

Electronic Supplementary Material (ESI) for Organic & Biomolecular Chemistry

Structures and inhibitory activity against breast cancer cells of new bufadienolides from the eggs of toad *Bufo bufo gargarizans*

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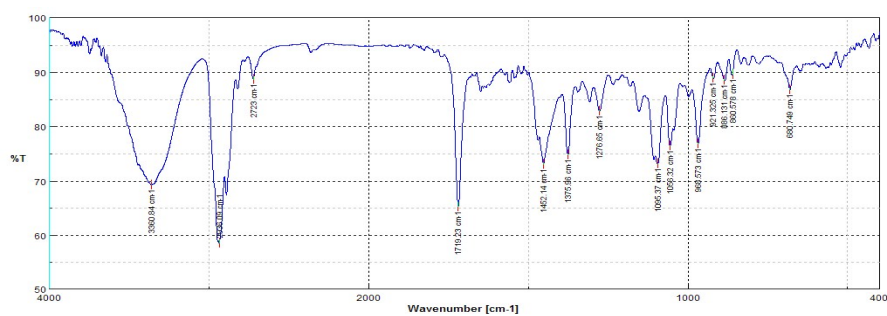


Fig.S1. IR spectrum of **1**

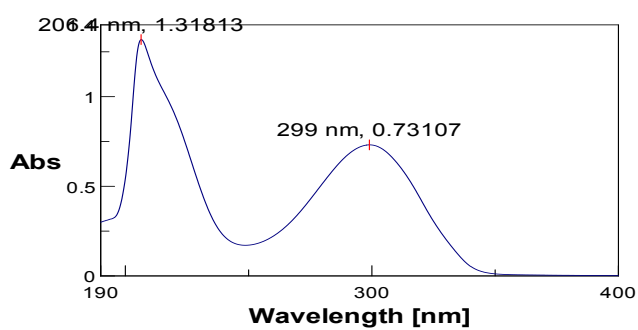


Fig.S2. UV spectrum of **1**

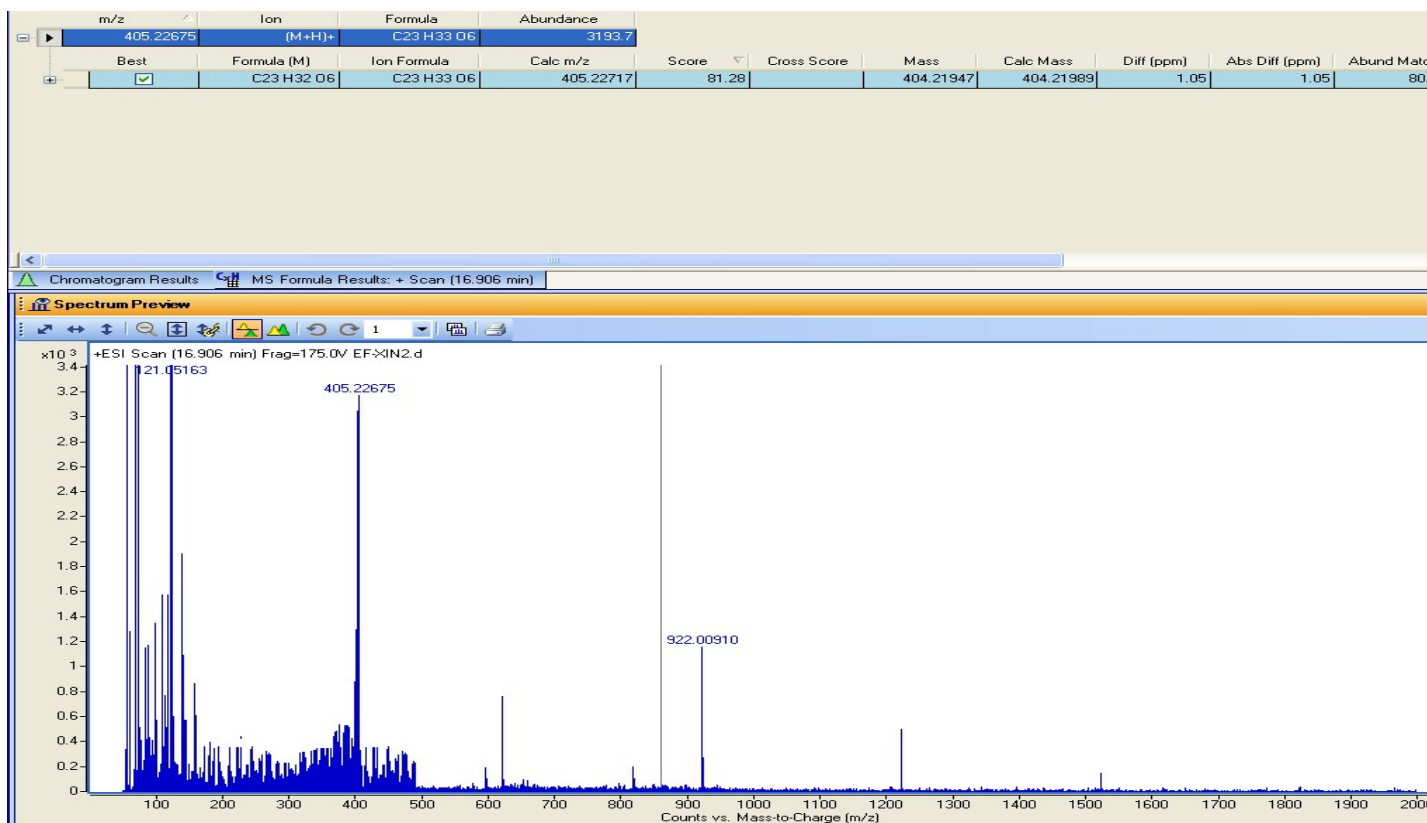


Fig.S3. HR-ESI-MS spectrum of **1**

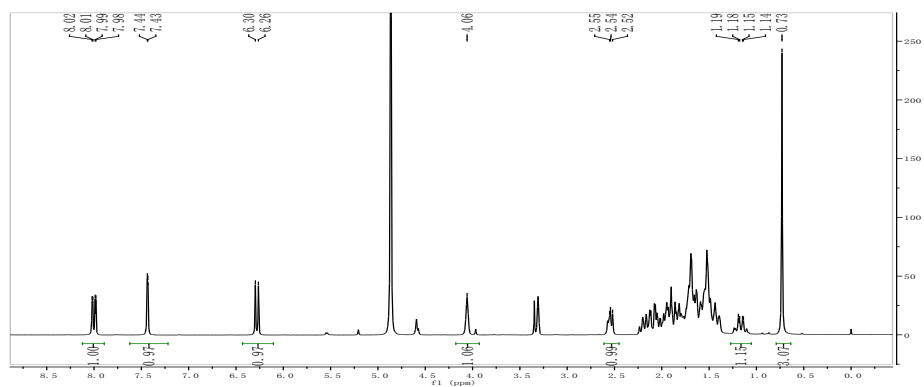


Fig.S4. ^1H NMR spectrum of **1**

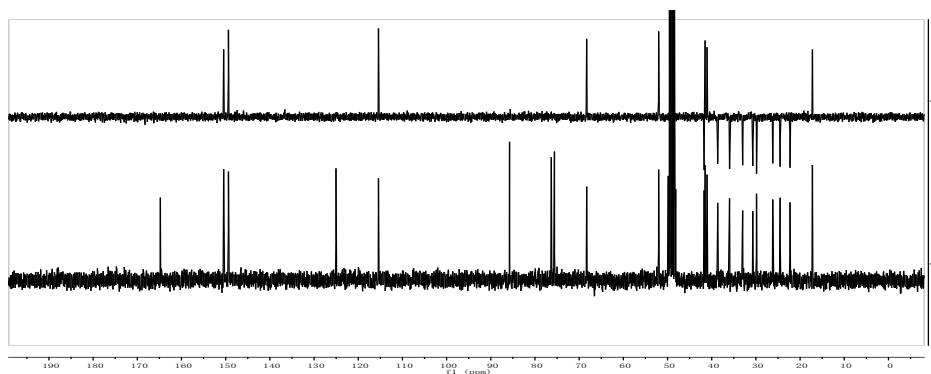


Fig.S5. ^{13}C NMR and DEPT135 spectrum of **1**

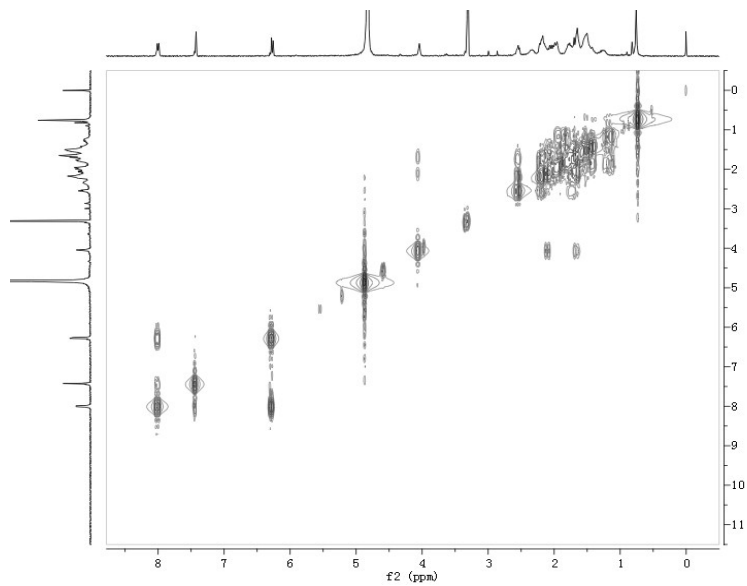


Fig.S6. ^1H - ^1H COSY spectrum of **1**

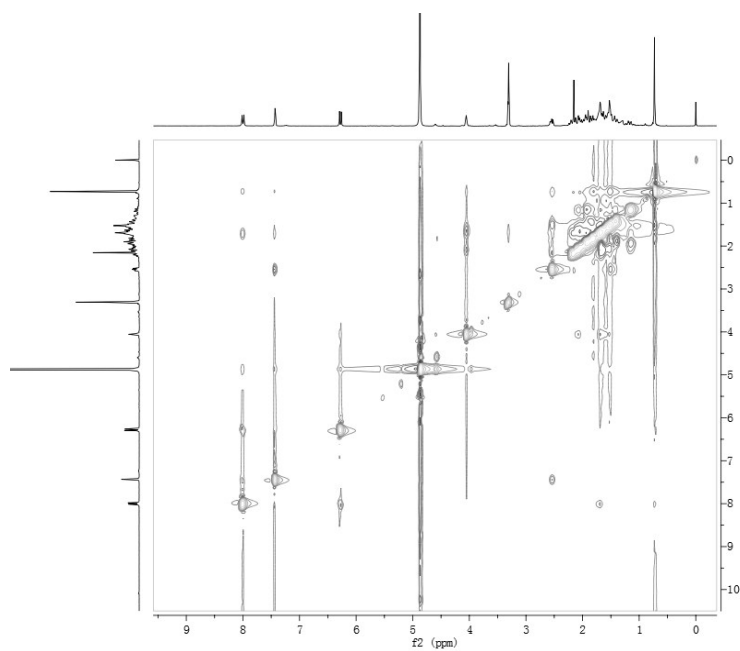


Fig.S7. NOESY spectrum of **1**

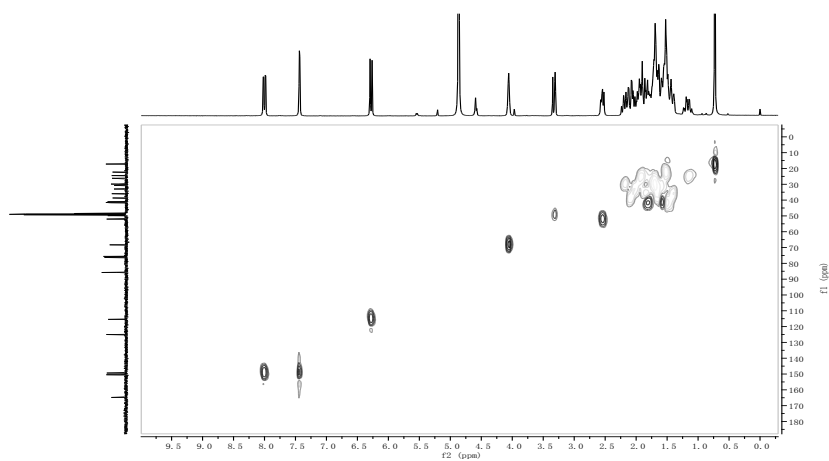


Fig.S8. HSQC spectrum of **1**

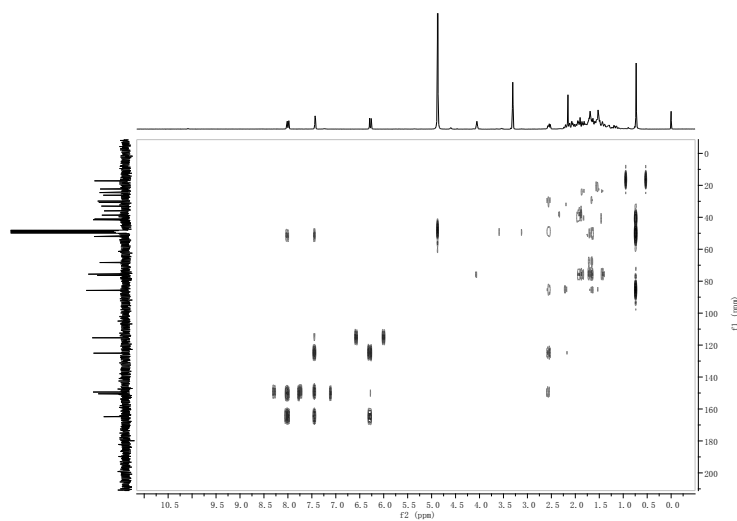


Fig.S9. HMBC spectrum of **1**

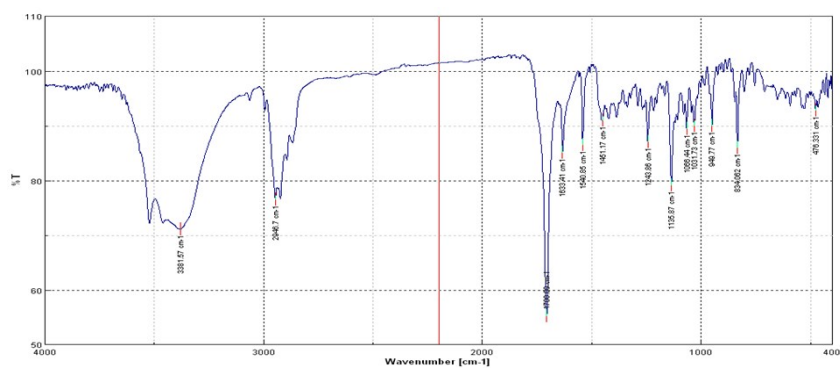


Fig.S10. IR spectrum of **2**

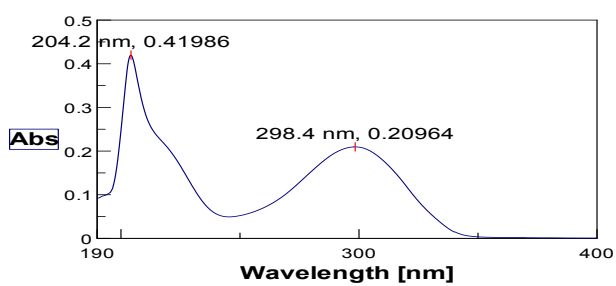


Fig.S11. UV spectrum of **2**

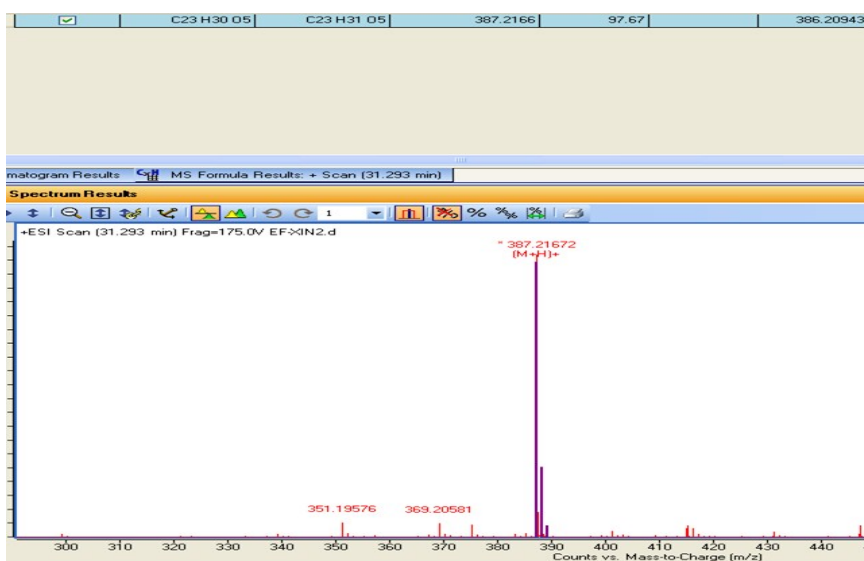


Fig.S12. HR-ESI-MS spectrum of **2**

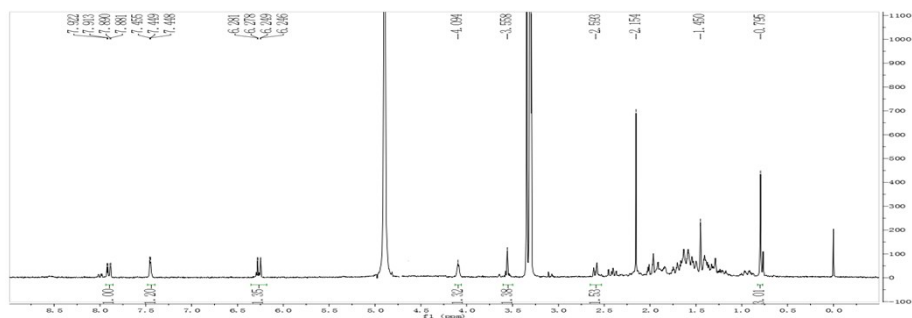


Fig.S13. ¹H NMR spectrum of **2**

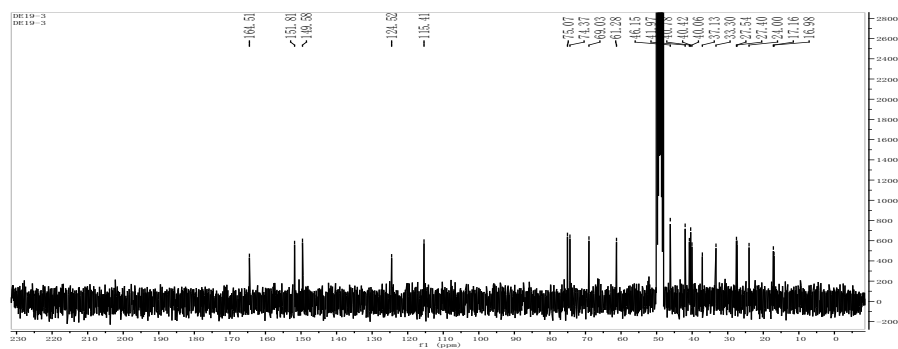


Fig.S14. ^{13}C NMR spectrum of **2**

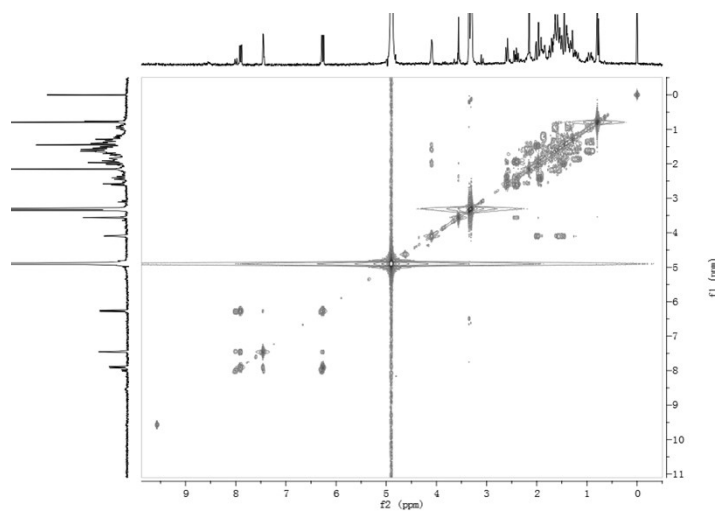


Fig.S15. ^1H - ^1H COSY spectrum of **2**

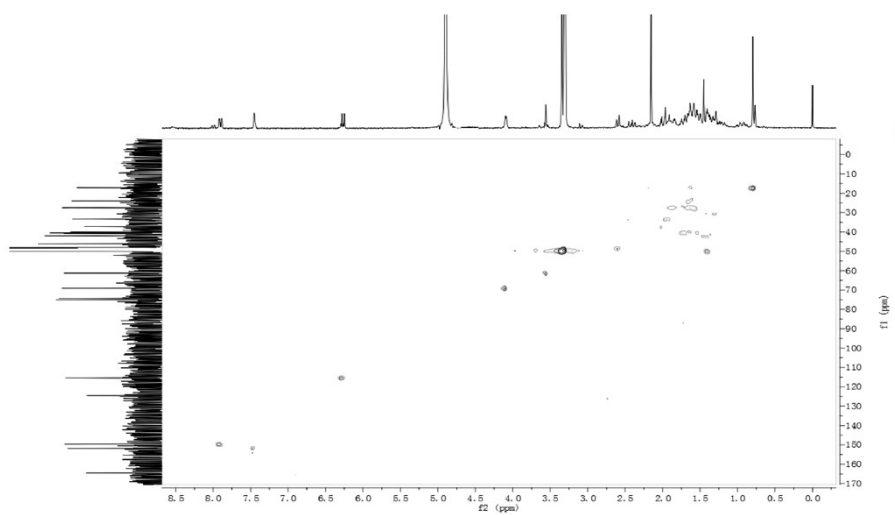


Fig.S16. HSQC spectrum of **2**

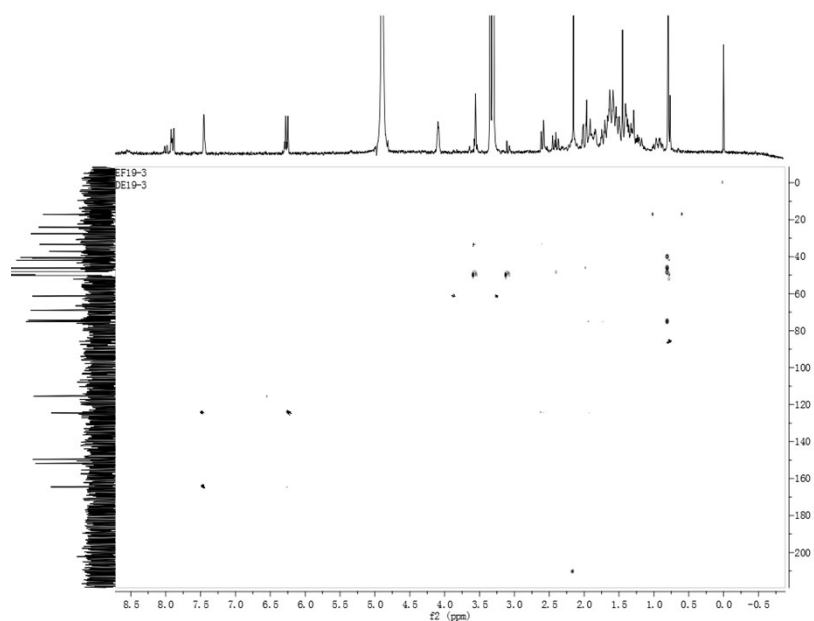


Fig.S17. HMBC spectrum of **2**

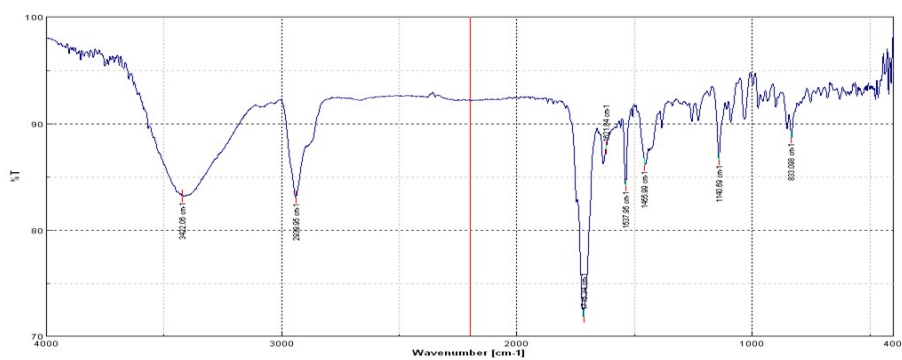


Fig.S18. IR spectrum of **3**

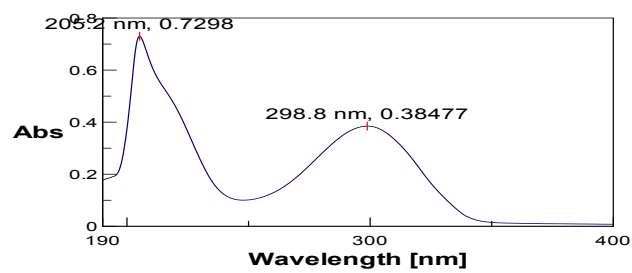


Fig.S19. UV spectrum of **3**

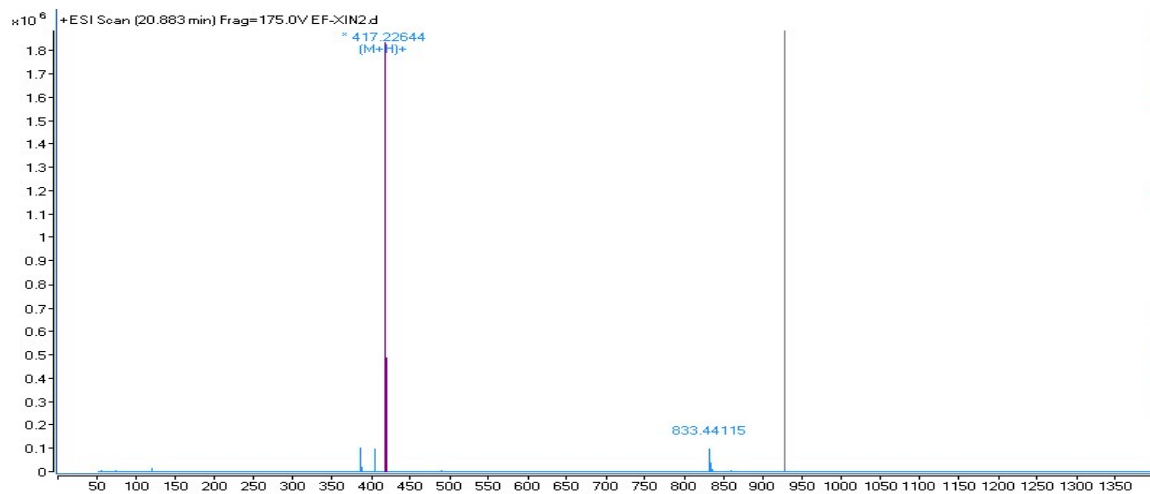


Fig.S20. HR-ESI-MS spectrum of **3**

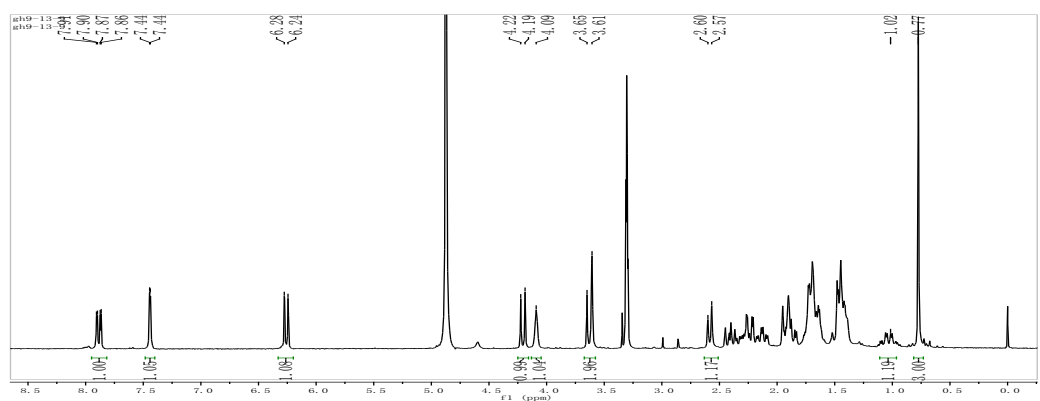


Fig.S21. ¹H-NMR spectrum of **3**

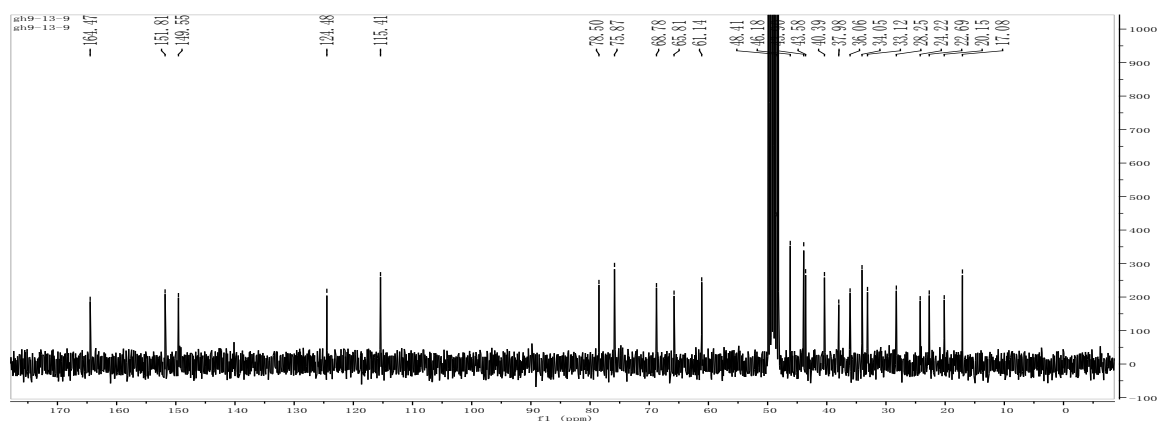


Fig.S22. ^{13}C NMR spectrum of **3**

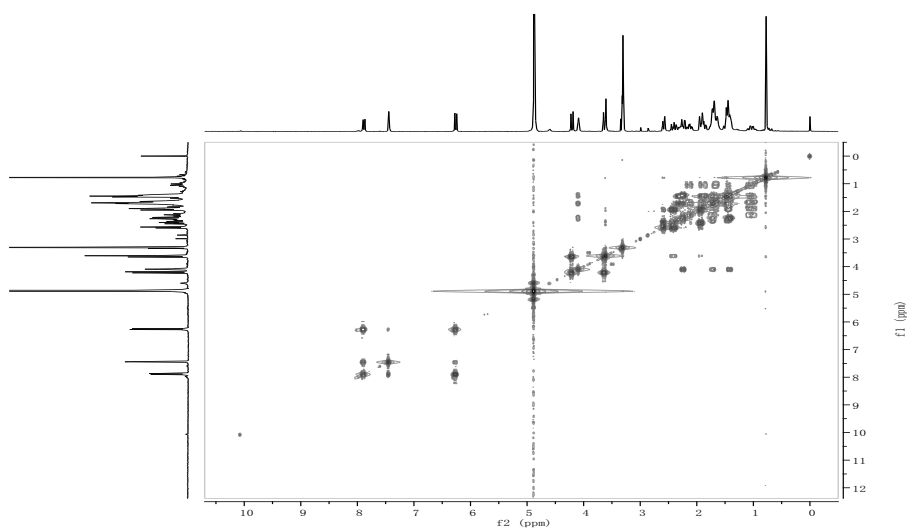


Fig.S23. ^1H - ^1H COSY spectrum of **3**

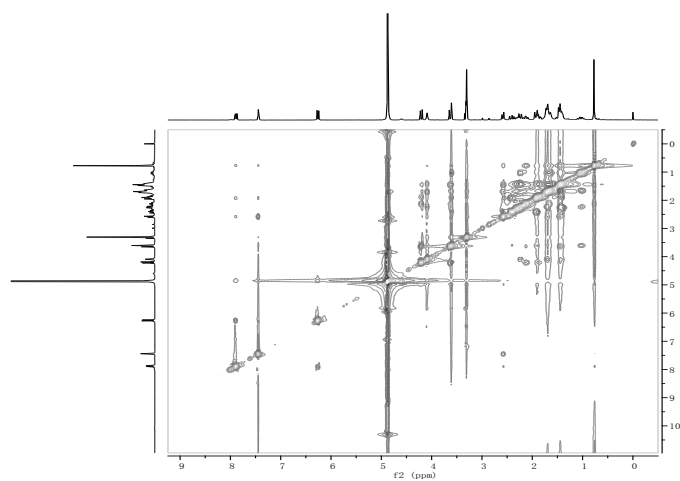


Fig.S24. NOESY spectrum of **3**

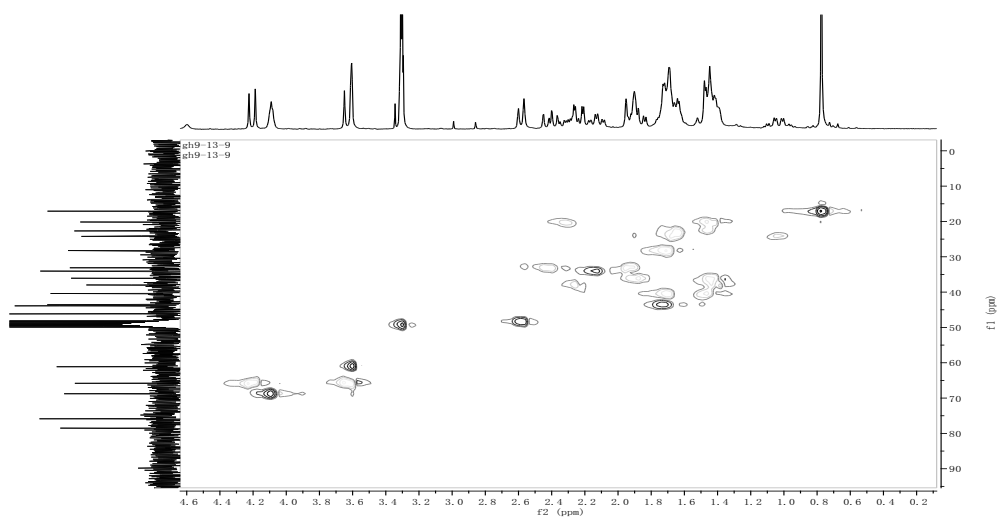


Fig.S25. HSQC spectrum of **3**

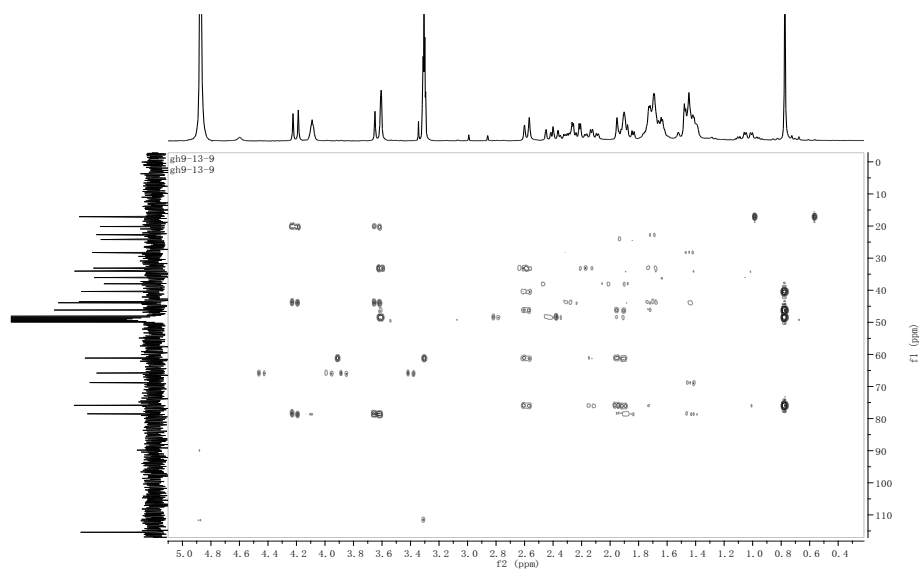


Fig.S26. HMBC spectrum of **3**

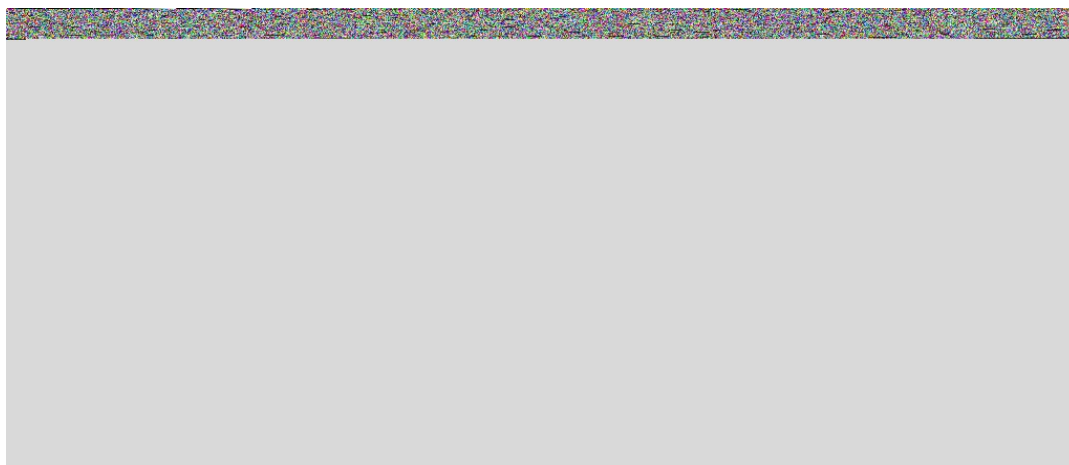


Fig. S27. IR spectrum of **4**

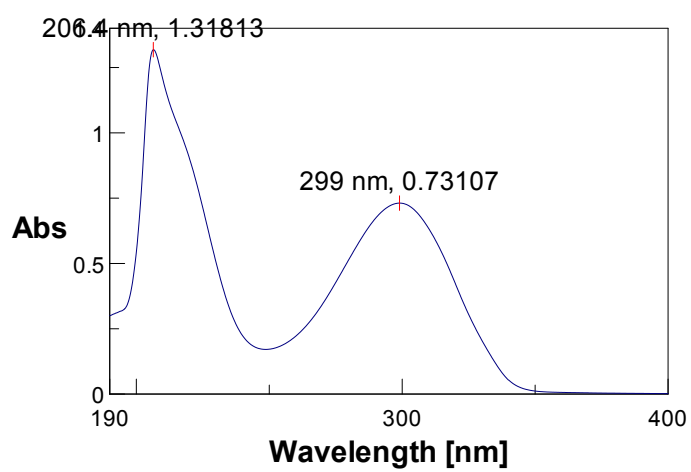


Fig. S28. UV spectrum of **4**

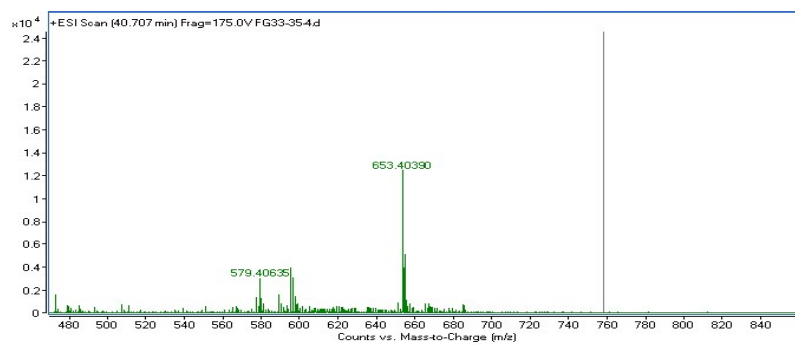


Fig. S29. HR-ESI-MS spectrum of **4**

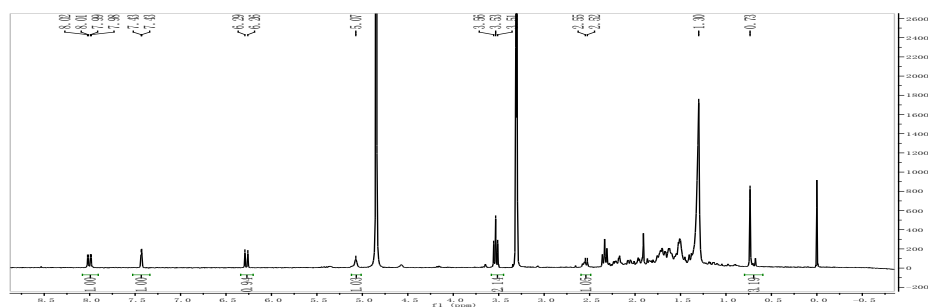


Fig. S30. ¹H NMR spectrum of **4**

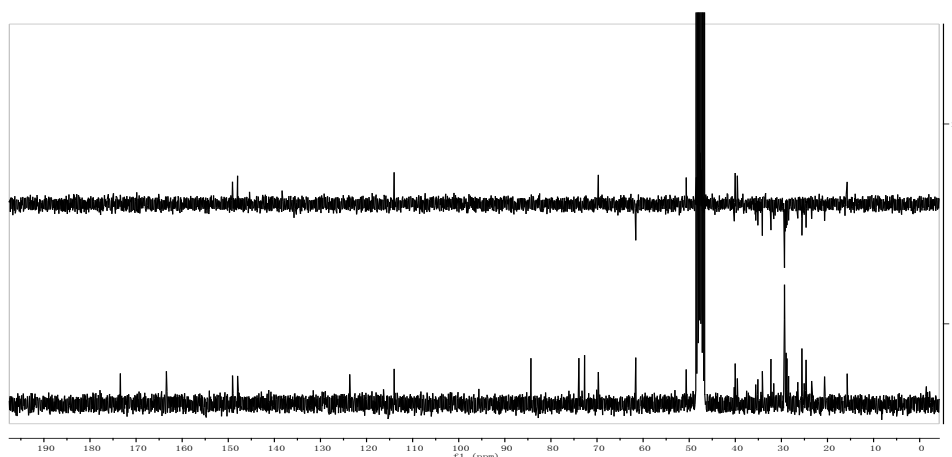


Fig. S31. ¹³C NMR spectrum of **4**

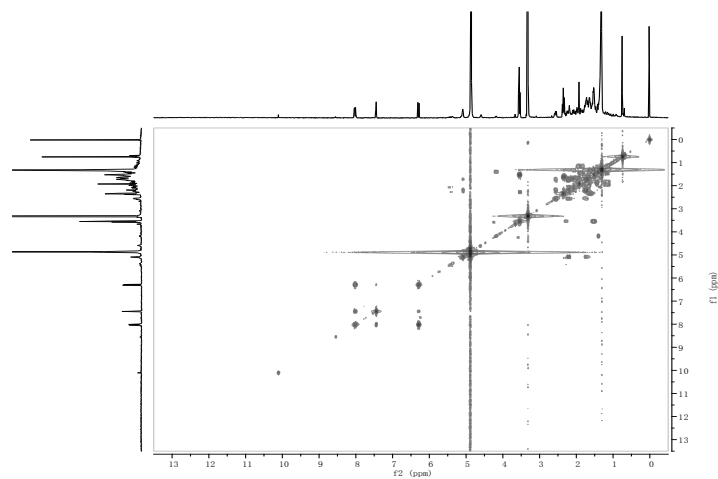


Fig. S32. ^1H - ^1H COSY spectrum of **4**

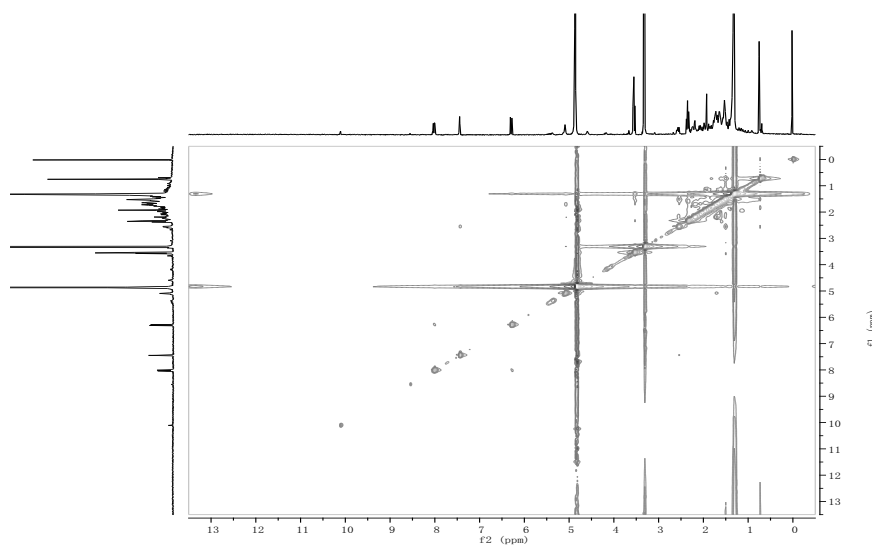


Fig. S33. NOESY spectrum of **4**

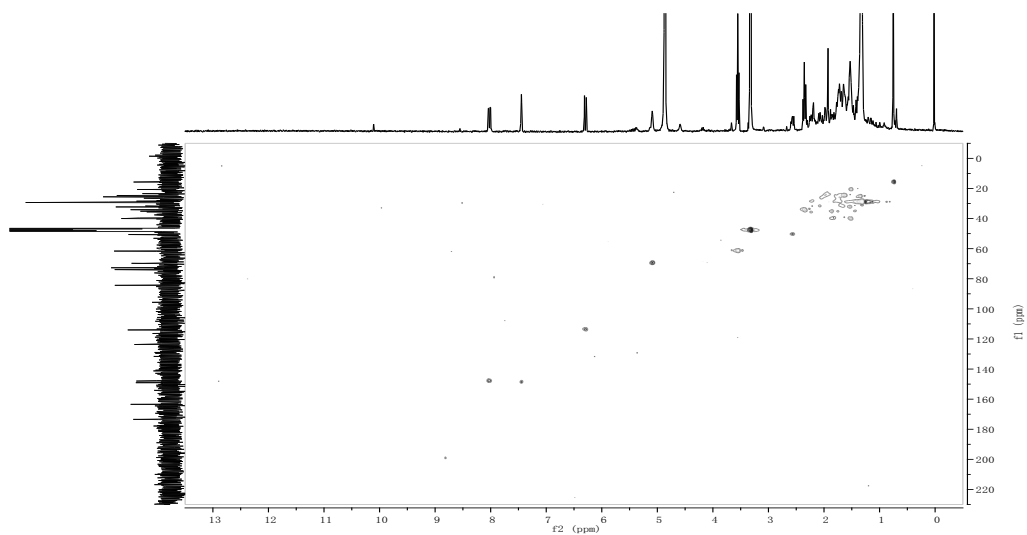


Fig. S34. HSQC spectrum of **4**

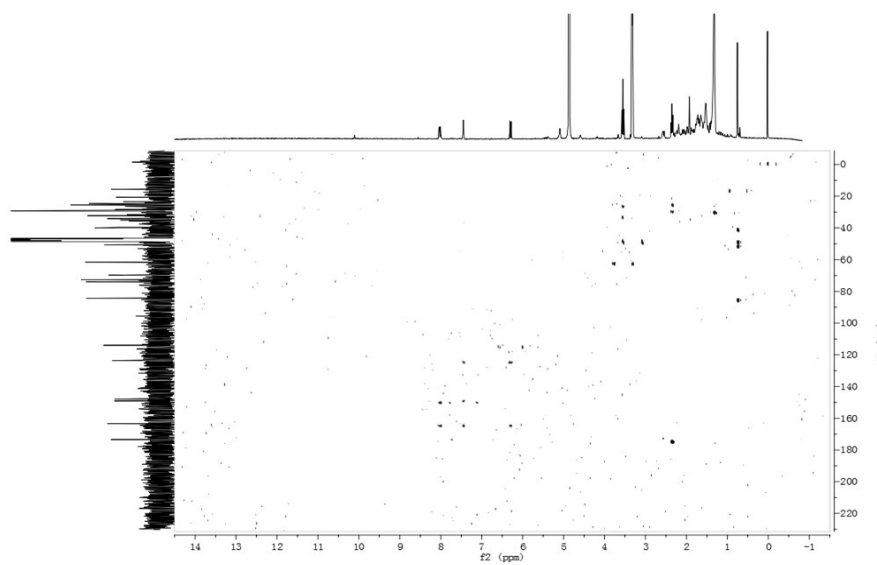


Fig. S35. HMBC spectrum of **4**

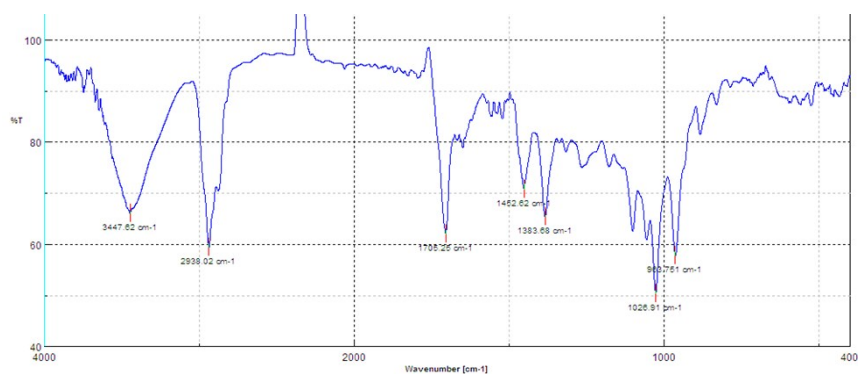


Figure S36. IR spectrum of **5**

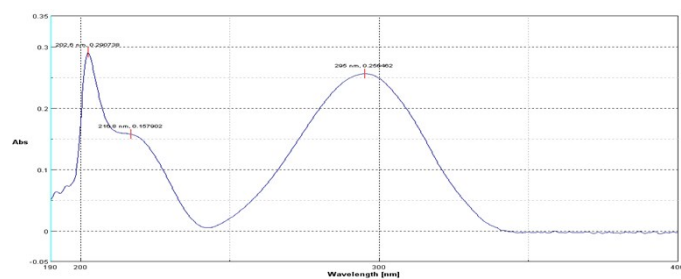


Figure S37. UV spectrum of **5**

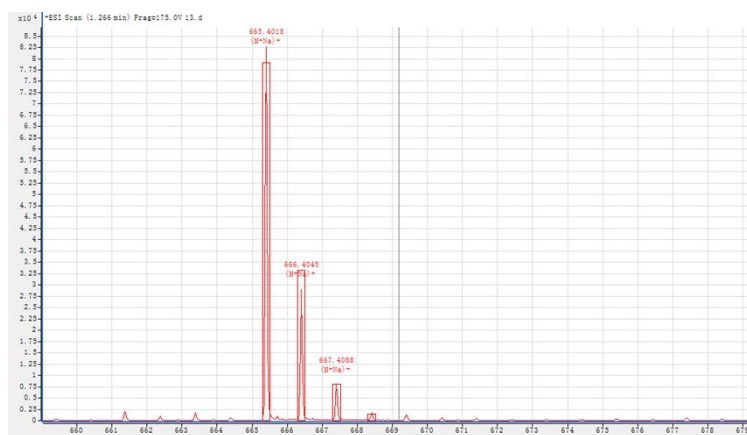


Figure S38. HRESIMS spectrum of **5**

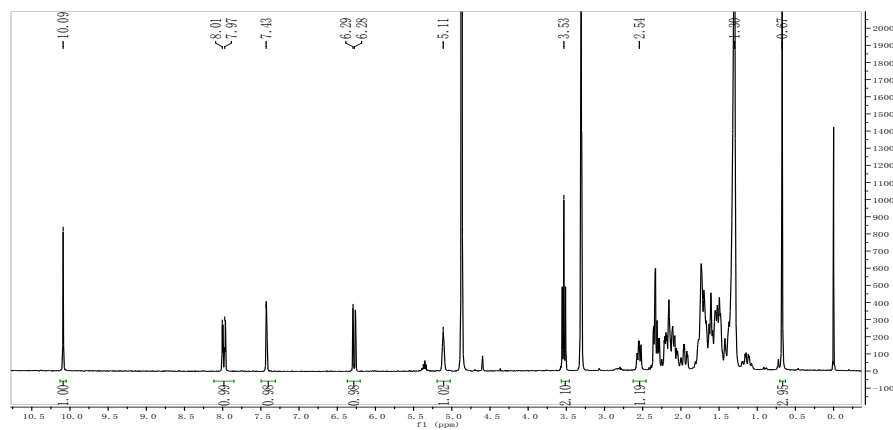


Figure S39. ¹H NMR spectrum of spectrum of **5**

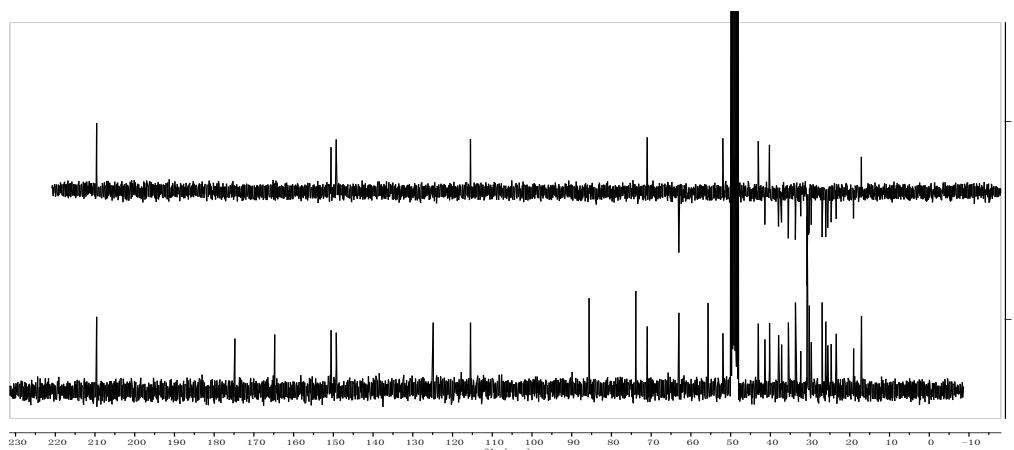


Figure S40. ^{13}C NMR spectrum of **5**

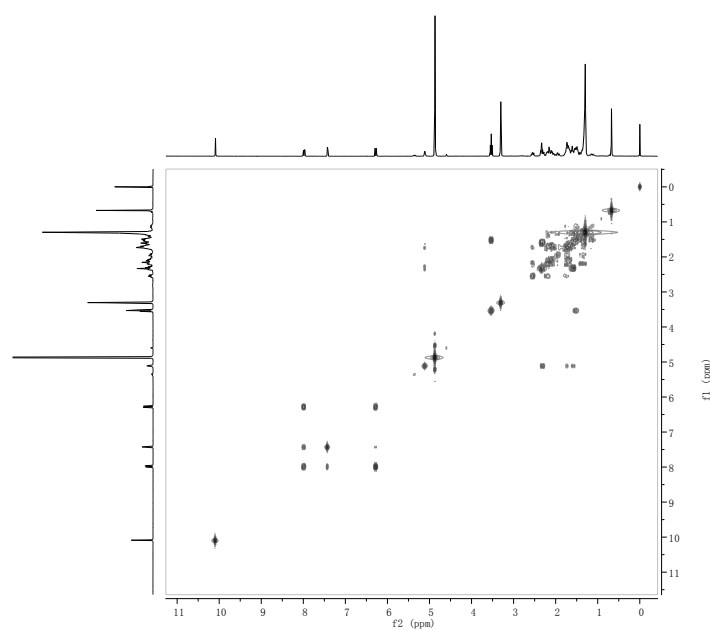


Fig.S41. ^1H - ^1H COSY spectrum of **5**

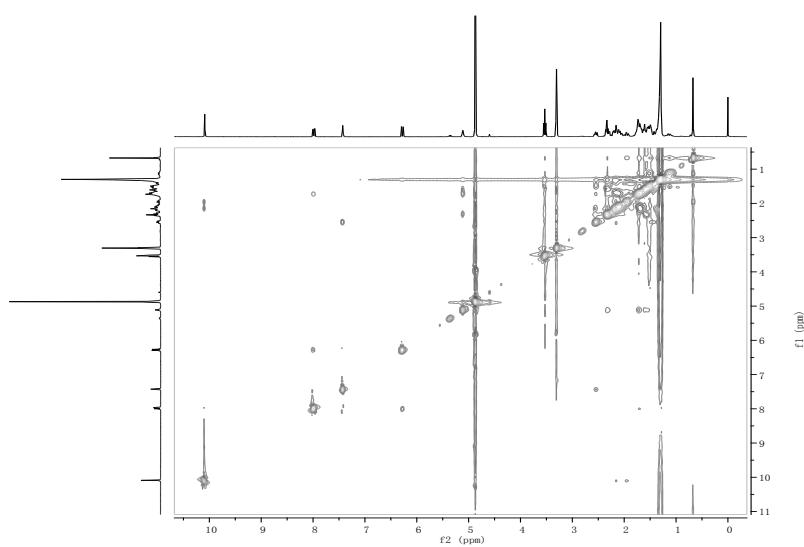


Fig.S42. NOESY spectrum of **5**

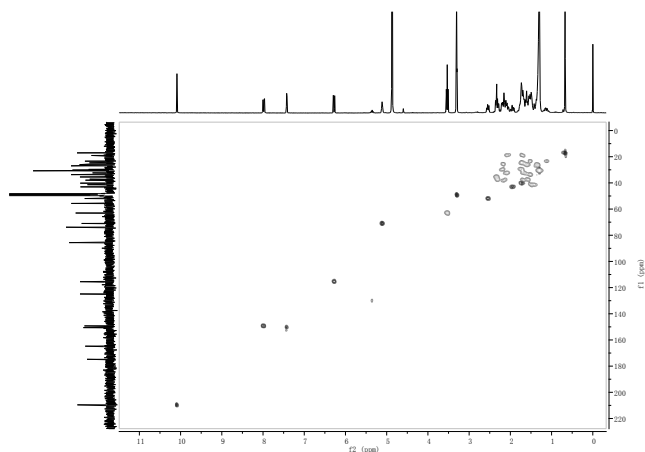


Fig.S43. HSQC spectrum of **5**

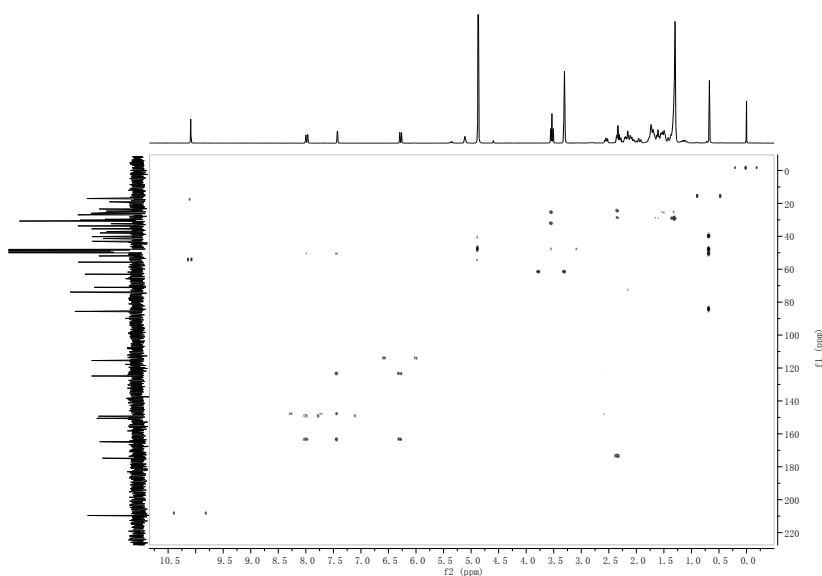


Fig.S44. HMBC spectrum of **5**

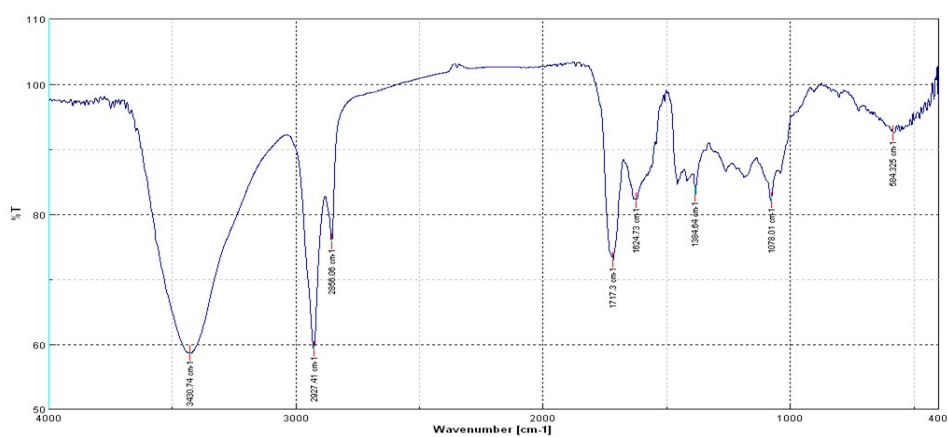


Fig.S45 IR spectrum of **6**

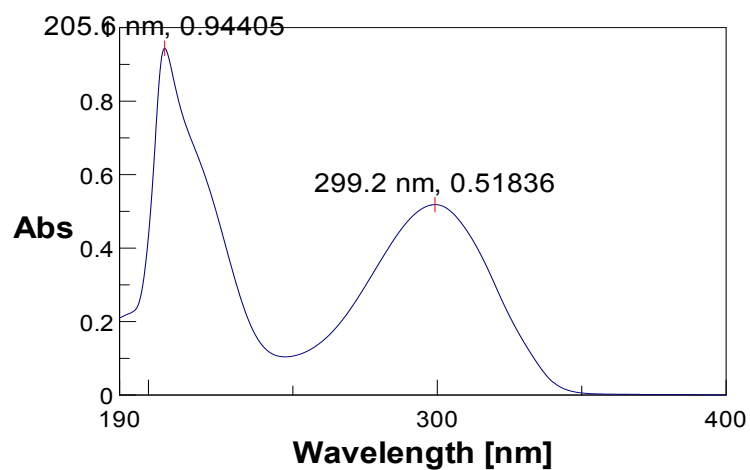


Fig.S46. UV spectrum of 6

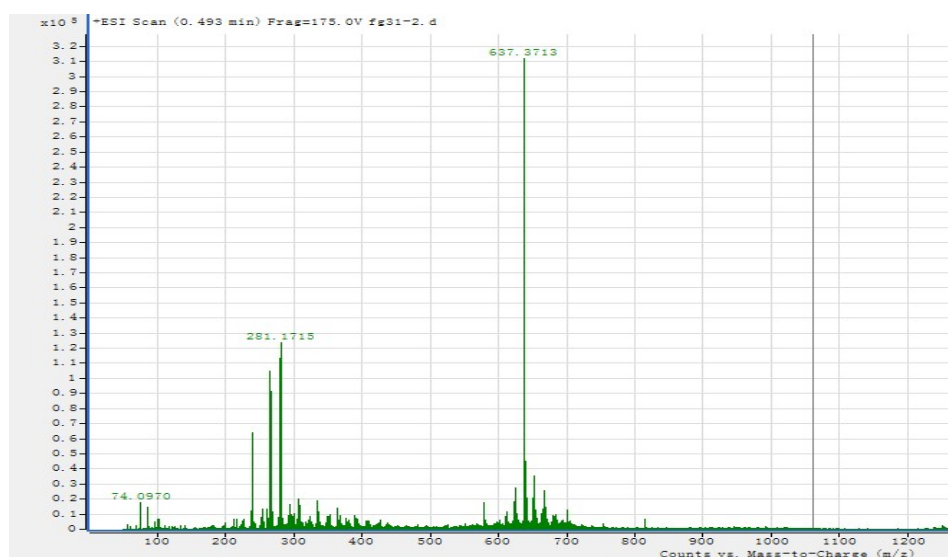


Fig.S47. HRESIMS spectrum of 6

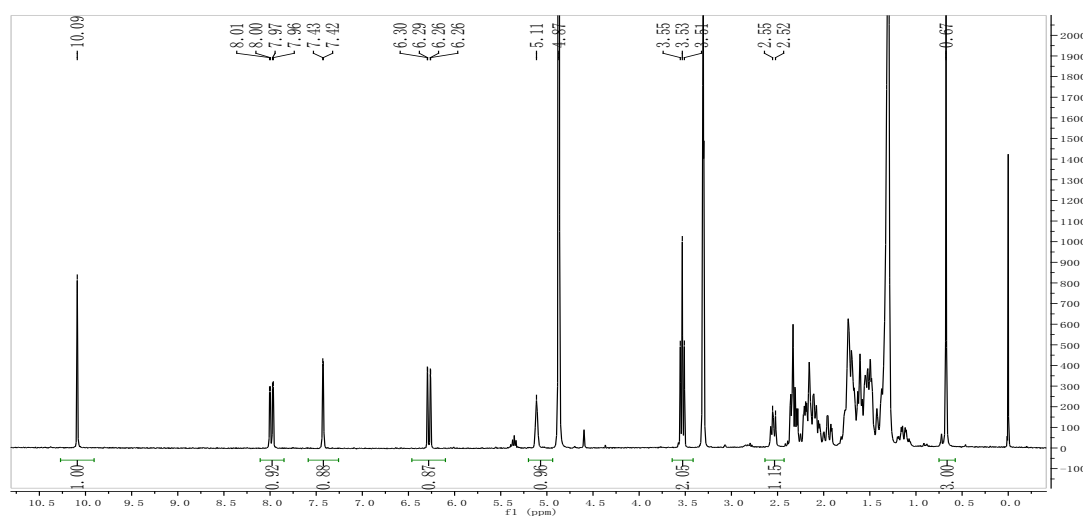


Fig.S48. ¹H NMR spectrum of 6

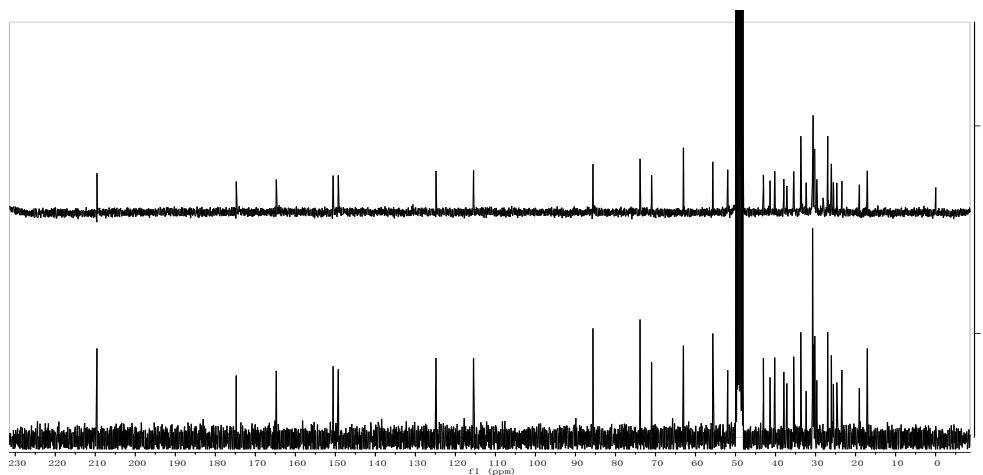


Fig.S49. ^{13}C NMR spectrum of **6**

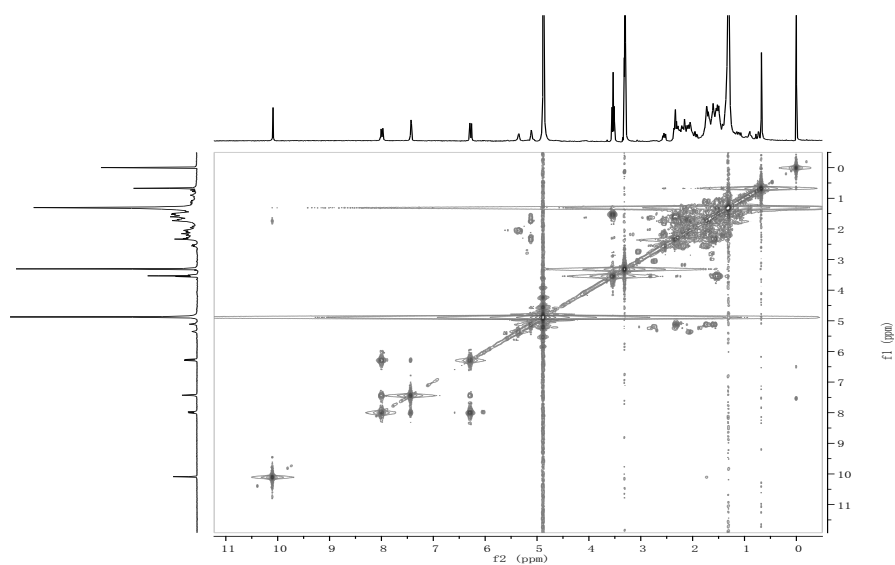


Fig.S50. ^1H - ^1H COSY spectrum of **6**

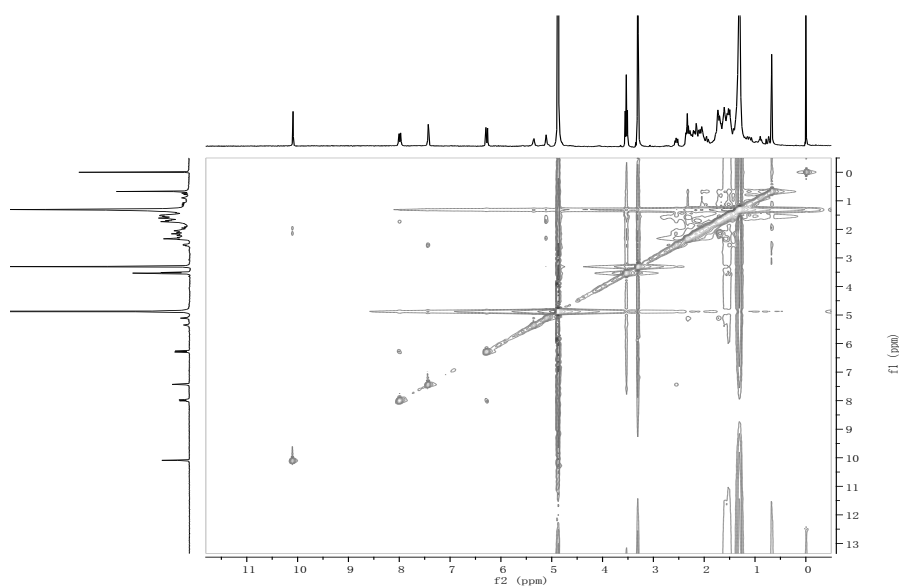


Fig.S51. NOESY spectrum of **6**

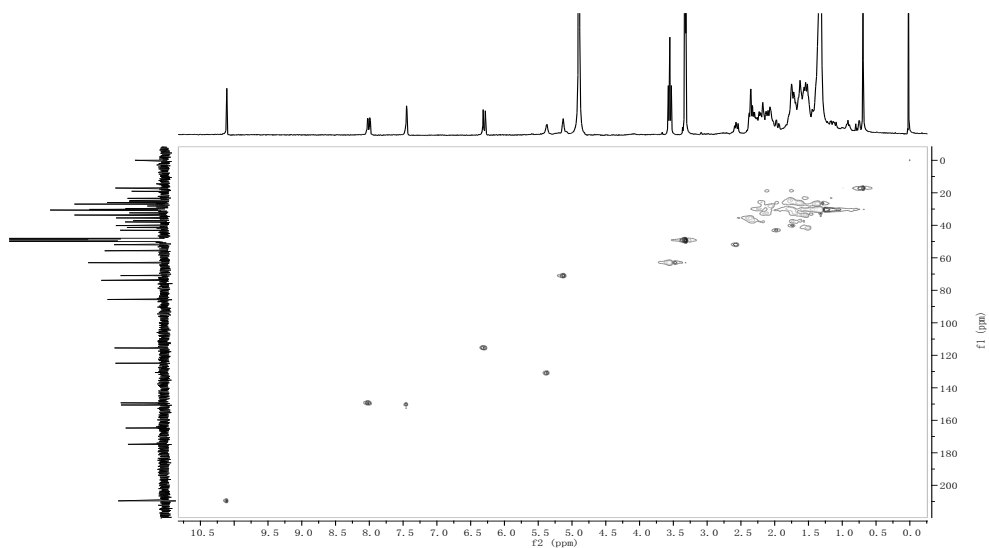


Fig.S52. HSQC spectrum of **6**

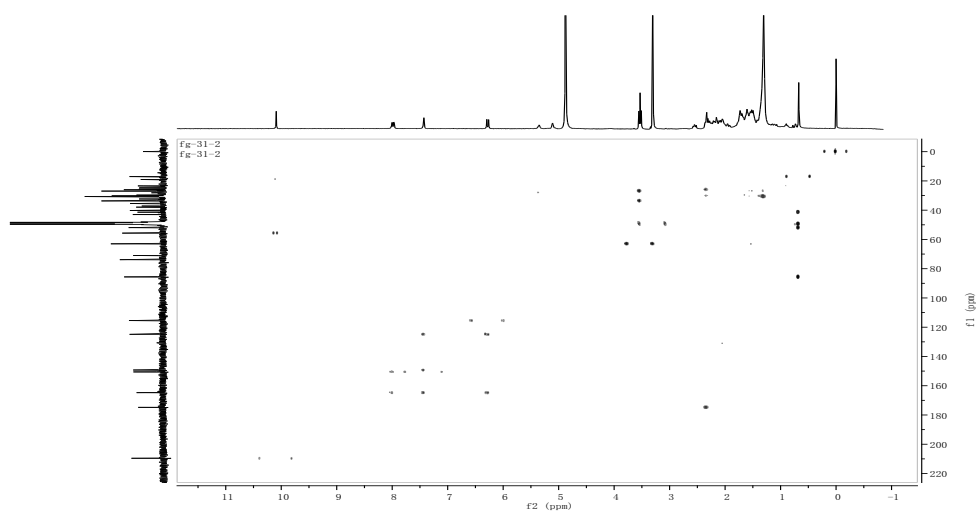


Fig.S53. HMBC spectrum of **6**

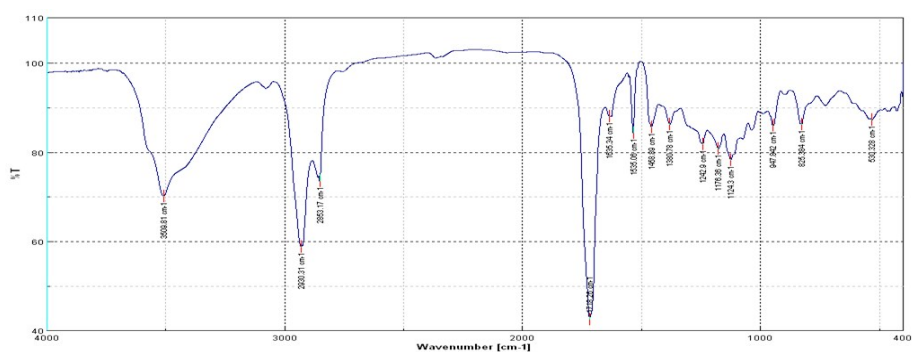


Fig.S54. IR spectrum of **7**

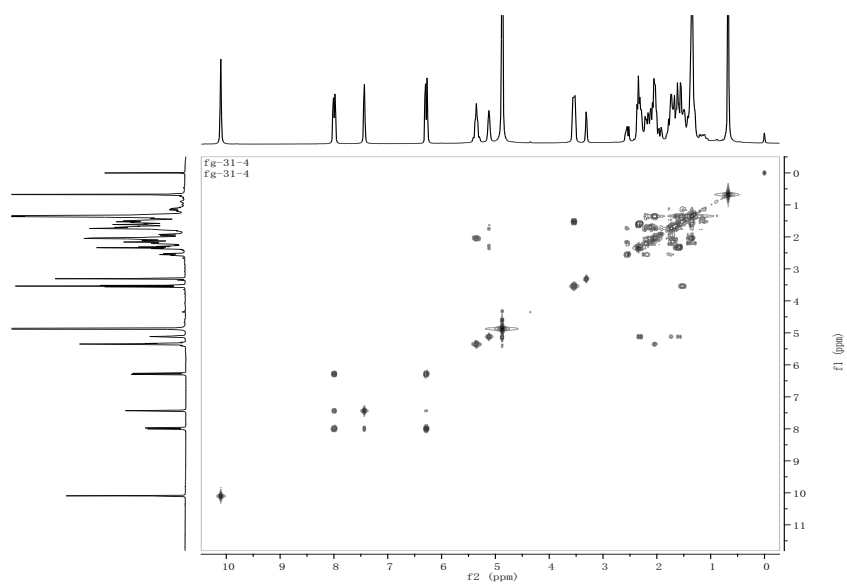


Fig.S59. ^1H - ^1H COSY spectrum of **7**

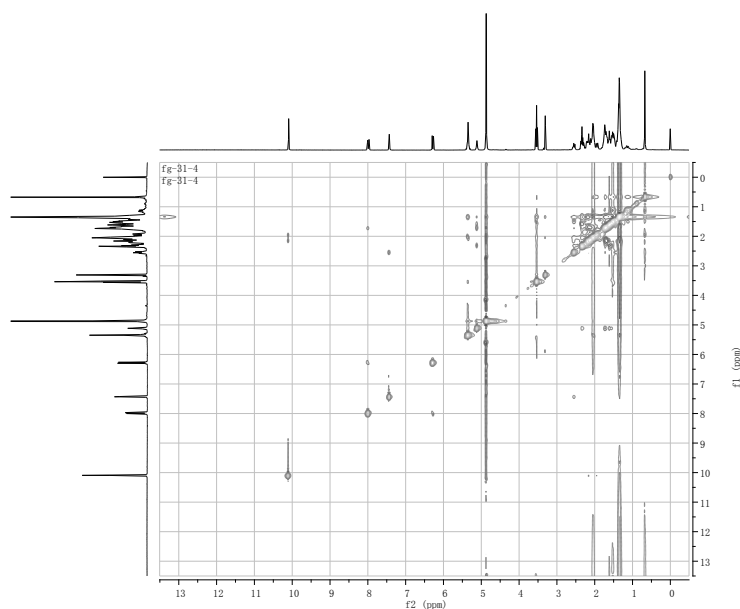


Fig.S60. NOESY spectrum of **7**

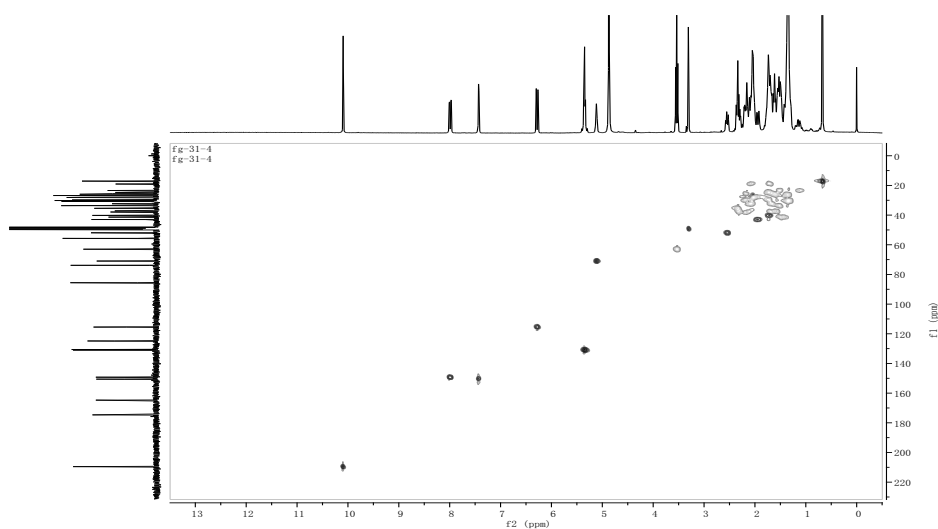


Fig.S61. HSQC spectrum of **7**

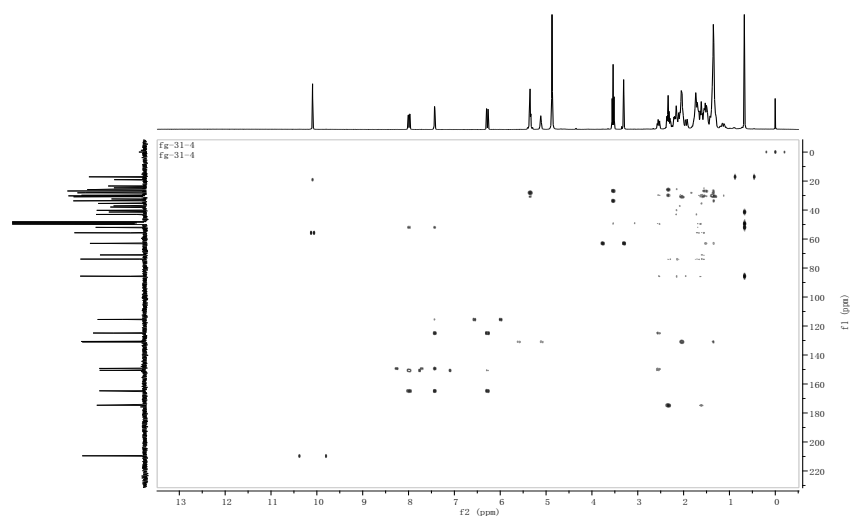


Fig.S62. HMBC spectrum of **7**

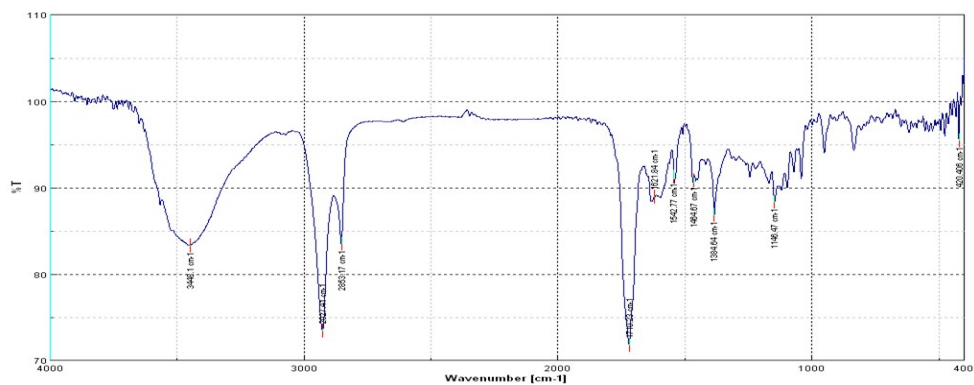


Fig. S63. IR spectrum of **8**

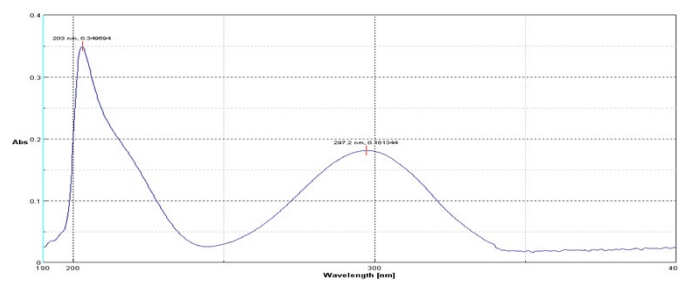


Fig. S64. UV spectrum of **8**

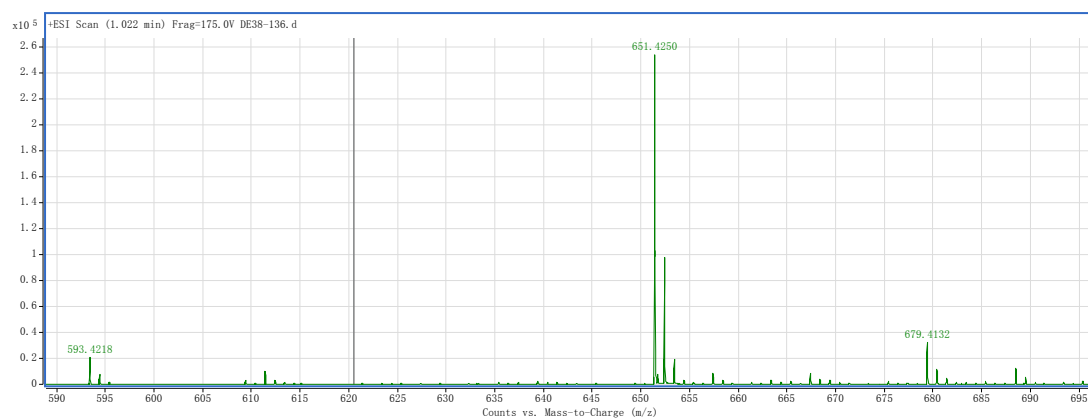


Fig. S65. HRMSIMS of **8**

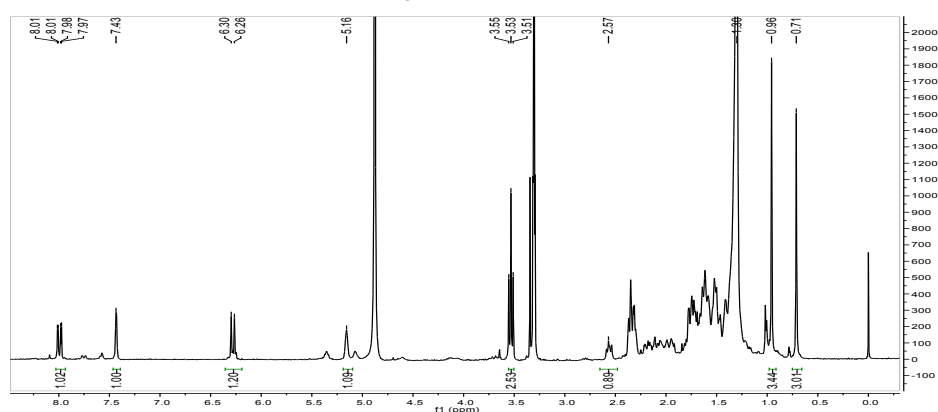


Fig.S66. ¹H NMR spectrum of **8**

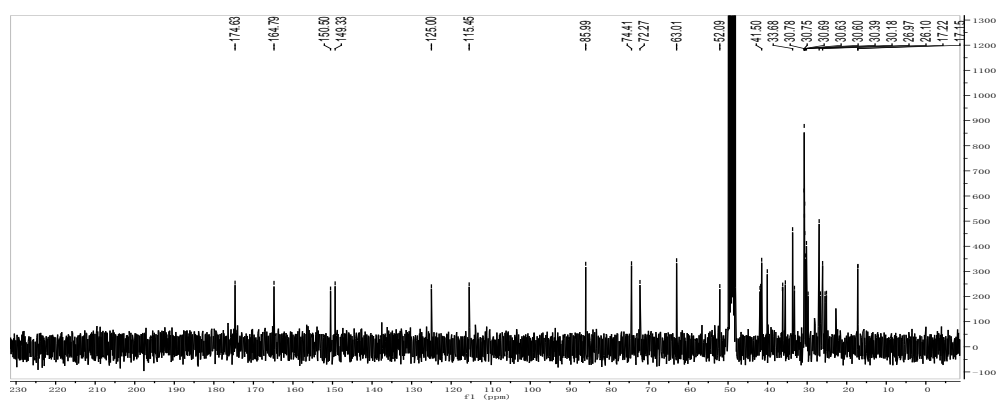


Fig.S67. ¹³C NMR spectrum of **8**

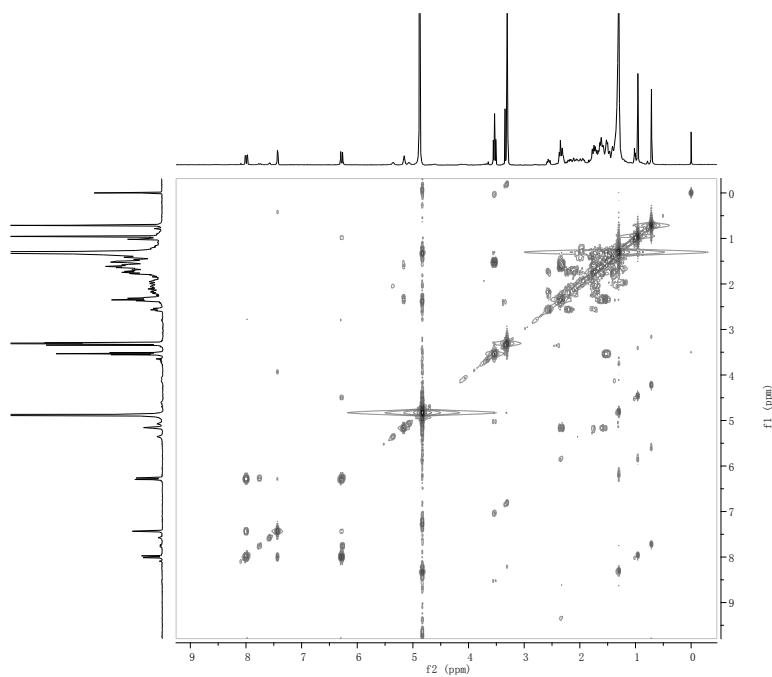


Fig. S68. ^1H - ^1H COSY spectrum of **8**

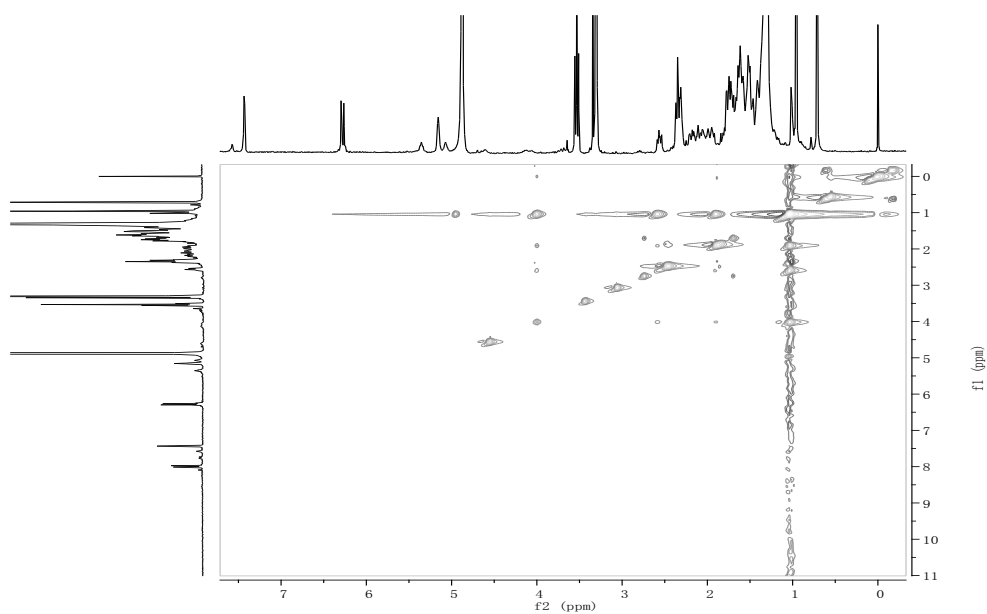


Fig. S69. NOESY spectrum of **8**

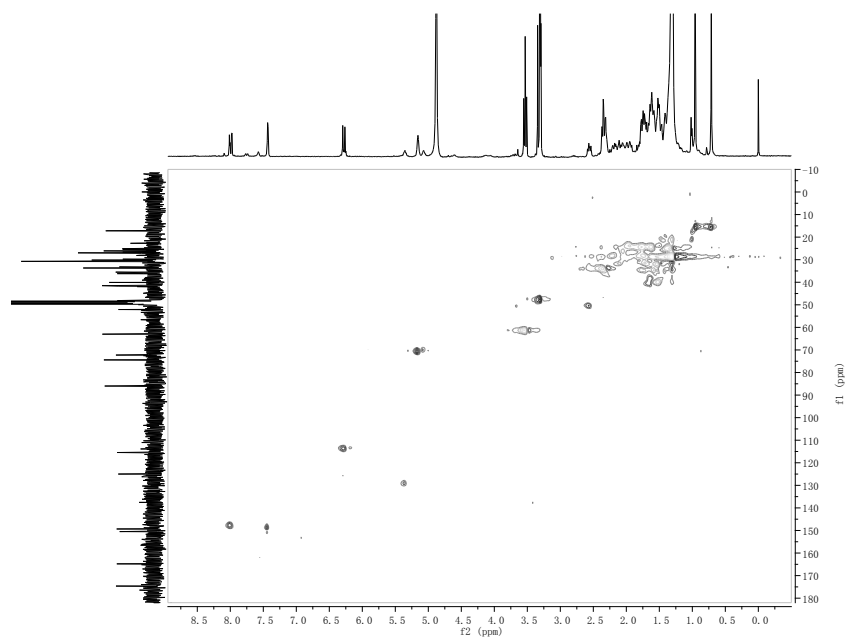


Fig. S70. HSQC spectrum of **8**

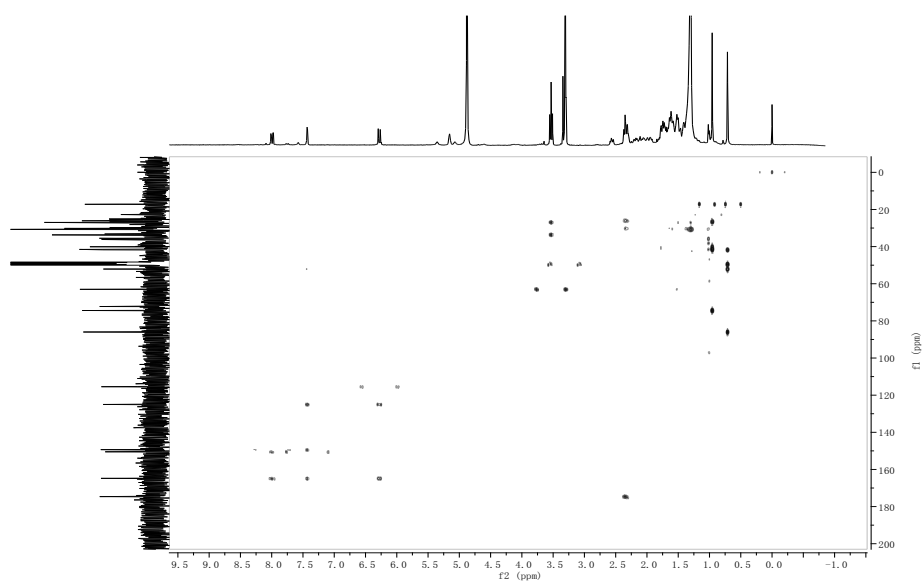


Fig. S71. HMBC spectrum of **8**

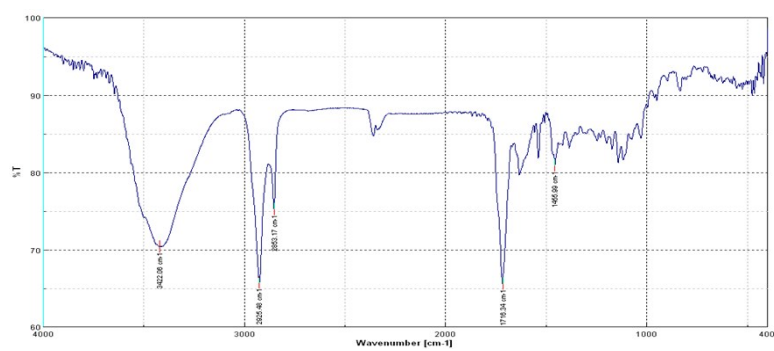


Fig.S72. IR spectrum of **9**

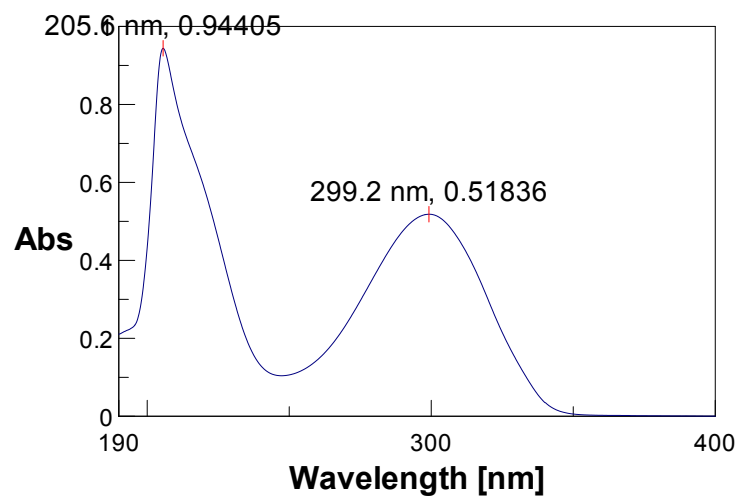


Fig. S73. UV spectrum of **9**

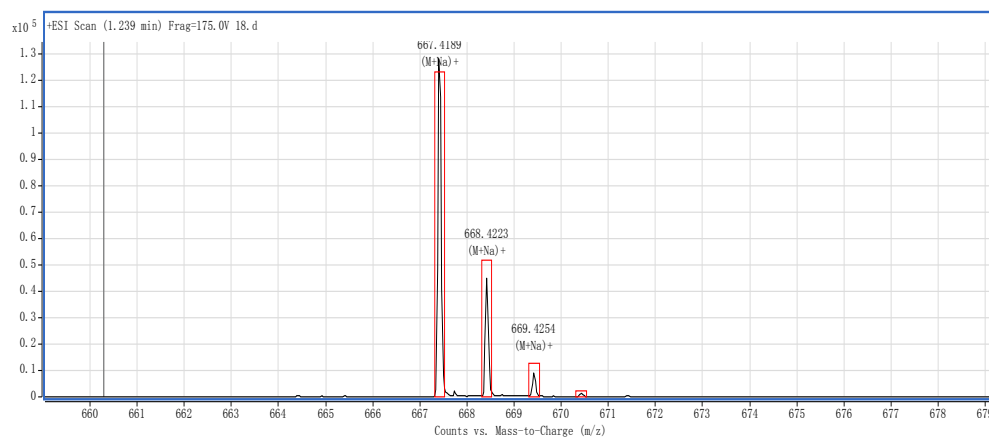


Fig.S74. HR-ESI-MS spectrum of **9**

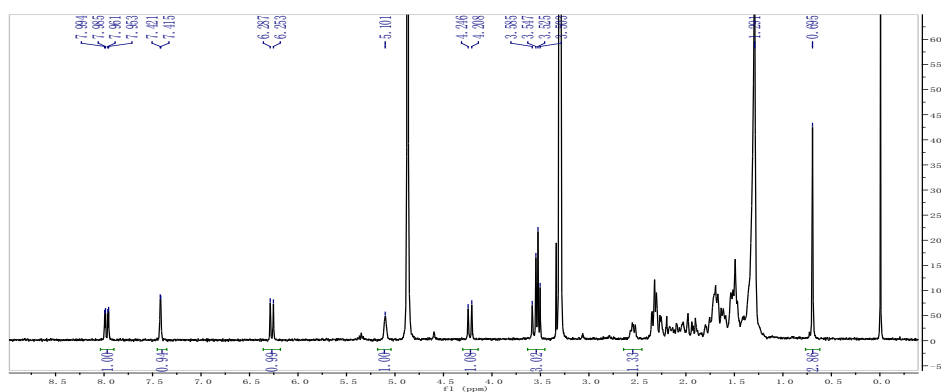


Fig. S75. ¹H NMR spectrum of **9**

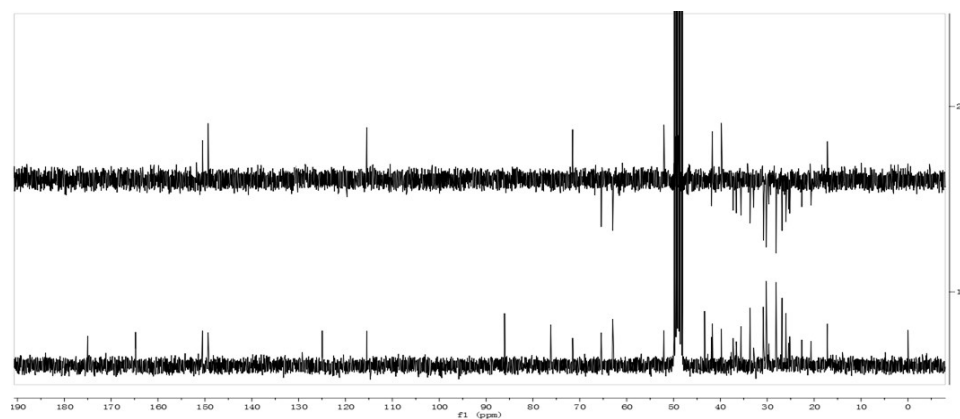


Fig. S76. ^{19}C NMR spectrum of **9**

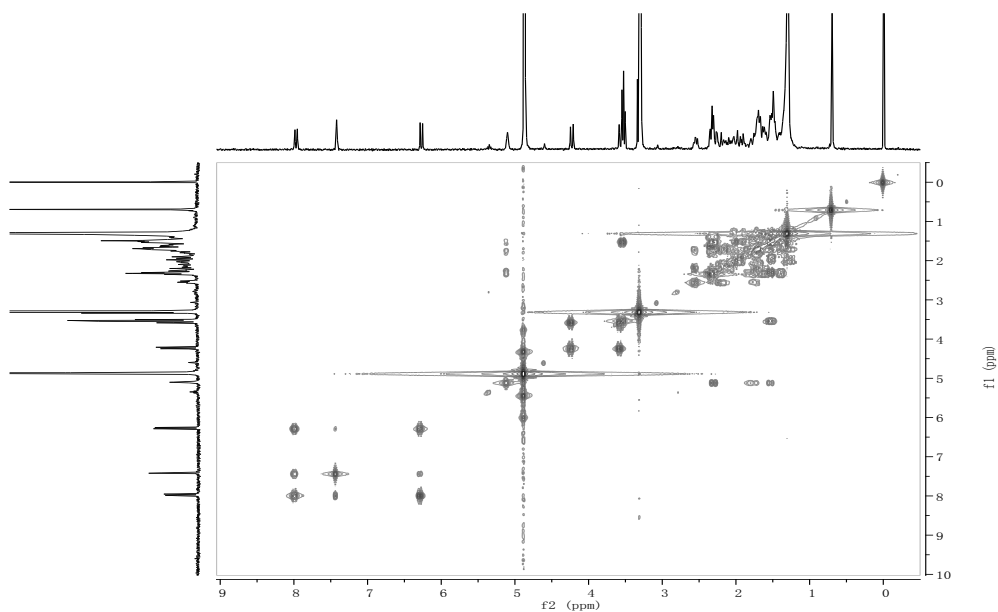


Fig. S77. ^1H - ^1H COSY spectrum of **9**

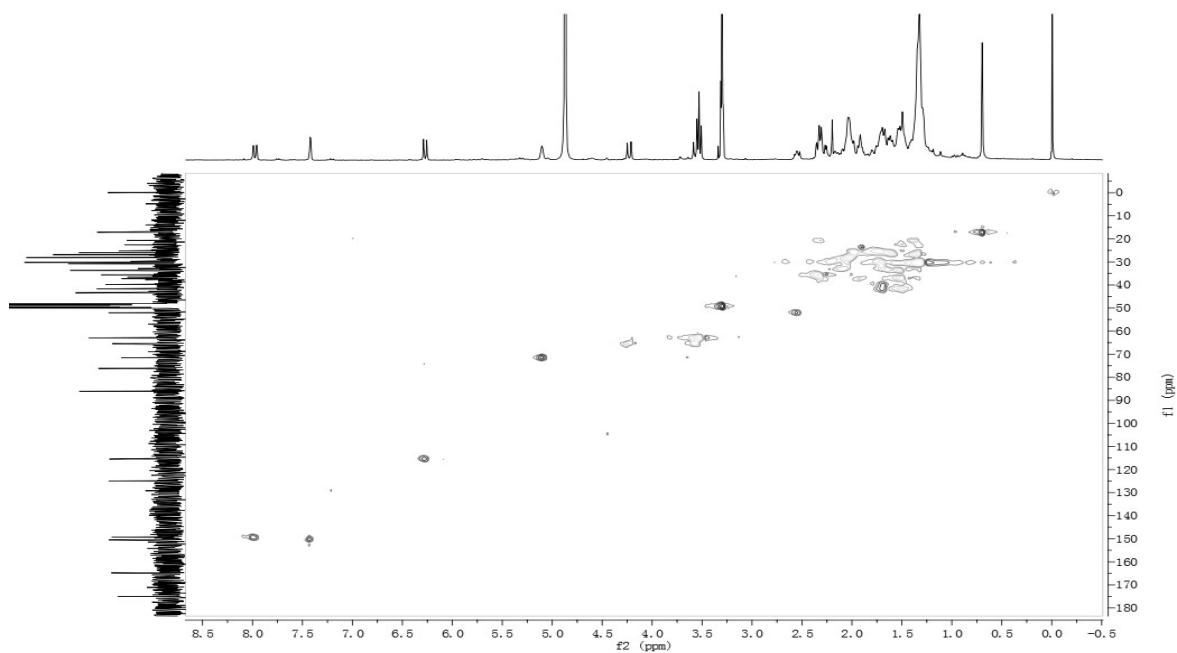


Fig. S78. HSQC spectrum of **9**

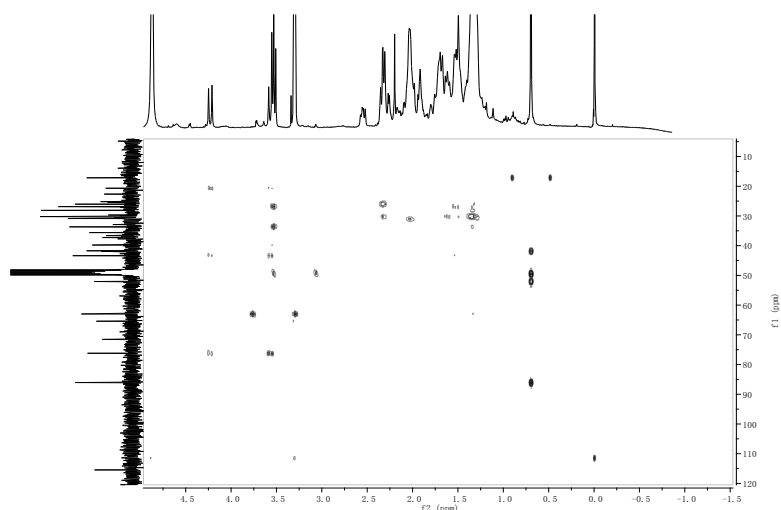


Fig. S79. HMBC spectrum of **9**

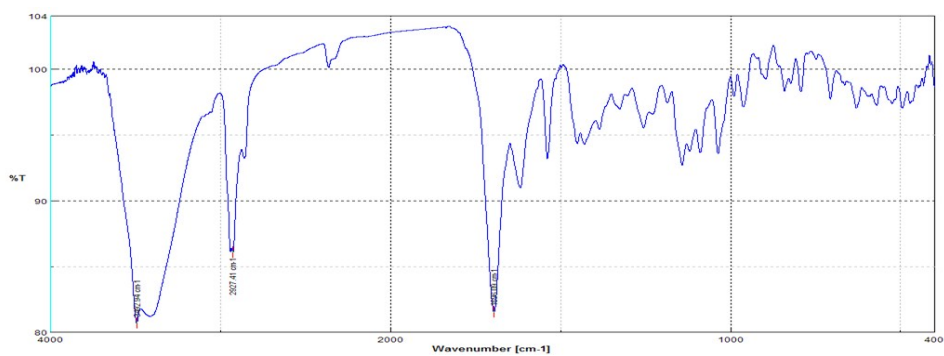


Fig. S80. IR spectrum of **10**

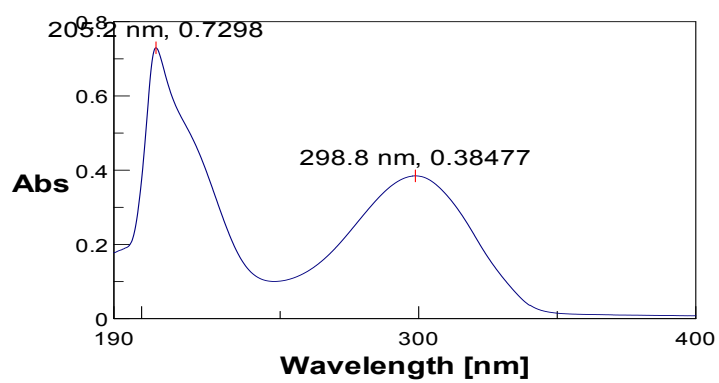


Fig. S81. UV spectrum of **10**

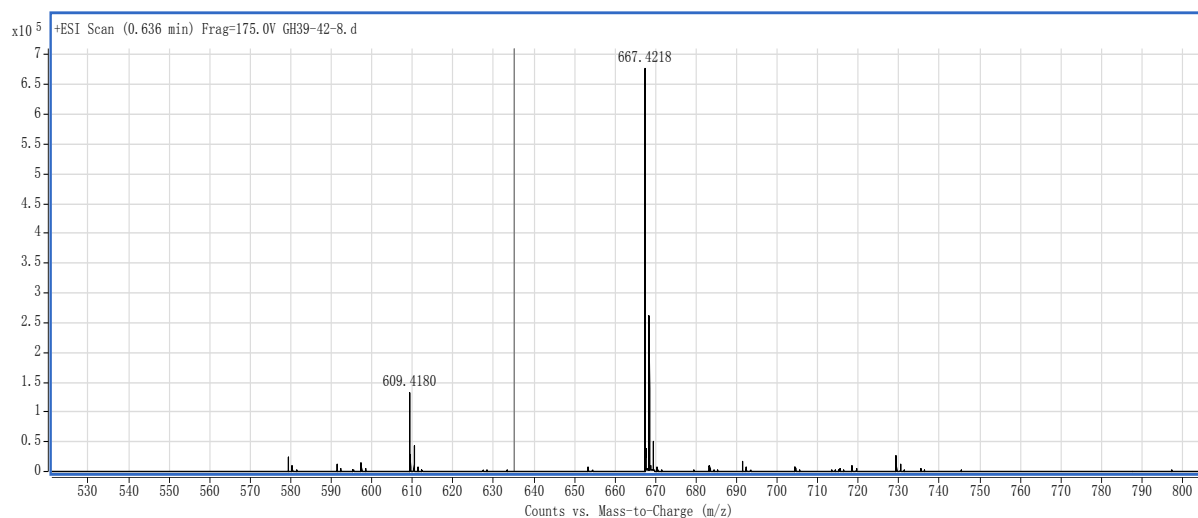


Fig. S82. HRESIMS spectrum of **10**

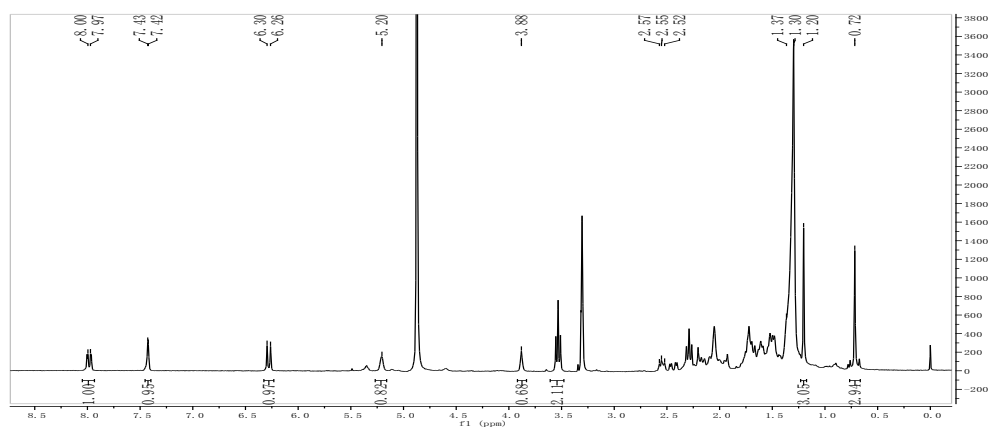


Fig. S83. ^1H NMR spectrum of **10**

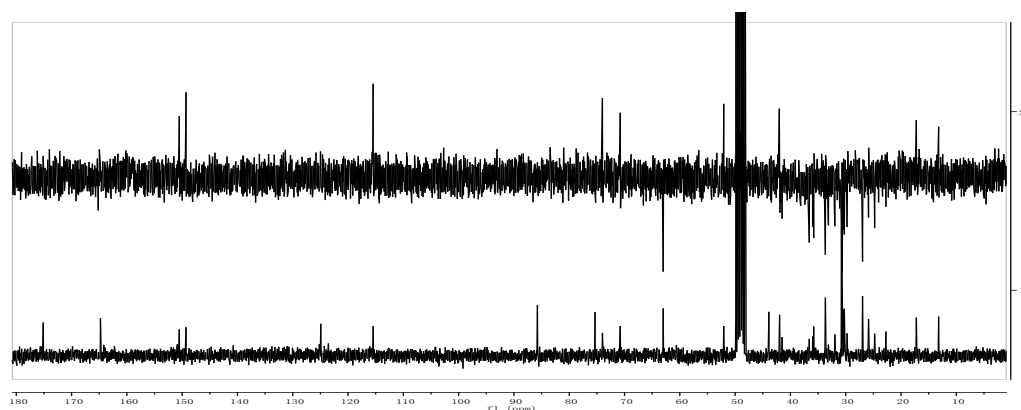


Fig. S84. ^{13}C NMR and DEPT1310 spectrum of **10**

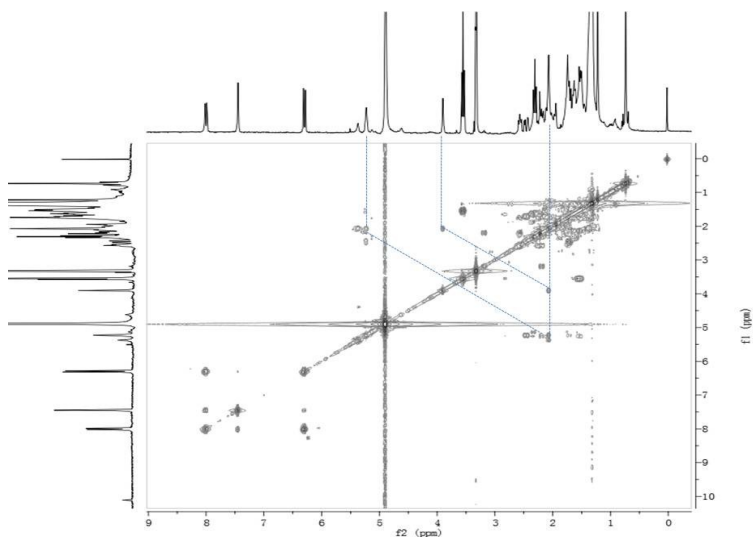


Fig. S85. ^1H - ^1H COSY spectrum of **10**

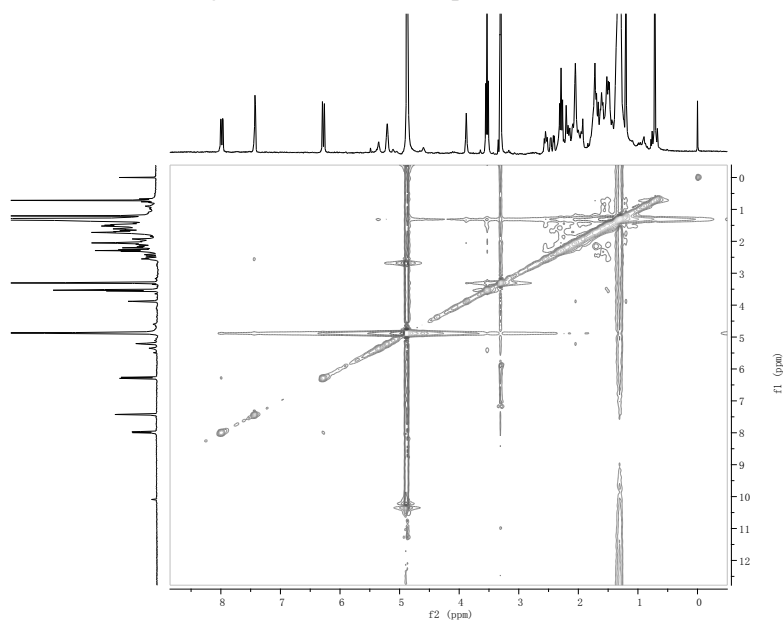


Fig. S86. NOESY spectrum of **10**

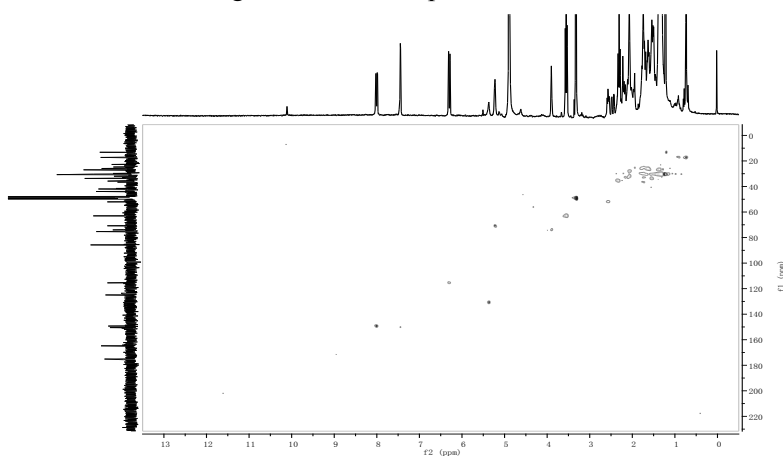


Fig. S87. HSQC spectrum of **10**

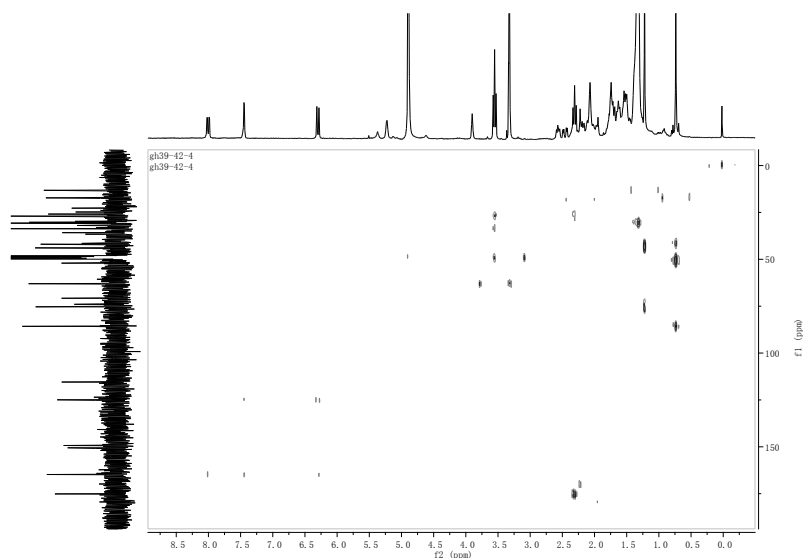


Fig. S88. HMBC spectrum of **10**

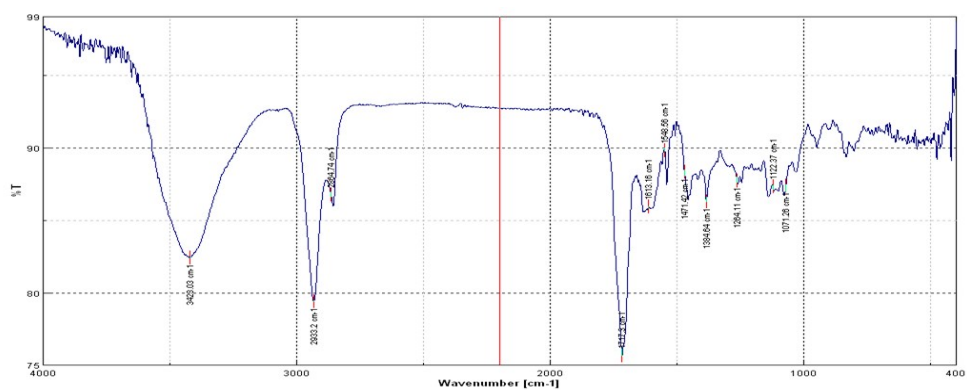


Fig. S89. IR spectrum of **11**

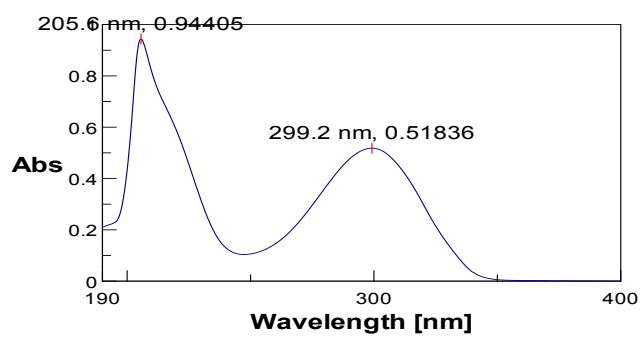


Fig. S90. UV spectrum of **11**

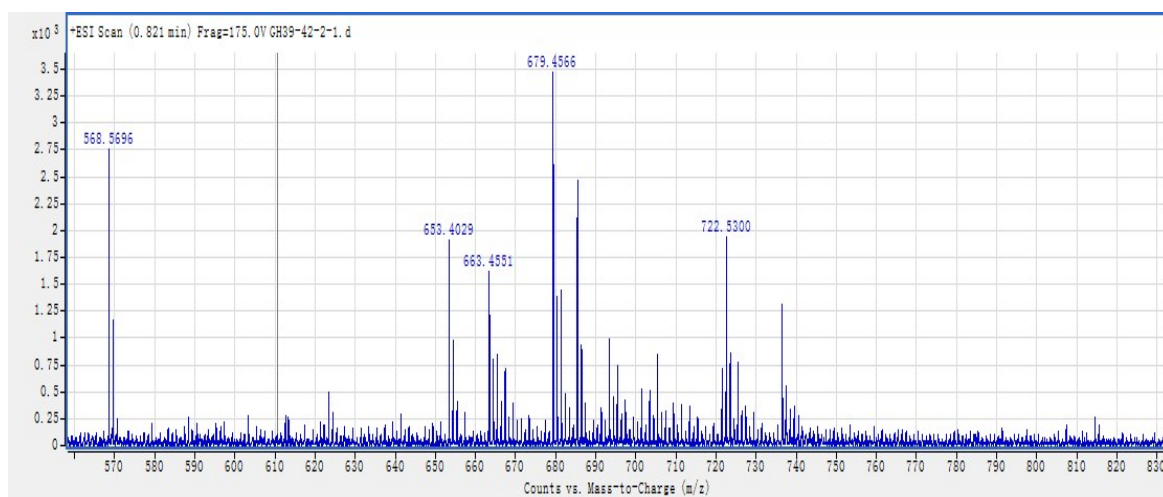


Fig. S91. HR-ESI-MS spectrum of **11**

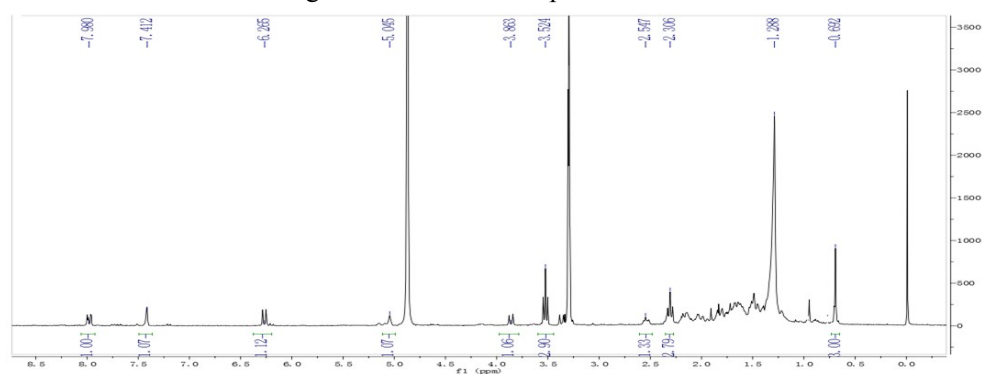


Fig. S92. ¹H NMR spectrum of **11**

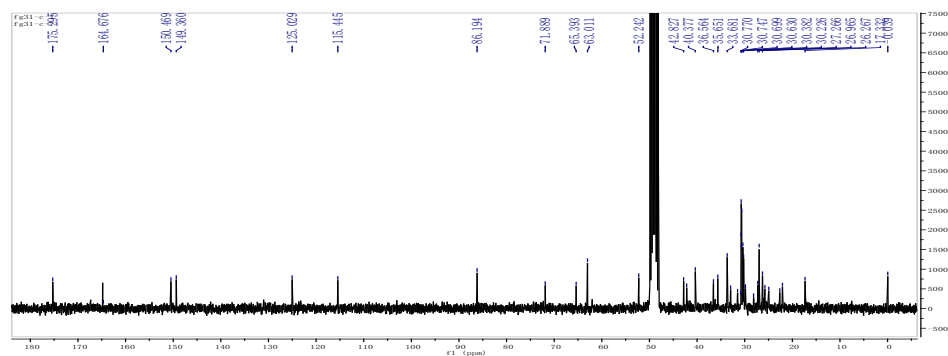


Fig. S93. ¹³C NMR spectrum of **11**

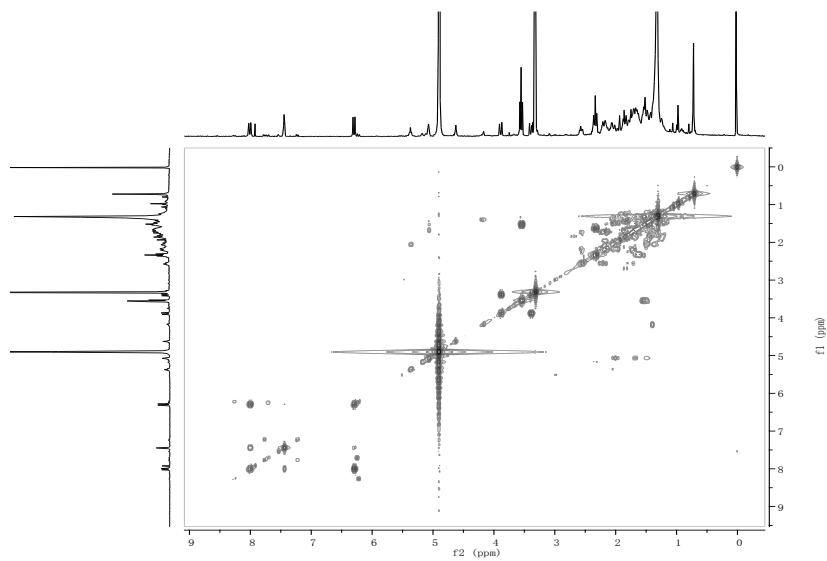


Fig. S94. ^1H - ^1H COSY spectrum of **11**

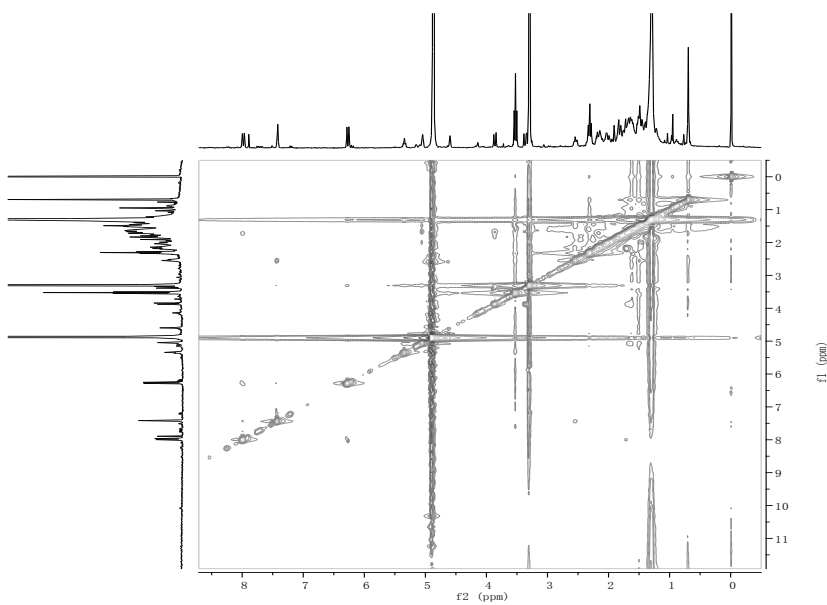


Fig. S95. NOESY spectrum of **11**

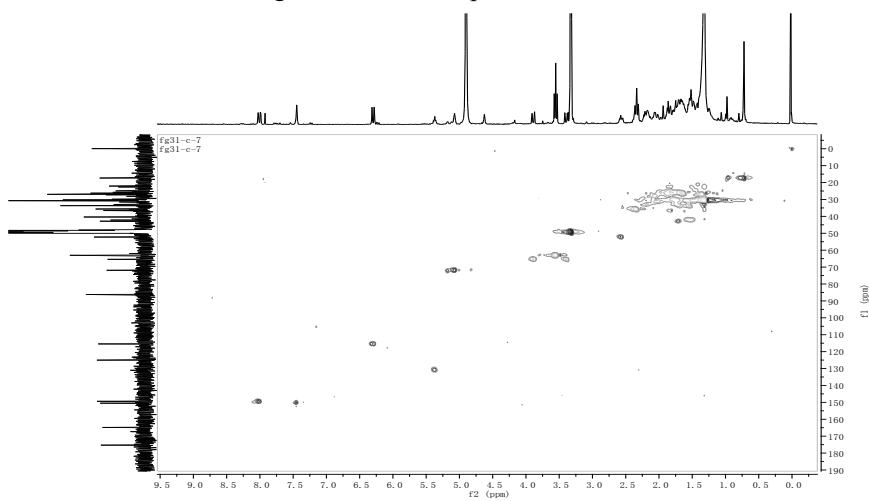


Fig.S96. HSQC spectrum of **11**

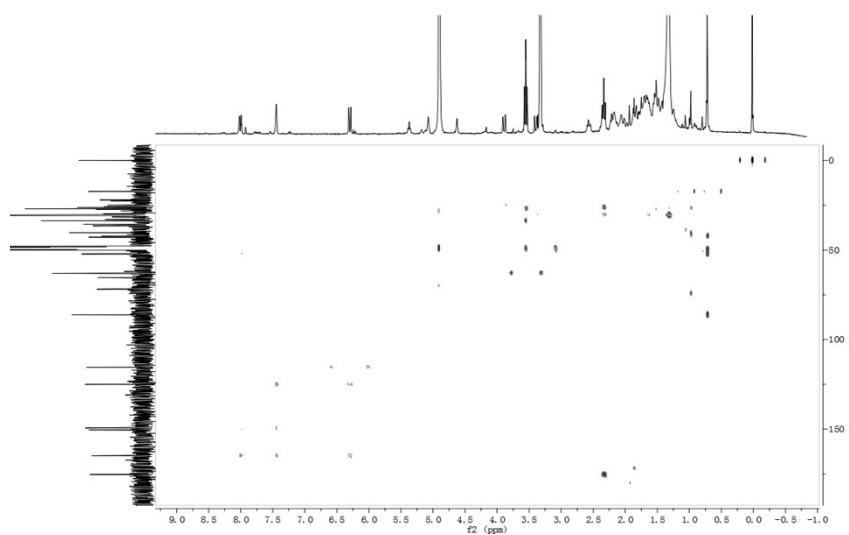


Fig. S97. HMBC spectrum of **11**

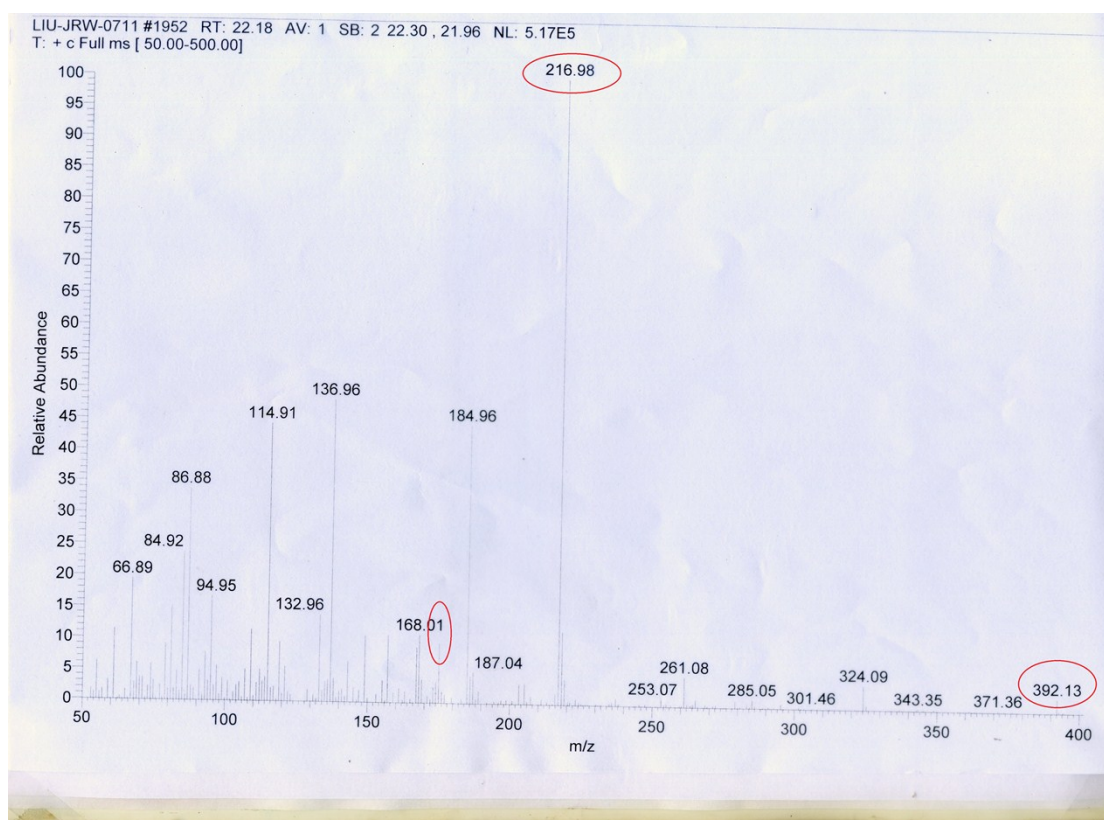


Fig.S98. EI-MS/MS of DMDS adduct analysis of **7**

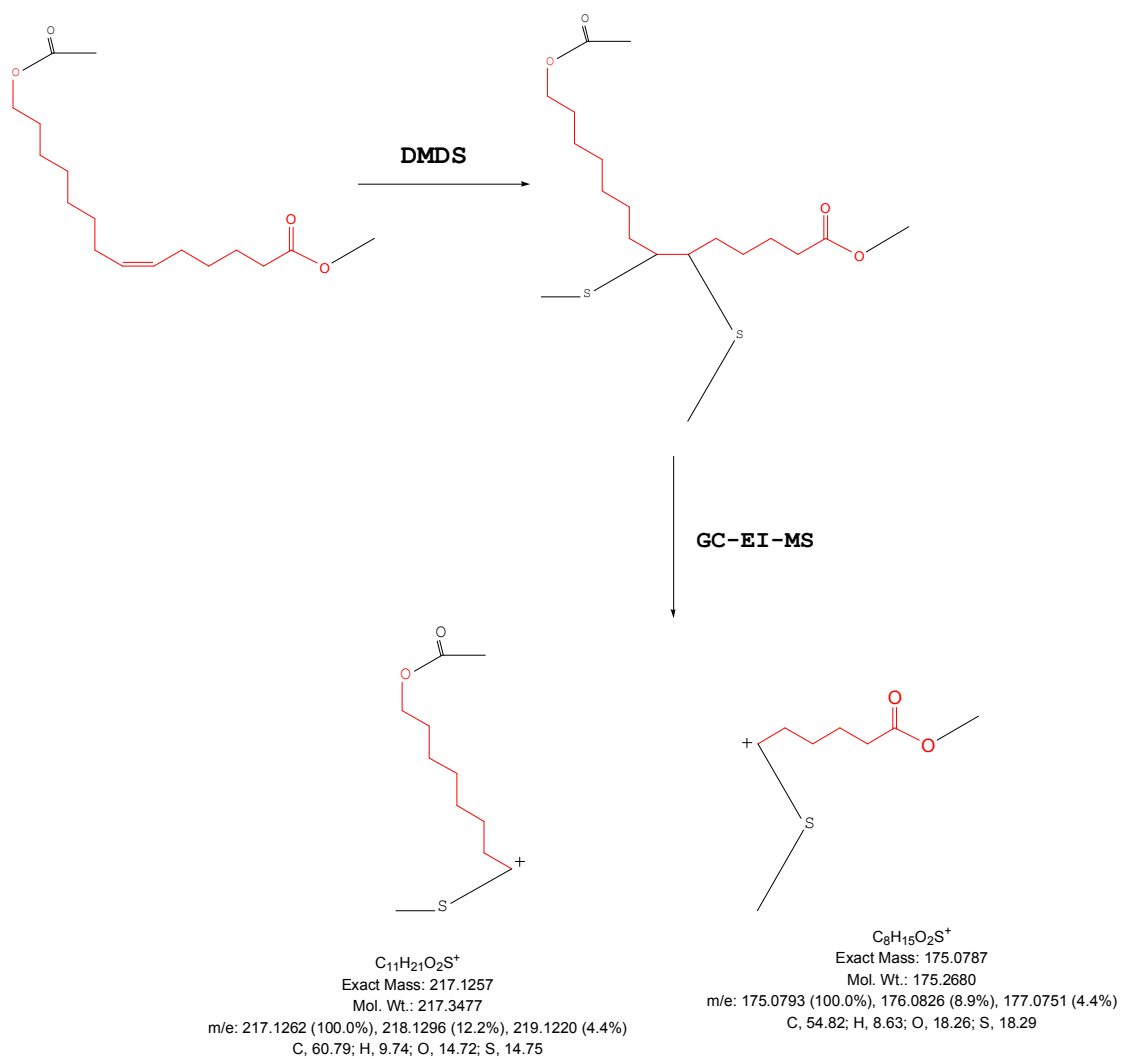


Fig.S99.Fragmentation pathway of the DMDS adduct of the fatty acid side chain of 7