

Supporting Information for

**Antimicrobial Furancarboxylic Acids from a
Penicillium sp.**

Jin-Ling Chang,^{†, #} Hong-Zhe Xu,^{†, #} Jia Zhou,[†] Ming Zhou,[†] Xuke Zhang,[‡]

Yuanqiang Guo,[‡] and Han-Li Ruan^{†*}

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

[‡]State Key Laboratory of Medicinal Chemical Biology, College of Pharmacy, and Tianjin Key Laboratory of Molecular Drug Research, Nankai University, Tianjin 300350, People's Republic of China

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

T: FTMS + p ESI Full ms [100.00-800.00]

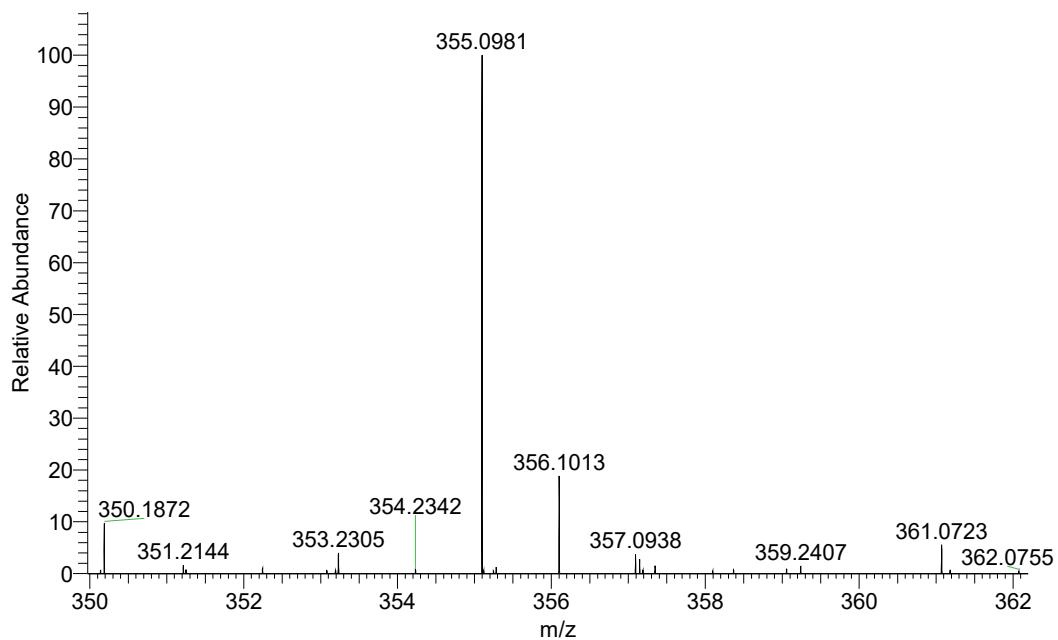


Figure S2. ^1H NMR (400 MHz, CDCl_3) spectrum of **1**

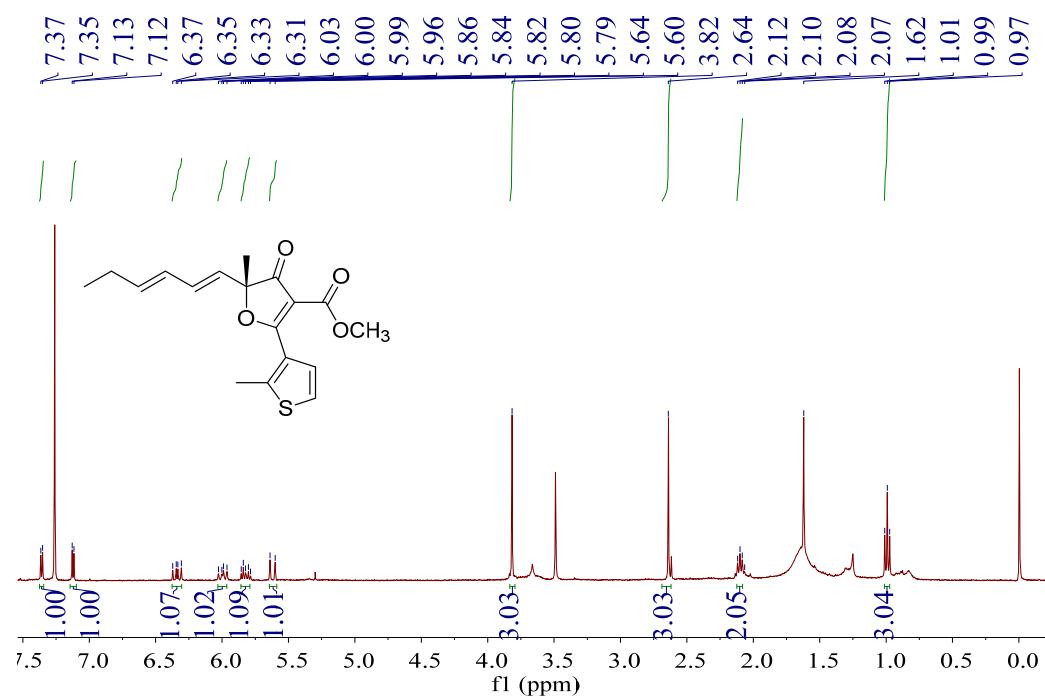


Figure S3. ^{13}C NMR (100 MHz, CDCl_3) spectrum of **1**

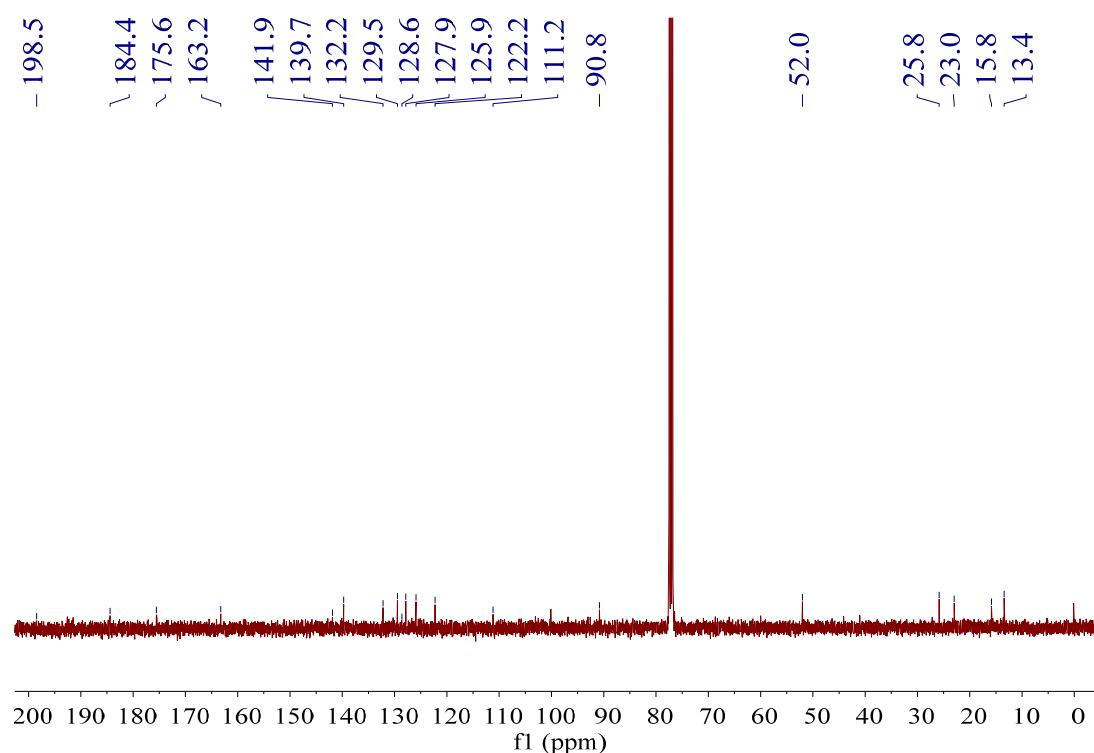


Figure S4. DEPT 135 (100 MHz, CDCl_3) spectrum of **1**

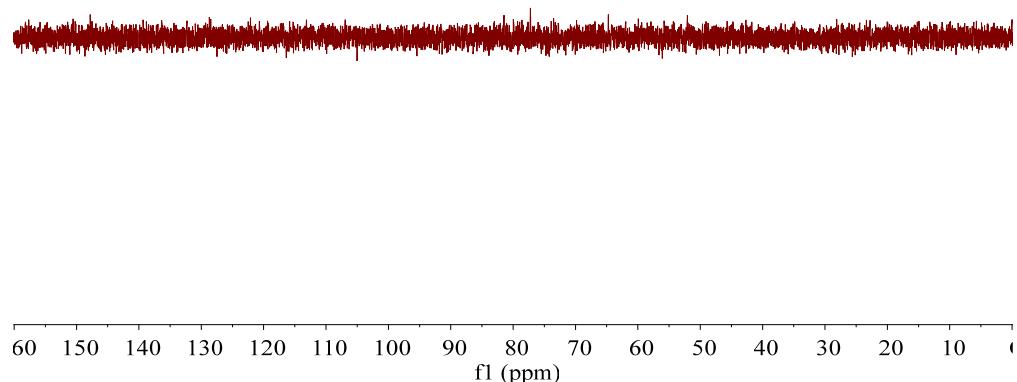


Figure S5. HSQC spectrum of **1** in CDCl_3

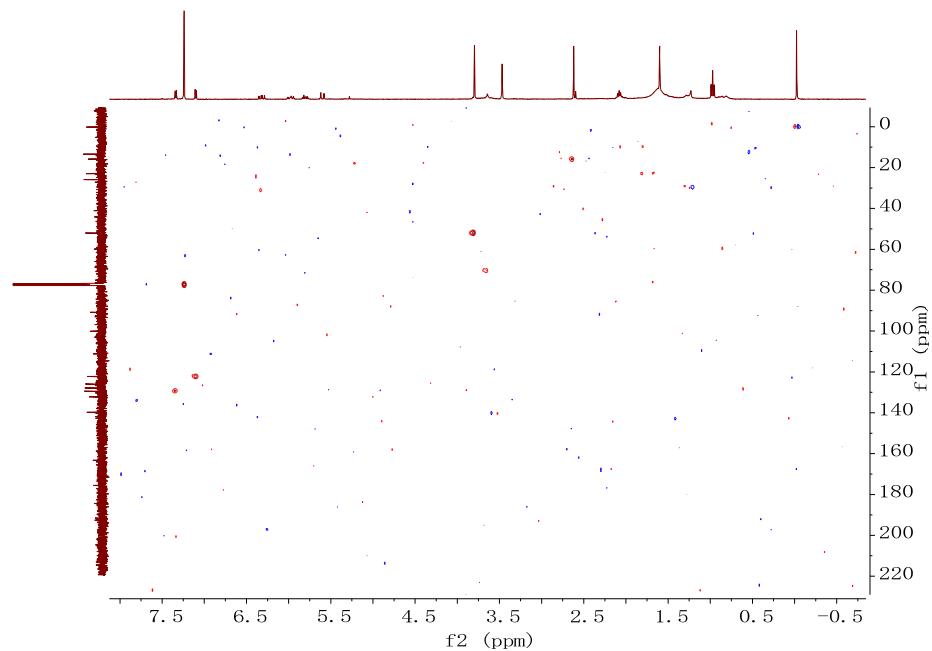


Figure S6. ^1H - ^1H COSY spectrum of **1** in CDCl_3

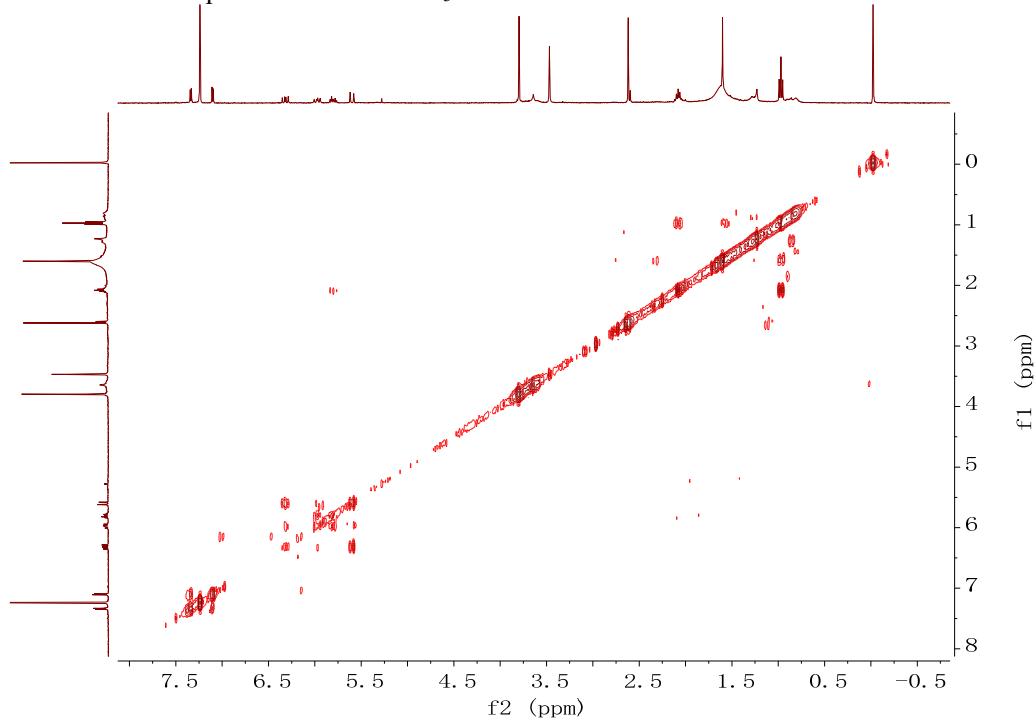


Figure S7. HMBC spectrum of **1** in CDCl_3

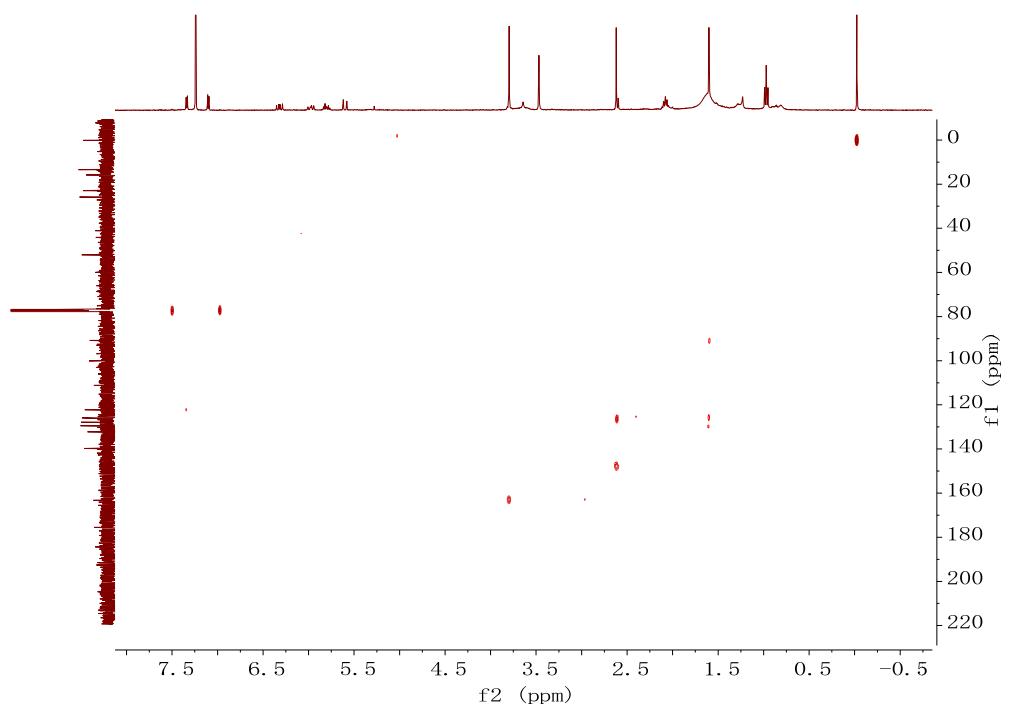


Figure S8. NOESY spectrum of **1** in CDCl_3

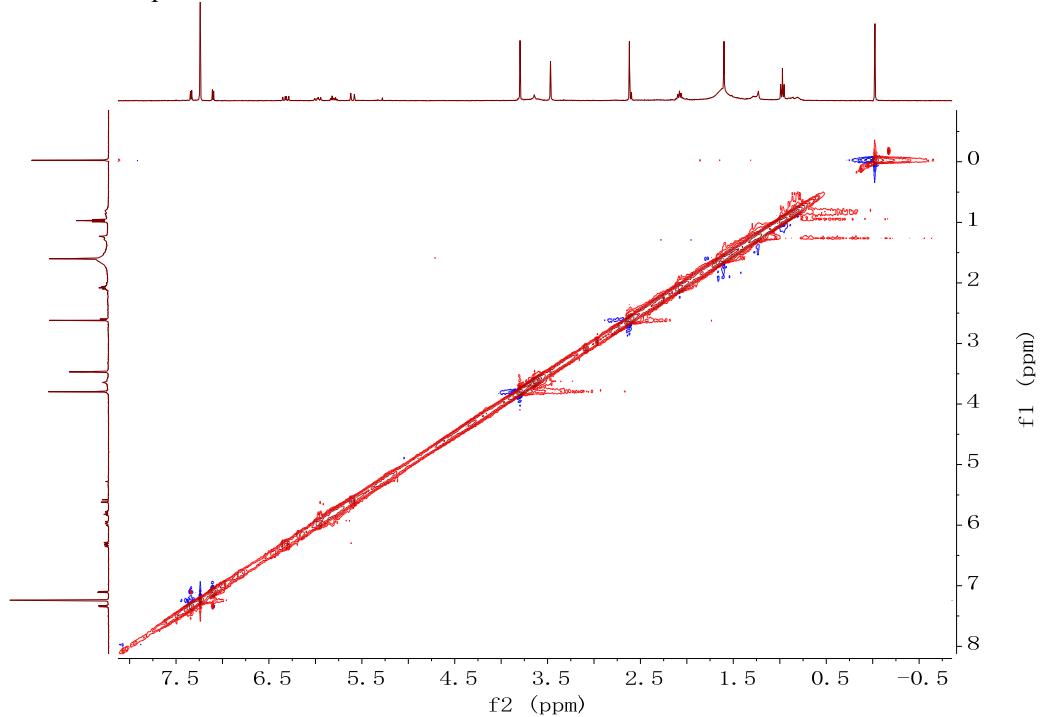


Figure S9. Experimental ECD spectrum of **1**

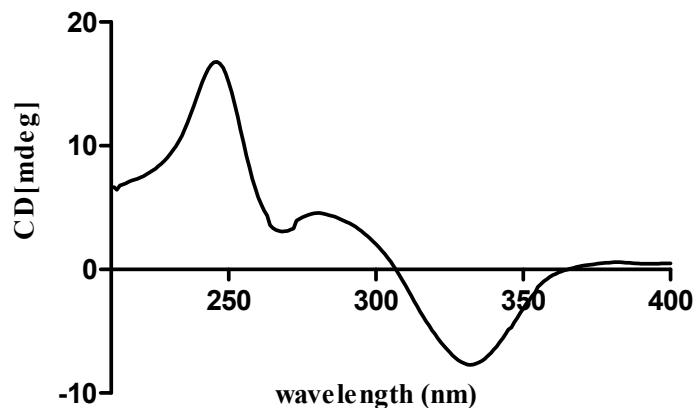


Figure S10. UV spectrum of **1**

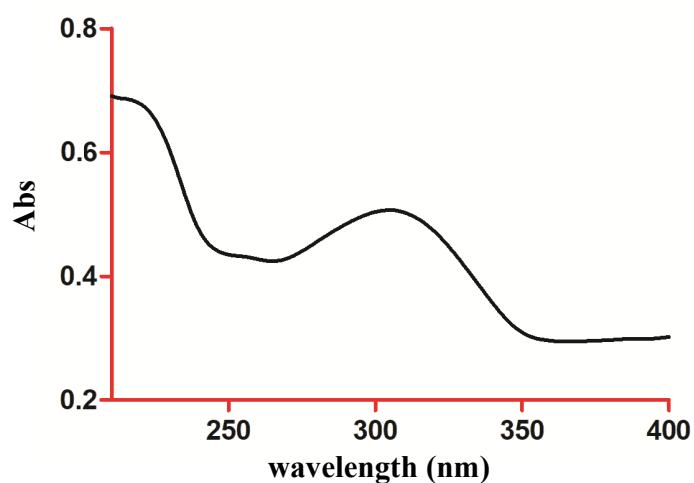


Figure S11. IR spectrum of 1

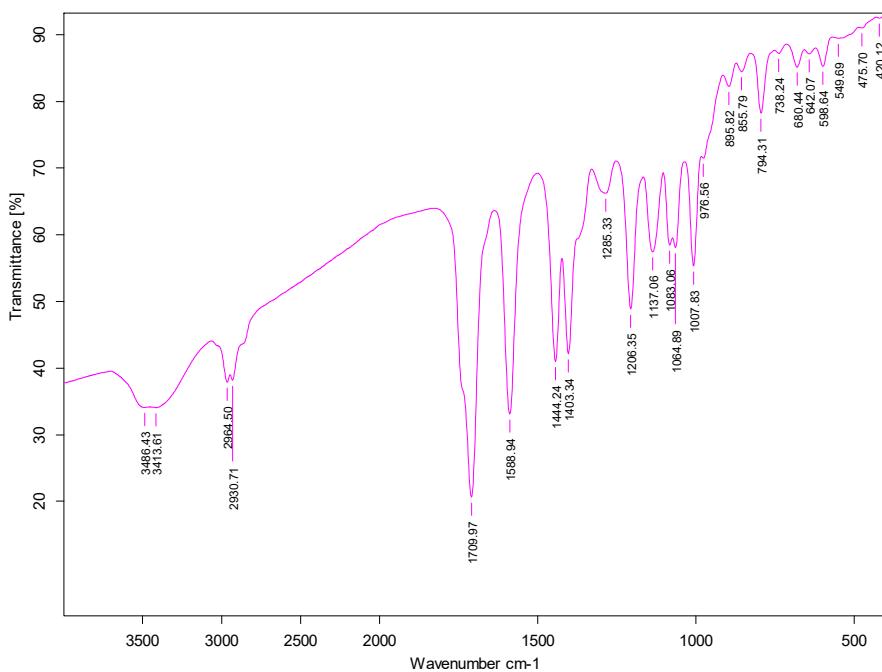


Figure S12. (+)-HR-ESI-MS spectrum of 2

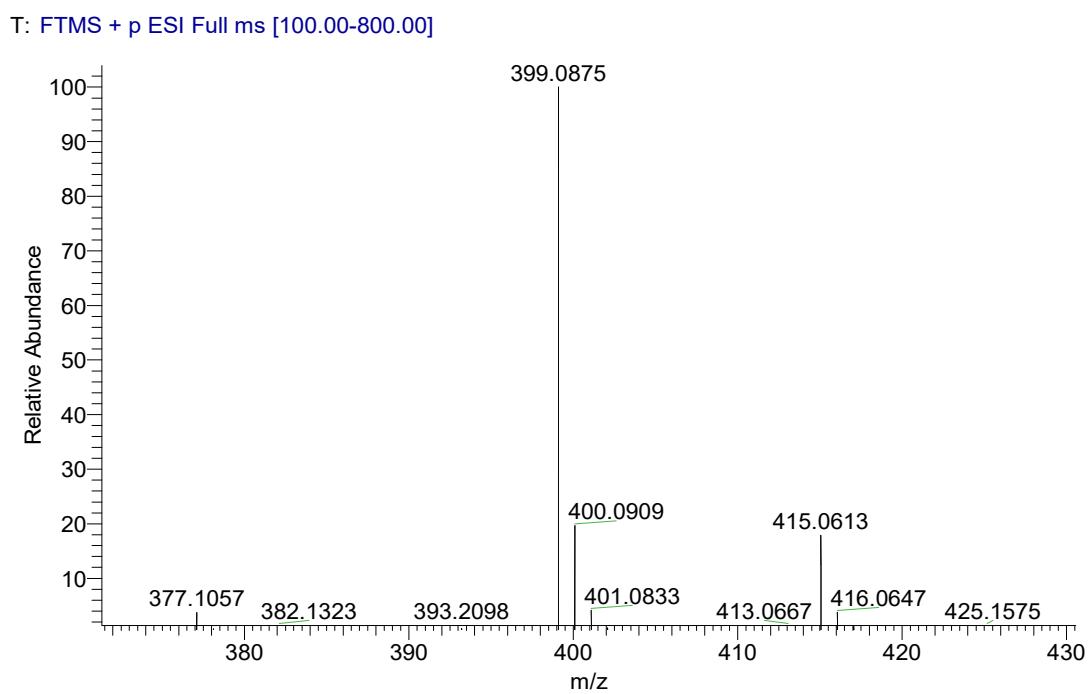


Figure S13. ^1H NMR (400 MHz, CDCl_3) spectrum of **2**

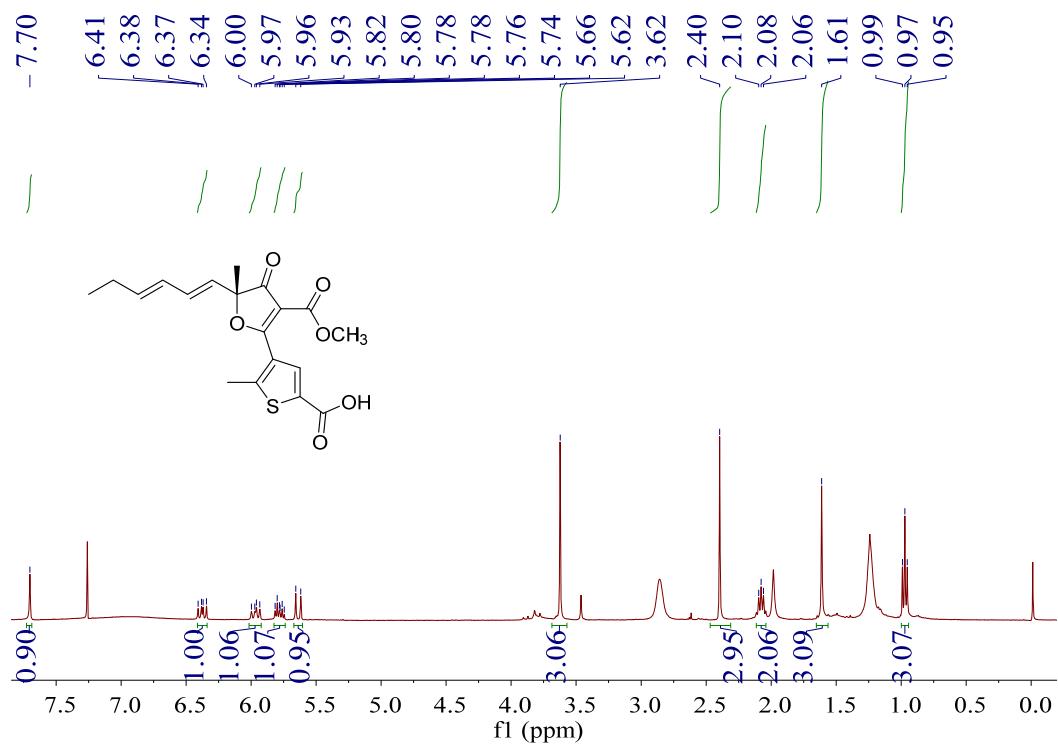


Figure S14. ^{13}C NMR (100 MHz, CDCl_3) spectrum of **2**

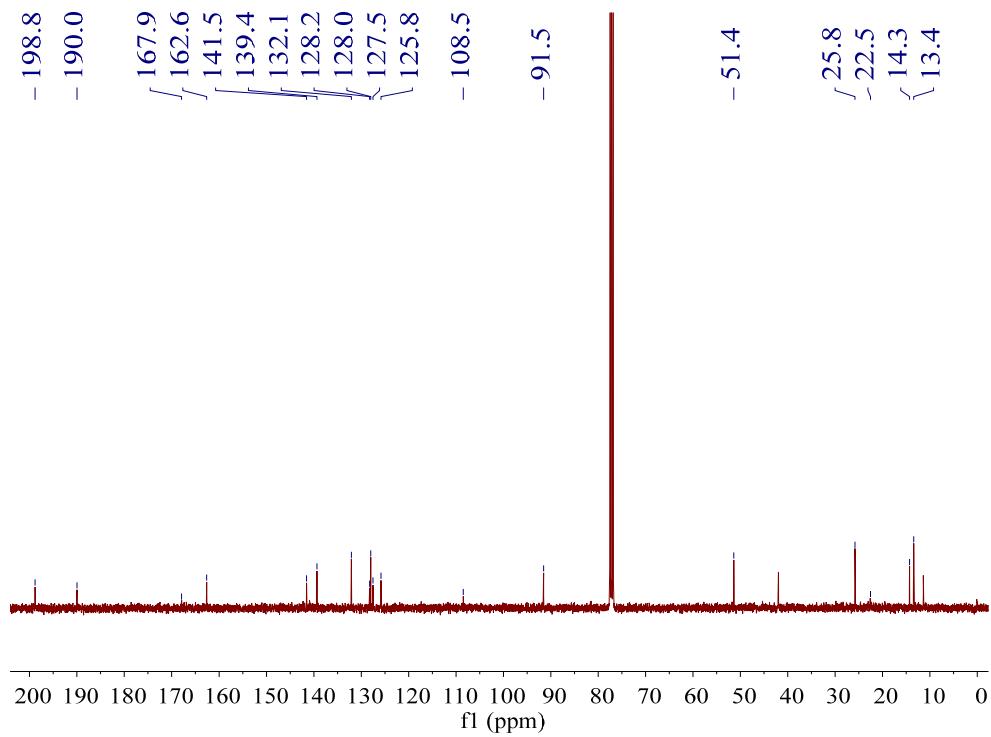


Figure S15. DEPT 135 (100 MHz, CDCl_3) spectrum of **2**

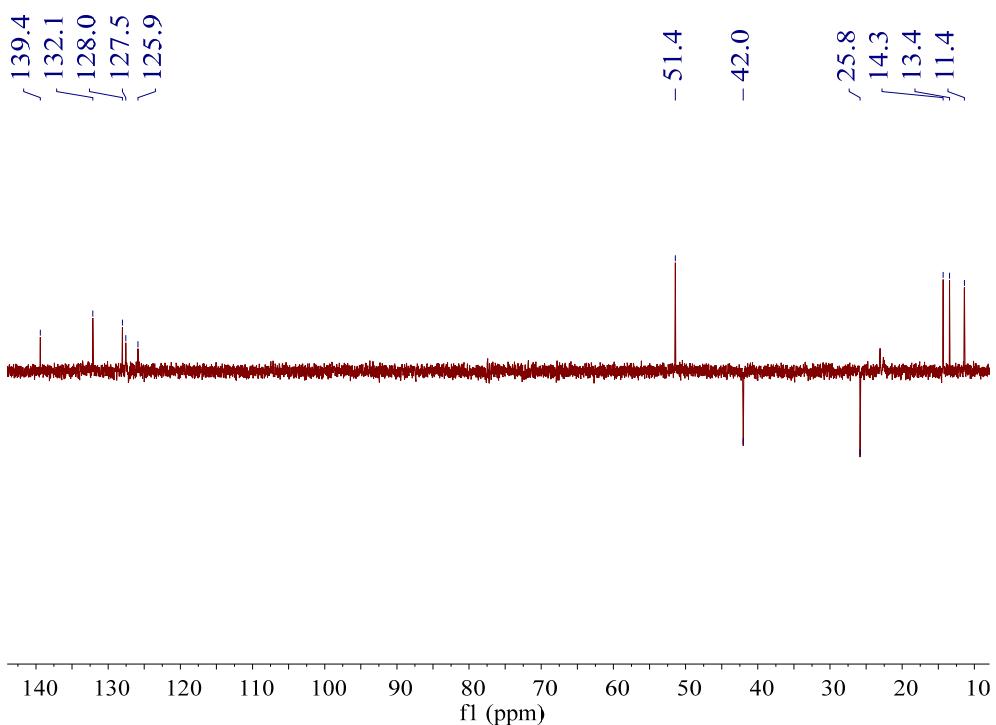


Figure S16. HSQC spectrum of **2** in CDCl_3

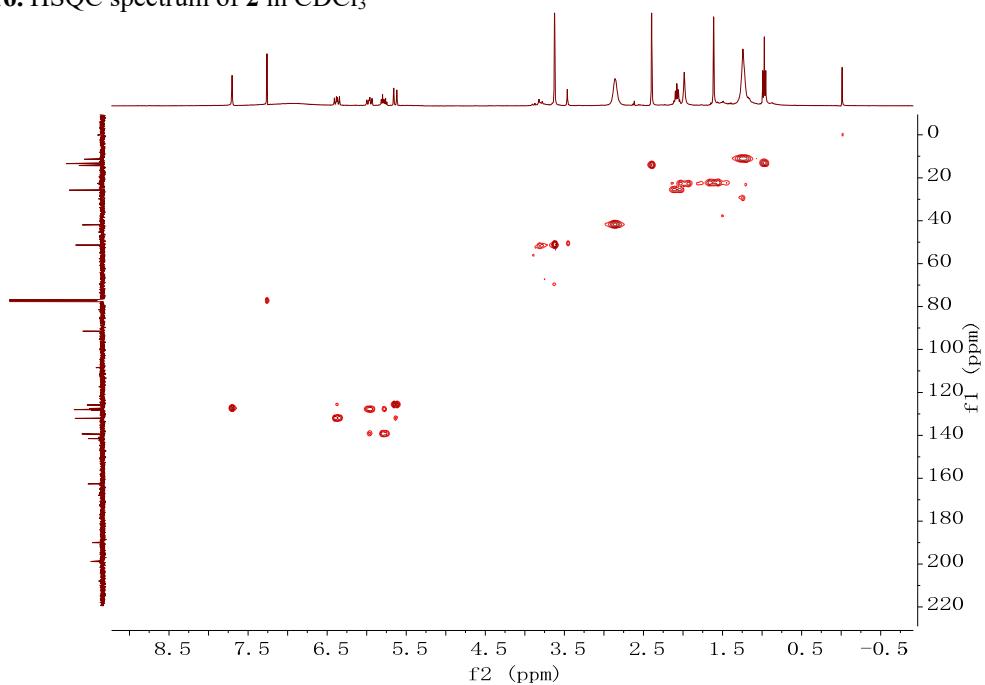


Figure S17. ^1H - ^1H COSY spectrum of **2** in CDCl_3

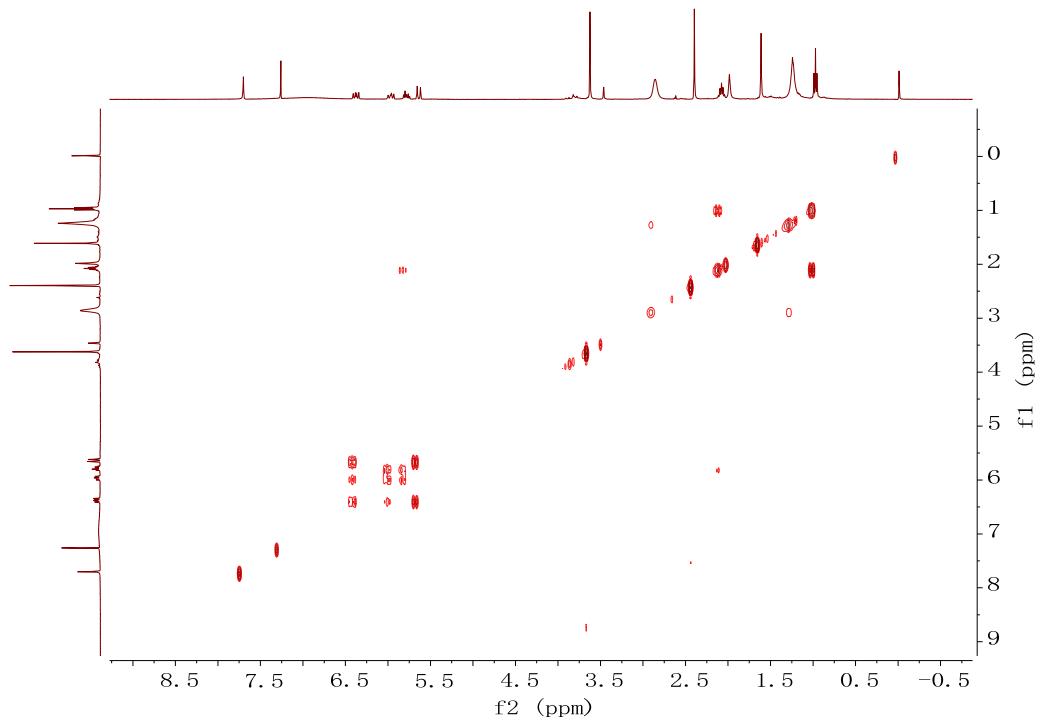


Figure S18. HMBC spectrum of **2** in CDCl_3

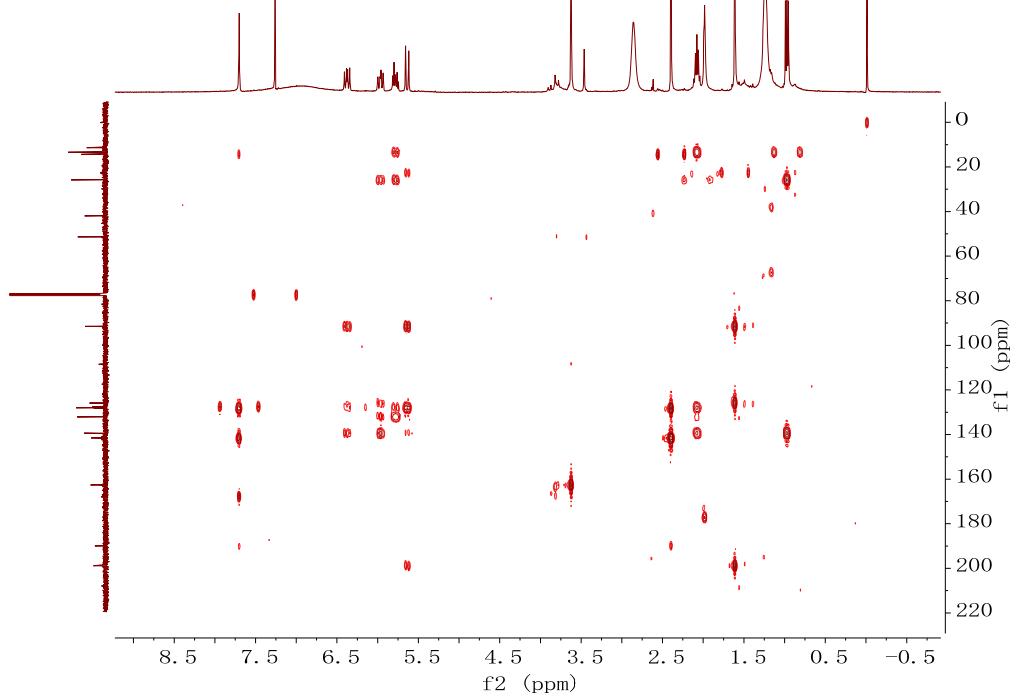


Figure S19. NOESY spectrum of **2** in CDCl_3

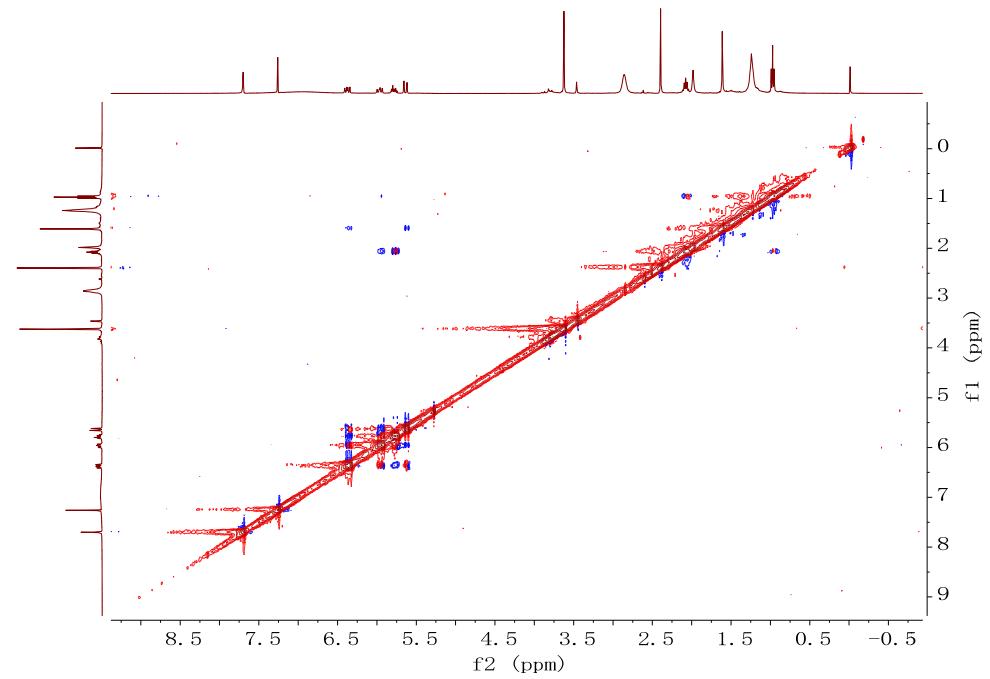


Figure S20. Experimental ECD spectrum of **2**

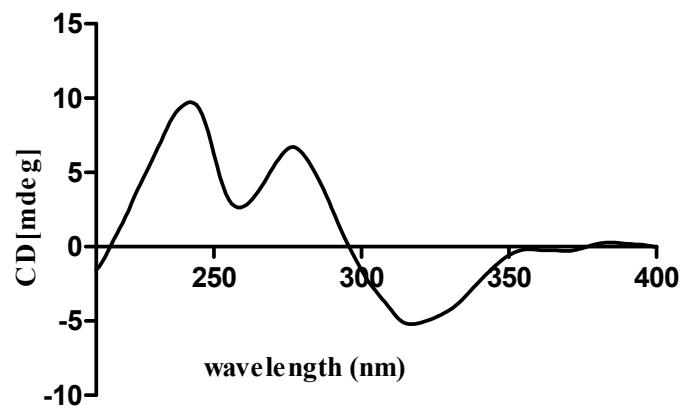


Figure S21. UV spectrum of **2**

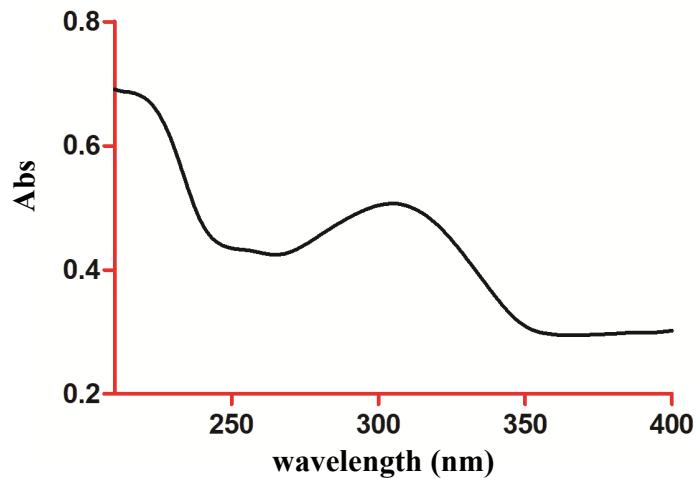


Figure S22. IR spectrum of **2**

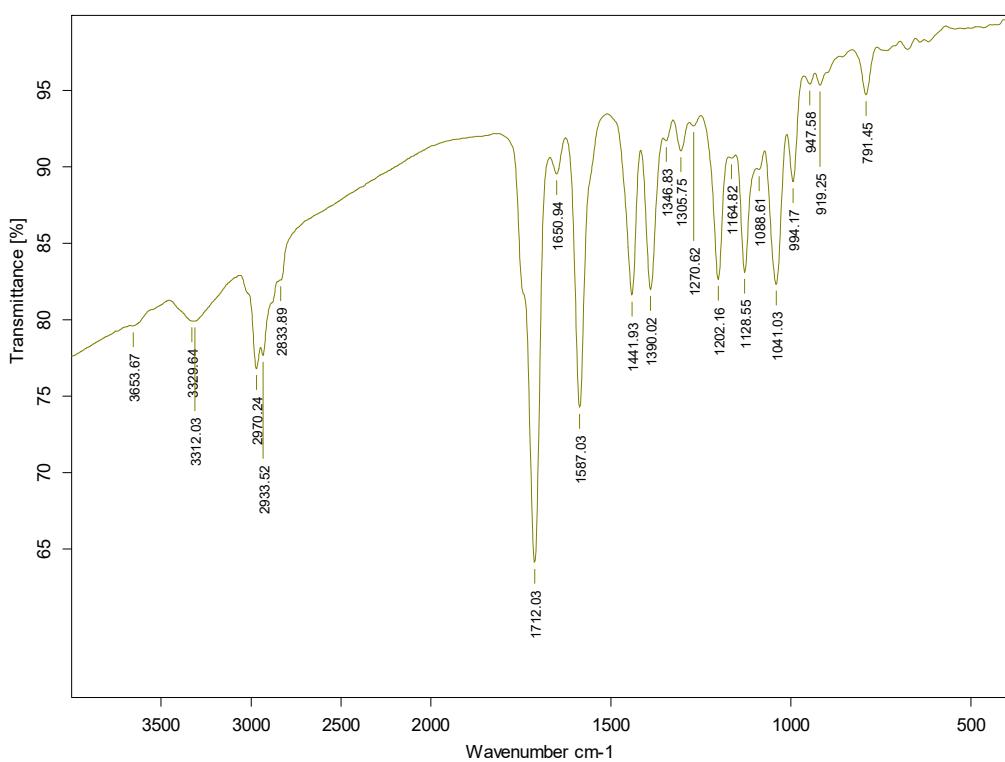


Figure S23. (+)-HR-ESI-MS spectrum of 3

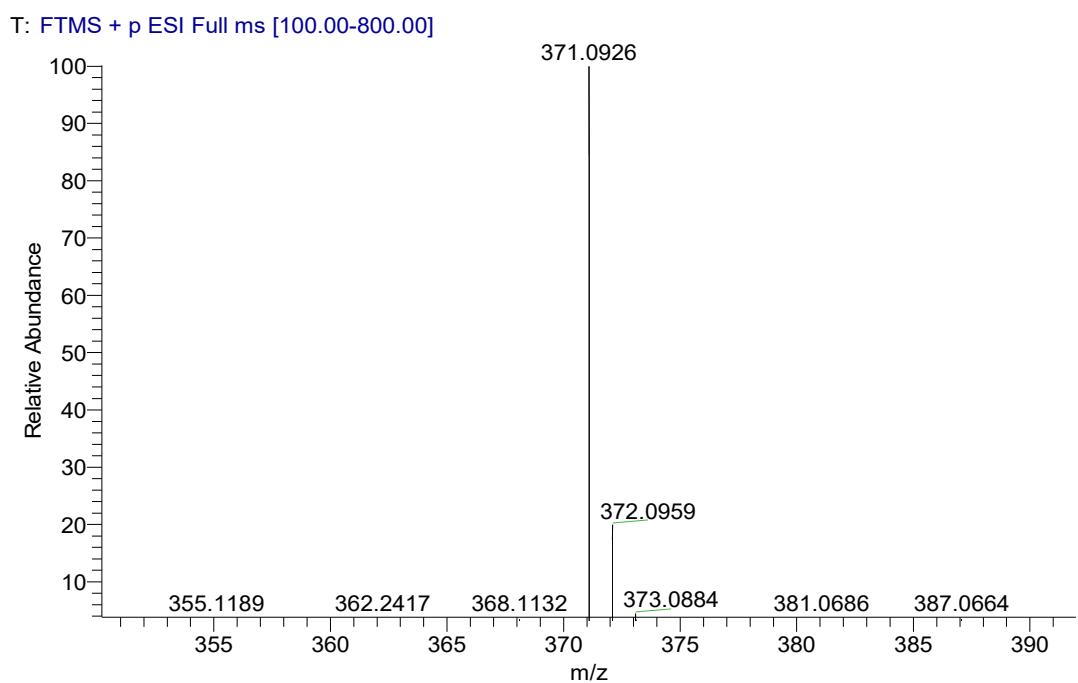


Figure S24. ^1H NMR (400 MHz, CDCl_3) spectrum of 3

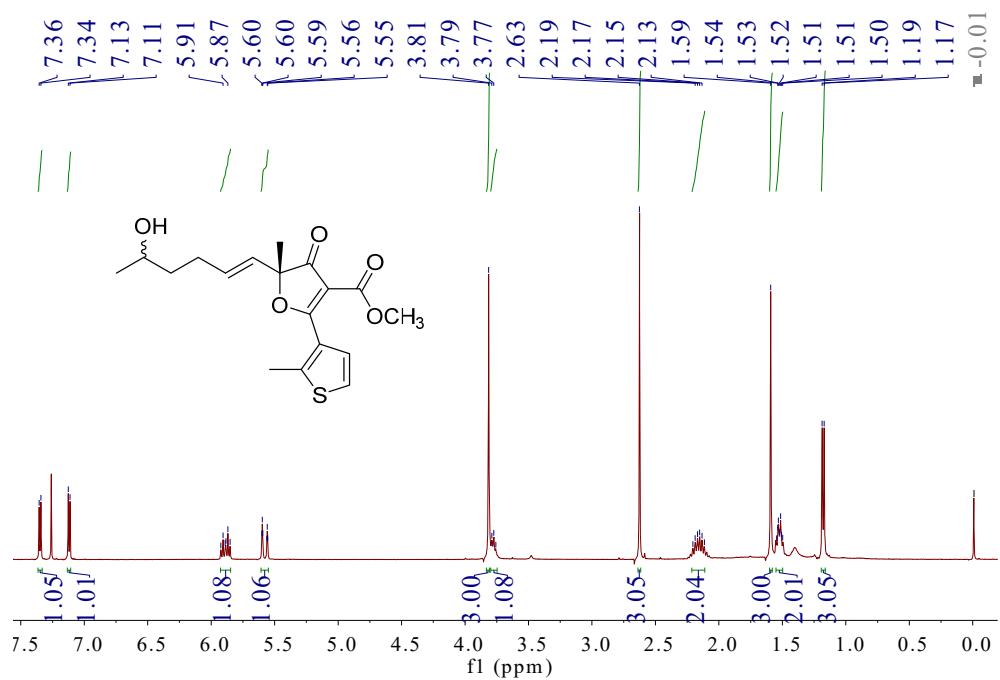


Figure S25. ^1H NMR (400 MHz, CDCl_3) spectra of **3a** and **3b**

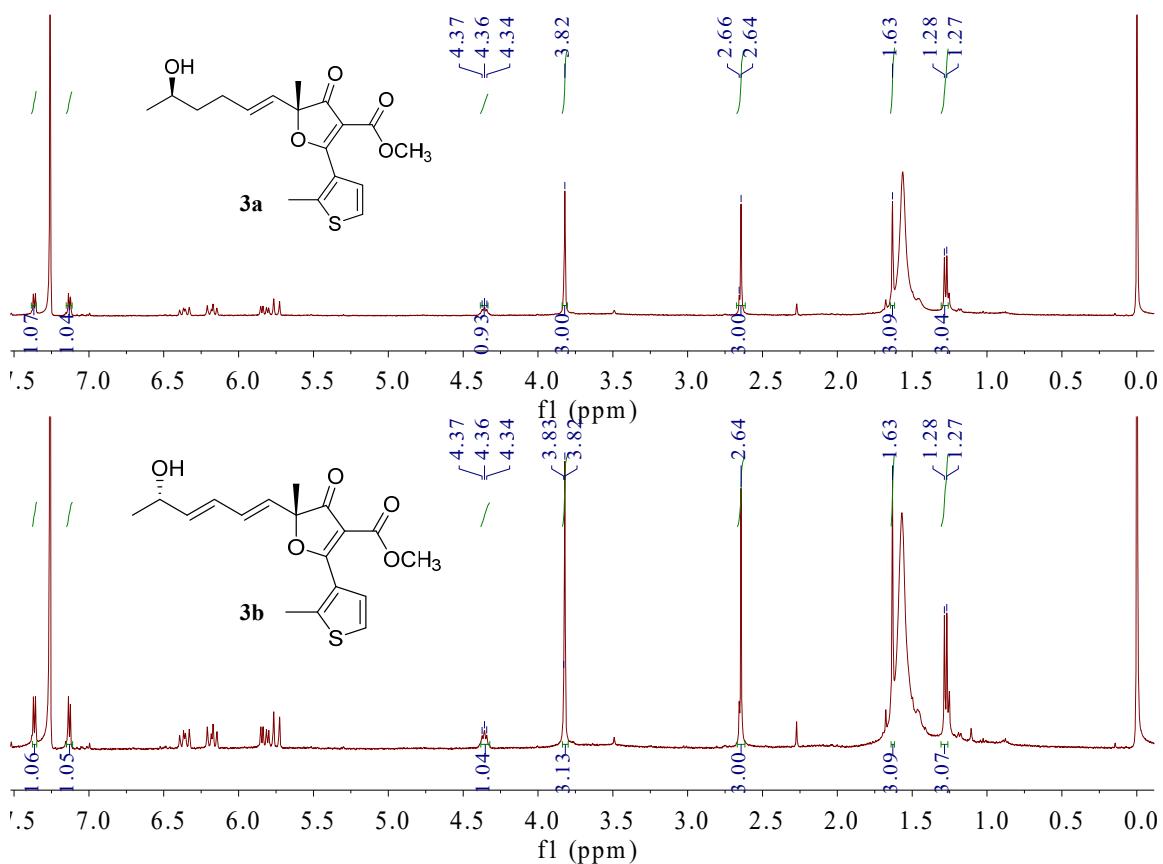


Figure S26. ^{13}C NMR (100 MHz, CDCl_3) spectrum of **3**

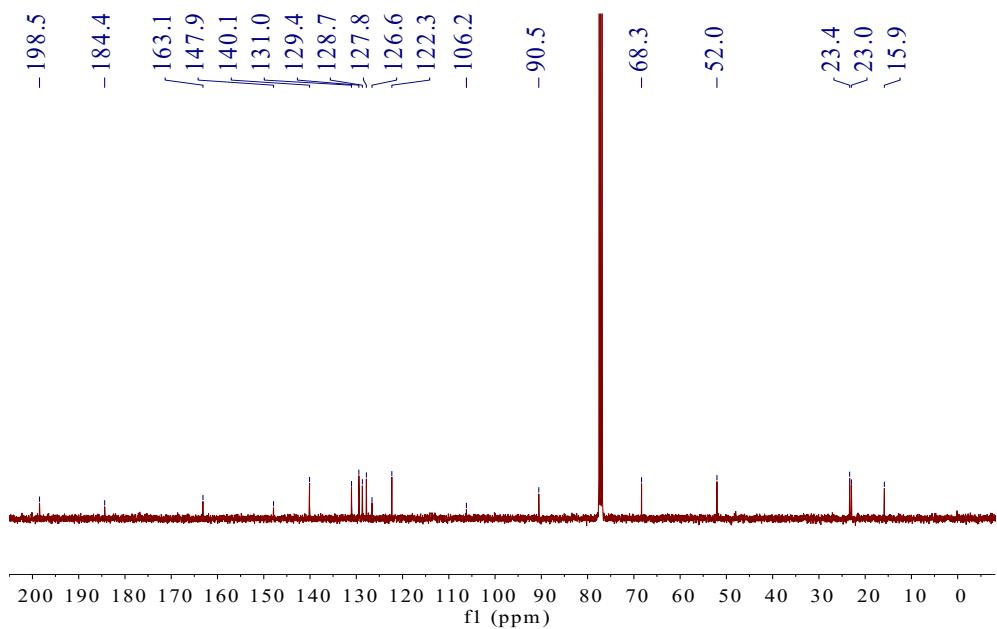


Figure S27. DEPT 135 (100 MHz, CDCl_3) spectrum of **3**

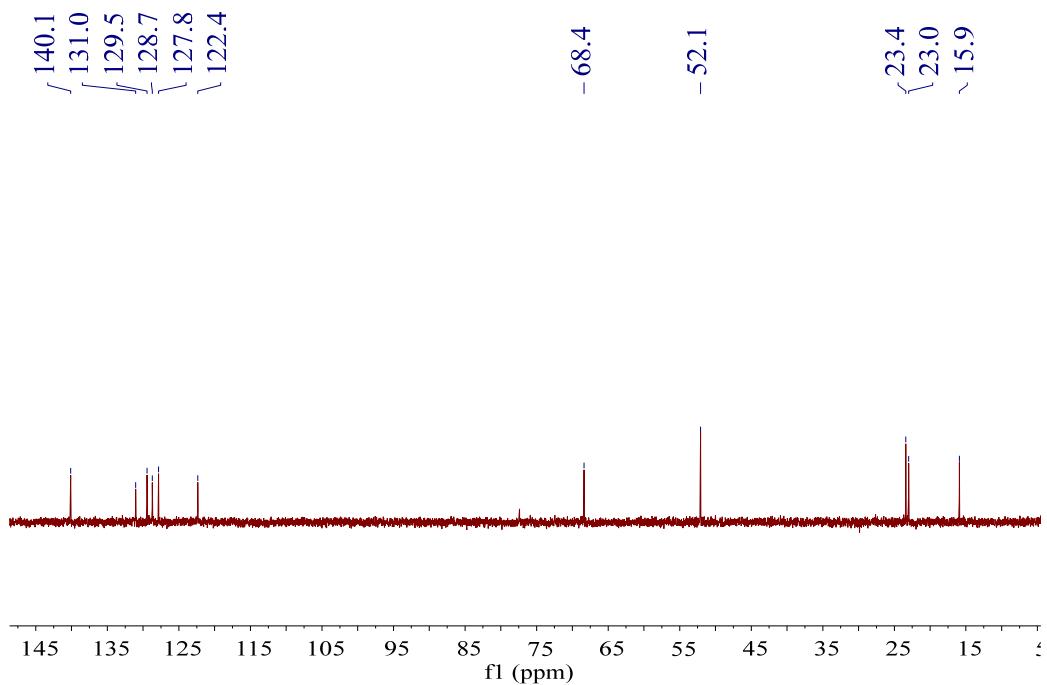


Figure S28. HSQC spectrum of **3** in CDCl_3

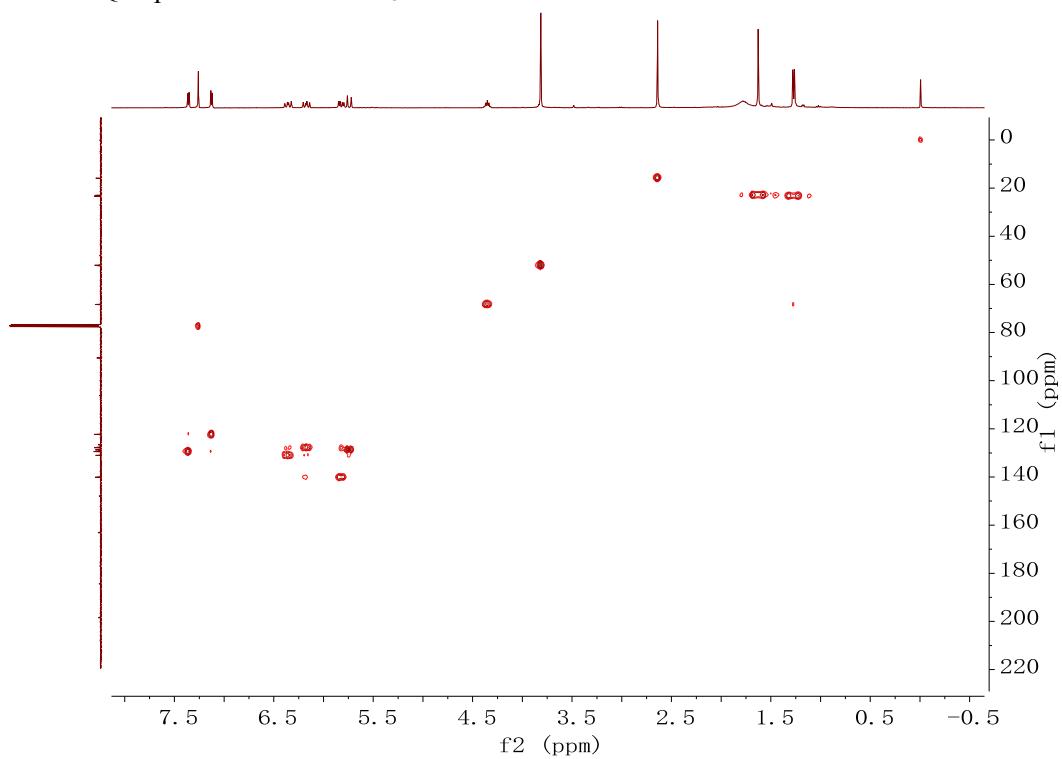


Figure S29. ^1H - ^1H COSY spectrum of **3** in CDCl_3

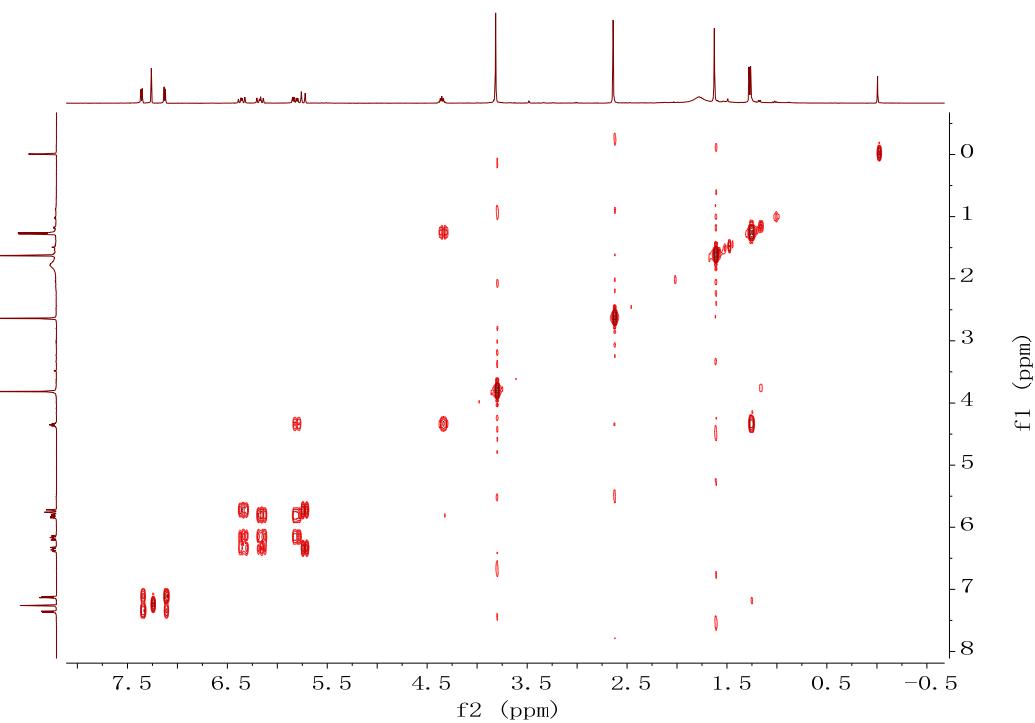


Figure S30. HMBC spectrum of **3** in CDCl_3

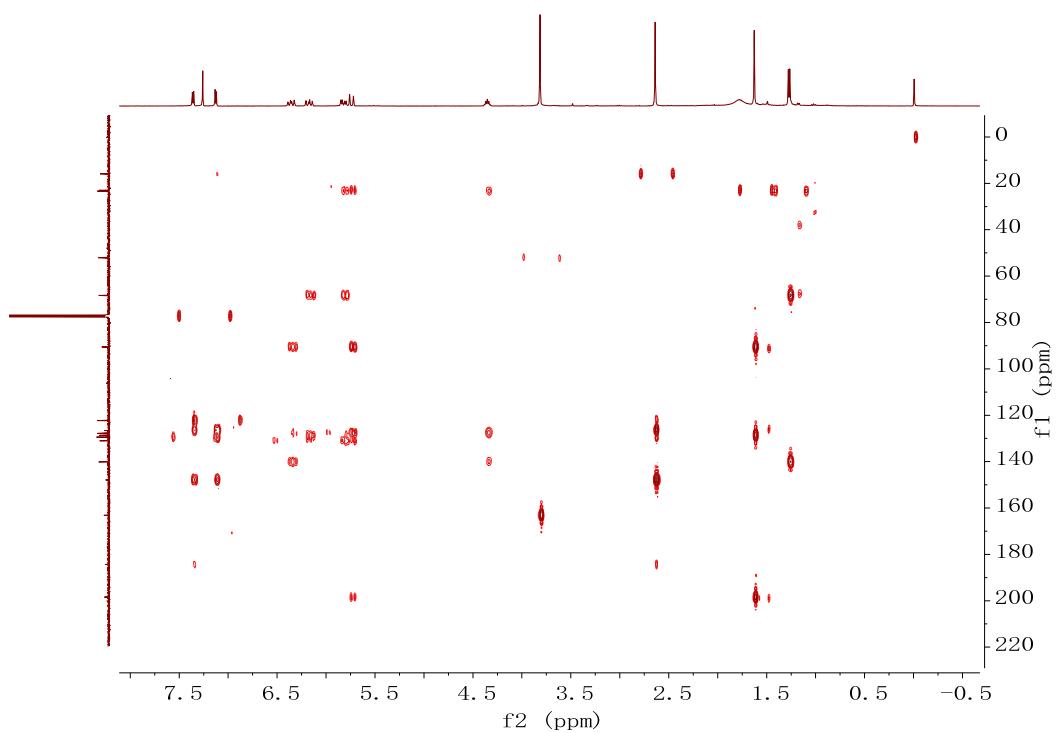


Figure S31. NOESY spectrum of **3** in CDCl_3

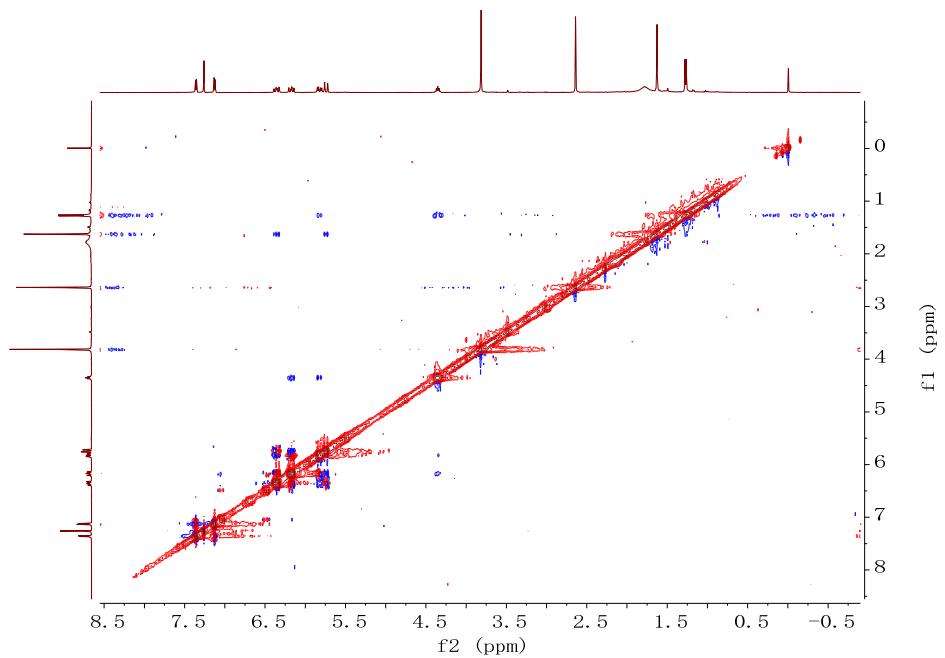


Figure S32. Experimental ECD spectrum of **3a**

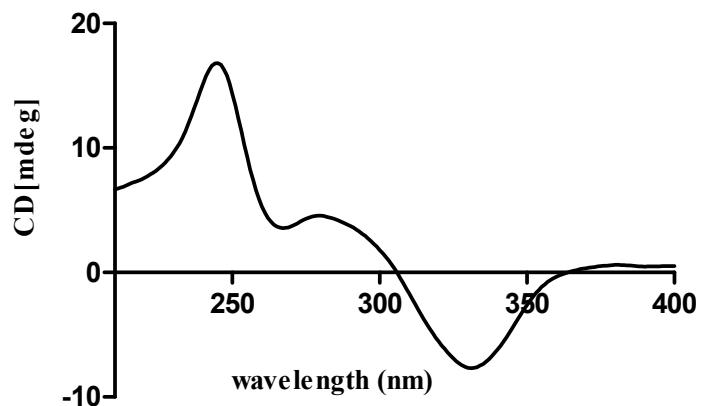


Figure S33. Experimental ECD spectrum of **3b**

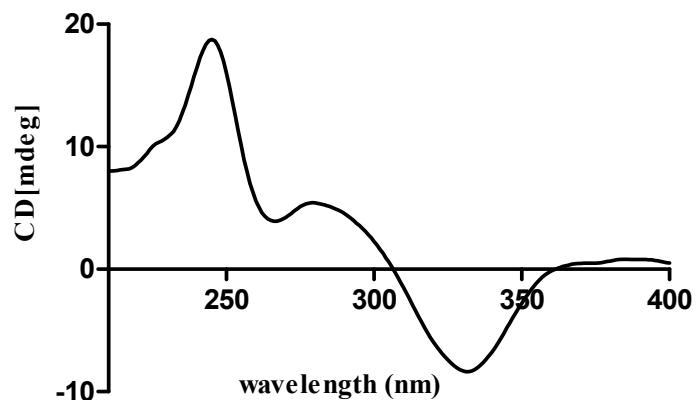


Figure S34. UV spectrum of **3**

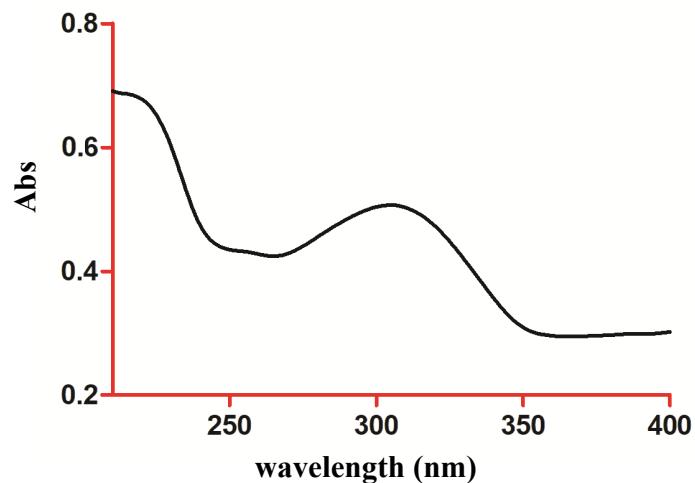


Figure S35. IR spectrum of **3**

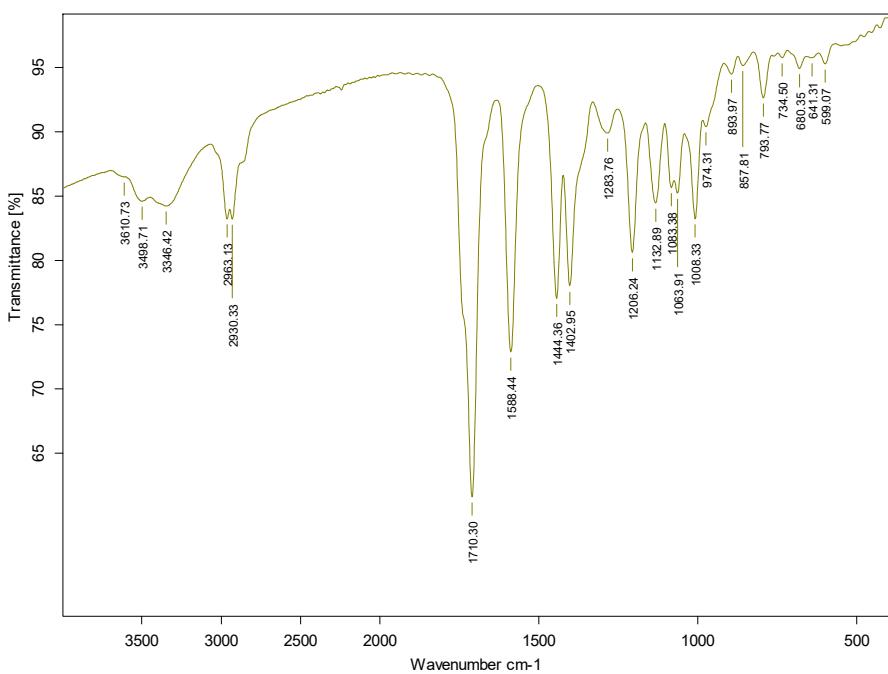


Figure S36. ^1H NMR Spectroscopic for *S*-MTPA ester of **3a**

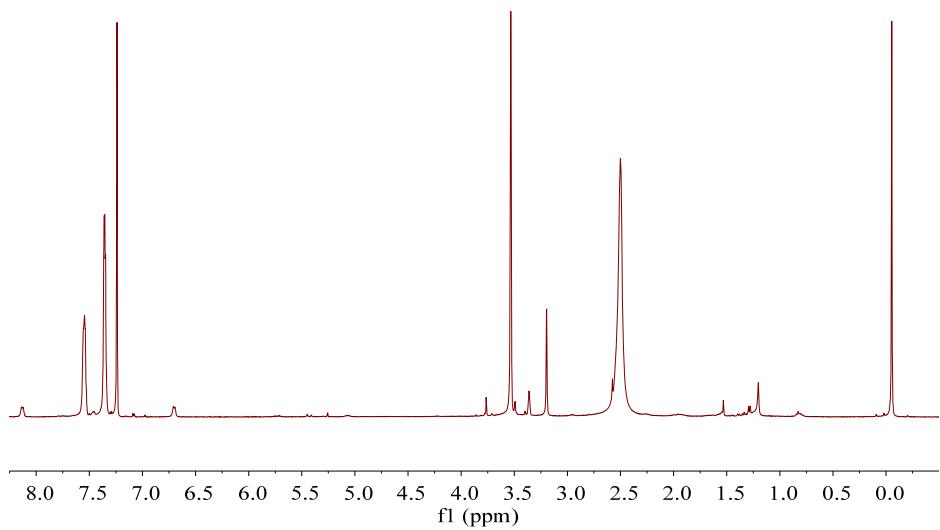


Figure S37. ^1H NMR Spectroscopic for *R*-MTPA ester of **3a**

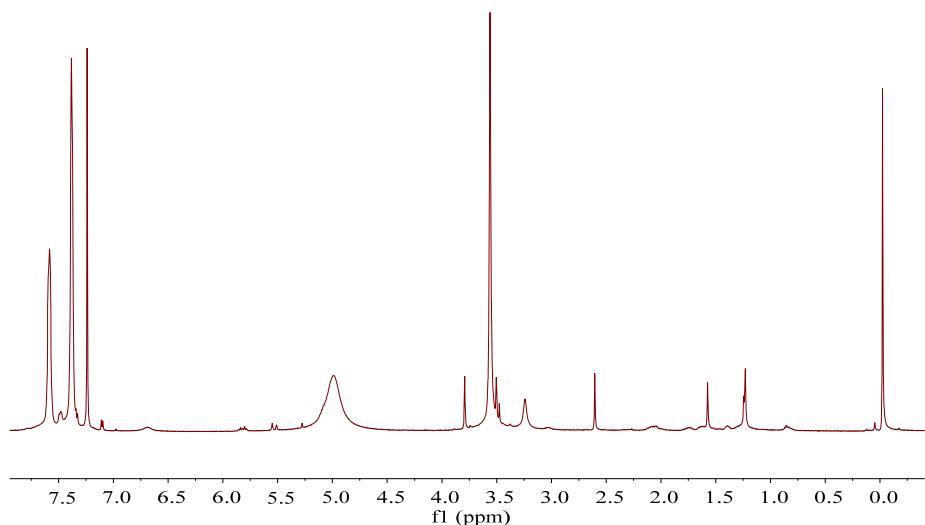


Figure S38. Chiral HPLC separation profiles of **3** (n-hexane-ethanol-Acetic acid, 75:25:0.1; flow: 1.0mL/min)

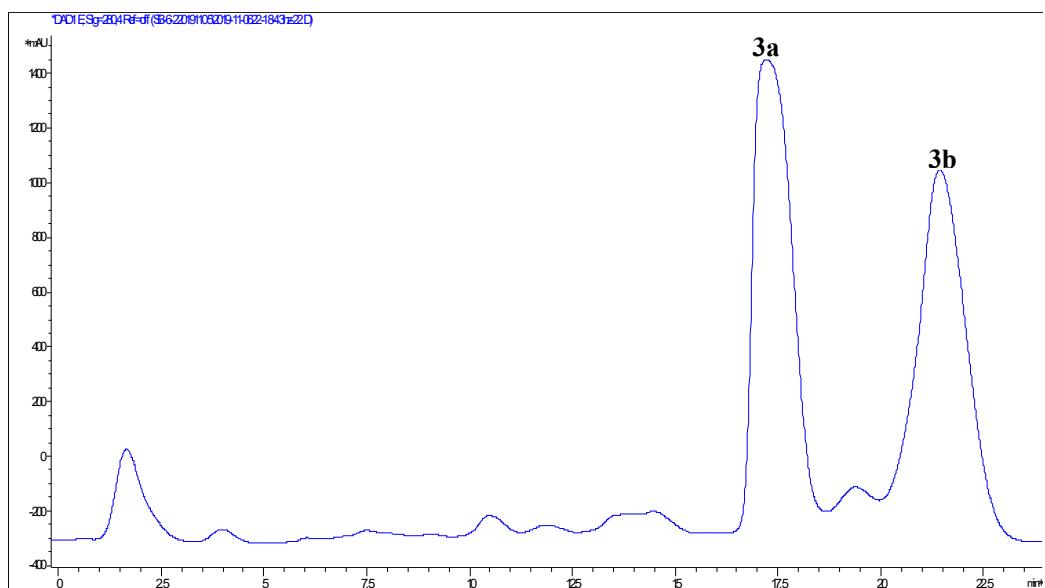


Figure S39. (+)-HR-ESI-MS spectrum of 4

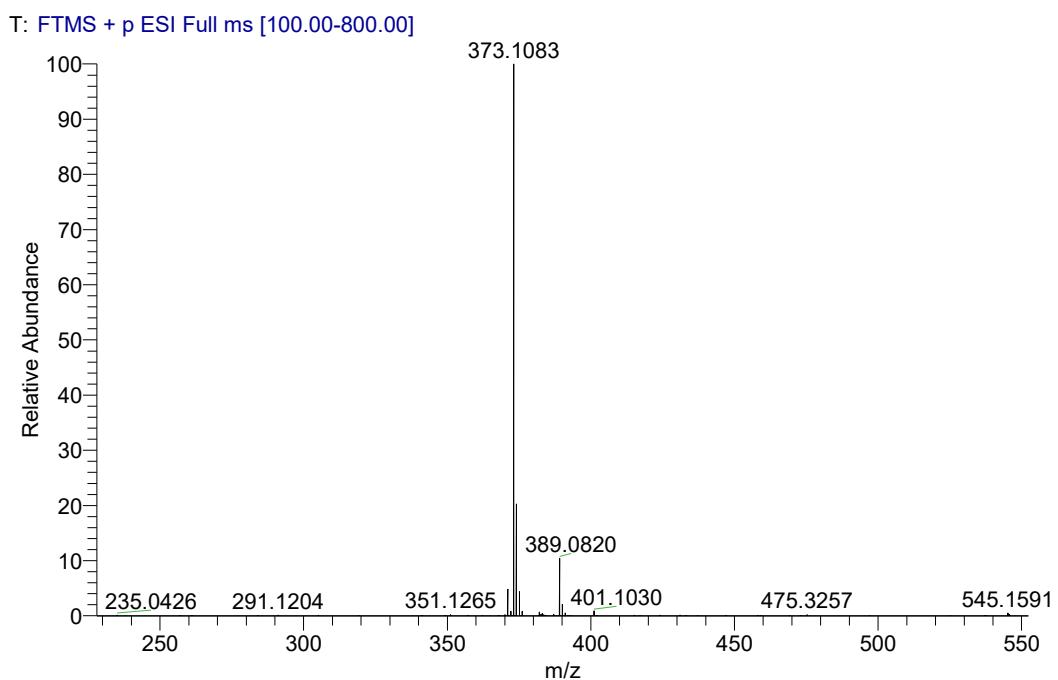


Figure S40. ^1H NMR (400 MHz, CDCl_3) spectrum of 4

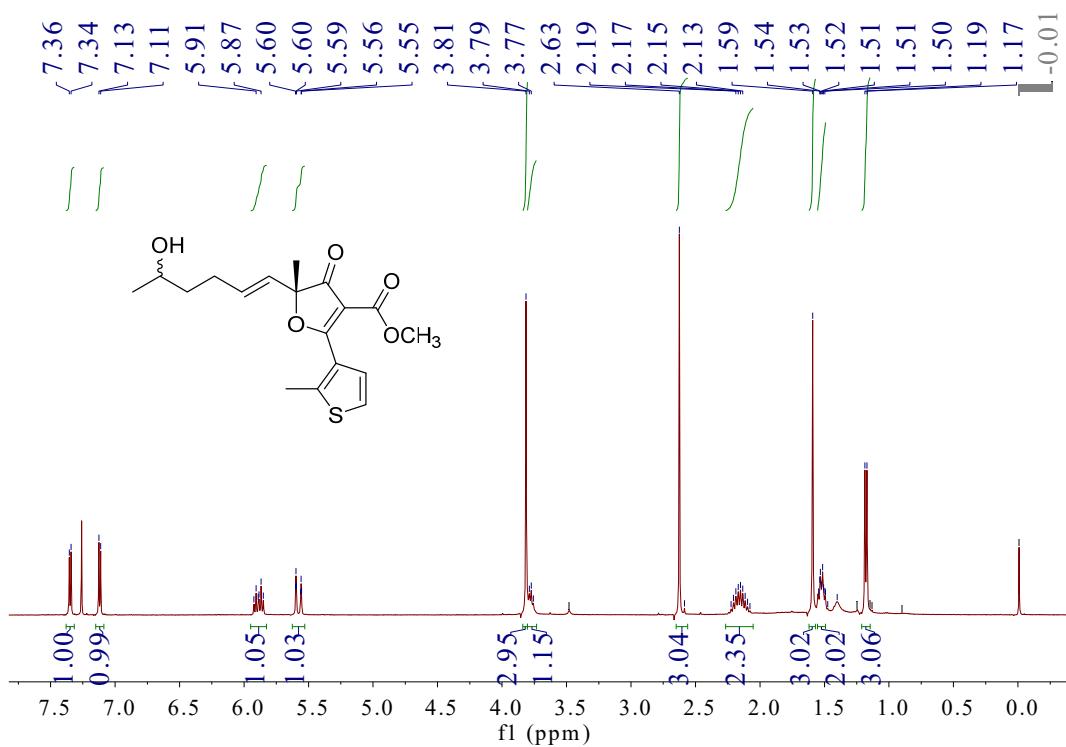


Figure S41. ^1H NMR (400 MHz, CDCl_3) spectra of **4a** and **4b**

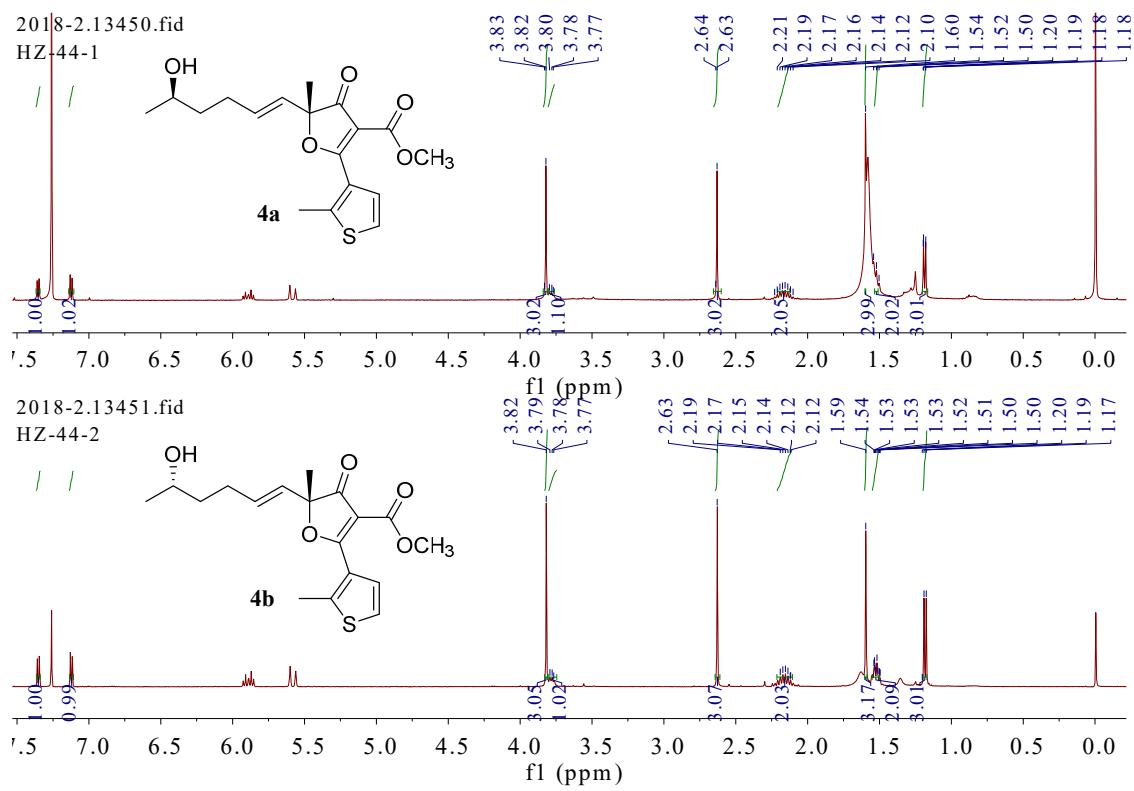


Figure S42. ^{13}C NMR (100 MHz, CDCl_3) spectrum of **4**

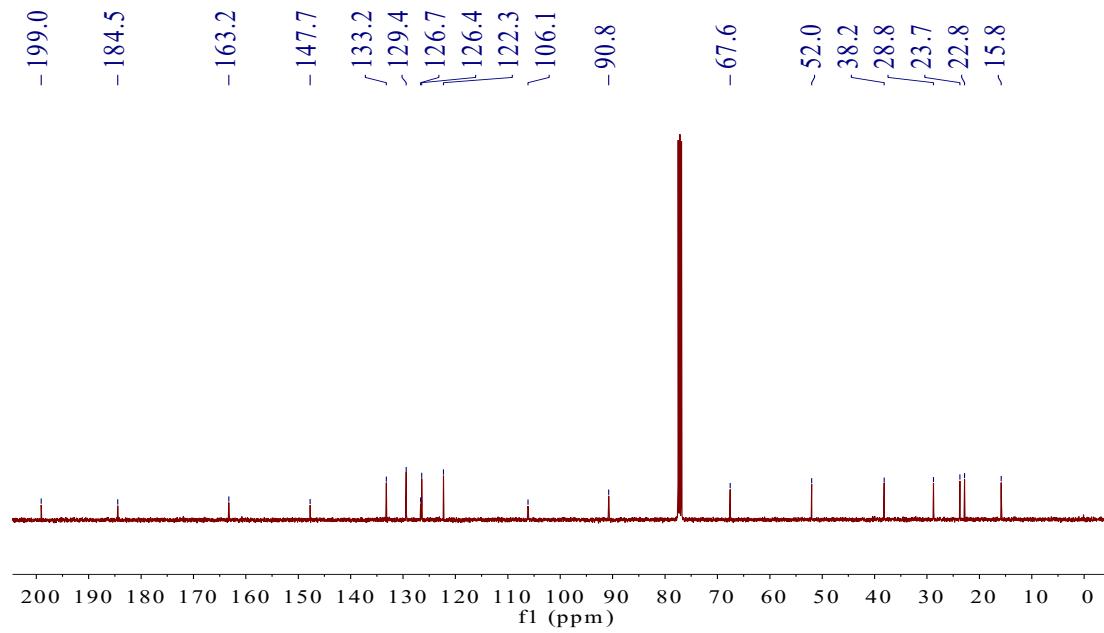


Figure S43. DEPT 135 (100 MHz, CDCl_3) spectrum of **4**

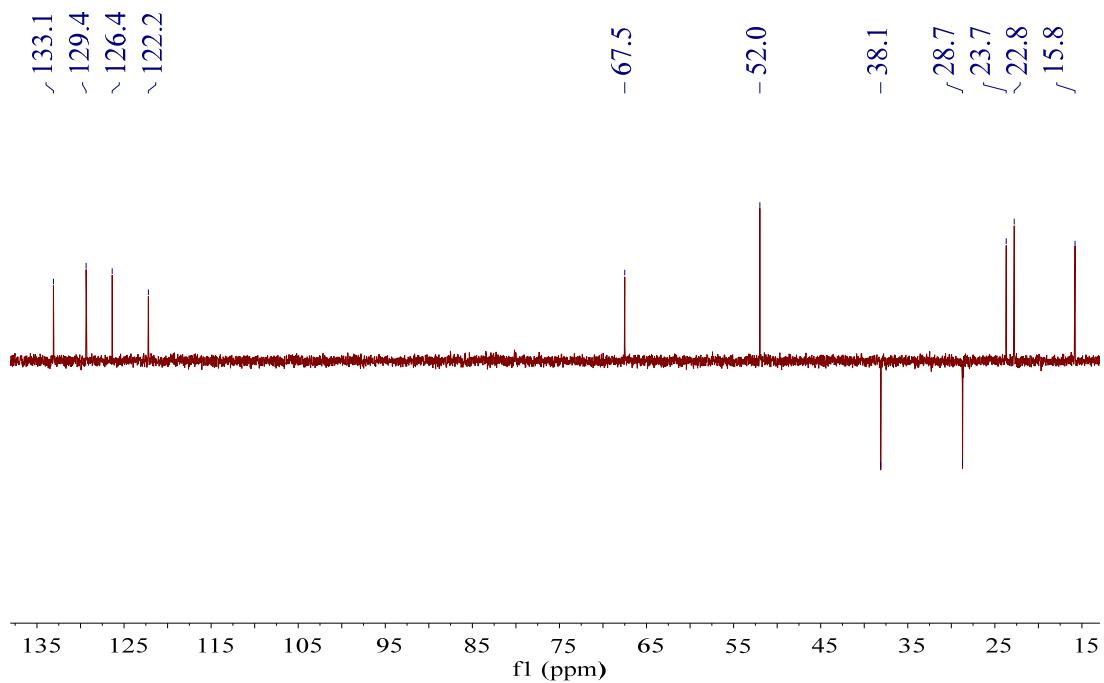


Figure S44. HSQC spectrum of **4** in CDCl_3

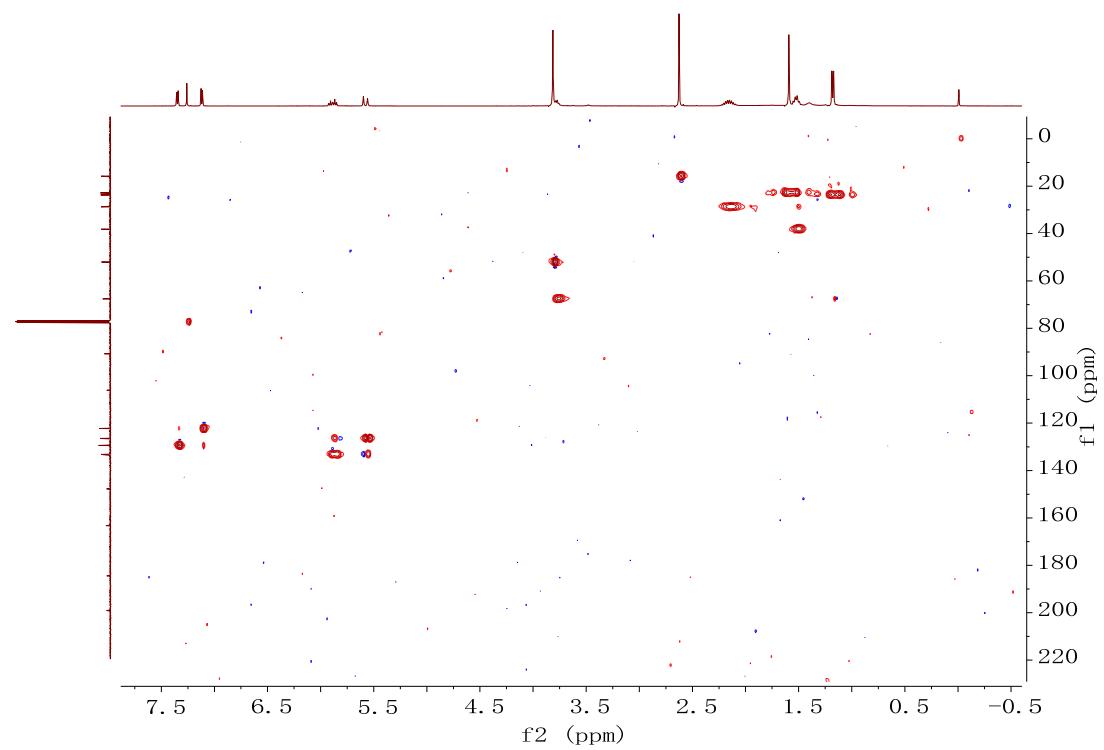


Figure S45. ^1H - ^1H COSY spectrum of **4** in CDCl_3

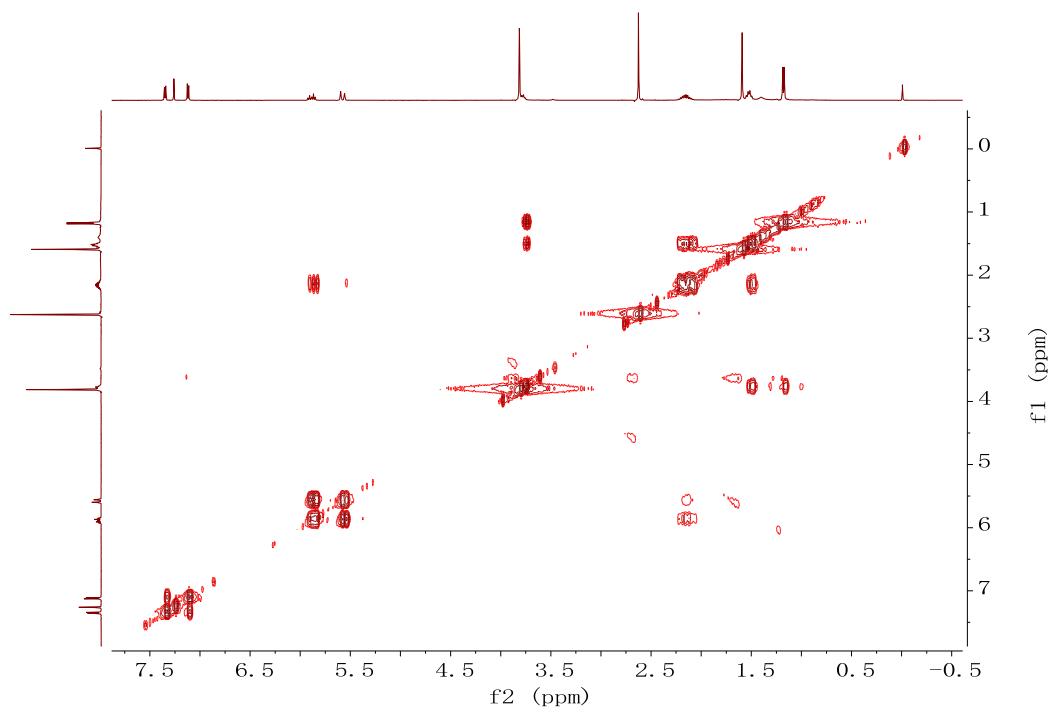


Figure S46. HMBC spectrum of **4** in CDCl_3

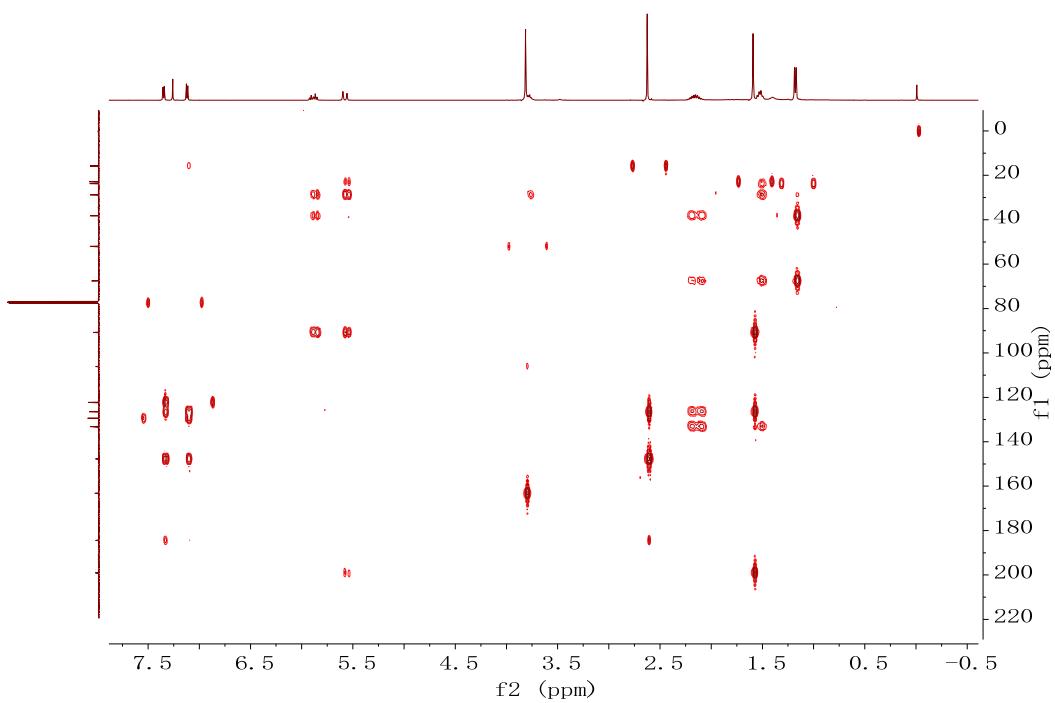


Figure S47. Experimental ECD spectrum of **4a**

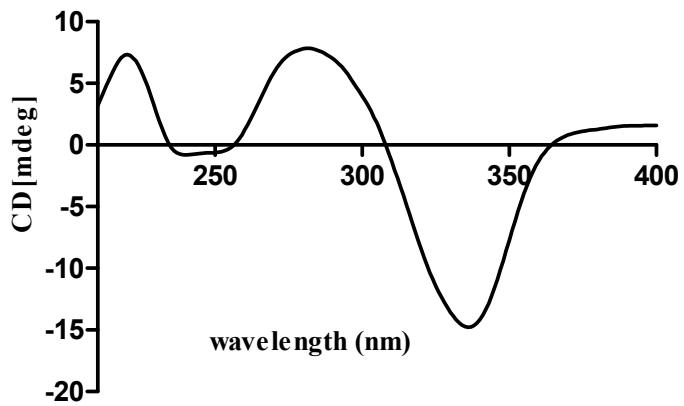


Figure S48. Experimental ECD spectrum of **4b**

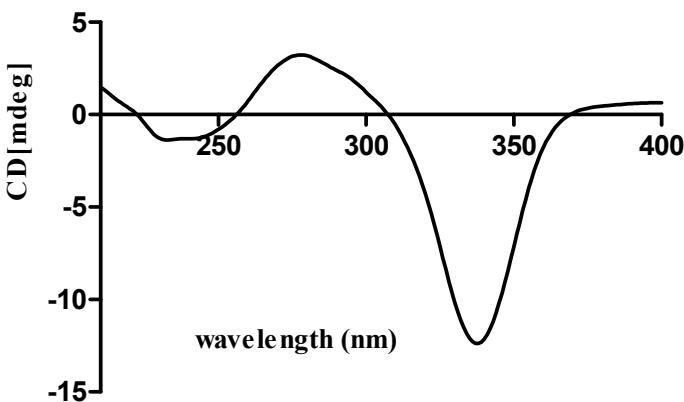


Figure S49. UV spectrum of **4**

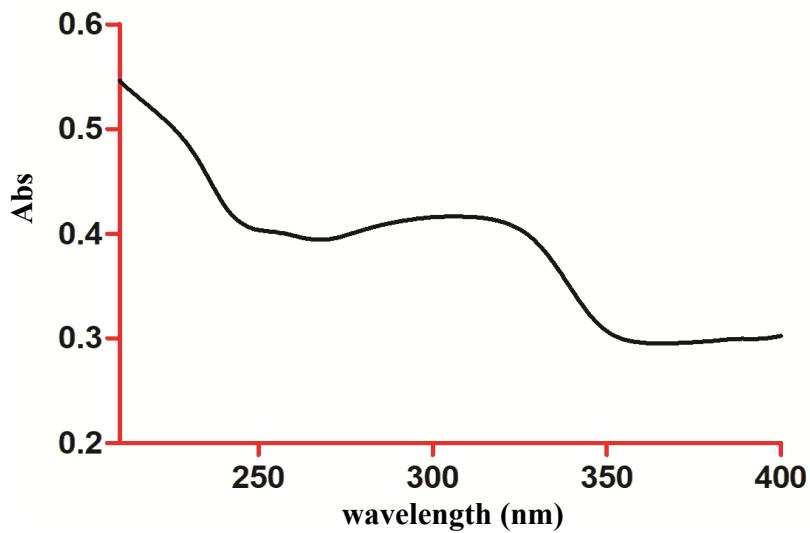


Figure S50. IR spectrum of **4**

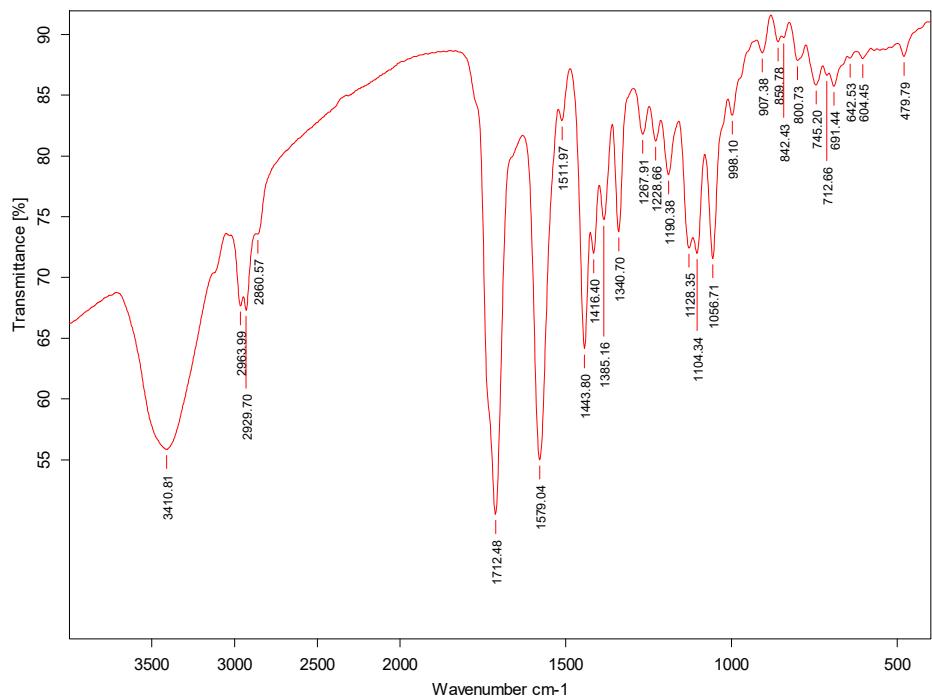


Figure S51. ¹H NMR Spectroscopic for *S*-MTPA ester of **4a**

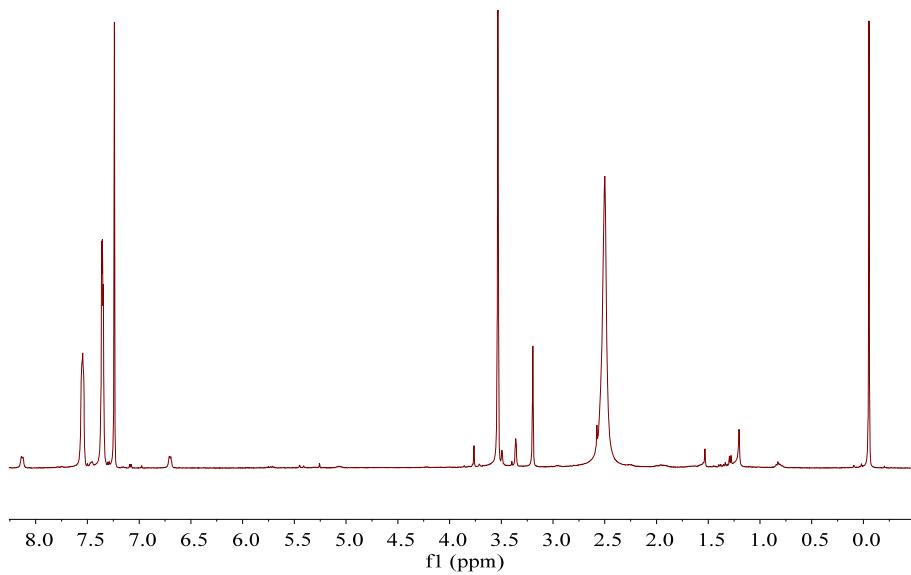


Figure S52. ^1H NMR Spectroscopic for *R*-MTPA ester of **4a**

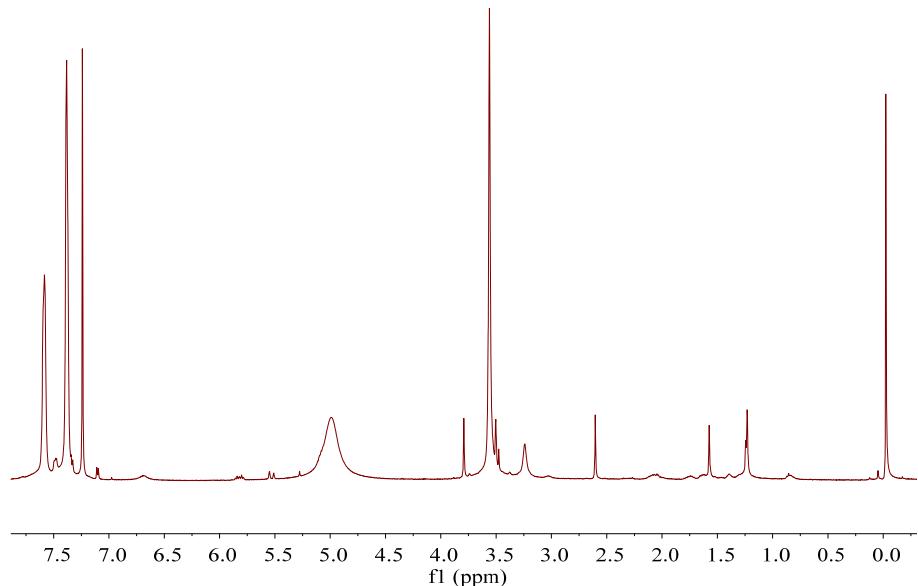


Figure S53. Chiral HPLC separation profiles of **4** (n-hexane-ethanol-Acetic acid, 75:25:0.1; flow: 1.0mL/min)

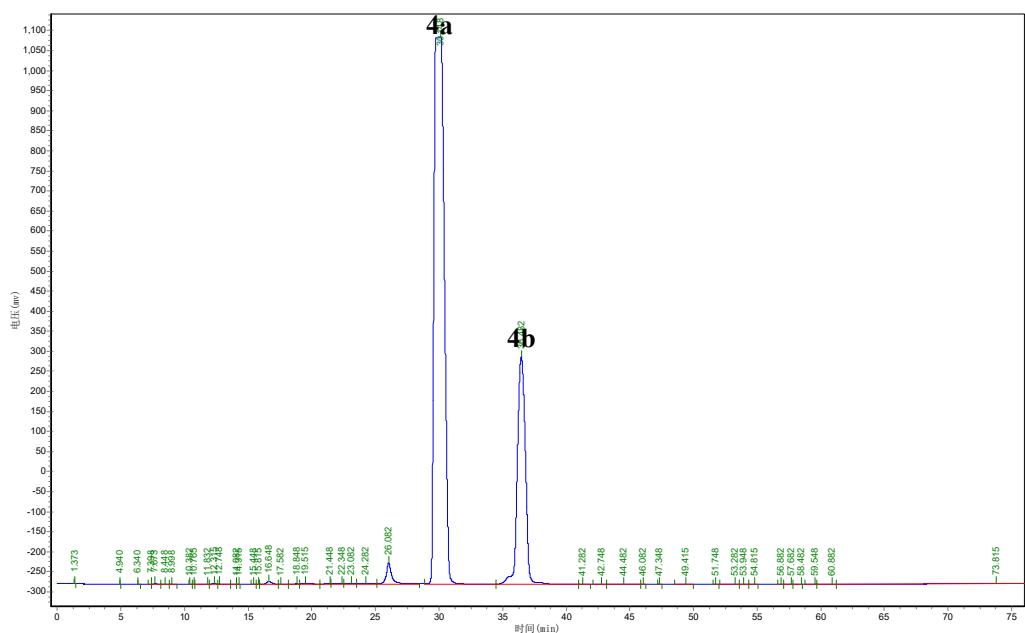


Figure S54. (+)-HR-ESI-MS spectrum of **5**

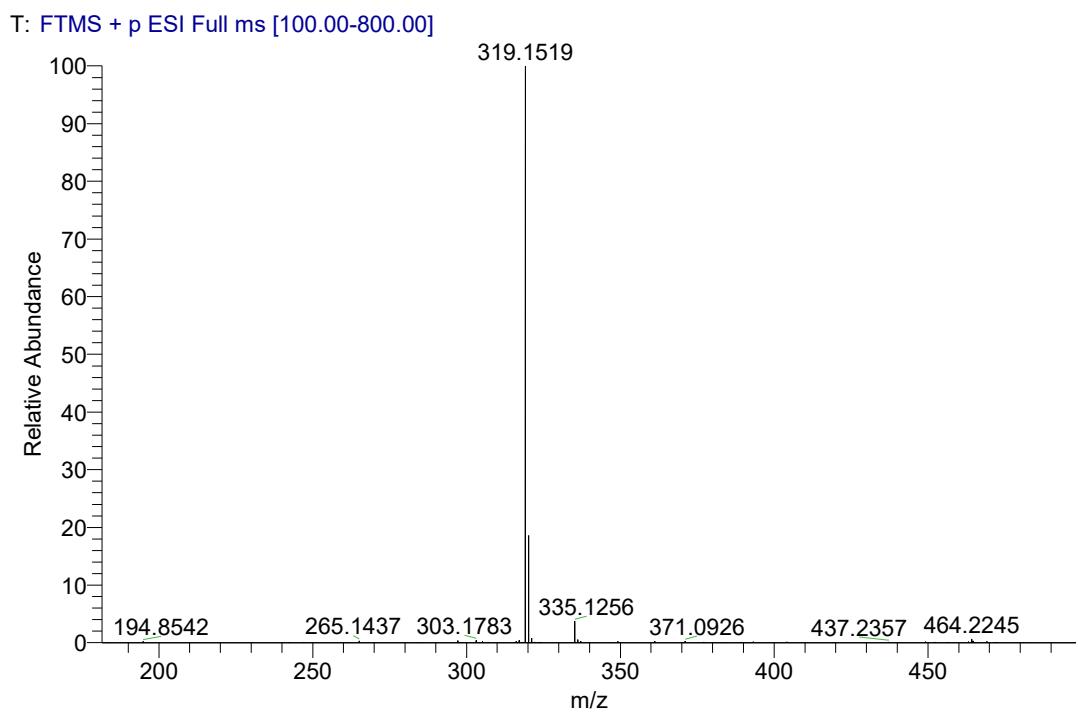


Figure S55. ^1H NMR (400 MHz, CDCl_3) spectrum of **5**

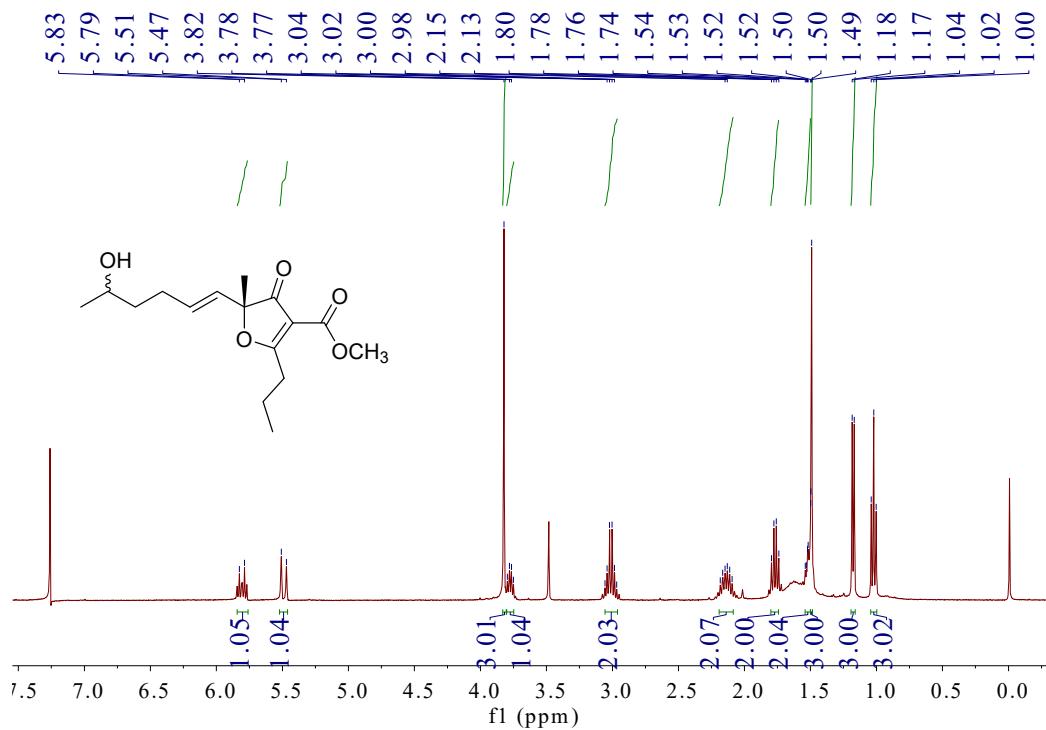


Figure S56. ^1H NMR (400 MHz, CDCl_3) spectra of **5a** and **5b**

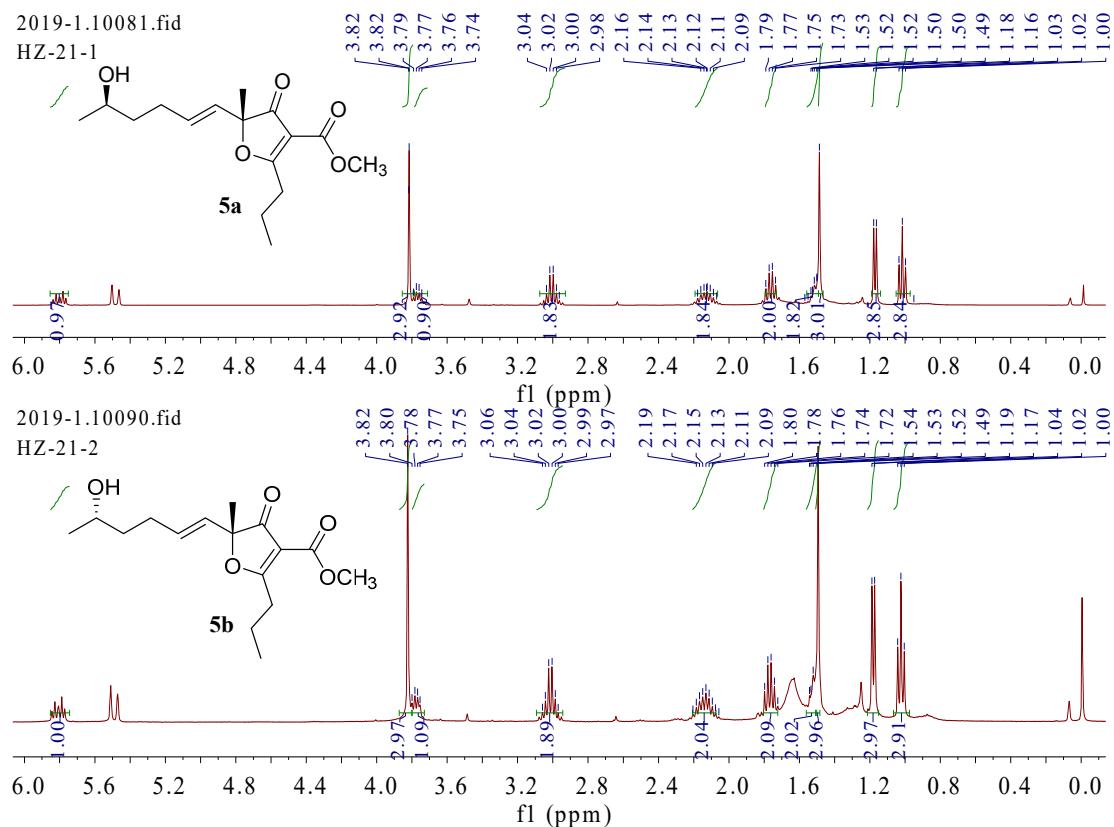


Figure S57. ^{13}C NMR (100 MHz, CDCl_3) spectrum of **5**

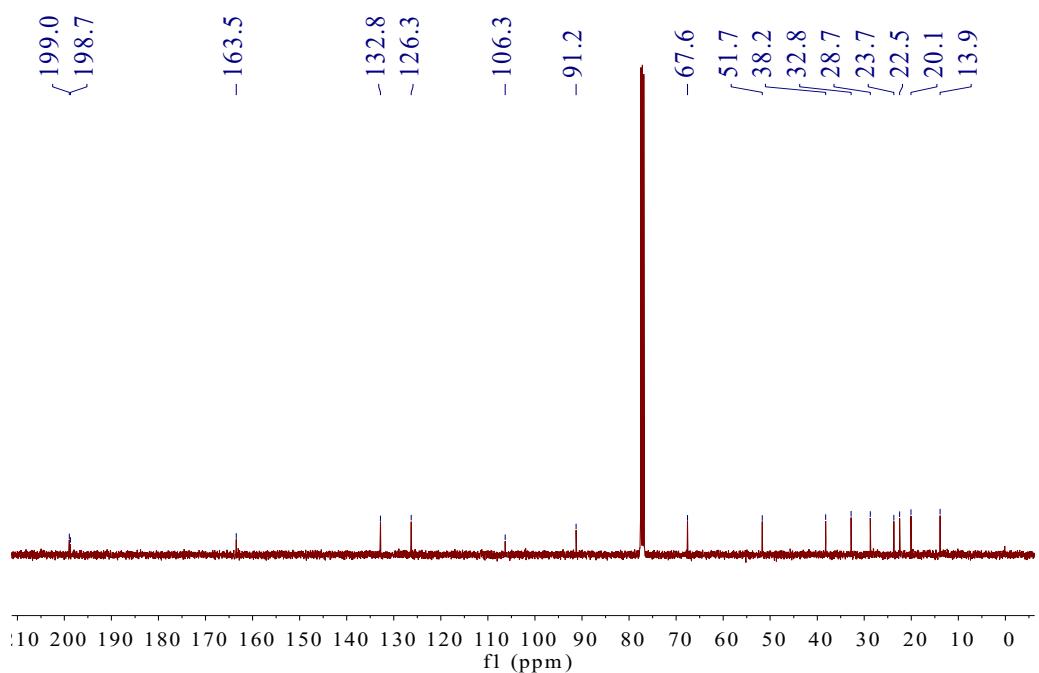


Figure S58. ^{13}C NMR (100 MHz, CDCl_3) spectra of **5a** and **5b**

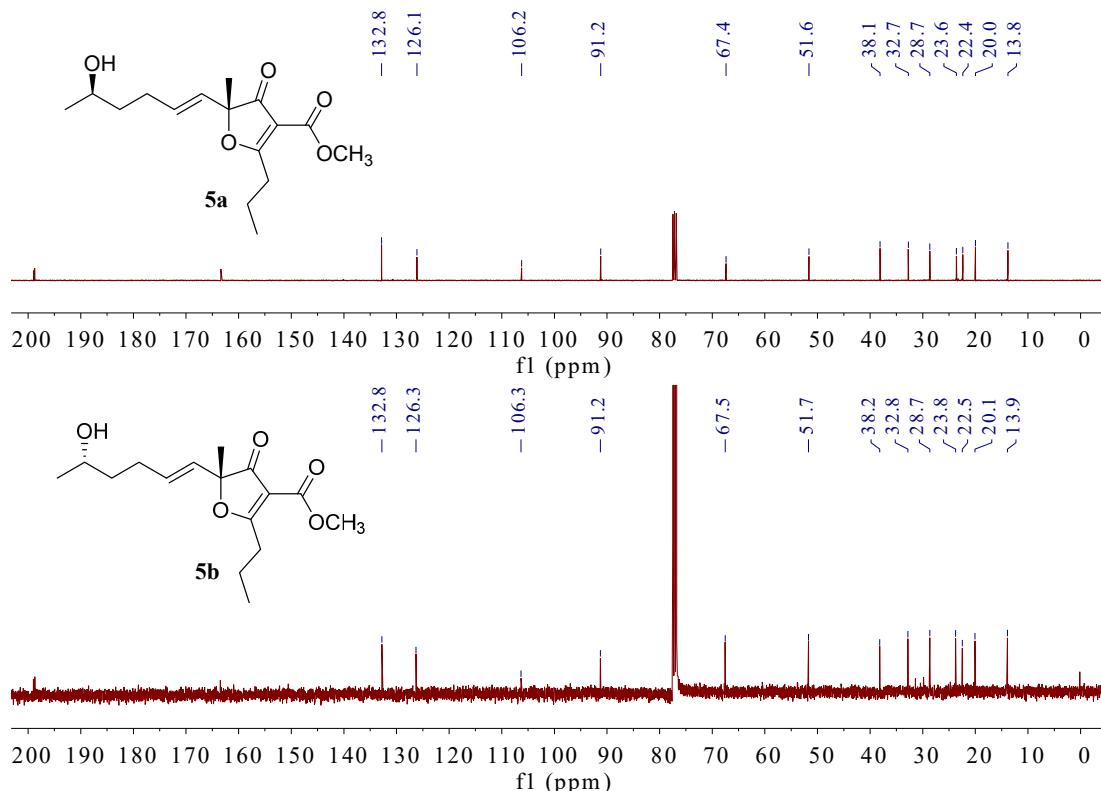


Figure S59. DEPT 135 (100 MHz, CDCl_3) spectrum of **5**

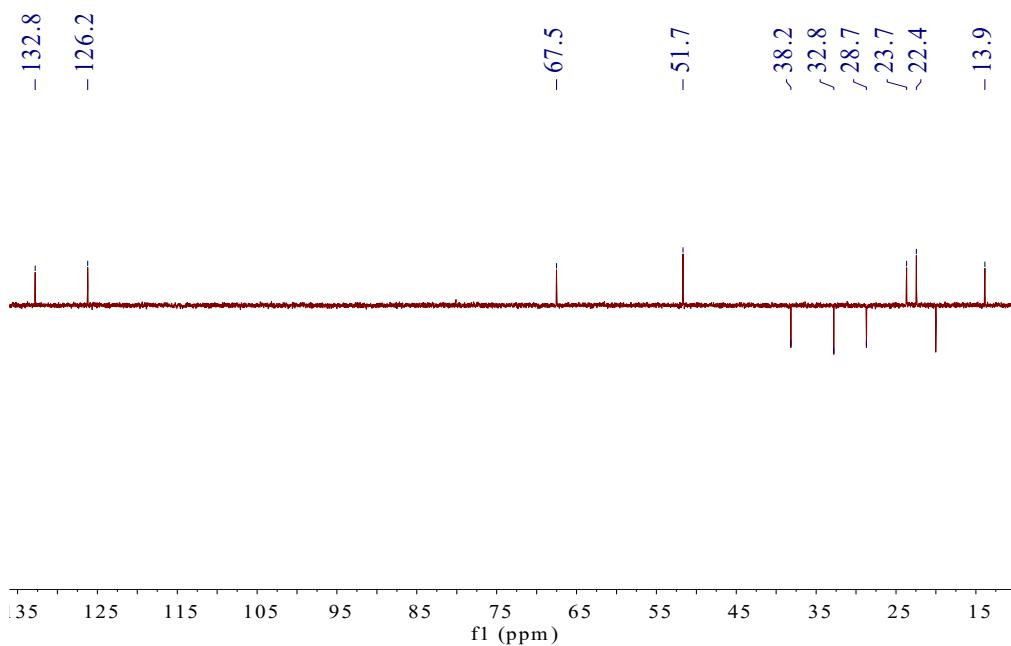


Figure S60. HSQC spectrum of **5** in CDCl_3

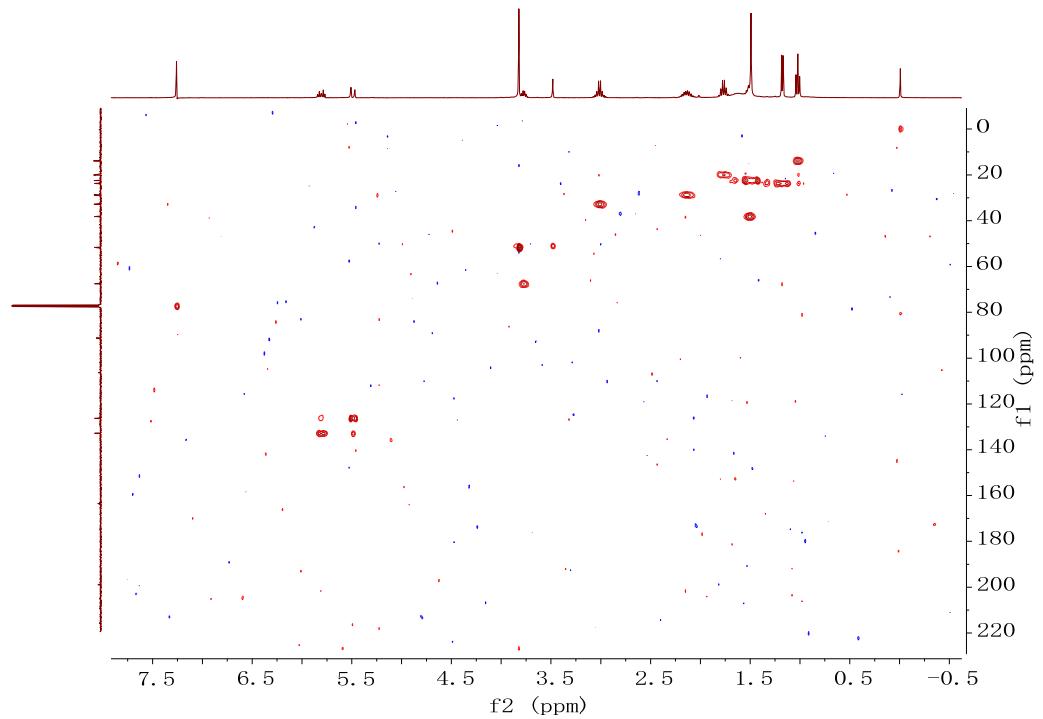


Figure S61. ^1H - ^1H COSY spectrum of **5** in CDCl_3

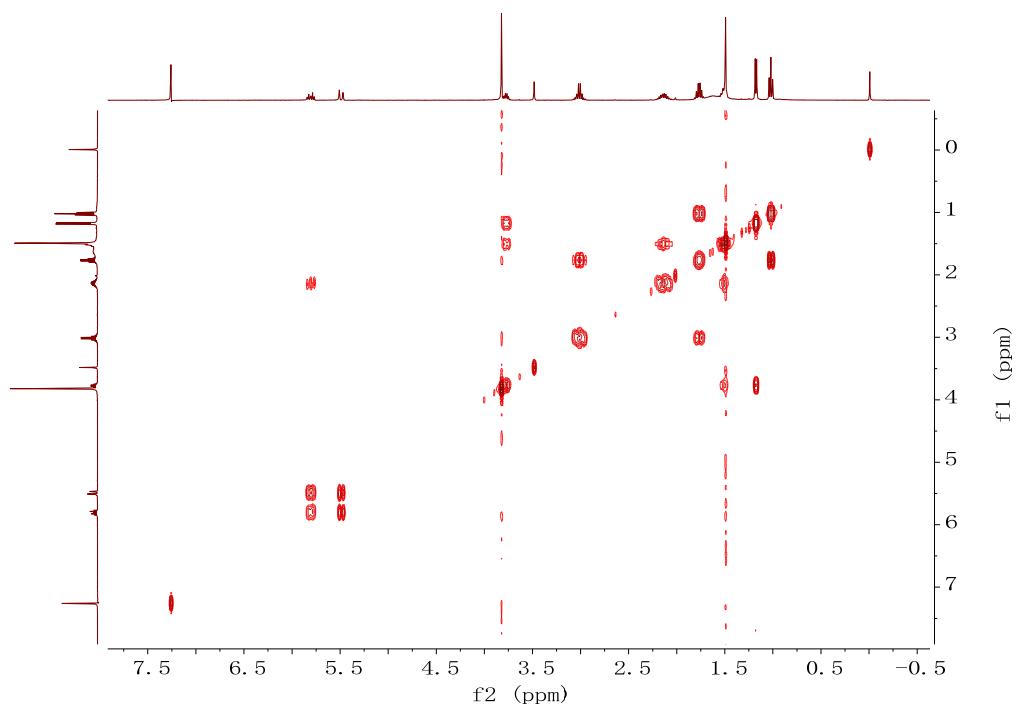


Figure S62. HMBC spectrum of **5** in CDCl_3

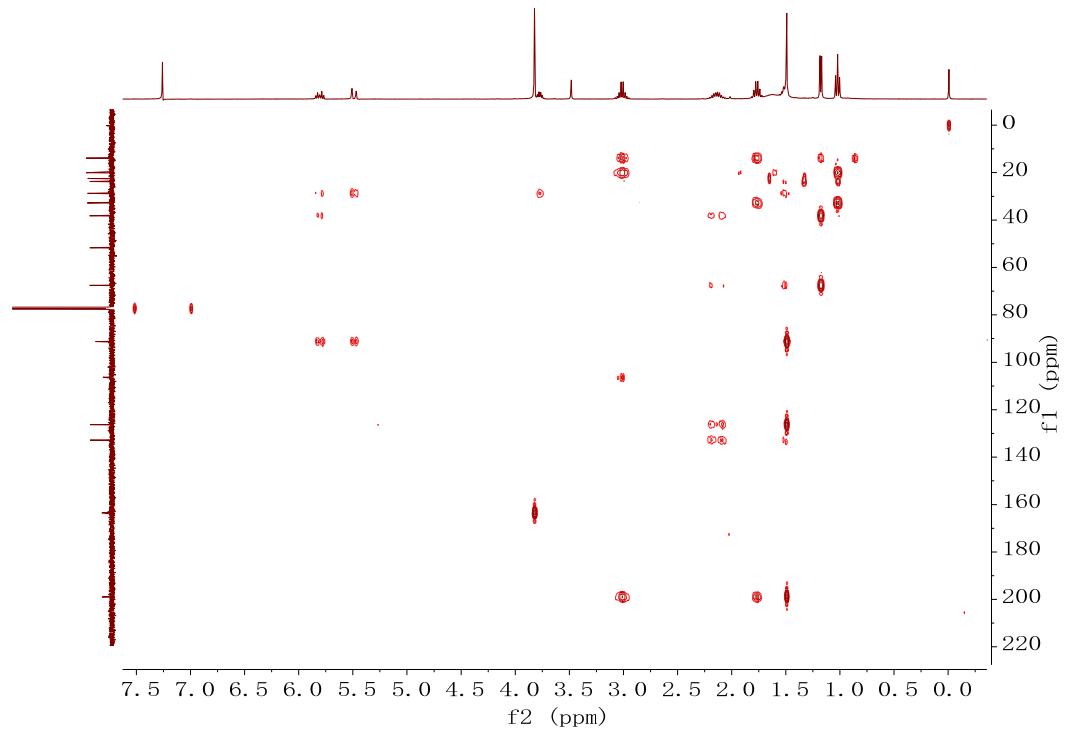


Figure S63. NOESY spectrum of **5** in CDCl_3

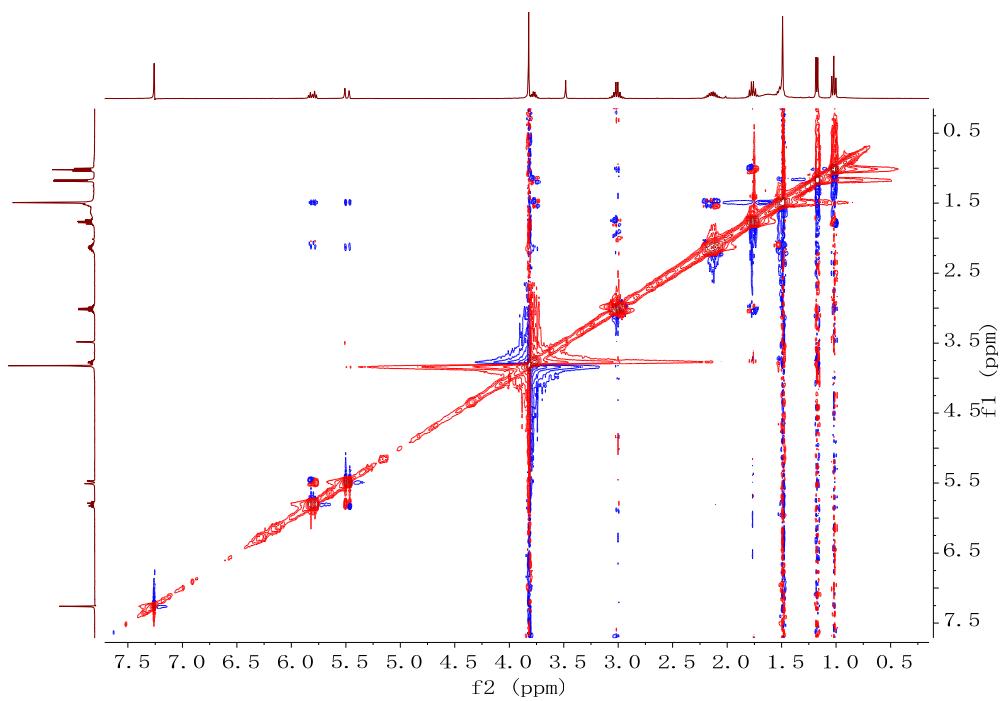


Figure S64. Experimental ECD spectrum of **5a**

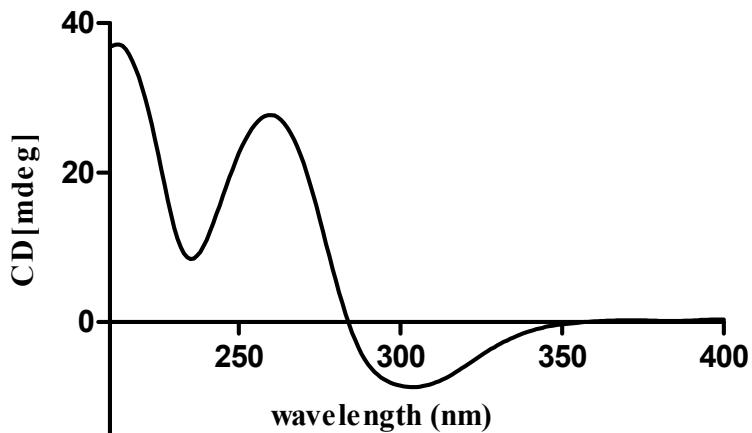


Figure S65. Experimental ECD spectrum of **5b**

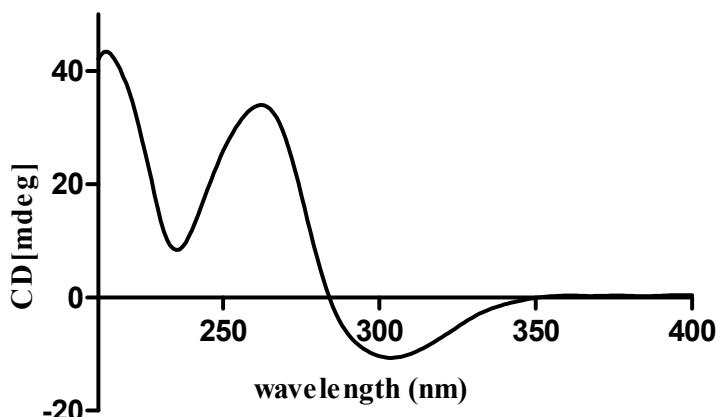


Figure S66. UV spectrum of **5**

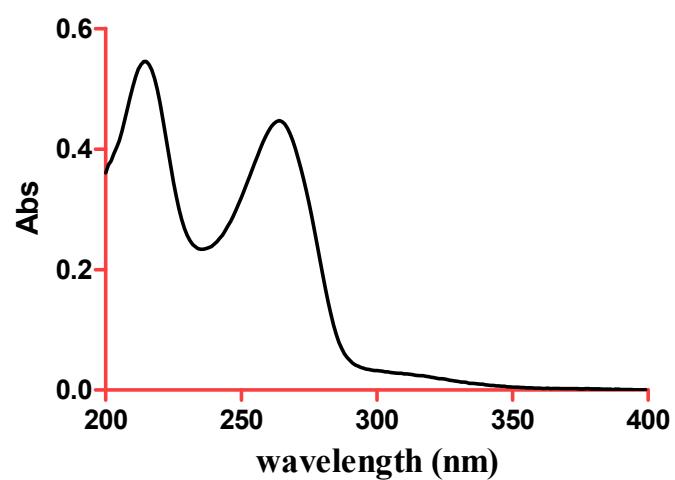


Figure S67. IR spectrum of **5**

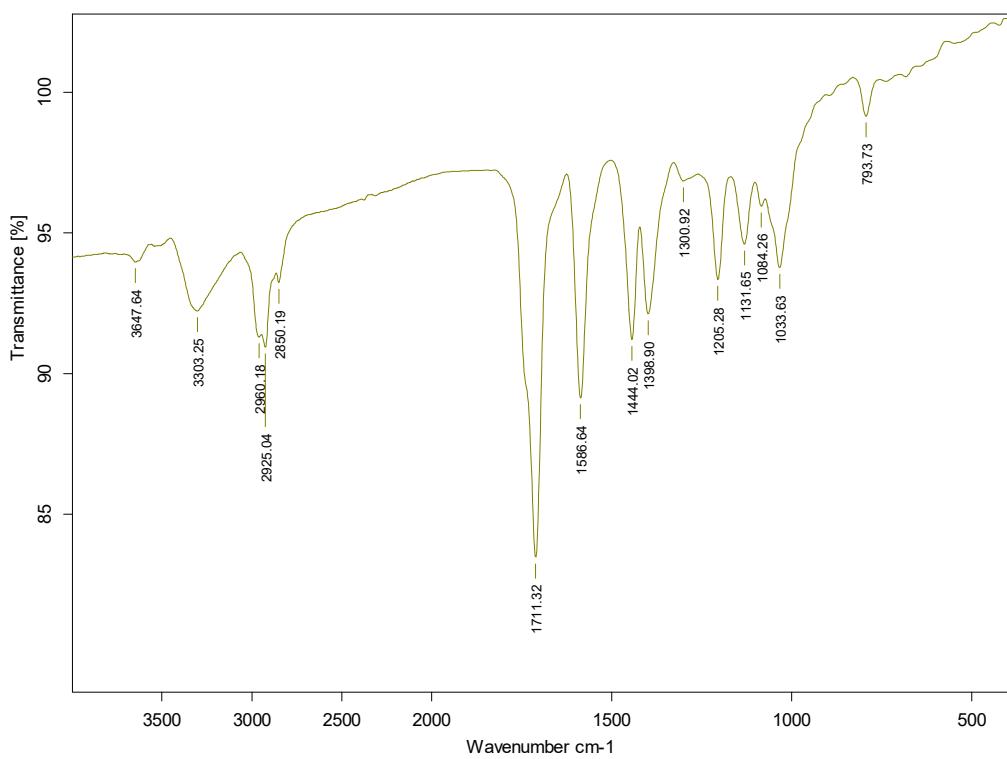


Figure S68. ^1H NMR Spectroscopic for S-MTPA ester of **5a**

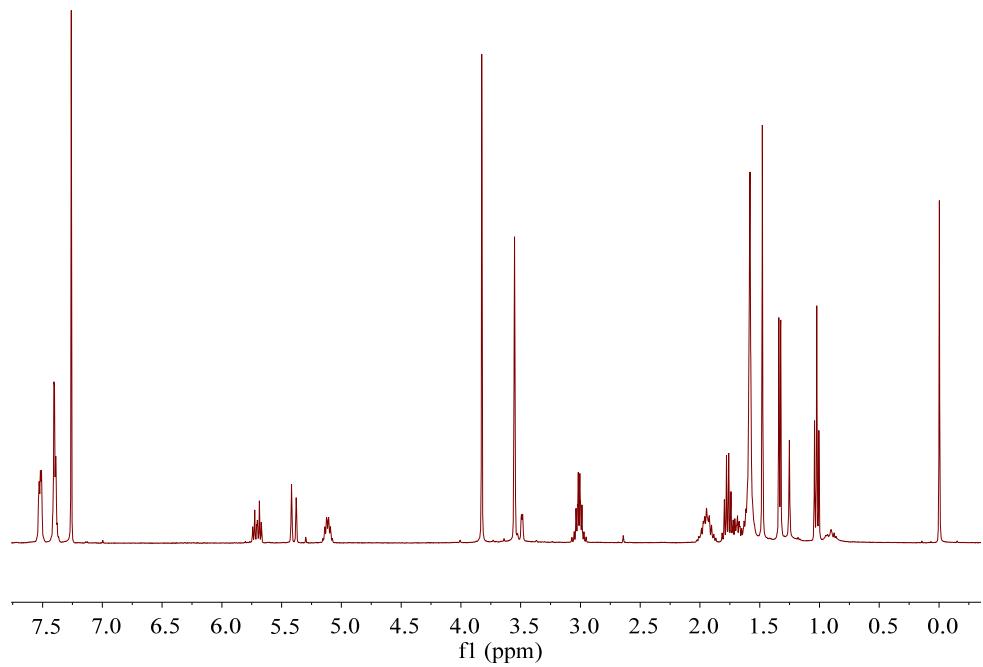


Figure S69. ^1H NMR Spectroscopic for *R*-MTPA ester of **5a**

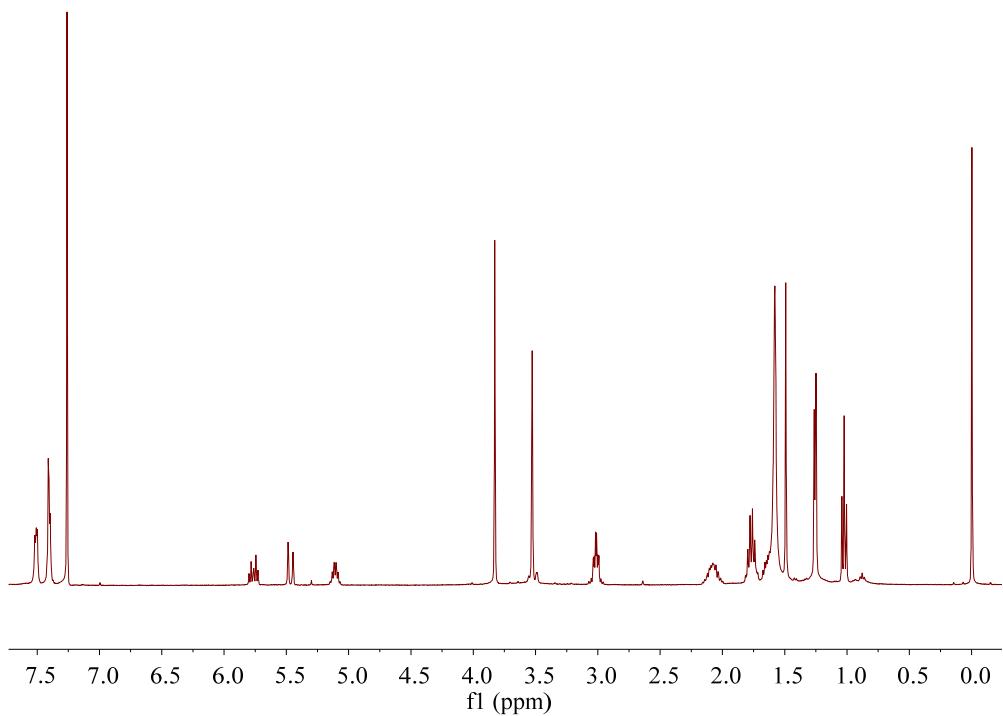


Figure S70. ^1H NMR Spectroscopic for *S*-MTPA ester of **5b**

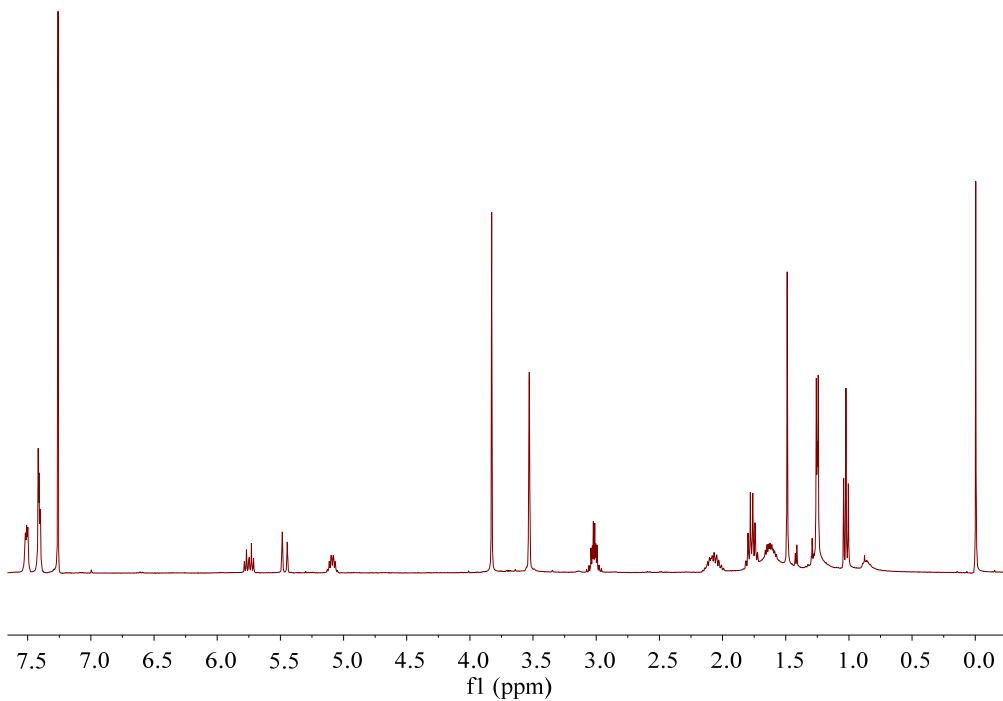


Figure S71. ^1H NMR Spectroscopic for *R*-MTPA ester of **5b**

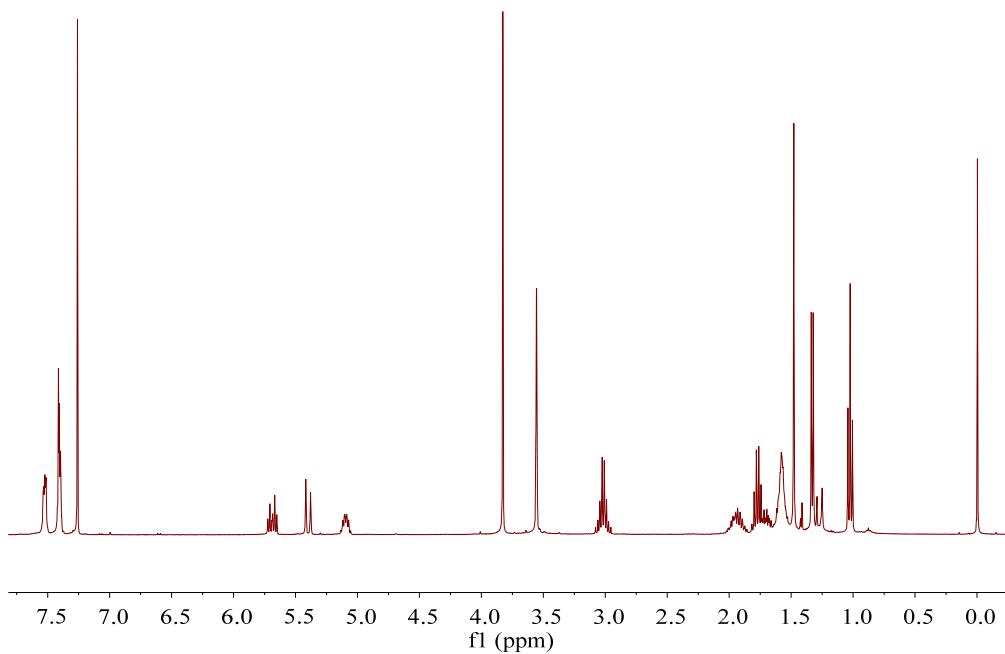


Figure S72. Chiral HPLC separation profiles of **5** (n-hexane-ethanol-Acetic acid, 75:25:0.1; flow: 1.0mL/min)

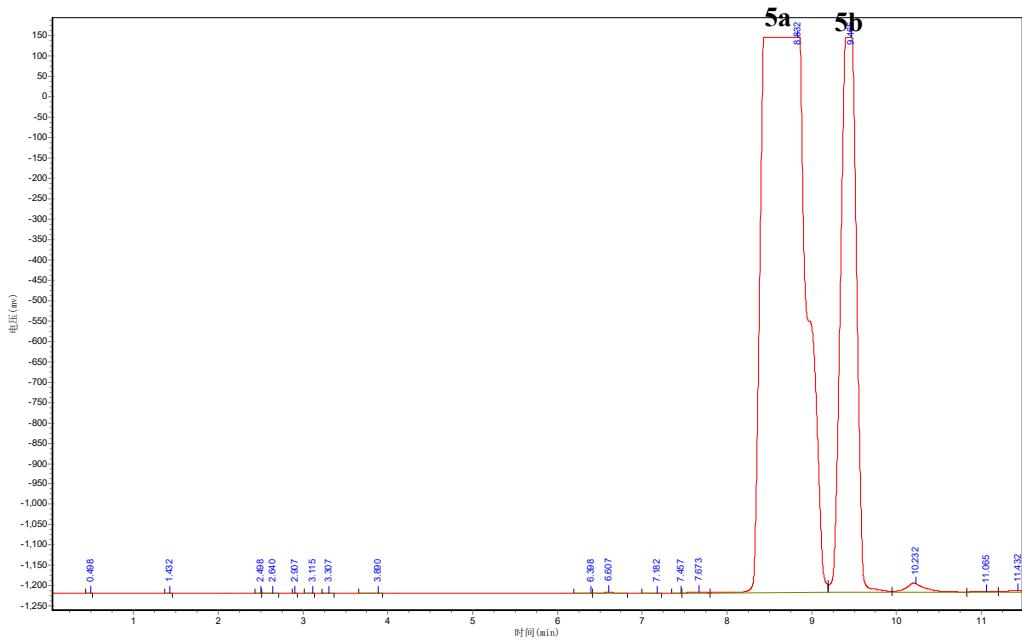


Figure S73. (+)-HR-ESI-MS spectrum of **6**

T: FTMS + p ESI Full ms [100.00-800.00]

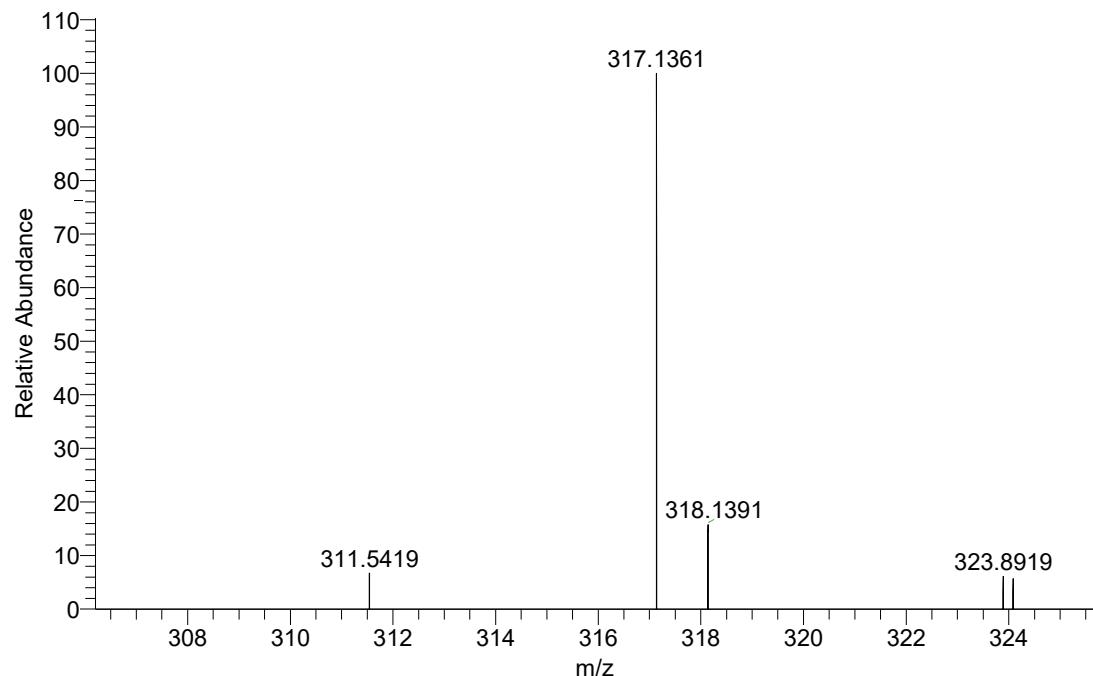


Figure S74. ^1H NMR (400 MHz, CDCl_3) spectrum of **6**

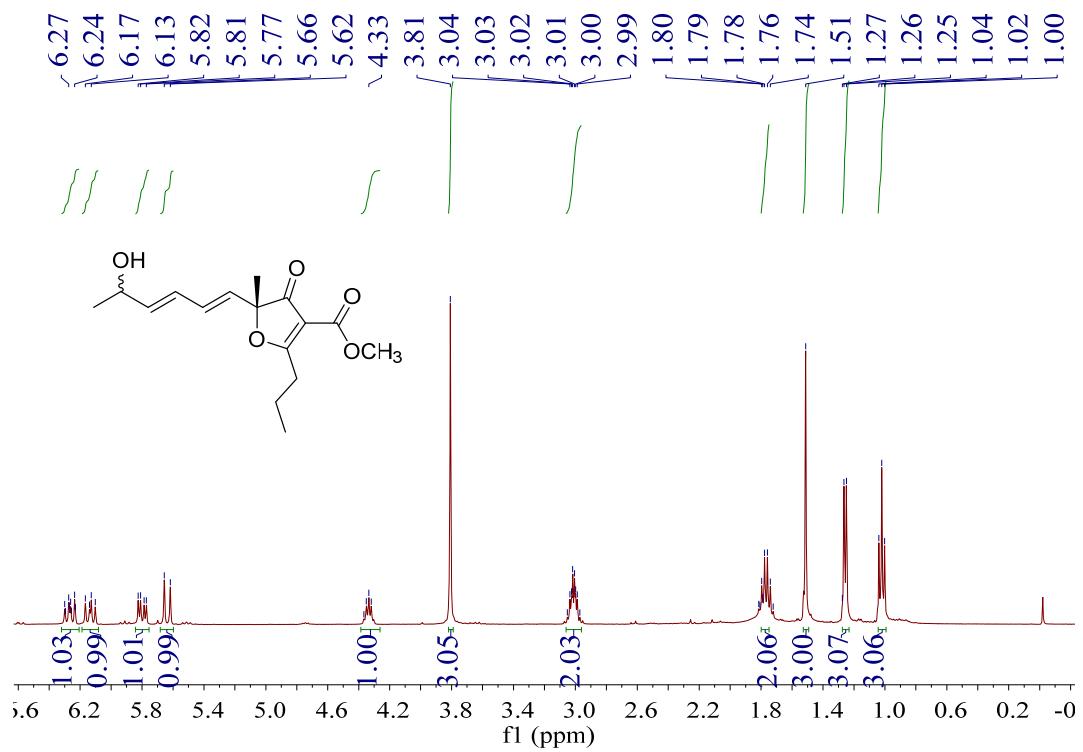


Figure S75. ^1H NMR (400 MHz, CDCl_3) spectra of **6a** and **6b**

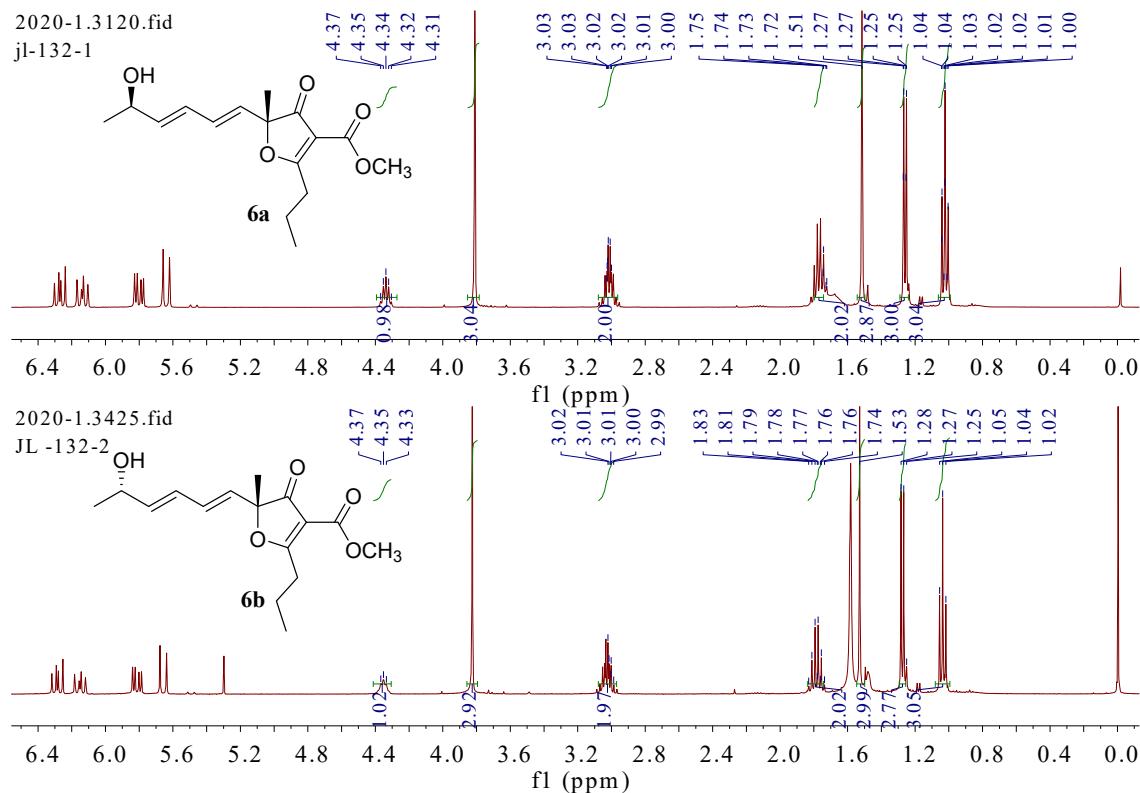


Figure S76. ^{13}C NMR (100 MHz, CDCl_3) spectrum of **6**

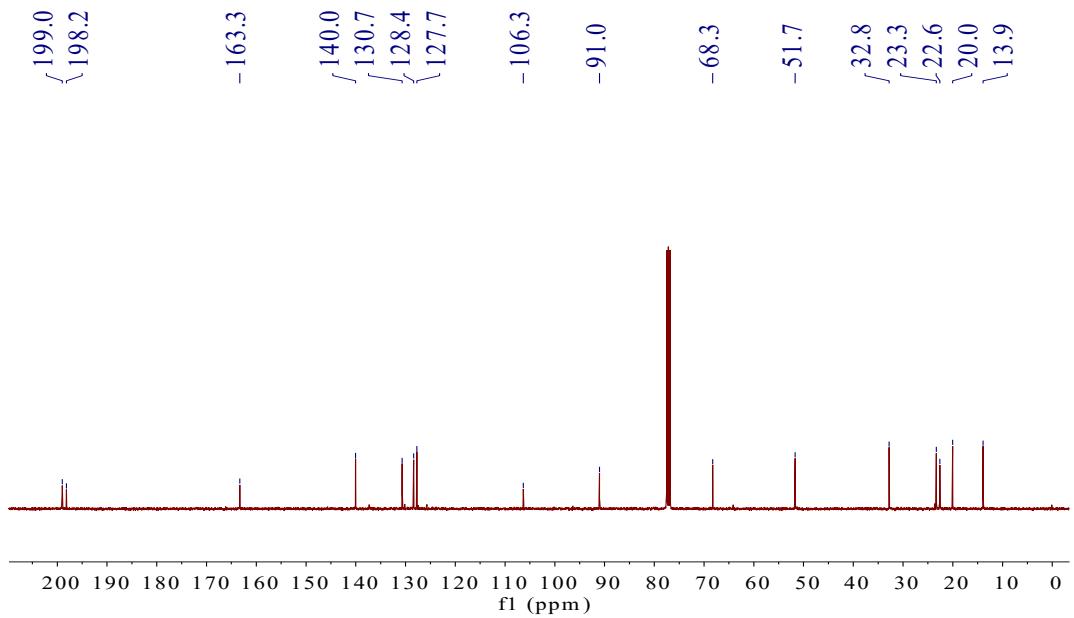


Figure S77. DEPT 135 (100 MHz, CDCl_3) spectrum of **6**

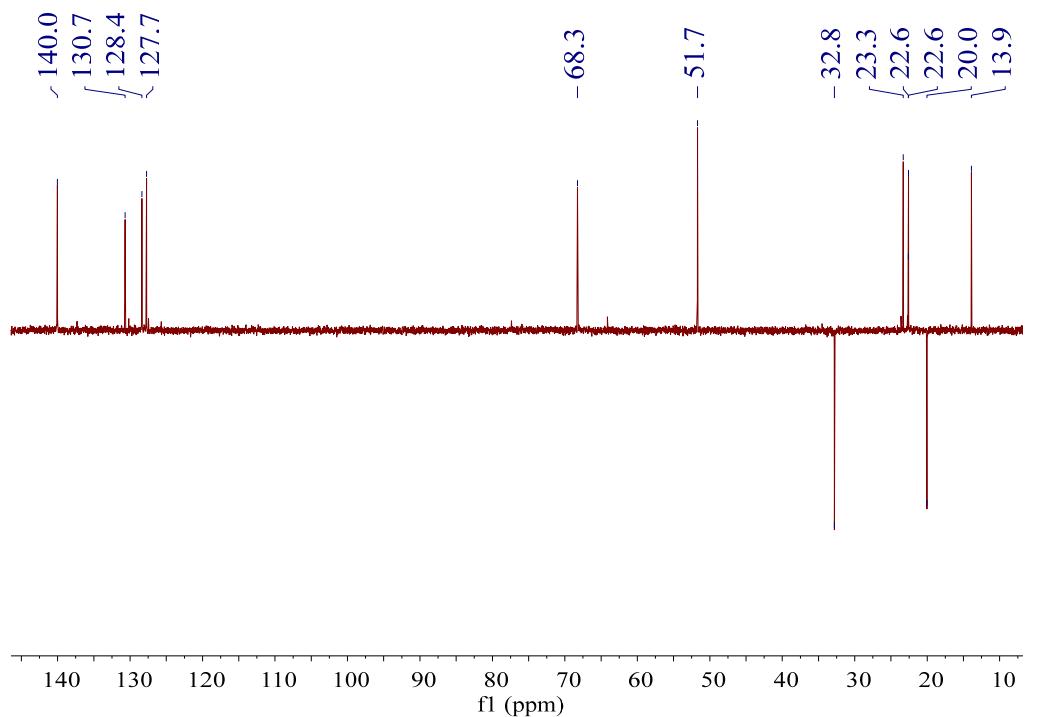


Figure S78. HSQC spectrum of **6** in CDCl_3

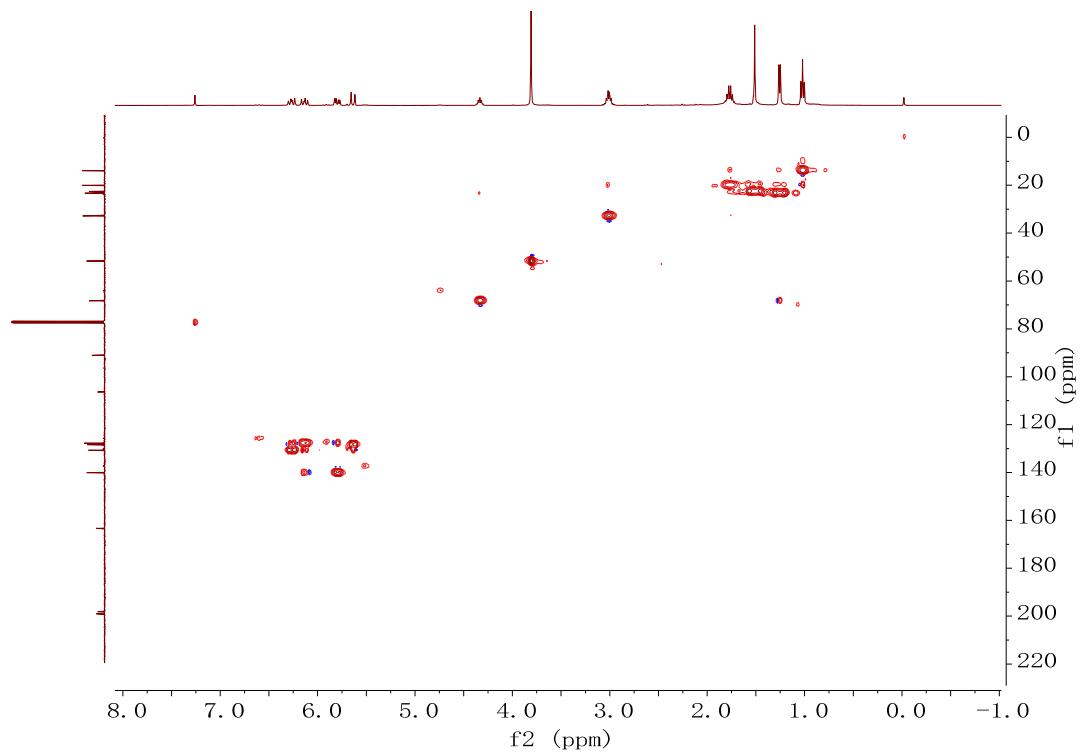


Figure S79. ^1H - ^1H COSY spectrum of **6** in CDCl_3

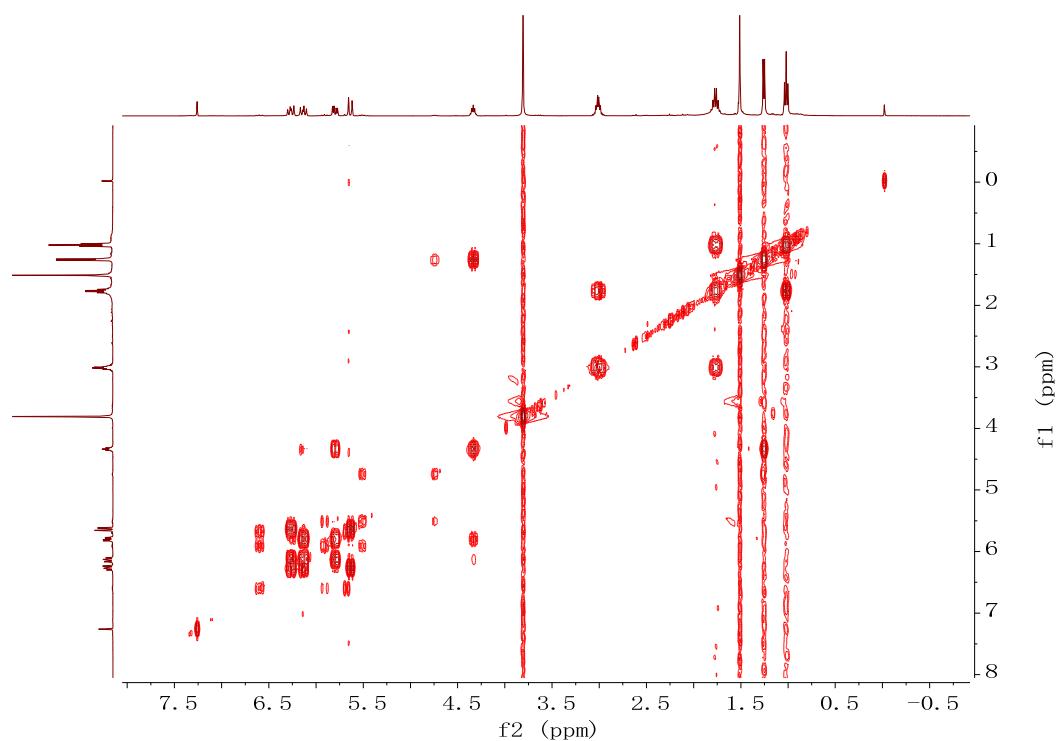


Figure S80. HMBC spectrum of **6** in CDCl_3

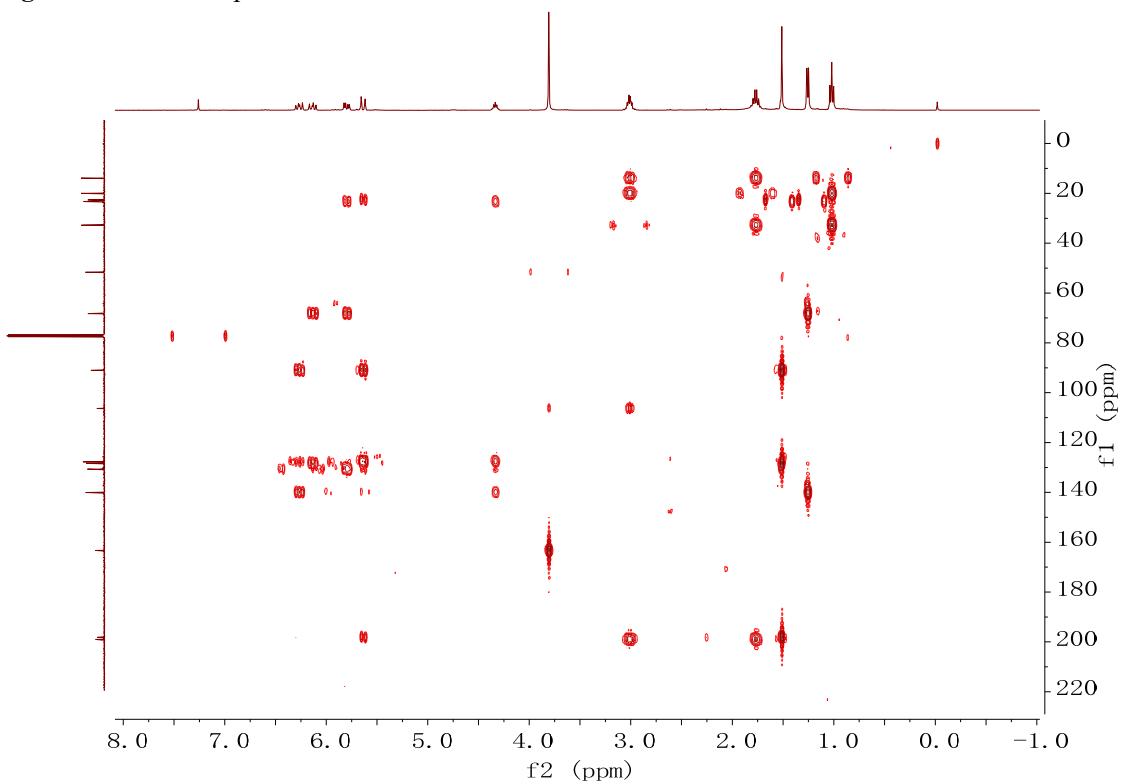


Figure S81. NOESY spectrum of **6** in CDCl_3

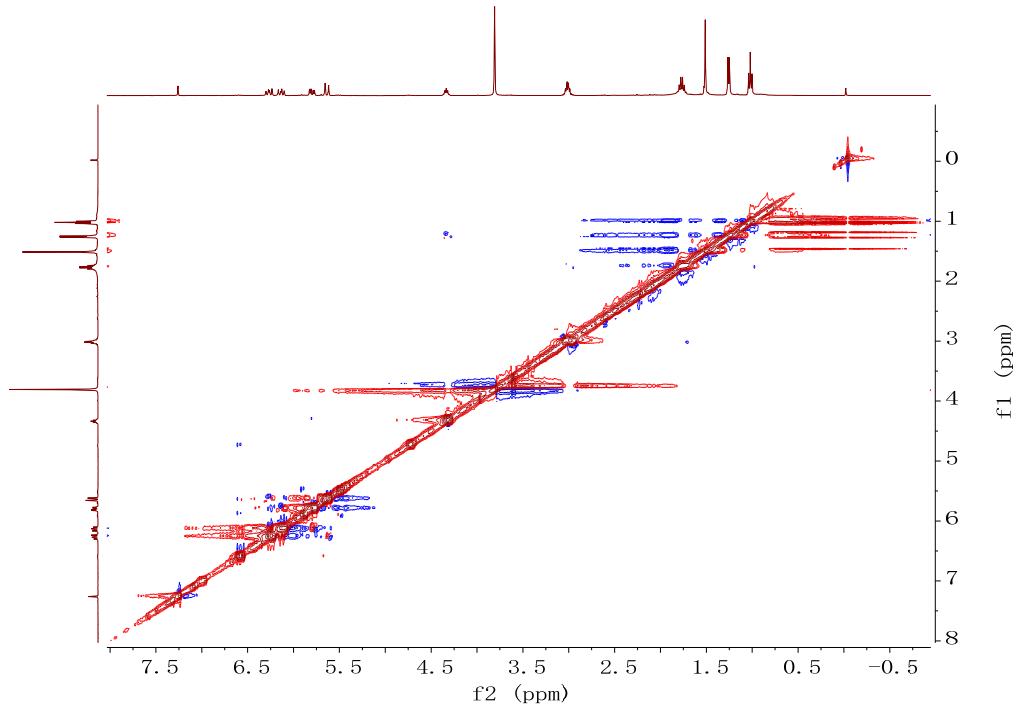


Figure S82. Experimental ECD spectrum of **6a**

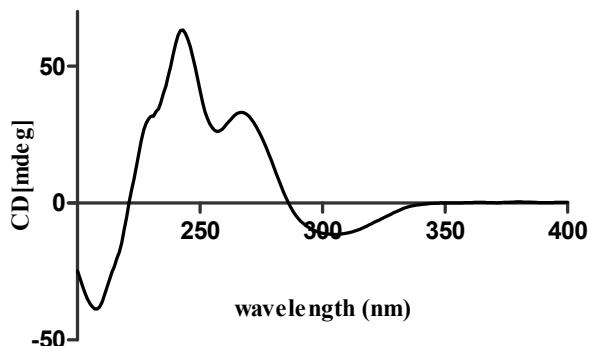


Figure S83. Experimental ECD spectrum of **6b**

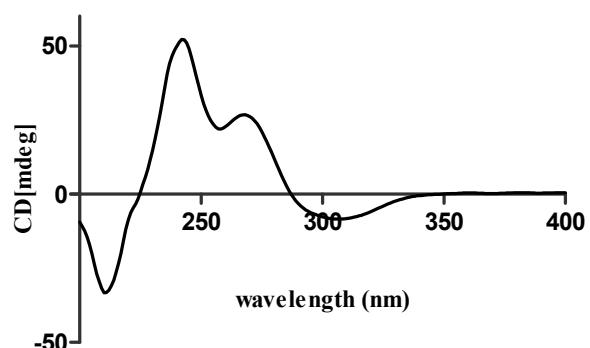


Figure S84. UV spectrum of **6**

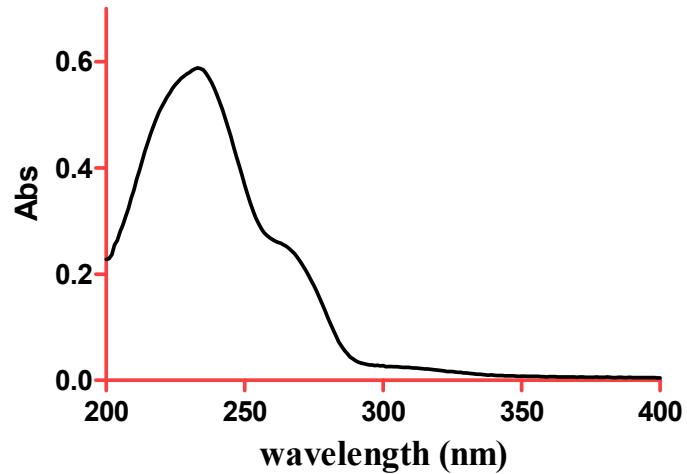


Figure S85. IR spectrum of **6**

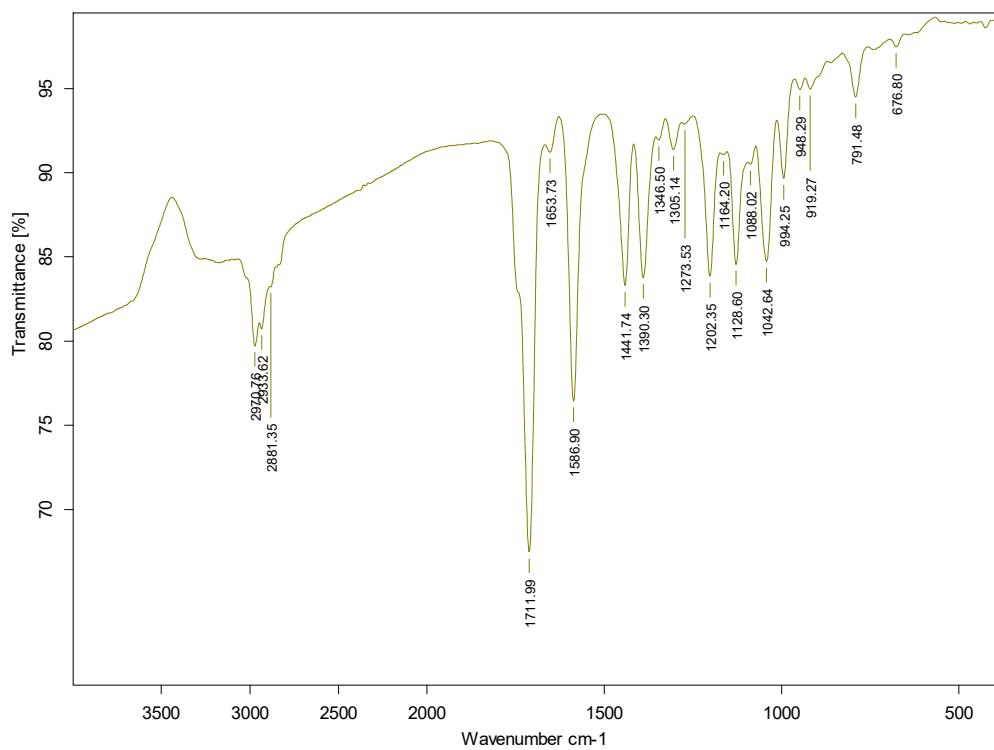


Figure S86. ^1H NMR Spectroscopic for *S*-MTPA ester of **6a**

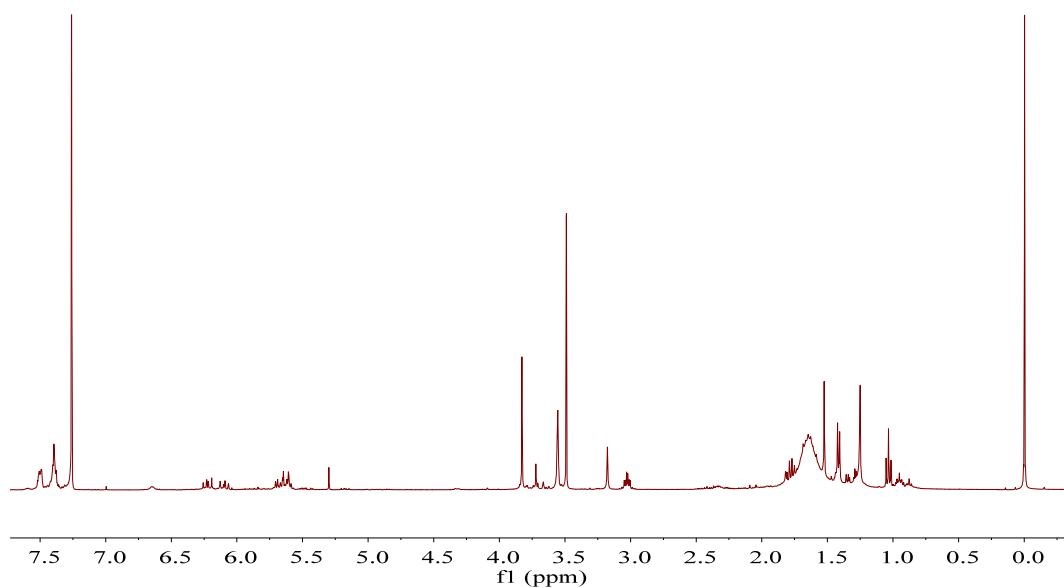


Figure S87. ^1H NMR Spectroscopic for *R*-MTPA ester of **6a**

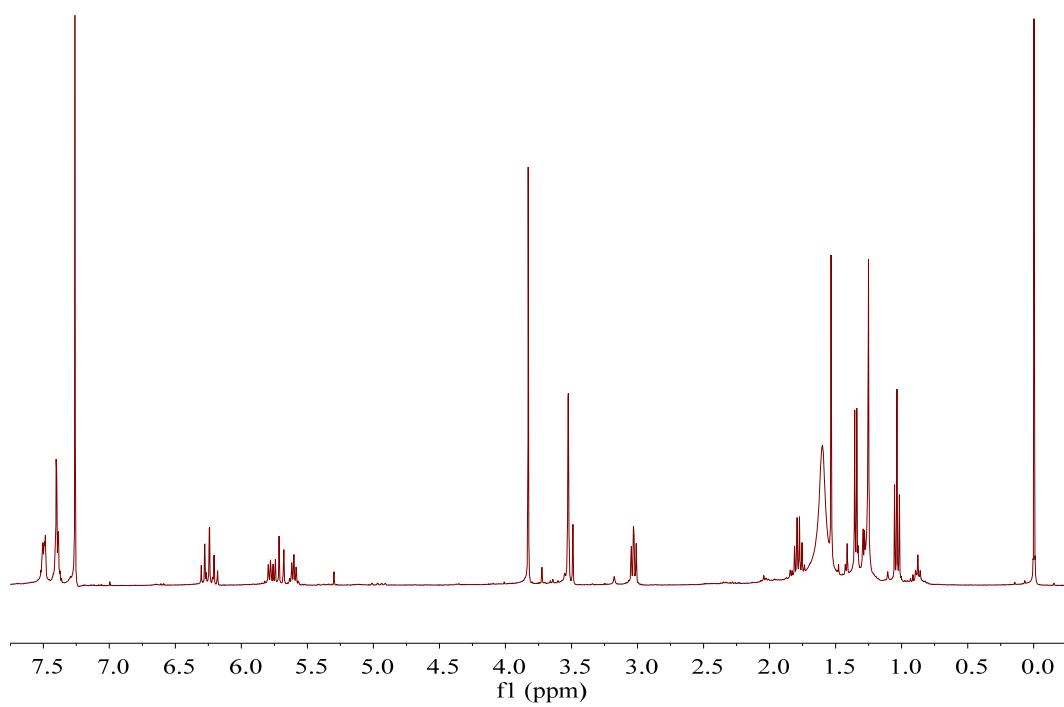


Figure S88. ^1H NMR Spectroscopic for *S*-MTPA ester of **6b**

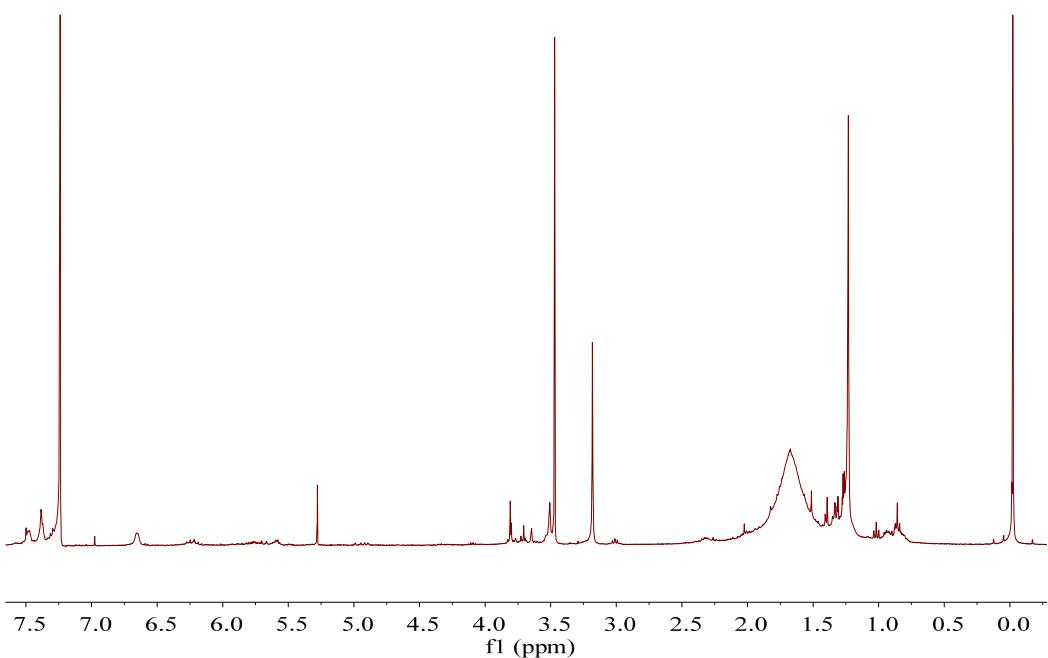


Figure S89. ^1H NMR Spectroscopic for *R*-MTPA ester of **6b**

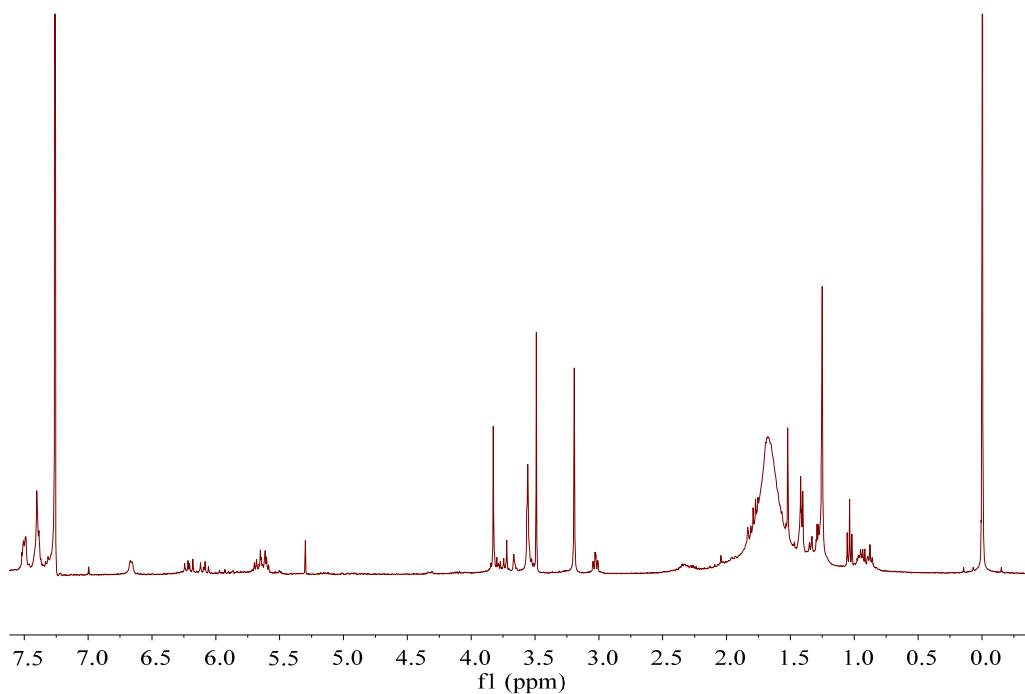


Figure S90. Chiral HPLC analysis profiles of **6** (n-hexane-ethanol-Acetic acid, 80:20:0.1; flow: 1.0mL/min)

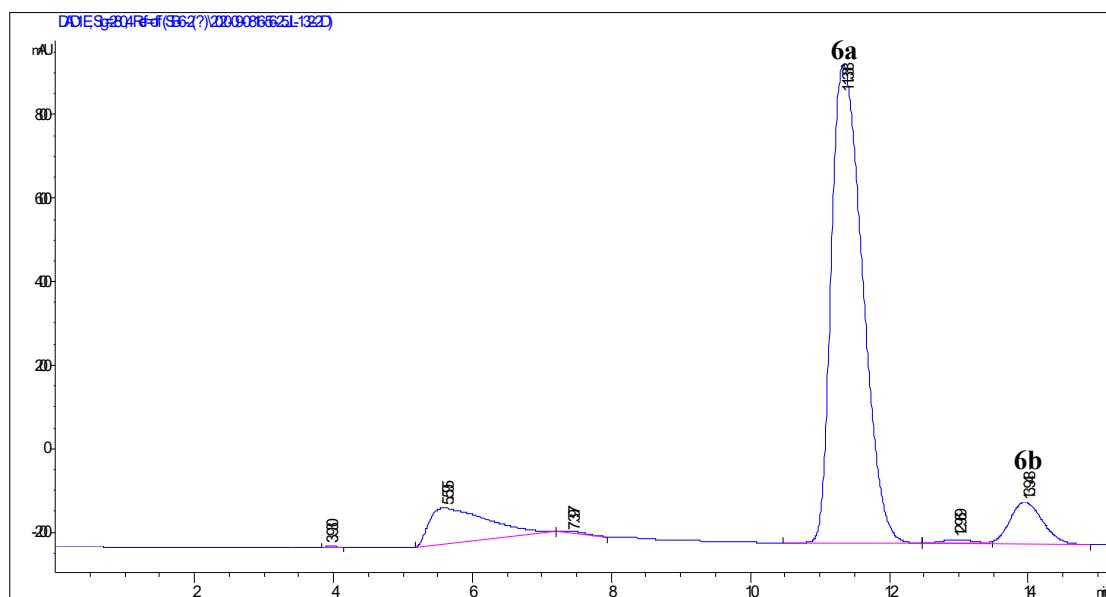


Figure S91. (+)-HR-ESI-MS spectrum of **7**

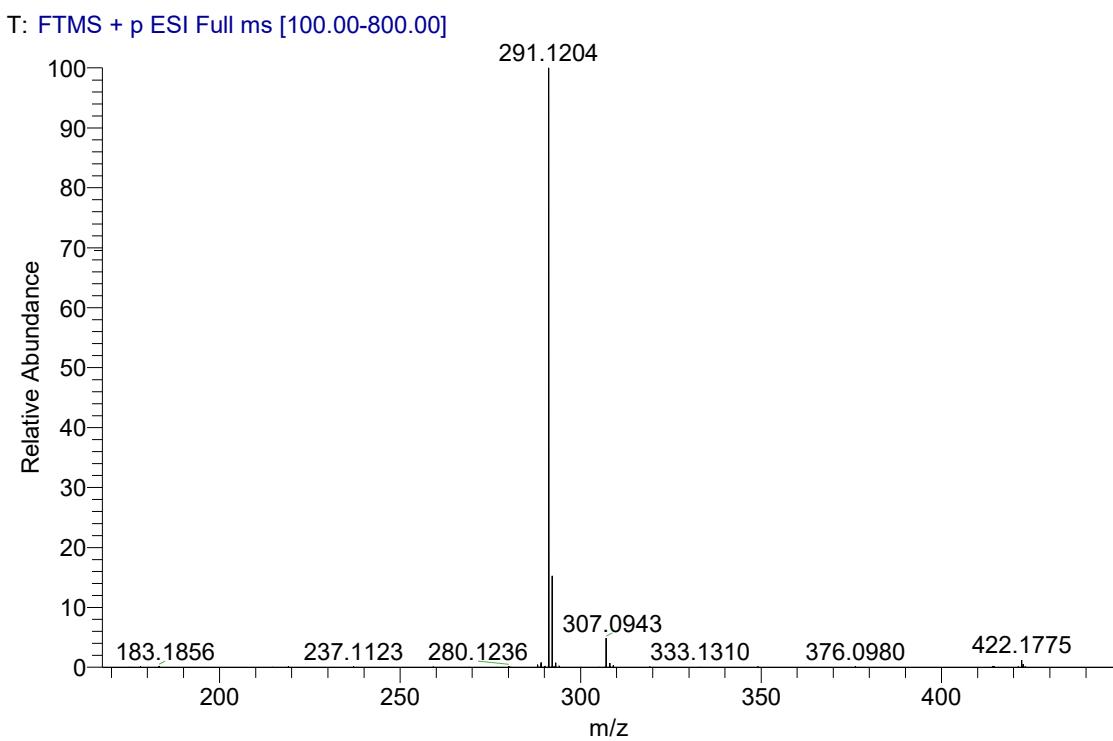


Figure S92. ^1H NMR (400 MHz, CD_3OD) spectrum of 7

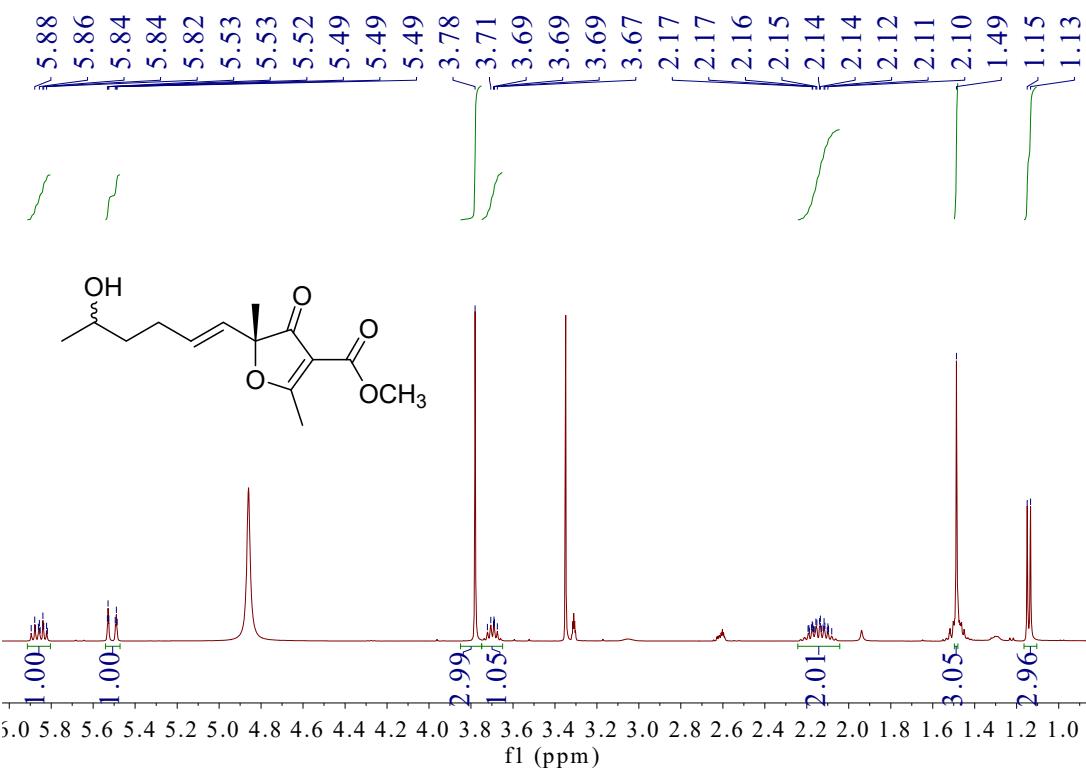


Figure S93. ^1H NMR (400 MHz, CD_3OD) spectra of **7a** and **7b**

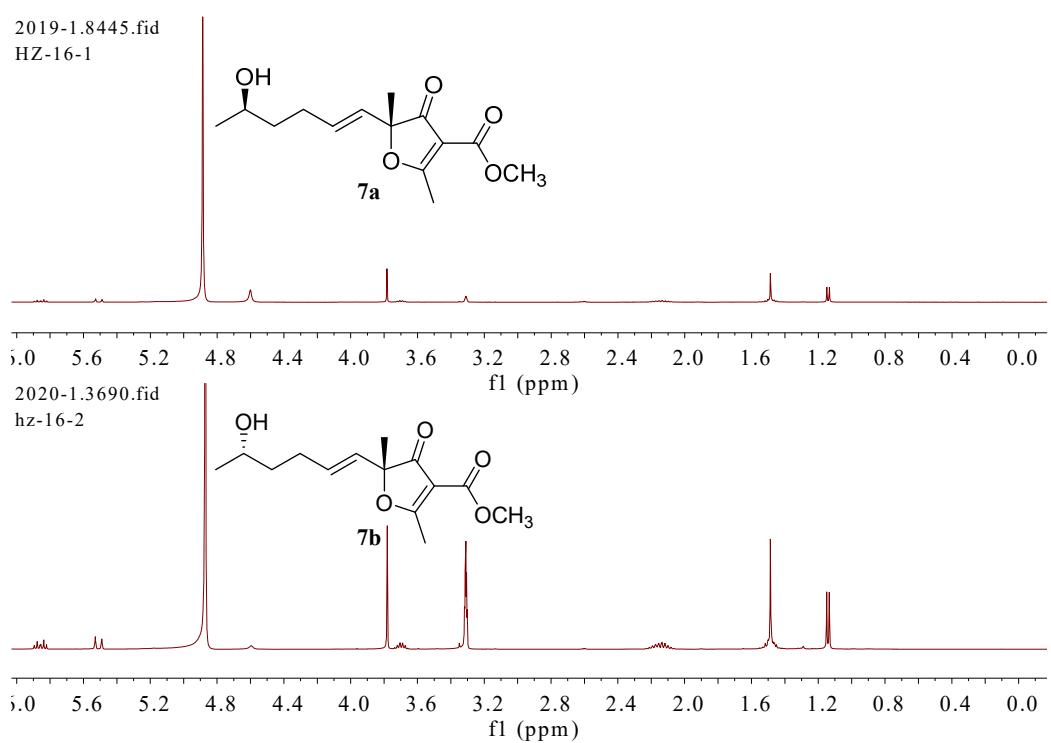


Figure S94. ^{13}C NMR (100 MHz, CD_3OD) spectrum of **7**

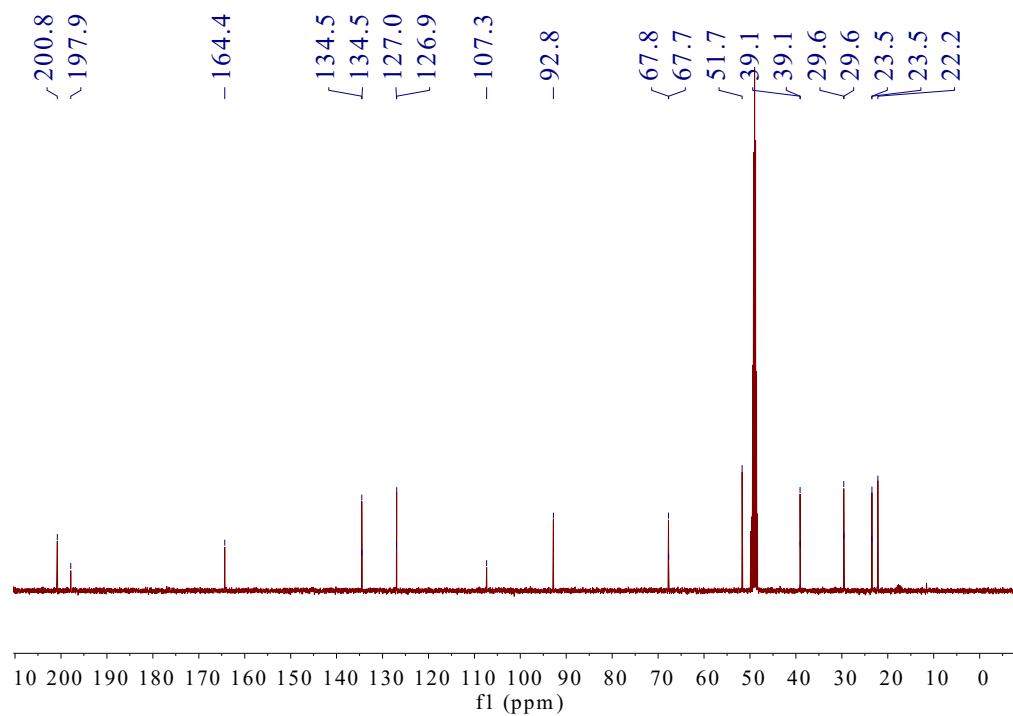


Figure S95. ^{13}C NMR (100 MHz, CD_3OD) spectra of **7a** and **7b**

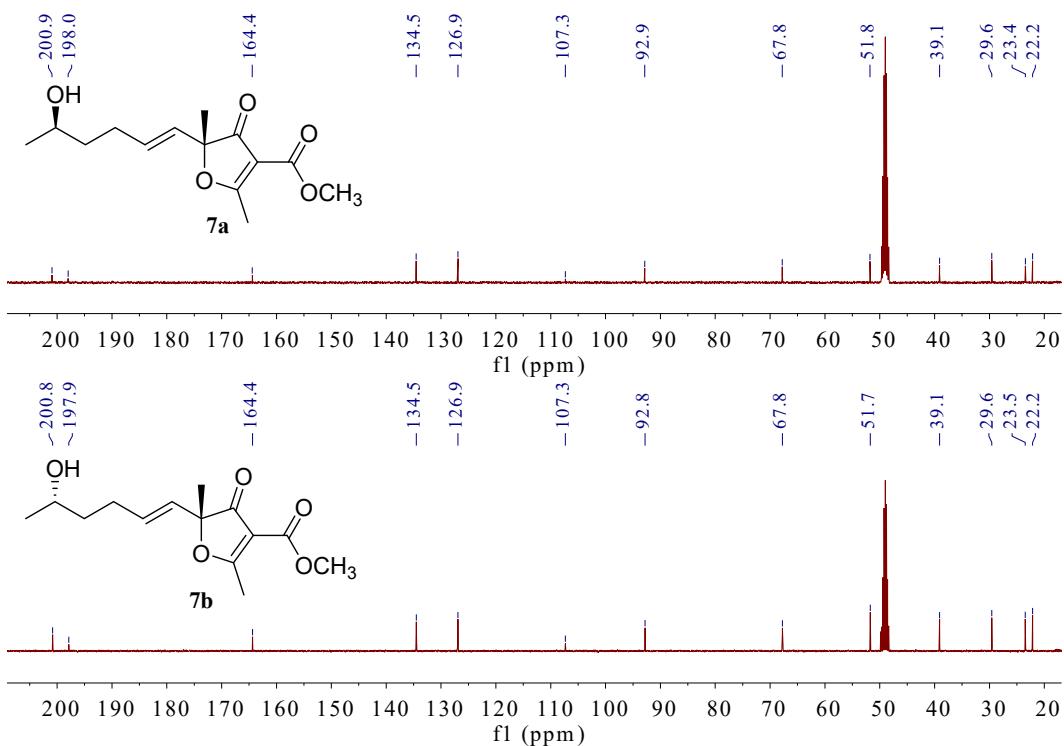


Figure S96. Experimental ECD spectrum of **7a**

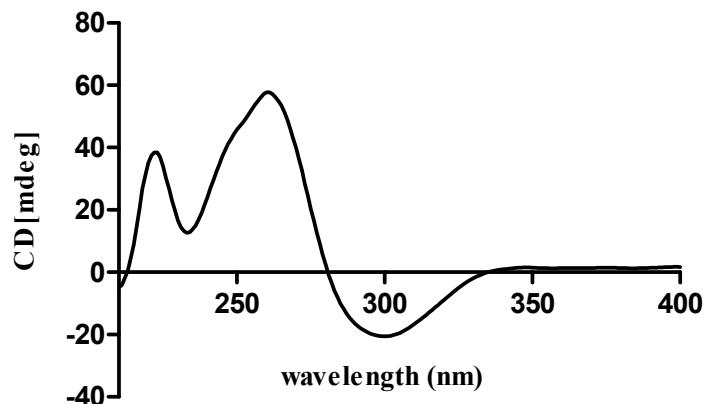


Figure S97. Experimental ECD spectrum of **7b**

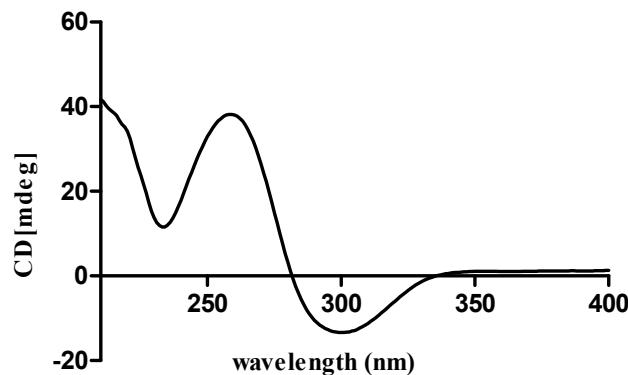


Figure S98. ^1H NMR Spectroscopic for *S*-MTPA ester of **7a**

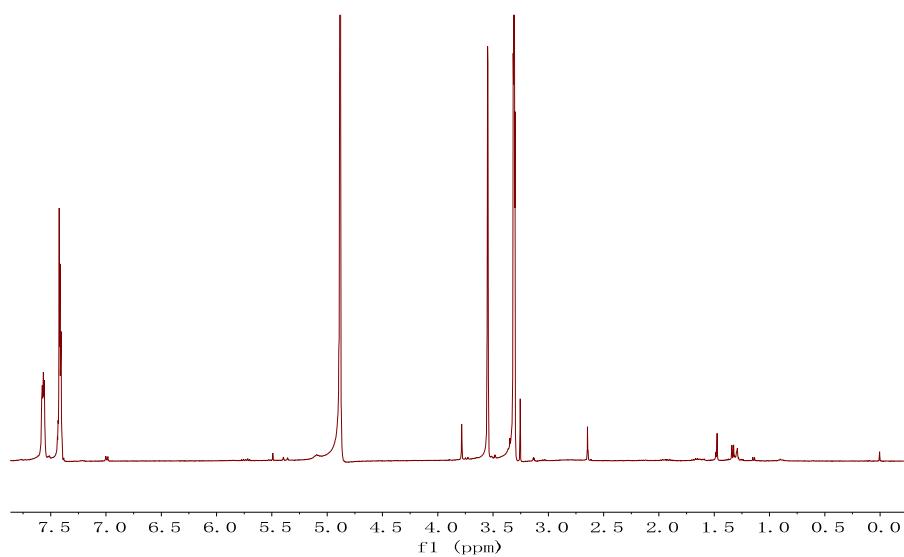


Figure S99. ^1H NMR Spectroscopic for *R*-MTPA ester of **7a**

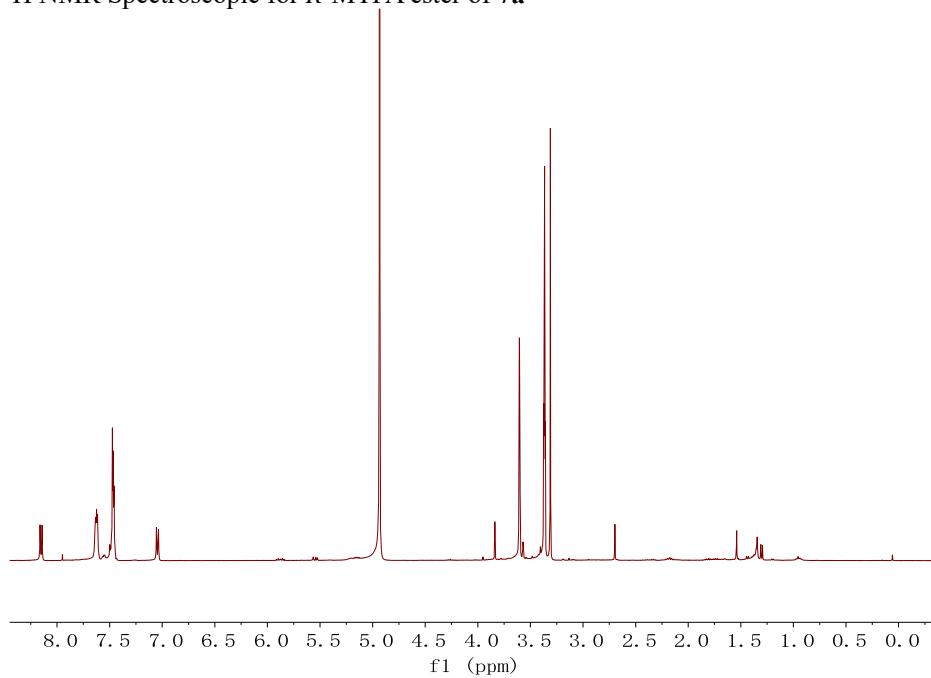


Figure S100. ^1H NMR Spectroscopic for *S*-MTPA ester of **7b**

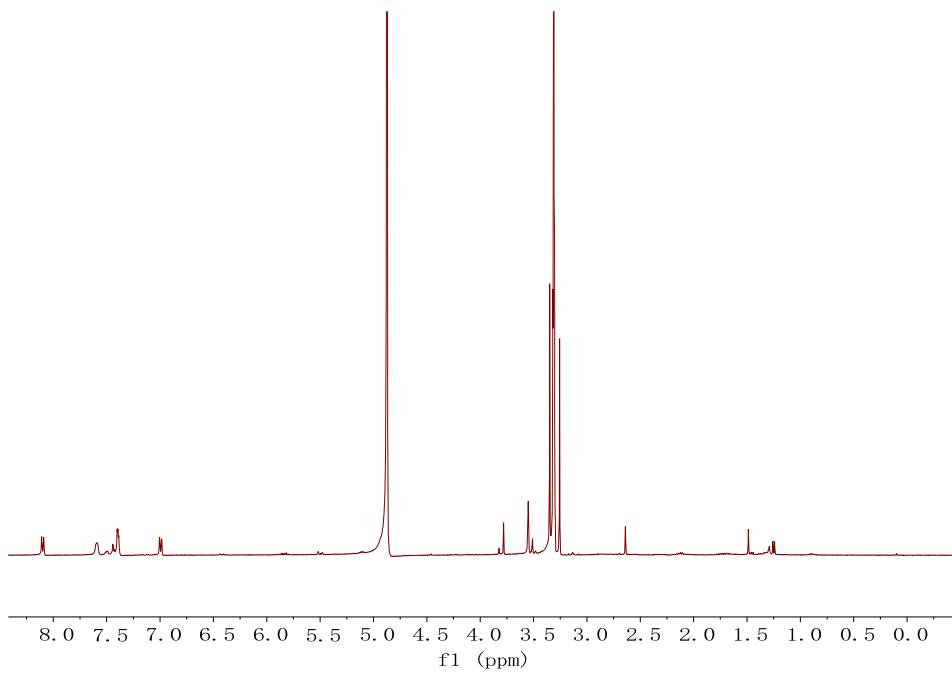


Figure S101. ^1H NMR Spectroscopic for *R*-MTPA ester of **7b**

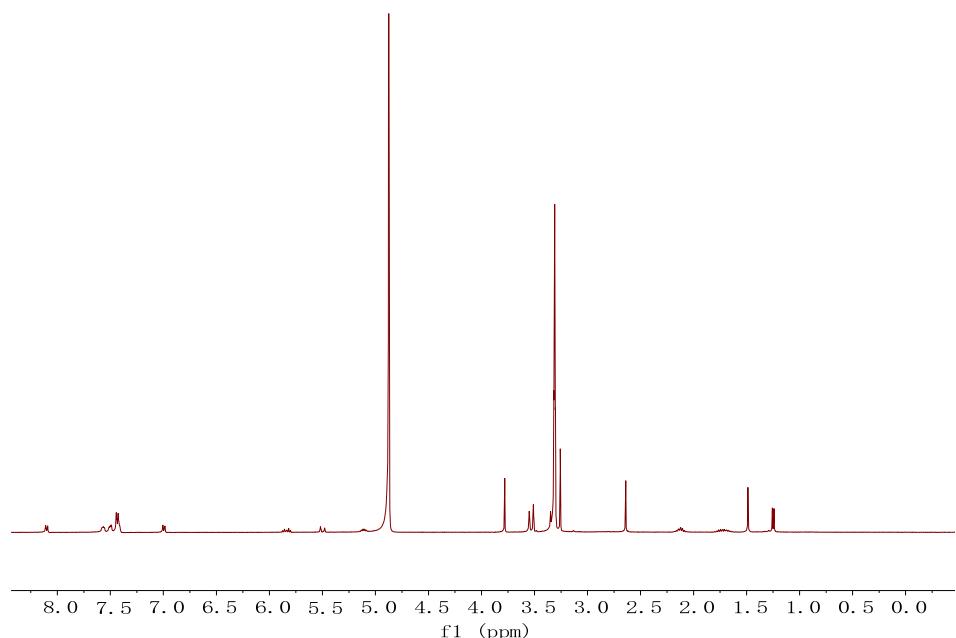


Figure S102. Chiral HPLC separation profiles of **7** (n-hexane-ethanol-Acetic acid, 75:25:0.1; flow:1.0mL/min)

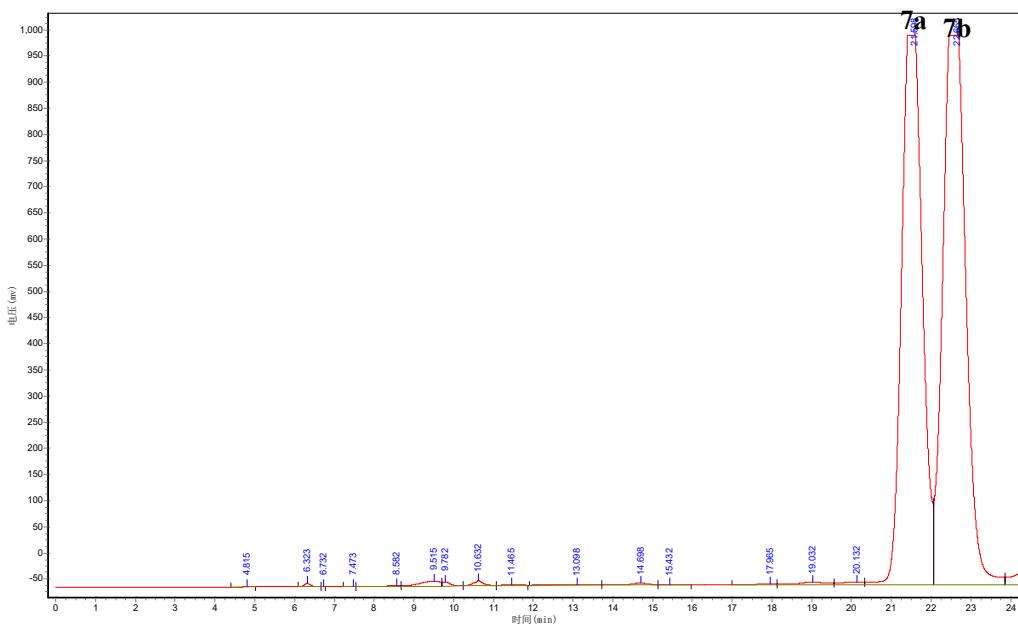


Figure S103. (+)-HR-ESI-MS spectrum of **8**

T: FTMS + p ESI Full ms [100.00-800.00]

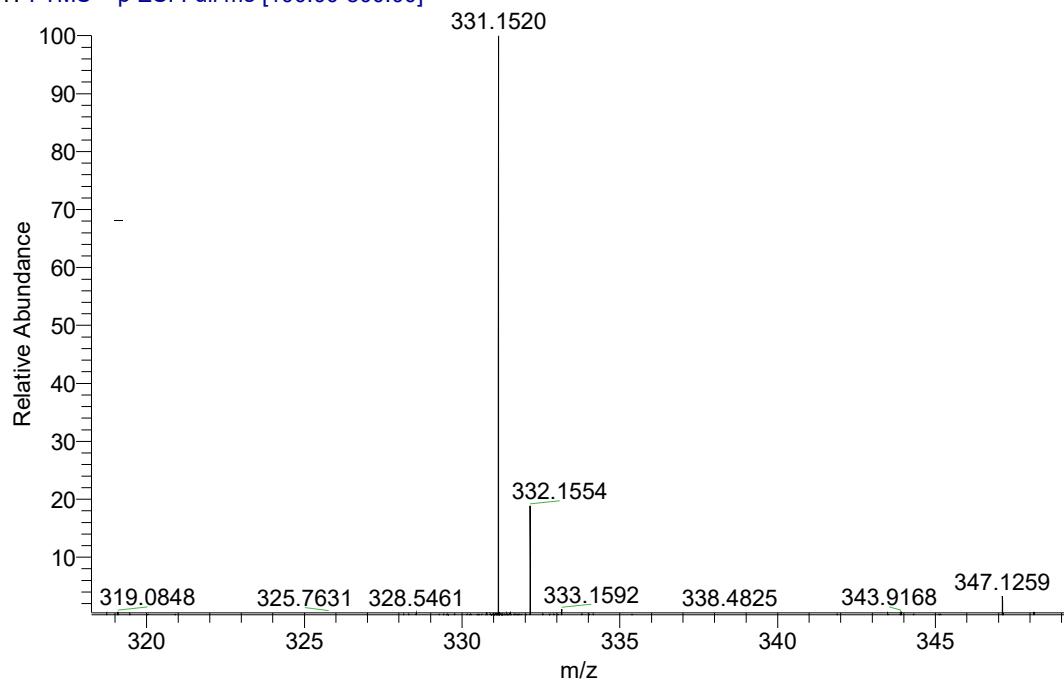


Figure S104. Chiral HPLC analysis profiles of **8** (n-hexane-ethanol-Acetic acid, 75:25:0.1; flow: 1.0mL/min)

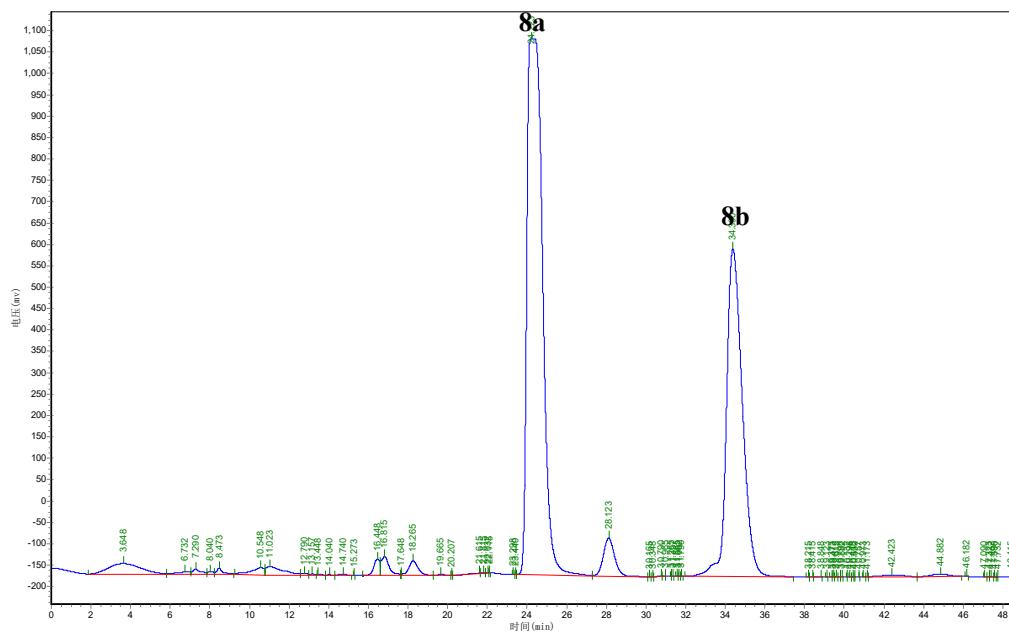


Figure S105. The total ionic chromatogram of MeOH extract (A) and selected ionic chromatograms at m/z 331.1506-331.1536 [M+H]⁺ of MeOH extract (B)

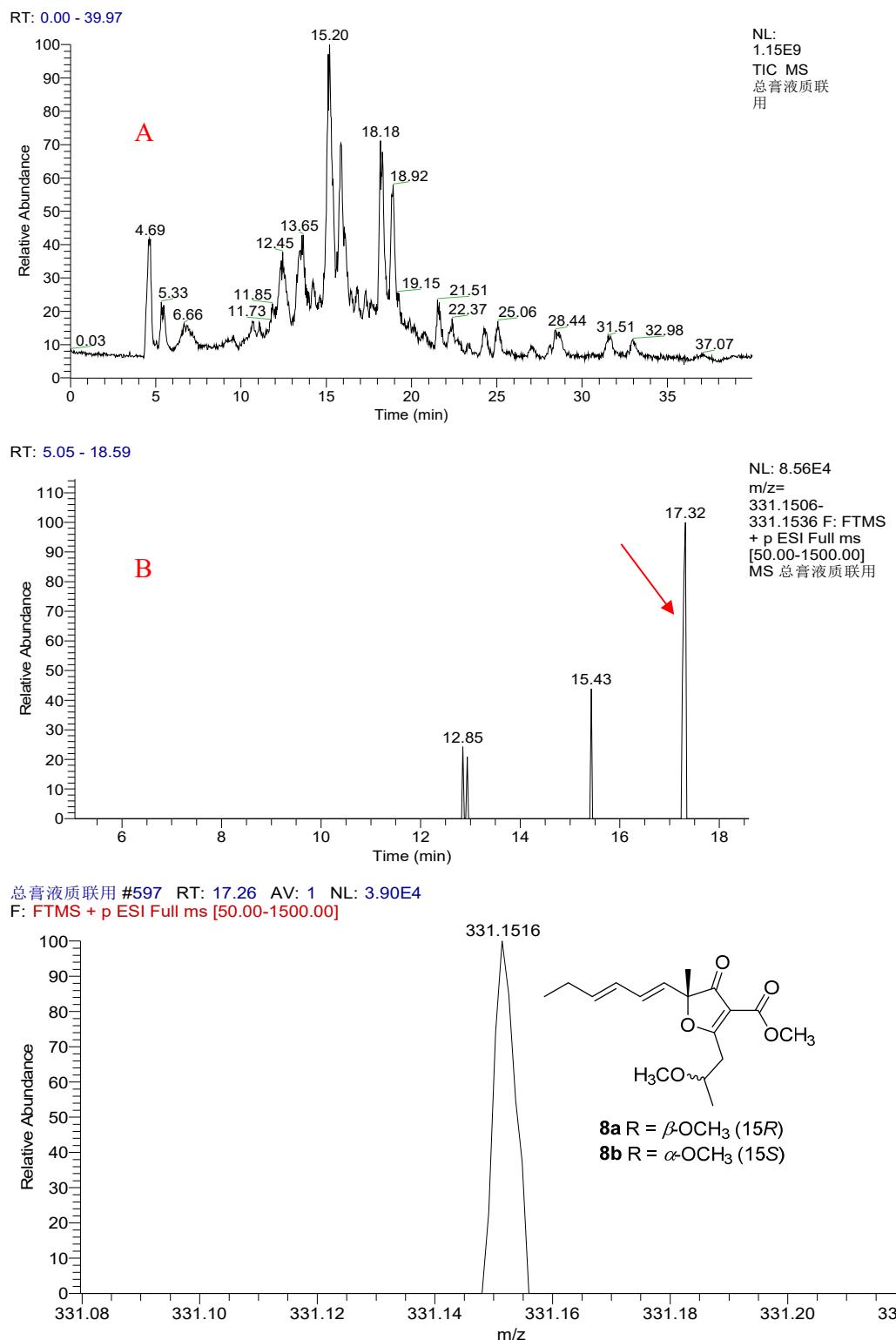


Table S1. Antimicrobial Activity of Compounds 1–7

In the process of antimicrobial experiment, the initial gradient screening concentration generally was 50 μM. Subsequently, in order to get the MICs (minimum inhibitory concentrations) of each compound, eight gradient concentrations (30, 25, 20, 15, 10, 5, 2.5, and 1 μM) for compounds 1–7 were set for the antimicrobial activity tests. And the MICs were observed by naked eyes, which represent the lowest concentration that inhibit the visible growth of a microorganism. For each isomeric pair, the MICs are exactly the same, which means the isomerization has very slight impact on the antimicrobial activities of those compounds.

Compound	MIC ^a		
	Bacteria		Fungi
	<i>Escherichia coli</i> μM (μg/mL)	<i>Staphylococcus aureus</i> μM (μg/mL)	<i>Candida albicans</i> μM (μg/mL)
1	5 (1.7)	5 (1.7)	10 (3.3)
2	2.5 (0.9)	5 (1.9)	10 (3.8)
3a	20 (7.0)	10 (3.5)	20 (7.0)
3b	20 (7.0)	10 (3.5)	20 (7.0)
4a	10 (3.5)	10 (3.5)	20 (7.0)
4b	10 (3.5)	10 (3.5)	20 (7.0)
5a	10 (3.0)	10 (3.0)	20 (5.9)
5b	10 (3.0)	10 (3.0)	20 (5.9)
6a	10 (2.9)	10 (2.9)	15 (4.4)
6b	10 (2.9)	10 (2.9)	15 (4.4)
7a	20 (5.4)	10 (2.7)	20 (5.4)
7b	20 (5.4)	10 (2.7)	20 (5.4)
Reference drugs			
Streptomycin	2.3 μg/mL	0.1 μg/mL	NT ^b
Amphotericin B	NT	NT	0.1 μg/mL

^a MIC: Minimal inhibitory concentration values.

^b NT: Not tested.

Scheme S1. Hypothetical Biogenetic Pathway of Compounds 1–4

