

Supporting Information II

Spectral data

Interpretation of Unusual Chemical Behaviors of Oxygenated theonellastrols using Quantum Mechanical Calculations and Stereochemical reassignment of 7α - hydroxytheonellasterol

A-Young Shin,^{1,2} Hyi-Seung Lee,^{1,2} Yeon-Ju Lee,^{1,2} Jong Seok Lee,^{1,2} Arang Son,³ Changhoon Cho,³

and Jihoon Lee^{1,2}*

¹Korea Institute of Ocean Science and Technology (KIOST), Busan 49111, Republic of Korea

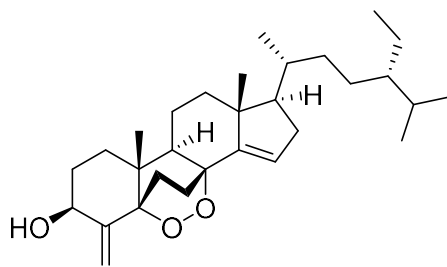
²Department of Marine Biotechnology, University of Science and Technology (UST), Daejeon 34113, Republic of Korea

³Department of Radiation Oncology, Samsung Medical Center, Seoul 06351, Republic of Korea

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1

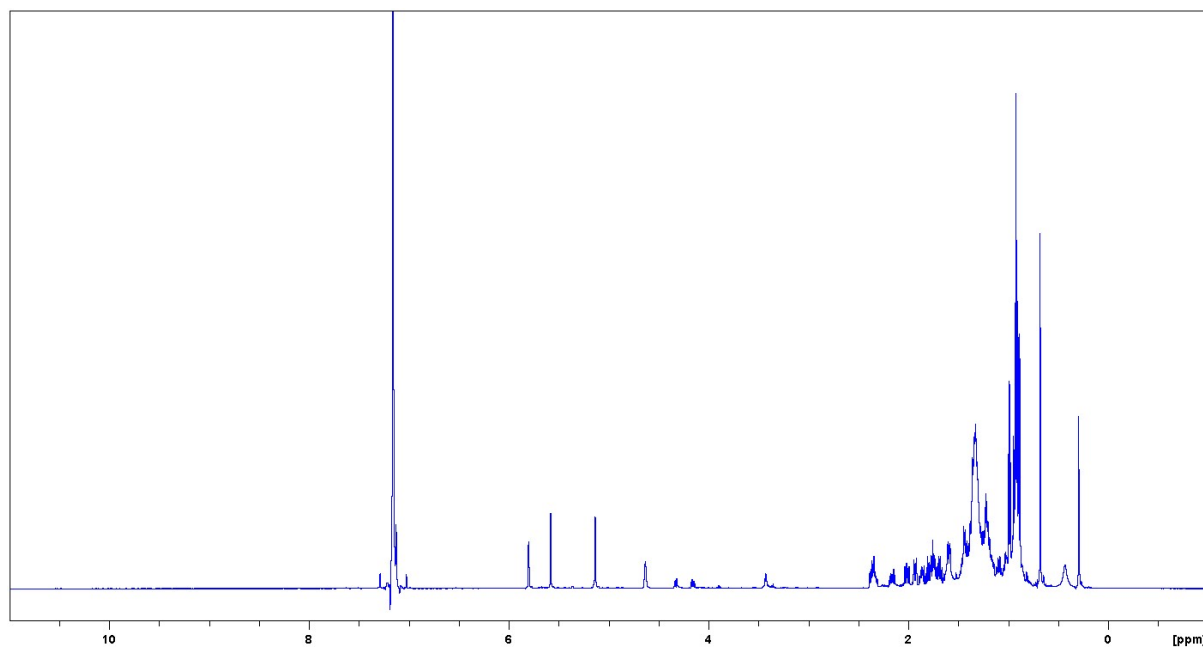


Figure SII-1. ^1H NMR spectrum of compound **1** (CDCl_3 , 600 MHz).

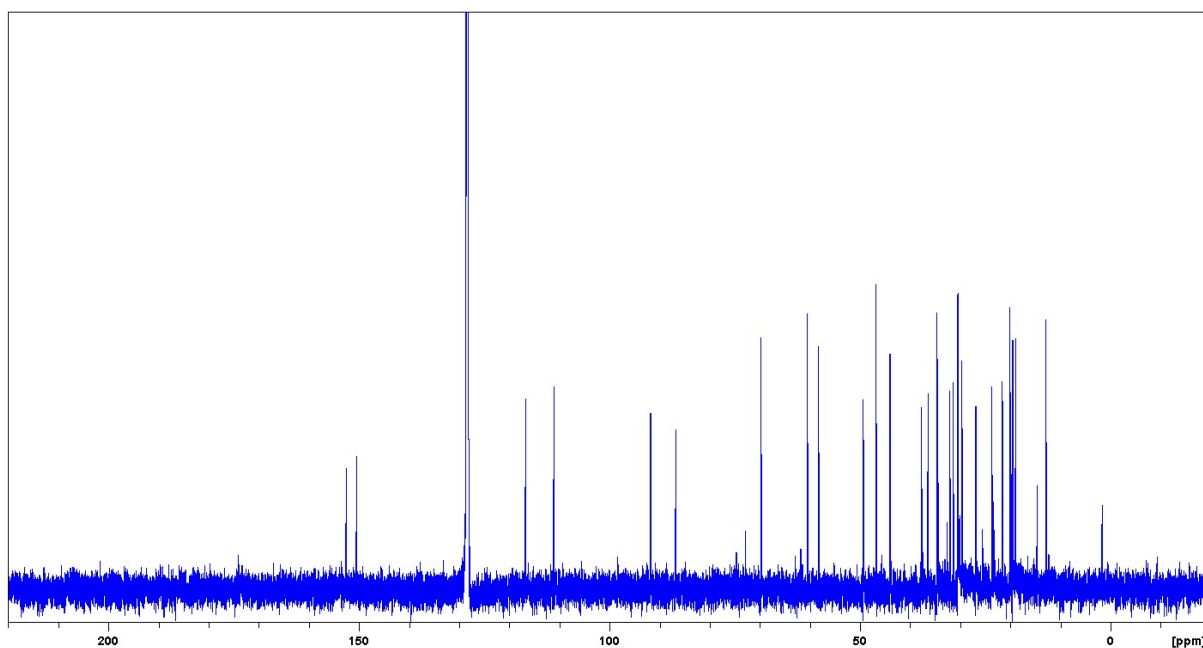


Figure SII-2. ^{13}C NMR spectrum of compound **1** (CDCl_3 , 150 MHz).

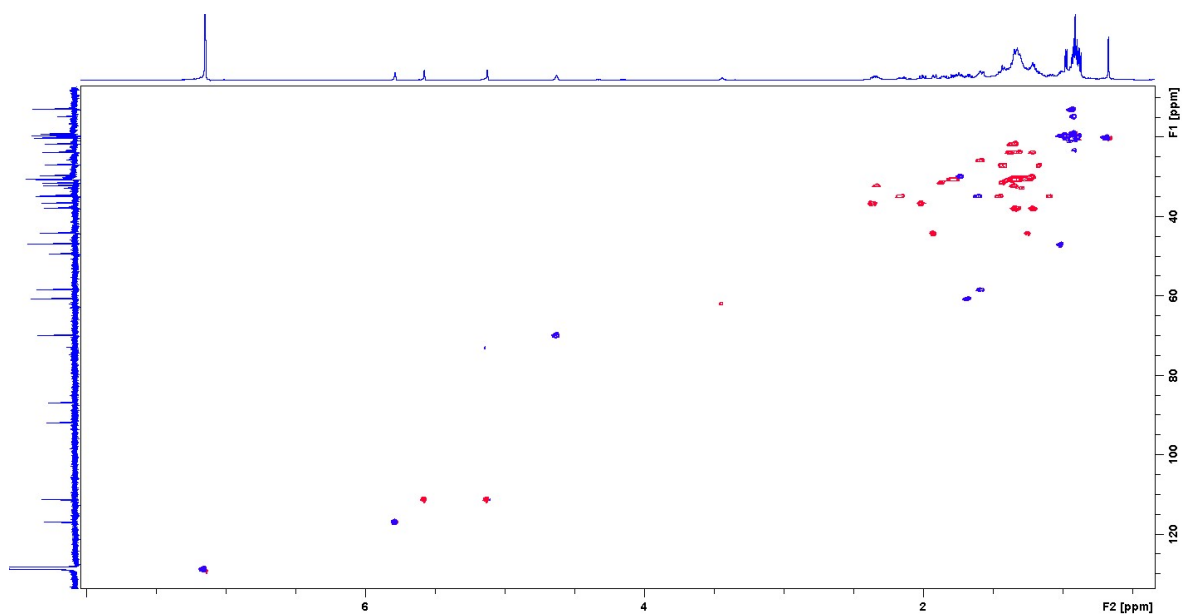


Figure SII-3. HSQC spectrum of compound **1** (C_6D_6 , 600 MHz).

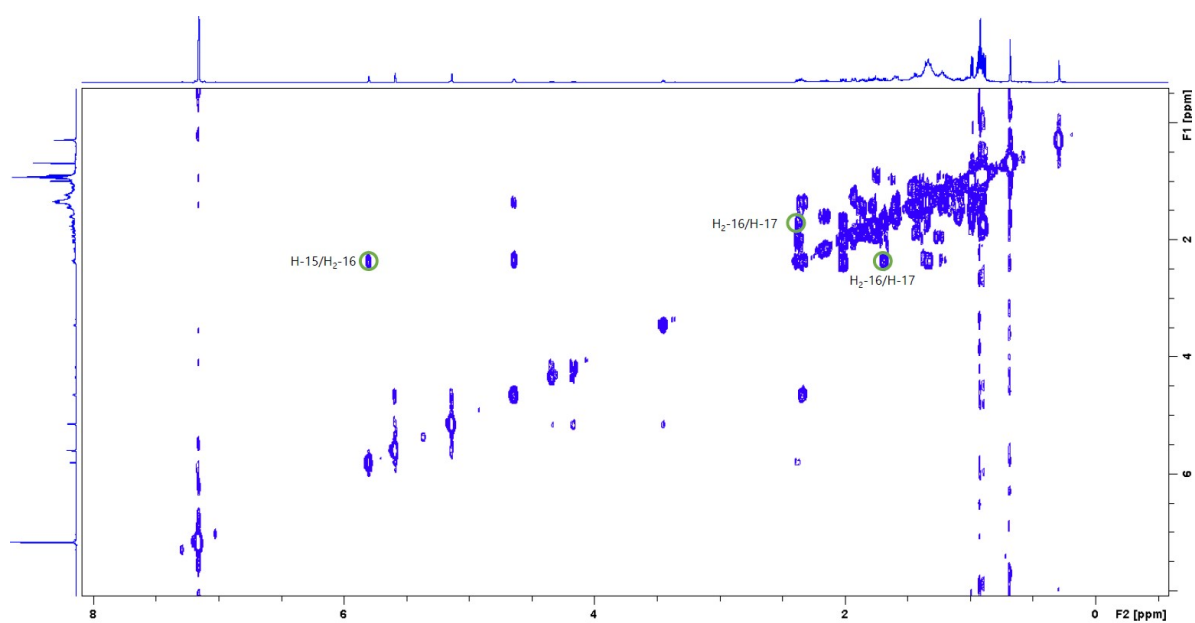


Figure SII-4. 1H - 1H COSY spectrum of compound **1** (C_6D_6 , 600 MHz).

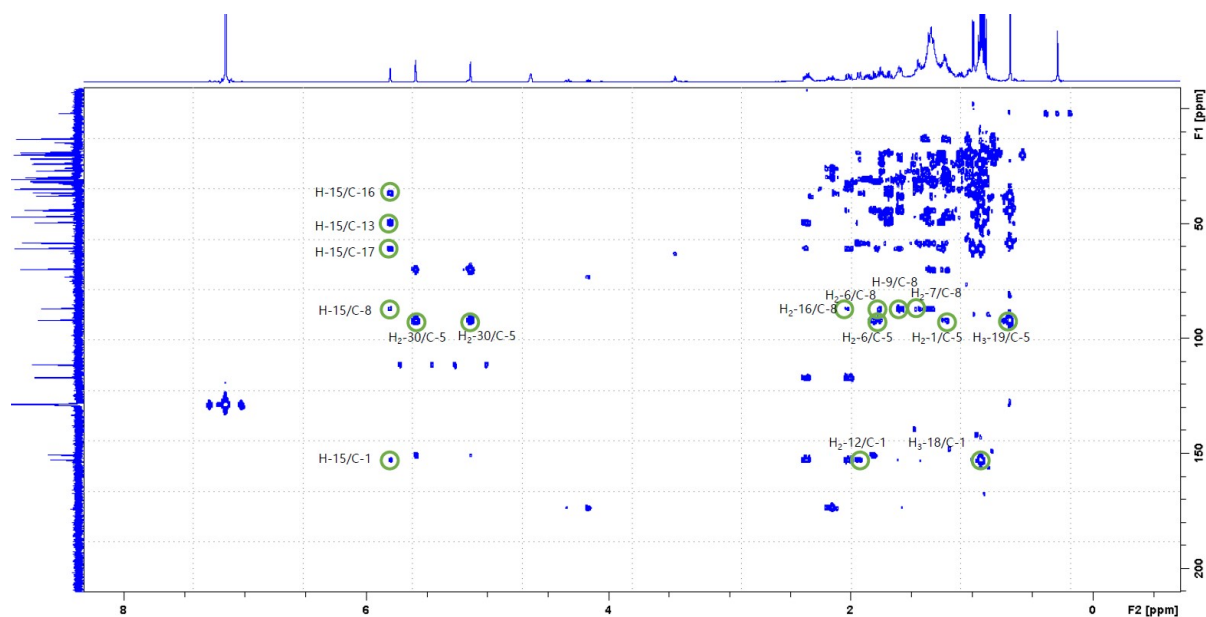


Figure SII-5. HMBC spectrum of compound **1** (C_6D_6 , 600 MHz).

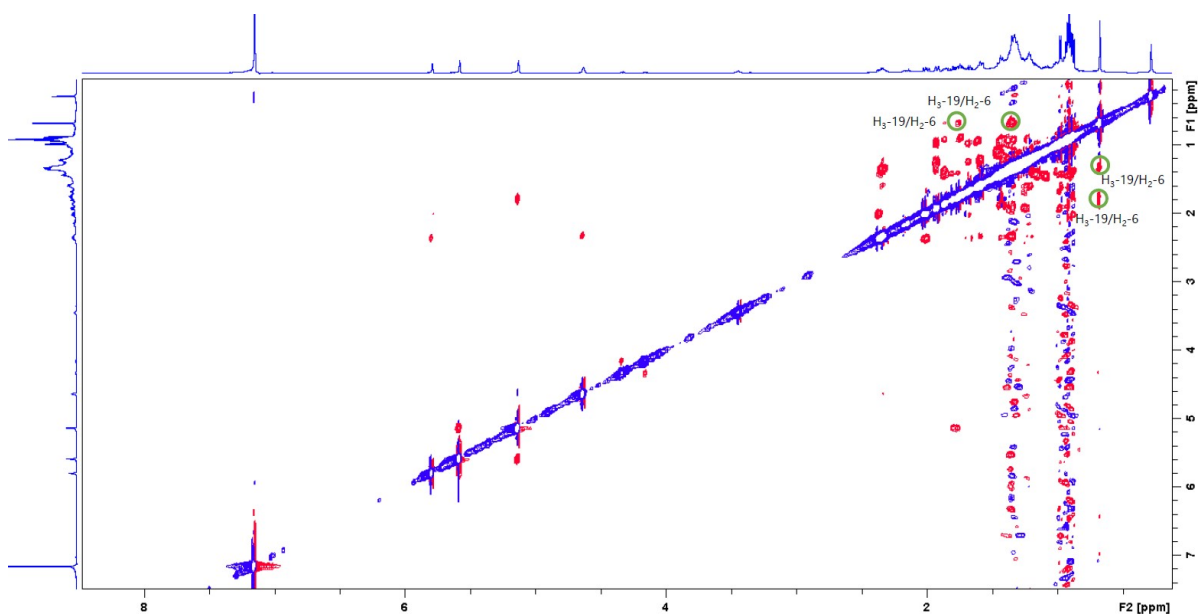


Figure SII-6. NOESY spectrum of compound **1** (C_6D_6 , 600 MHz).

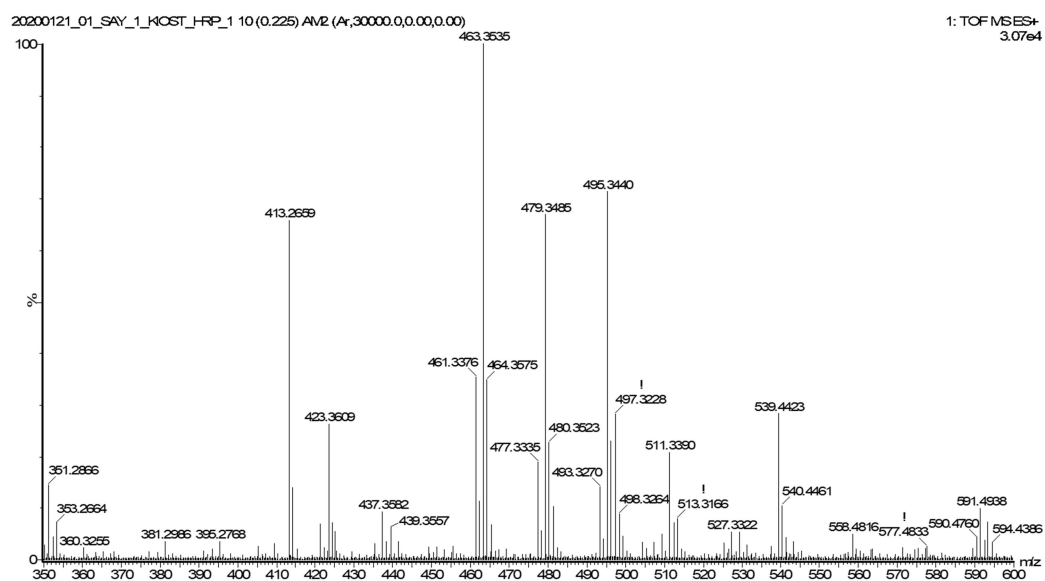
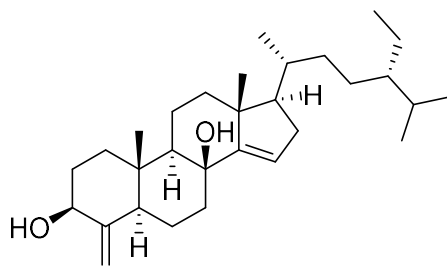


Figure SII-7. HRMS spectrum of compound **1**.



2

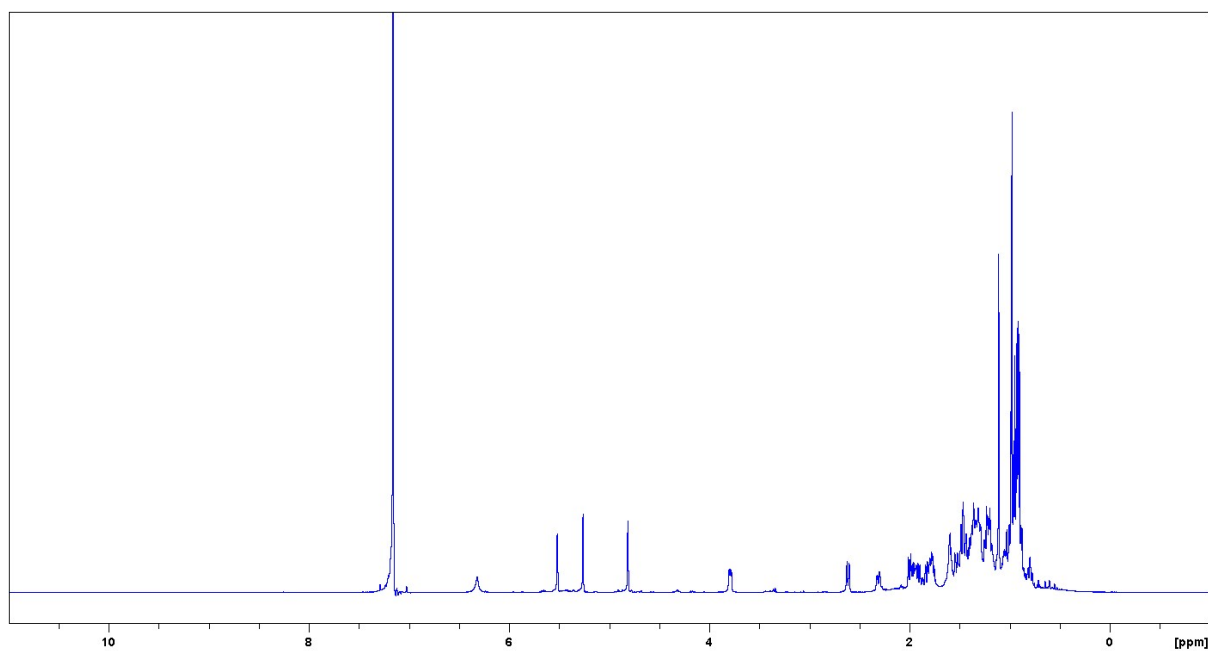


Figure SII-8. ^1H NMR spectrum of compound 2 (C_6D_6 , 600 MHz).

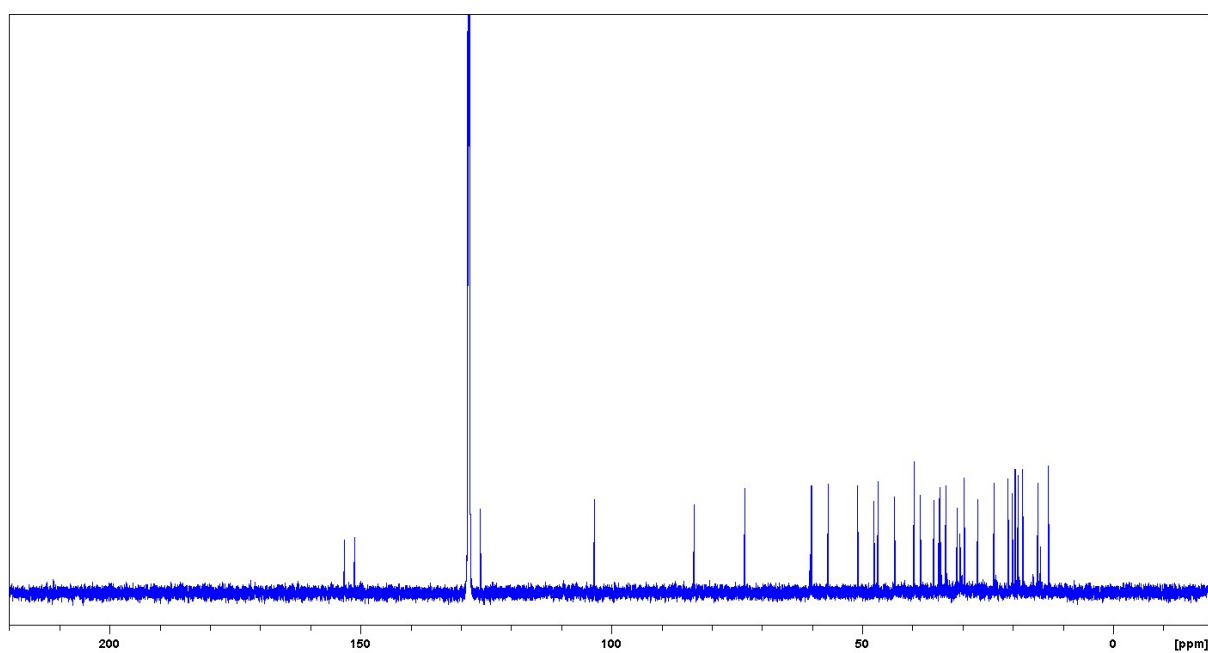


Figure SII-9. ^{13}C NMR spectrum of compound 2 (C_6D_6 , 150 MHz).

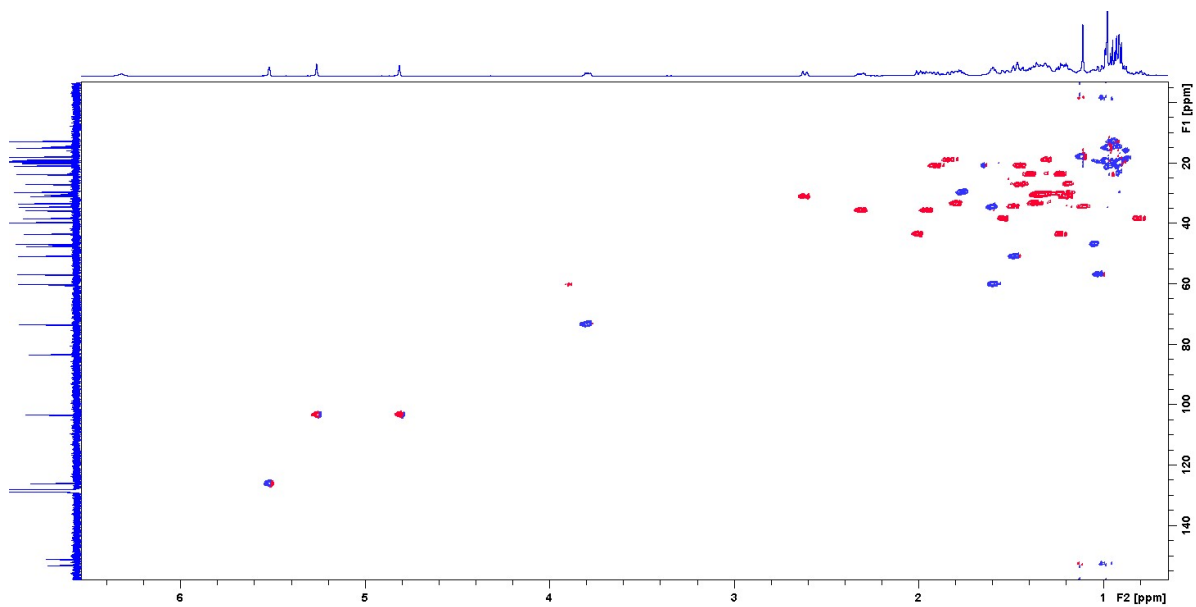


Figure SII-10. HSQC spectrum of compound **2** (C₆D₆, 600 MHz).

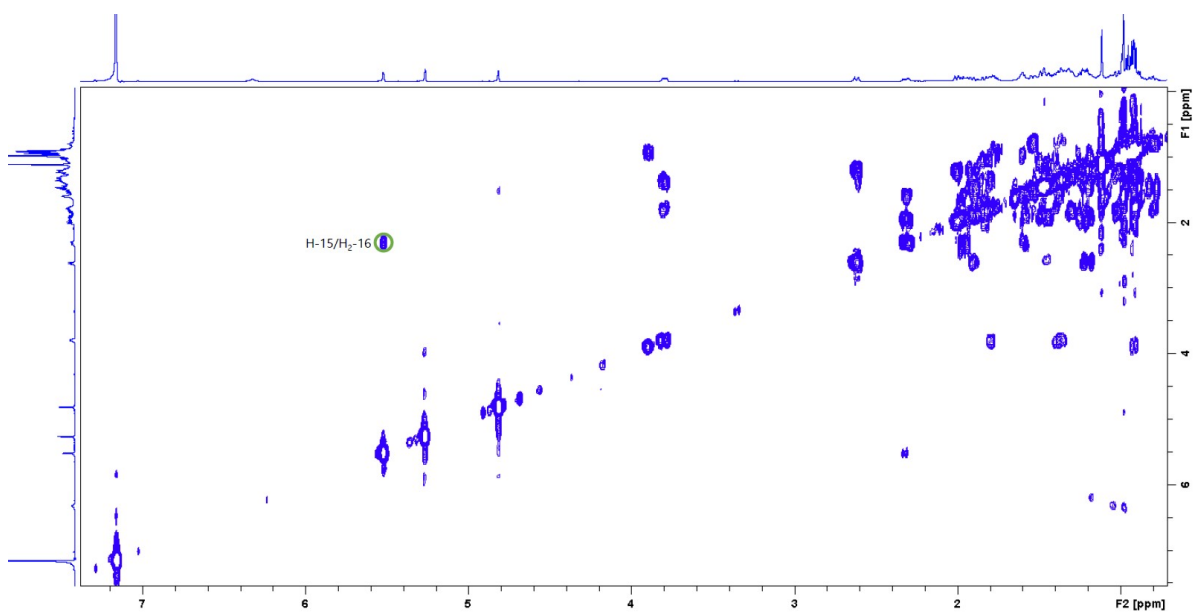


Figure SII-11. ¹H-¹H COSY spectrum of compound **2** (C₆D₆, 600 MHz).

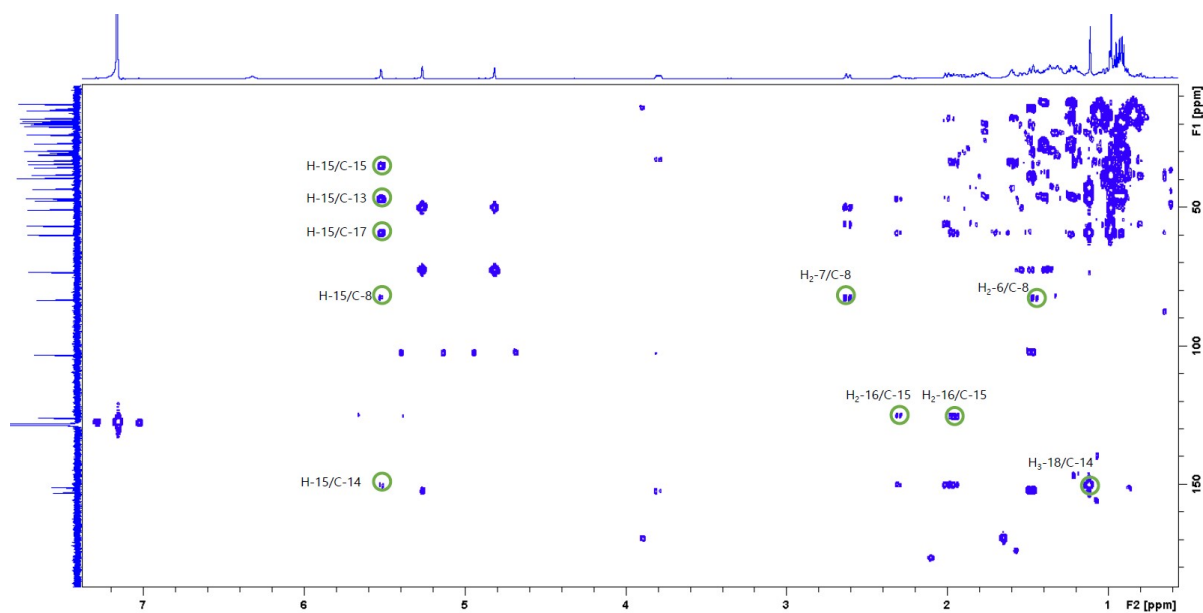


Figure SII-12. HMBC spectrum of compound 2 (C_6D_6 , 600 MHz).

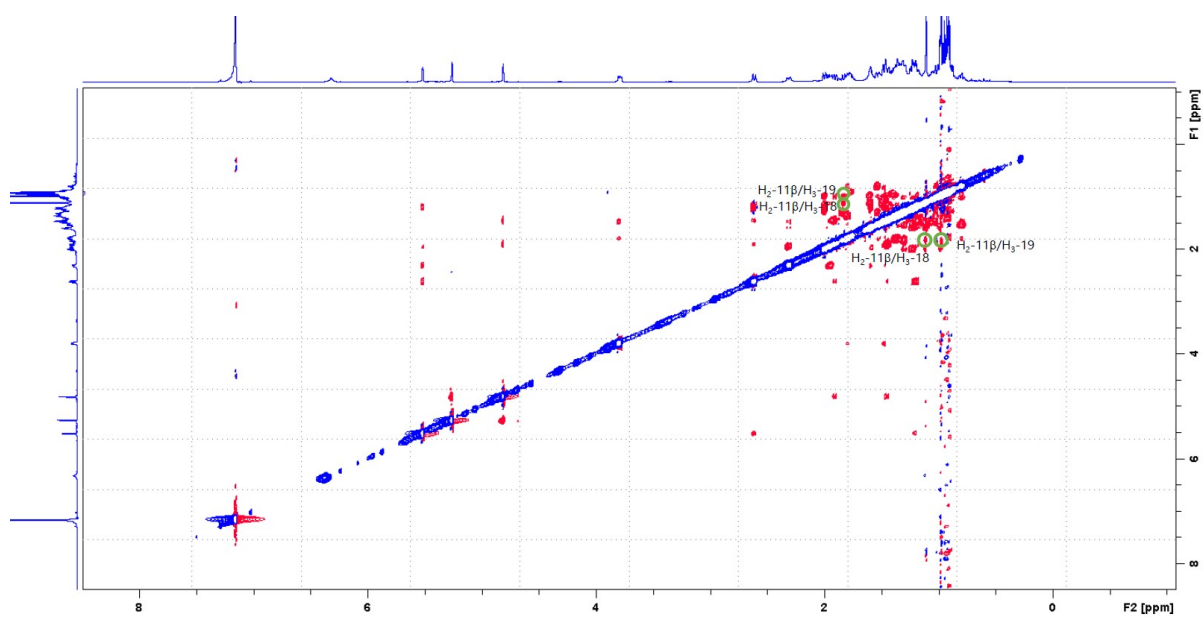


Figure SII-13. NOESY spectrum of compound 2 (C_6D_6 , 600 MHz).

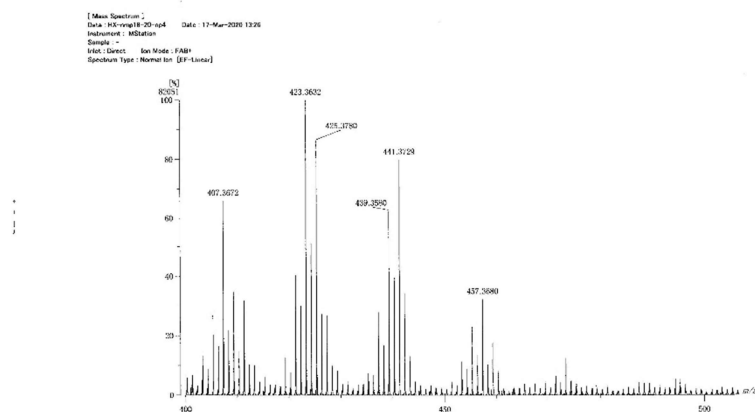
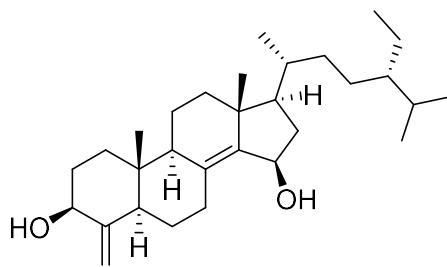


Figure SII-14. HRMS spectrum of compound **2**.



3

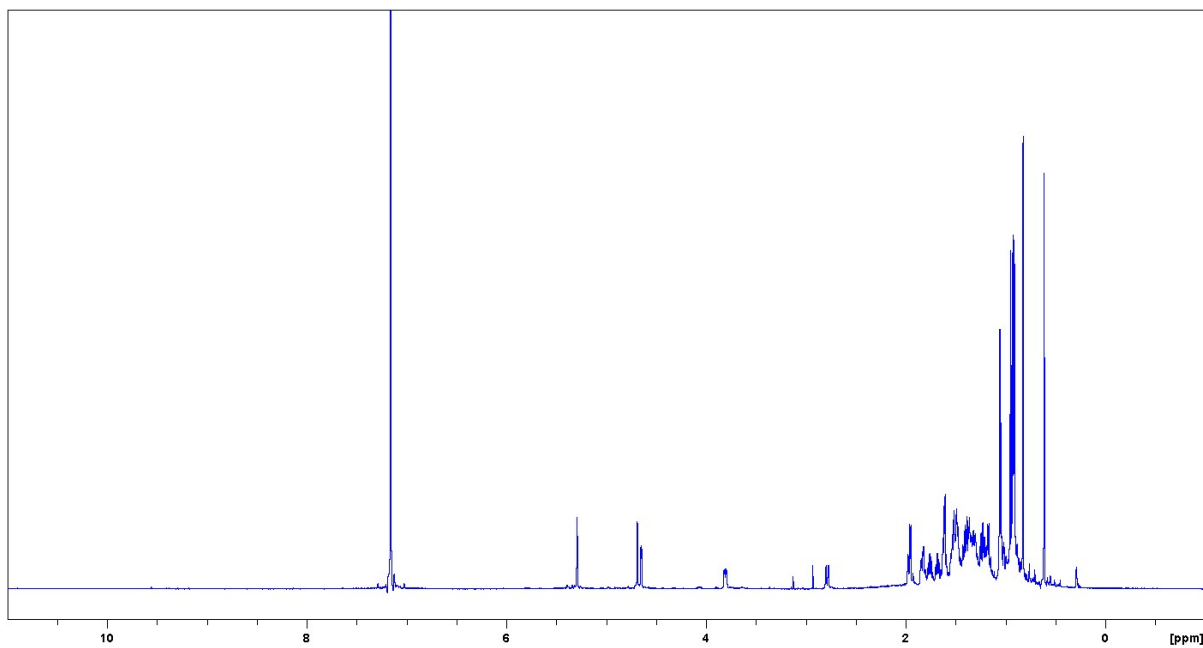


Figure SII-15. ^1H NMR spectrum of compound **3** (CDCl_3 , 600 MHz).

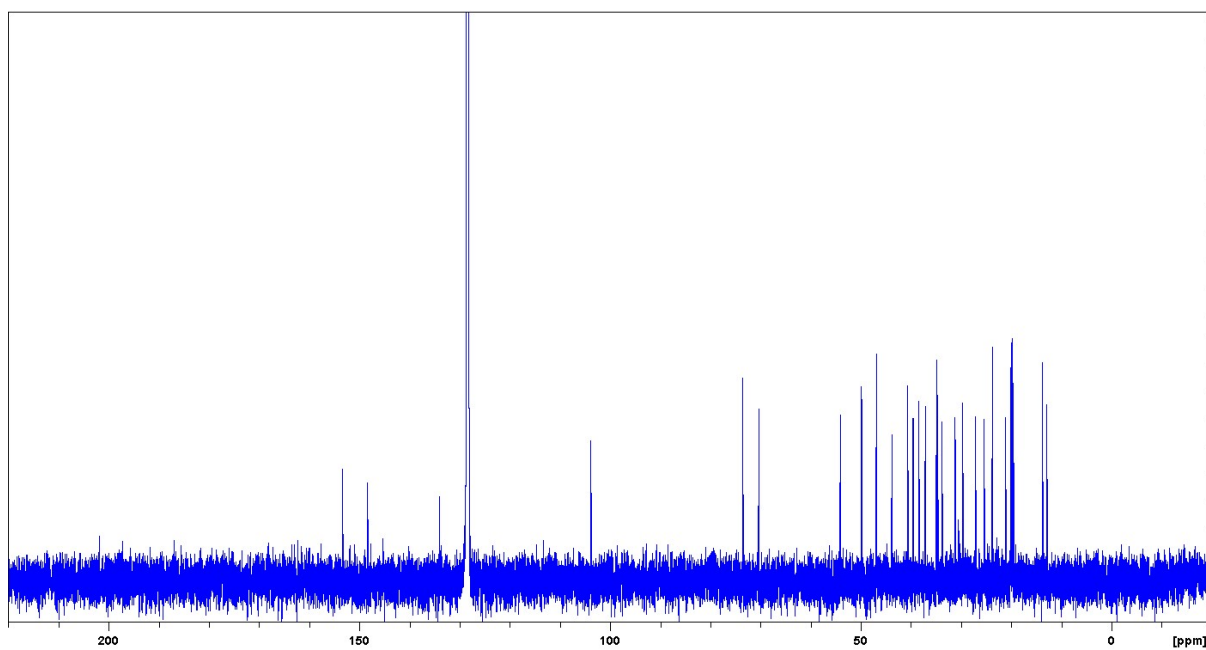


Figure SII-16. ^{13}C NMR spectrum of compound **3** (CDCl_3 , 150 MHz).

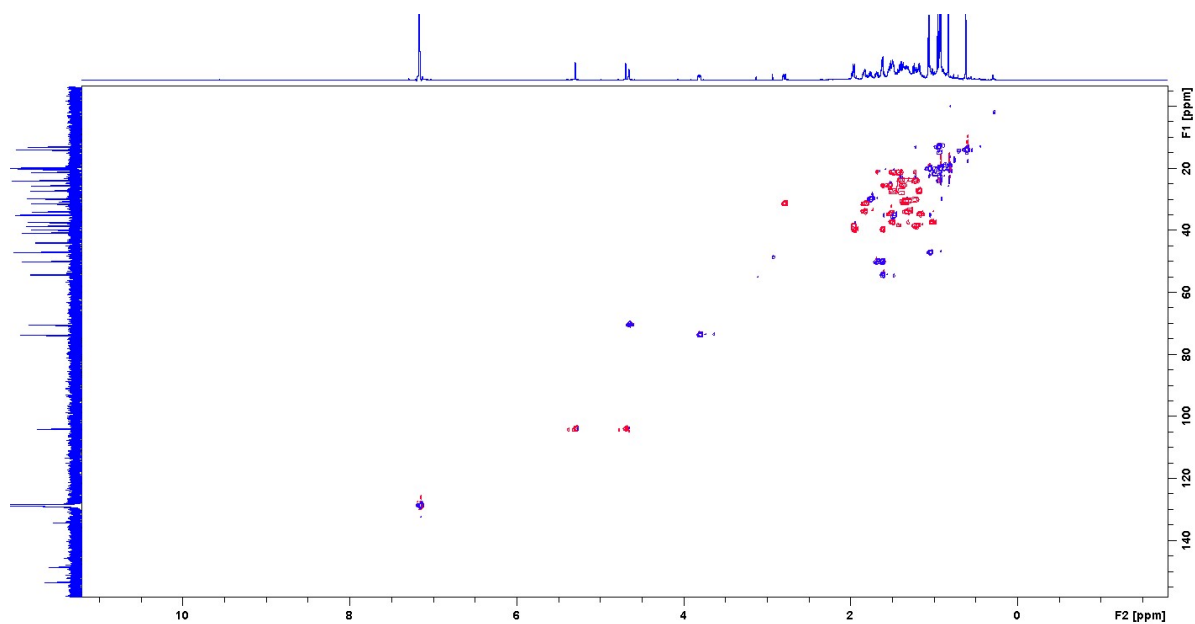


Figure SII-17. HSQC spectrum of compound **3** (C_6D_6 , 600 MHz).

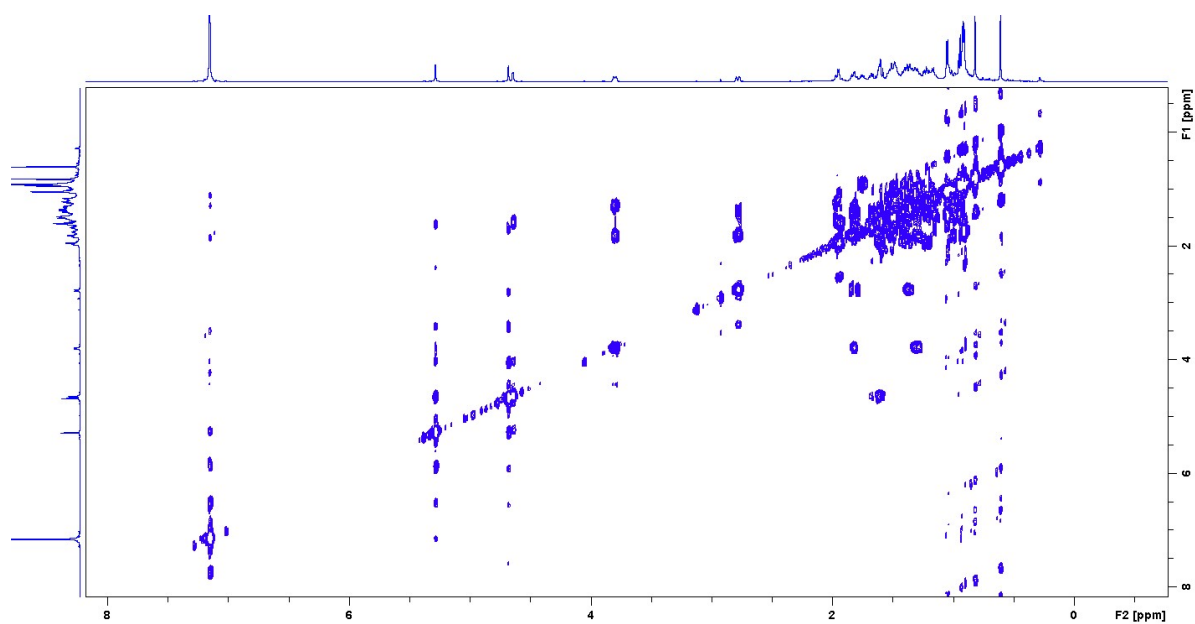


Figure SII-18. ^1H - ^1H COSY spectrum of compound **3** (C_6D_6 , 600 MHz).

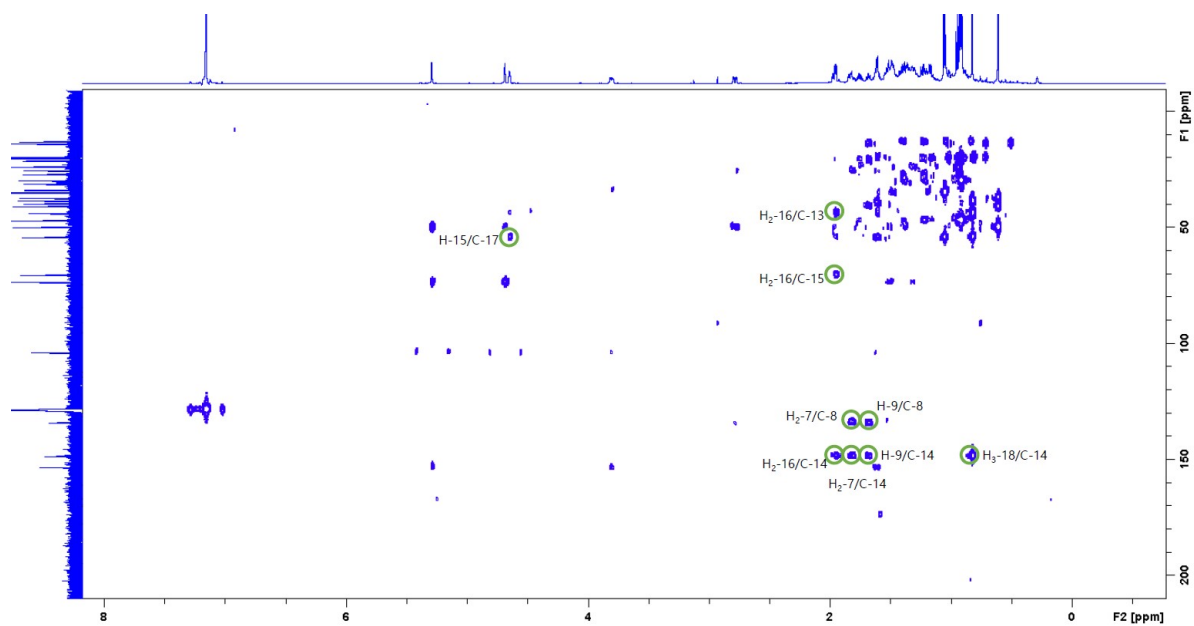


Figure SII-19. HMBC spectrum of compound **3** (C_6D_6 , 600 MHz).

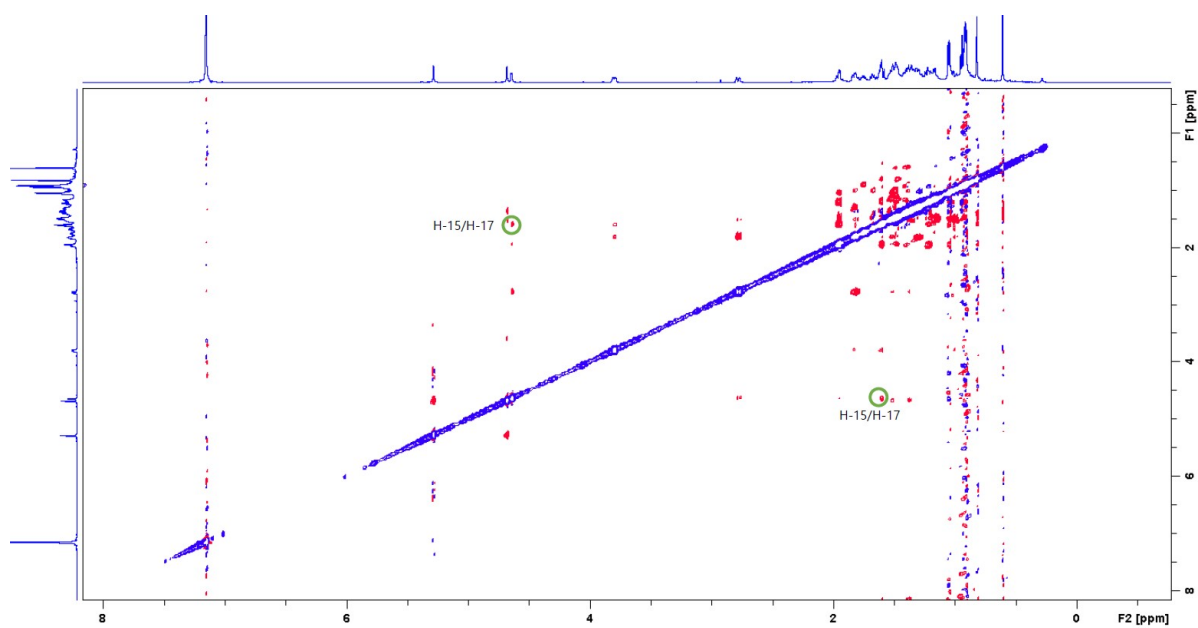


Figure SII-20. NOESY spectrum of compound **3** (C_6D_6 , 600 MHz).

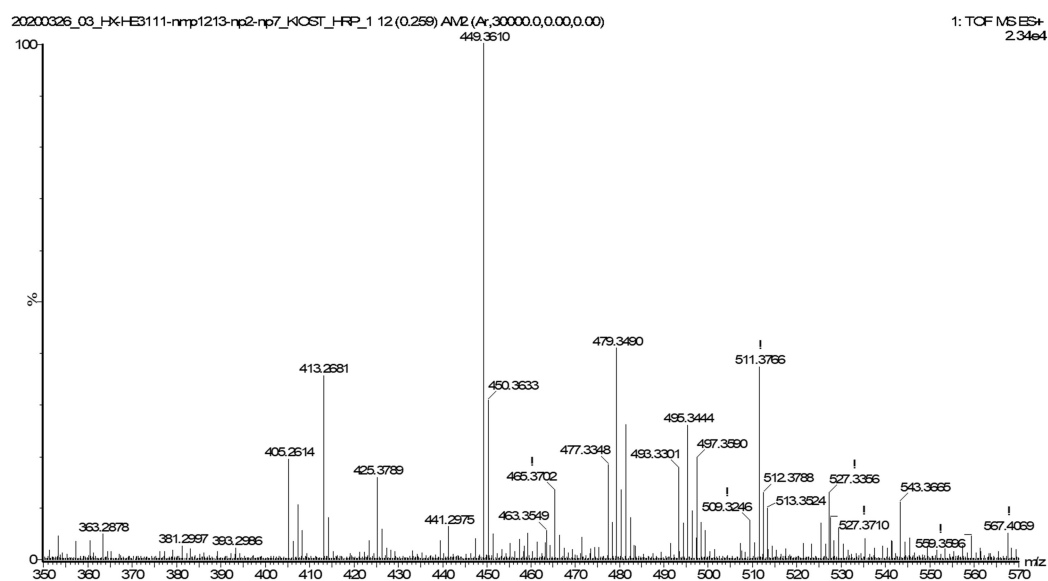
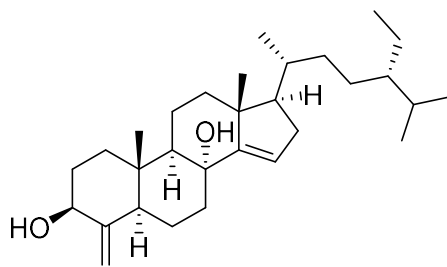


Figure SII-21. HRMS spectrum of compound **3**.



4

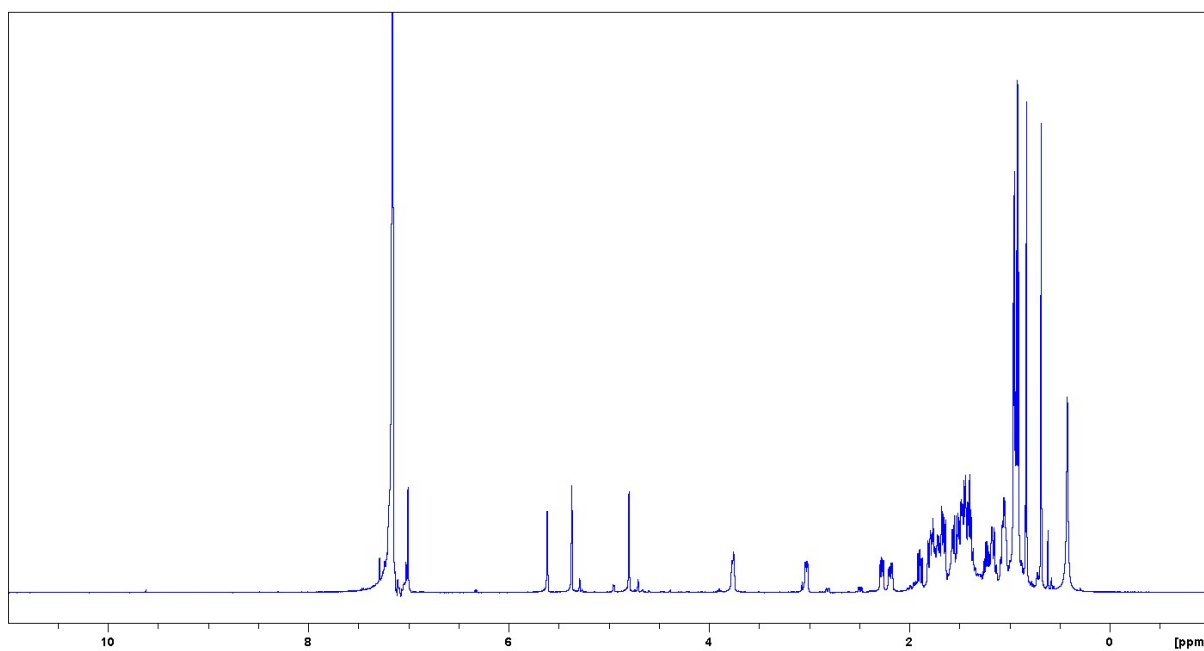


Figure SII-22. ^1H NMR spectrum of compound **4** (C_6D_6 , 600 MHz).

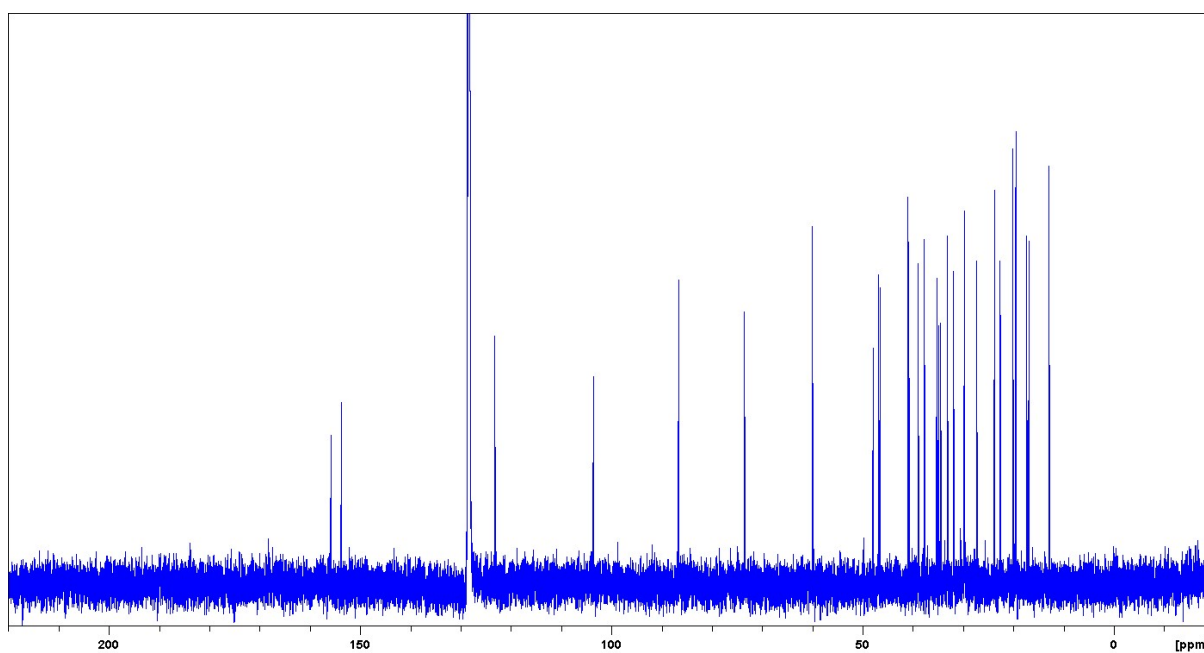


Figure SII-23. ^{13}C NMR spectrum of compound **4** (C_6D_6 , 150 MHz).

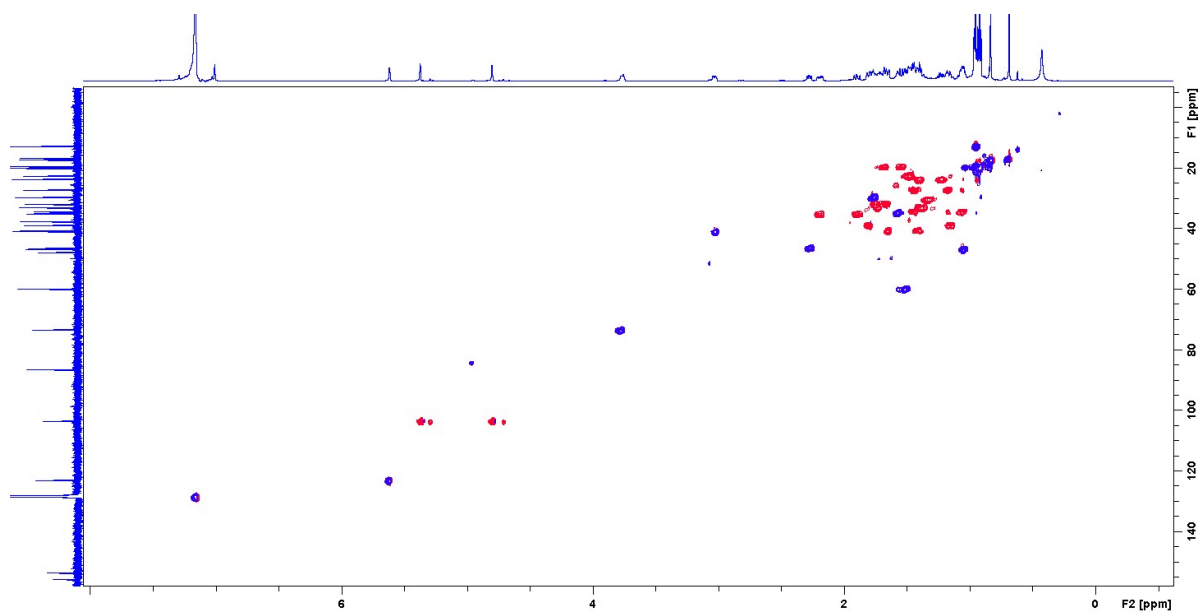


Figure SII-24. HSQC spectrum of compound **4** (C_6D_6 , 600 MHz).

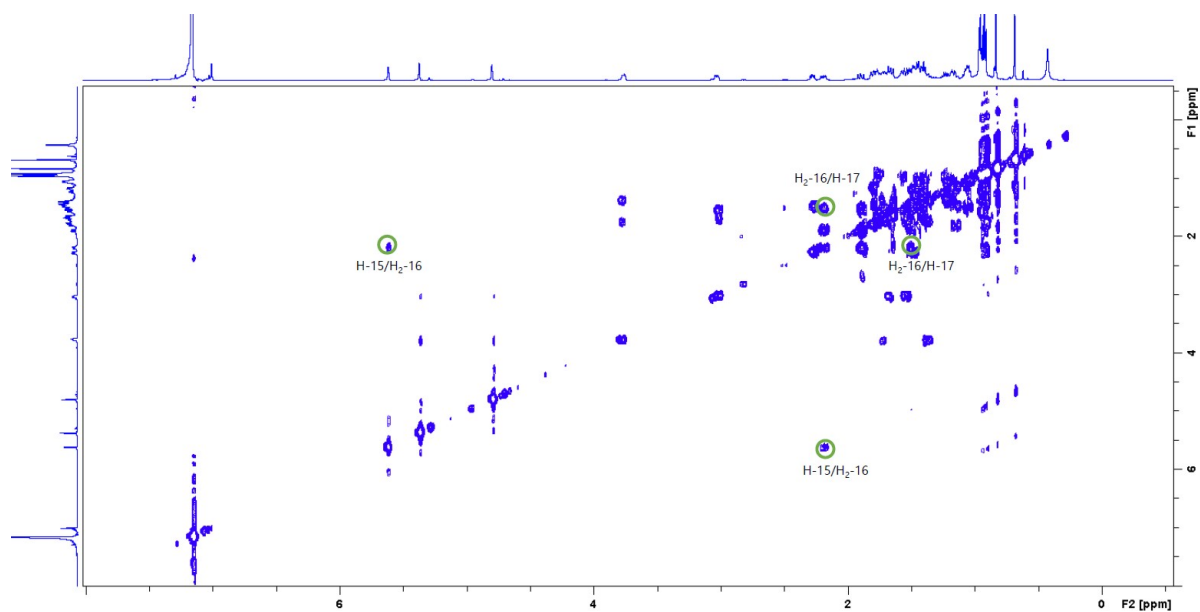


Figure SII-25. ^1H - ^1H COSY spectrum of compound **4** (C_6D_6 , 600 MHz).

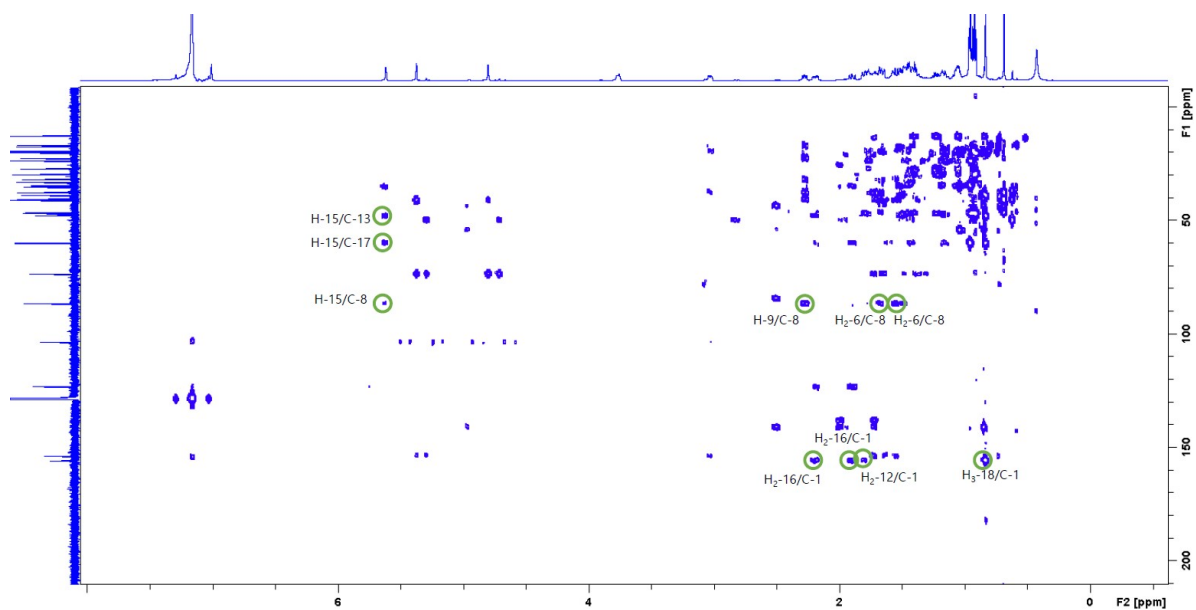


Figure SII-26. HMBC spectrum of compound **4** (C_6D_6 , 600 MHz).

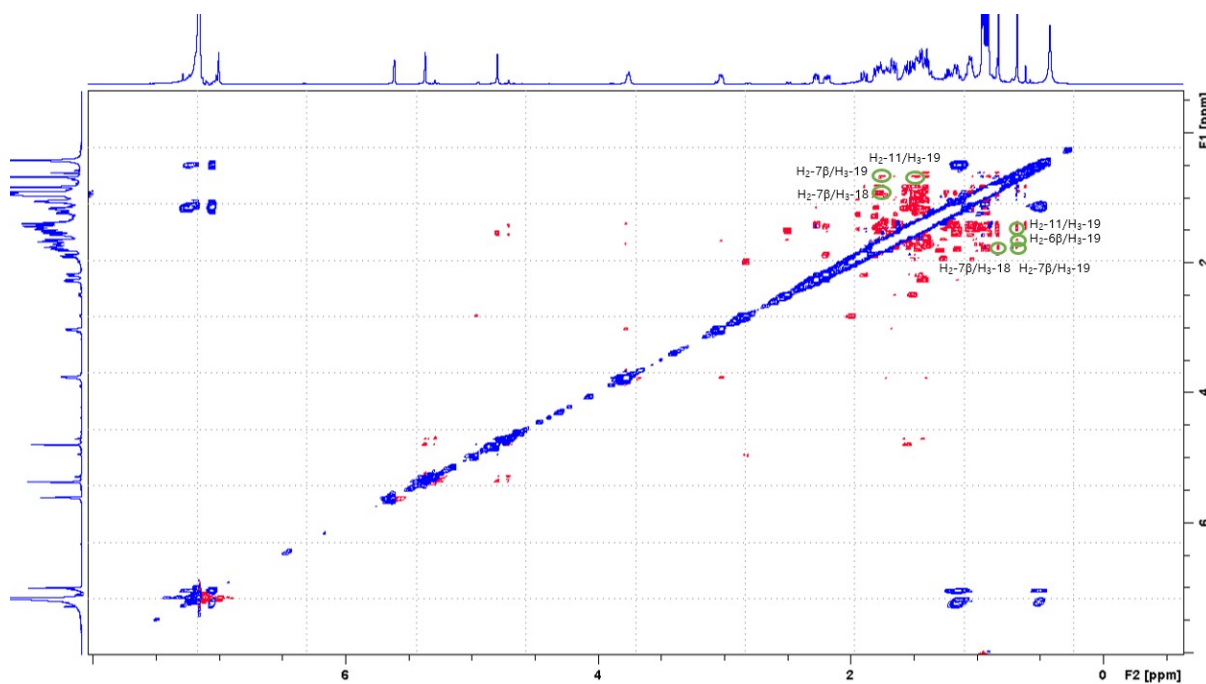
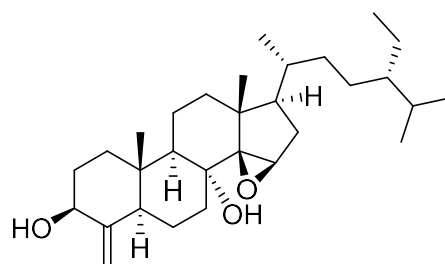


Figure SII-27. NOESY spectrum of compound **4** (C_6D_6 , 600 MHz).



5

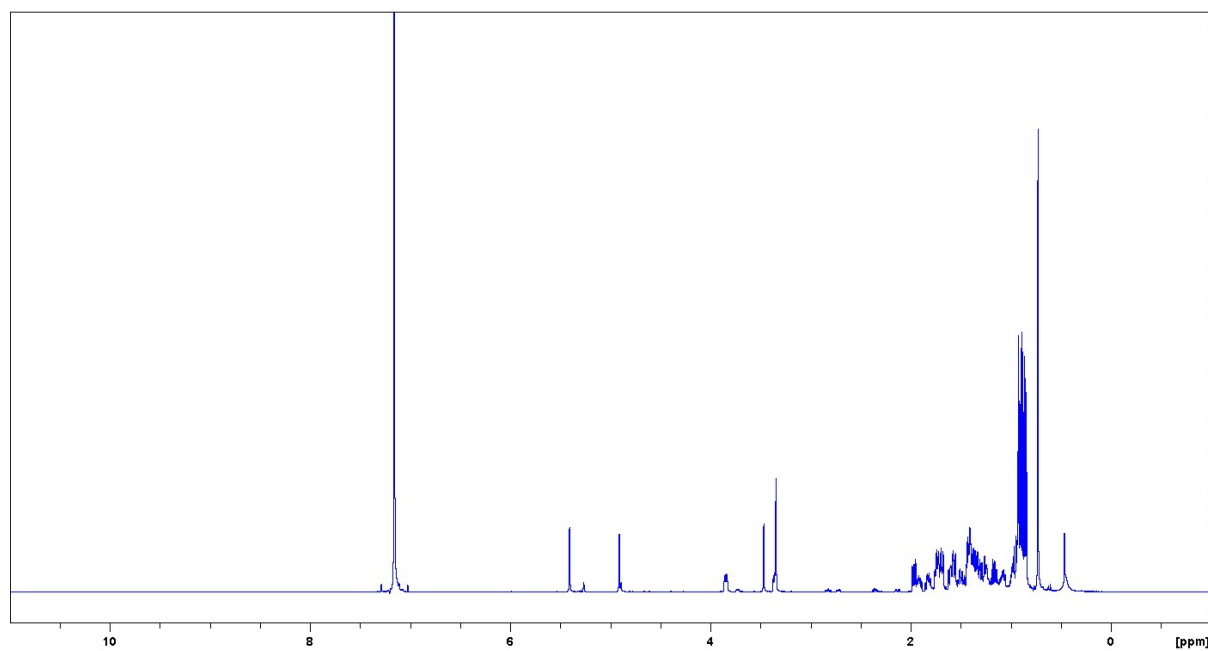


Figure SII-28. ^1H NMR spectrum of compound **5** (C_6D_6 , 600 MHz).

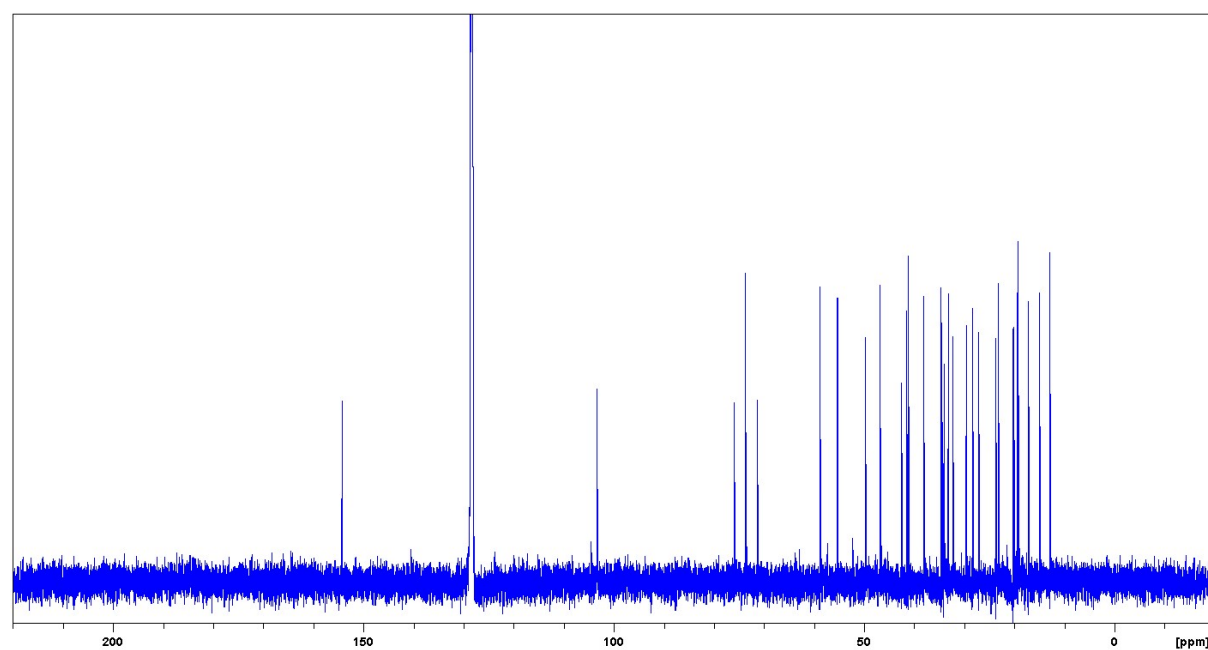


Figure SII-29. ^{13}C NMR spectrum of compound **5** (C_6D_6 , 150 MHz).

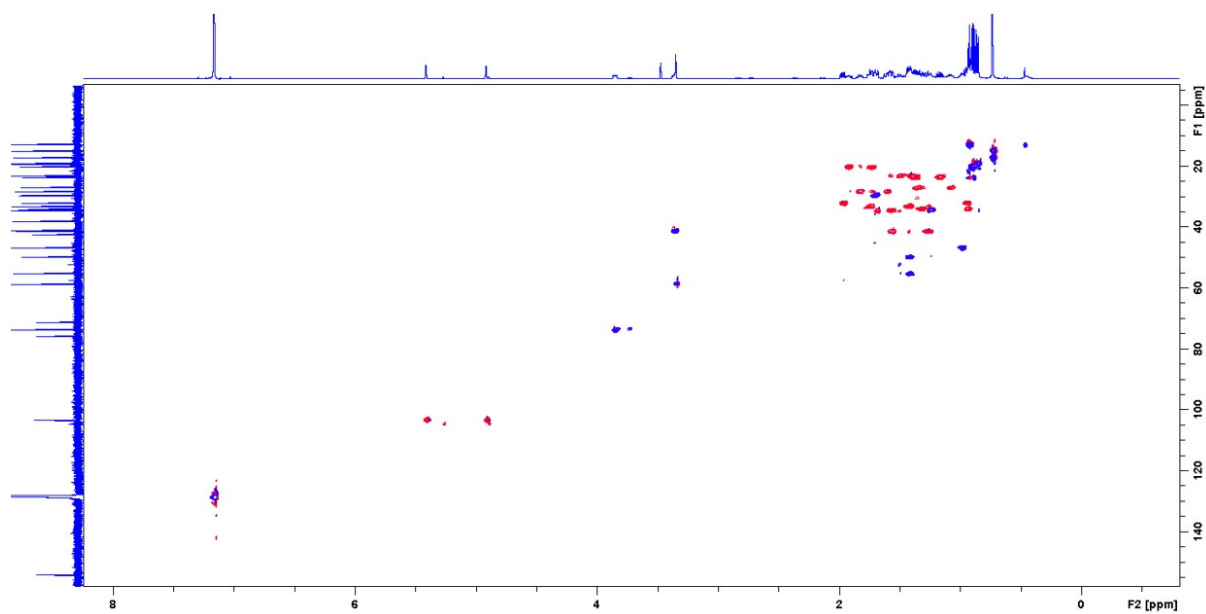


Figure SII-30. HSQC spectrum of compound **5** (C_6D_6 , 600 MHz).

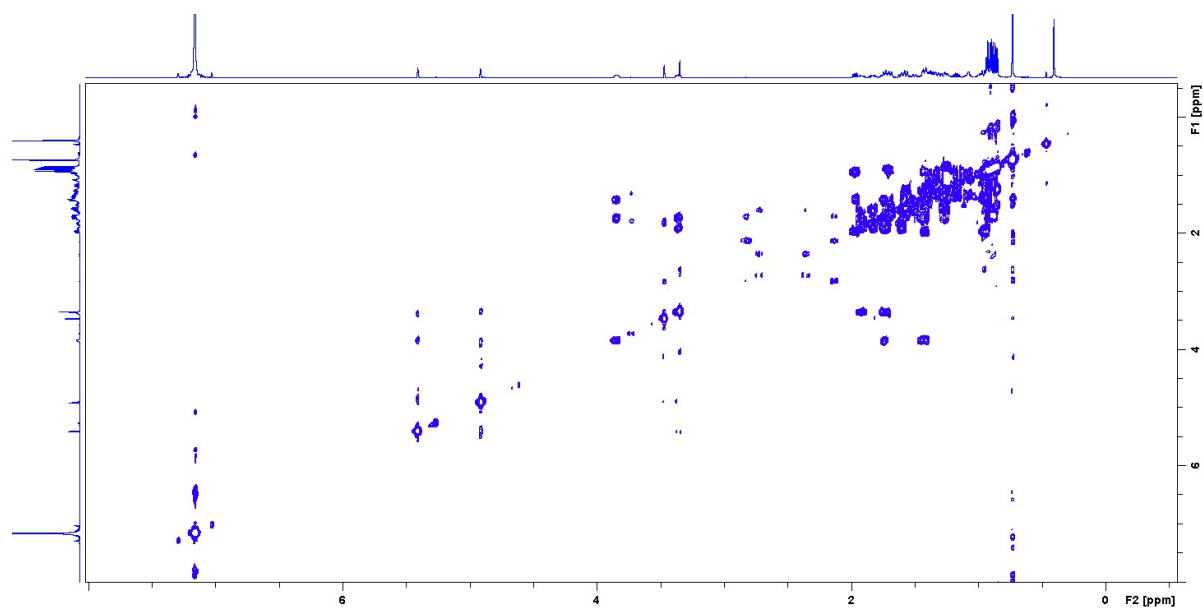


Figure SII-31. ^1H - ^1H COSY spectrum of compound **5** (C_6D_6 , 600 MHz).

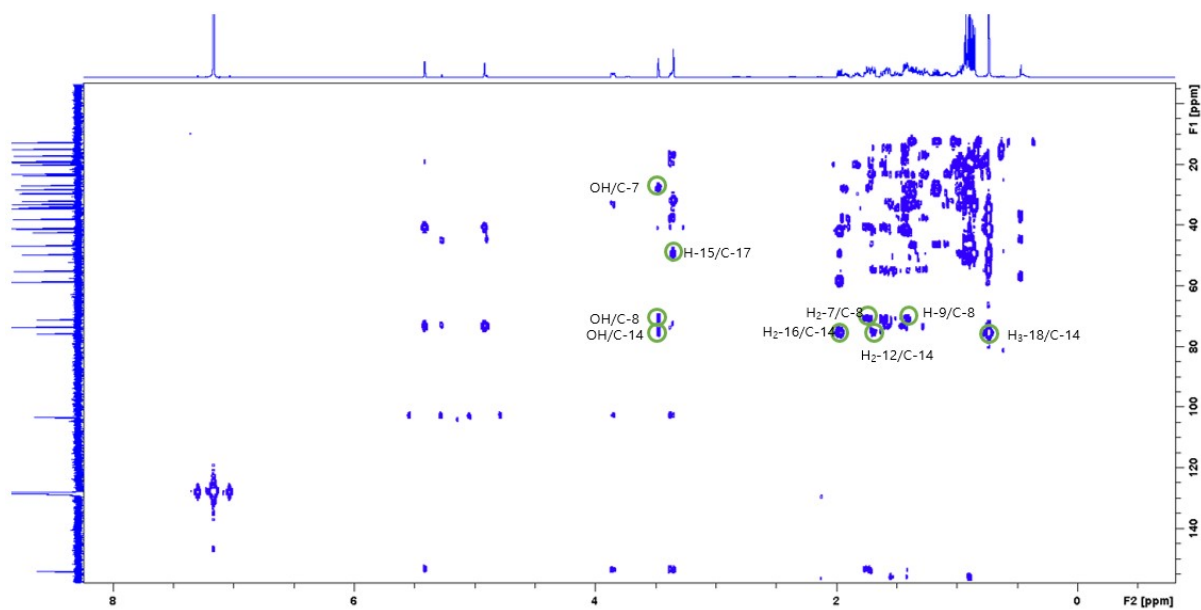


Figure SII-32. HMBC spectrum of compound **5** (C_6D_6 , 600 MHz).

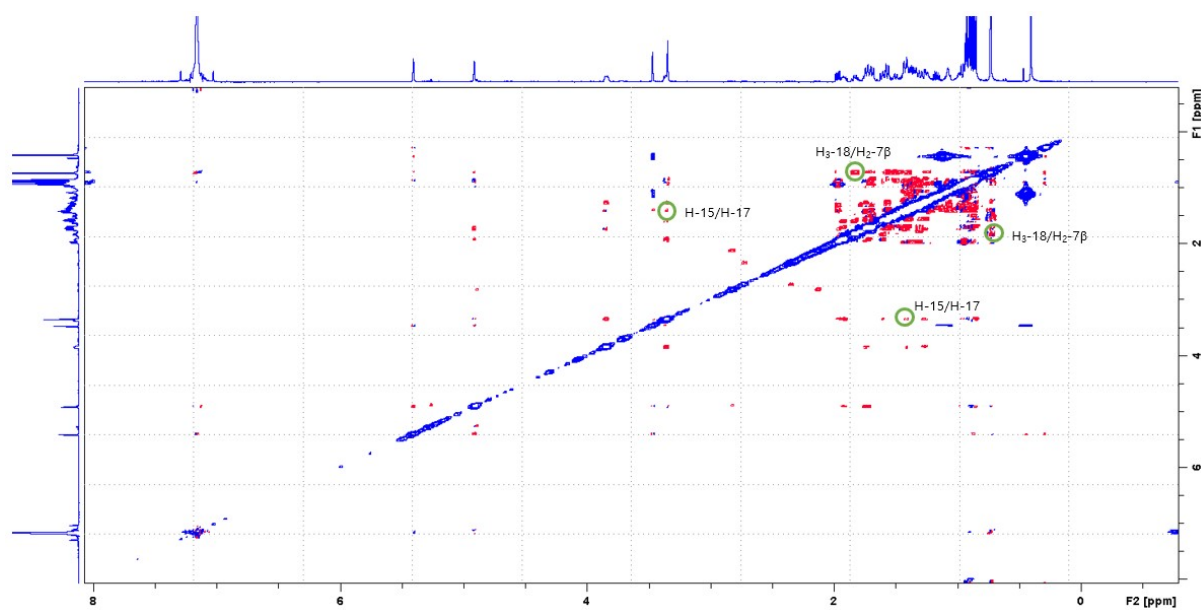


Figure SII-33. NOESY spectrum of compound **5** (C_6D_6 , 600 MHz).

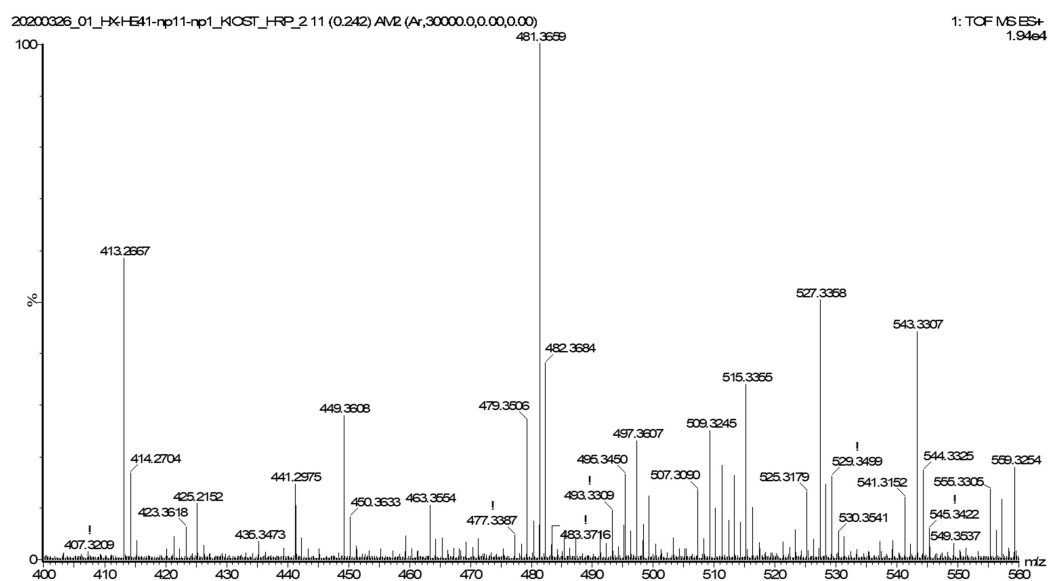
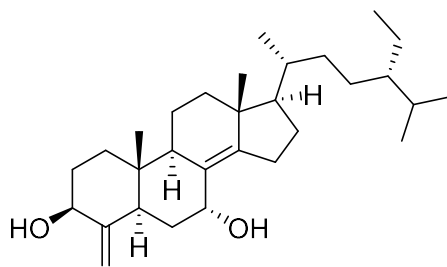


Figure SII-34. HRMS spectrum of compound **5**.



6

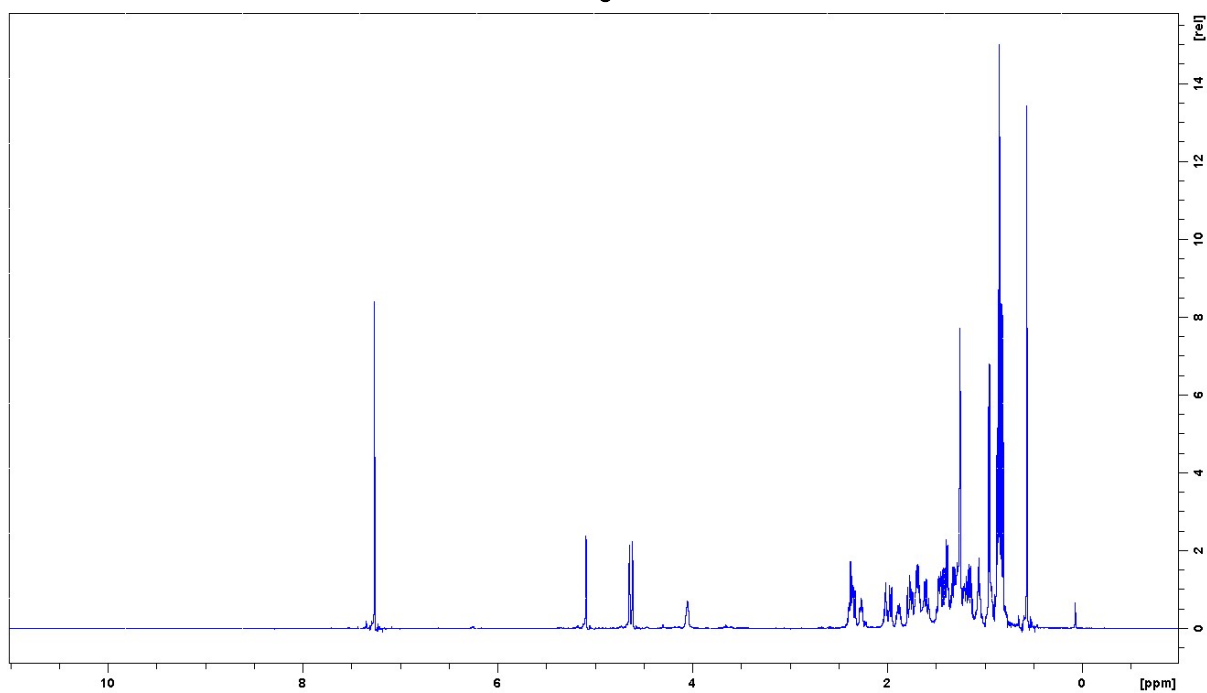


Figure SII-35. ^1H NMR spectrum of compound **6** (CDCl_3 , 600 MHz).

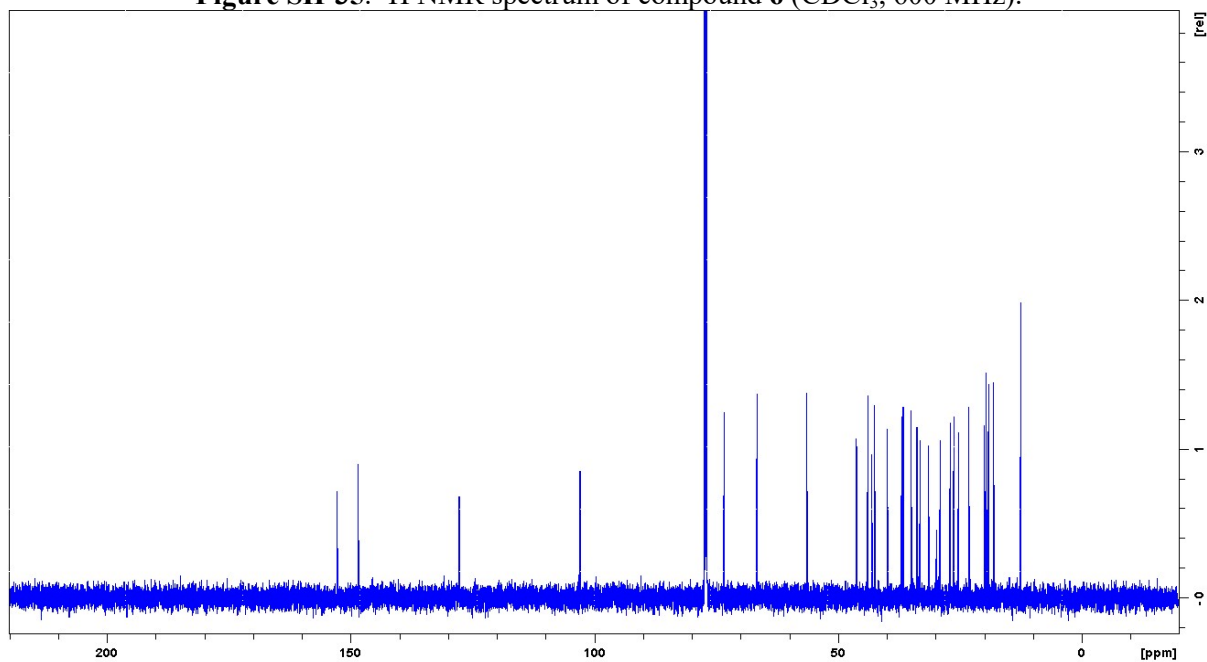


Figure SII-36. ^{13}C NMR spectrum of compound **6** (CDCl_3 , 150 MHz).

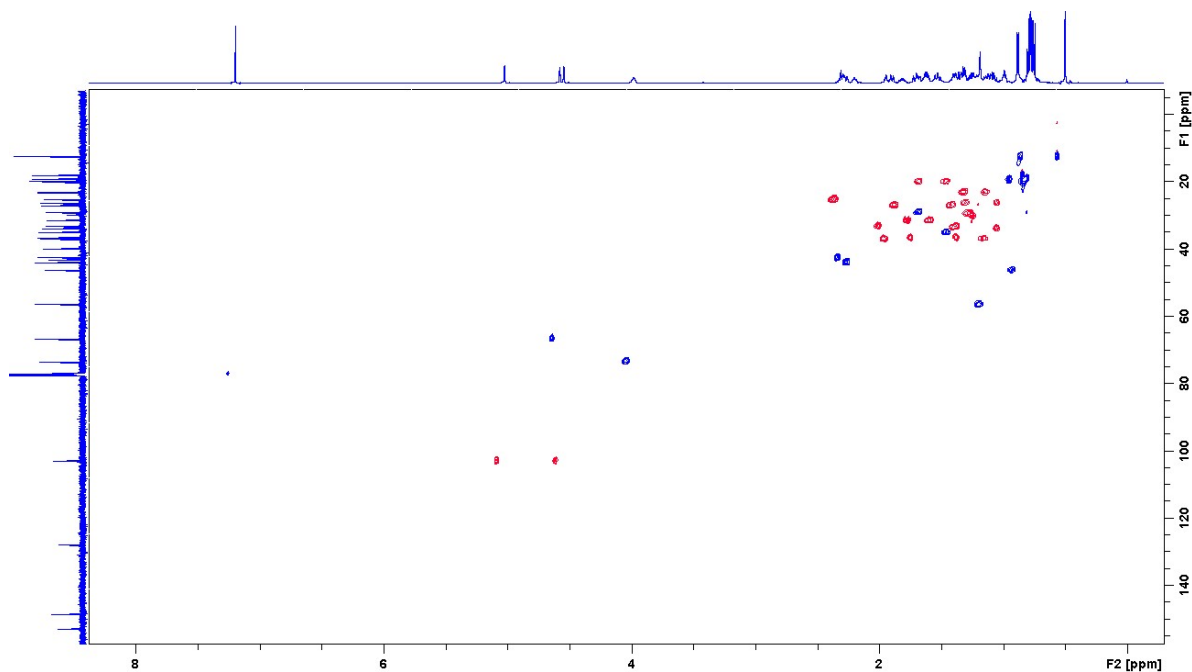


Figure SII-37. HSQC spectrum of compound **6** (CDCl₃, 600 MHz).

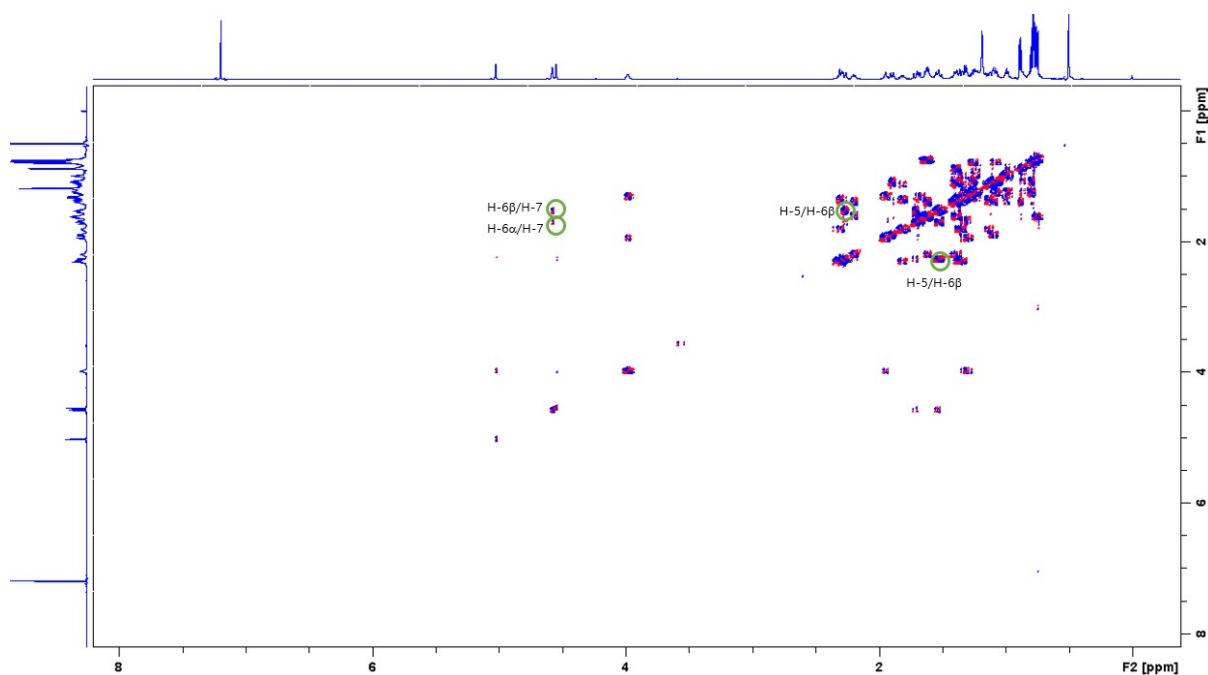


Figure SII-38. ¹H-¹H COSY spectrum of compound **6** (CDCl₃, 600 MHz).

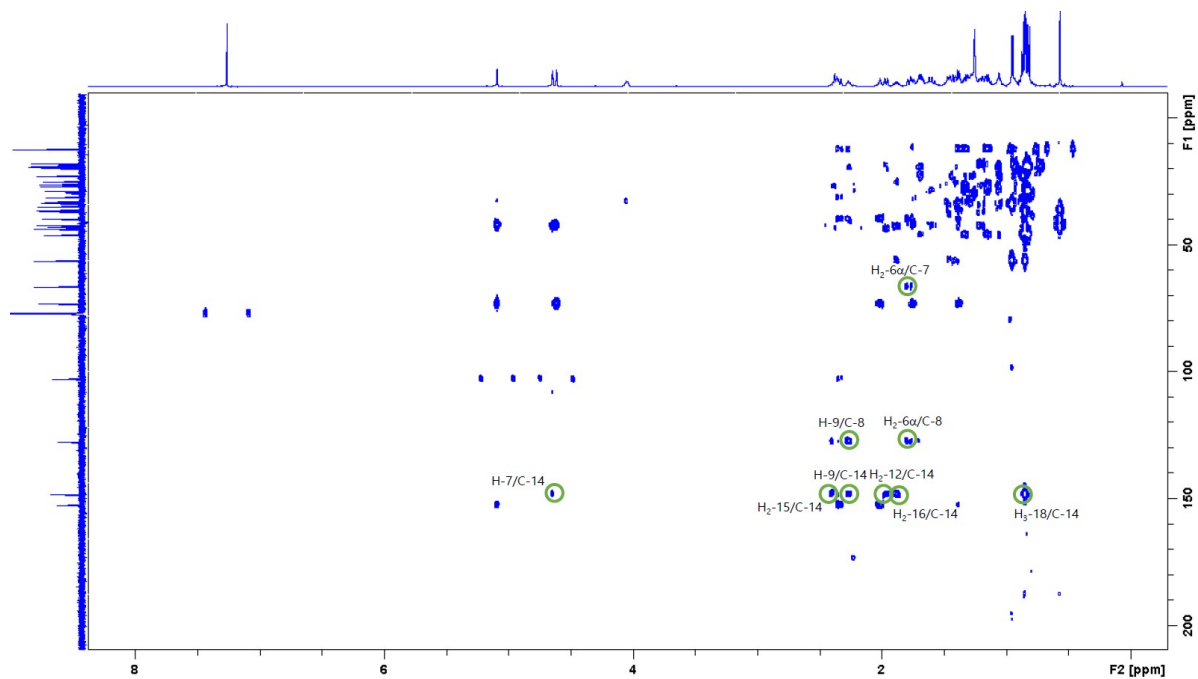


Figure SII-39. HMBC spectrum of compound **6** (CDCl₃, 600 MHz).

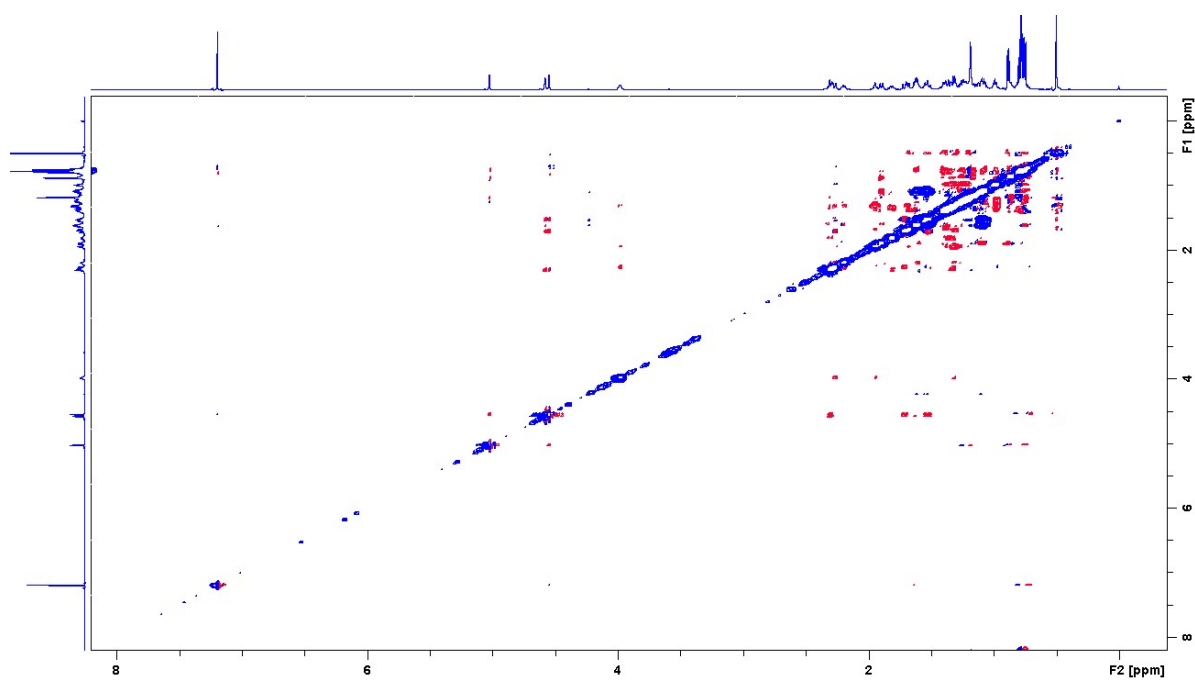


Figure SII-40. NOESY spectrum of compound **6** (CDCl₃, 600 MHz).

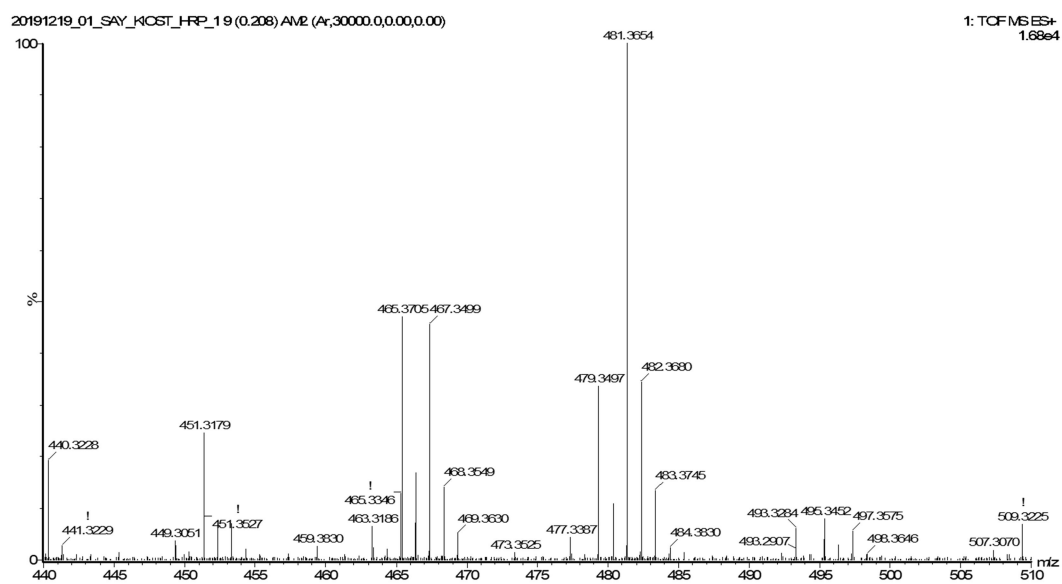
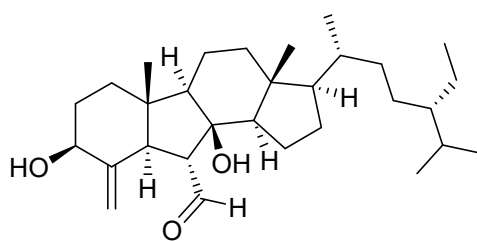


Figure SII-41. HRMS spectrum of compound 6.



7

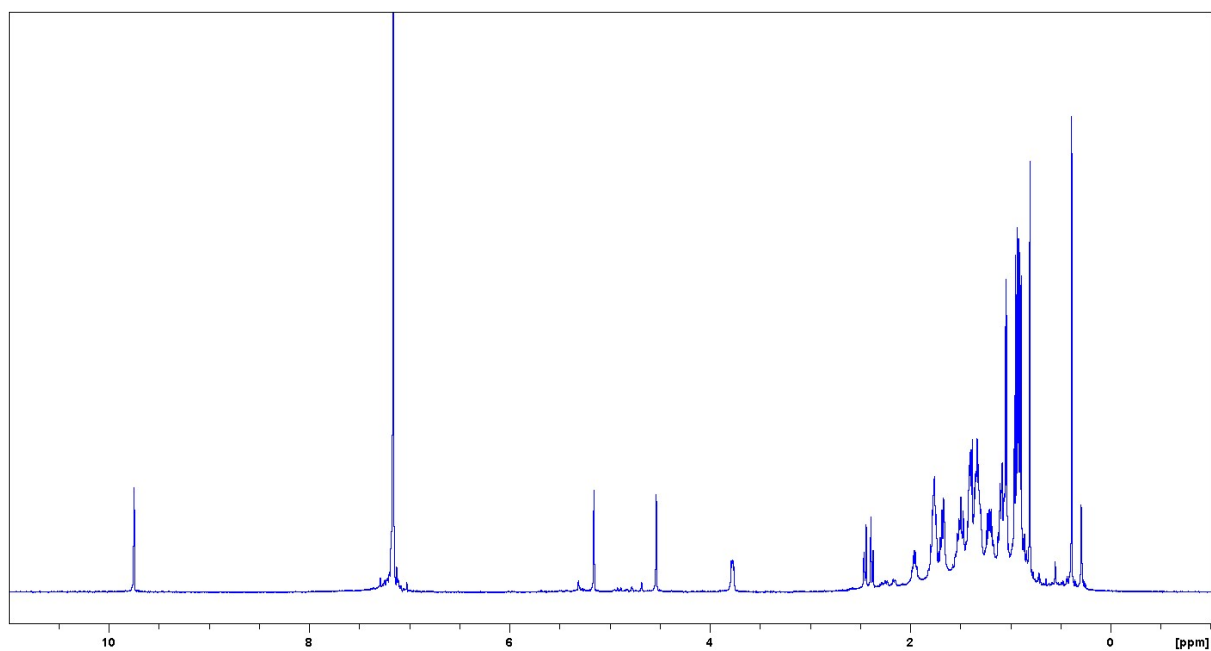


Figure SII-42. ^1H NMR spectrum of compound **7** (C_6D_6 , 600 MHz).

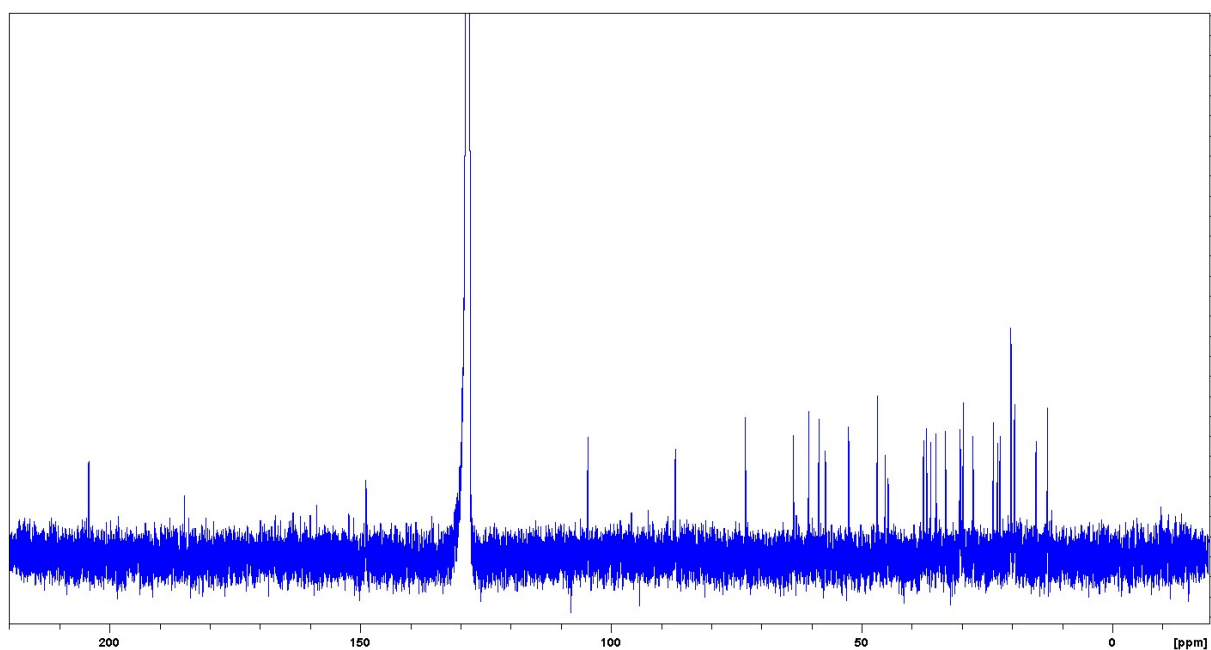


Figure SII-43. ^{13}C NMR spectrum of compound **7** (C_6D_6 , 150 MHz).

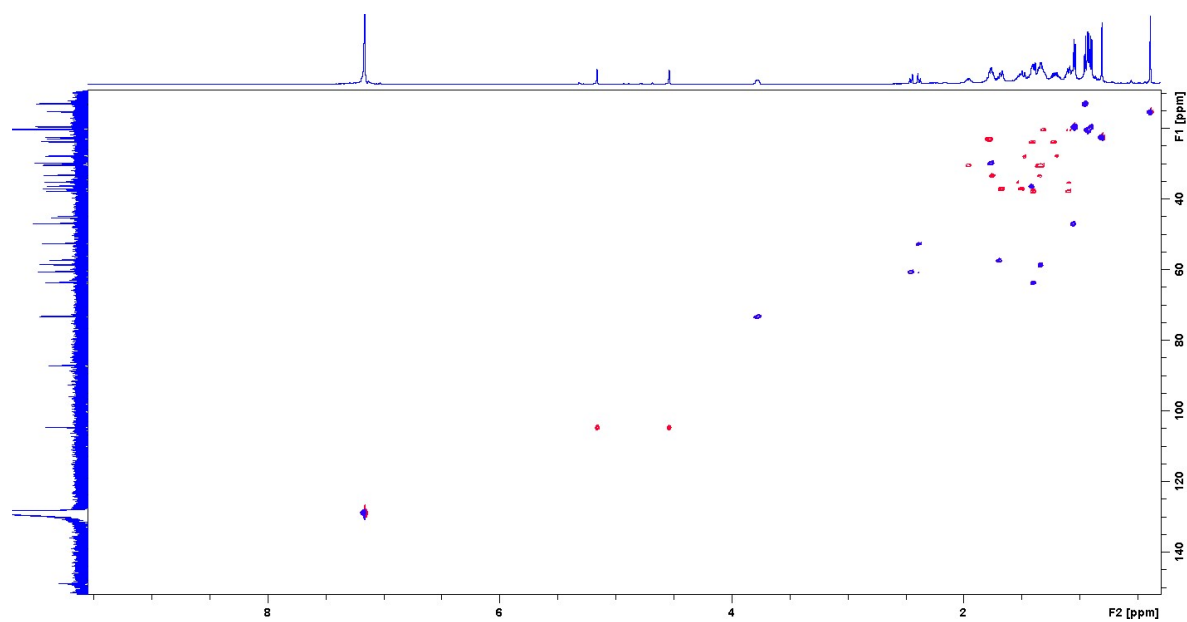


Figure SII-44. HSQC spectrum of compound **7** (C_6D_6 , 600 MHz).

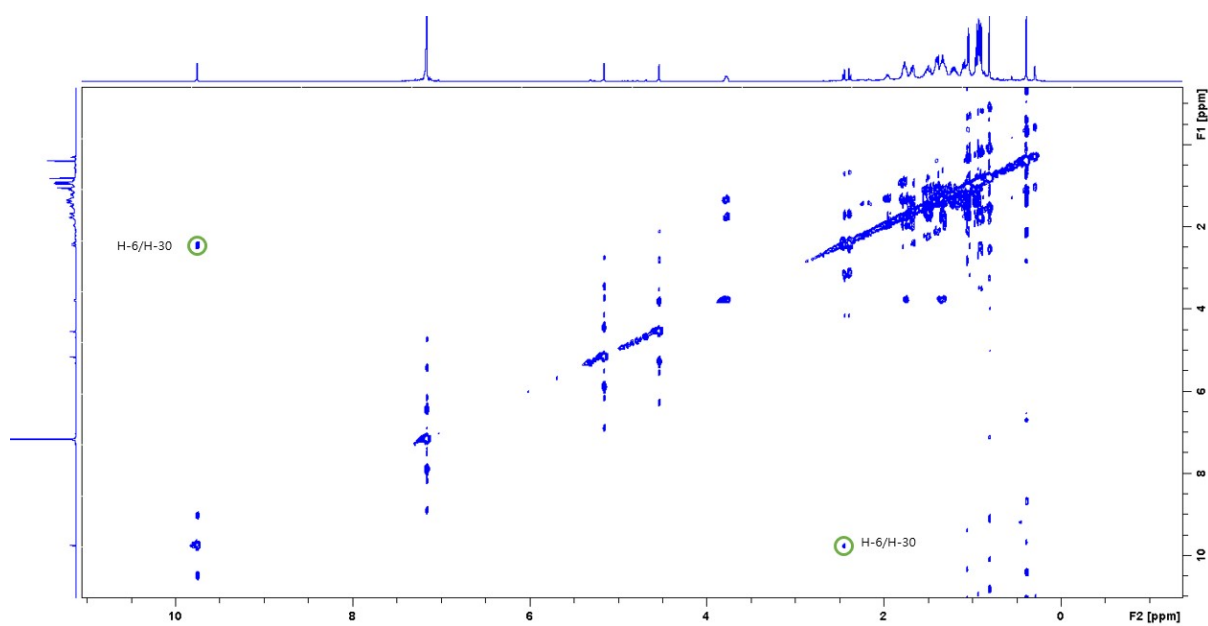


Figure SII-45. ^1H - ^1H COSY spectrum of compound **7** (C_6D_6 , 600 MHz).

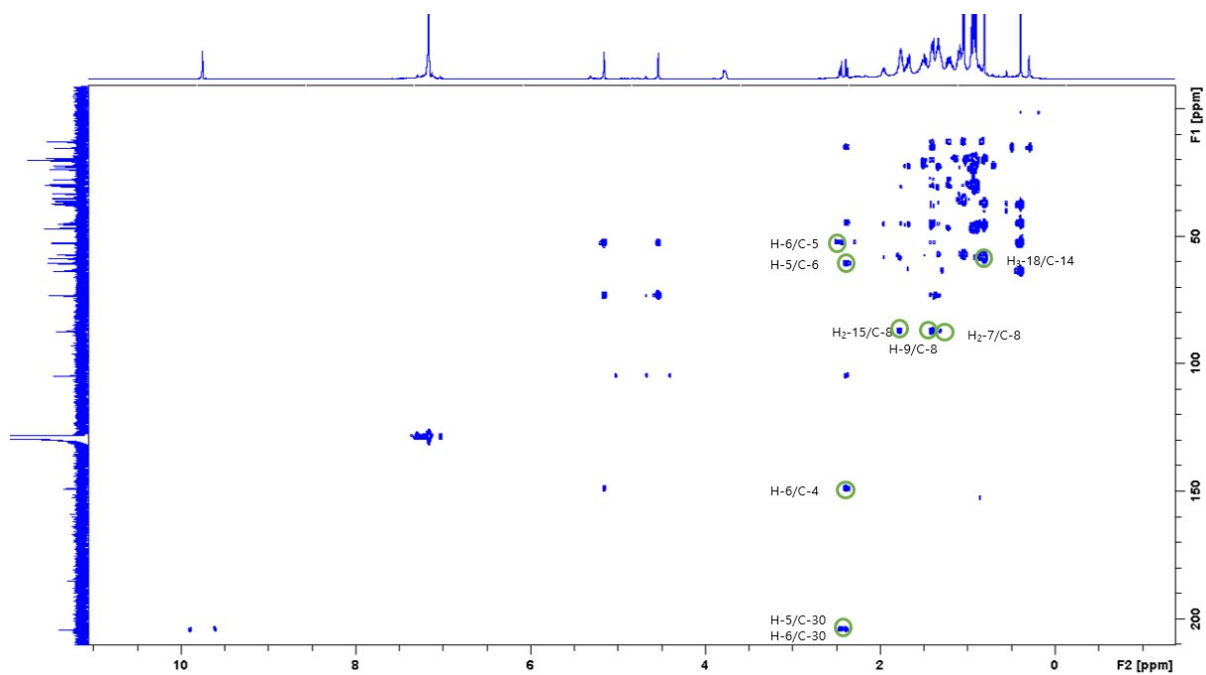


Figure SII-46. HMBC spectrum of compound **7** (C_6D_6 , 600 MHz).

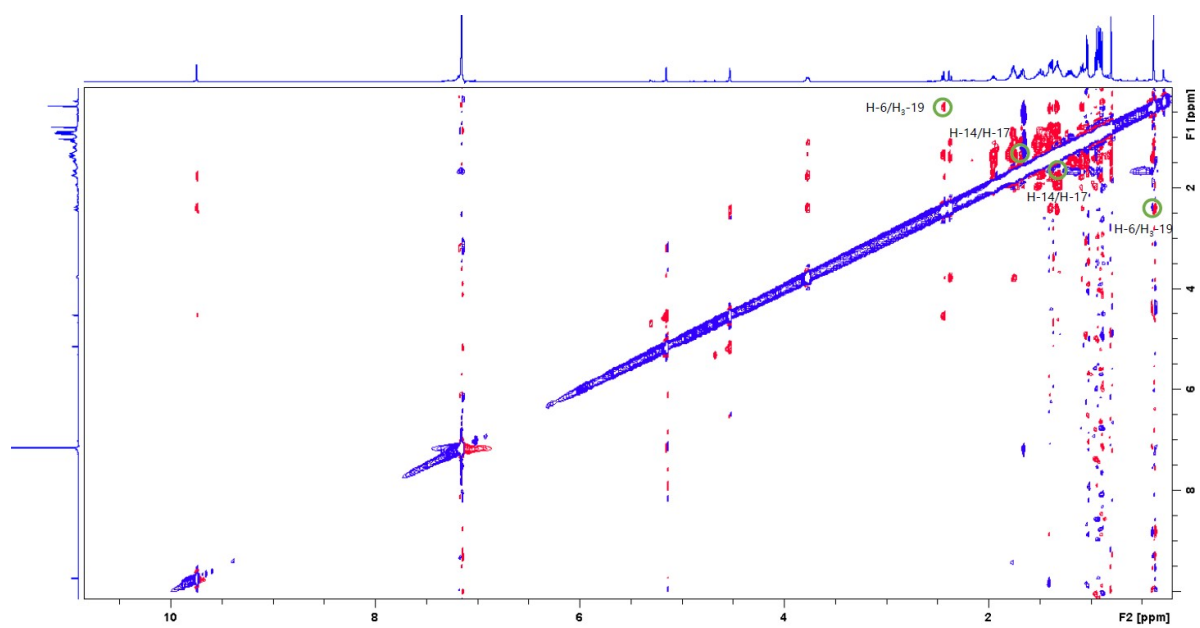


Figure SII-47. NOESY spectrum of compound **7** (C_6D_6 , 600 MHz).

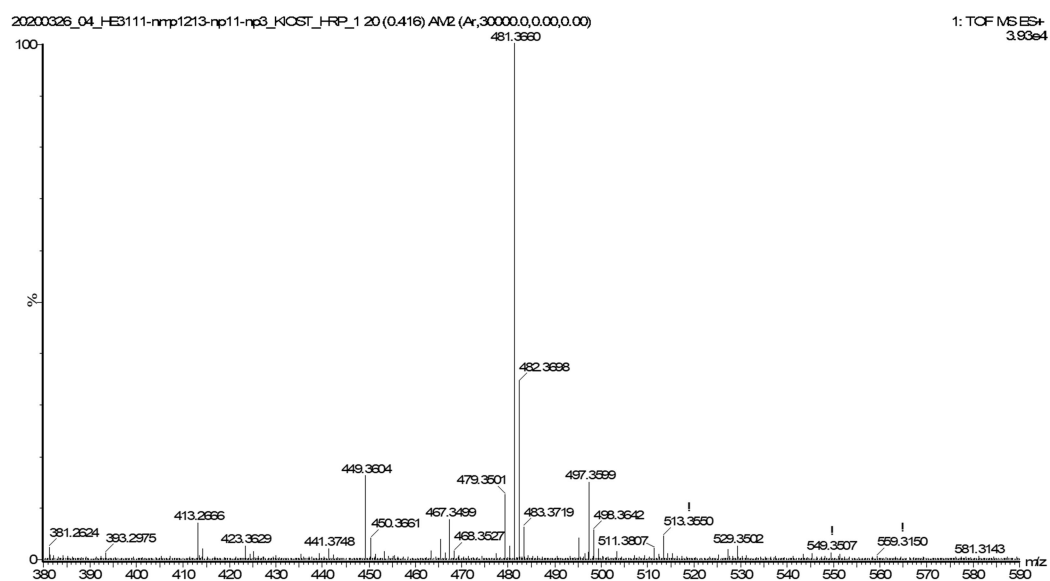


Figure SII-48. HRMS spectrum of compound **7**.

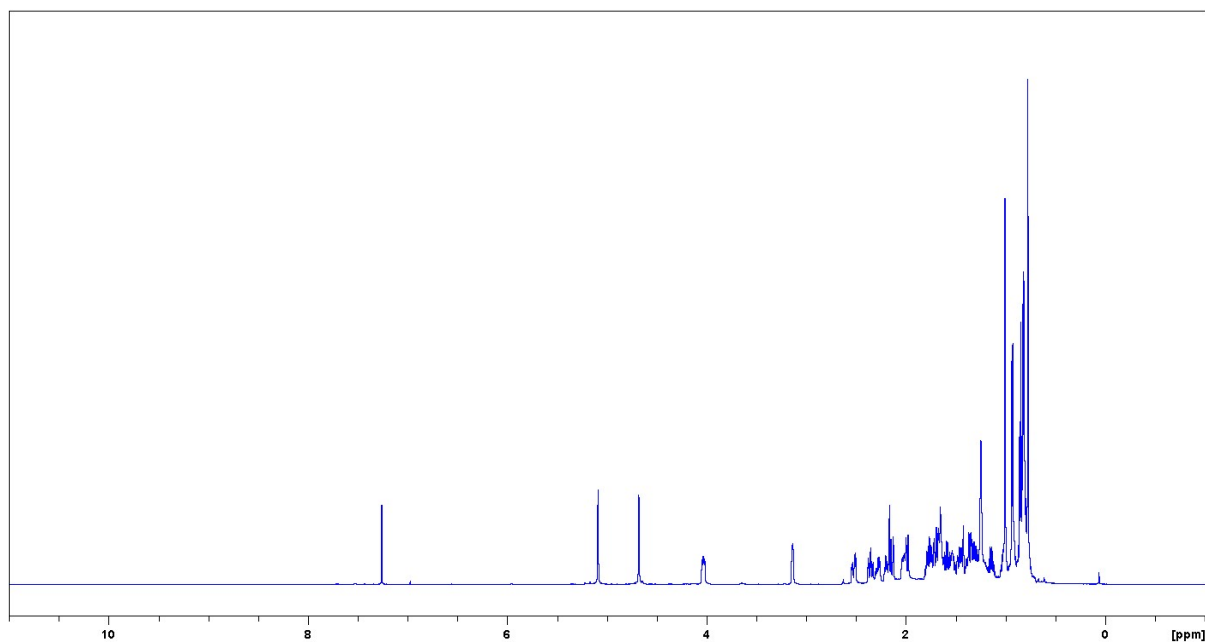
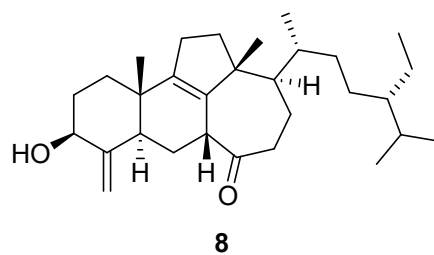


Figure SII-49. ^1H NMR spectrum of compound **8** (CDCl_3 , 600 MHz).

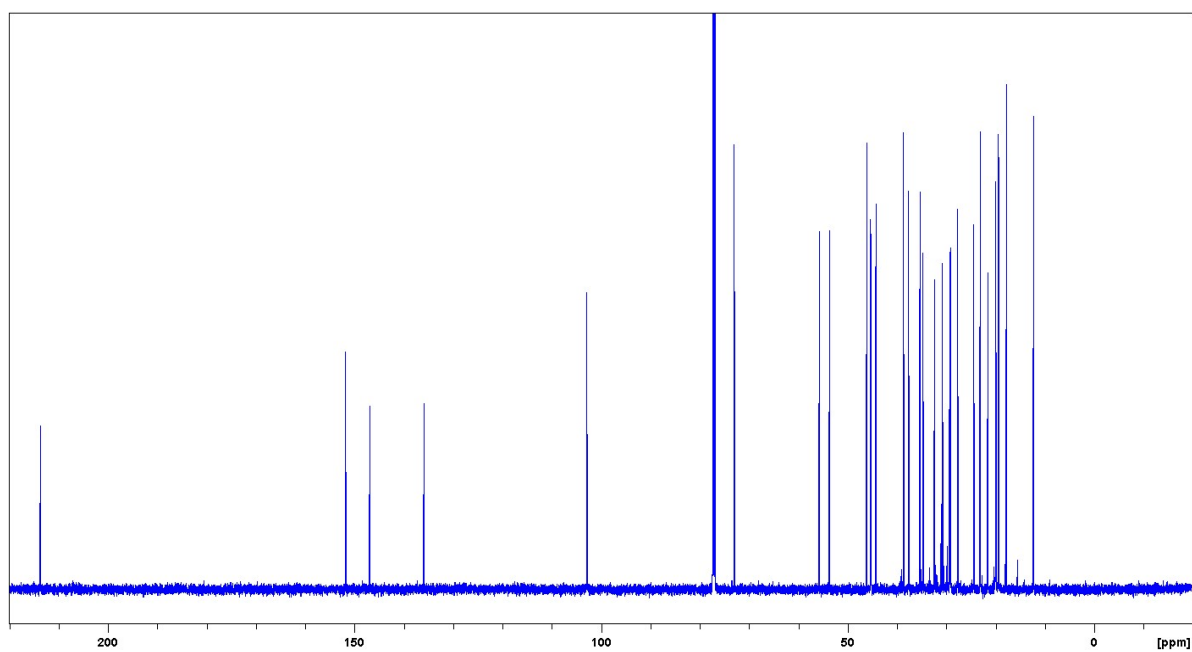


Figure SII-50. ^{13}C NMR spectrum of compound **8** (CDCl_3 , 150 MHz).

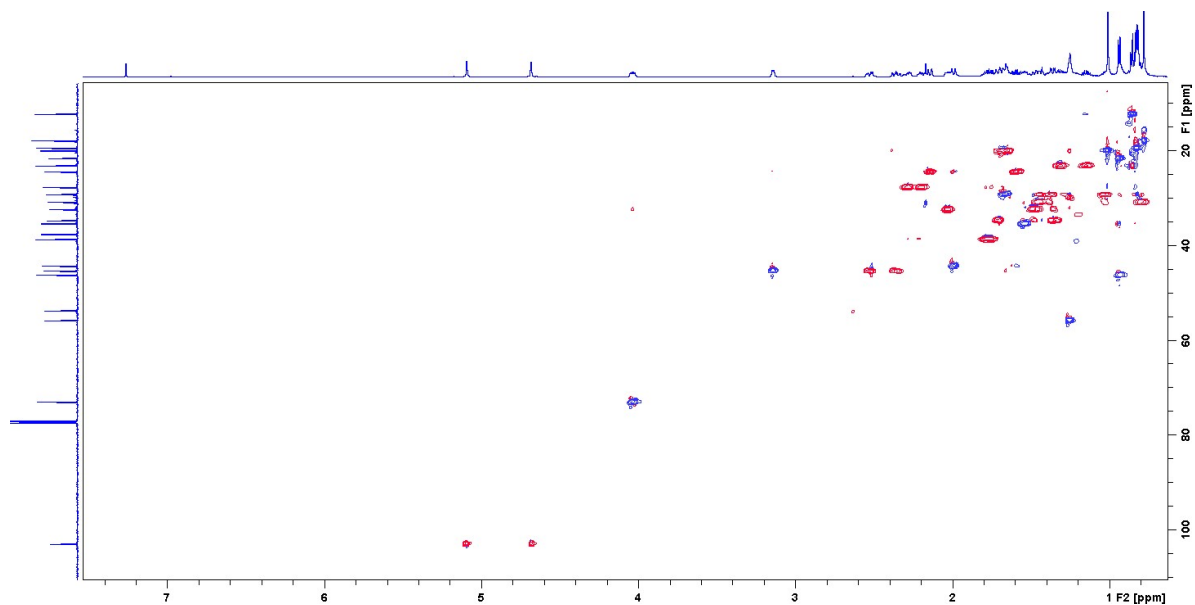


Figure SII-51. HSQC spectrum of compound **8** (CDCl₃, 600 MHz).

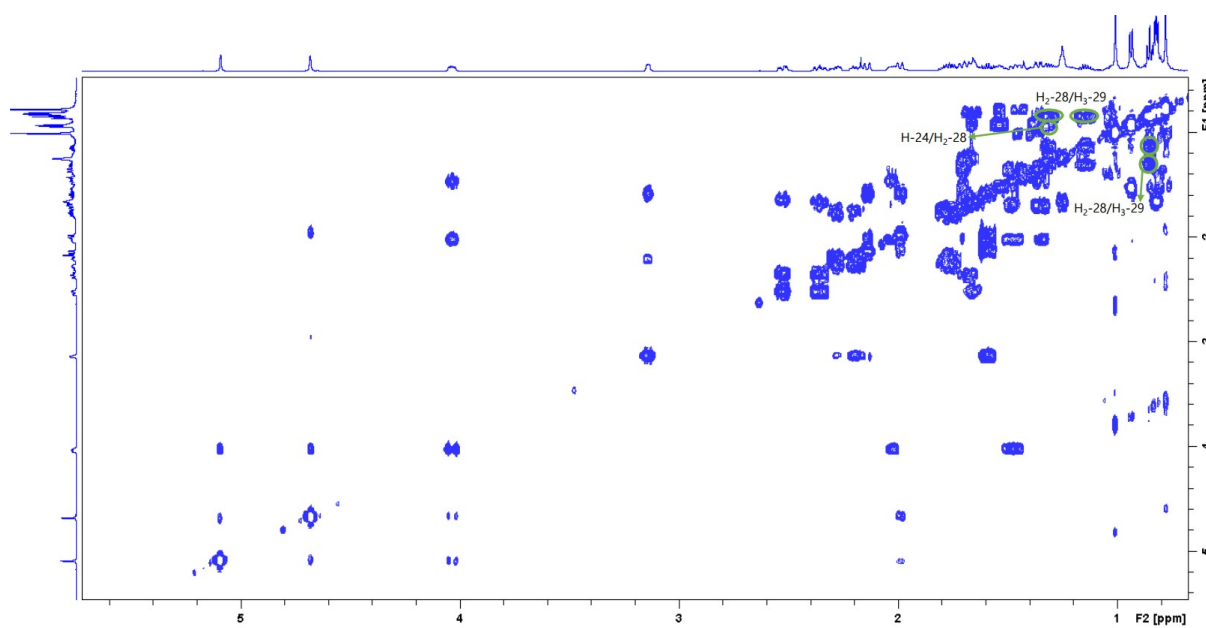


Figure SII-52. ¹H-¹H COSY spectrum of compound **8** (CDCl₃, 600 MHz).

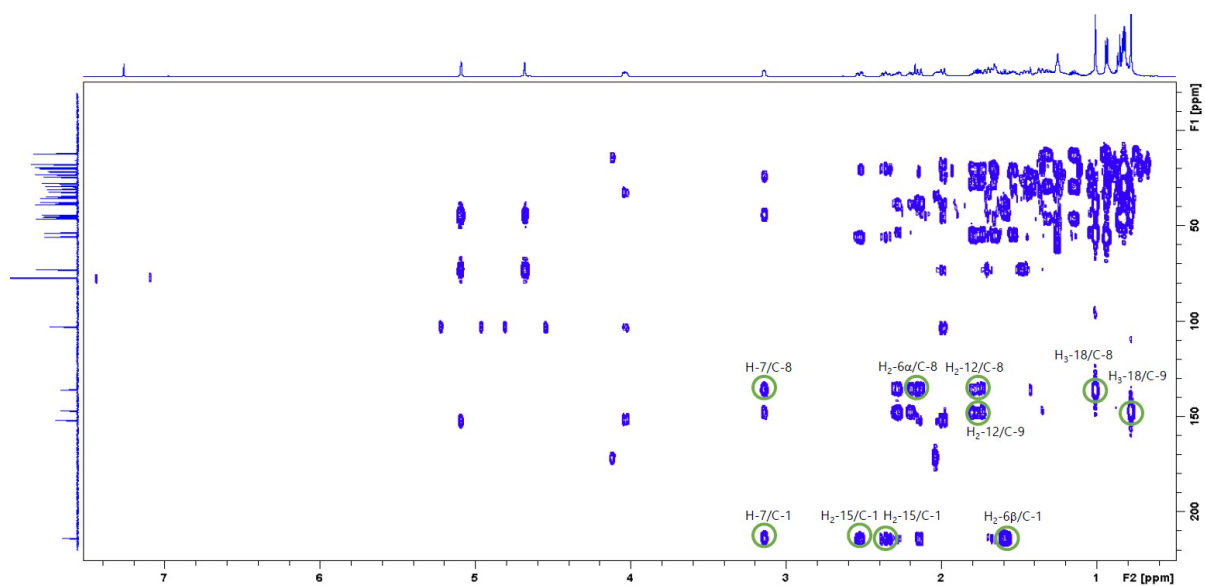


Figure SII-53. HMBC spectrum of compound **8** (CDCl₃, 600 MHz).

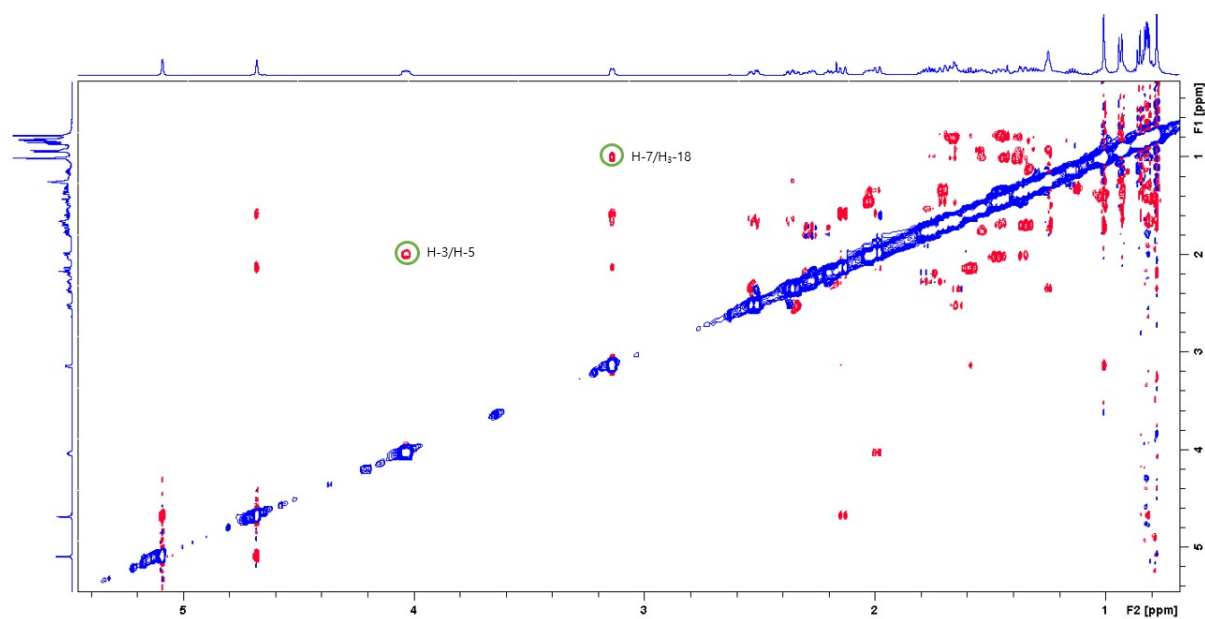


Figure SII-54. NOESY spectrum of compound **8** (CDCl₃, 600 MHz).

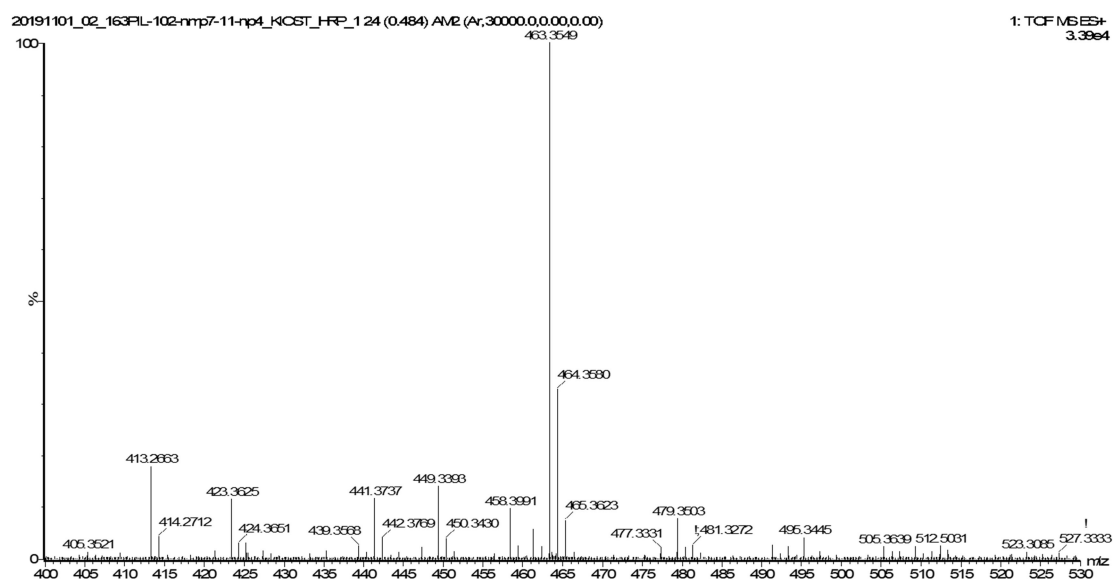
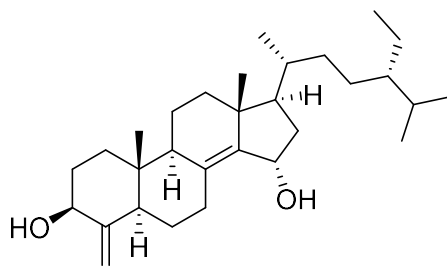


Figure SII-55. HRMS spectrum of compound **8**.



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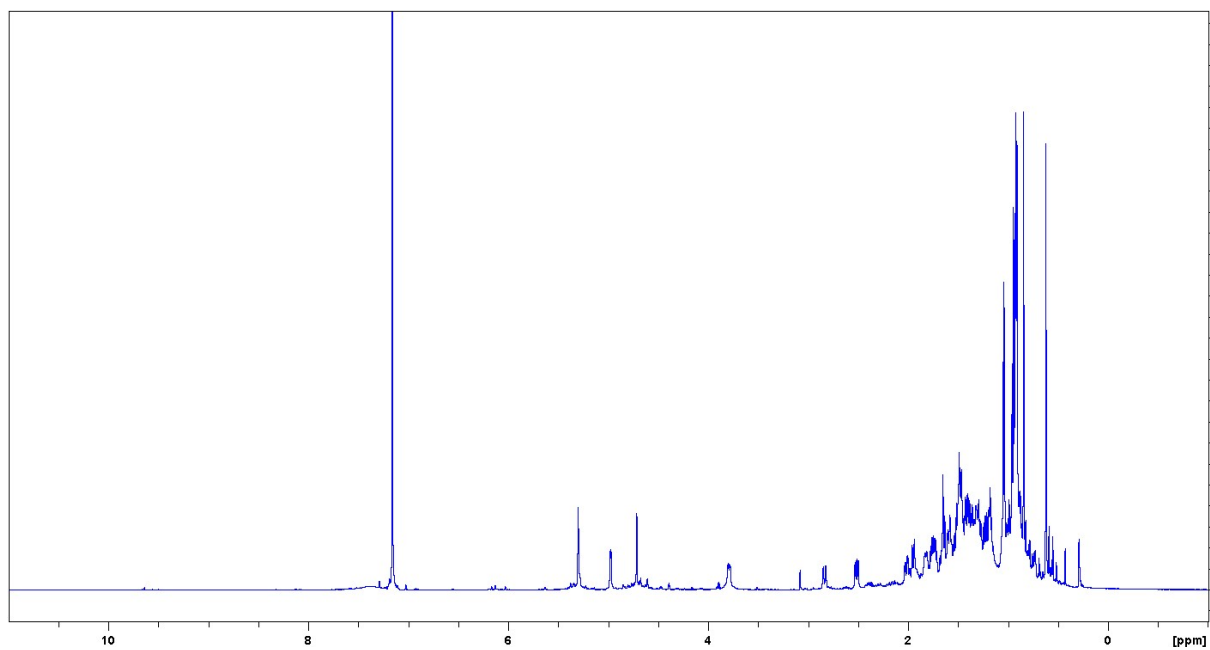


Figure SII-56. ^1H NMR spectrum of compound **9** (C_6D_6 , 600 MHz).

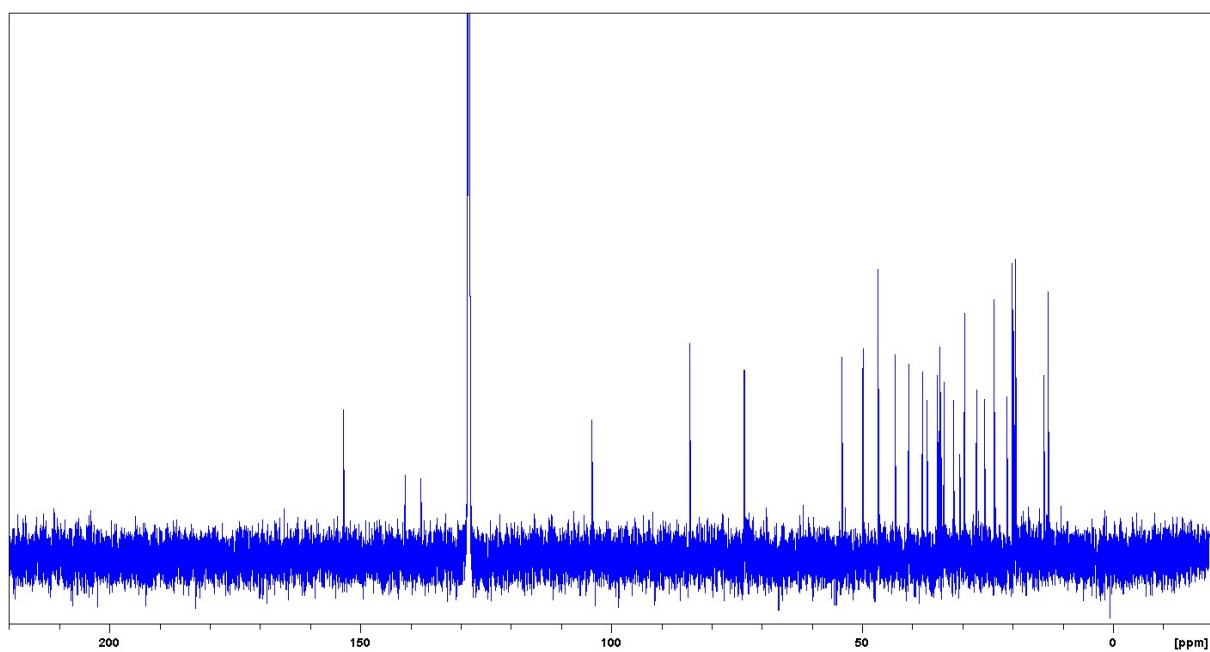


Figure SII-57. ^{13}C NMR spectrum of compound **9** (C_6D_6 , 150 MHz).

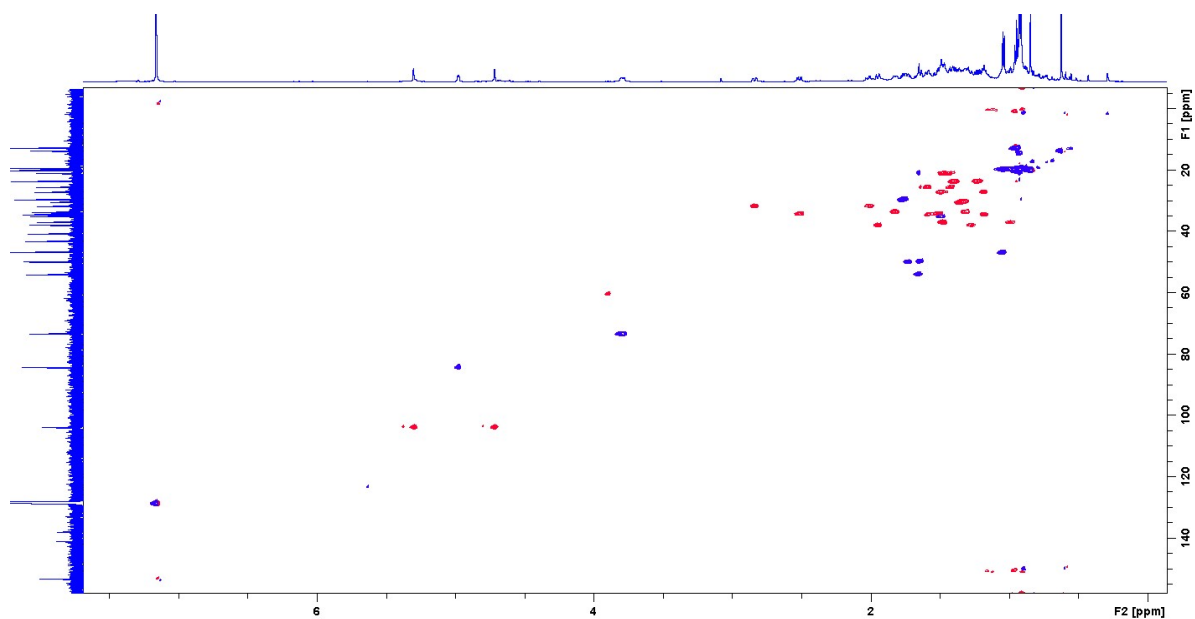


Figure SII-58. HSQC spectrum of compound **9** (C_6D_6 , 600 MHz).

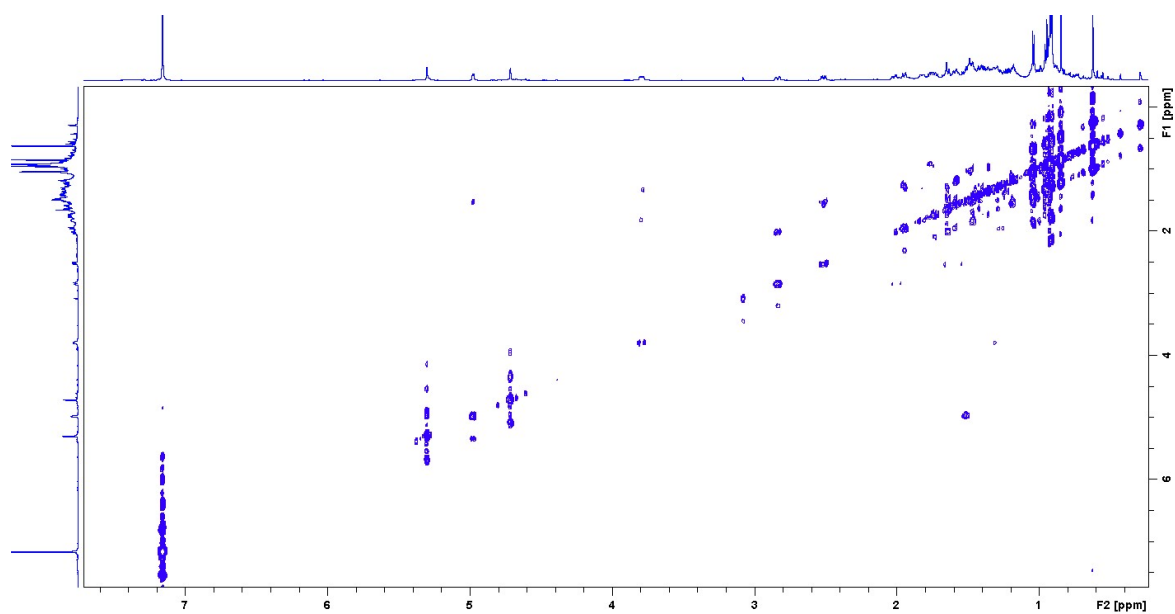


Figure SII-59. ^1H - ^1H COSY spectrum of compound **9** (C_6D_6 , 600 MHz).

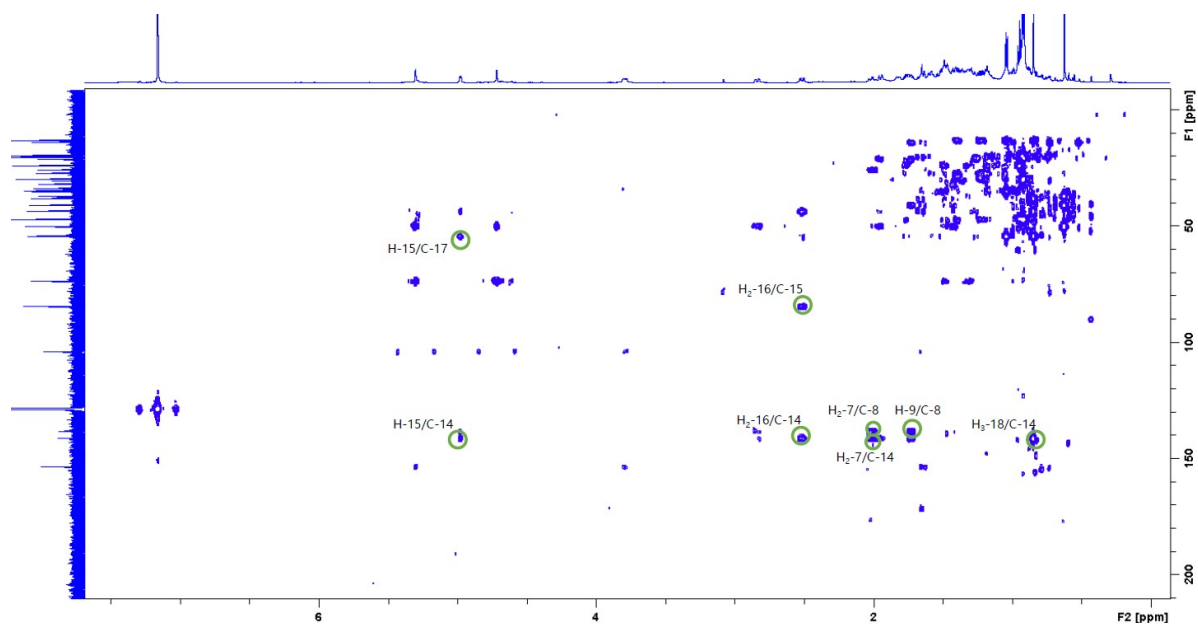


Figure SII-60. HMBC spectrum of compound **9** (C_6D_6 , 600 MHz).

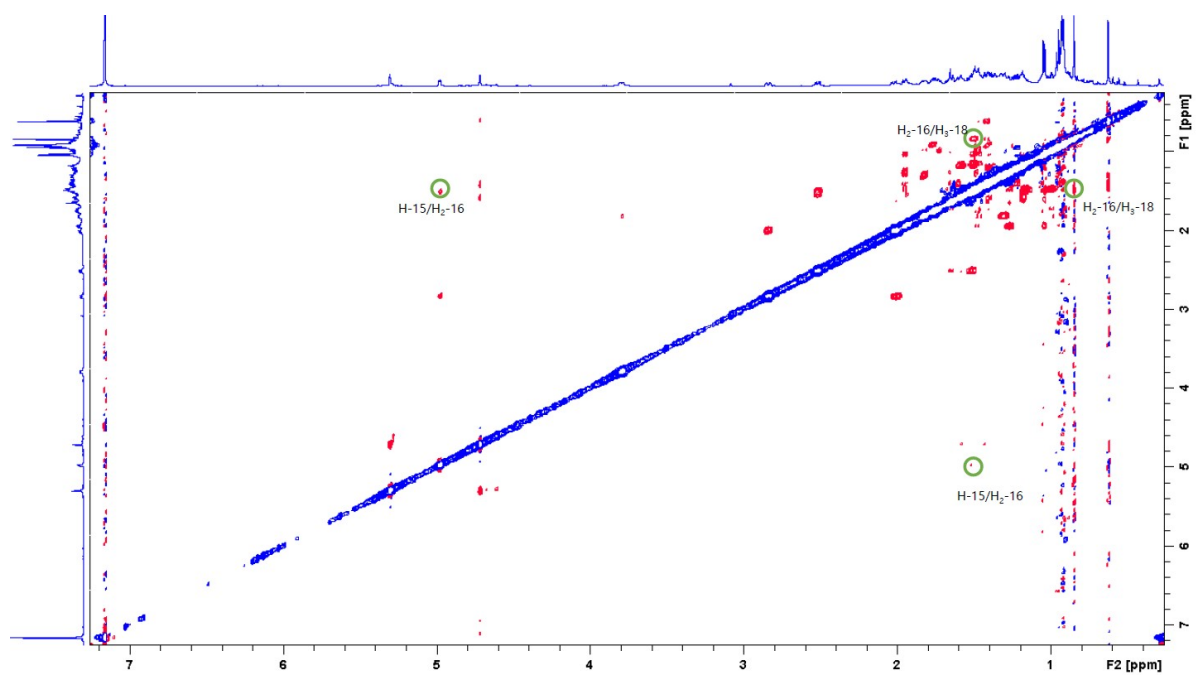
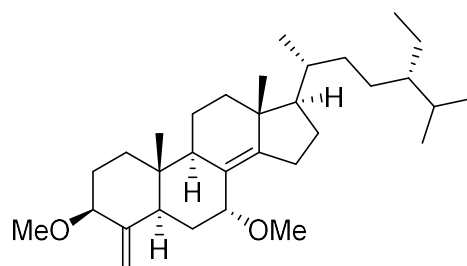


Figure SII-61. NOESY spectrum of compound **9** (C_6D_6 , 600 MHz).



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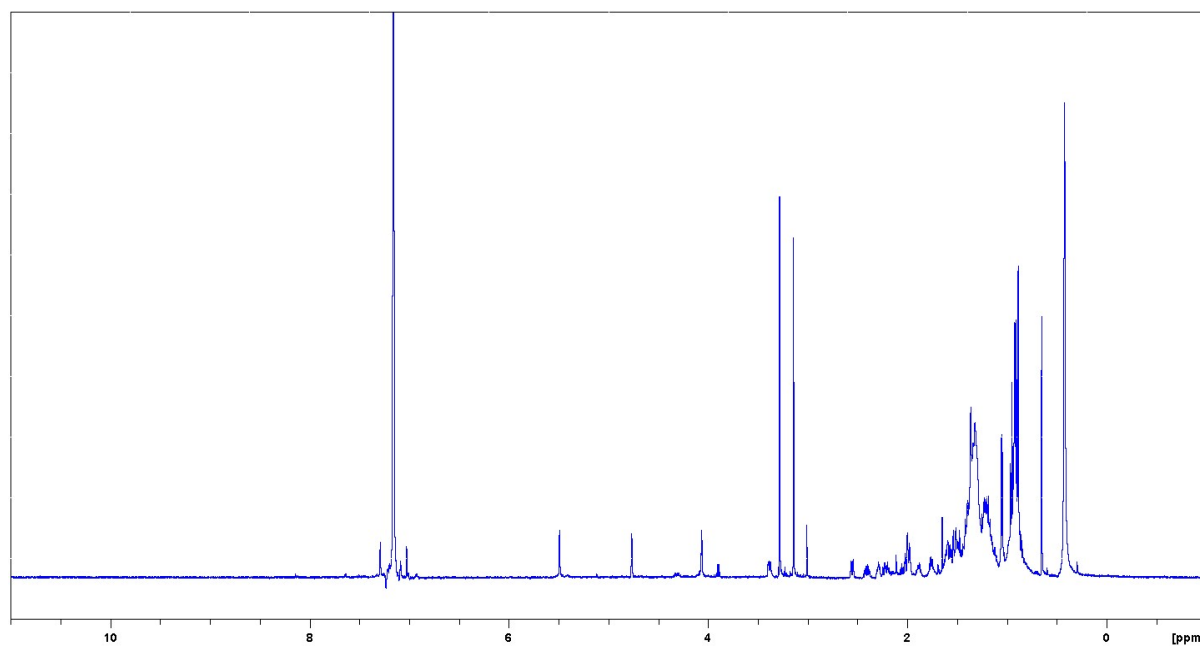


Figure SII-62. ^1H NMR spectrum of 3-Ome-swinhosterol C **10** (C_6D_6 , 600 MHz).

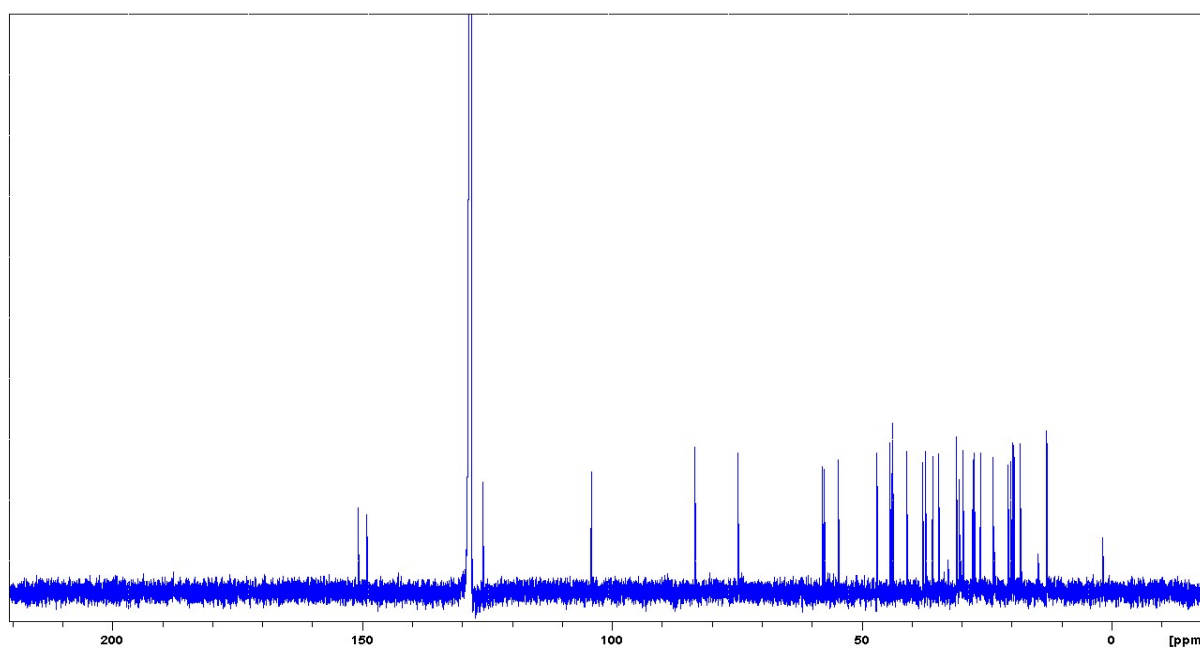


Figure SII-63. ^{13}C NMR spectrum of 3-Ome-swinhosterol C **10** (C_6D_6 , 150 MHz).

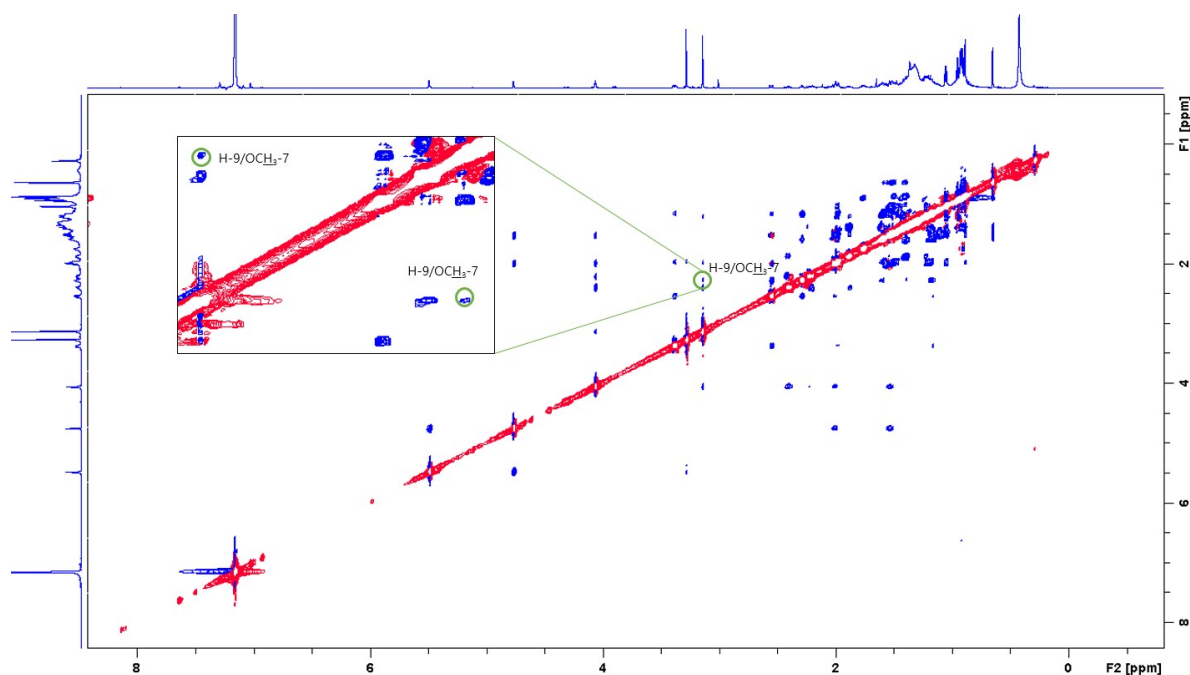


Figure SII-64. NOESY spectrum of 3-OMe-swinhosterol C **10** (C_6D_6 , 600 MHz).

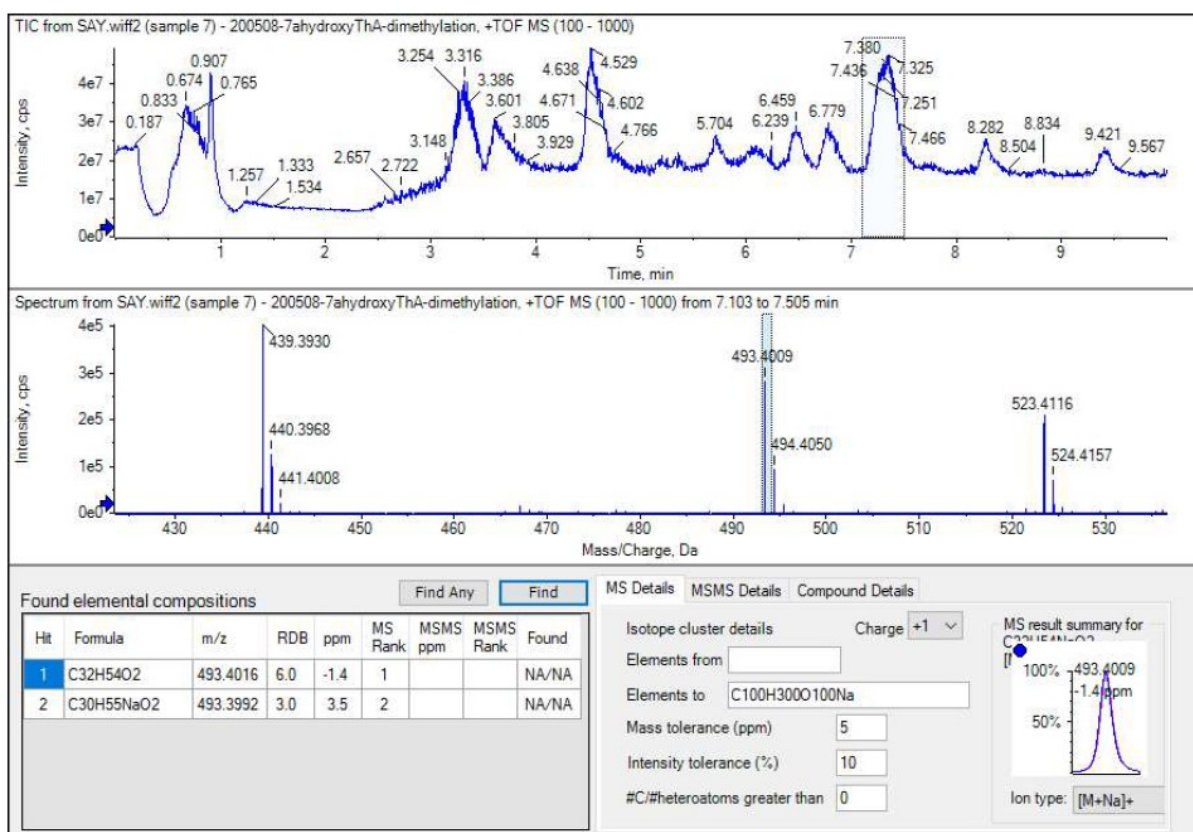


Figure SII-65. HRMS spectrum of compound **10**.