

Discovery of lipid peroxidation inhibitors from *Bacopa* species prioritized through multivariate data analysis and multi-informative molecular networking

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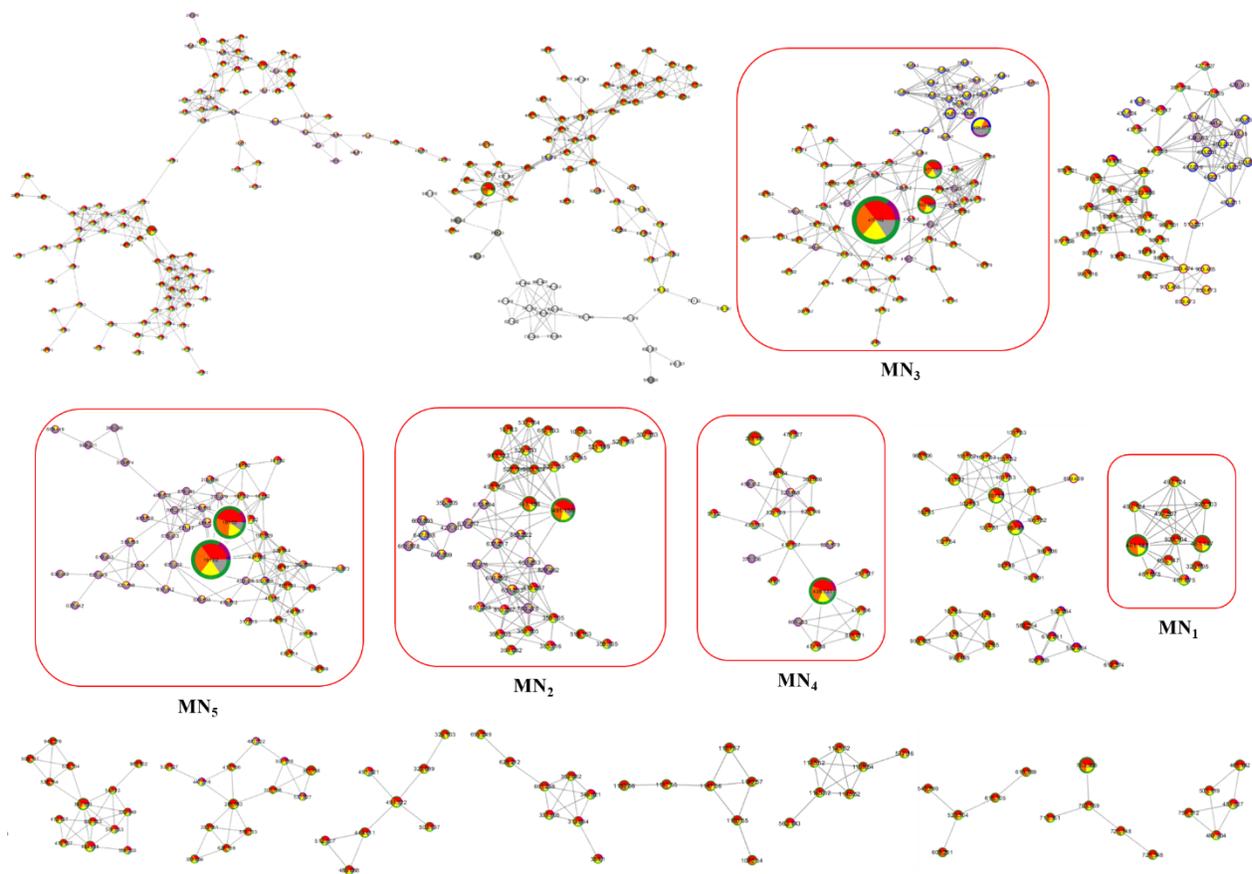


Figure S1. Twenty candidate bioactive clusters with a minimum of five nodes observed by visual inspection based on dominant red color tag and five selected bioactive clusters in red square box (MN₁–MN₅) were nominated based on node size.

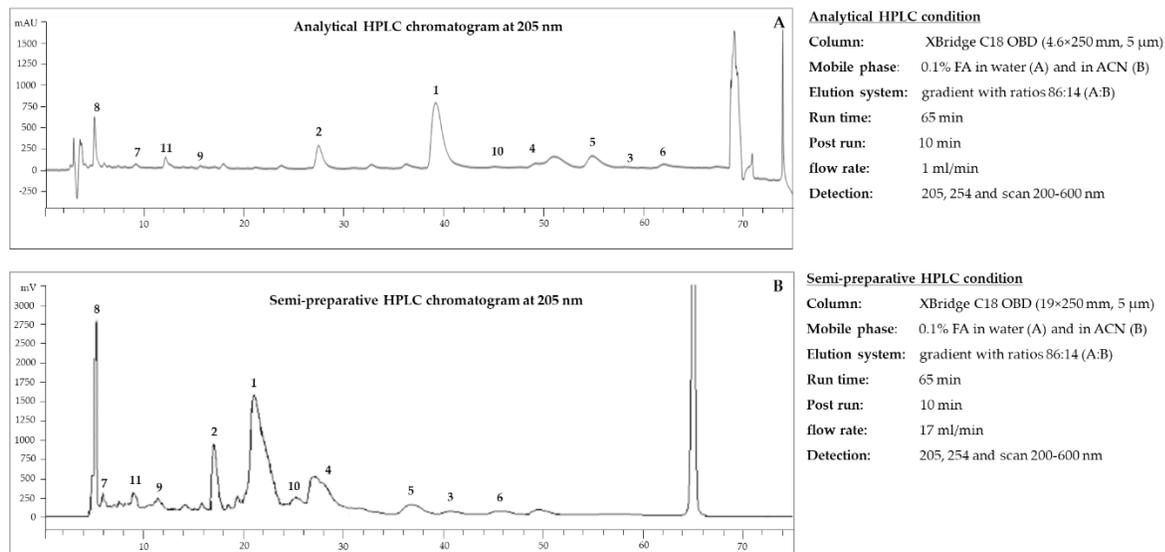


Figure S2. Representative HPLC chromatograms from method transfer between HPLC (A) and semi-preparative HPLC (B) for separation of compounds 1–11 in fraction 3 of MPLC of *B. monnieri* extract

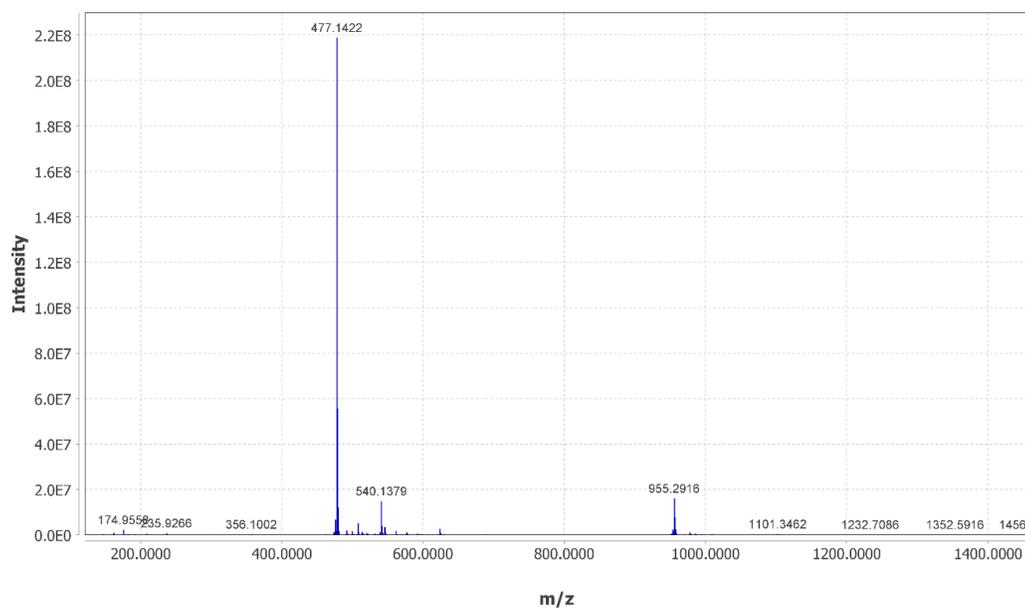


Figure S3. HRESIMS spectrum of compound 4 (negative ionization)

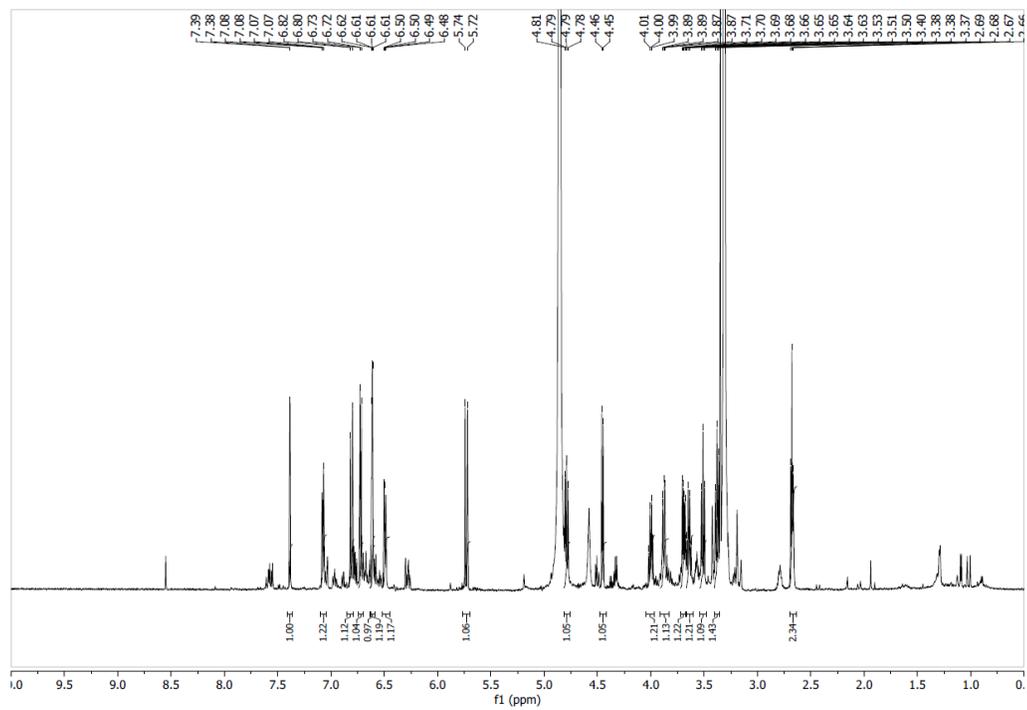


Figure S4. ^1H NMR spectrum of compound **4** in CD_3OD at 600 MHz

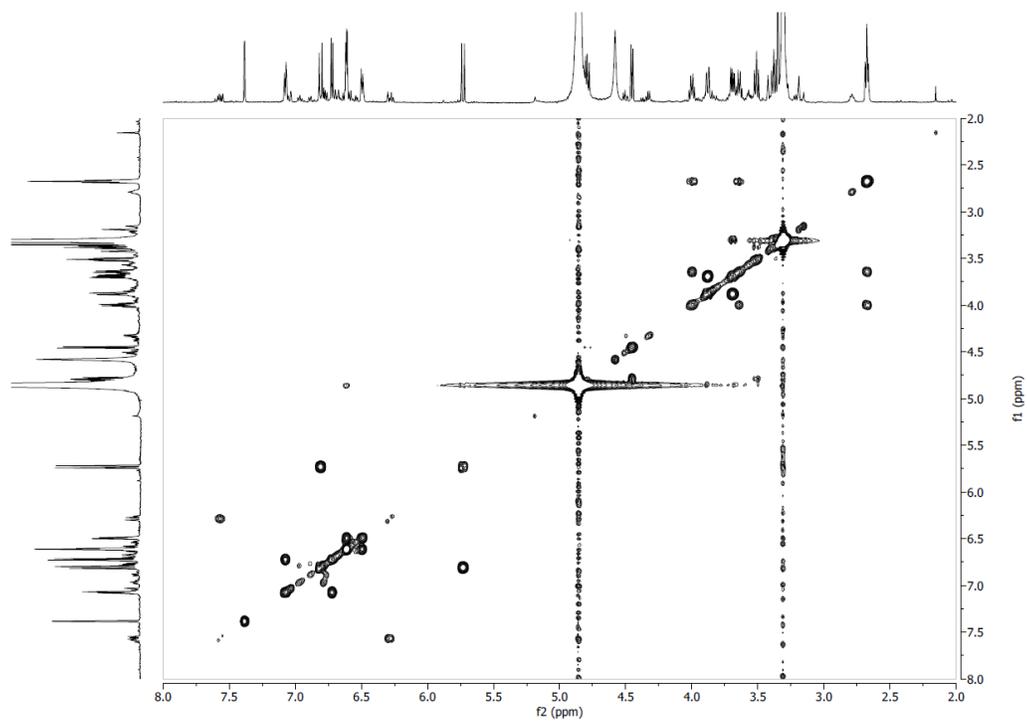


Figure S5. COSY NMR spectrum of compound **4** in CD_3OD

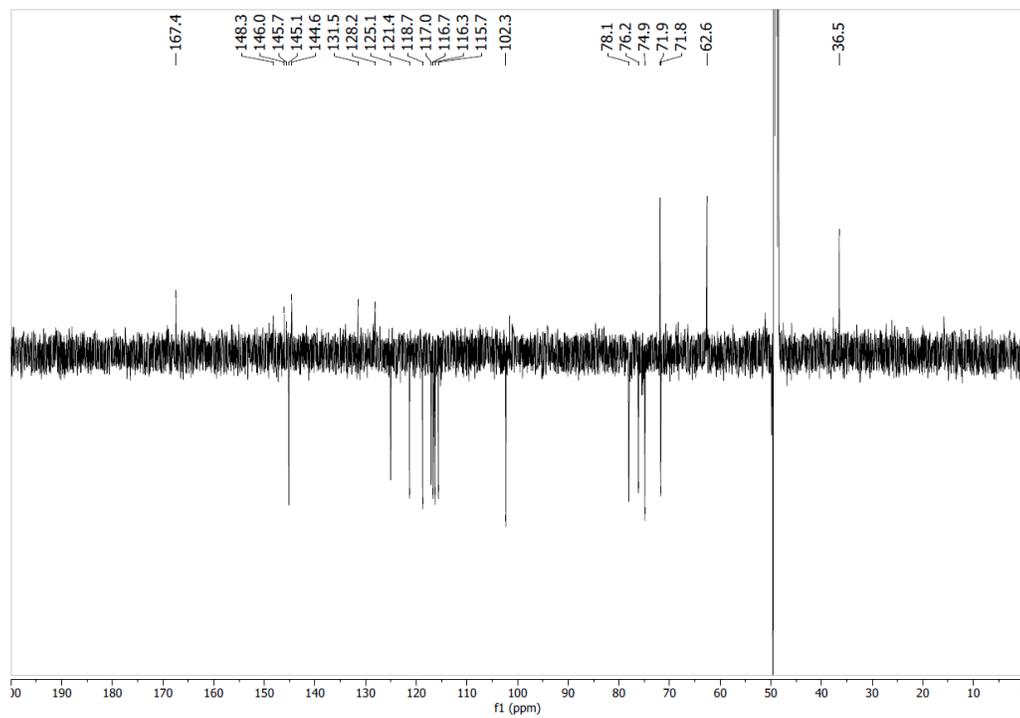


Figure S6. ^{13}C -DEPTQ NMR spectrum of compound **4** in CD_3OD at 151 MHz

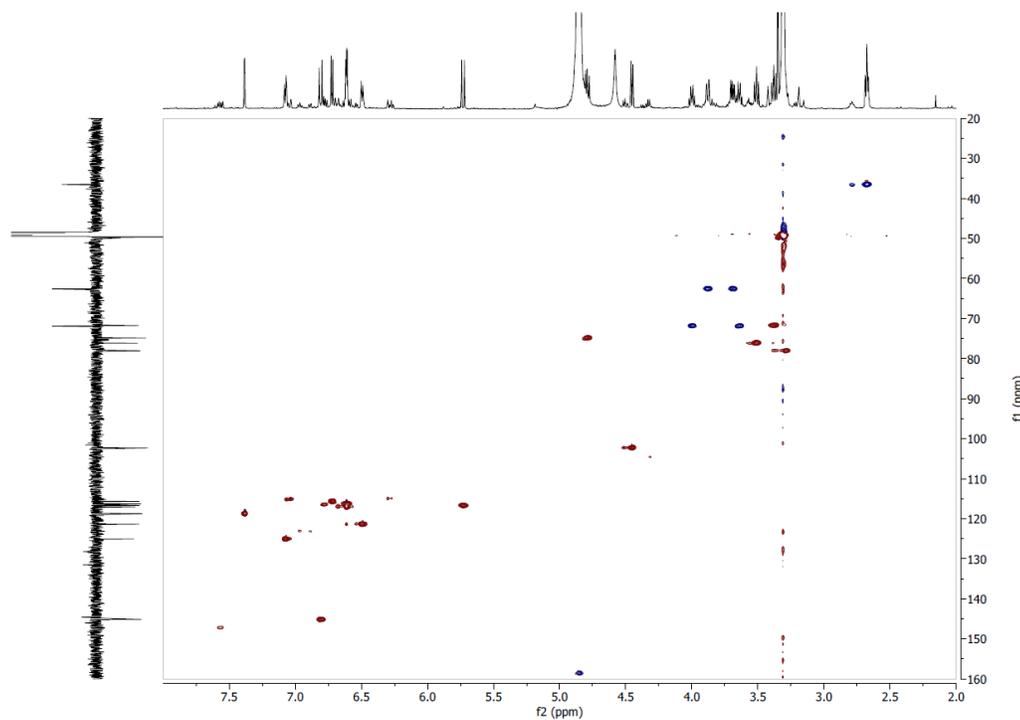


Figure S7. Edited-HSQC NMR spectrum of compound **4** in CD_3OD

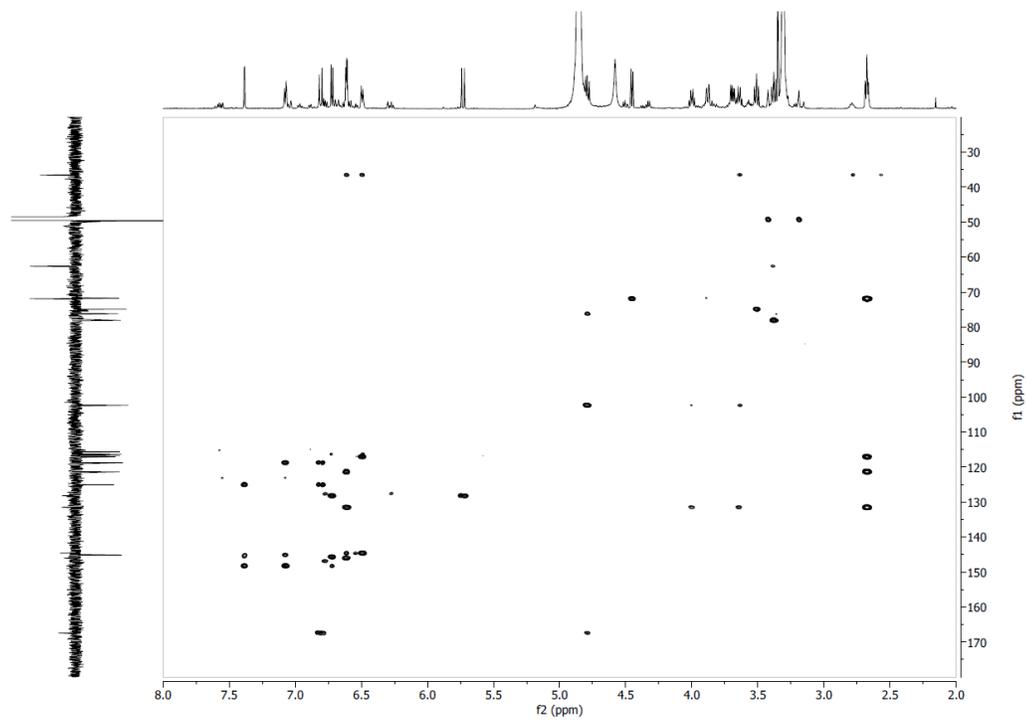


Figure S8. HMBC NMR spectrum of compound 4 in CD₃OD

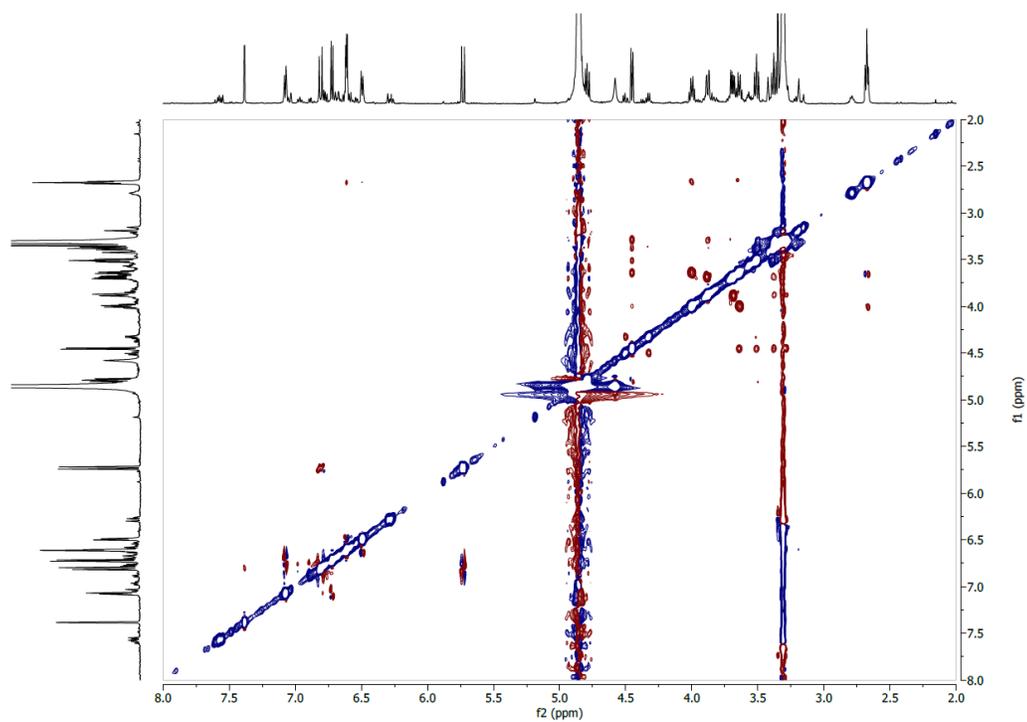


Figure S9. ROESY NMR spectrum of compound 4 in CD₃OD

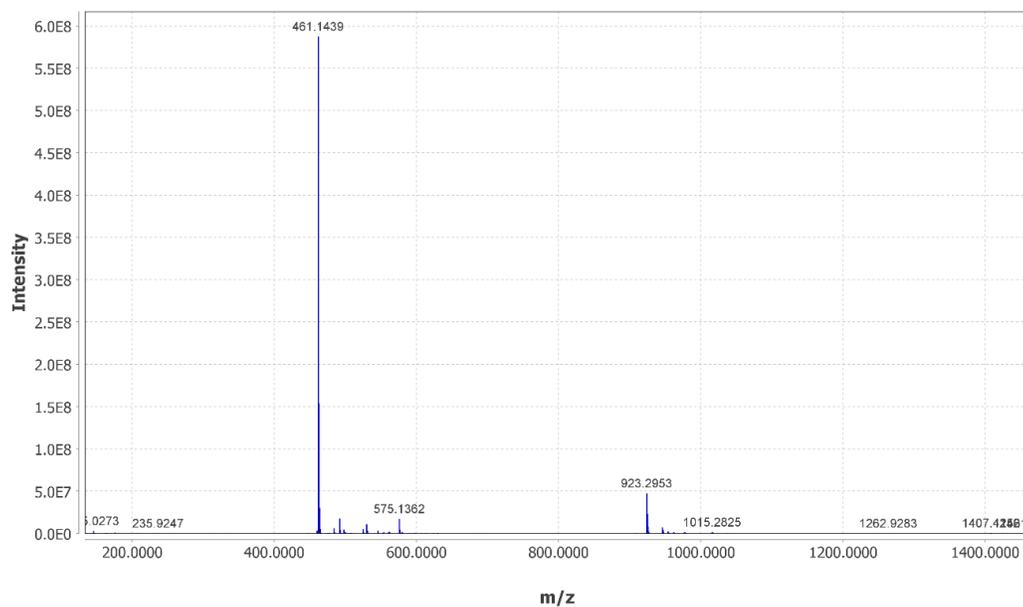


Figure S10. HRESIMS spectrum of compound 5 (negative ionization)

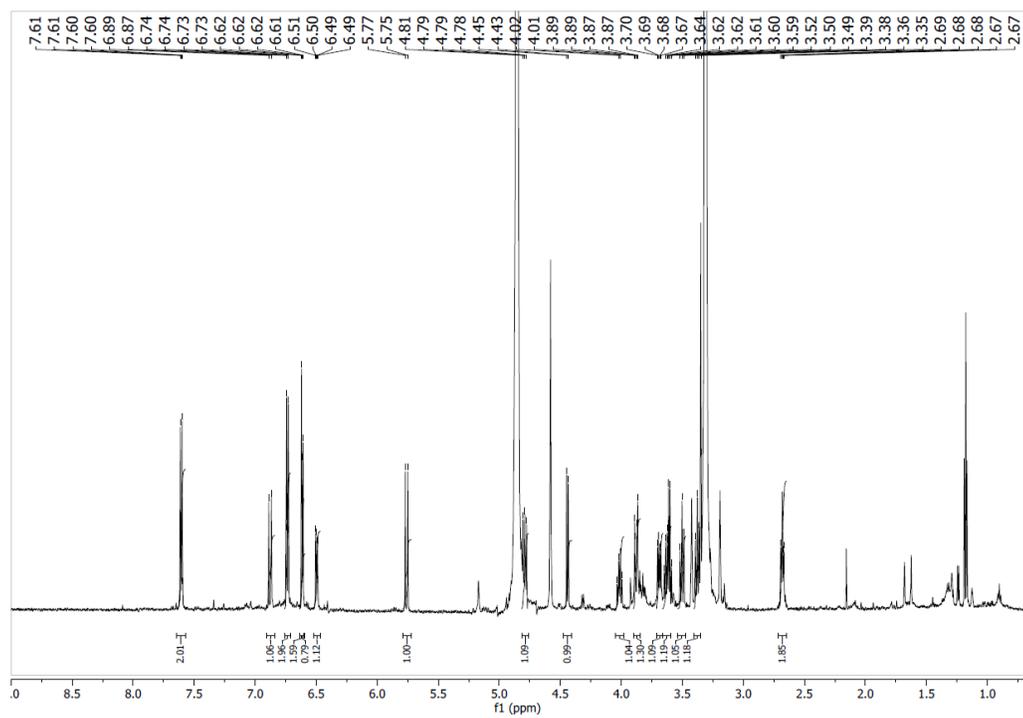


Figure S11. ¹H NMR spectrum of compound 5 in CD₃OD at 600 MHz

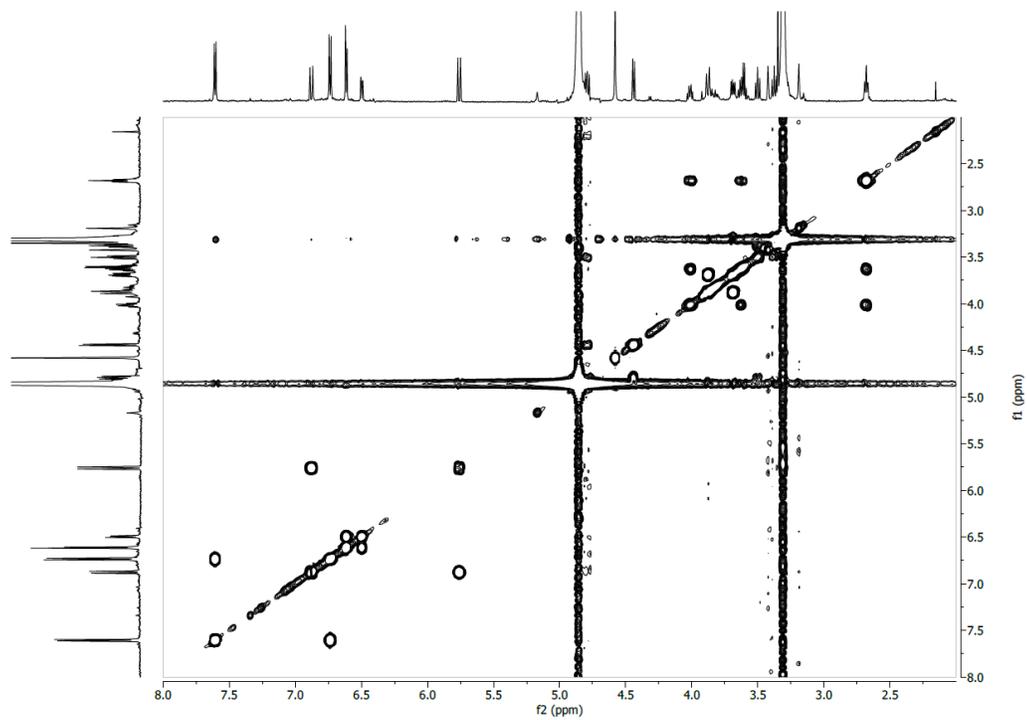


Figure S12. COSY NMR spectrum of compound 5 in CD₃OD

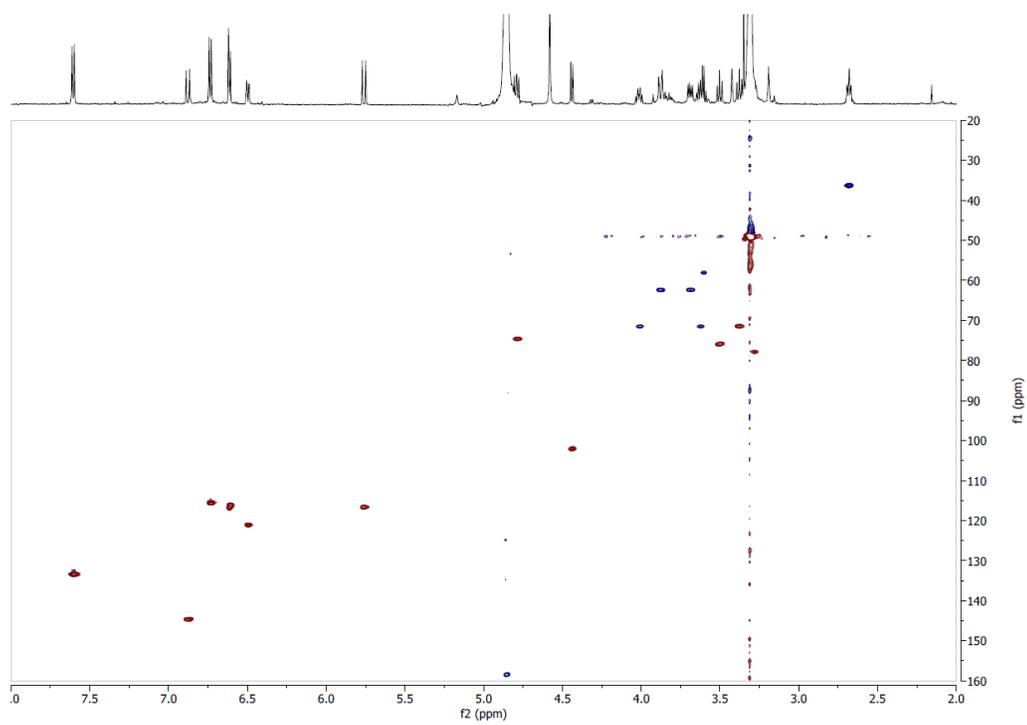


Figure S13. Edited-HSQC NMR spectrum of compound 5 in CD₃OD

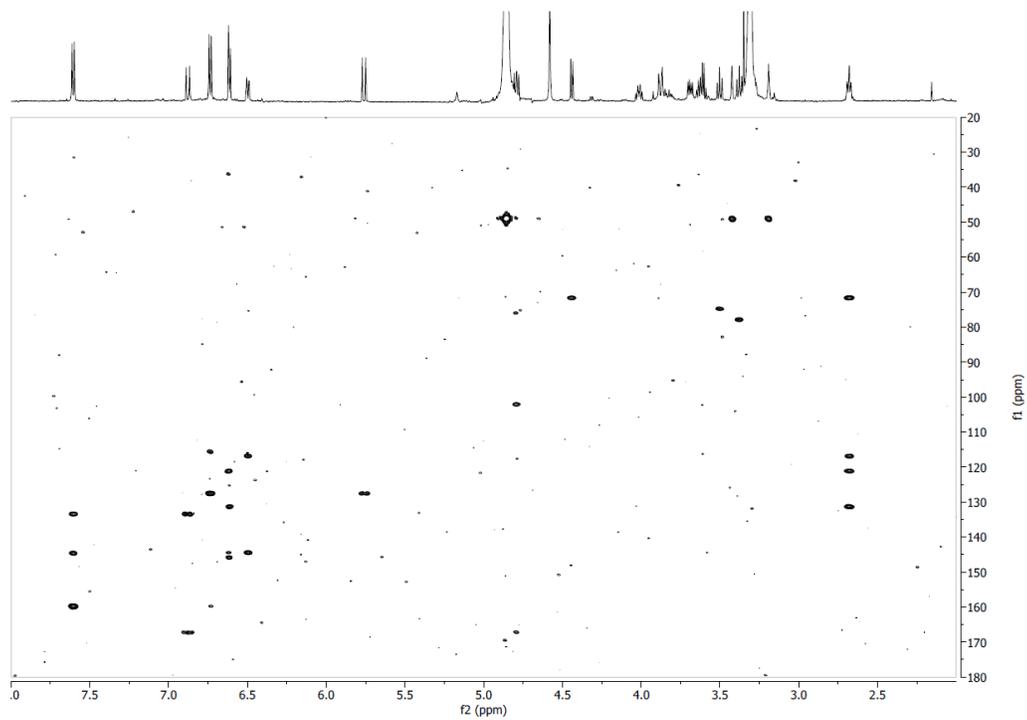


Figure S14. HMBC NMR spectrum of compound 5 in CD₃OD

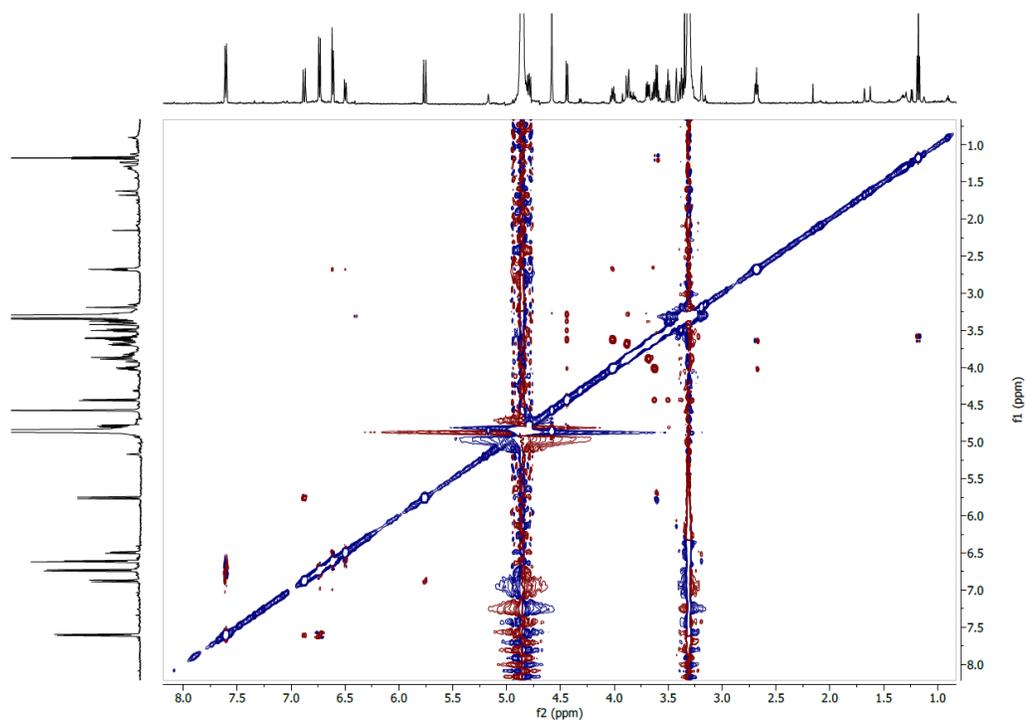


Figure S15. ROESY NMR spectrum of compound 5 in CD₃OD

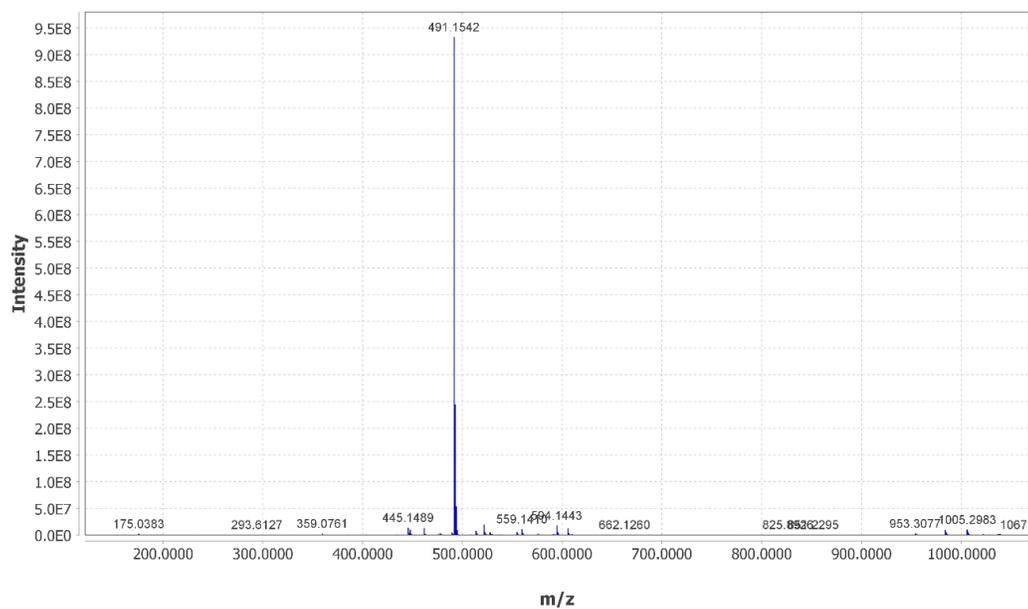


Figure S16. HRESIMS spectrum of compound 6 (negative ionization)

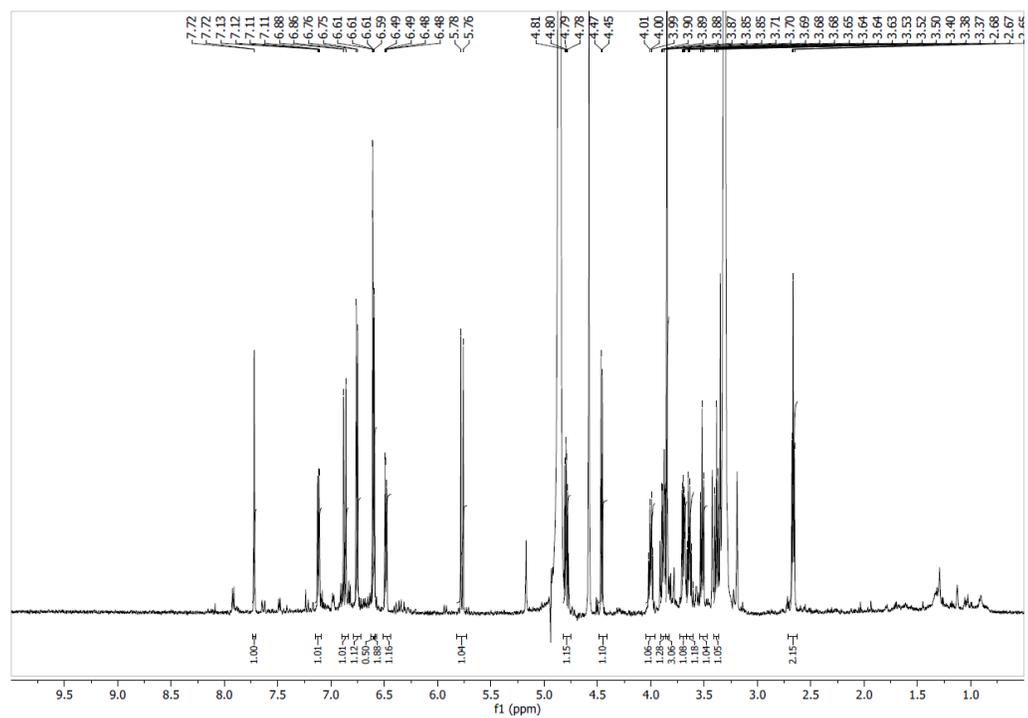


Figure S17. ¹H NMR spectrum of compound 6 in CD₃OD at 600 MHz

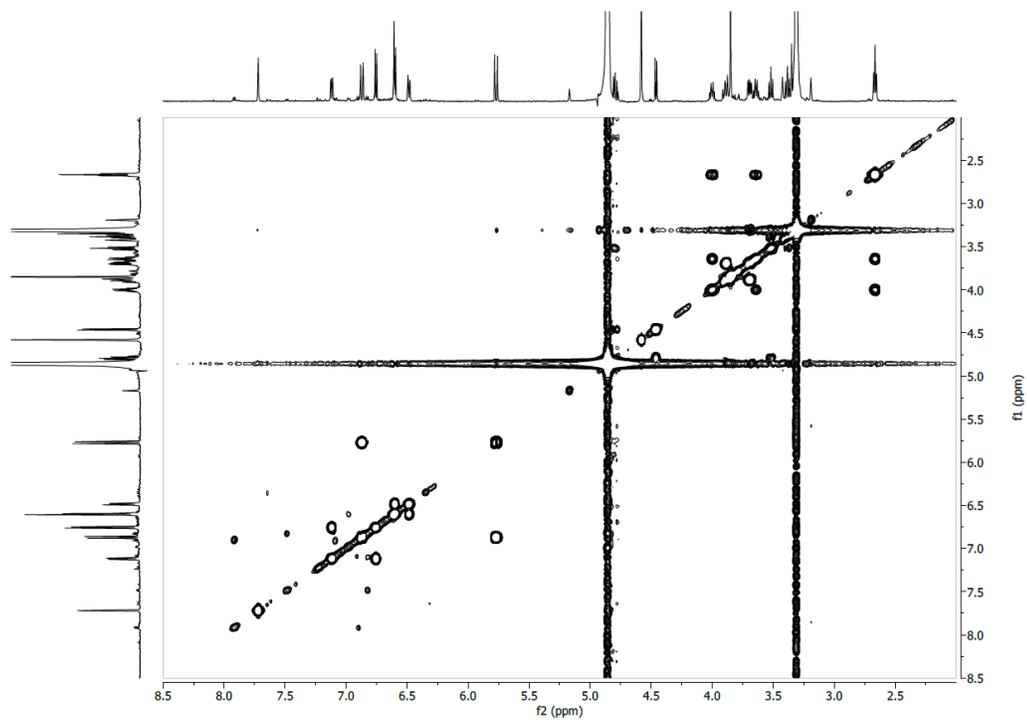


Figure S18. COSY NMR spectrum of compound 6 in CD₃OD

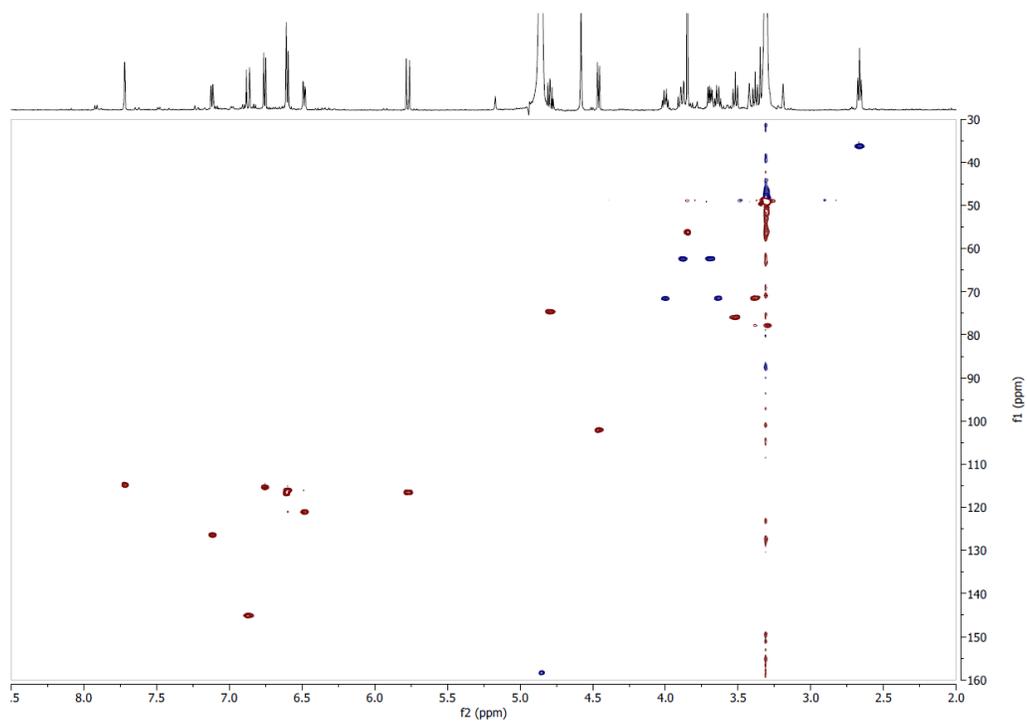


Figure S19. Edited-HSQC NMR spectrum of compound 6 in CD₃OD

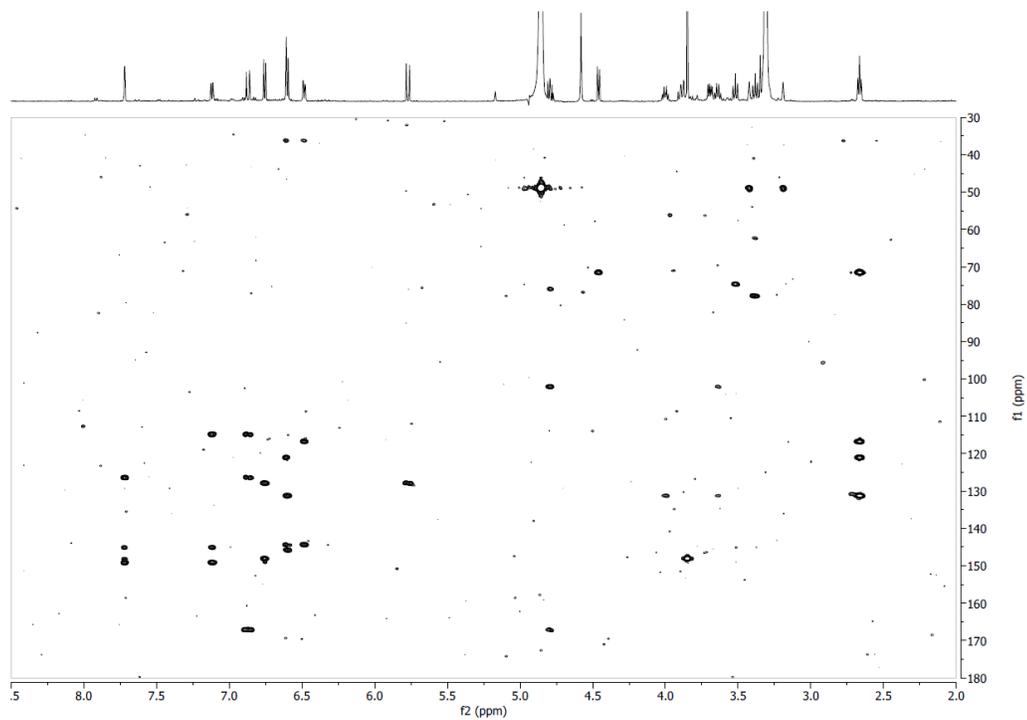


Figure S20. HMBC NMR spectrum of compound 6 in CD₃OD

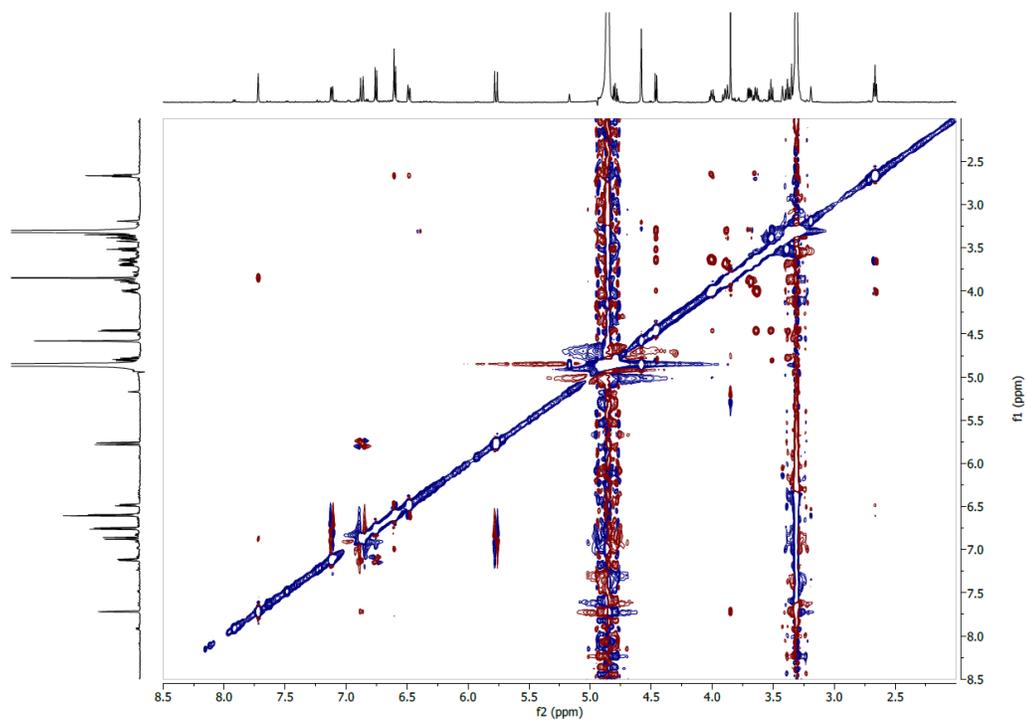


Figure S21. ROESY NMR spectrum of compound 6 in CD₃OD