

Talaromarins A-F: Six New Isocoumarins from Mangrove-Derived Fungus *Talaromyces flavus* TGGP35

Jin Cai^{1,2,†}, Xiao-Chen Zhu^{3,†}, Wei-Nv Zeng^{1,2}, Bin Wang^{1,2}, You-Ping Luo^{1,2}, Jing Liu^{1,2}, Min-Jing Chen^{1,2}, Gao-Yu Li^{1,2}, Guo-Lei Huang^{1,2}, Guang-Ying Chen^{1,2}, Jing Xu^{3,*} and Cai-Juan Zheng^{1,2,*}

1 Key Laboratory of Tropical Medicinal Resource Chemistry of Ministry of Education, College of Chemistry and Chemical Engineering, Hainan Normal University, Haikou, Hainan, 571158, People's Republic of China; caijin20210207@163.com (J.C.); z17889949296@163.com (W. - N.Z.); 15180328507@163.com (B.W.); lyp188089688692022@163.com (Y.-P.L.); liujing3182799099@163.com (J.L.); cmj19151835730@163.com (M.-J. C.); qqwbma_999@163.com (G.-Y.L.); 070333@hainnu.edu.cn (G.-L.H.); chgying@163.com (G.-Y.C.)

2 Key Laboratory of Tropical Medicinal Plant Chemistry of Hainan Province, Haikou, Hainan, 571158, People's Republic of China

3 Key Laboratory of Advanced Materials of Tropical Island Resources of Ministry of Education, School of Chemical Engineering and Technology, Hainan University, Haikou 570228, China; zhuxiaochenlucky@163.com (X.-C.Z.)

* Correspondence: caijuan2002@163.com (C.-J. Z.); happyjing3@163.com (J. X.)

† These authors contributed equally to this work.

List of contents

Figure S1. ^1H NMR spectrum of **1** in CDCl_3

Figure S2. ^{13}C NMR spectrum of **1** in CDCl_3

Figure S3. 135-DEPT spectrum of **1** in CDCl_3

Figure S4. HMQC spectrum of **1** in CDCl_3

Figure S5. ^1H - ^1H COSY spectrum of **1** in CDCl_3

Figure S6. HMBC spectrum of **1** in CDCl_3

Figure S7. HR-ESI-MS spectrum of **1**

Figure S8. ^1H NMR spectrum of **2** in CDCl_3

Figure S9. ^{13}C NMR spectrum of **2** in CDCl_3

Figure S10. 135-DEPT spectrum of **2** in CDCl_3

Figure S11. HMQC spectrum of **2** in CDCl_3

Figure S12. ^1H - ^1H COSY spectrum of **2** in CDCl_3

Figure S13. HMBC spectrum of **2** in CDCl_3

Figure S14. HR-ESI-MS spectrum of **2**

Figure S15. ^1H NMR spectrum of **3** in CDCl_3

Figure S16. ^{13}C NMR spectrum of **3** in CDCl_3

Figure S17. 135-DEPT spectrum of **3** in CDCl_3

Figure S18. HMQC spectrum of **3** in CDCl_3

Figure S19. ^1H - ^1H COSY spectrum of **3** in CDCl_3

Figure S20. HMBC spectrum of **3** in CDCl_3

Figure S21. HR-ESI-MS spectrum of **3**

Figure S22. ^1H NMR spectrum of **4** in CDCl_3

Figure S23. ^{13}C NMR spectrum of **4** in CDCl_3

Figure S24. 135-DEPT spectrum of **4** in CDCl_3

Figure S25. HMQC spectrum of **4** in CDCl_3

Figure S26. ^1H - ^1H COSY spectrum of **4** in CDCl_3

Figure S27. HMBC spectrum of **4** in CDCl_3

Figure S28. HR-ESI-MS spectrum of **4**

Figure S29. ^1H NMR spectrum of **5** in CDCl_3

Figure S30. ^{13}C NMR spectrum of **5** in CDCl_3

Figure S31. 135-DEPT spectrum of **5** in CDCl_3

Figure S32. HMQC spectrum of **5** in CDCl_3

Figure S33. ^1H - ^1H COSY spectrum of **5** in CDCl_3

Figure S34. HMBC spectrum of **5** in CDCl_3

Figure S35. HR-ESI-MS spectrum of **5**

Figure S36. ^1H NMR spectrum of **6** in CDCl_3

Figure S37. ^{13}C NMR spectrum of **6** in CDCl_3

Figure S38. 135-DEPT spectrum of **6** in CDCl_3

Figure S39. HMQC spectrum of **6** in CDCl_3

Figure S40. ^1H - ^1H COSY spectrum of **6** in CDCl_3

Figure S41. HMBC spectrum of **6** in CDCl_3

Figure S42. HR-ESI-MS spectrum of **6**

Figure S43. ^1H NMR (CDCl_3 , 400 MHz) of Hydrolysate of **1a**

Figure S44. ^{13}C NMR (CDCl_3 , 400 MHz) of Hydrolysate of **1a**

Figure S45. ESI-MS spectrum of **1a**

Figure S46. ^1H NMR (CDCl_3 , 600 MHz) of *S*-MTPA ester of **1a**

Figure S47. ESI-MS spectrum of **1a**

Figure S48. ^1H NMR (CDCl_3 , 600 MHz) of *R*-MTPA ester of **1a**

Figure S49. ESI-MS spectrum of **1a**

Figure S50. ^1H NMR (CDCl_3 , 600 MHz) of *S*-MTPA ester of **2**

Figure S51. ESI-MS spectrum of **2**

Figure S52. ^1H NMR (CDCl_3 , 600 MHz) of *R*-MTPA ester of **2**

Figure S53. ESI-MS spectrum of **2**

Figure S54. ^1H NMR (CDCl_3 , 400 MHz) of *S*-MTPA ester of **3**

Figure S55. ESI-MS spectrum of **3**

Figure S56. ^1H NMR (CDCl_3 , 400 MHz) of *R*-MTPA ester of **3**

Figure S57. ESI-MS spectrum of **3**

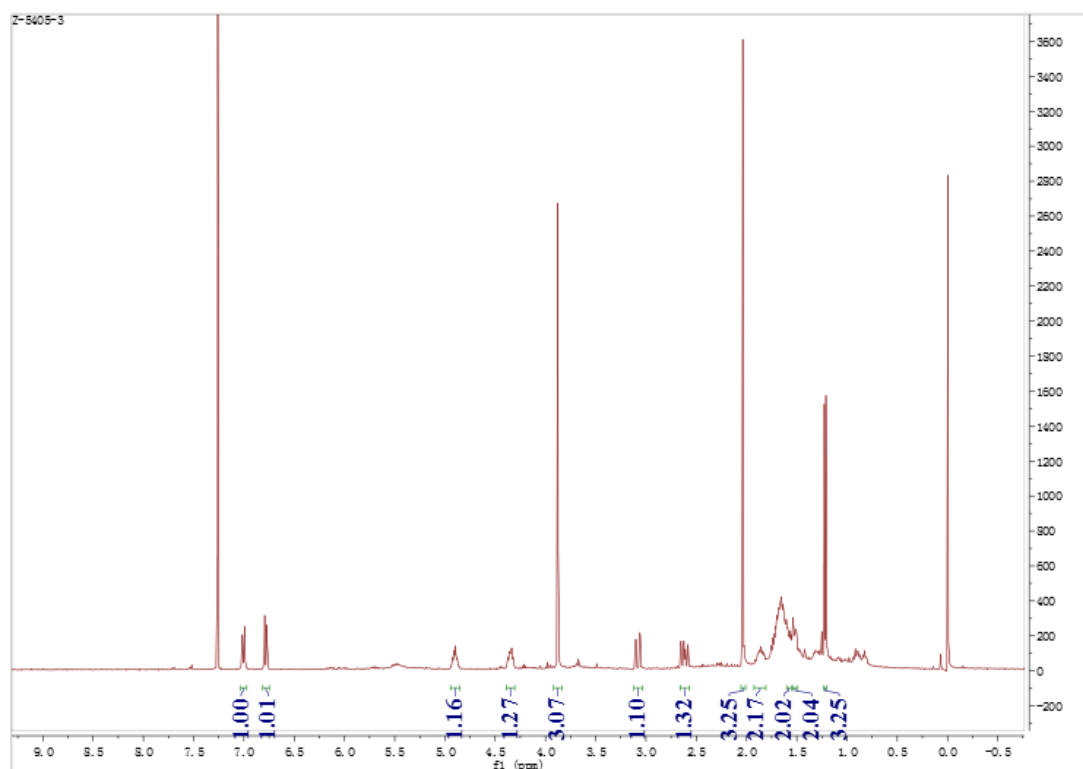


Figure S1. ¹H NMR spectrum of **1** in CDCl₃

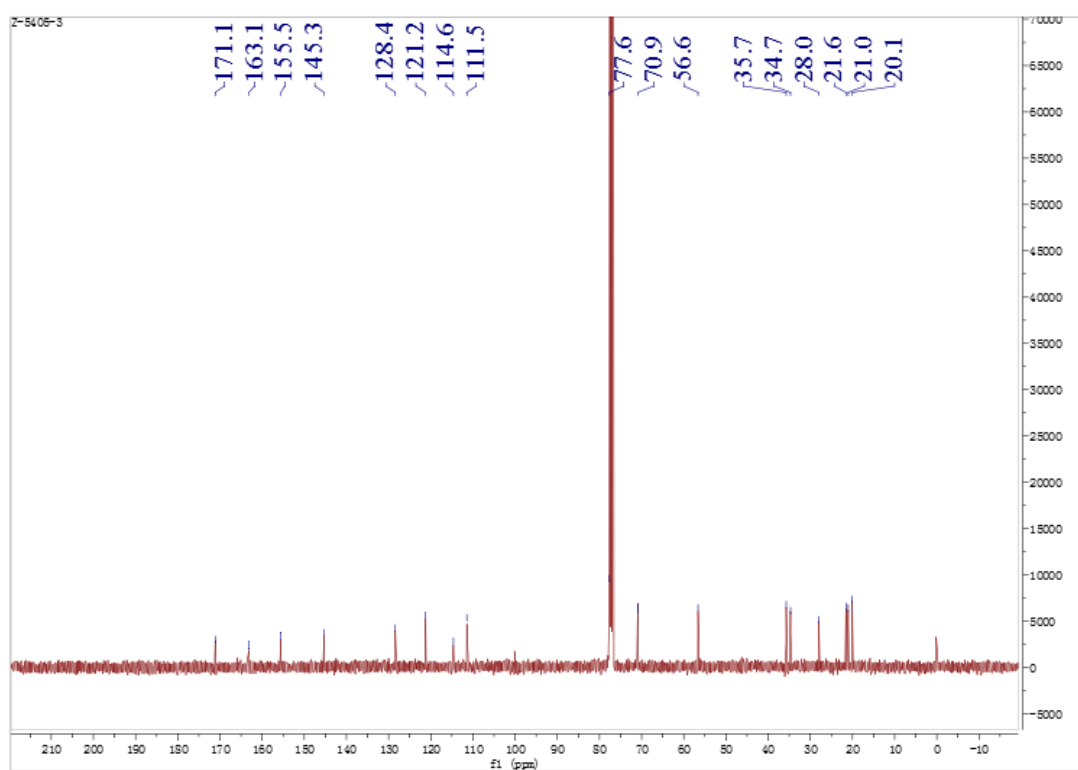


Figure S2. ¹³C NMR spectrum of **1** in CDCl₃

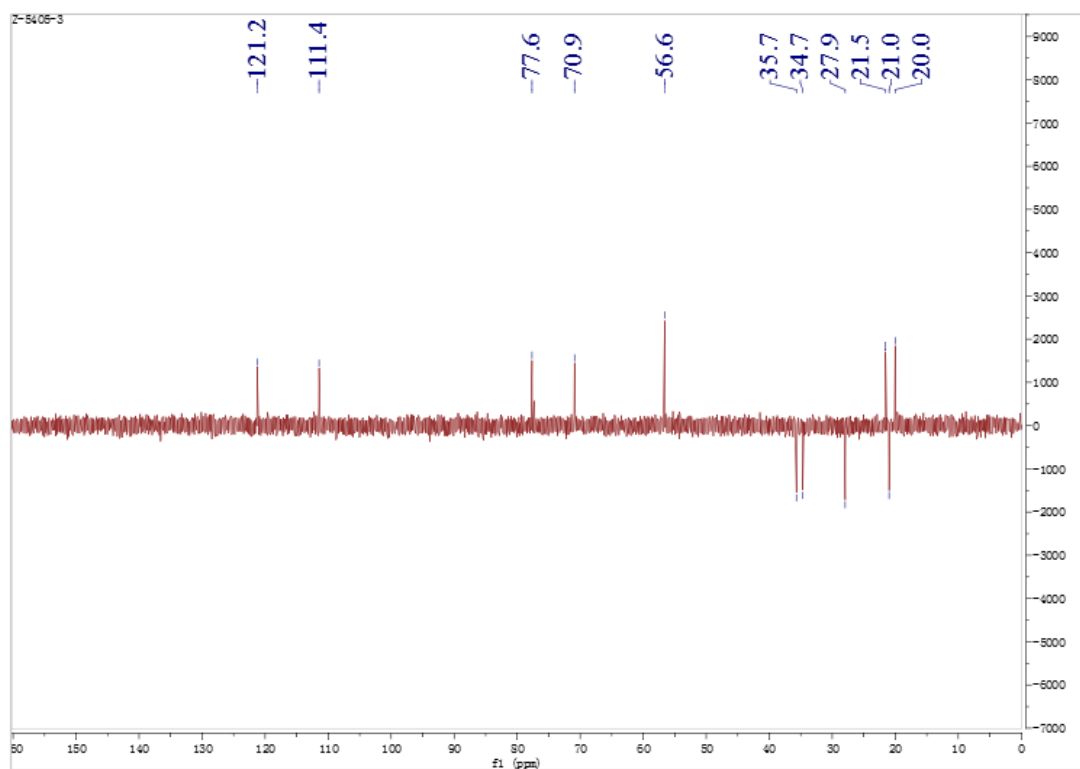


Figure S3. 135-DEPT spectrum of **1** in CDCl_3

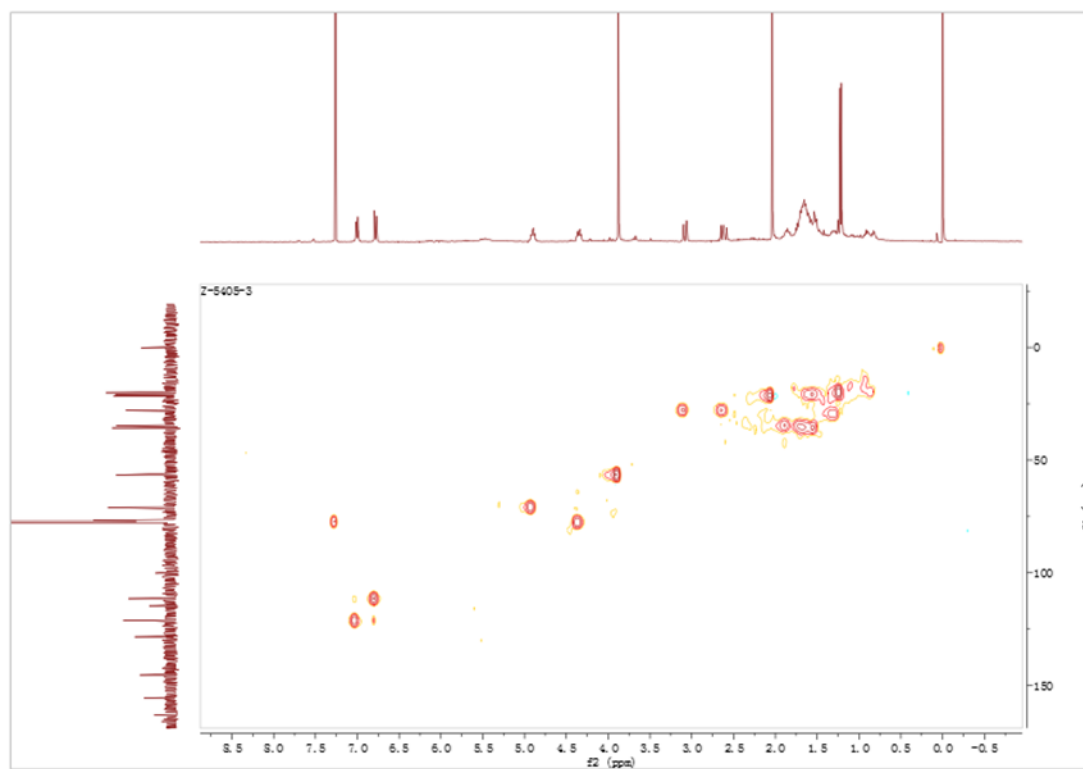


Figure S4. HMQC spectrum of **1** in CDCl_3

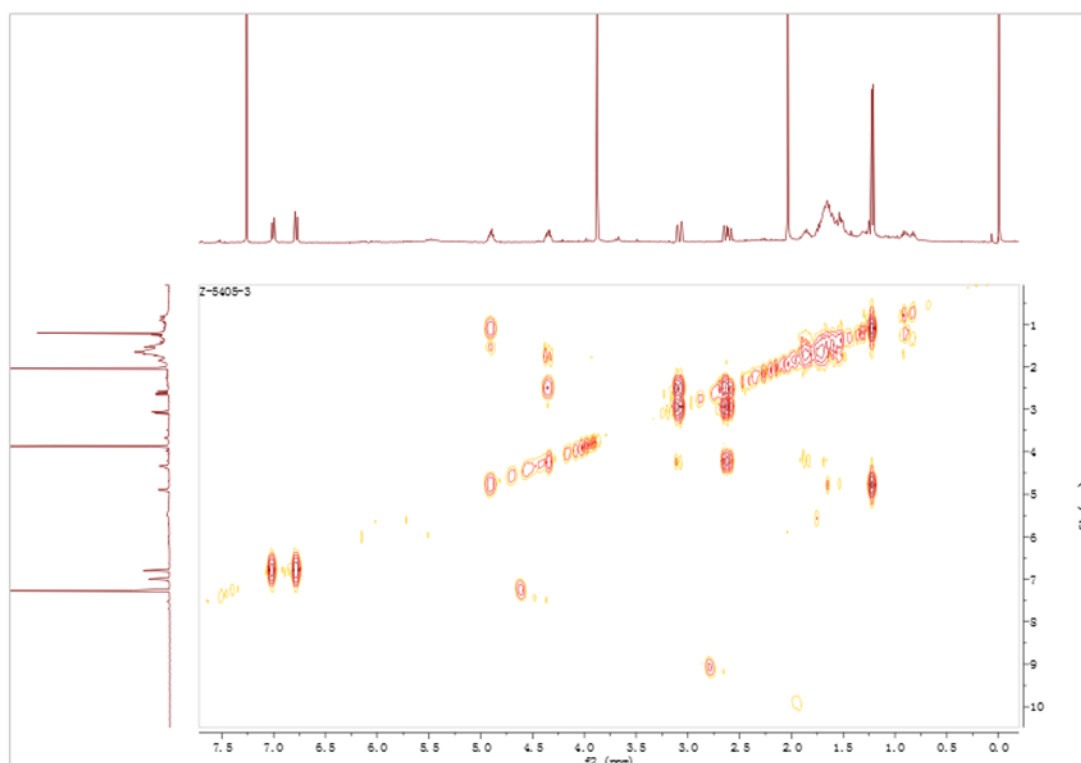


Figure S5. ^1H - ^1H COSY spectrum of **1** in CDCl_3

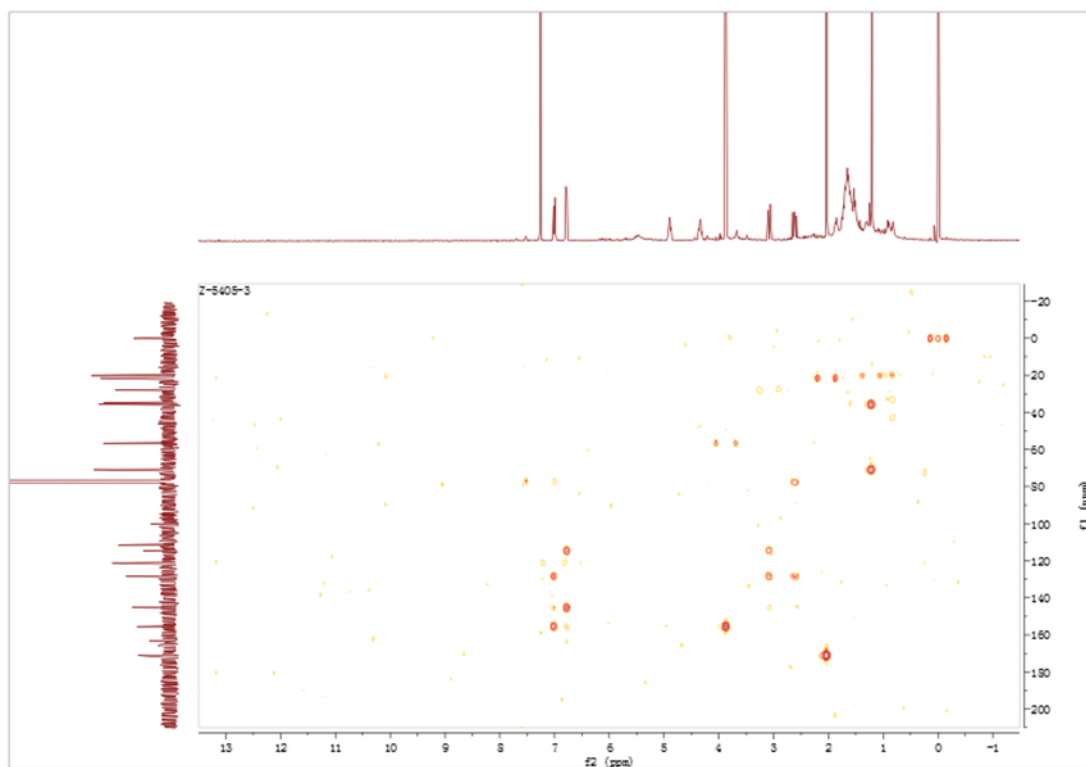


Figure S6. HMBC spectrum of **1** in CDCl_3

20201210-4-Z-5405-3 #1 RT: 0.00 AV: 1 NL: 3.66E6
T: FTMS + p ESI Full ms [170.0000-430.0000]

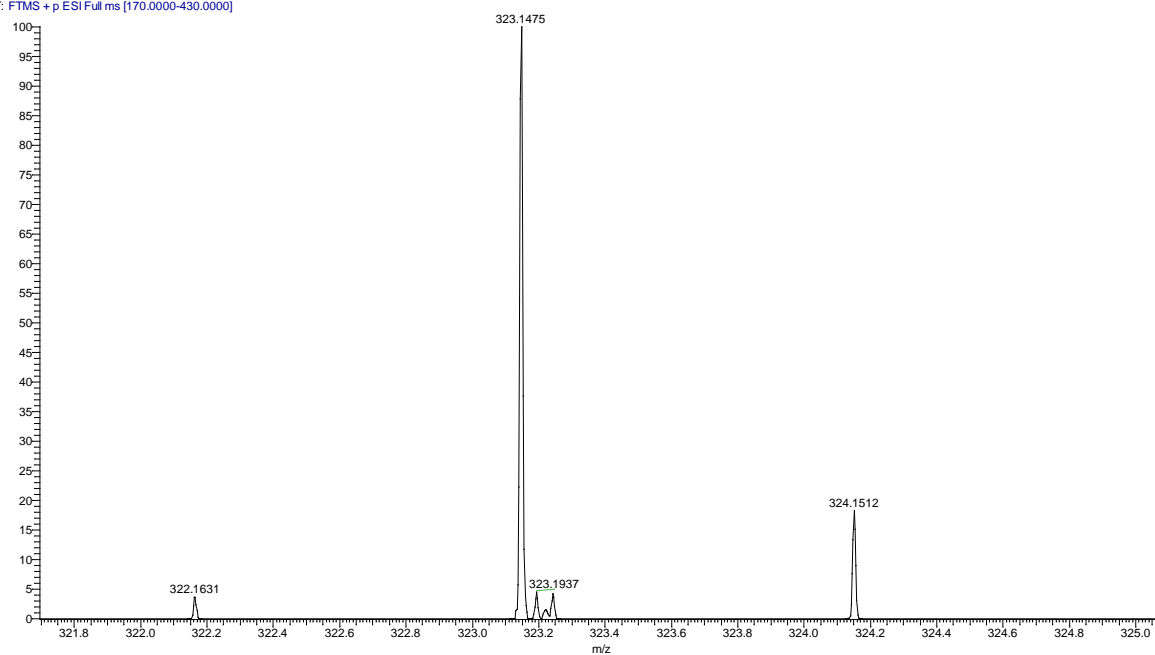


Figure S7. HR-ESI-MS spectrum of **1**

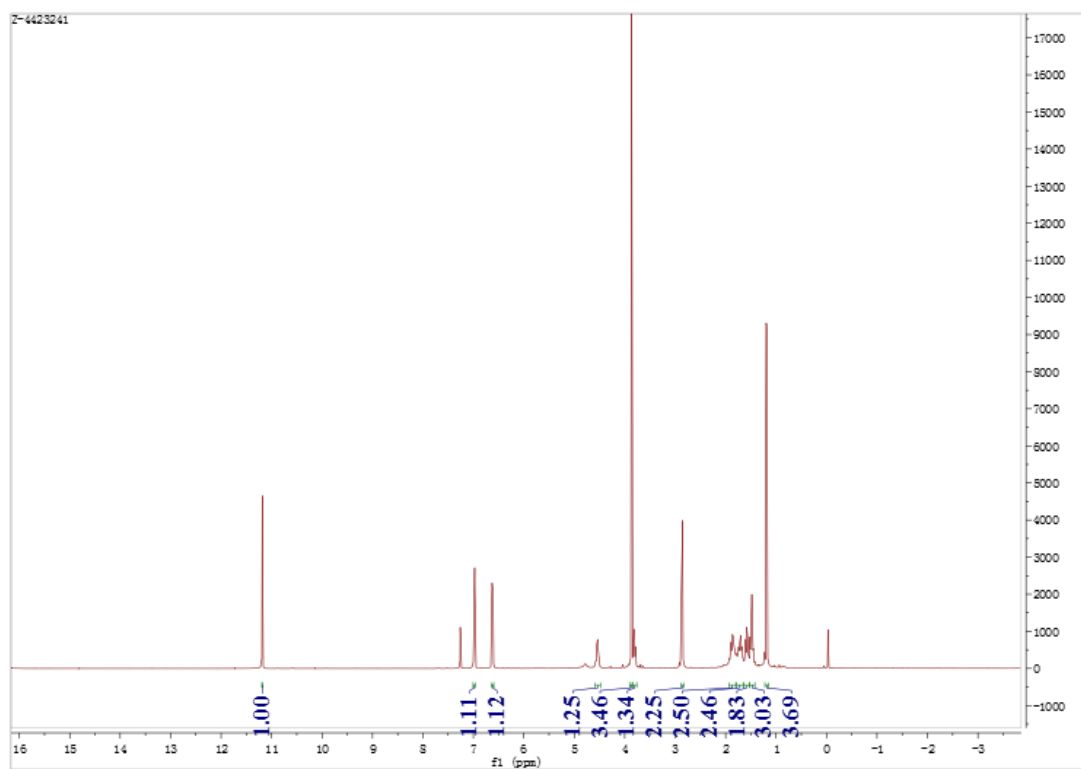


Figure S8. ¹H NMR spectrum of **2** in CDCl₃

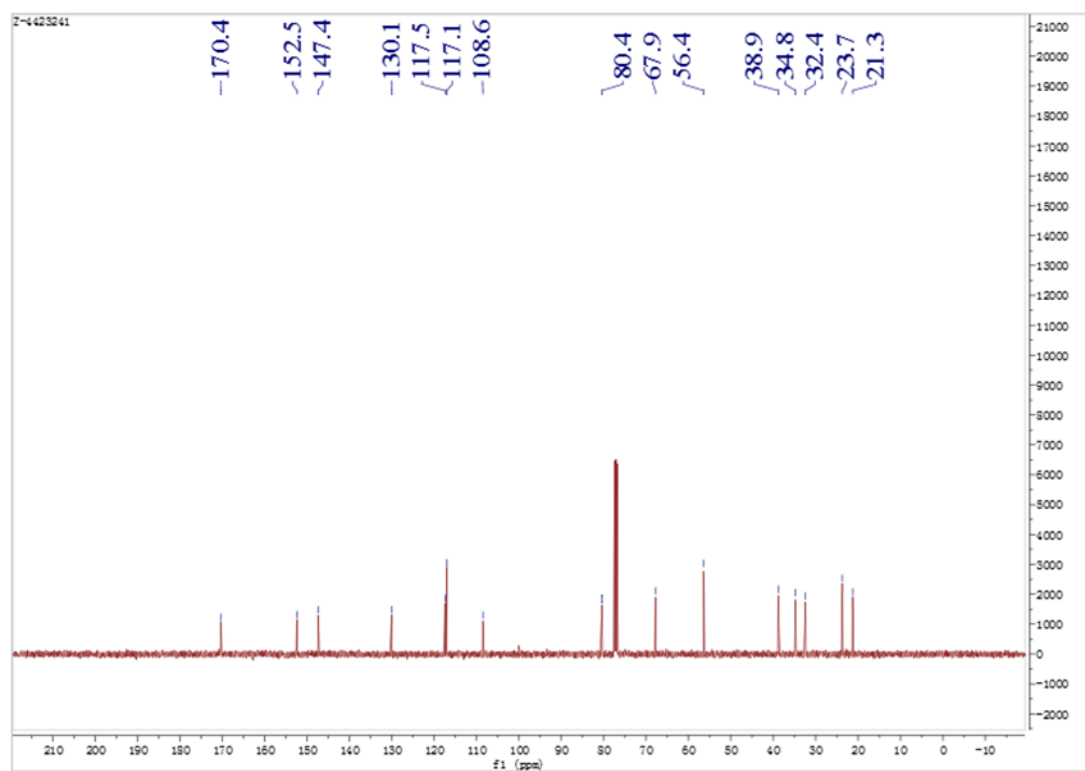


Figure S9. ¹³C NMR spectrum of **2** in CDCl₃

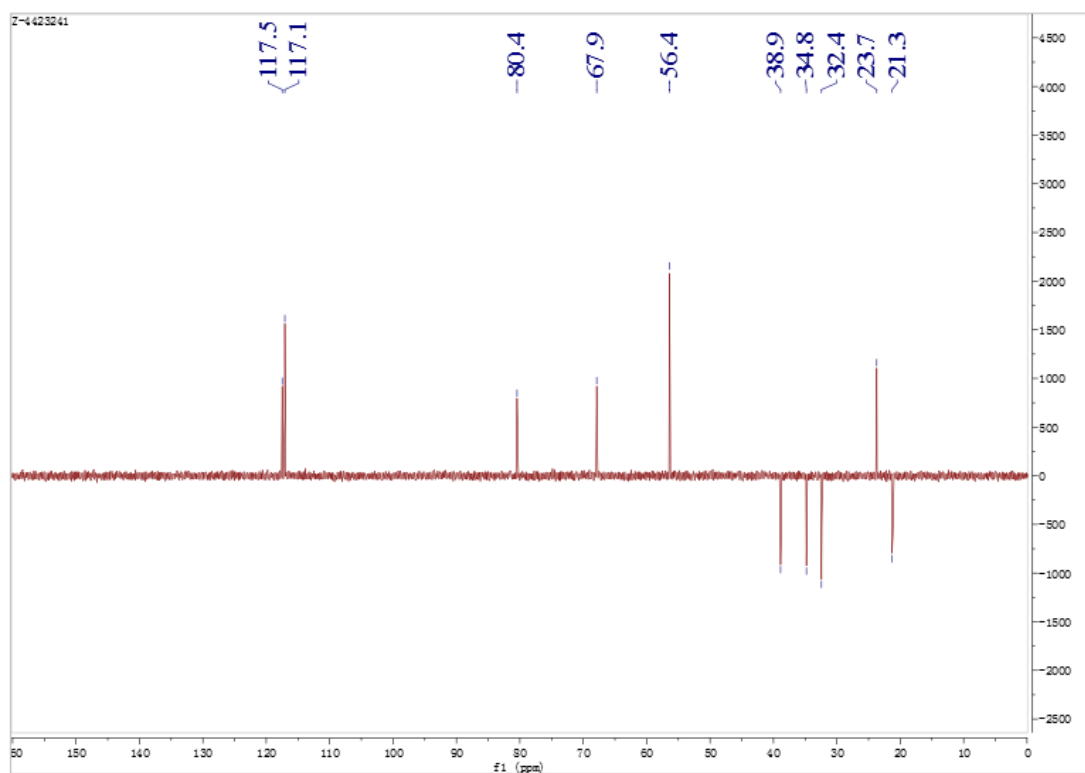


Figure S10. ¹³⁵-DEPT spectrum of **2** in CDCl₃

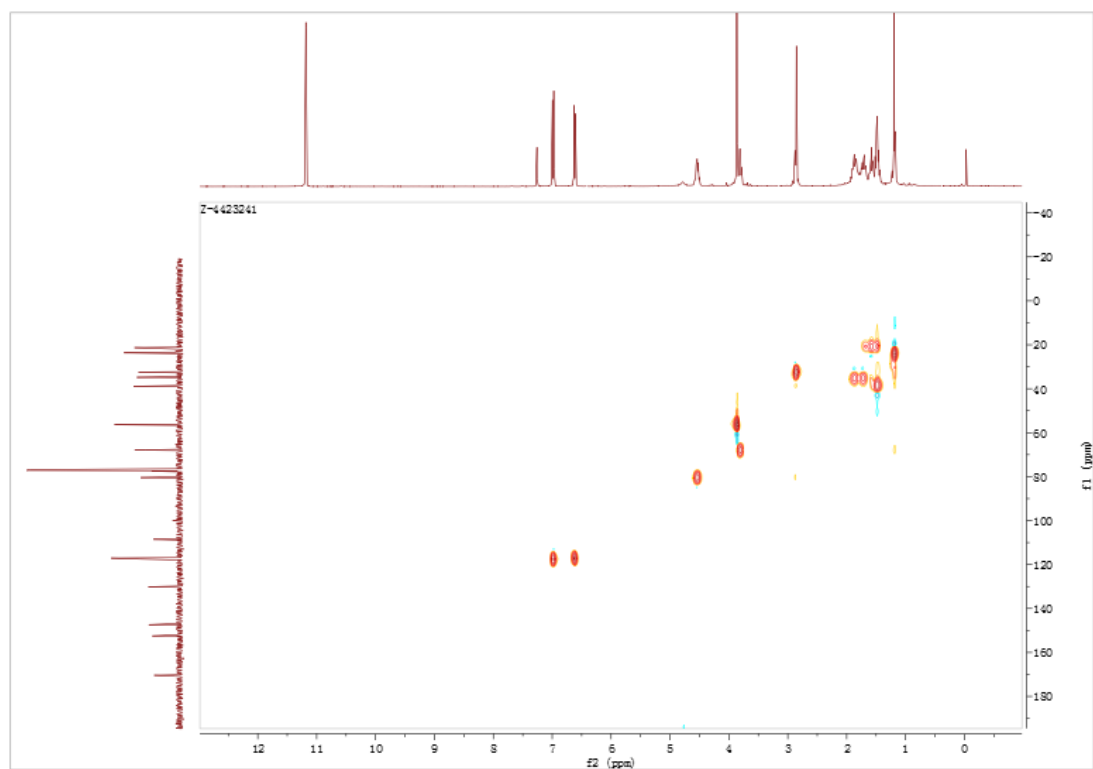


Figure S11. HMQC spectrum of **2** in CDCl_3

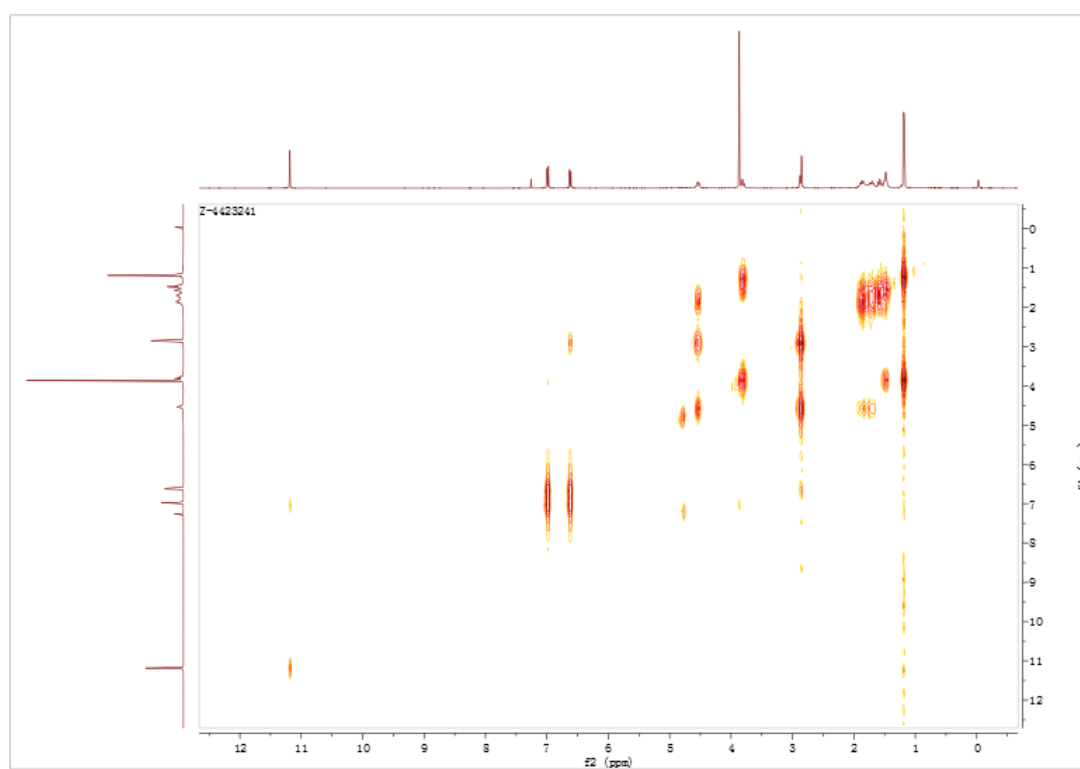


Figure S12. ^1H - ^1H COSY spectrum of **2** in CDCl_3

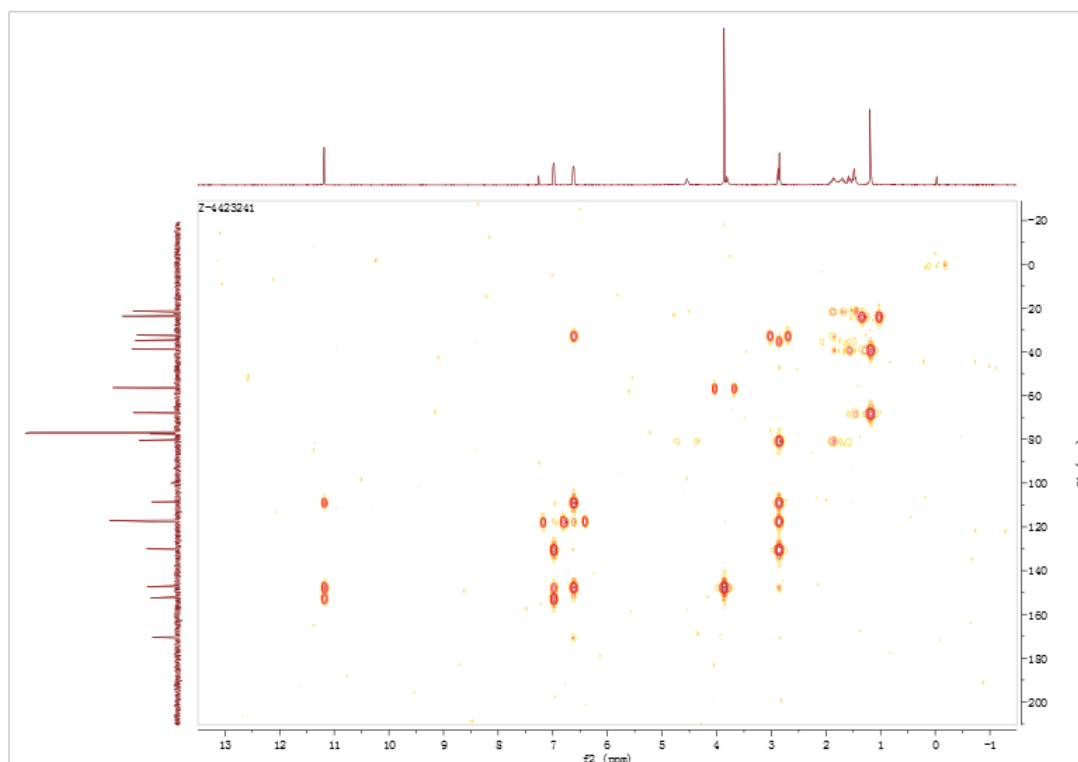


Figure S13. HMBC spectrum of **2** in CDCl_3

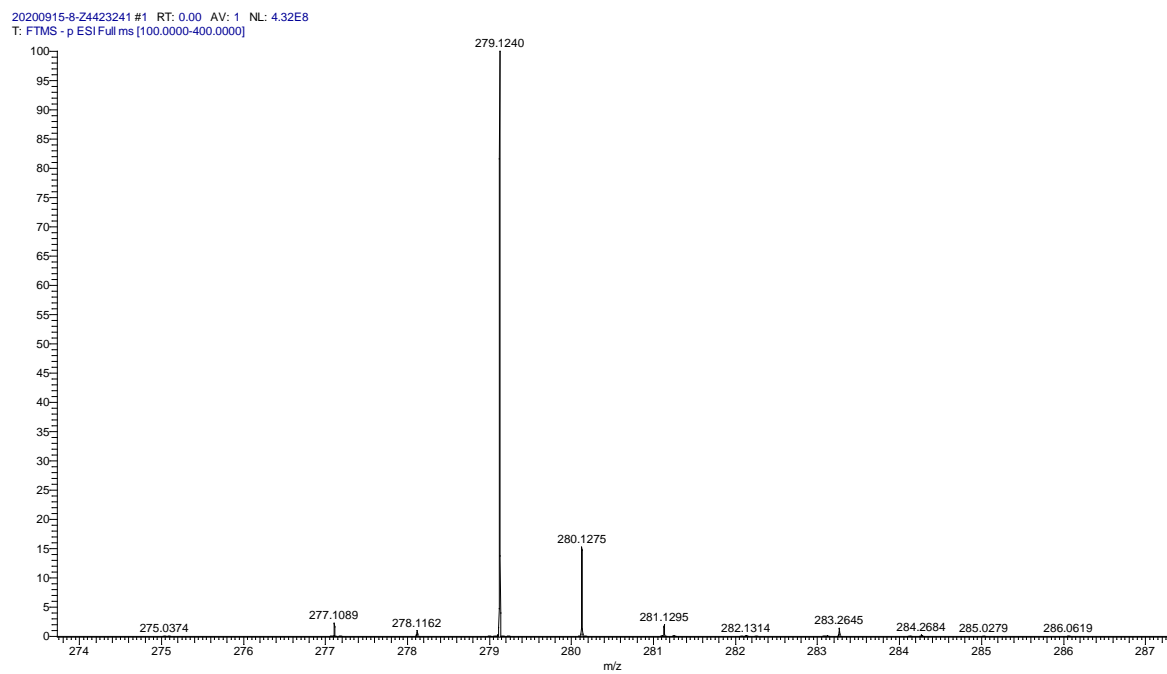


Figure S14. HR-ESI-MS spectrum of **2**

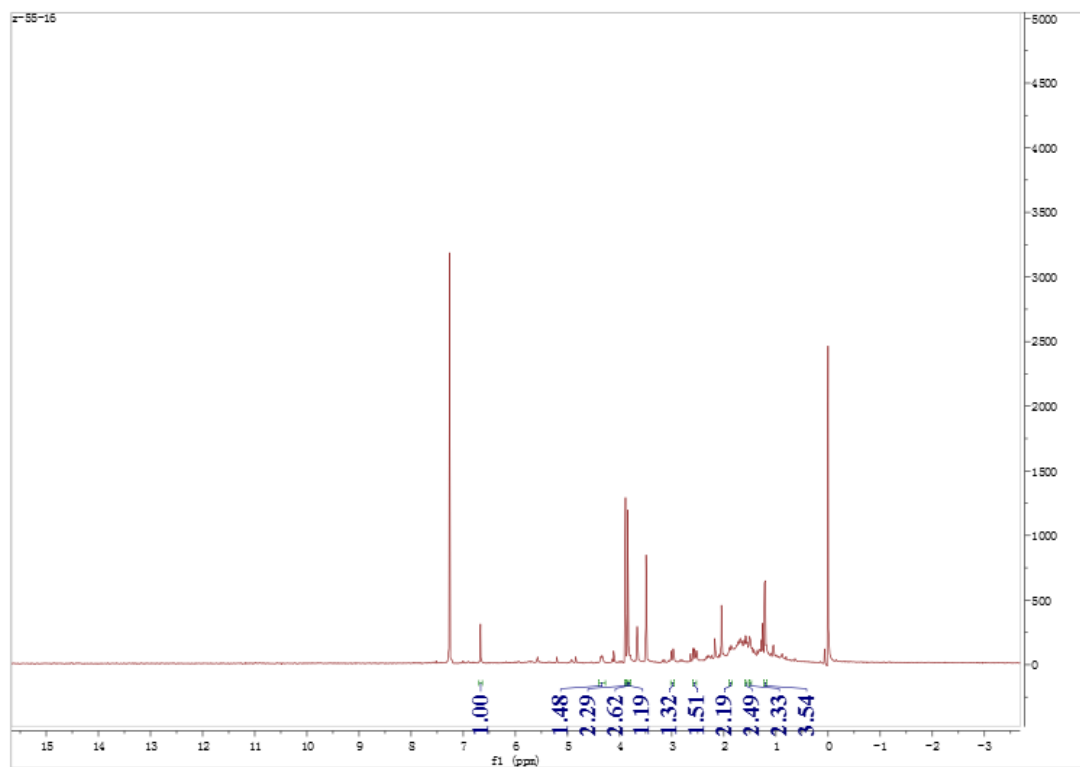


Figure S15. ¹H NMR spectrum of **3** in CDCl₃

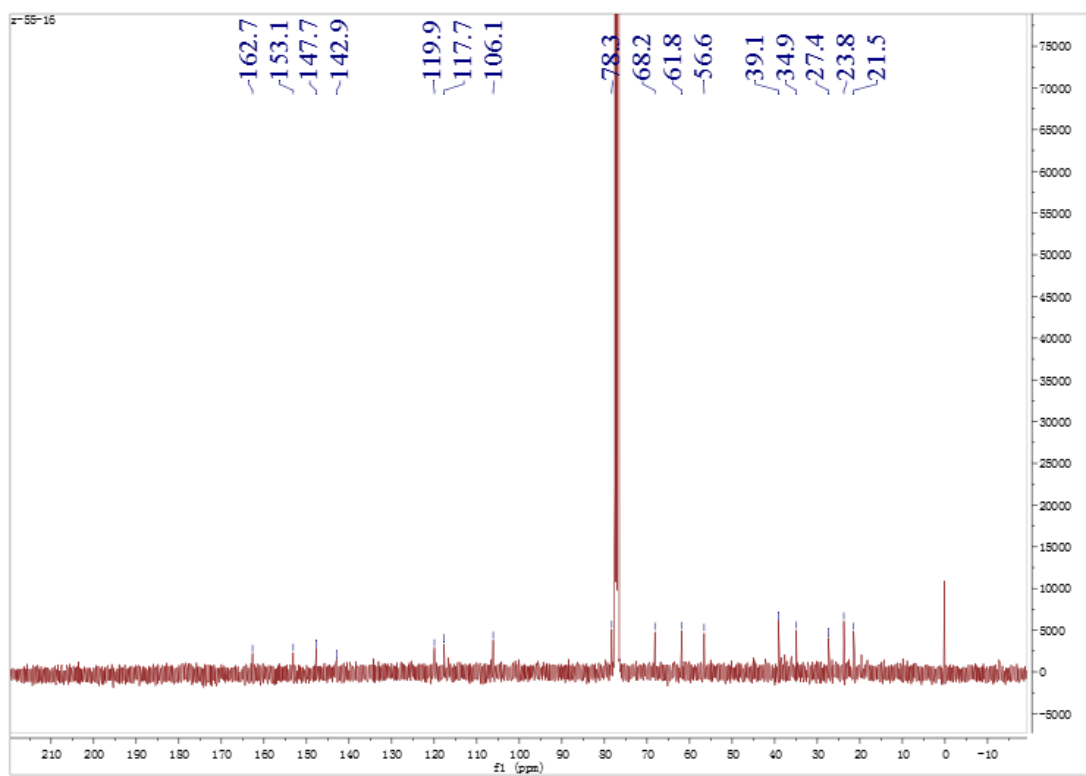


Figure S16. ¹³C NMR spectrum of **3** in CDCl₃

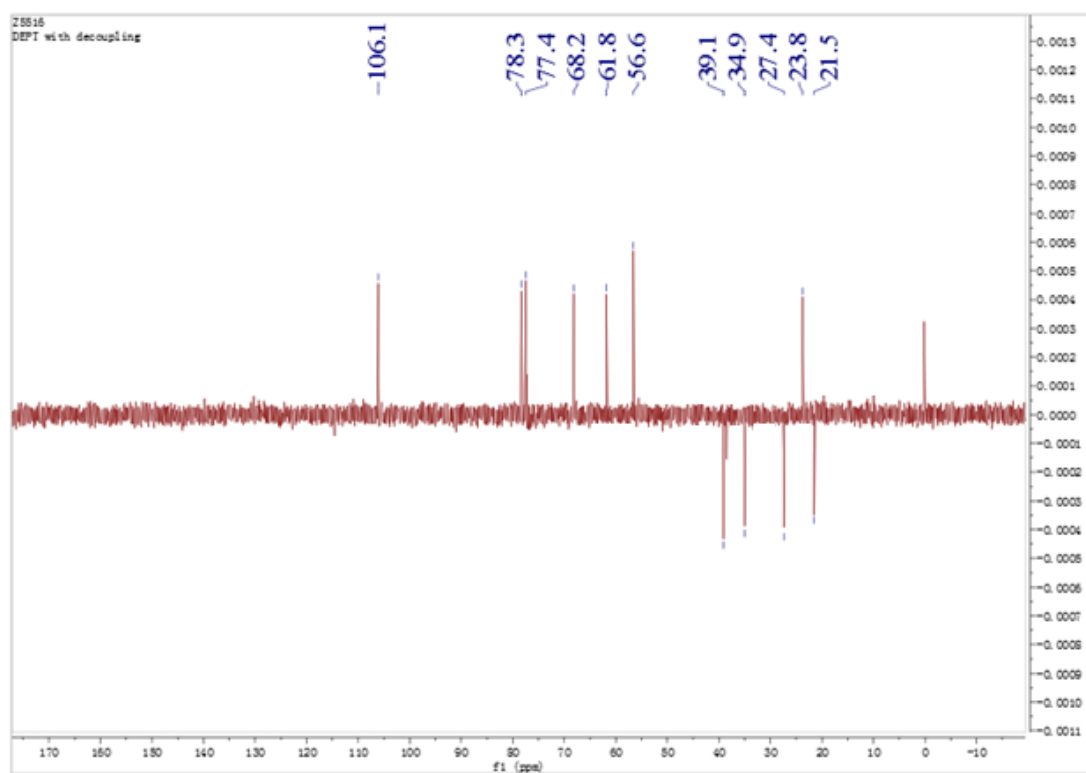


Figure S17. 135-DEPT spectrum of **2** in CDCl₃

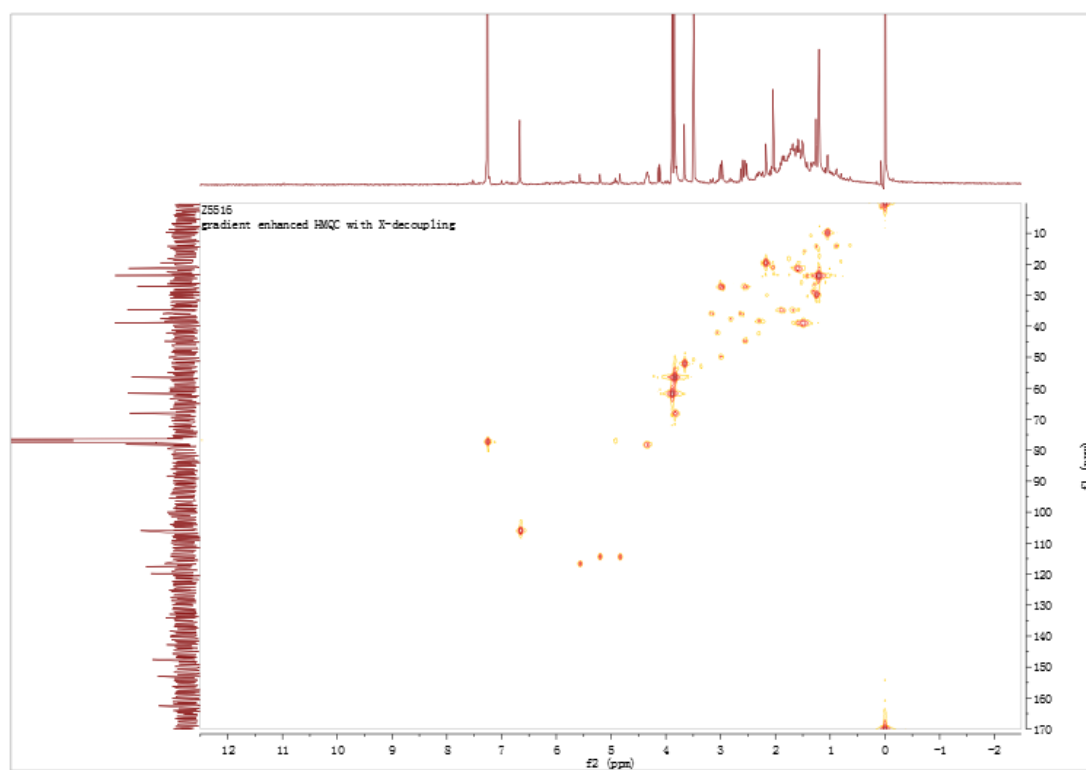


Figure S18. HMQC spectrum of **3** in CDCl₃

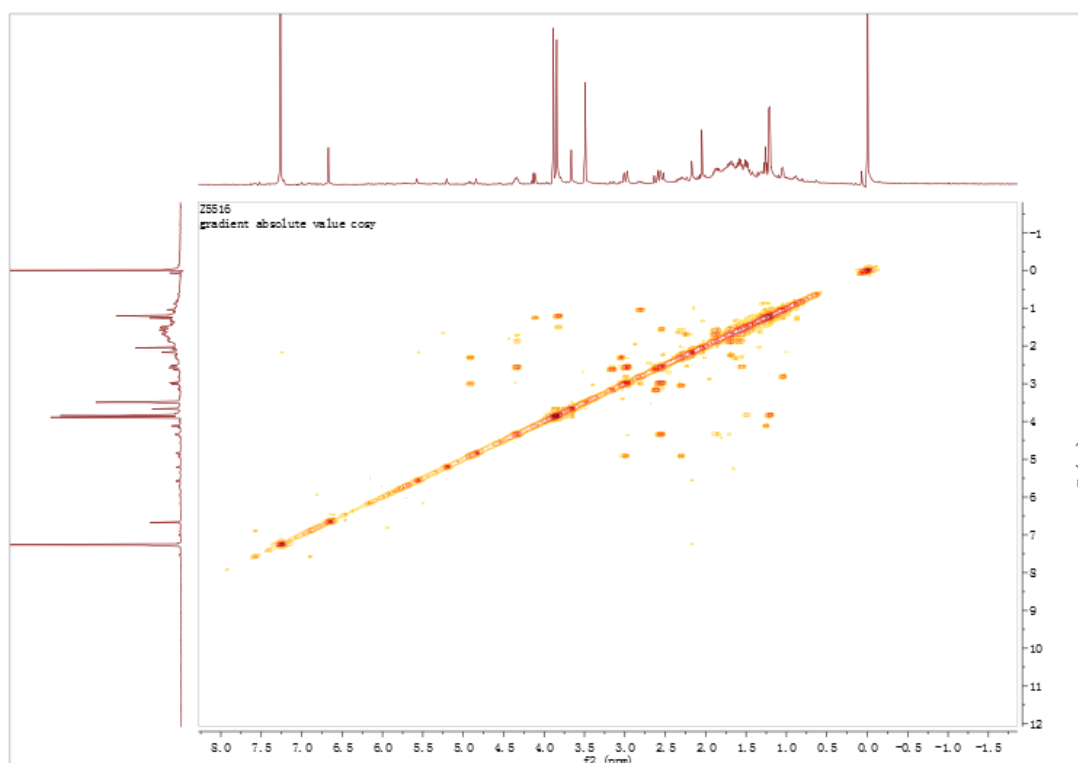


Figure S19. ^1H - ^1H COSY spectrum of **2** in CDCl_3

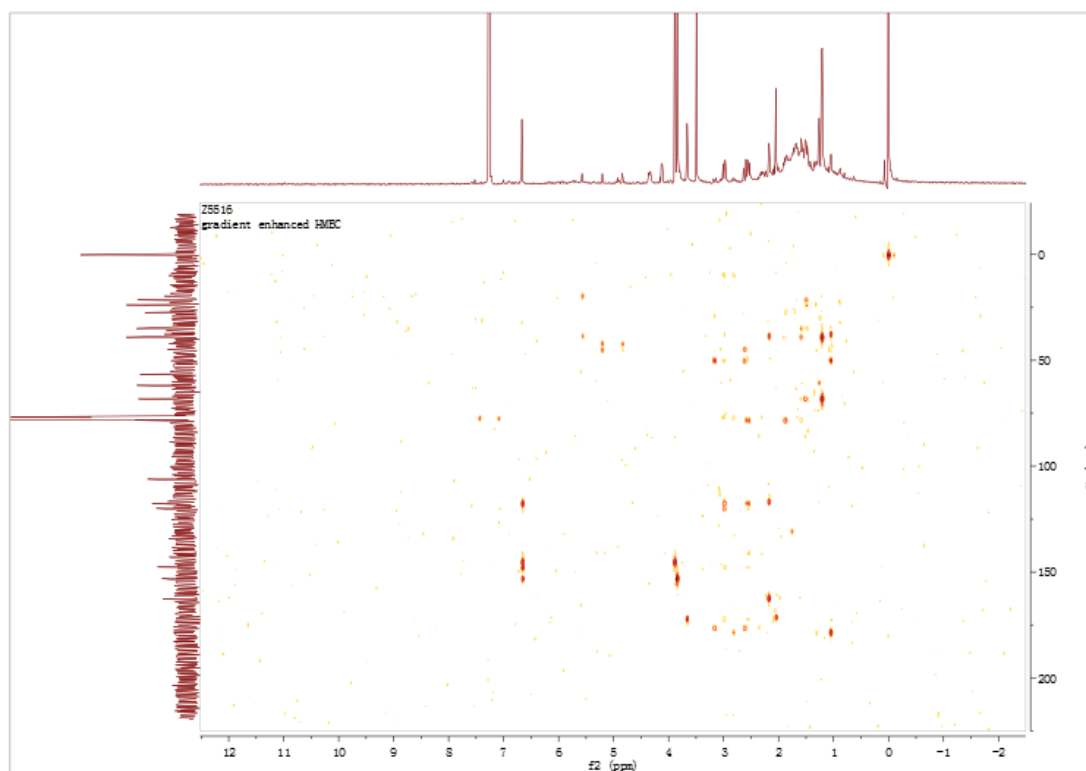


Figure S20. HMBC spectrum of **3** in CDCl_3

20200915-16-Z-55-16 #1 RT: 0.00 AV: 1 NL: 9.79E7
T: FTMS + p ESI Full ms [200.0000-600.0000]

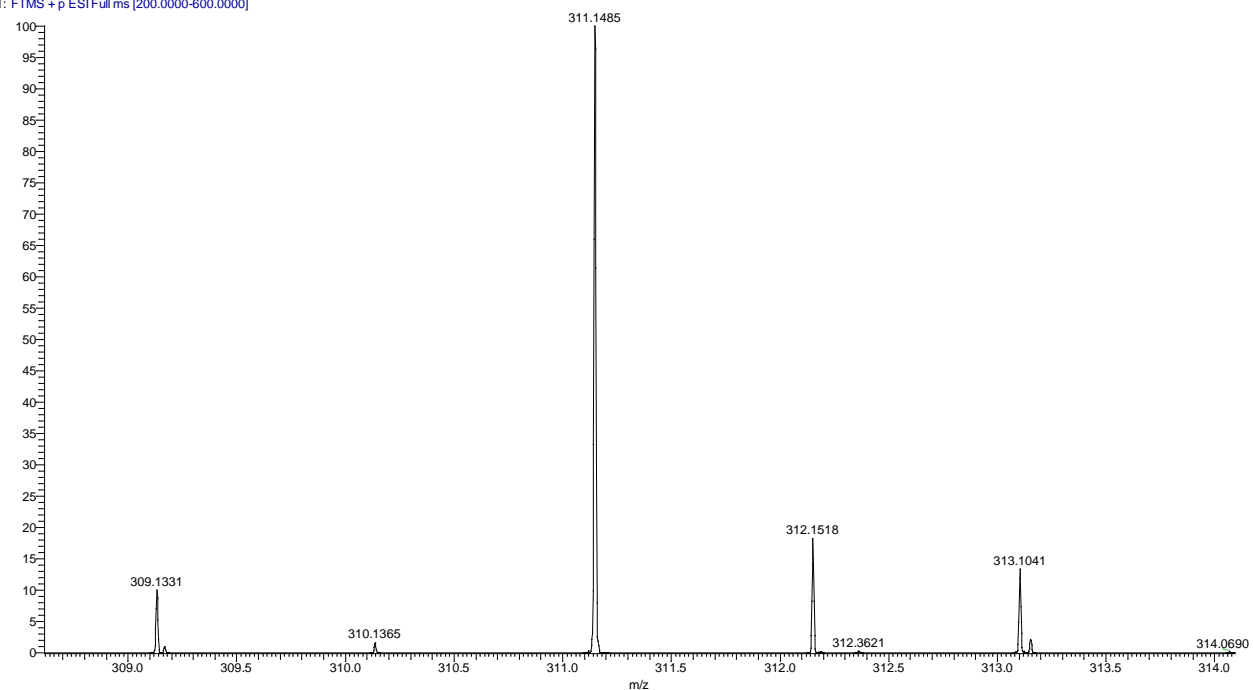


Figure S21. HR-ESI-MS spectrum of **3**

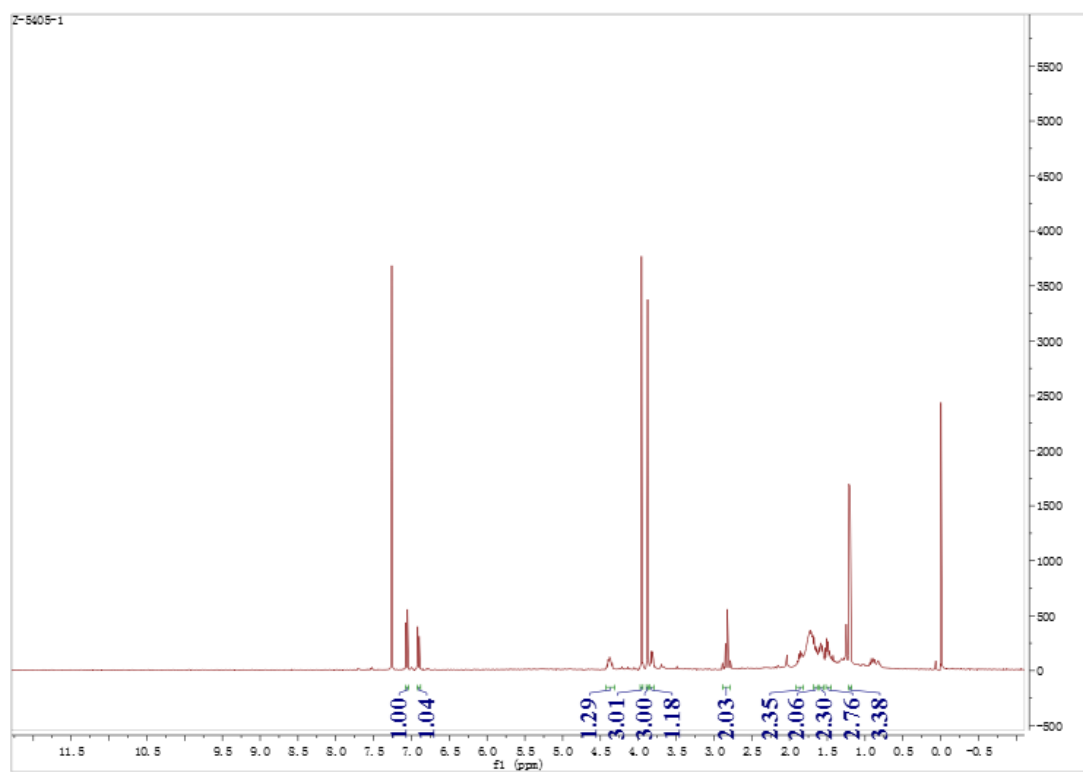


Figure S22. ^1H NMR spectrum of **4** in CDCl_3

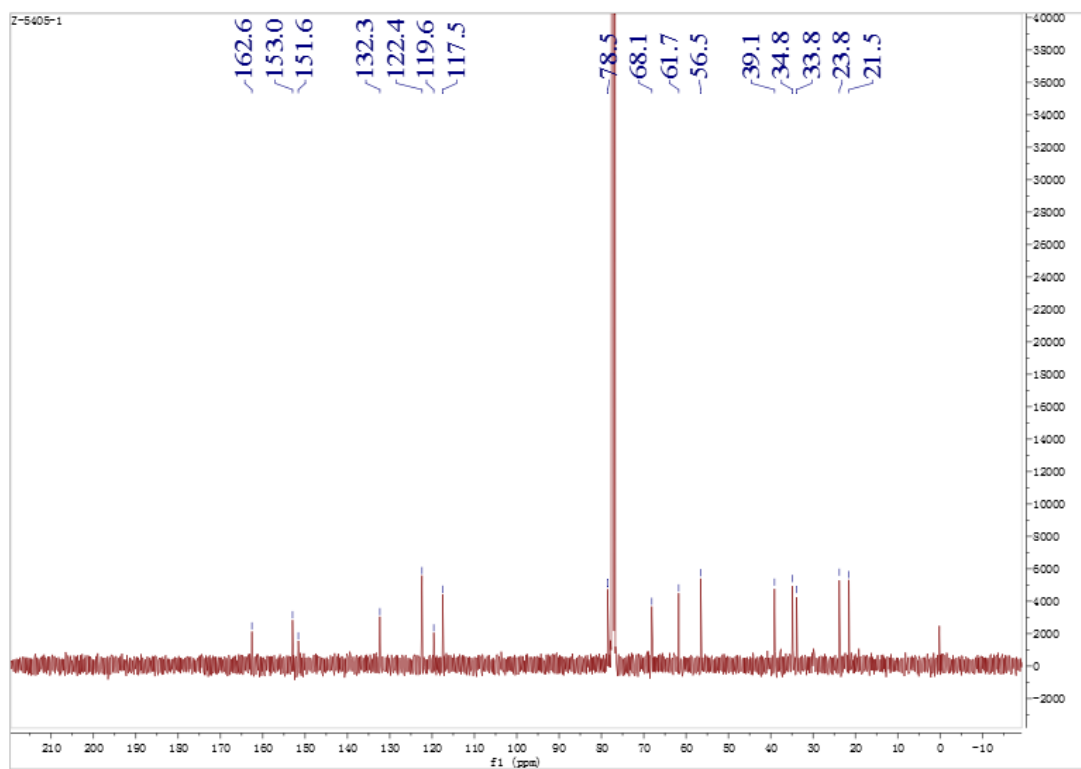


Figure S23. ¹³C NMR spectrum of **4** in CDCl₃

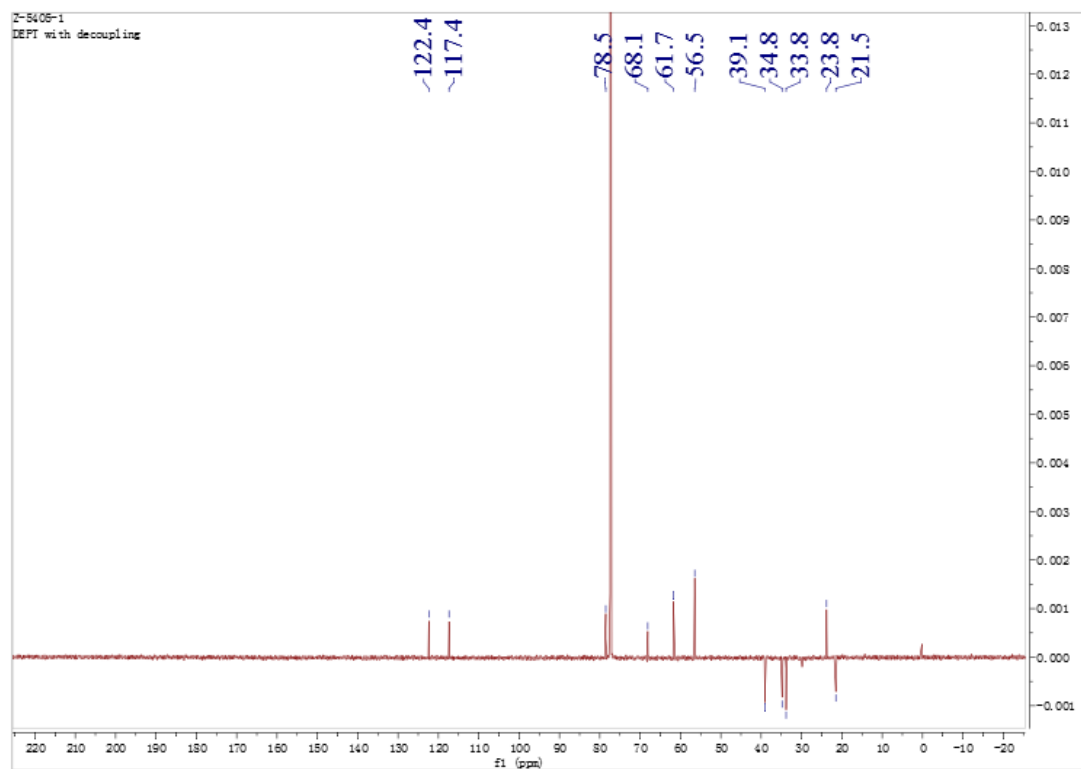


Figure S24. ¹³⁵-DEPT spectrum of **4** in CDCl₃

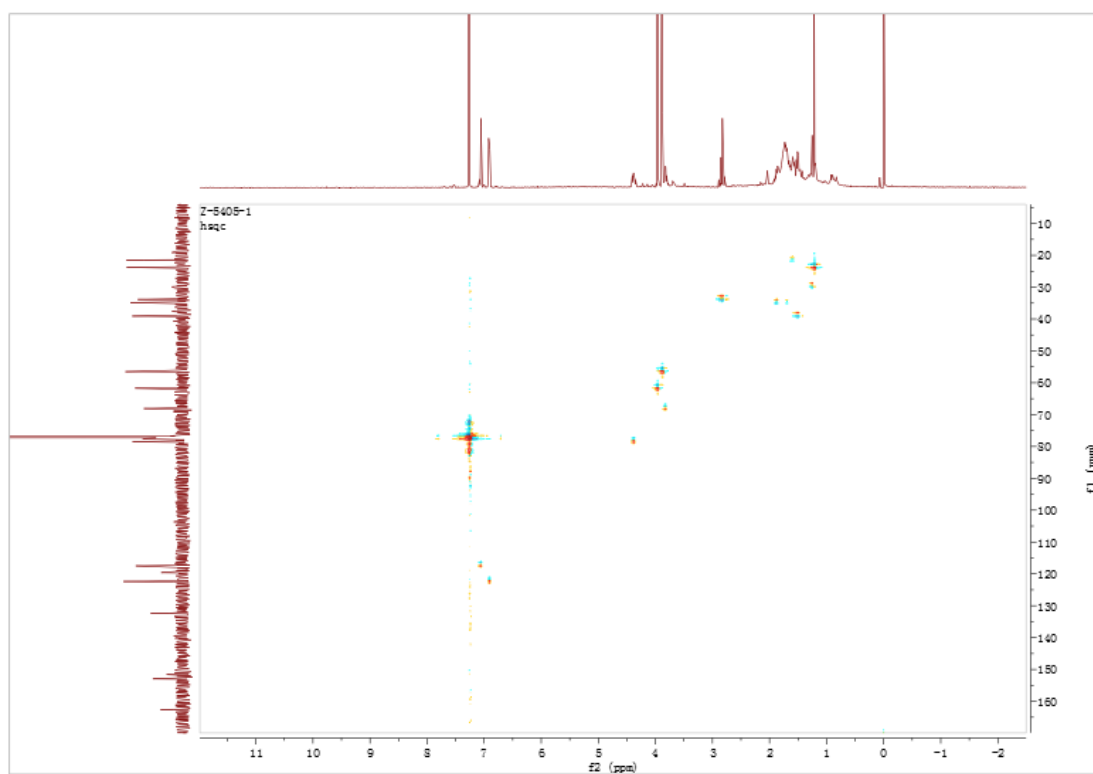


Figure S25. HMQC spectrum of **4** in CDCl₃

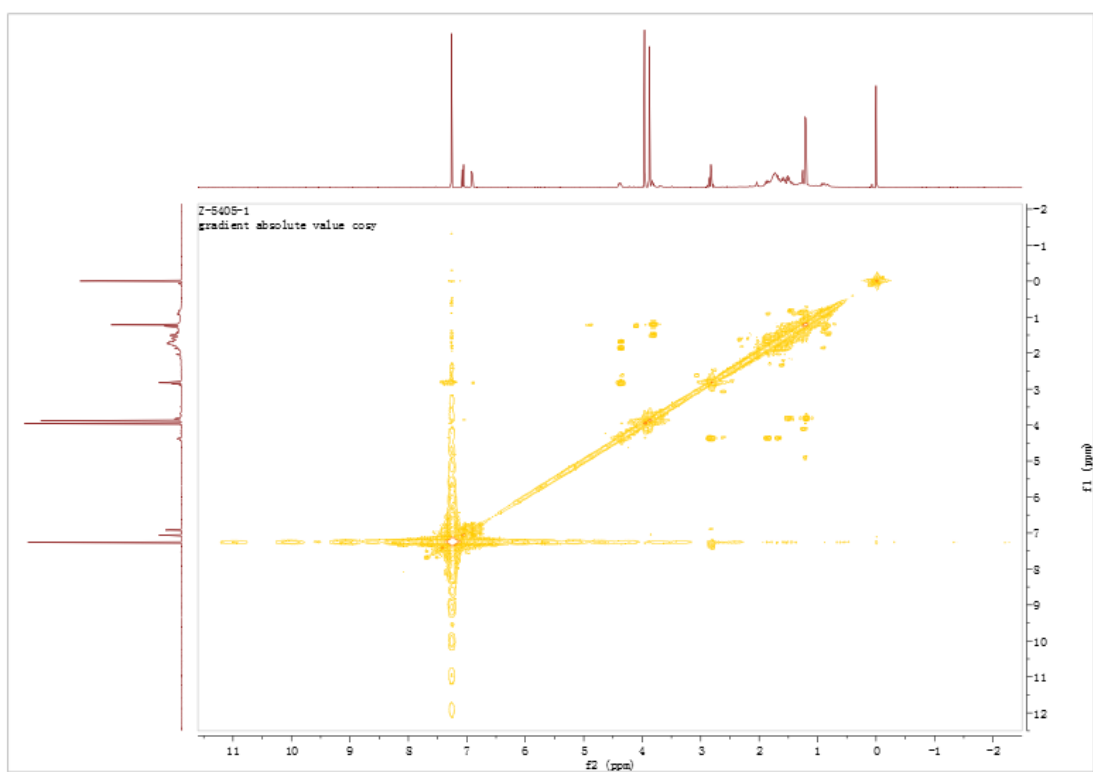


Figure S26. ¹H-¹H COSY spectrum of **4** in CDCl₃

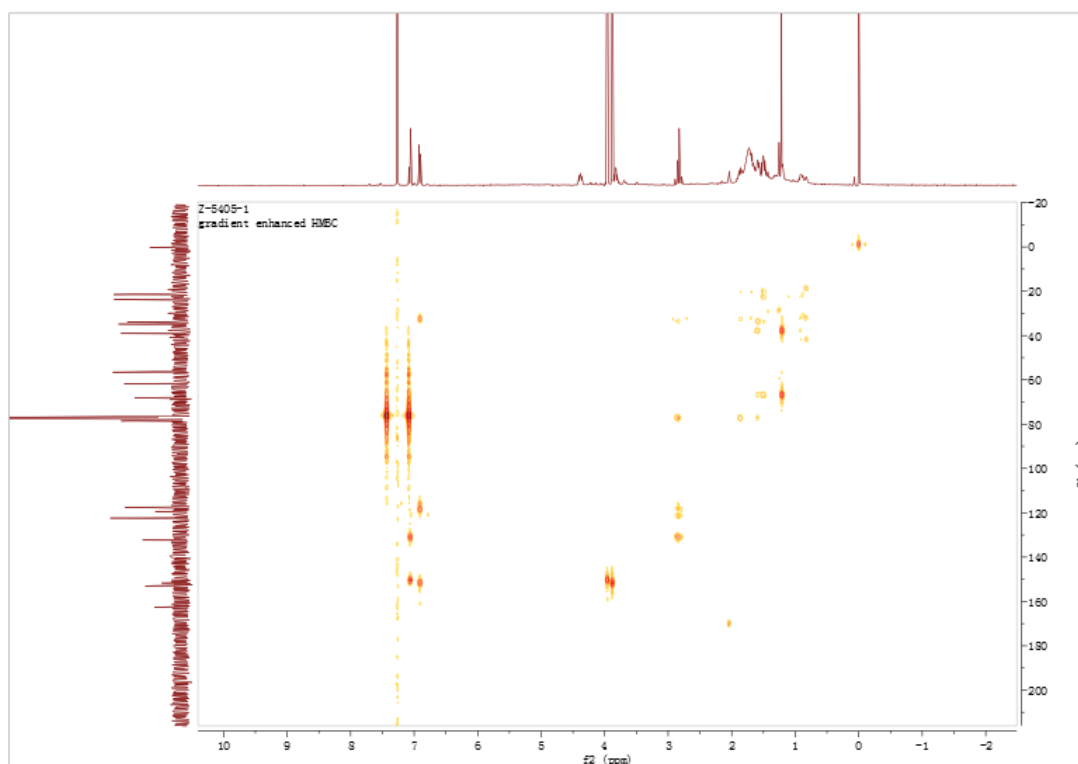


Figure S27. HMBC spectrum of **4** in CDCl_3

20201210-3-Z-5405-1 #1 RT: 0.00 AV: 1 NL: 1.51E7
T: FTMS + p ESI Full ms [200.0000-400.0000]

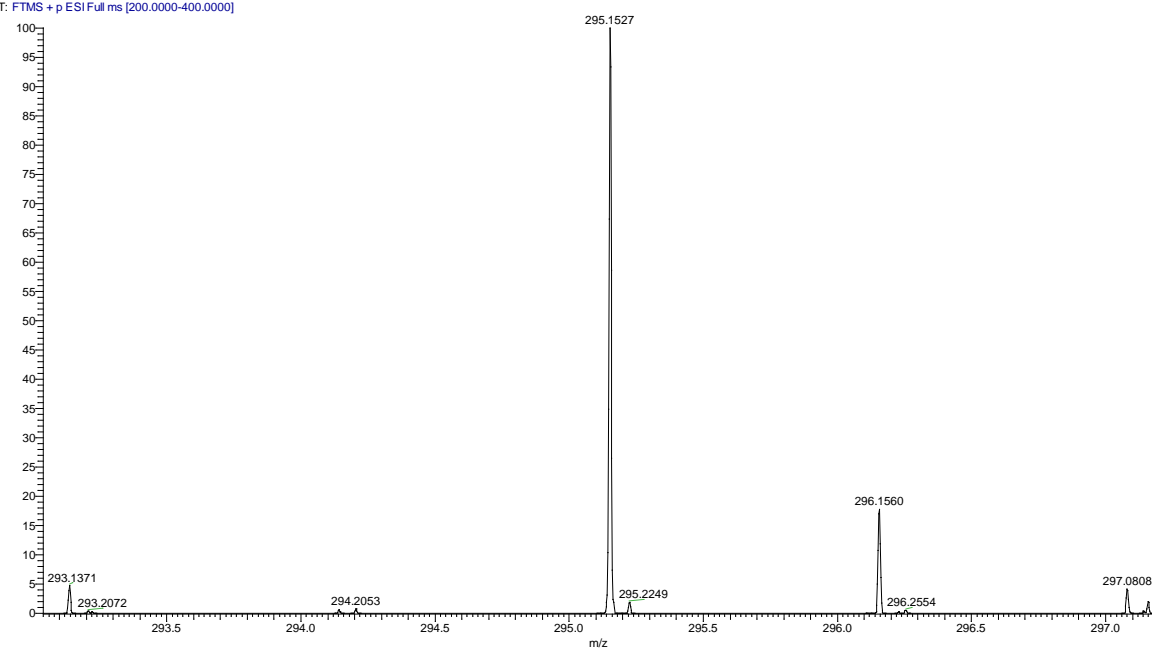


Figure S28. HR-ESI-MS spectrum of **4**

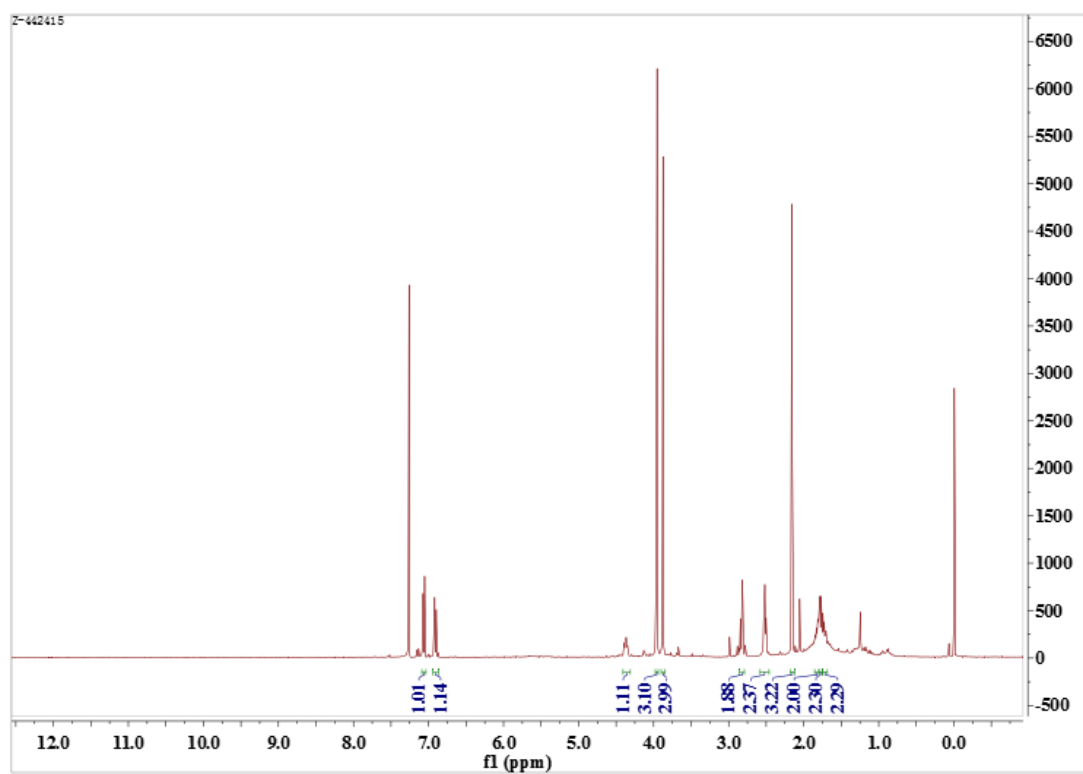


Figure S29. ¹H NMR spectrum of **5** in CDCl₃

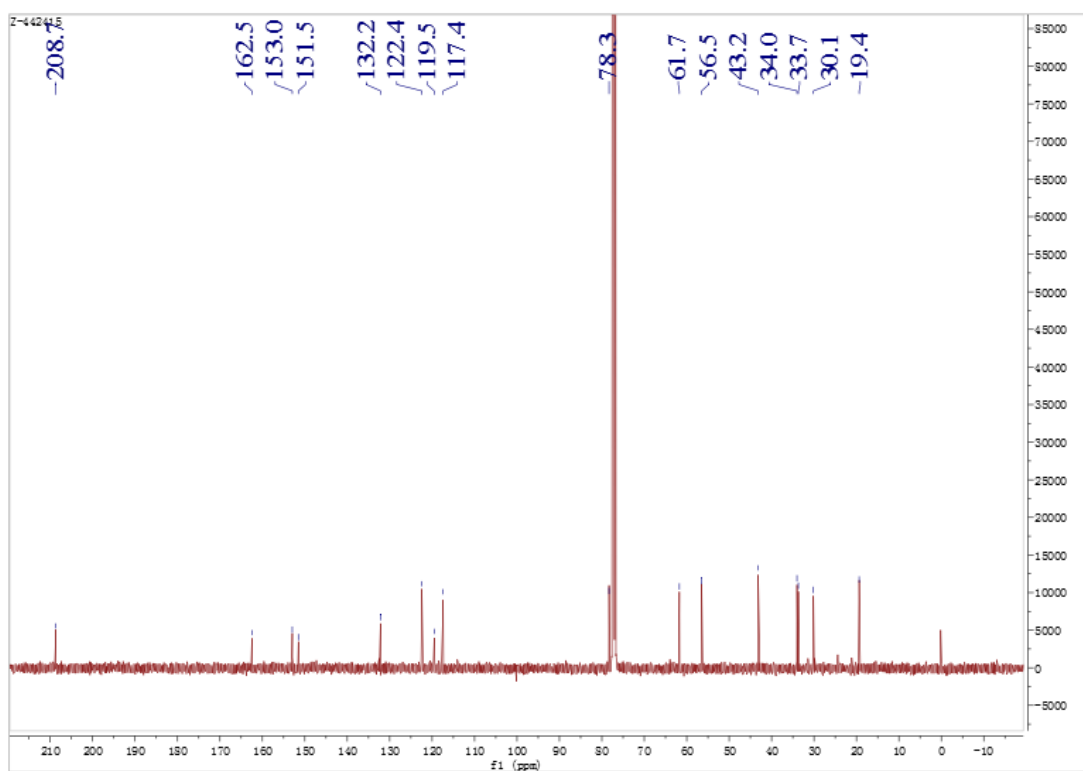


Figure S30. ¹³C NMR spectrum of **5** in CDCl₃

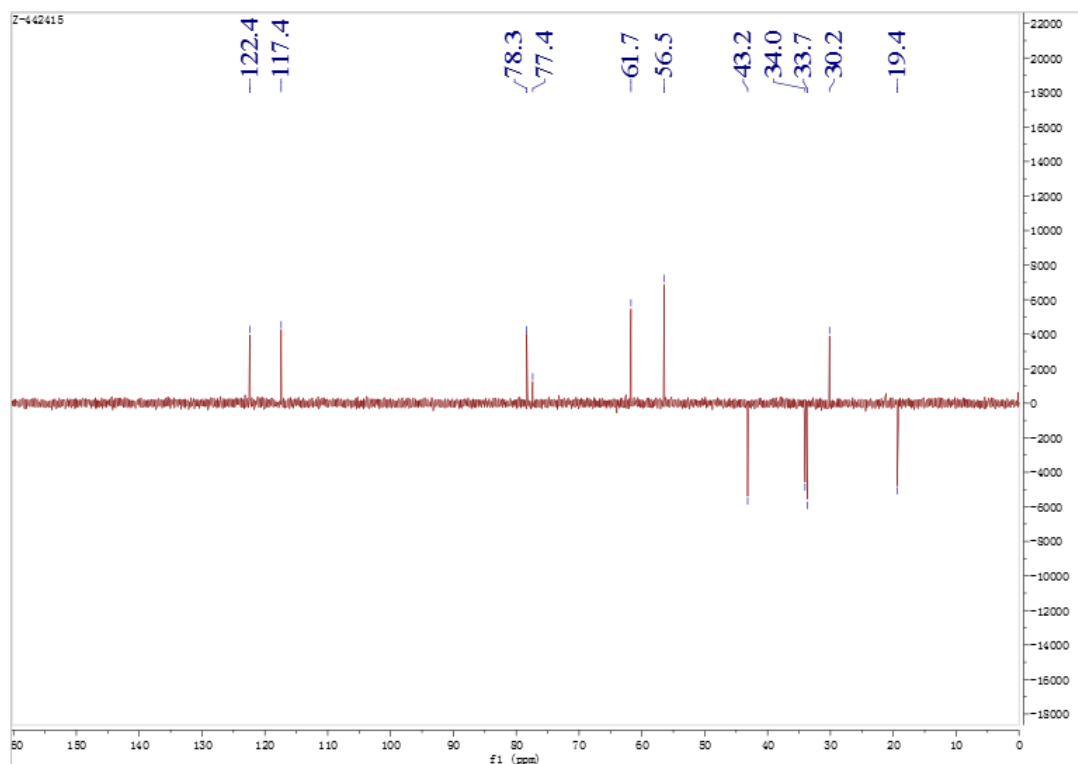


Figure S31. $^{135}\text{-DEPT}$ spectrum of **5** in CDCl_3

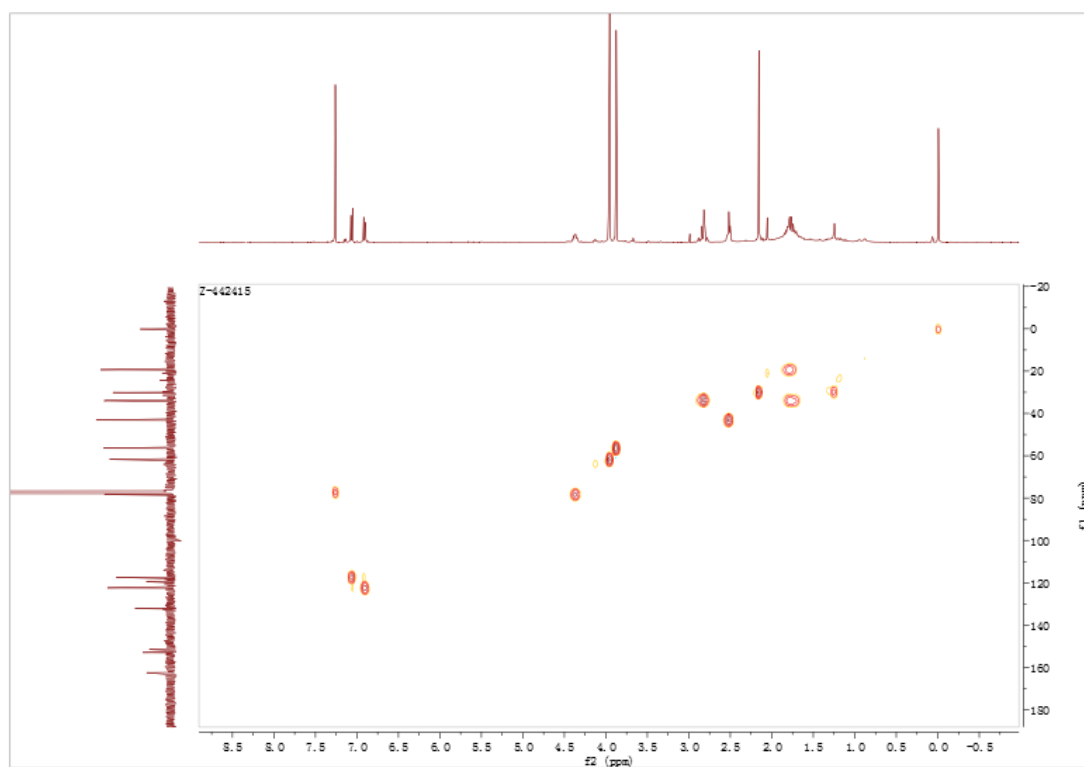


Figure S32. HMQC spectrum of **5** in CDCl_3

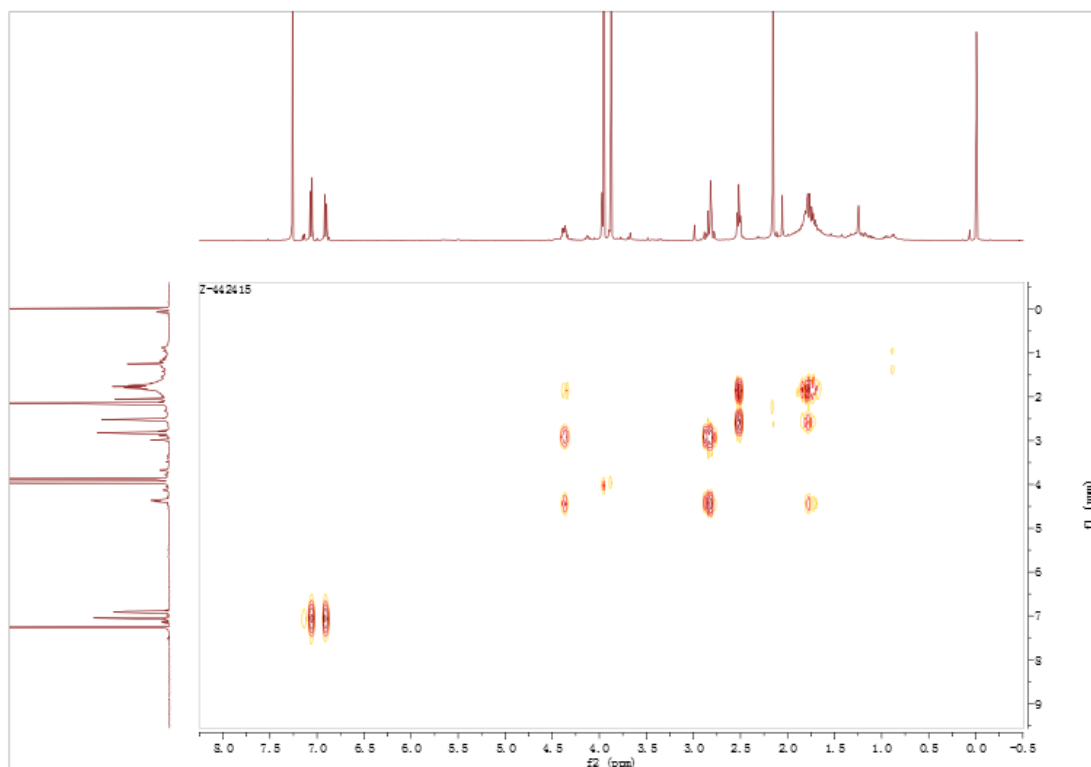


Figure S33. ^1H - ^1H COSY spectrum of **5** in CDCl_3

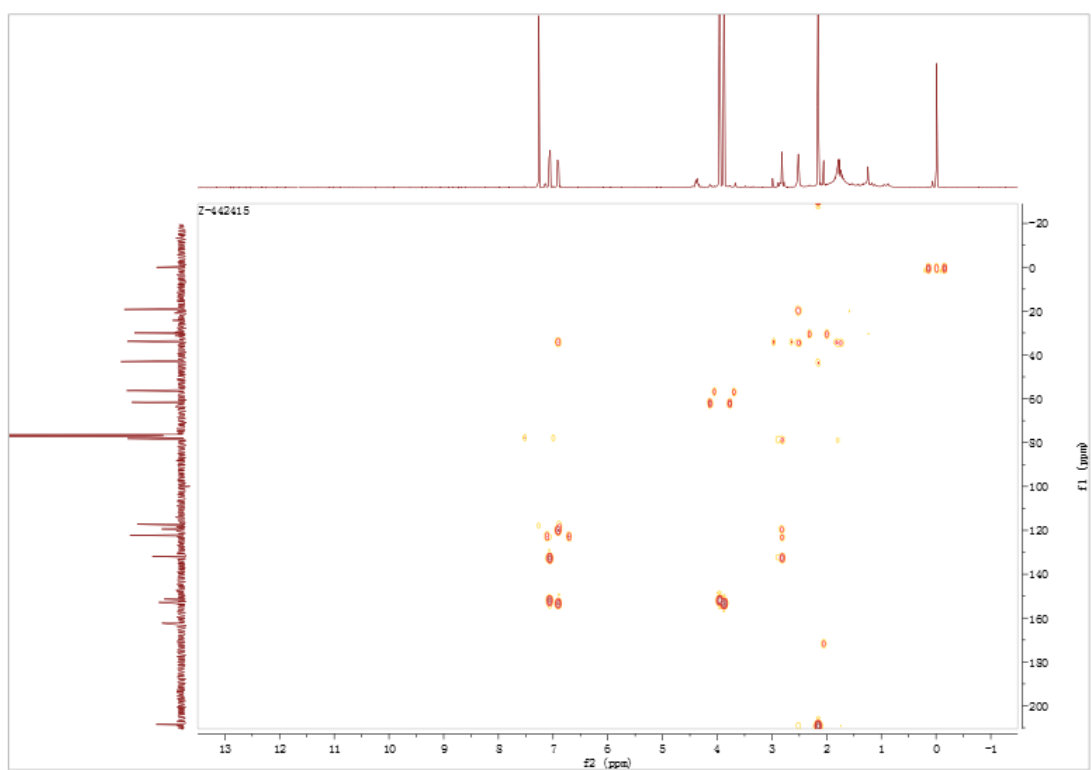


Figure S34. HMBC spectrum of **5** in CDCl_3

20201210-5-Z-442415 #1 RT: 0.00 AV: 1 NL: 1.93E8
T: FTMS + p ESI Full ms [170.0000-430.0000]

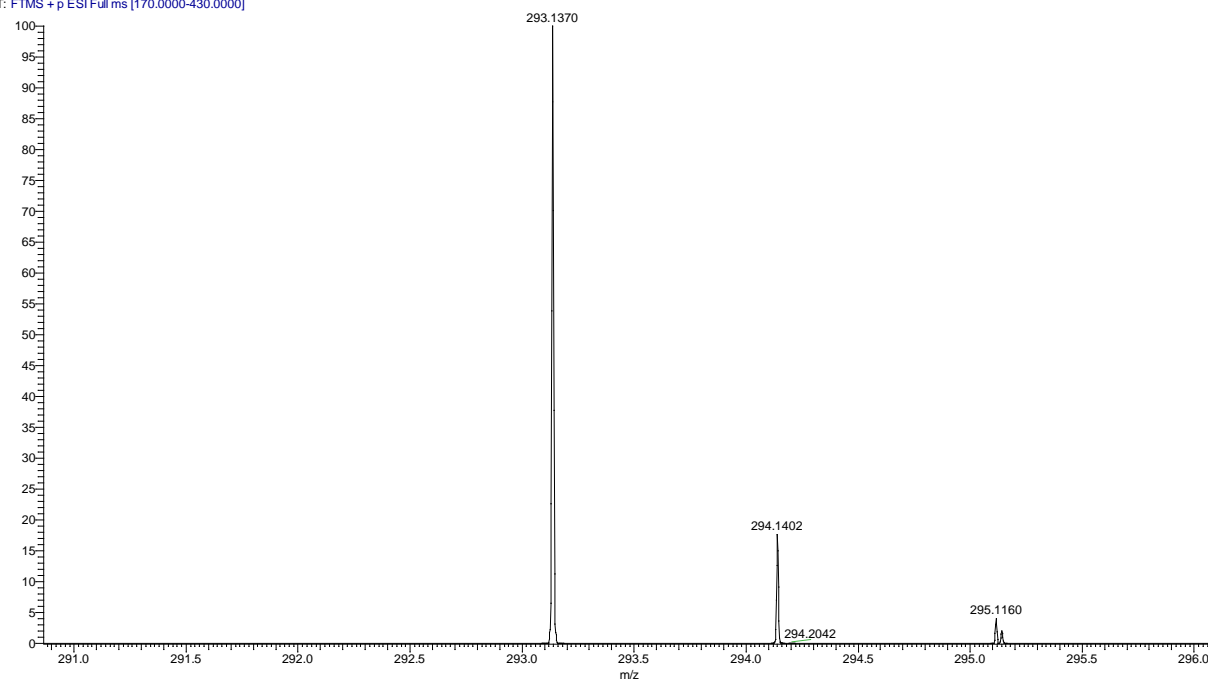


Figure S35. HR-ESI-MS spectrum of **5**

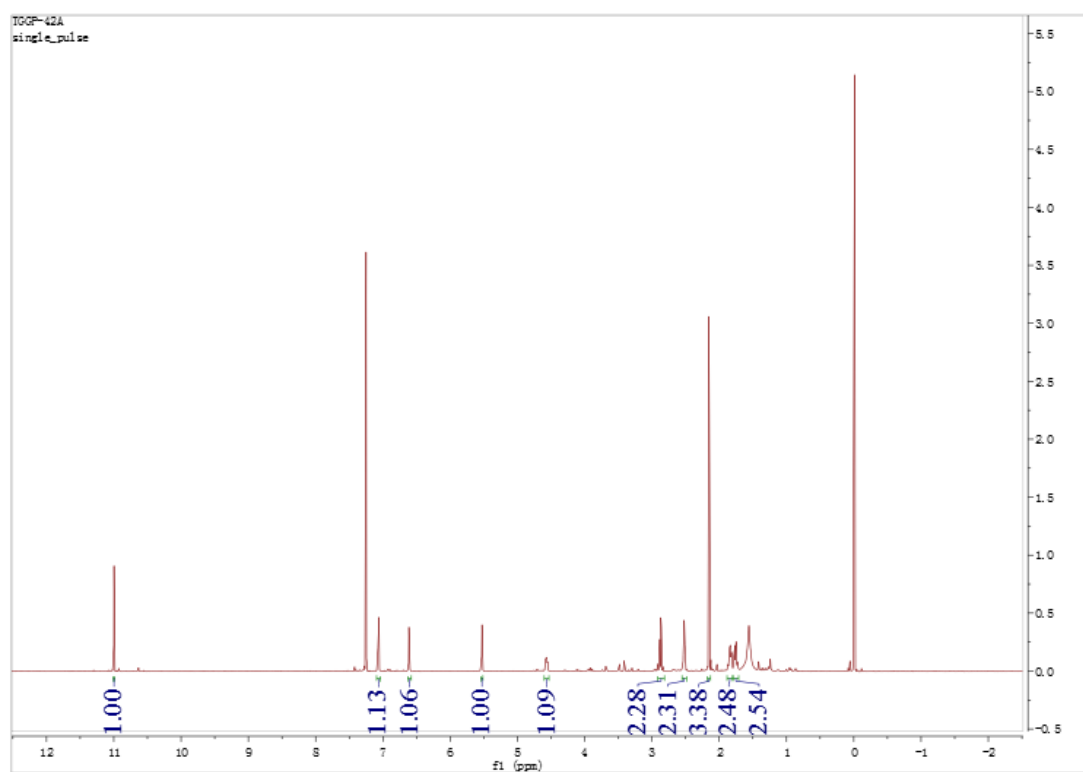


Figure S36. ¹H NMR spectrum of **6** in CDCl₃

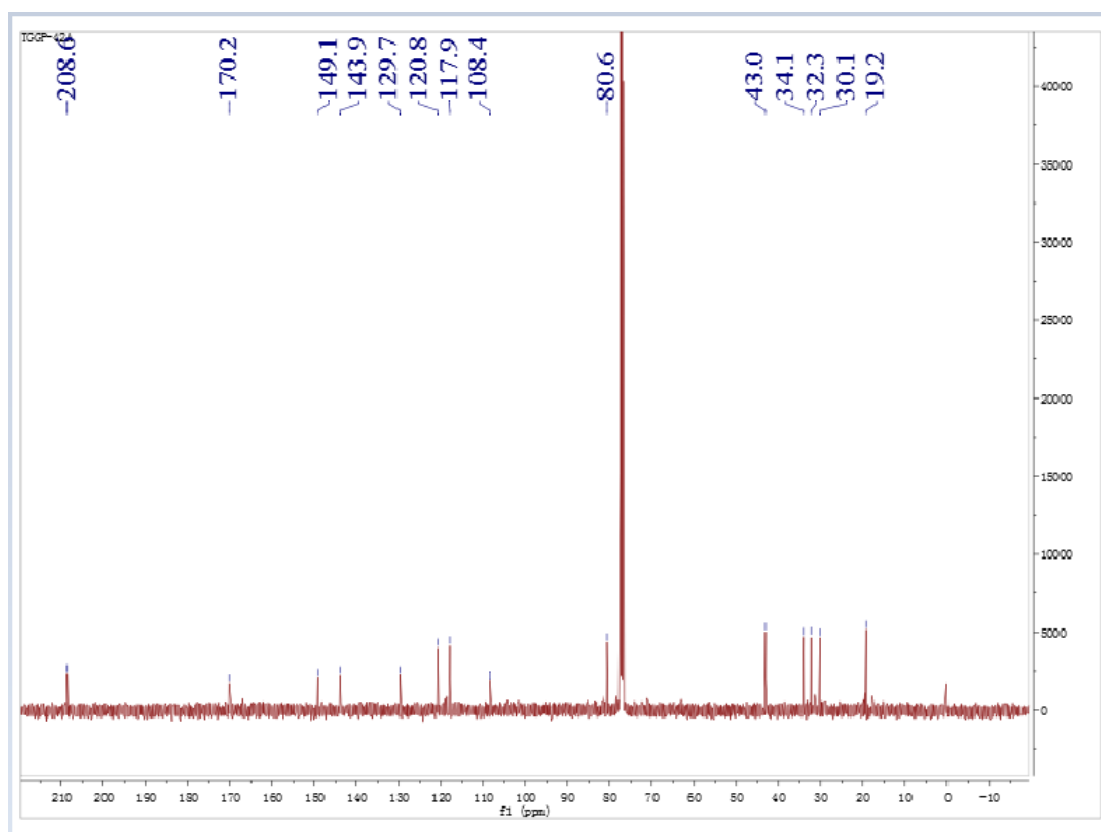


Figure S37. ¹³C NMR spectrum of 6 in CDCl₃

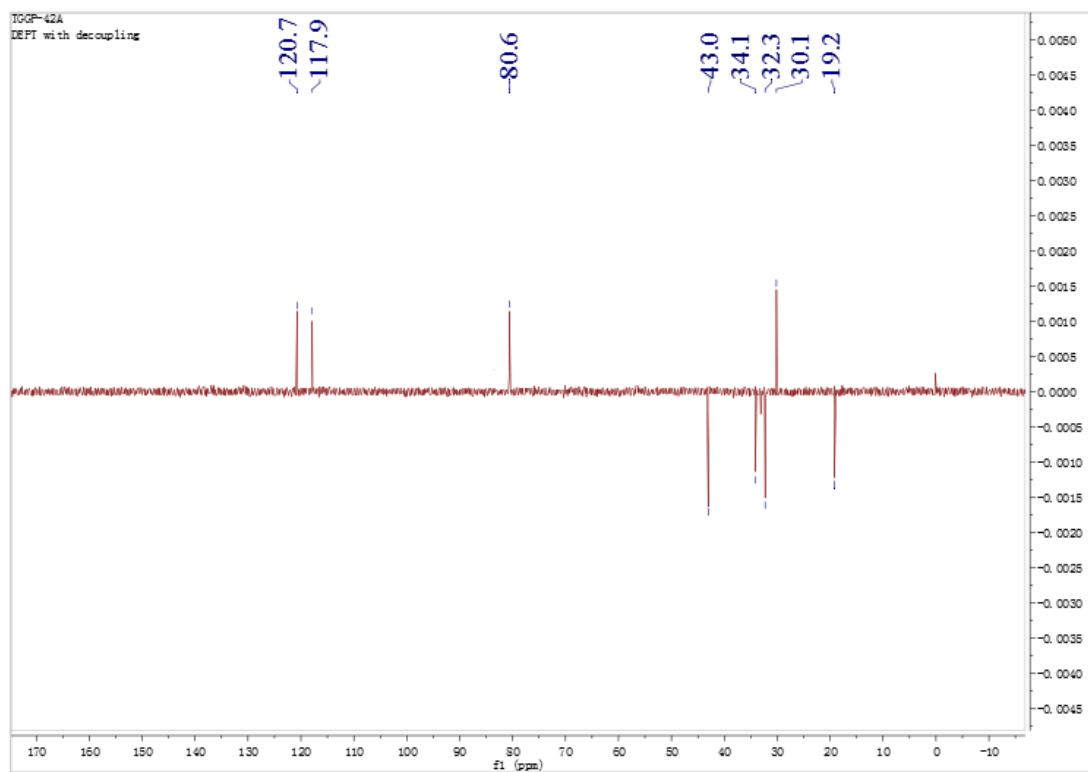


Figure S38. ¹³⁵-DEPT spectrum of 6 in CDCl₃

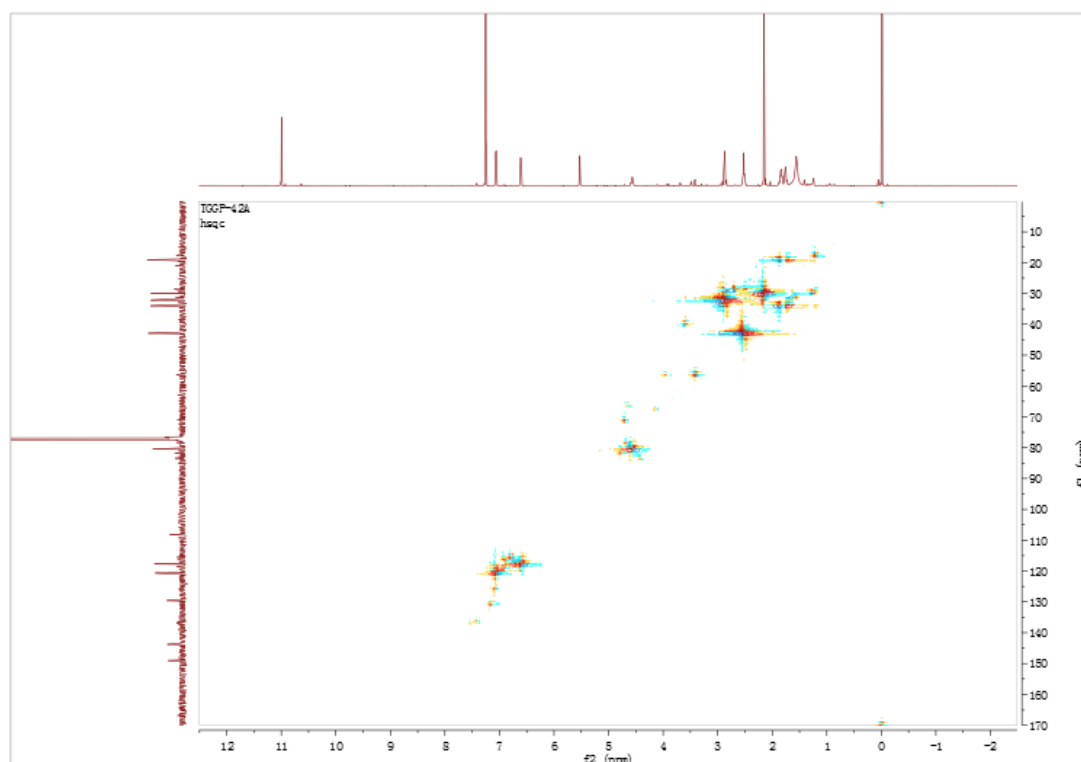


Figure S39. HMQC spectrum of **6** in CDCl_3

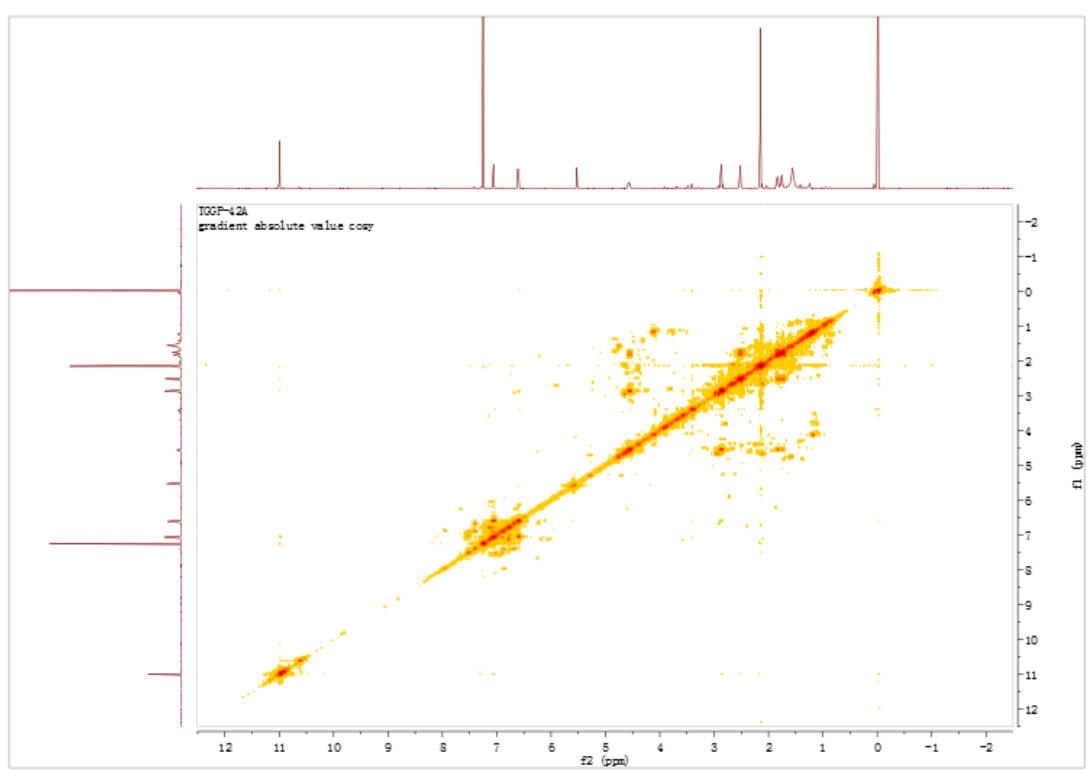


Figure S40. ^1H - ^1H COSY spectrum of **6** in CDCl_3

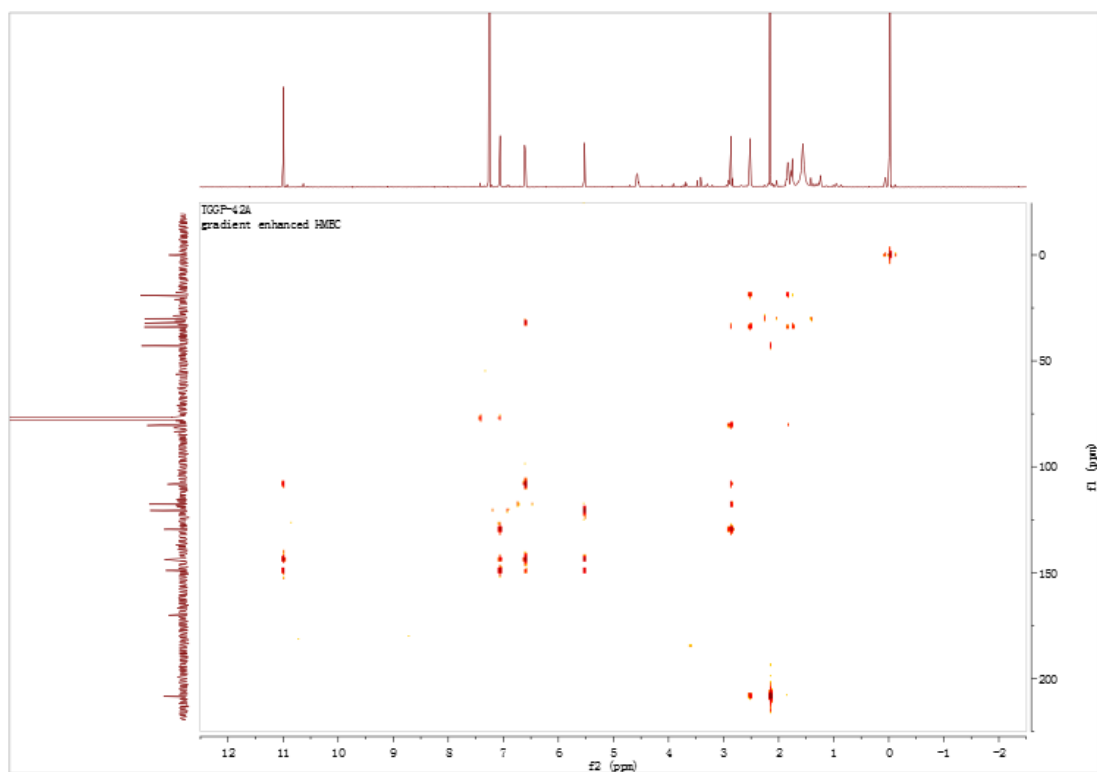


Figure S41. HMBC spectrum of **6** in CDCl_3

20201230-1-TGPP-42A+ #1 RT: 0.00 AV: 1 NL: 9.95E5
T: FTMS + p ESI Full ms [178.0000-378.0000]

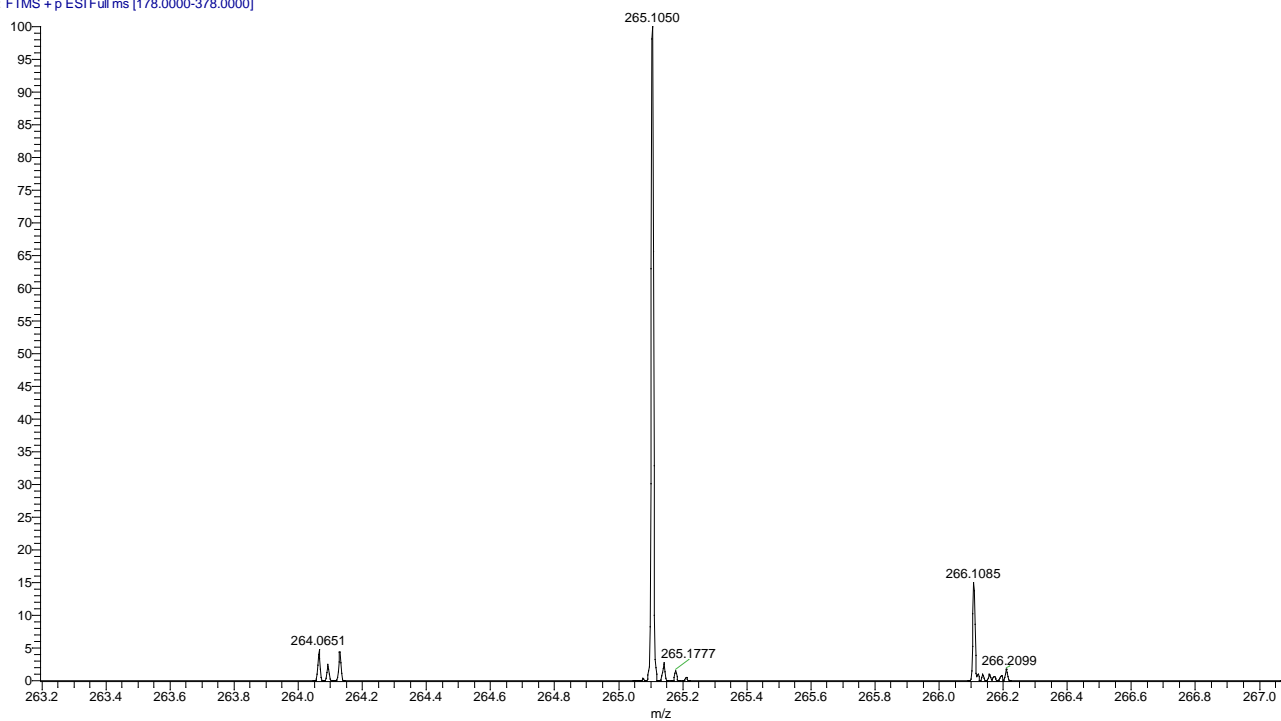


Figure S42. HR-ESI-MS spectrum of **6**

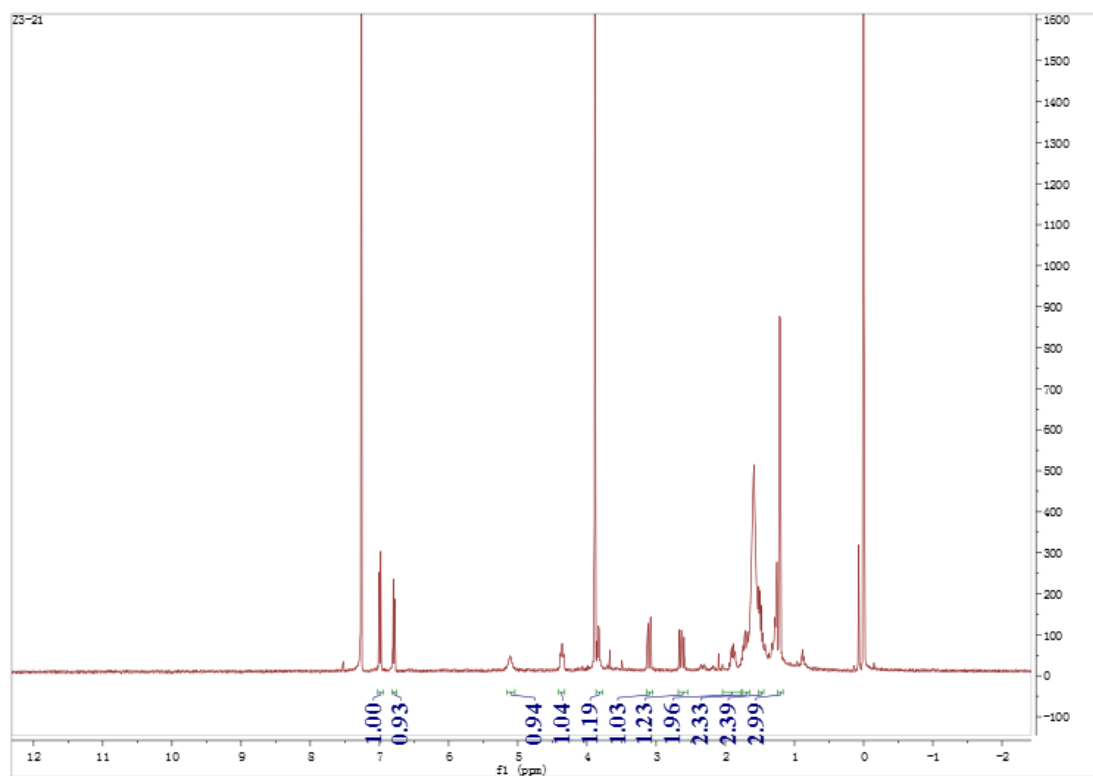


Figure S43. ¹H NMR (CDCl₃, 400 MHz) of Hydrolysate of **1** (**1a**)

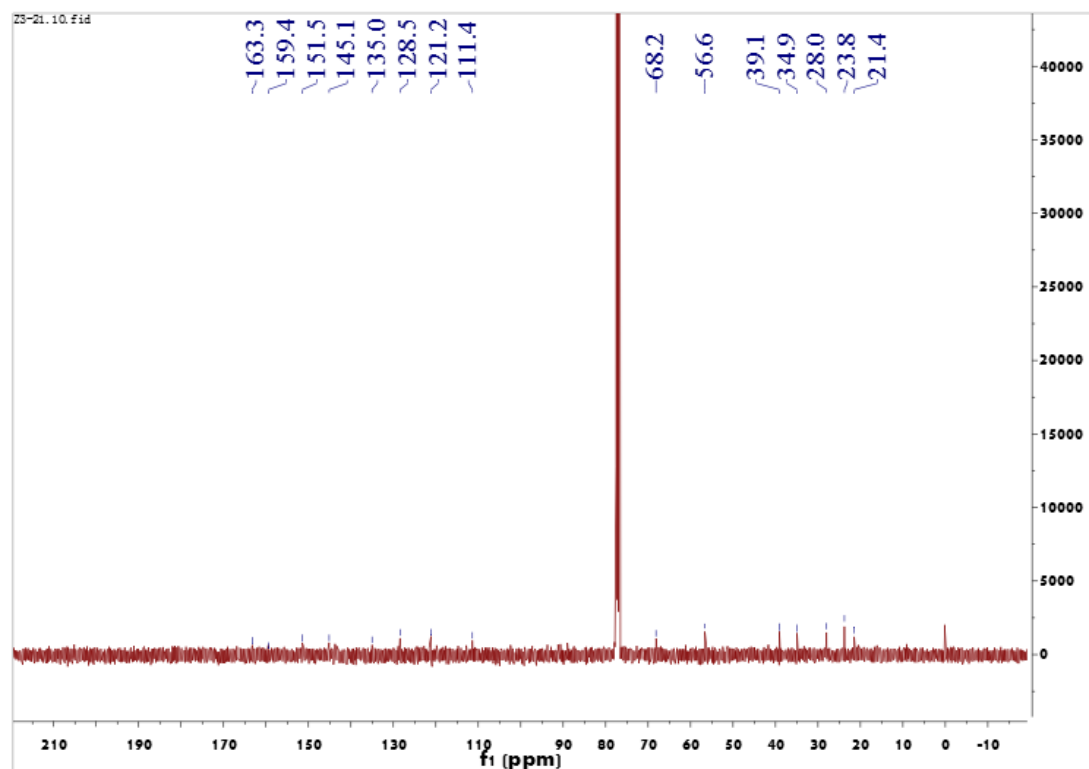


Figure S44. ¹³C NMR (CDCl₃, 400 MHz) of Hydrolysate of **1** (**1a**)

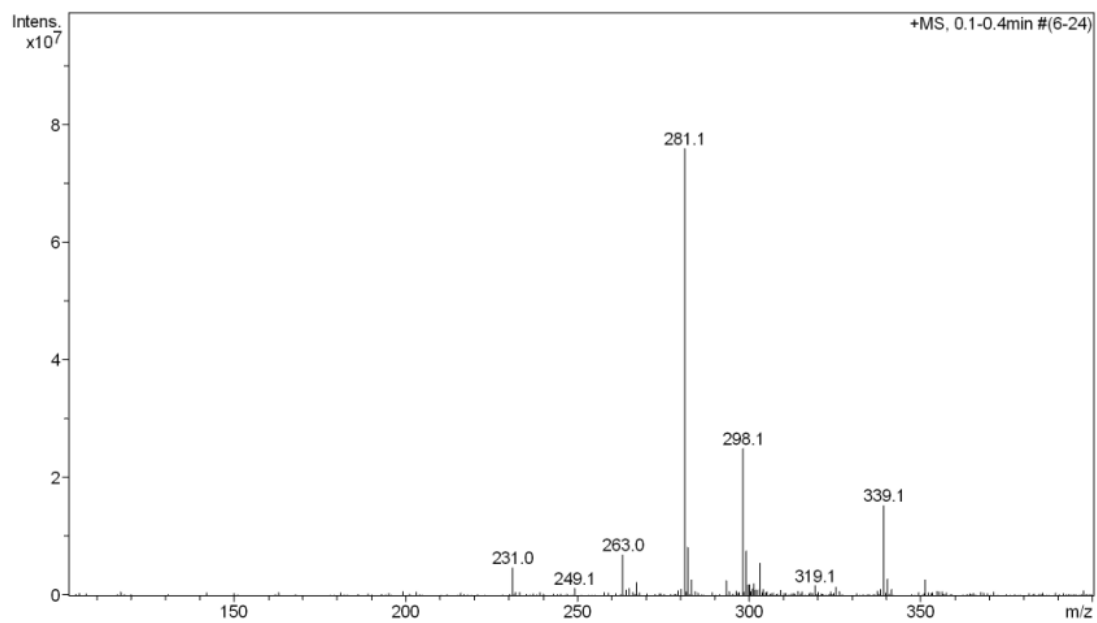


Figure S45. ESI-MS spectrum of **1a**

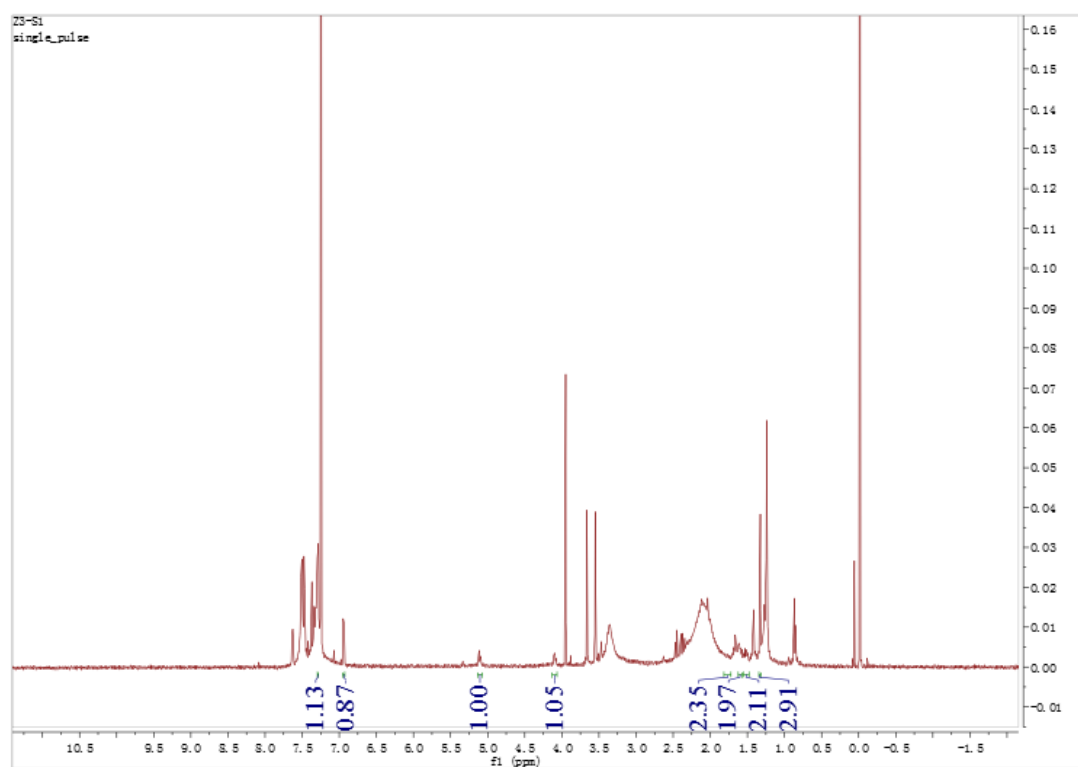


Figure S46. ^1H NMR (CDCl_3 , 600 MHz) of *S*-MTPA ester of **1** (**1b**)

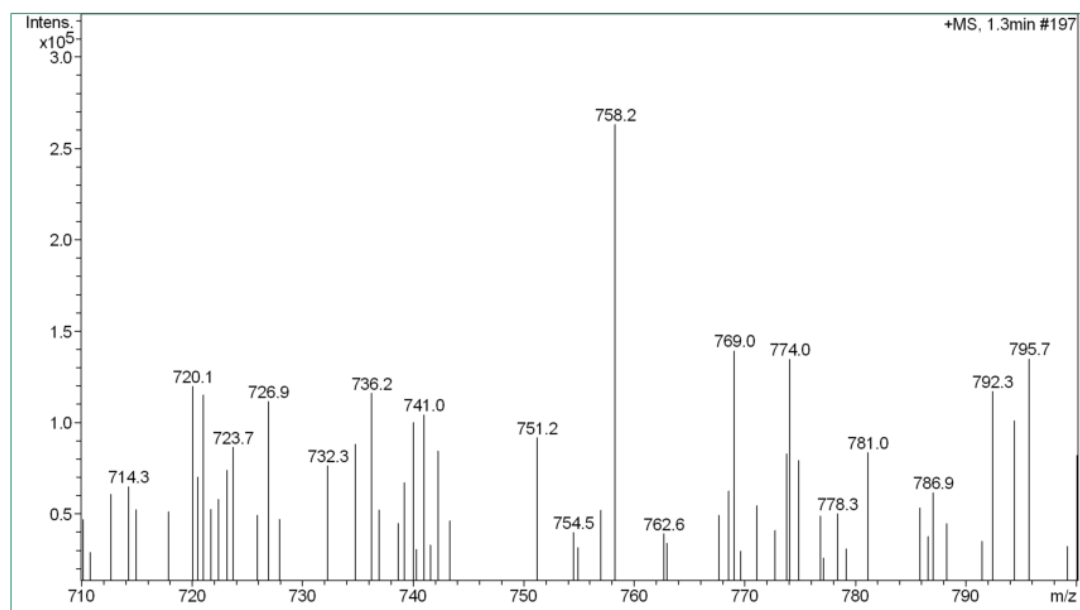


Figure S47. ESI-MS spectrum of **1b**

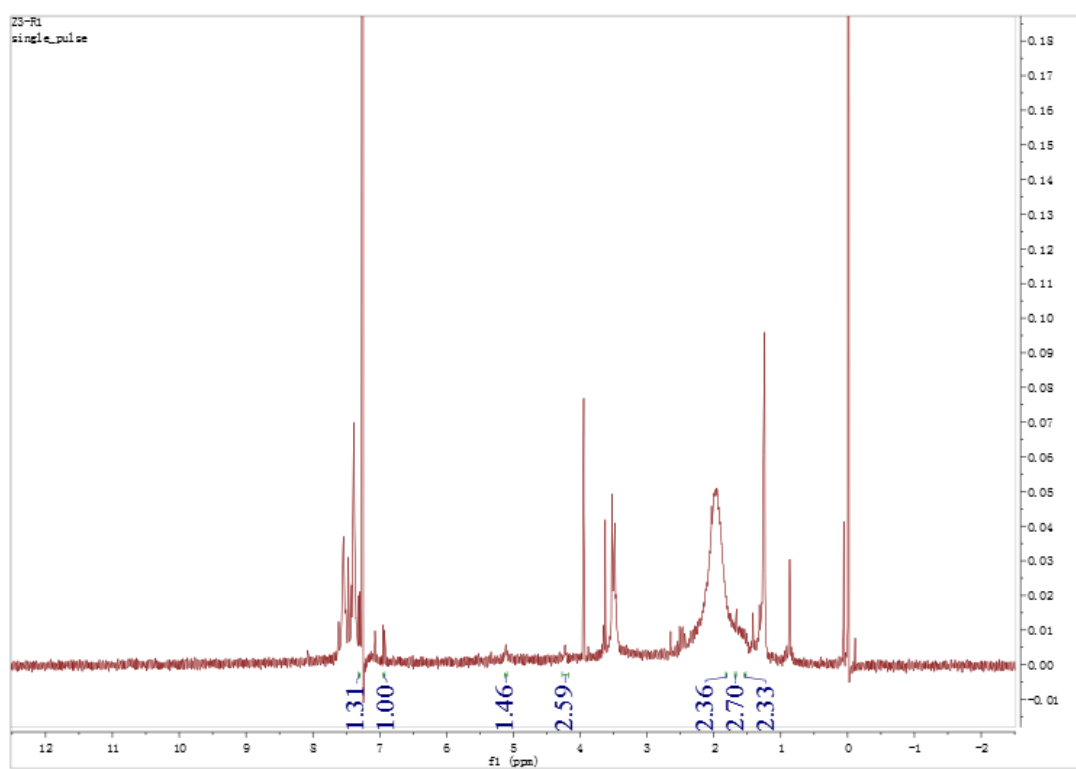


Figure S48. ^1H NMR (CDCl_3 , 600 MHz) of *R*-MTPA ester of **1** (**1c**)

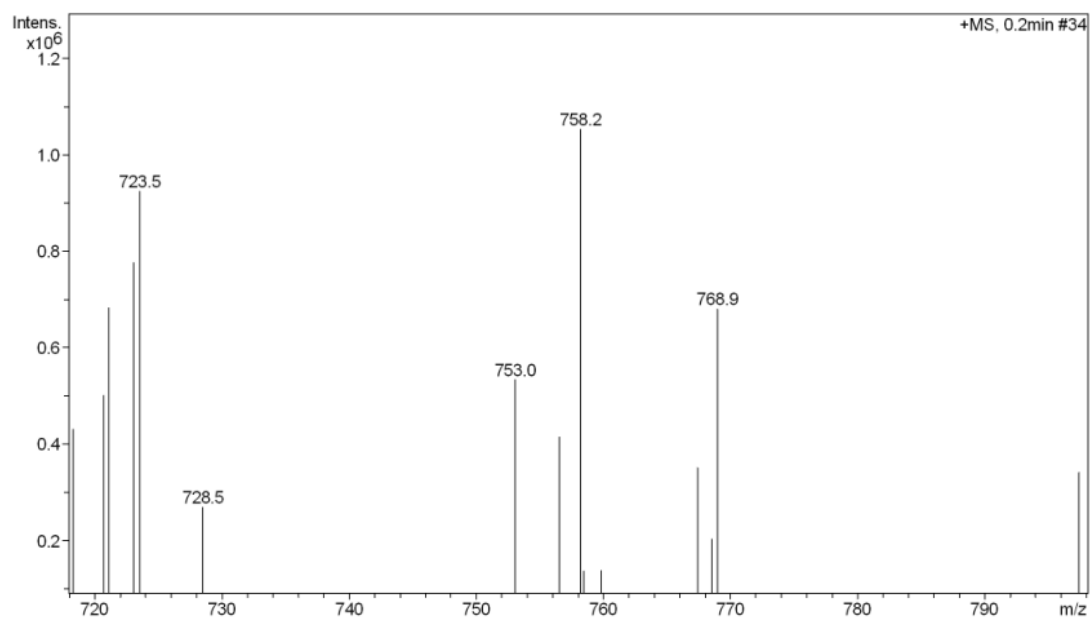


Figure S49. ESI-MS spectrum of **1c**

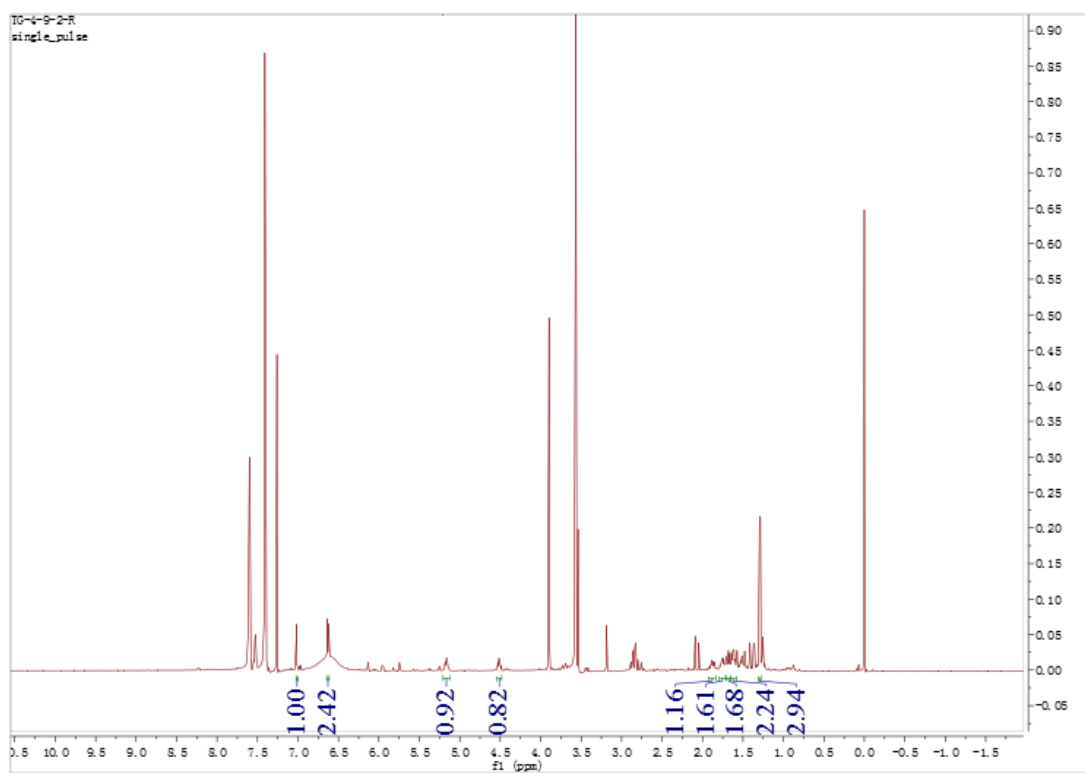


Figure S50. ^1H NMR (CDCl_3 , 600 MHz) of *S*-MTPA ester of **2** (**2a**)

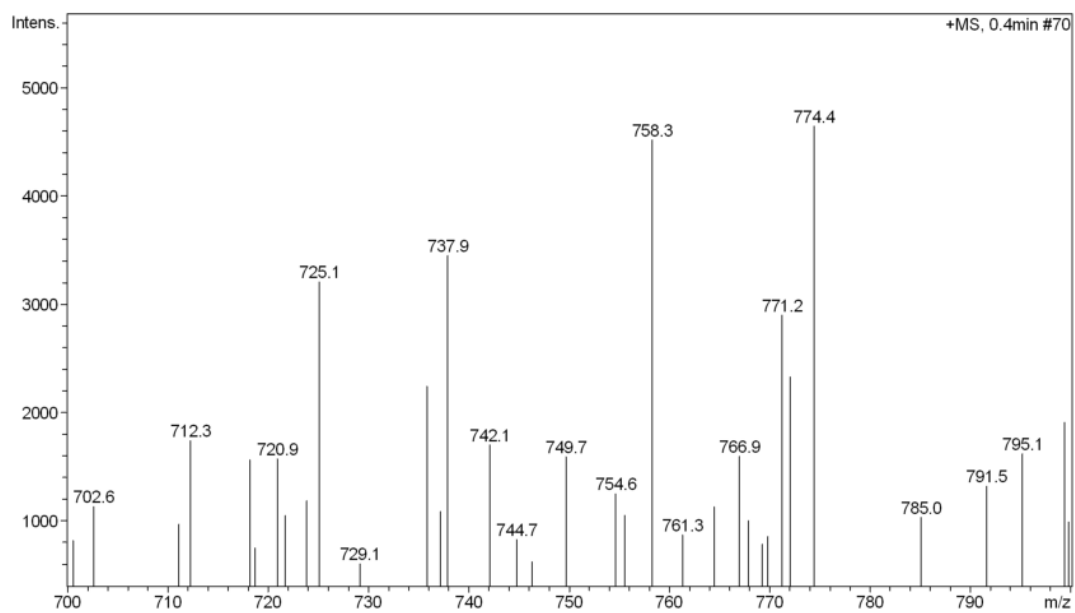


Figure S51. ESI-MS spectrum of **2a**

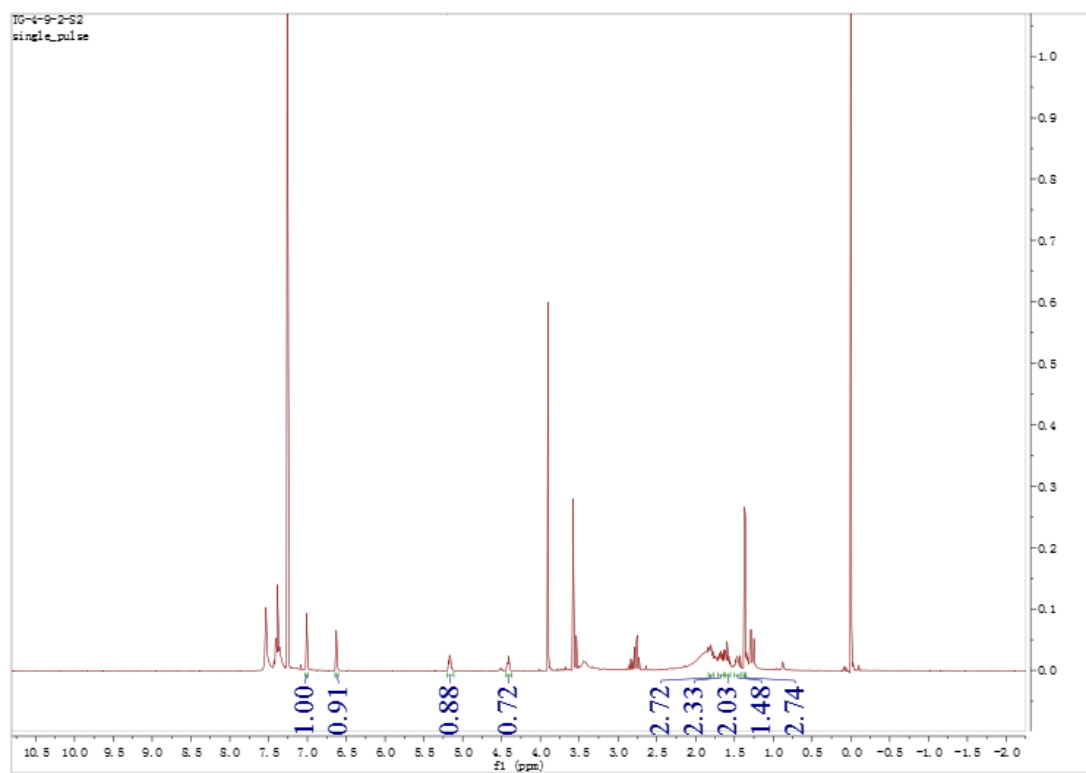


Figure S52. ¹H NMR (CDCl₃, 600 MHz) of *R*-MTPA ester of **2** (**2b**)

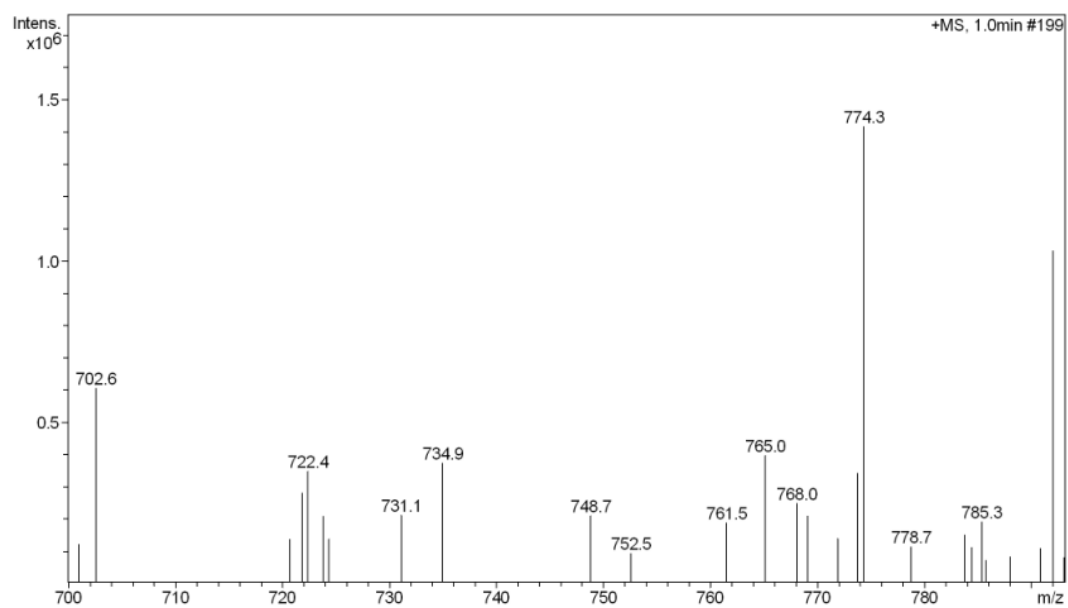


Figure S53. ESI-MS spectrum of **2a**

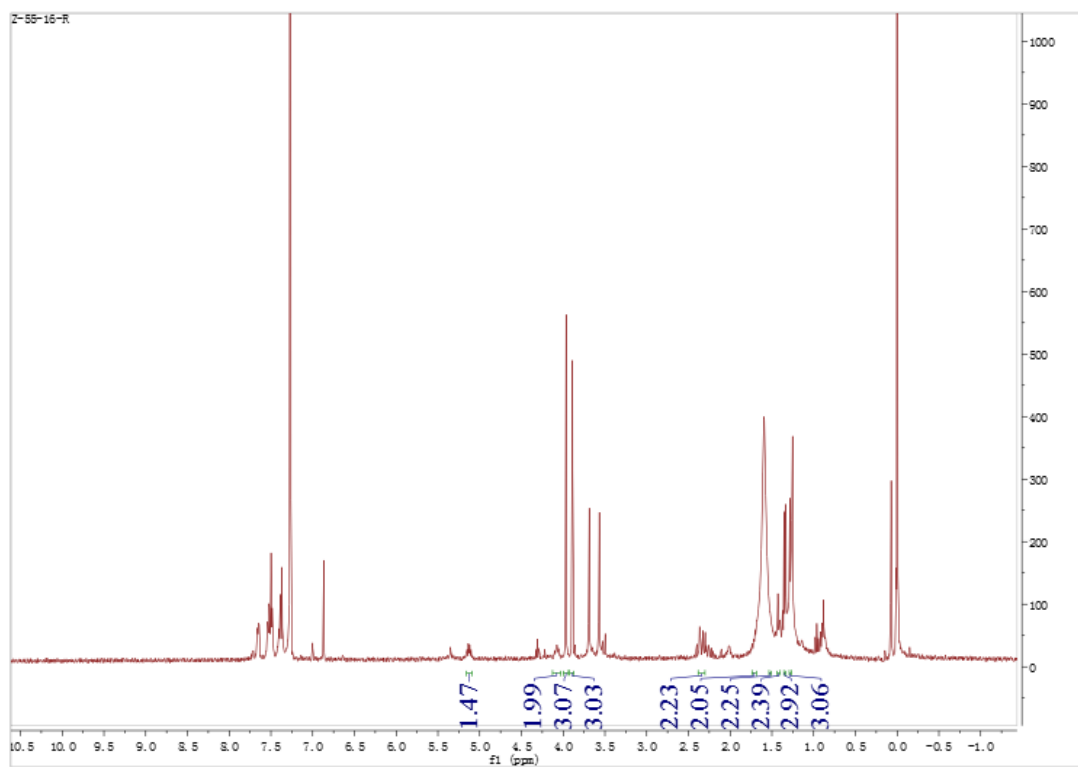


Figure S54. ^1H NMR (CDCl_3 , 400 MHz) of *S*-MTPA ester of **3** (**3a**)

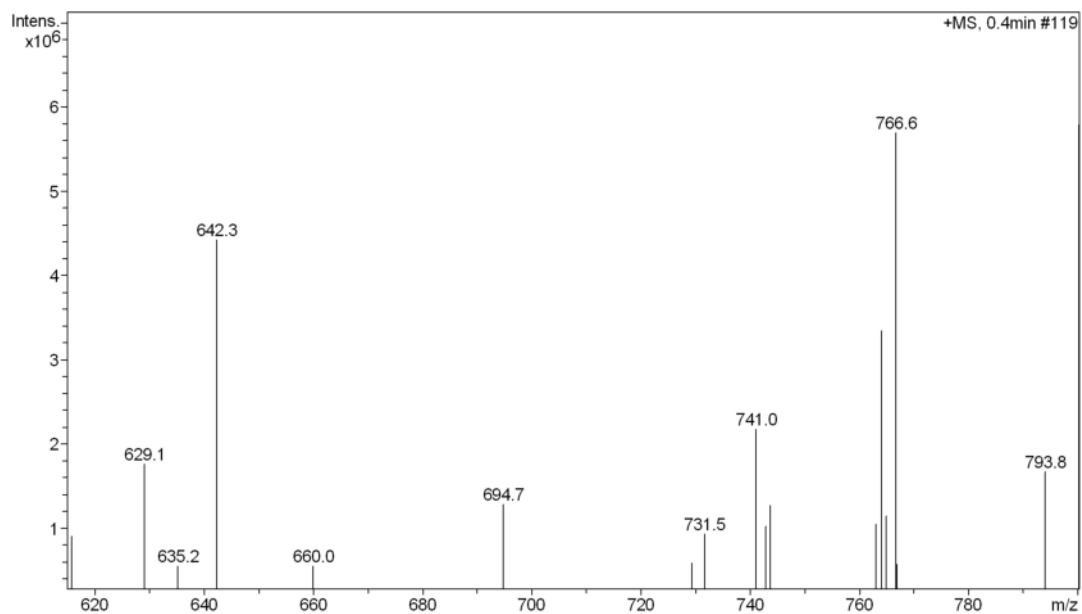


Figure S55. ESI-MS spectrum of **3a**

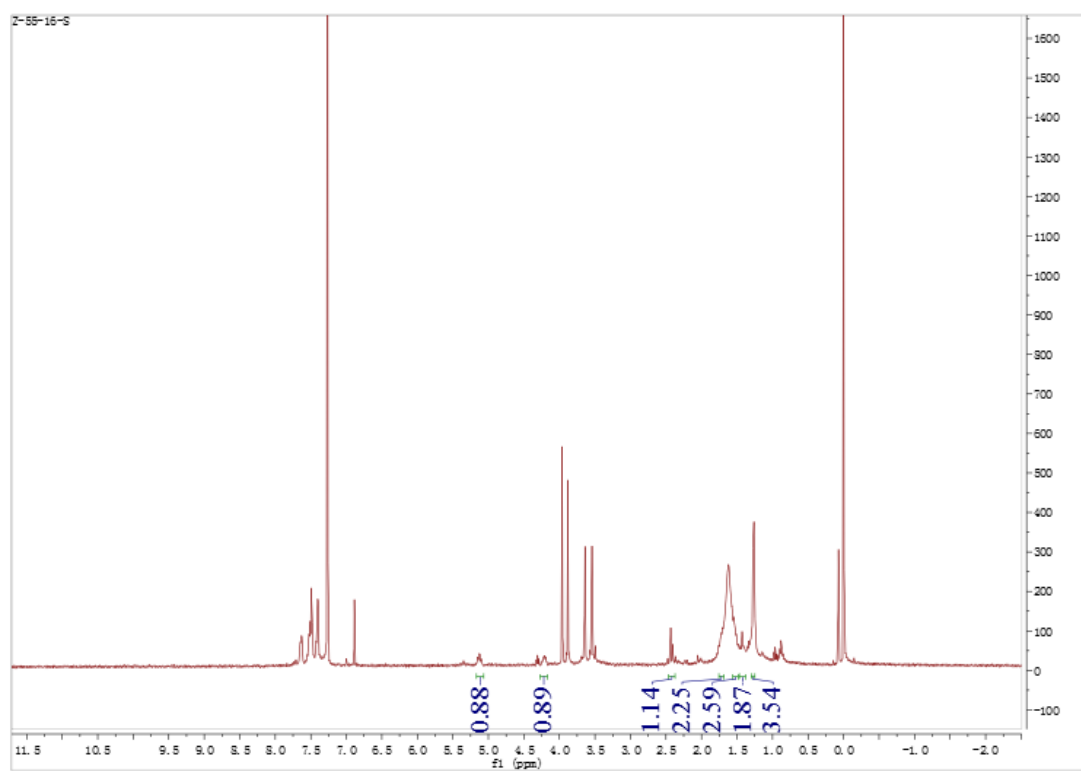


Figure S56. ¹H NMR (CDCl₃, 400 MHz) of *R*-MTPA ester of **3** (**3b**)

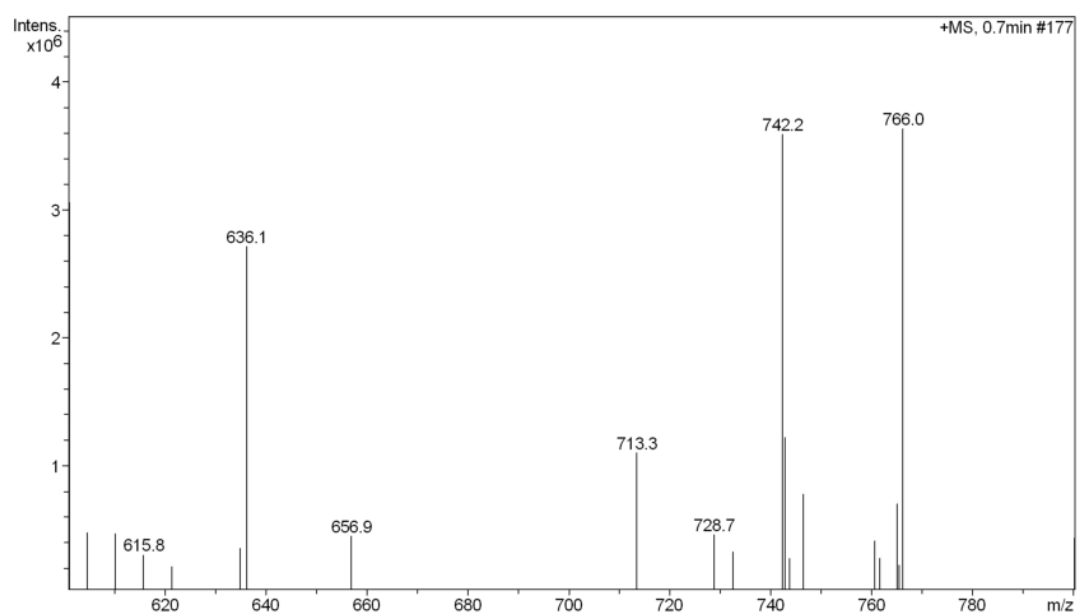


Figure S57. ESI-MS spectrum of **3b**