

Chemical Investigation of the Indonesian Tunicate *Polycarpa aurata* and Evaluation of the Effects Against *Schistosoma mansoni* of the Novel Alkaloids Polyaurines A and B.

Marcello Casertano¹, Concetta Imperatore¹, Paolo Luciano¹, Anna Aiello¹, Masteria Yunovilsa Putra², Roberto Gimmelli³, Giovina Ruberti³ and Marialuisa Menna^{1,*}

- ¹ The NeaNat Group, Department of Pharmacy, University of Naples "Federico II", Via D. Montesano 49, 80131 Napoli, Italy; marcello.casertano@unina.it (M.C.); cimperat@unina.it (C.I.); pluciano@unina.it (P.L.); aiello@unina.it (A.A.)
 - ² Research Center for Oceanography, Indonesian Institute of Sciences. Jl Pasir Putih Raya 1, DKI Jakarta 14430, Indonesia; mast001@lipi.go.id (M.Y.P.)
 - ³ Institute of Cell biology and Neurobiology, National Research Council, Campus A. Buzzati-Traverso, Via E. Ramarini, 32, 00015 Monterotondo (Roma), Italy; roberto.gimmelli@ibcn.cnr.it (R.G.); giovina.ruberti@cnr.it (G.R.)
- * Correspondence: mlmenna@unina.it (M.M.); Tel.: +39-081-678518

TABLE OF CONTENTS

| | |
|---|----|
| Figure S1. HRESIMS spectrum of polyaurine A (1)..... | 3 |
| Figure S2. ¹ H NMR spectrum of polyaurine A (1) in CDCl ₃ (500 MHz)..... | 3 |
| Figure S3. ¹³ C NMR spectrum of polyaurine A (1) in CDCl ₃ (500 MHz)..... | 4 |
| Figure S4. HSQC spectrum of polyaurine A (1) in CDCl ₃ (500 MHz)..... | 4 |
| Figure S5. COSY spectrum of polyaurine A (1) in CDCl ₃ (500 MHz)..... | 5 |
| Figure S6. HMBC spectrum of polyaurine A (1) in CDCl ₃ (500 MHz)..... | 5 |
| Figure S7. HRESI-MS spectrum of polyaurine B (2)..... | 6 |
| Figure S8. ¹ H NMR spectrum of polyaurine B (2) in CDCl ₃ (700 MHz)..... | 6 |
| Figure S9. ¹³ C NMR spectrum of polyaurine B (2) in CDCl ₃ (700 MHz)..... | 7 |
| Figure S10. HSQC spectrum of polyaurine B (2) in CDCl ₃ (700 MHz)..... | 7 |
| Figure S11. COSY spectrum of polyaurine B (2) in CDCl ₃ (700 MHz)..... | 8 |
| Figure S12. HMBC spectrum of polyaurine B (2) in CDCl ₃ (700 MHz)..... | 8 |
| Figure S13. HRESI-MS spectrum of compound 3..... | 9 |
| Figure S14. ¹ H NMR spectrum of compound 3 in CDCl ₃ (700 MHz)..... | 9 |
| Figure S15. COSY spectrum of compound 3 in CDCl ₃ (700 MHz)..... | 10 |
| Figure S16. HRESI-MS spectrum of compound 4 | 10 |
| Figure S17. ¹ H NMR spectrum of compound 4 in CDCl ₃ (700 MHz)..... | 11 |
| Figure S18. HSQC spectrum of compound 4 in CDCl ₃ (700 MHz)..... | 11 |
| Figure S19. COSY spectrum of compound 4 in CDCl ₃ (700 MHz)..... | 12 |
| Figure S20. HMBC spectrum of compound 4 in CDCl ₃ (700 MHz)..... | 12 |
| Figure S21. HRESI-MS spectrum of compound 5 | 13 |
| Figure S22. ¹ H NMR spectrum of compound 5 in CDCl ₃ (700 MHz)..... | 13 |
| Figure S23. HRESI-MS spectrum of compound 6 | 14 |
| Figure S24. ¹ H NMR spectrum of compound 6 in CDCl ₃ (500 MHz)..... | 14 |
| Figure S25. HRESI-MS spectrum of compound 7 | 15 |
| Figure S26. ¹ H NMR spectrum of compound 7 in CDCl ₃ (500 MHz)..... | 15 |
| Figure S27. HRESI-MS spectrum of compound 8 | 16 |
| Figure S28. ¹ H NMR spectrum of compound 8 in CDCl ₃ (700 MHz)..... | 16 |

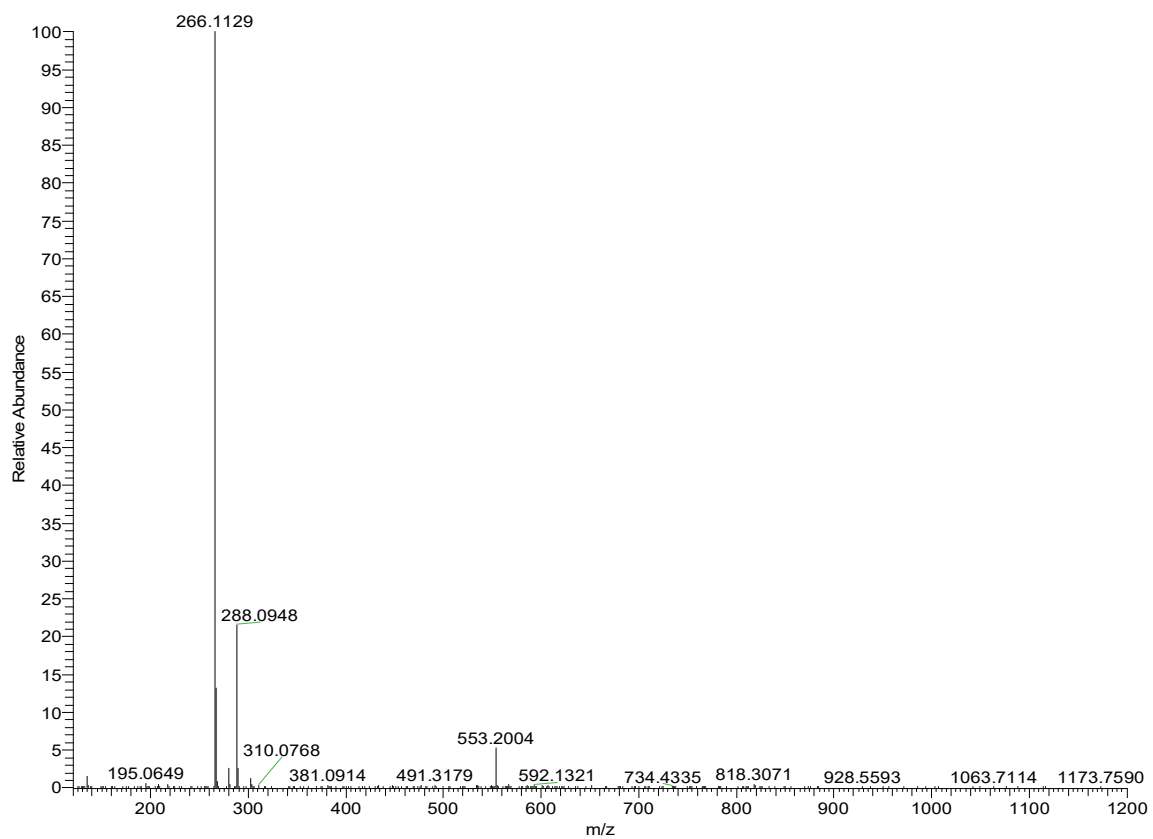


Figure S1. HRESI-MS spectrum of polyaurine A (1)

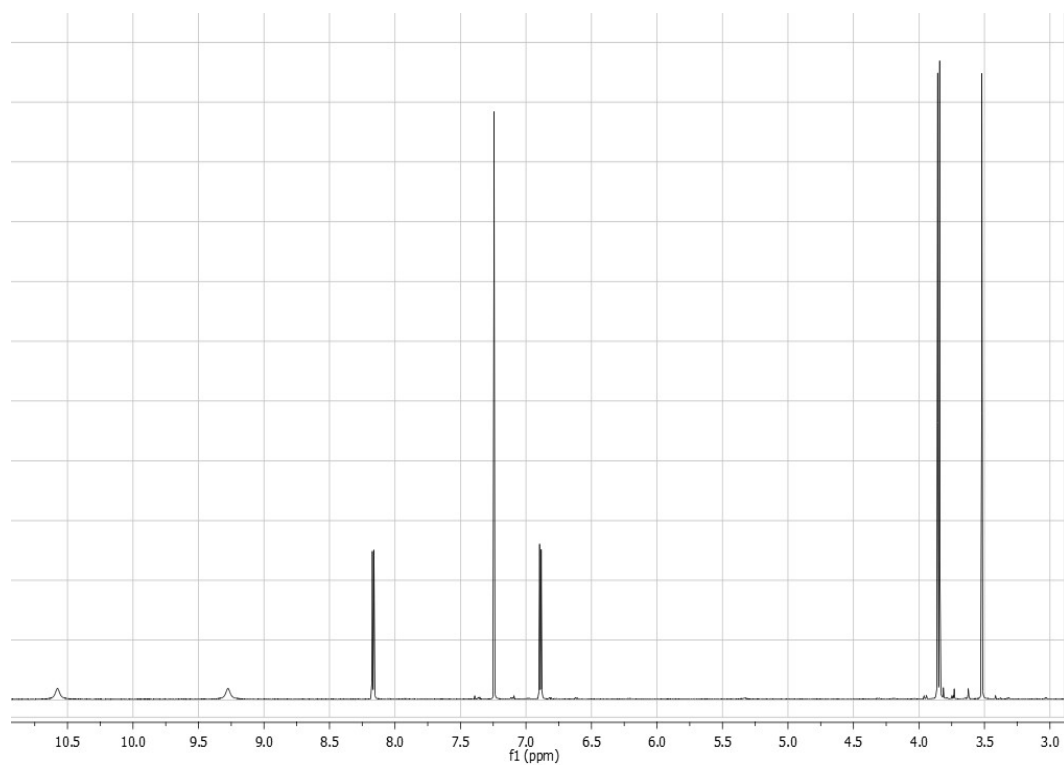


Figure S2. ¹H NMR spectrum of polyaurine A (1) in CDCl₃ (500 MHz)

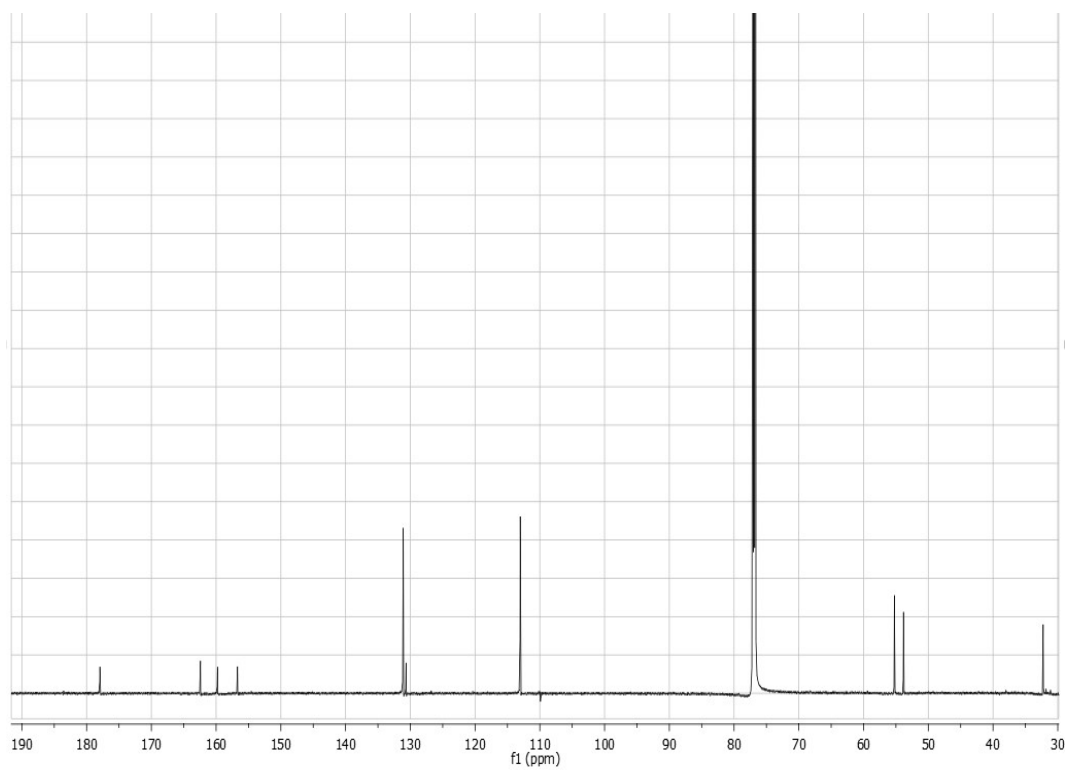


Figure S3. ^{13}C NMR spectrum of polyaurine A (1) in CDCl_3 (500 MHz)

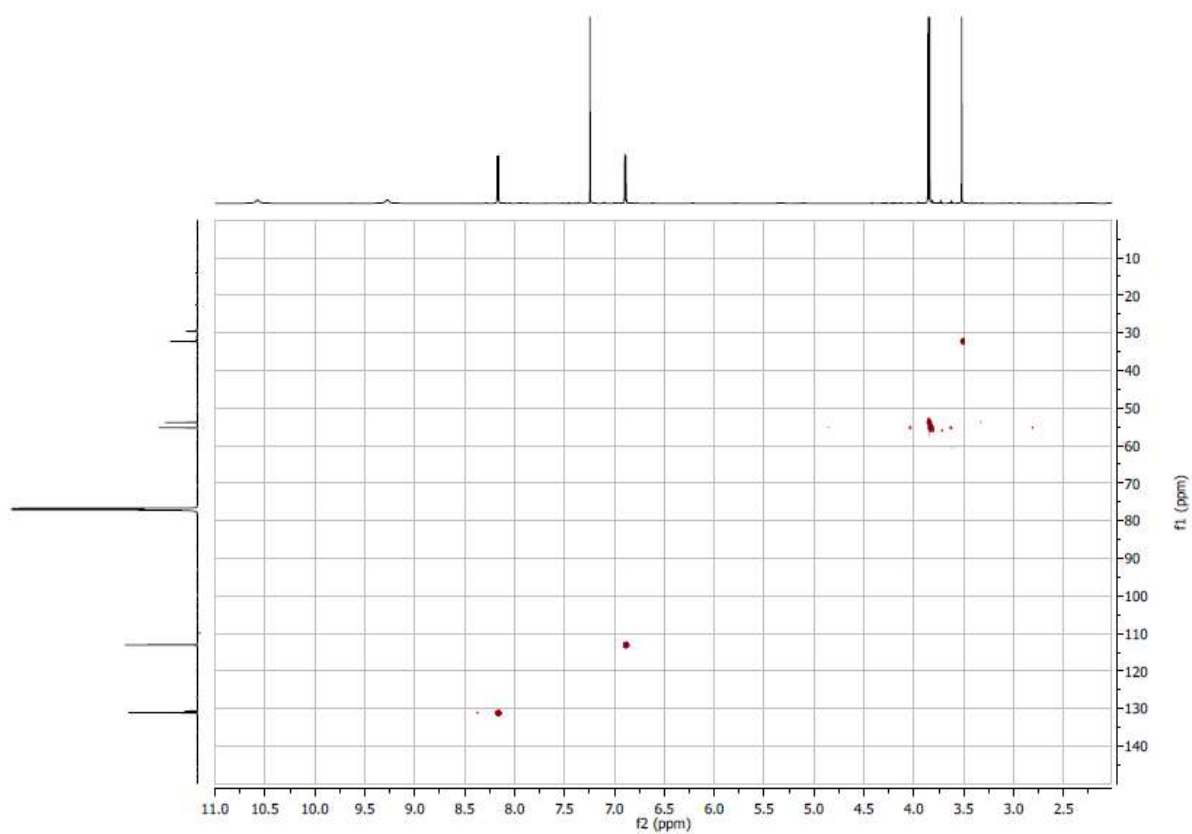


Figure S4. HSQC spectrum of polyaurine A (1) in CDCl_3 (500 MHz)

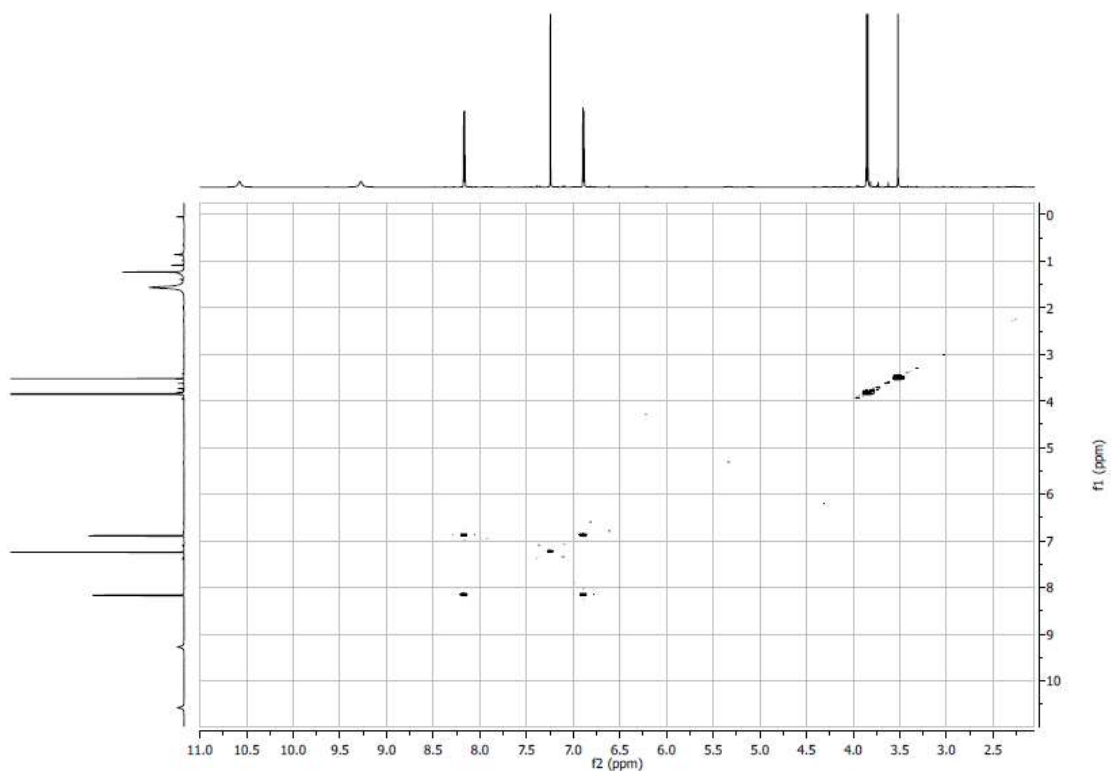


Figure S5. COSY spectrum of polyaurine A (**1**) in CDCl₃ (500 MHz)

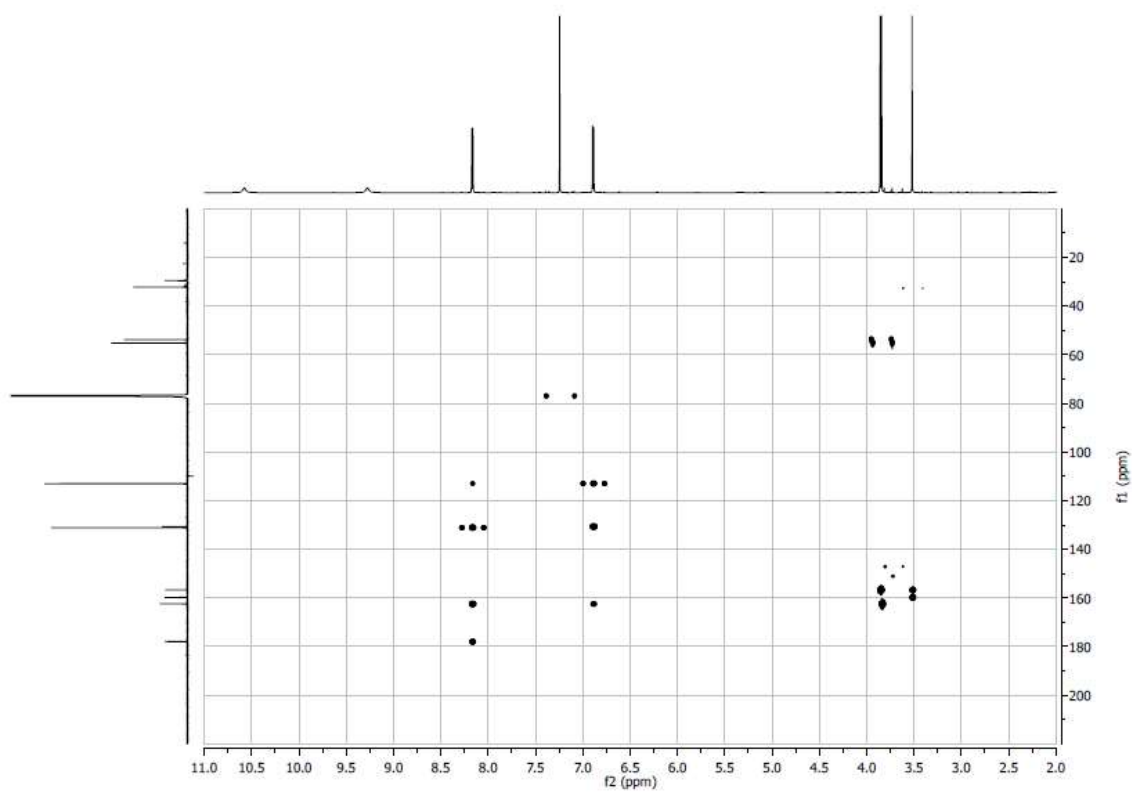


Figure S6. HMBC spectrum of polyaurine A (**1**) in CDCl₃ (500 MHz)

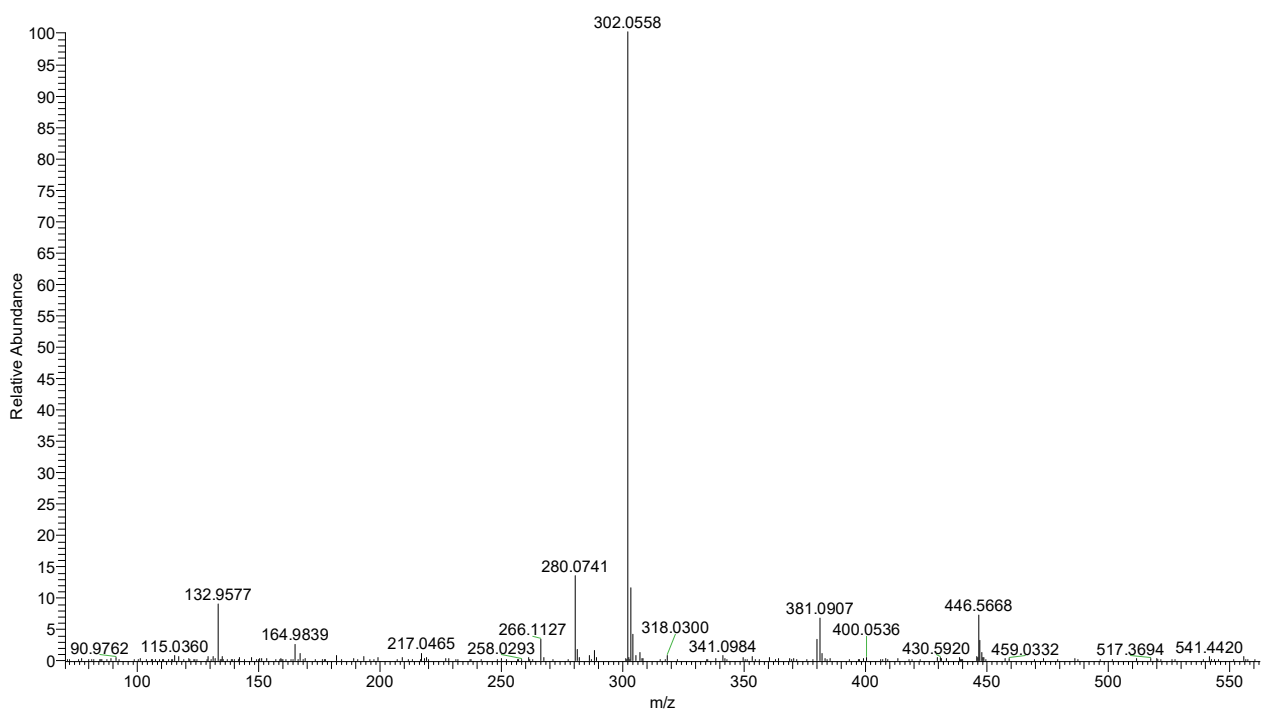


Figure S7. HRESI-MS spectrum of polyaurine B (2)

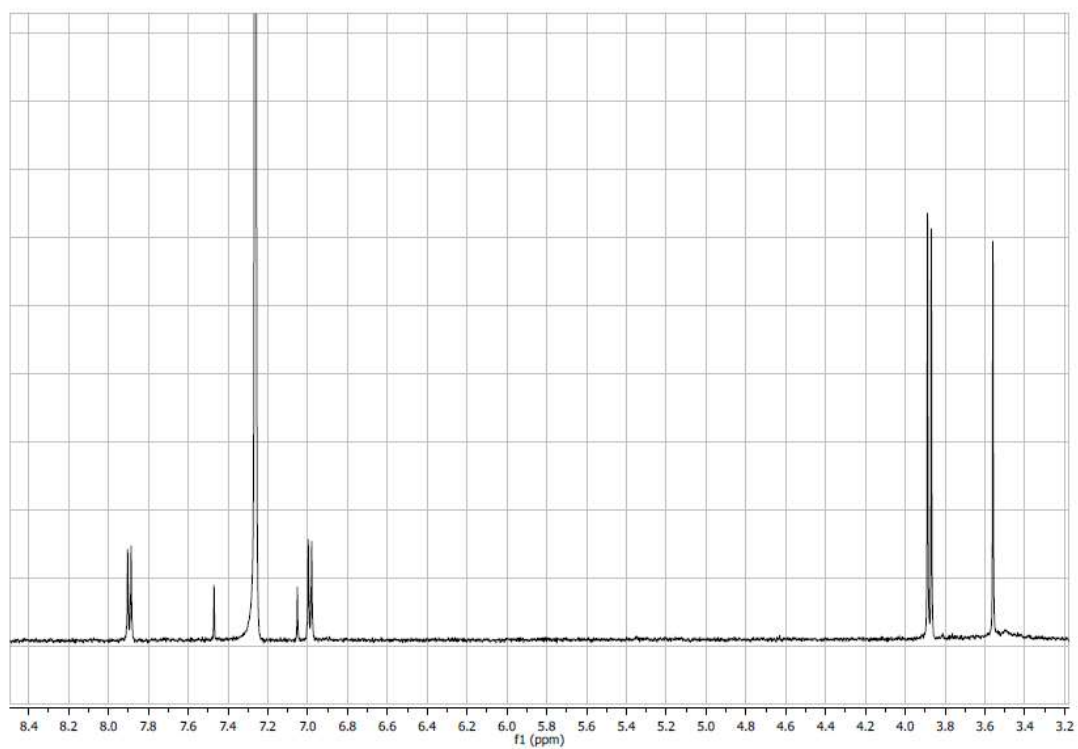


Figure S8. ¹H NMR spectrum of polyaurine B (2) in CDCl₃ (700 MHz)

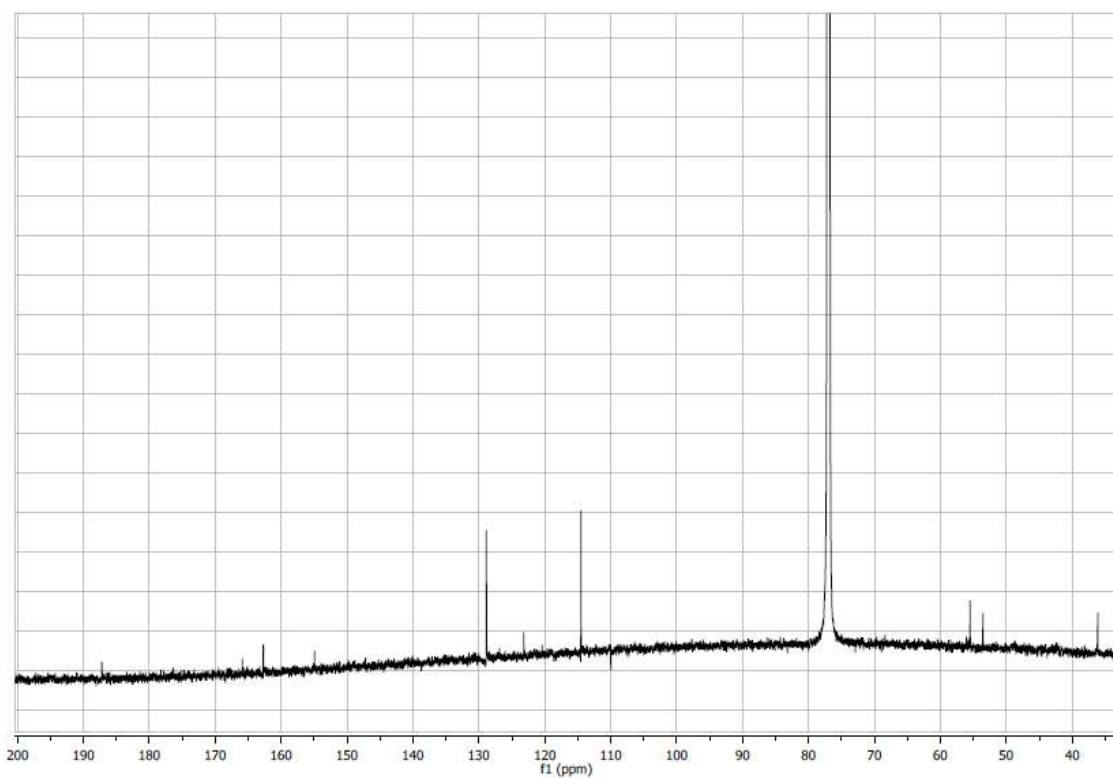


Figure S9. ^{13}C NMR spectrum of polyaurine B (**2**) in CDCl_3 (700 MHz)

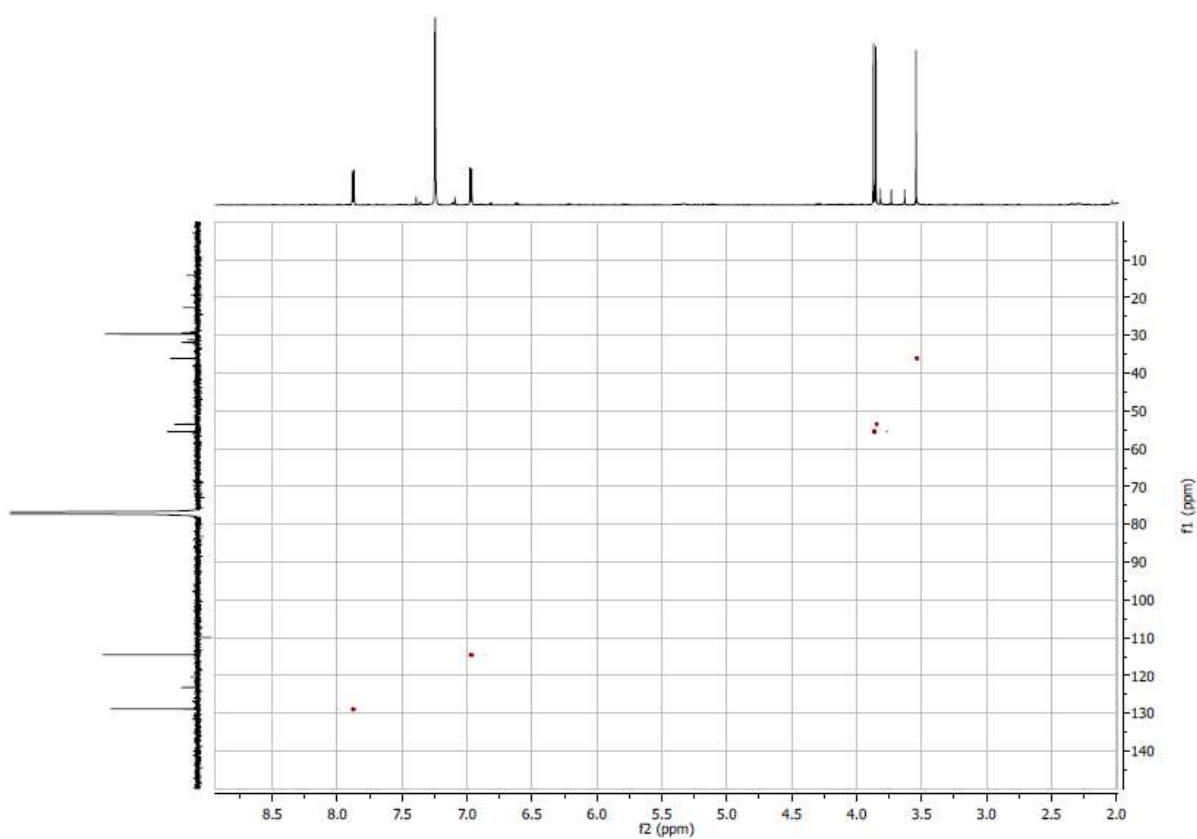


Figure S10. HSQC spectrum of polyaurine B (**2**) in CDCl_3 (700 MHz)

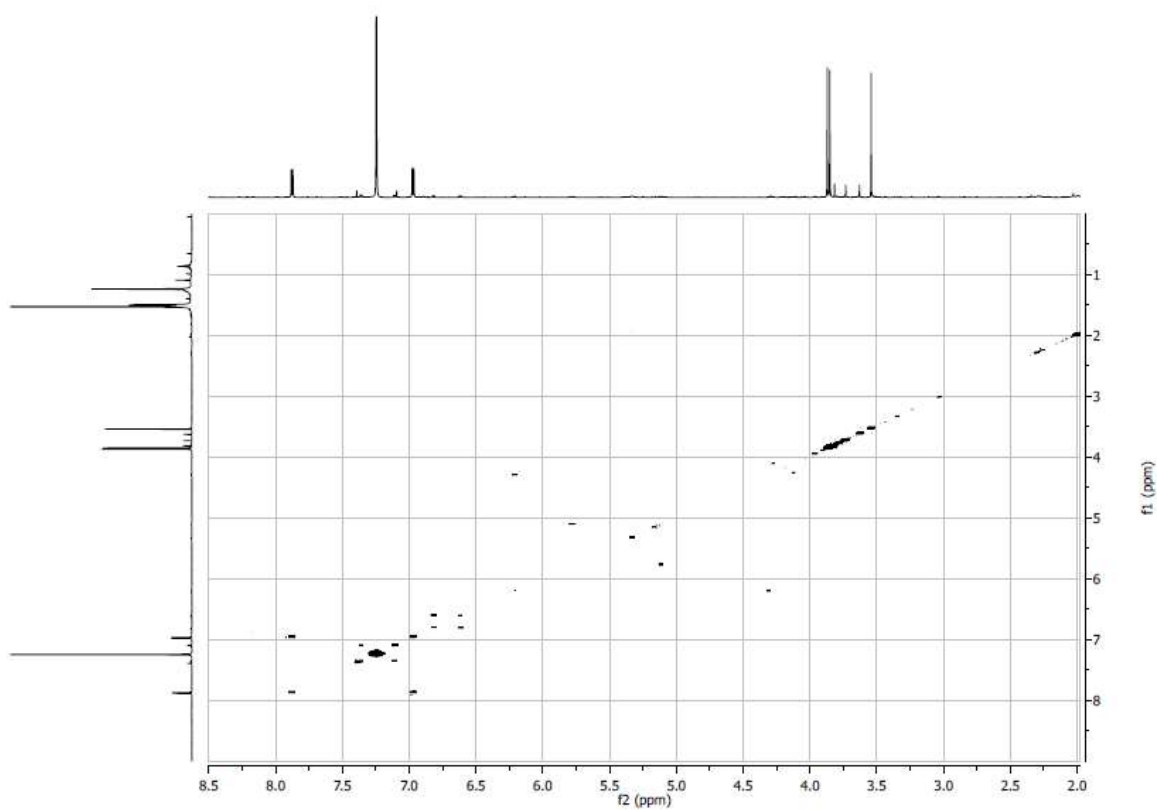


Figure S11. COSY spectrum of polyaurine B (**2**) in CDCl₃ (700 MHz)

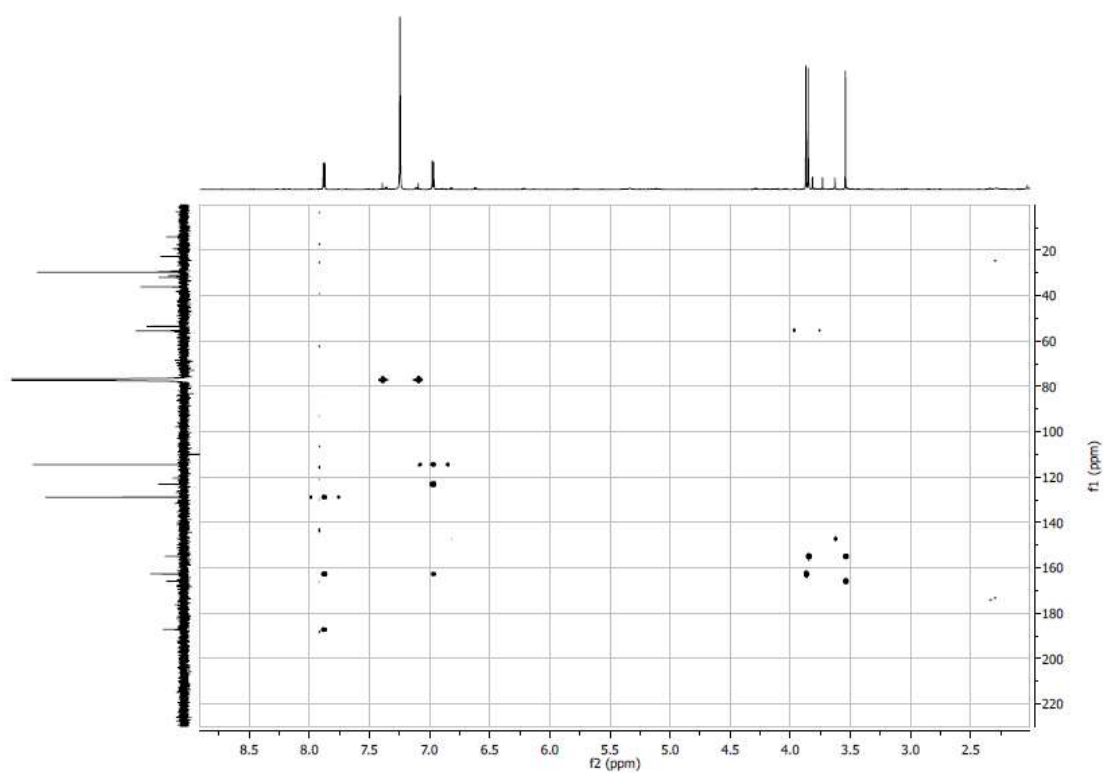


Figure S12. HMBC spectrum of polyaurine B (**2**) in CDCl₃ (700 MHz)

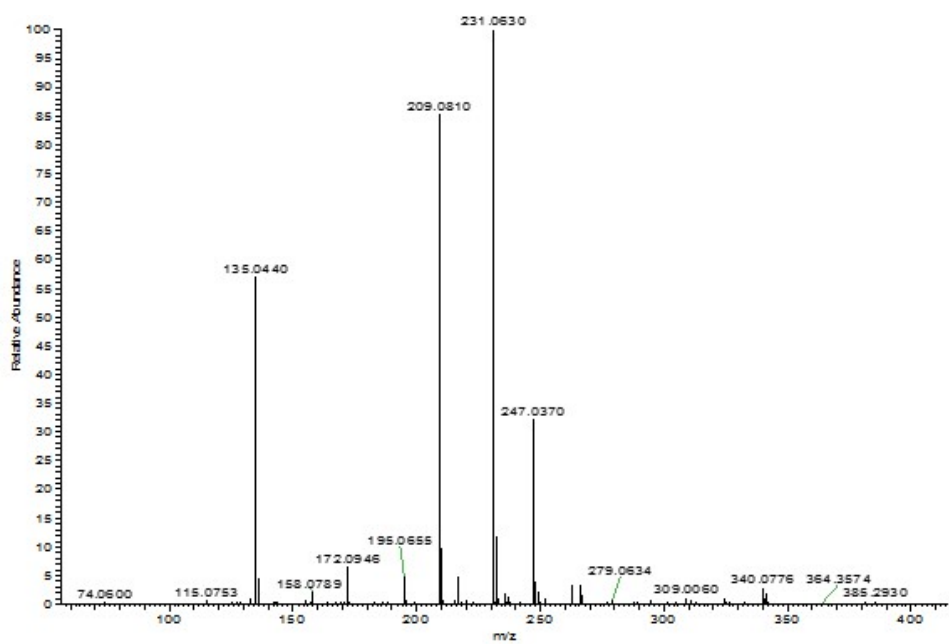


Figure S13. HRESI-MS spectrum of compound 3

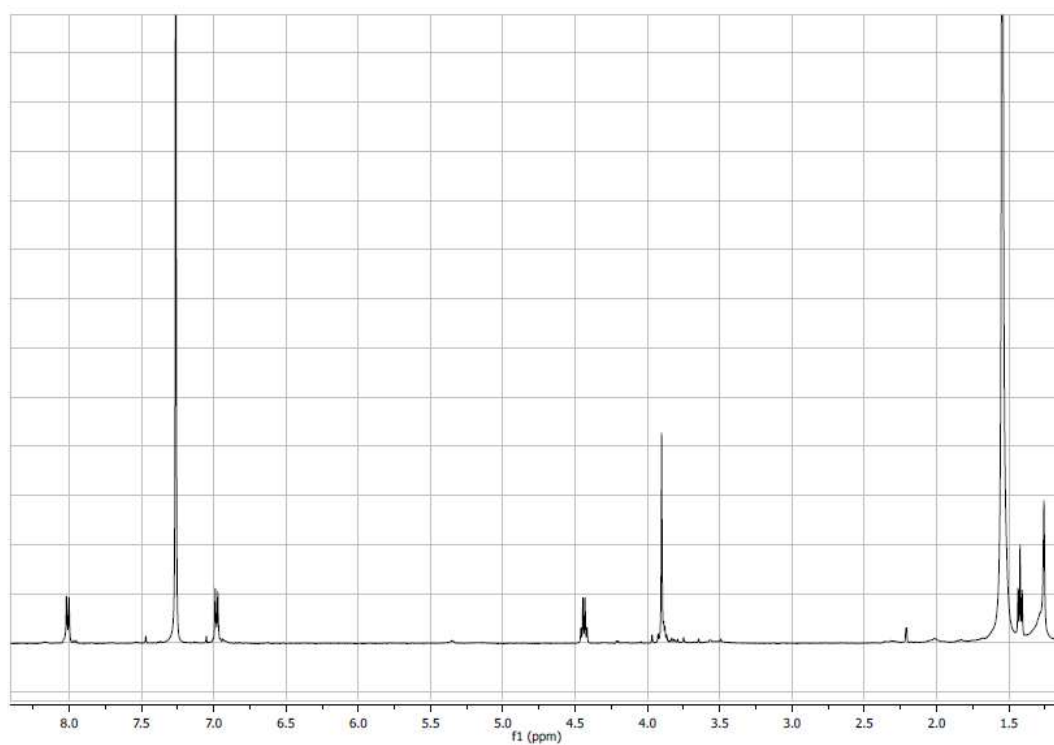


Figure S14. ¹H NMR spectrum of compound 3 in CDCl₃ (700 MHz)

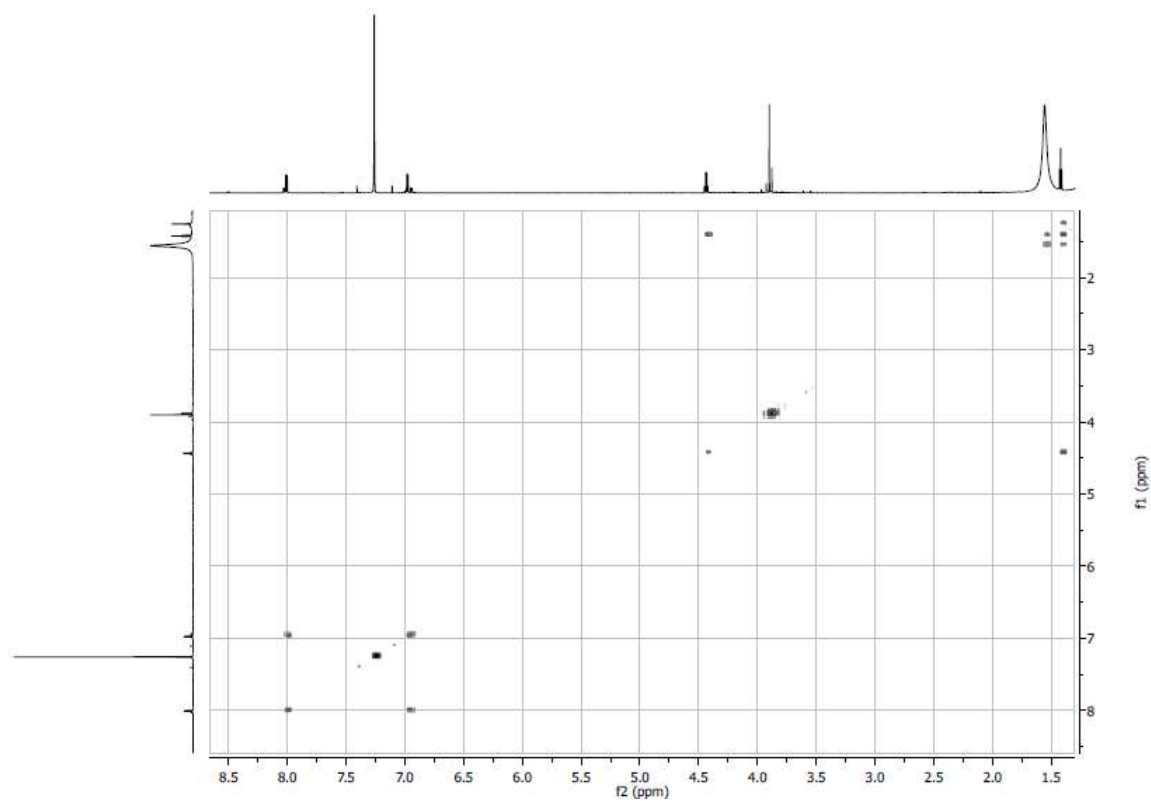


Figure S15. COSY spectrum of compound **3** in CDCl_3 (700 MHz)

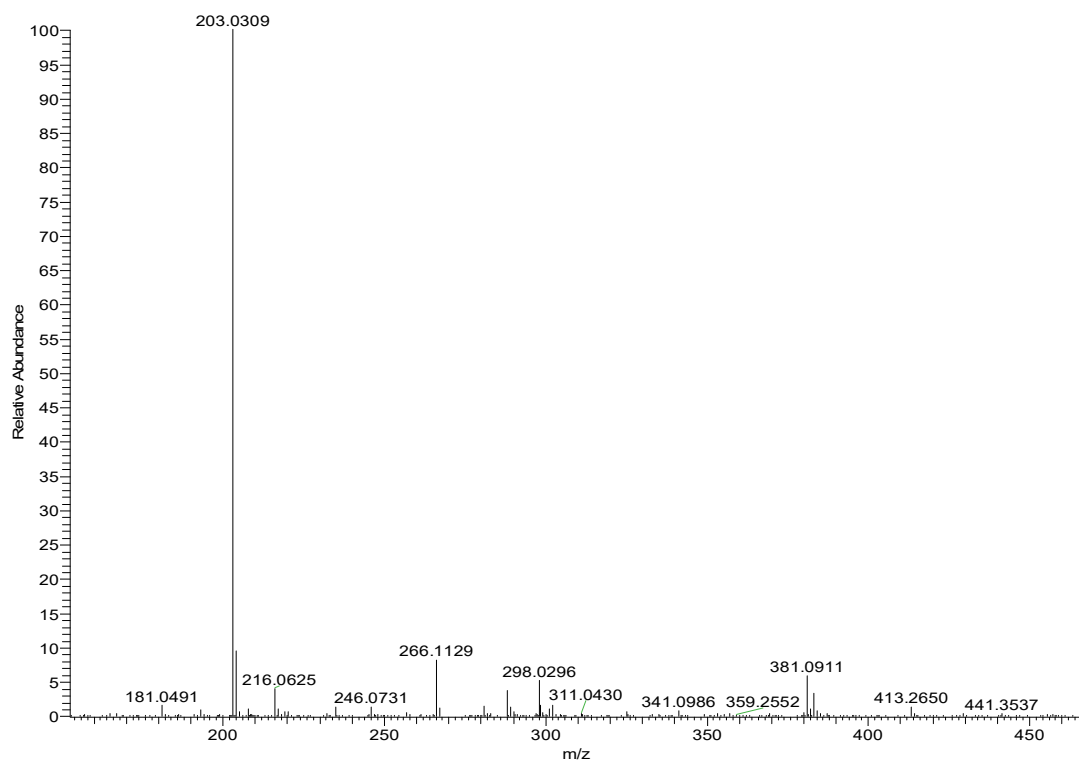


Figure S16. HRESI-MS spectrum of compound **4**

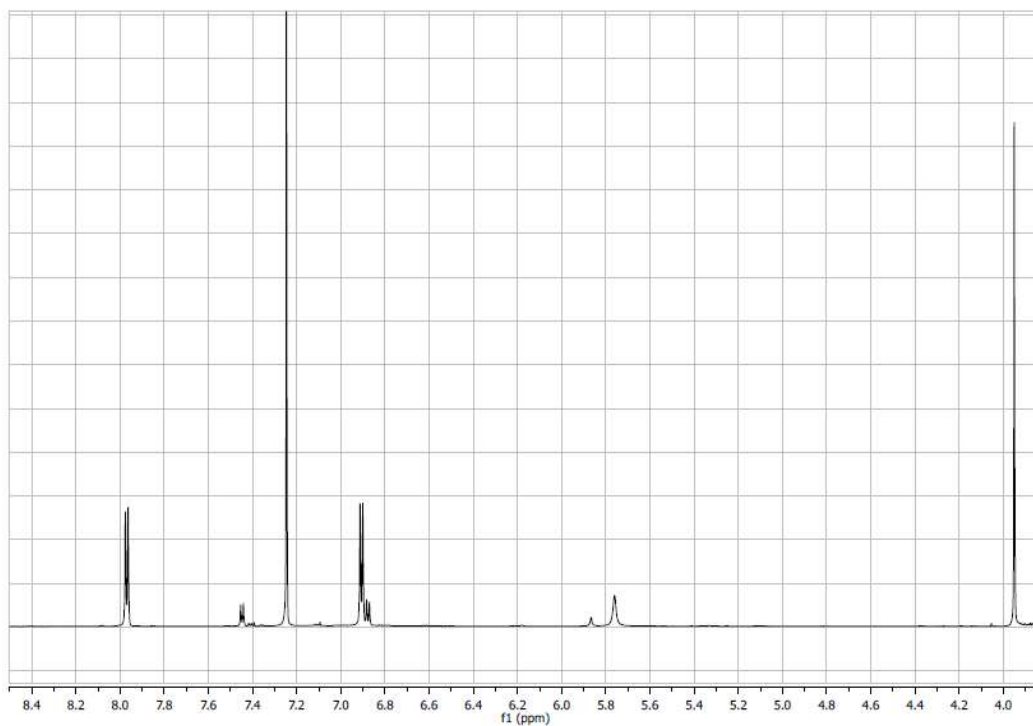


Figure S17. ^1H NMR spectrum of compound **4** in CDCl_3 (700 MHz)

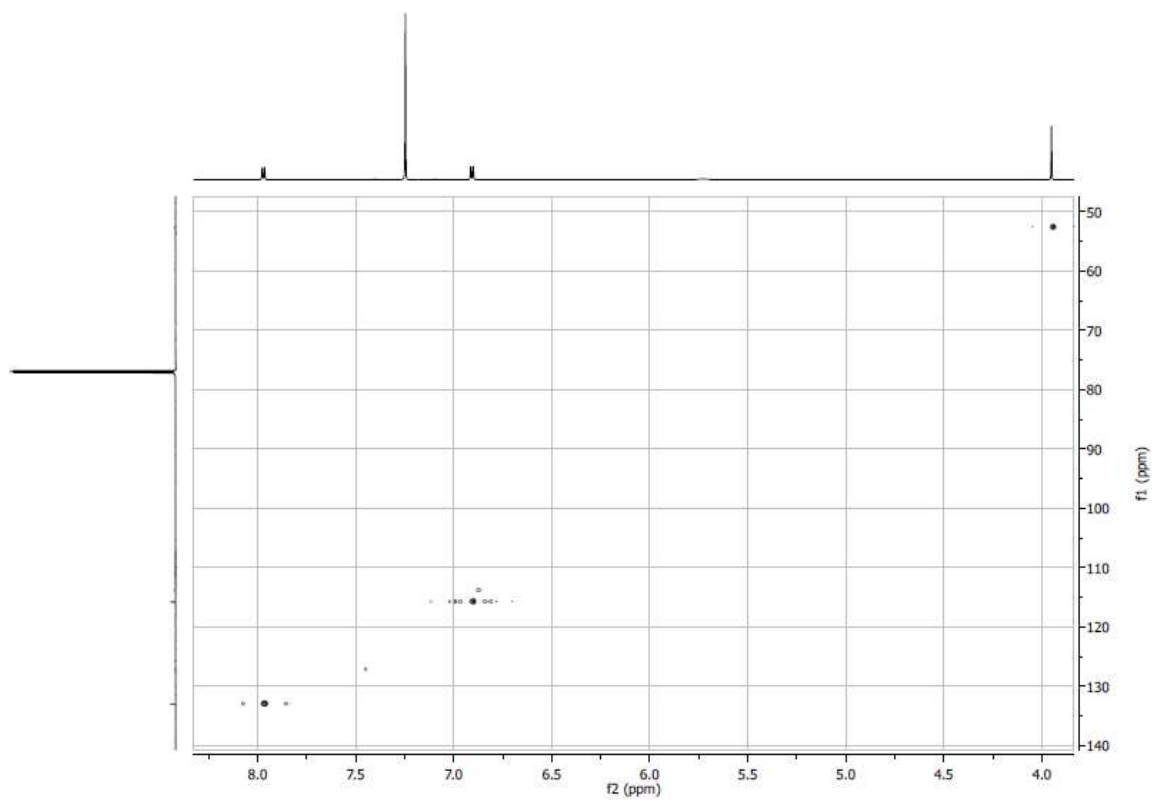


Figure S18. HSQC spectrum of compound **4** in CDCl_3 (700 MHz)

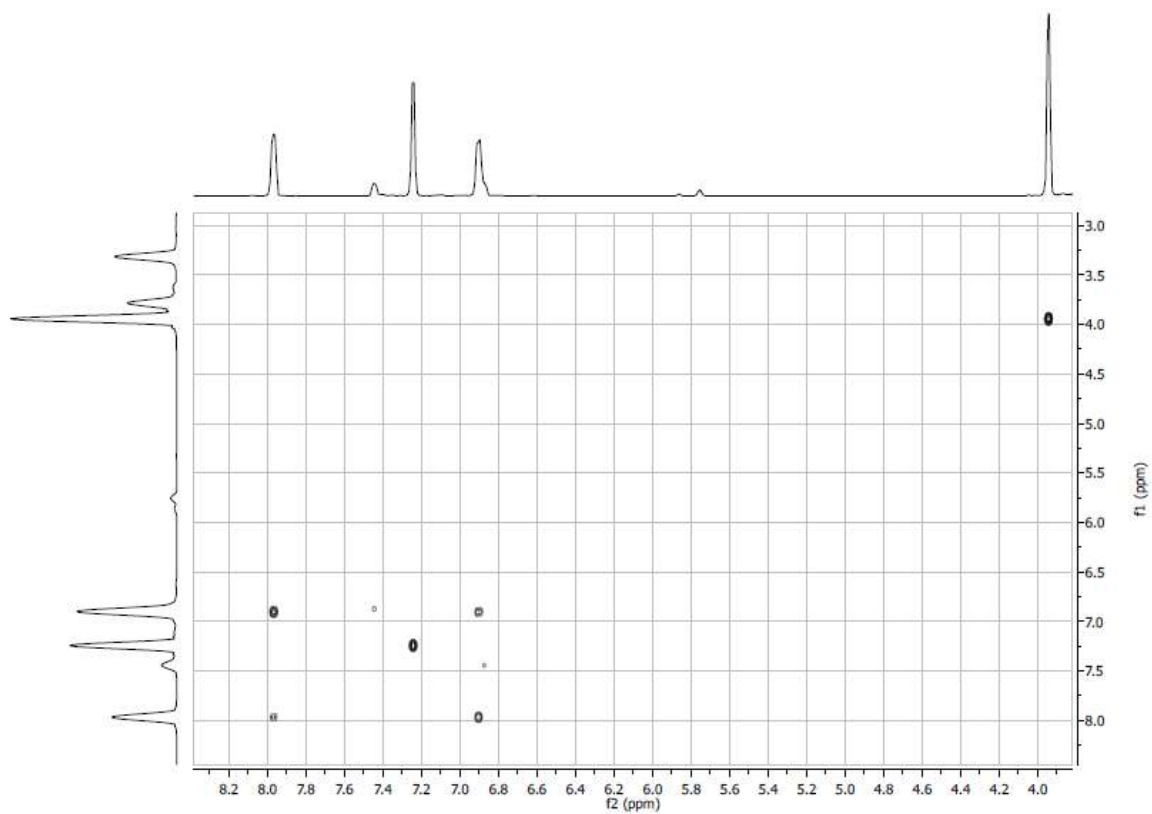


Figure S19. COSY spectrum of compound **4** in CDCl₃ (700 MHz)

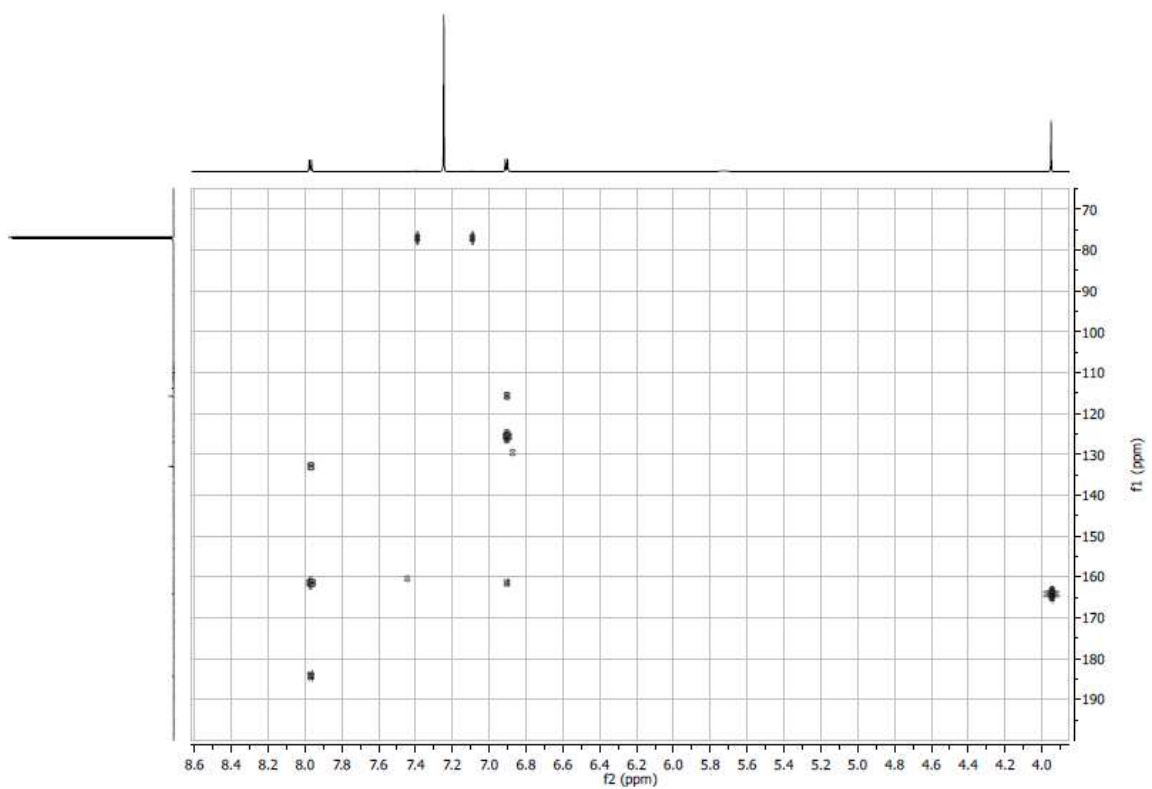


Figure S20. HMBC spectrum of compound **4** in CDCl₃ (700 MHz)

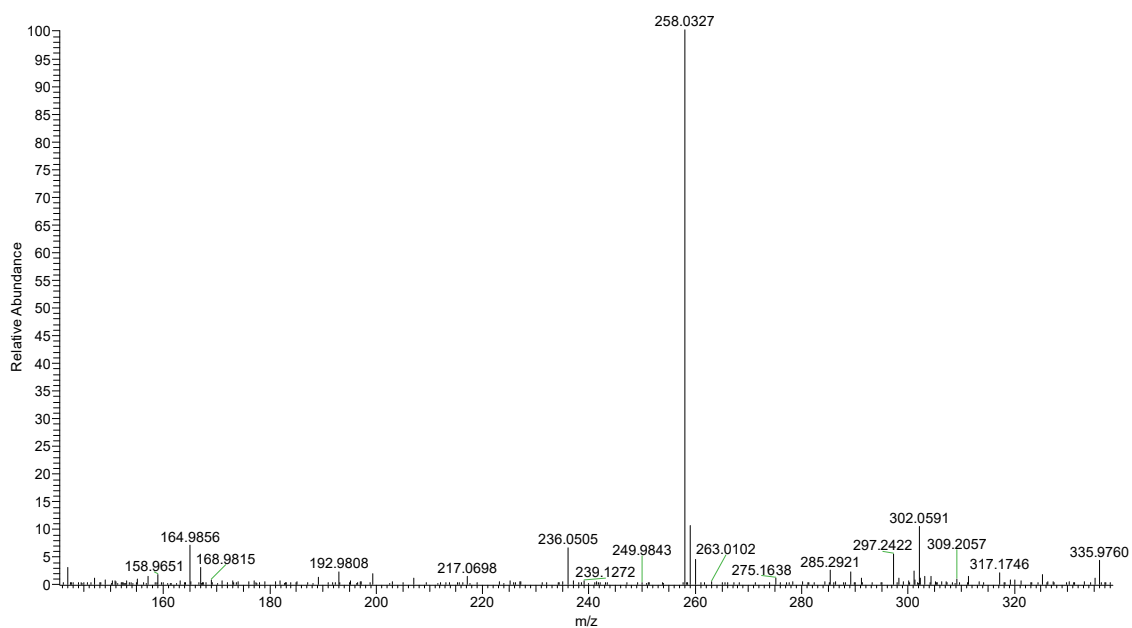


Figure S21. HRESI-MS spectrum of compound 5

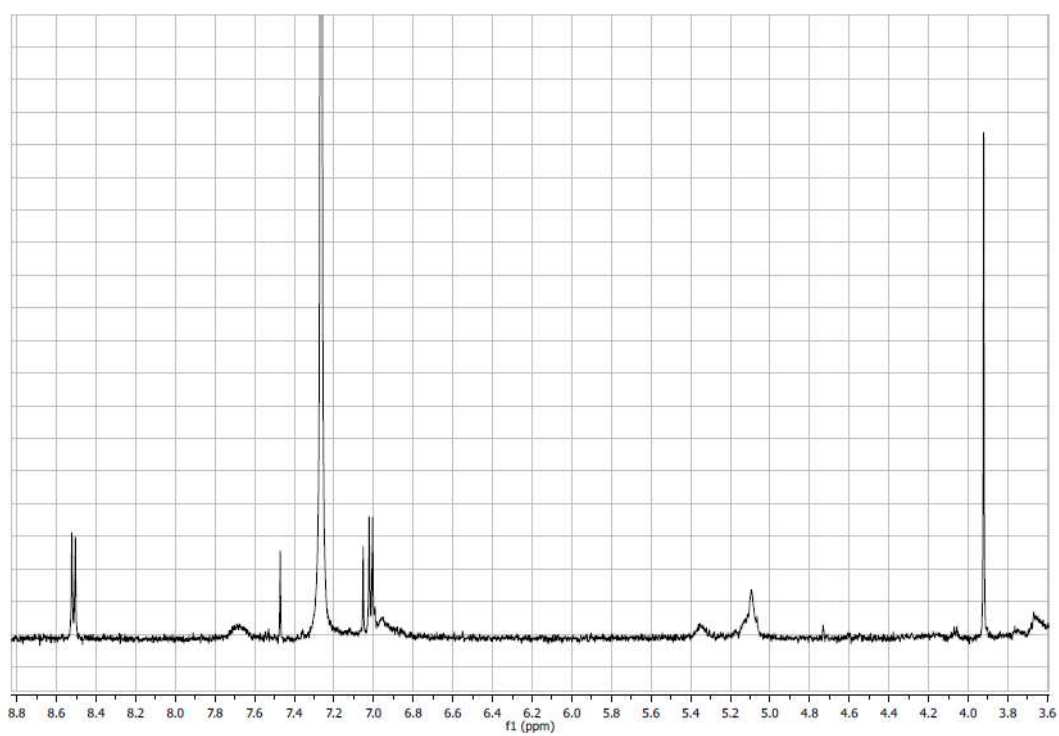


Figure S22. ¹H NMR spectrum of compound 5 in CDCl₃ (700 MHz)

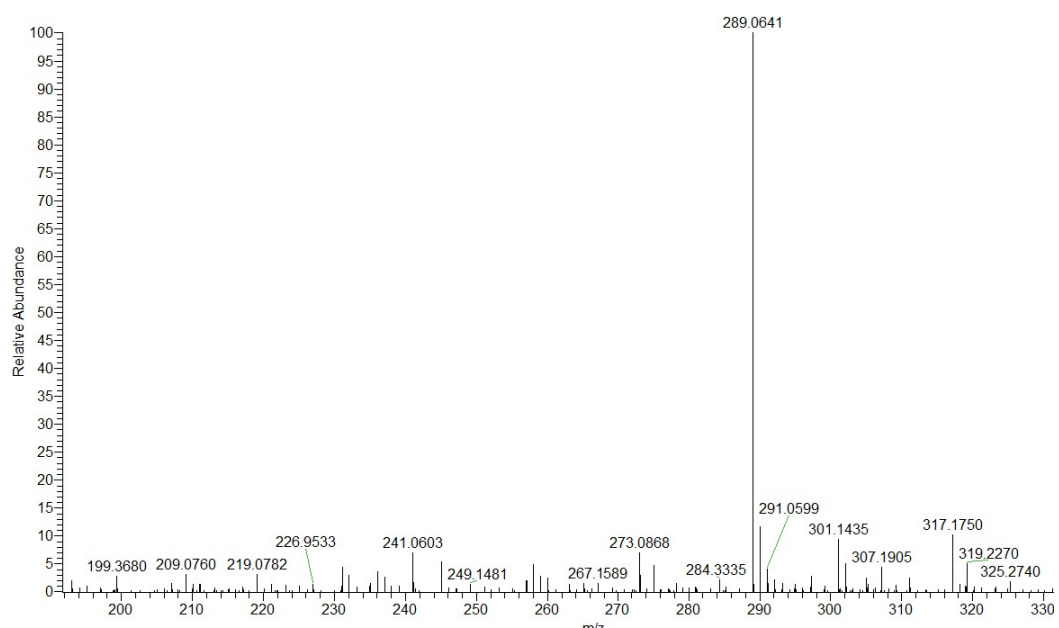


Figure S23. HRESI-MS spectrum of compound **6**

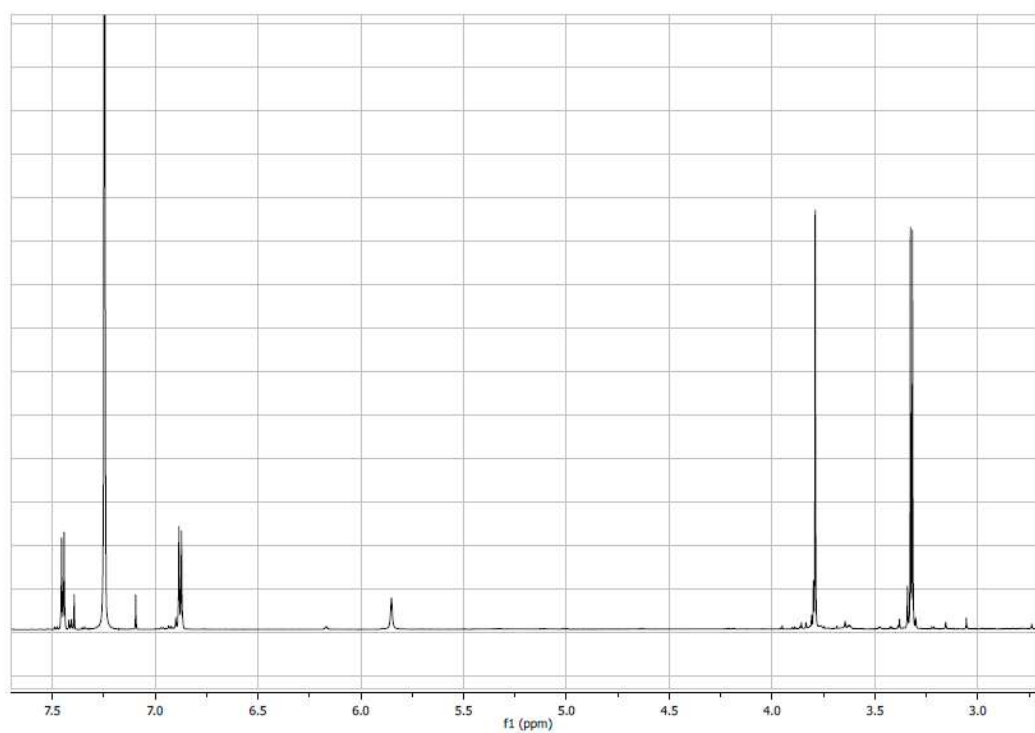


Figure S24. ¹H NMR spectrum of compound **6** in CDCl₃ (500 MHz)

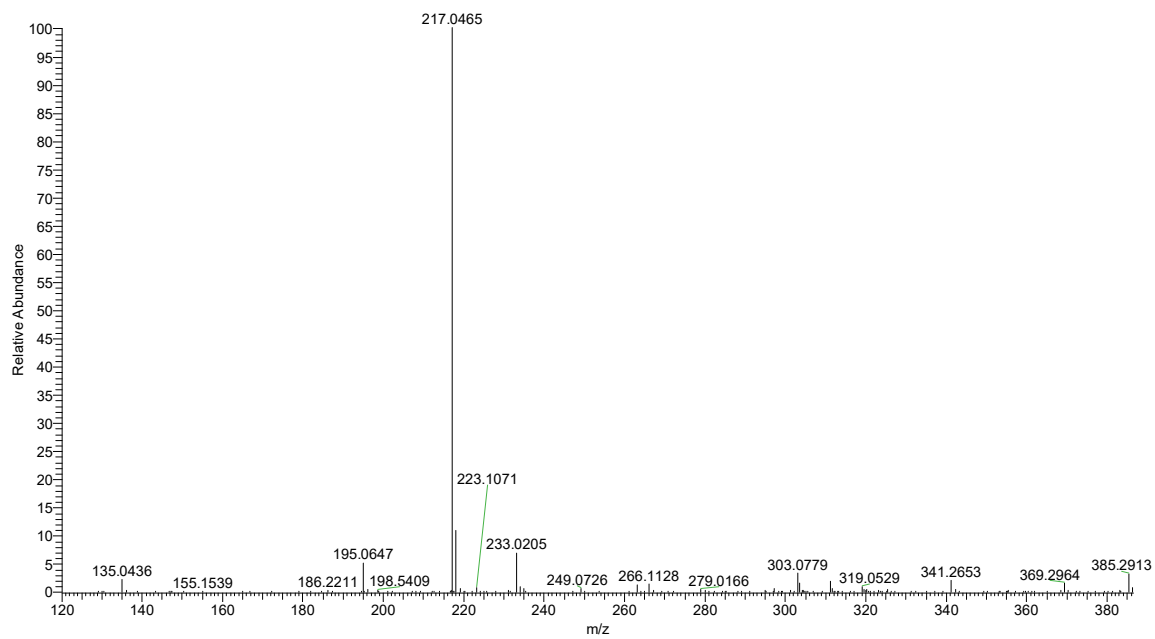


Figure S25. HRESI-MS spectrum of compound 7

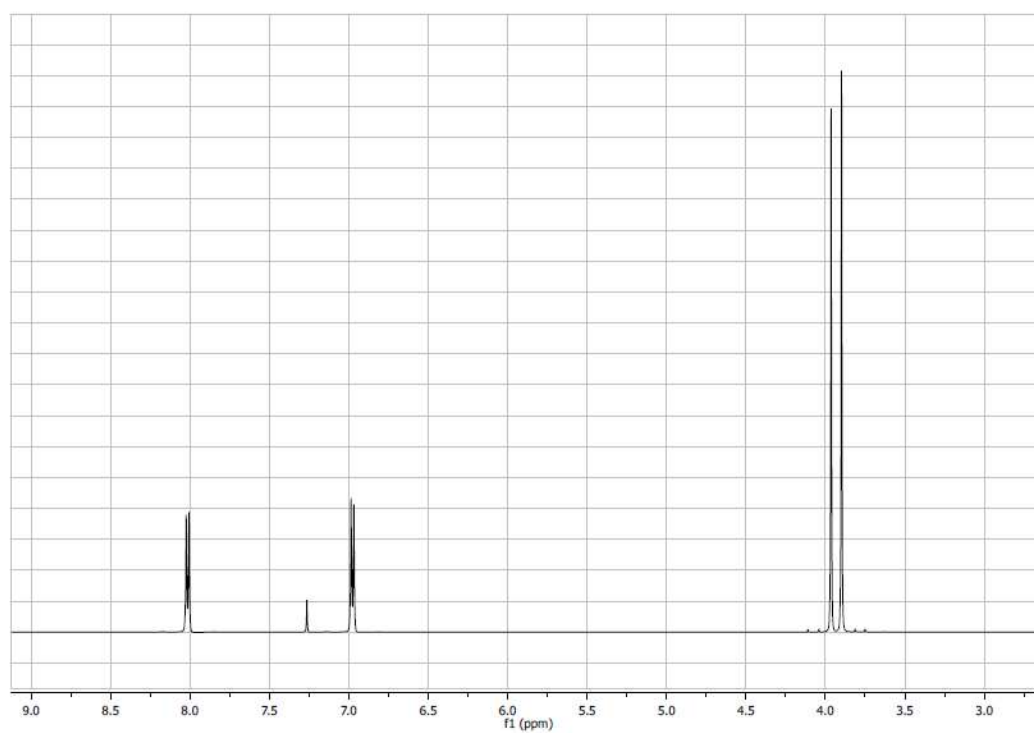


Figure S26. ¹H NMR spectrum of compound 7 in CDCl₃ (500 MHz)

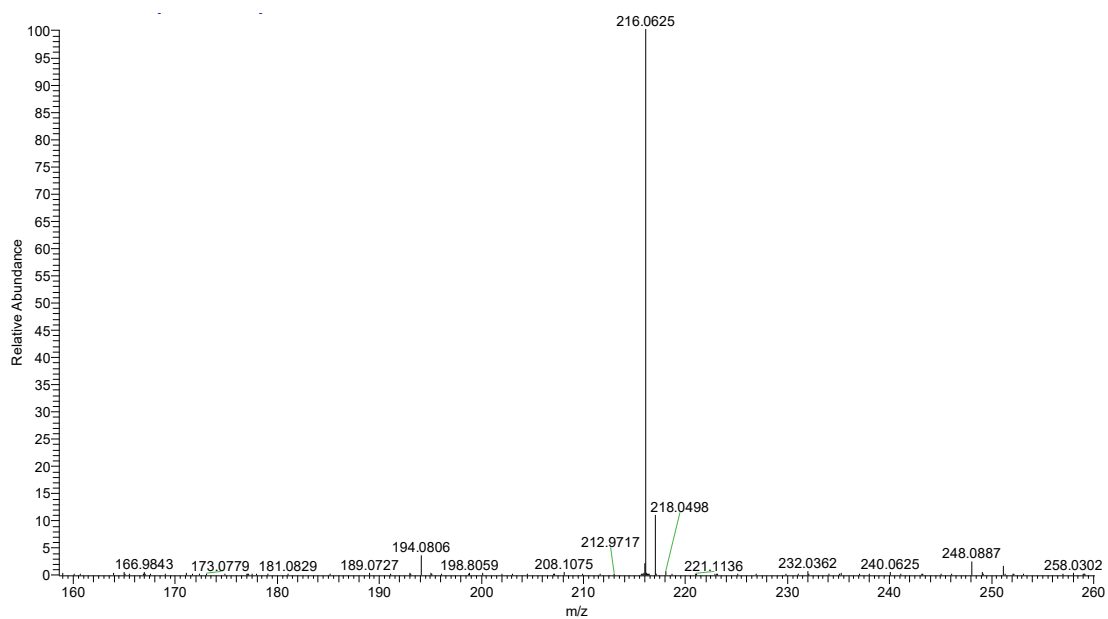


Figure S27. HRESI-MS spectrum of compound **8**

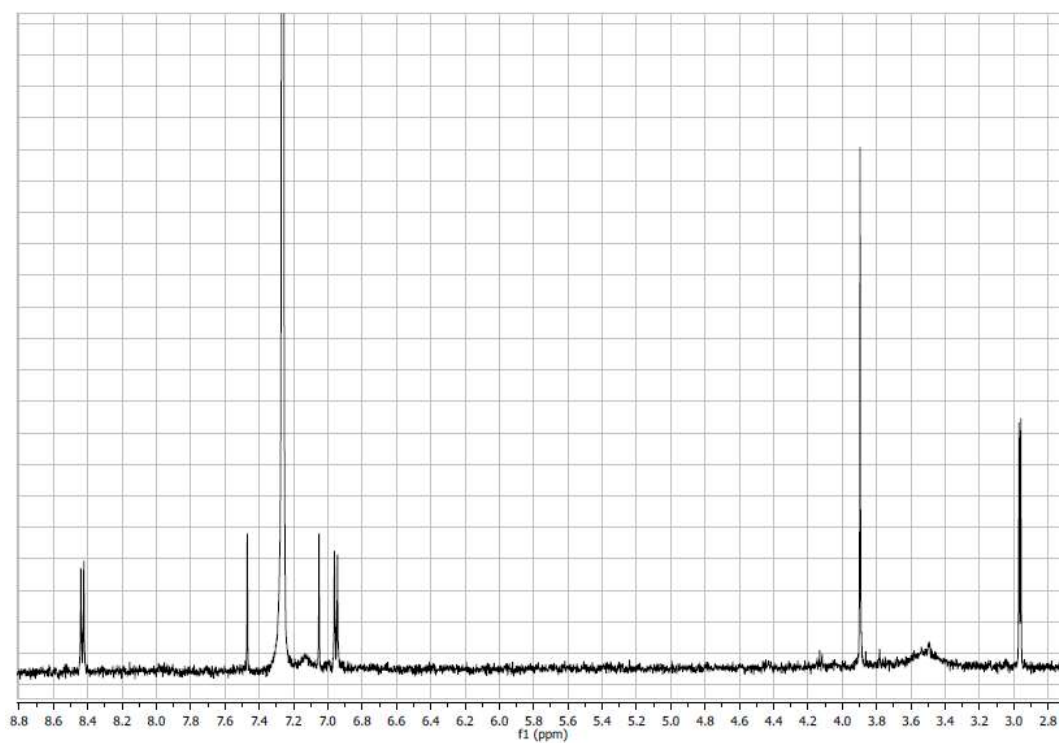


Figure S28. ¹H NMR spectrum of compound **8** in CDCl₃ (700 MHz)