Antioxidant Lignans and Neolignans from Acorus tatarinowii

Yuanyuan Lu,[1,2] Yongbo Xue,[1] Shenjie Chen,[1] Hucheng Zhu,[1] Jinwen Zhang,[2] Xiao-Nian Li,[3] Jianping Wang,[1] JunJun Liu,[1] Changxing Qi,[1] Guang Du[2,*] & Yonghui Zhang[1,*]

[1]Hubei Key Laboratory of Natural Medicinal Chemistry and Resource Evaluation, School of Pharmacy, Tongji Medical College, Huazhong University of Science and Technology, Wuhan 430030, Hubei Province, People's Republic of China

[2]Tongji Hospital Affiliated to Tongji Medical College, Huazhong University of Science and Technology, Wuhan 430030, Hubei Province, People's Republic of China

[3]State Key Laboratory of Phytochemistry and Plant Resources in West China, Kunming Institute of Botany, Chinese Academy of Sciences, Kunming 650204, People's Republic of China

* **Corresponding Authors**

* Tel./fax: +86-027-83692892

Emails: zhangyh@mails.tjmu.edu.cn (Y.Z.);

tjyxb@sina.com (G.D.)

Figure S1. (+)-HR-ESI-MS spectrum of **1** (**1a/1b**)

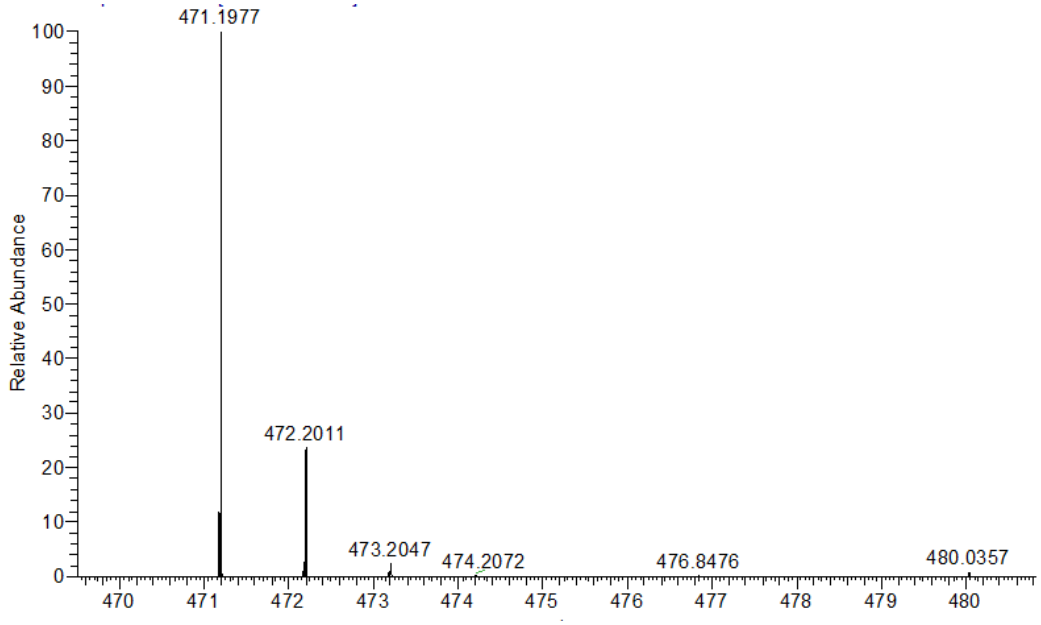


Figure S2. IR spectrum of **1** (**1a/1b**)

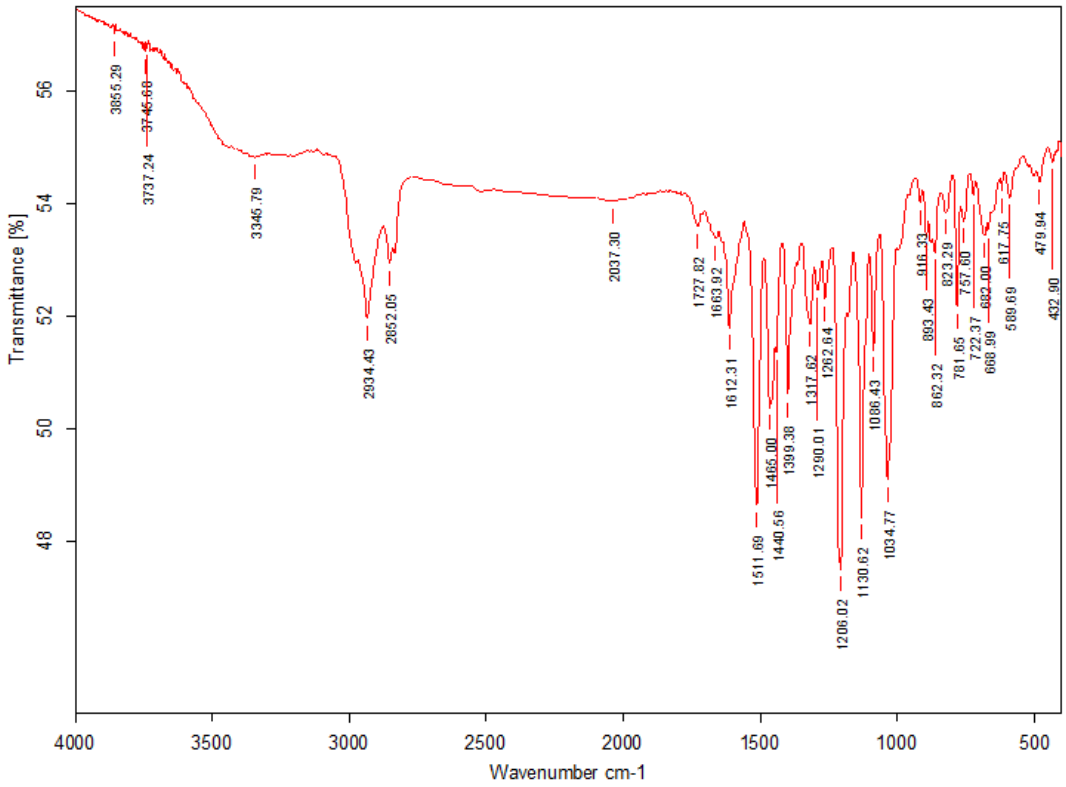


Figure S3. UV spectrum of **1** (**1a/1b**)

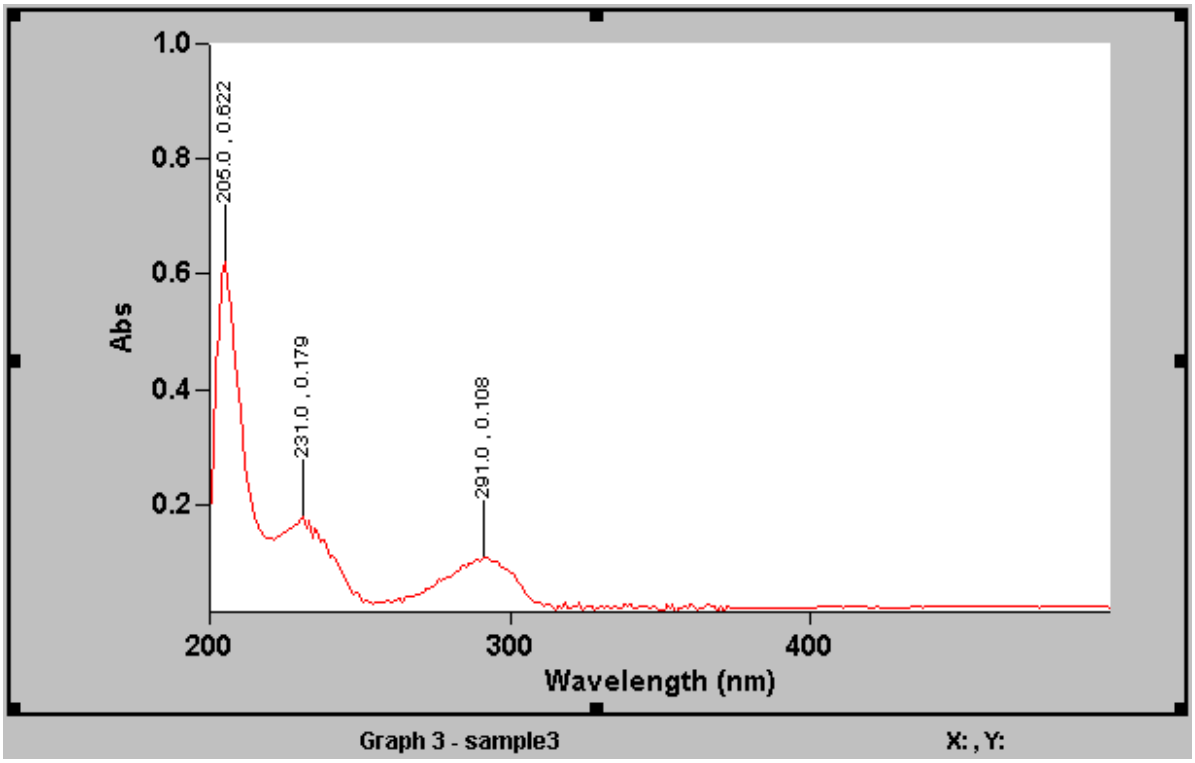


Figure S4. ^{1}H NMR spectrum of **1** (**1a/1b**) in $CDCl_3$

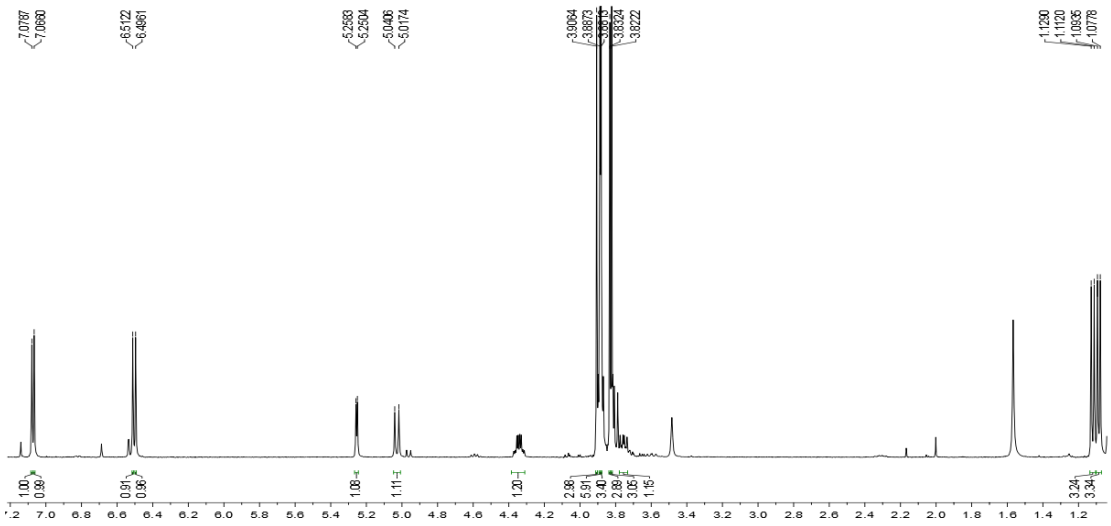


Figure S5. ^{13}C NMR spectrum of **1**(**1a/1b**) in $CDCl_3$

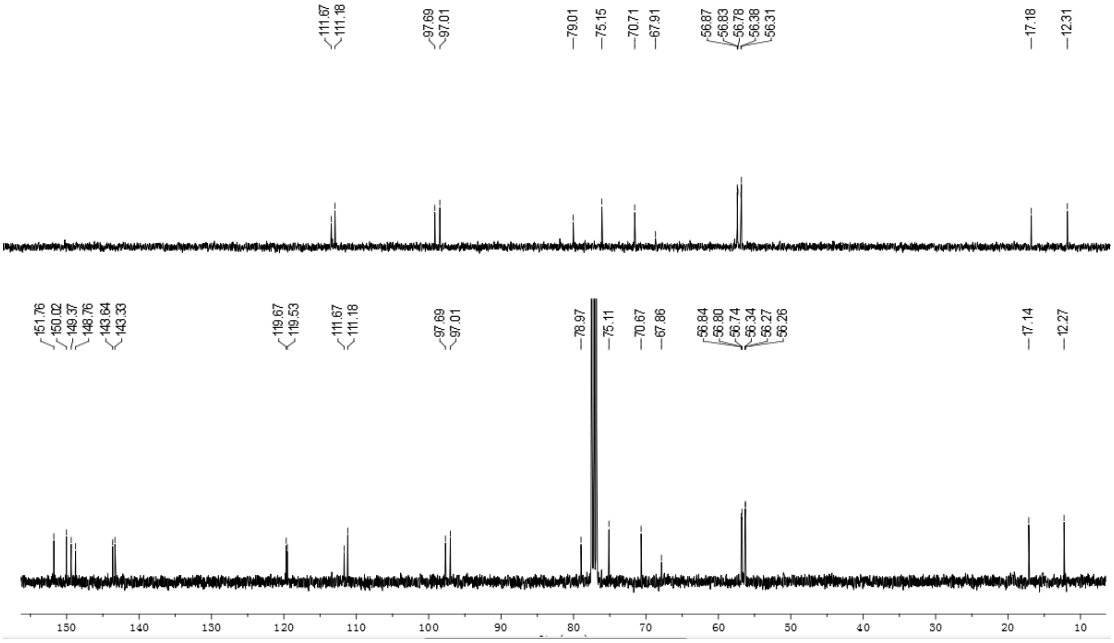


Figure S6. HSQC spectrum of **1** (**1a/1b**) in $CDCl_3$

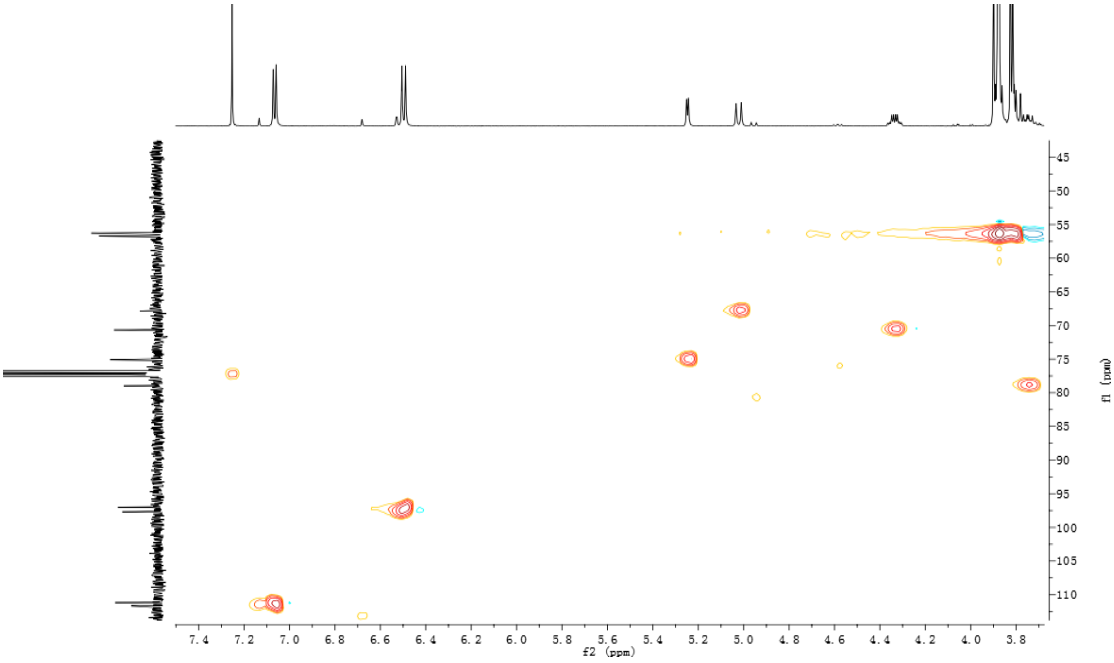


Figure S7. HMBC spectrum of **1** (**1a/1b**) in $CDCl_3$

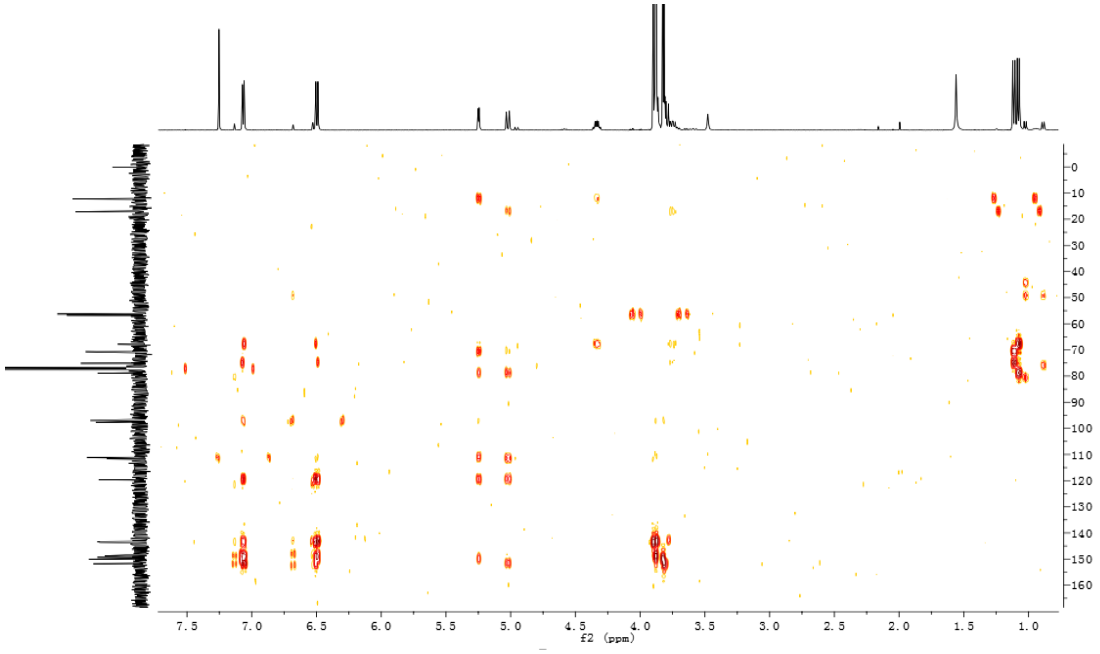


Figure S8. ^{1}H-^{1}H COSY spectrum of **1** (**1a/1b**) in $CDCl_3$

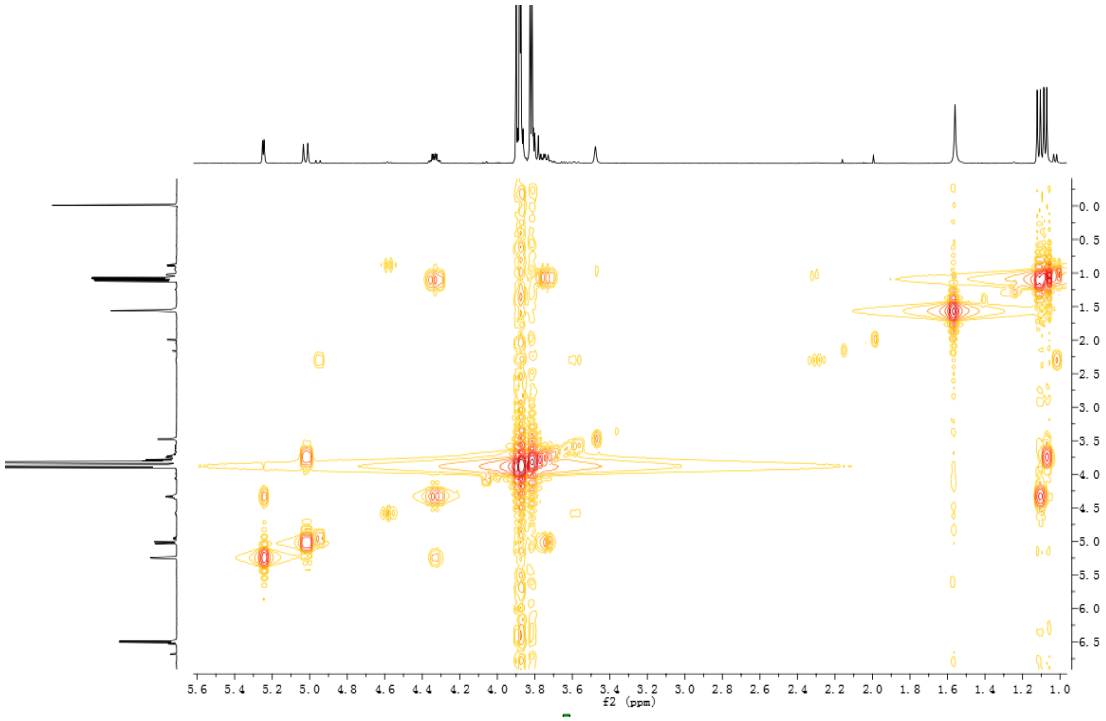


Figure S9. NOESY spectrum of **1** (**1a/1b**) in $CDCl_3$

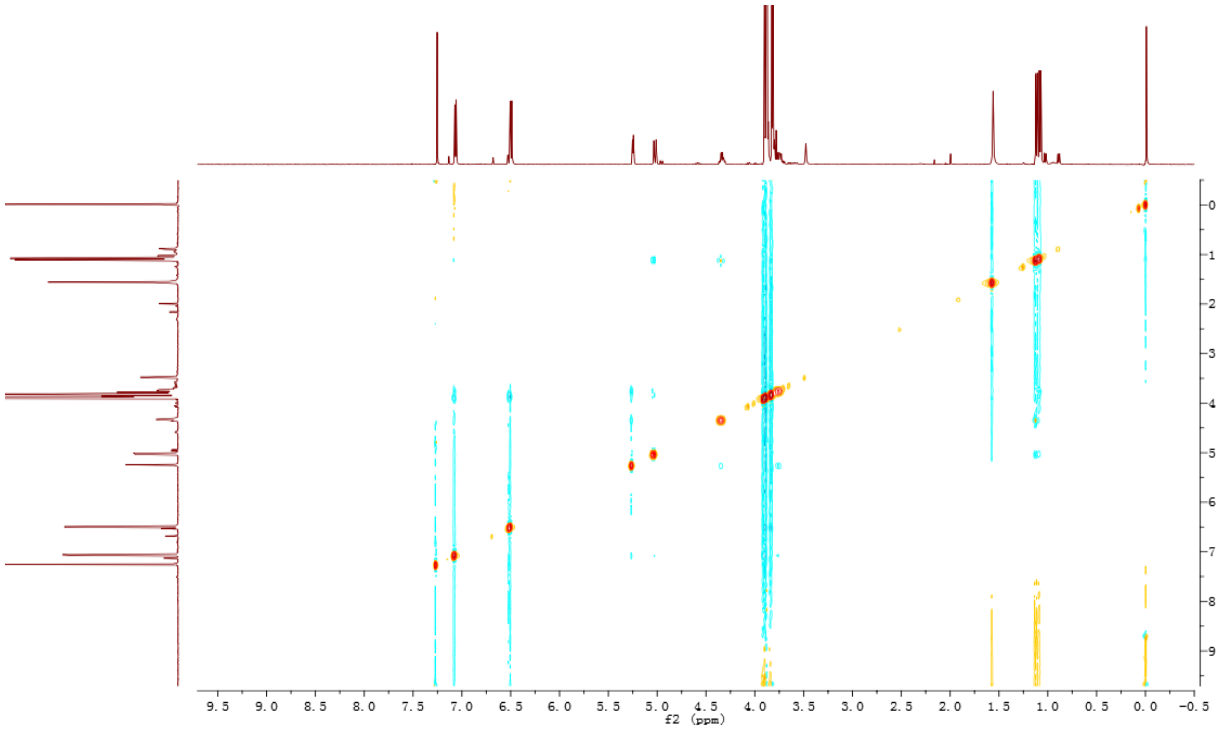


Figure S10. (+)-HR-ESI-MS spectrum of **2** (**2a/2b**)

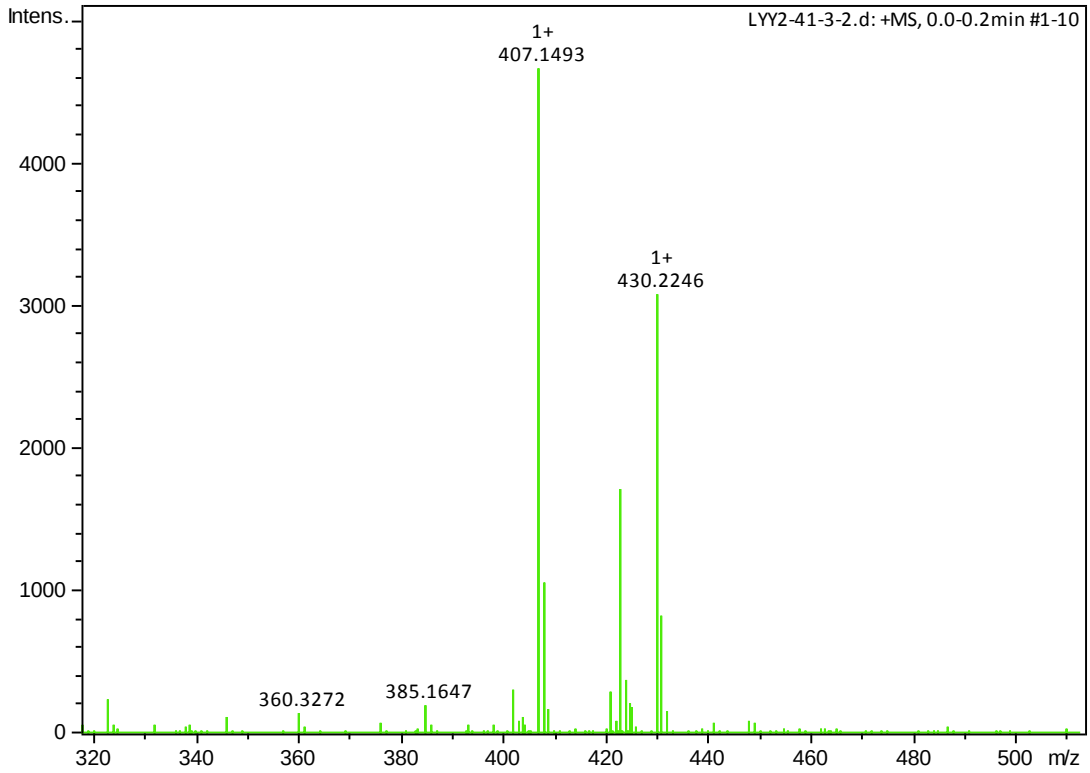


Figure S11. IR spectrum of **2** (**2a/2b**)

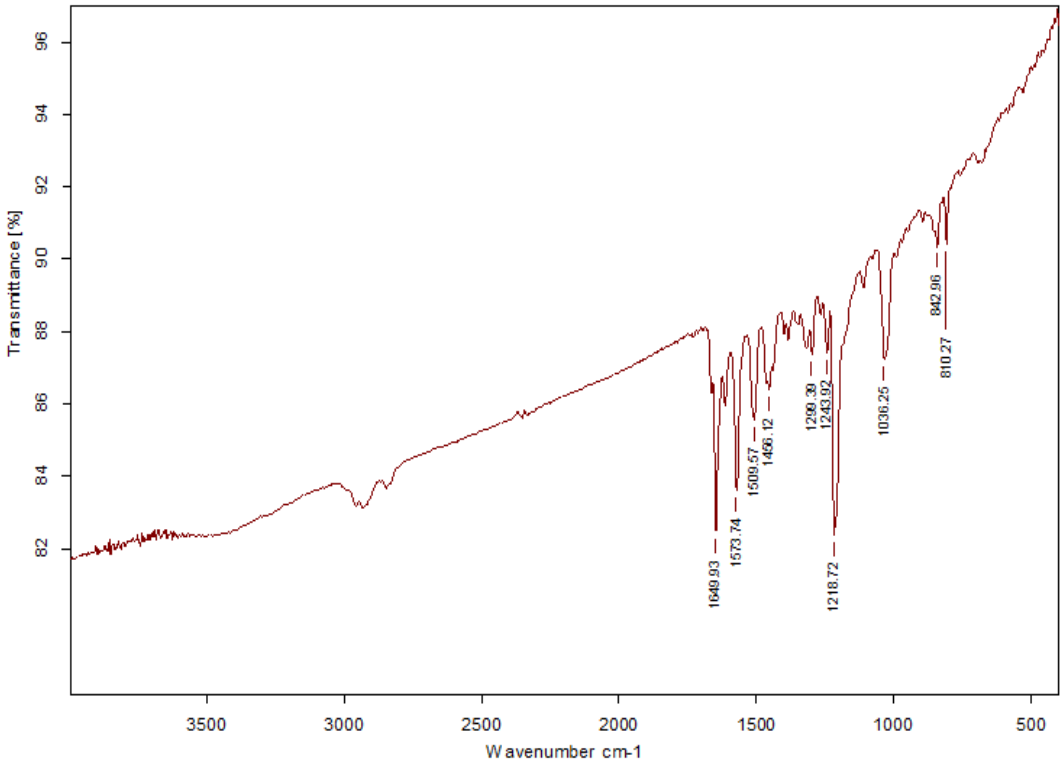


Figure S12. UV spectrum of **2** (**2a/2b**)

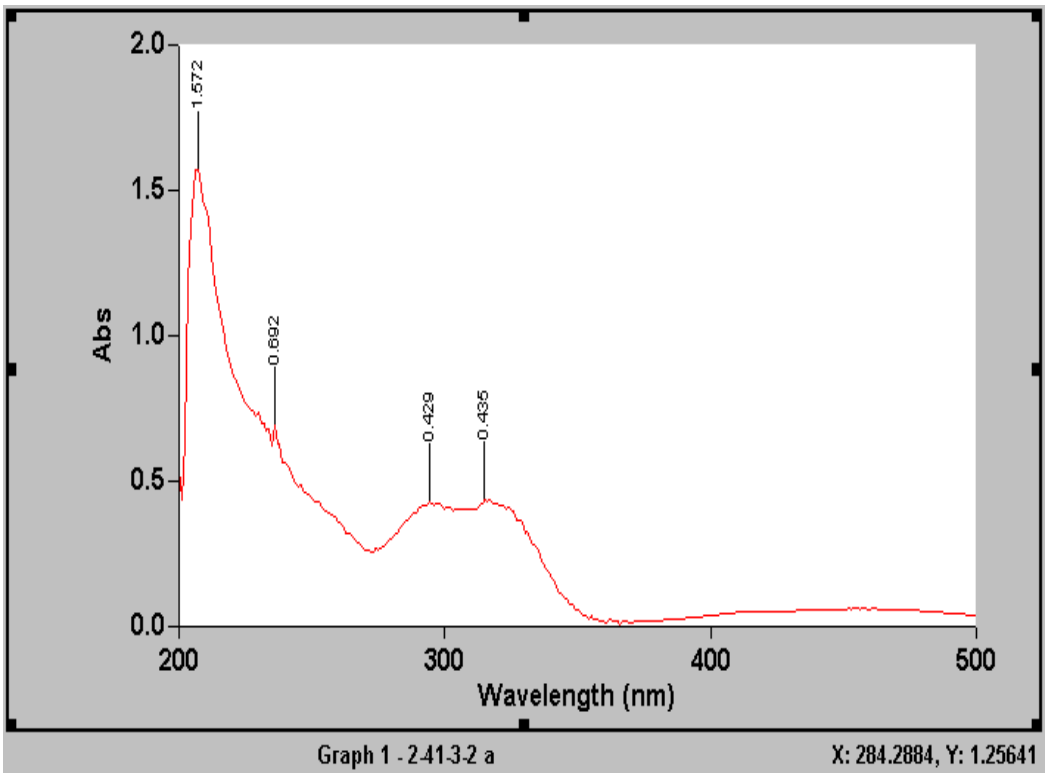


Figure S13. ^{1}H NMR spectrum of **2** (**2a/2b**) in $CDCl_3$

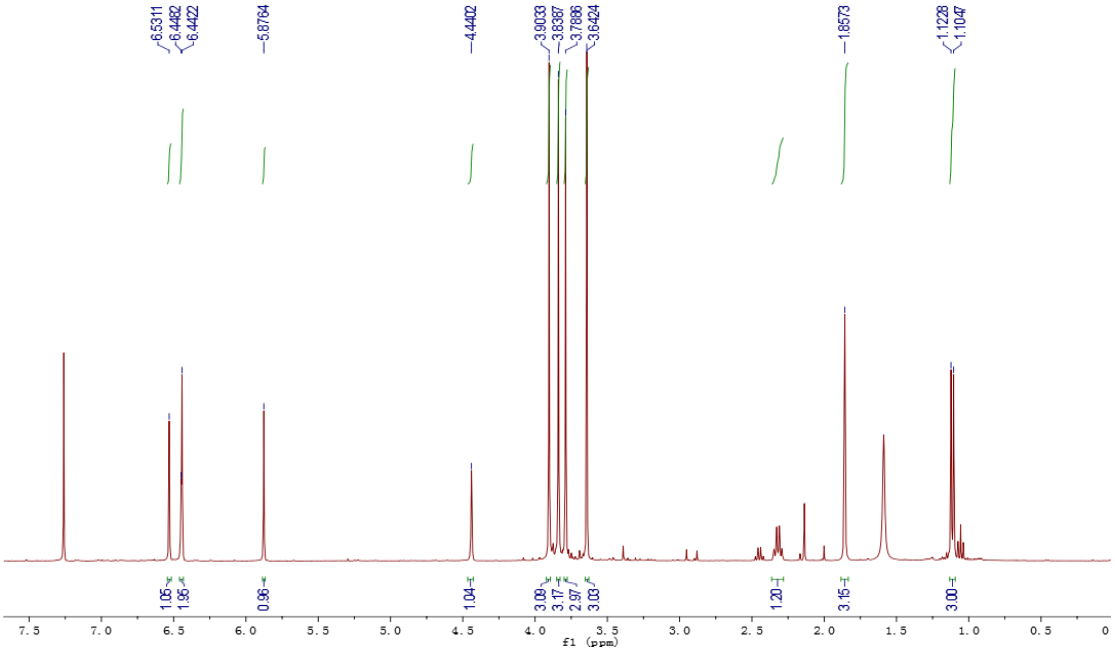


Figure S14.^{13}C NMR spectrum of **2** (**2a/2b**) in $CDCl_3$

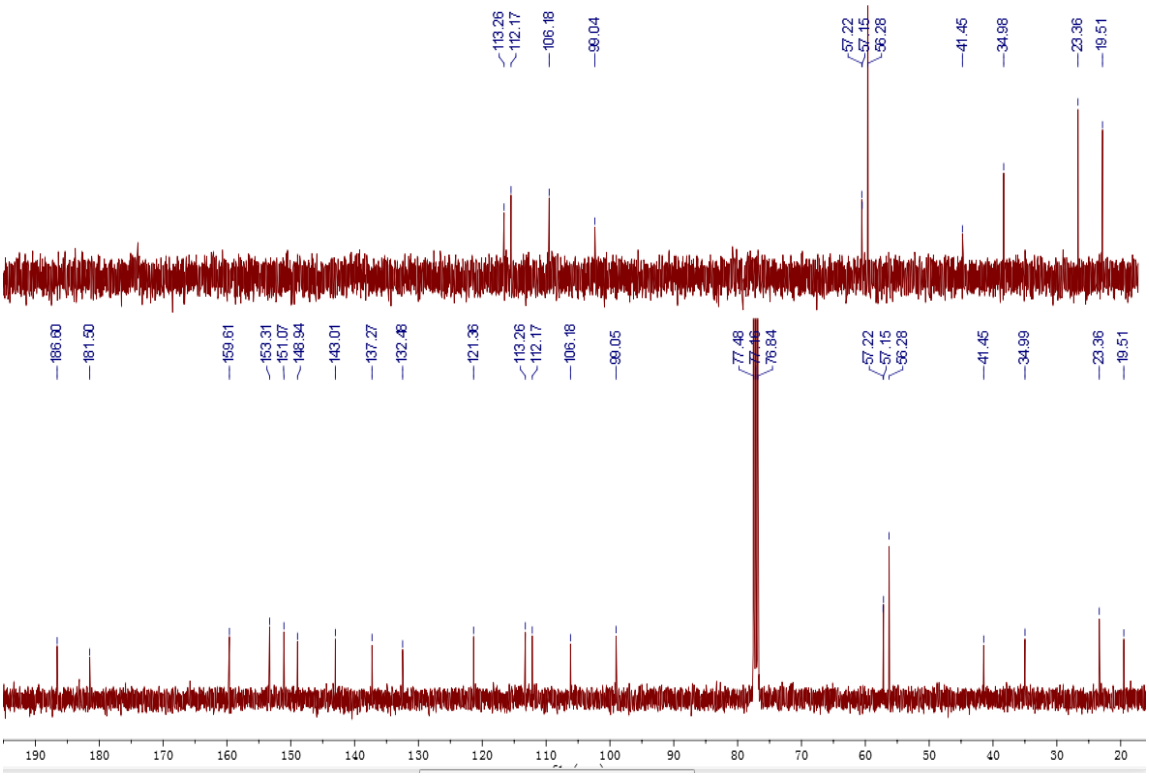


Figure S15. HSQC spectrum of **2** (**2a/2b**) in $CDCl_3$

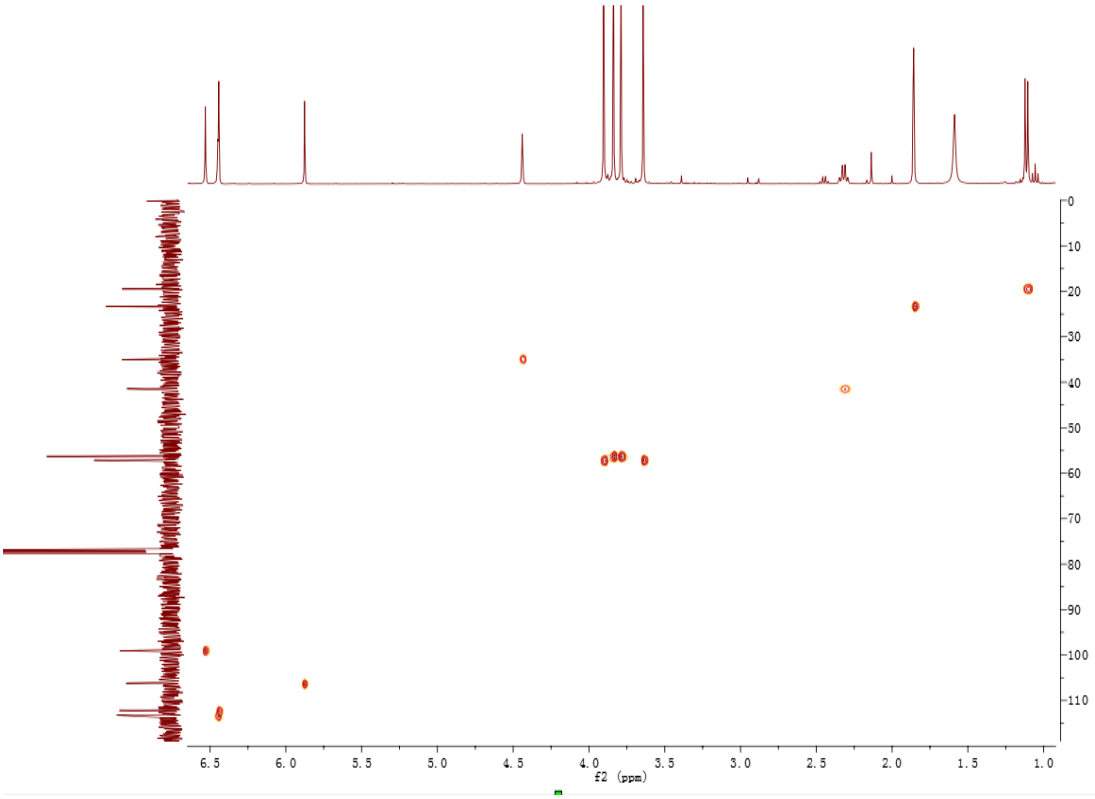


Figure S16. HMBC spectrum of **2** (**2a/2b**) in $CDCl_3$

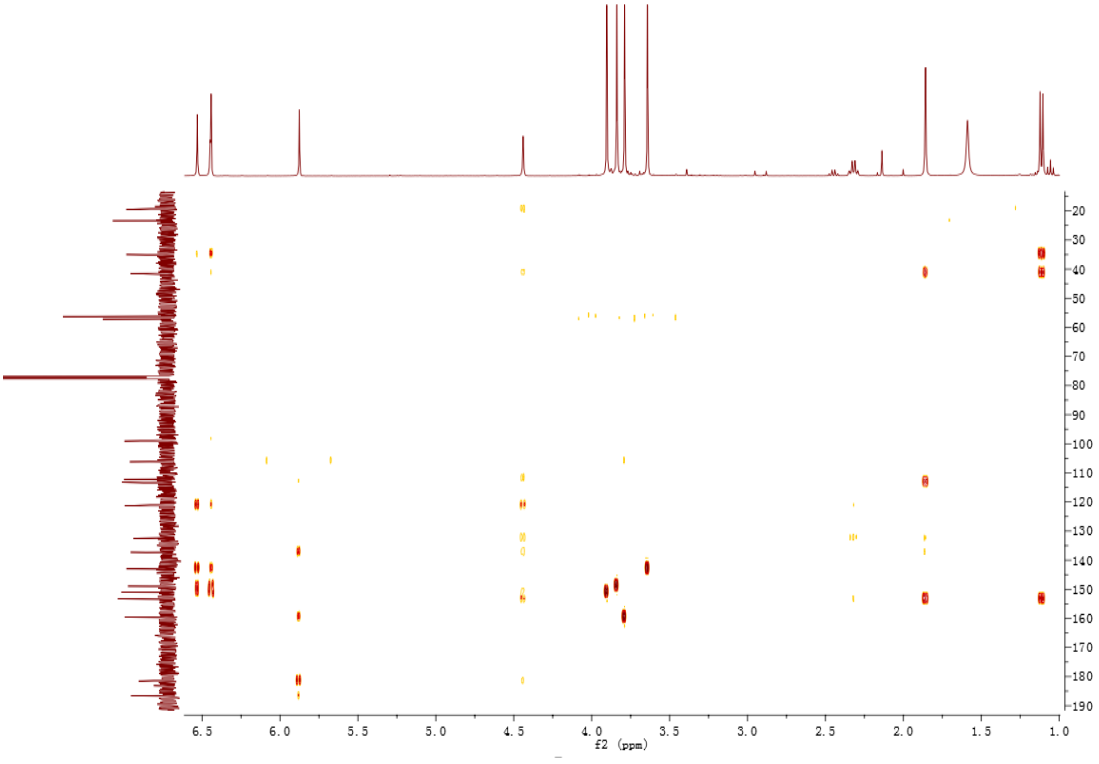


Figure S17. ^{1}H-^{1}H COSY spectrum of **2** (**2a/2b**) in $CDCl_3$

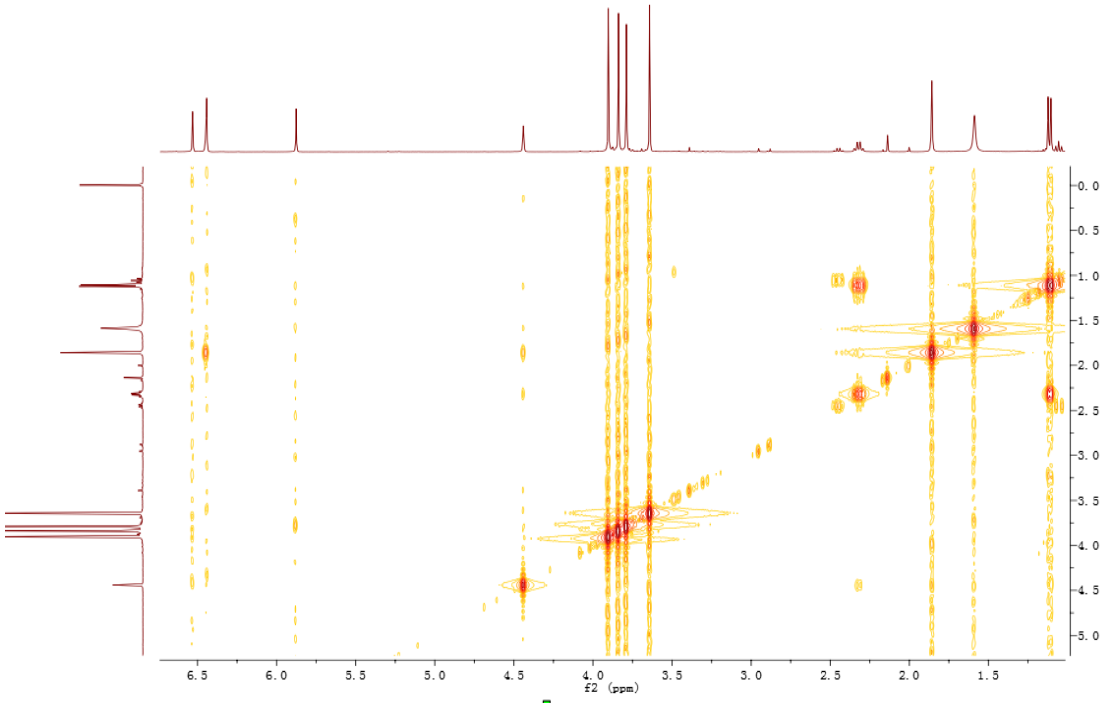


Figure S18. NOESY spectrum of **2** (**2a/2b**) in $CDCl_3$

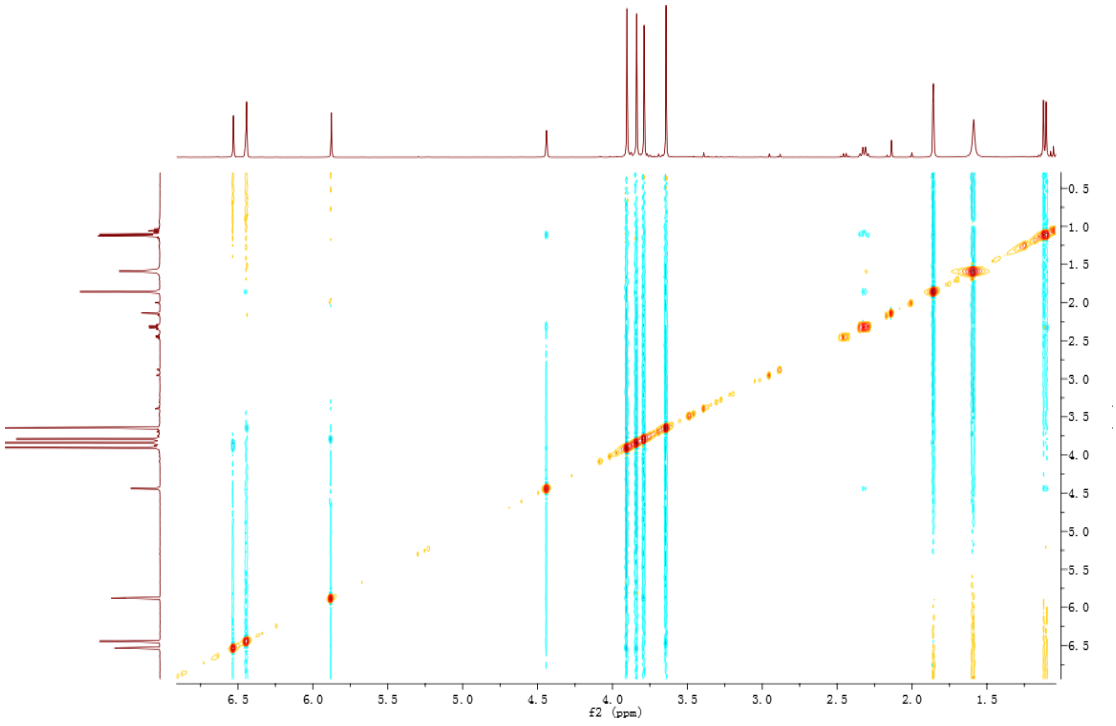


Figure S19. (+)-HR-ESI-MS spectrum of **3** (**3a/3b**)

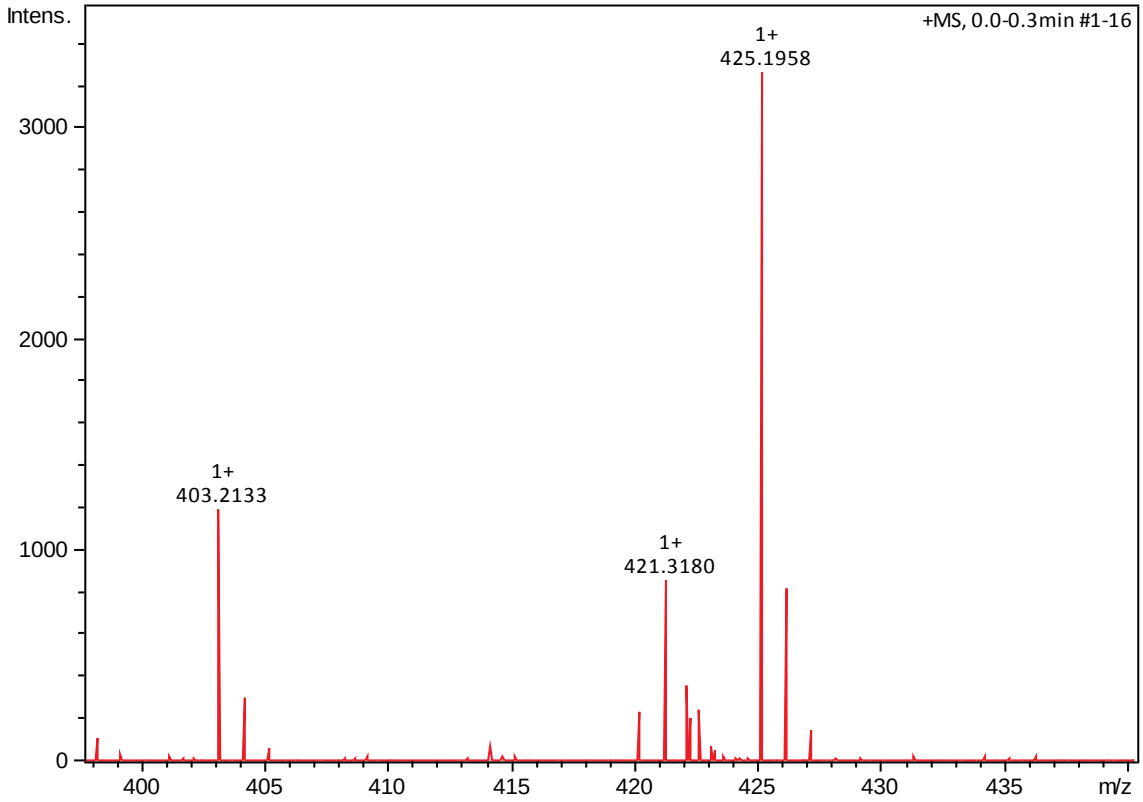


Figure S20. IR spectrum of **3** (**3a/3b**)

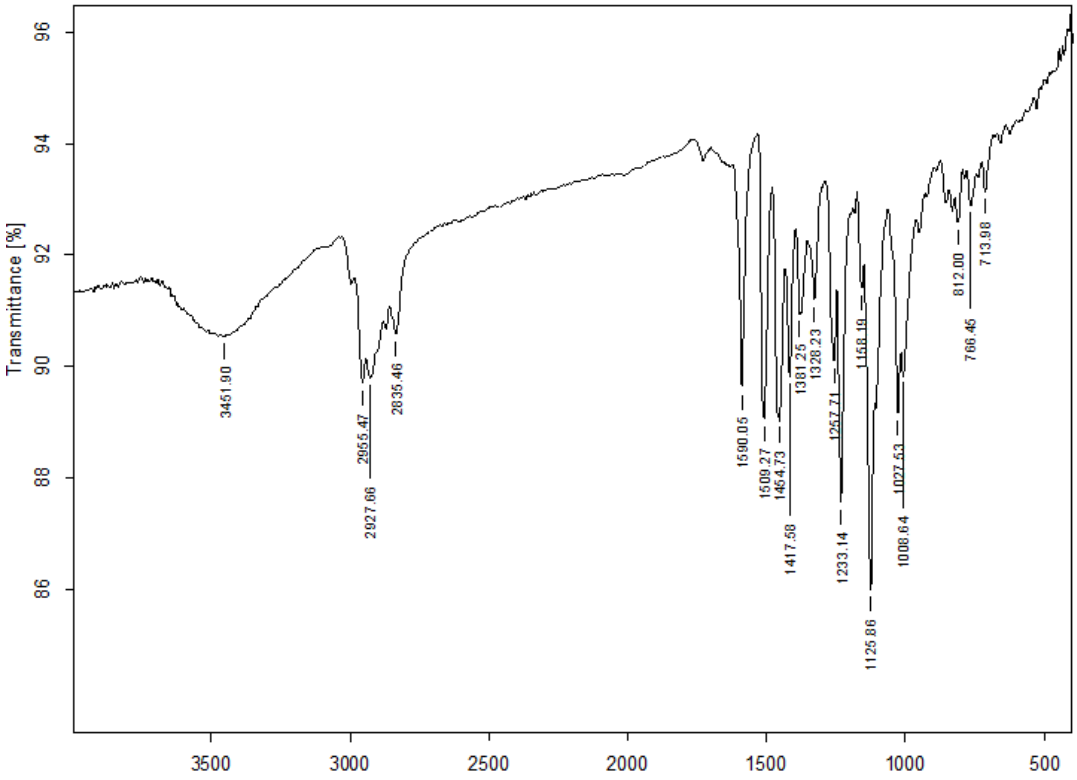


Figure S21. UV spectrum of **3** (**3a/3b**)

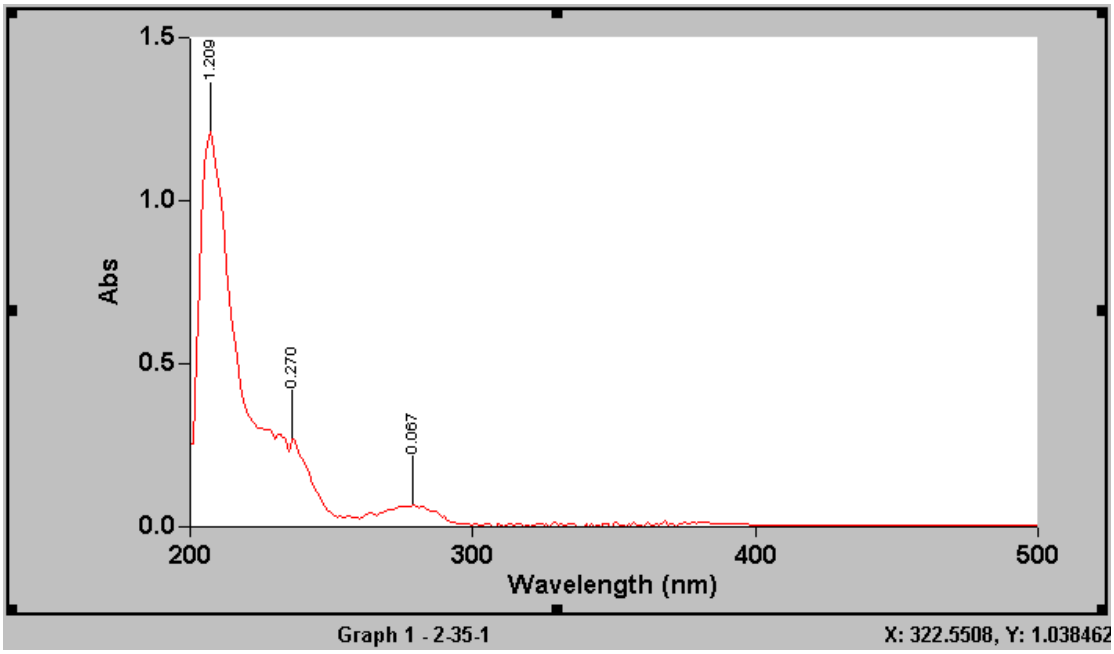


Figure S22. ^{1}H NMR spectrum of **3** (**3a/3b**) in CD_3OD

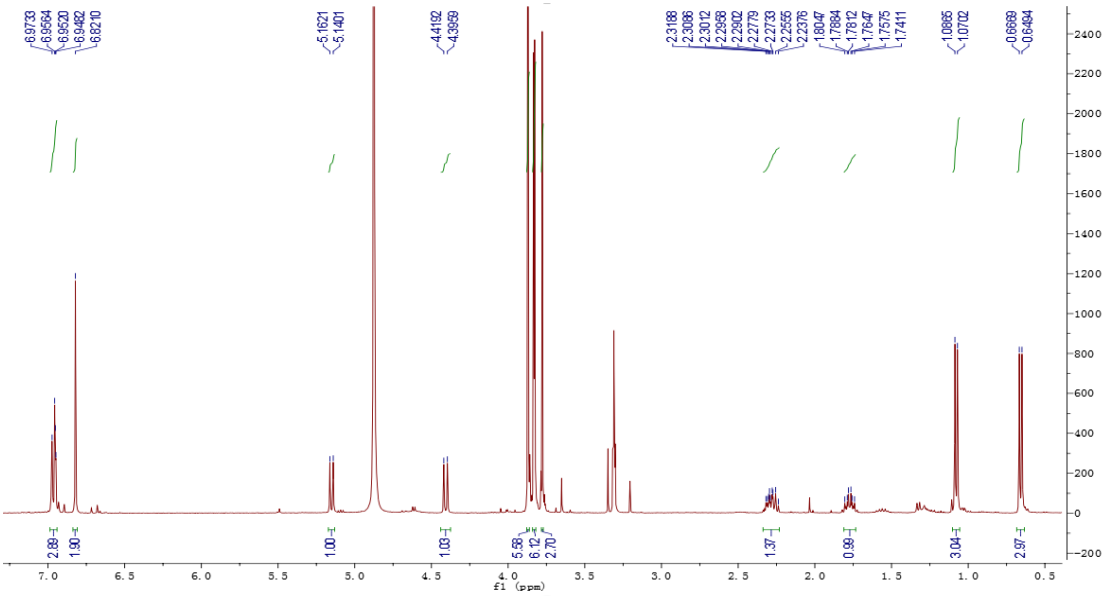


Figure S23.[13]C NMR spectrum of **3** (**3a/3b**) in CD_3OD

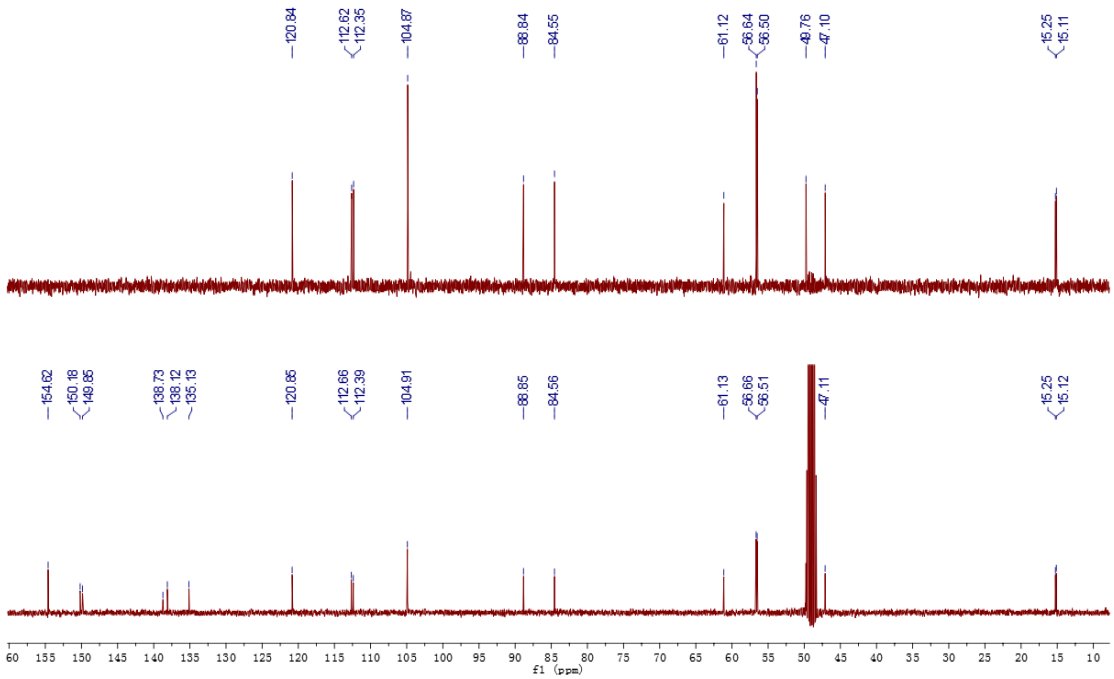


Figure S24. HSQC spectrum of **3** (**3a/3b**) in CD_3OD

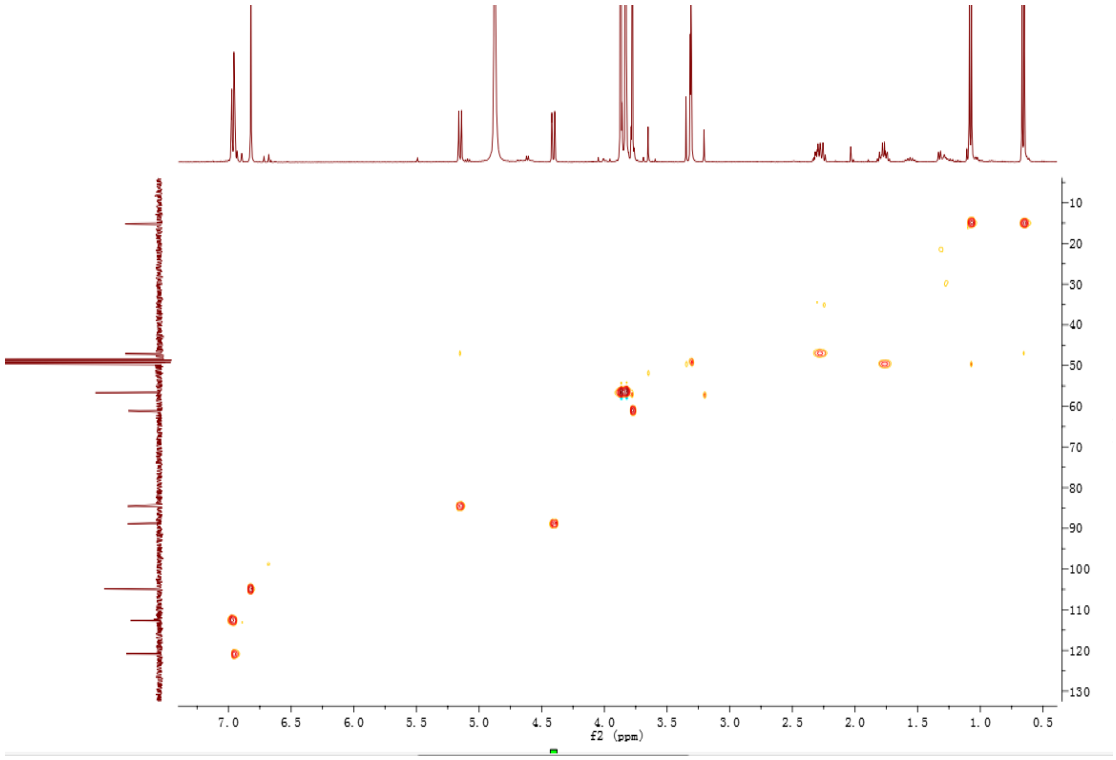


Figure S25. HMBC spectrum of **3** (**3a/3b**) in CD_3OD

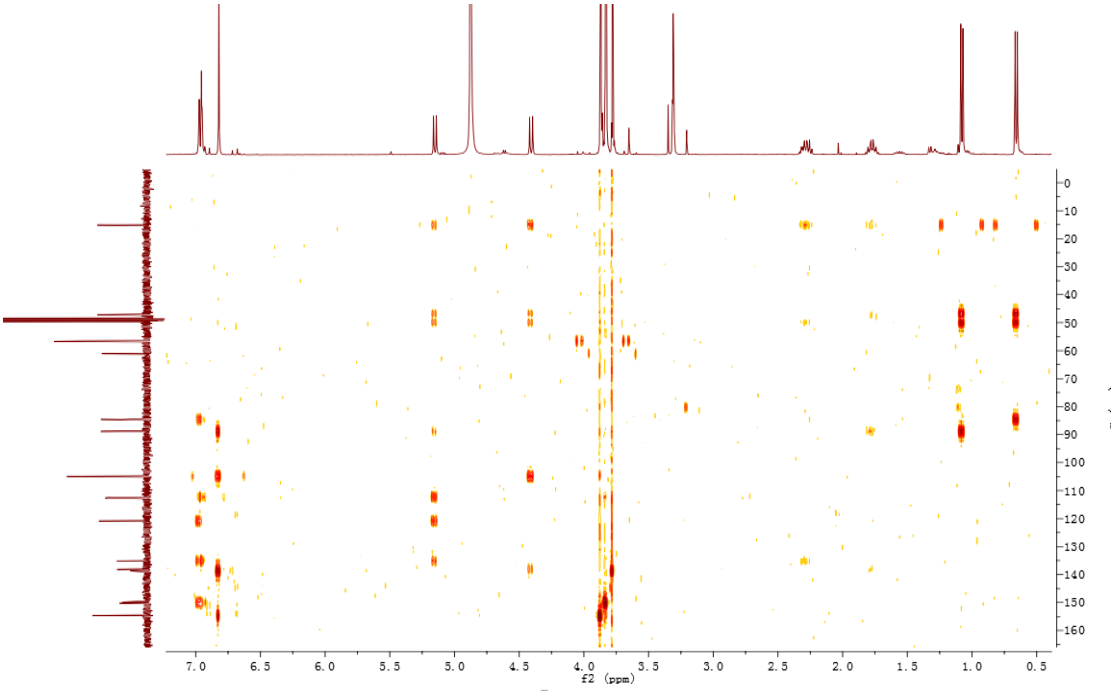


Figure S26. ^{1}H-^{1}H COSY spectrum of **3** (**3a/3b**) in CD_3OD

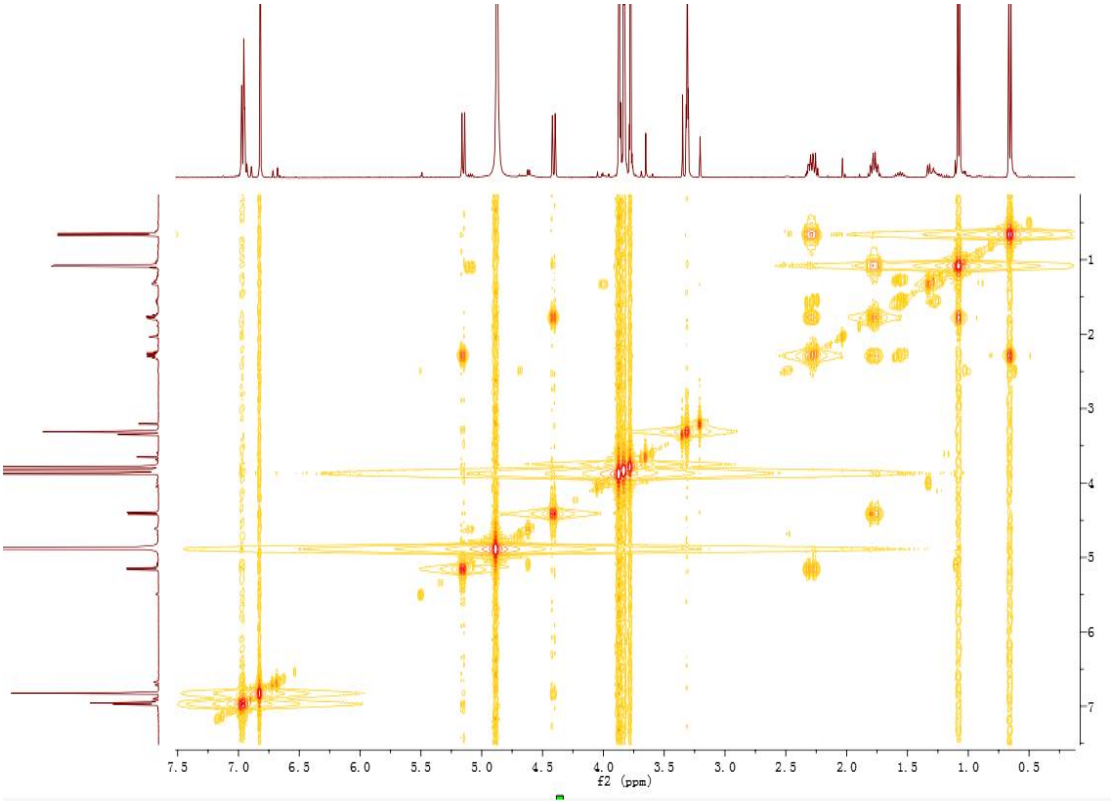


Figure S27. NOESY spectrum of **3** (**3a/3b**) in CD_3OD

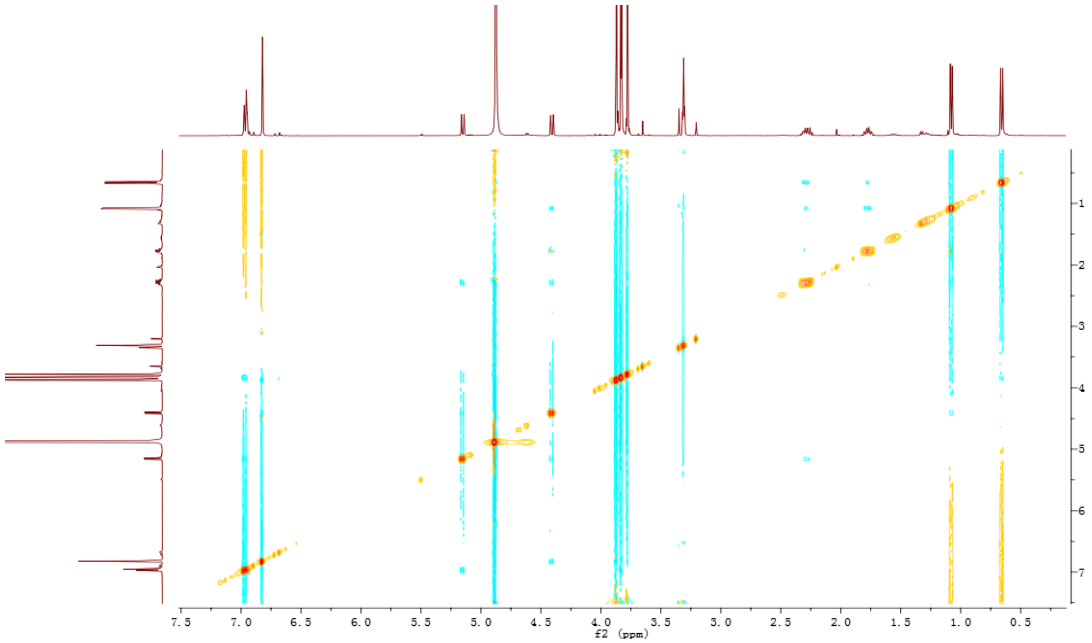


Figure S28. (+)-HR-ESI-MS spectrum of **4**

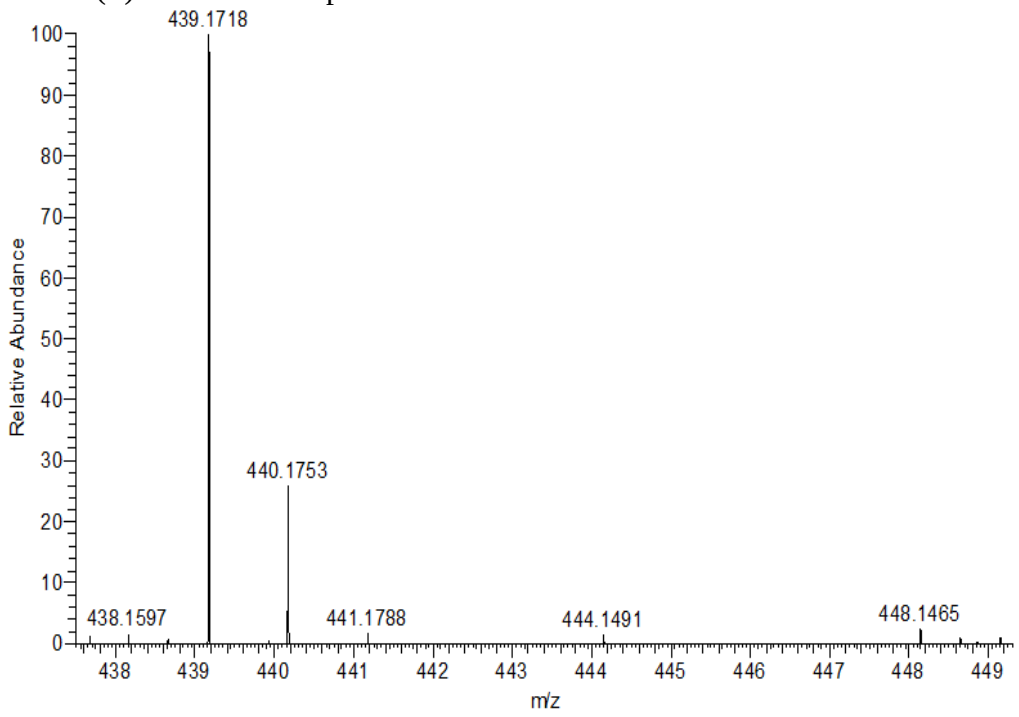


Figure S29. IR spectrum of **4**

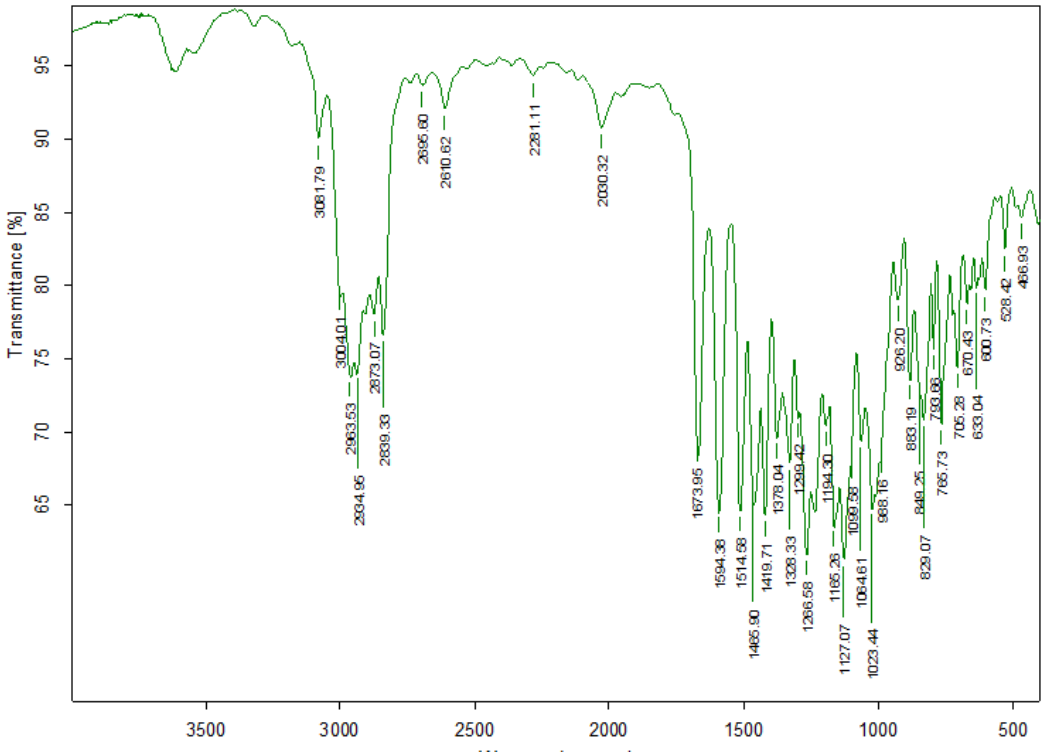


Figure S30. UV spectrum of **4**

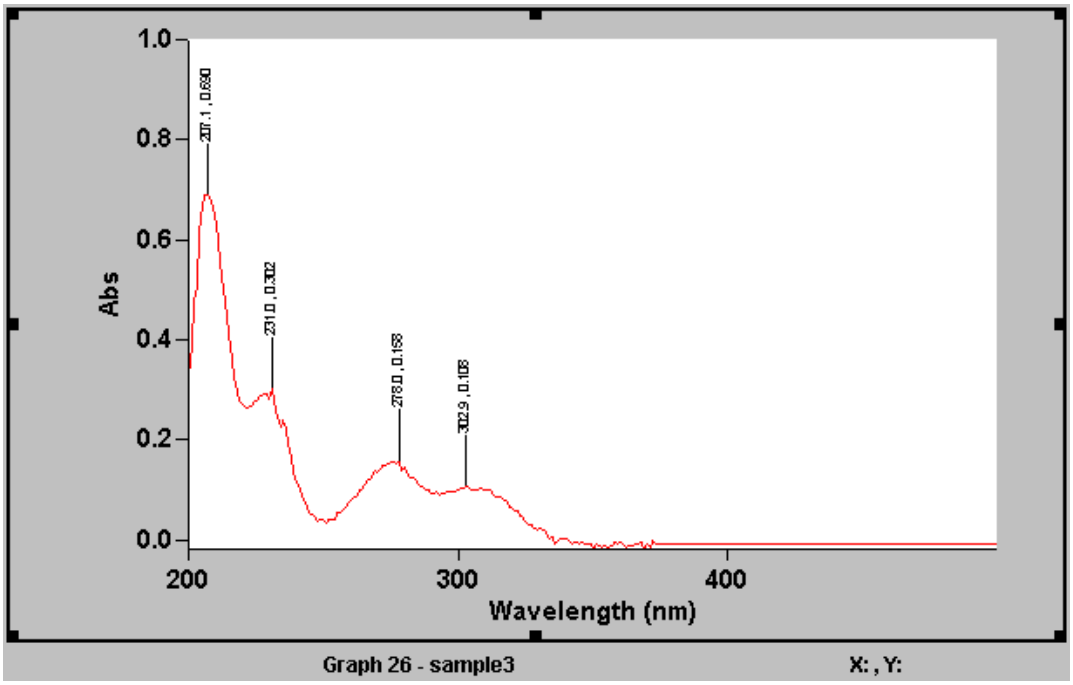


Figure S31. ^{1}H NMR spectrum of **4** in $CDCl_3$

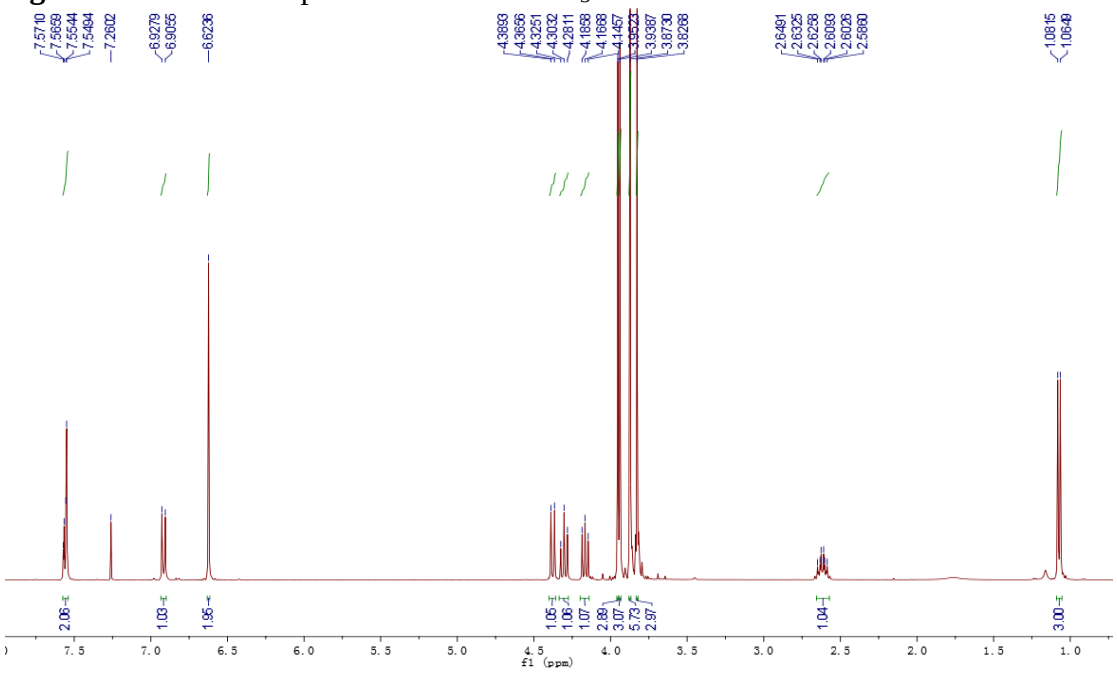


Figure S32. ^{13}C NMR spectrum of **4** in $CDCl_3$

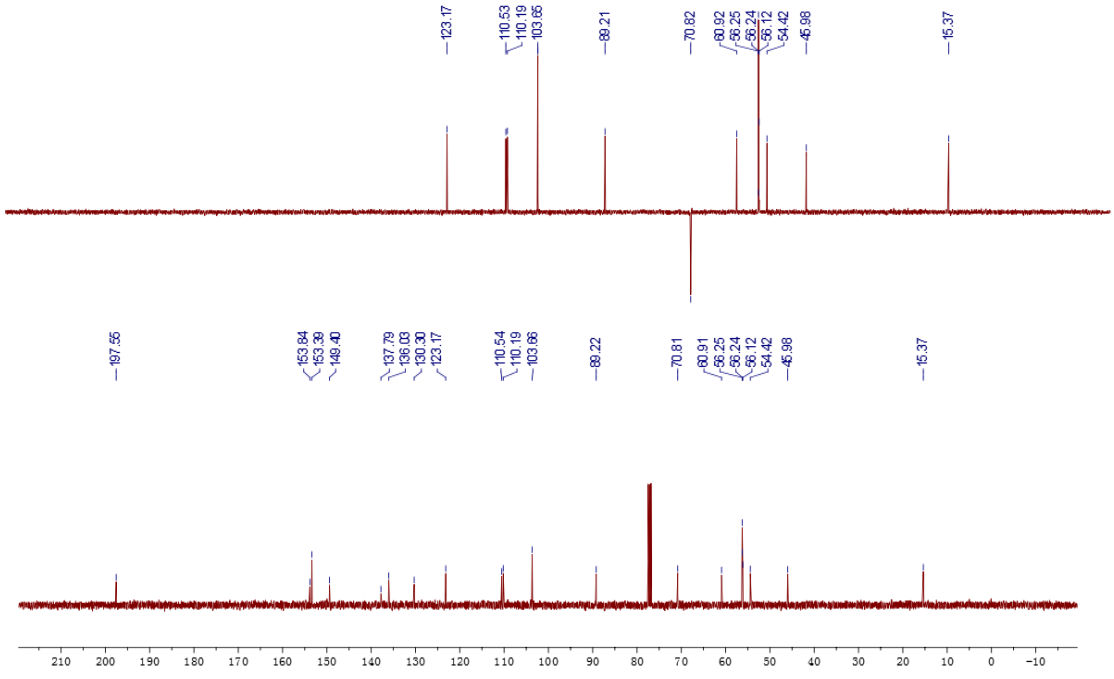


Figure S33. HSQC spectrum of **4** in $CDCl_3$

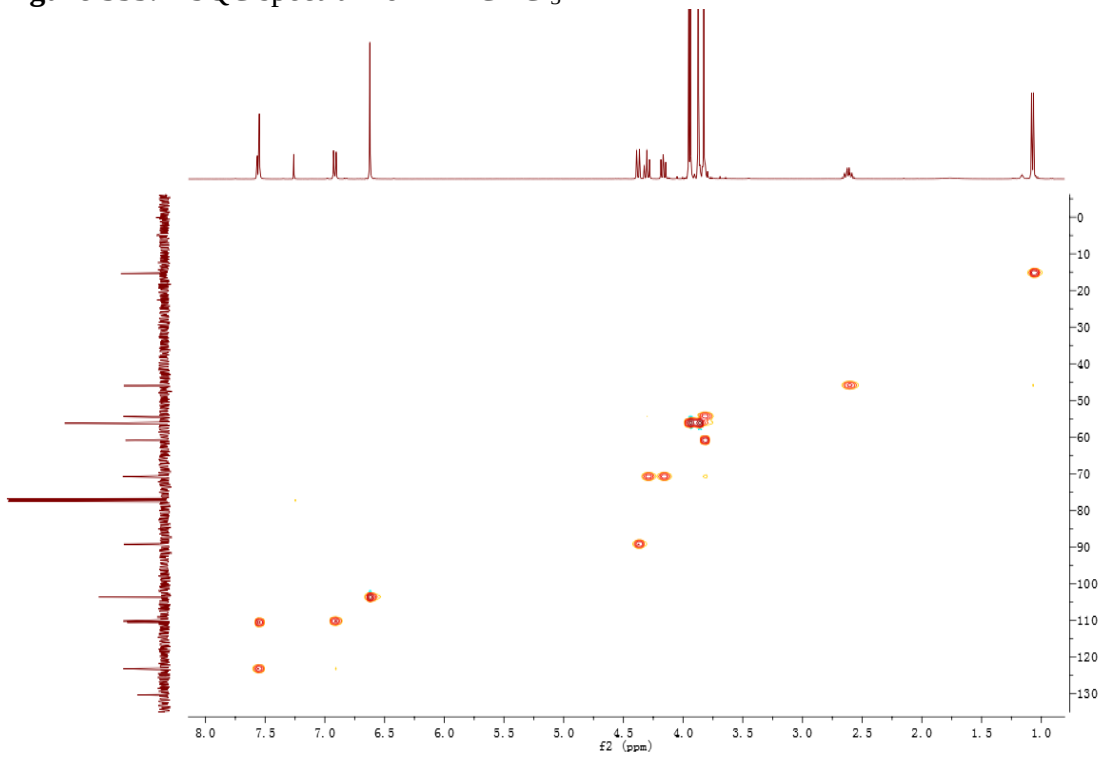


Figure S34. HMBC spectrum of **4** in $CDCl_3$

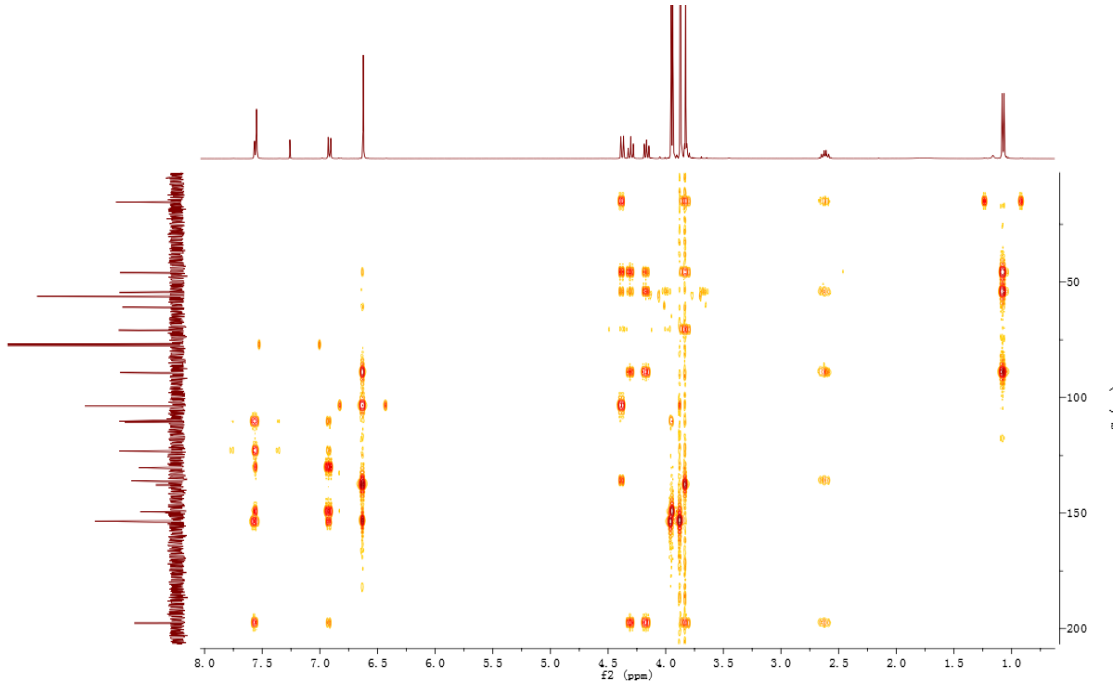


Figure S35. ^{1}H-^{1}H COSY spectrum of **4** in $CDCl_3$

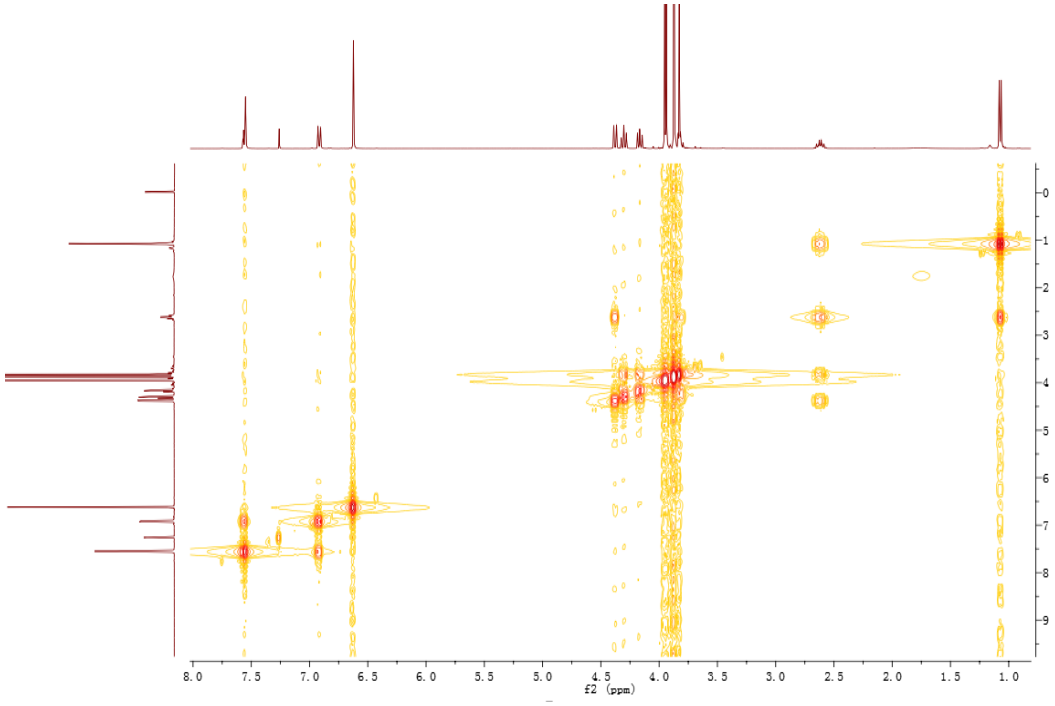


Figure S36. NOESY spectrum of **4** in $CDCl_3$

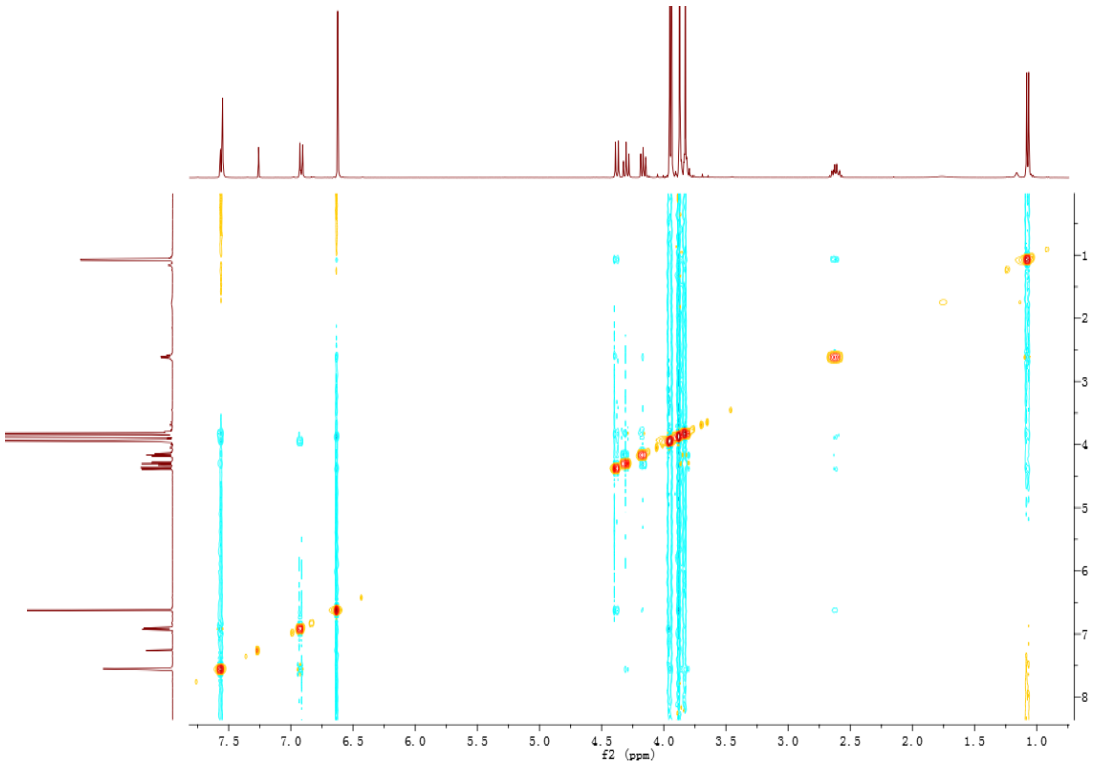


Figure S37. ECD spectrum of **4** in MeOH

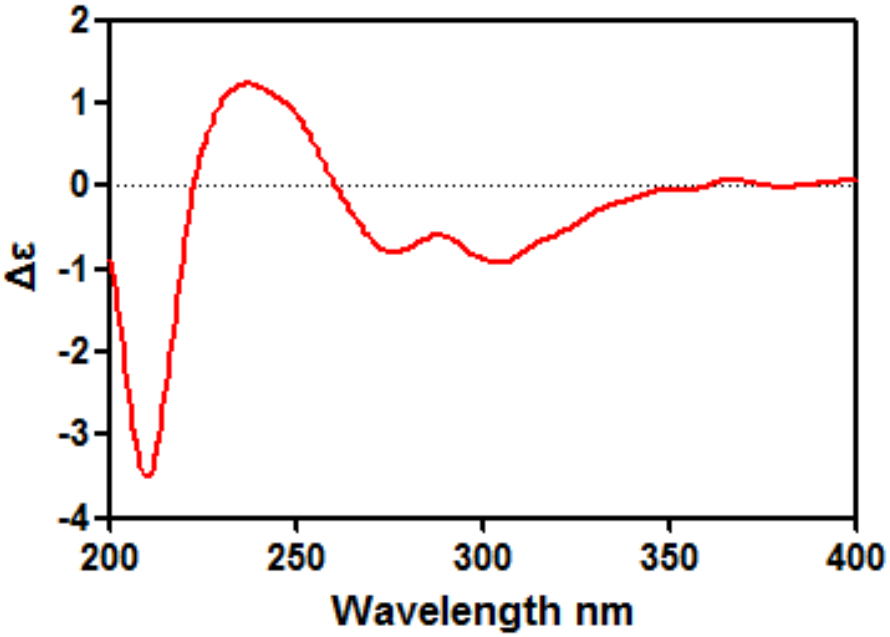


Figure S38. (+)-HR-ESI-MS spectrum of **5**

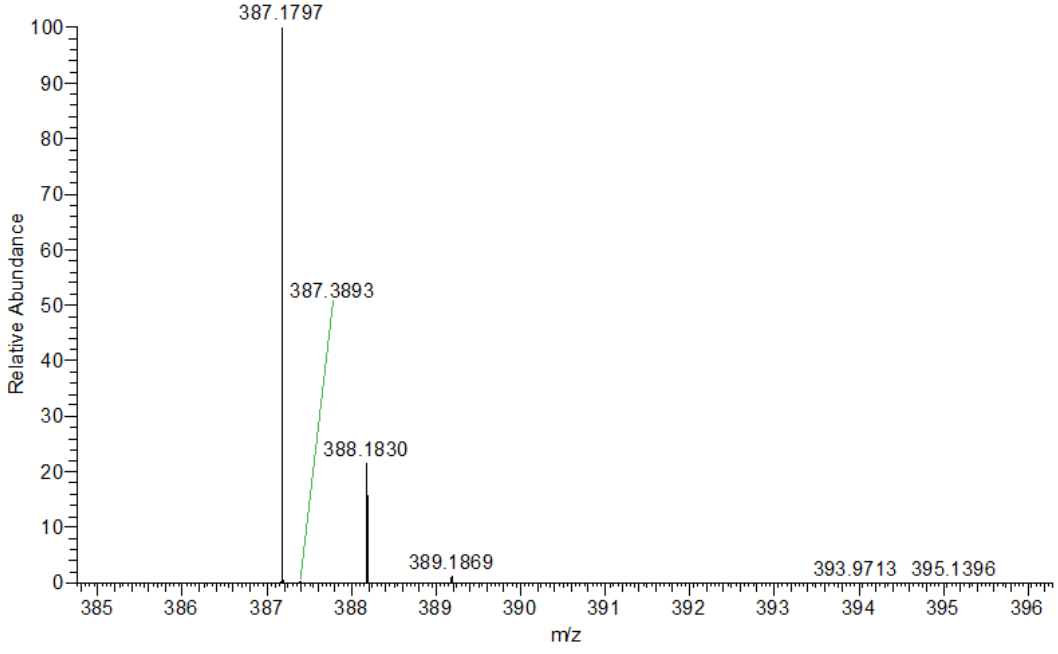


Figure S39. IR spectrum of **5**

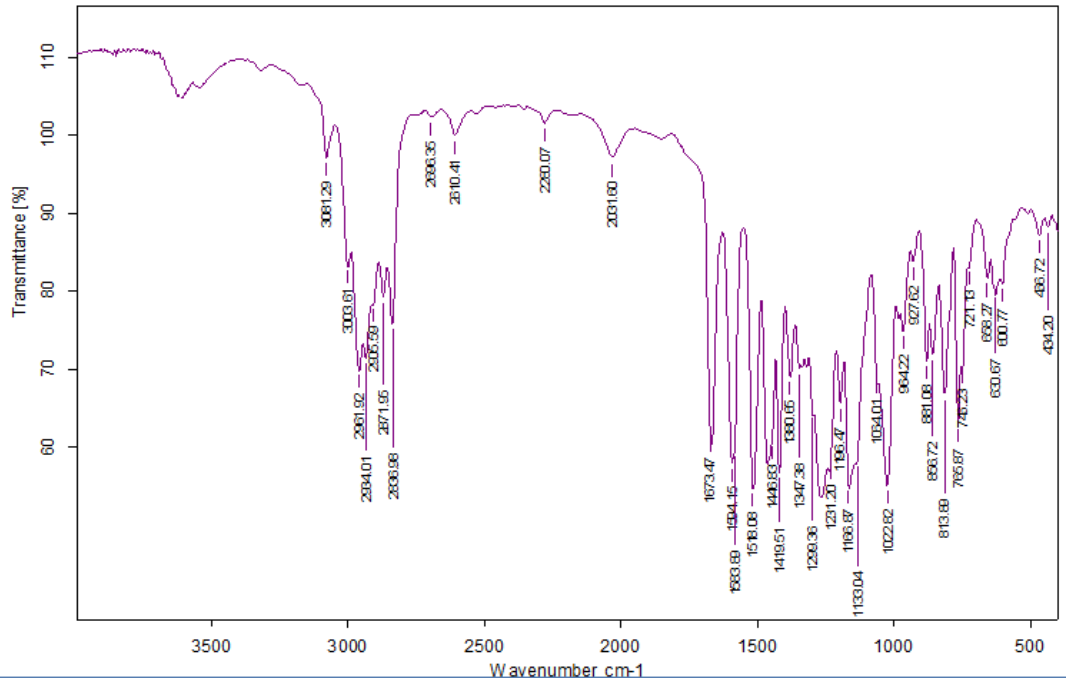


Figure S40. UV spectrum of **5**

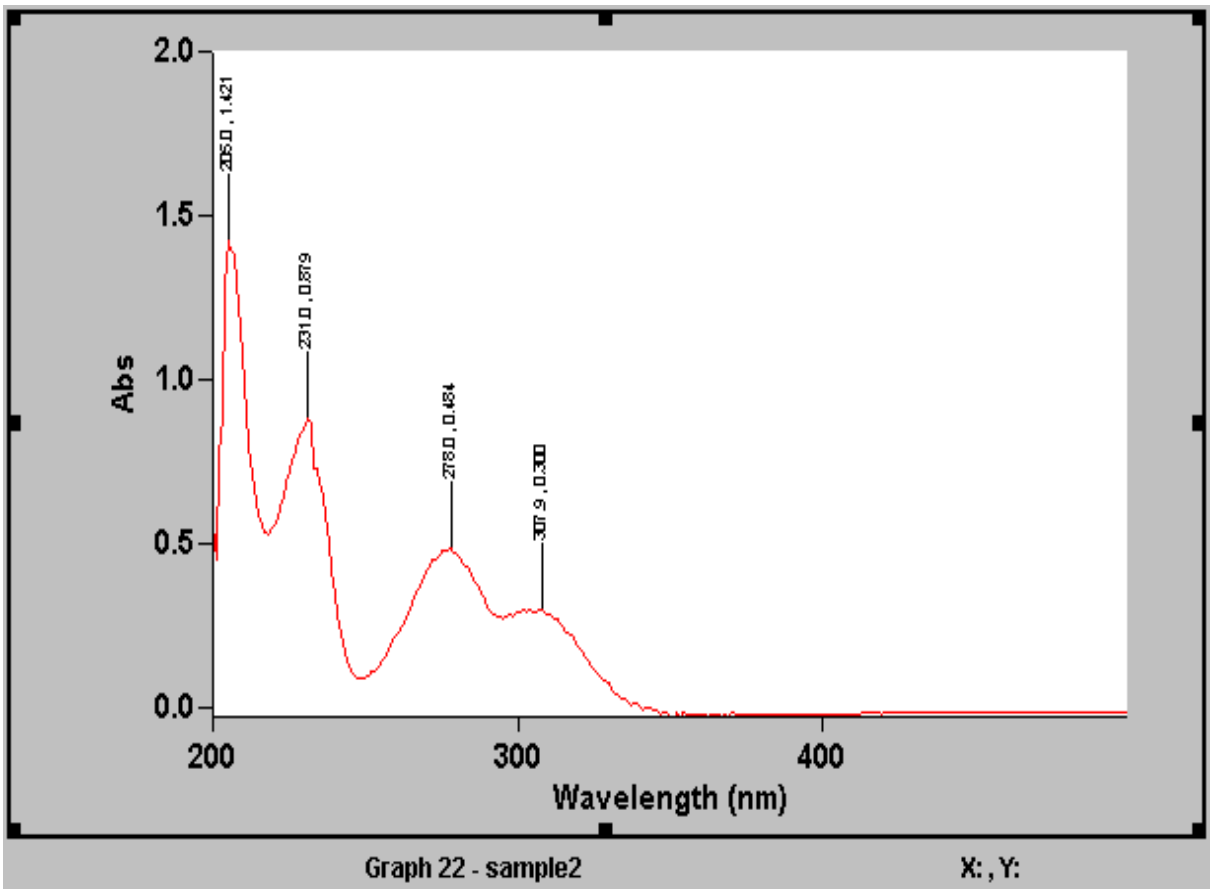


Figure S41. ^{1}H NMR spectrum of **5** in CD_3OD

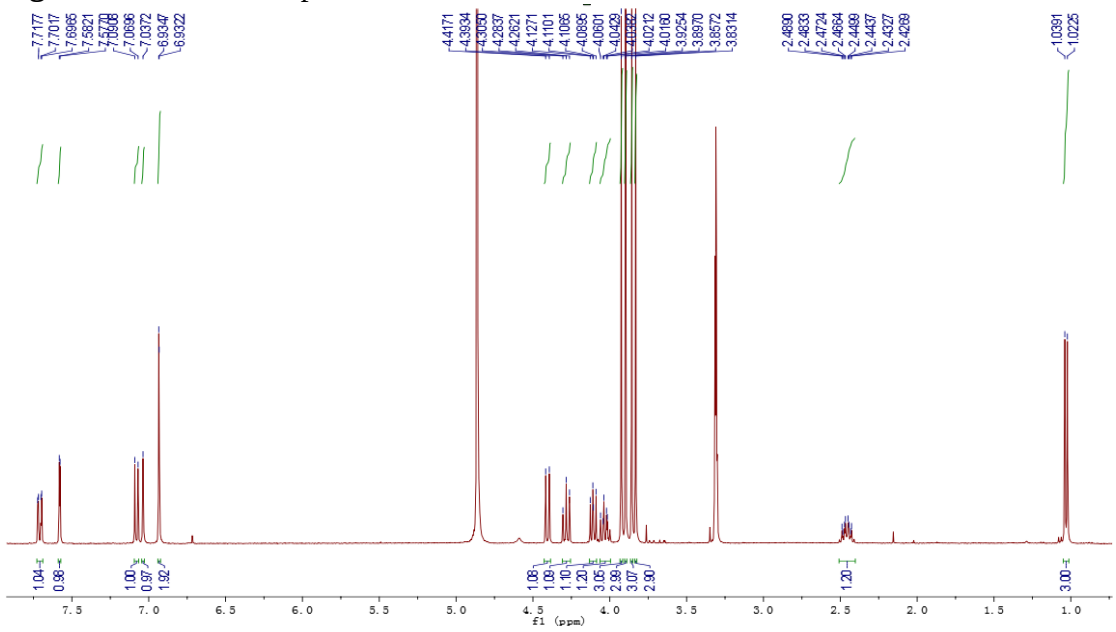


Figure S42. ^{13}C NMR spectrum of **5** in CD_3OD

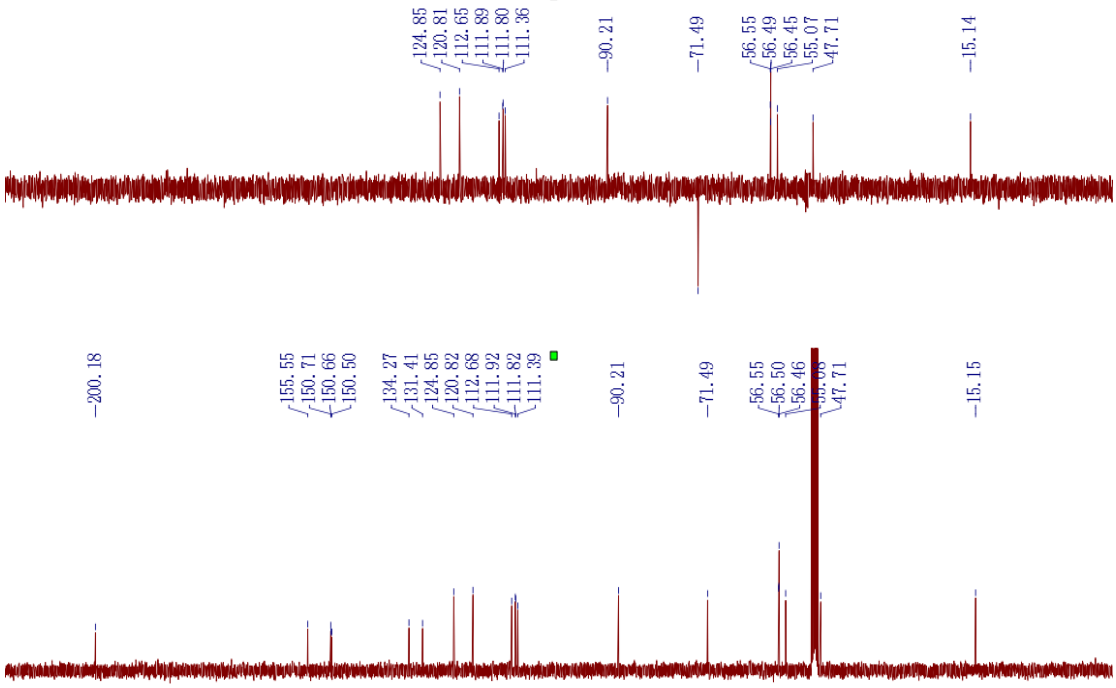


Figure S43. HSQC spectrum of **5** in CD_3OD

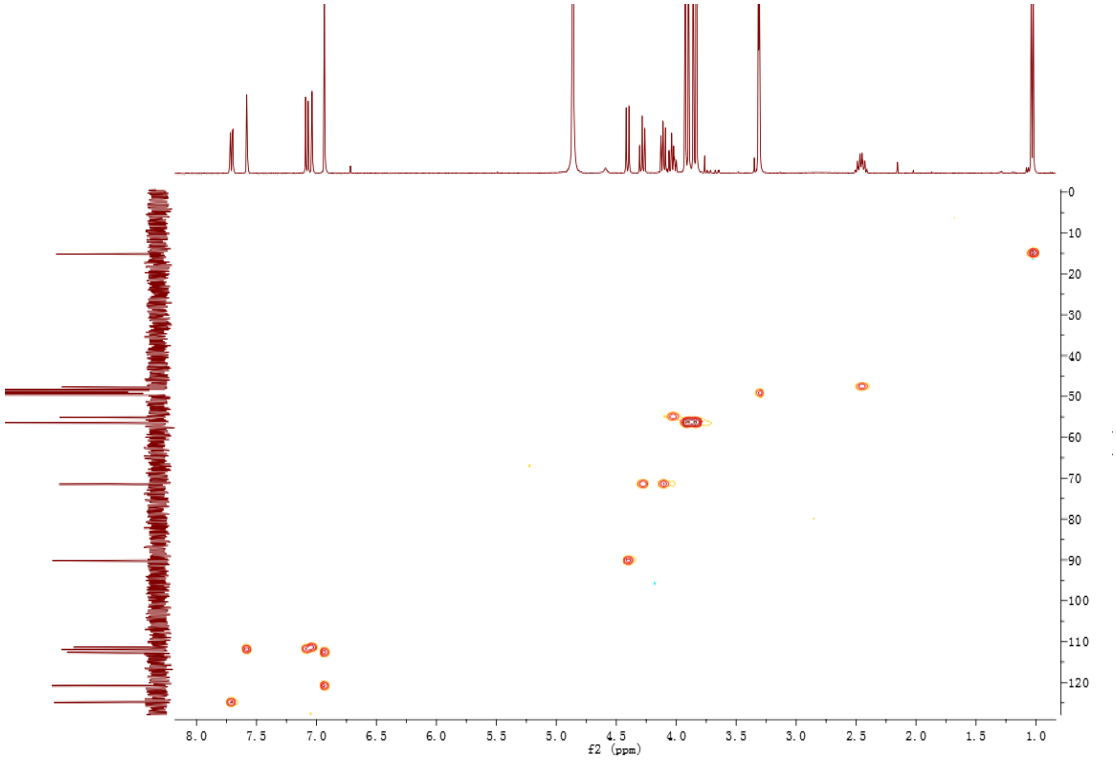


Figure S44. HMBC spectrum of **5** in CD_3OD

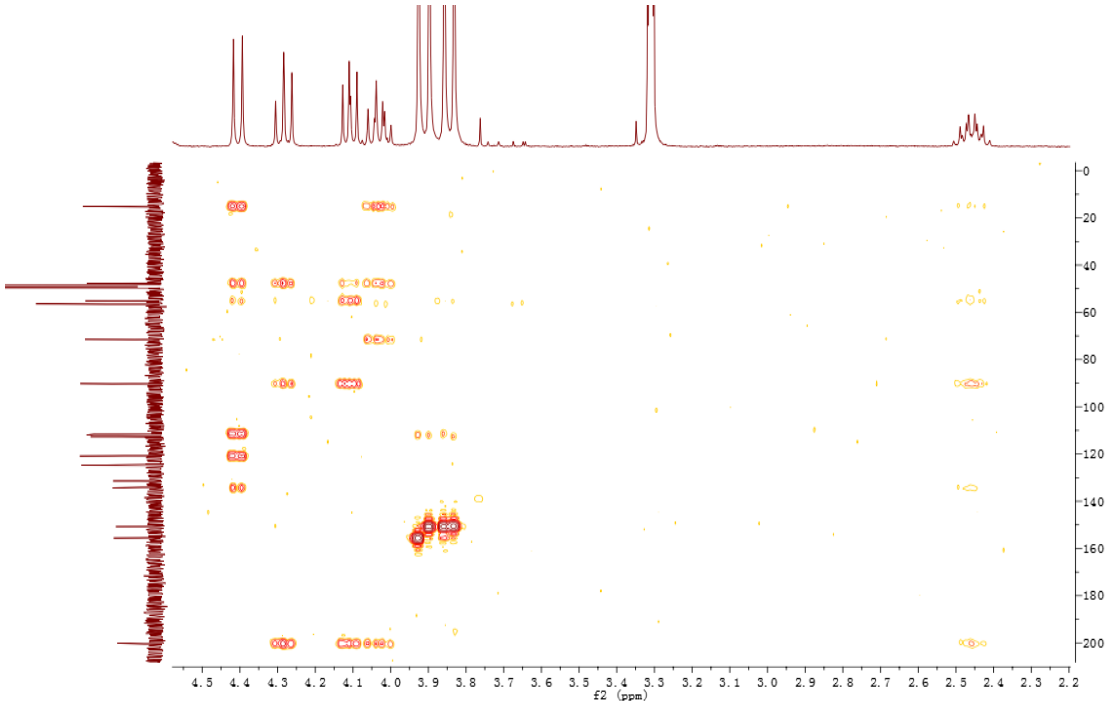


Figure S45. ^{1}H-^{1}H COSY spectrum of **5** in CD_3OD

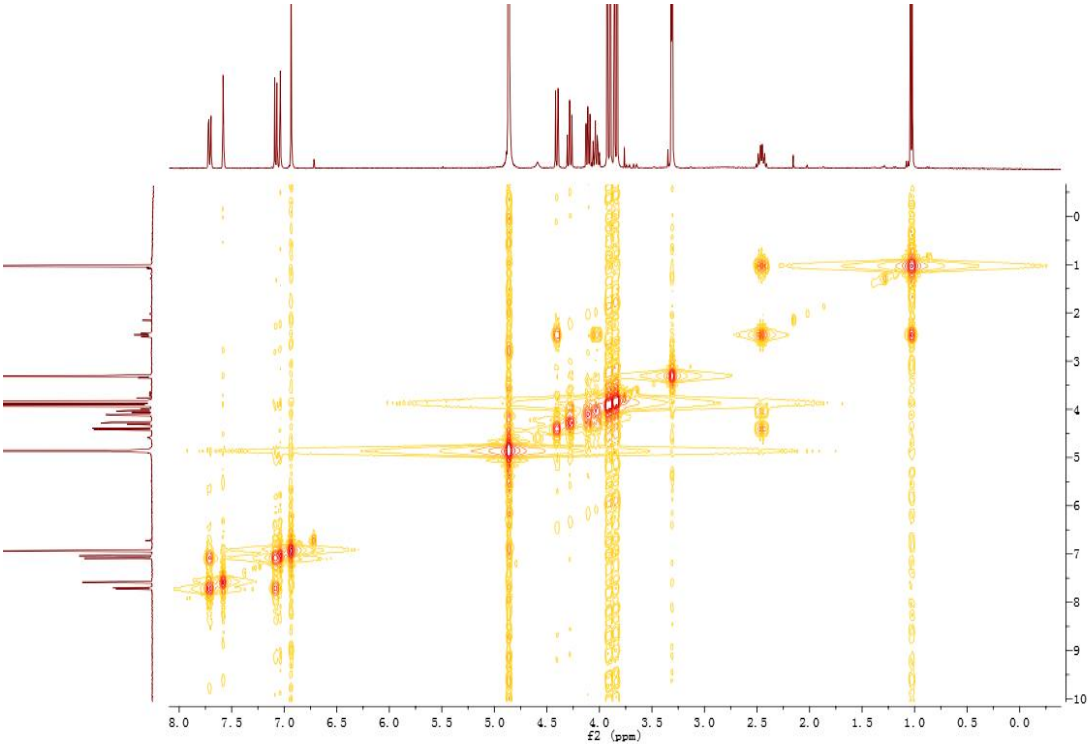


Figure S46. NOSEY spectrum of **5** in CD_3OD

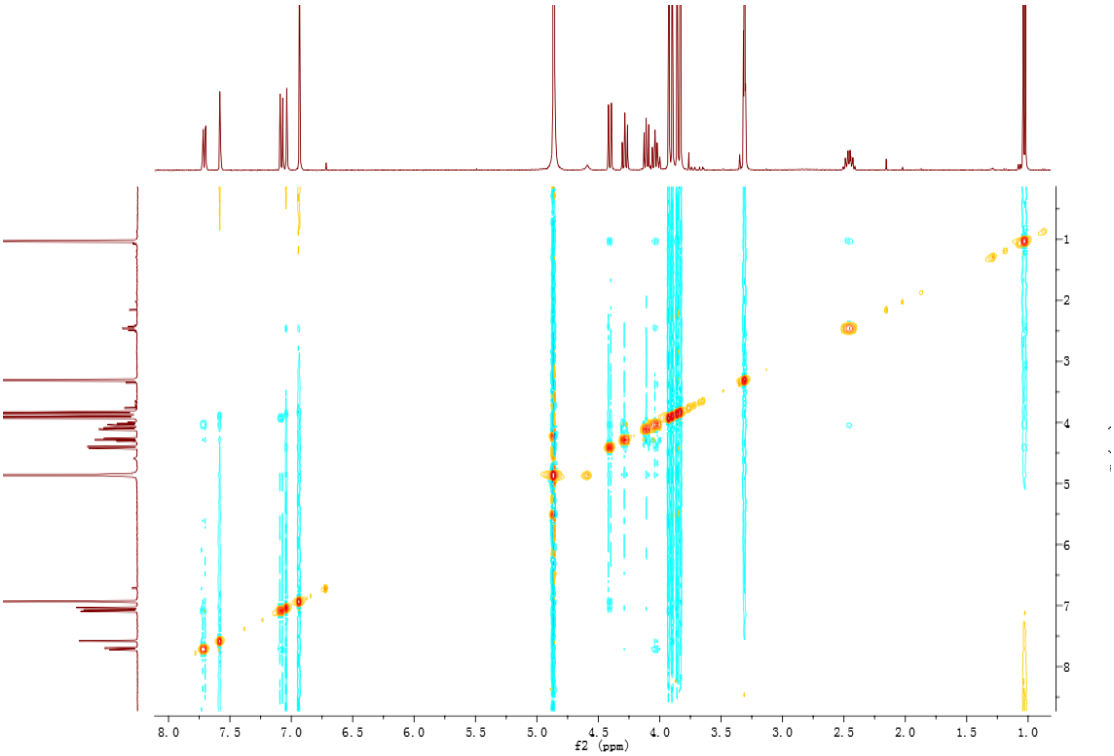


Figure S47. ECD spectrum of **5** in MeOH

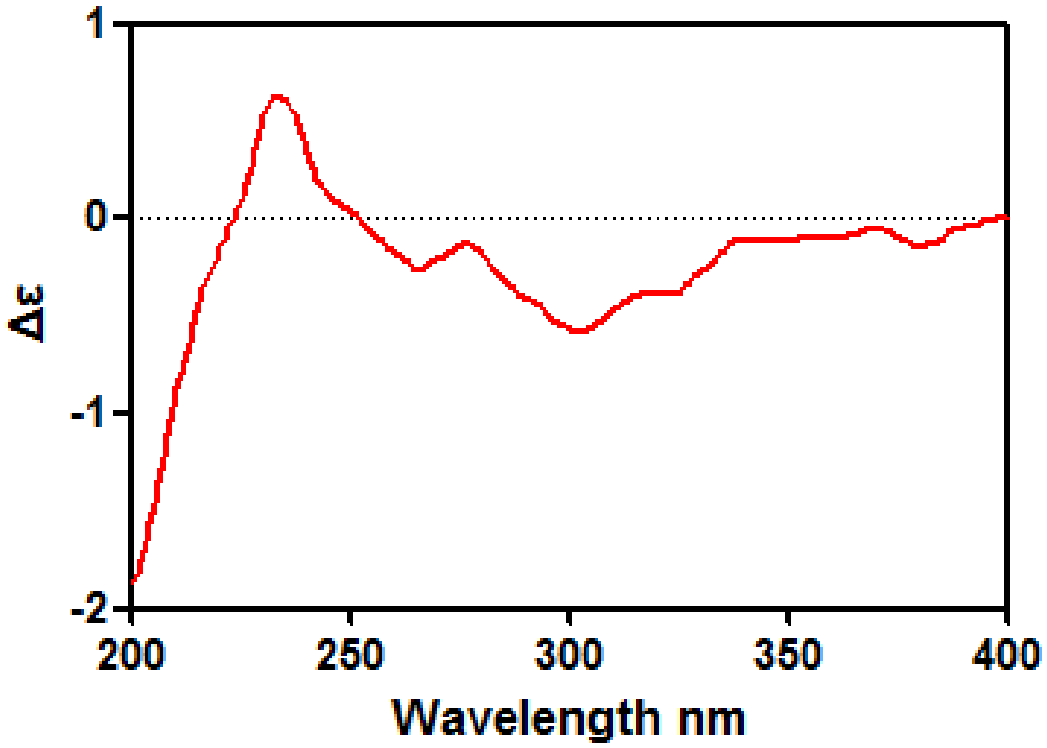


Figure S48. (+)-HR-ESI-MS spectrum of **6**

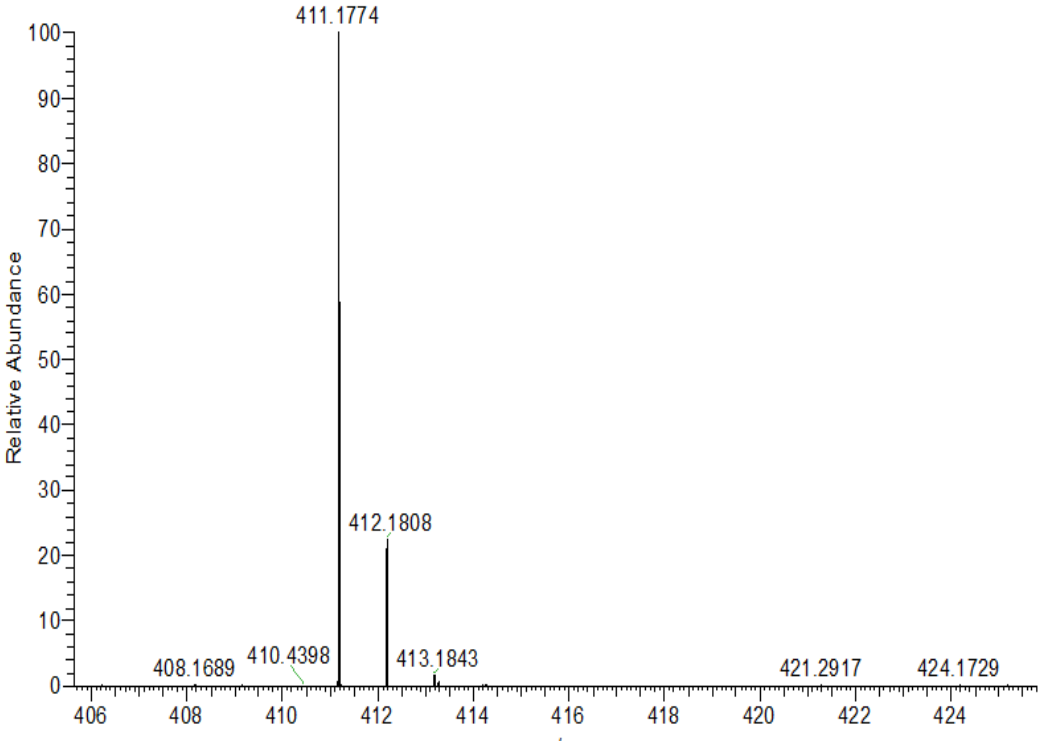


Figure S49. IR spectrum of **6** (**6a/6b**)

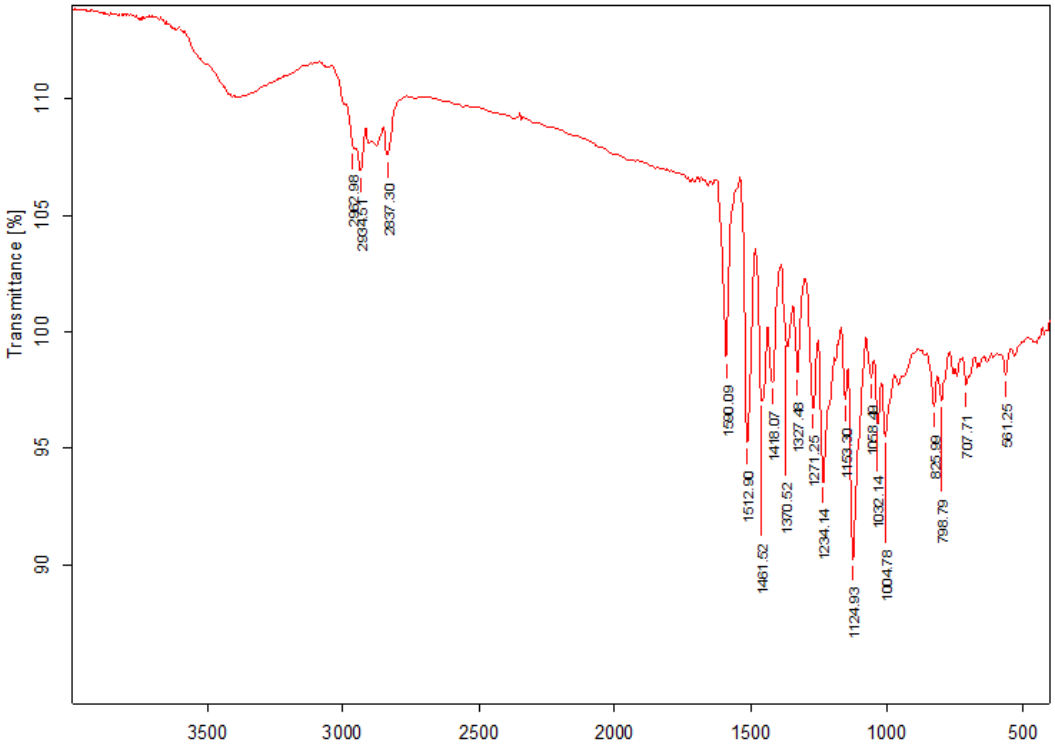


Figure S50. UV spectrum of **6**

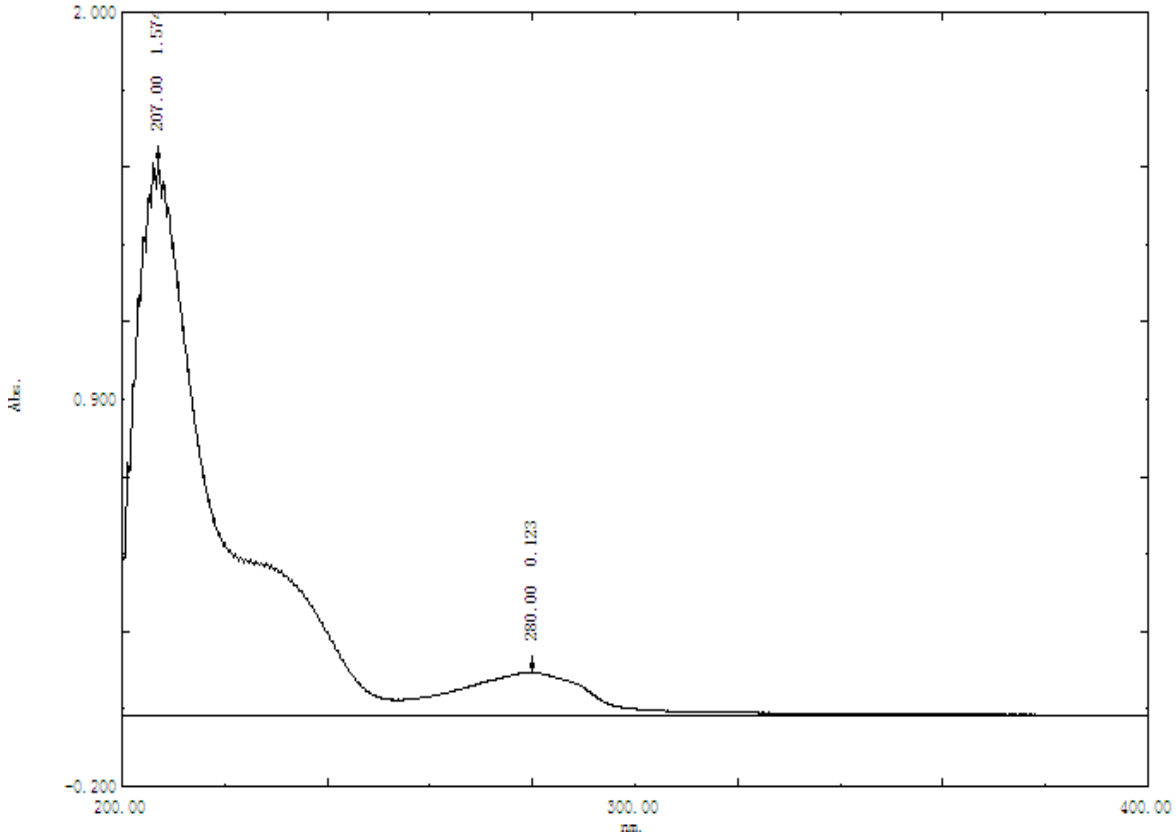


Figure S51. ^{1}H NMR spectrum of **6** in CD_3OD

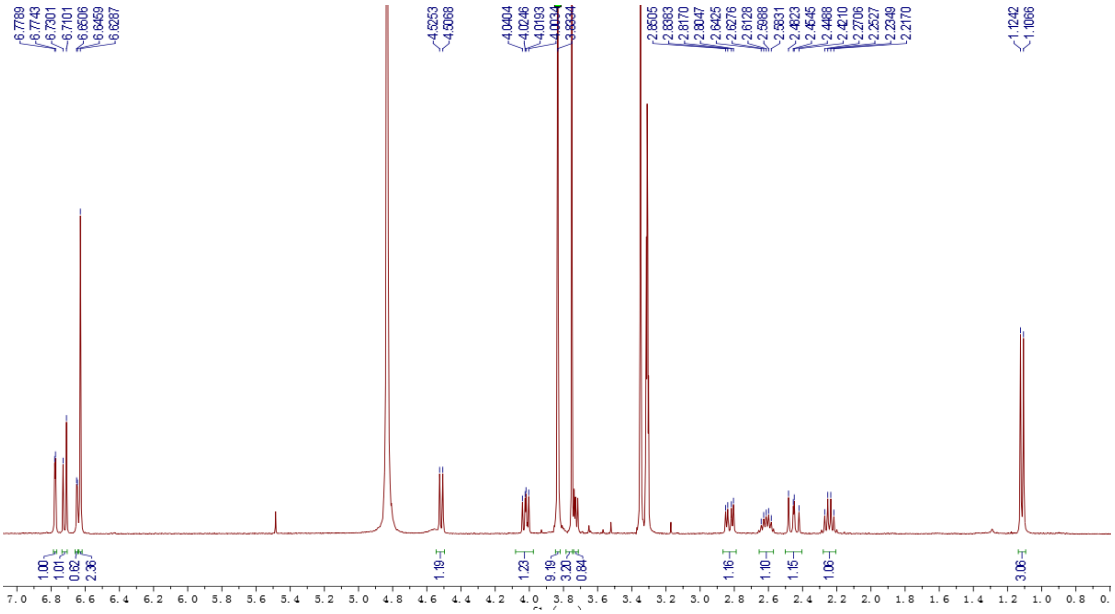


Figure S52. ^{13}C NMR spectrum of **6** in CD_3OD

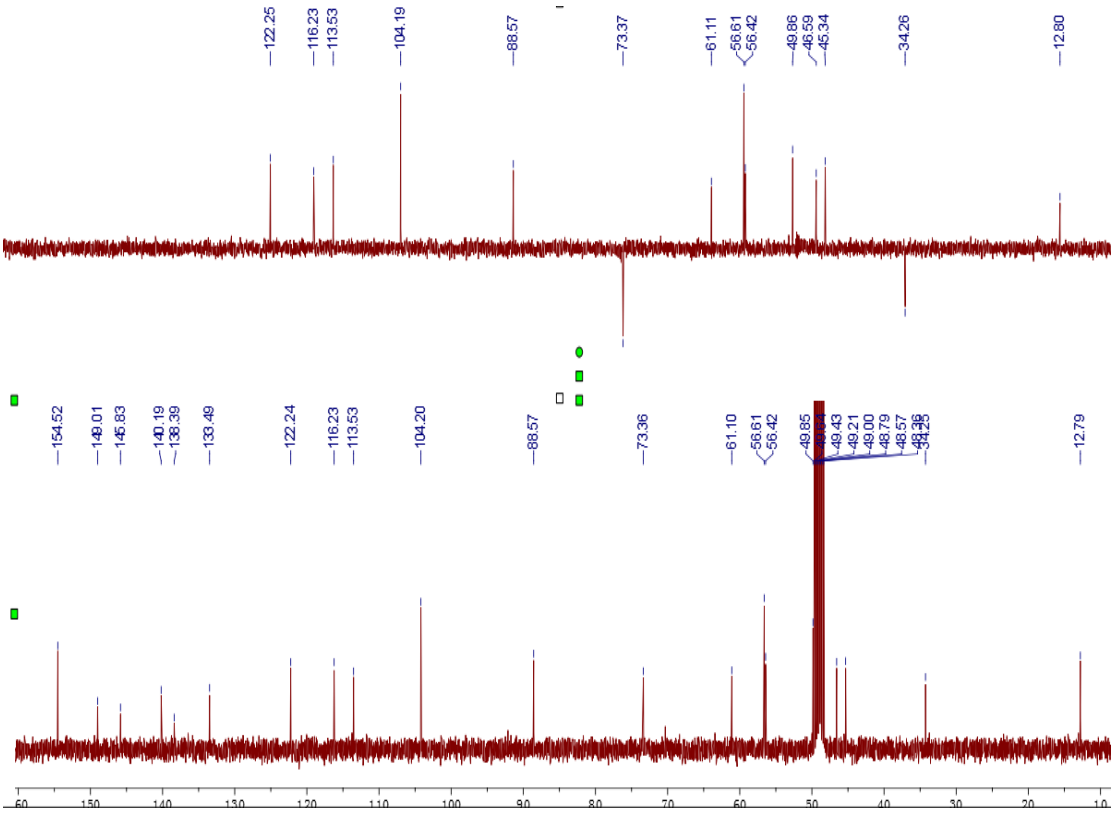


Figure S53. HSQC spectrum of **6** in CD_3OD

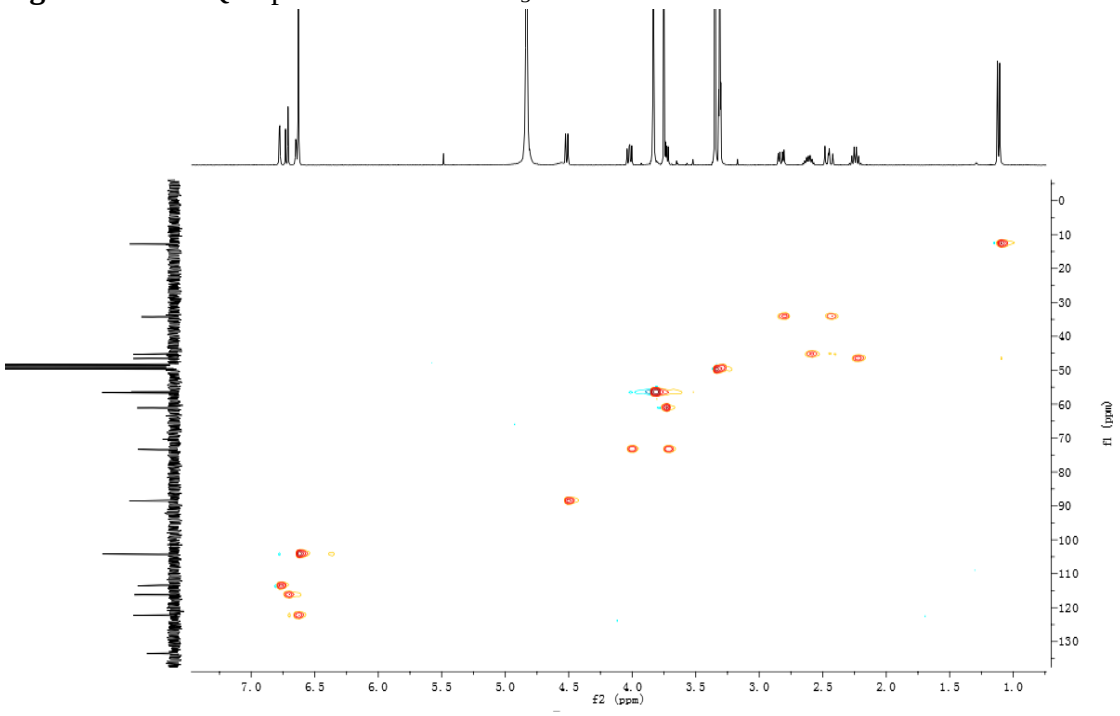


Figure S54. HMBC spectrum of **6** in CD_3OD

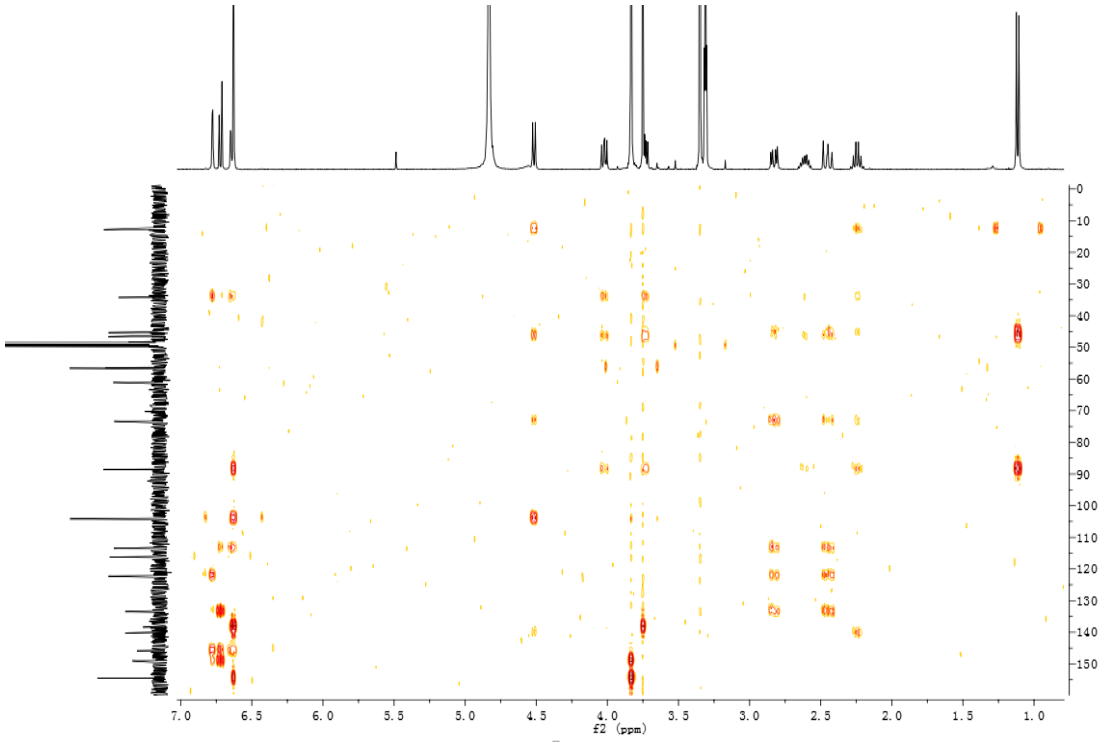


Figure S55. ^{1}H-^{1}H COSY spectrum of **6** in CD_3OD

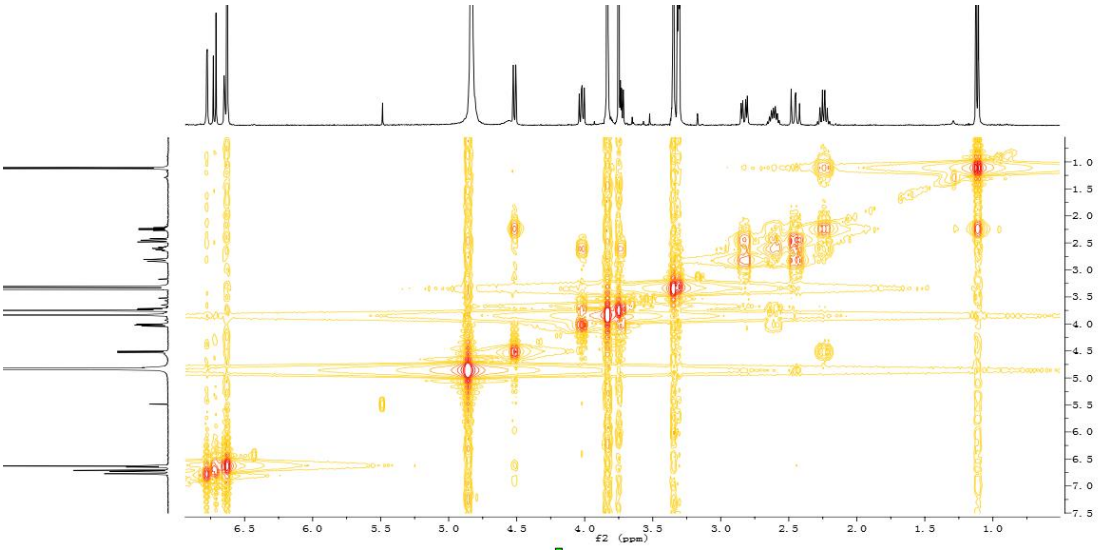


Figure S56. NOESY spectrum of **6** in CD_3OD

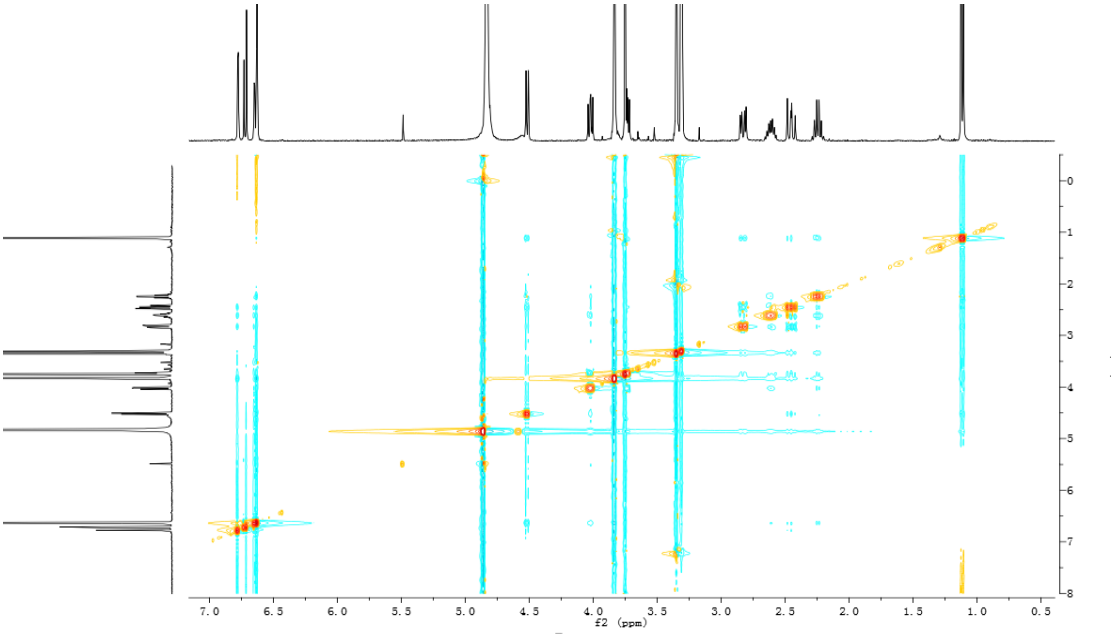


Figure S57. ECD spectrum of **6** in MeOH

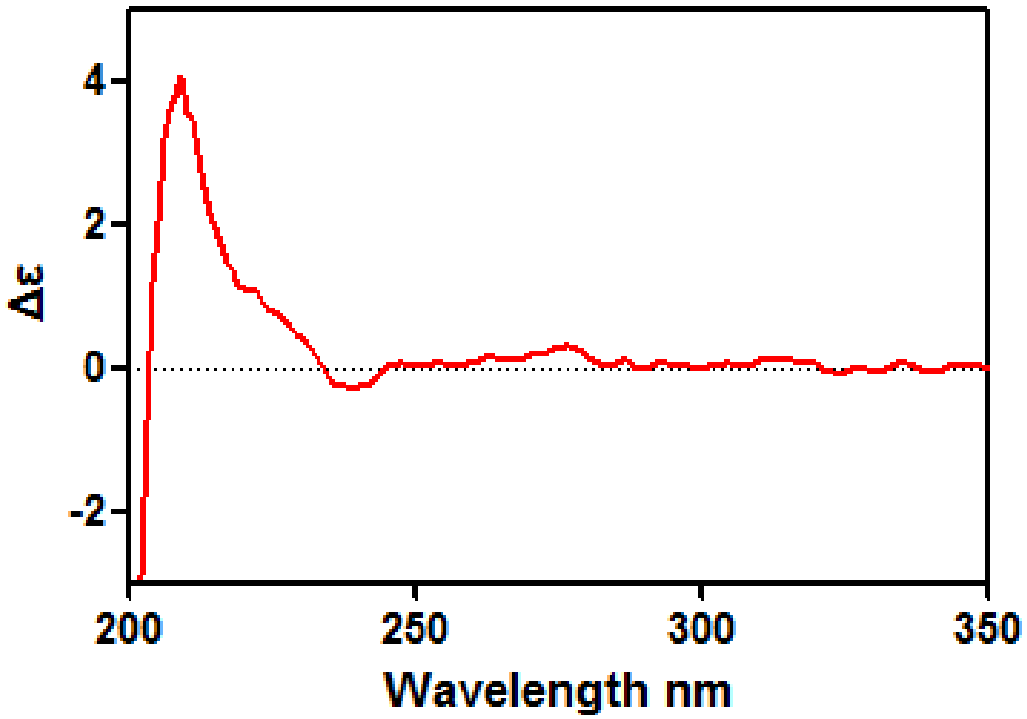


Figure S58. (+)-HR-ESI-MS spectrum of **7**

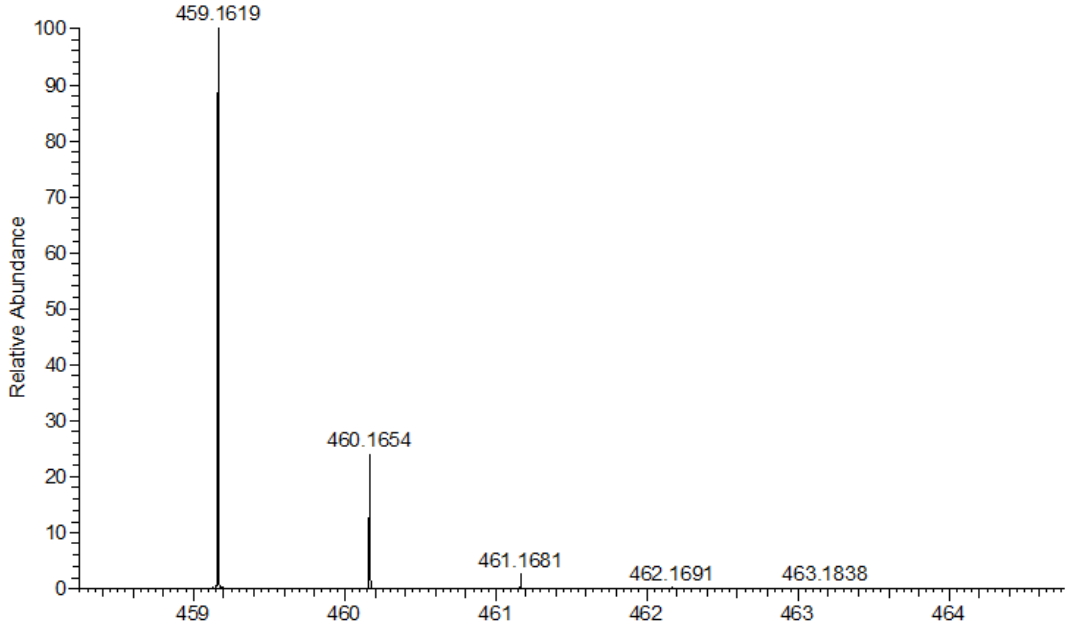


Figure S59. IR spectrum of **7**

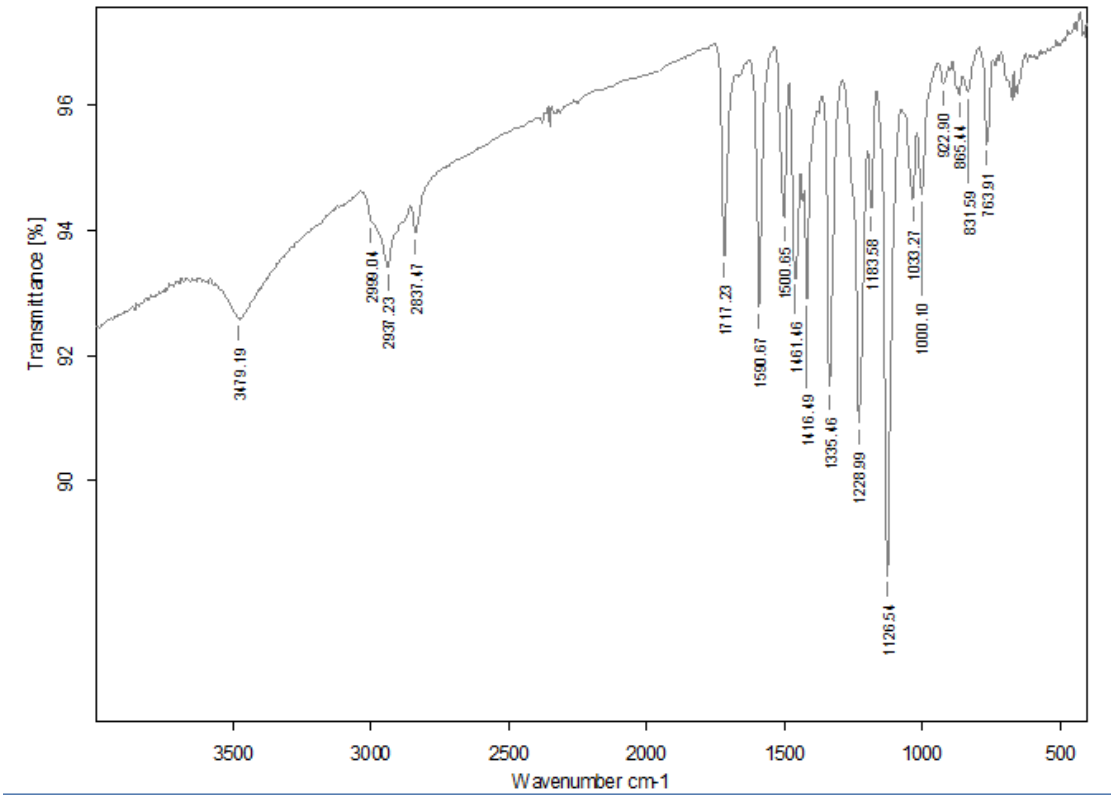


Figure S60. UV spectrum of **7**

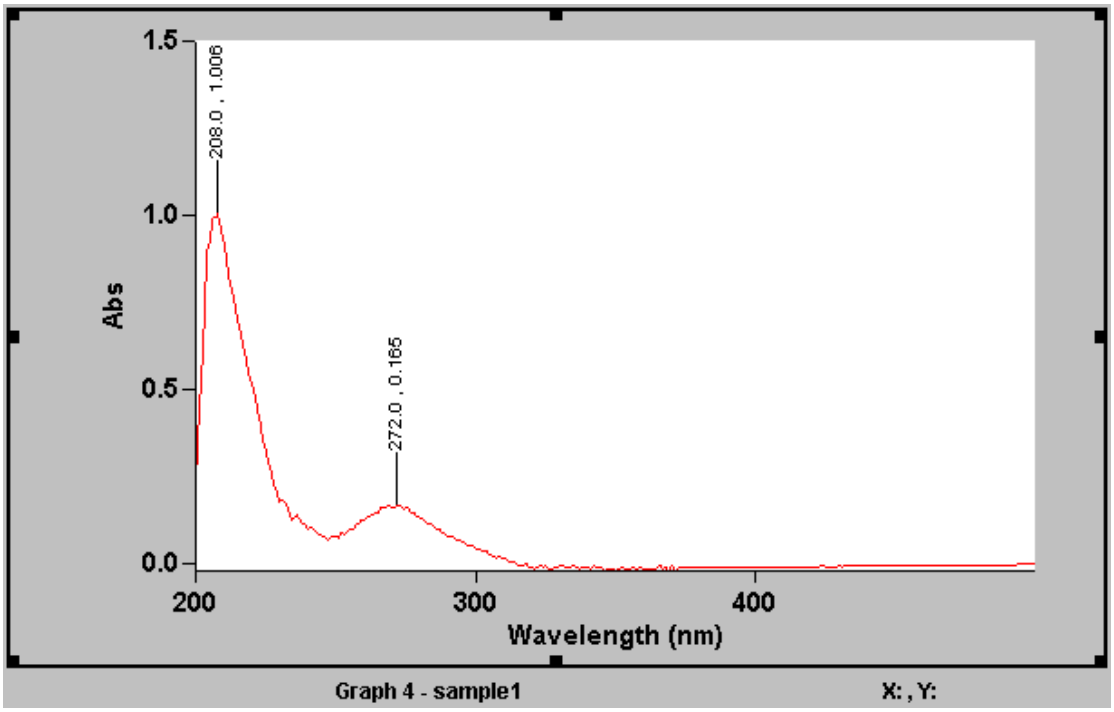


Figure S61. ^{1}H NMR spectrum of **7** in CD_3OD

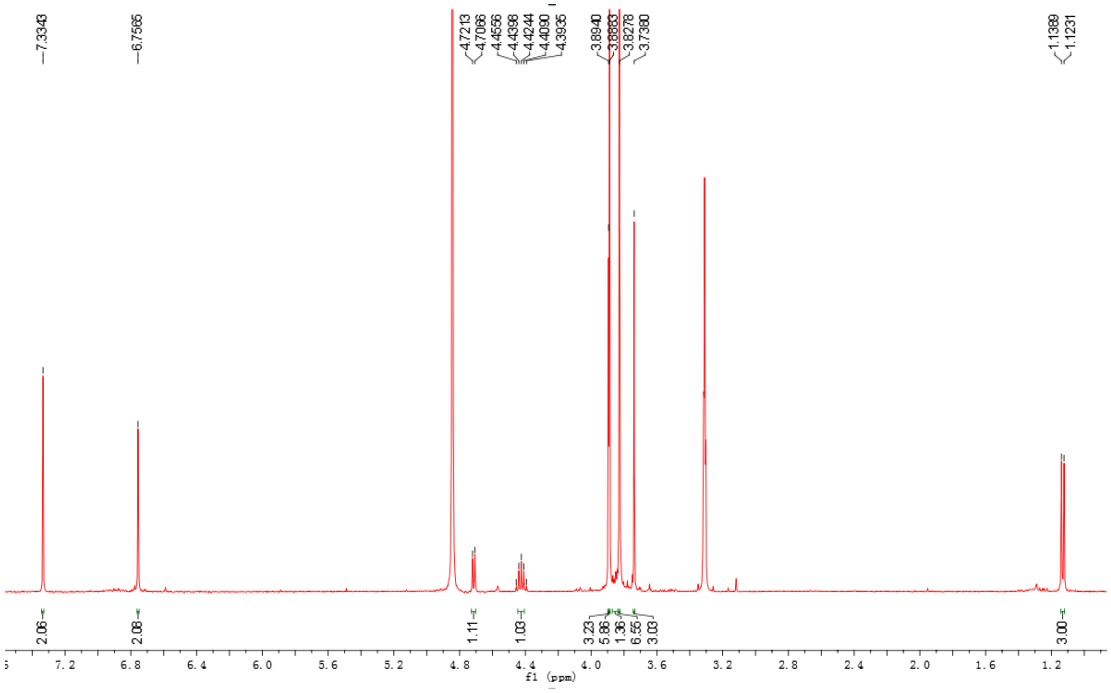


Figure S62. ^{13}C NMR spectrum of **7** in CD_3OD

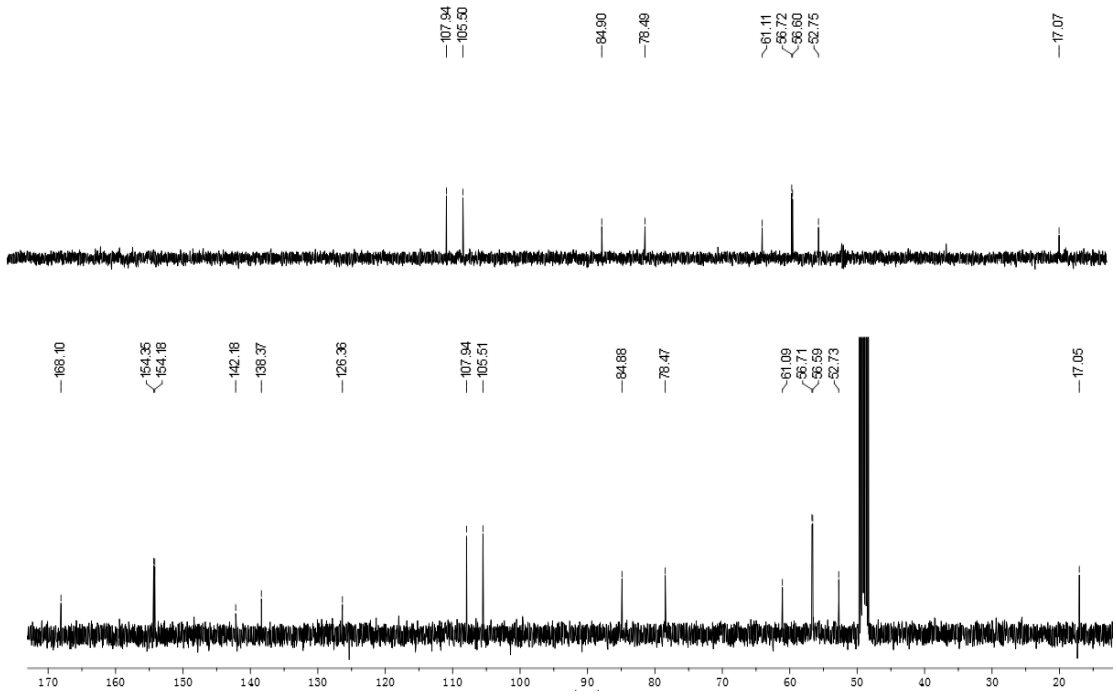


Figure S63. HSQC spectrum of **7** in CD_3OD

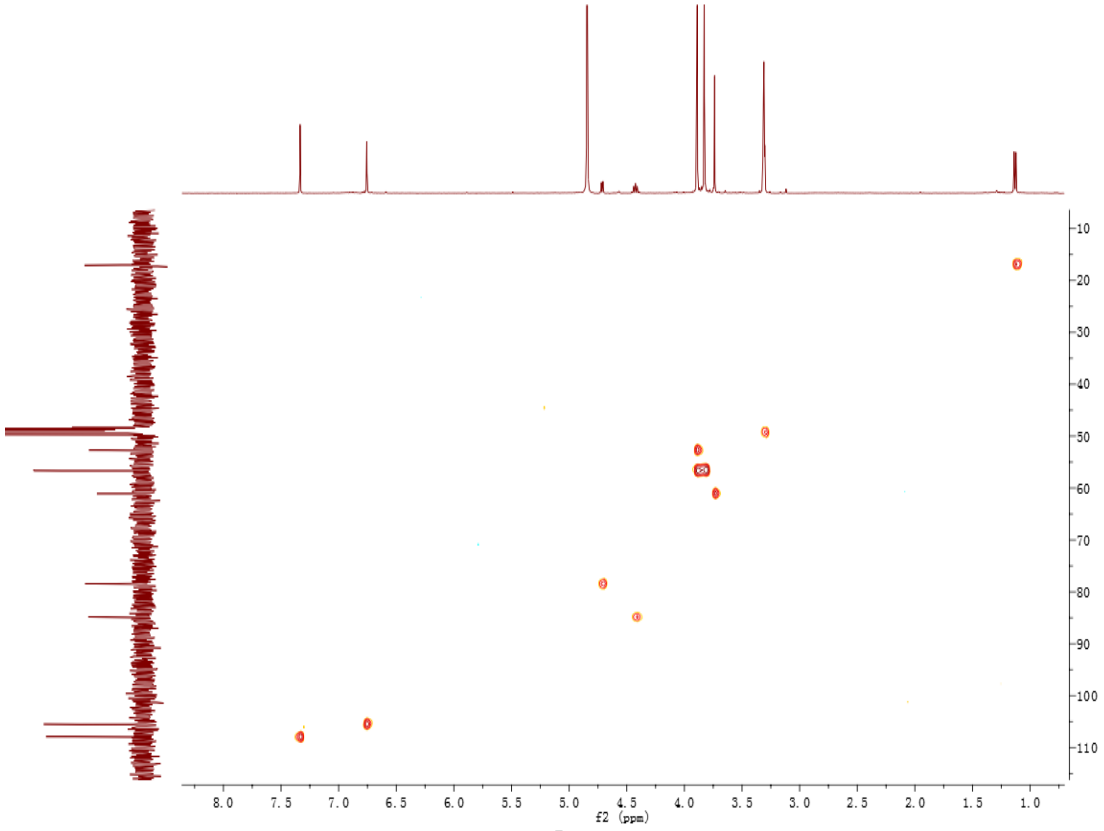


Figure S64. HMBC spectrum of **7** in CD_3OD

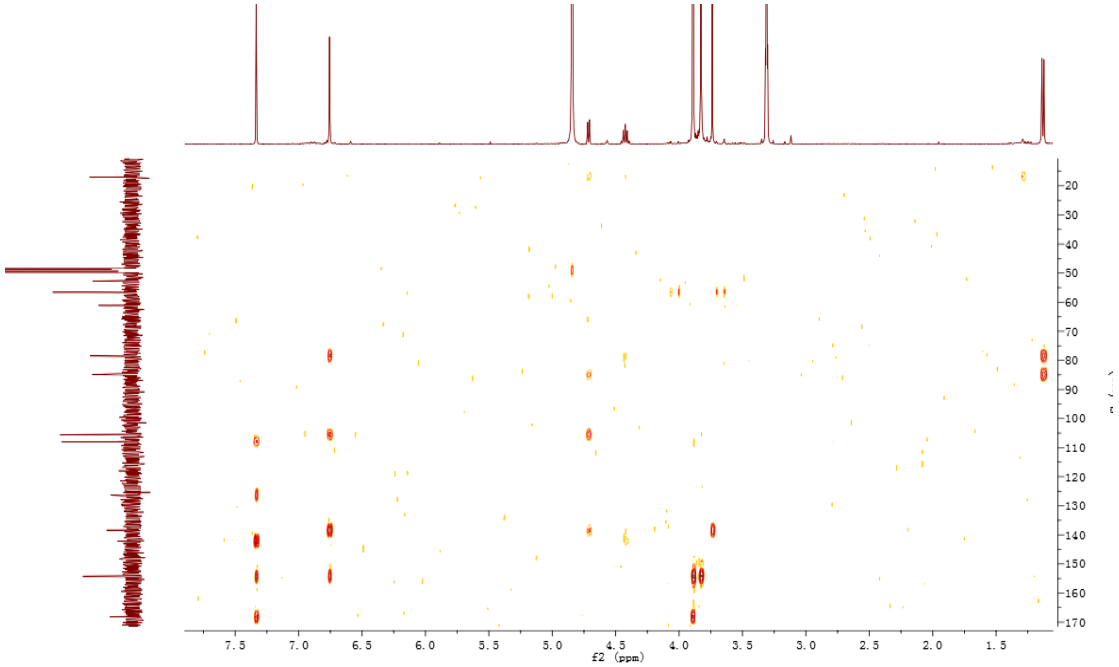


Figure S65. ^{1}H-^{1}H COSY spectrum of **7** in CD_3OD

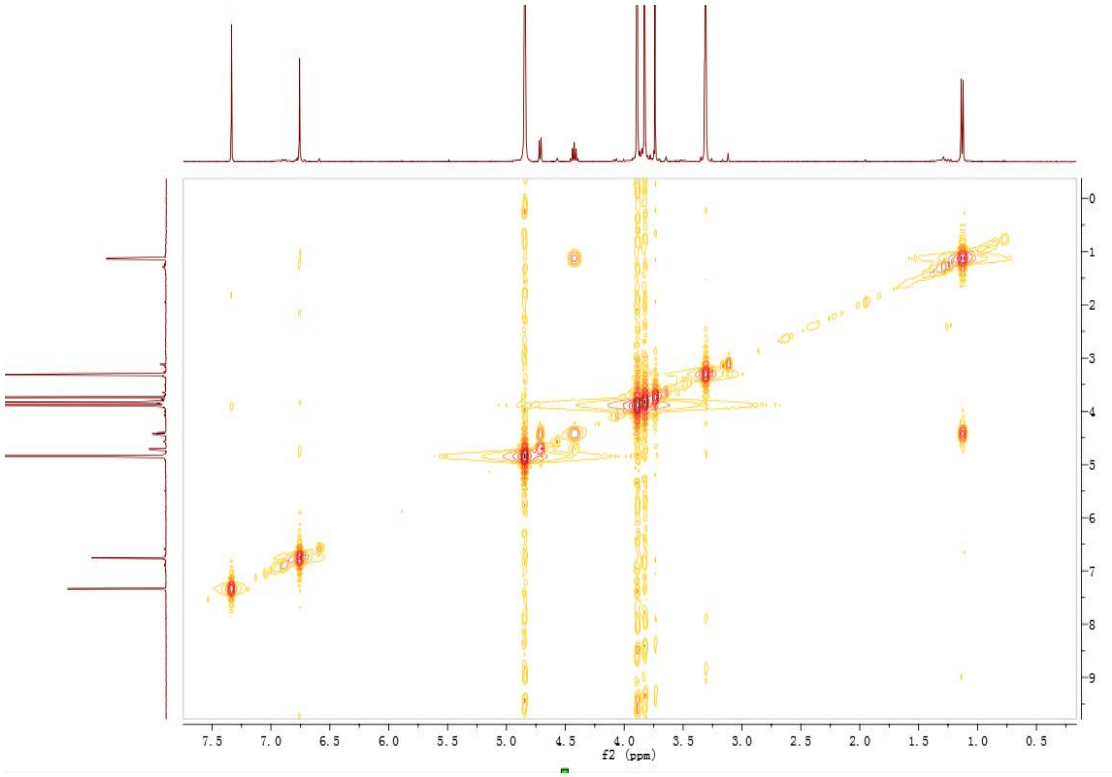


Figure S66. NOESY spectrum of **7** in CD_3OD

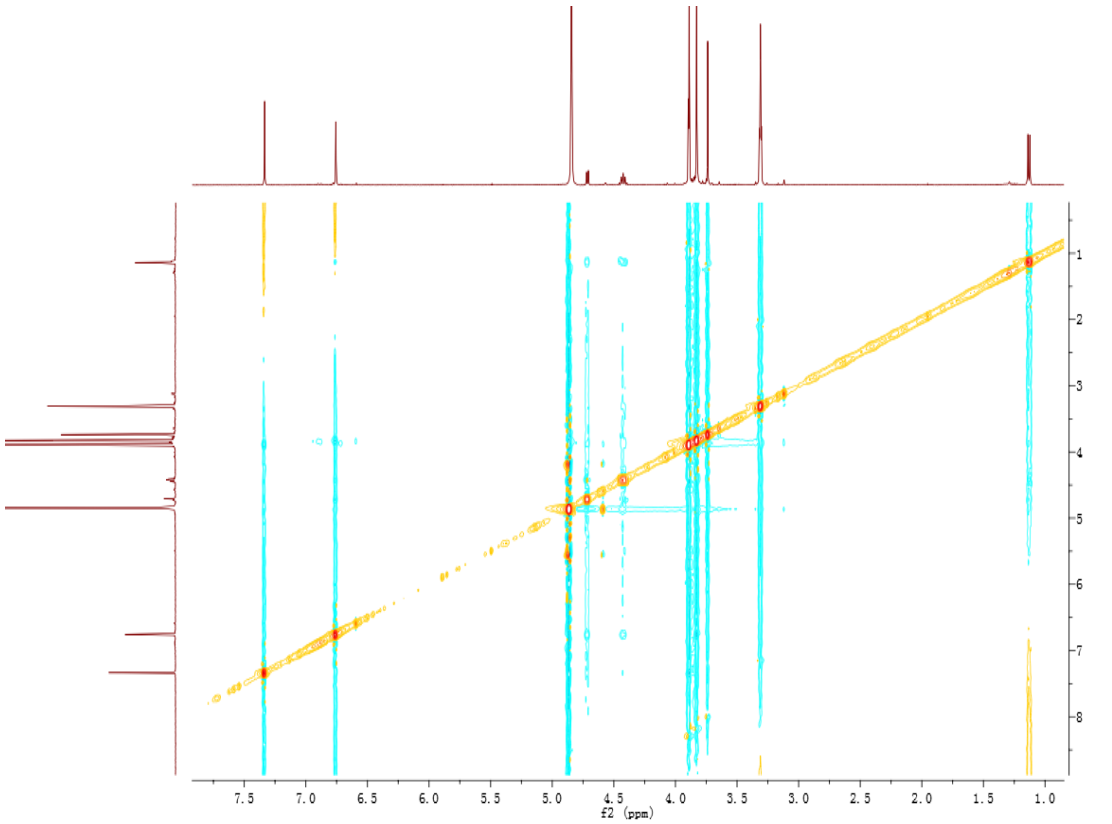


Figure S67. ECD spectrum of **7** in MeOH

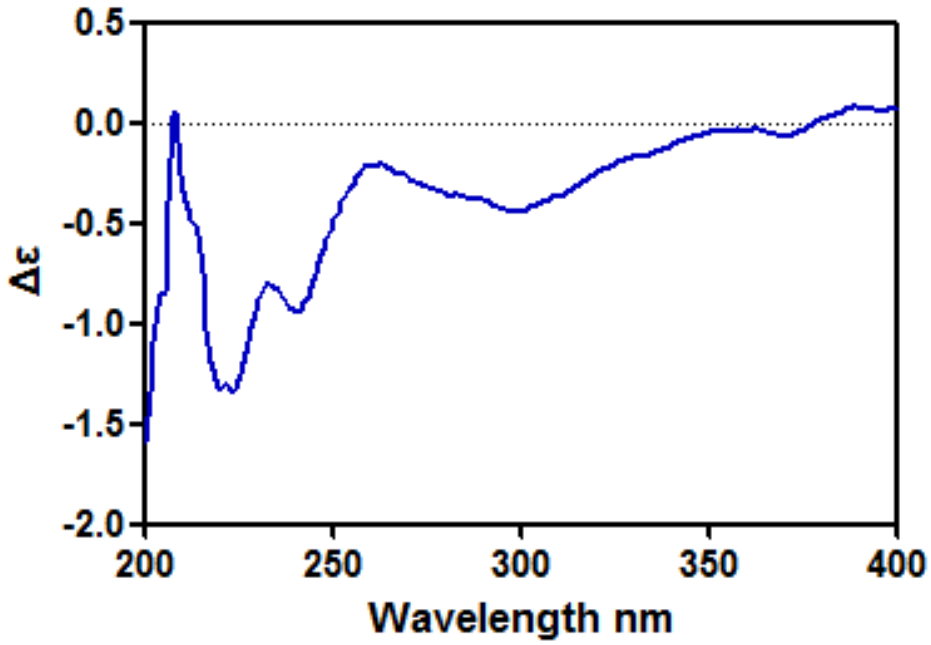


Figure S68. (+)-HR-ESI-MS spectrum of **8**

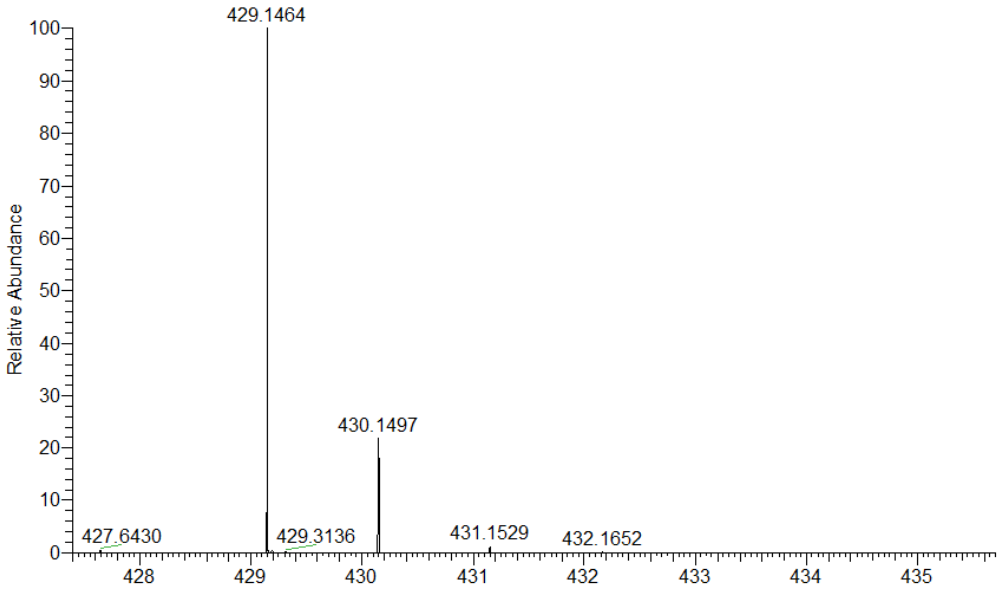


Figure S69. IR spectrum of **8**

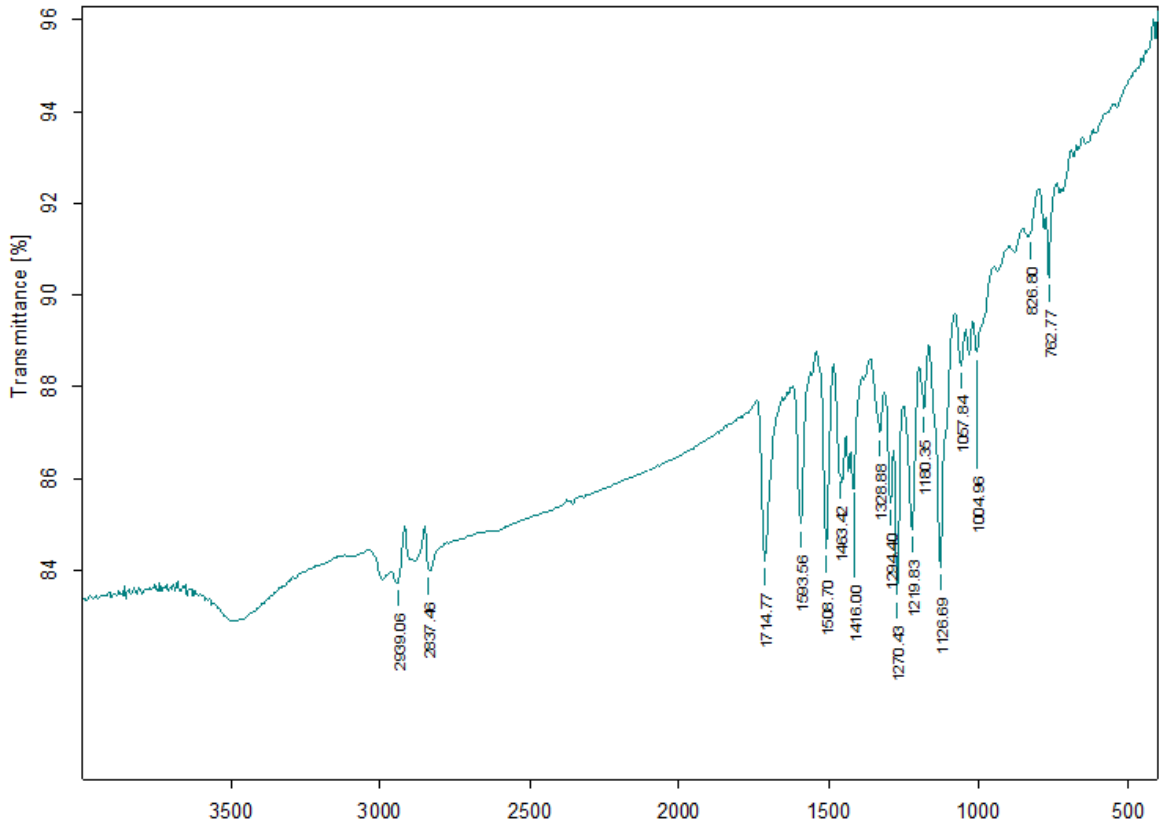


Figure S70. UV spectrum of **8**

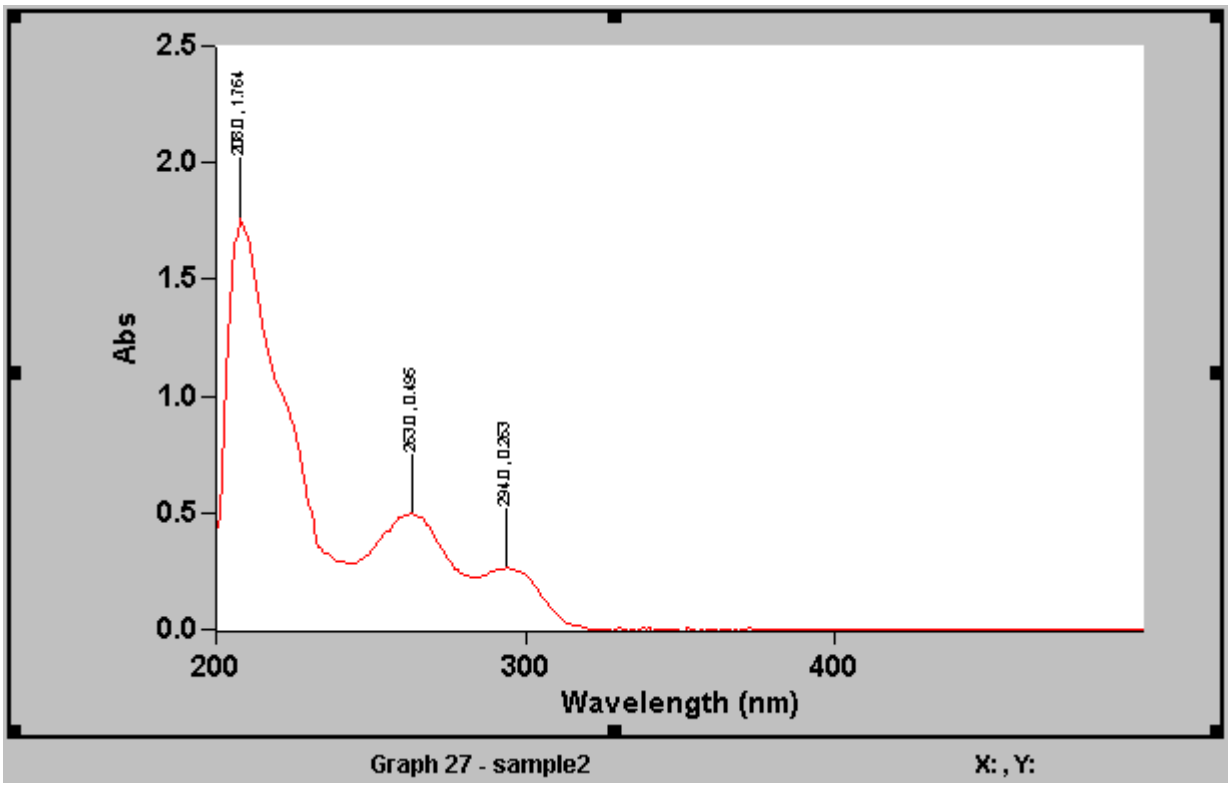


Figure S71. ^{1}H NMR spectrum of **8** in CD_3OD

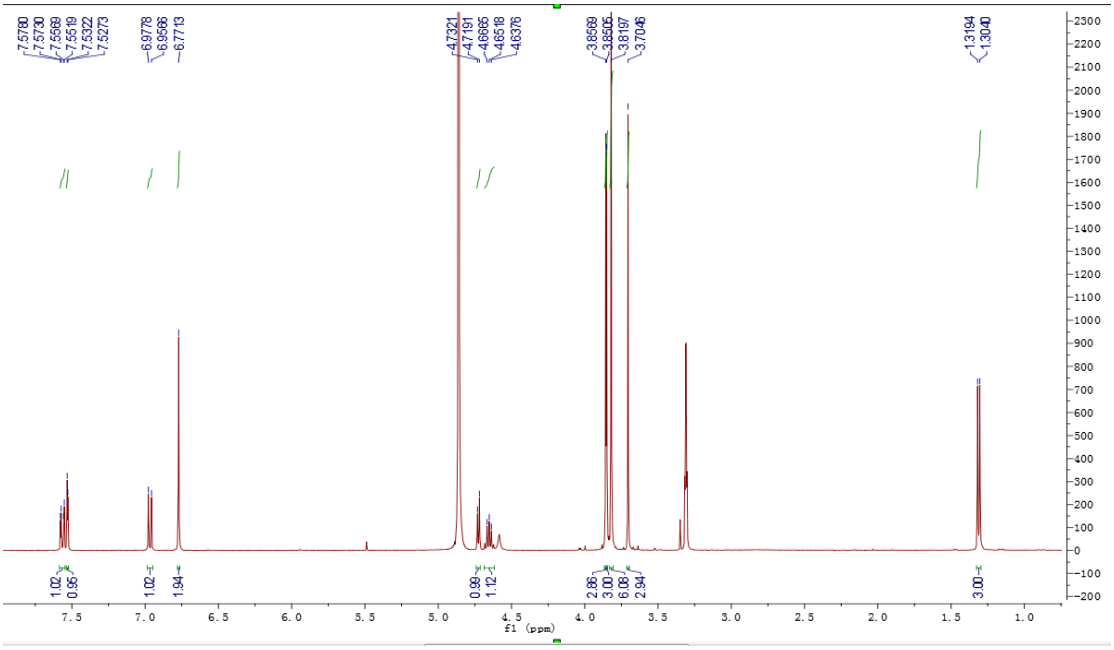


Figure S72. ^{13}C NMR spectrum of **8** in CD_3OD

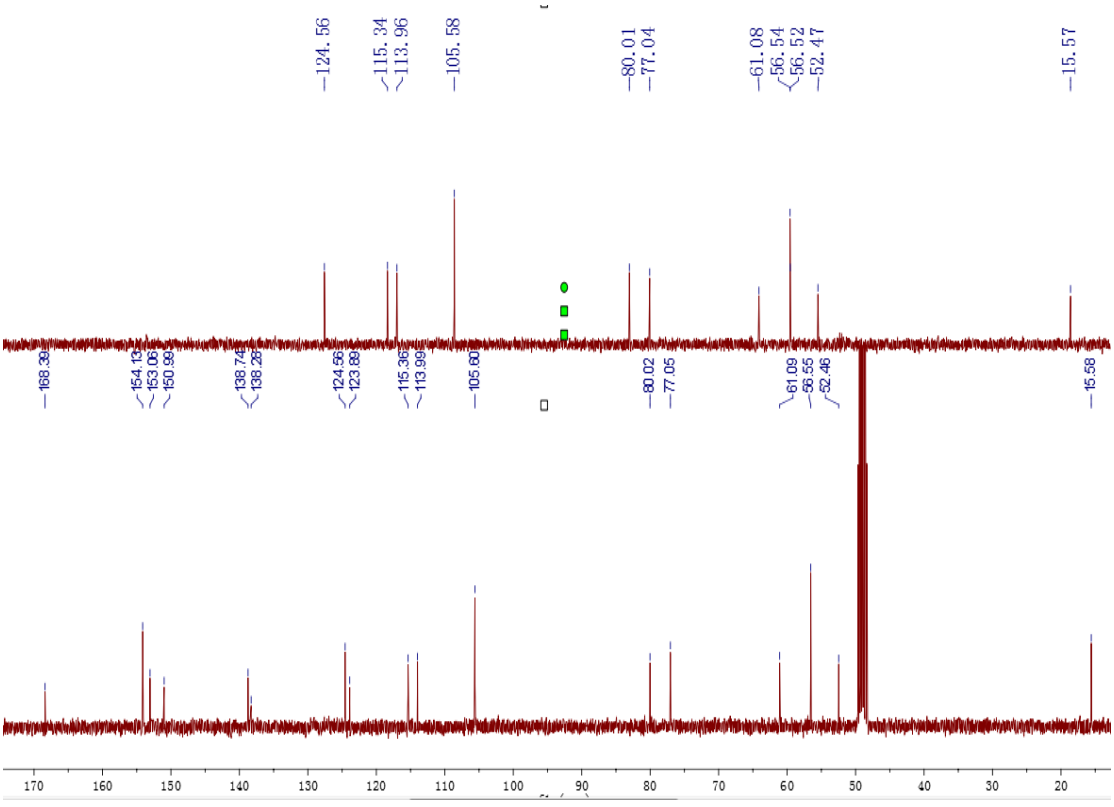


Figure S73. HSQC spectrum of **8** in CD_3OD

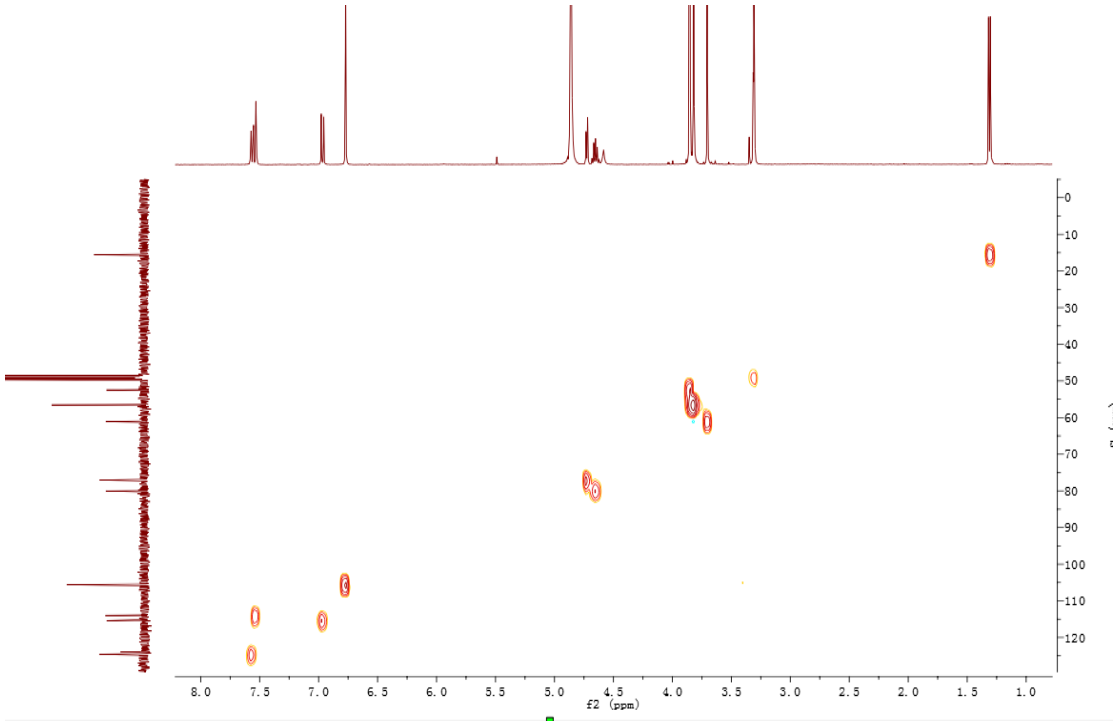


Figure S74. HMBC spectrum of **8** in CD_3OD

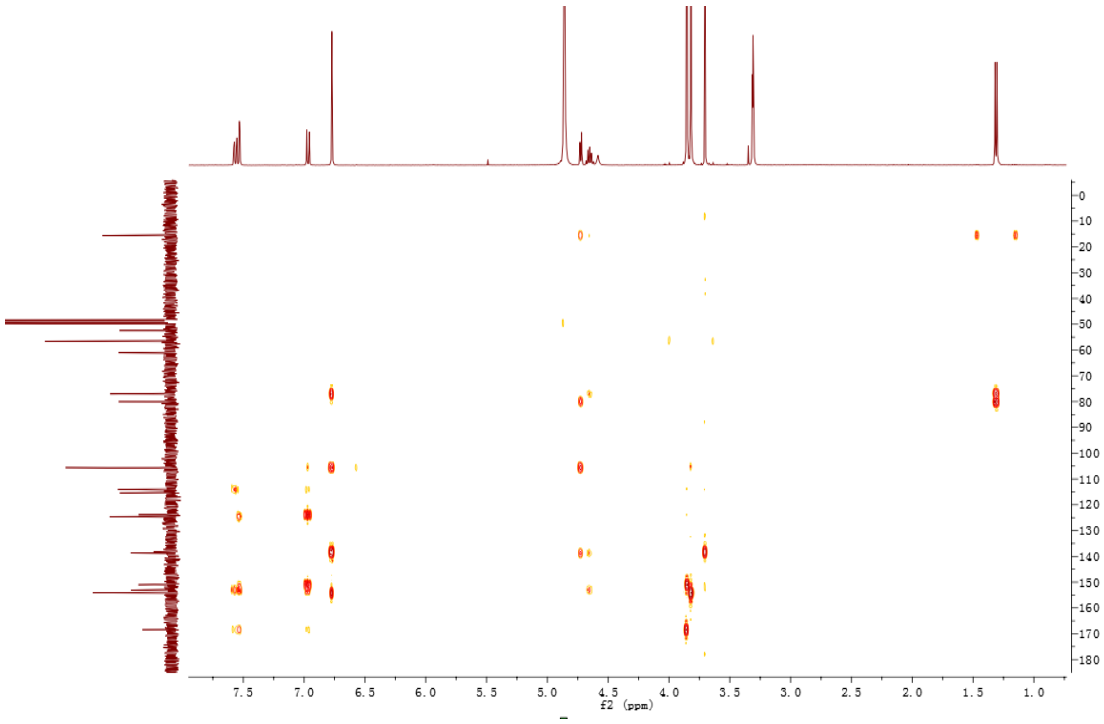


Figure S75. ^{1}H-^{1}H COSY spectrum of **8** in CD_3OD

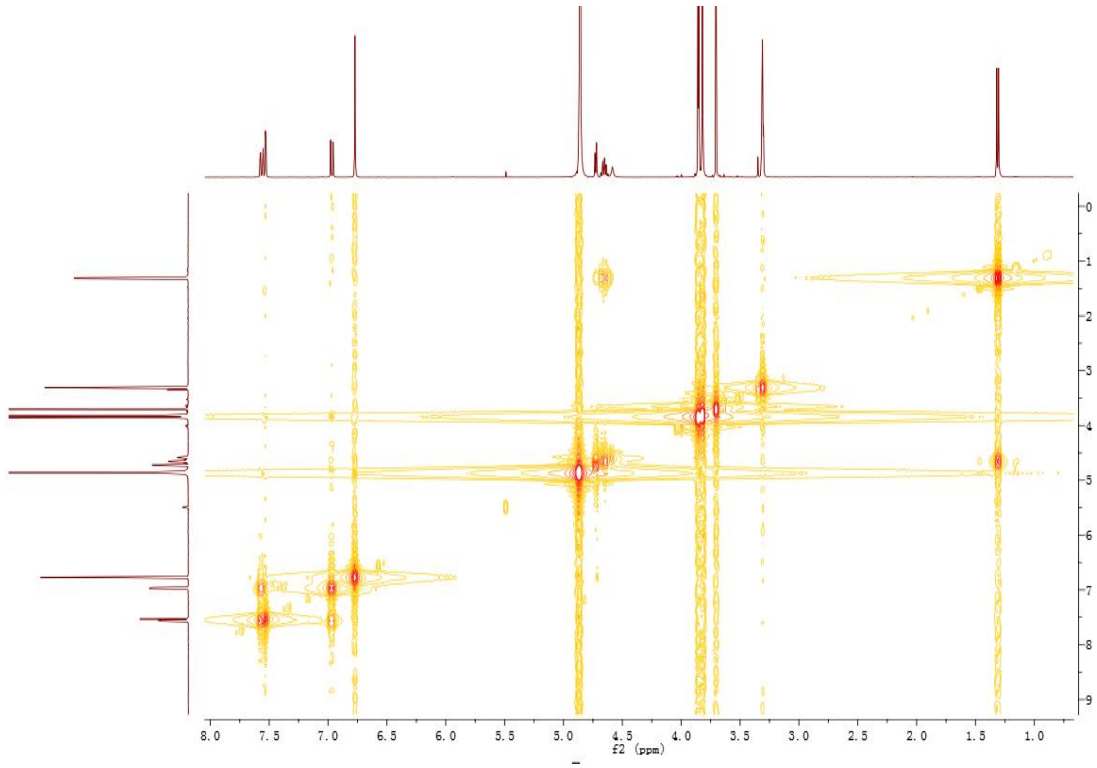


Figure S76. NOESY spectrum of **8** in CD_3OD

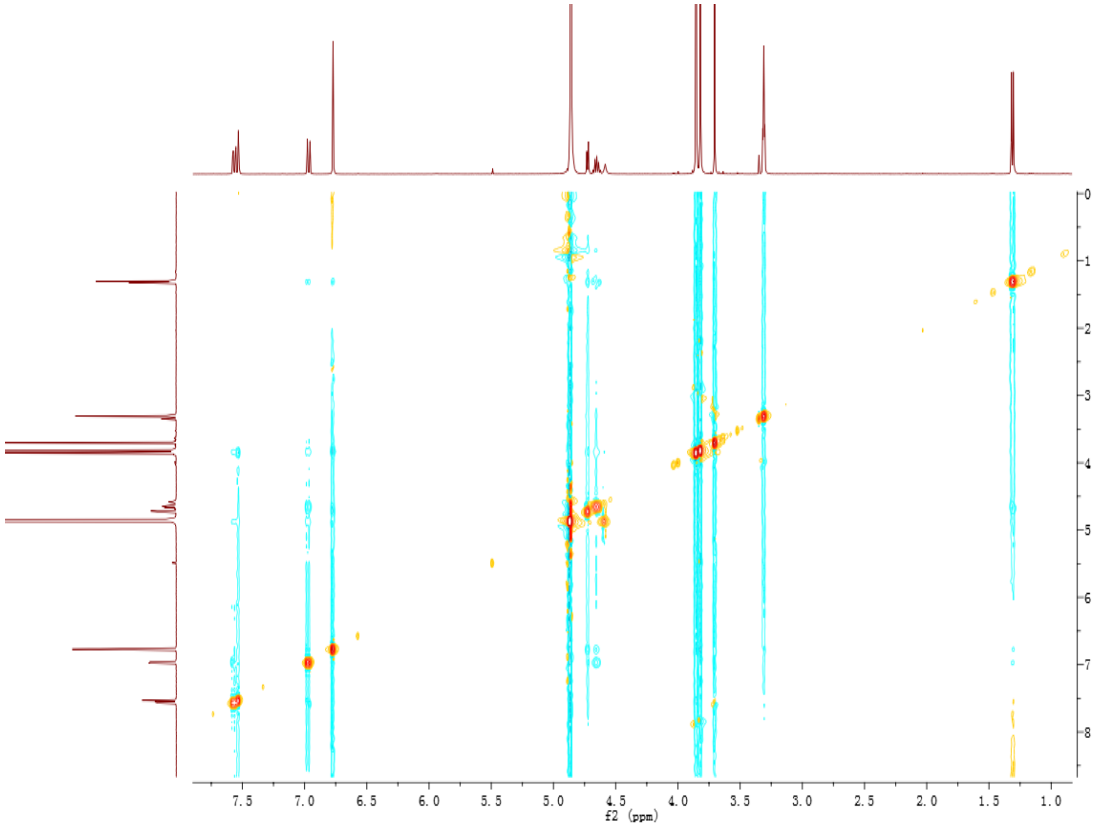


Figure S77. ECD spectrum of **8** in MeOH

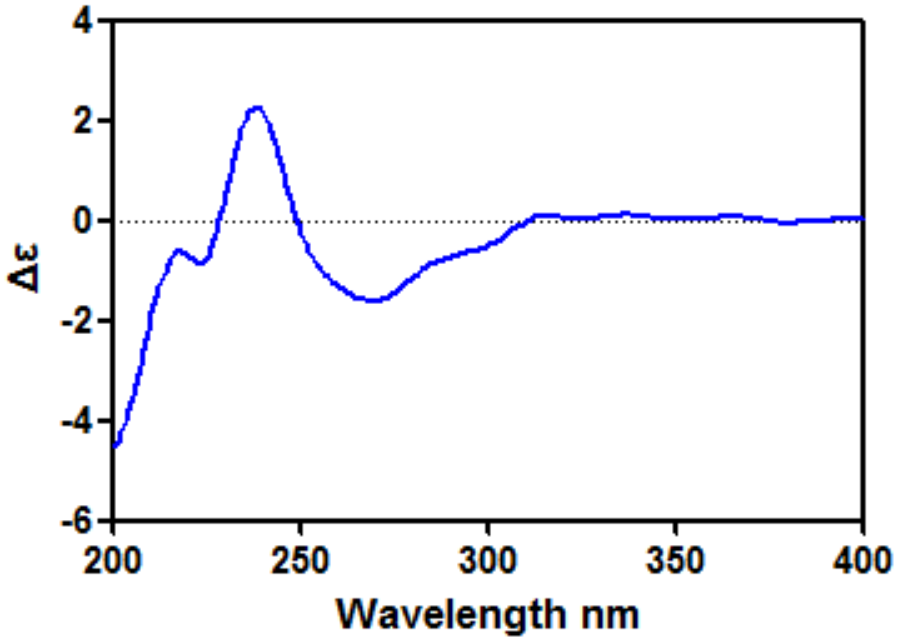


Figure S78. (+)-HR-ESI-MS spectrum of *S*-MTPA-**7** ester

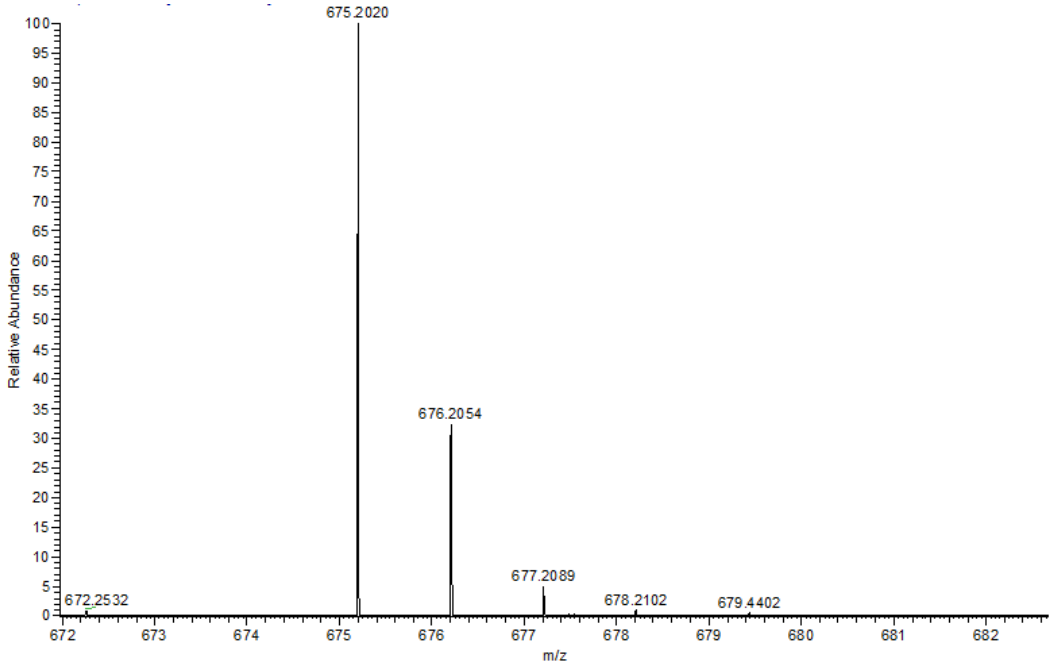


Figure S79. (+)-HR-ESI-MS spectrum of *R*-MTPA-**7** ester

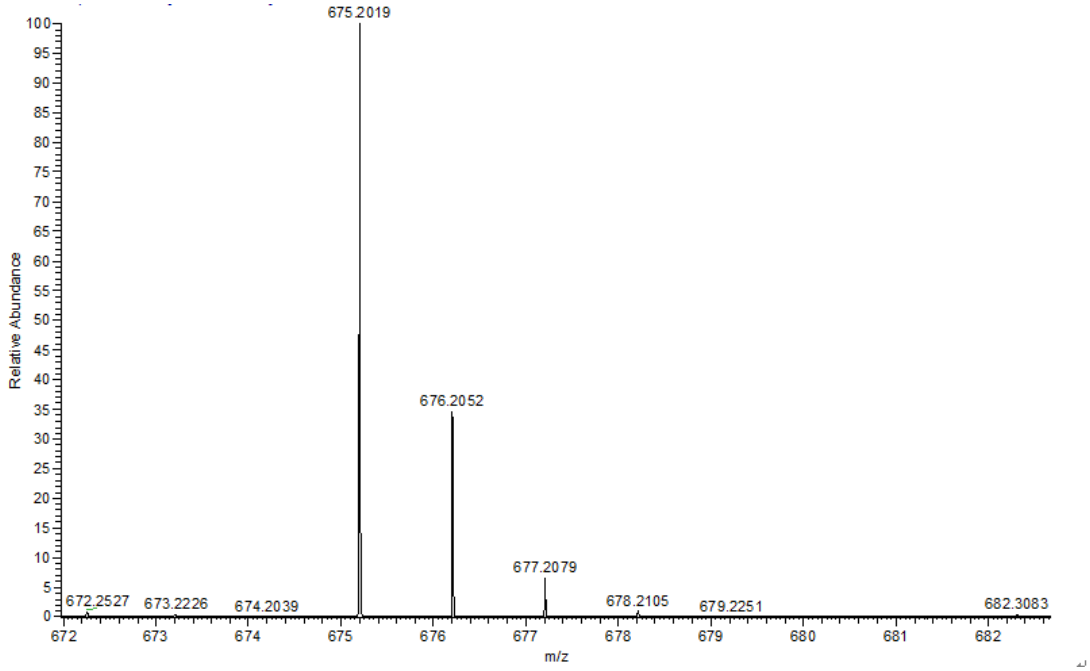


Figure S80. ^{1}H NMR spectrum of *R*/*S*-MTPA-**7** ester in CD_3OD

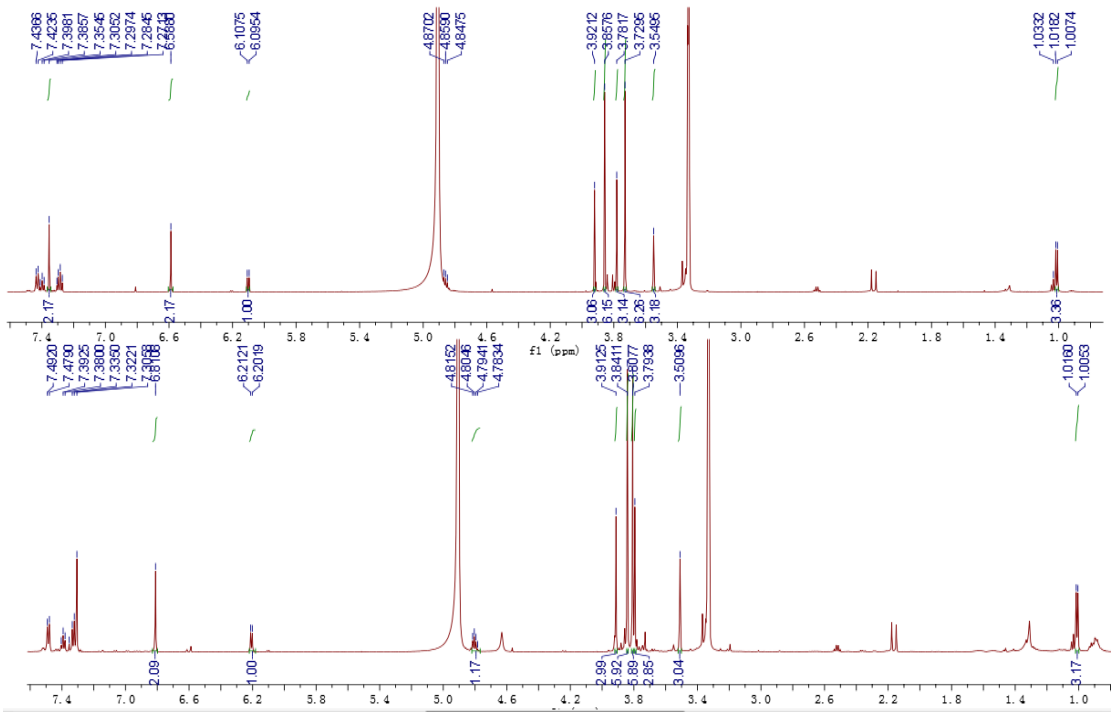
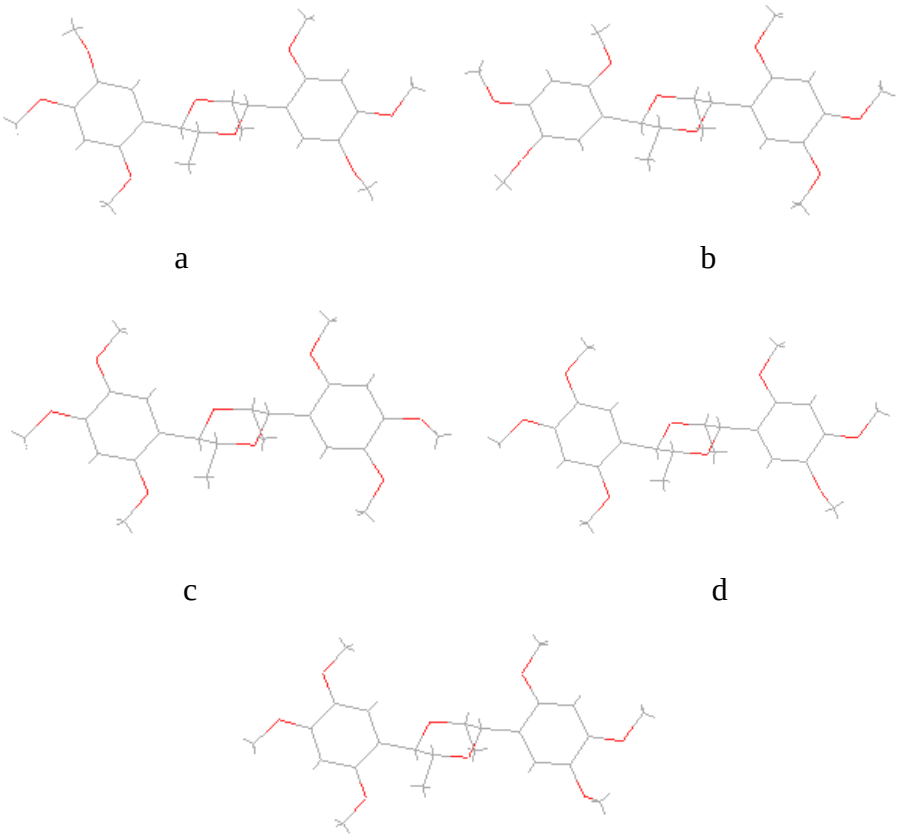


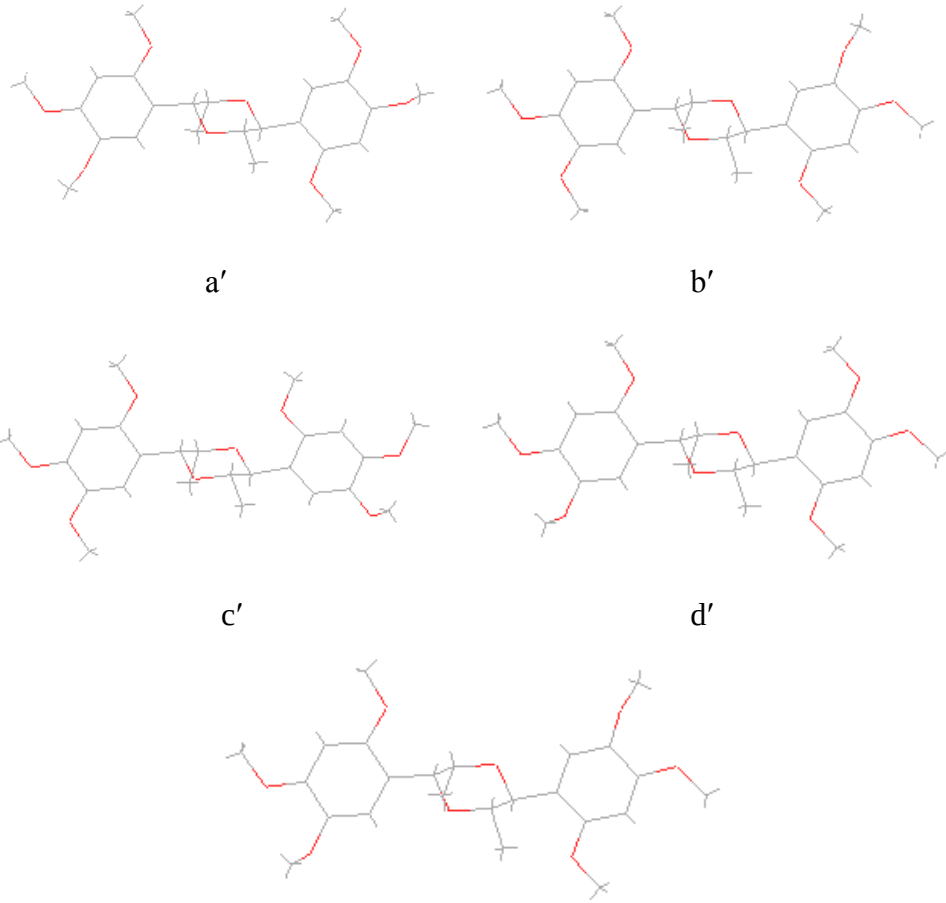
Figure S81. ECD spectra calculation

The conformational analyses were carried out for compounds **1a/1b** using BALLOON11 and confab12 programs. The theoretical calculation of ECD was performed using time-dependent density functional theory (TDDFT) at the B3LYP/6-31G (d, p) level in methanol with a PCM model. The calculated ECD curve was generated using SpecDis 1.51.

Figure S82. Five lowest energy conformers of the isomer 7*S*,7′*R*,8*S*,8′*S* and five lowest energy conformers of the 7*R*,7′*S*,8*R*,8′*R* isomer of compound **1**.



a-e: Five lowest energy conformers of the7*S*, 7′*R*, 8*S*, 8′*S* isomer.



a′ b′ c′ d′ e′

a′-e′: Five lowest energy conformers of the 7*R*, 7′*S*, 8*R*, 8′*R* isomer.

Table S1. Relative free energies (ΔG) and equilibrium populations (P) of the conformers of the (7*S*,7′*R*,8*S*,8′*S*)-**1** and (7*R*,7′*S*,8*R*,8′*R*)-**1**

conformer	isomer 7*S*,7′*R*,8*S*,8′*S*		conformer	Isomer 7*R*,7′*S*,8*R*,8′*R*	
	ΔG (kcal/mol)	P (%)		ΔG (kcal/mol)	P (%)
a	0.7975	9.96%	a′	1.4749	3.98%
b	1.5650	2.73%	b′	0.0000	47.89%
c	0.6379	13.05%	c′	1. 4666	4.03%
d	0.0000	38.27%	d′	0.2589	30.94%
e	0.0365	35.99%	e′	0.7650	13.17%