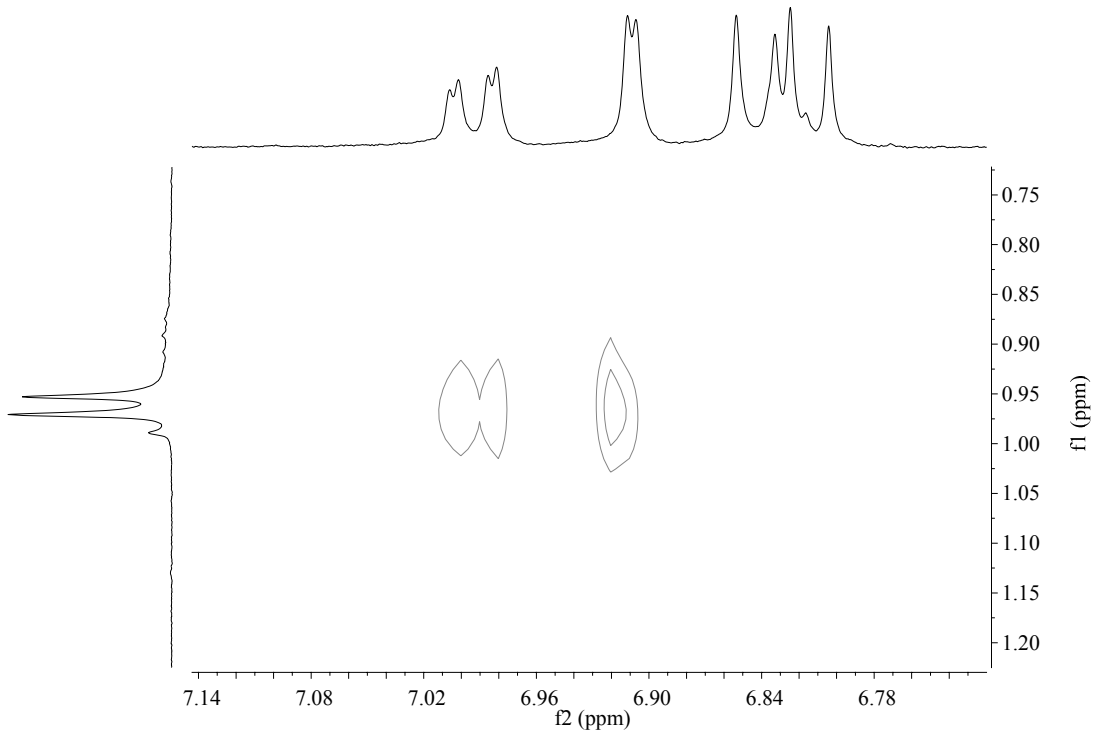


Figure S26. Partially intercepted NOESY (400 MHz, $CDCl_3$) spectrum of compound **2**



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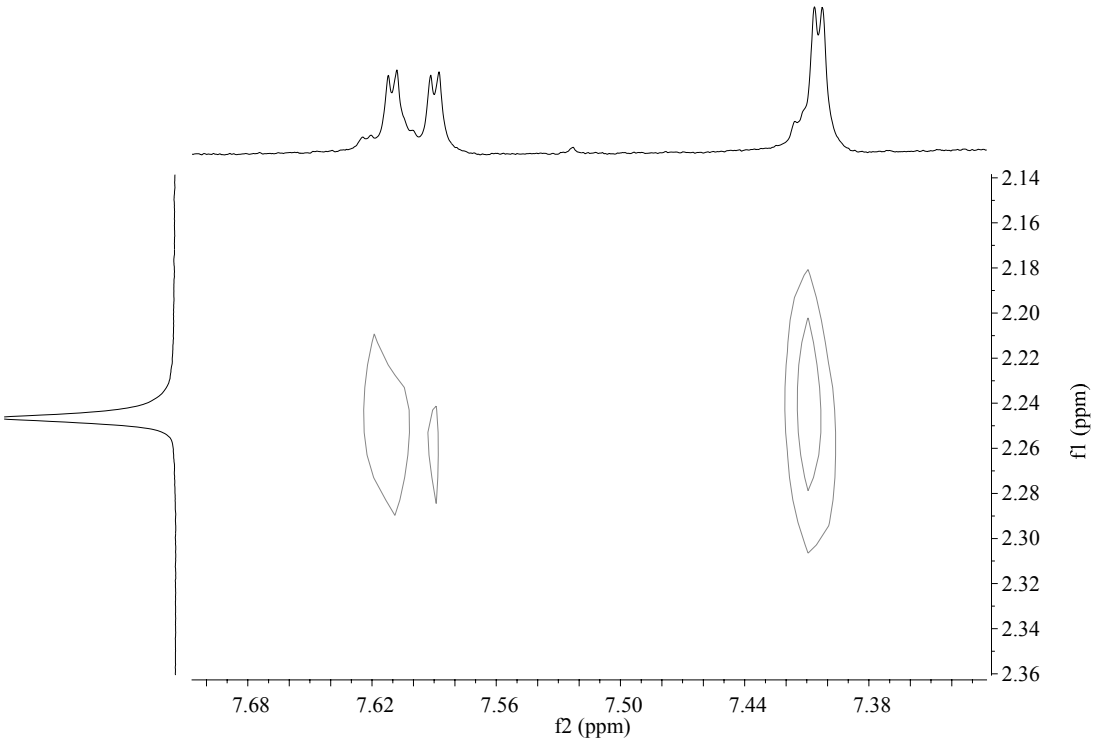
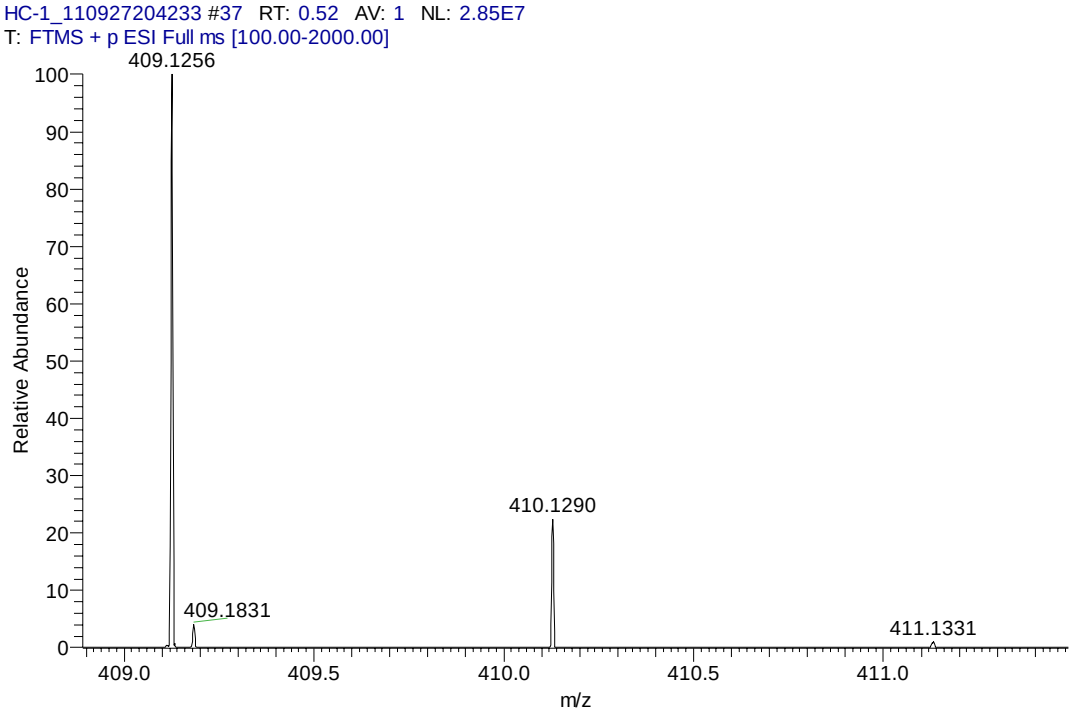


Figure S28. HRESIMS spectrum of compound **2**



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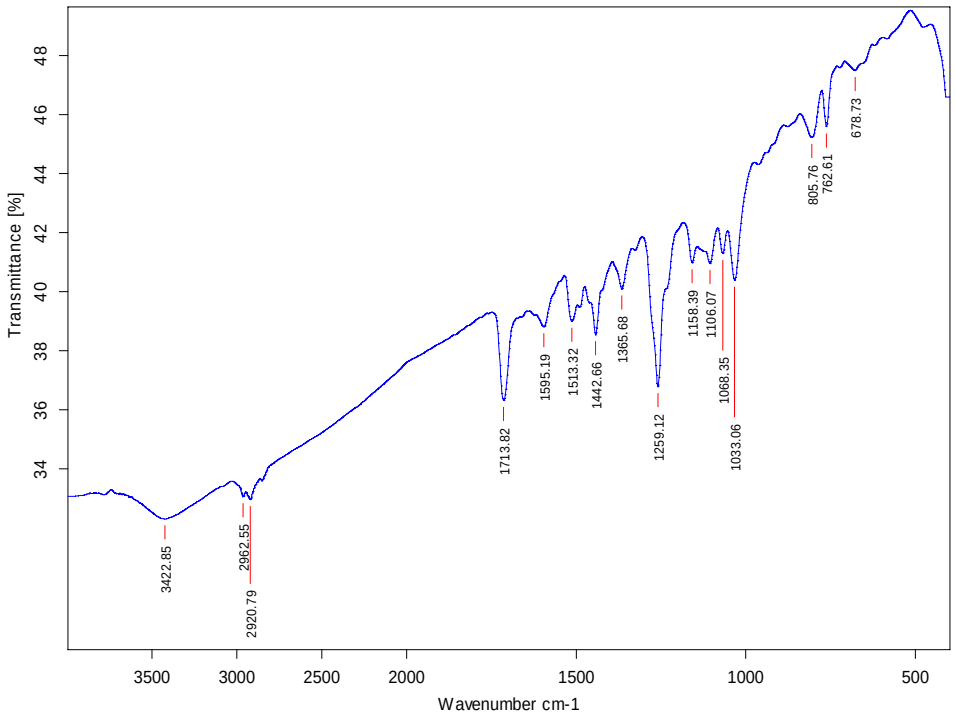
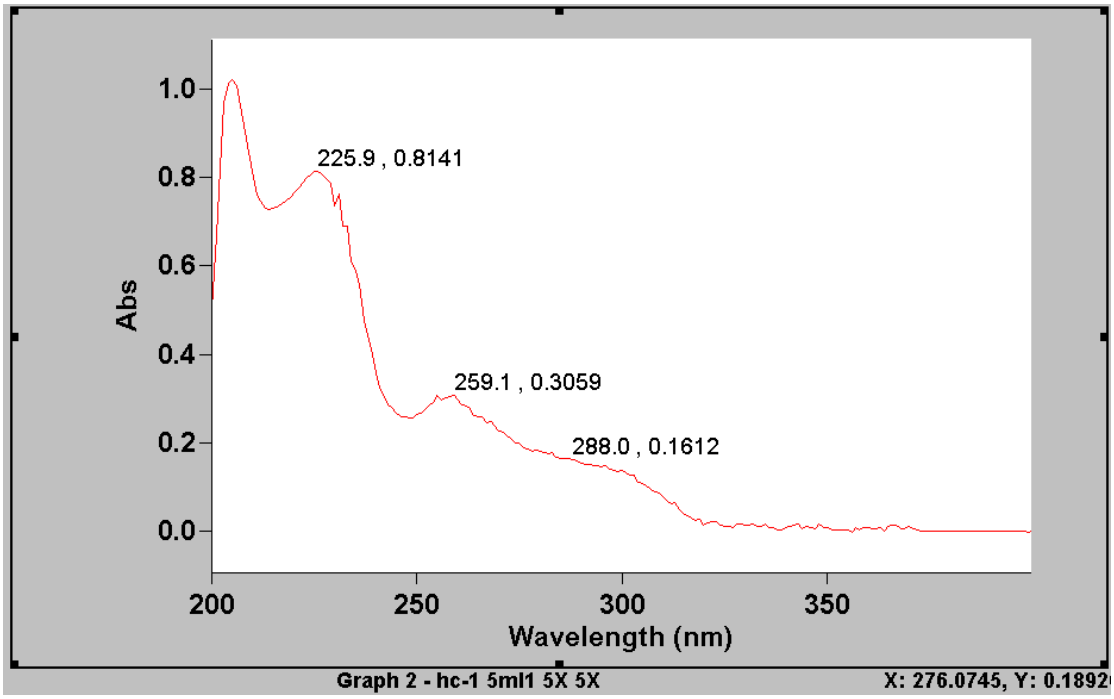


Figure S30. UV spectrum of compound **2**



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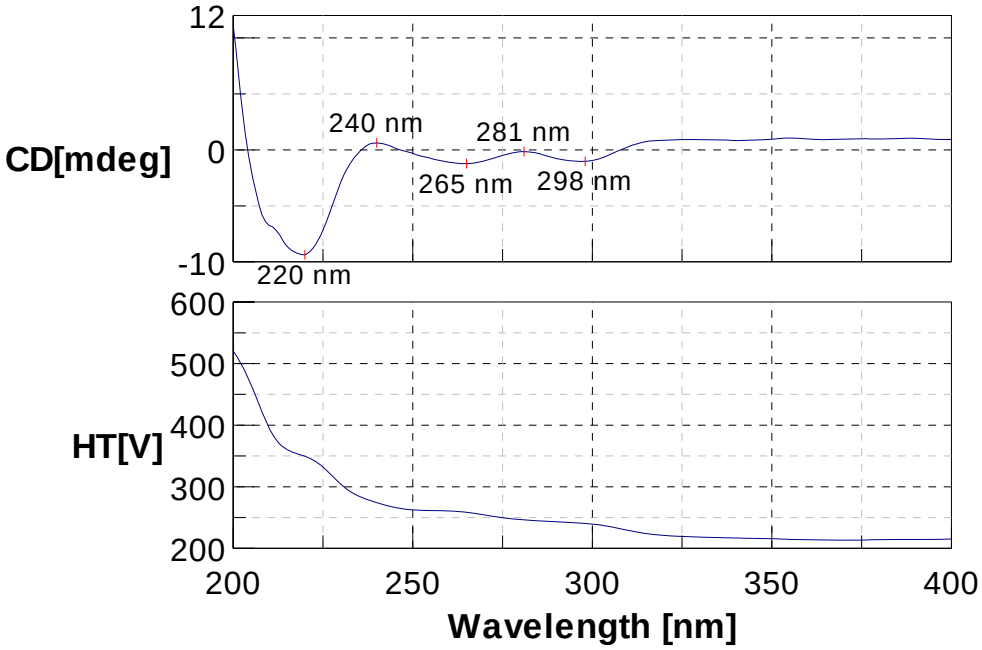


Figure S32. ^{1}H NMR (400 MHz, CD_3OD) spectrum of compound **3**

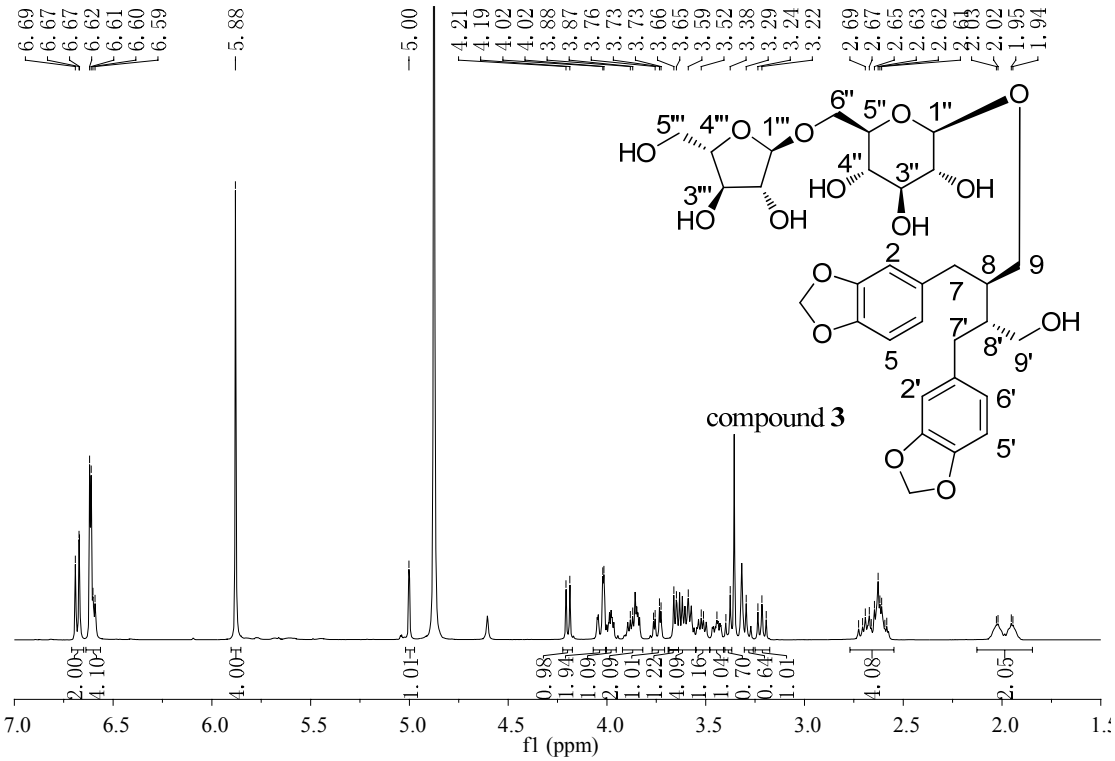


Figure S33. Partially intercepted ^{1}H NMR (400 MHz, CD_3OD) spectrum of compound **3**

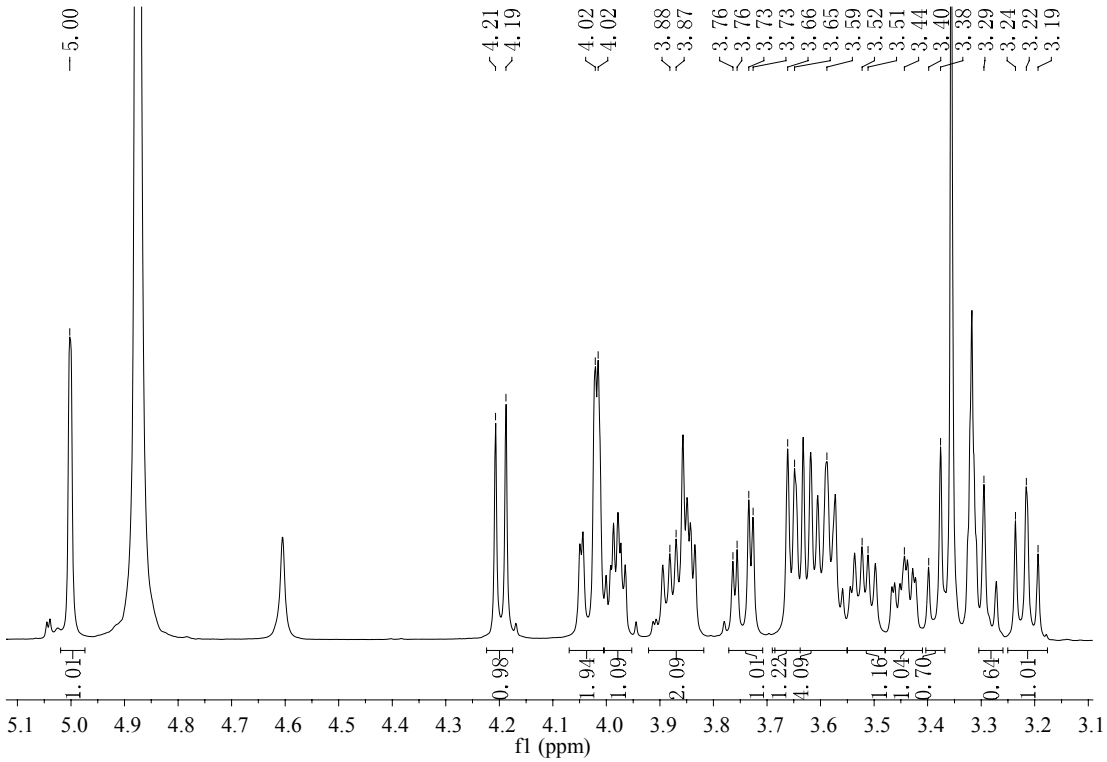
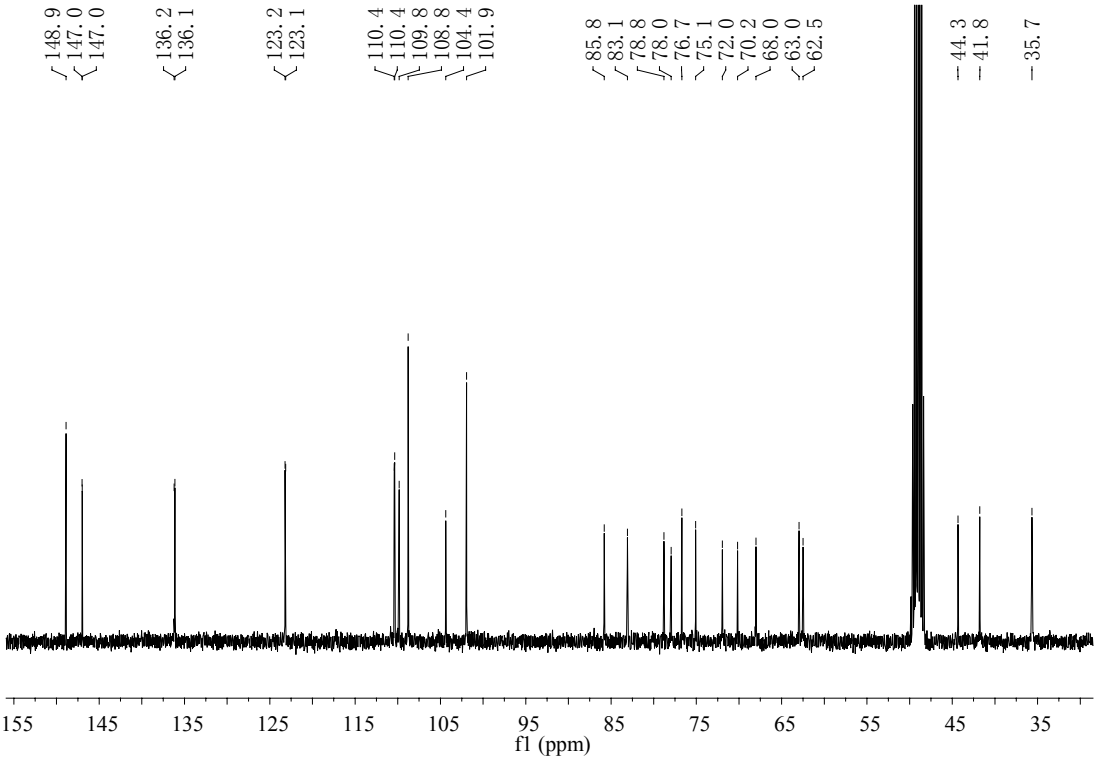


Figure S34. ^{13}C NMR (100 MHz, CD_3OD) spectrum of compound **3**



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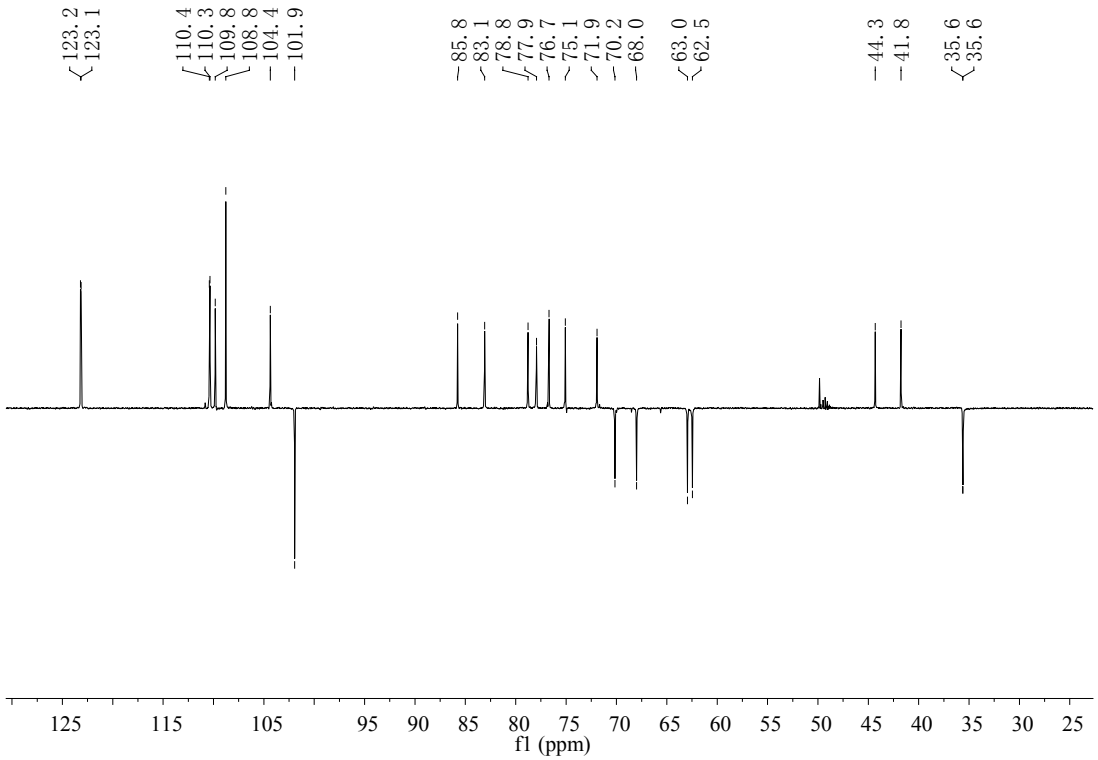


Figure S36. HSQC (400 MHz, CD_3OD) spectrum of compound **3**

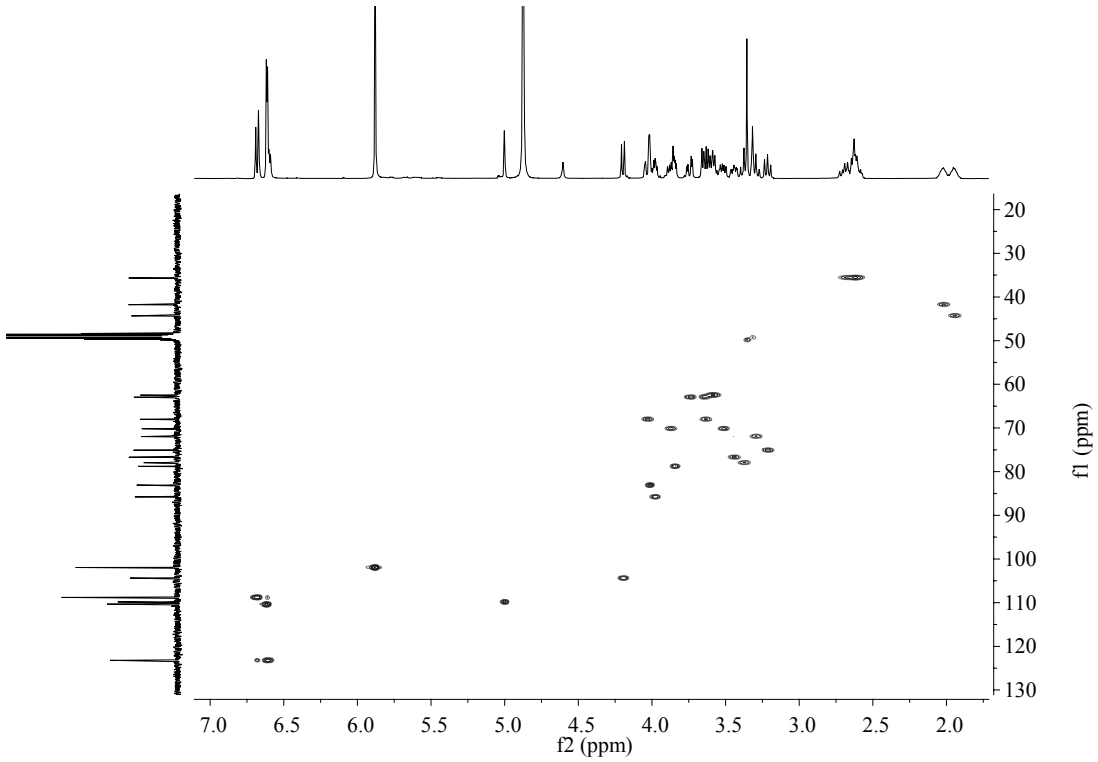


Figure S37. HMBC (400 MHz, CD_3OD) spectrum of compound **3**

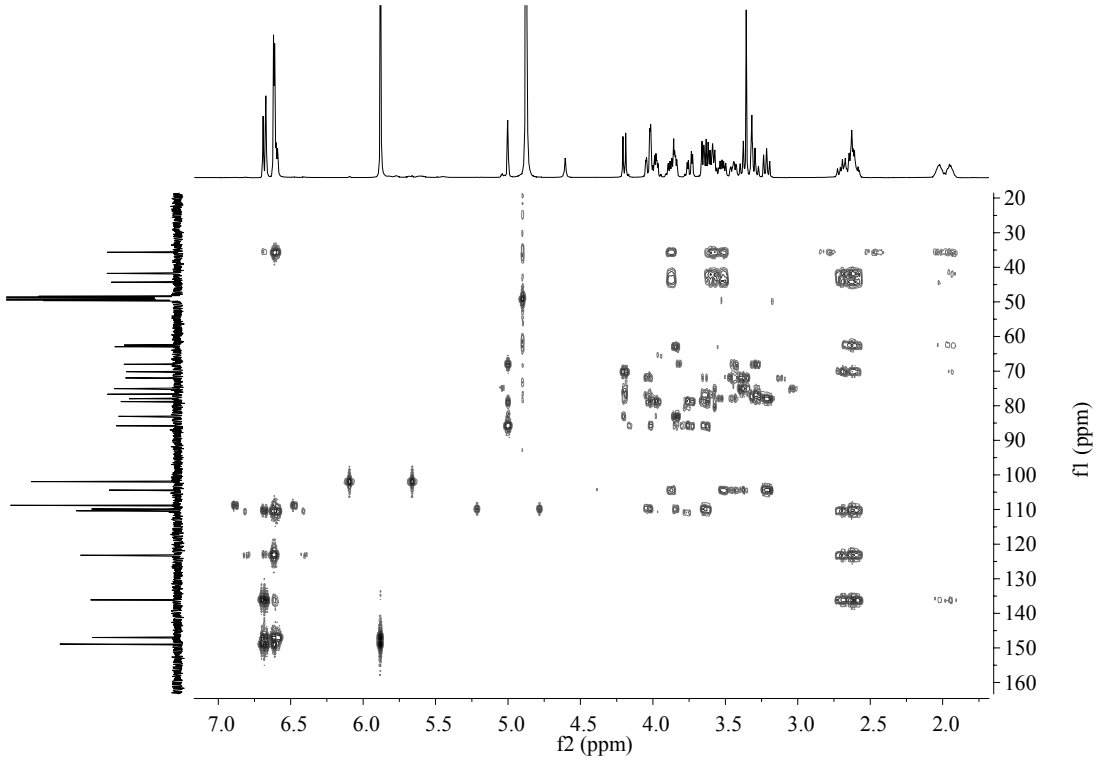


Figure S38. Partially intercepted HMBC (400 MHz, CD_3OD) spectrum of compound **3**

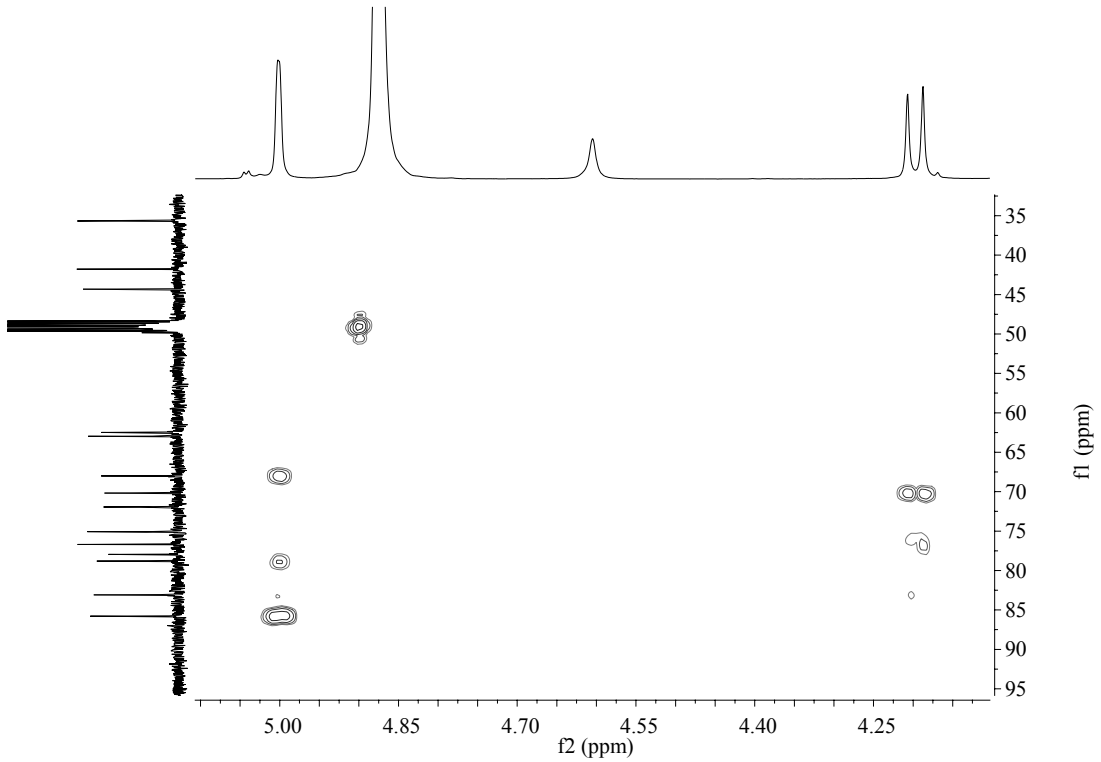


Figure S39. ^{1}H-^{1}H COSY (400 MHz, CD_3OD) spectrum of compound **3**

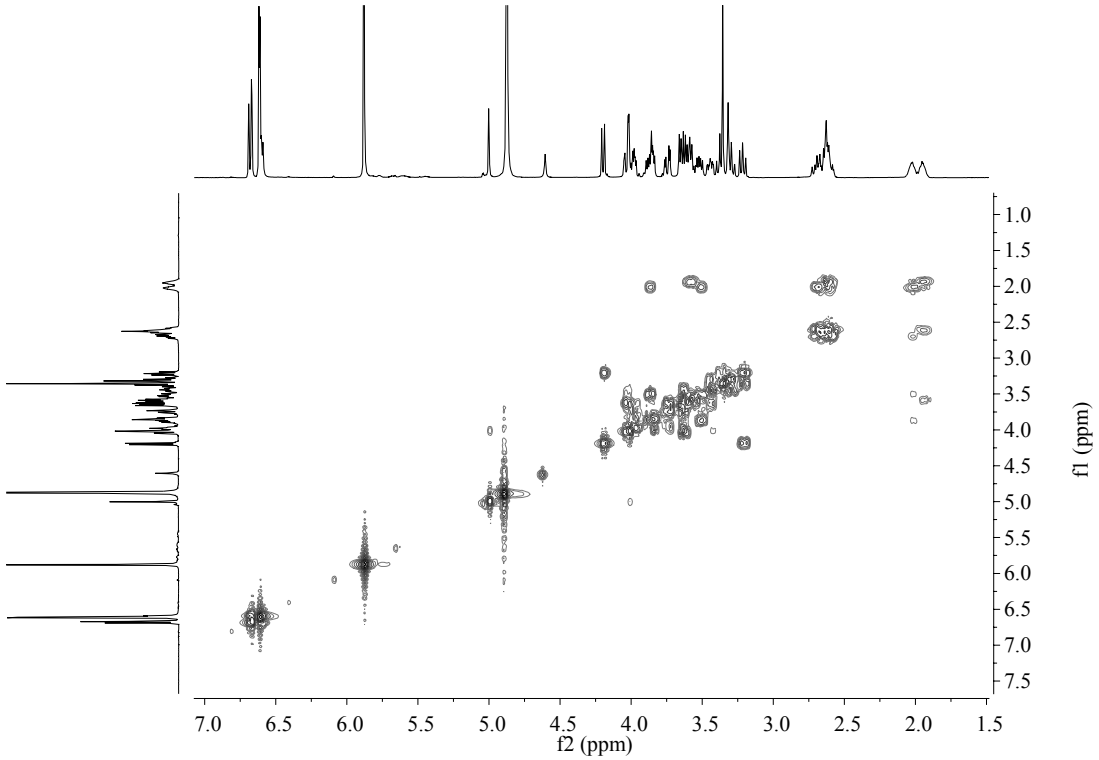


Figure S40. NOESY (400 MHz, CD_3OD) spectrum of compound **3**

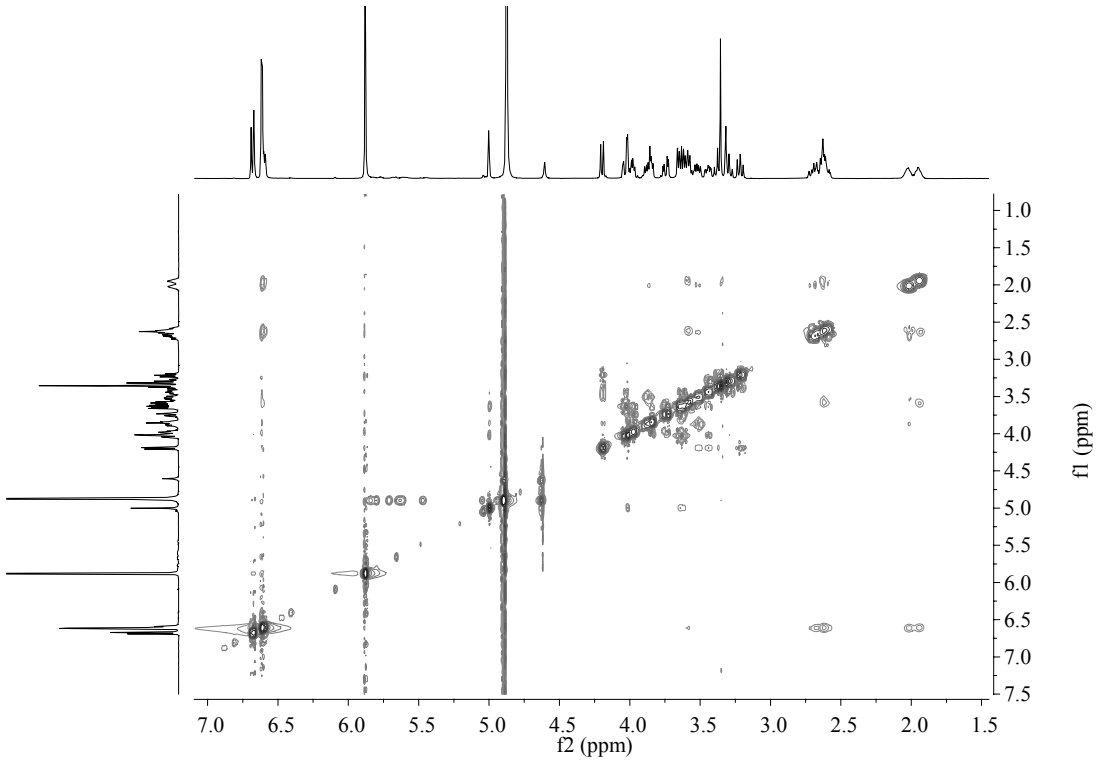


Figure S41. HRESIMS spectrum of compound **3**

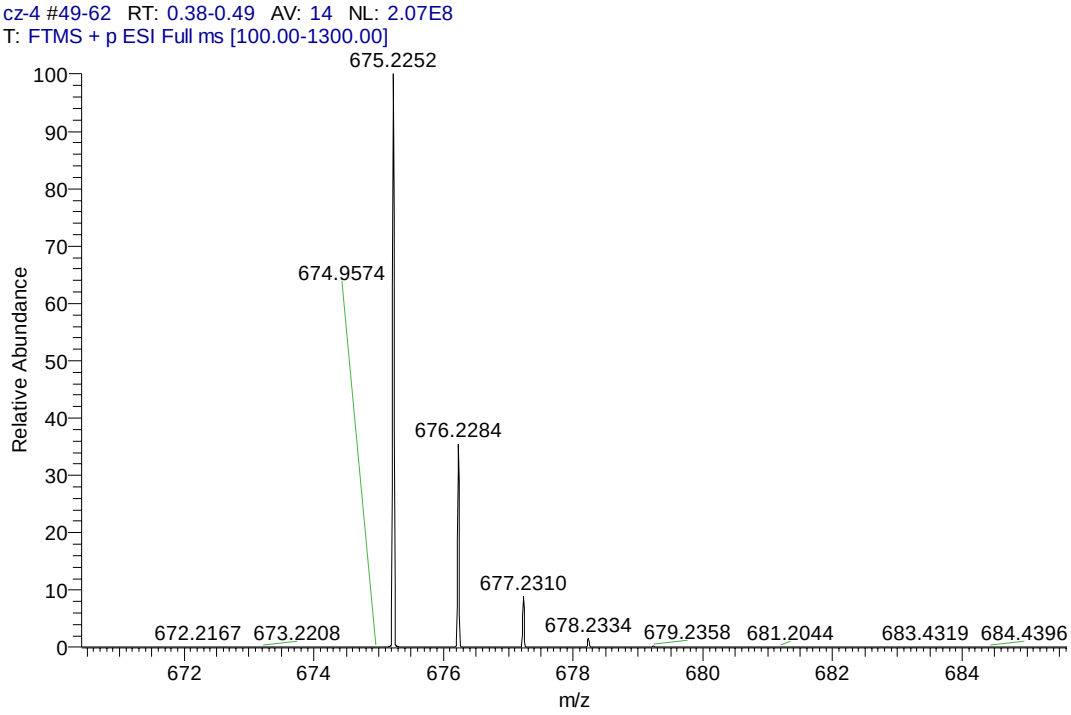


Figure S42. IR spectrum of compound **3**

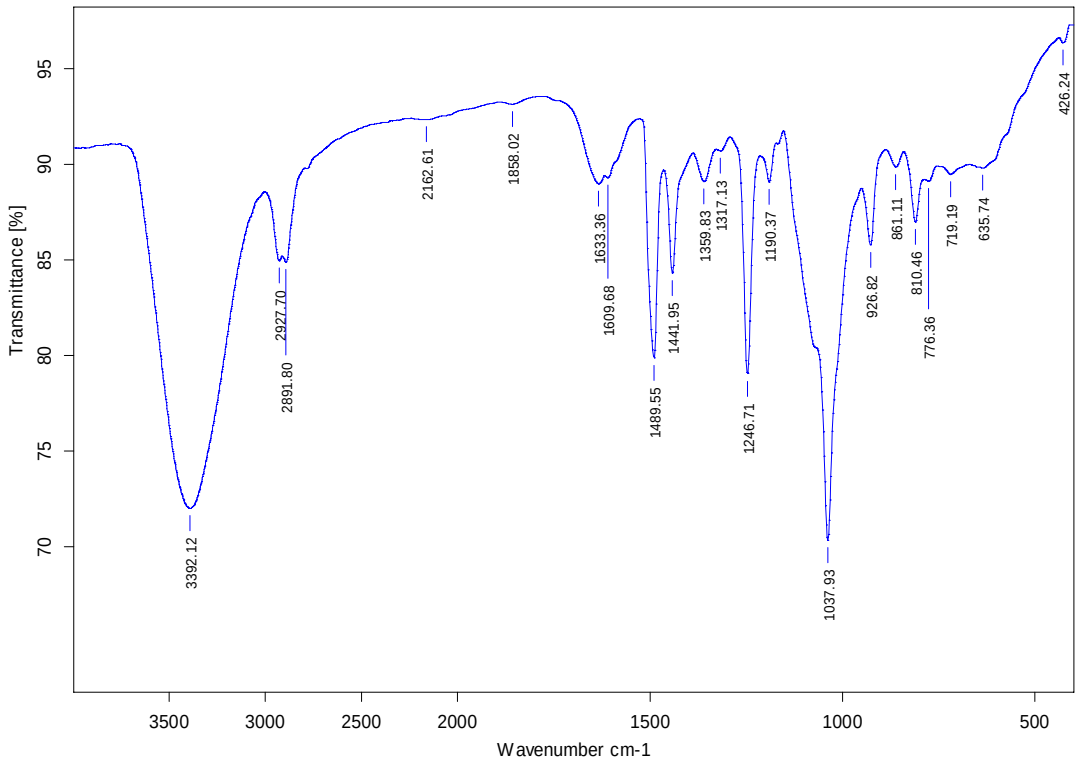


Figure S43. UV spectrum of compound **3**

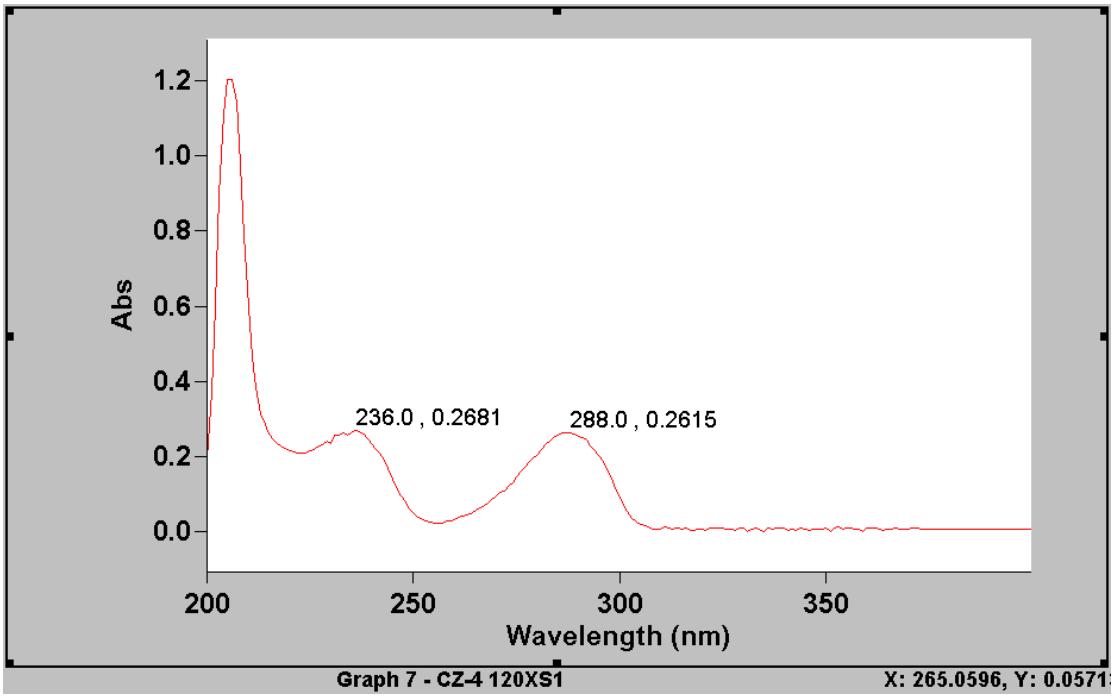


Figure S44. ECD spectrum of compound **3**

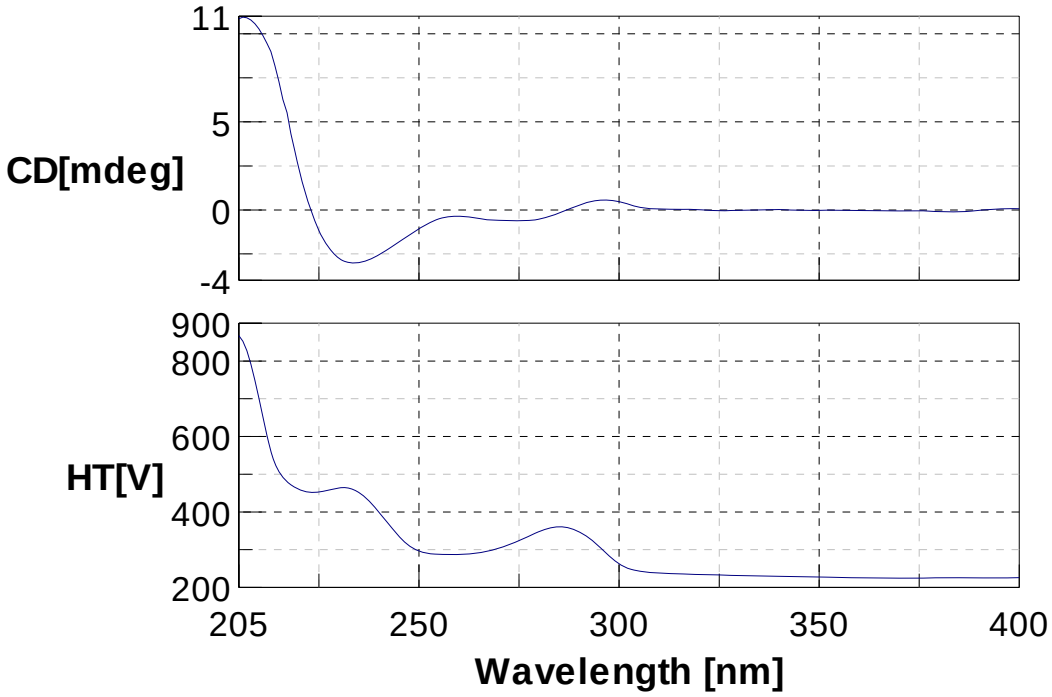


Figure S45. ^{1}H NMR (400 MHz, CD_3OD) spectrum of compound **4**

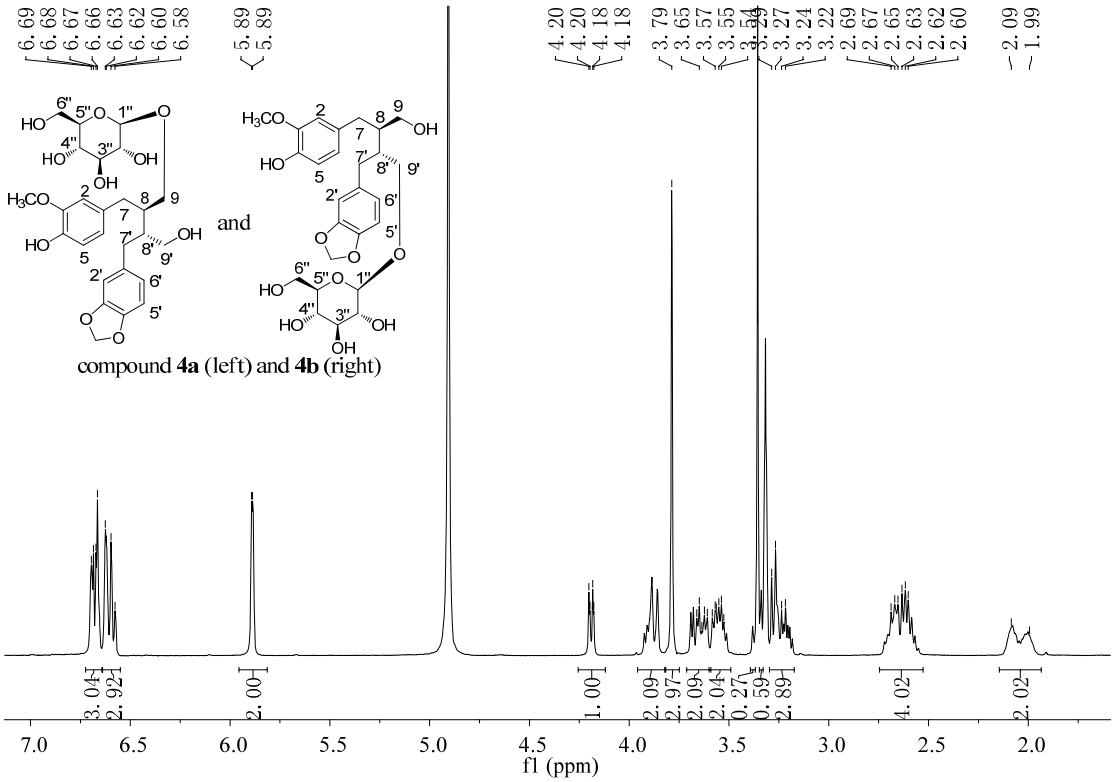


Figure S46. Partially intercepted ^{1}H NMR (400 MHz, CD_3OD) spectrum of compound **4**

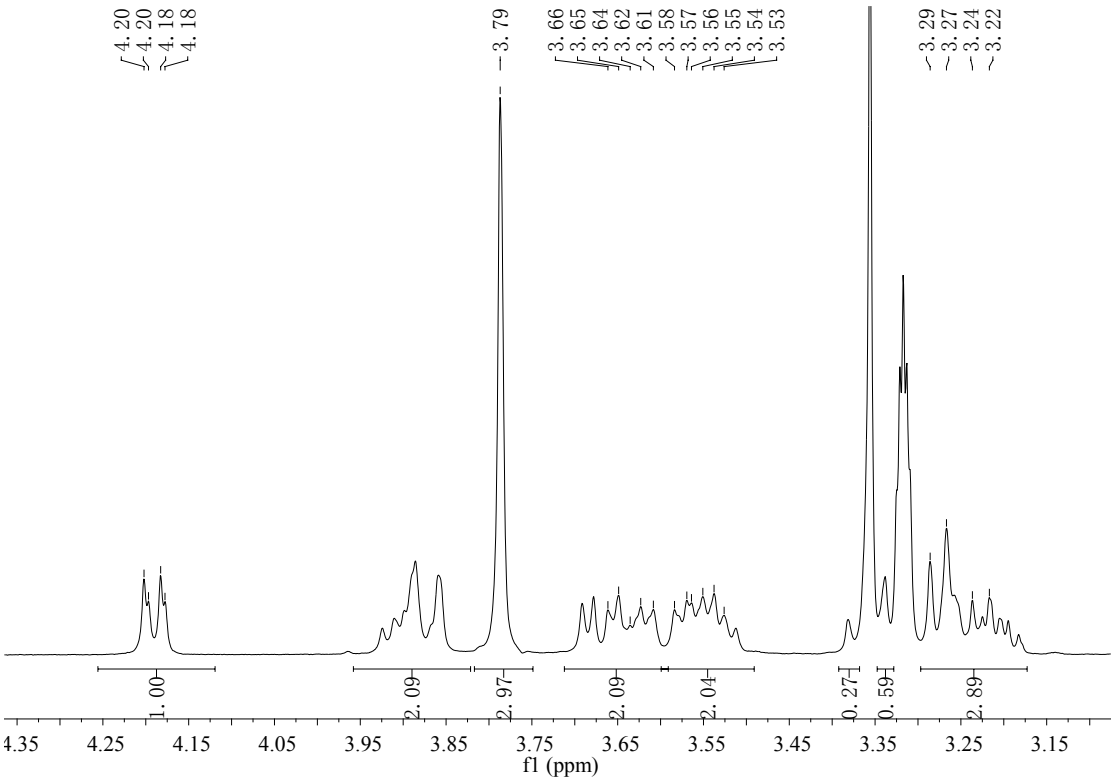


Figure S47. ^{13}C NMR (100 MHz, CD_3OD) spectrum of compound **4**

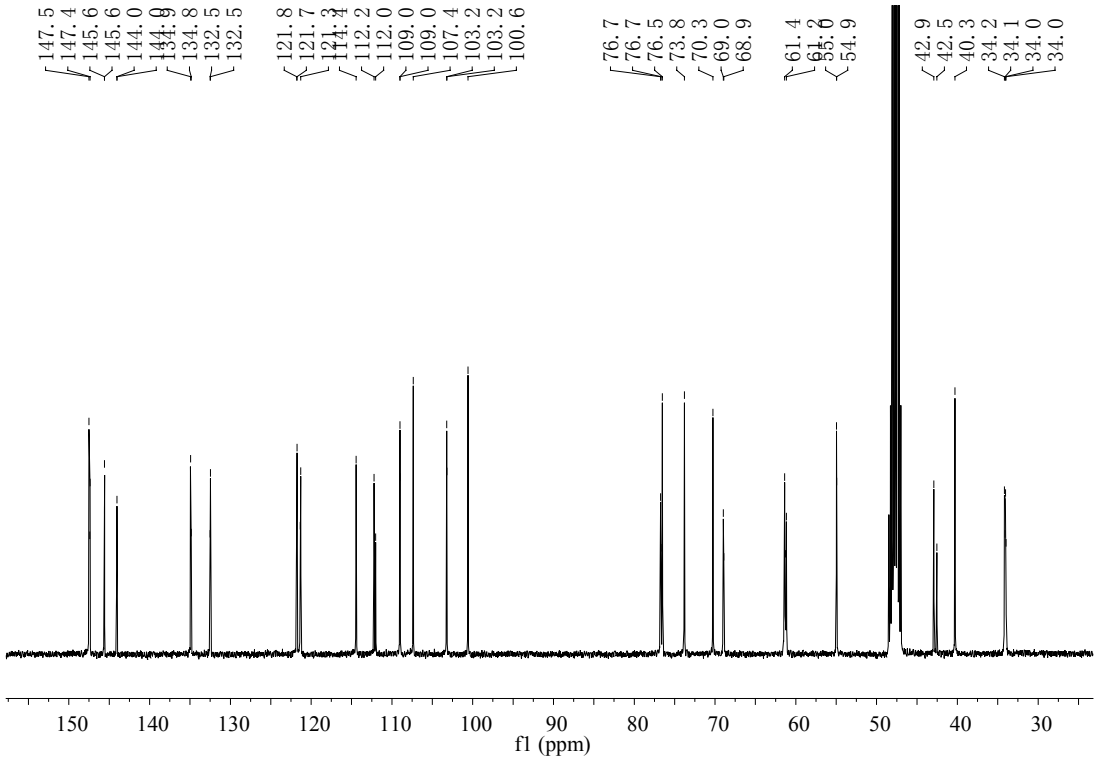


Figure S48. Partially intercepted ^{13}C NMR (100 MHz, CD_3OD) spectrum of compound **4**

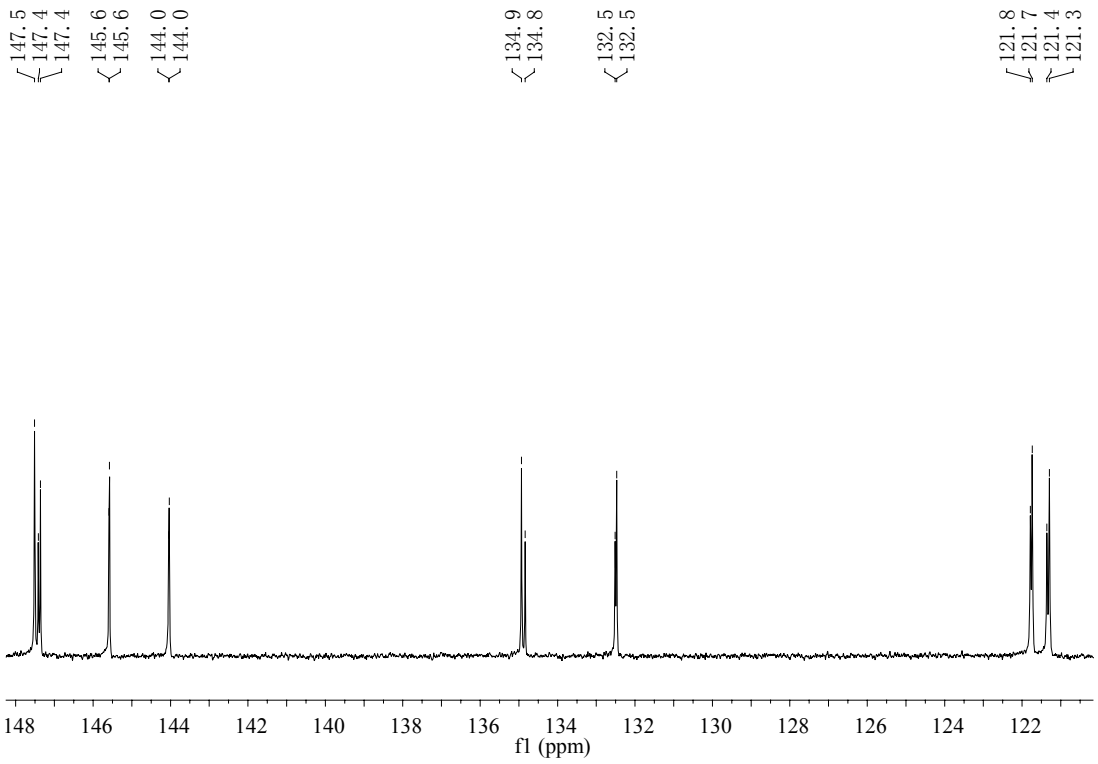


Figure S49. Partially intercepted ^{13}C NMR (100 MHz, CD_3OD) spectrum of compound **4**

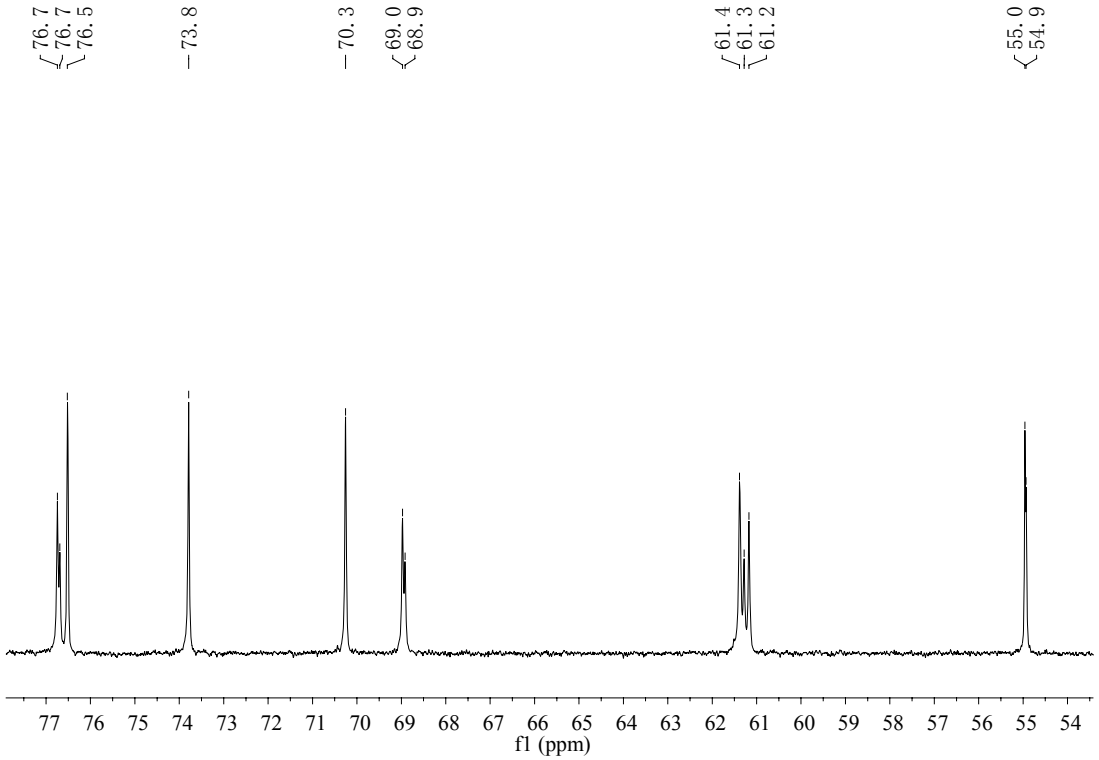


Figure S50. DEPT135 (100 MHz, CD_3OD) spectrum of compound **4**

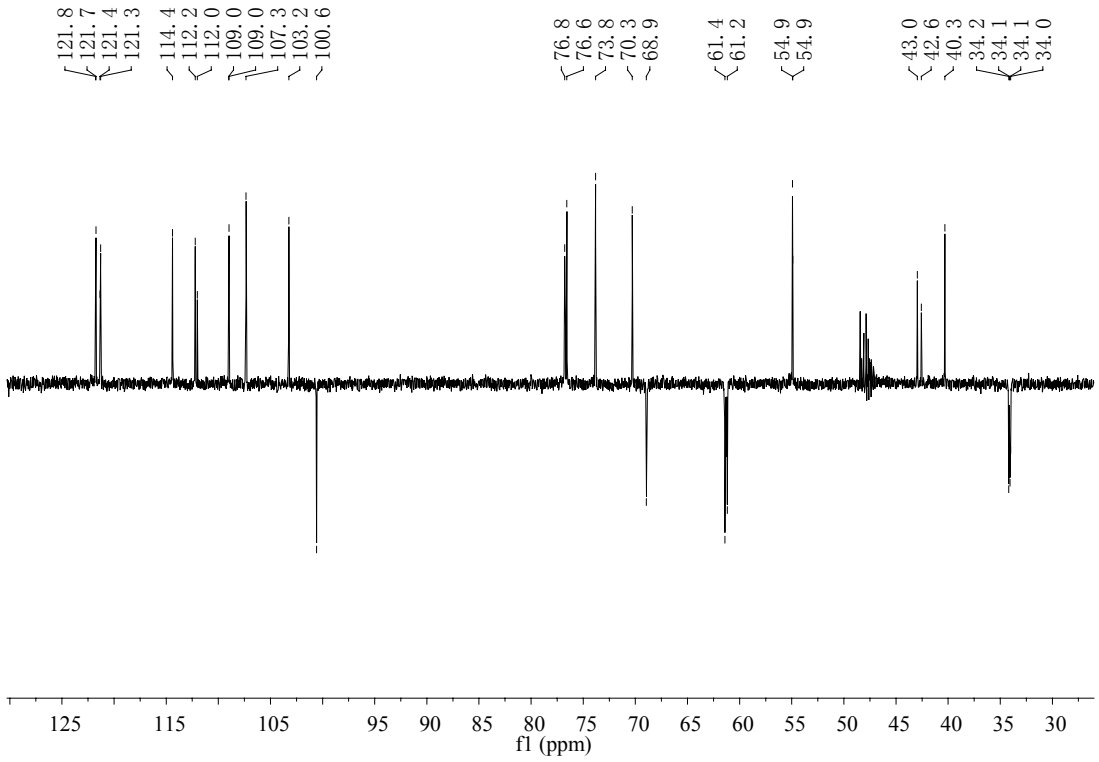


Figure S51. HSQC (400 MHz, CD_3OD) spectrum of compound **4**

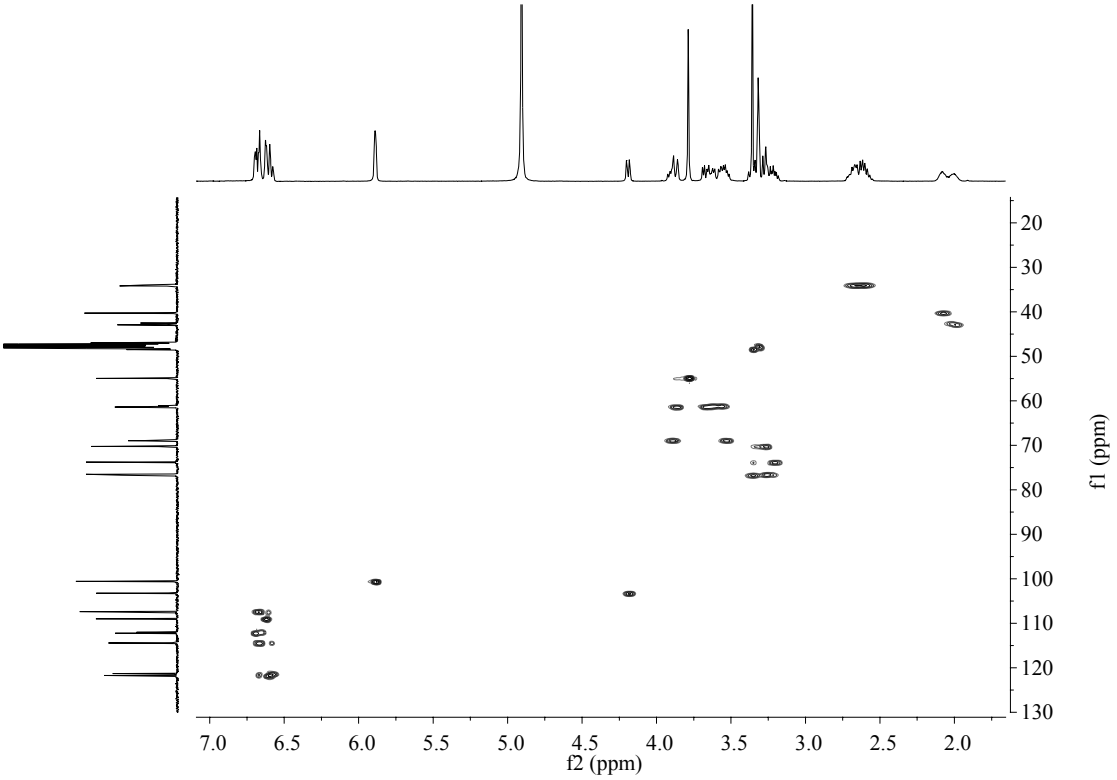


Figure S52. HMBC (400 MHz, CD_3OD) spectrum of compound **4**

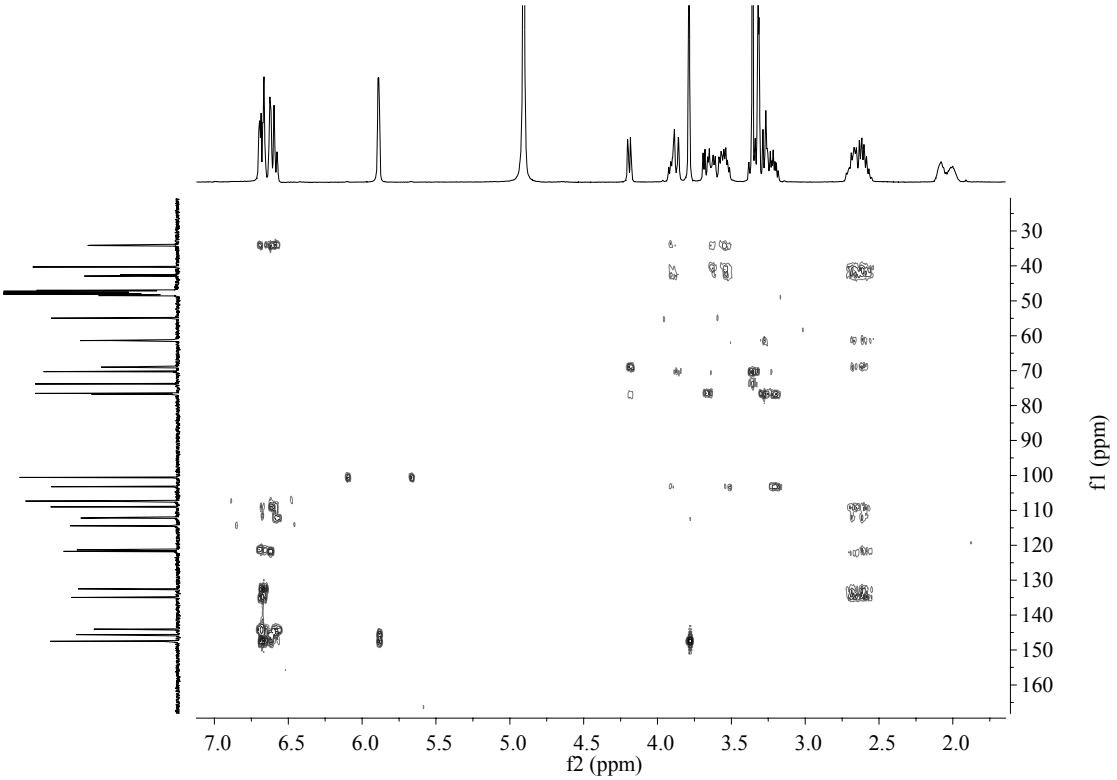


Figure S53. ^{1}H-^{1}H COSY (400 MHz, CD_3OD) spectrum of compound **4**

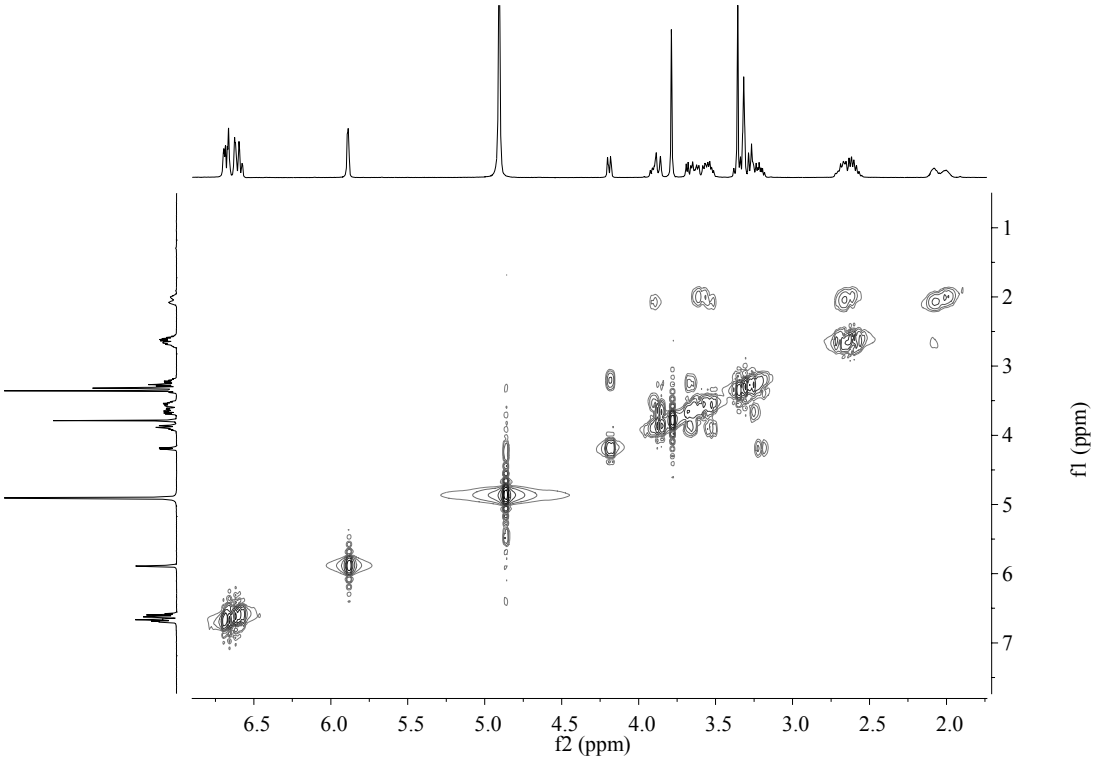


Figure S54. NOESY (400 MHz, CD_3OD) spectrum of compound **4**

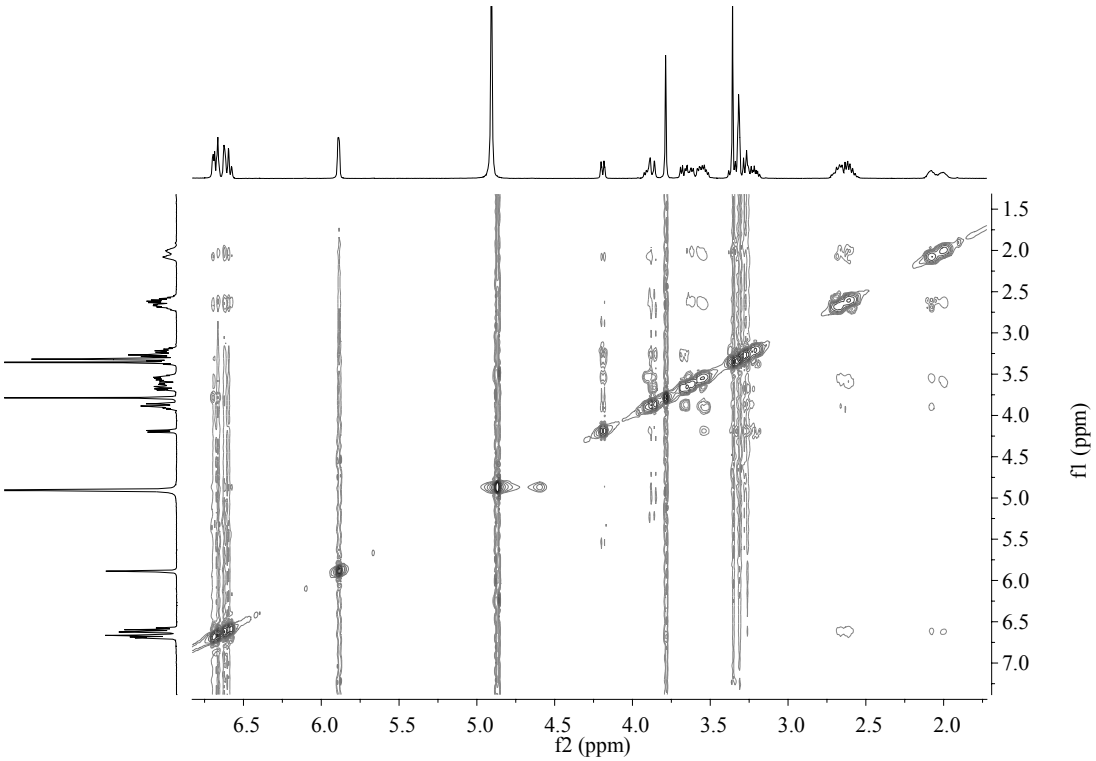


Figure S55. HRESIMS spectrum of compound **4**

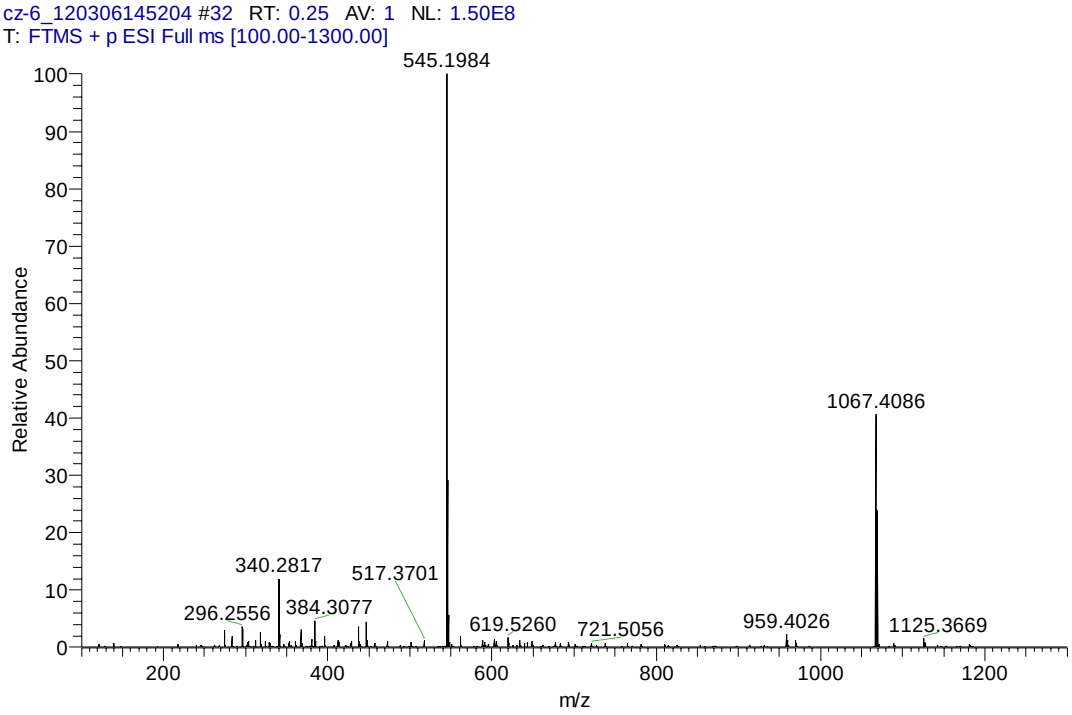


Figure S56. IR spectrum of compound **4**

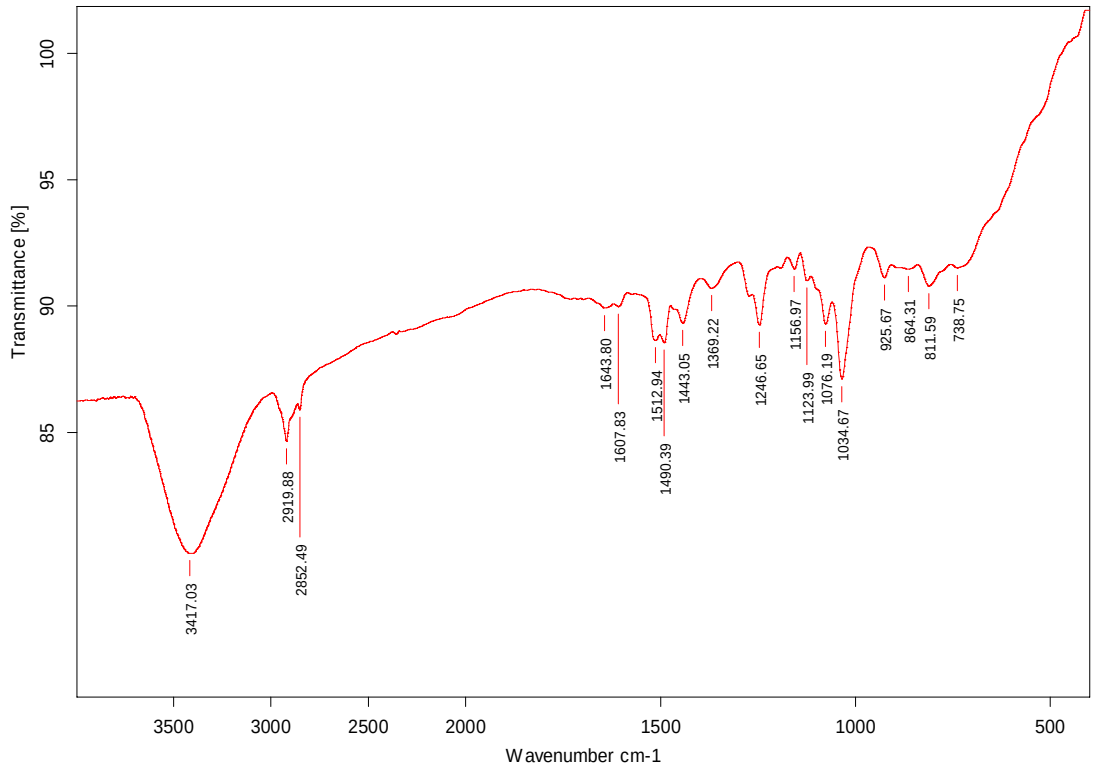


Figure S57. UV spectrum of compound **4**

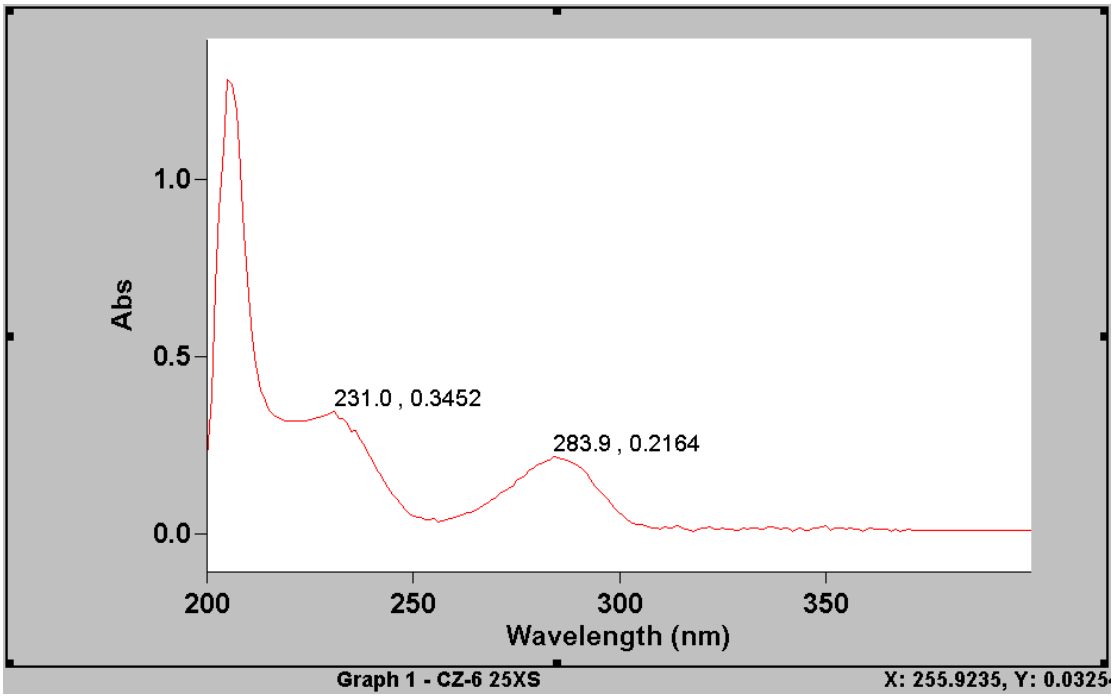


Figure S58. ECD spectrum of compound **4**

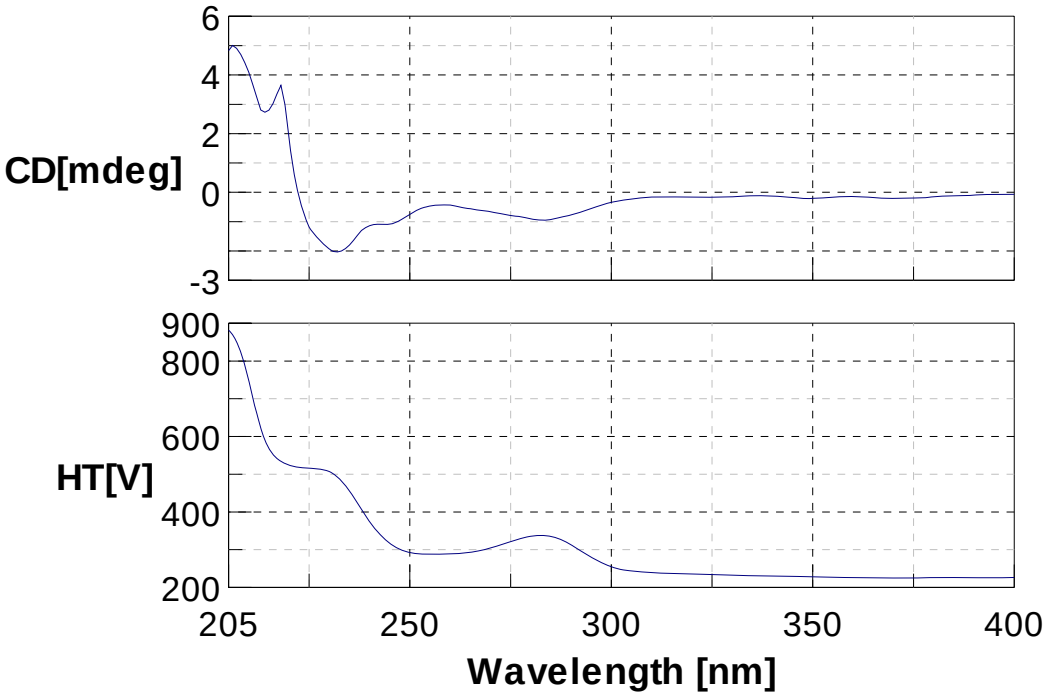


Figure S59. ^{1}H NMR (400 MHz, $CDCl_3$) spectrum of (−)-dihydrocubebin

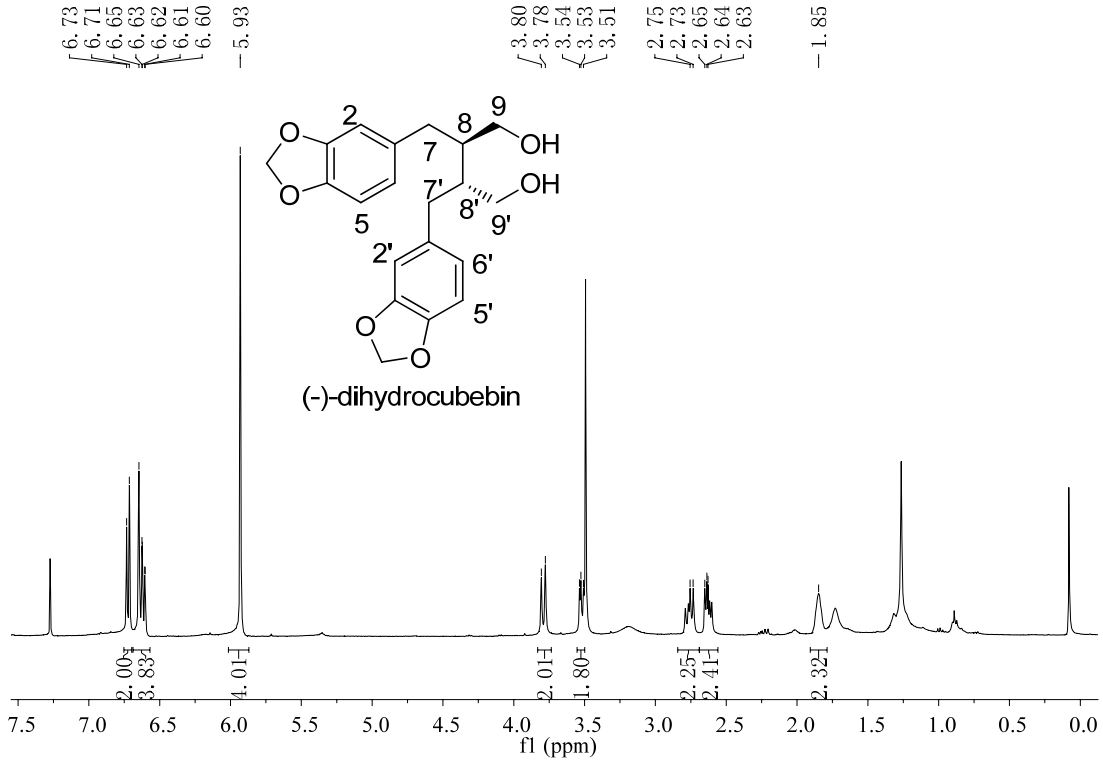


Figure S60. ^{13}C NMR (100 MHz, $CDCl_3$) spectrum of (−)-dihydrocubebin

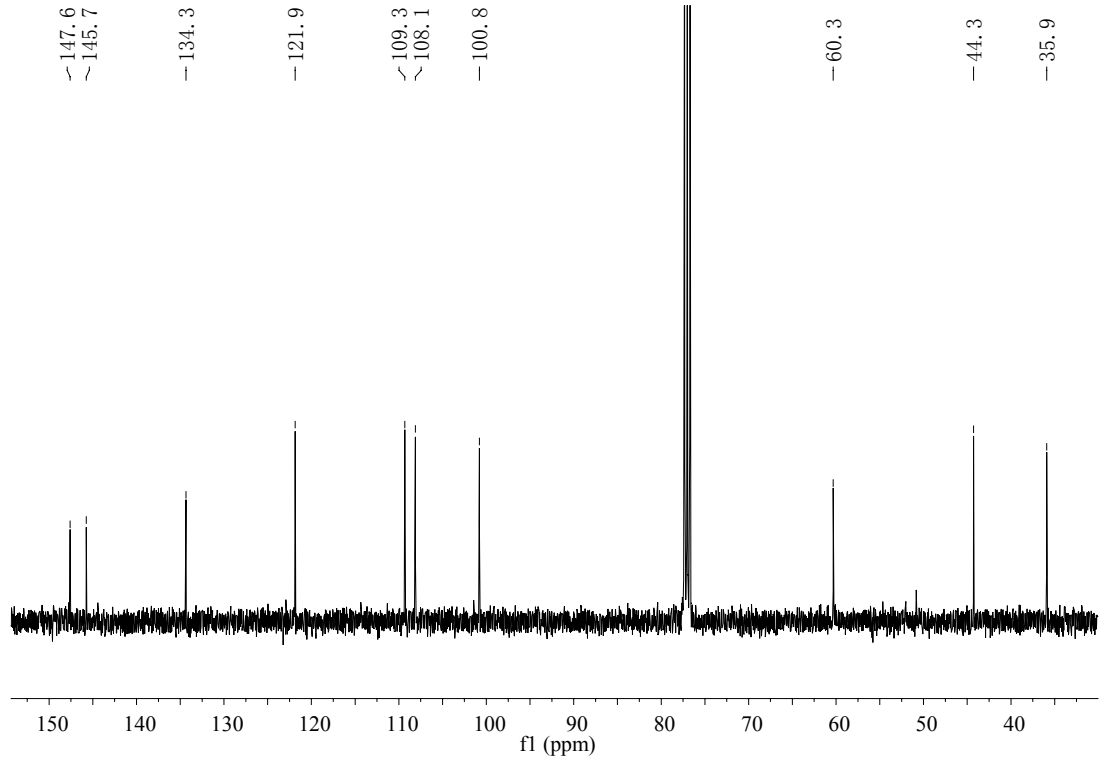


Figure S61. ECD spectrum of (–)-dihydrocubebin

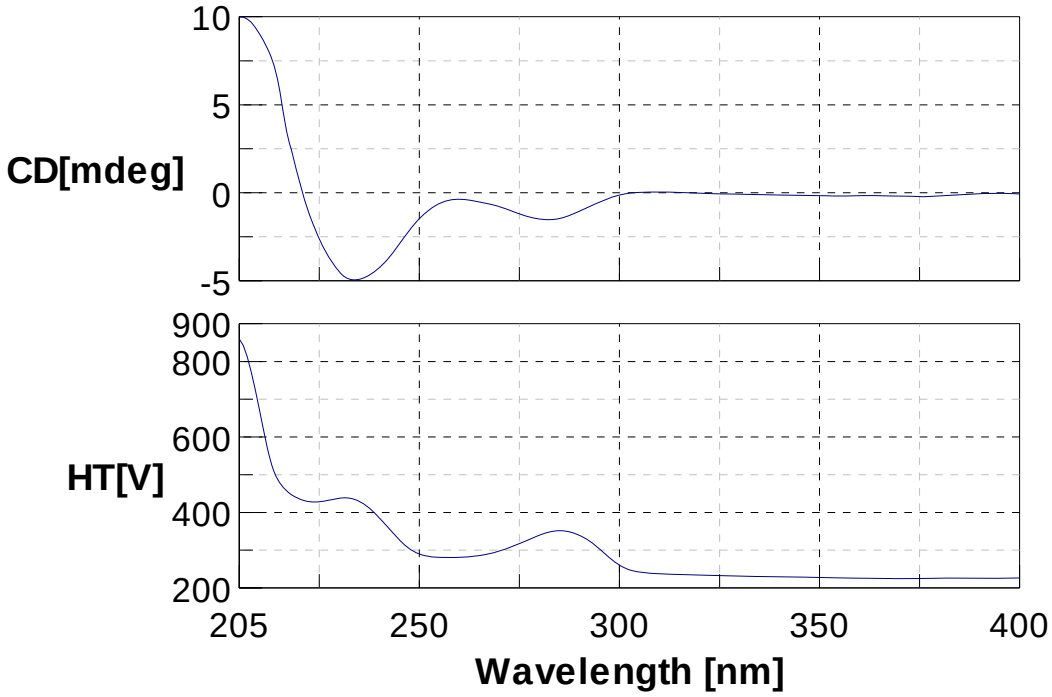


Figure S62. ^{1}H NMR (400 MHz, $CDCl_3$) spectrum of piperphilippinin VI

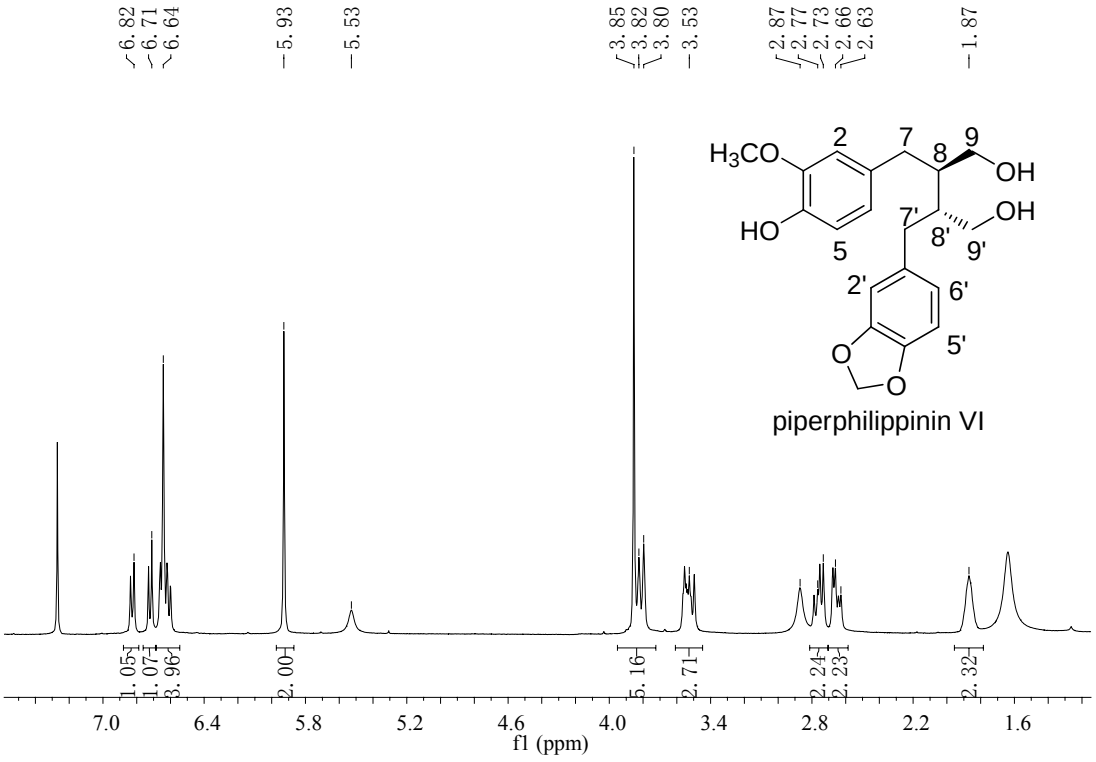


Figure S63. ^{13}C NMR (100 MHz, $CDCl_3$) spectrum of piperphilippinin VI

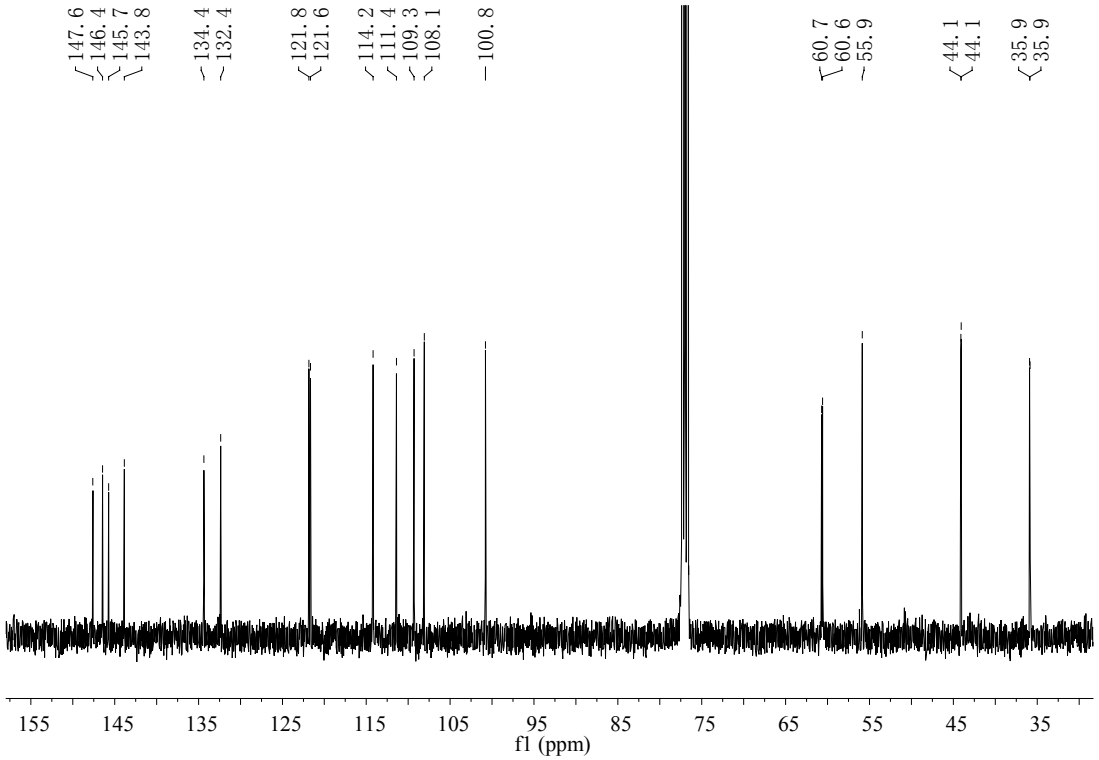


Figure S64. ECD spectrum of piperphilippinin VI

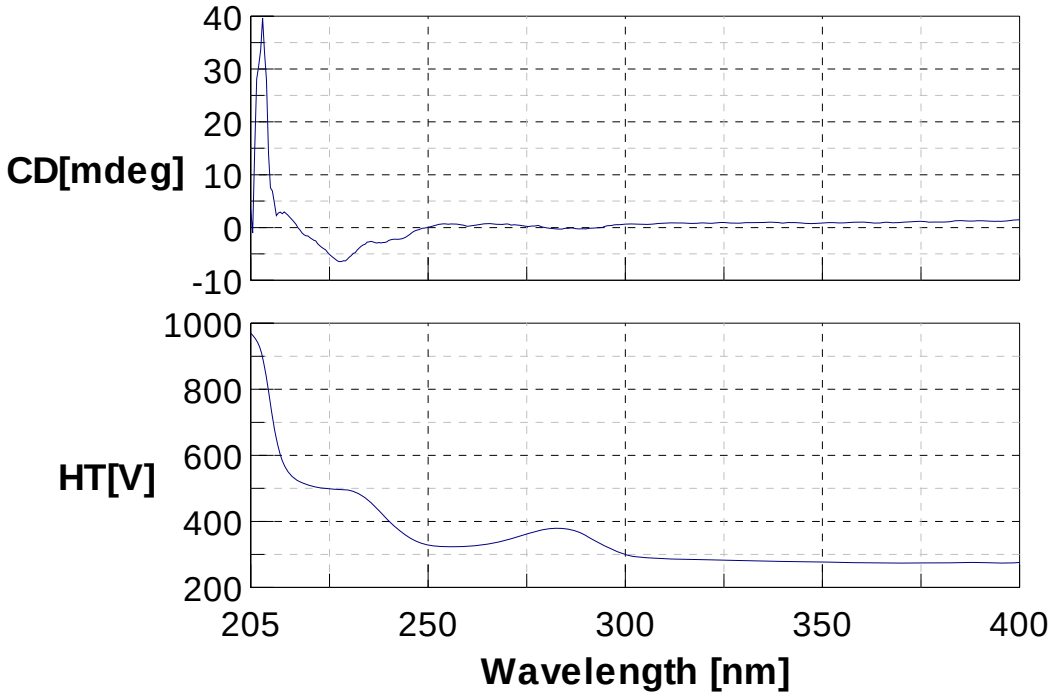


Figure S65. DPPH radical scavenging activity of an ethanol extract of the fruit of *S. glaucescens* Diels. DPPH (150 μM) was added to the ethanol extract of *S. glaucescens* fruit at various concentrations (62.5, 125, 250, 750, and 1000 μg/mL). Vitamin C (100 μM) was used as the positive control. DPPH radical scavenging rate (%) = $[(A_{control} - A_{sample})/A_{control}] \times 100$.

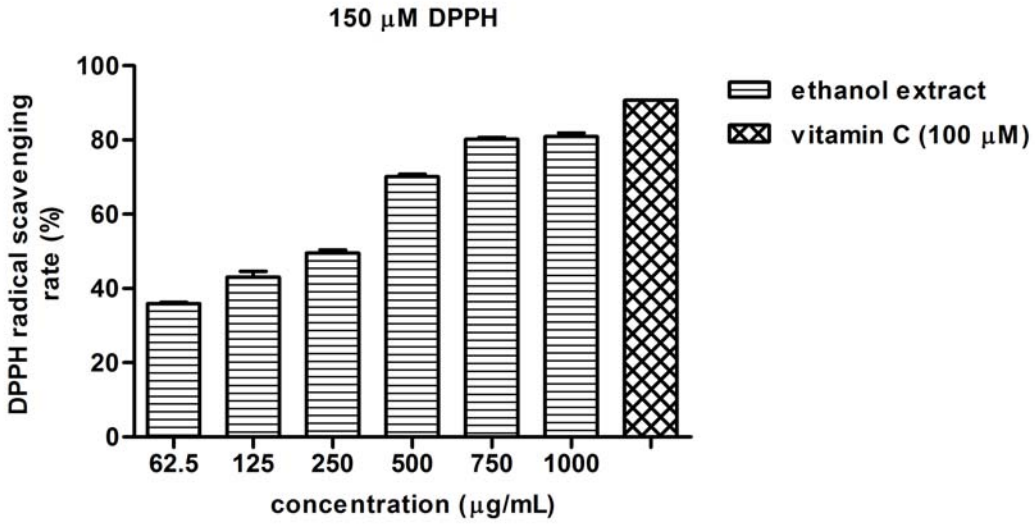


Figure S66. Neuroprotective effect of an ethanol extract of *S. glaucescens* fruit against A$\beta_{25\text{-}35}$-induced SH-SY5Y cell death. Three independent experiments were performed. $^{*}p < 0.05$, $^{**}p < 0.01$, $^{***}p < 0.001$, compared with the A$\beta_{25\text{-}35}$-treated group. Vitamin C (10 μM) was used as the positive control.

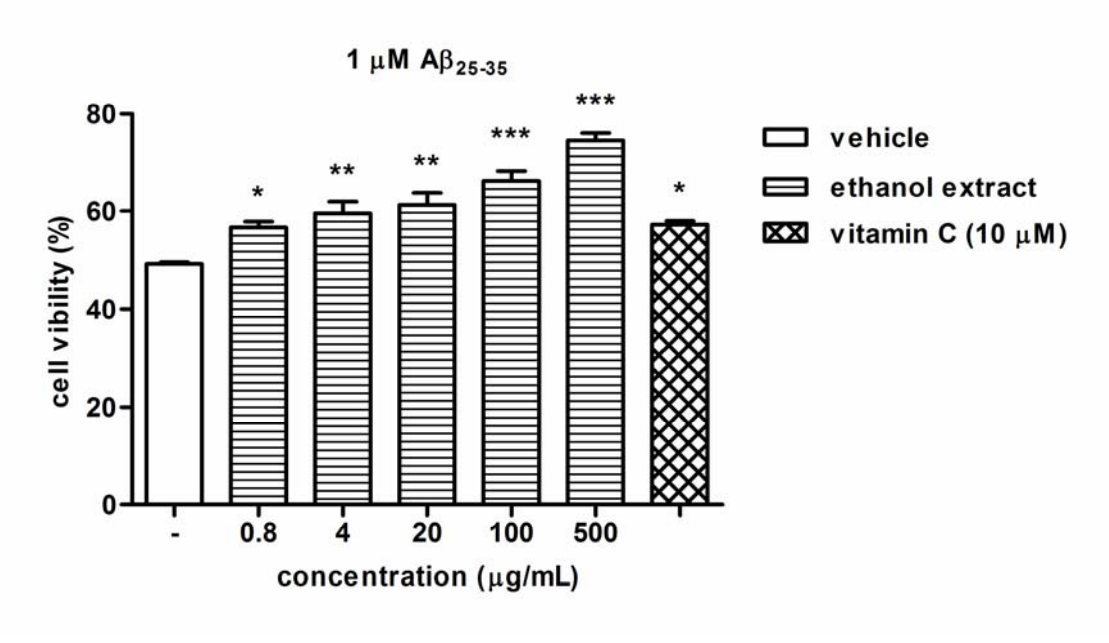


Figure S67. HPLC analysis of the EtOAc layer of the enzymatic hydrolysis reaction of compound **3**. Chromatographic conditions: 75% methanol; 1.0 mL/min; 254 nm.

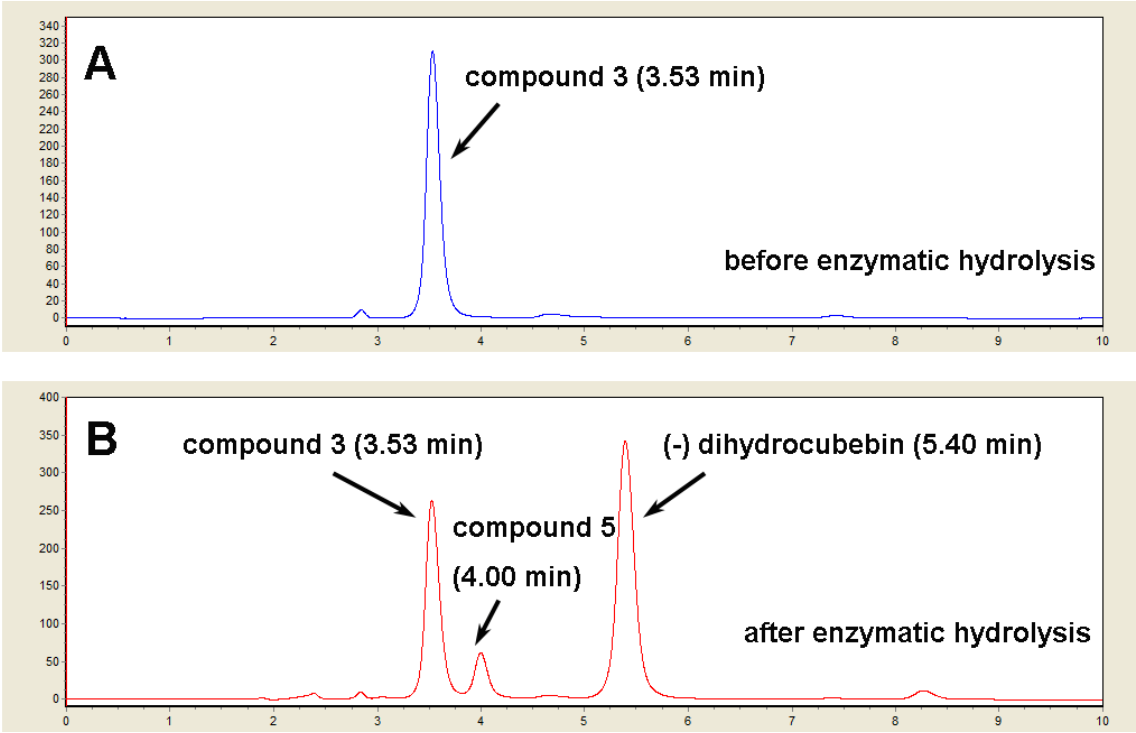


Figure S68. HPLC analysis of the EtOAc layer of the enzymatic hydrolysis reaction of compound **4**. Chromatographic conditions: 75% methanol; 1.0 mL/min; 254 nm.

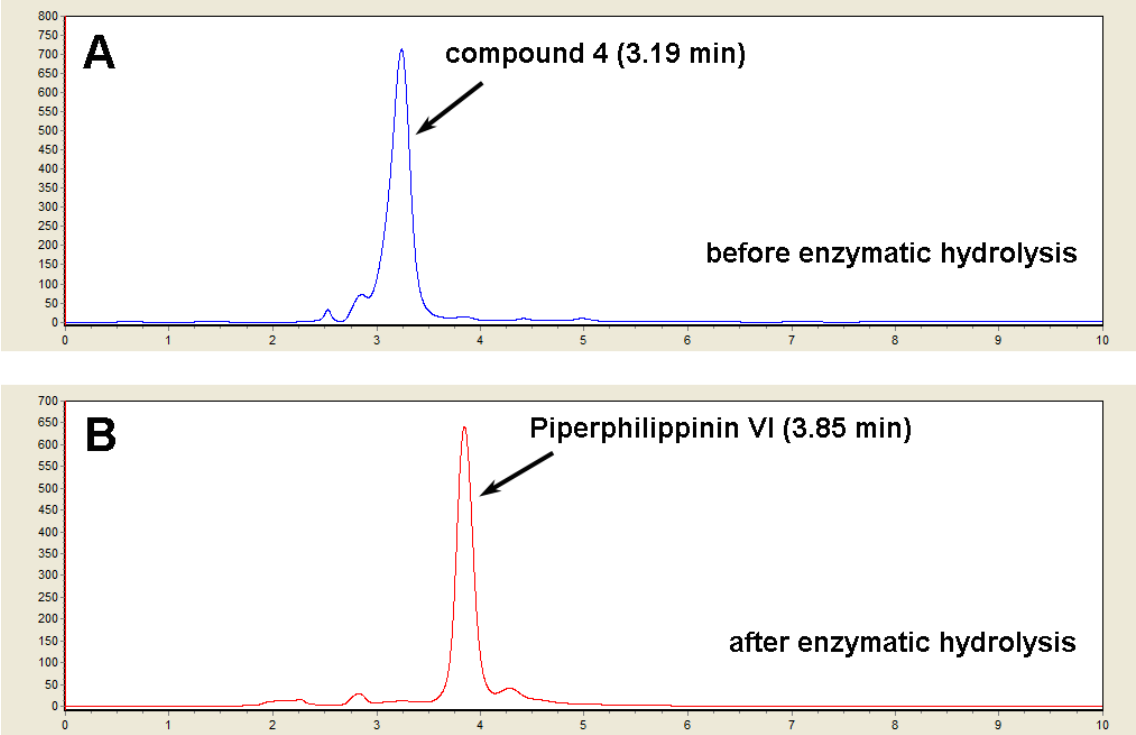
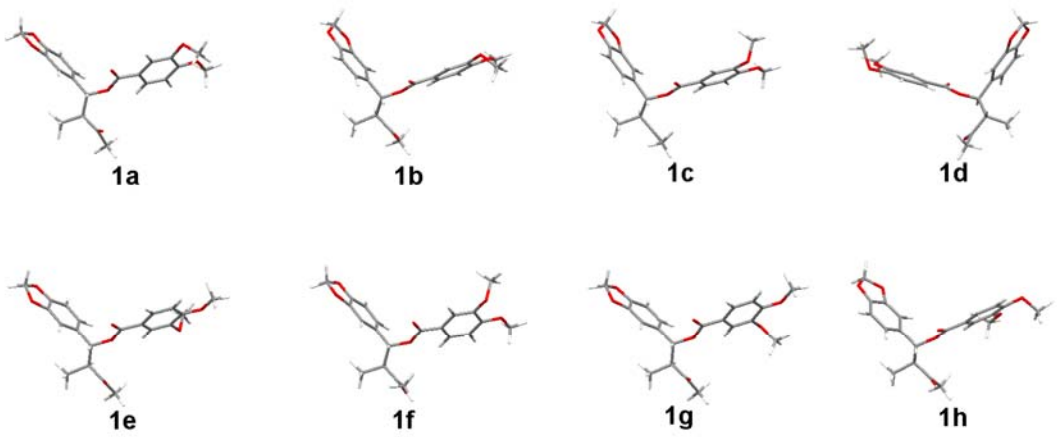
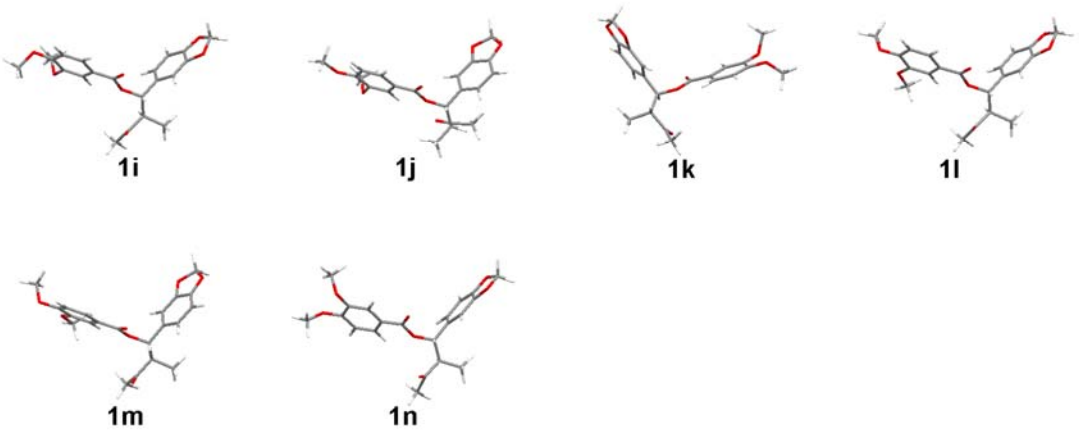


Figure S69. Eight lowest energy conformers of the 7′*R*,8′*S* isomer and six lowest energy conformers of the 7′*S*,8′*R* isomer of compound **1**.

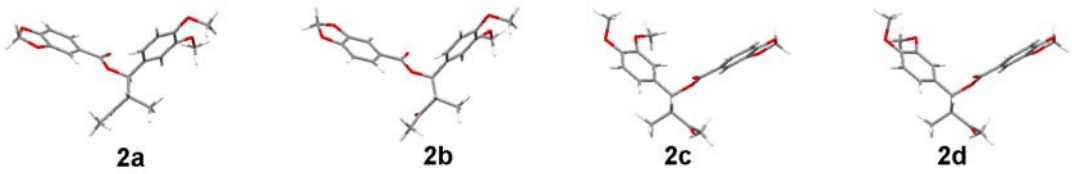


1a-1h: eight lowest energy conformers of isomer 7'*R*, 8'*S* of compound **1.**

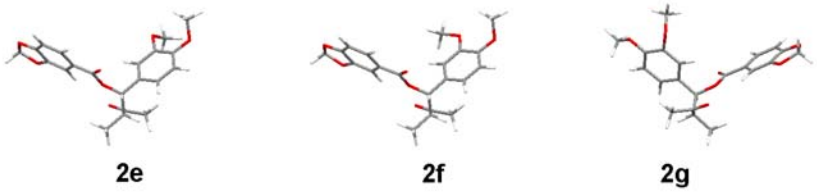


1i-1n: six lowest energy conformers of isomer 7'*S*, 8'*R* of compound **1.**

Figure S70. Four lowest energy conformers of the 7′*R*,8′*S* isomer and three lowest energy conformers of the 7′*S*,8′*R* isomer of compound **2**.



2a-2d: four lowest energy conformers of isomer 7'*R*,8'*S* of compound **2**.



2e-2g: three lowest energy conformers of isomer 7'*S*,8'*R* of compound **2**.

Table S1. Relative free energies (Δ*G*) and equilibrium populations (*P*) of the conformers of the 7′*R*,8′*S* and 7′*S*,8′*R* isomers of compound **1**.

	isomer 7′*R*,8′*S* of **1**			isomer 7′*S*,8′*R* of **1**	
conformer	ΔG (kcal/mol)	*P* (%)	conformer	ΔG (kcal/mol)	*P* (%)
1a	0.89	10.9	**1i**	1.65	3.4
1b	0.00	49.2	**1j**	1.94	2.0
1c	1.85	2.2	**1k**	0.90	12.0
1d	1.07	8.0	**1l**	0.48	24.0
1e	1.10	7.7	**1m**	0.00	54.4
1f	2.26	1.1	**1n**	1.52	4.2
1g	0.85	11.6			
1h	0.98	9.5			

Table S2. Relative free energies (Δ*G*) and equilibrium populations (*P*) of the conformers of the 7′*R*,8′*S* and 7′*S*,8′*R* isomers of compound **2**.

	isomer 7′*R*,8′*S* of **2**			isomer 7′*S*,8′*R* of **2**	
conformer	ΔG (kcal/mol)	*P* (%)	conformer	ΔG (kcal/mol)	*P* (%)
2a	0.15	28.4	**2e**	0.19	37.3
2b	0.17	27.6	**2f**	0.00	51.2
2c	0.00	36.6	**2g**	0.88	11.5
2d	0.94	7.5			