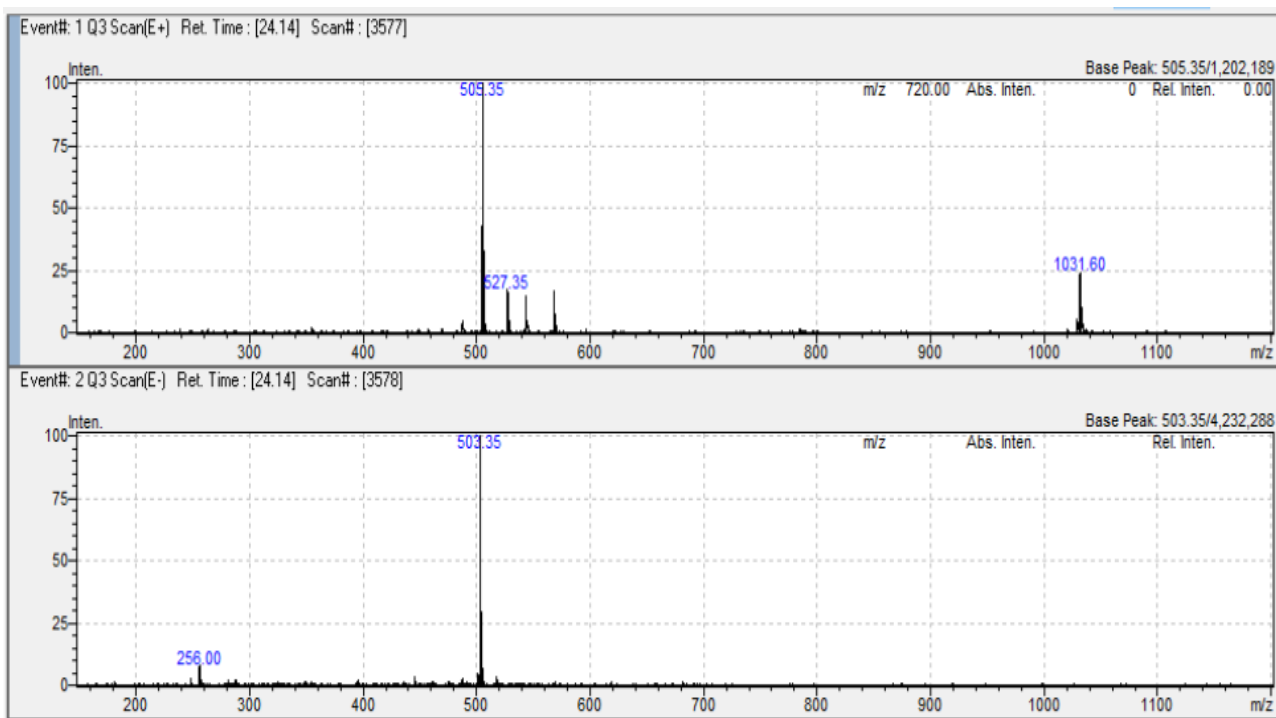


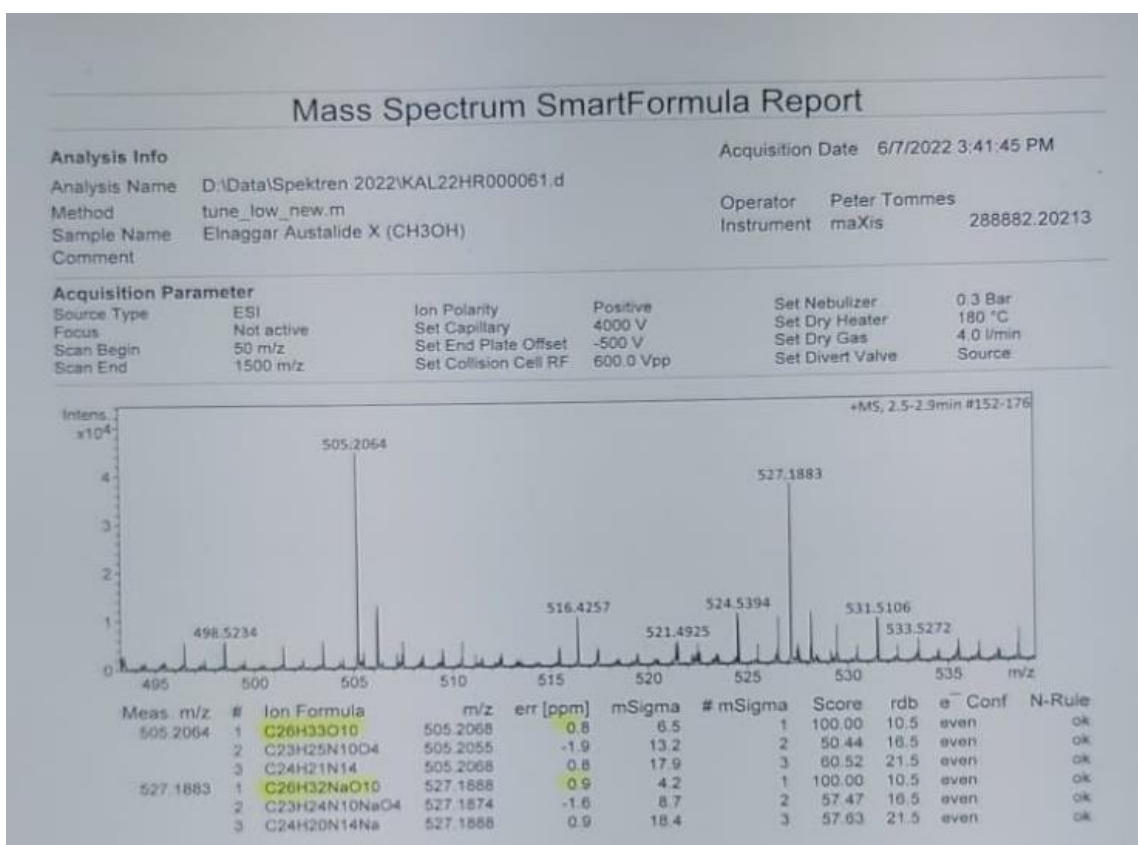
Supporting information

An austalide derivative from the marine-derived *Aspergillus* *sp.* and evaluation of its cytotoxic and ADME/TOPKAT properties

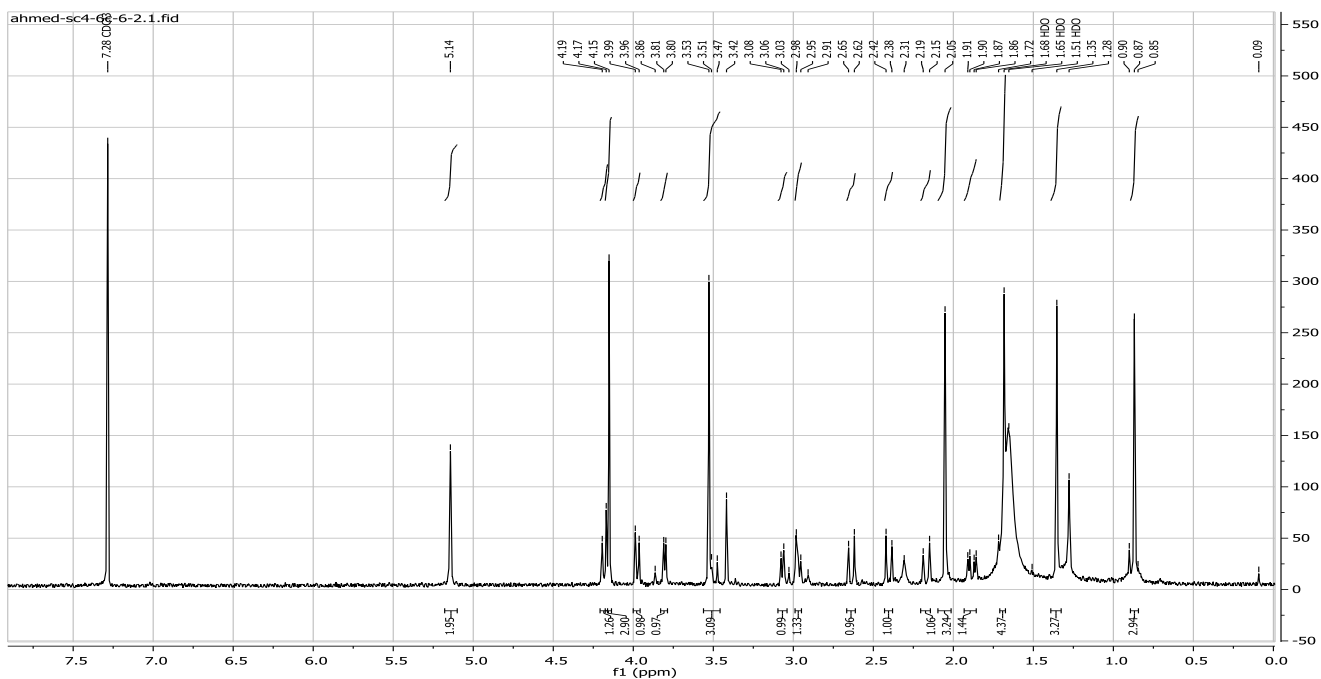
Mohamed S. Elnaggar^{a,c#}, Ahmed M. Elissawy^{a,b,#*}, Fadia S. Youssef^a, Máté Kicsák^d, Tibor Kurtán^d, Abdel Nasser B. Singab^{a,b*}, and Rainer Kalscheuer^c



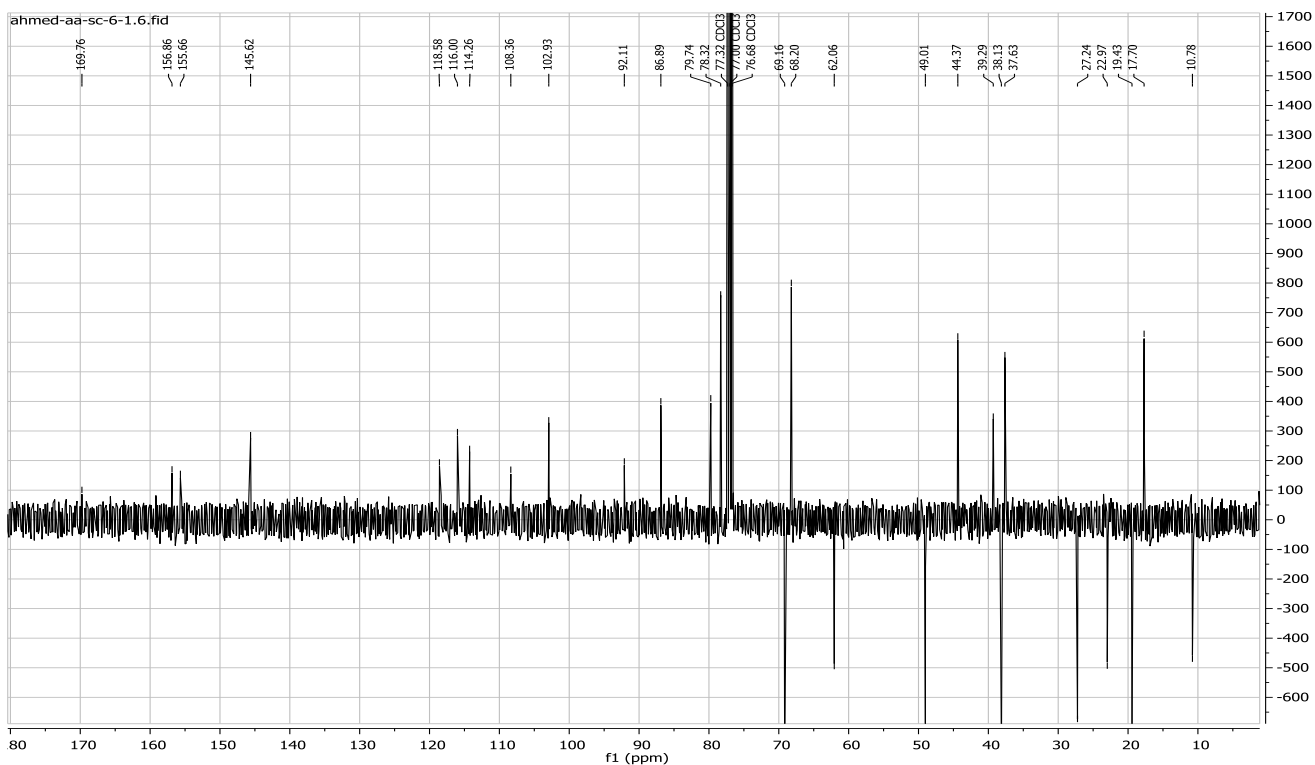
S1A. Low resolution +ve/-ve ESIMS of compound 1



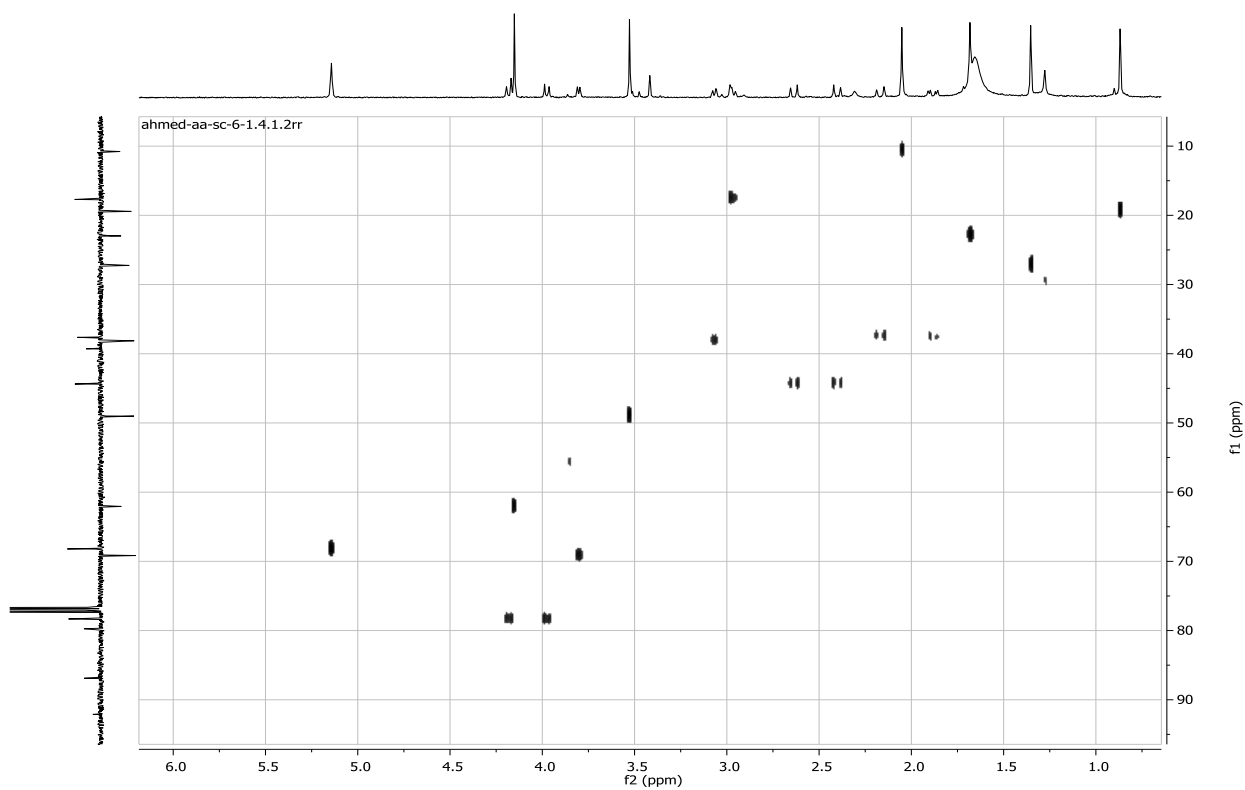
S1B. High-resolution +ve ESIMS of compound 1



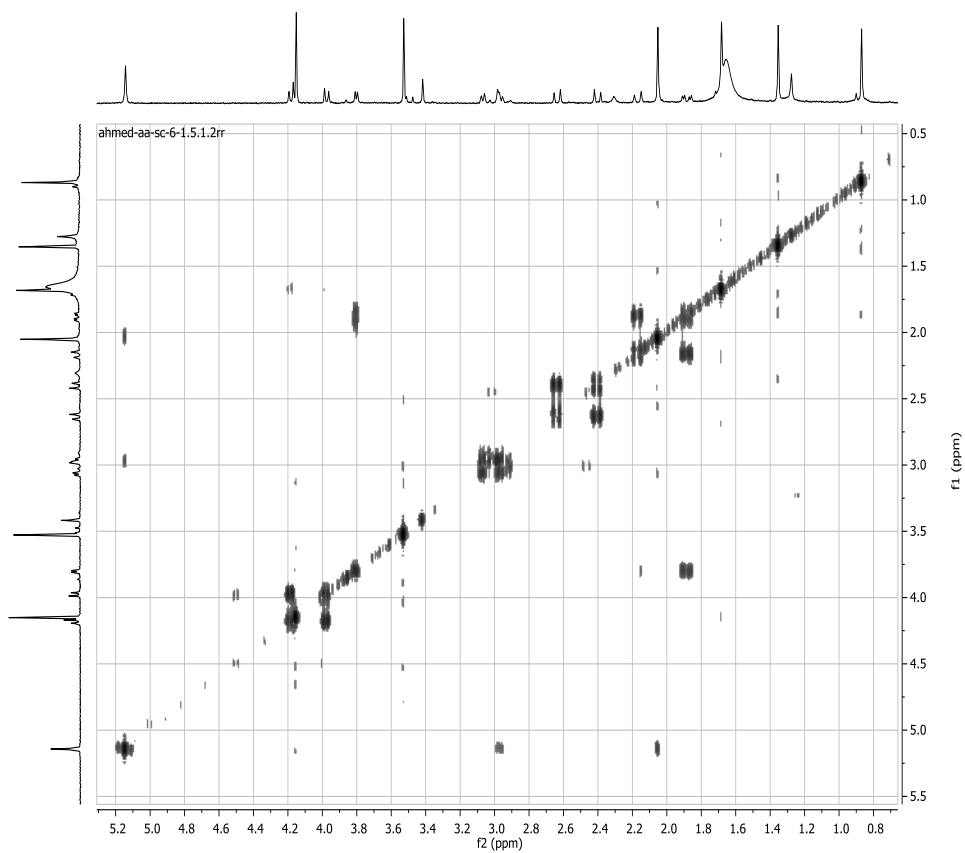
S2. ¹H NMR spectrum of compound 1



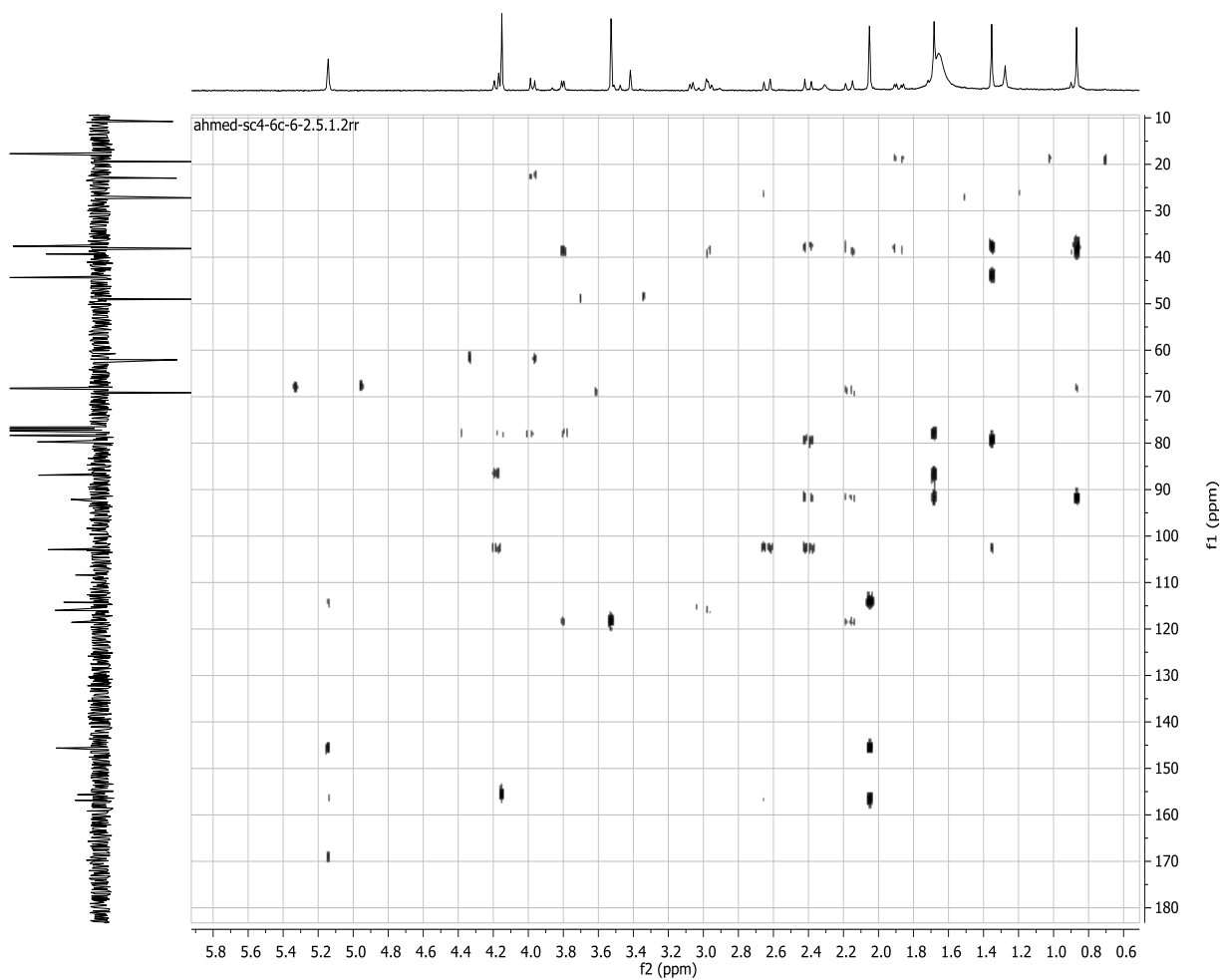
S3. APT NMR spectrum of compound 1



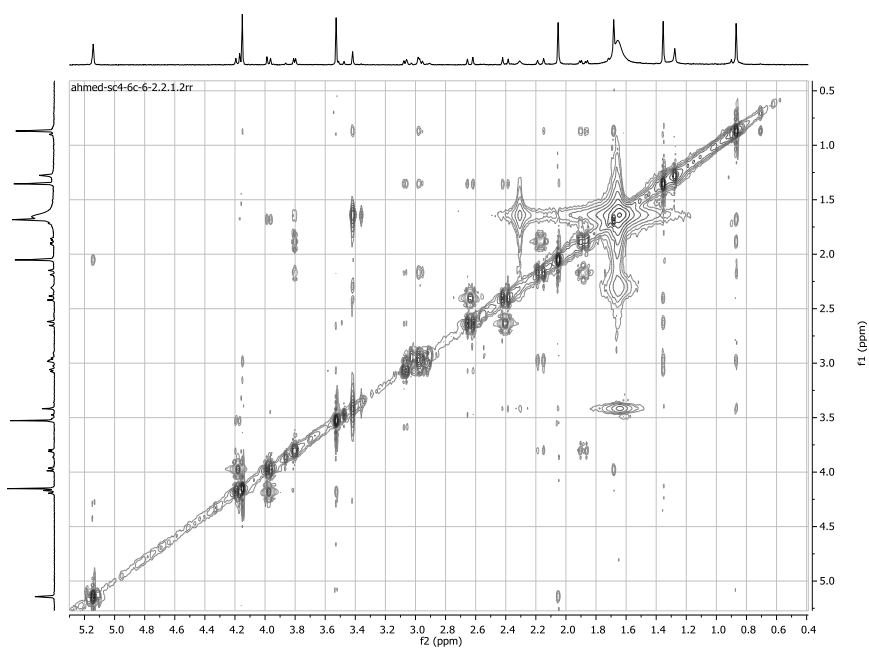
S4. HSQC spectrum of compound 1



S5. COSY spectrum of compound 1

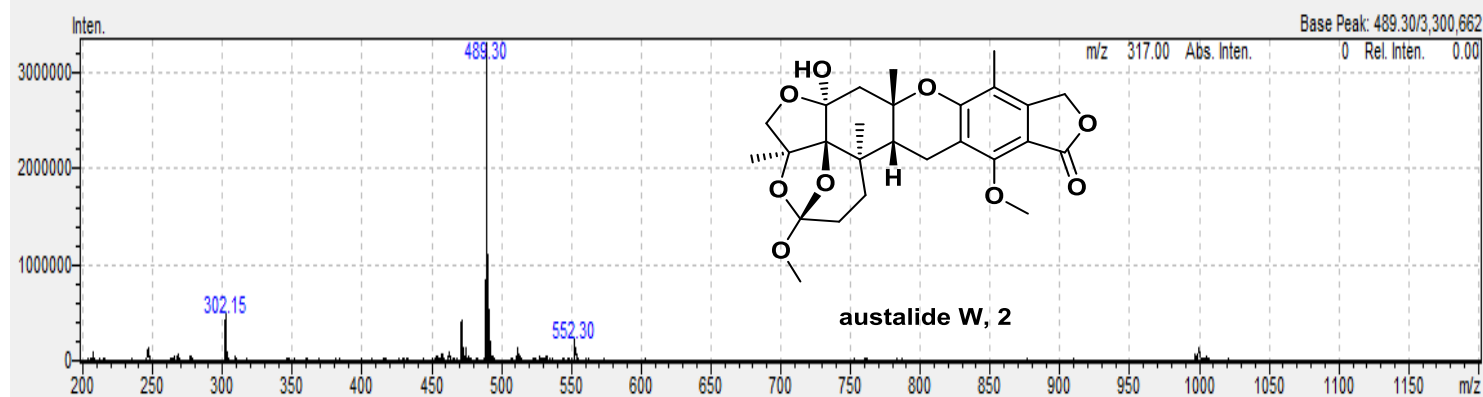


S6. HMBC spectrum of compound 1

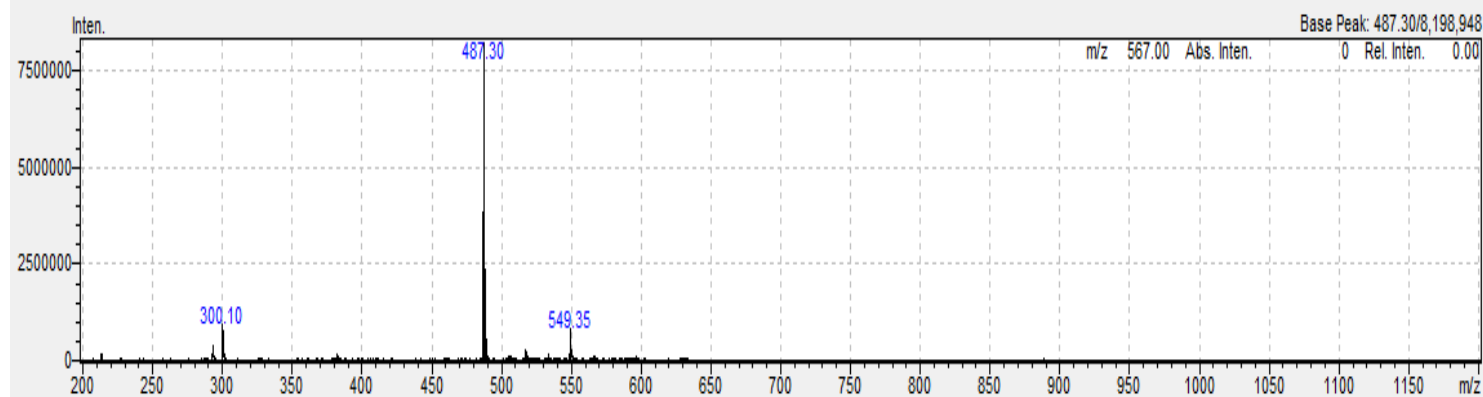


S7. NOESY NMR spectrum of compound 1

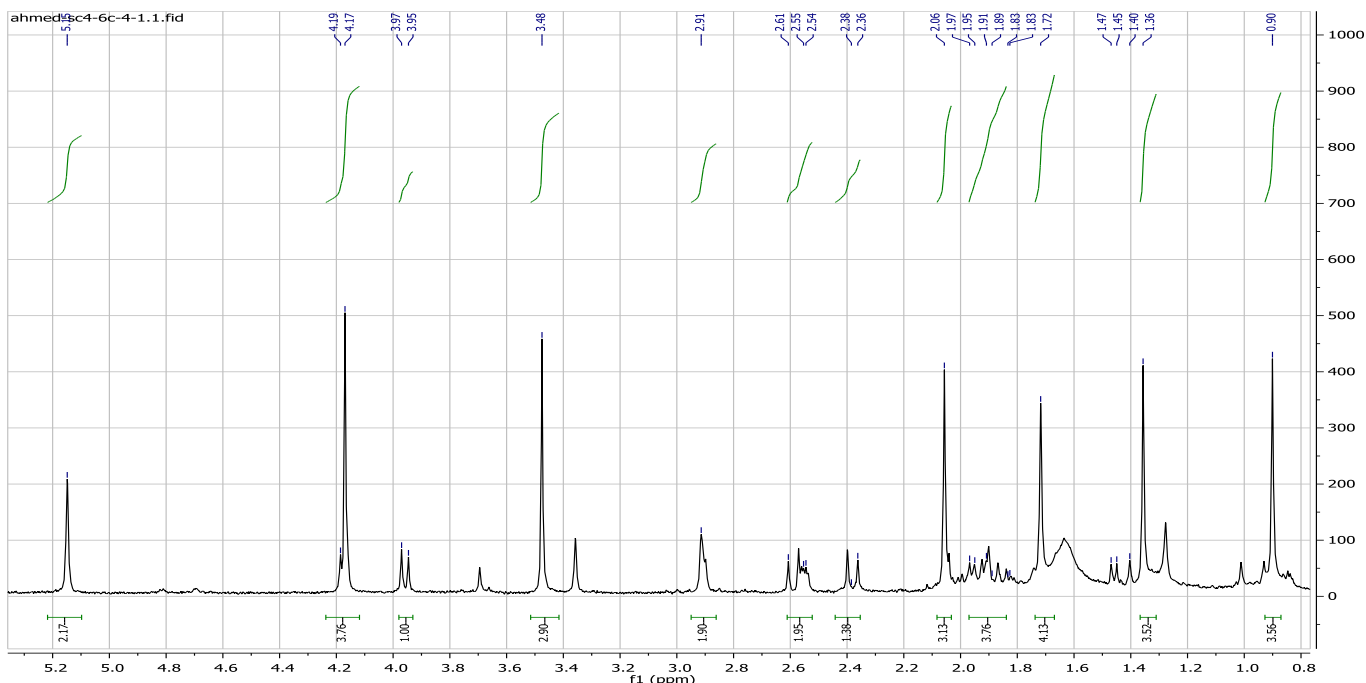
Event#: 1 Q3 Scan(E+) Ret. Time: [11.12] Scan#: [1649]



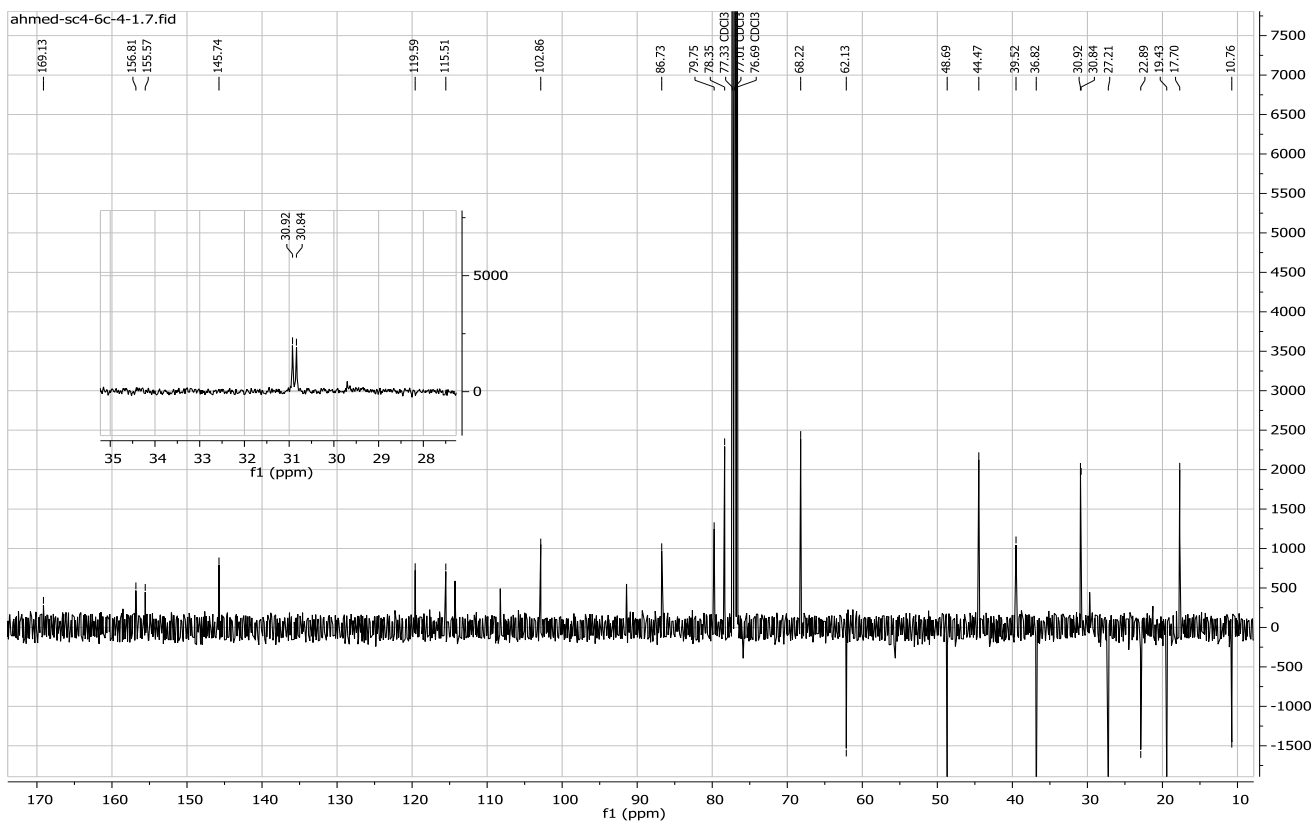
Event#: 2 Q3 Scan(E-) Ret. Time: [11.13] Scan#: [1650]



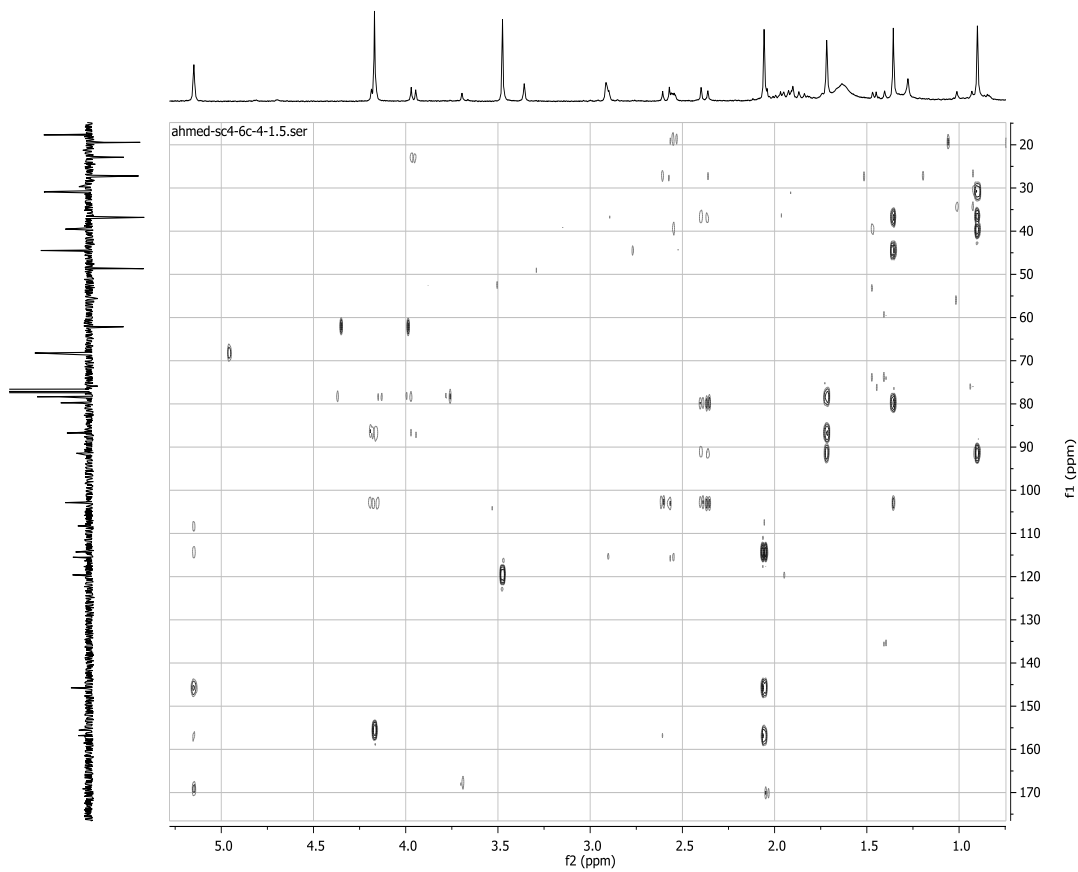
S8. +/- ESIMS spectrum of Compound 2



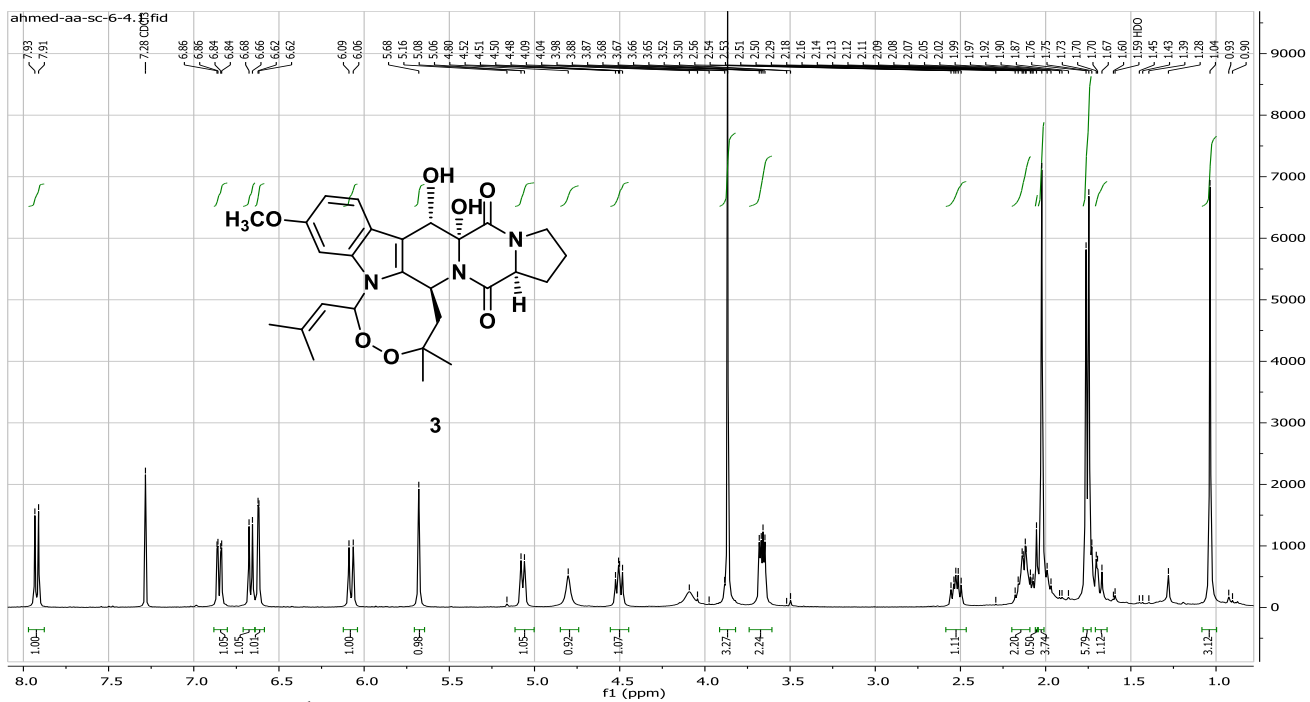
S9. ¹H NMR spectrum of compound 2 (CDCl₃)



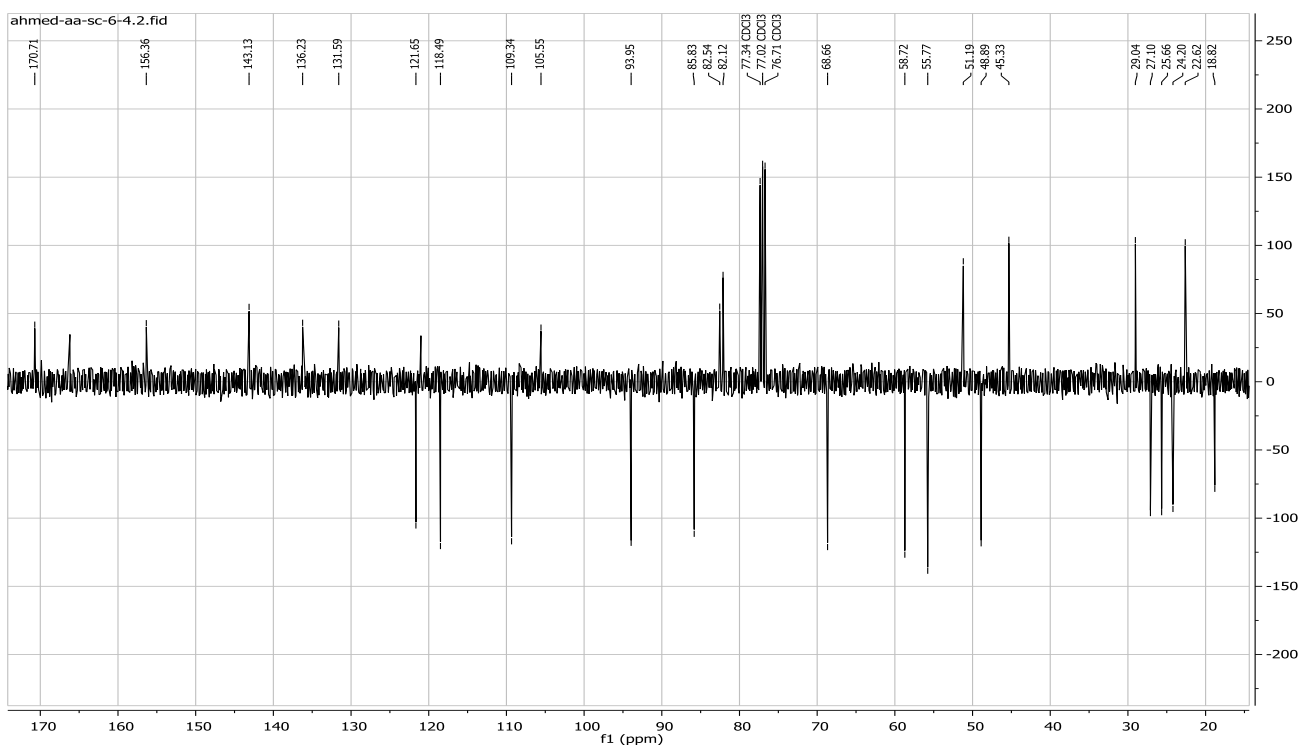
S10. APT NMR spectrum of compound 2



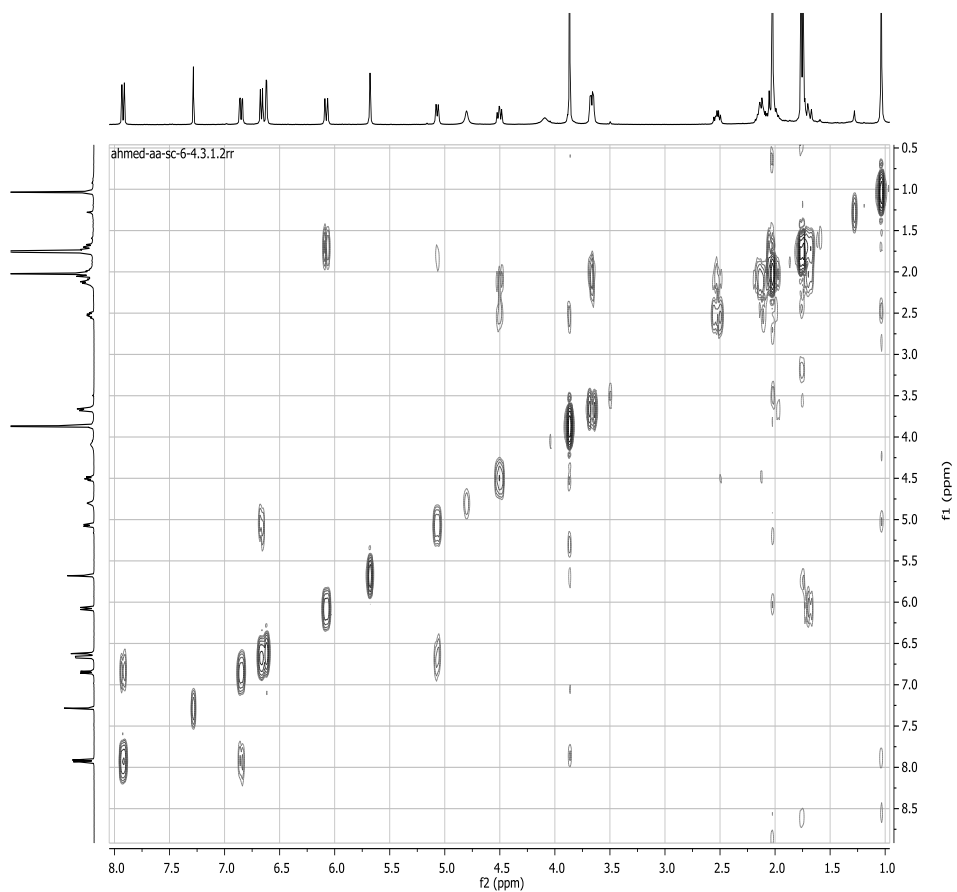
S11. HMBC spectrum of compound 2



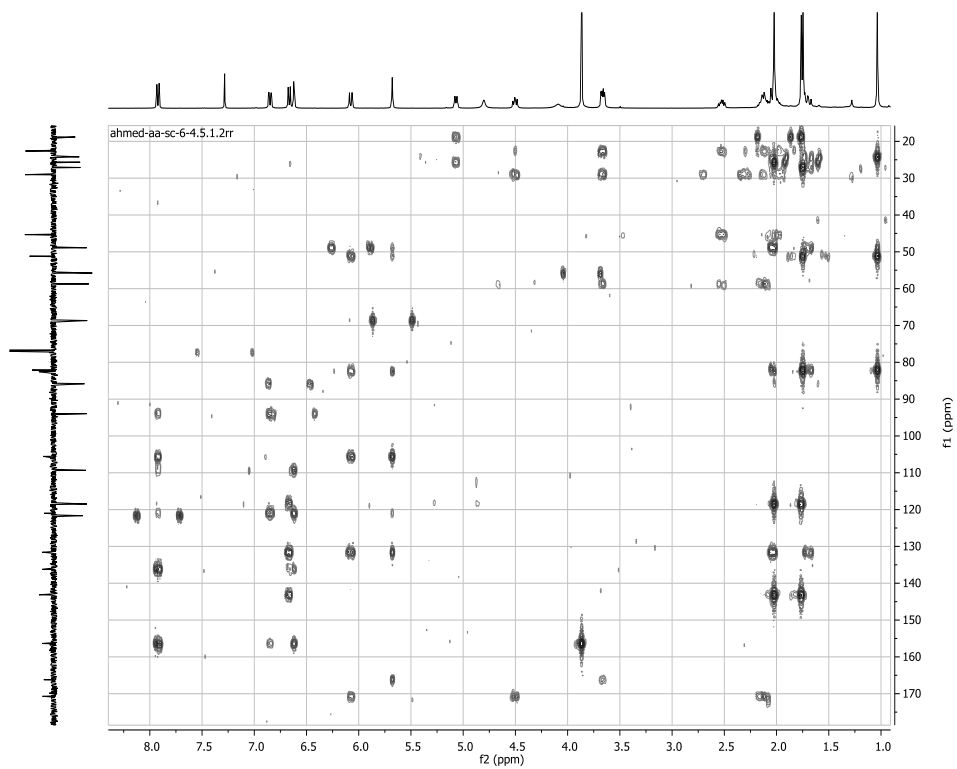
S12. ¹H NMR spectrum of compound 3 (CDCl₃)



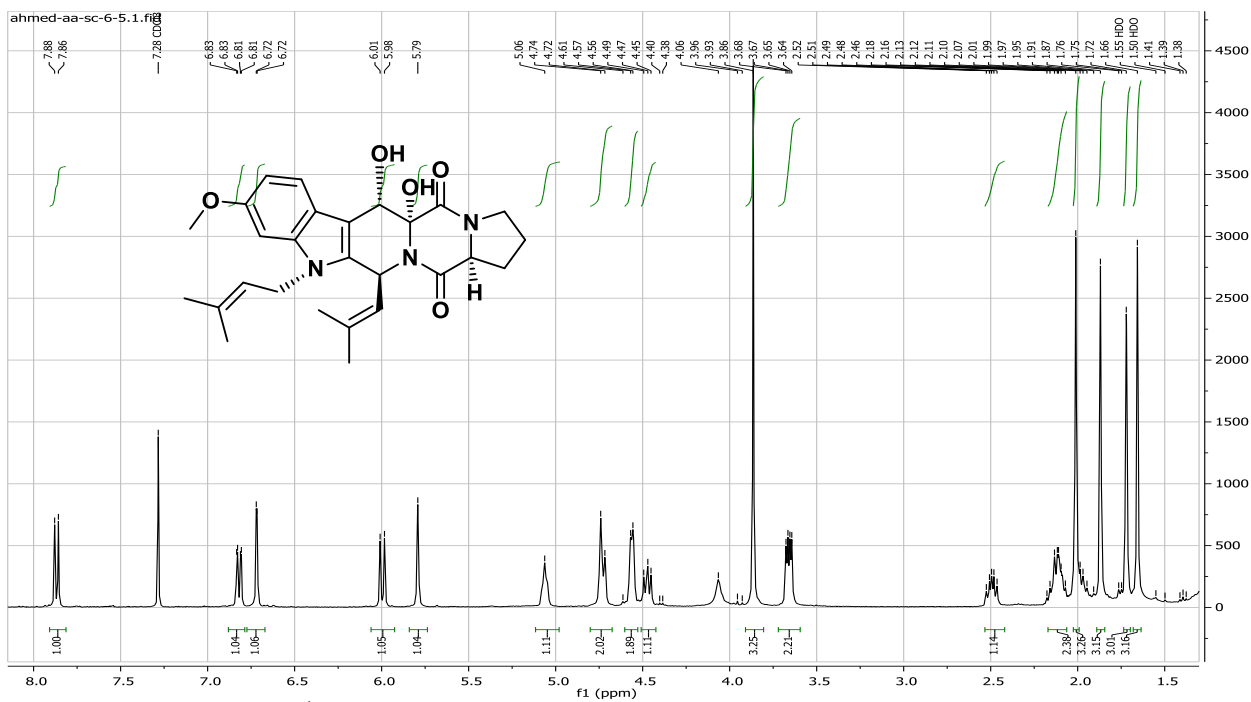
S13. APT NMR spectrum of compound 3



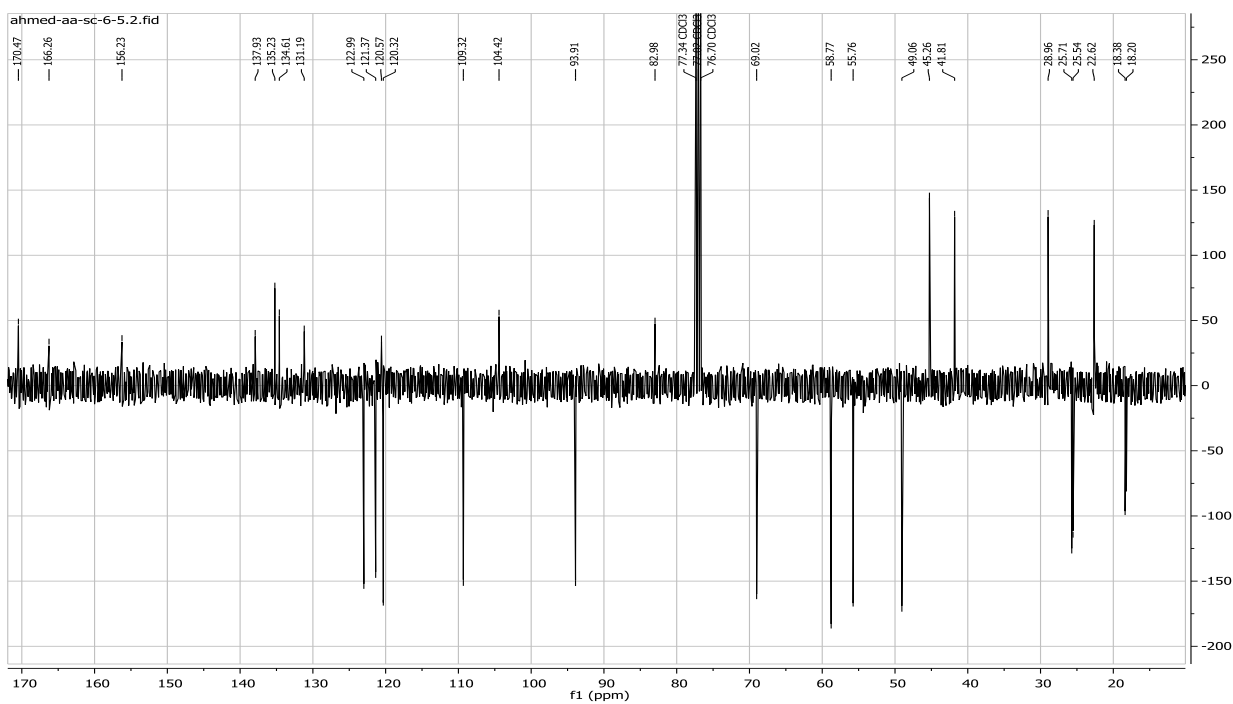
S14.COSY spectrum of compound 3



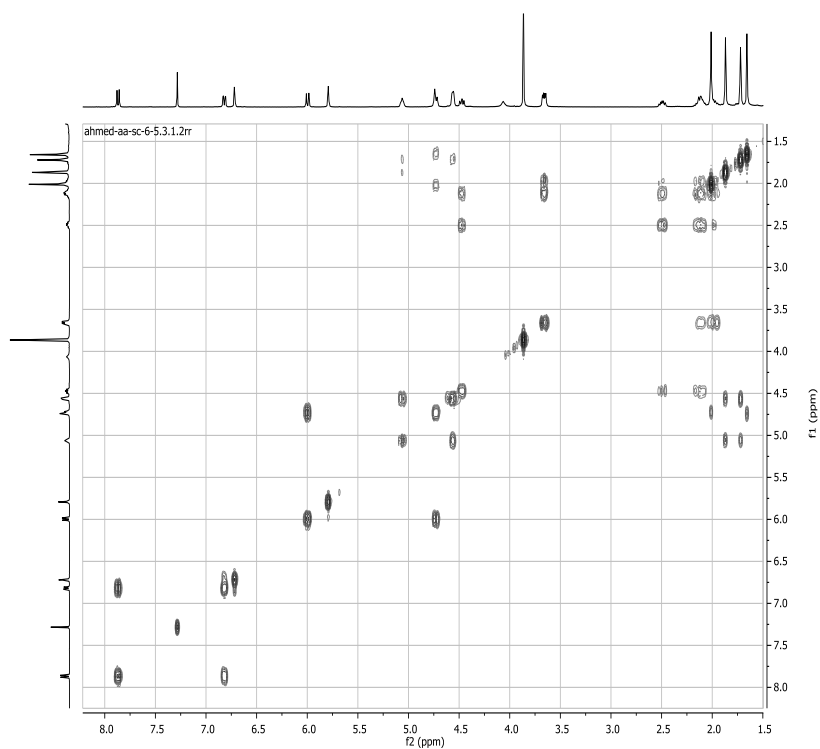
S15. HMBC spectrum of compound 3



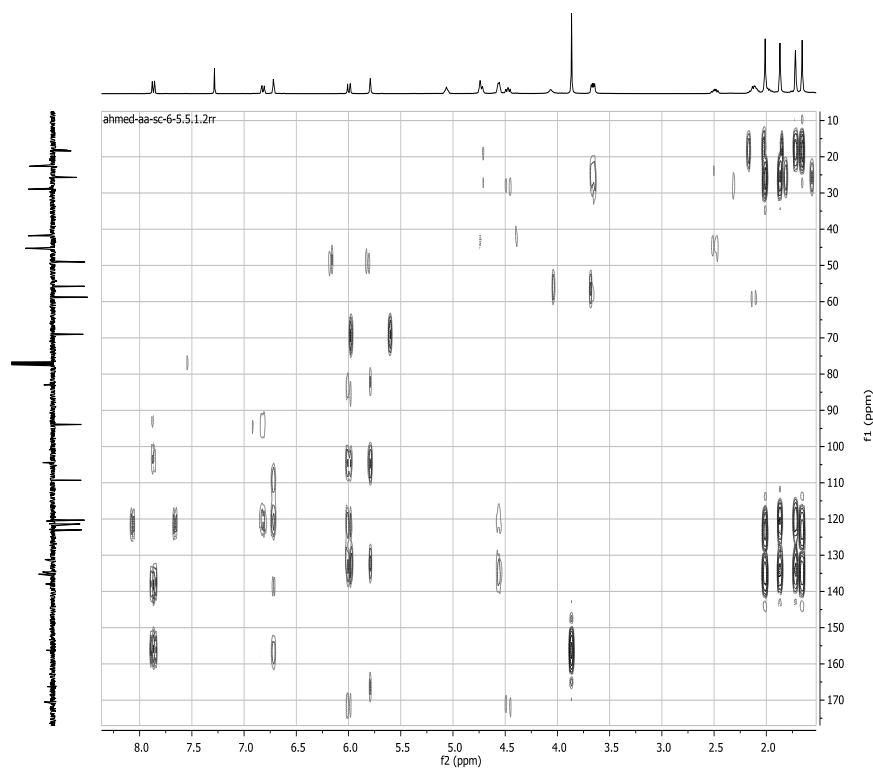
S16. ¹H NMR spectrum of compound 4 (CDCl₃)



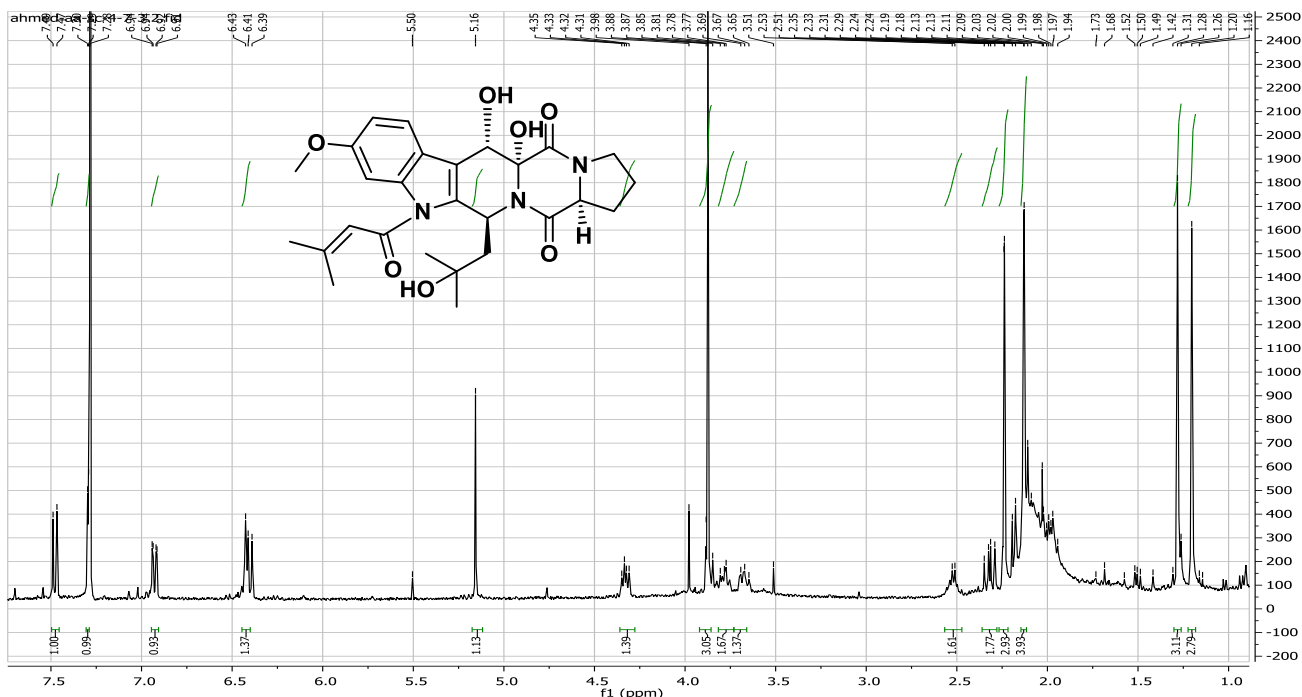
S17. APT NMR spectrum of compound 4



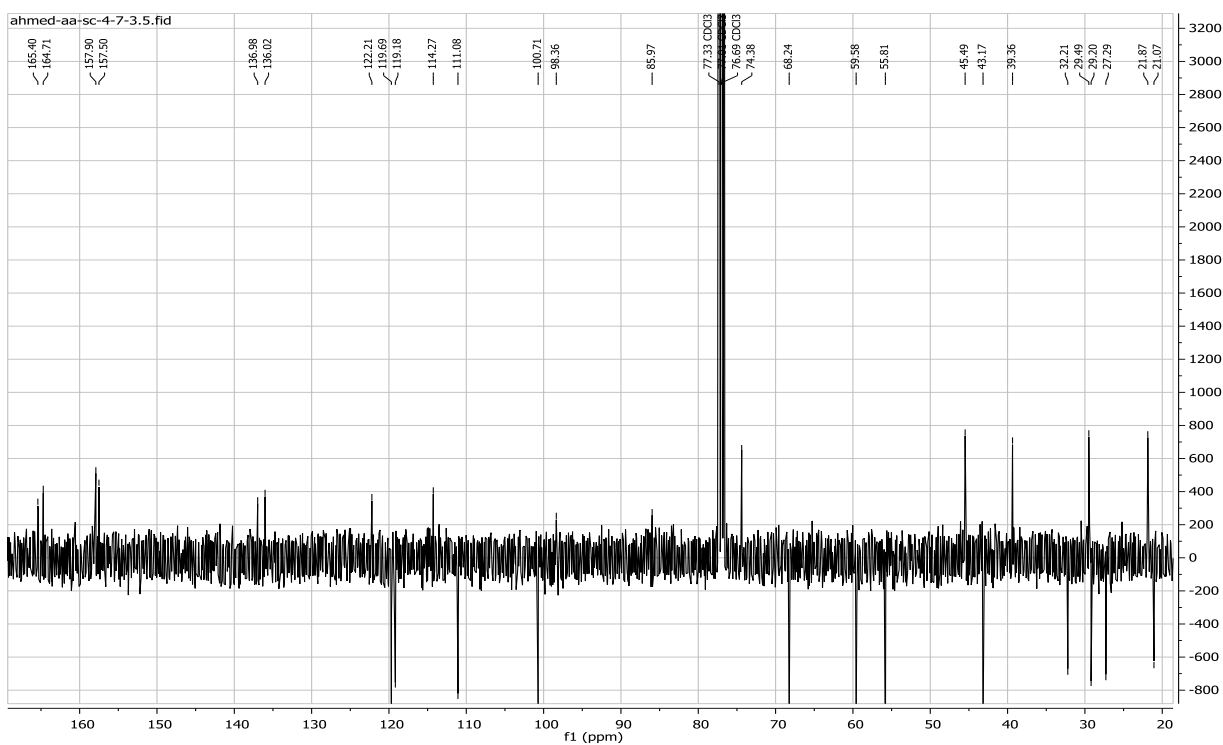
S18.COSY spectrum of compound 4



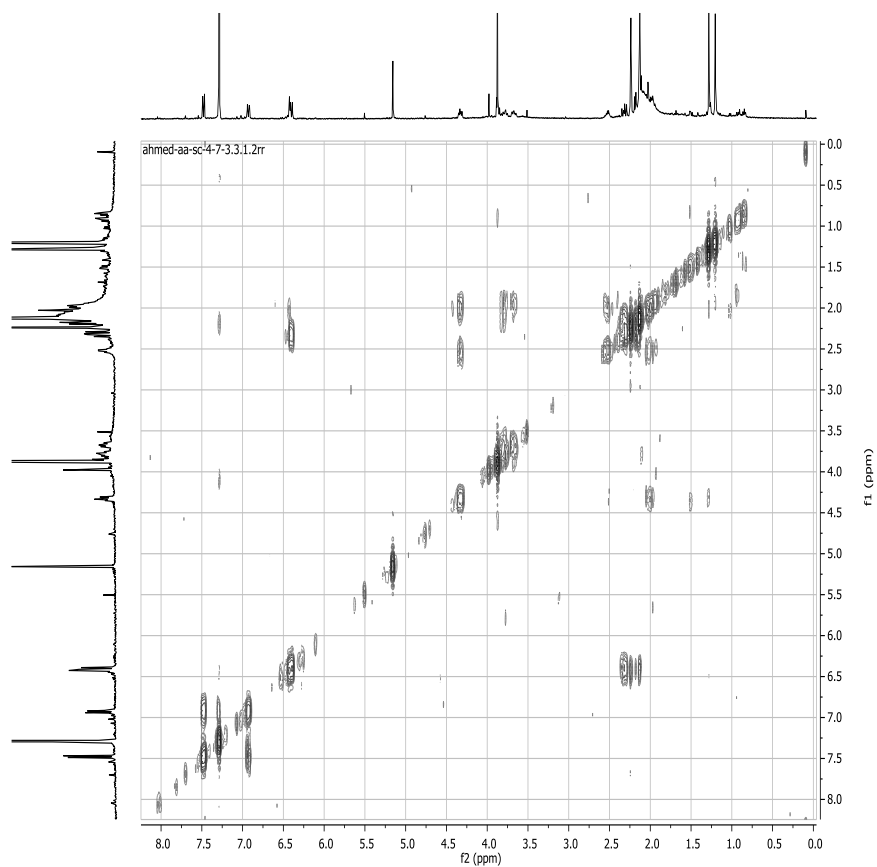
S19. HMBC spectrum of compound 4



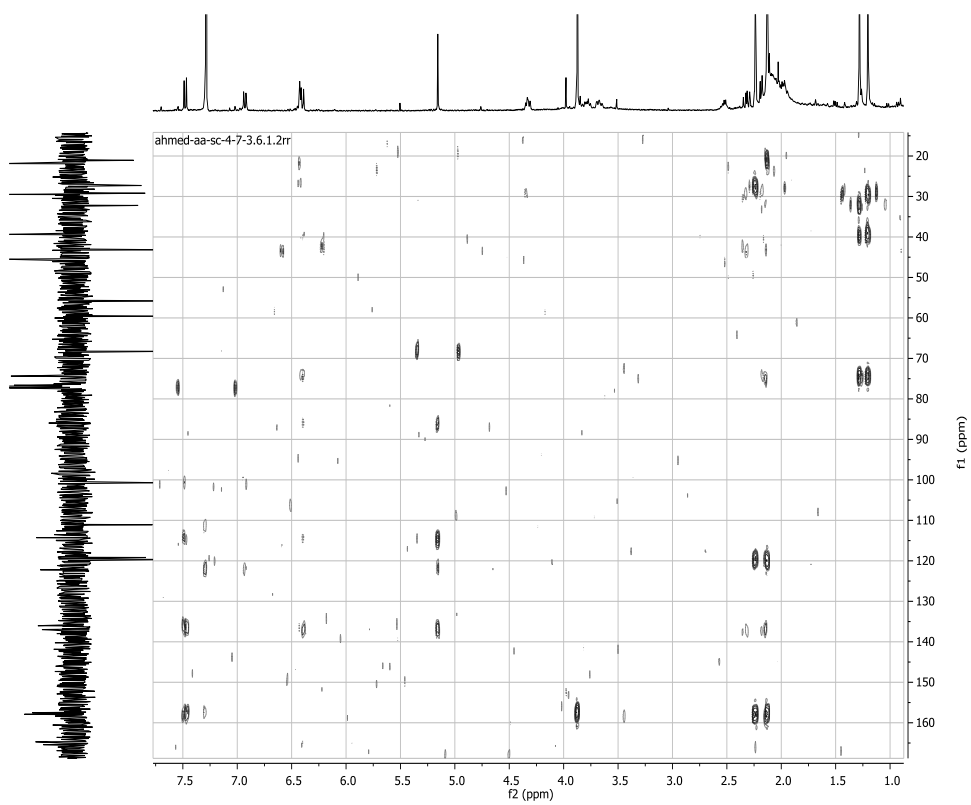
S20. ¹H NMR spectrum of compound 5 (CDCl₃)



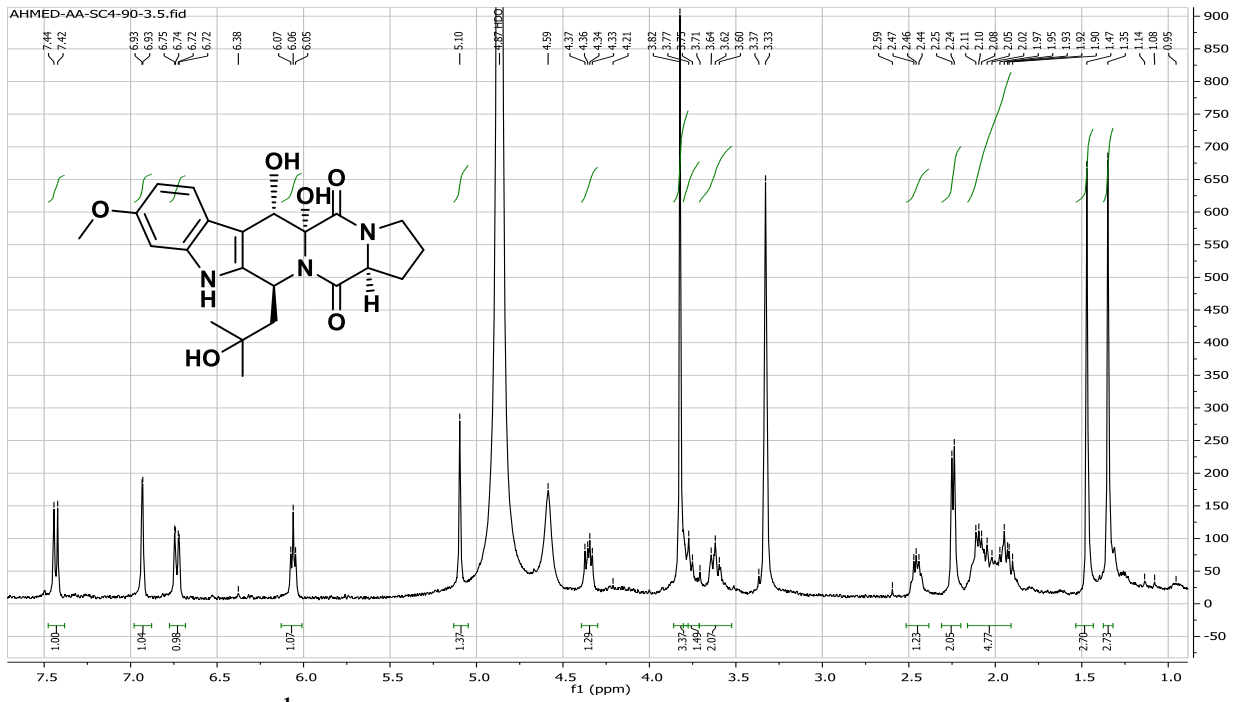
S21. APT NMR spectrum of compound 5



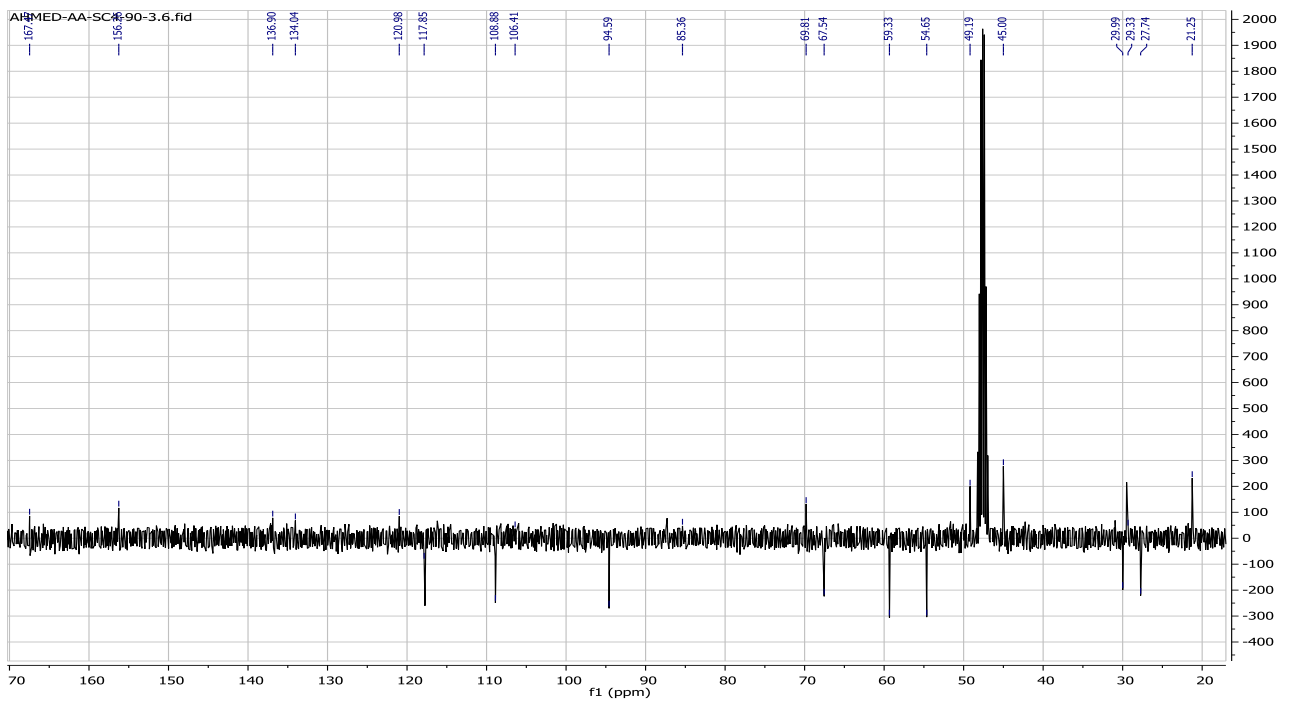
S22. COSY spectrum of compound 5



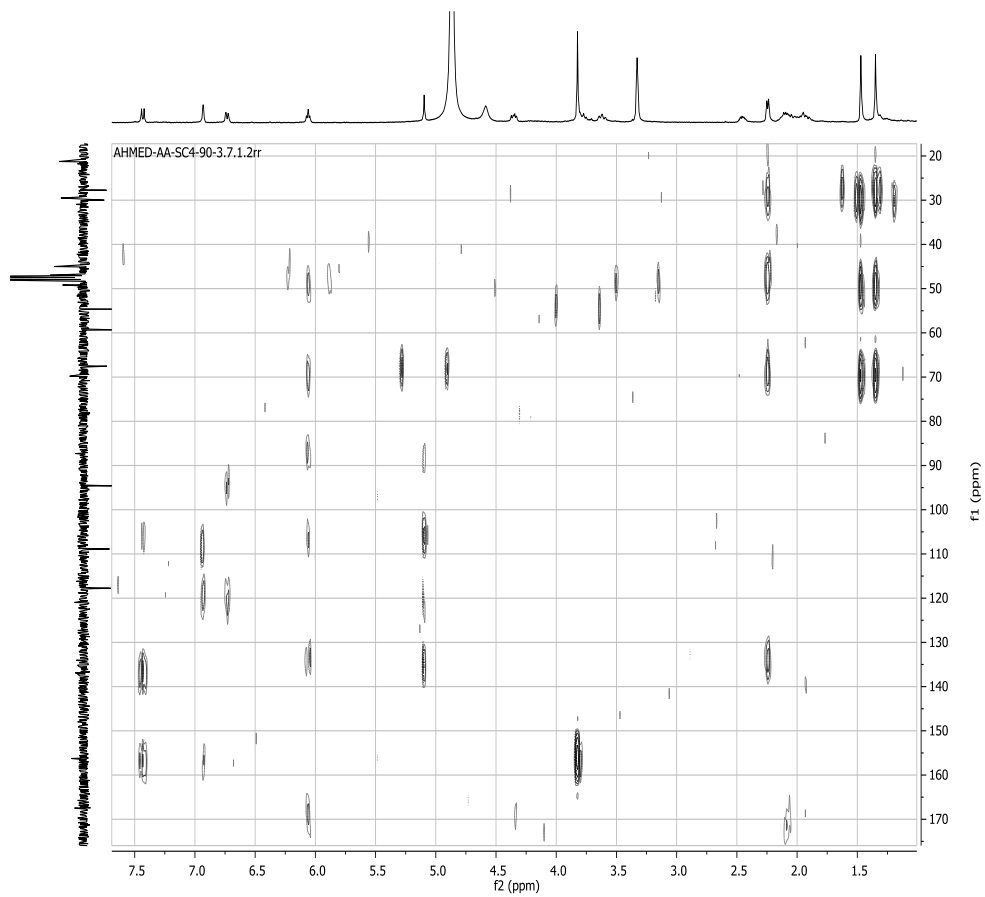
S23. HMBC spectrum of compound 5



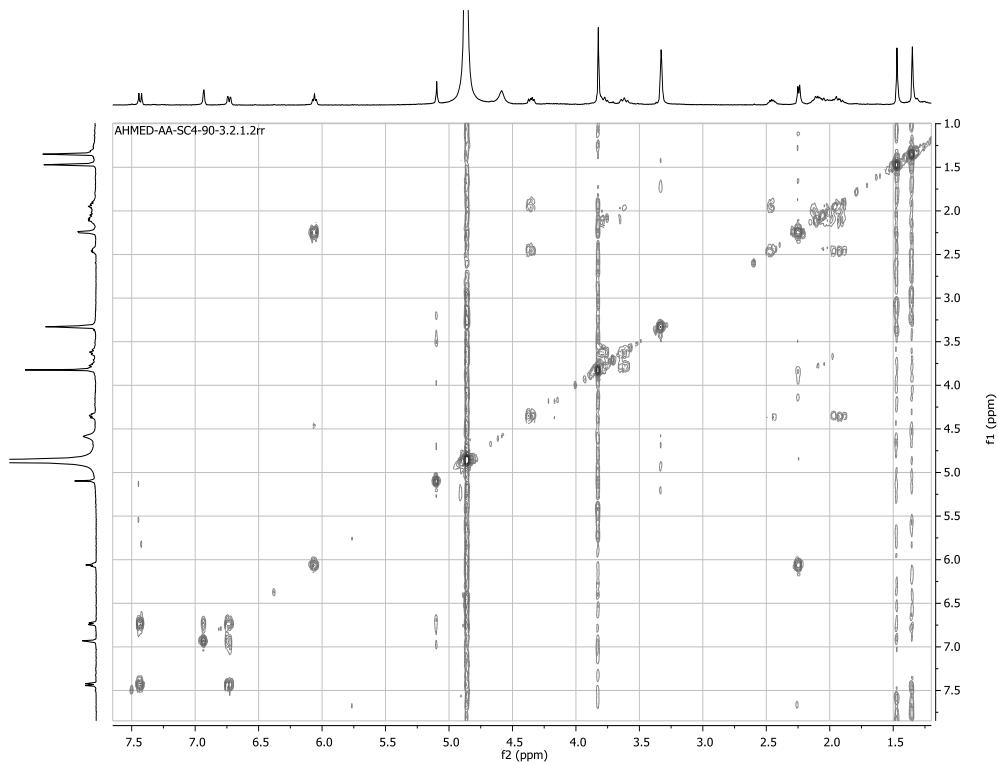
S24. ^1H NMR spectrum of compound 6 (CD_3OD)



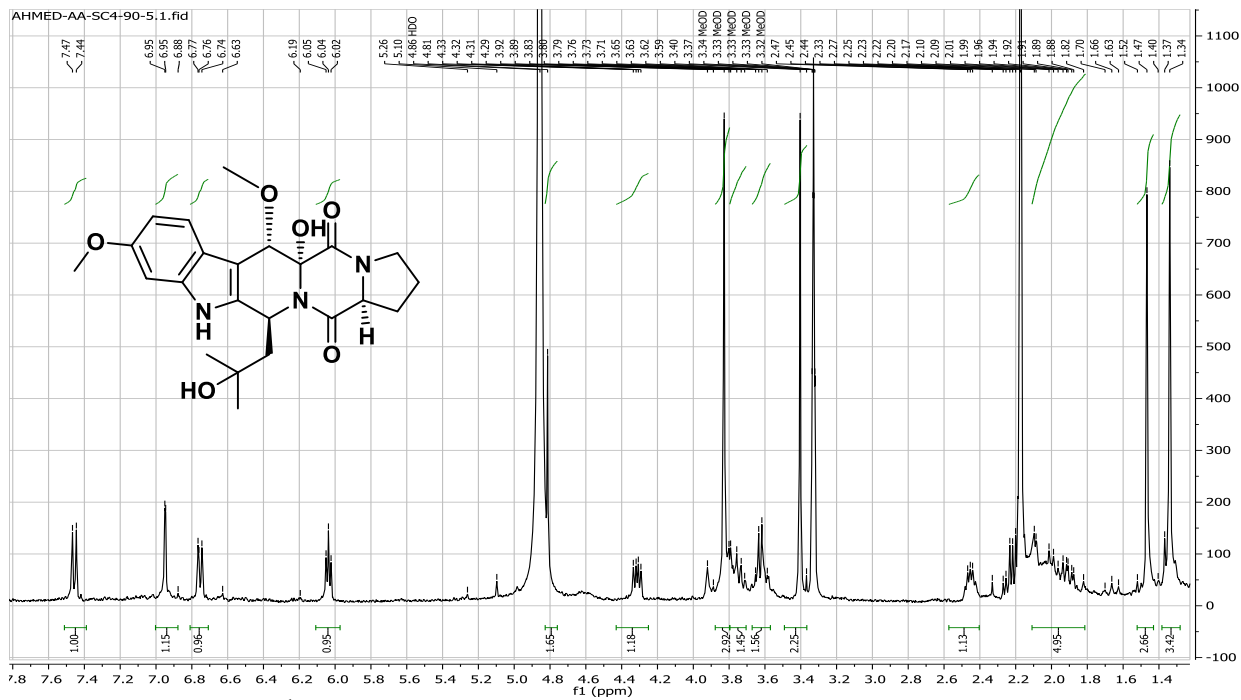
S25. APT spectrum of compound 6



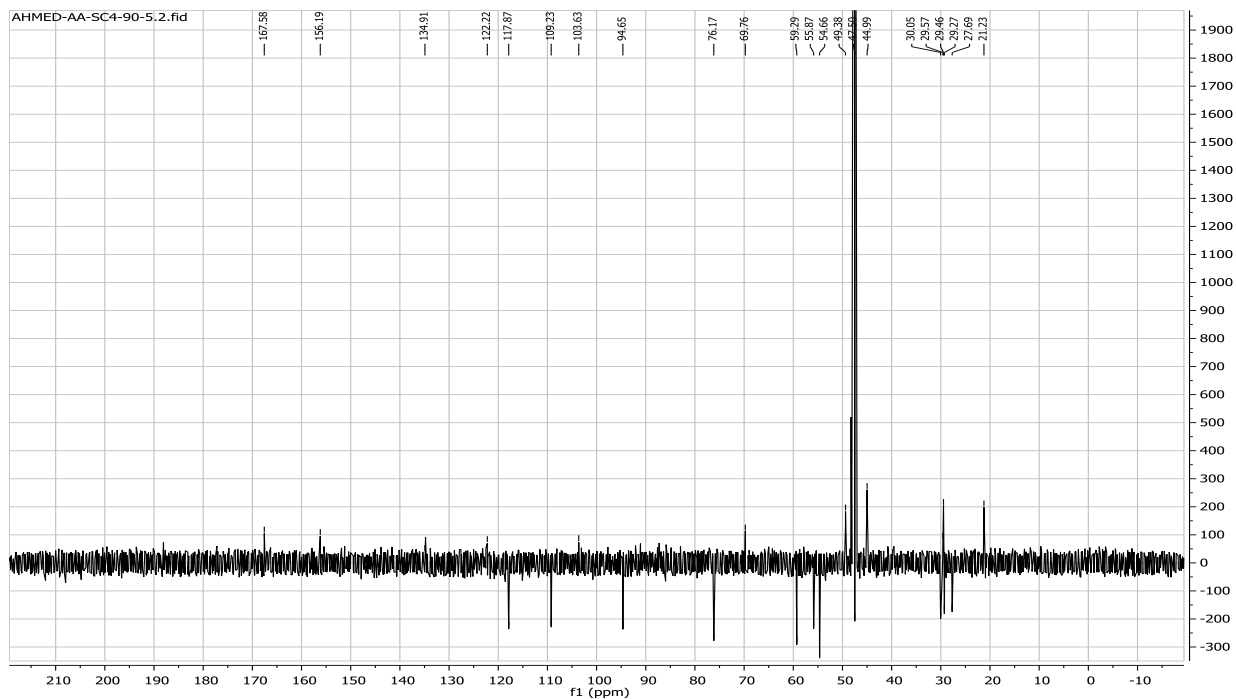
S27. HMBC spectrum of compound 6



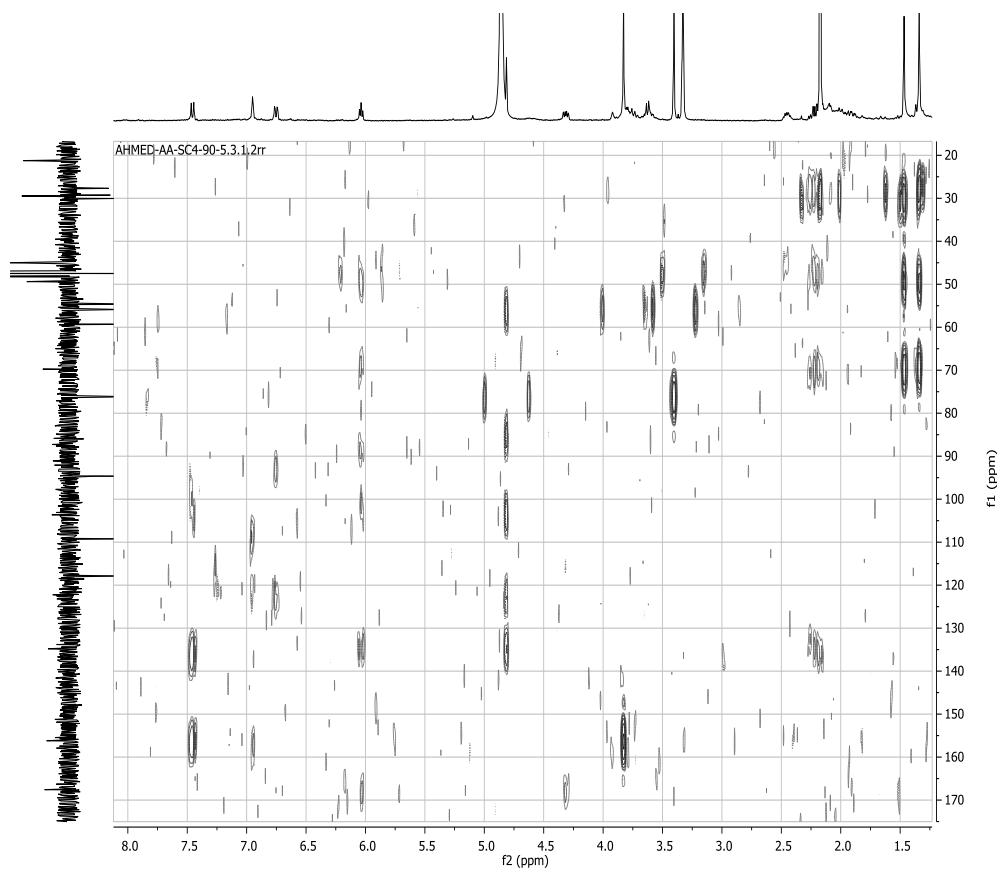
S28. COSY spectrum of compound 6



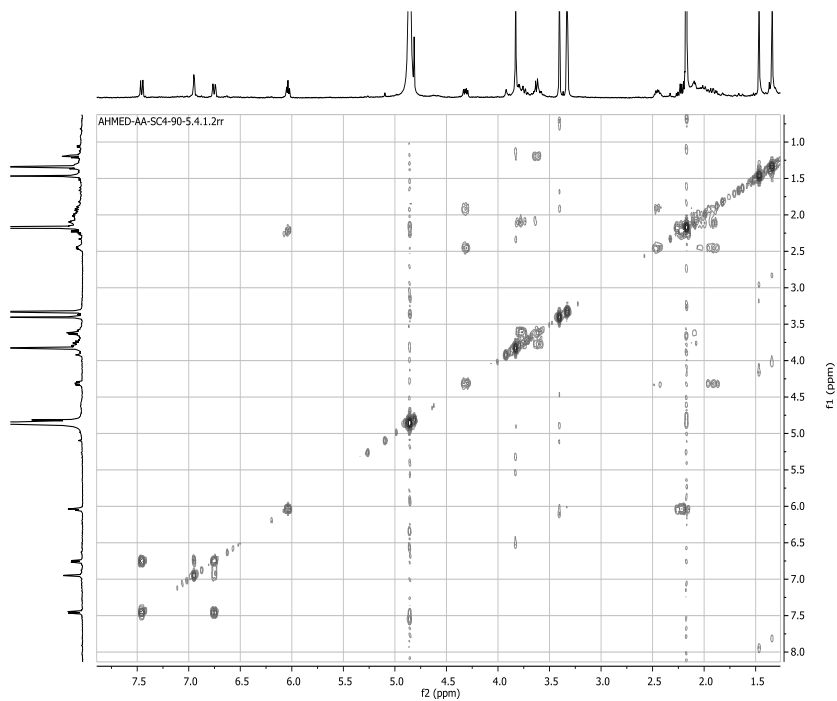
S29. ¹H NMR spectrum of compound 7 (CD₃OD)



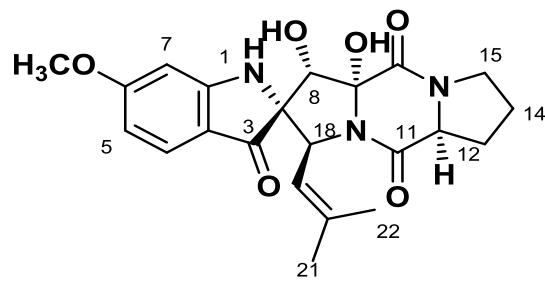
S30. APT NMR spectrum of compound 7



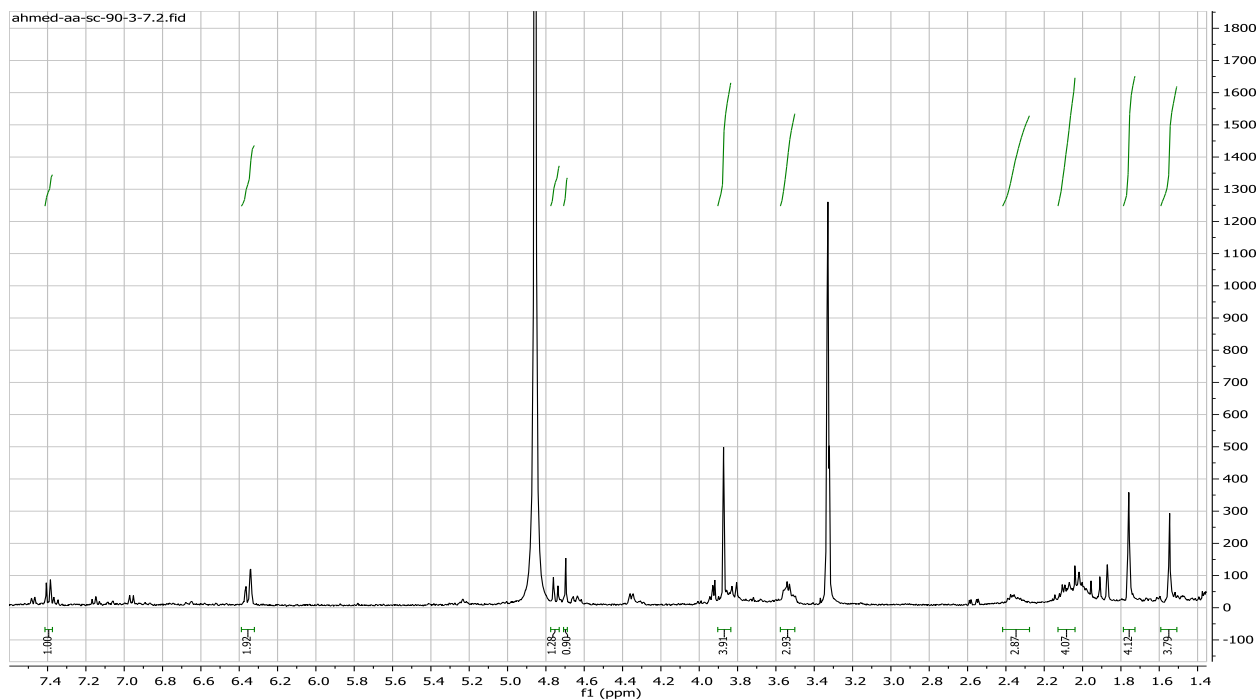
S31. HMBC spectrum of compound 7



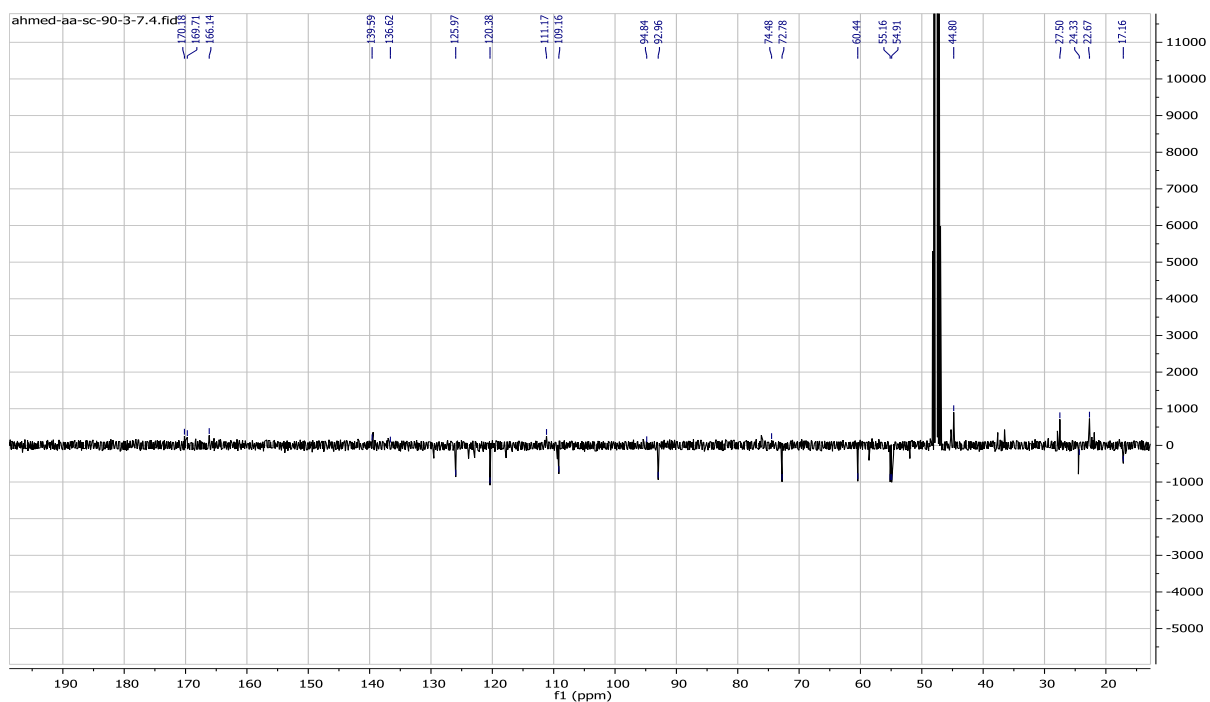
S32. COSY spectrum of compound 7



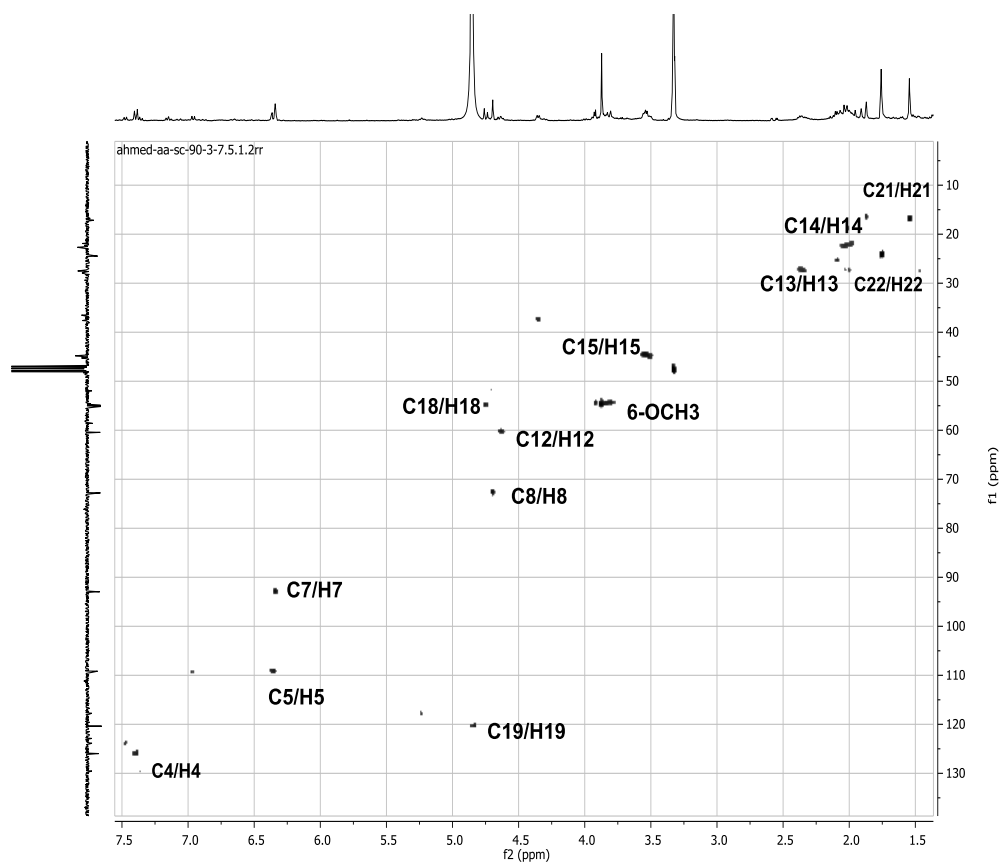
Compound 8



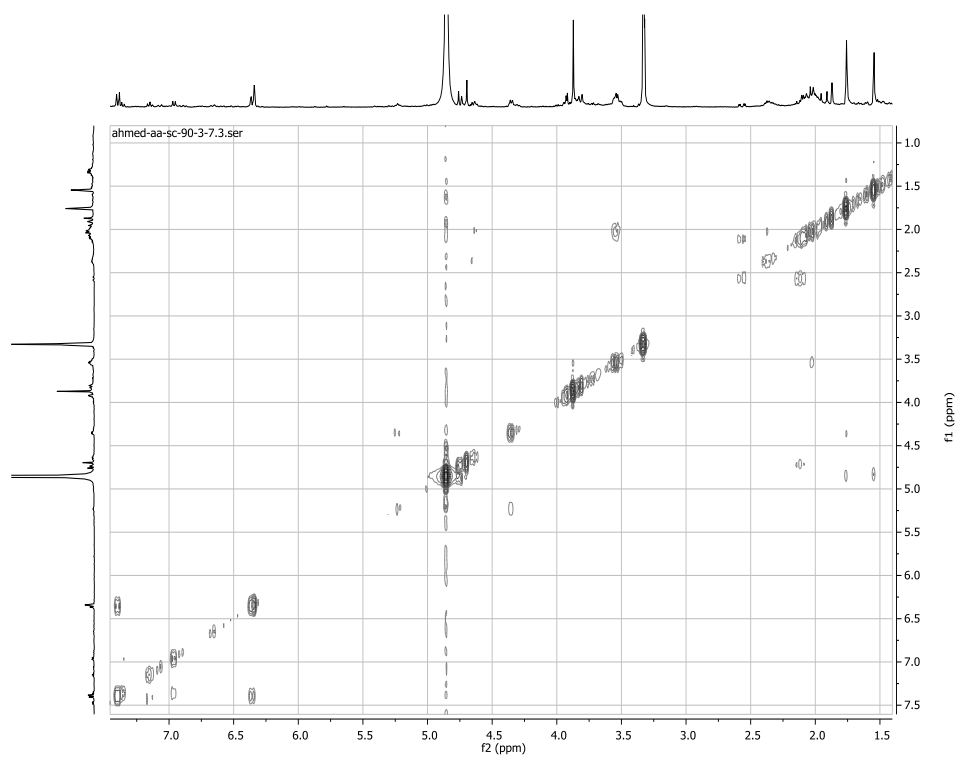
S33. ¹H NMR spectrum of compound 8 (CD₃OD)



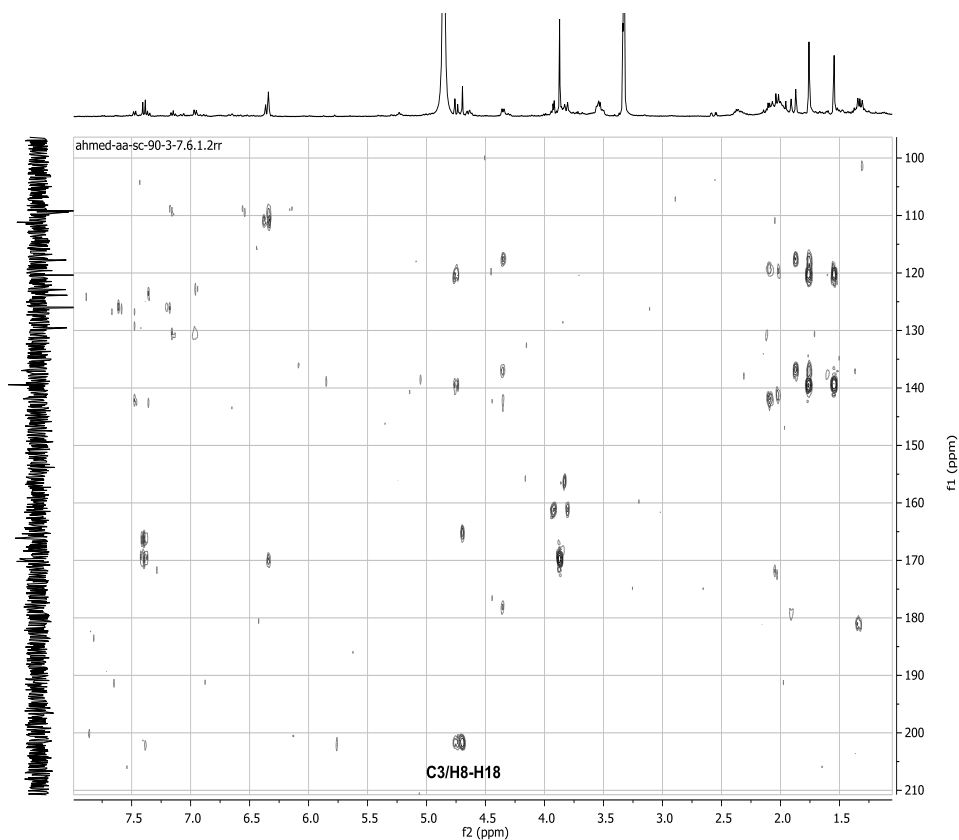
S34. APT NMR spectrum of compound 8



S35. HSQC NMR spectrum of compound 8

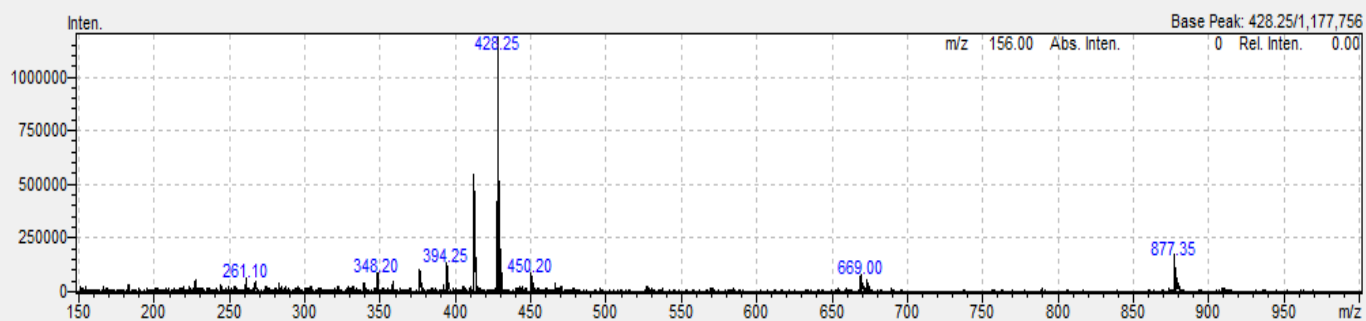


S36. COSY NMR spectrum of compound 8

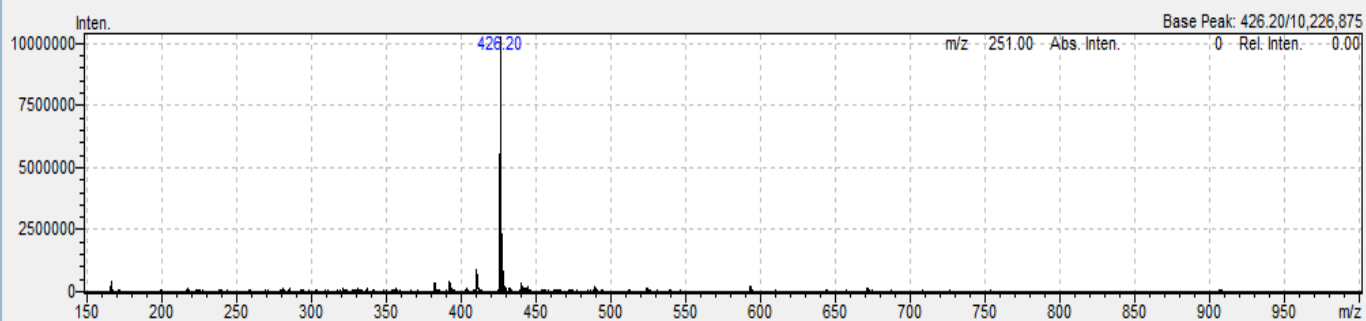


S37. HMBC NMR spectrum of compound 8

Event#: 1 Q3 Scan(E+) Ret. Time: [6.98] Scan#: [1035]



Event#: 2 Q3 Scan(E-) Ret. Time: [6.99] Scan#: [1036]



S38. +/- ESIMS spectrum of Compound 8