



Supporting Information

for

Non-peptide compounds from *Kronopolites svenhedini* (Verhoeff) and their antitumor and iNOS inhibitory activities

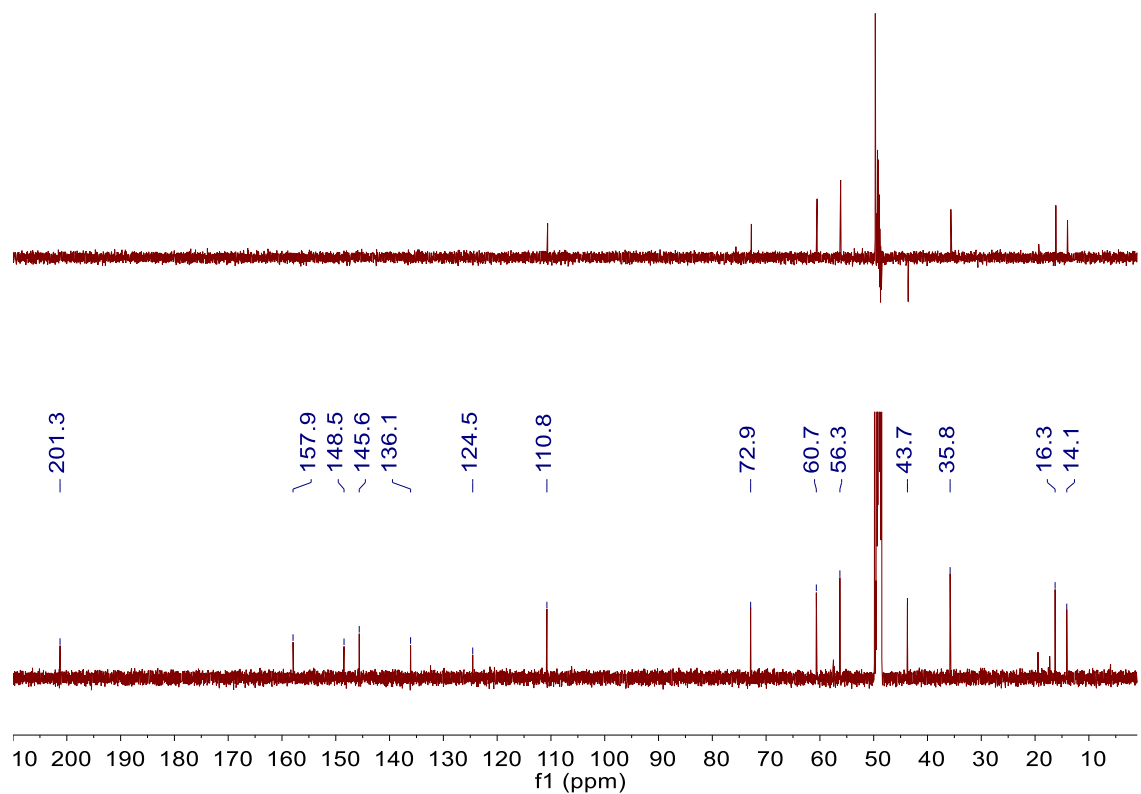
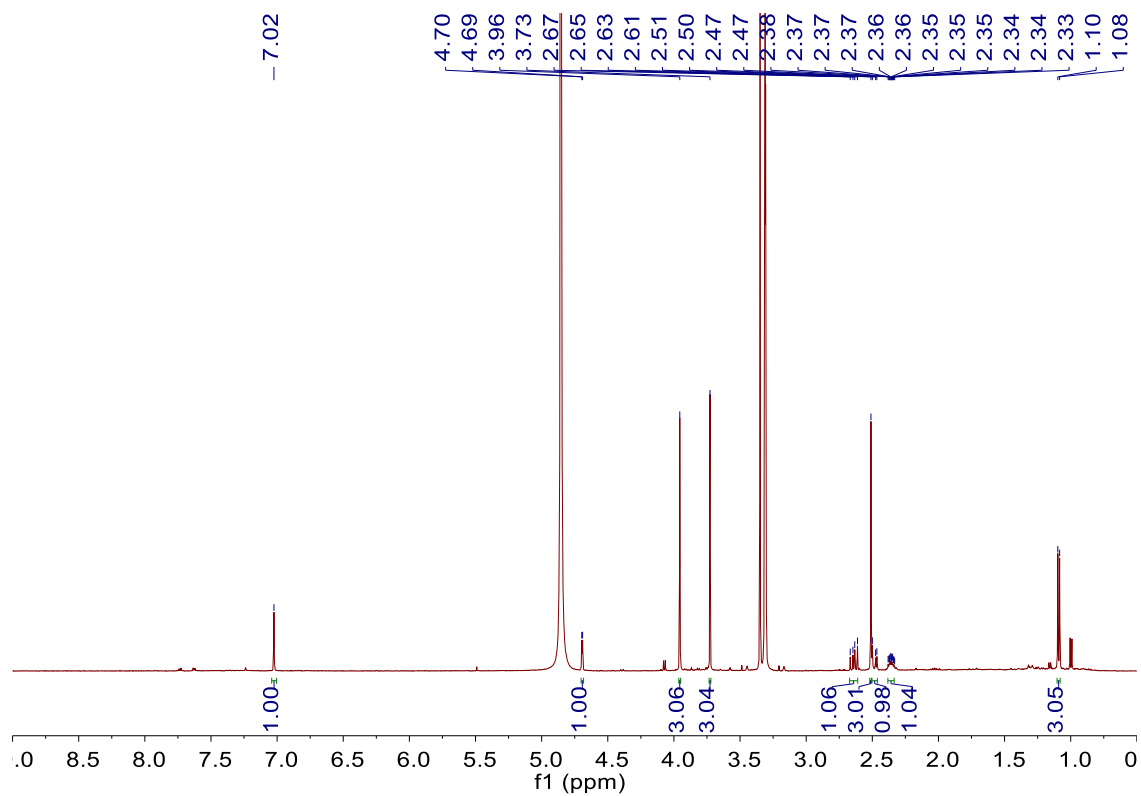
Yuan-Nan Yuan, Jin-Qiang Li, Hong-Bin Fang, Shao-Jun Xing, Yong-Ming Yan
and Yong-Xian Cheng

Beilstein J. Org. Chem. **2023**, 19, 789–799. doi:10.3762/bjoc.19.59

NMR, HRESIMS, and CD spectra for new compounds and the figures of antitumor activity assay of CD8⁺ T cells in vitro

Table of contents

Figure S1. ^1H NMR spectrum of 1 in methanol- d_4
Figure S2. ^{13}C NMR and DEPT spectrum of 1 in methanol- d_4
Figure S3. ^1H - ^1H COSY spectrum of 1 in methanol- d_4
Figure S4. HSQC spectrum of 1 in methanol- d_4
Figure S5. HMBC spectrum of 1 in methanol- d_4
Figure S6. HRESIMS spectrum of 1
Figure S7. CD spectrum of 1 in MeOH
Figure S8. ^1H NMR spectrum of 2 in methanol- d_4
Figure S9. ^{13}C NMR and DEPT spectrum of 2 in methanol- d_4
Figure S10. ^1H - ^1H COSY spectrum of 2 in methanol- d_4
Figure S10. HSQC spectrum of 2 in methanol- d_4
Figure S12. HMBC spectrum of 2 in methanol- d_4
Figure S13. HRESIMS spectrum of 2
Figure S14. ^1H NMR spectrum of 3 in methanol- d_4
Figure S15. ^{13}C NMR and DEPT spectrum of 3 in methanol- d_4
Figure S16. ^1H - ^1H COSY spectrum of 3 in methanol- d_4
Figure S17. HSQC spectrum of 3 in methanol- d_4
Figure S18. HMBC spectrum of 3 in methanol- d_4
Figure S19. HRESIMS spectrum of 3
Figure S20. ^1H NMR spectrum of 4 in methanol- d_4
Figure S21. ^{13}C NMR and DEPT spectrum of 4 in methanol- d_4
Figure S22. ^1H - ^1H COSY spectrum of 4 in methanol- d_4
Figure S23. HSQC spectrum of 4 in methanol- d_4
Figure S24. HMBC spectrum of 4 in methanol- d_4
Figure S25. HRESIMS spectrum of 4
Figure S26. CD spectrum of 4 in MeOH
Figure S27. ^1H NMR spectrum of 7 in methanol- d_4
Figure S28. ^{13}C NMR and DEPT spectrum of 7 in methanol- d_4
Figure S29. ^1H - ^1H COSY spectrum of 7 in methanol- d_4
Figure S30. HSQC spectrum of 7 in methanol- d_4
Figure S31. HMBC spectrum of 7 in methanol- d_4
Figure S32. ROESY spectrum of 7 in methanol- d_4
Figure S33. HRESIMS spectrum of 7
Figure S34. ^1H NMR spectrum of 8 in methanol- d_4
Figure S35. ^{13}C NMR and DEPT spectrum of 8 in methanol- d_4
Figure S36. ^1H - ^1H COSY spectrum of 8 in methanol- d_4
Figure S37. HSQC spectrum of 8 in methanol- d_4
Figure S38. HMBC spectrum of 8 in methanol- d_4
Figure S39. ROESY spectrum of 8 in methanol- d_4
Figure S40. HRESIMS spectrum of 8
Figure S41. Compounds inhibited cell proliferation of Panc02-h7-GP-GFP cells.
Figure S42. Purification of CD8 ⁺ T cells in vitro.
Figure S43. Compounds affected the antitumor activity of CD8 ⁺ T cells in vitro.



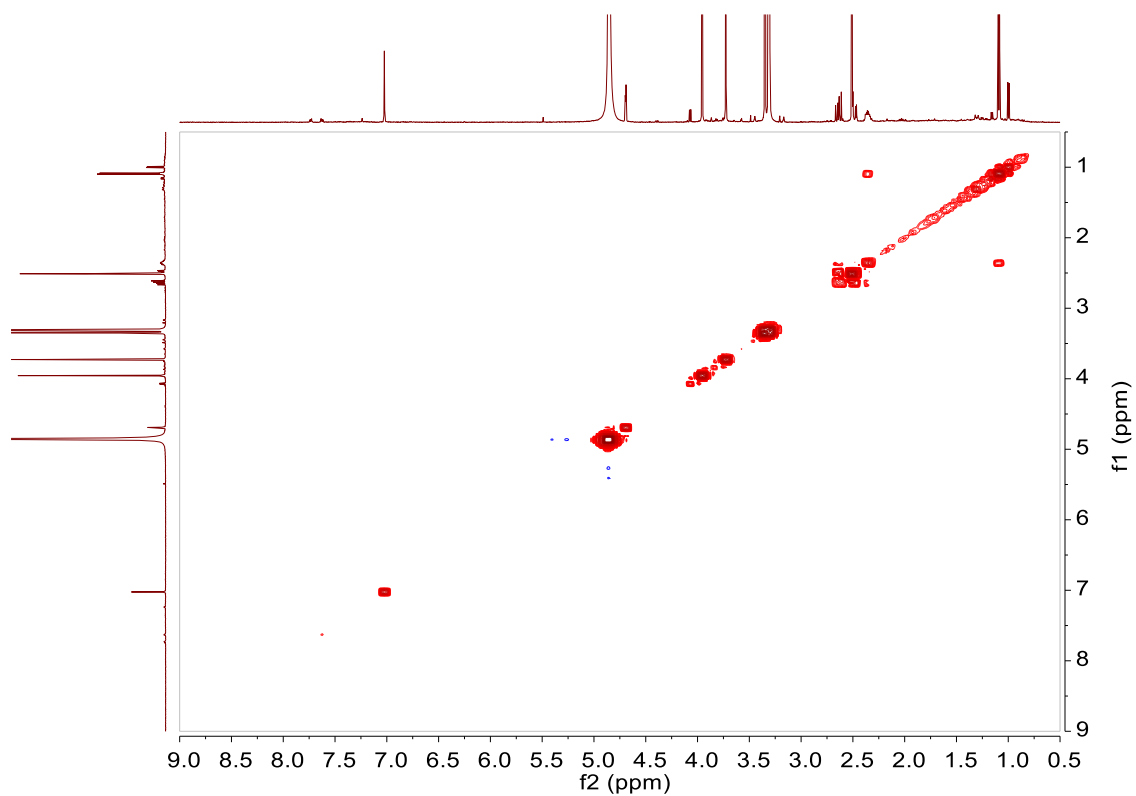


Figure S3: ^1H - ^1H COSY spectrum of **1** in methanol- d_4

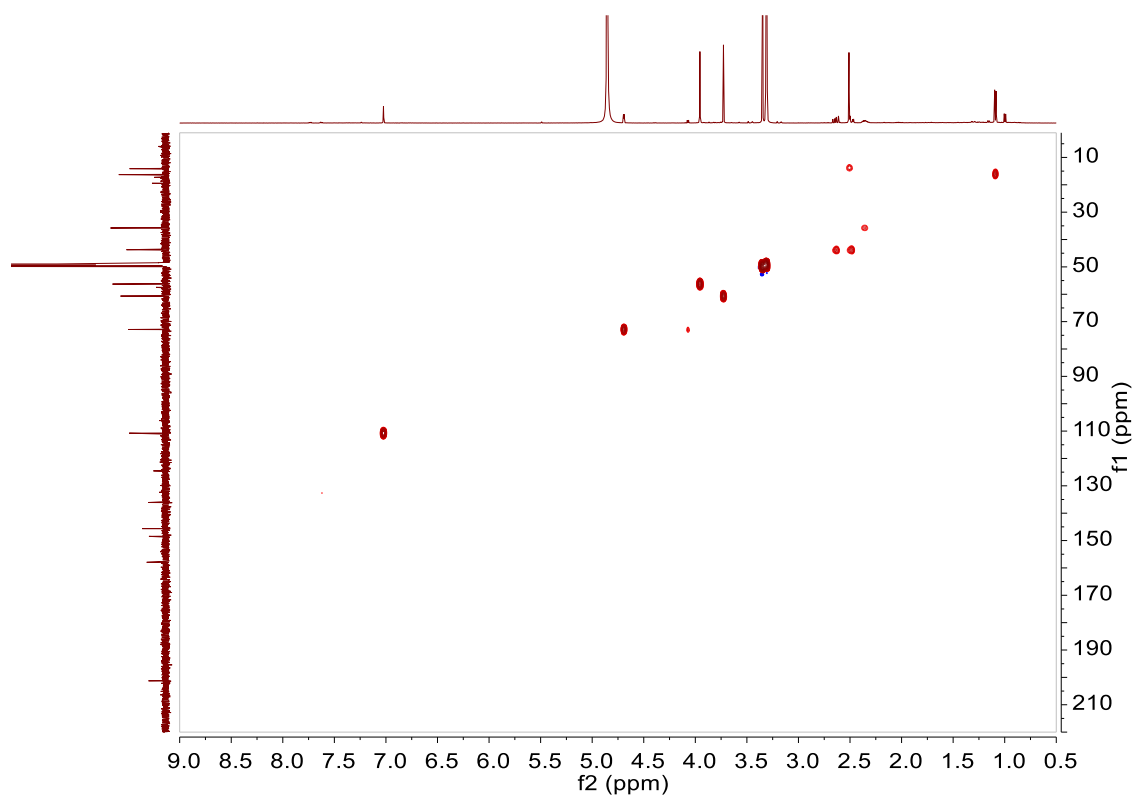


Figure S4: HSQC spectrum of **1** in methanol- d_4

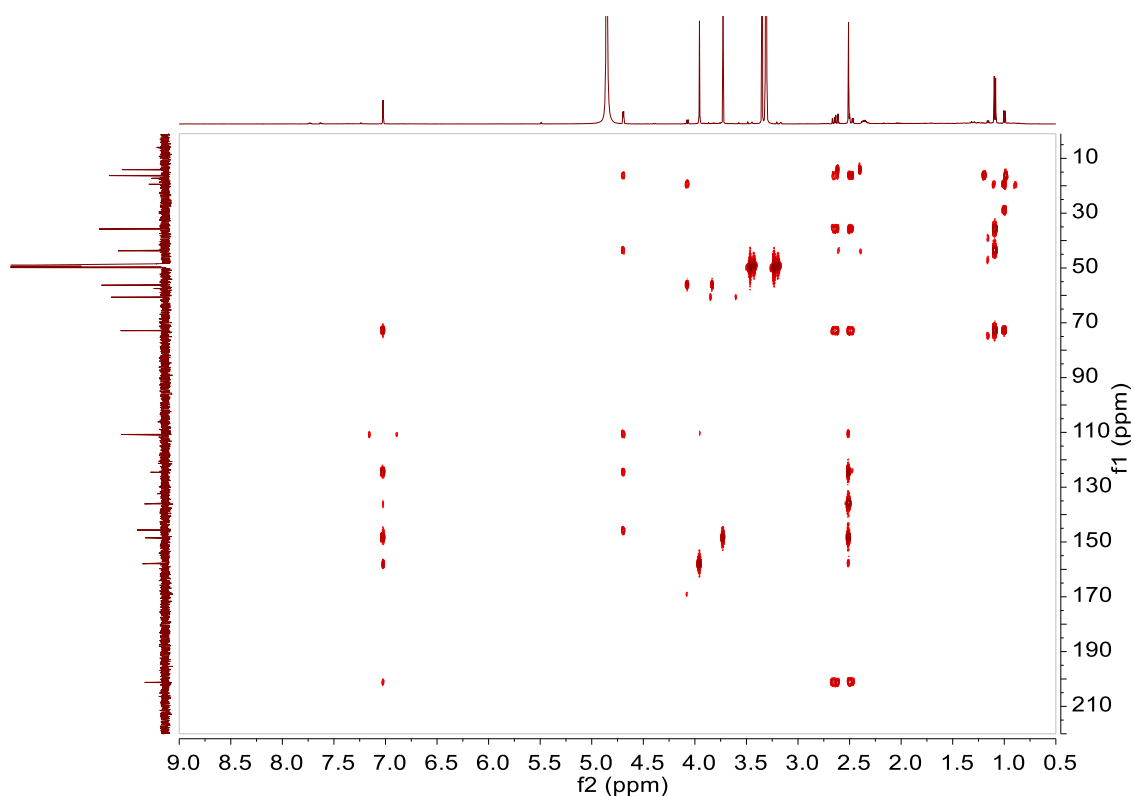


Figure S5: HMBC spectrum of **1** in methanol- d_4

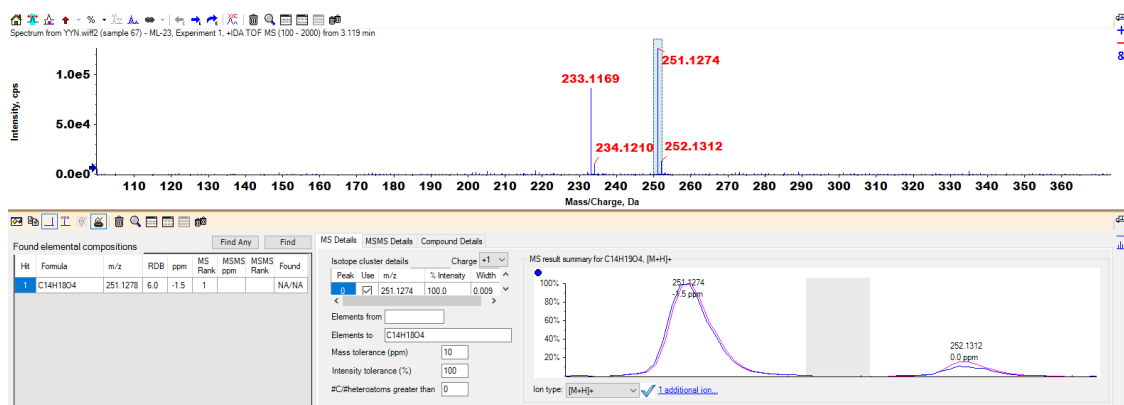


Figure S6: HRESIMS spectrum of **1**

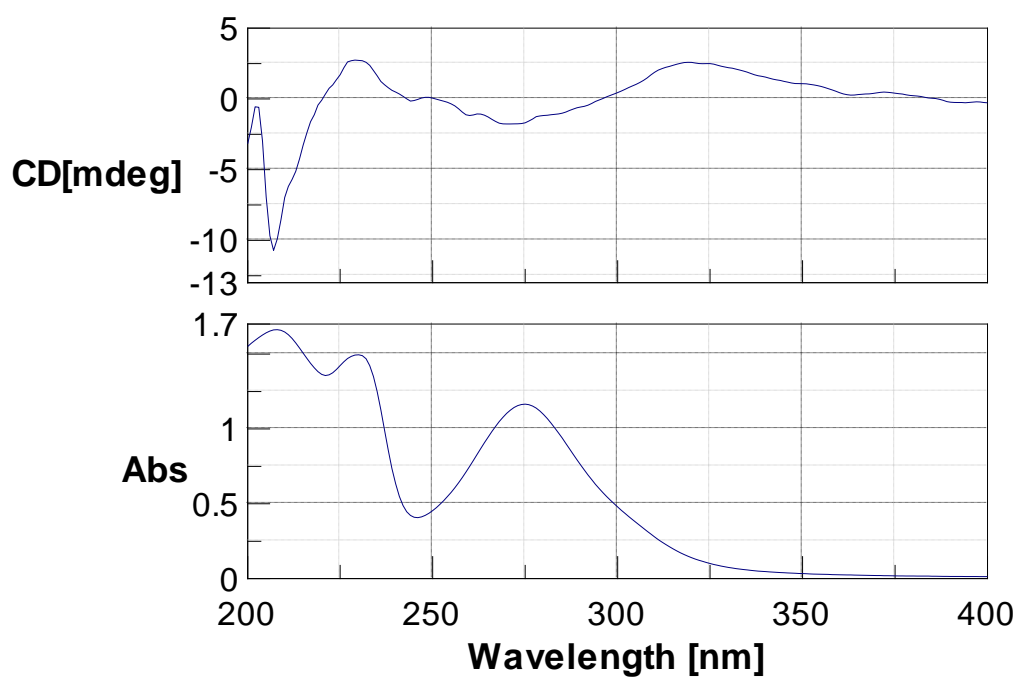


Figure S7: CD spectrum of **1** in MeOH

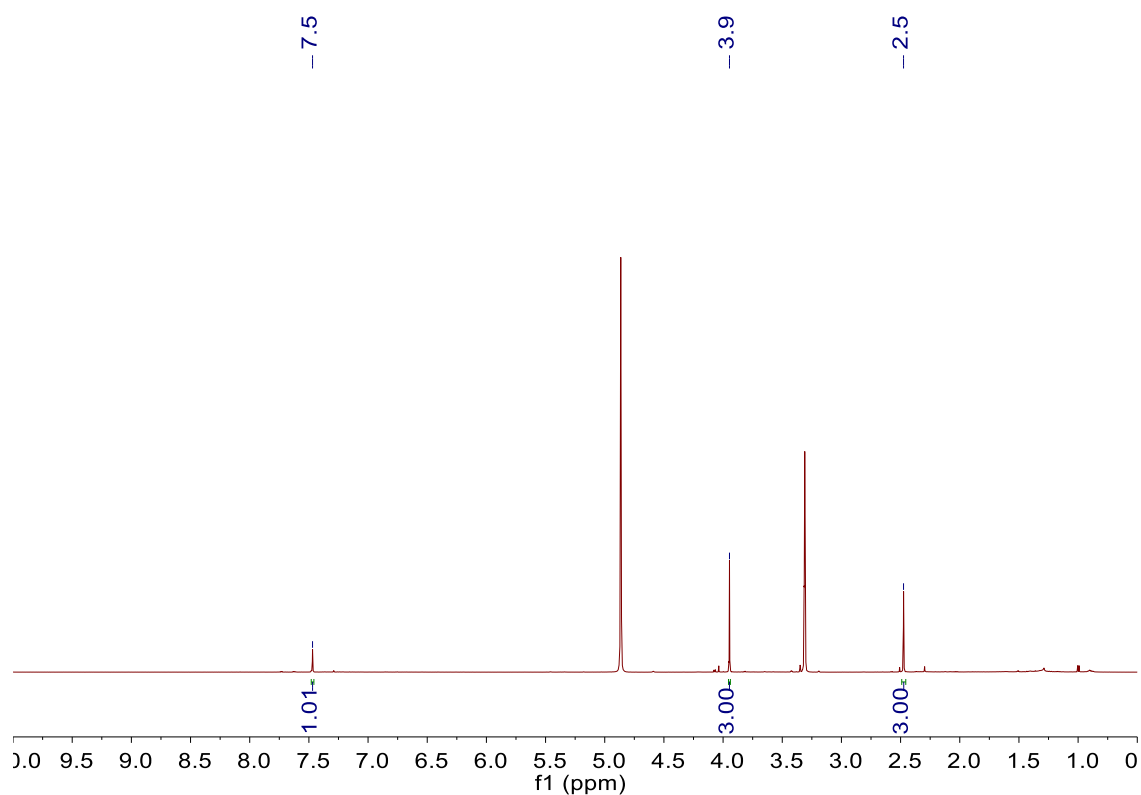


Figure S8: ¹H NMR spectrum of **2** in methanol-*d*₄

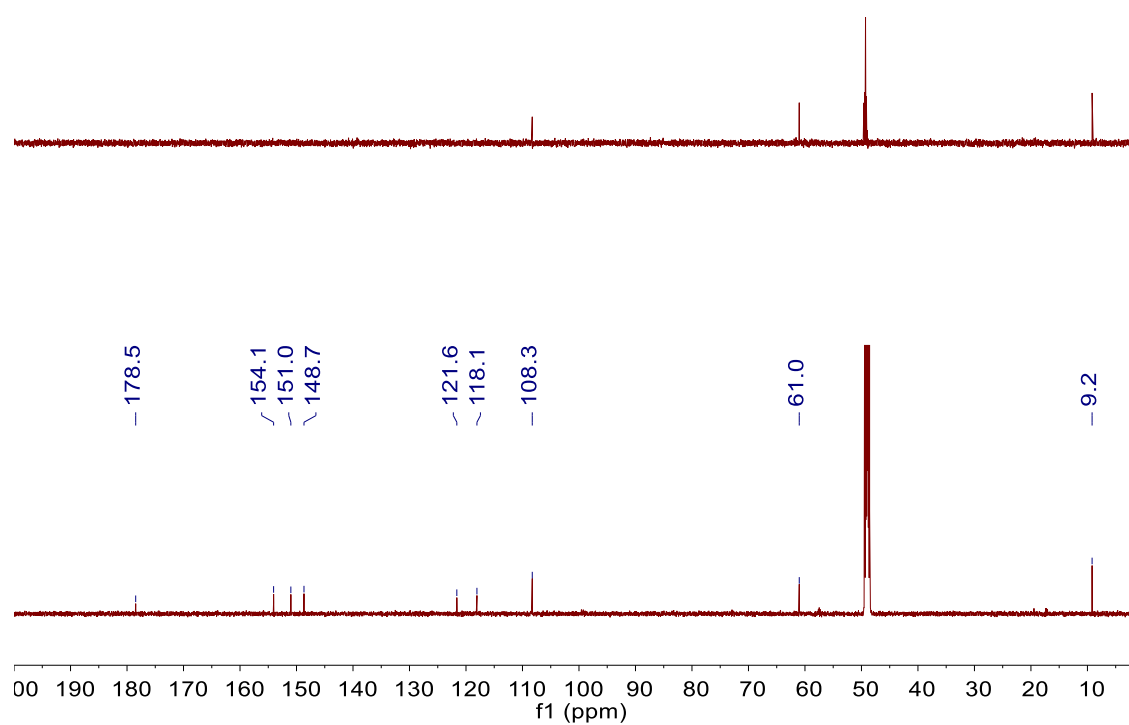


Figure S9: ^{13}C NMR and DEPT spectrum of **2** in methanol- d_4

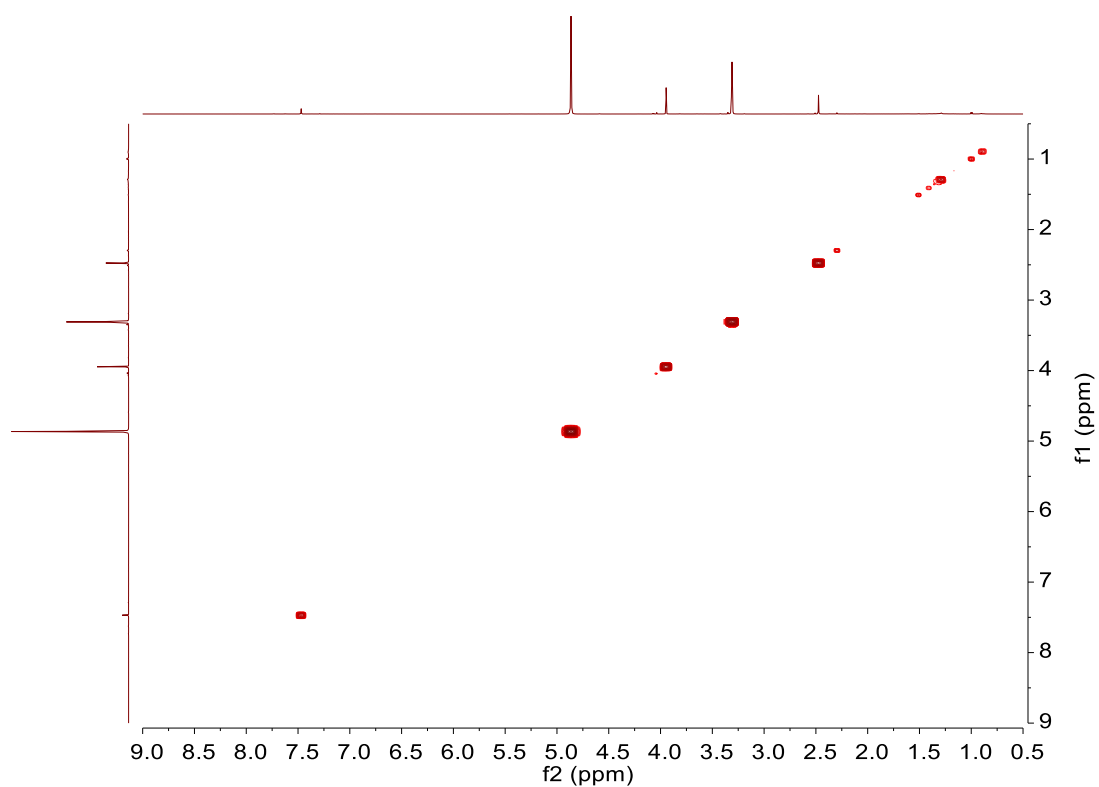


Figure S10: ^1H - ^1H COSY spectrum of **2** in methanol- d_4

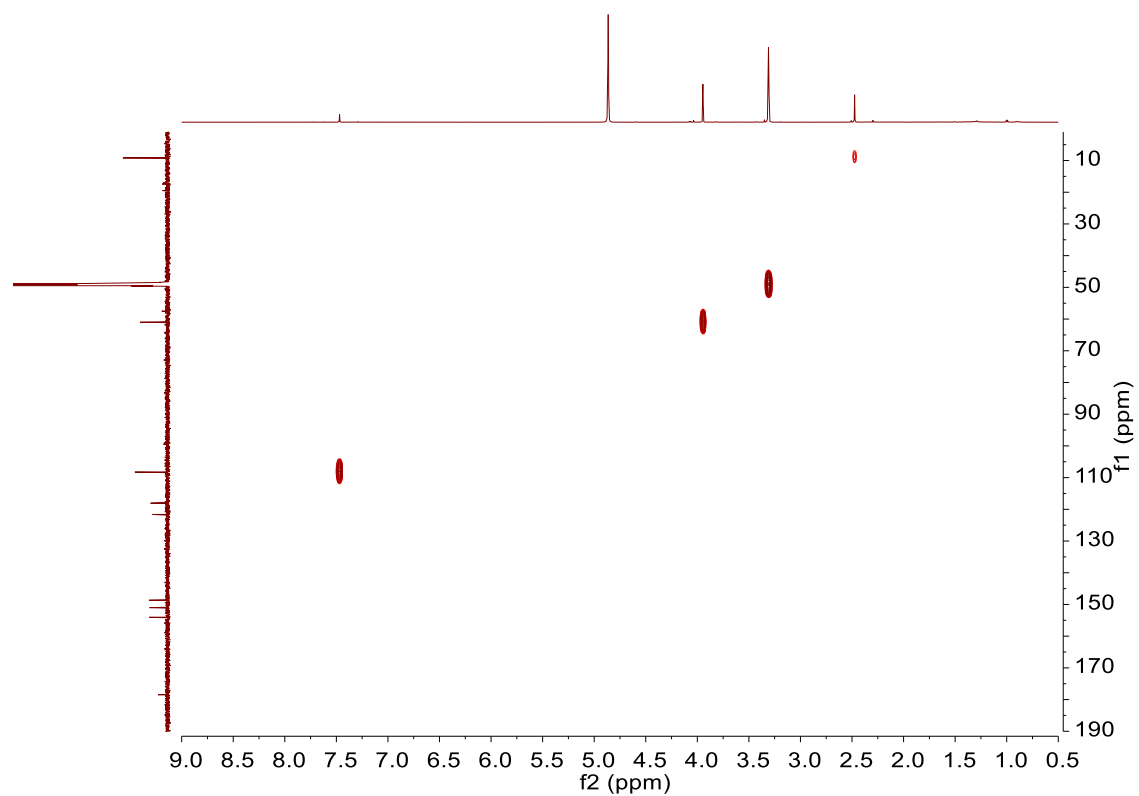


Figure S11: HSQC spectrum of **2** in methanol- d_4

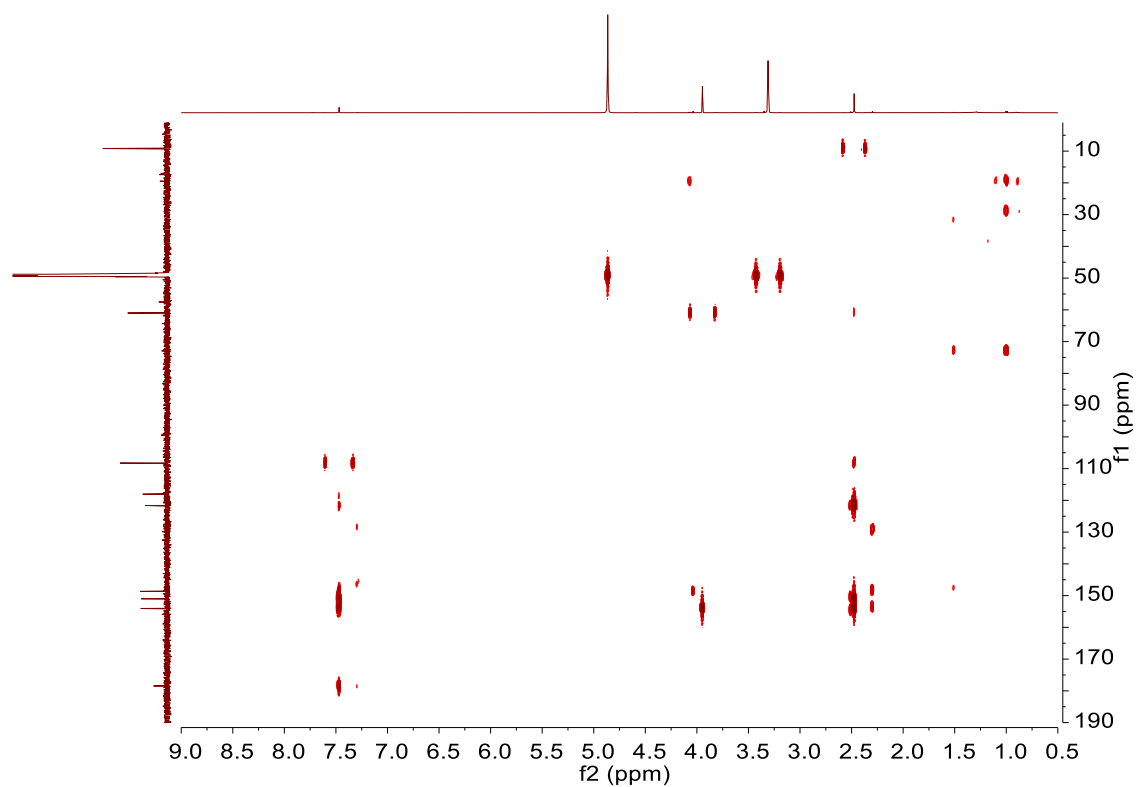


Figure S12: HMBC spectrum of **2** in methanol- d_4

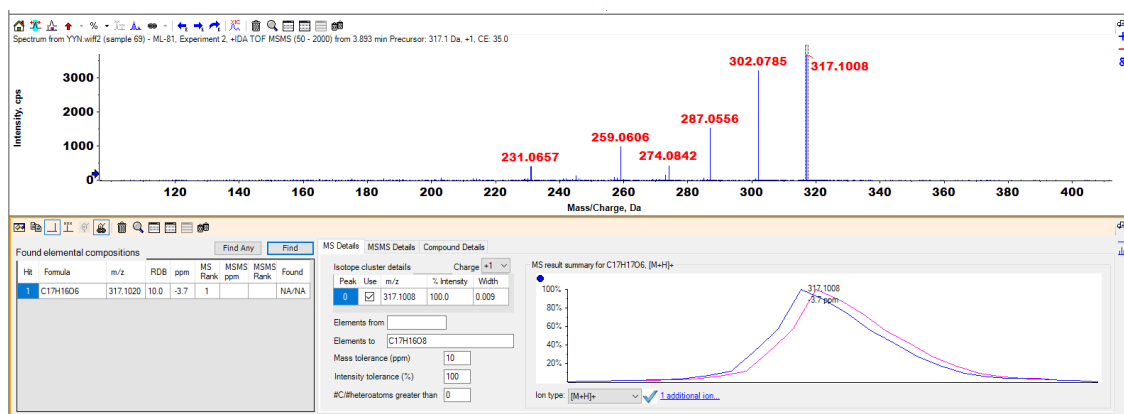


Figure S13: HRESIMS spectrum of 2

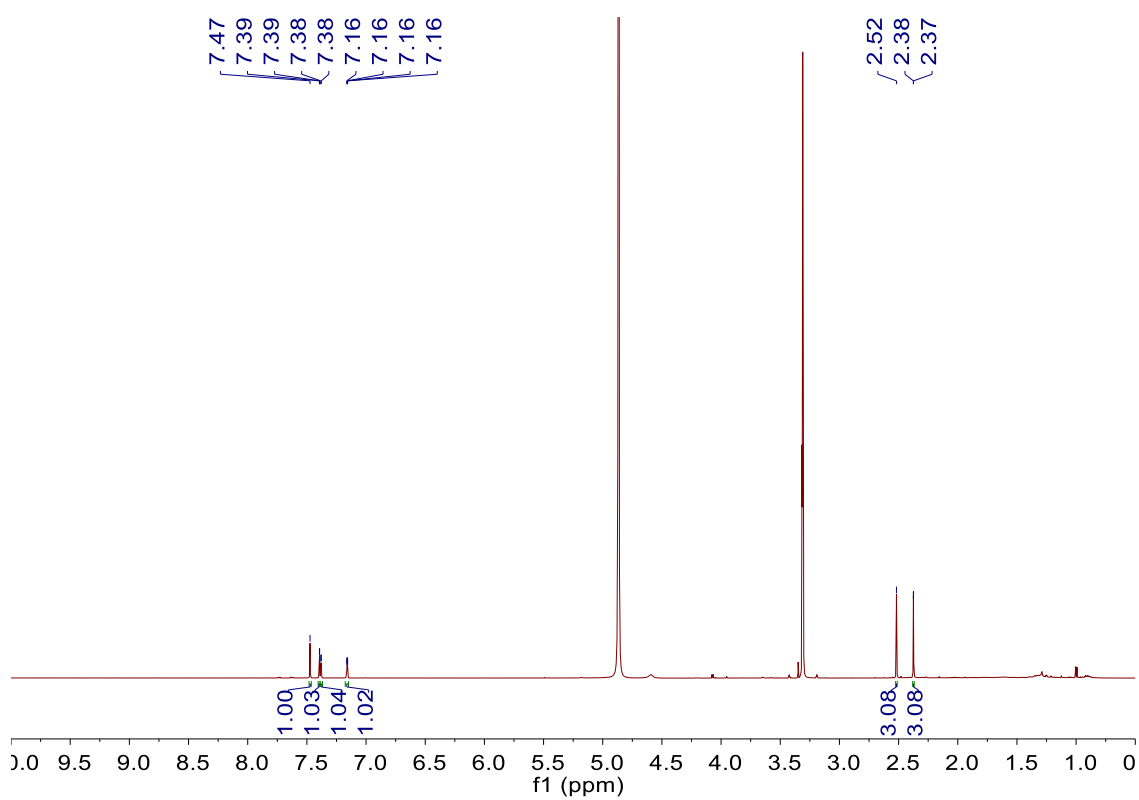


Figure S14: ¹H NMR spectrum of 3 in methanol-*d*₄

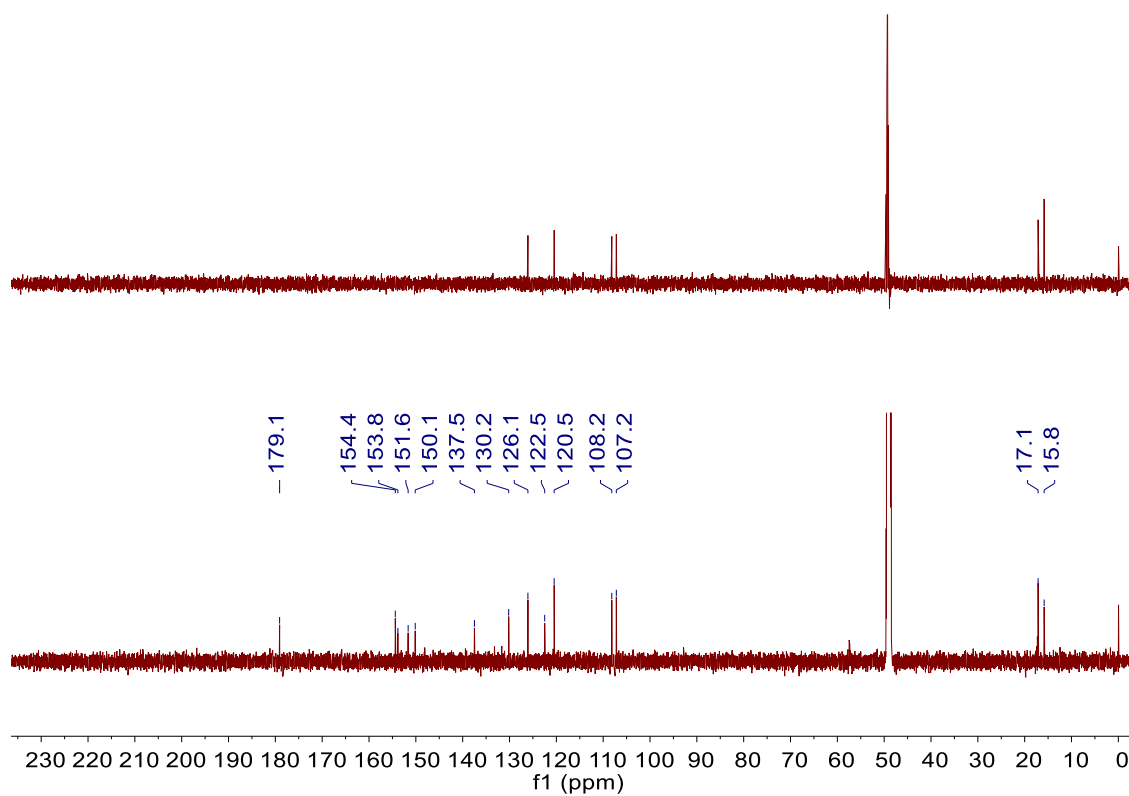


Figure S15: ^{13}C NMR and DEPT spectrum of **3** in methanol- d_4

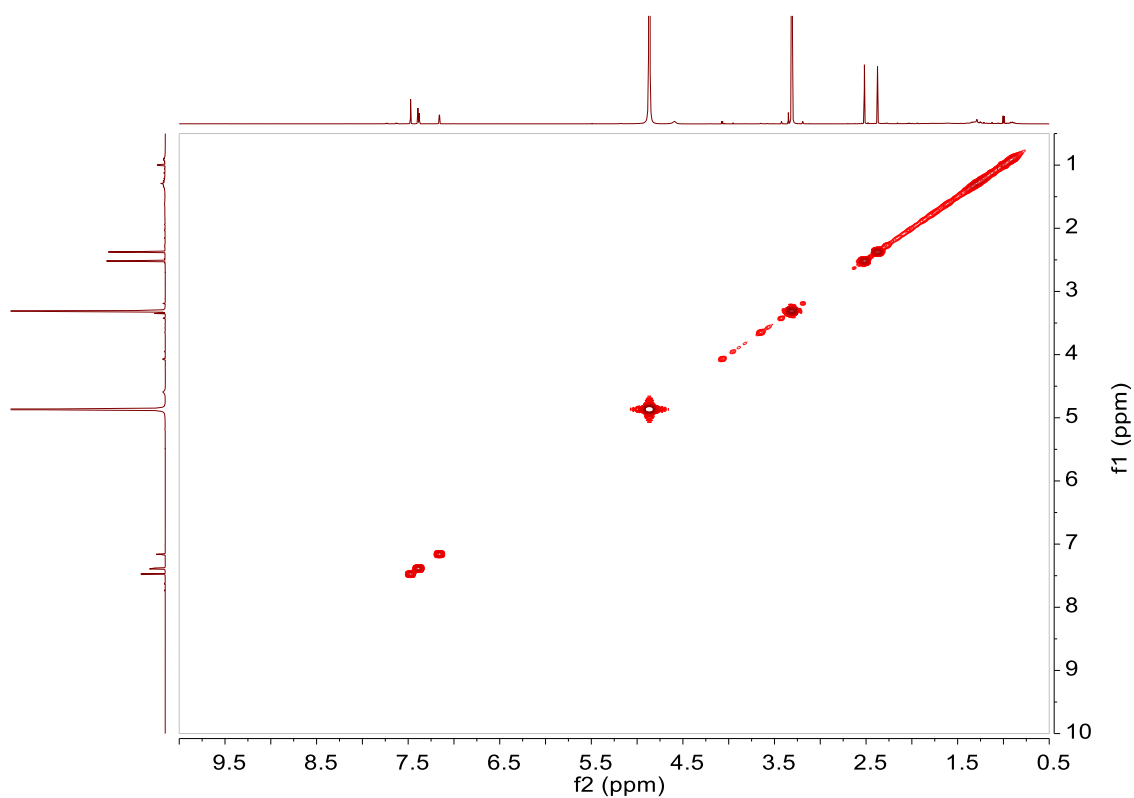


Figure S16: ^1H - ^1H COSY spectrum of **3** in methanol- d_4

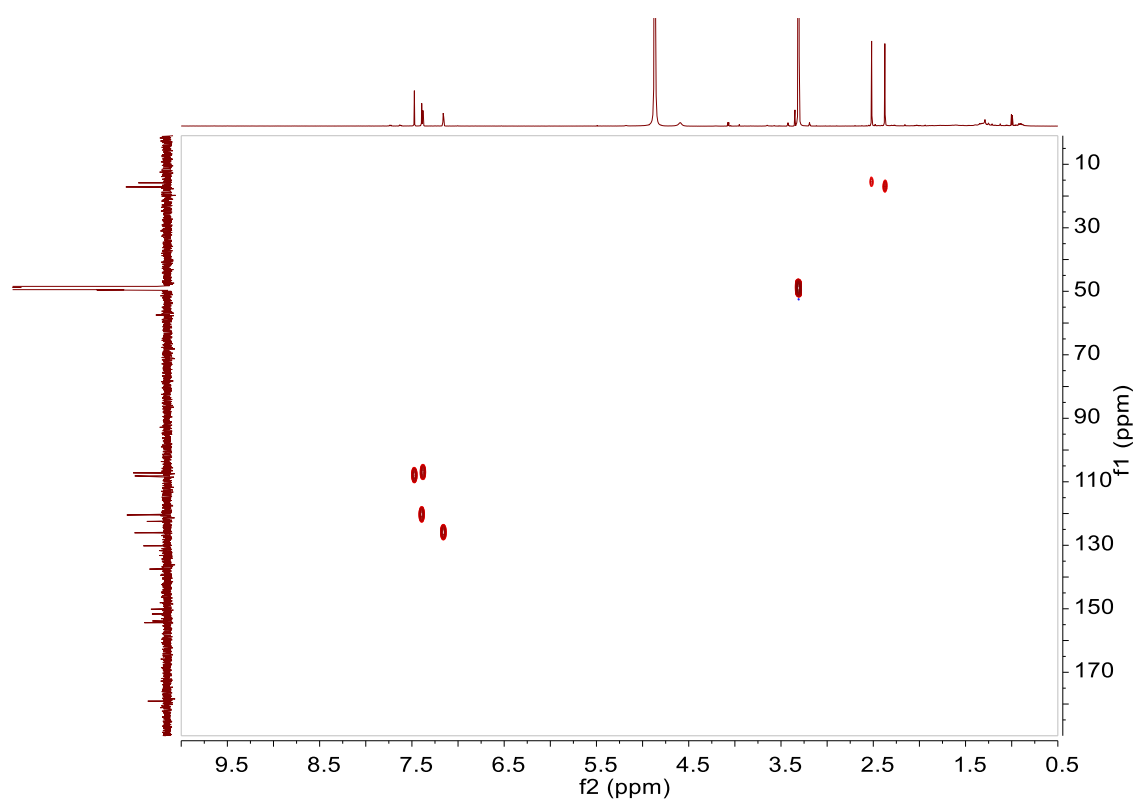


Figure S17: HSQC spectrum of **3** in methanol- d_4

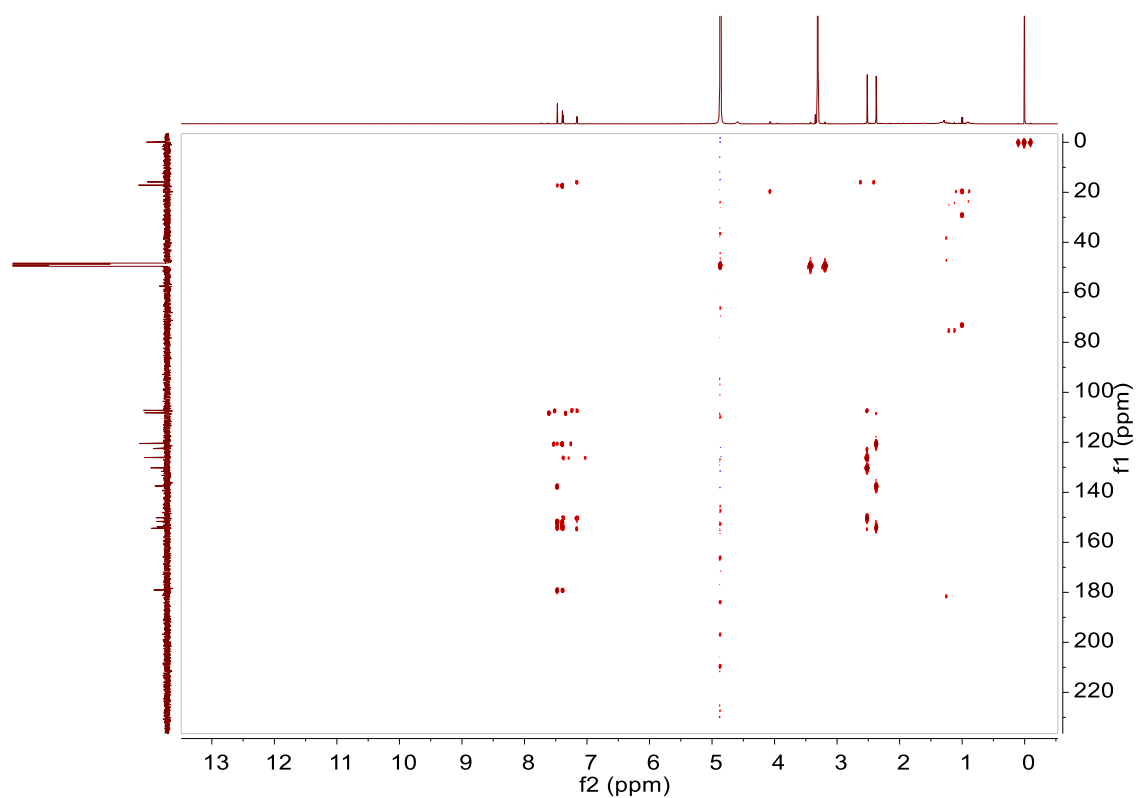


Figure S18: HMBC spectrum of **3** in methanol- d_4

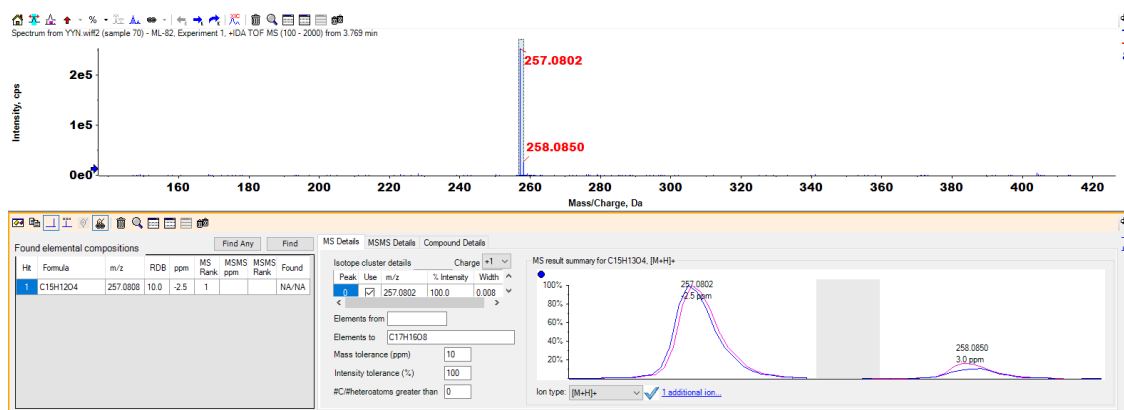


Figure S19: HRESIMS spectrum of **3**

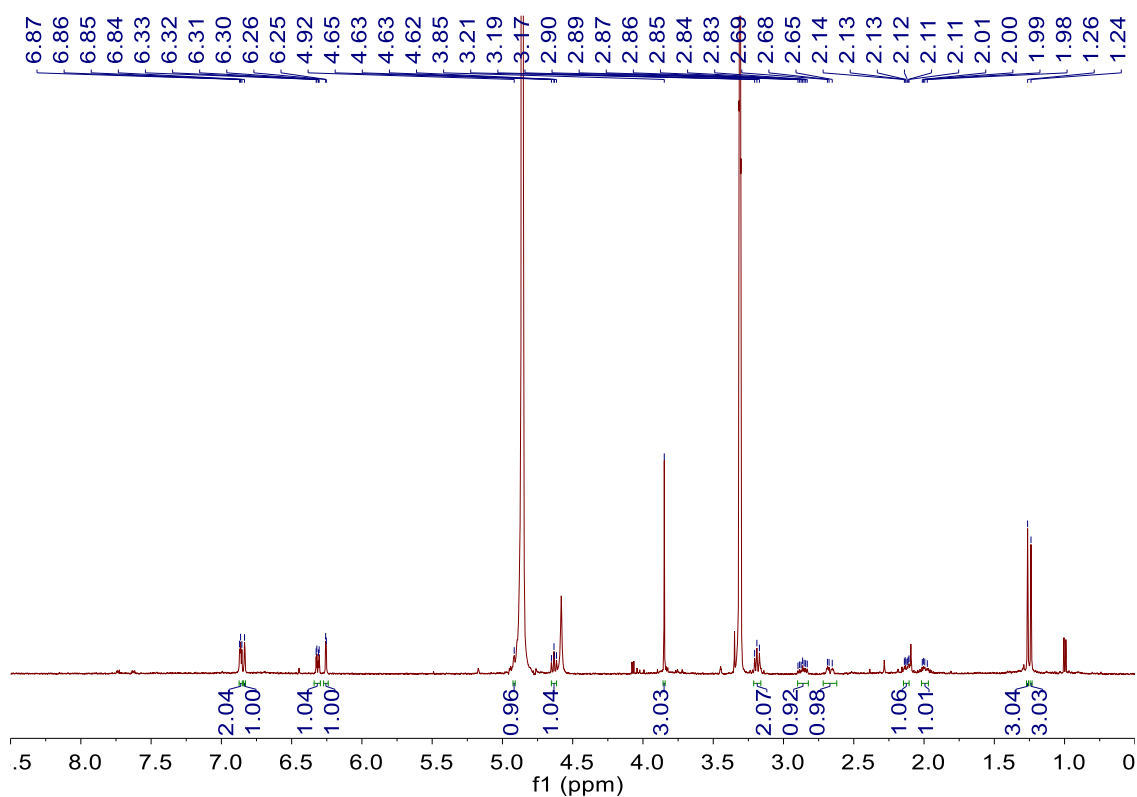


Figure S20: ¹H NMR spectrum of **4** in methanol-*d*₄

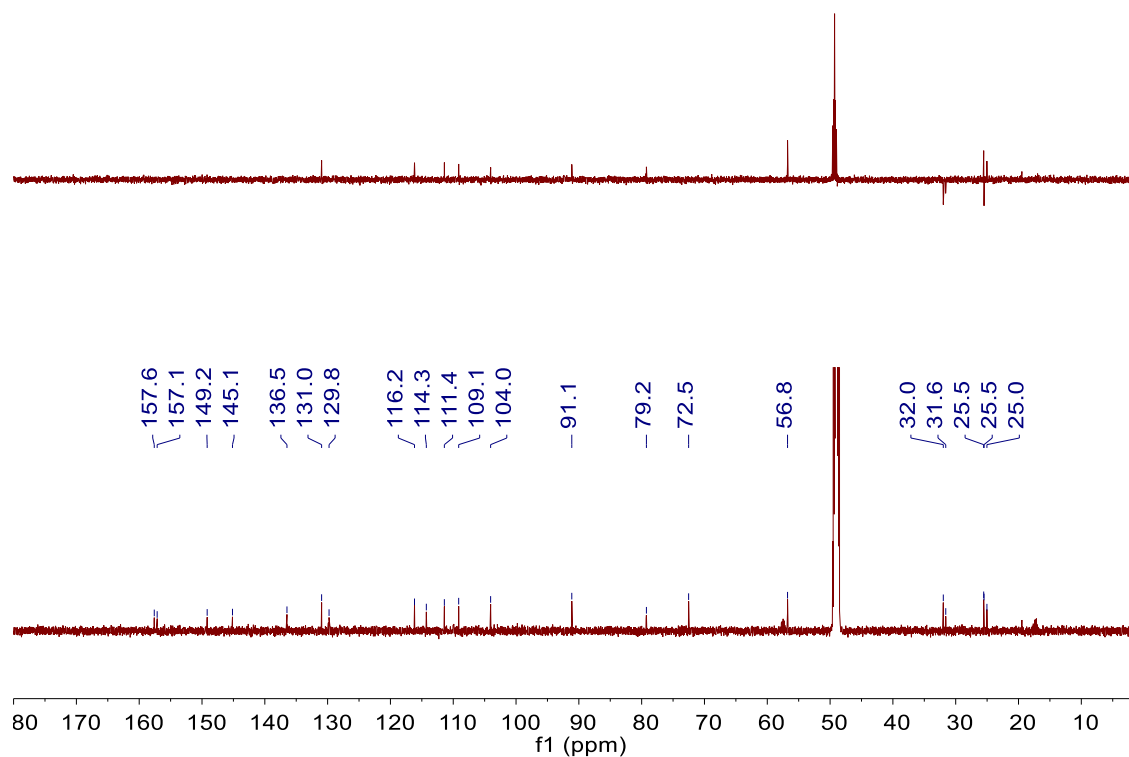


Figure S21: ^{13}C NMR and DEPT spectrum of **4** in methanol- d_4

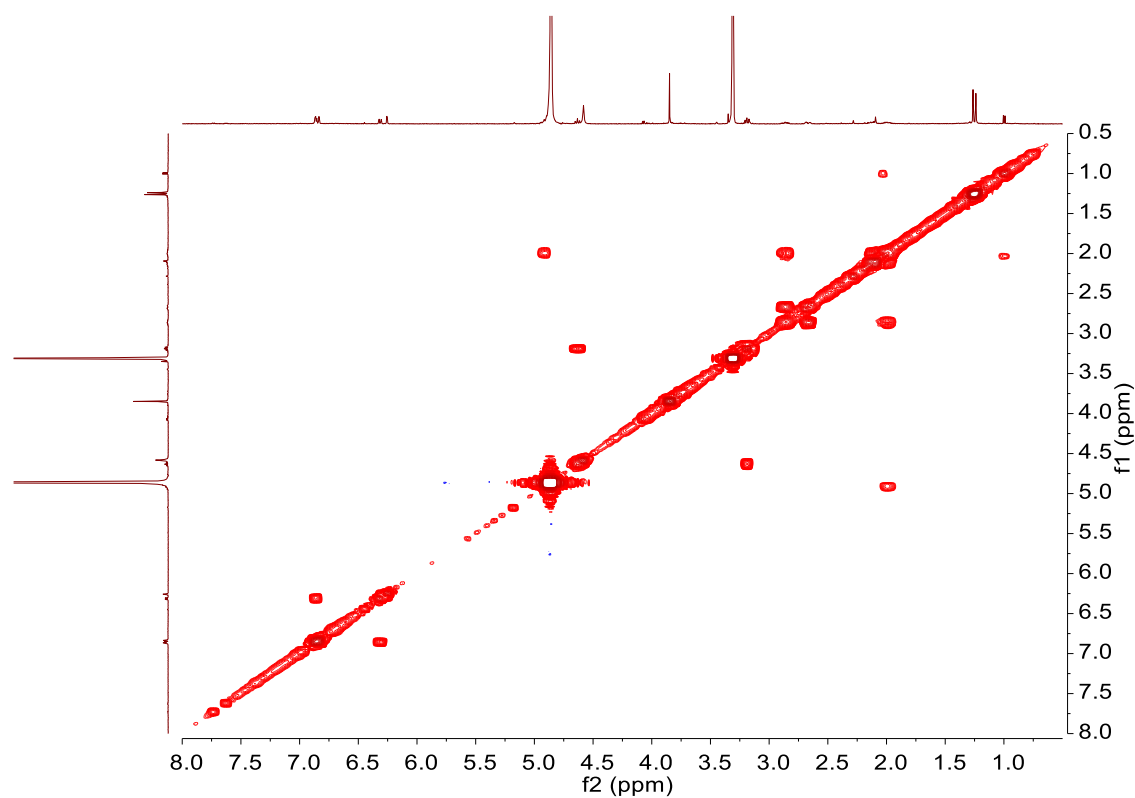


Figure S22: ^1H - ^1H COSY spectrum of **4** in methanol- d_4

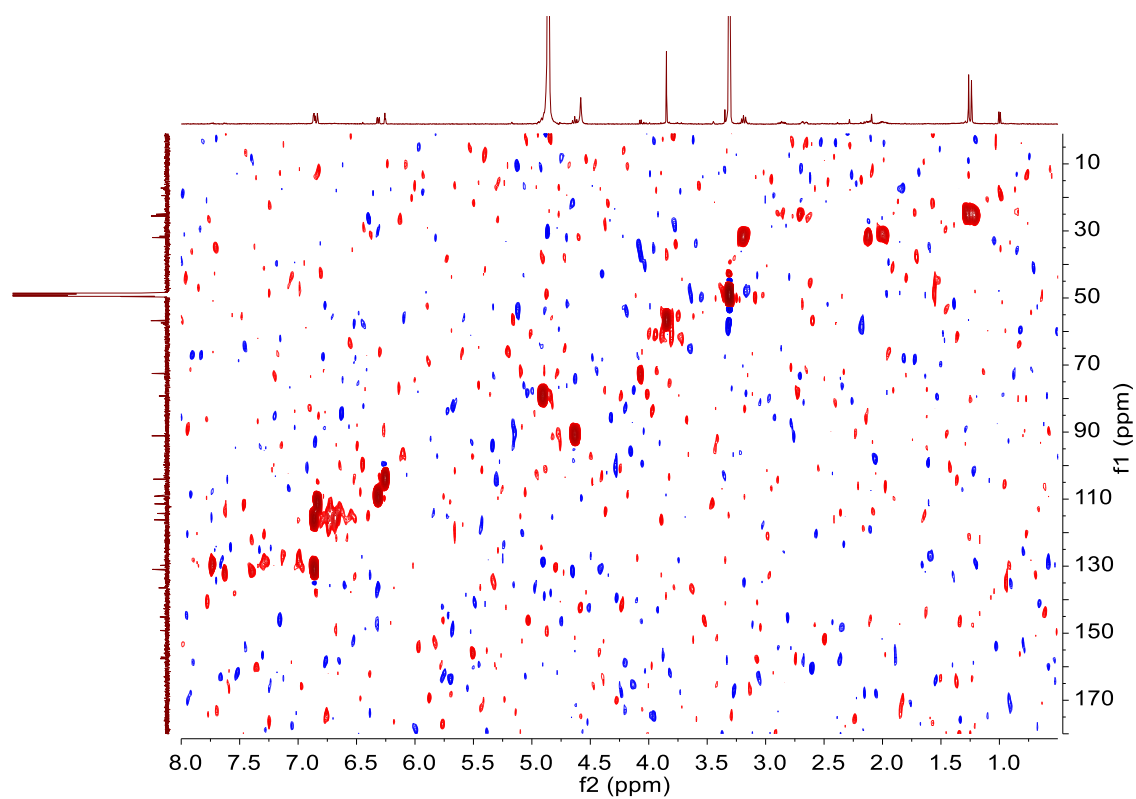


Figure S23: HSQC spectrum of **4** in methanol- d_4

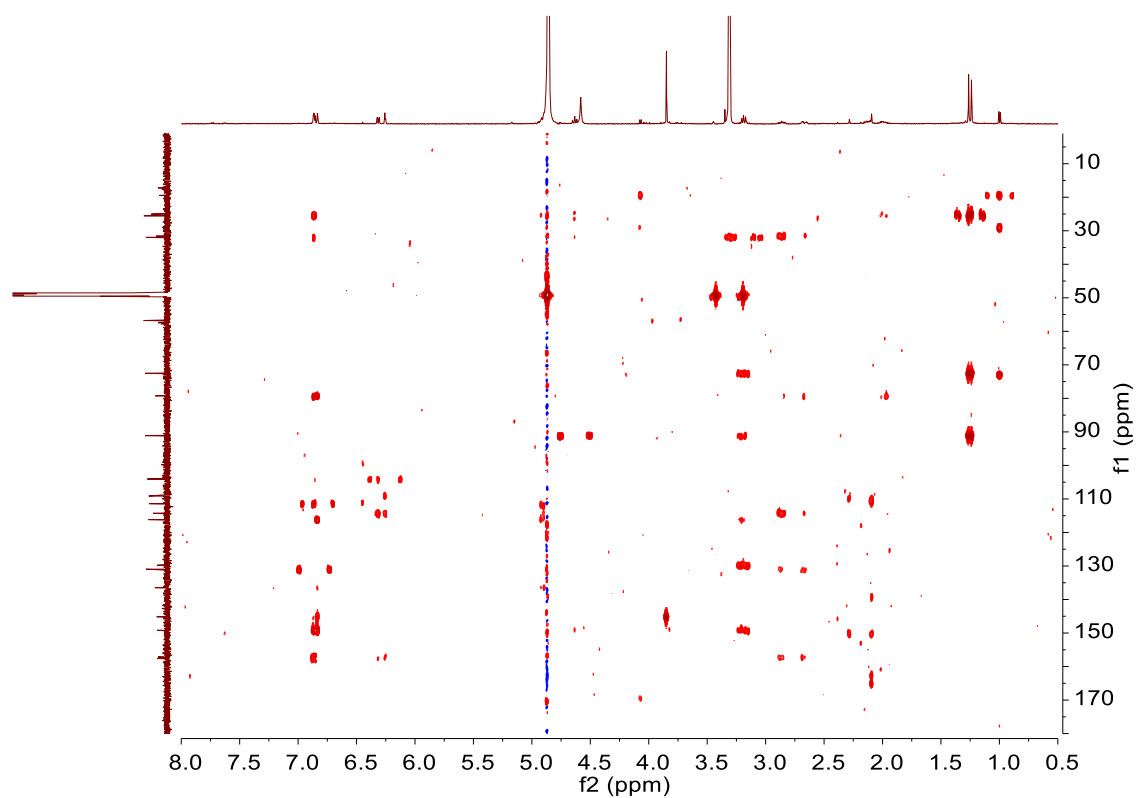


Figure S24: HMBC spectrum of **4** in methanol- d_4

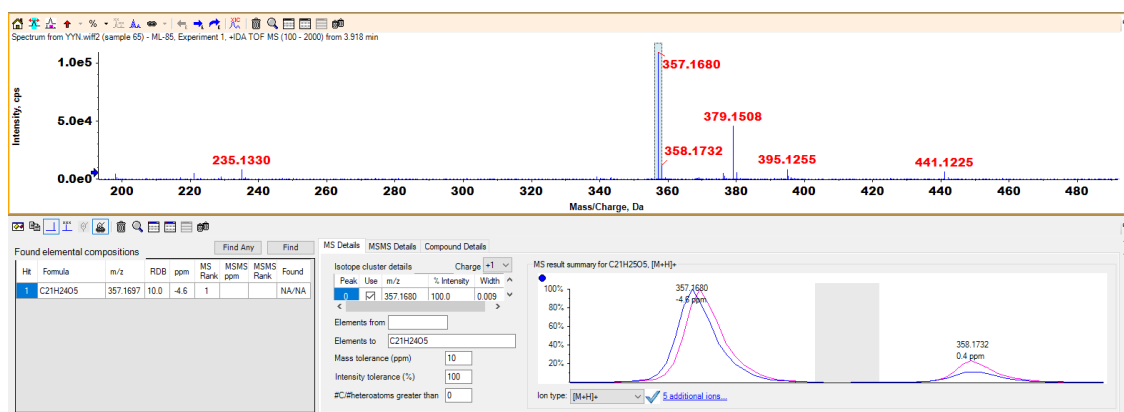


Figure S25: HRESIMS spectrum of **4**

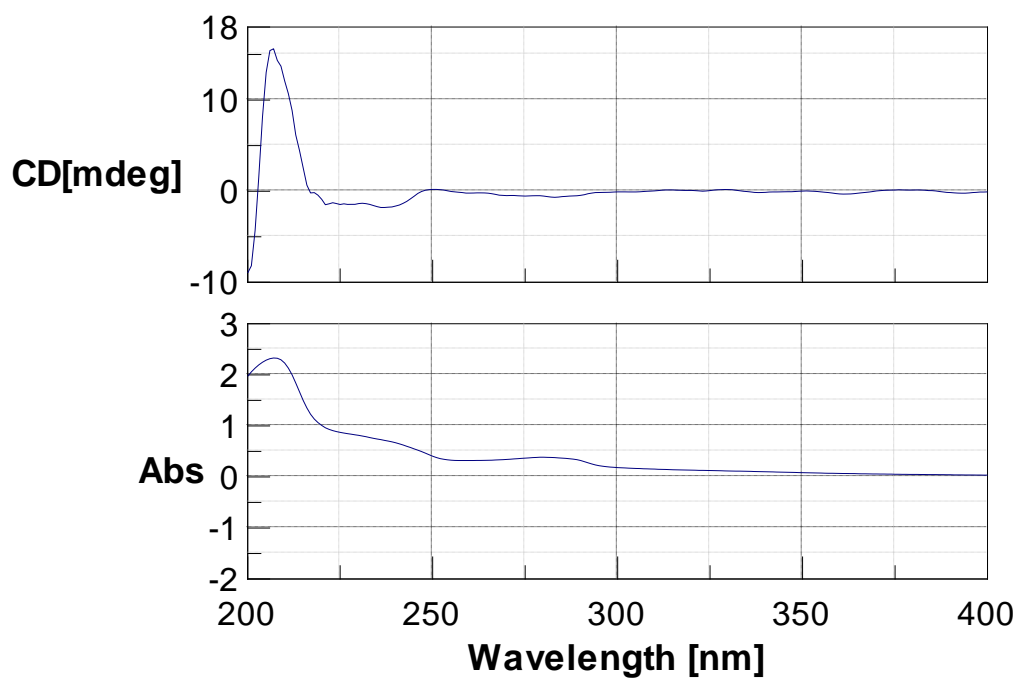


Figure S26: CD spectrum of **4** in MeOH

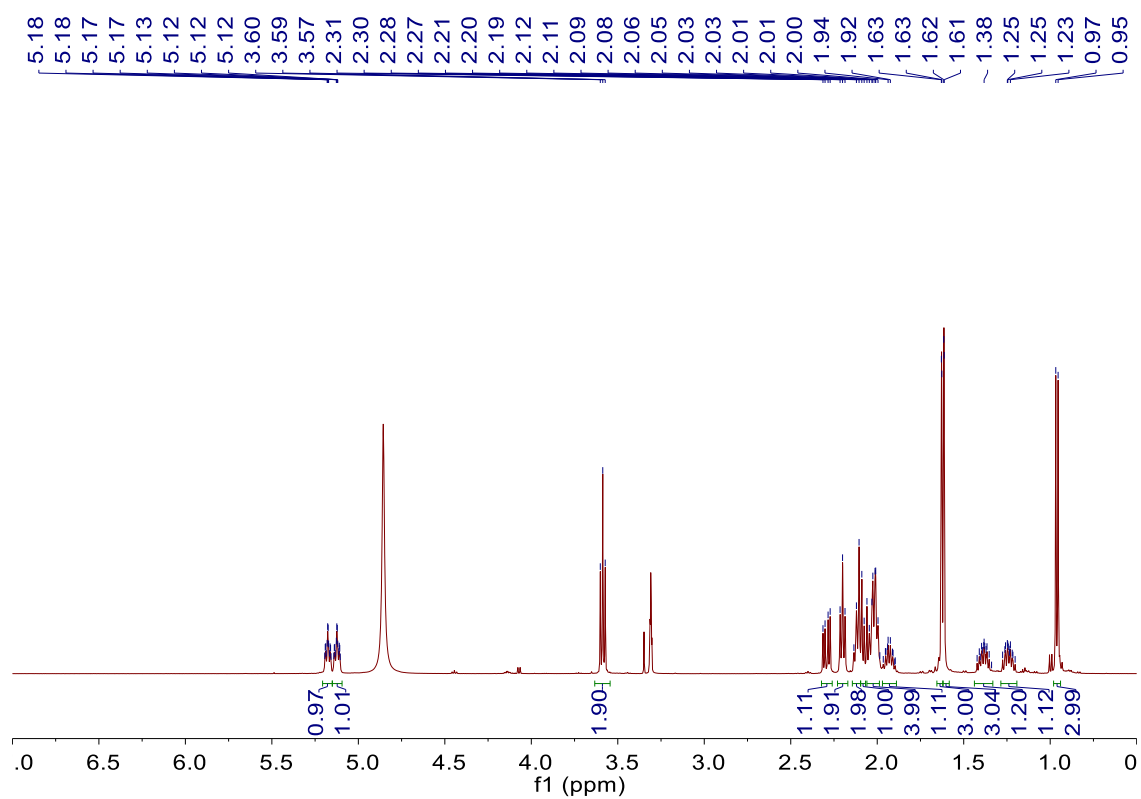


Figure S27: ^1H NMR spectrum of **7** in methanol- d_4

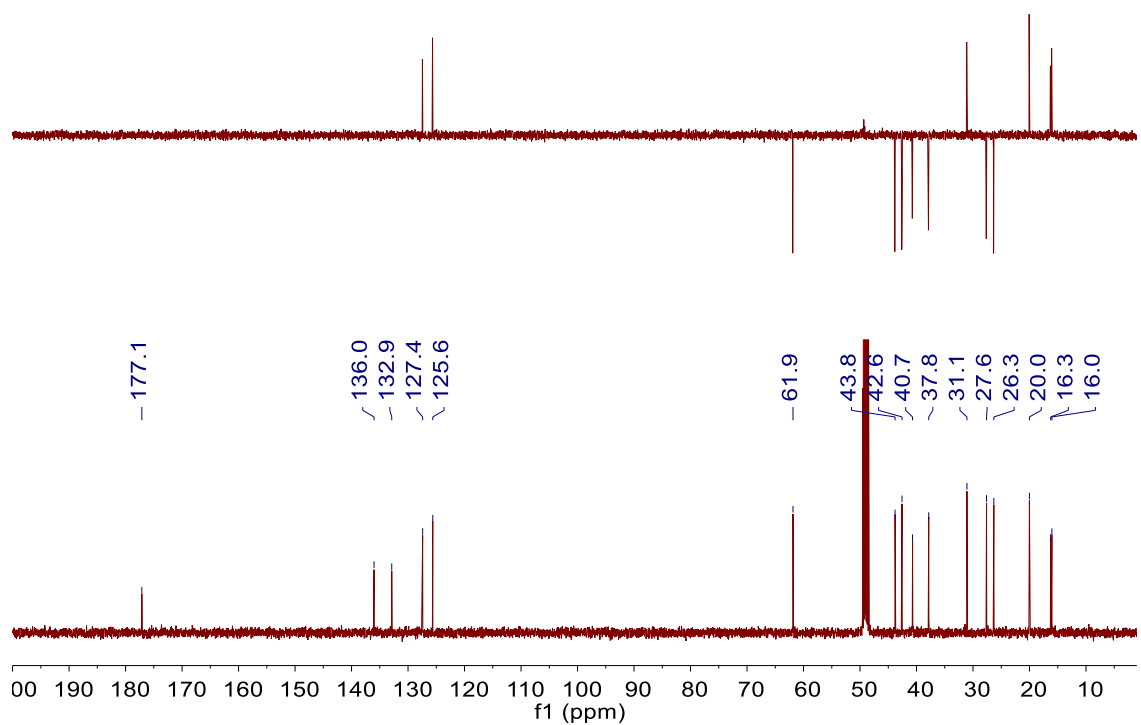


Figure S28: ^{13}C NMR and DEPT spectrum of **7** in methanol- d_4

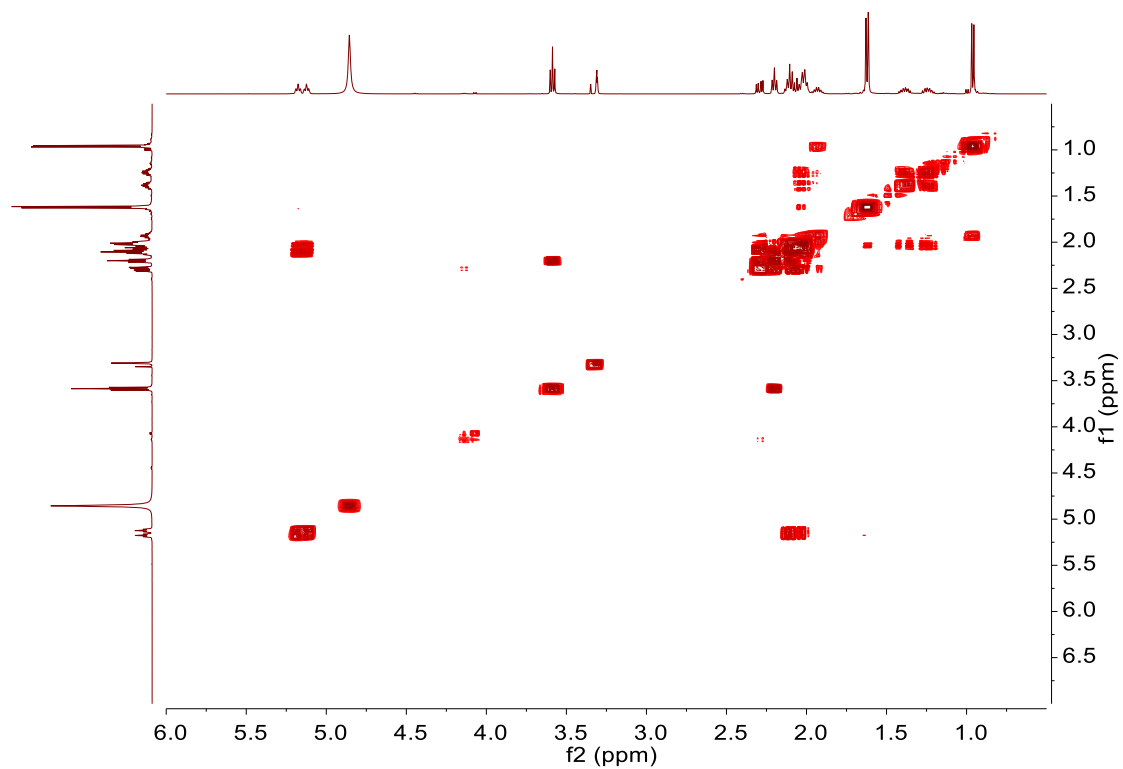


Figure S29: ^1H - ^1H COSY spectrum of **7** in methanol- d_4

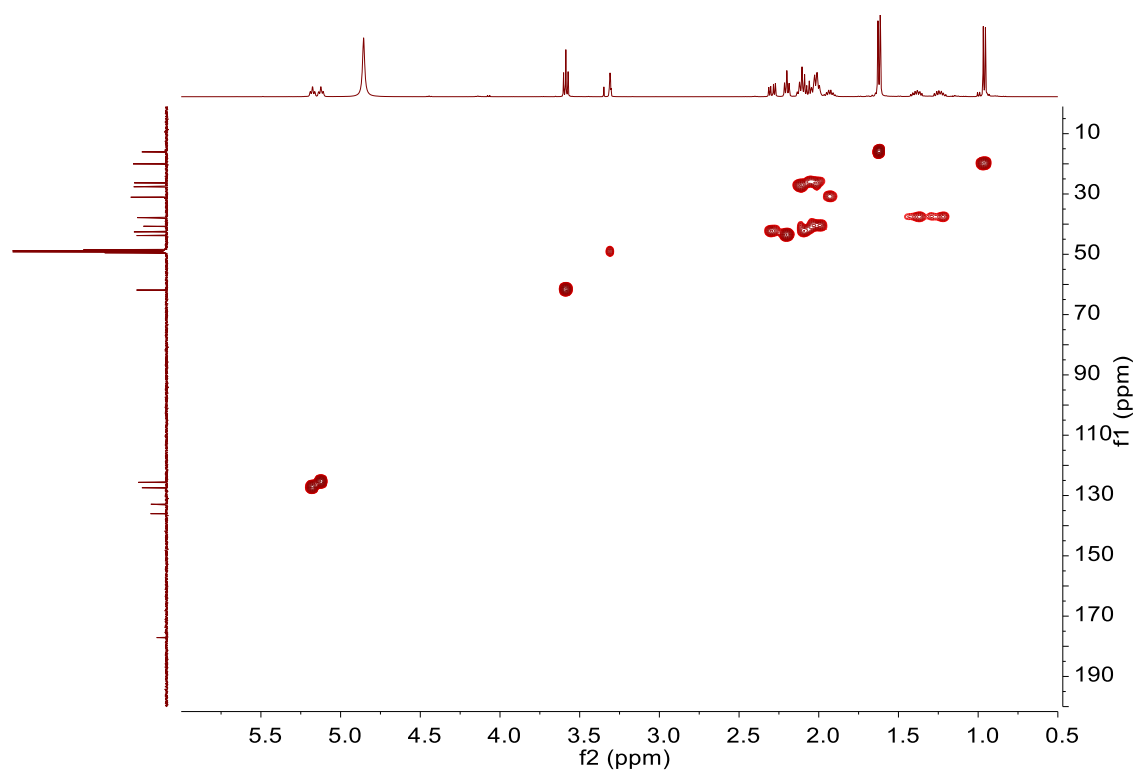


Figure S30: HSQC spectrum of **7** in methanol- d_4

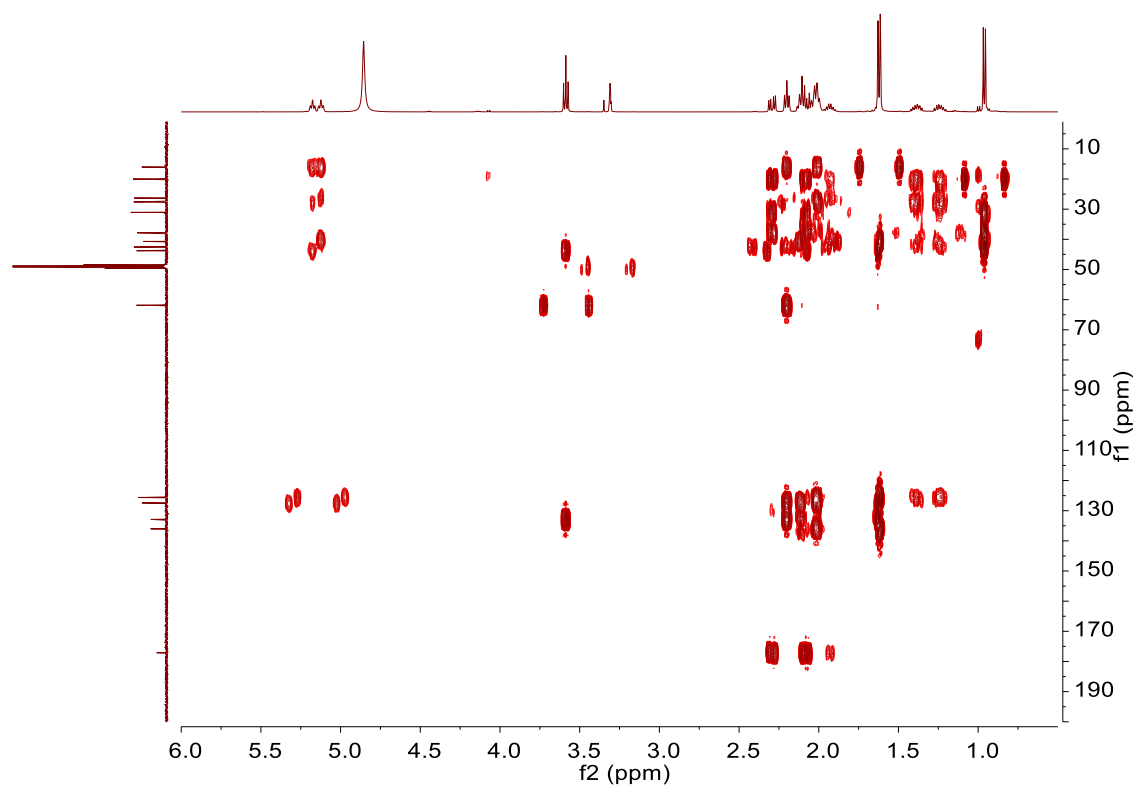


Figure S31: HMBC spectrum of **7** in methanol- d_4

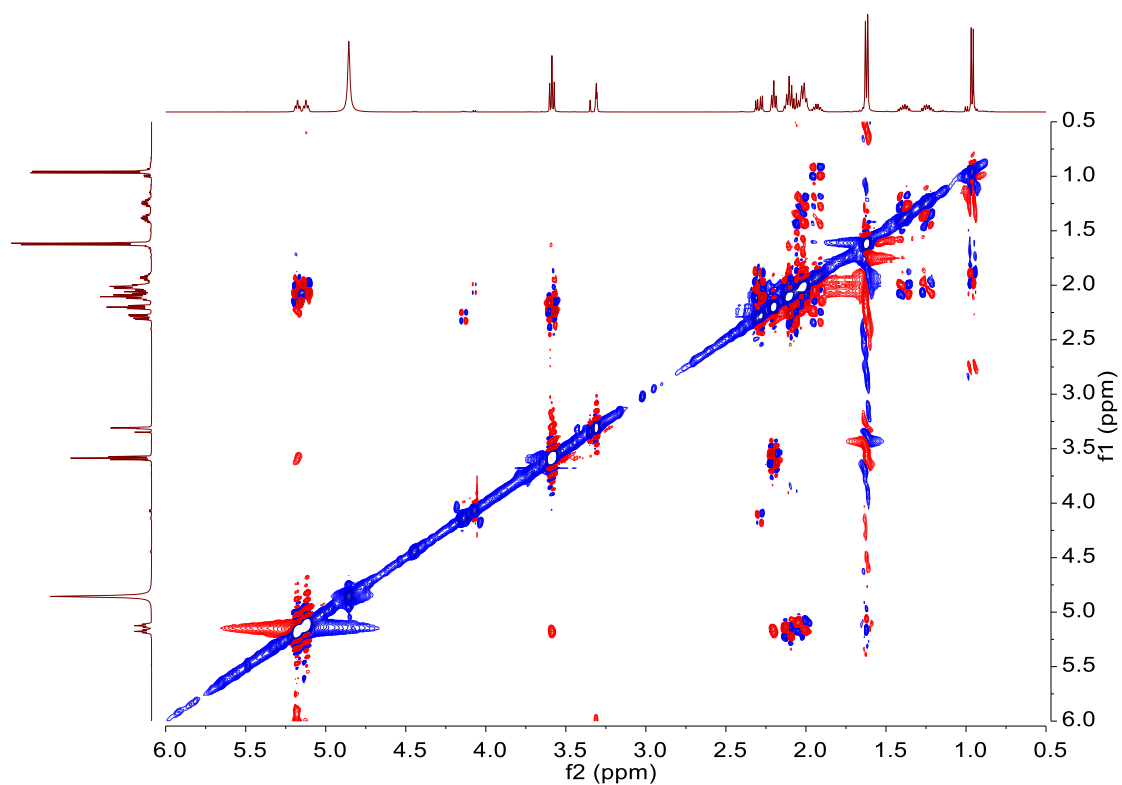


Figure S32: ROESY spectrum of **7** in methanol- d_4

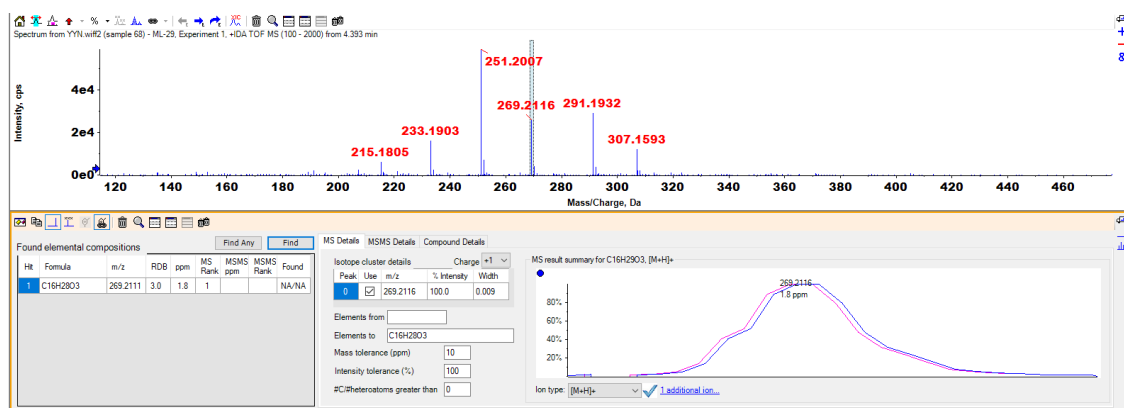


Figure S33: HRESIMS spectrum of **7**

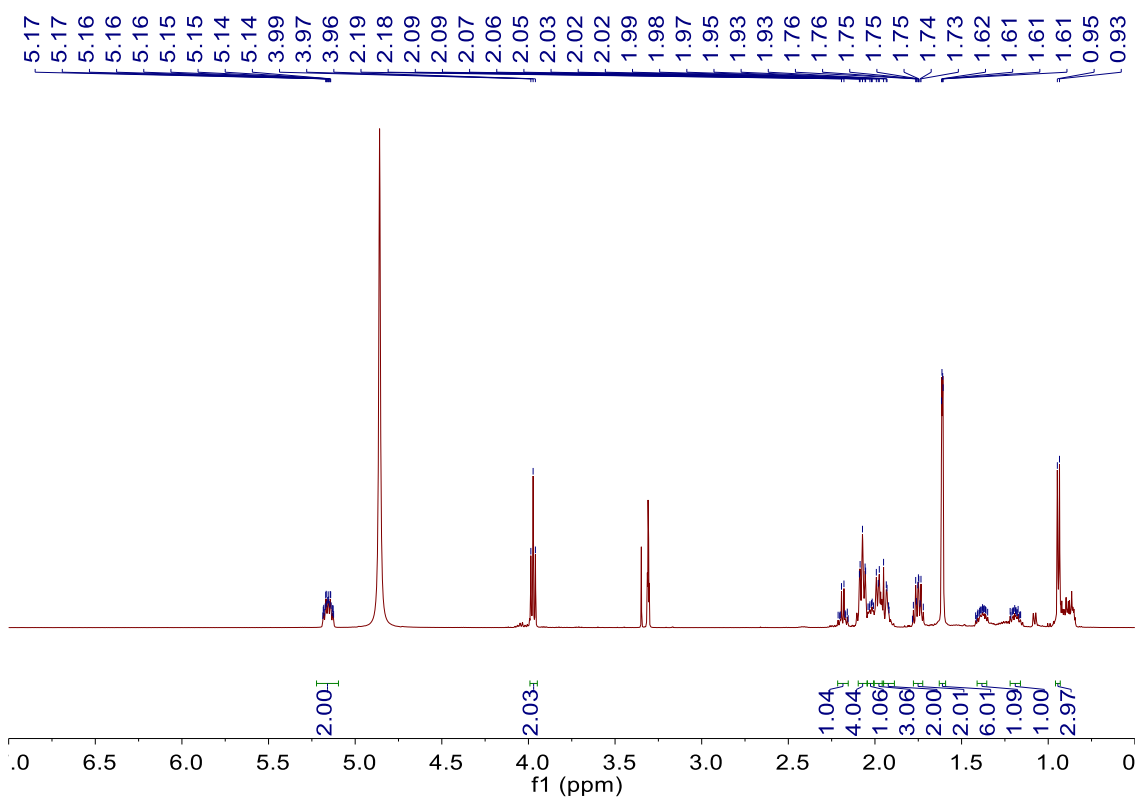


Figure S34: ¹H NMR spectrum of **8** in methanol-*d*₄

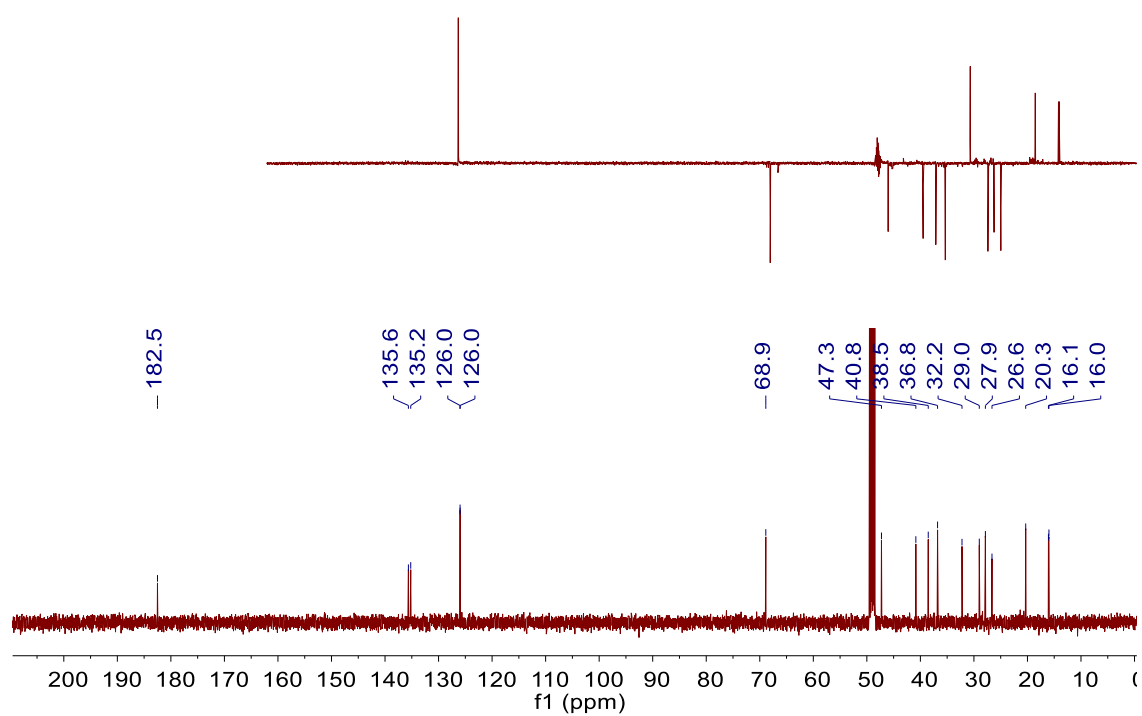


Figure S35: ¹³C NMR and DEPT spectrum of **8** in methanol-*d*₄

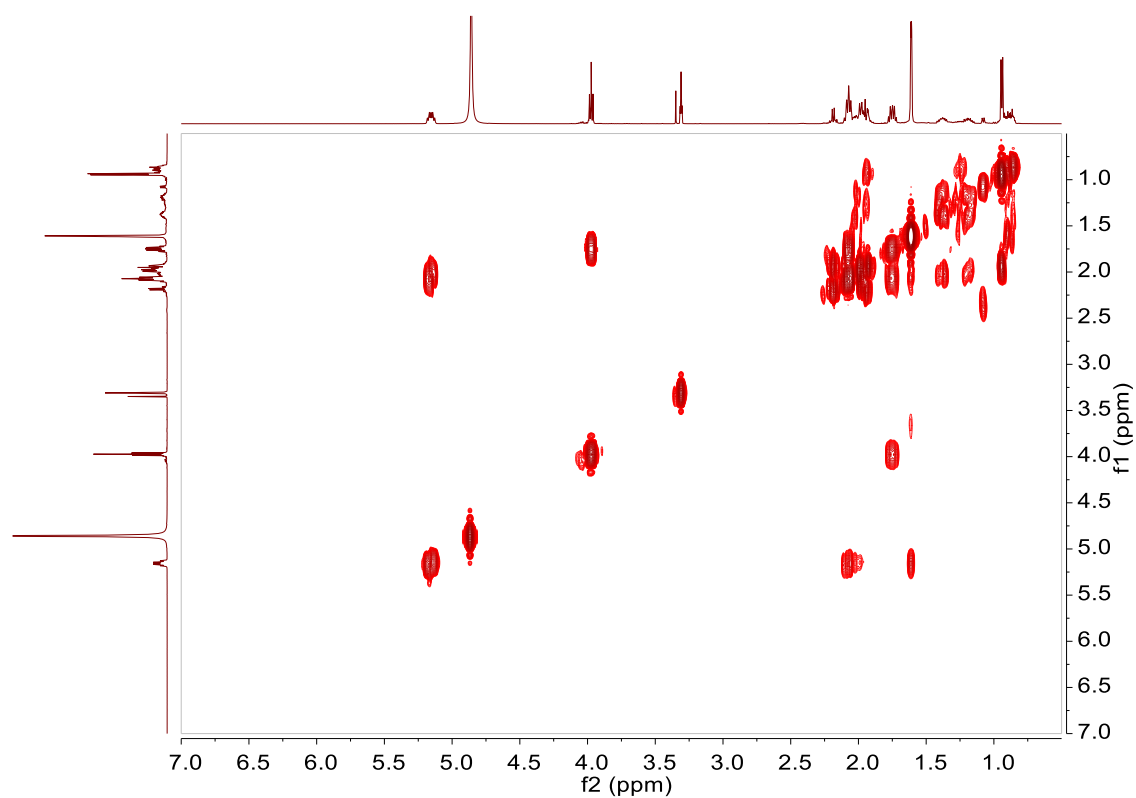


Figure S36: ¹H-¹H COSY spectrum of **8** in methanol-*d*₄

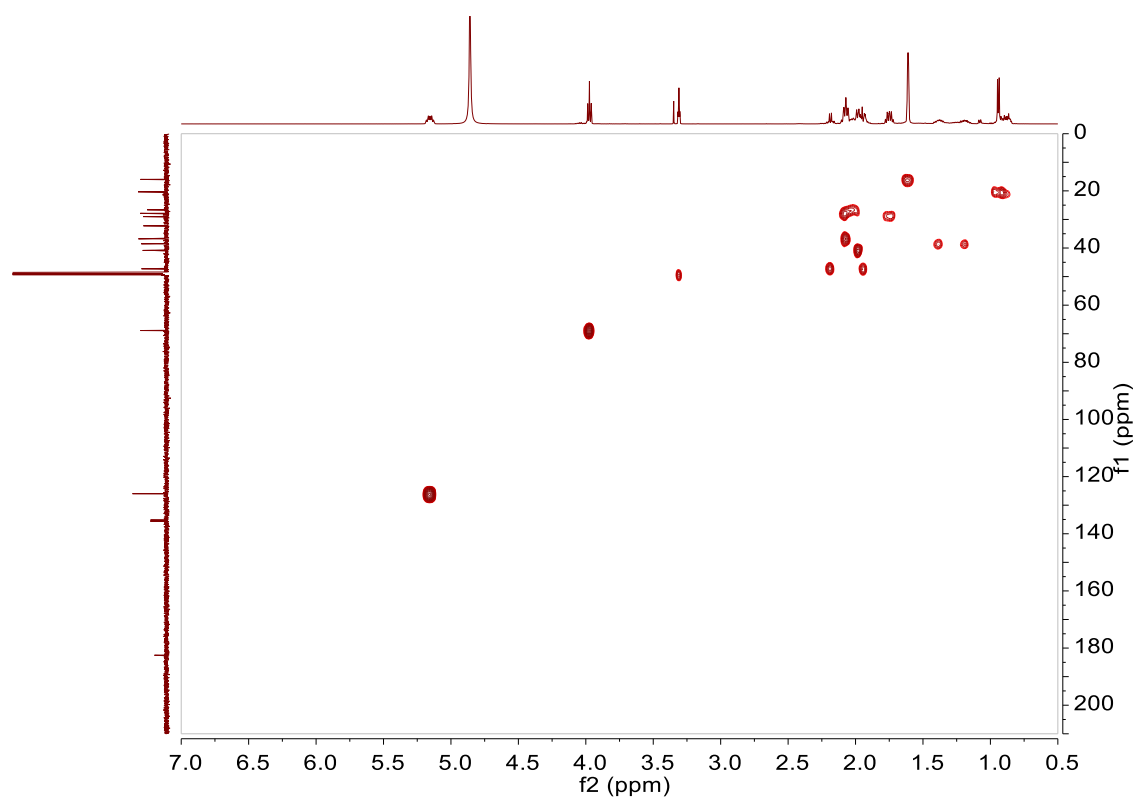


Figure S37: HSQC spectrum of **8** in methanol- d_4

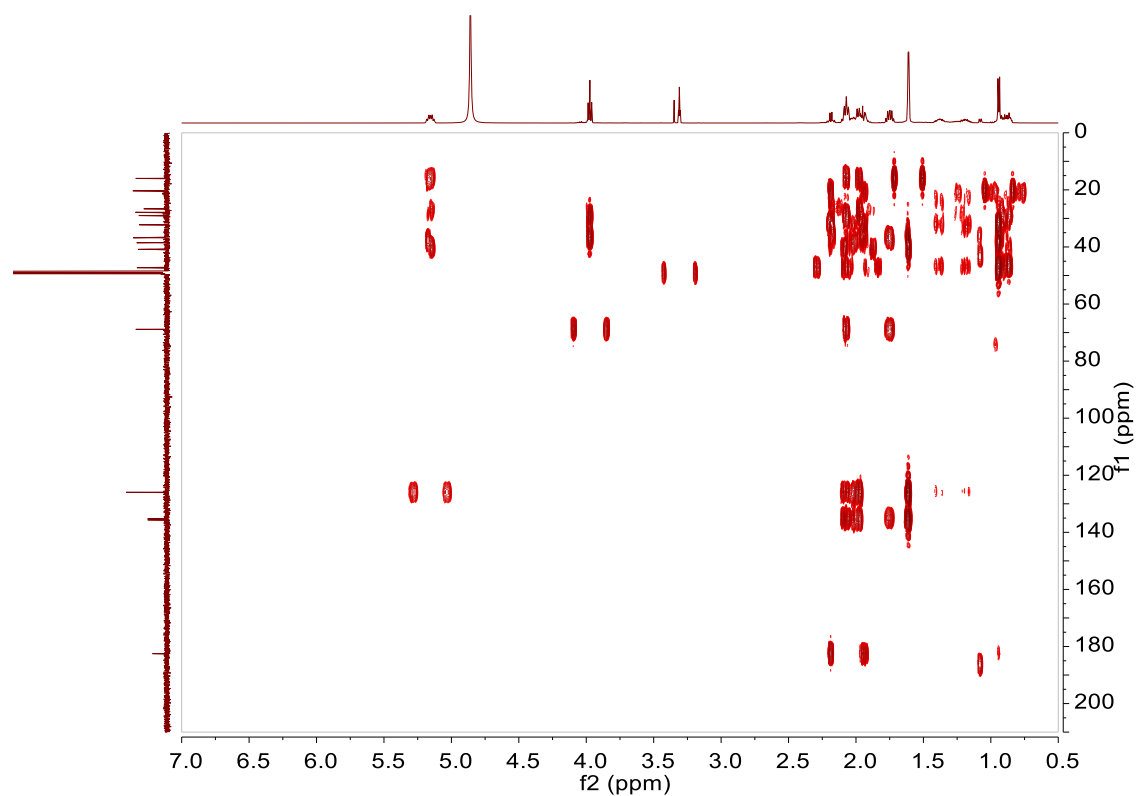


Figure S38: HMBC spectrum of **8** in methanol- d_4

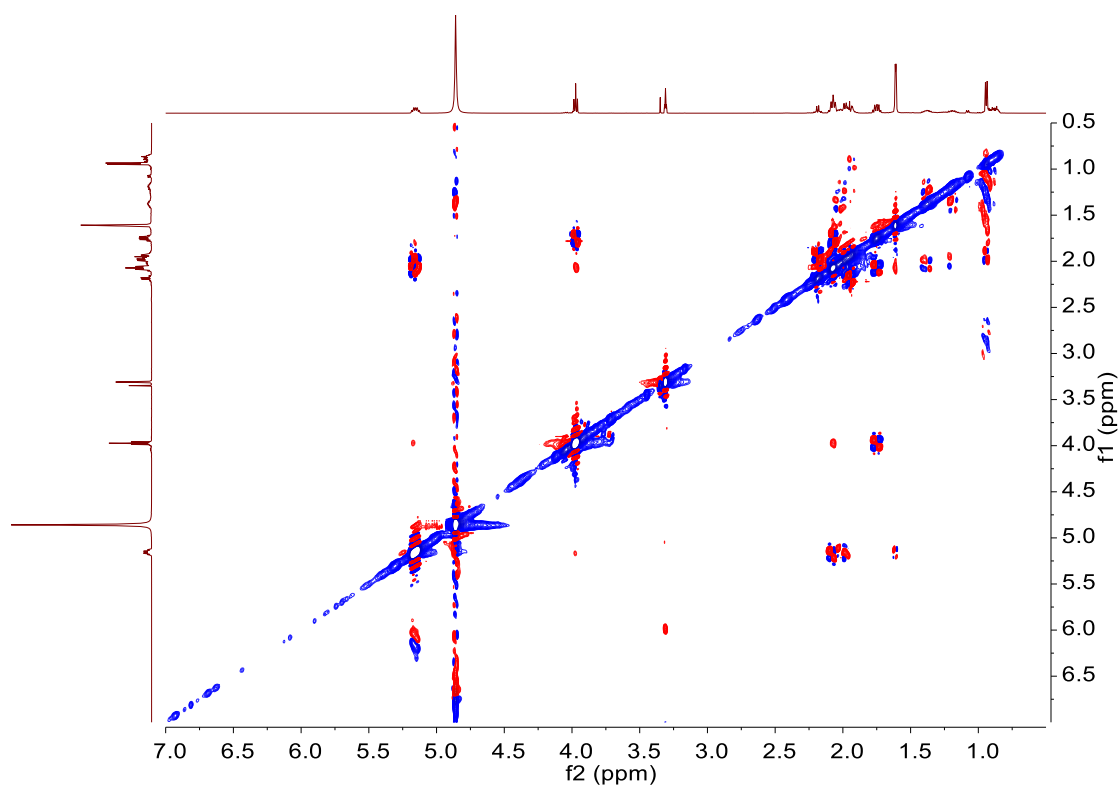


Figure S39: ROESY spectrum of **8** in methanol- d_4

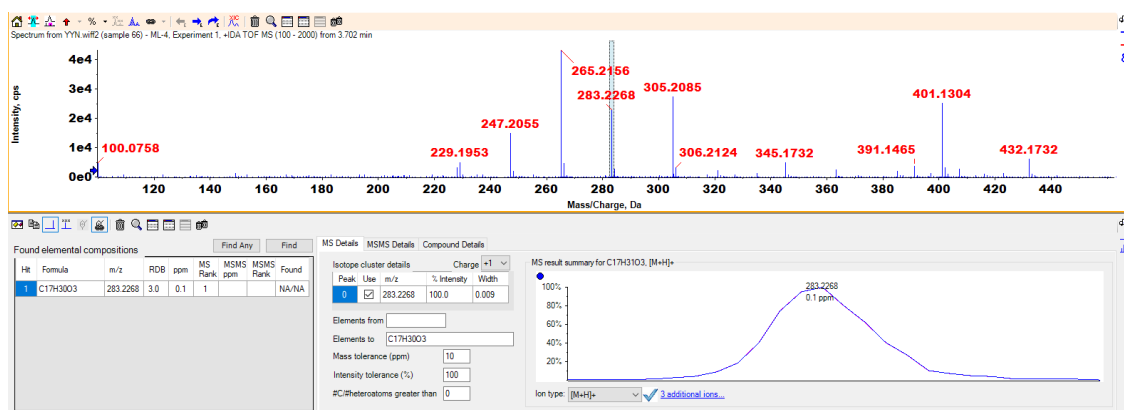


Figure S40: HRESIMS spectrum of **8**

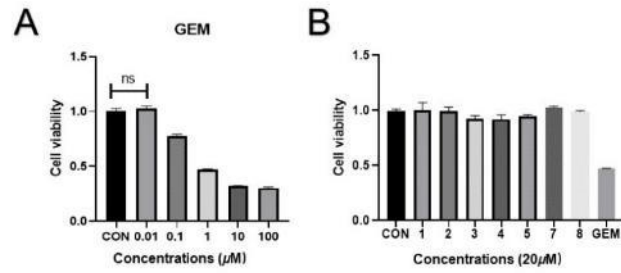


Figure S41. Compounds inhibited proliferation of Panc02-h7-GP-GFP cells. Cells were treated with gemcitabine, compounds at a 20 μM concentration, or DMSO for 48 h. The proliferation of Panc02-h7-GP-GFP cells in response to gemcitabine and the compounds was assessed by the CCK-8 assay. **A**, gemcitabine (GEM) inhibited proliferation of Panc02-h7-GP-GFP cells at 0.01, 0.1, 1, 10, and 100 μM concentrations. **B**, compounds were ineffective in inhibiting cell proliferation at 20 μM , using DMSO as a control and gemcitabine (GEM) at 1 μM as a positive control drug.

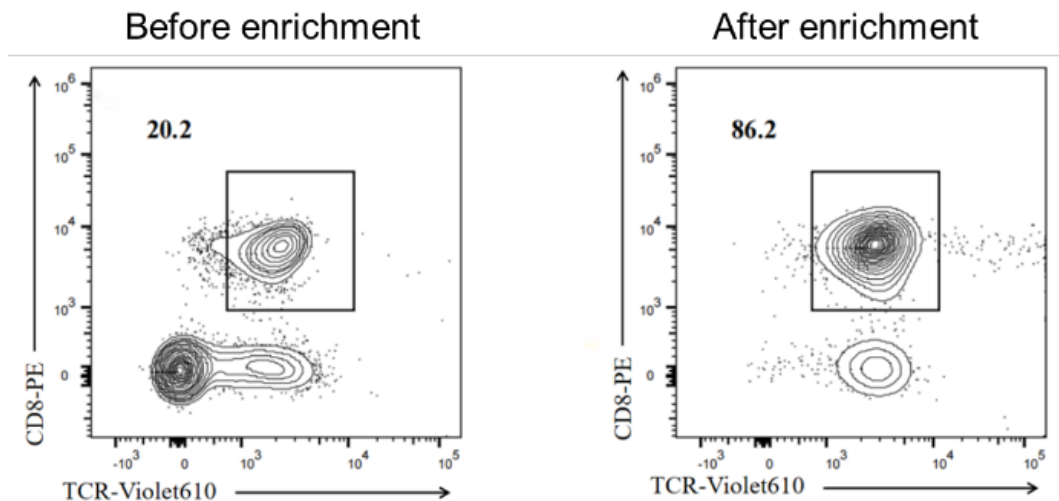


Figure S42: Purification of CD8⁺T cells in vitro.

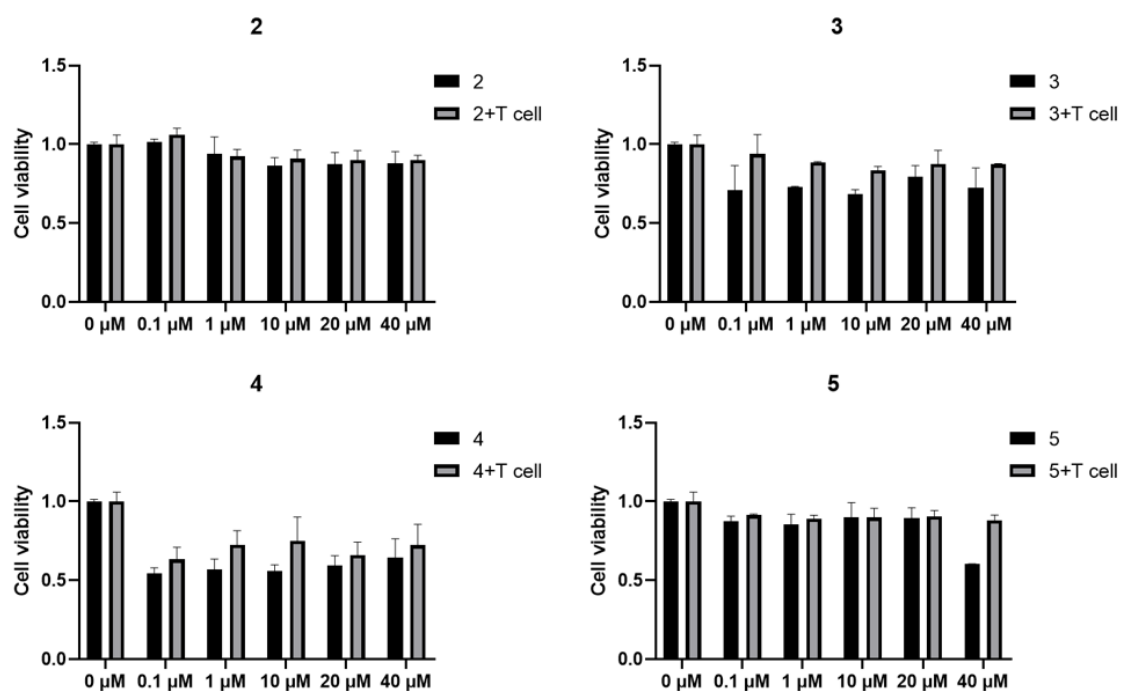


Figure S43: Compounds affected the antitumor activity of CD8⁺ T cells in vitro. Cells were incubated in the presence of the corresponding concentration of compounds or DMSO for 18 h and the fluorescence intensity was detected by a microplate reader (emission light 476 nm, excitation light 514 nm).