

New Thiodiketopiperazine and 3,4-Dihydroisocoumarin Derivatives from the Marine-derived Fungus *Aspergillus terreus*

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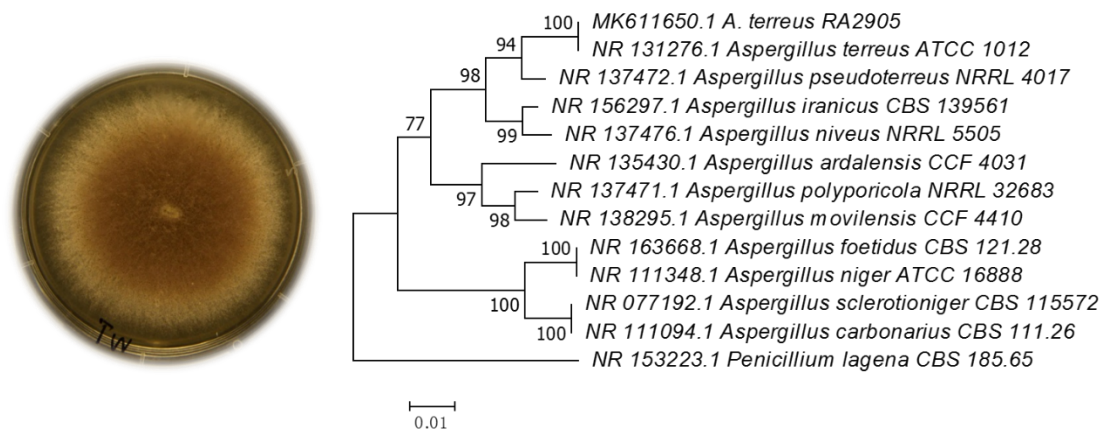


Figure S1. *Aspergillus terreus* RA2905 and its phylogenetic tree of ITS gene

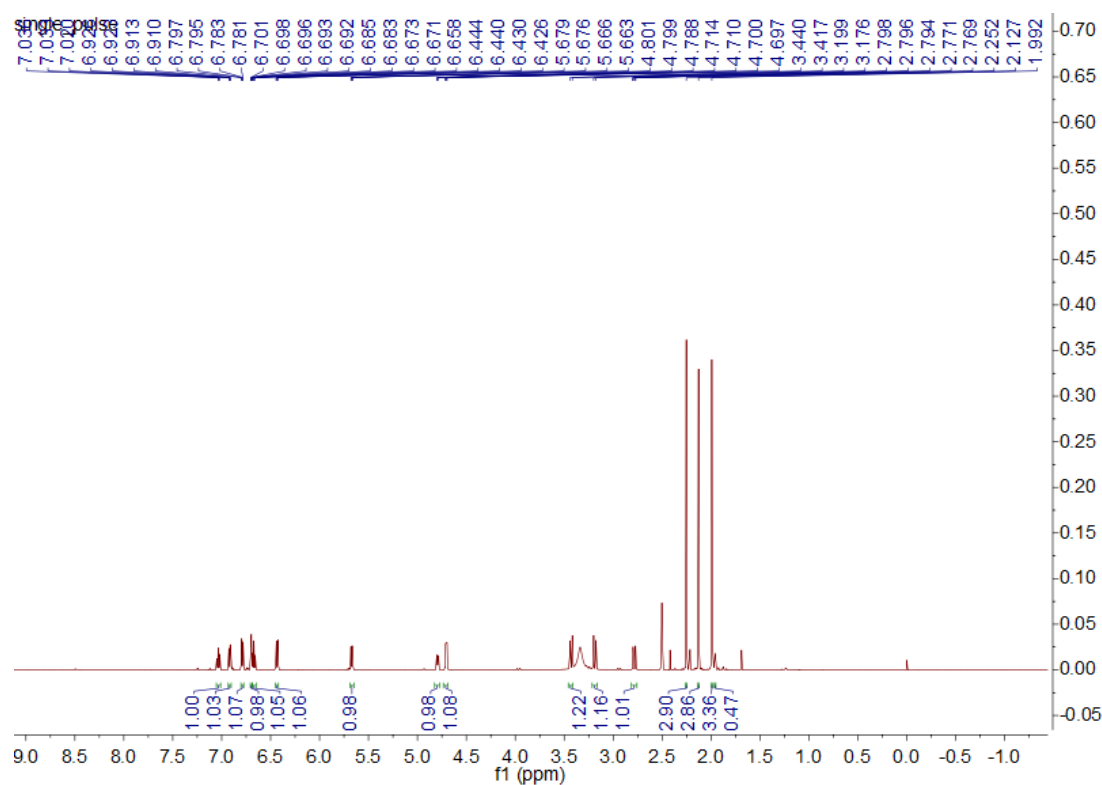


Figure S2. ¹H NMR (500 MHz, DMSO-*d*₆) spectrum of compound 1

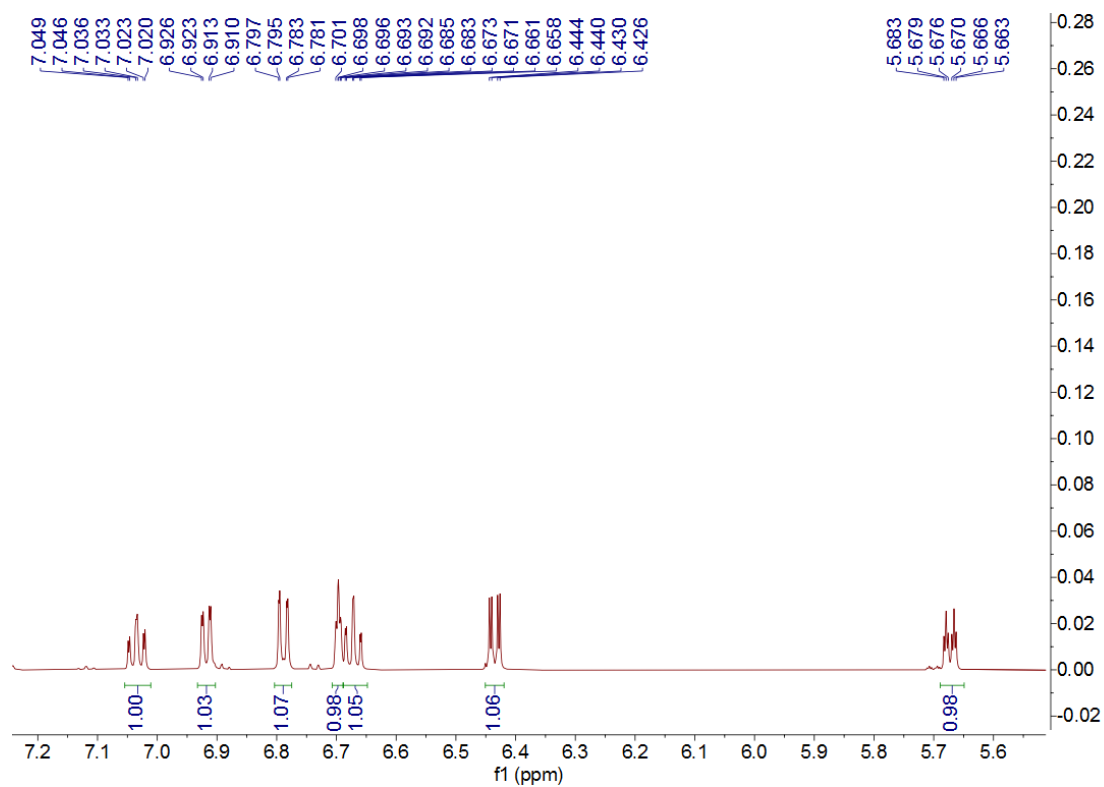


Figure S3. Partial ^1H NMR (500 MHz, $\text{DMSO}-d_6$) spectrum of compound **1**

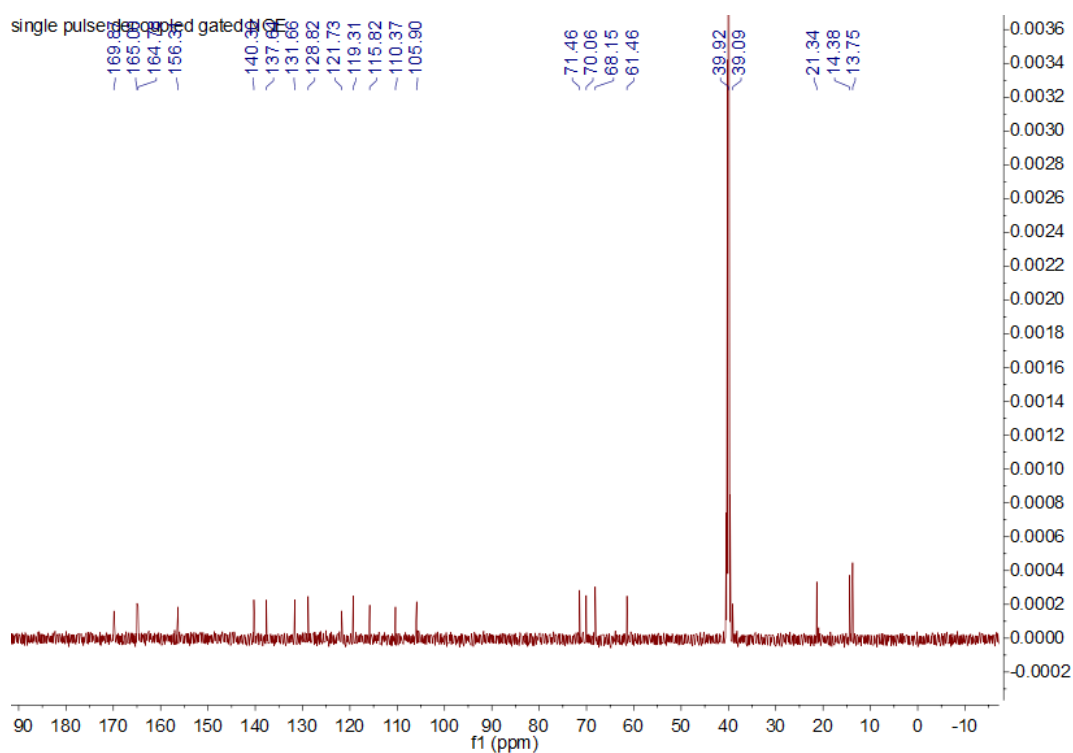


Figure S4. ^{13}C NMR (125 MHz, $\text{DMSO}-d_6$) spectrum of compound **1**

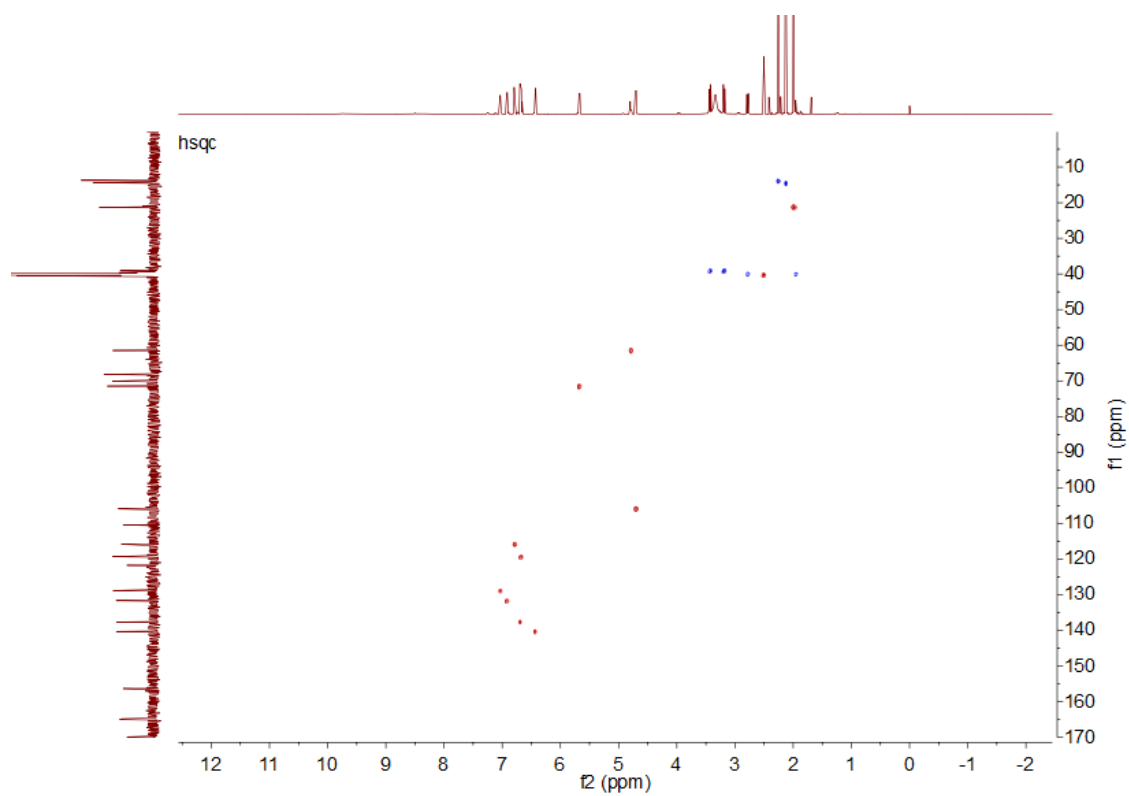


Figure S5. HSQC (DMSO- d_6) spectrum of compound **1**

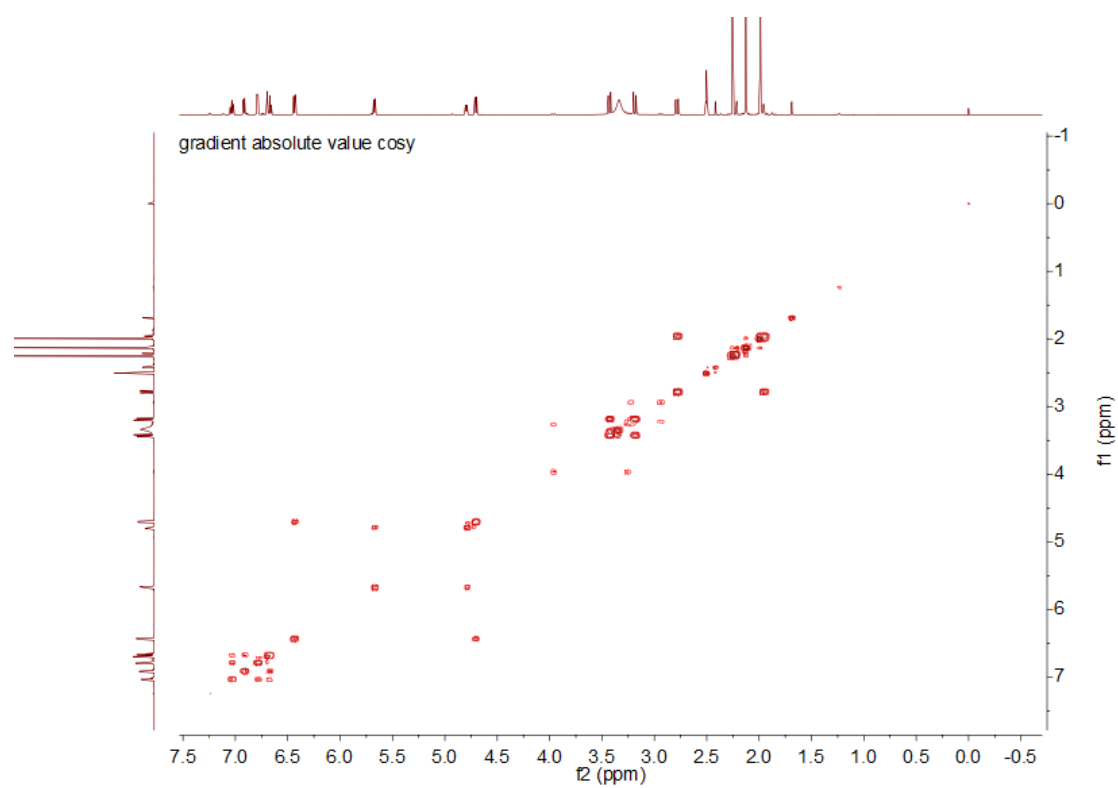


Figure S6. ^1H - ^1H COSY (DMSO- d_6) spectrum of compound **1**

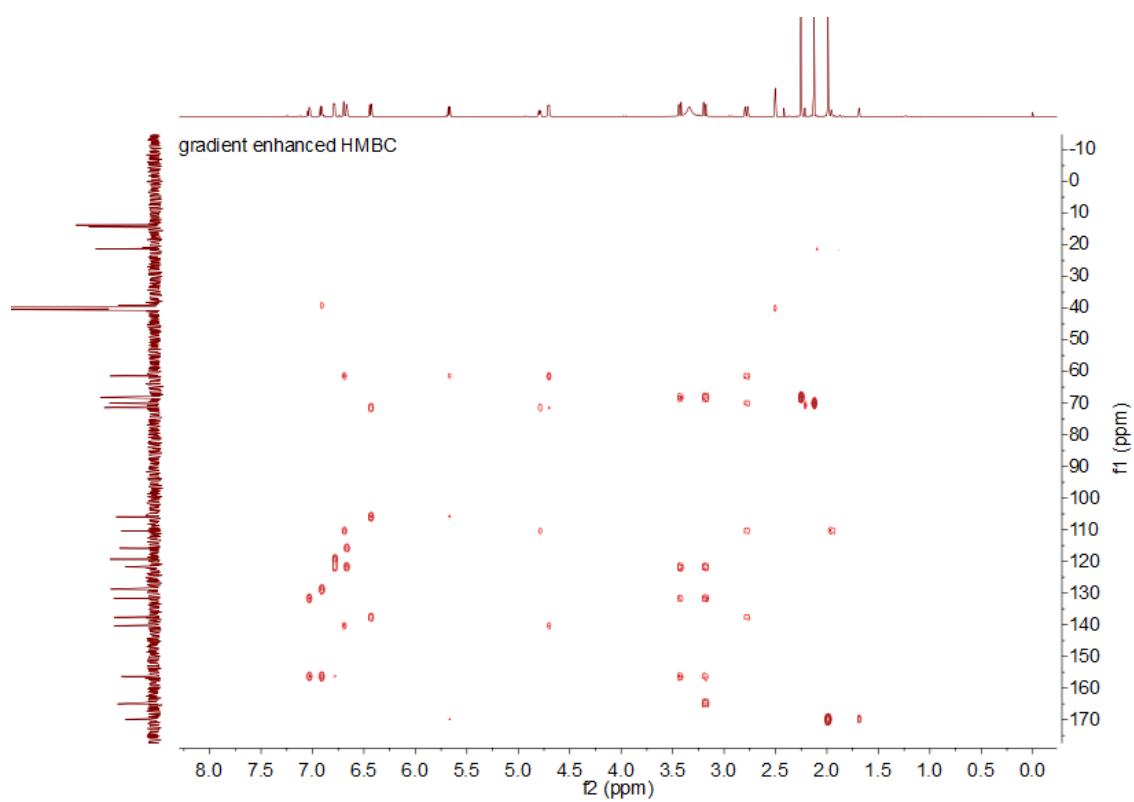


Figure S7. HMBC (DMSO- d_6) spectrum of compound **1**

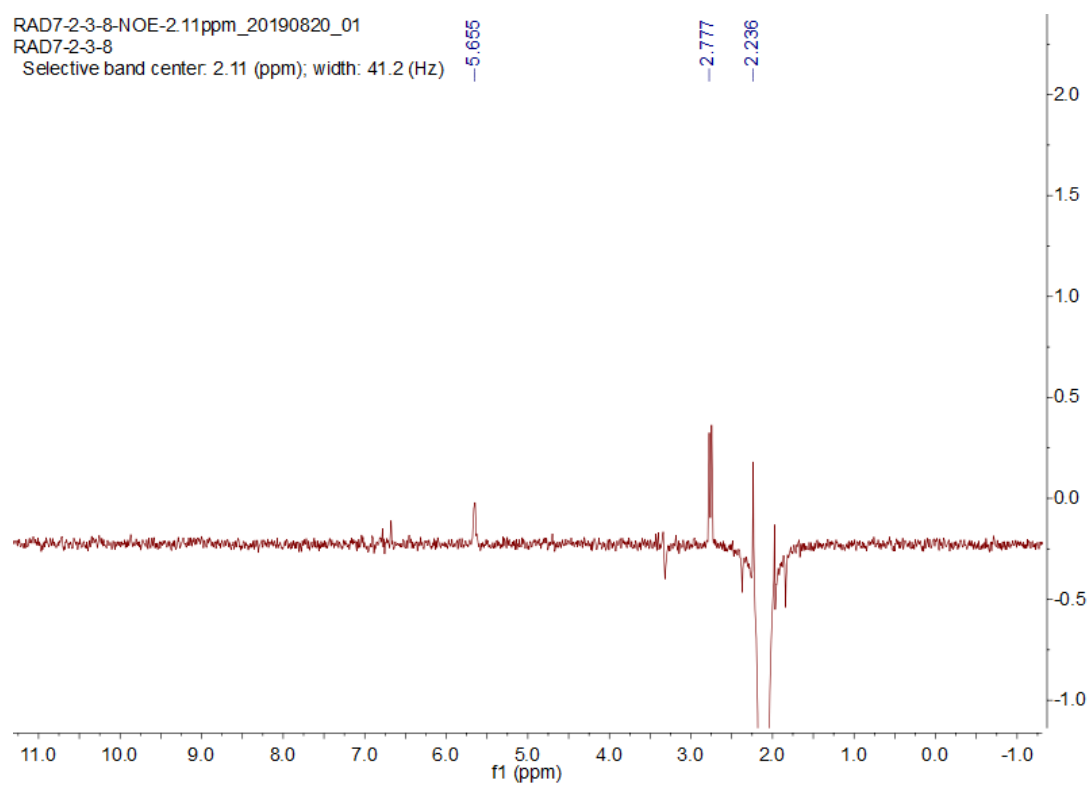


Figure S8. NOE (DMSO- d_6) spectrum of compound **1**

20190912-RAD7-2-3-8_190912085157 #52 RT: 0.79 AV: 1 NL: 1.61E6
T: FTMS - p ESI Full ms [100.00-2000.00]

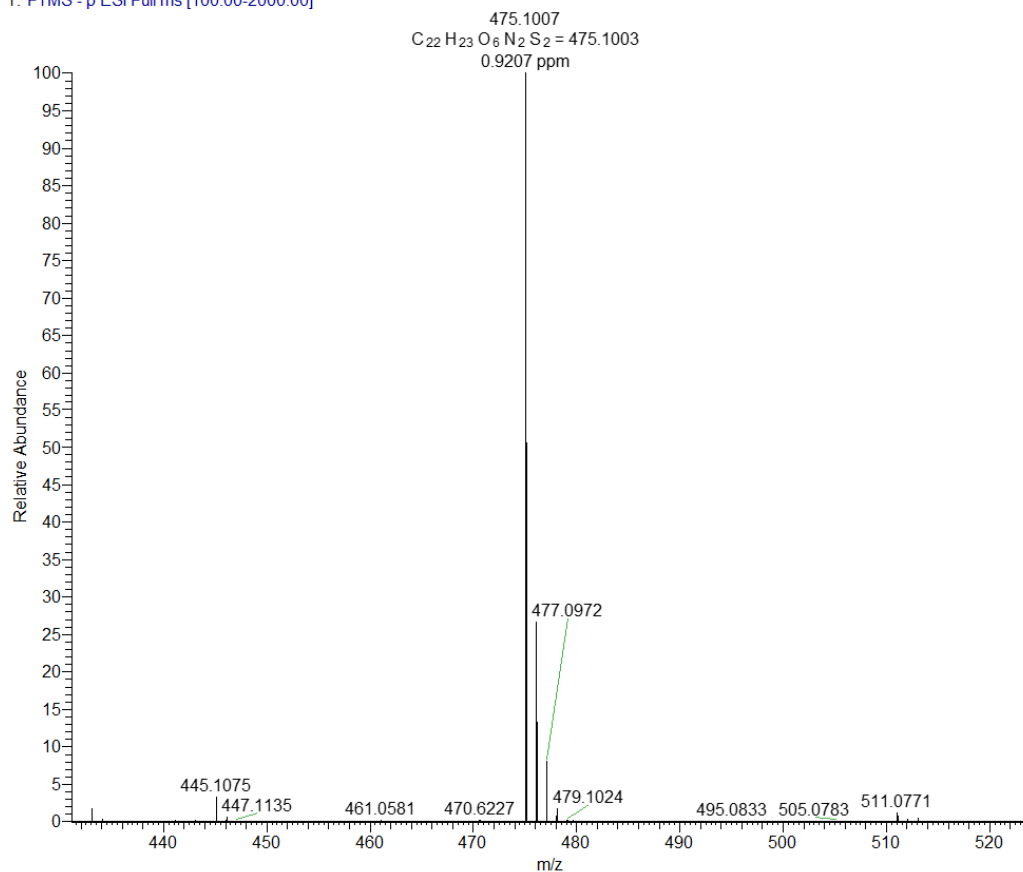


Figure S9. HRESIMS spectrum of compound 1

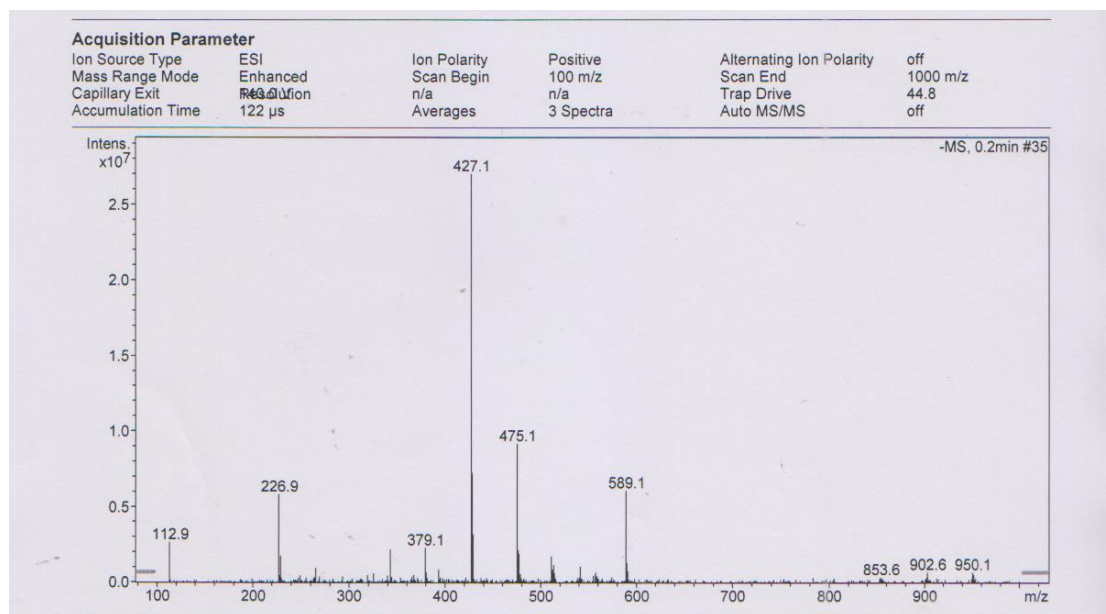


Figure S10. ESIMS spectrum of compound 1

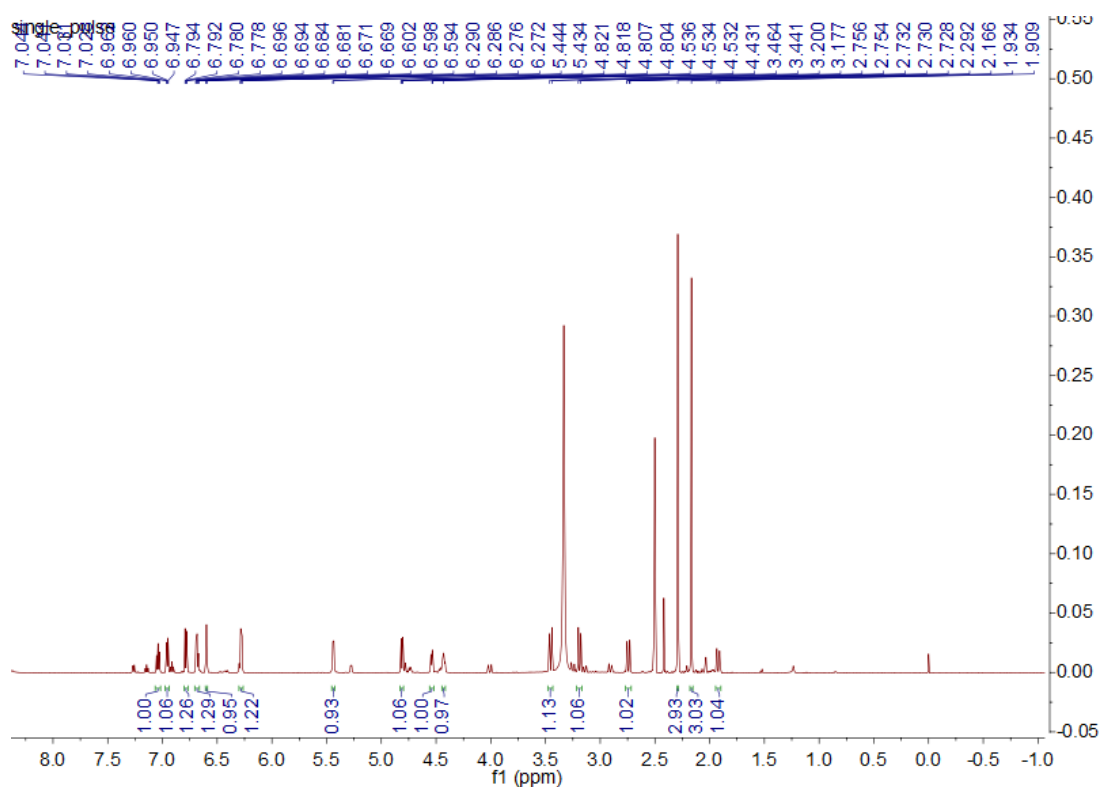


Figure S11. ^1H NMR (500 MHz, $\text{DMSO}-d_6$) spectrum of compound 2

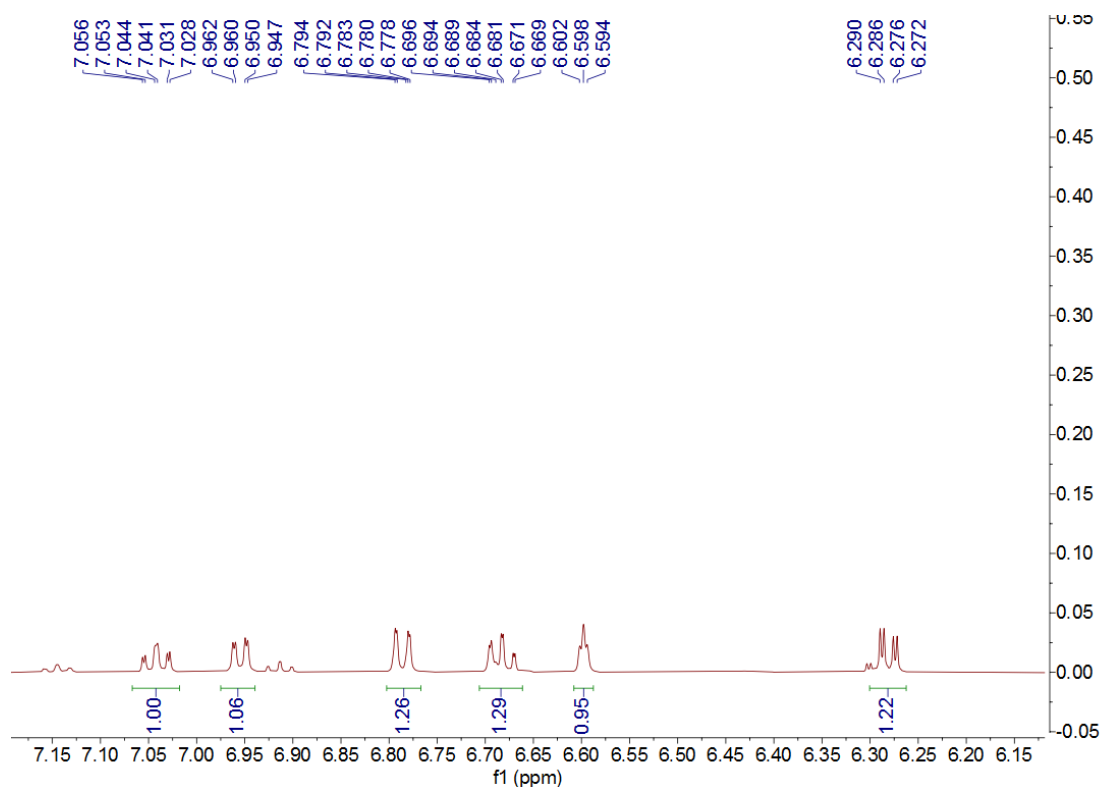


Figure S12. Partial ^1H NMR (500 MHz, $\text{DMSO}-d_6$) spectrum of compound 2

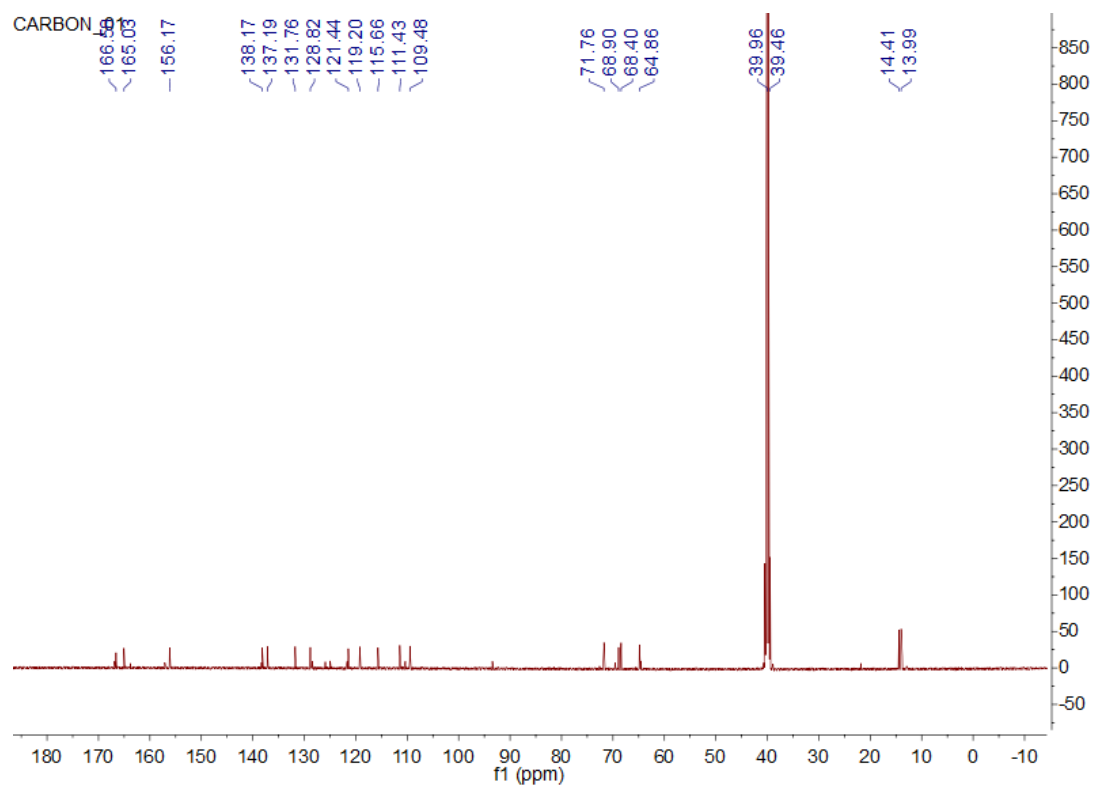


Figure S13. ^{13}C NMR (125 MHz, $\text{DMSO-}d_6$) spectrum of compound **2**

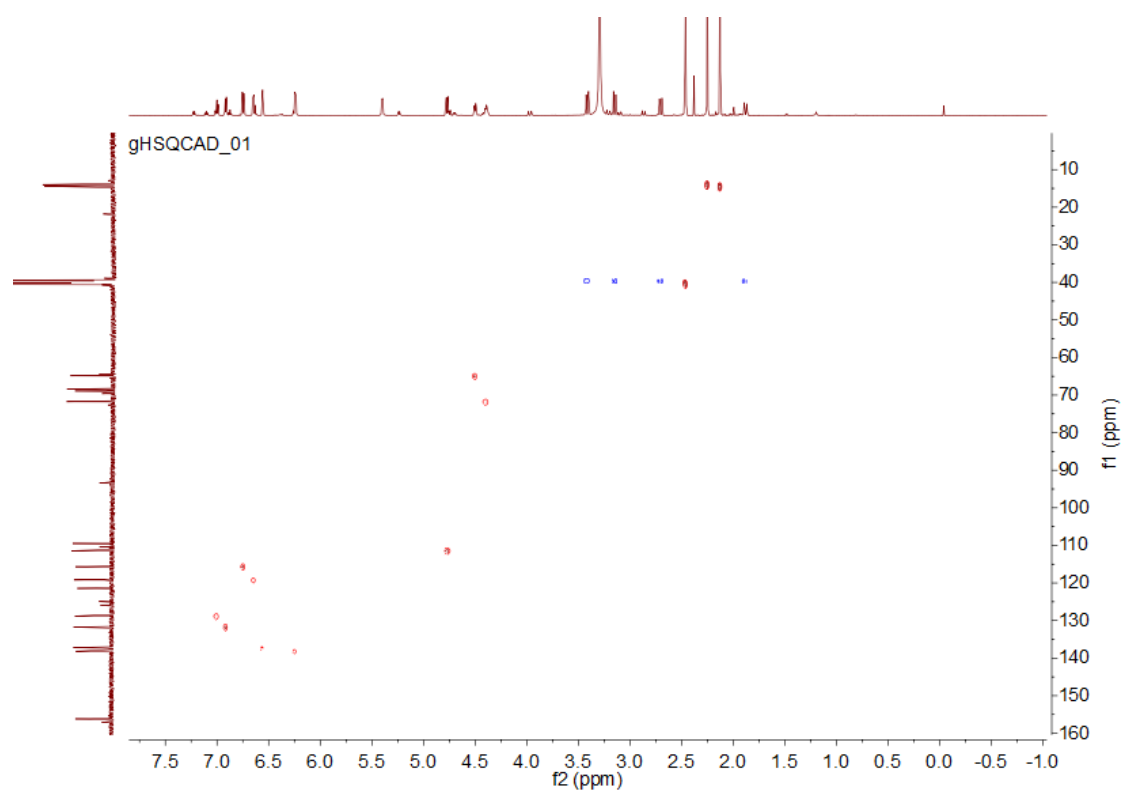


Figure S14. HSQC ($\text{DMSO-}d_6$) spectrum of compound **2**

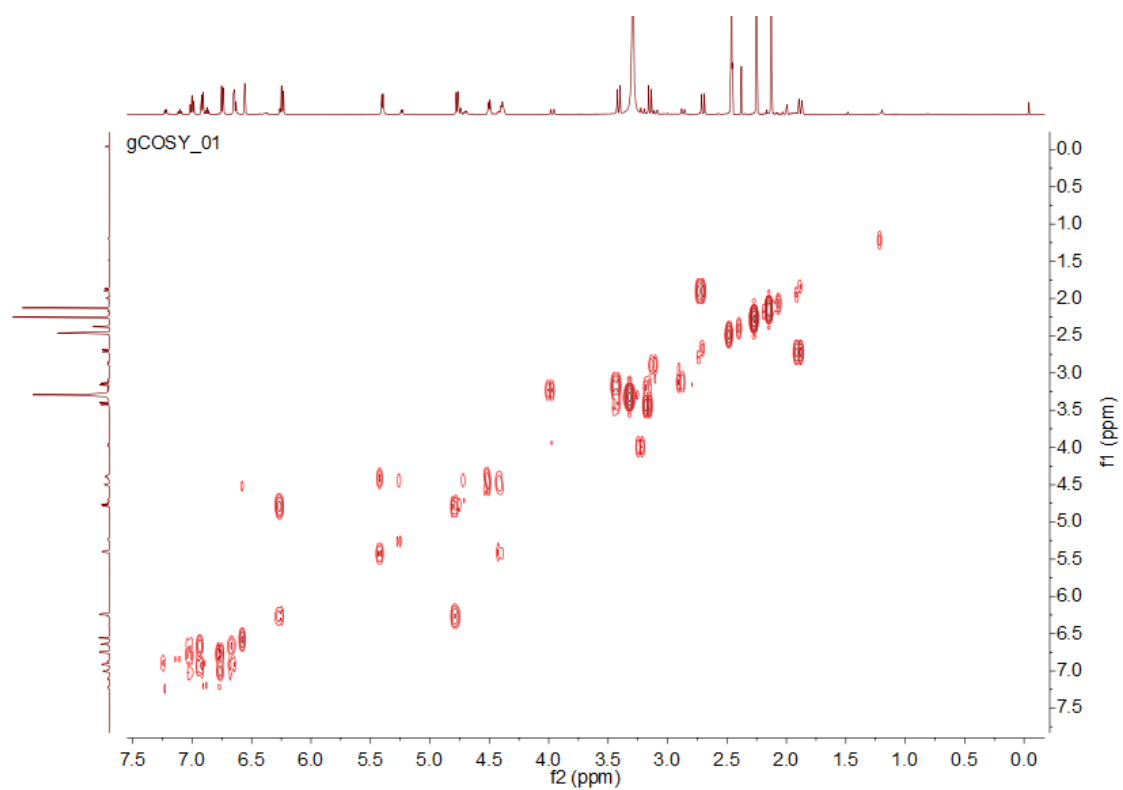


Figure S15. ^1H - ^1H COSY (DMSO- d_6) spectrum of compound **2**

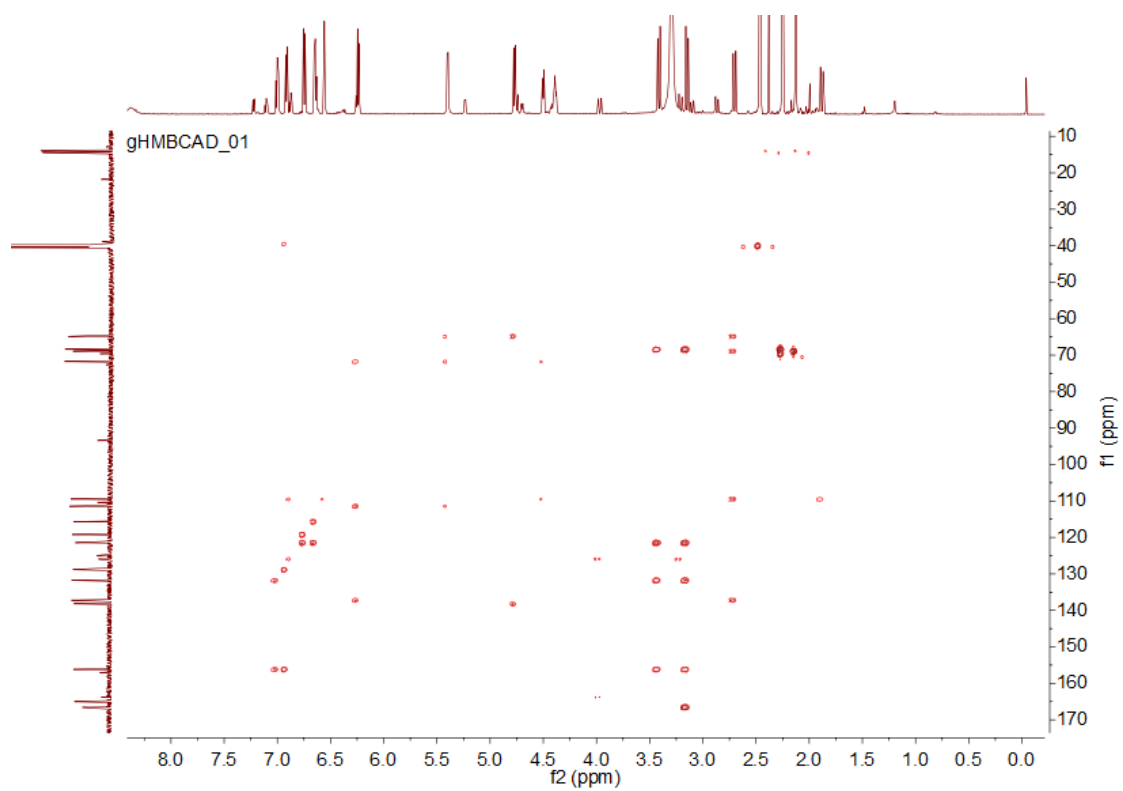


Figure S16. HMBC (DMSO- d_6) spectrum of compound **2**

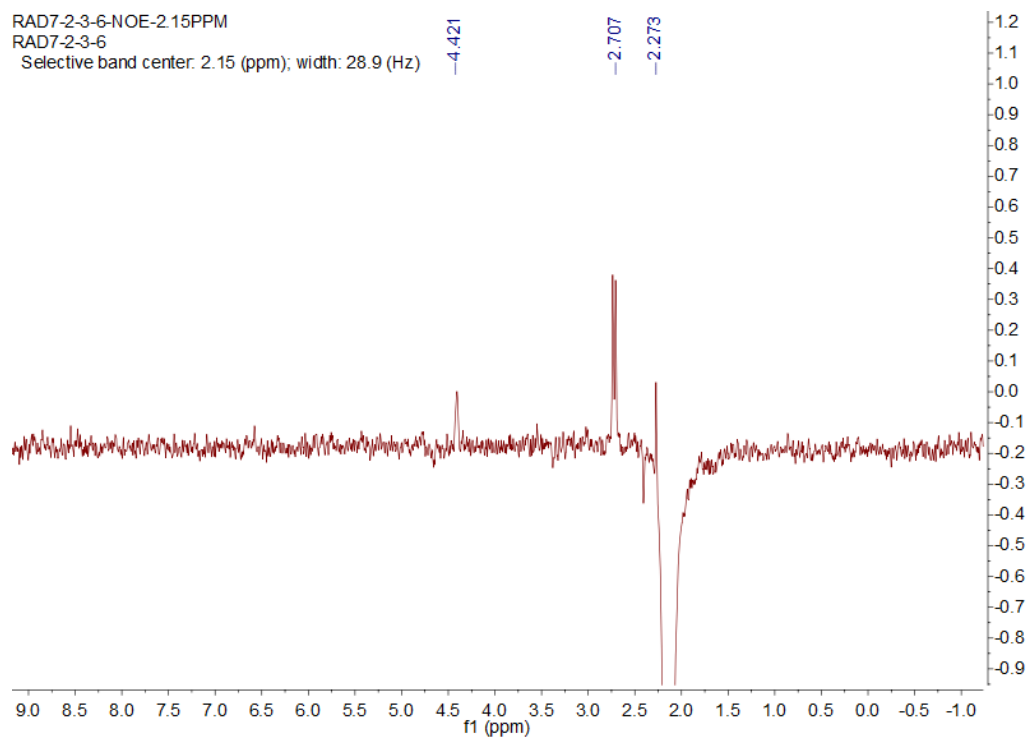


Figure S17. NOE (DMSO- d_6) spectrum of compound **2**

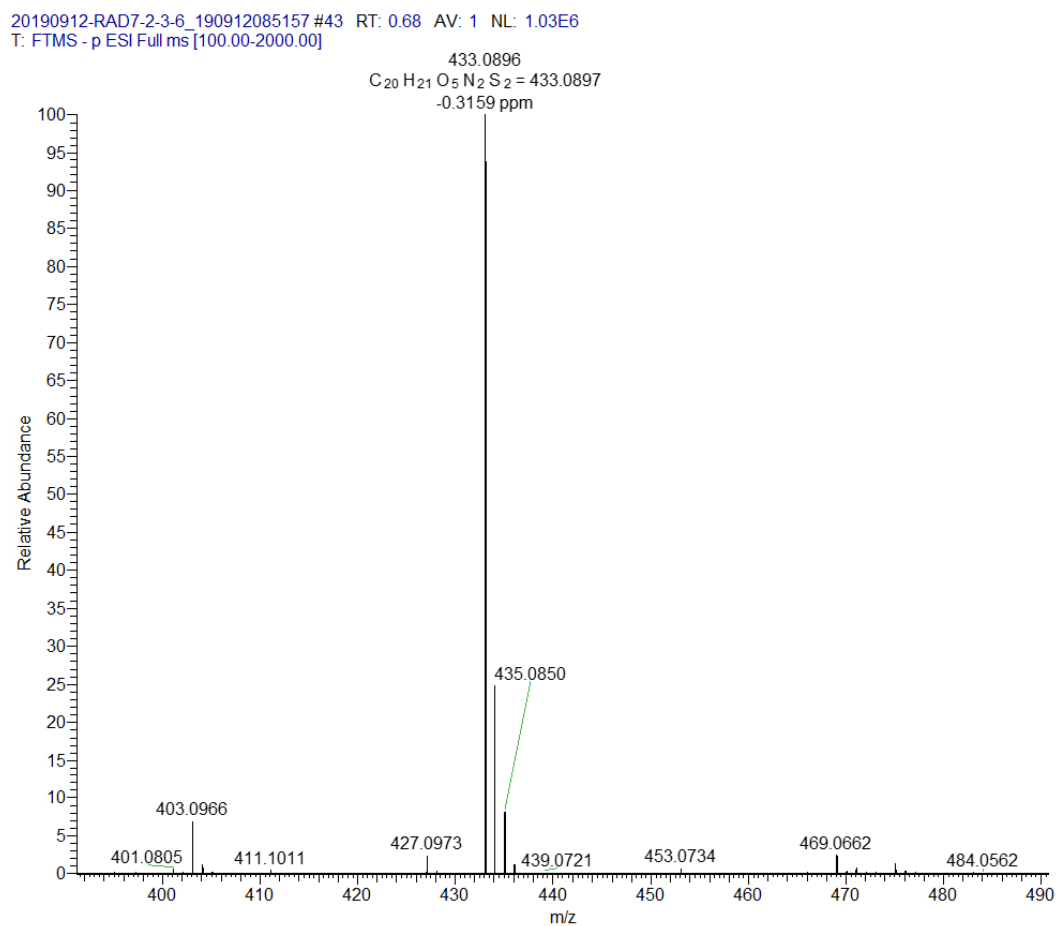


Figure S18. HRESIMS spectrum of compound **2**

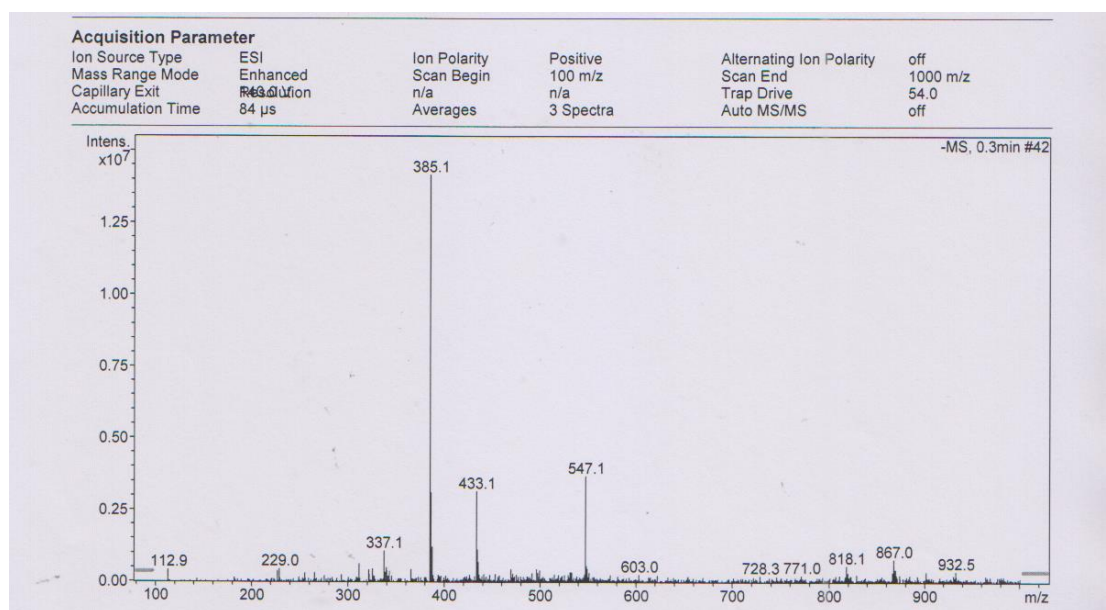


Figure S19. ESIMS spectrum of compound 2

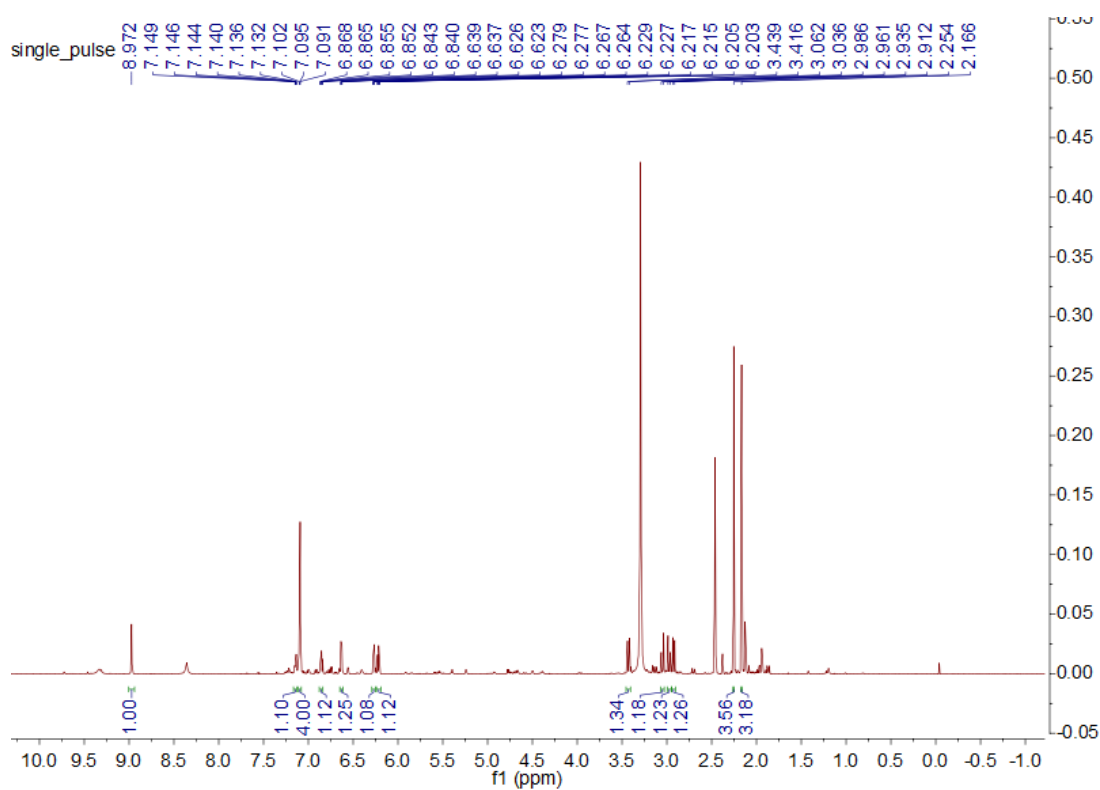


Figure S20. ¹H NMR (500 MHz, DMSO-*d*₆) spectrum of compound 3

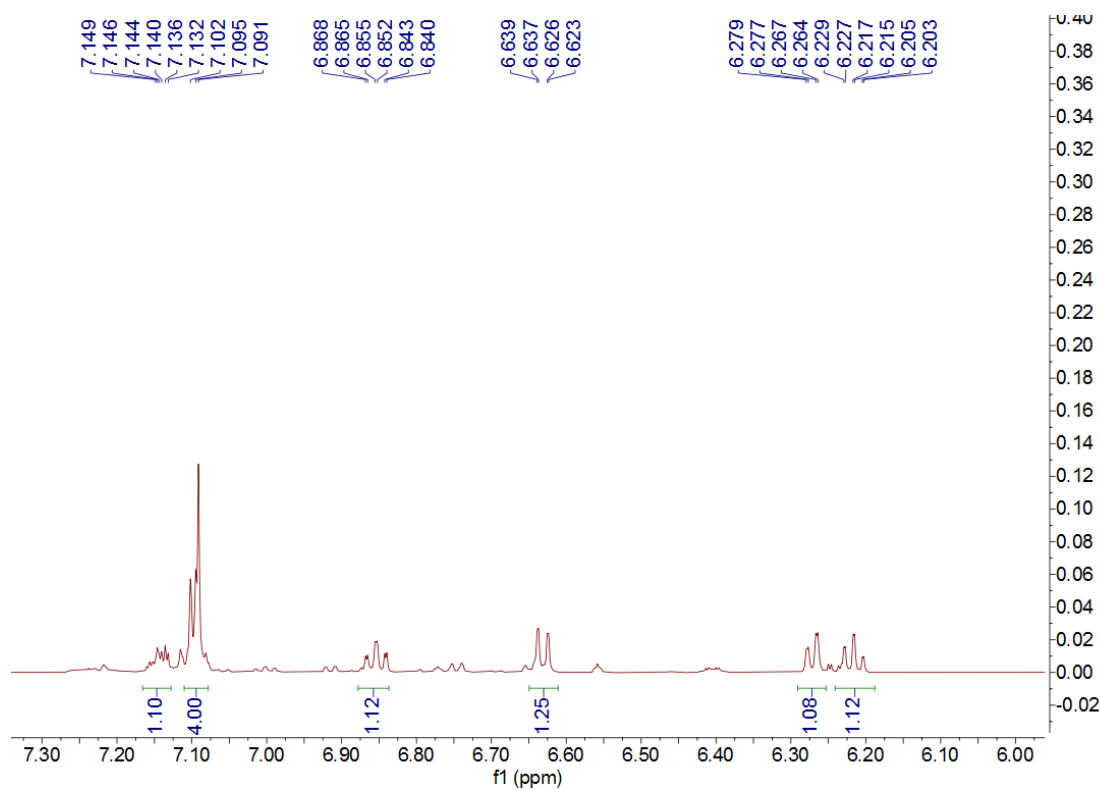


Figure S21. Partial ^1H NMR (500 MHz, $\text{DMSO-}d_6$) spectrum of compound **3**

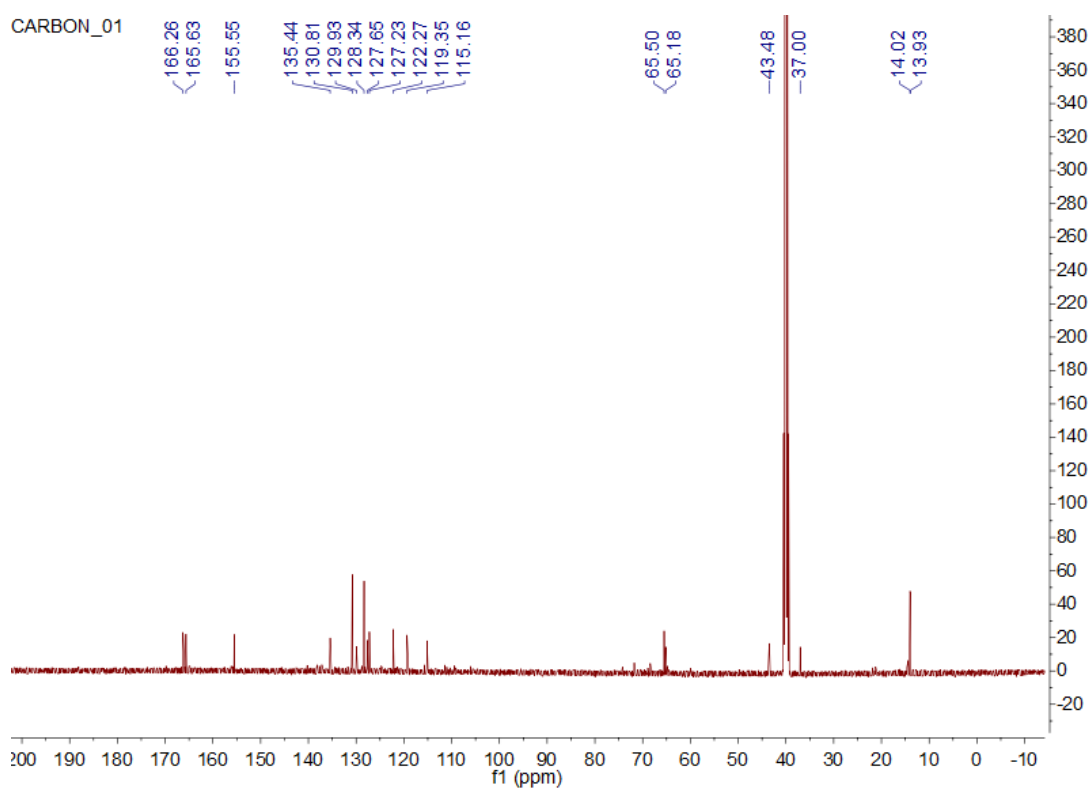


Figure S22. ^{13}C NMR (125 MHz, $\text{DMSO-}d_6$) spectrum of compound **3**

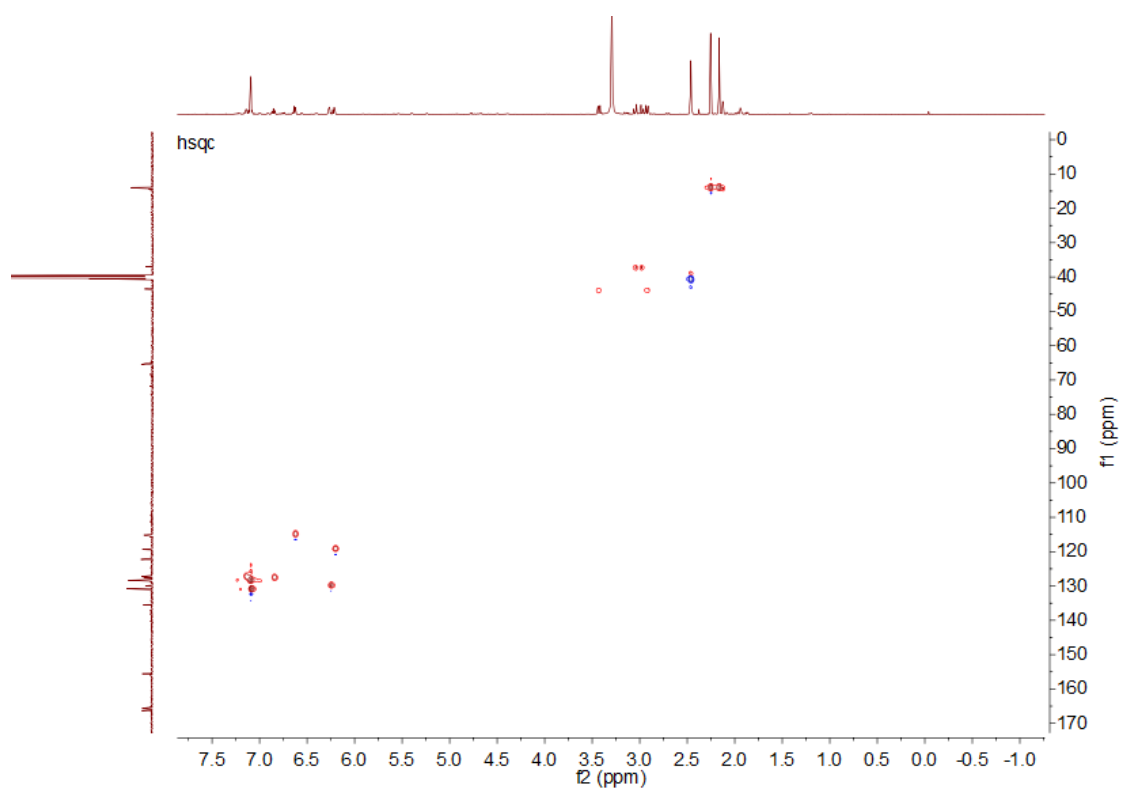


Figure S23. HSQC (DMSO- d_6) spectrum of compound **3**

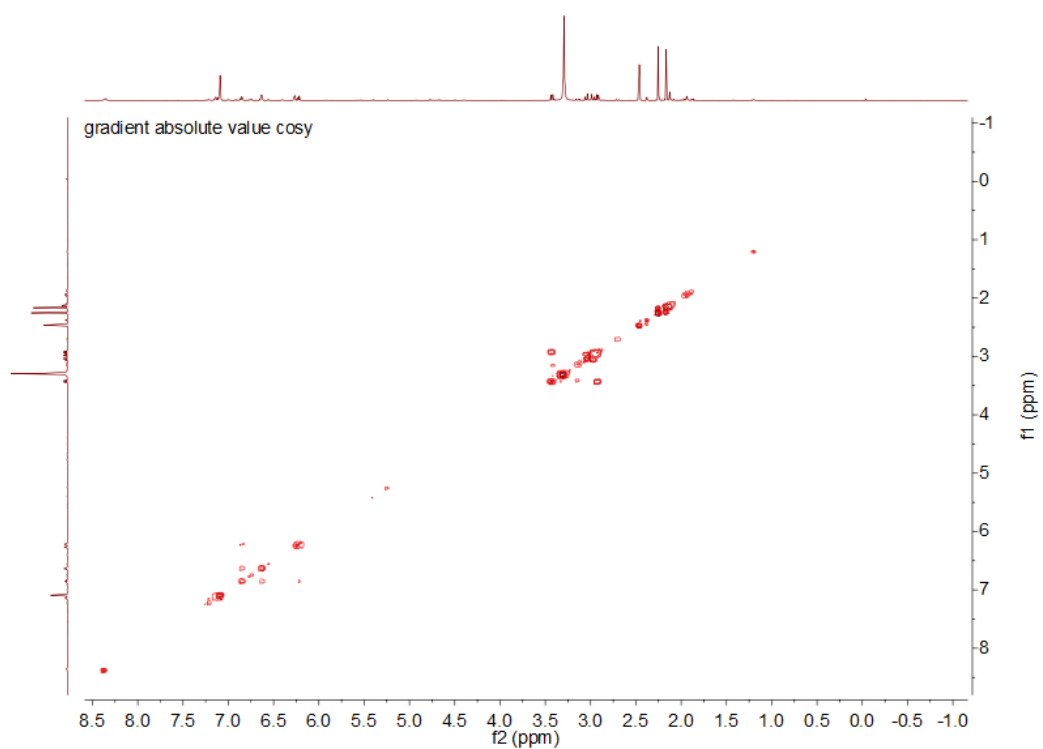


Figure S24. ^1H - ^1H COSY (DMSO- d_6) spectrum of compound **3**

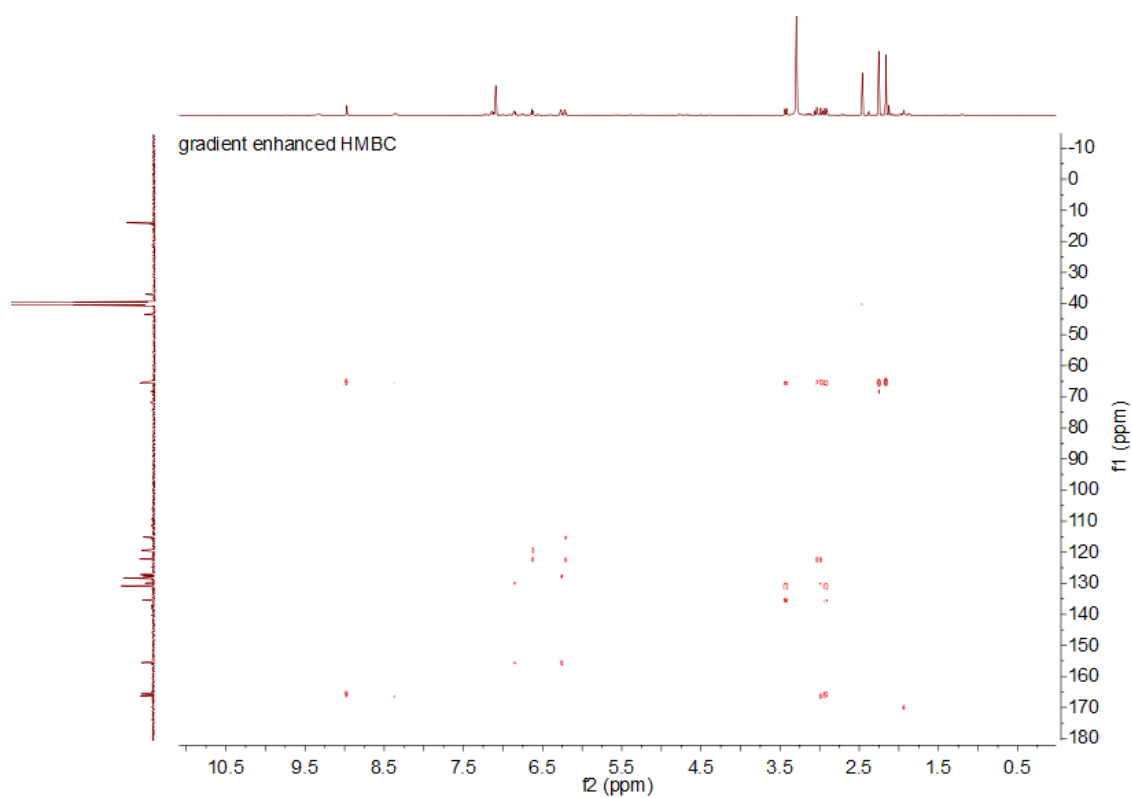


Figure S25. HMBC (DMSO- d_6) spectrum of compound **3**

20190912-RAD7-2-3-4_190912085157 #108-110 RT: 1.57-1.59 AV: 3 SB: 25 0.26-0.65 NL: 5.92E6
T: FTMS - p ESI Full ms [100.00-2000.00]

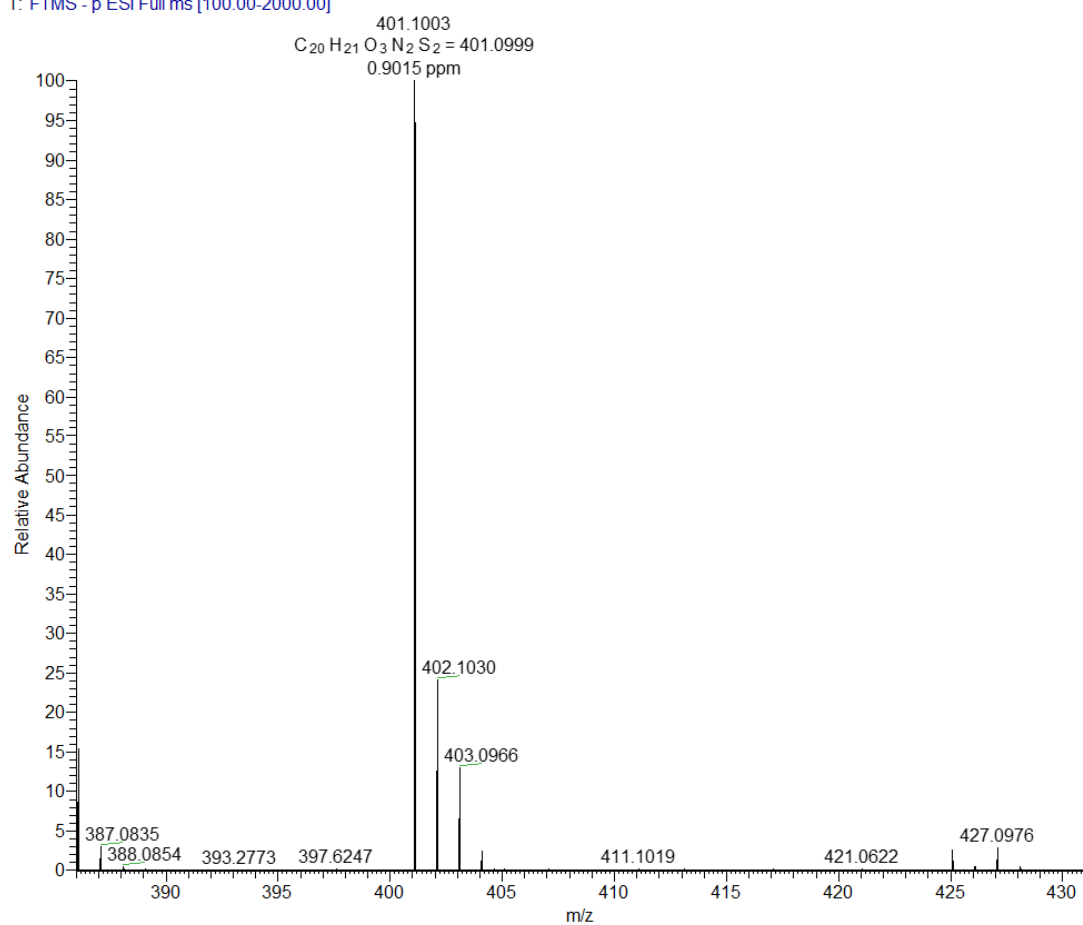


Figure S26. HRESIMS spectrum of compound **3**

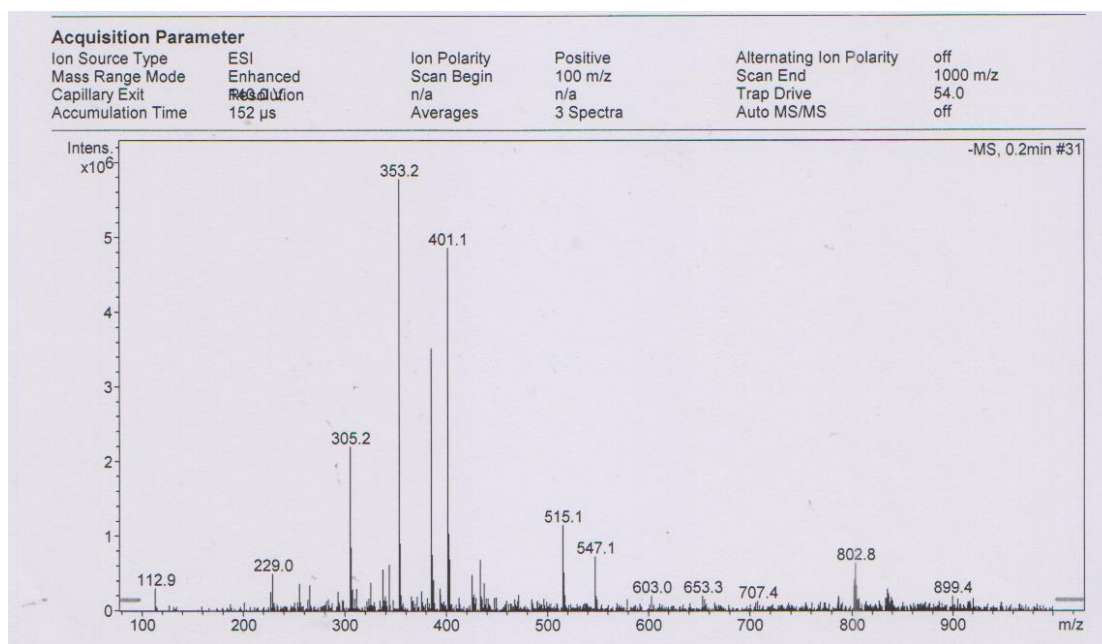


Figure S27. ESIMS spectrum of compound **3**

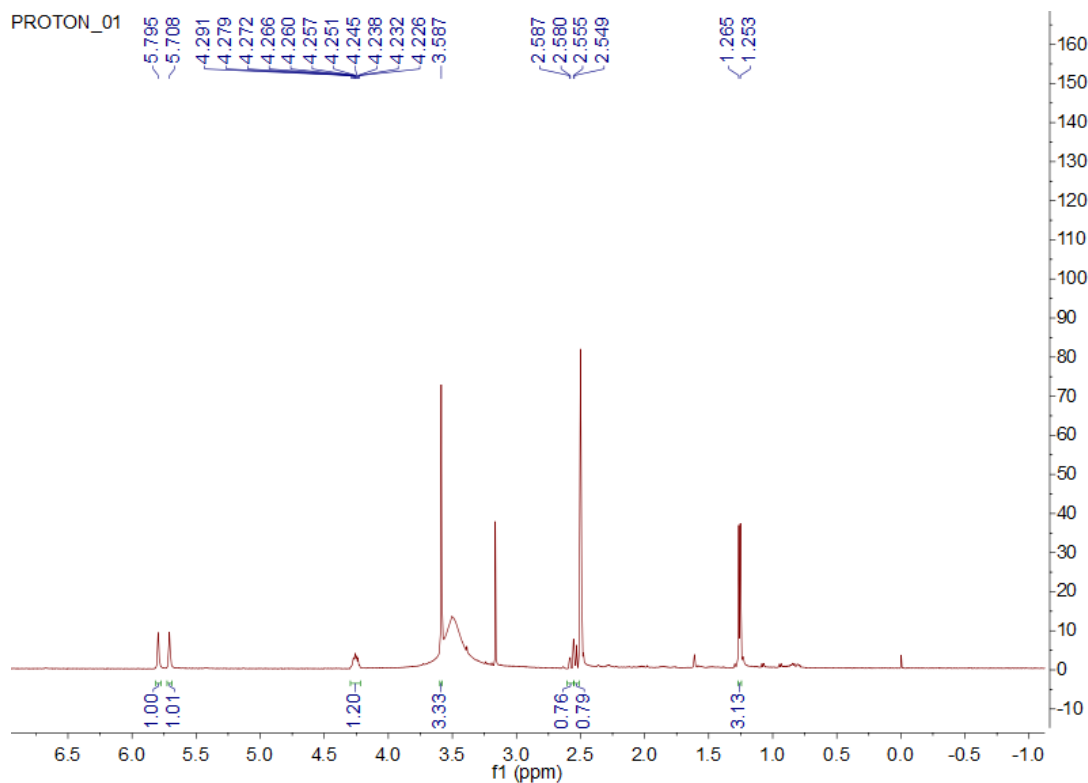


Figure S28. ^1H NMR (500 MHz, $\text{DMSO}-d_6$) spectrum of compound **8**

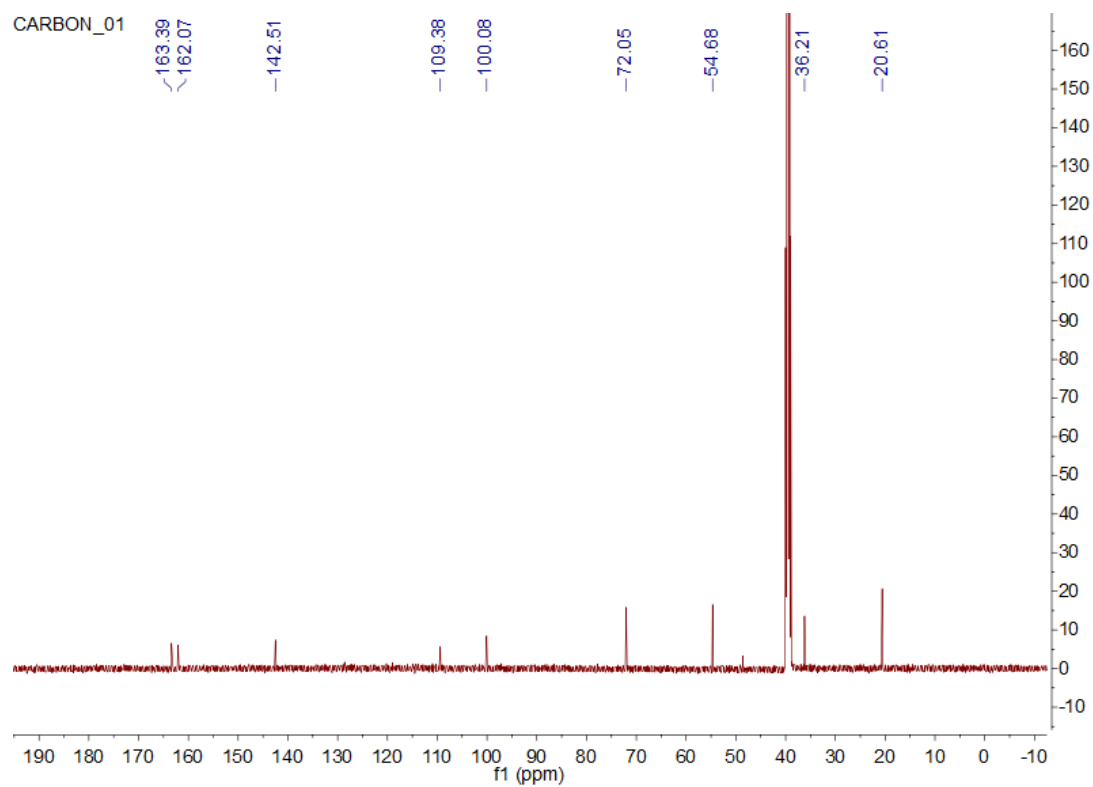


Figure S29. ^{13}C NMR (125MHz, $\text{DMSO}-d_6$) spectrum of compound **8**

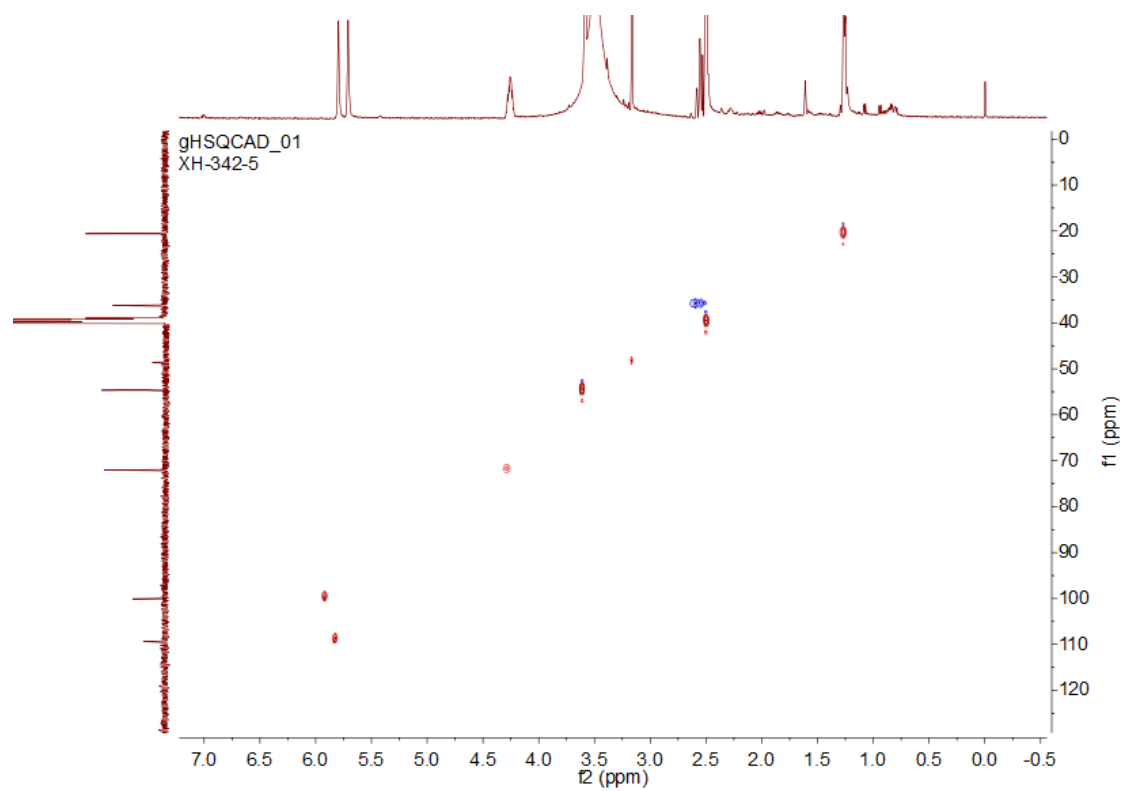


Figure S30. HSQC ($\text{DMSO}-d_6$) spectrum of compound **8**

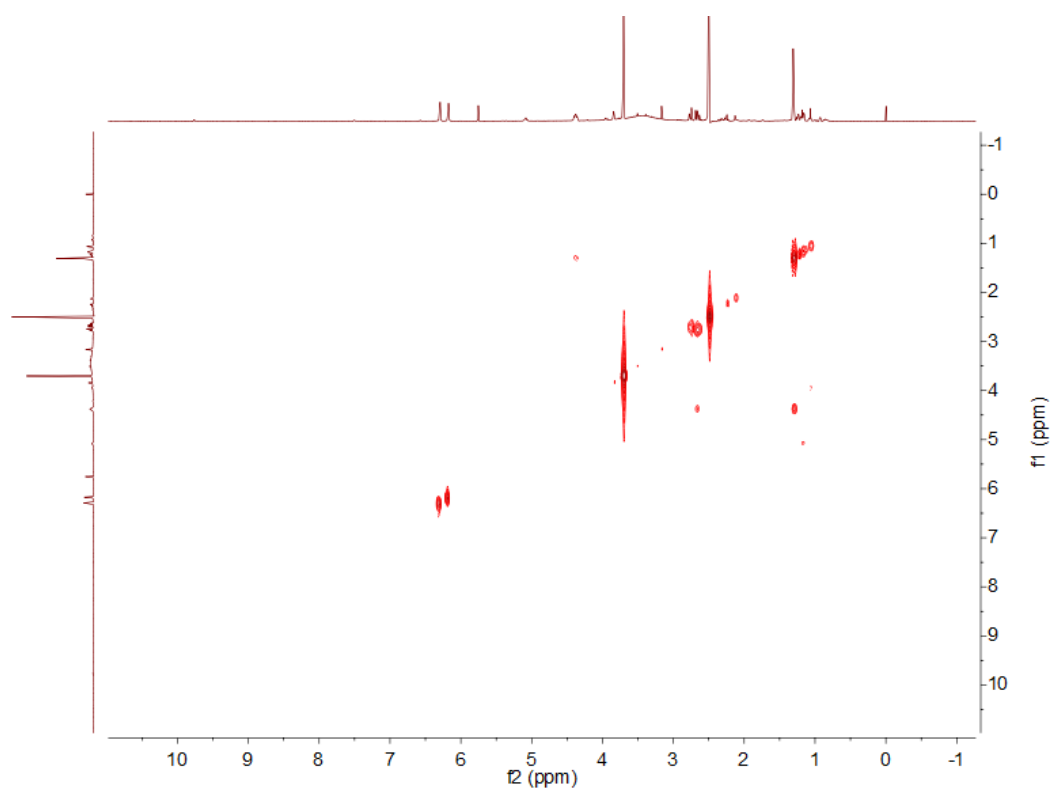


Figure S31. ^1H - ^1H COSY (DMSO- d_6) spectrum of compound **8**

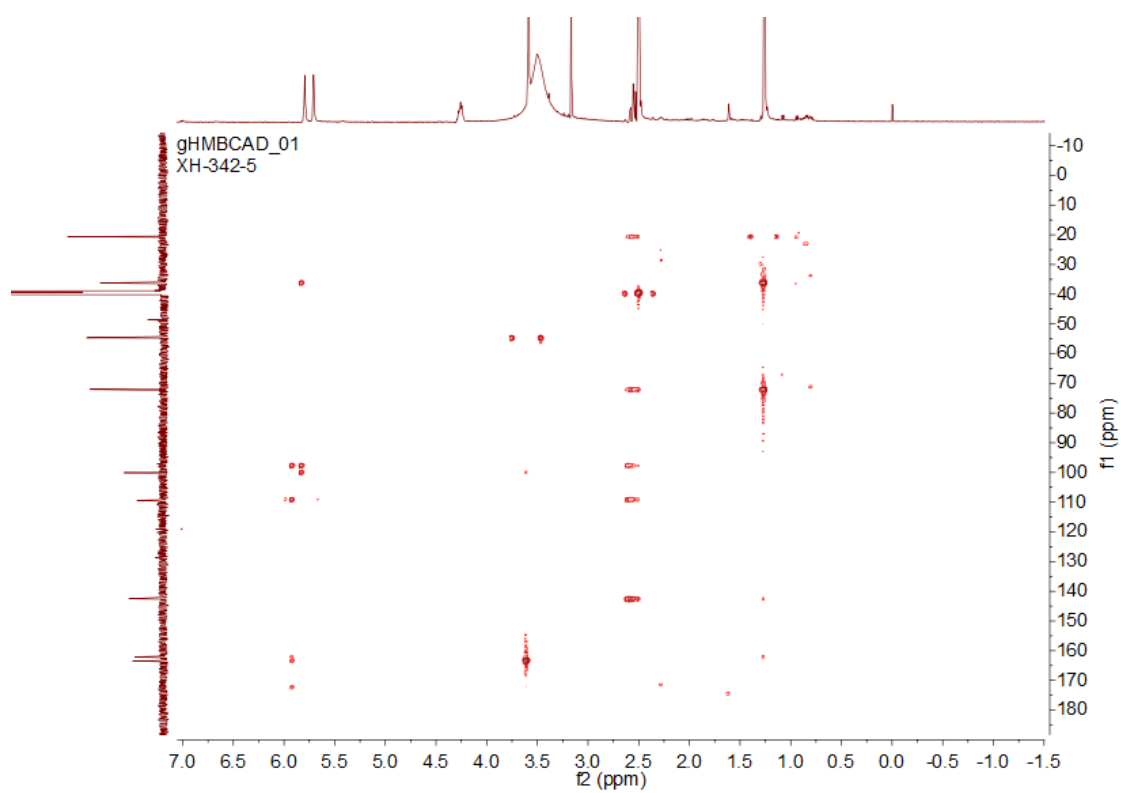


Figure S32. HMBC (DMSO- d_6) spectrum of compound **8**

20180704-XH-3425_180704113343#42 RT: 0.34 AV: 1 NL: 2.08E7
T: FTMS + p ESI Full ms [100.00-2000.00]

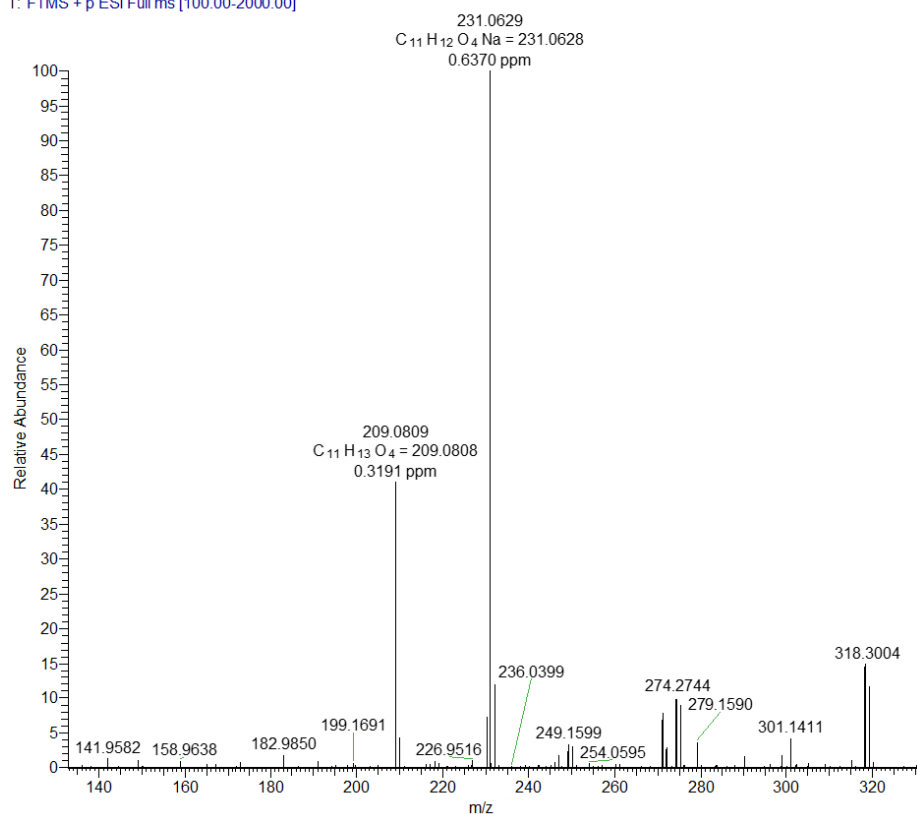


Figure S33. HRESIMS spectrum of compound **8**

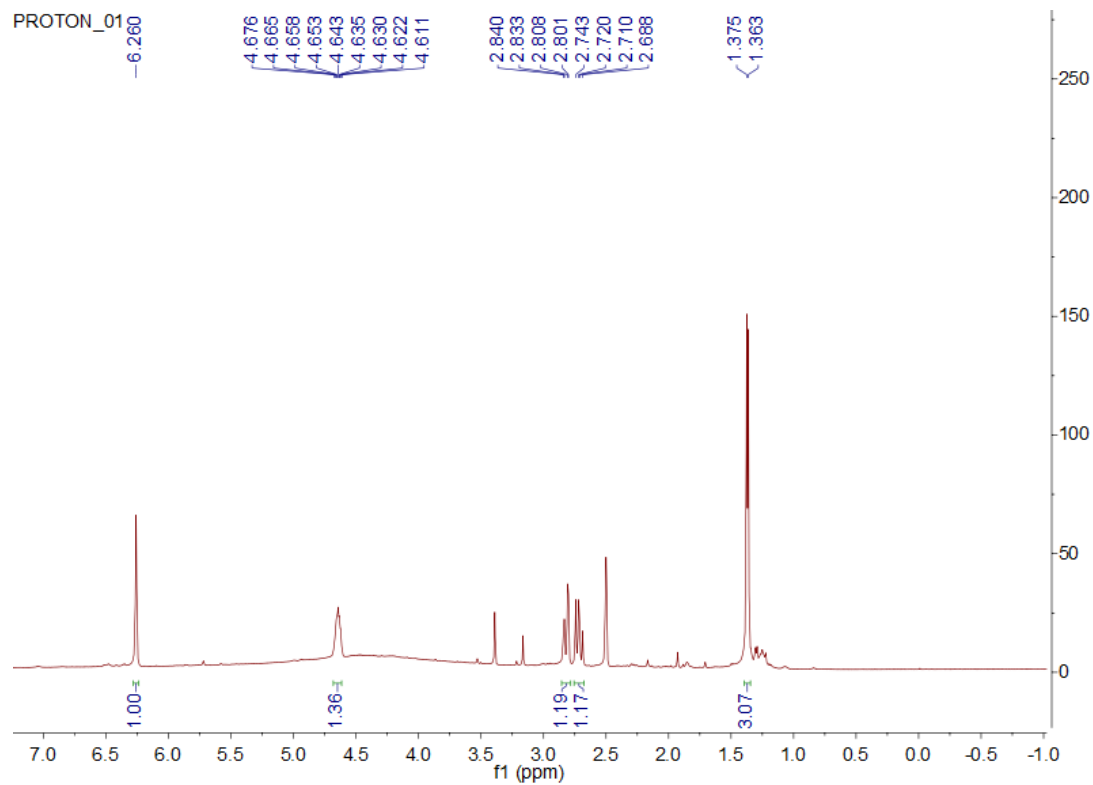


Figure S34. ¹H NMR (500 MHz, DMSO-*d*₆) spectrum of compound **9**

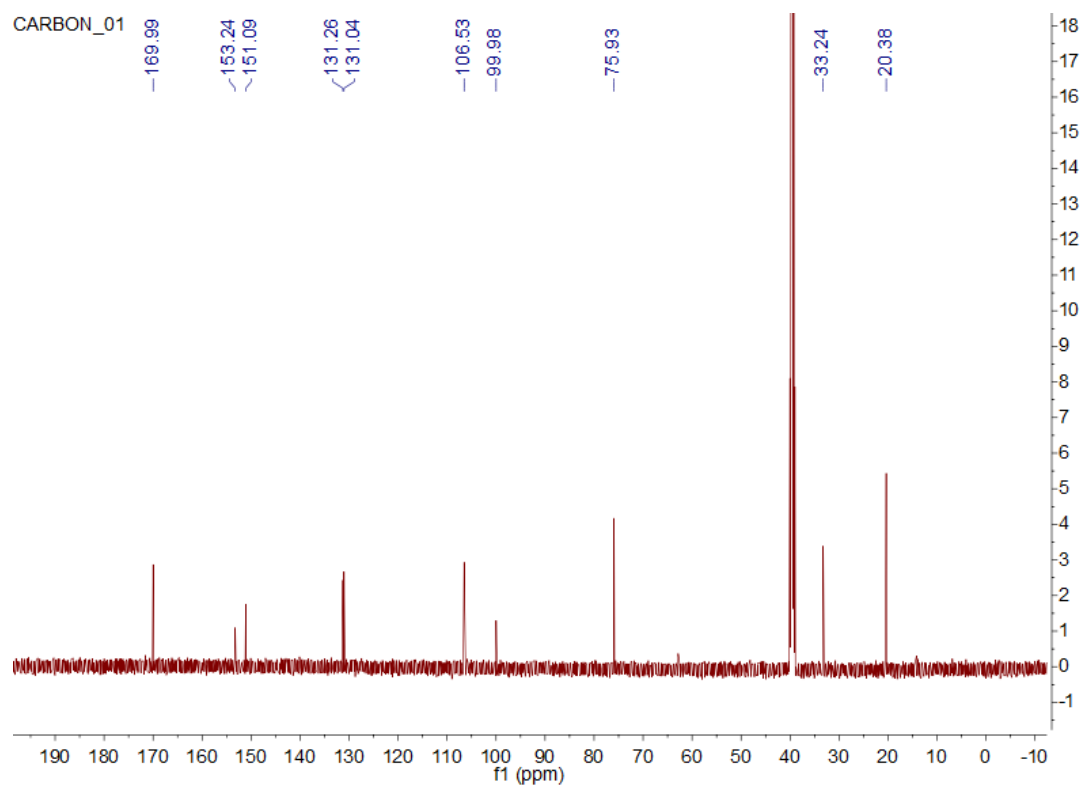


Figure S35. ^{13}C NMR (125MHz, $\text{DMSO}-d_6$) spectrum of compound **9**

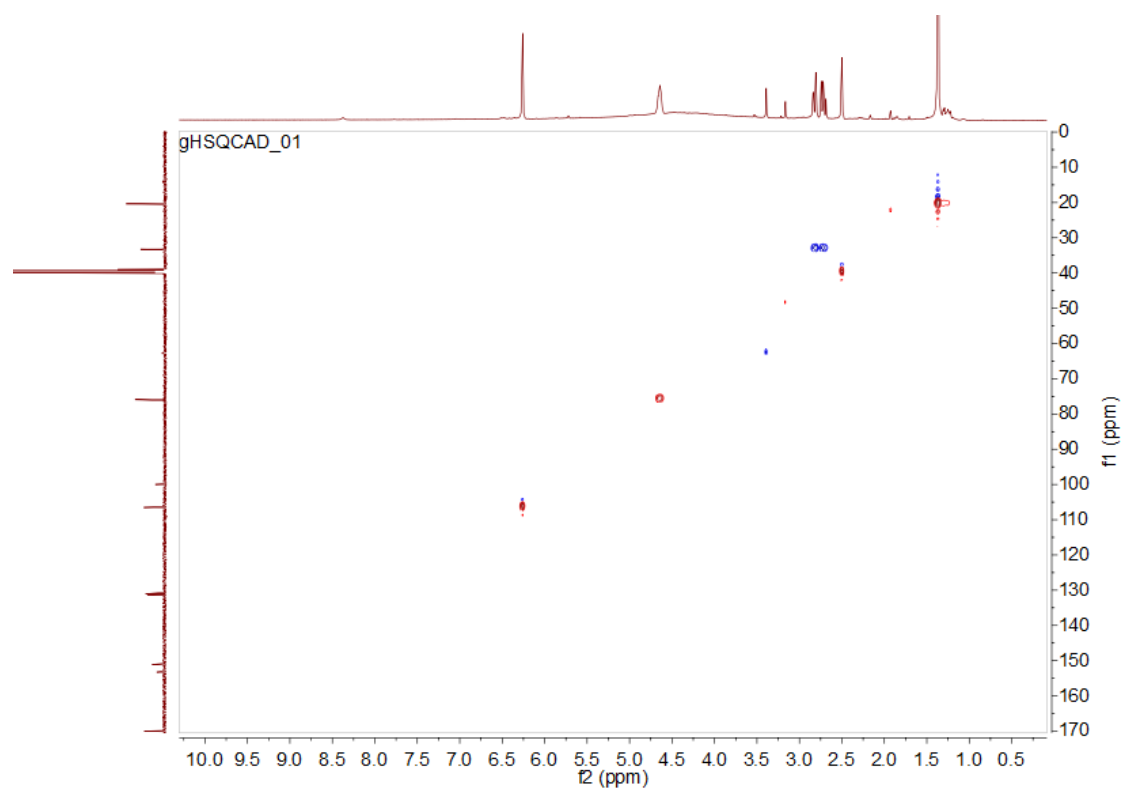


Figure S36. HSQC ($\text{DMSO}-d_6$) spectrum of compound **9**

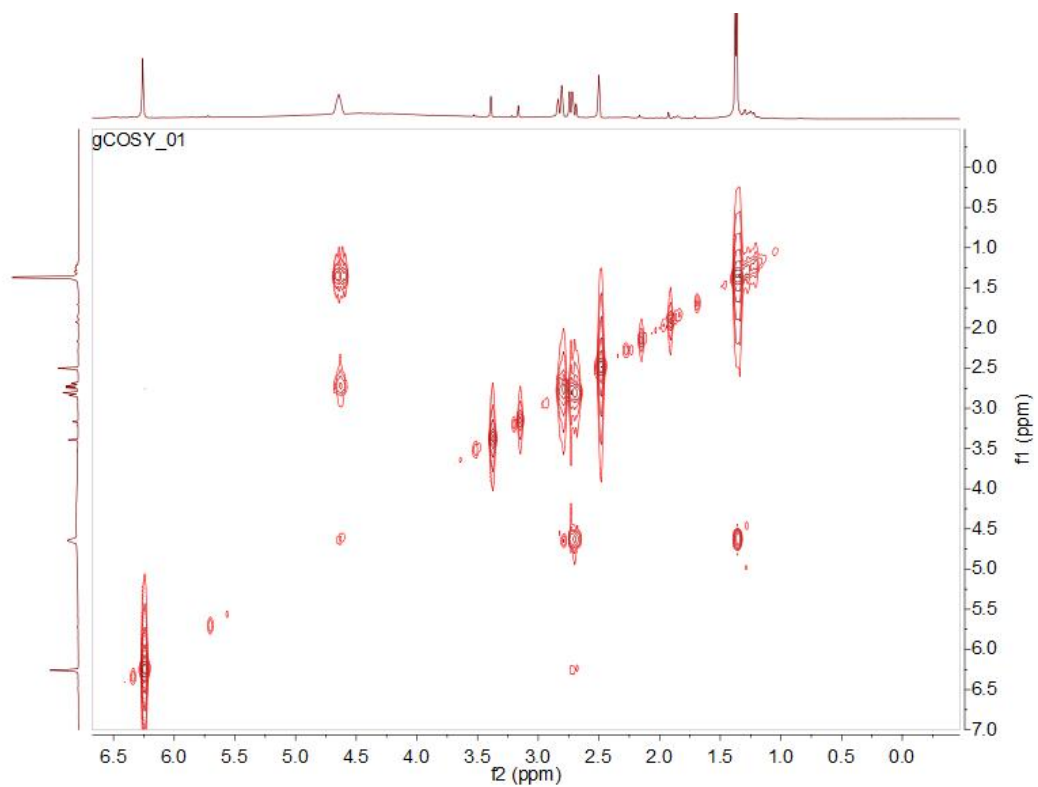


Figure S37. ^1H - ^1H COSY (DMSO- d_6) spectrum of compound **9**

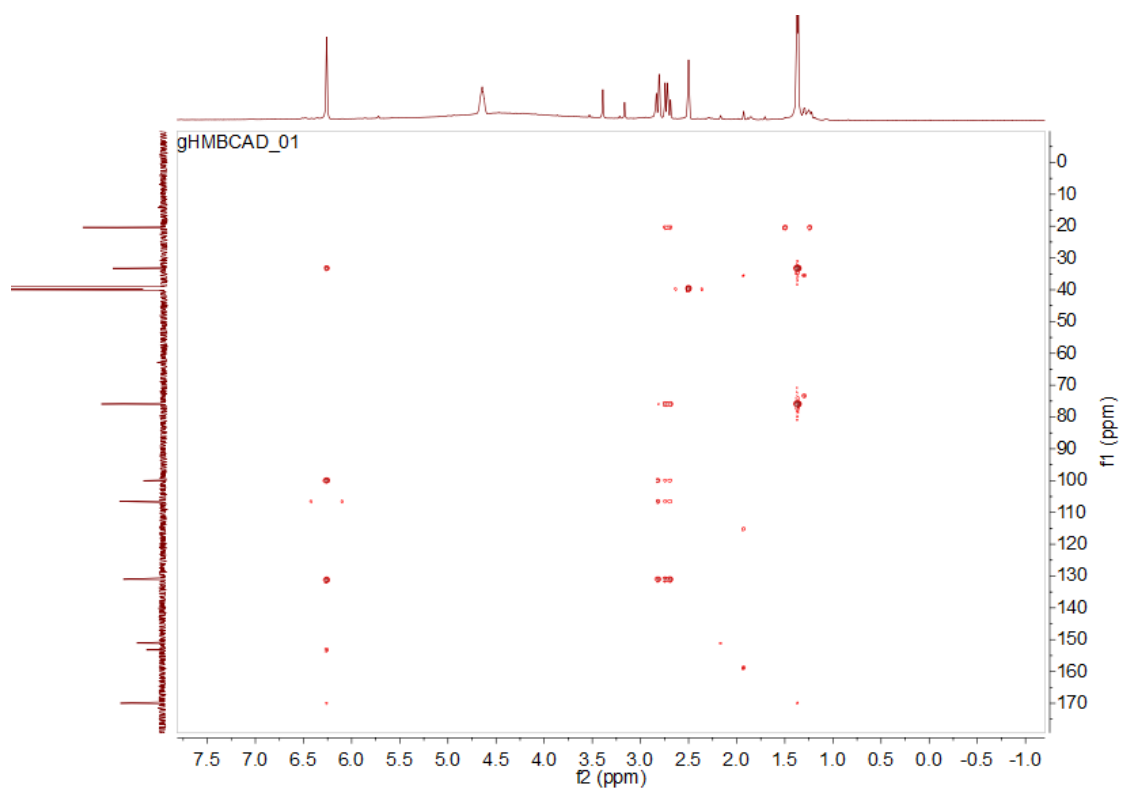


Figure S38. HMBC (DMSO- d_6) spectrum of compound **9**

201812045-XH-2253-1_181205084117 #111-114 RT: 1.22-1.26 AV: 4 SB: 12 0.04-0.18 NL: 6.31E5
T: FTMS - p ESI Full ms [150.00-1000.00]

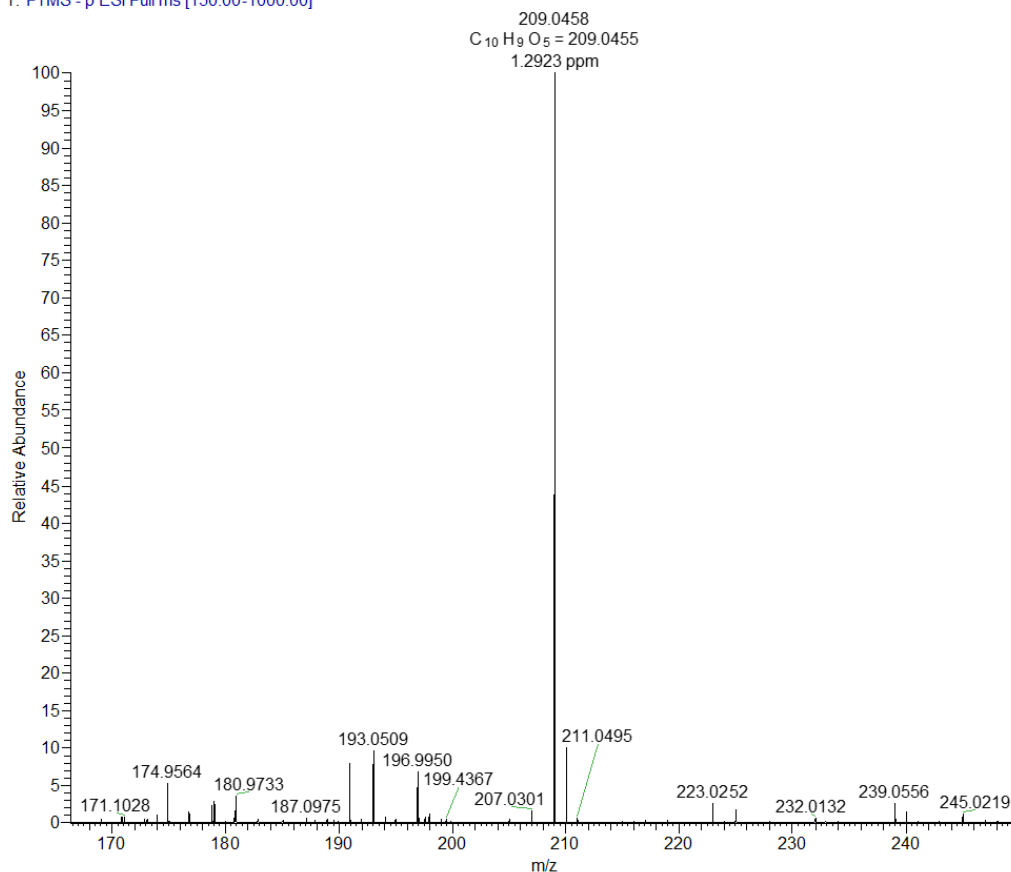


Figure S39. HRESIMS spectrum of compound **9**

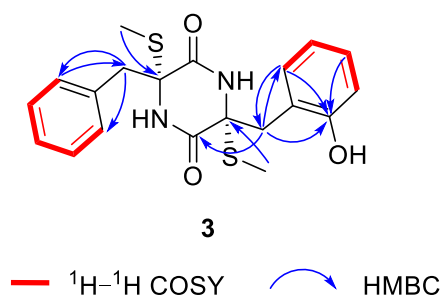


Figure S40. Key HMBC correlations of compound **3**

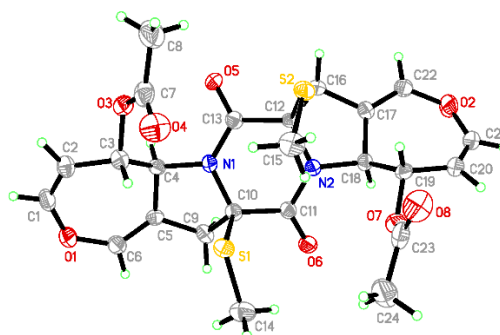


Figure S41. Crystal diagram of compound **6** (CCDC:1911625)

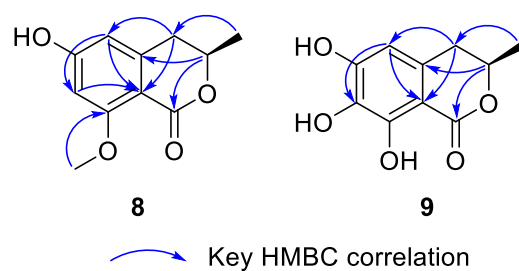


Figure S42. Key HMBC correlations of compounds **8** and **9**

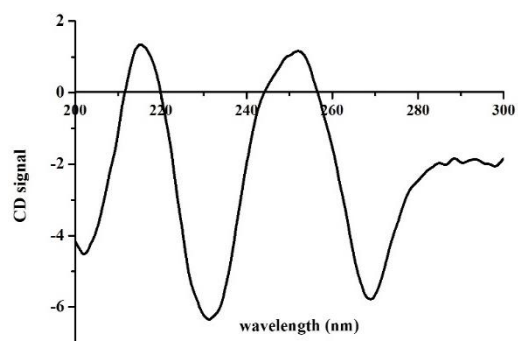


Figure S43. The CD spectrum of compound **8**

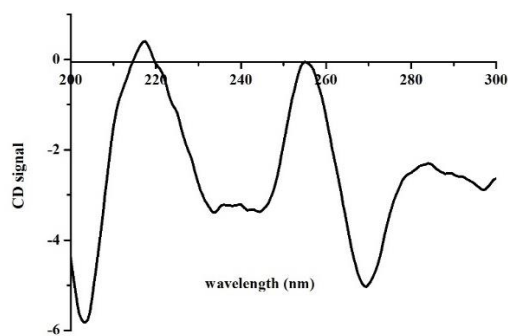


Figure S44. The CD spectrum of compound **9**