

Antioxidant Lignans and Neolignans from Acorus tatarinowii

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

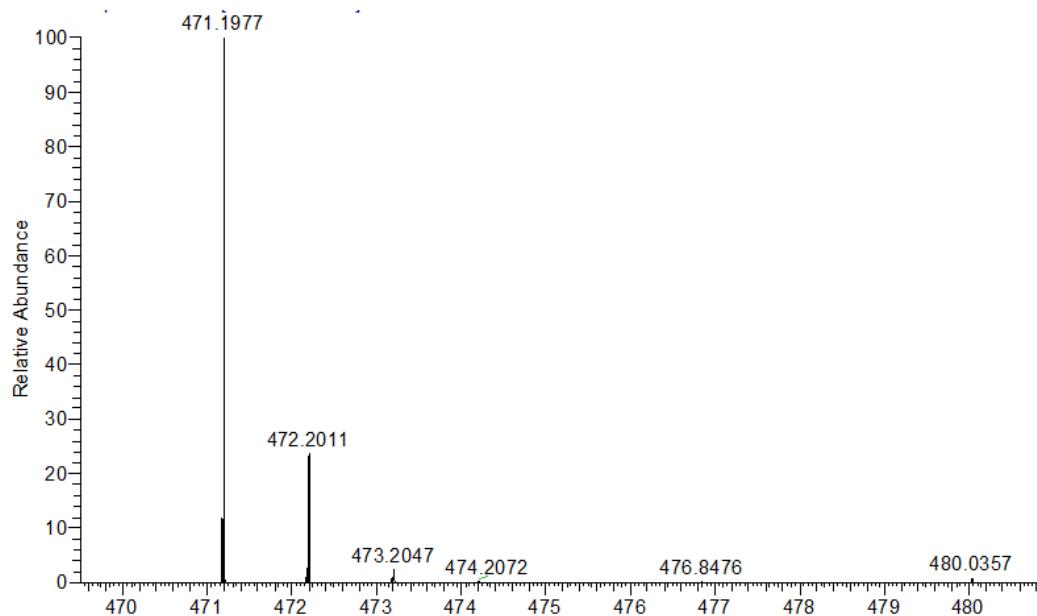


Figure S2. IR spectrum of **1** (**1a/1b**)

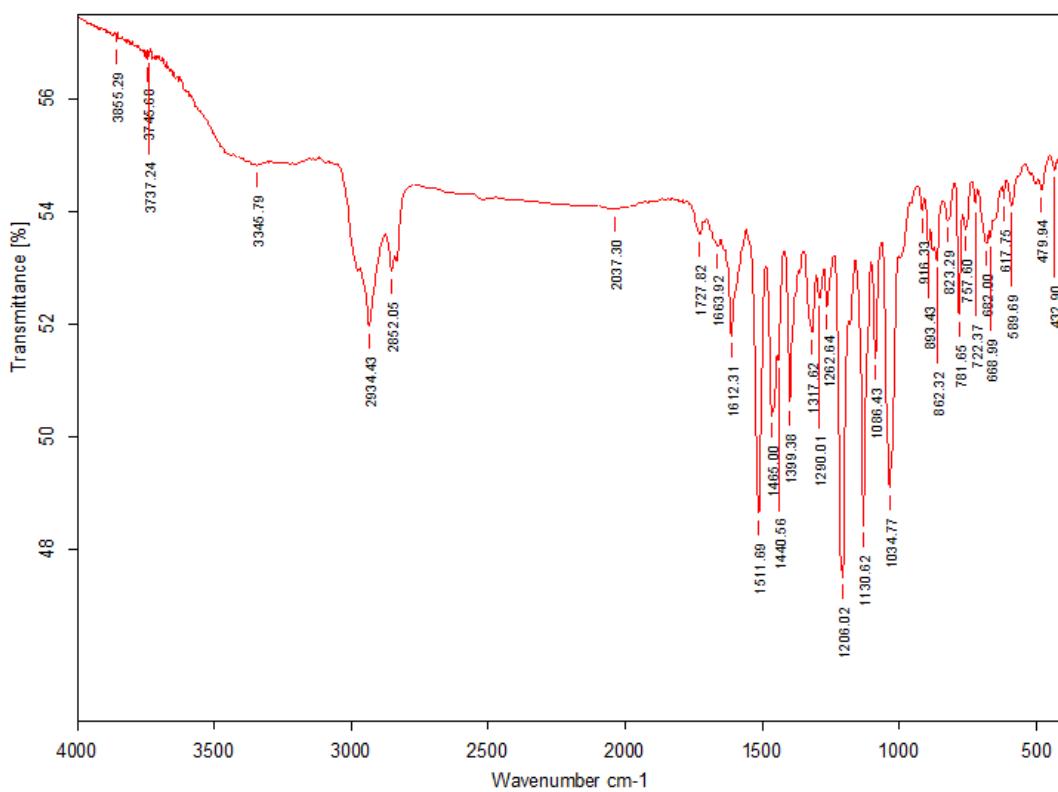


Figure S3. UV spectrum of **1** (**1a/1b**)

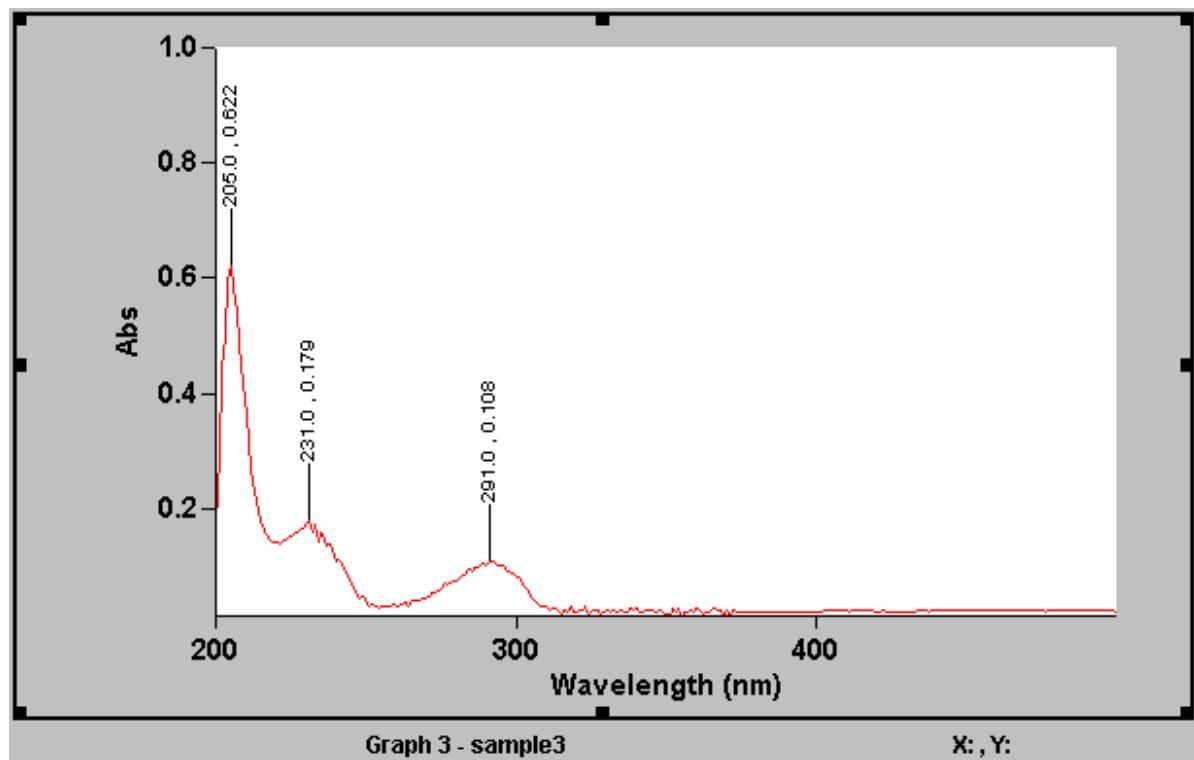


Figure S4. ^1H NMR spectrum of **1** (**1a/1b**) in CDCl_3

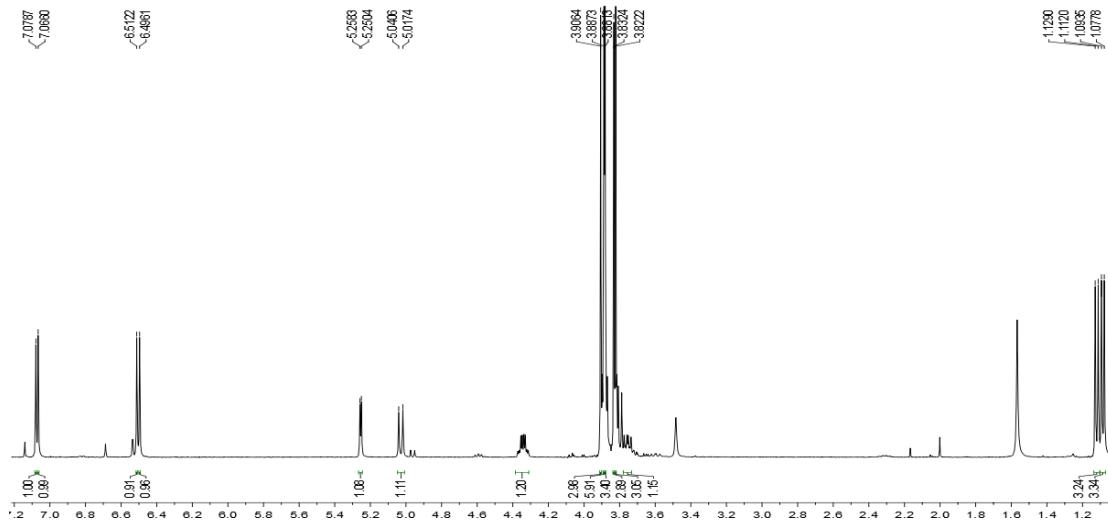


Figure S5. ^{13}C NMR spectrum of **1(1a/1b)** in CDCl_3

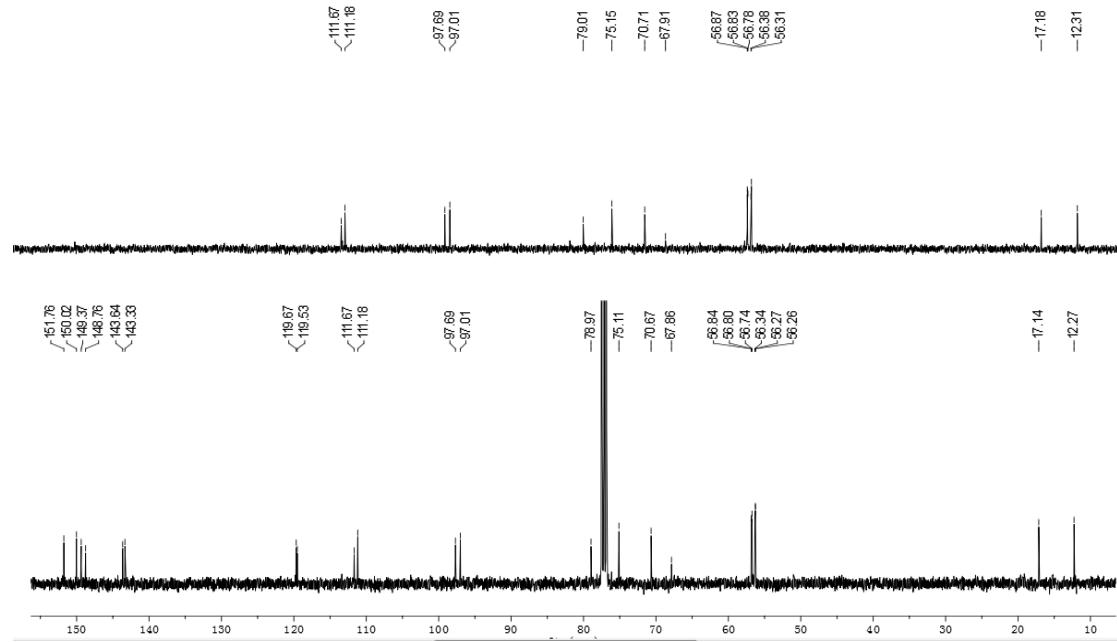


Figure S6. HSQC spectrum of **1 (1a/1b)** in CDCl_3

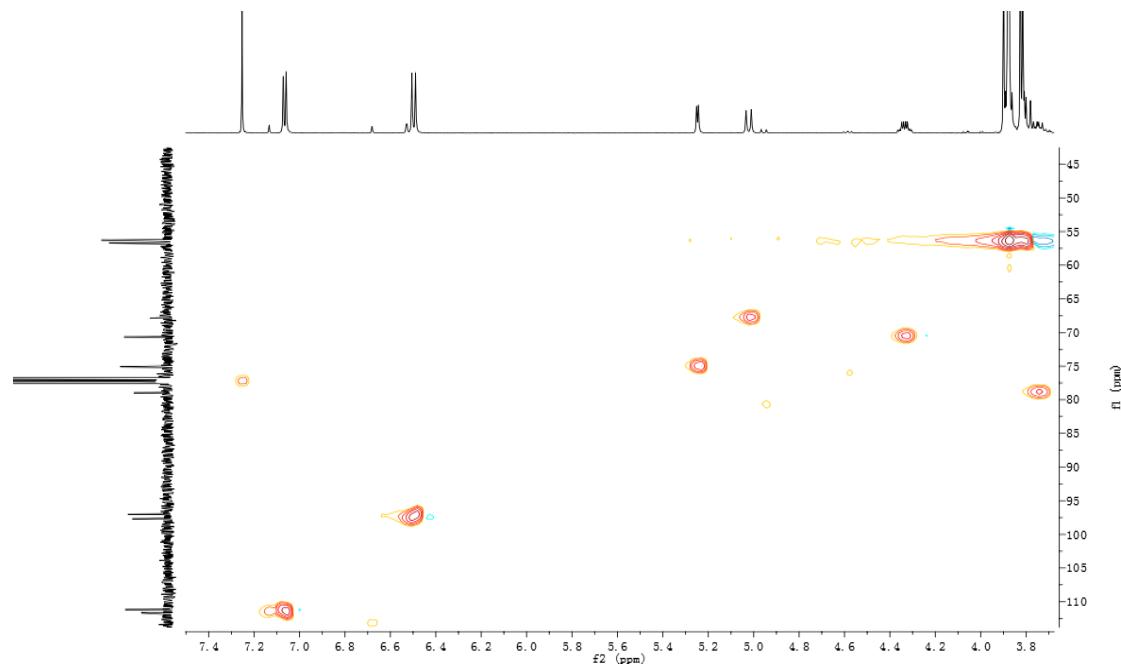


Figure S7. HMBC spectrum of **1** (**1a/1b**) in CDCl_3

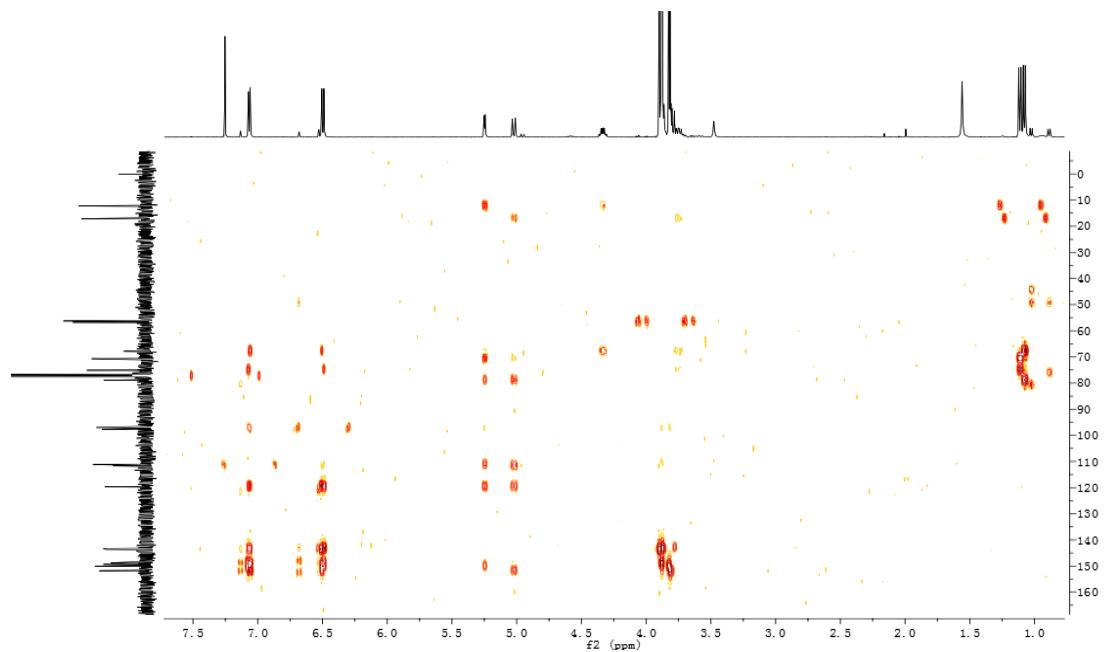


Figure S8. ^1H - ^1H COSY spectrum of **1** (**1a/1b**) in CDCl_3

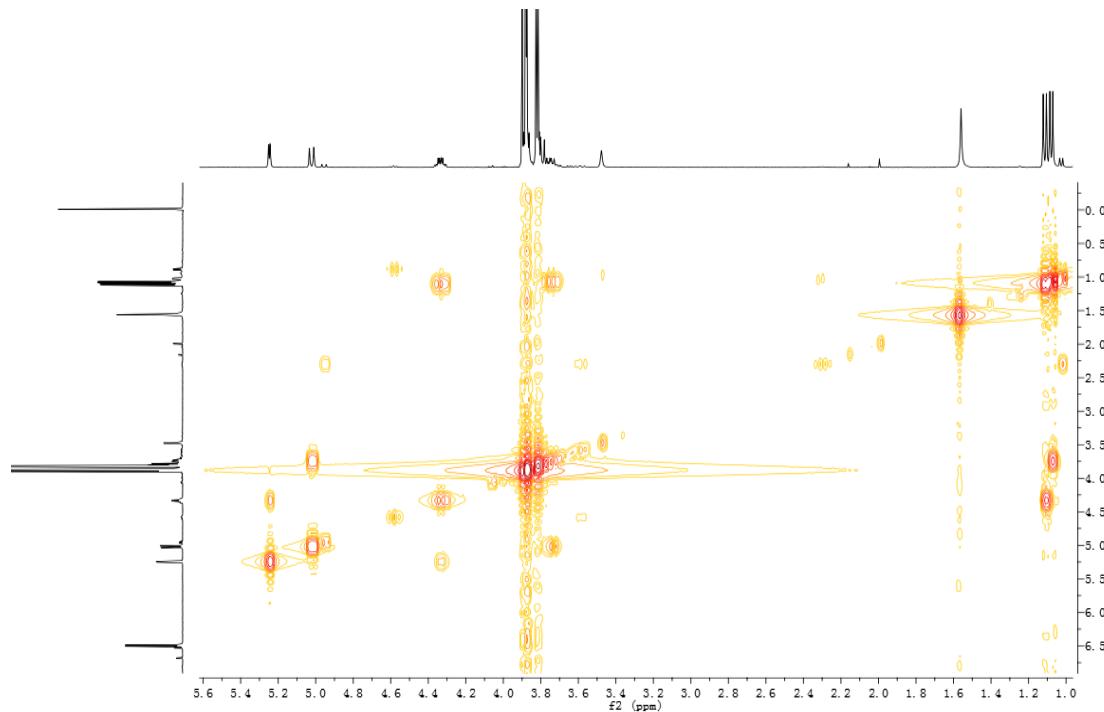


Figure S9. NOESY spectrum of **1** (**1a/1b**) in CDCl_3

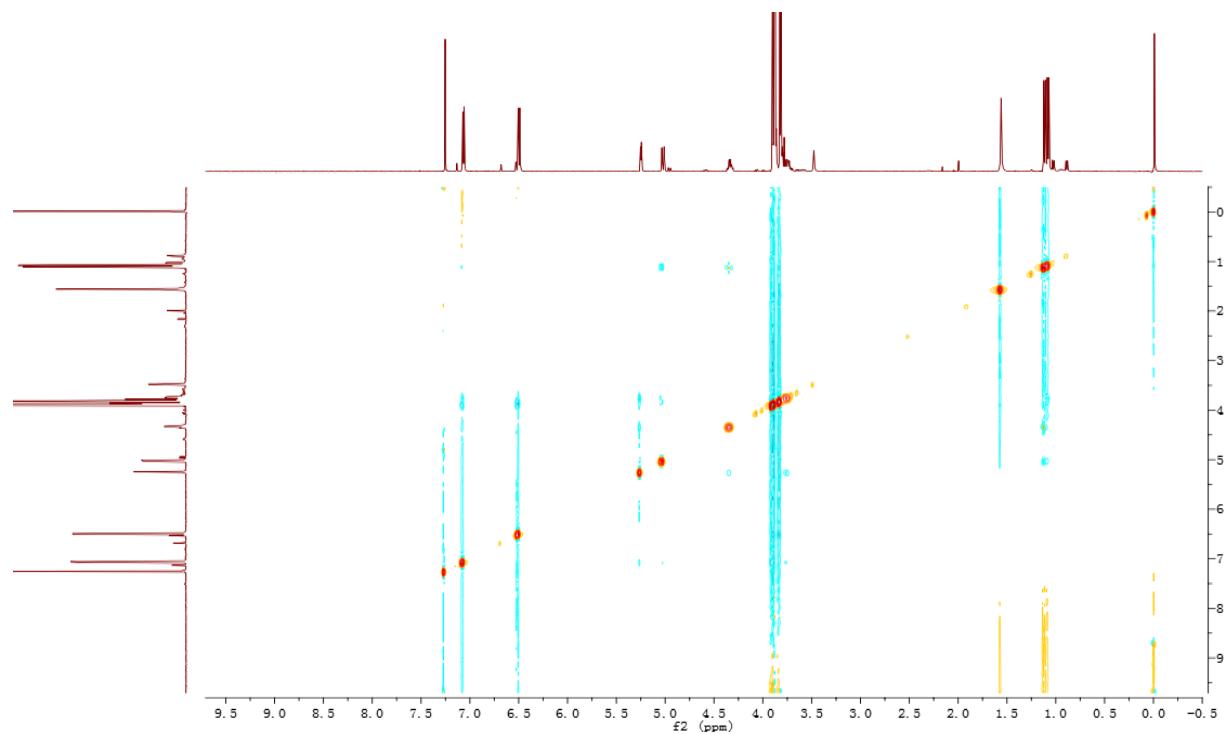


Figure S10. (+)-HR-ESI-MS spectrum of **2** (**2a/2b**)

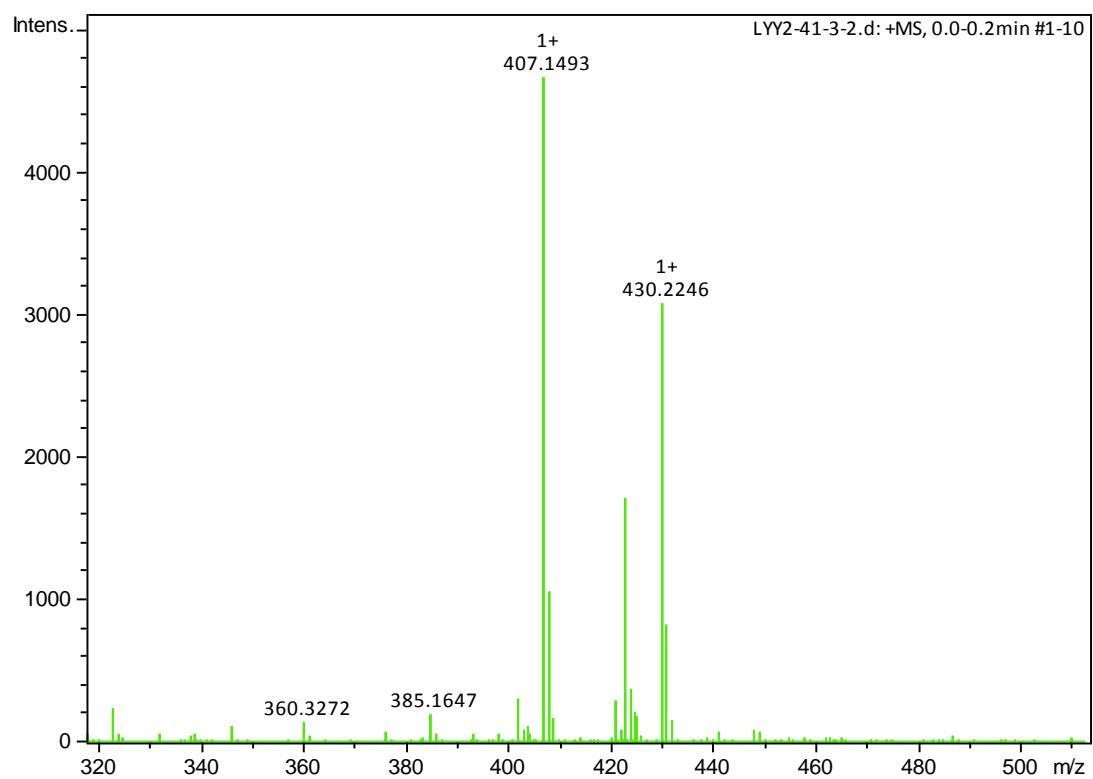


Figure S11. IR spectrum of **2** (2a/2b)

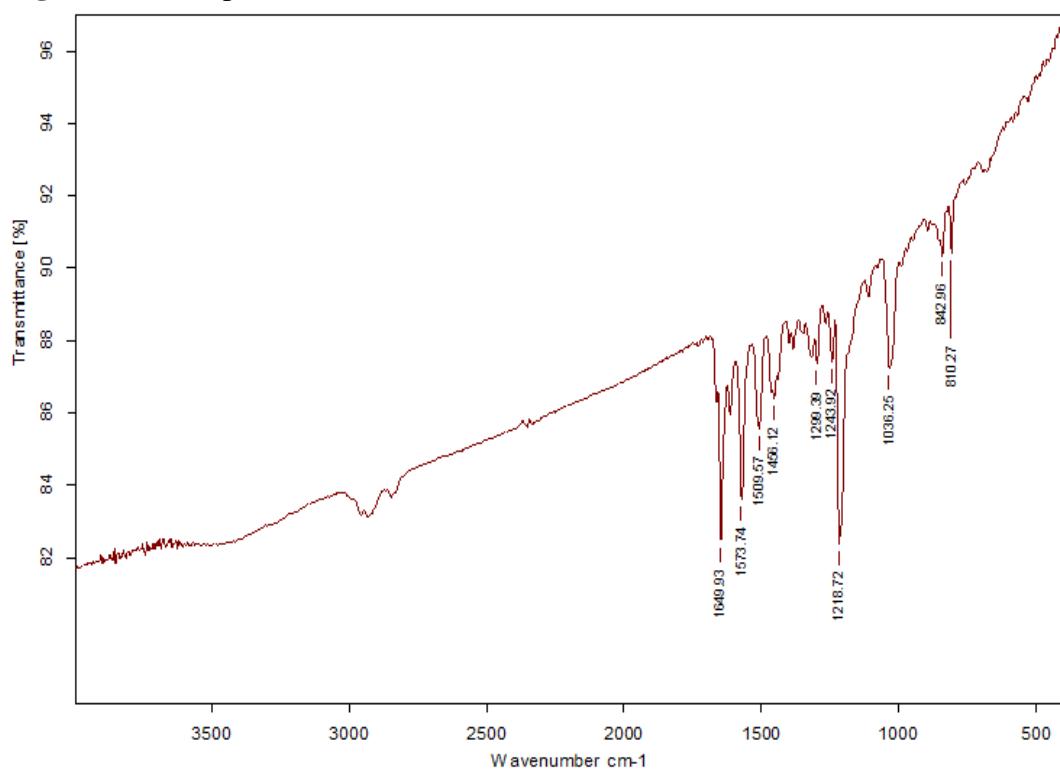


Figure S12. UV spectrum of **2** (2a/2b)

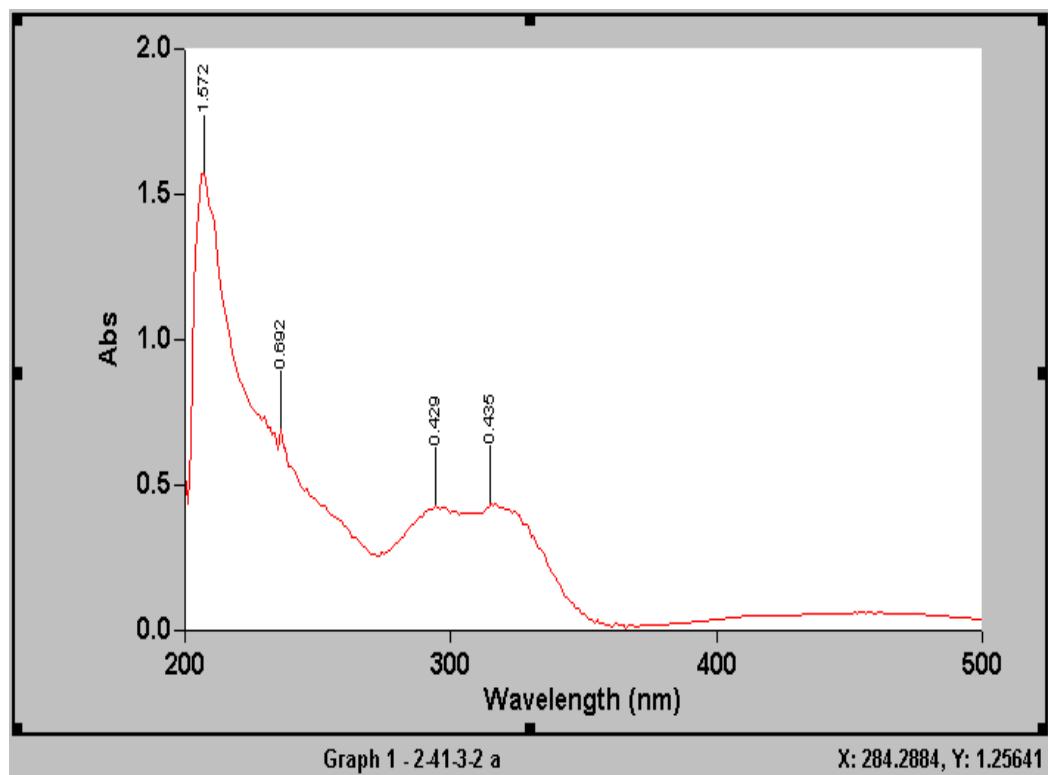


Figure S13. ^1H NMR spectrum of **2** (**2a/2b**) in CDCl_3

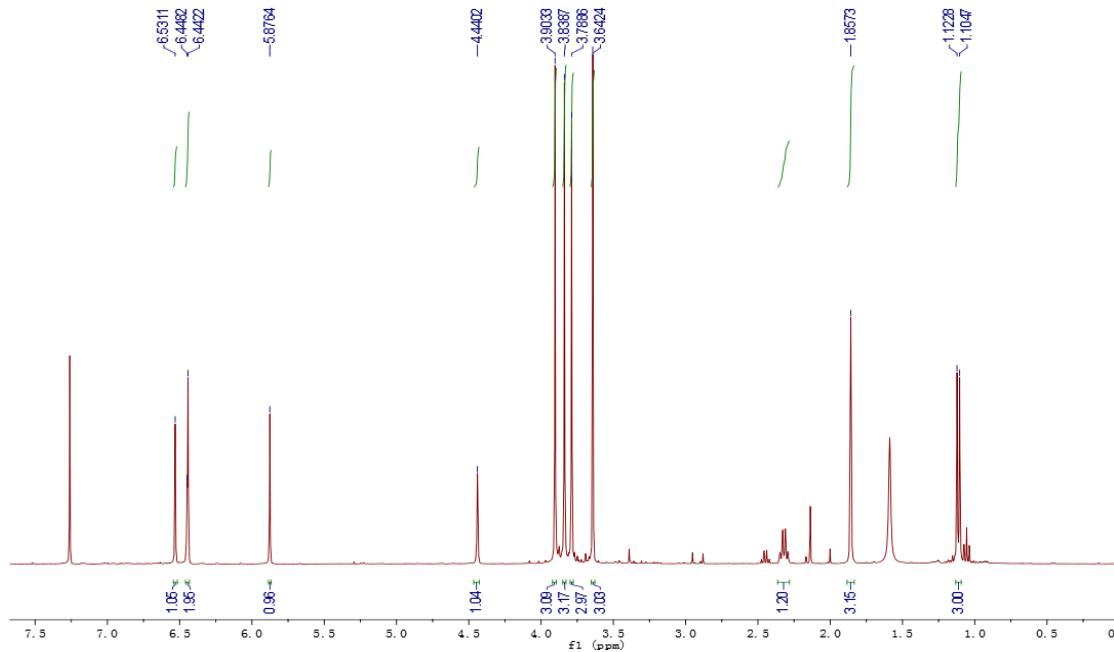


Figure S14. ^{13}C NMR spectrum of **2** (**2a/2b**) in CDCl_3

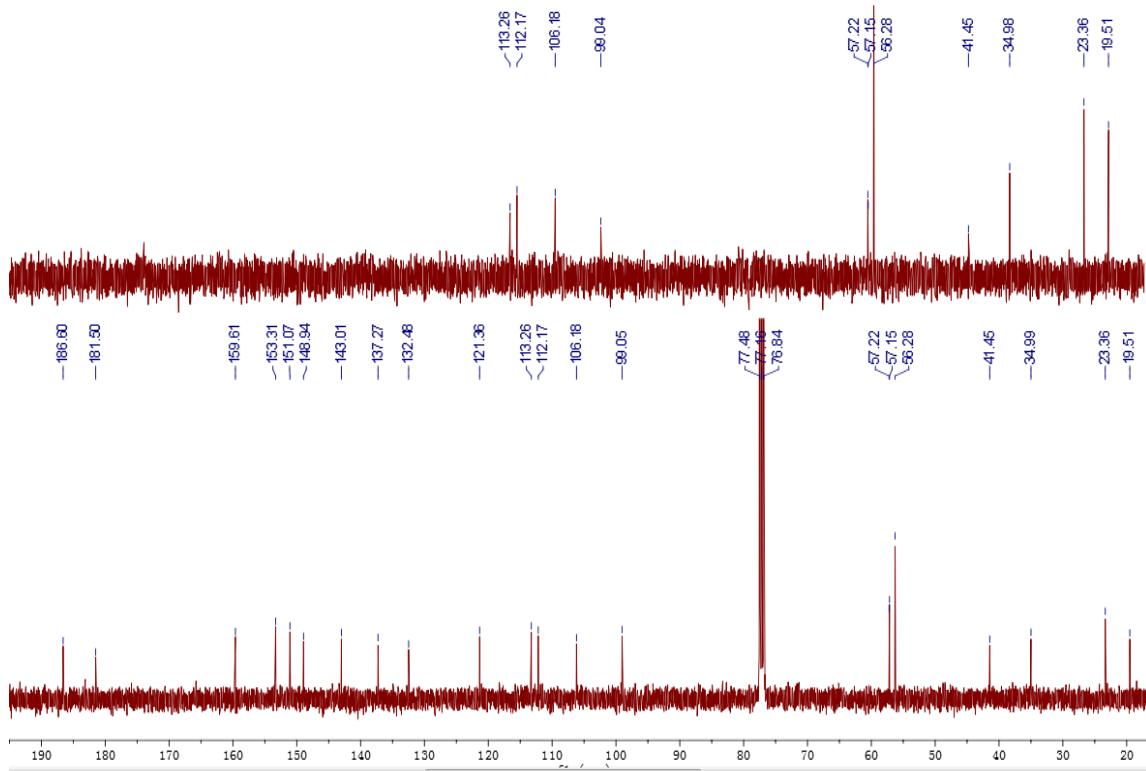


Figure S15. HSQC spectrum of **2** (**2a/2b**) in CDCl_3

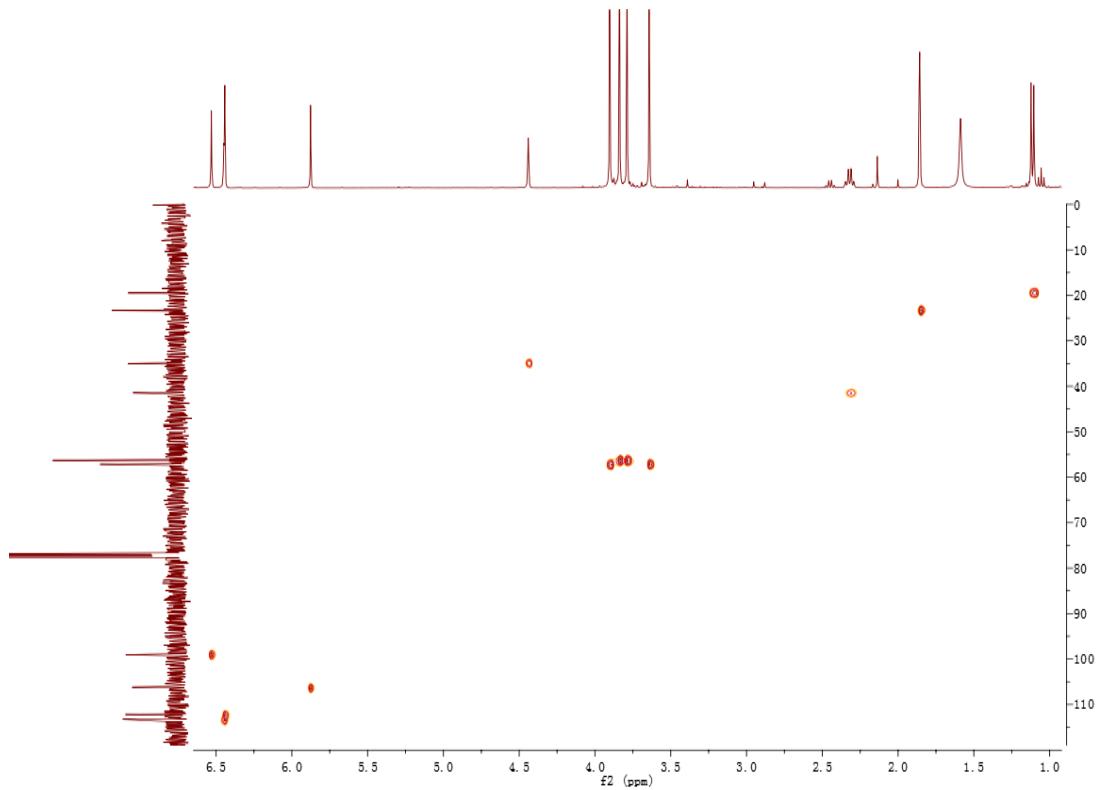


Figure S16. HMBC spectrum of **2** (**2a/2b**) in CDCl_3

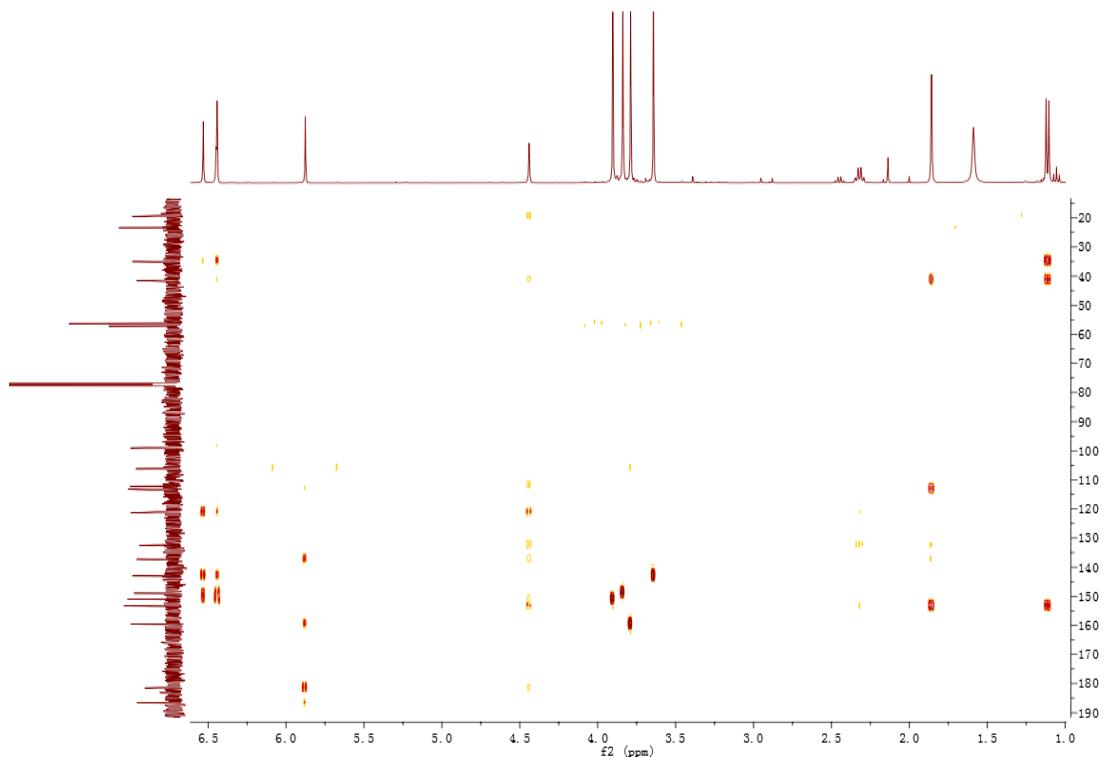


Figure S17. ^1H - ^1H COSY spectrum of **2** (**2a/2b**) in CDCl_3

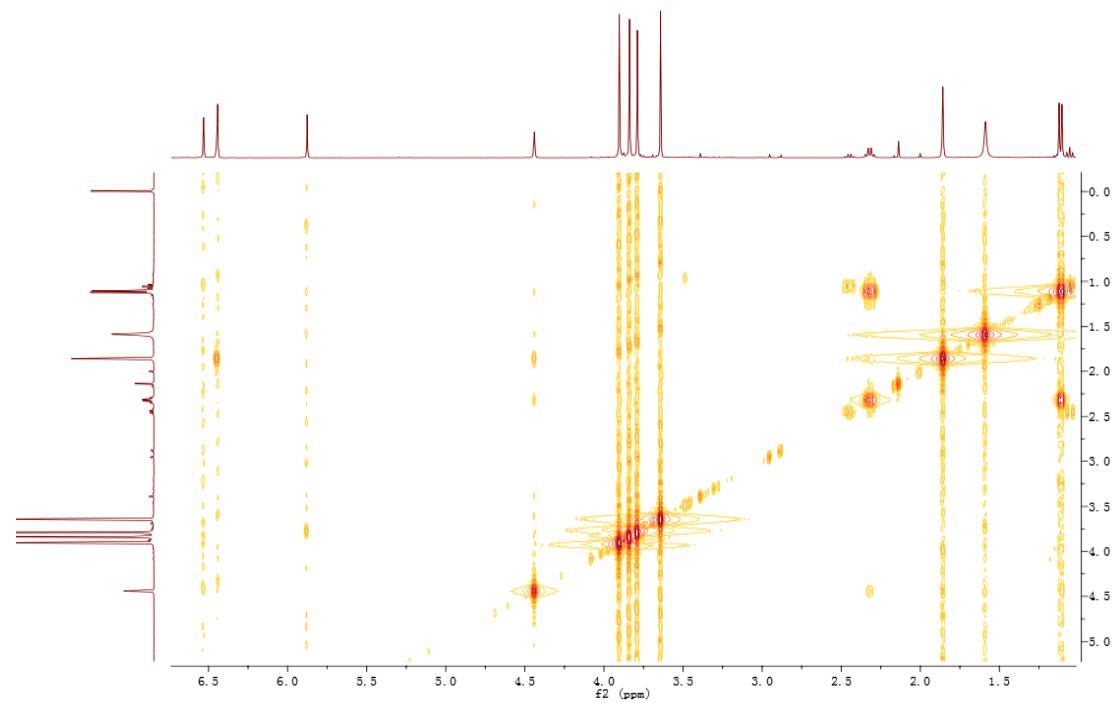


Figure S18. NOESY spectrum of **2** (**2a/2b**) in CDCl_3

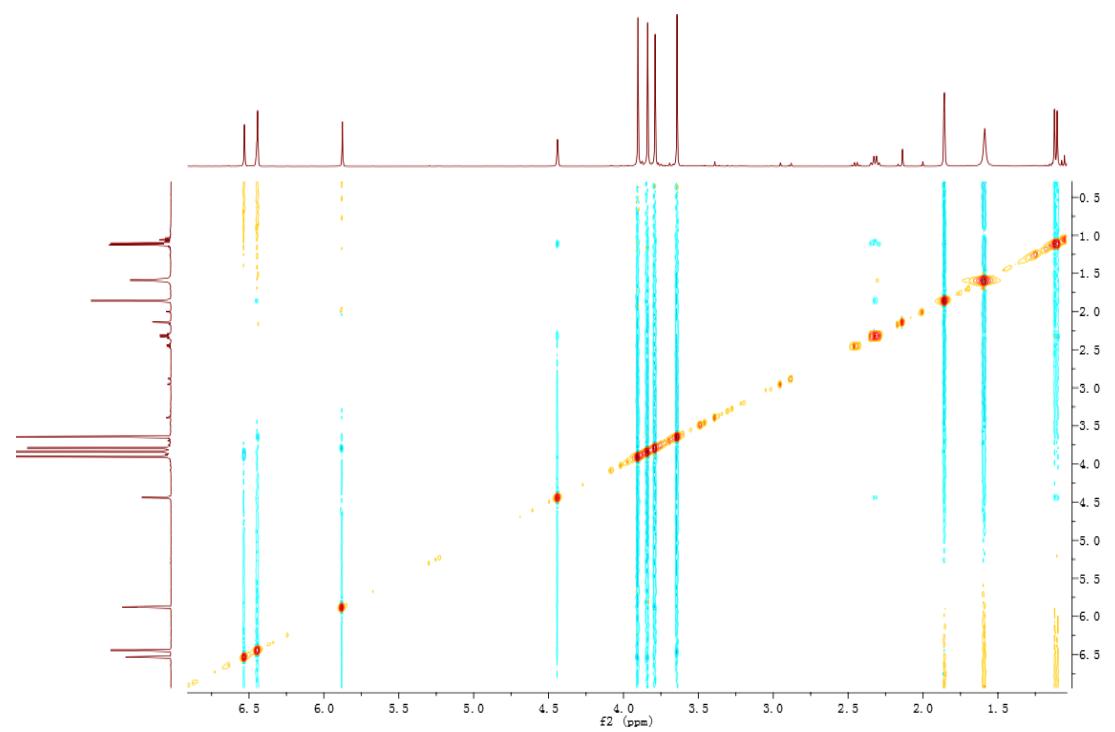


Figure S19. (+)-HR-ESI-MS spectrum of **3** (**3a/3b**)

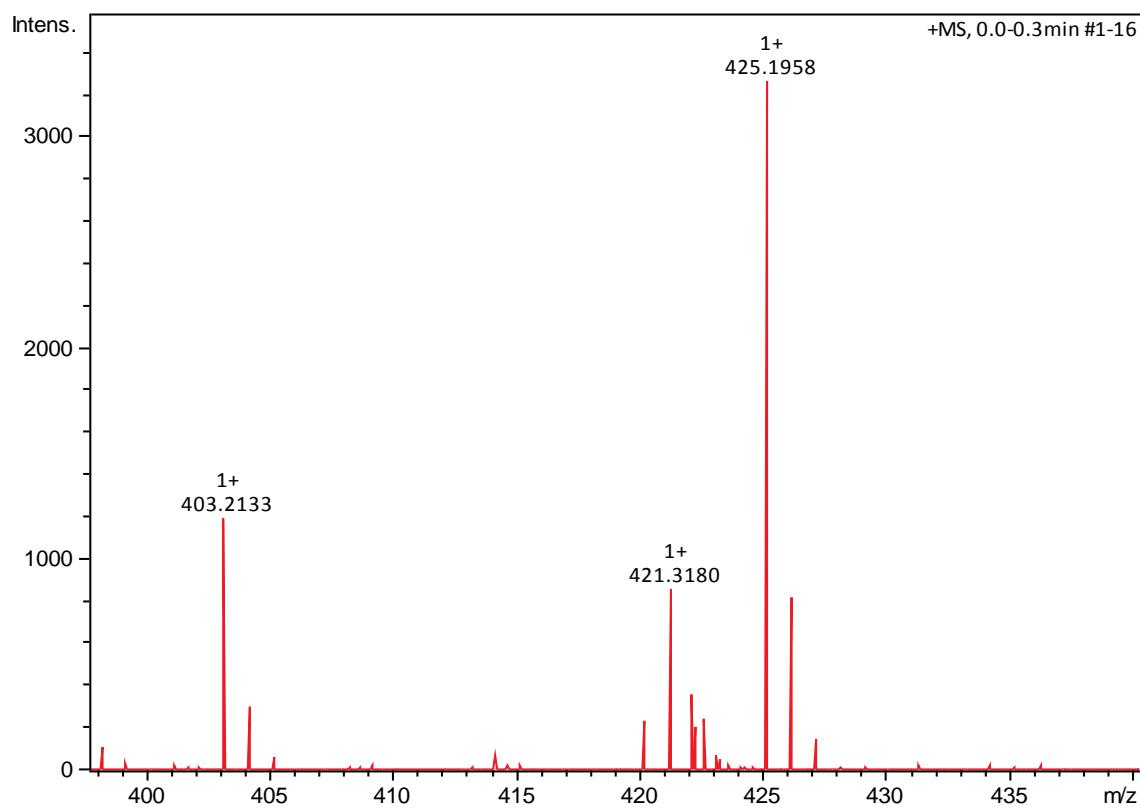


Figure S20. IR spectrum of **3** (**3a/3b**)

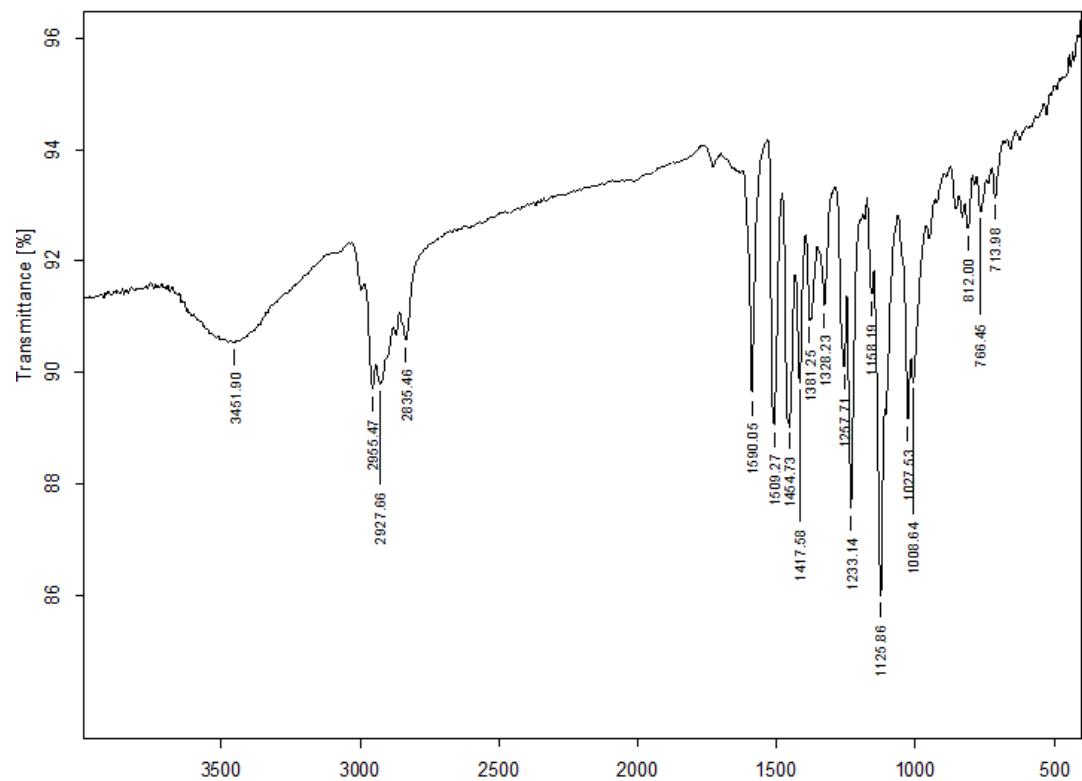


Figure S21. UV spectrum of **3** (**3a/3b**)

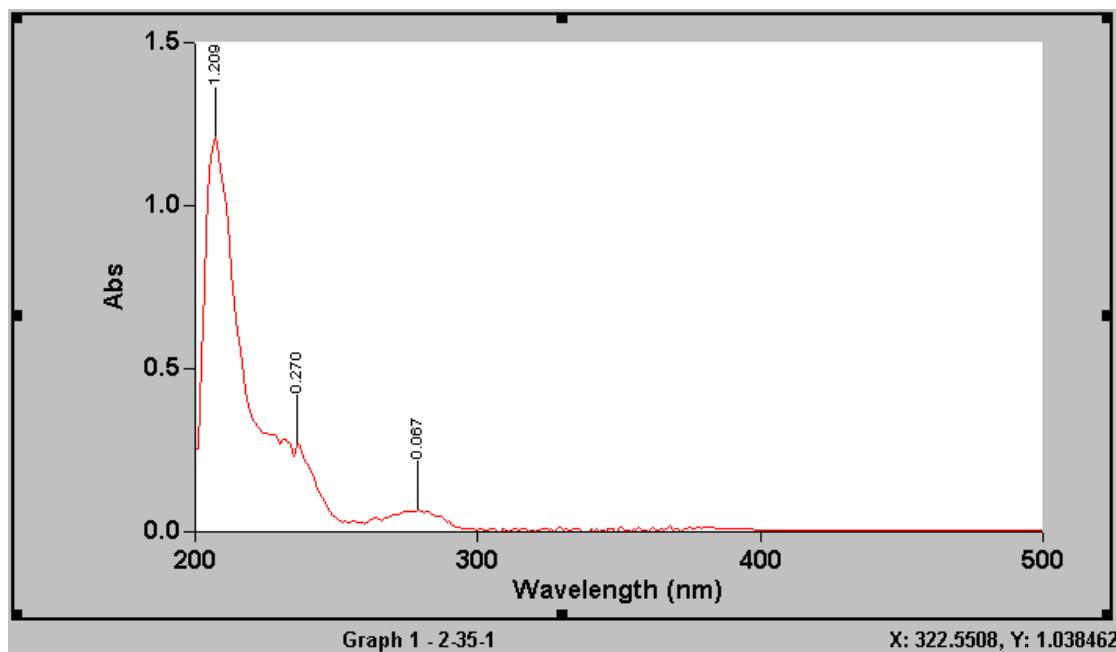


Figure S22. ^1H NMR spectrum of **3** (**3a/3b**) in CD_3OD

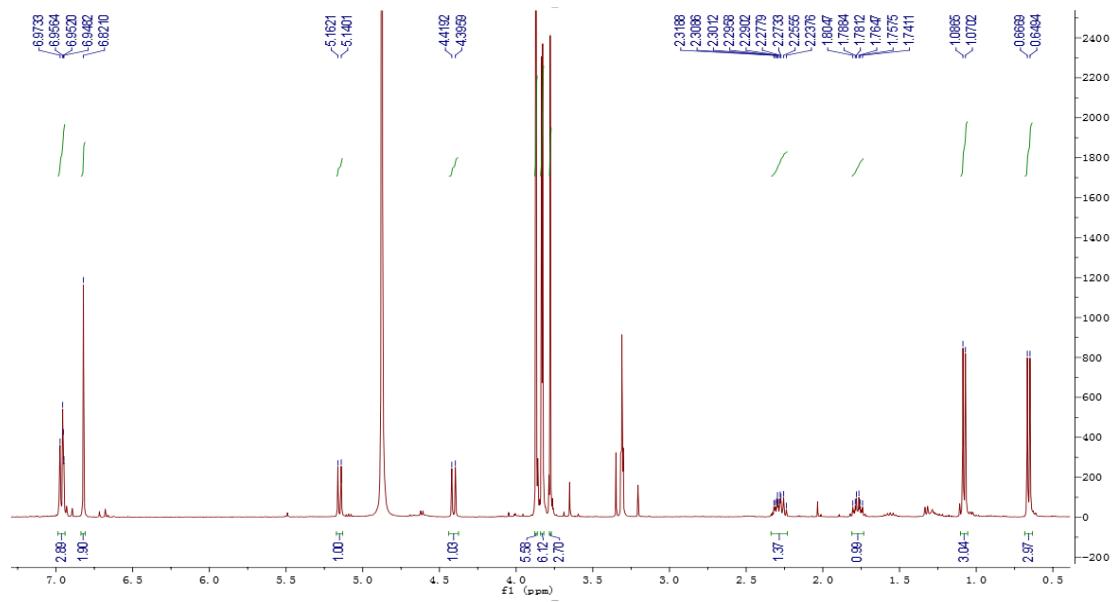


Figure S23. ^{13}C NMR spectrum of **3** (**3a/3b**) in CD_3OD

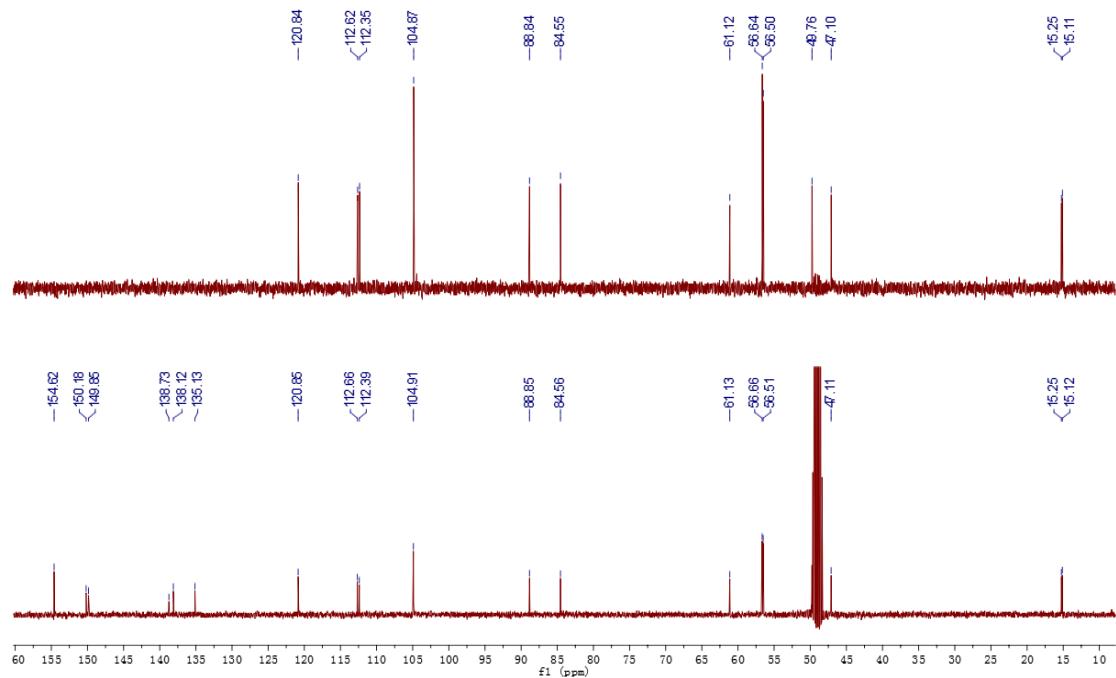


Figure S24. HSQC spectrum of **3** (**3a/3b**) in CD_3OD

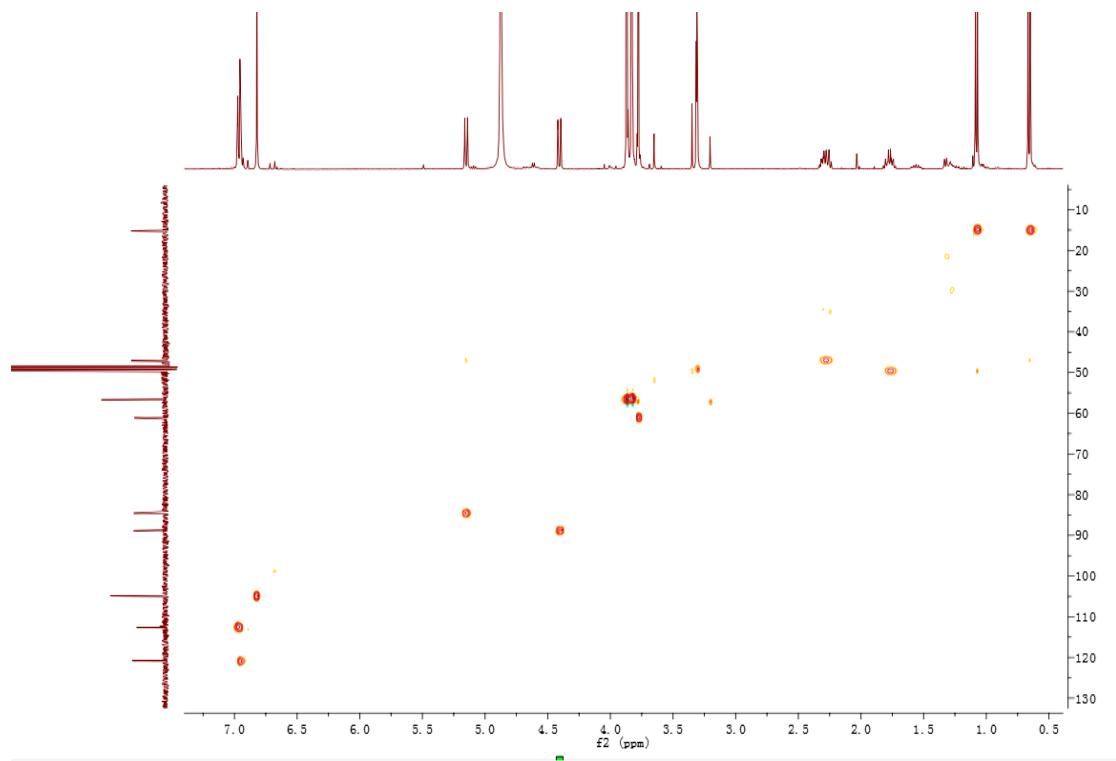


Figure S25. HMBC spectrum of **3** (**3a/3b**) in CD₃OD

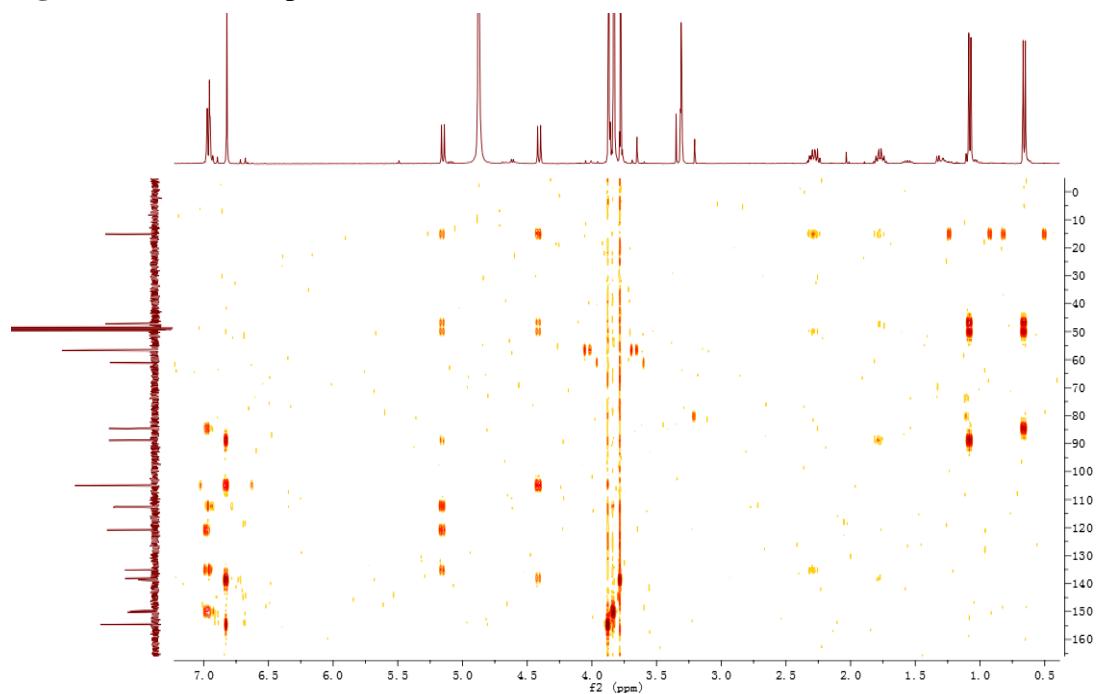


Figure S26. ^1H - ^1H COSY spectrum of **3** (**3a/3b**) in CD₃OD

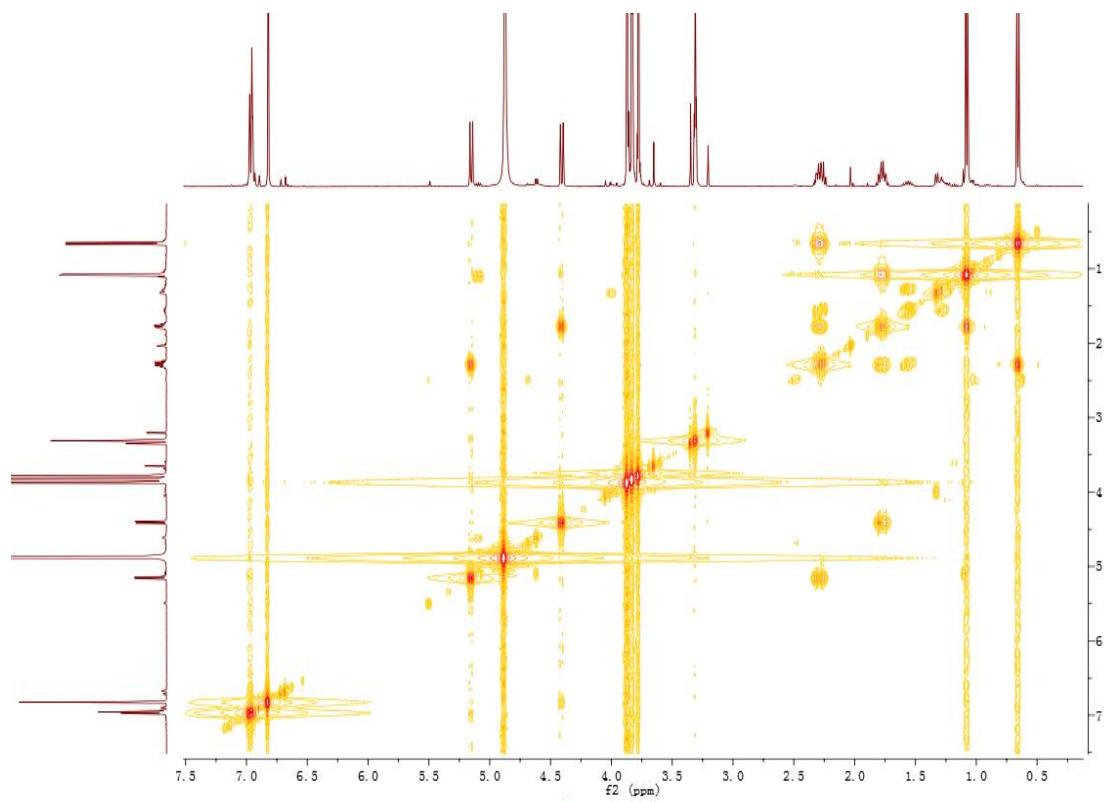


Figure S27. NOESY spectrum of **3** (**3a/3b**) in CD₃OD

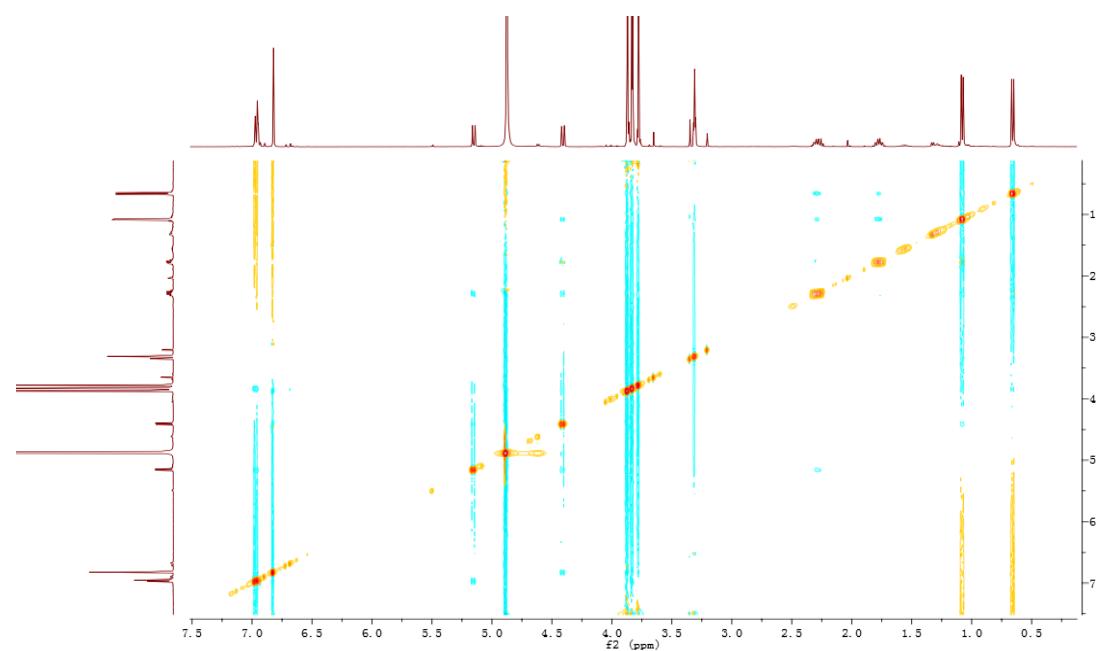


Figure S28. (+)-HR-ESI-MS spectrum of **4**

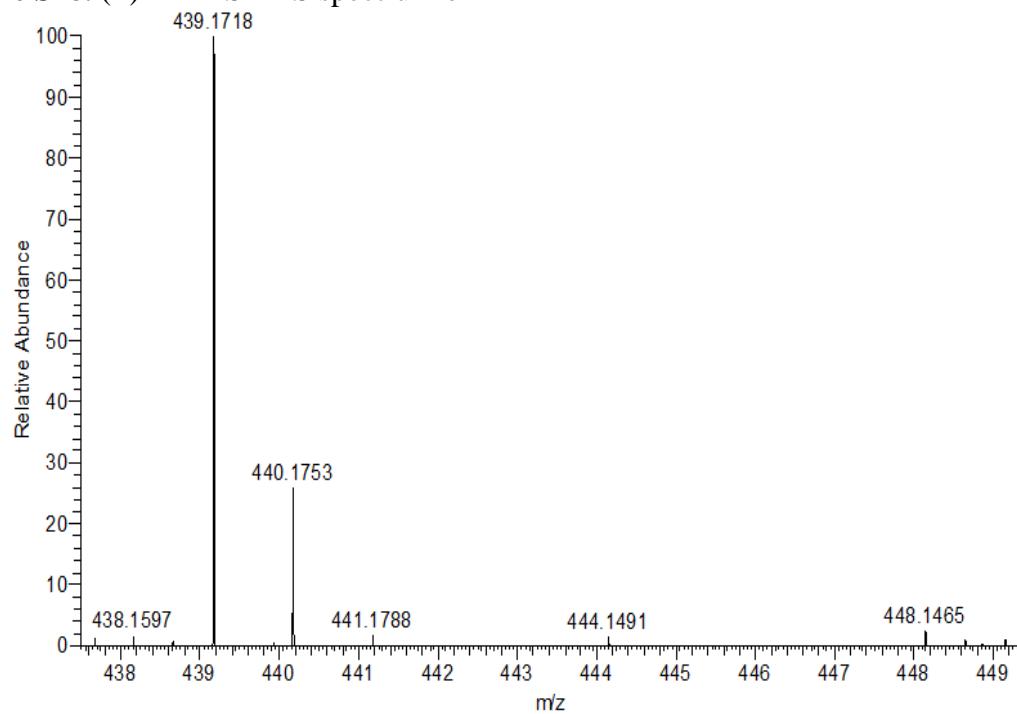


Figure S29. IR spectrum of 4

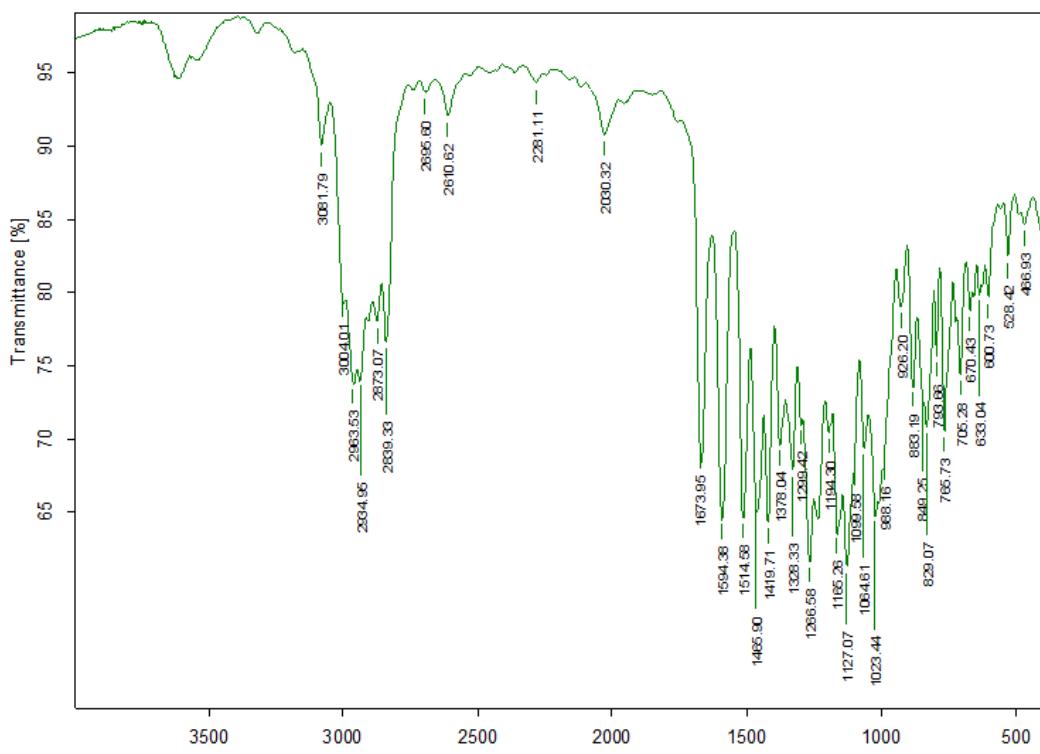


Figure S30. UV spectrum of 4

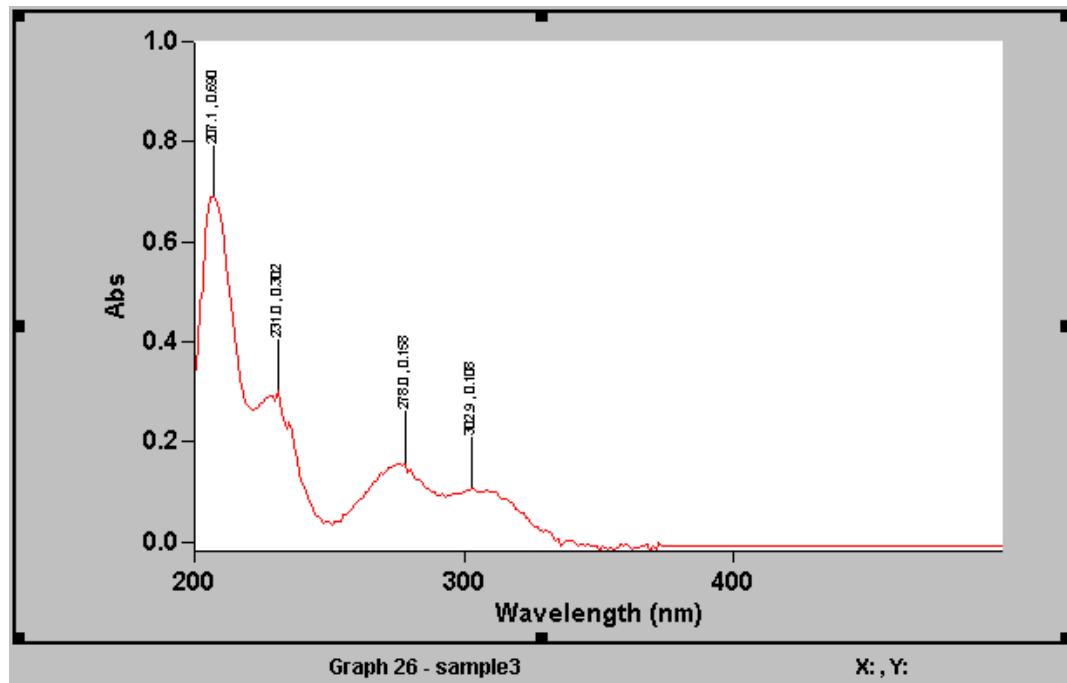


Figure S31. ^1H NMR spectrum of **4** in CDCl_3

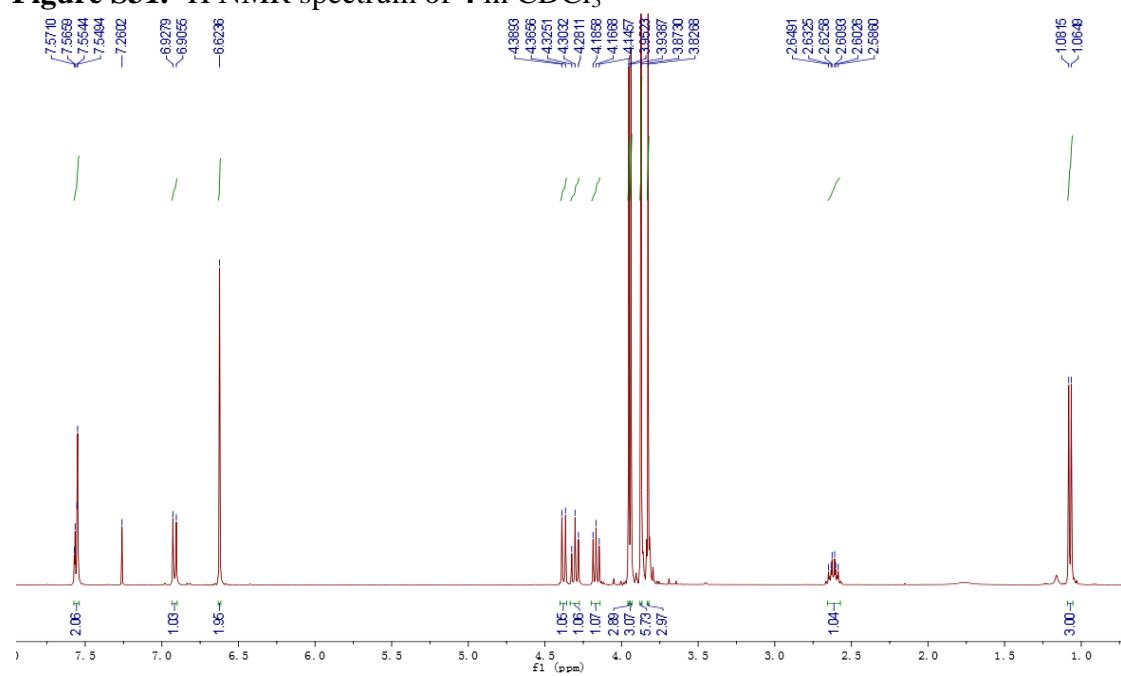


Figure S32. ^{13}C NMR spectrum of **4** in CDCl_3

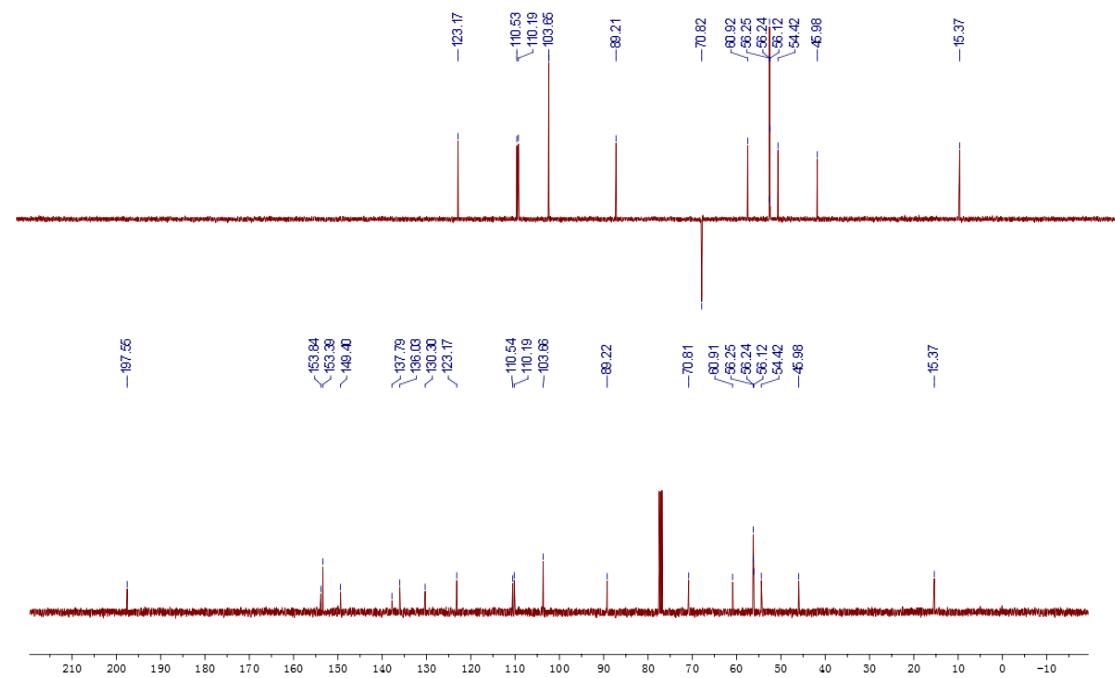


Figure S33. HSQC spectrum of **4** in CDCl_3

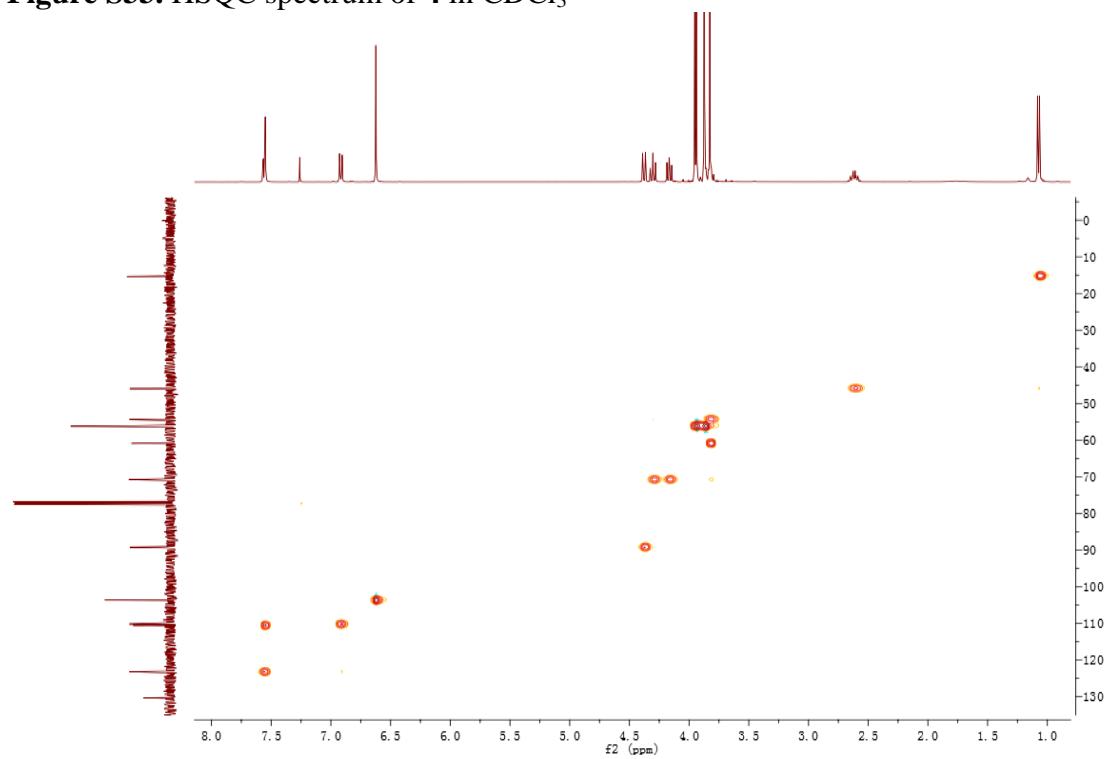


Figure S34. HMBC spectrum of **4** in CDCl_3

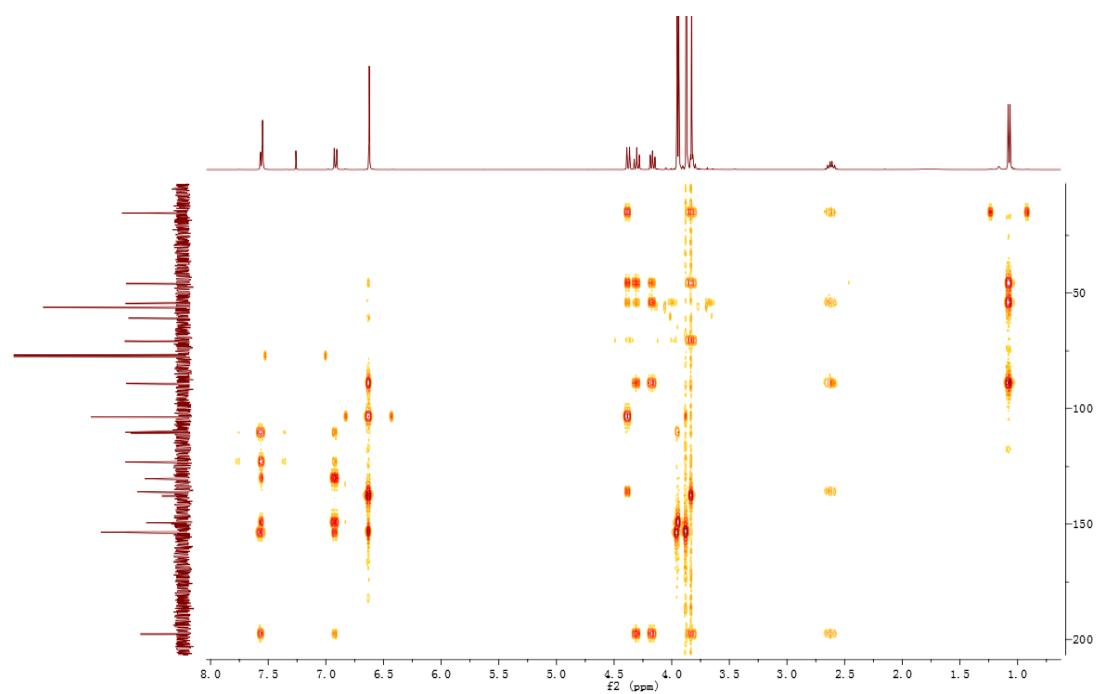


Figure S35. ^1H - ^1H COSY spectrum of **4** in CDCl_3

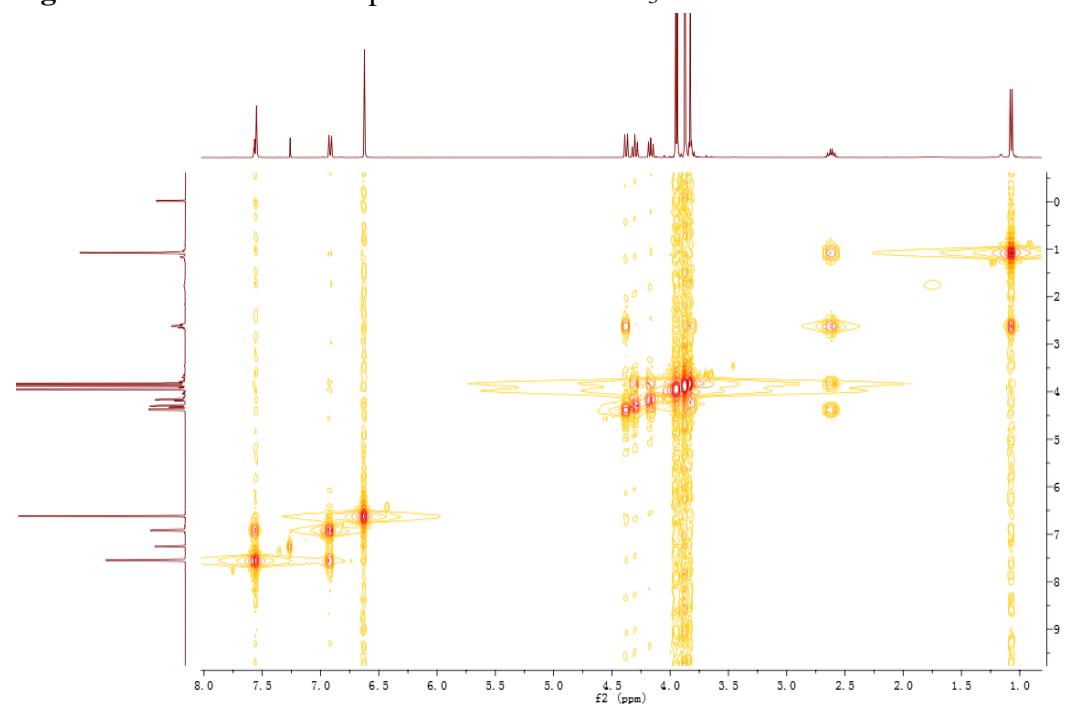


Figure S36. NOESY spectrum of **4** in CDCl_3

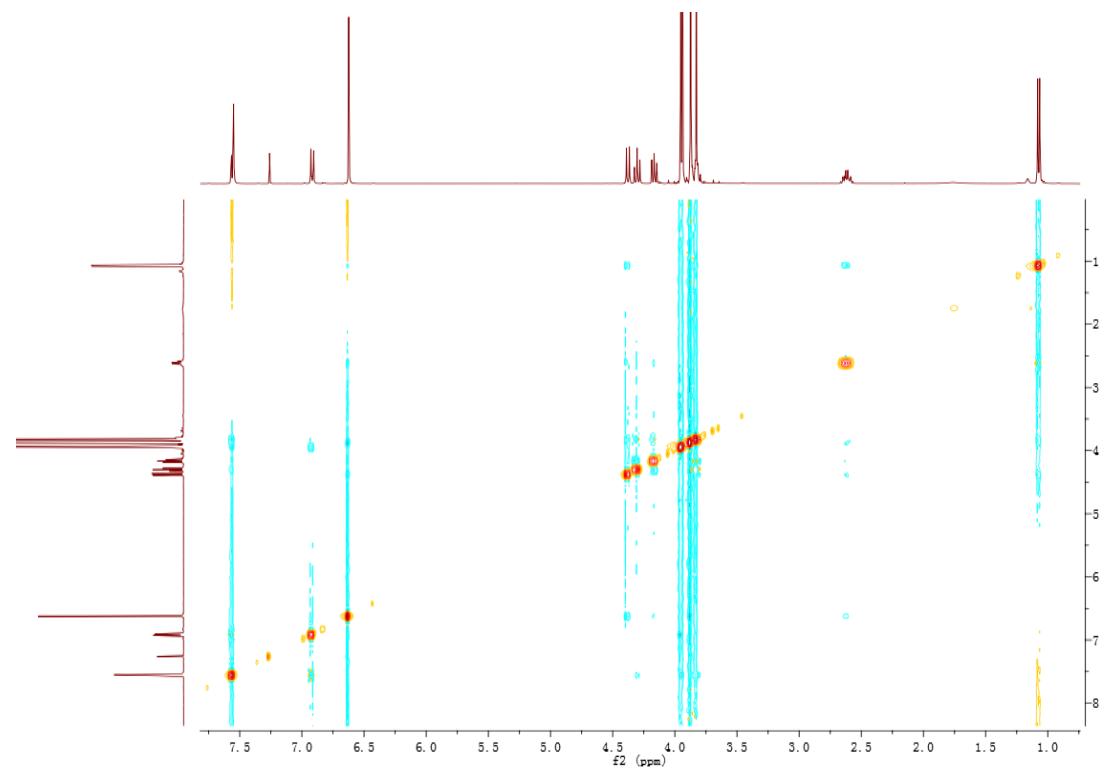


Figure S37. ECD spectrum of **4** in MeOH

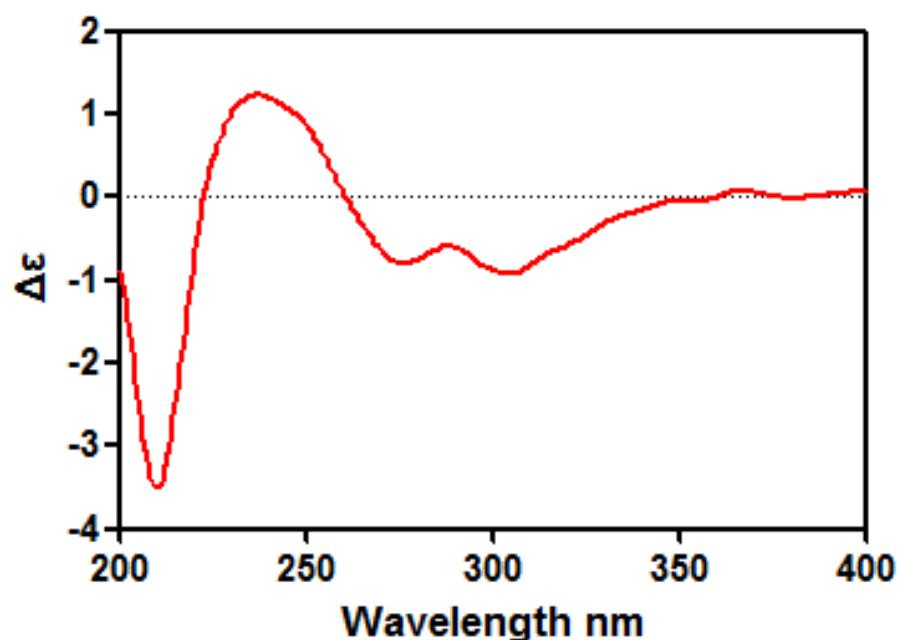


Figure S38. (+)-HR-ESI-MS spectrum of **5**

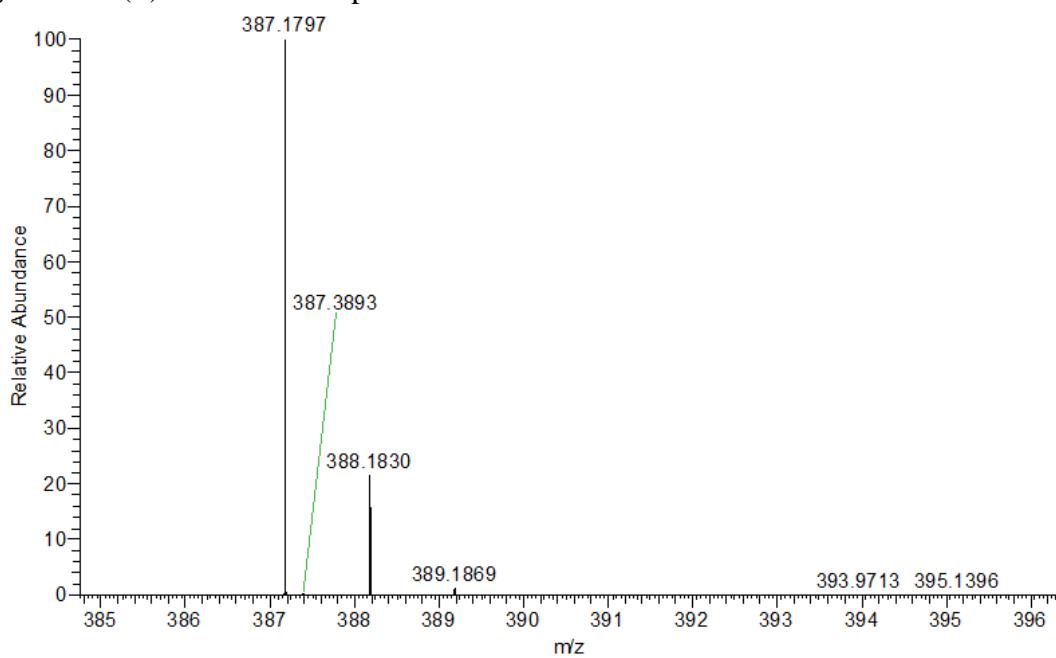


Figure S39. IR spectrum of **5**

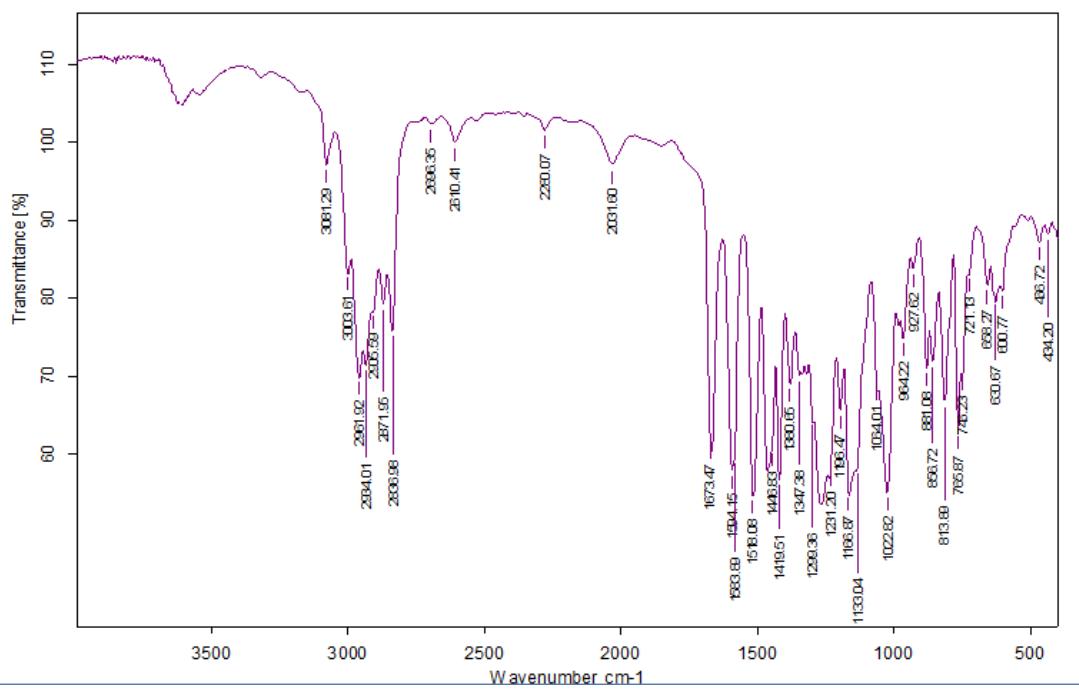


Figure S40. UV spectrum of **5**

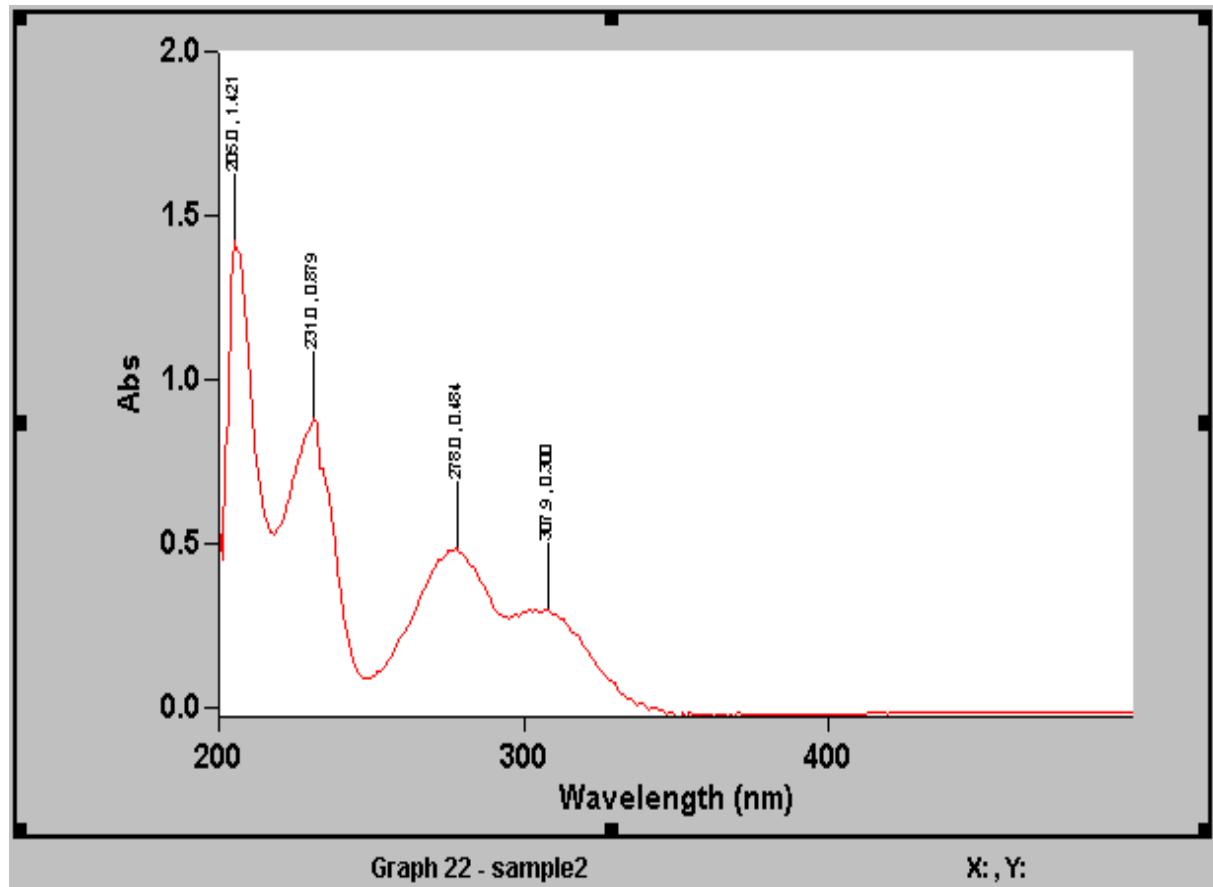


Figure S41. ^1H NMR spectrum of **5** in CD_3OD

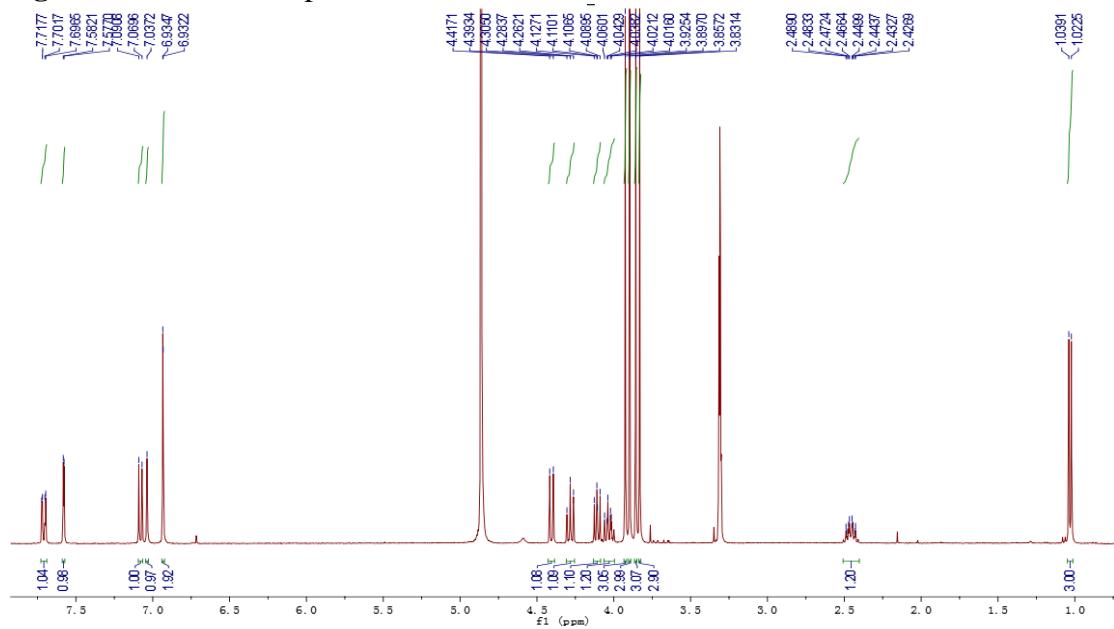


Figure S42. ^{13}C NMR spectrum of **5** in CD_3OD

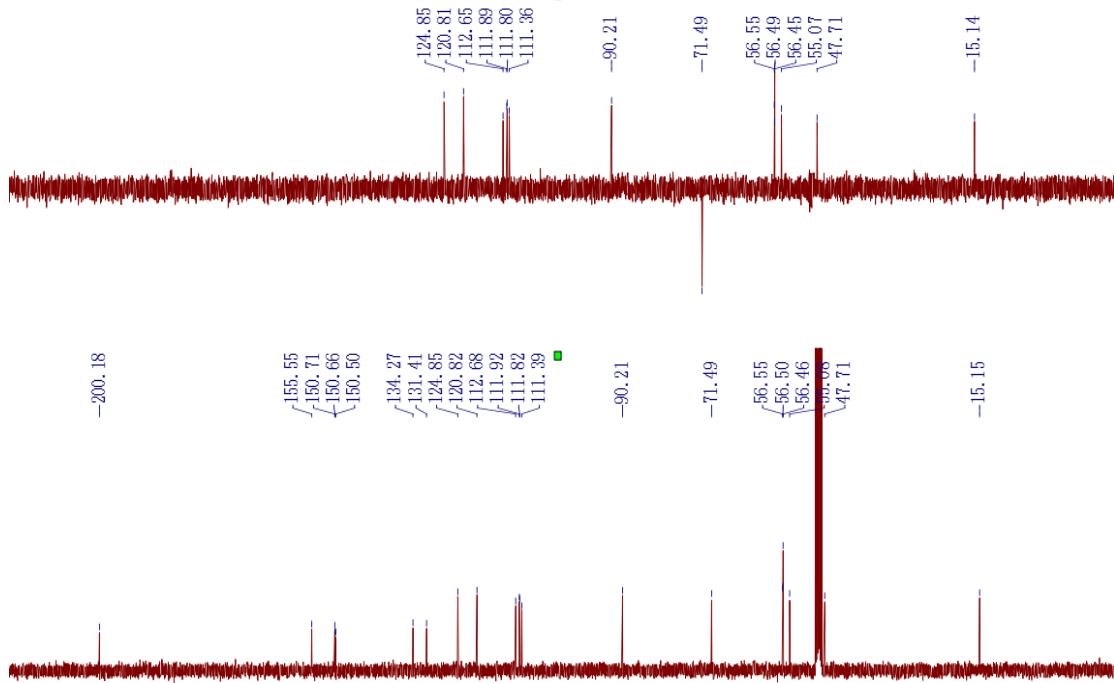


Figure S43. HSQC spectrum of **5** in CD₃OD

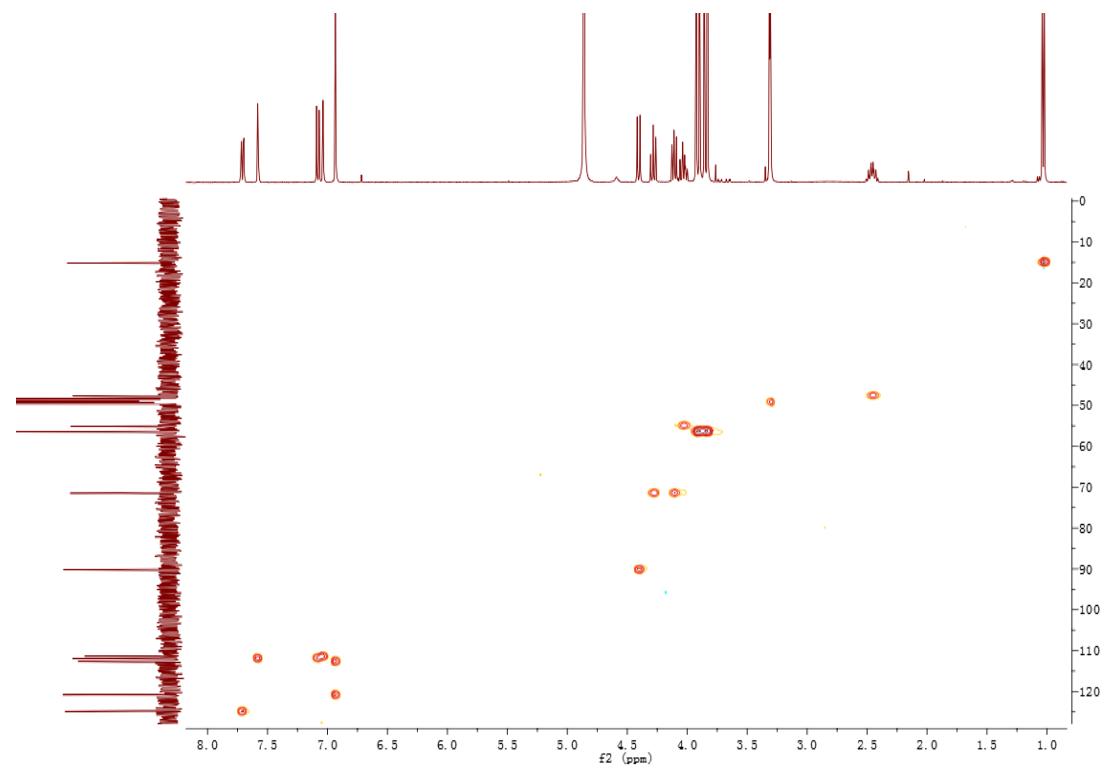


Figure S44. HMBC spectrum of **5** in CD₃OD

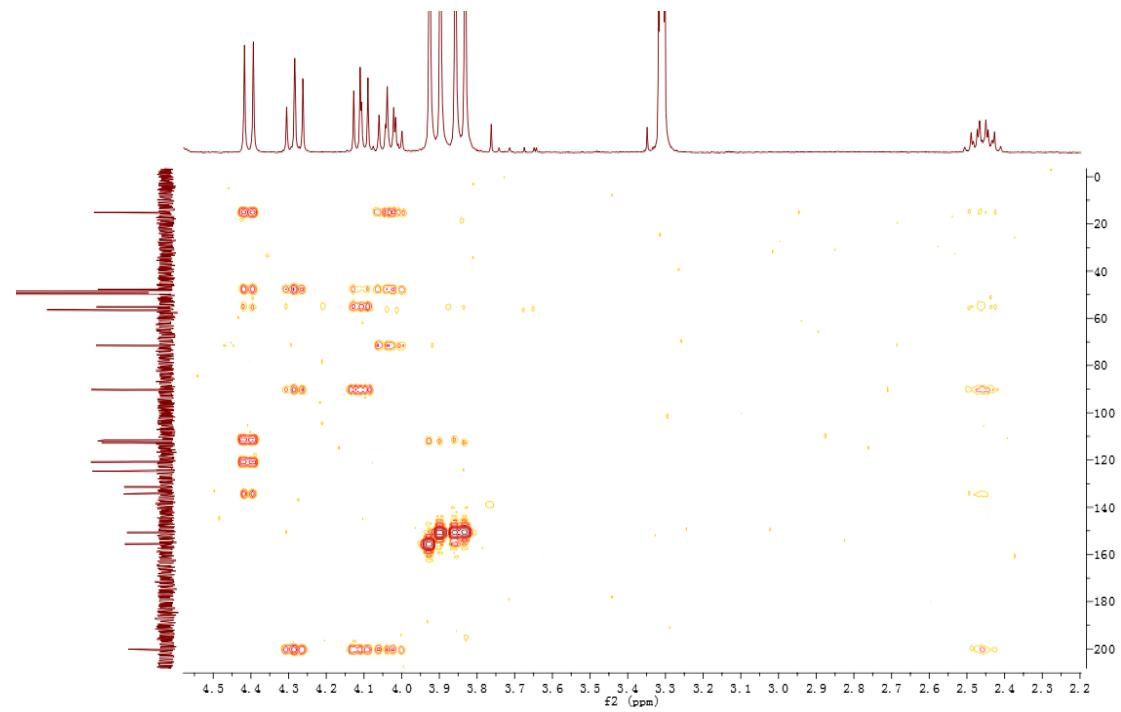


Figure S45. ^1H - ^1H COSY spectrum of **5** in CD_3OD

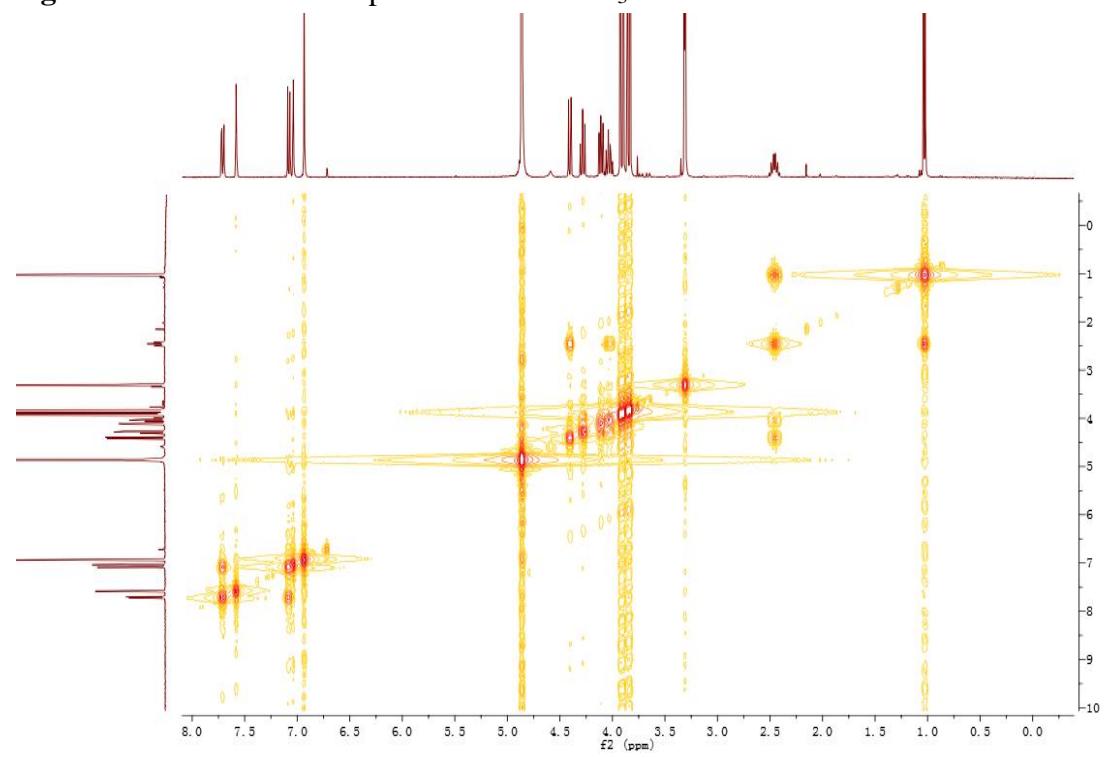


Figure S46. NOSEY spectrum of **5** in CD_3OD

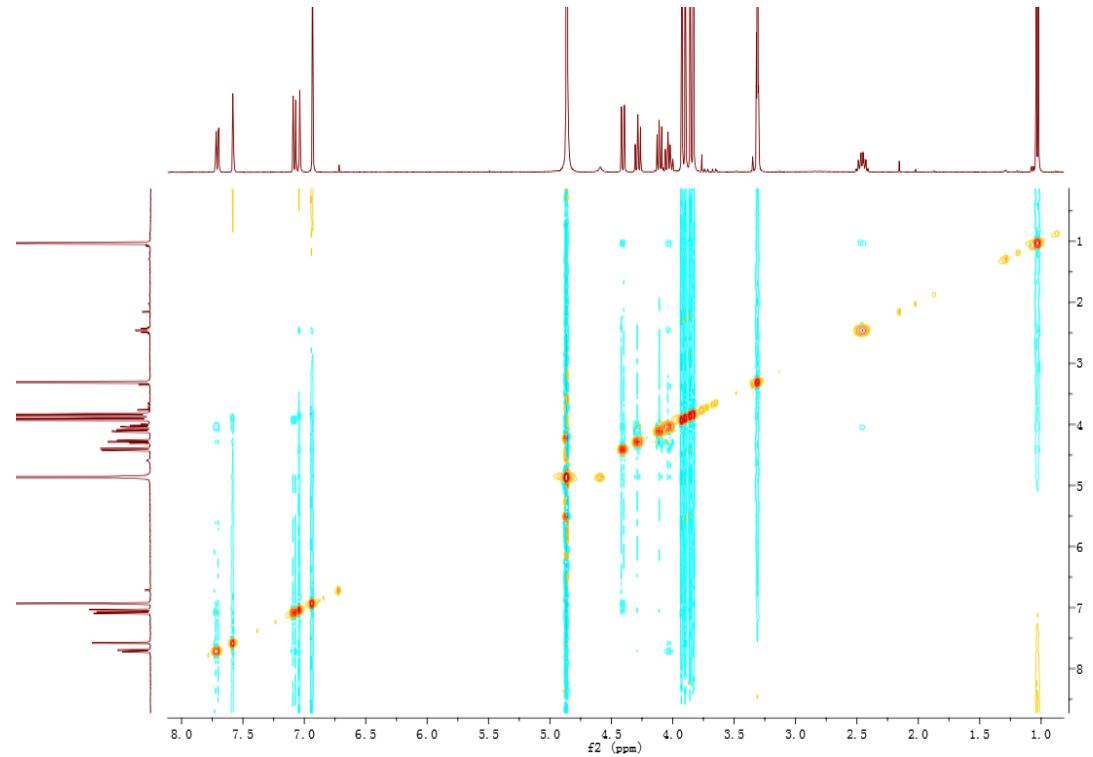


Figure S47. ECD spectrum of **5** in MeOH

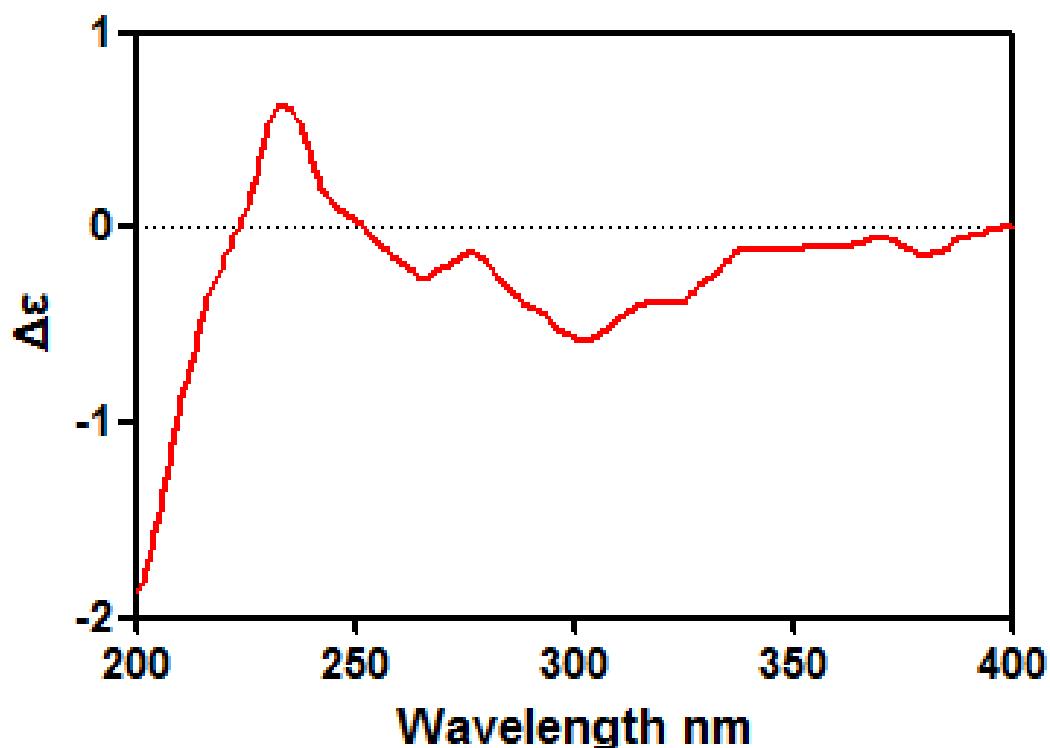


Figure S48. (+)-HR-ESI-MS spectrum of **6**

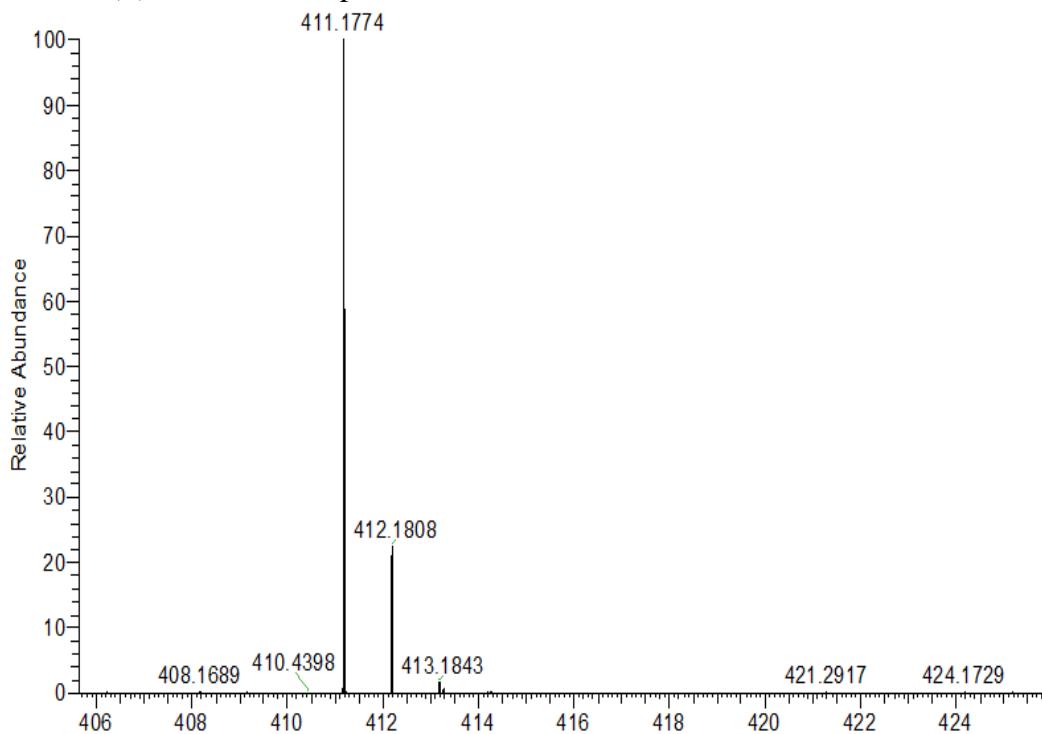


Figure S49. IR spectrum of **6** (**6a/6b**)

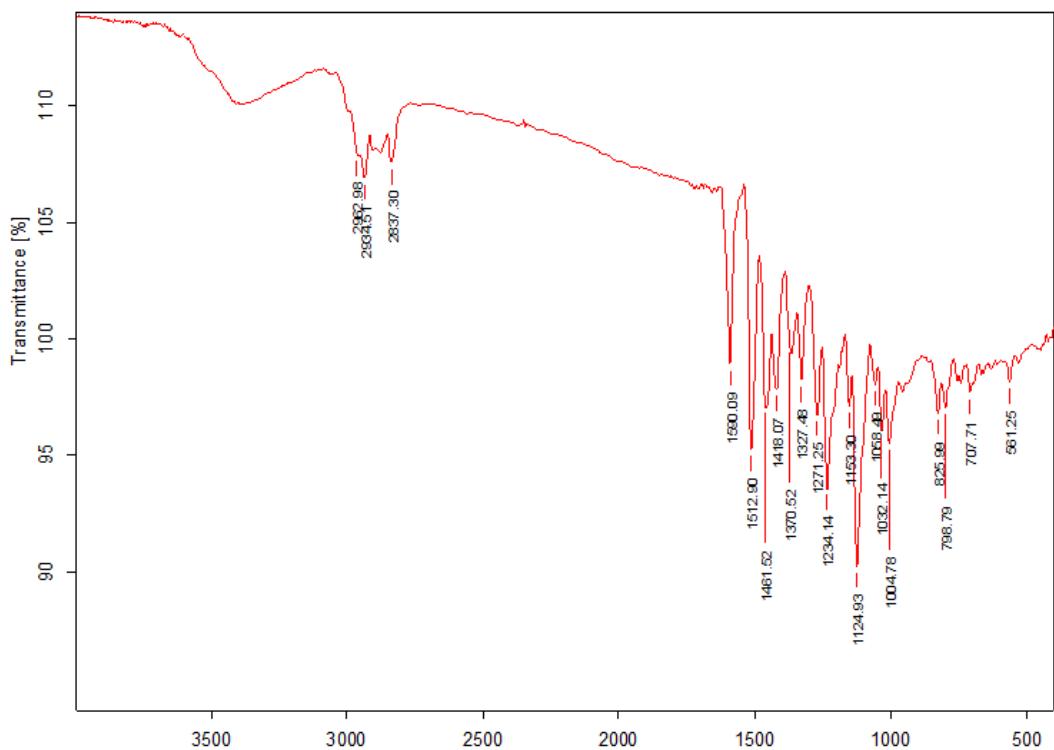


Figure S50. UV spectrum of **6**

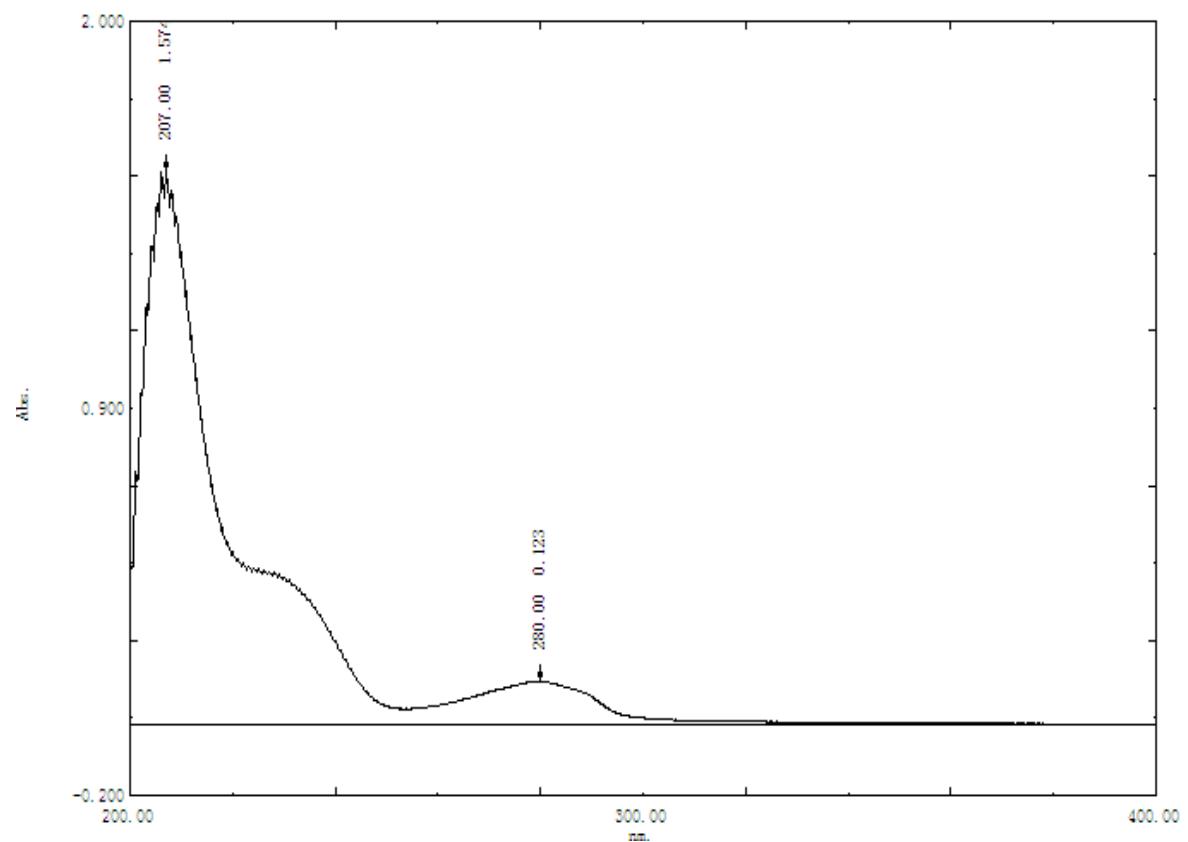


Figure S51. ^1H NMR spectrum of **6** in CD_3OD

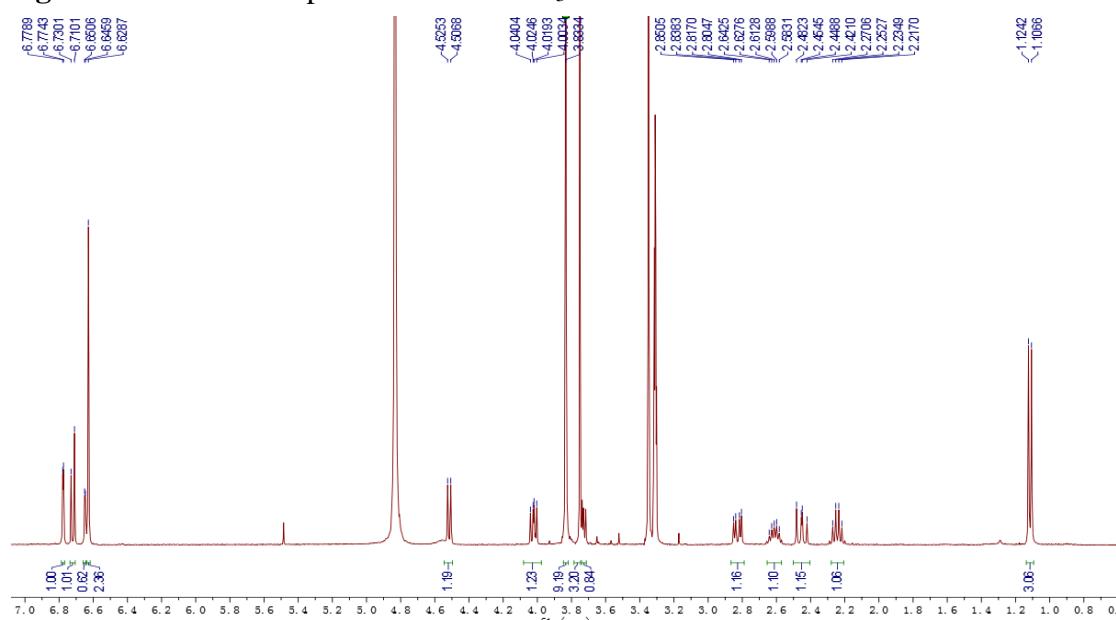


Figure S52. ^{13}C NMR spectrum of **6** in CD_3OD

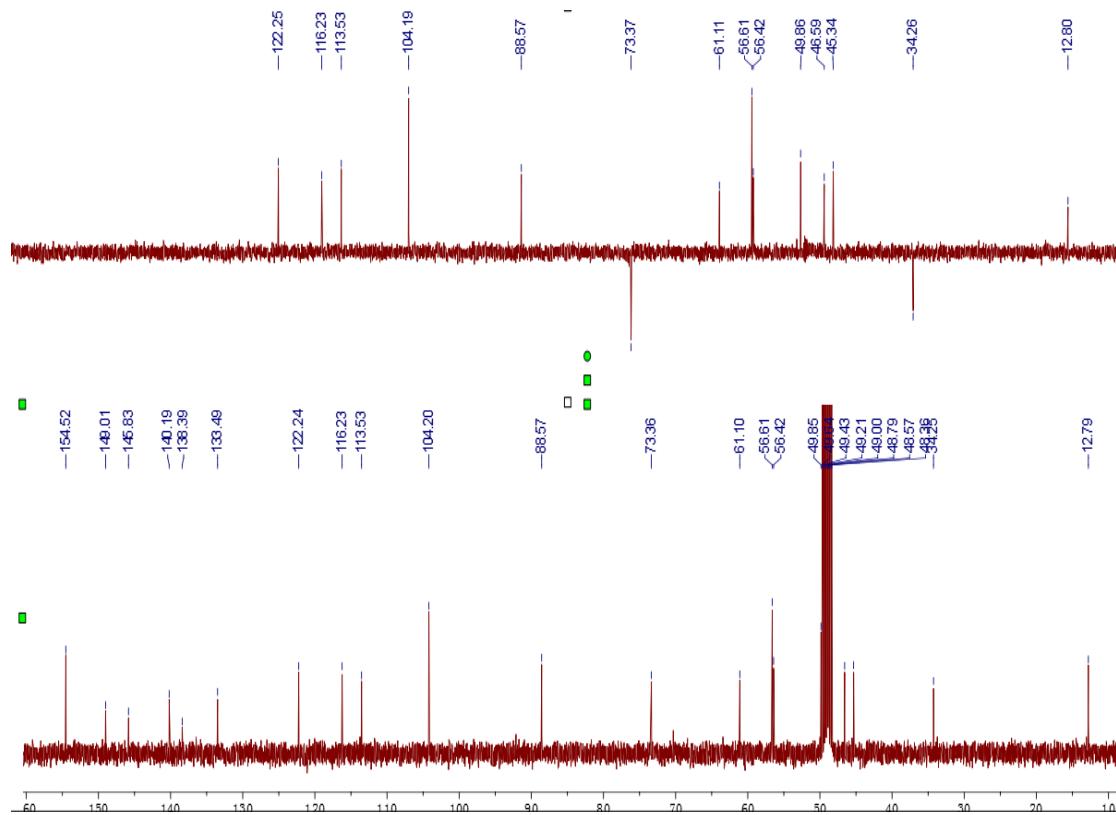


Figure S53. HSQC spectrum of **6** in CD₃OD

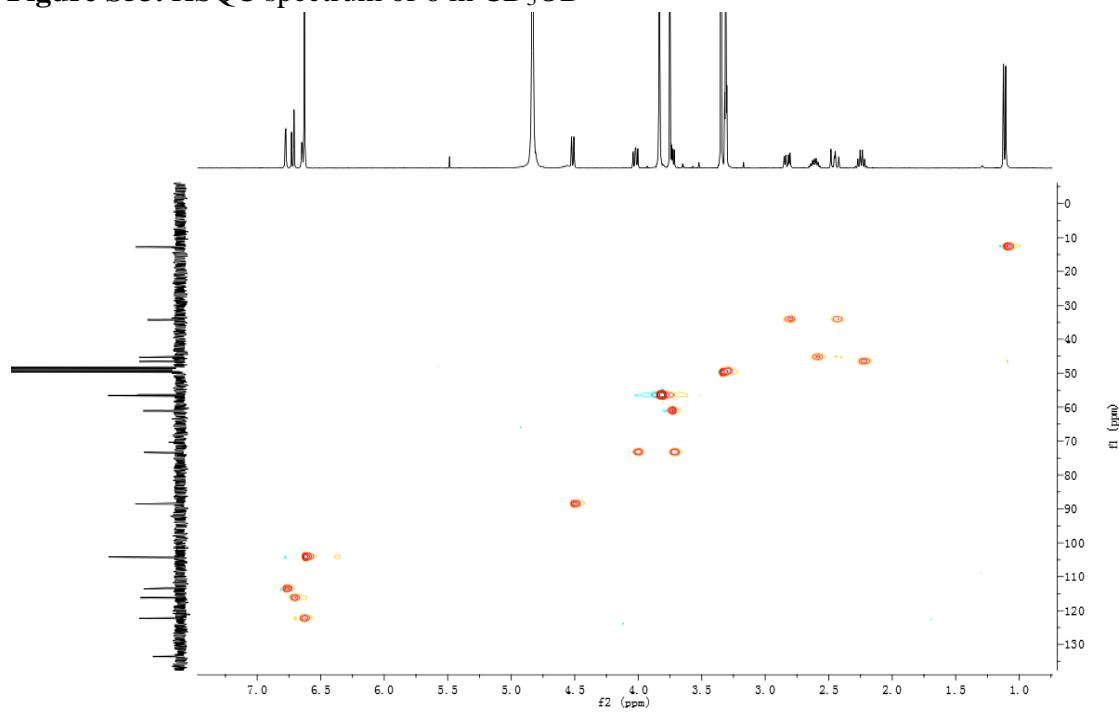


Figure S54. HMBC spectrum of **6** in CD₃OD

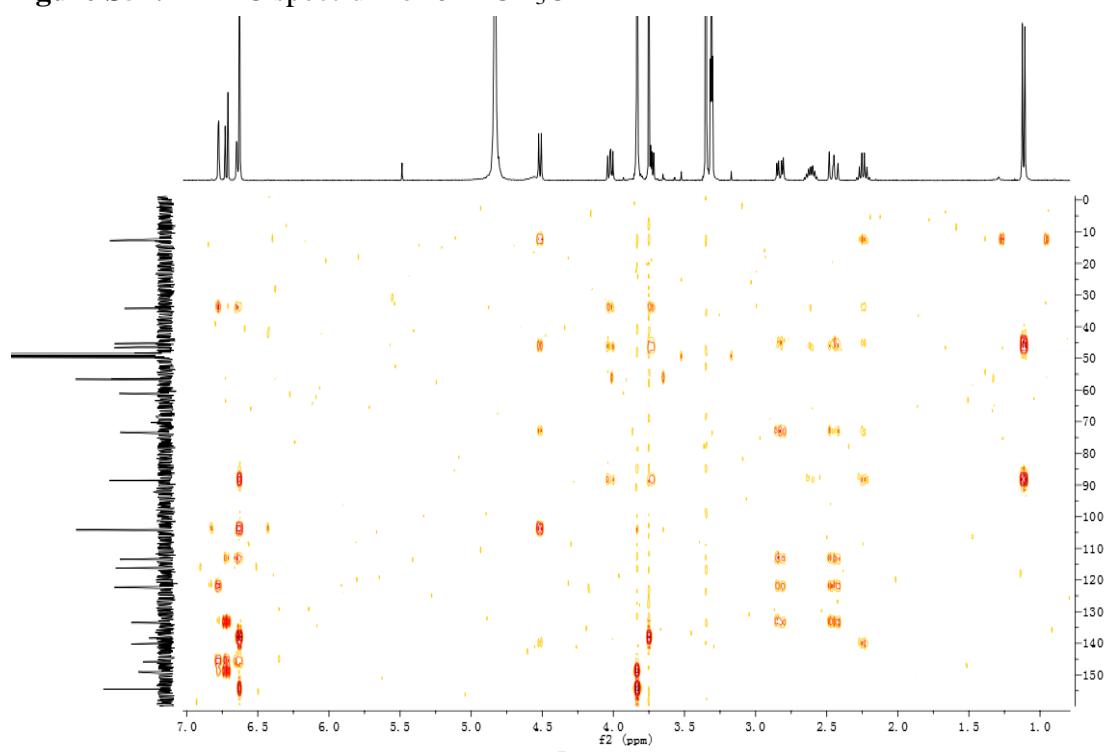


Figure S55. ^1H - ^1H COSY spectrum of **6** in CD_3OD

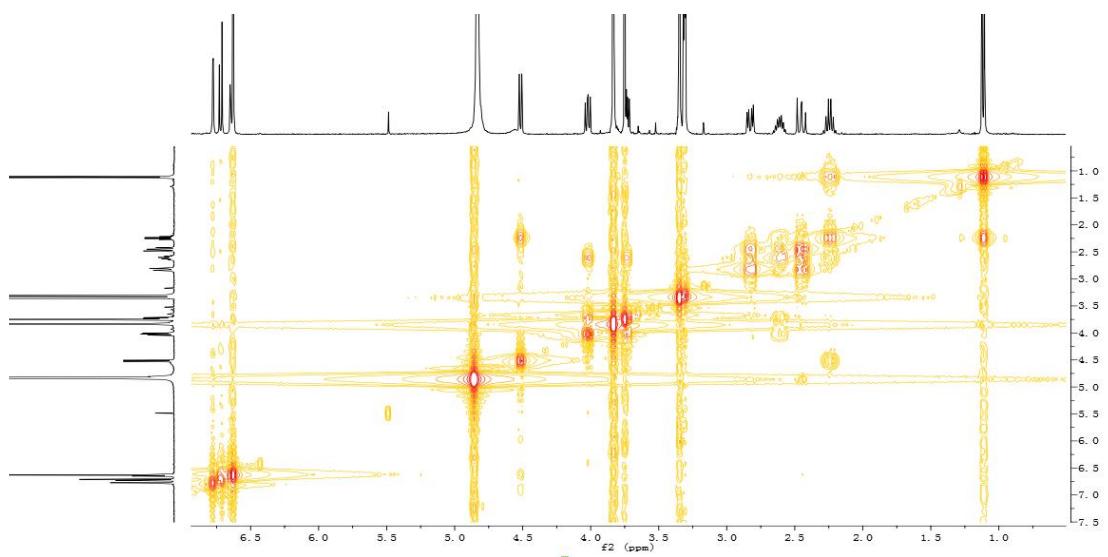


Figure S56. NOESY spectrum of **6** in CD_3OD

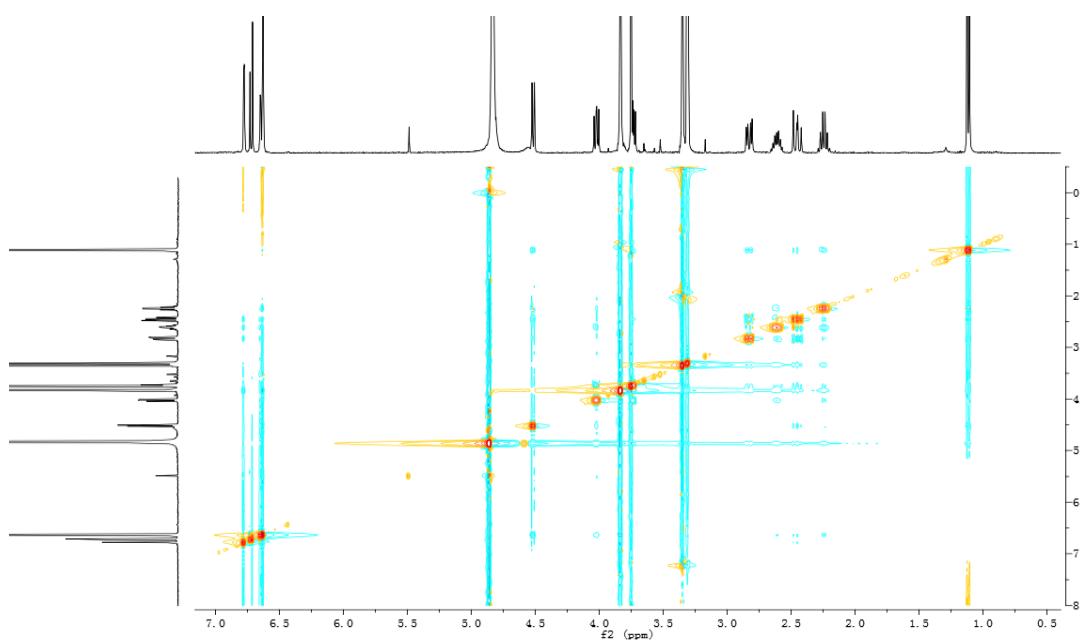


Figure S57. ECD spectrum of **6** in MeOH

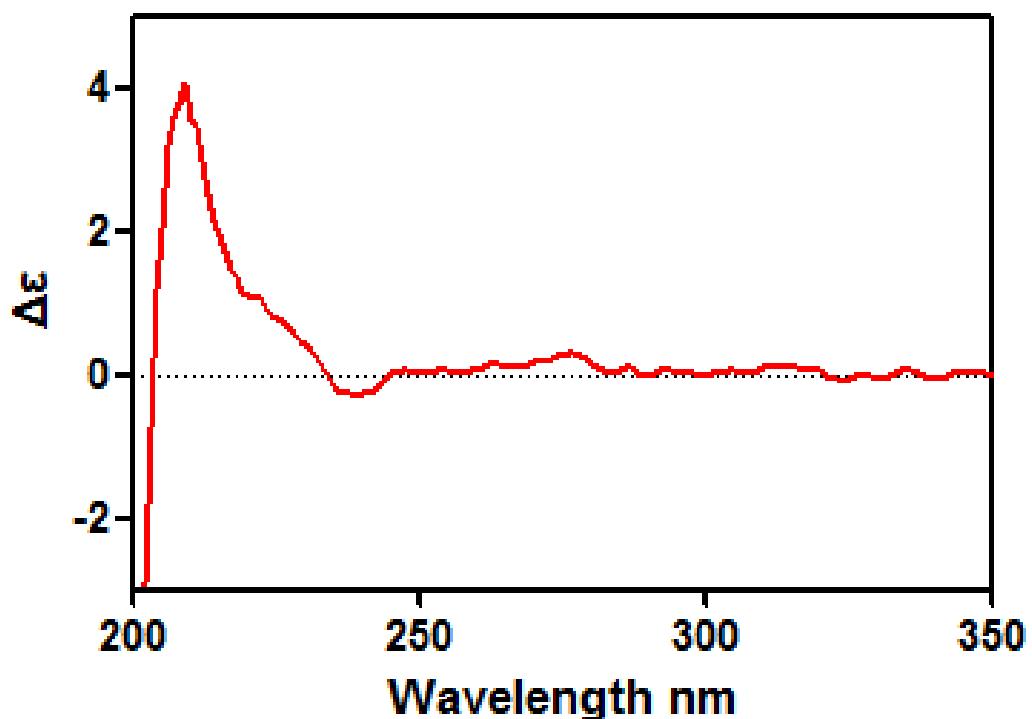


Figure S58. (+)-HR-ESI-MS spectrum of **7**

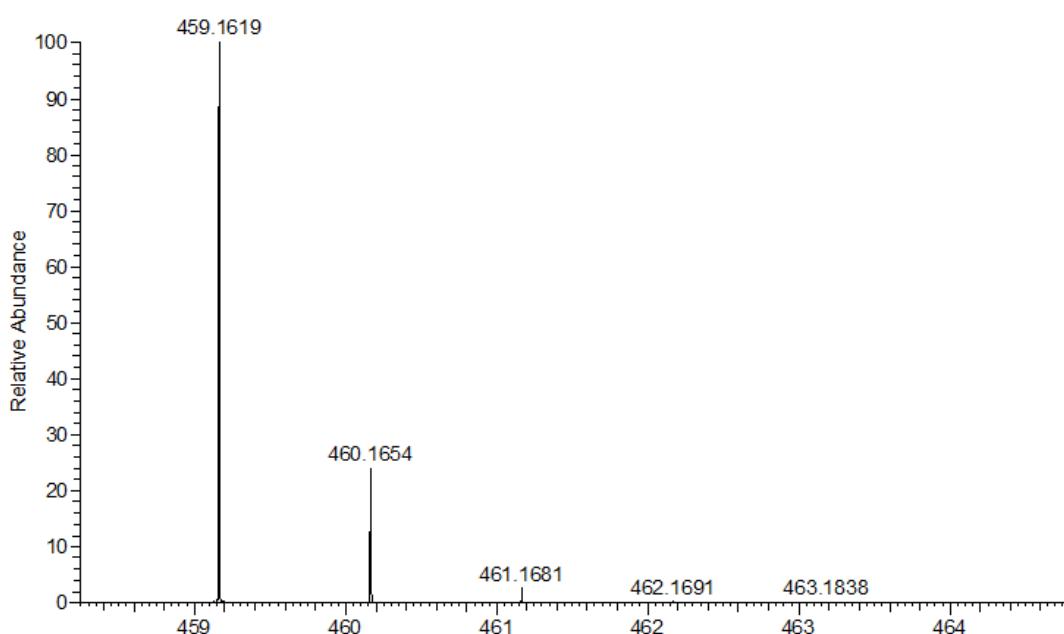


Figure S59. IR spectrum of 7

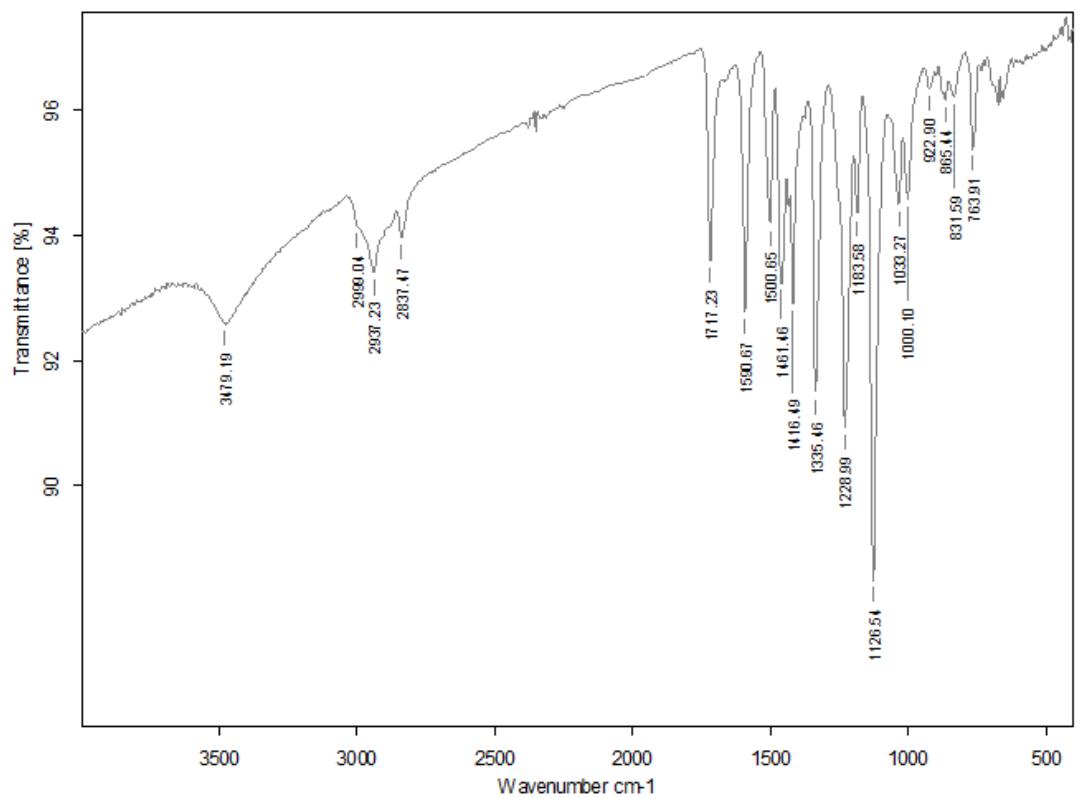


Figure S60. UV spectrum of 7

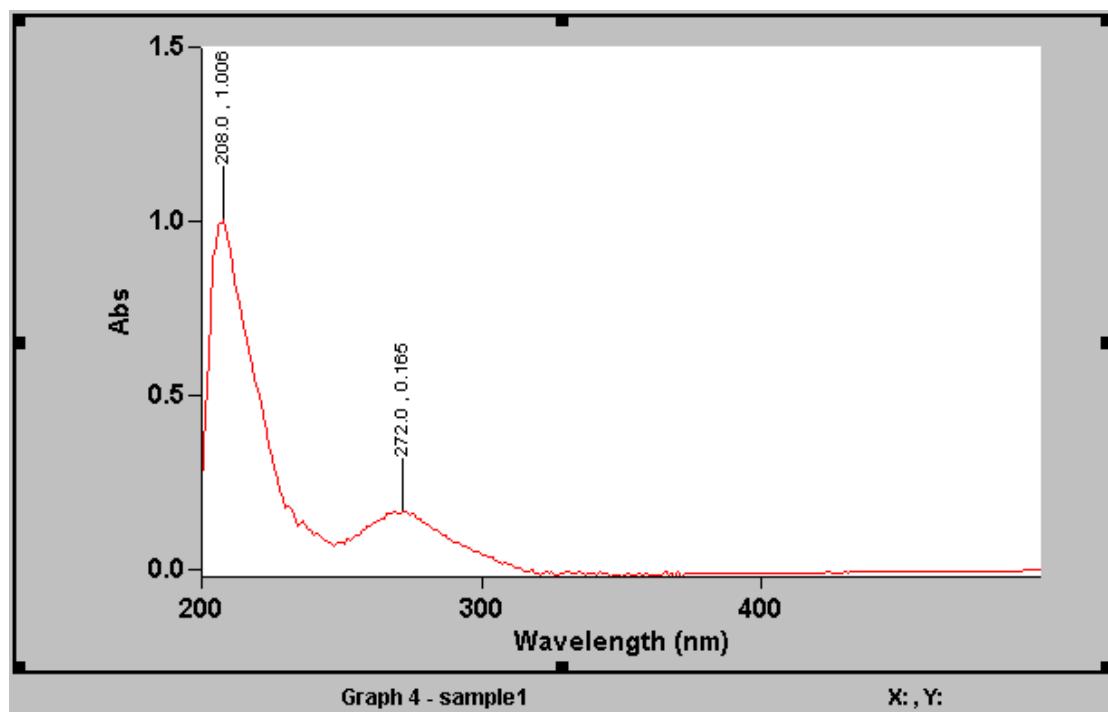


Figure S61. ^1H NMR spectrum of **7** in CD_3OD

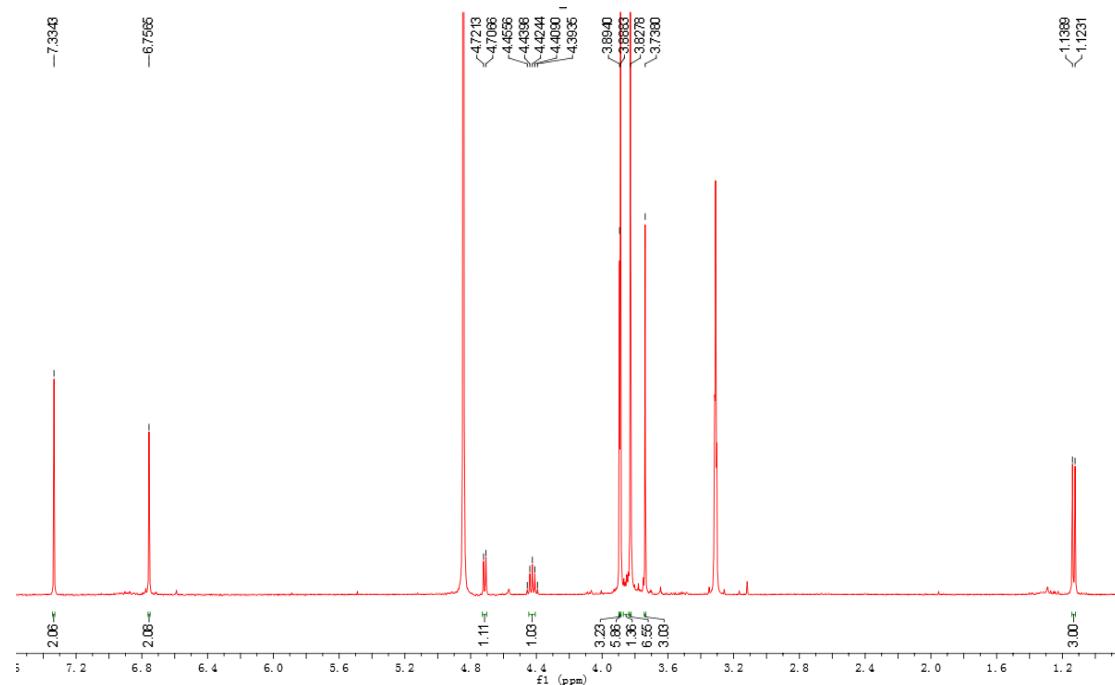


Figure S62. ^{13}C NMR spectrum of **7** in CD_3OD

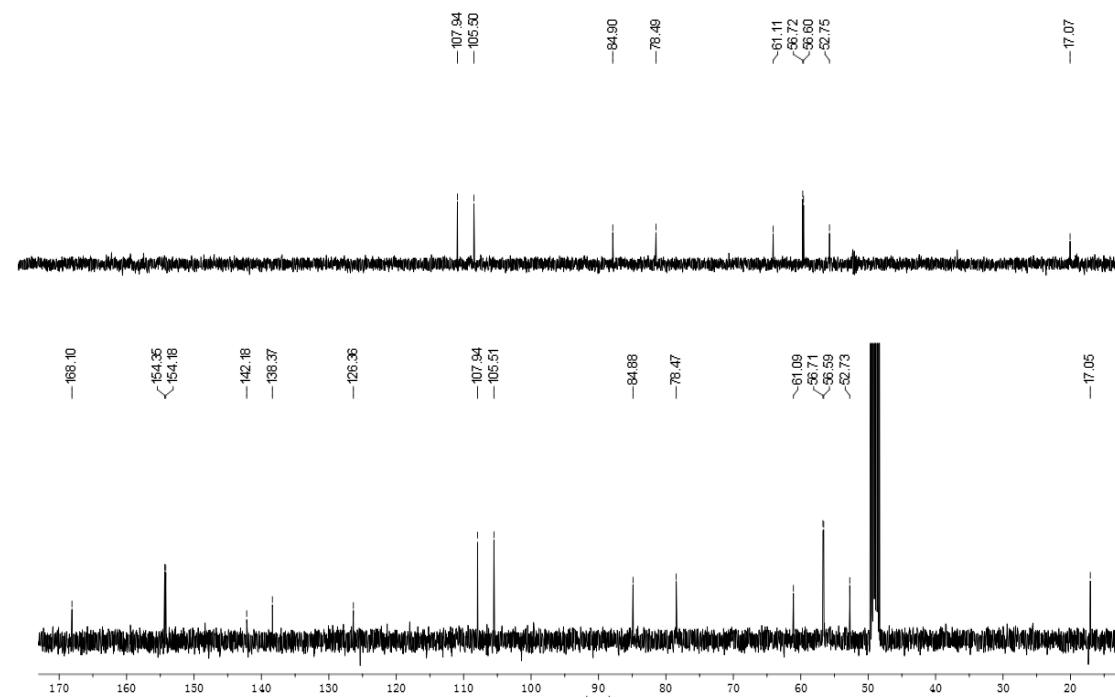


Figure S63. HSQC spectrum of 7 in CD₃OD

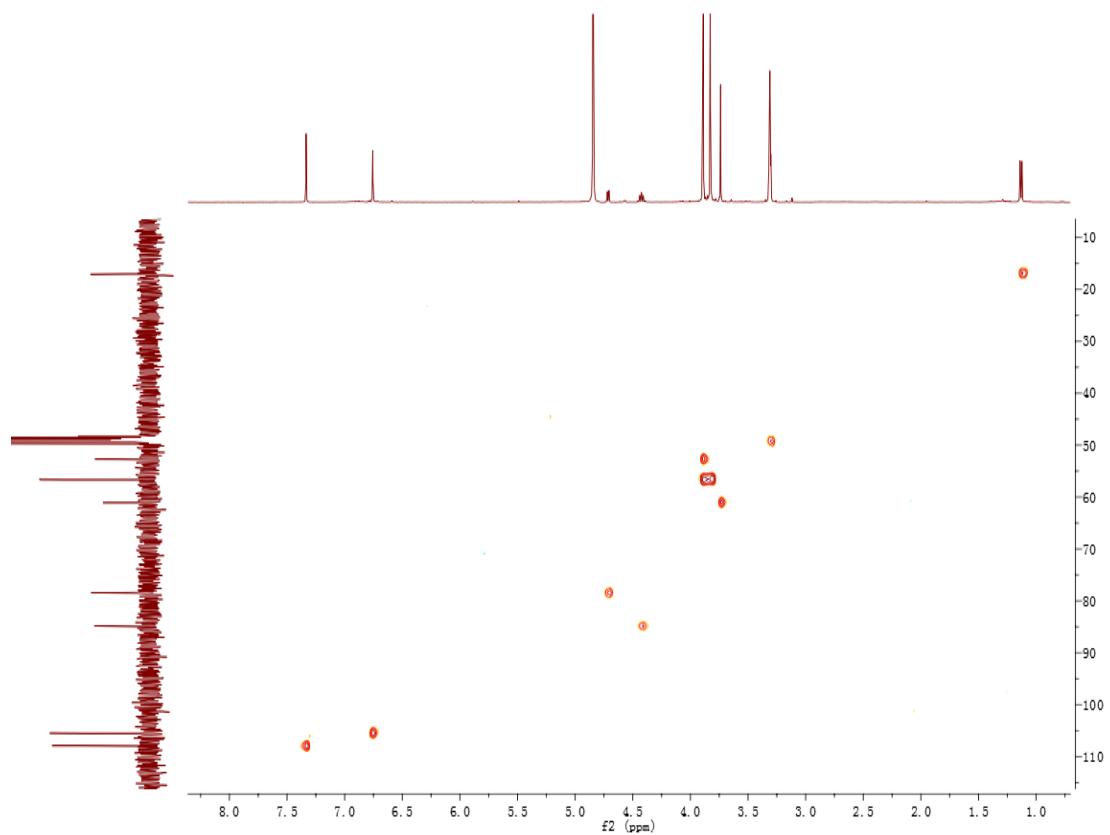


Figure S64. HMBC spectrum of 7 in CD₃OD

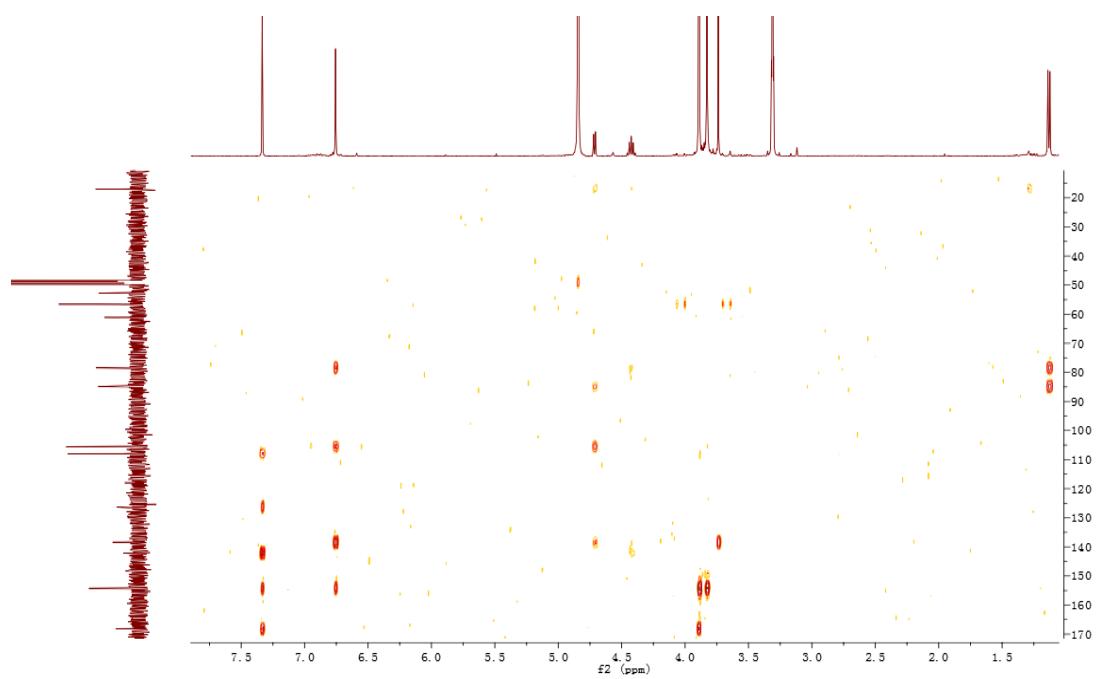


Figure S65. ^1H - ^1H COSY spectrum of **7** in CD_3OD

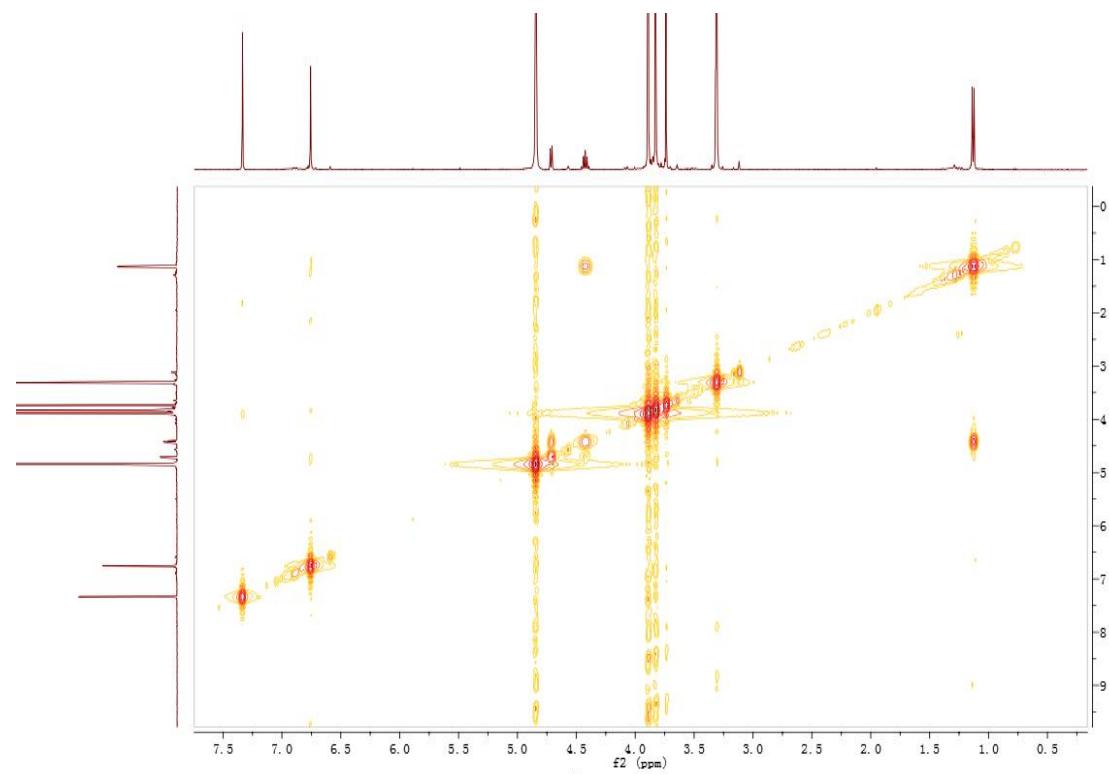


Figure S66. NOESY spectrum of **7** in CD_3OD

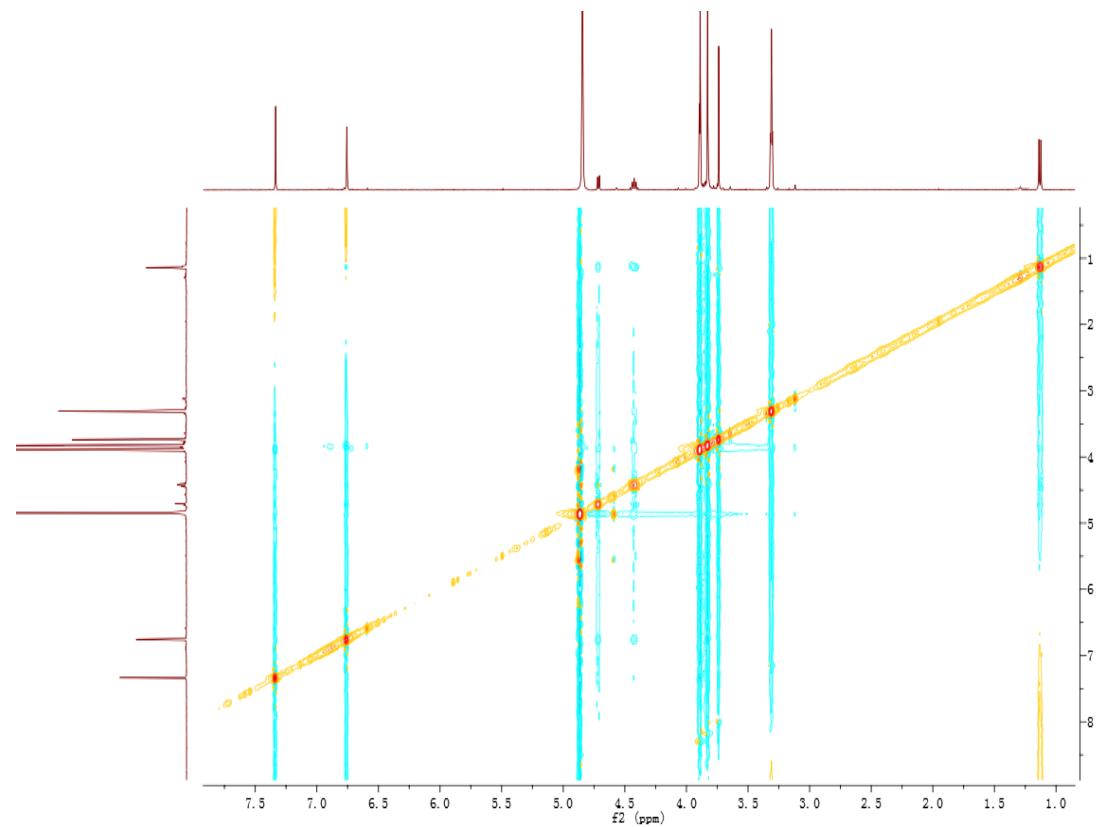


Figure S67. ECD spectrum of **7** in MeOH

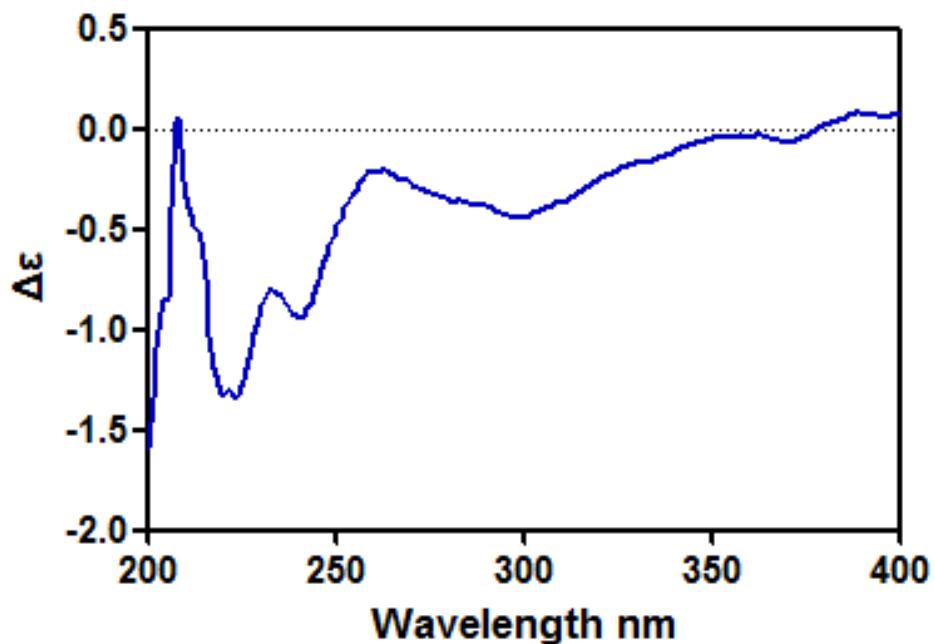


Figure S68. (+)-HR-ESI-MS spectrum of **8**

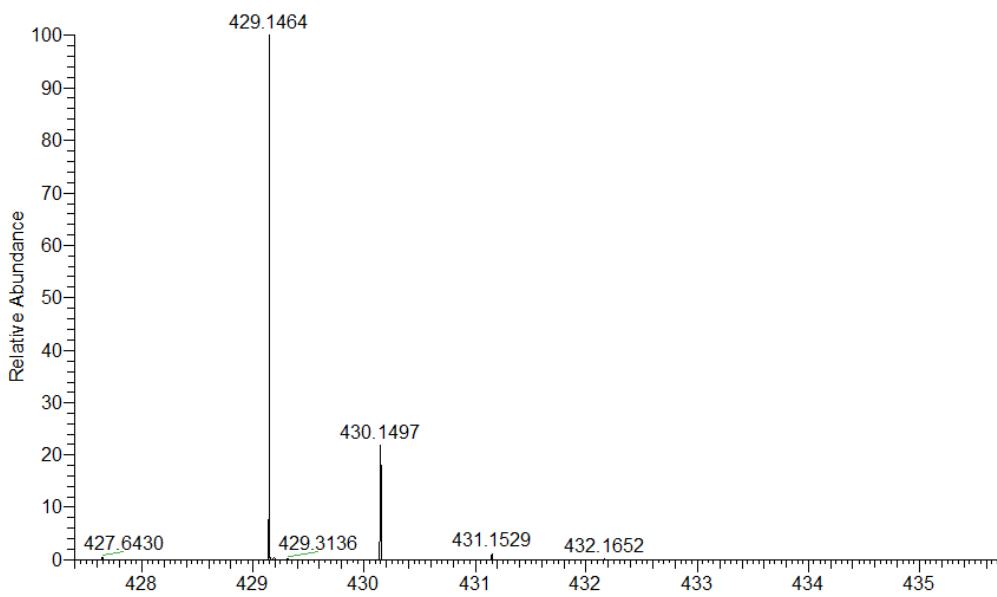


Figure S69. IR spectrum of **8**

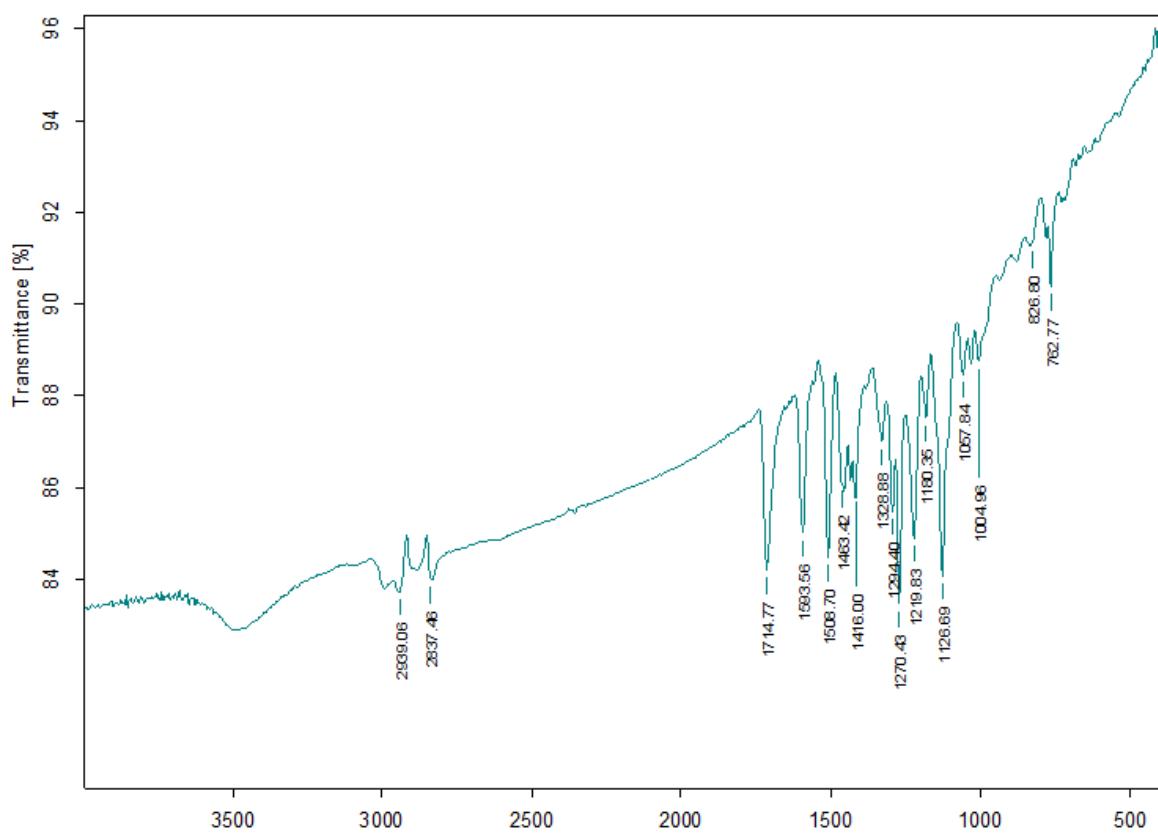


Figure S70. UV spectrum of **8**

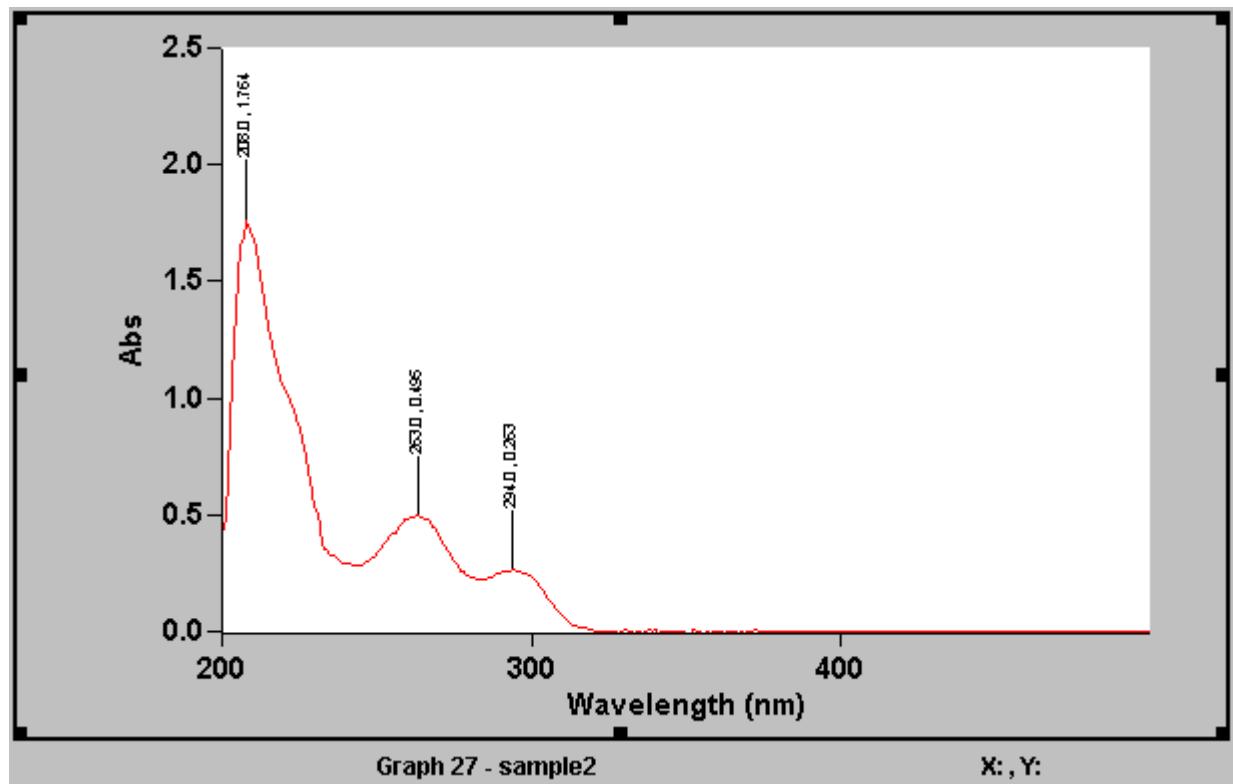


Figure S71. ^1H NMR spectrum of **8** in CD_3OD

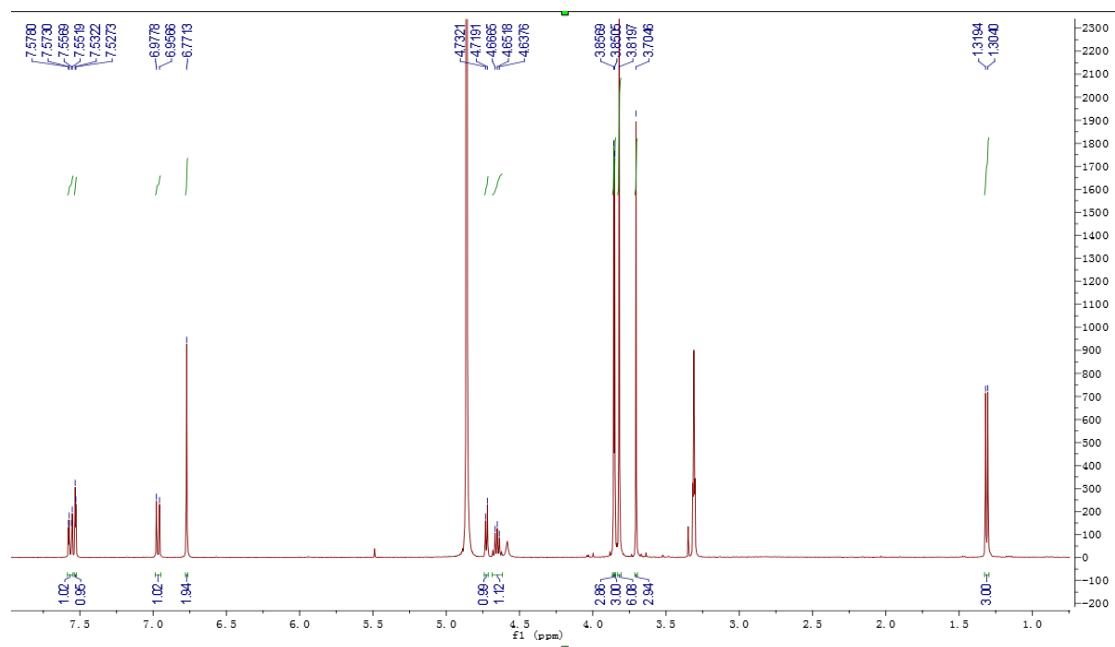


Figure S72. ^{13}C NMR spectrum of **8** in CD_3OD

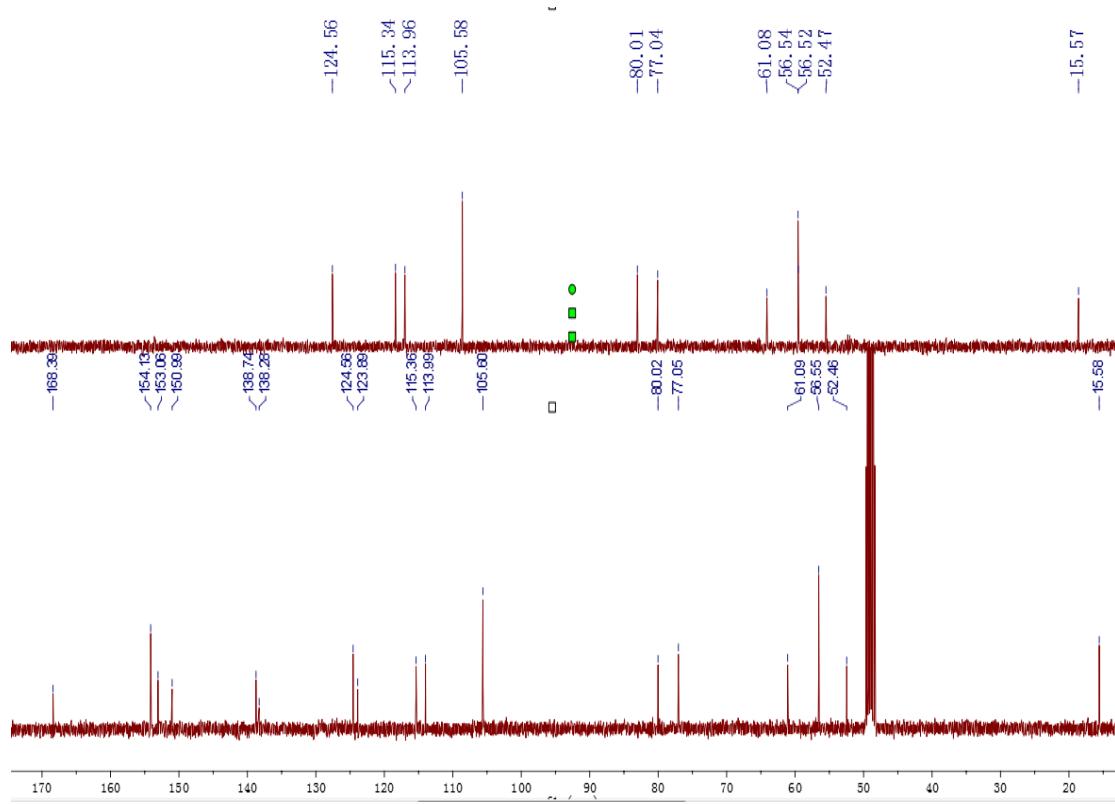


Figure S73. HSQC spectrum of **8** in CD₃OD

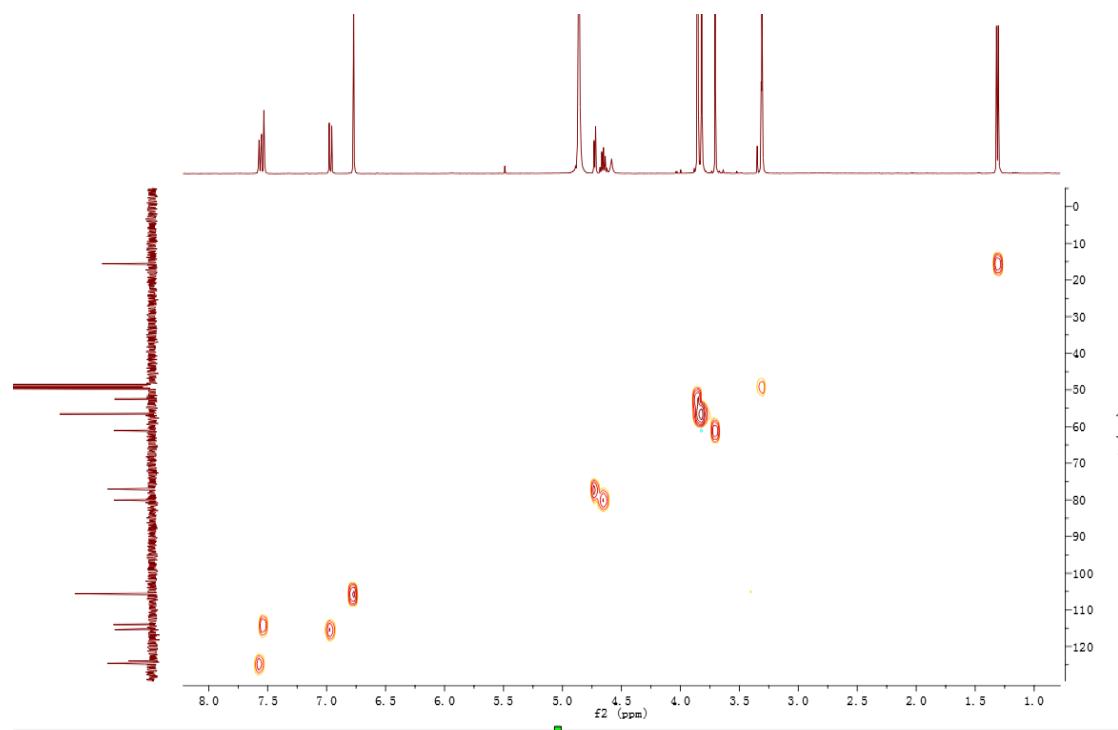


Figure S74. HMBC spectrum of **8** in CD₃OD

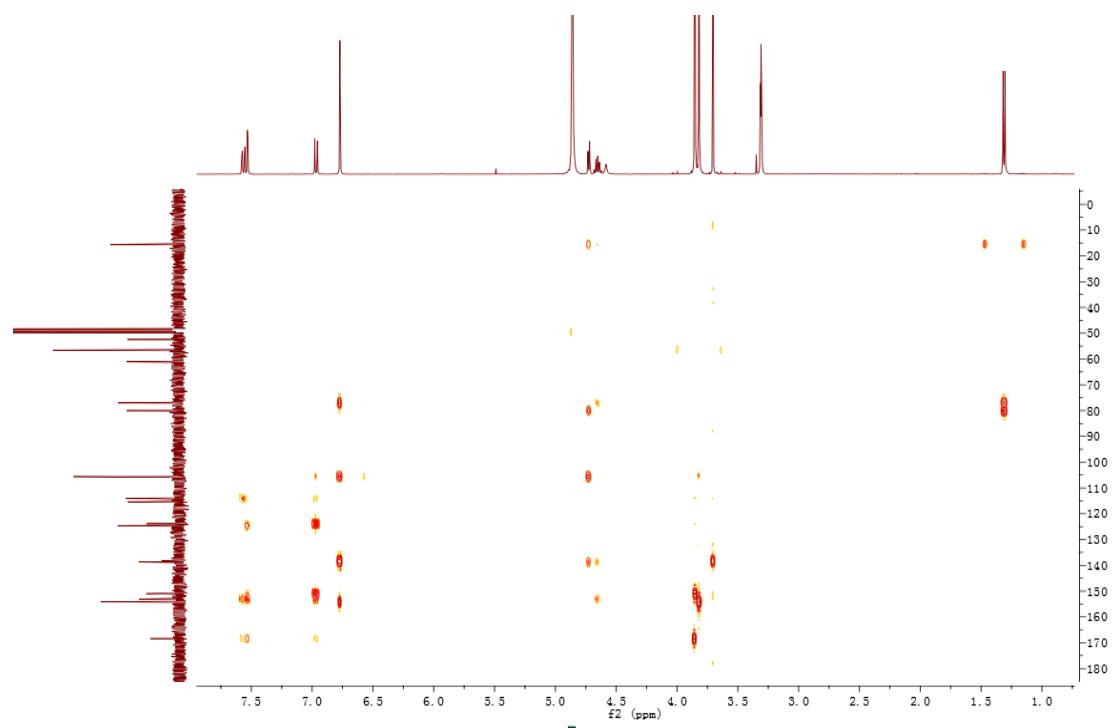


Figure S75. ^1H - ^1H COSY spectrum of **8** in CD_3OD

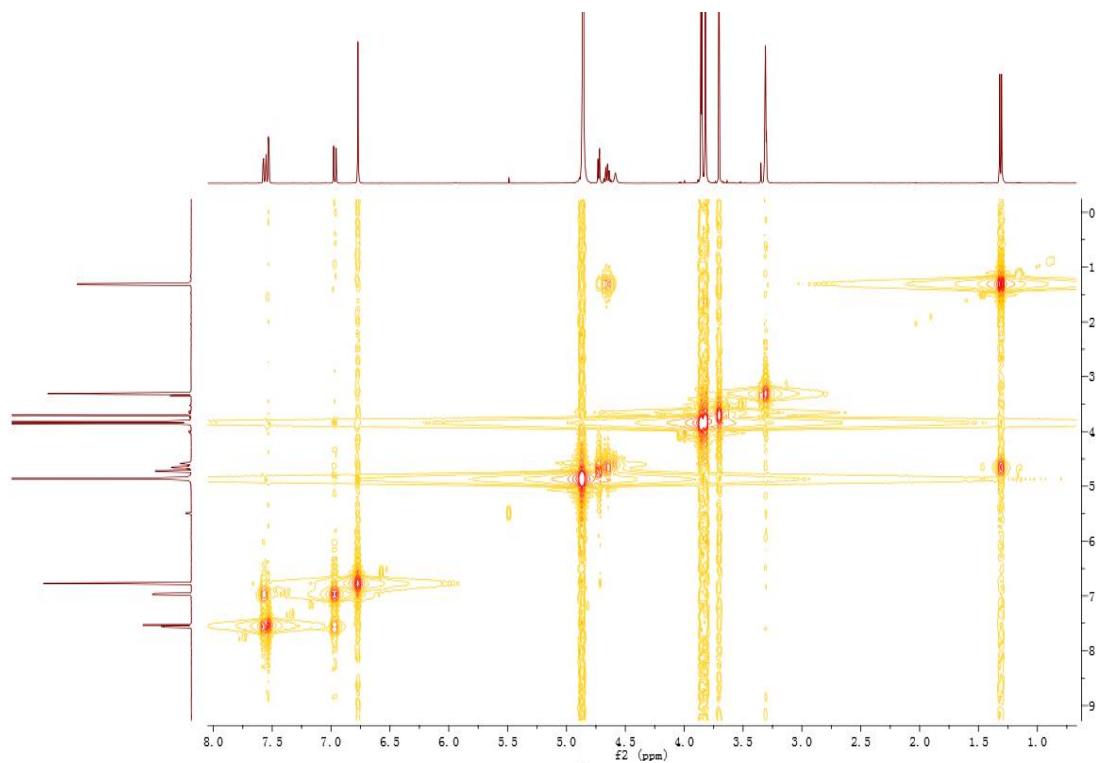


Figure S76. NOESY spectrum of **8** in CD_3OD

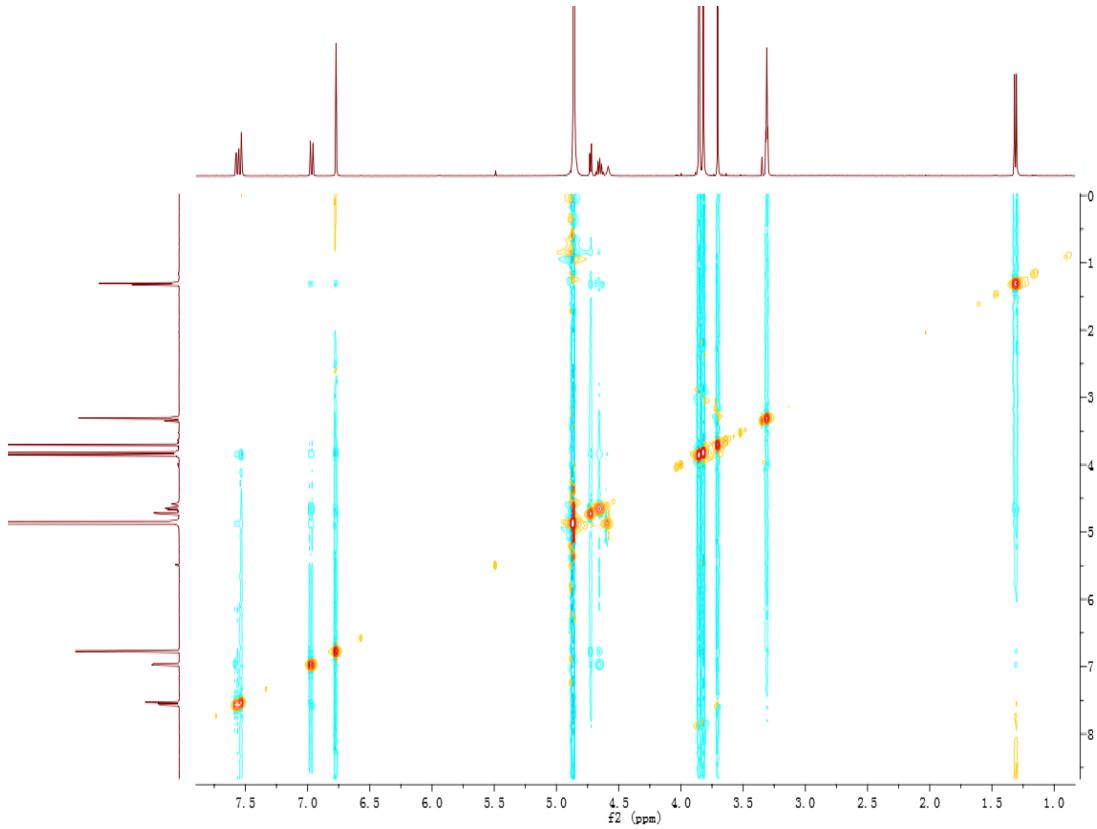


Figure S77. ECD spectrum of **8** in MeOH

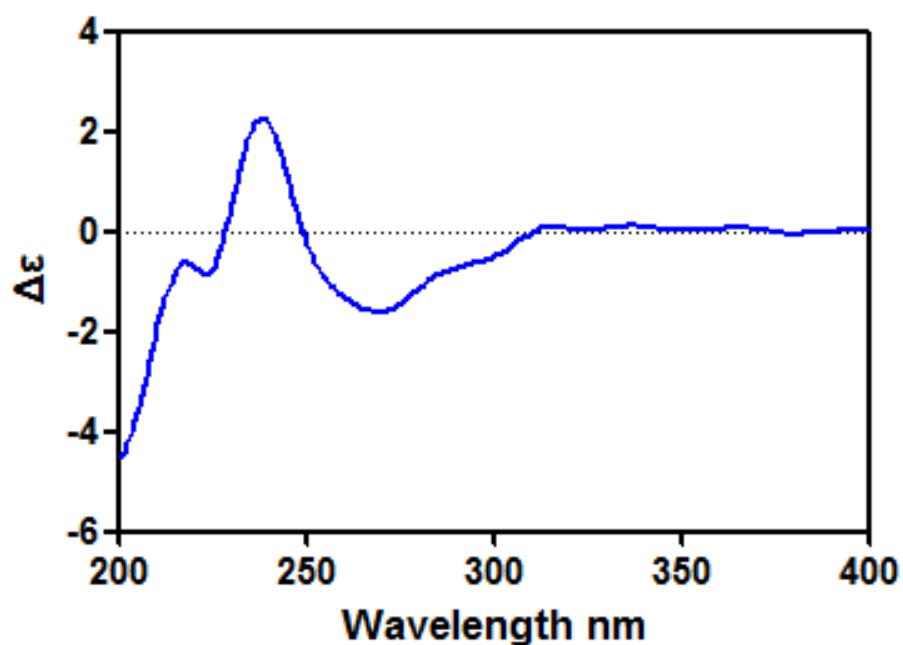


Figure S78. (+)-HR-ESI-MS spectrum of *S*-MTPA-**7** ester

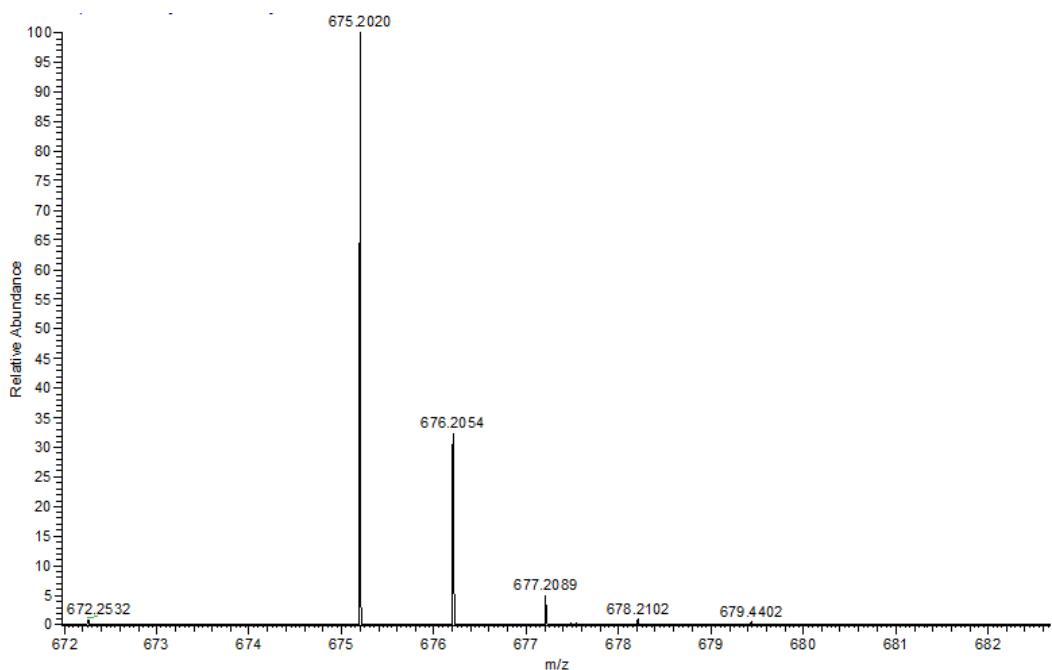


Figure S79. (+)-HR-ESI-MS spectrum of *R*-MTPA-7 ester

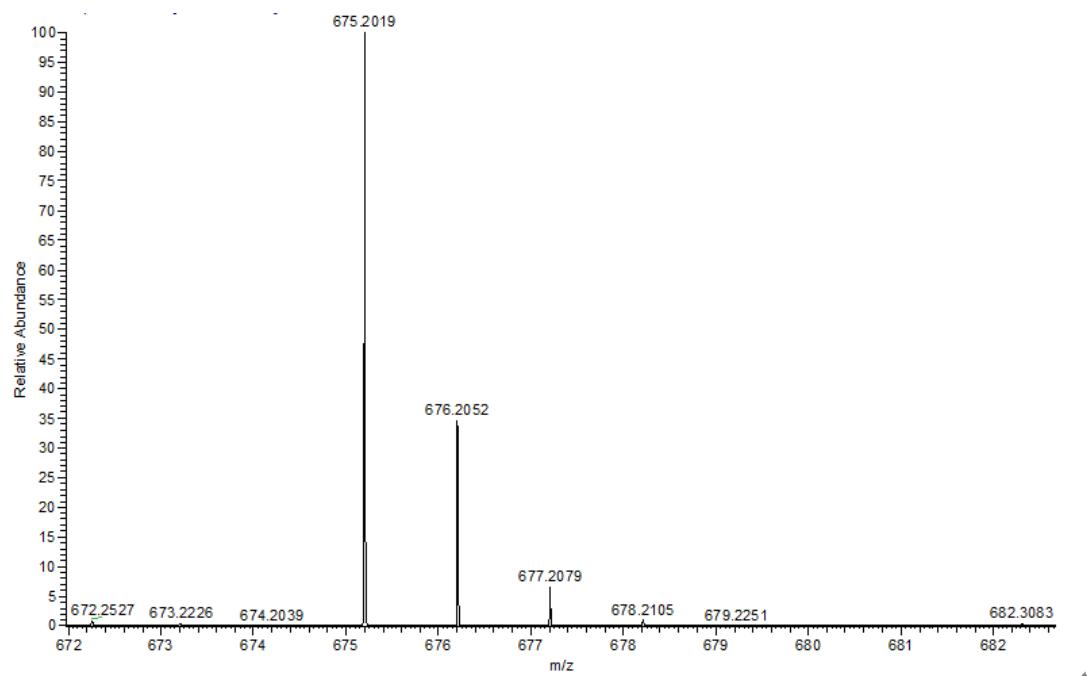


Figure S80. ^1H NMR spectrum of *R/S*-MTPA-7 ester in CD_3OD

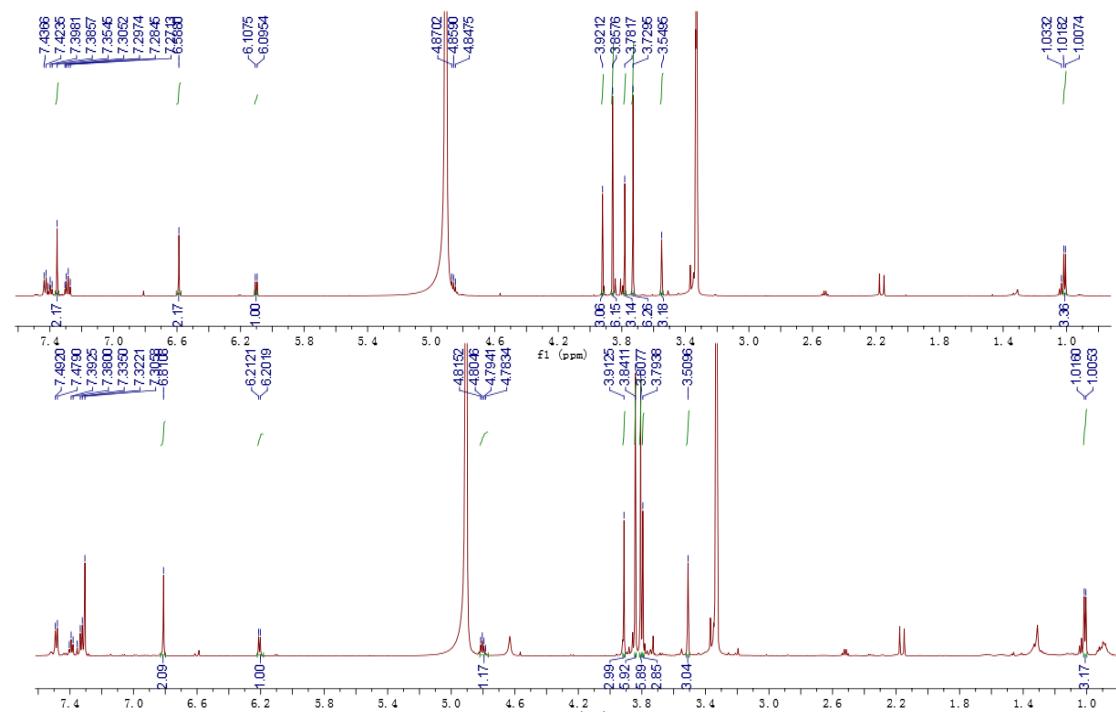
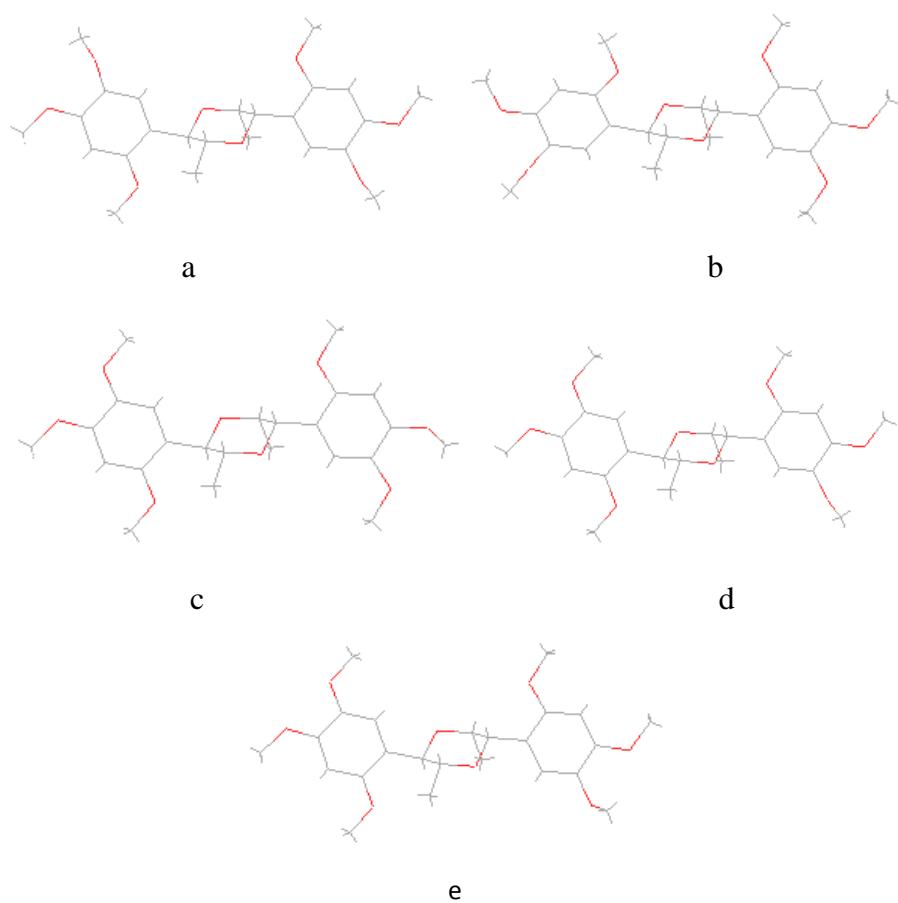


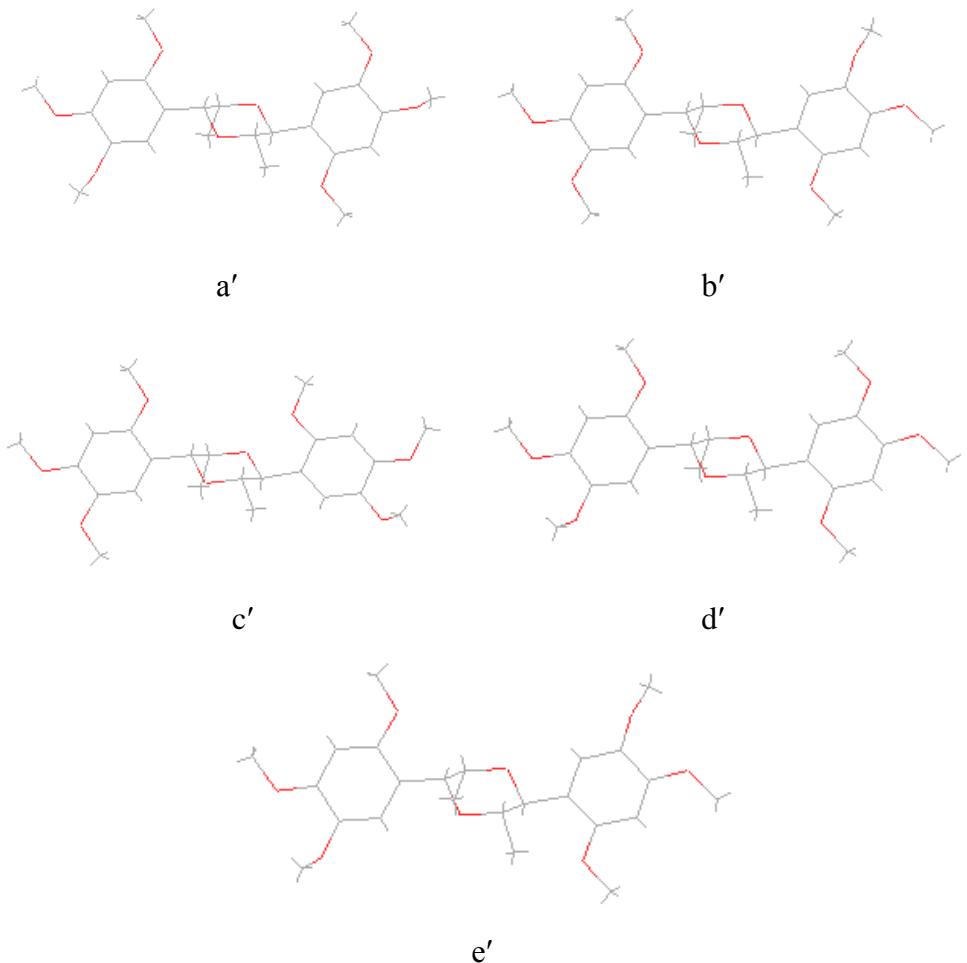
Figure S81. ECD spectra calculation

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 *7S,7'R,8S,8'S* and five lowest energy conformers of the *7R,7'S,8R,8'R* isomer of compound **1**.



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



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 <i>S</i> ,7'R,8 <i>S</i> ,8'S		conformer	Isomer 7 <i>R</i> ,7'S,8 <i>R</i> ,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%