

Supplementary Data

New ψ -santonin derivatives from *Crossostephium chinense* and their anti- proliferative activities against *Leishmania* *major* and human cancer cells A549

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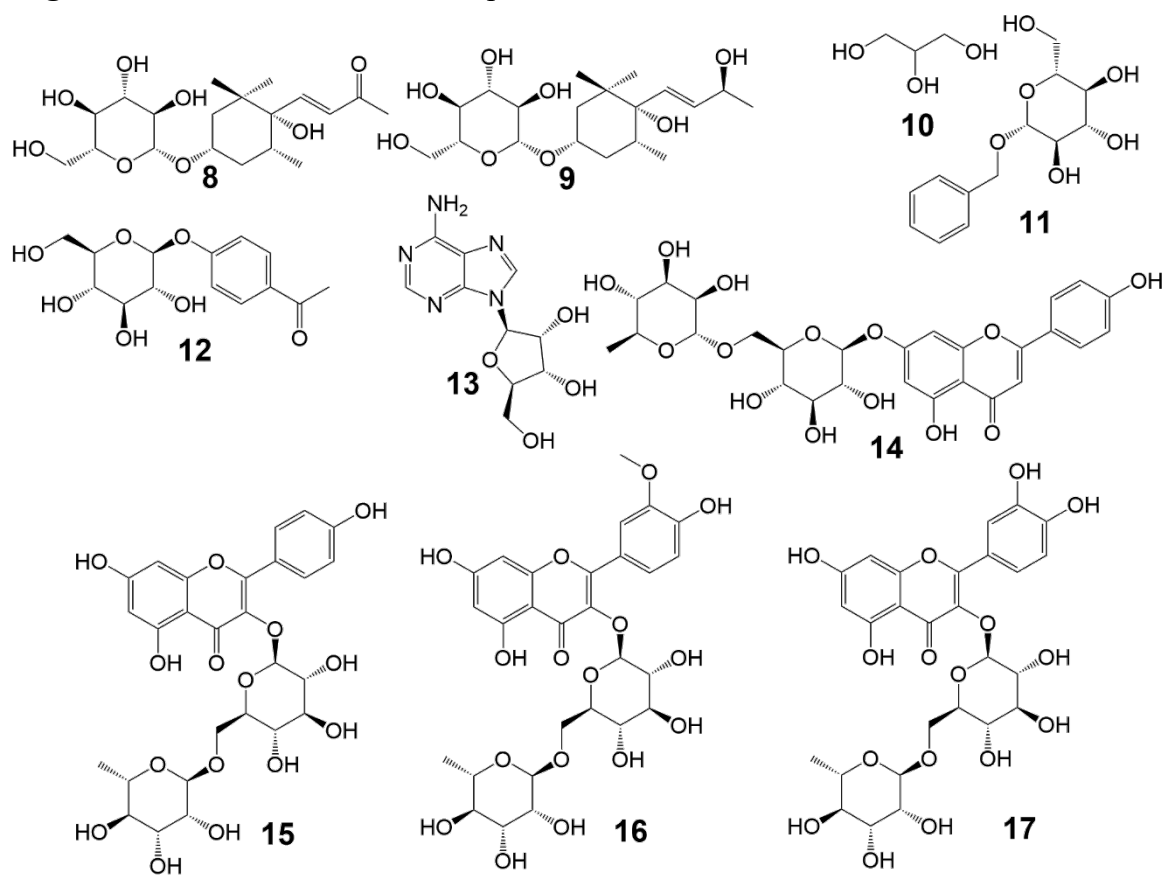
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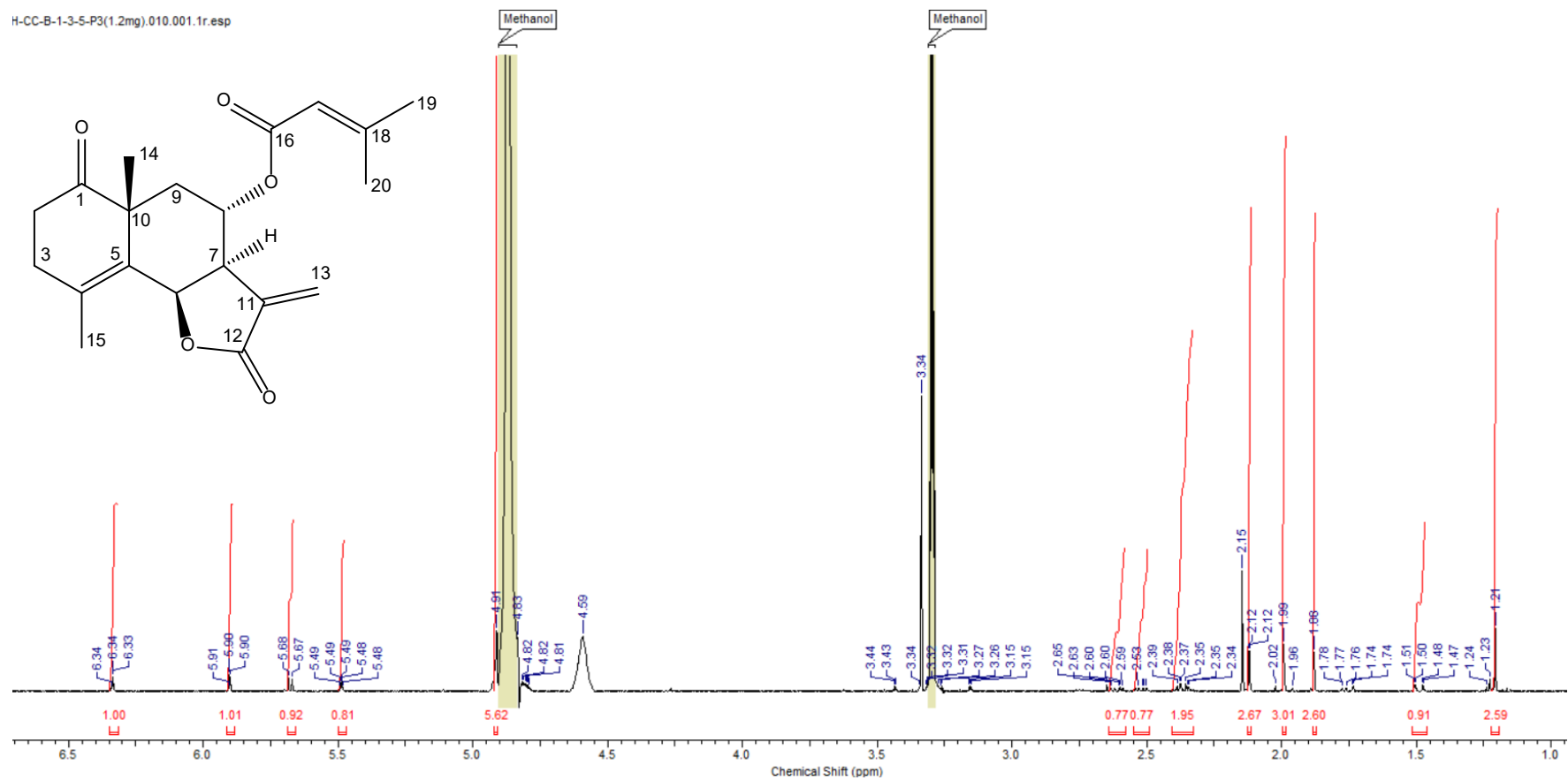


Figure S2. ¹H-NMR spectrum of **1** in MeOD (500 MHz)

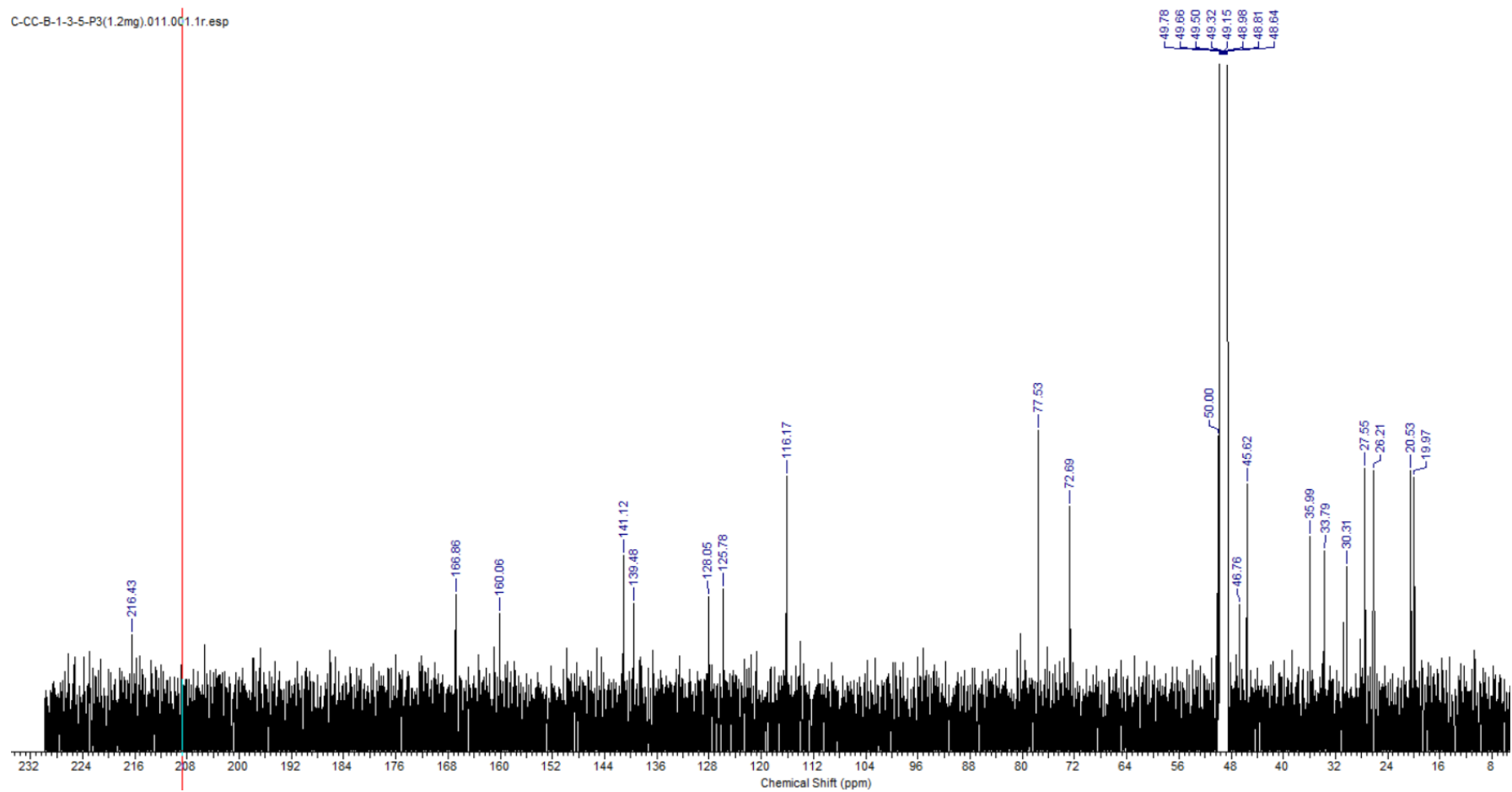


Figure S3. ^{13}C -NMR spectrum of **1** in MeOD (125 MHz)

T-CC-B-1-3-5P3(1.2mg)-2D.015.001.1r.esp

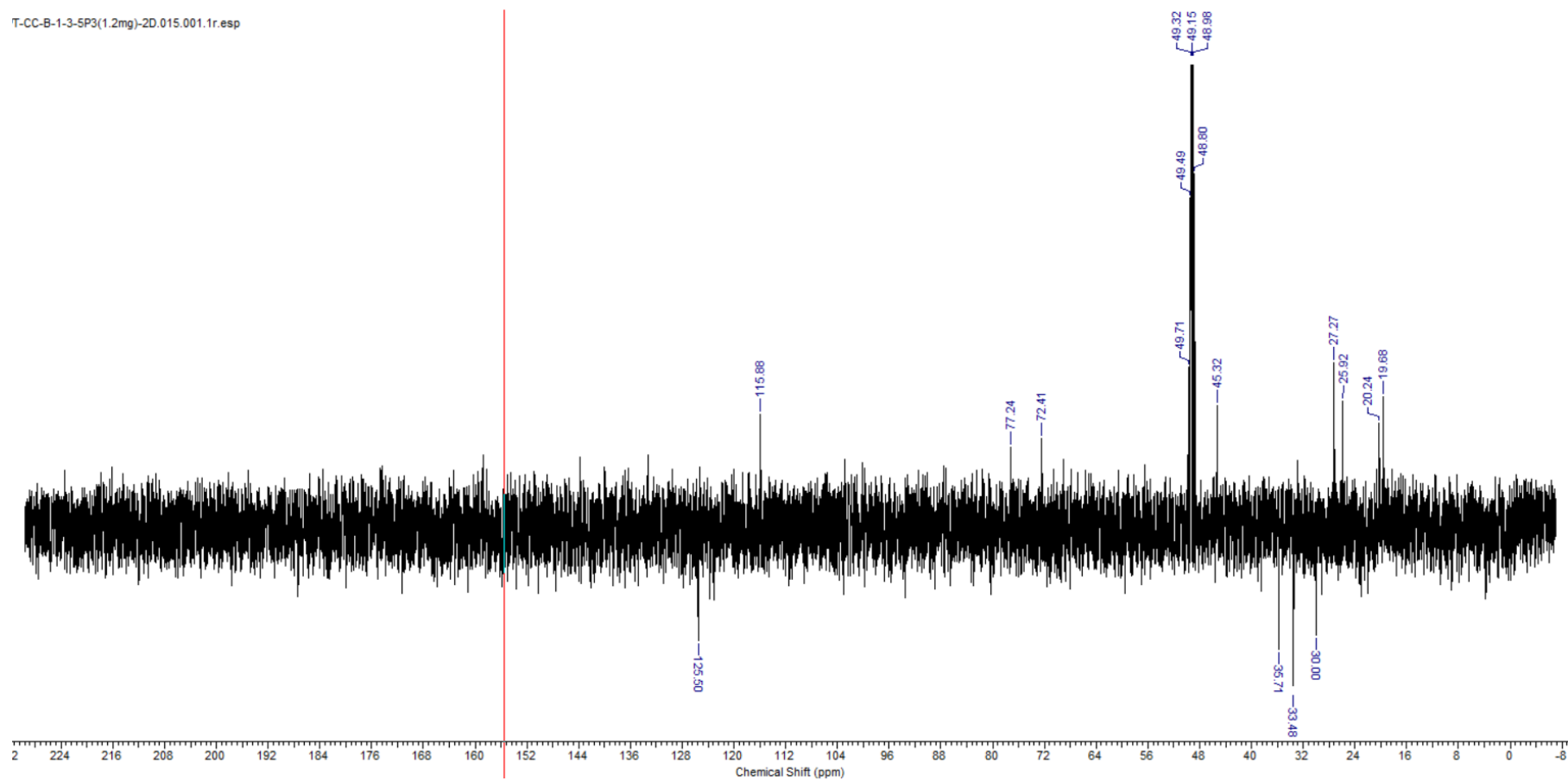


Figure S4. ¹³C DEPT135 NMR spectrum of **1** in MeOD (125 MHz)

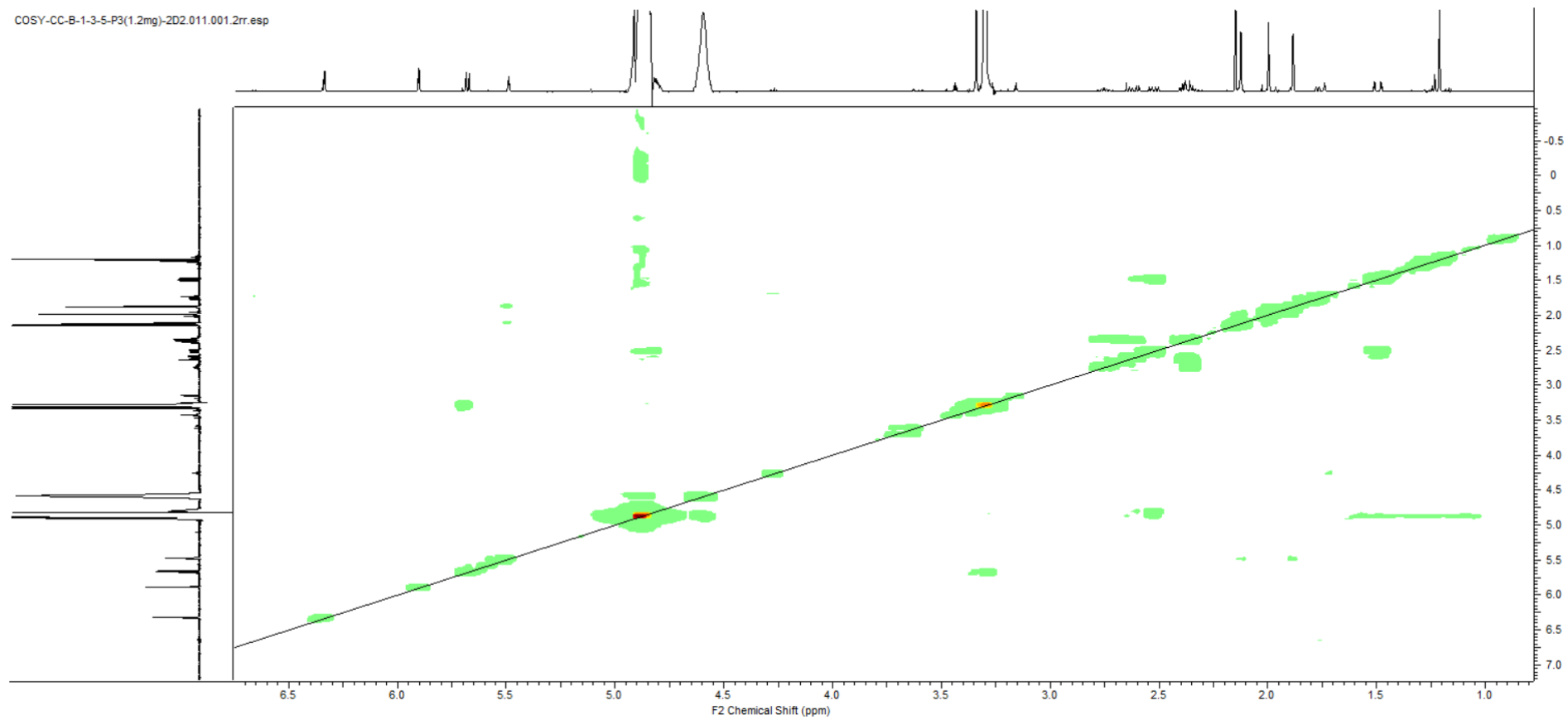


Figure S5. ¹H-¹H COSY spectrum of **1** in MeOD (500 MHz)

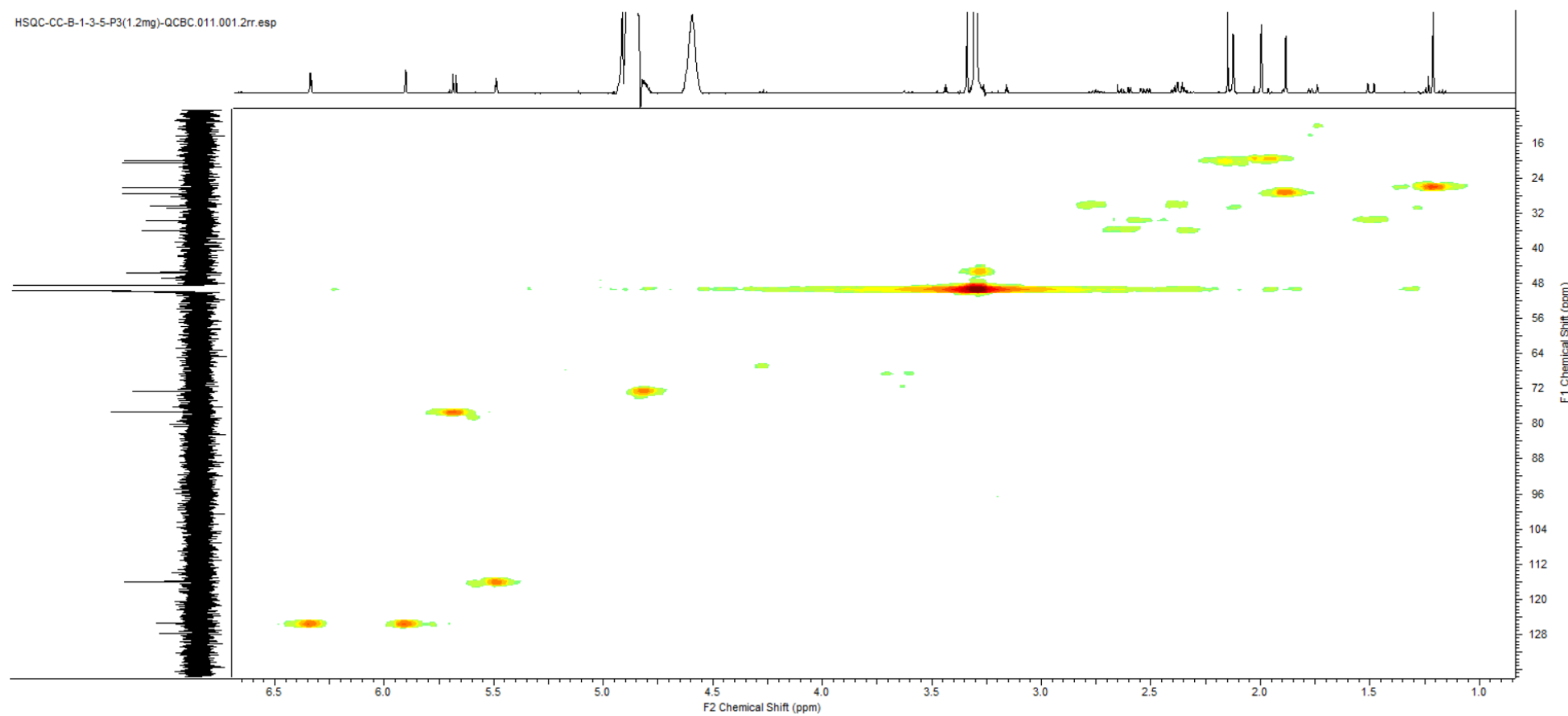


Figure S6. HSQC spectrum of **1** in MeOD (500 MHz)

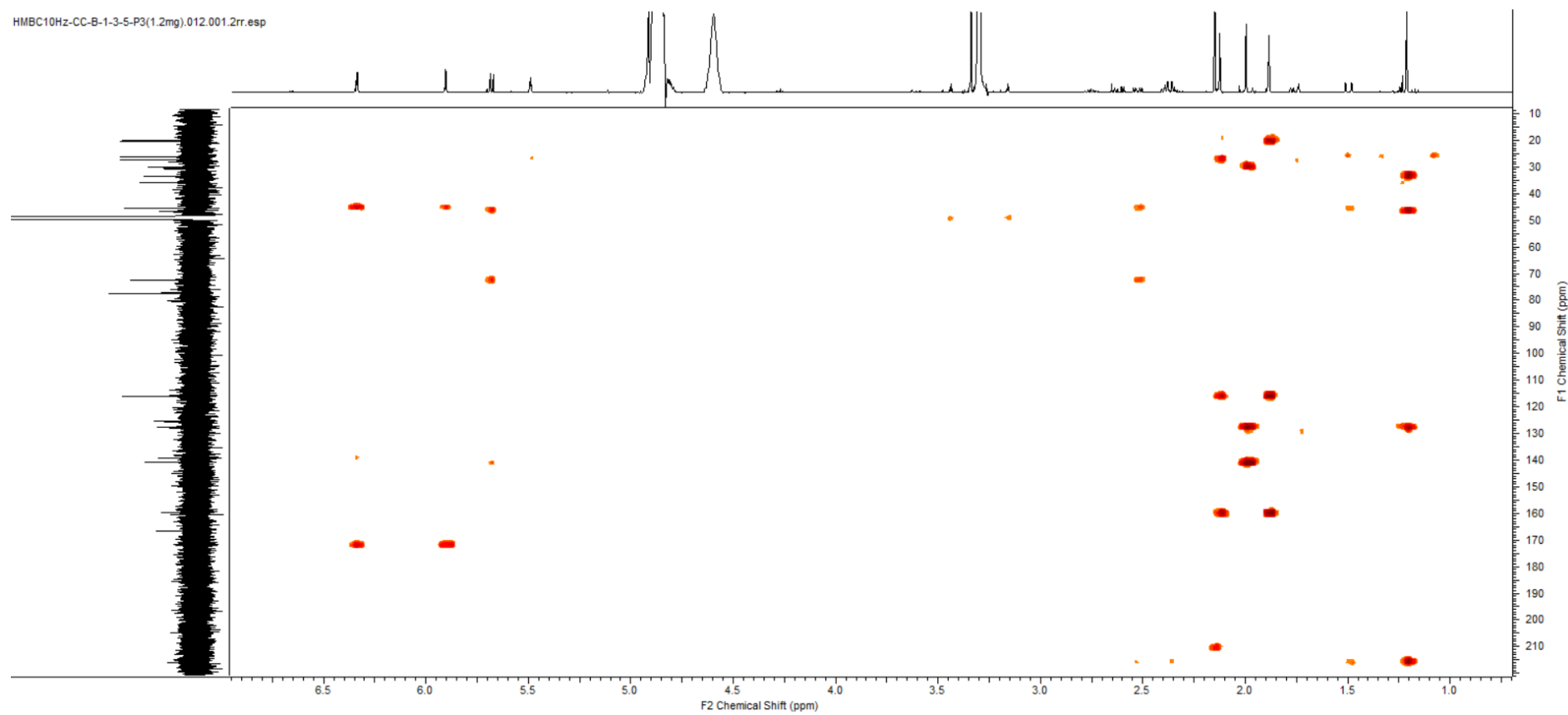


Figure S7. HMBC spectrum of **1** in MeOD (500 MHz)

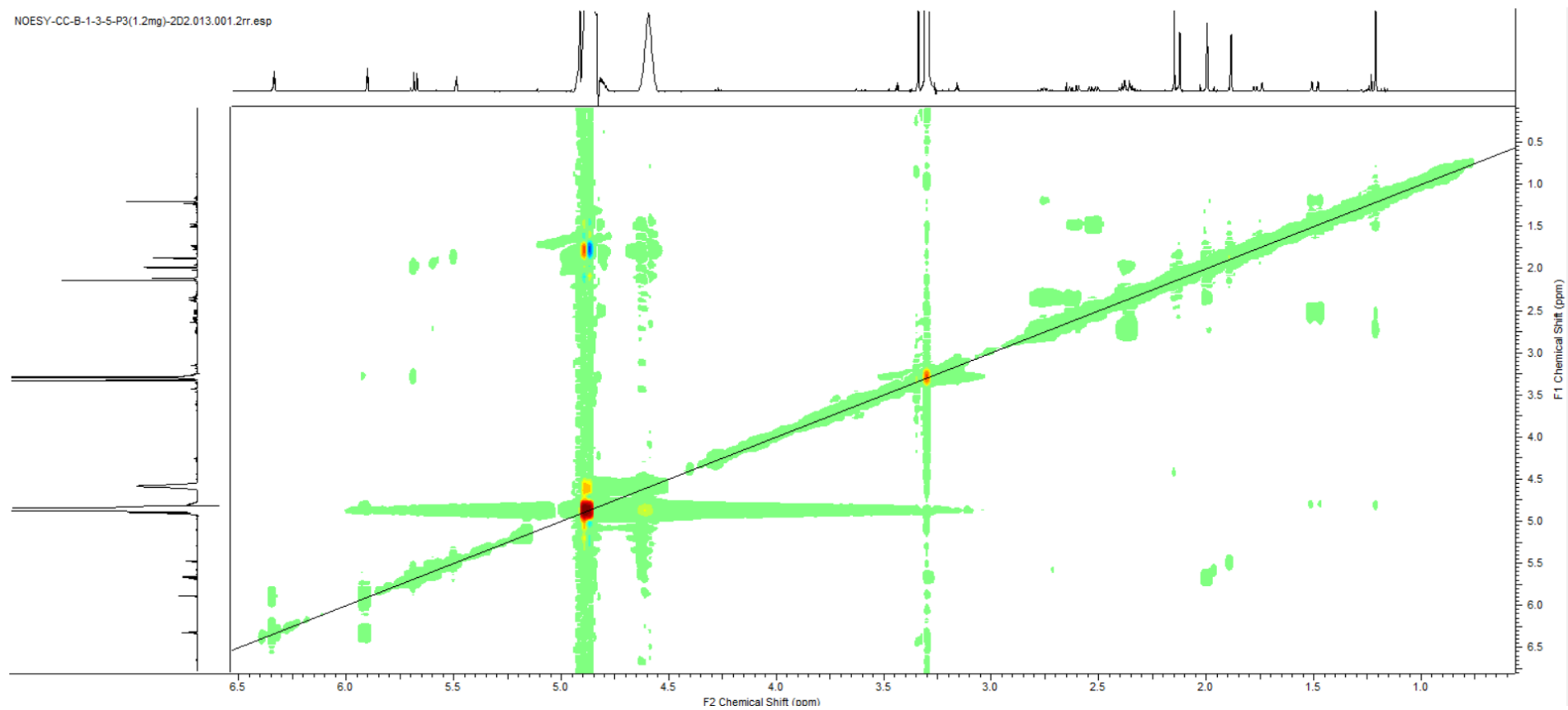


Figure S8. PS-NOESY spectrum of **1** in MeOD (500 MHz)

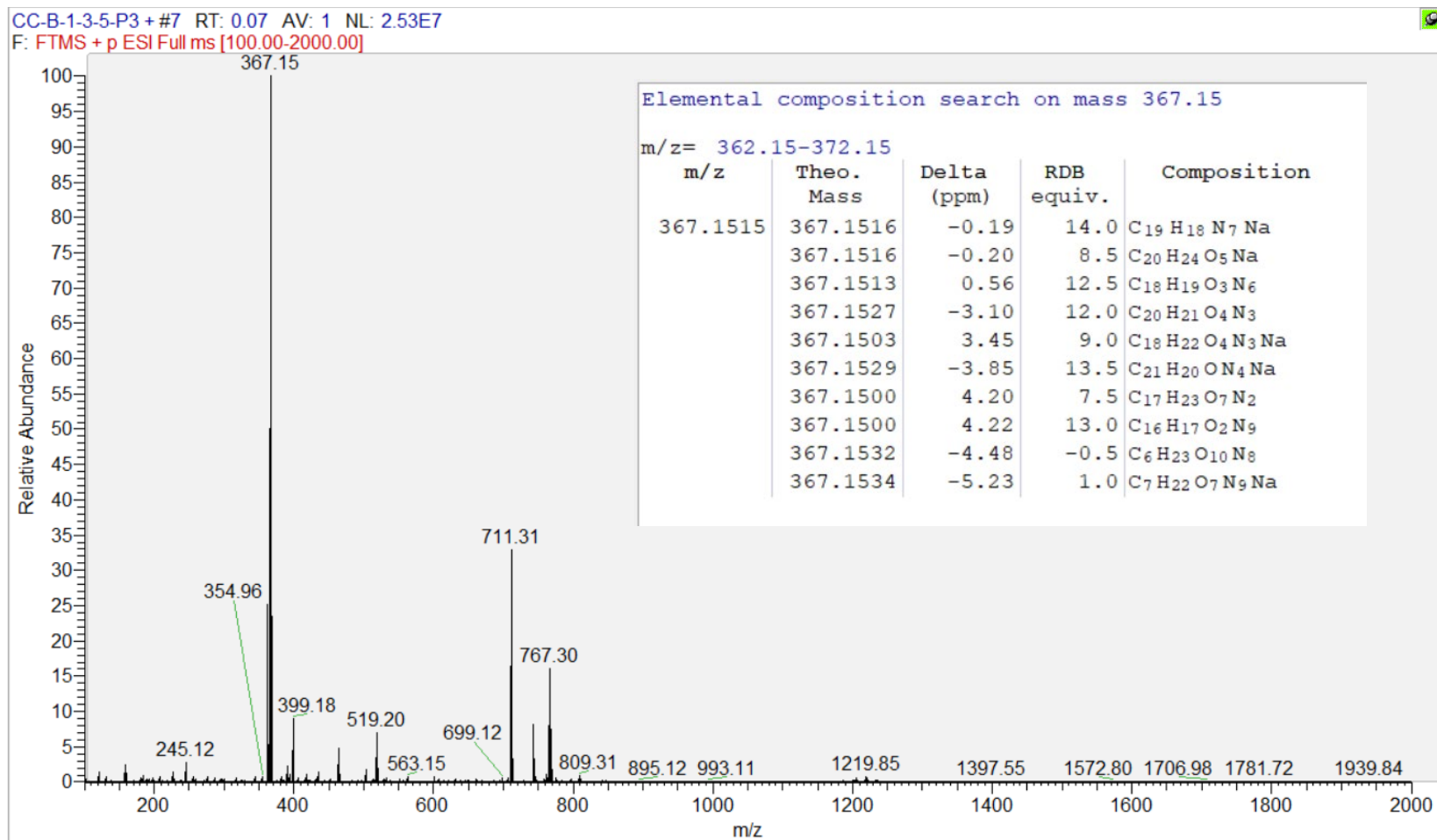


Figure S9. HR-ESI-MS spectrum of **1**

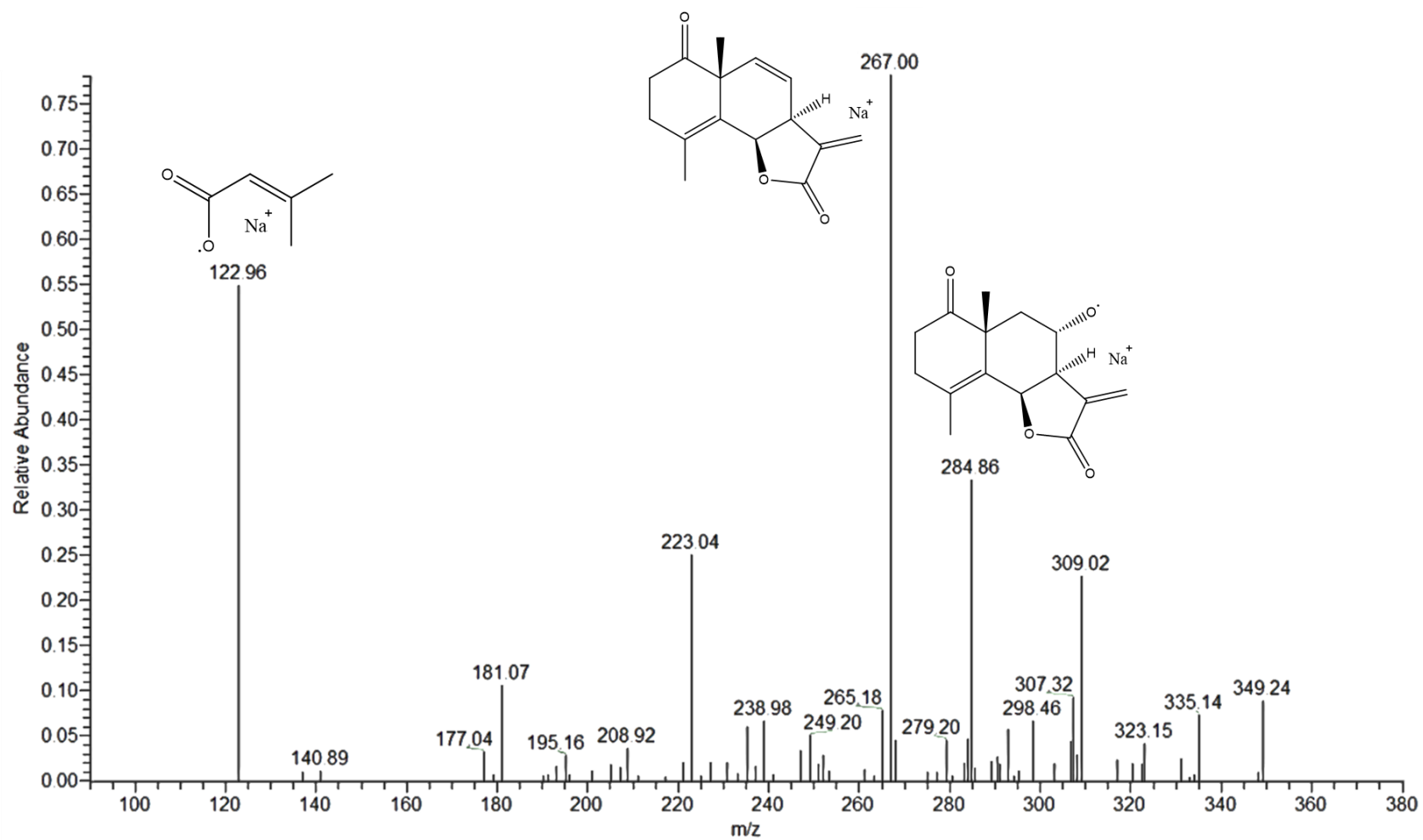


Figure S10. ESI-MS/MS spectrum of **1**

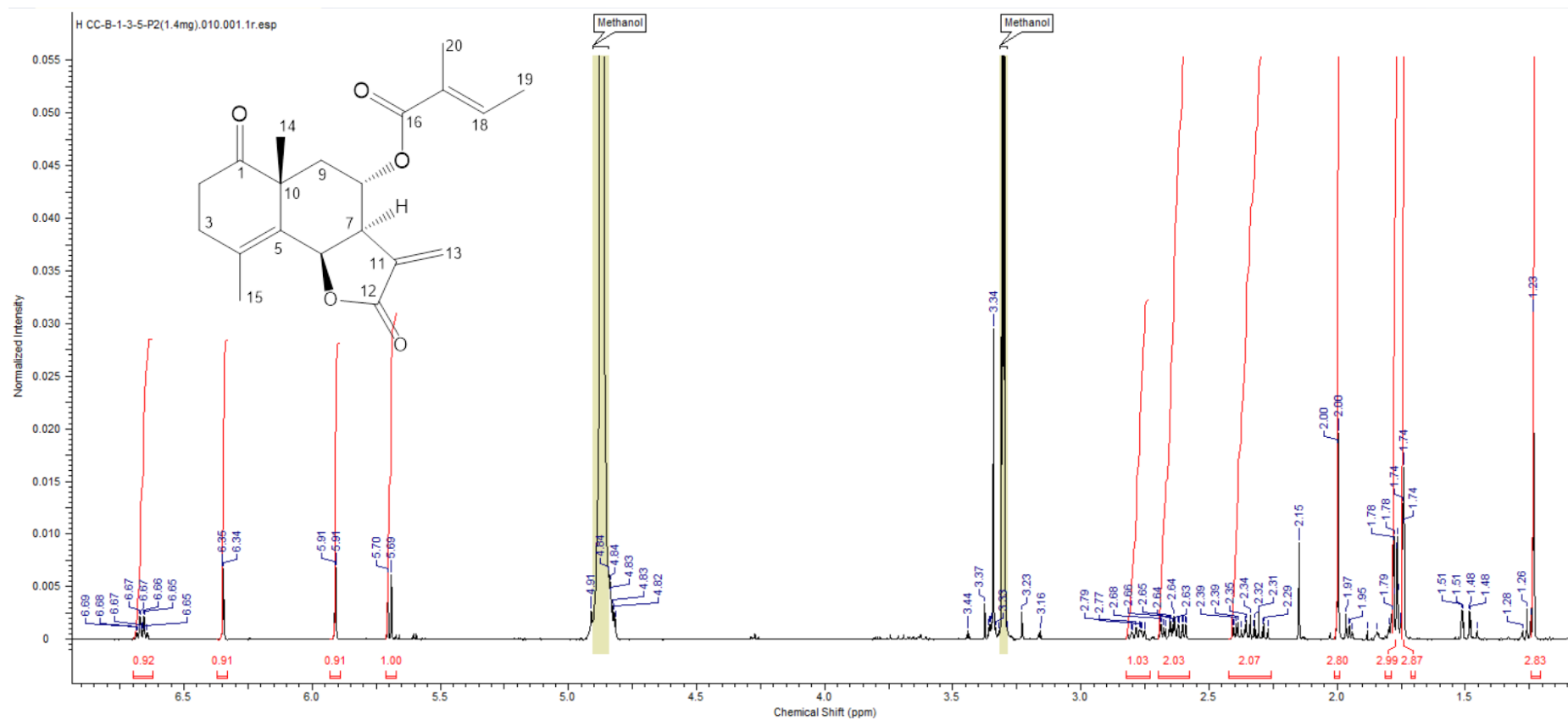


Figure S11. ^1H -NMR spectrum of **2** in MeOD (500 MHz)

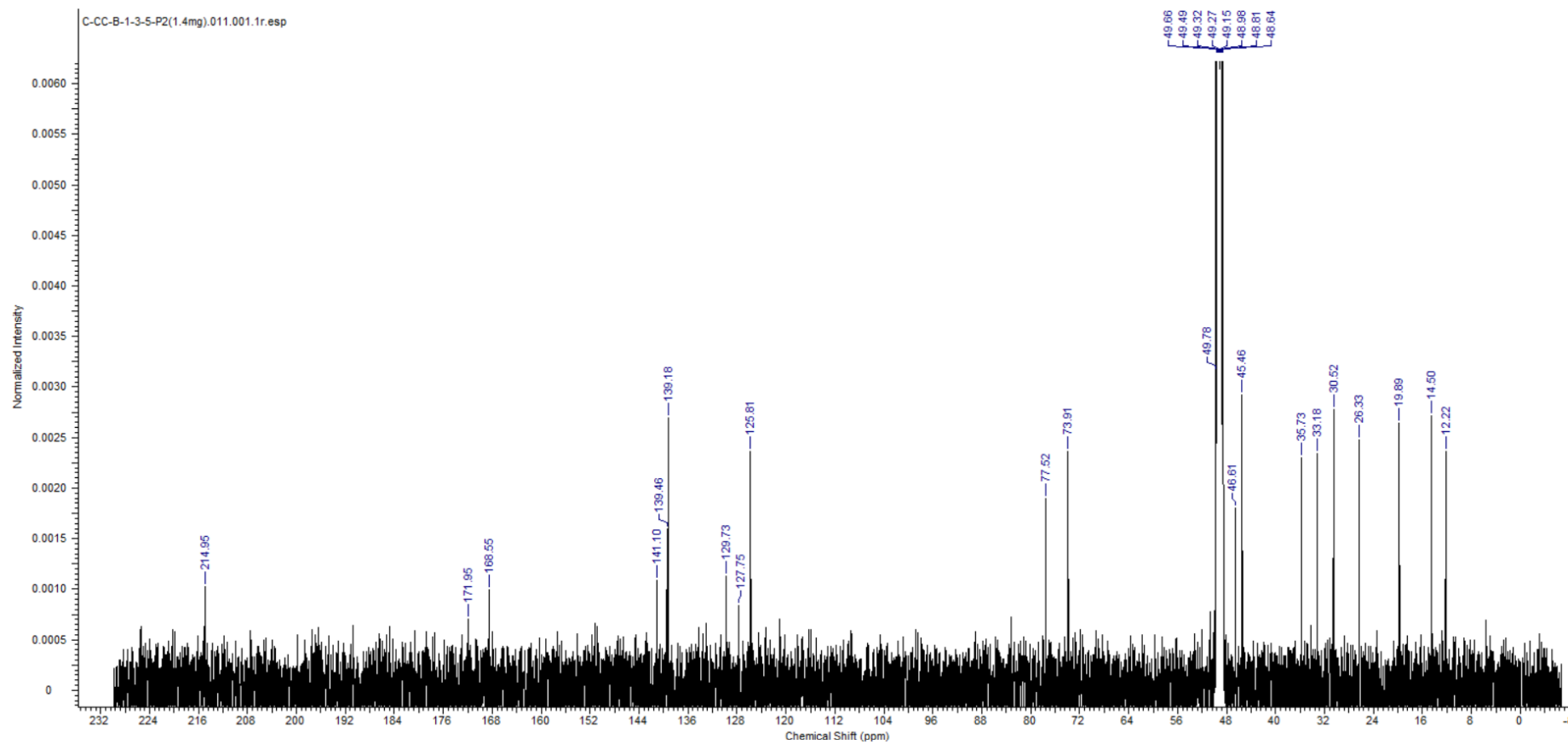


Figure S12. ^{13}C -NMR spectrum of **2** in MeOD (125 MHz)

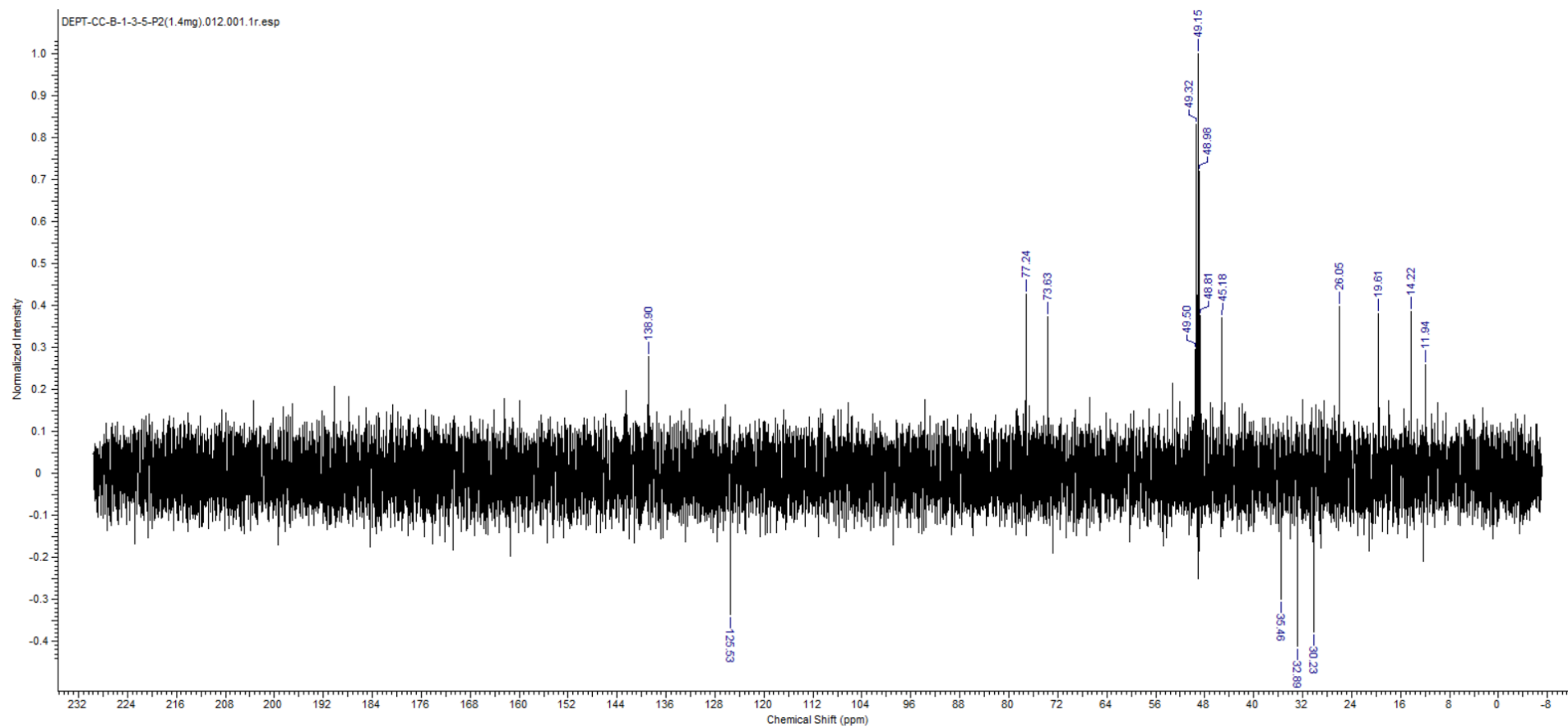


Figure S13. ^{13}C DEPT135 NMR spectrum of **2** in MeOD (125 MHz)

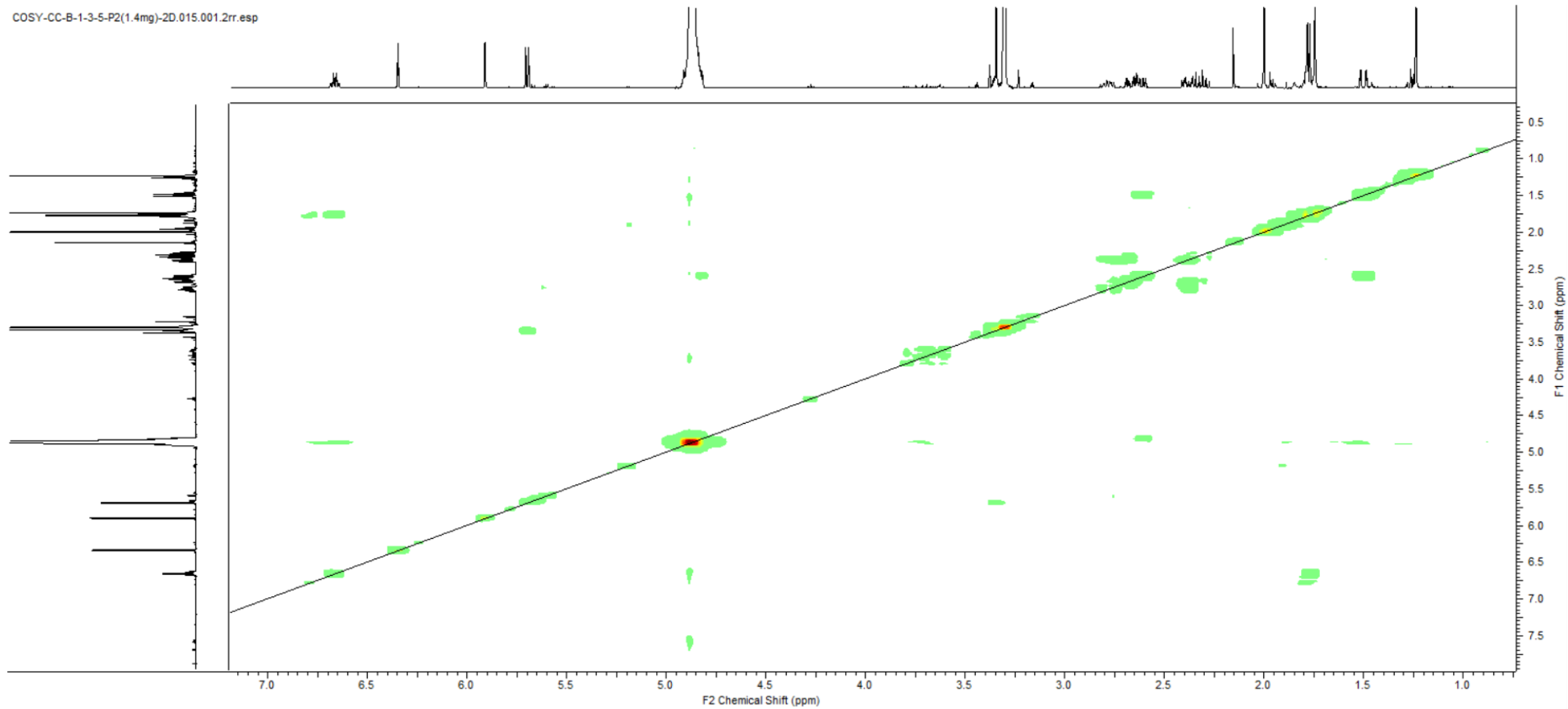


Figure S14. ¹H-¹H COSY spectrum of **2** in MeOD (500 MHz)

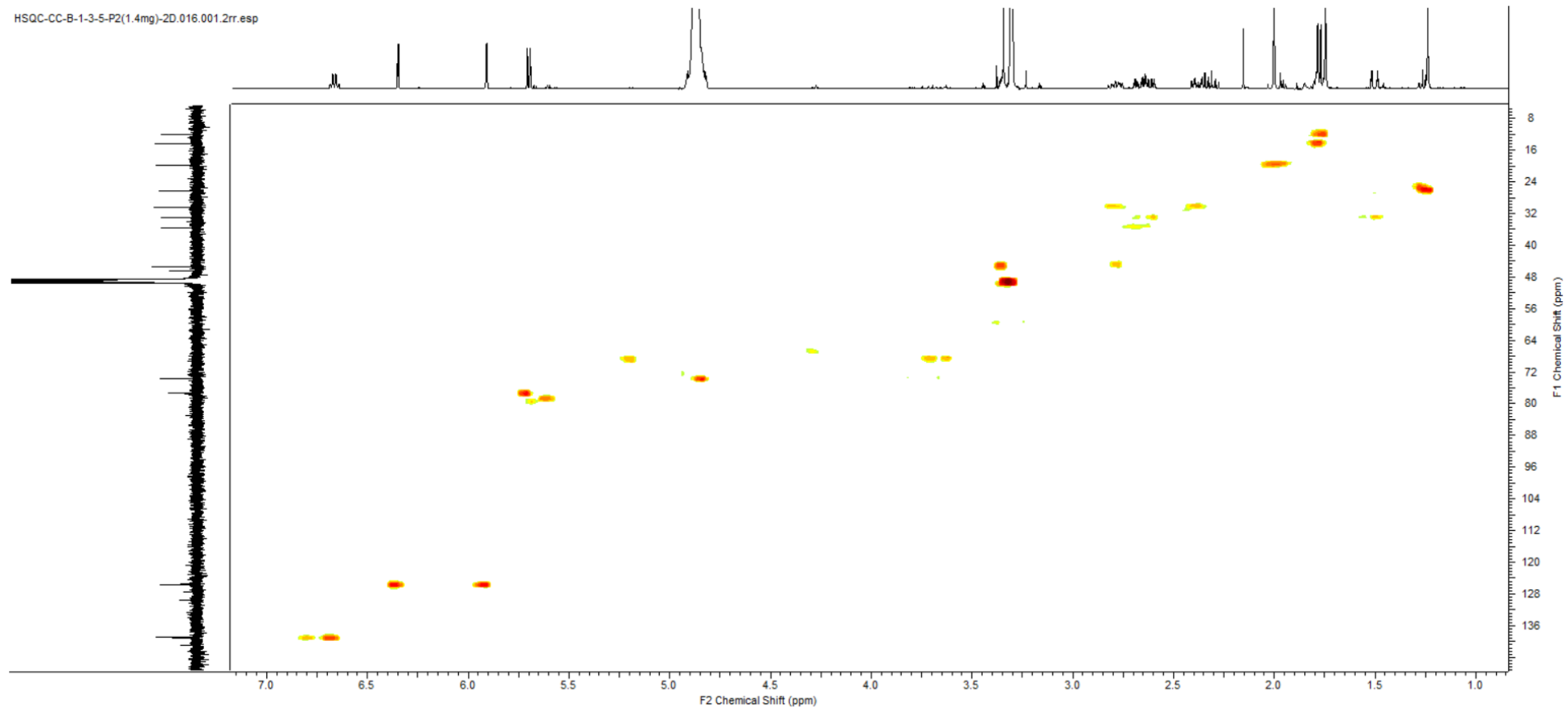


Figure S15. HSQC spectrum of **2** in MeOD (500 MHz)

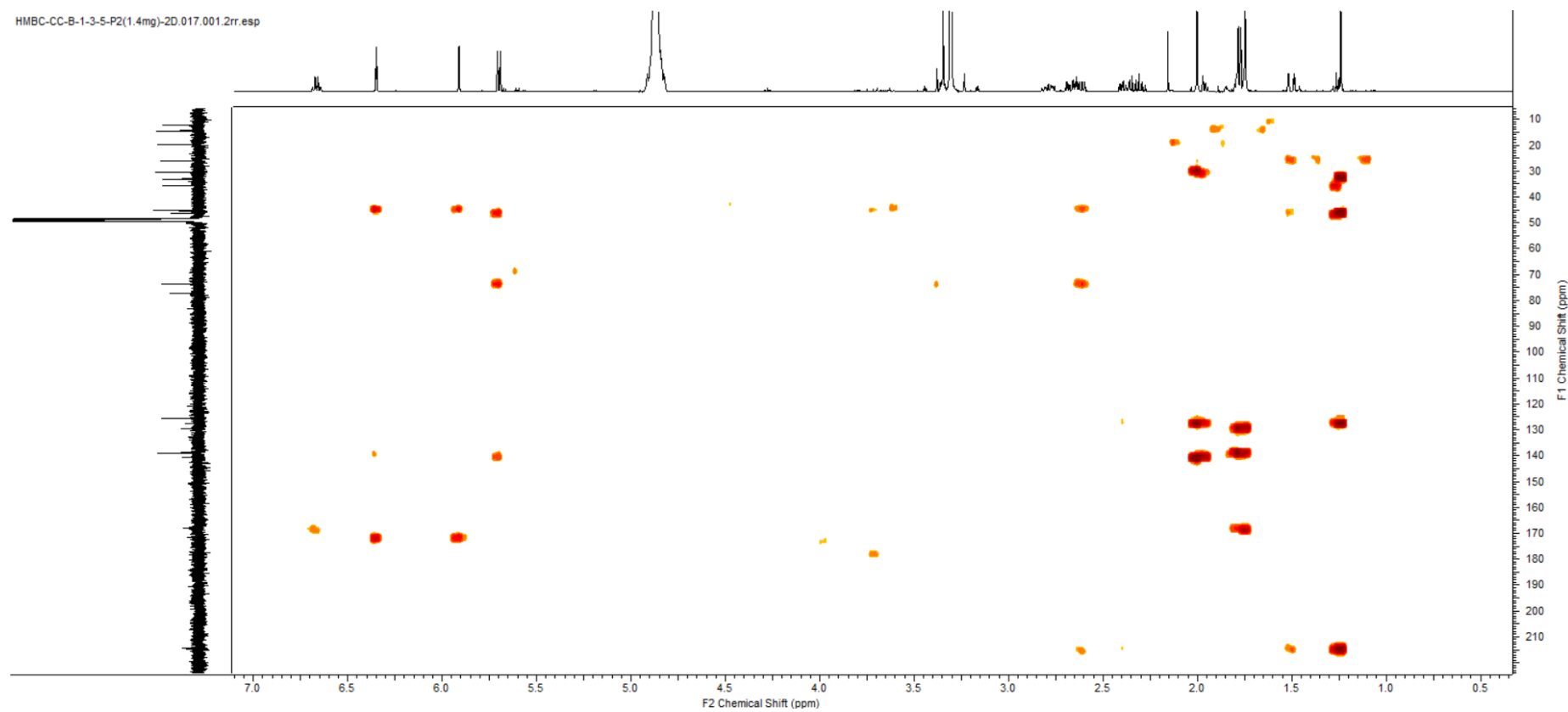


Figure S16. HMBC spectrum of **2** in MeOD (500 MHz)

CC-B-1-3-5-P2 + #4 RT: 0.04 AV: 1 NL: 3.17E7
 F: FTMS + p ESI Full ms [100.00-2000.00]

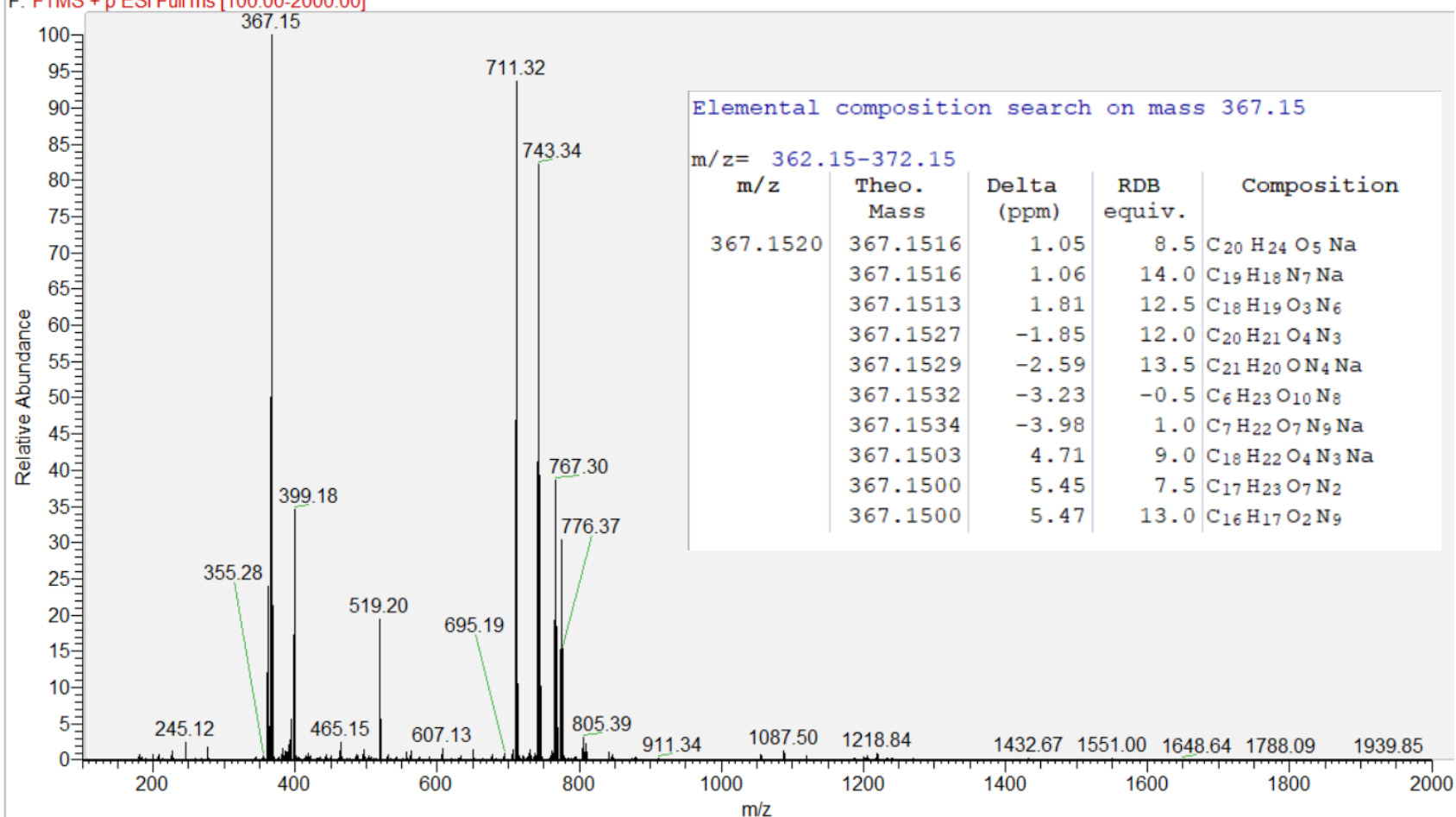


Figure S18. HR-ESI-MS spectrum of **2**

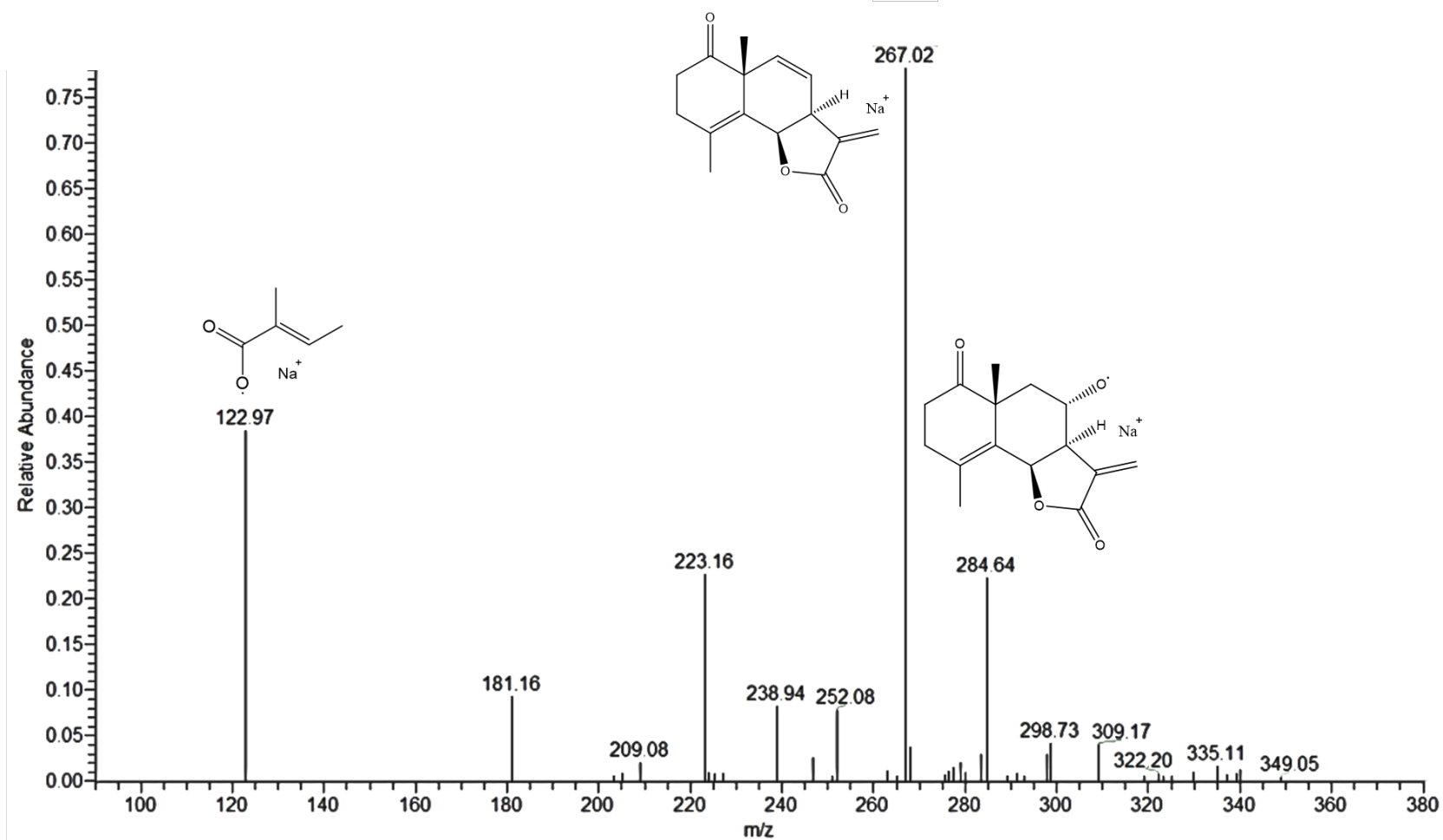


Figure S19. ESI-MS/MS spectrum of **2**

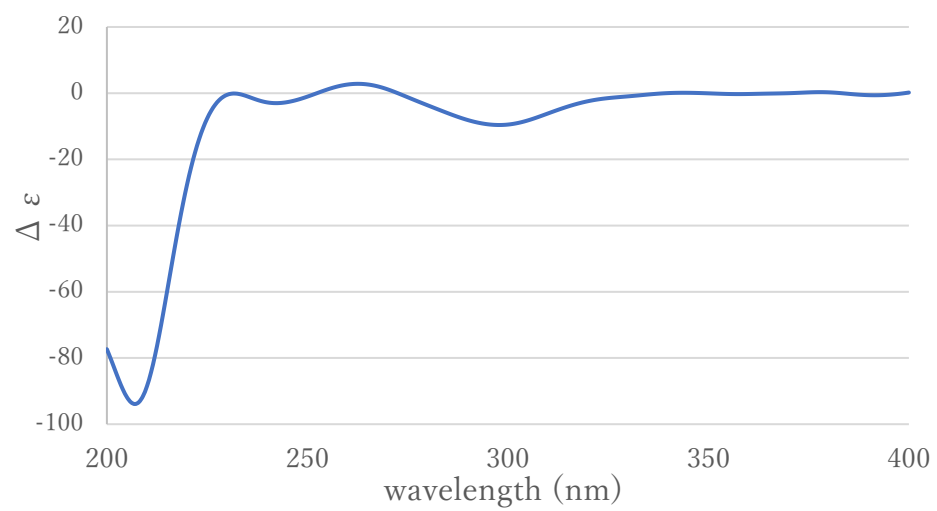


Figure S20. Experimental CD spectrum of **2** in CH₃CN

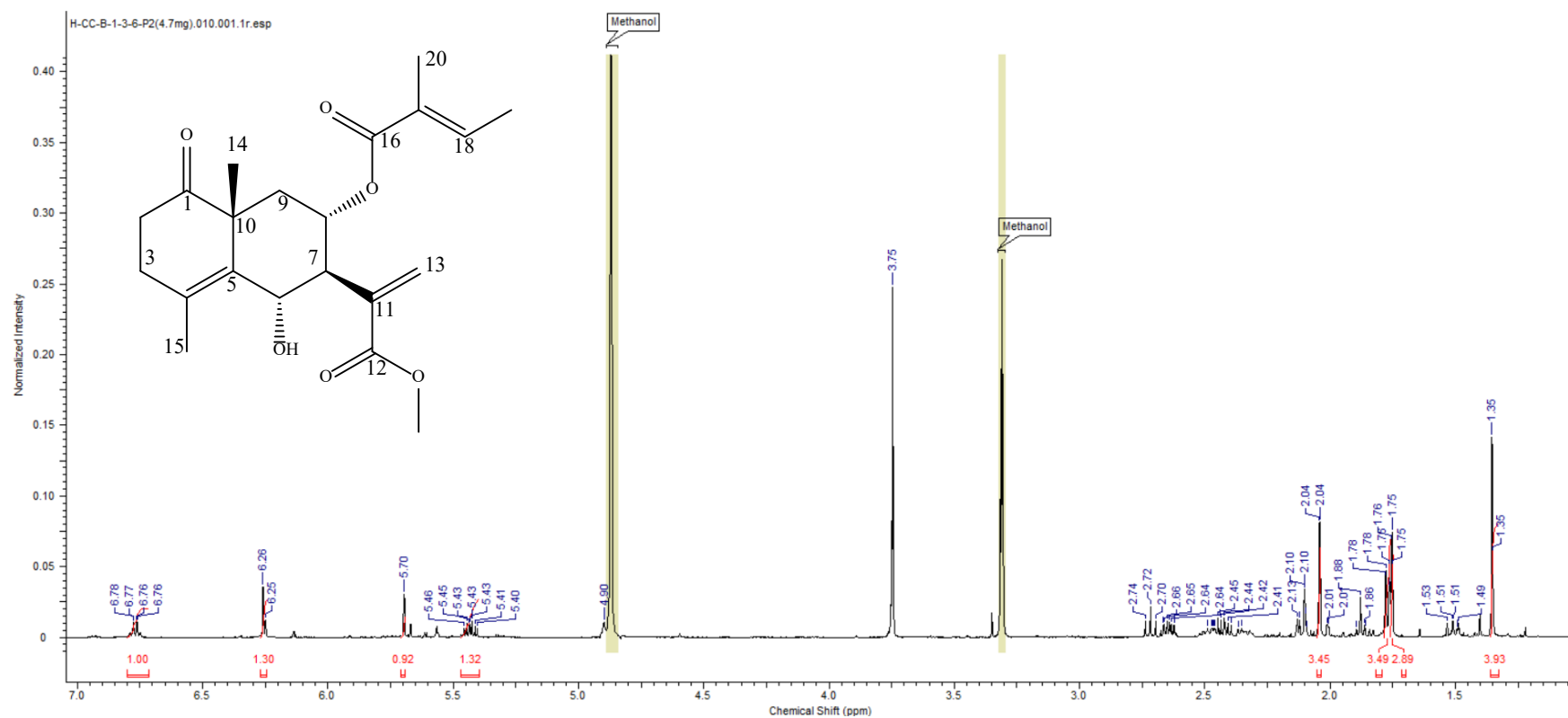


Figure S21. ^1H -NMR spectrum of **3** in MeOD (500 MHz)

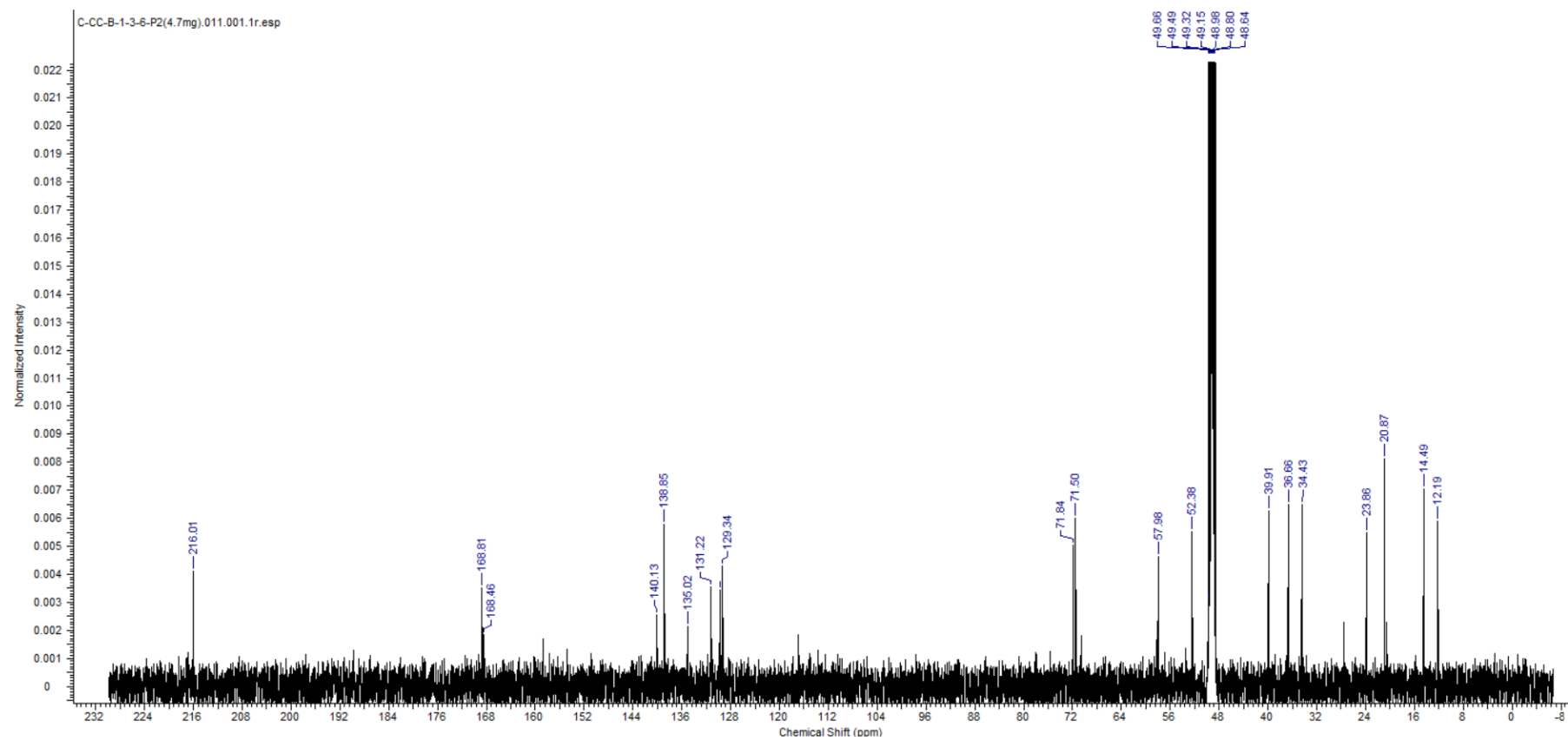


Figure S22. ^{13}C -NMR spectrum of **3** in MeOD (125 MHz)

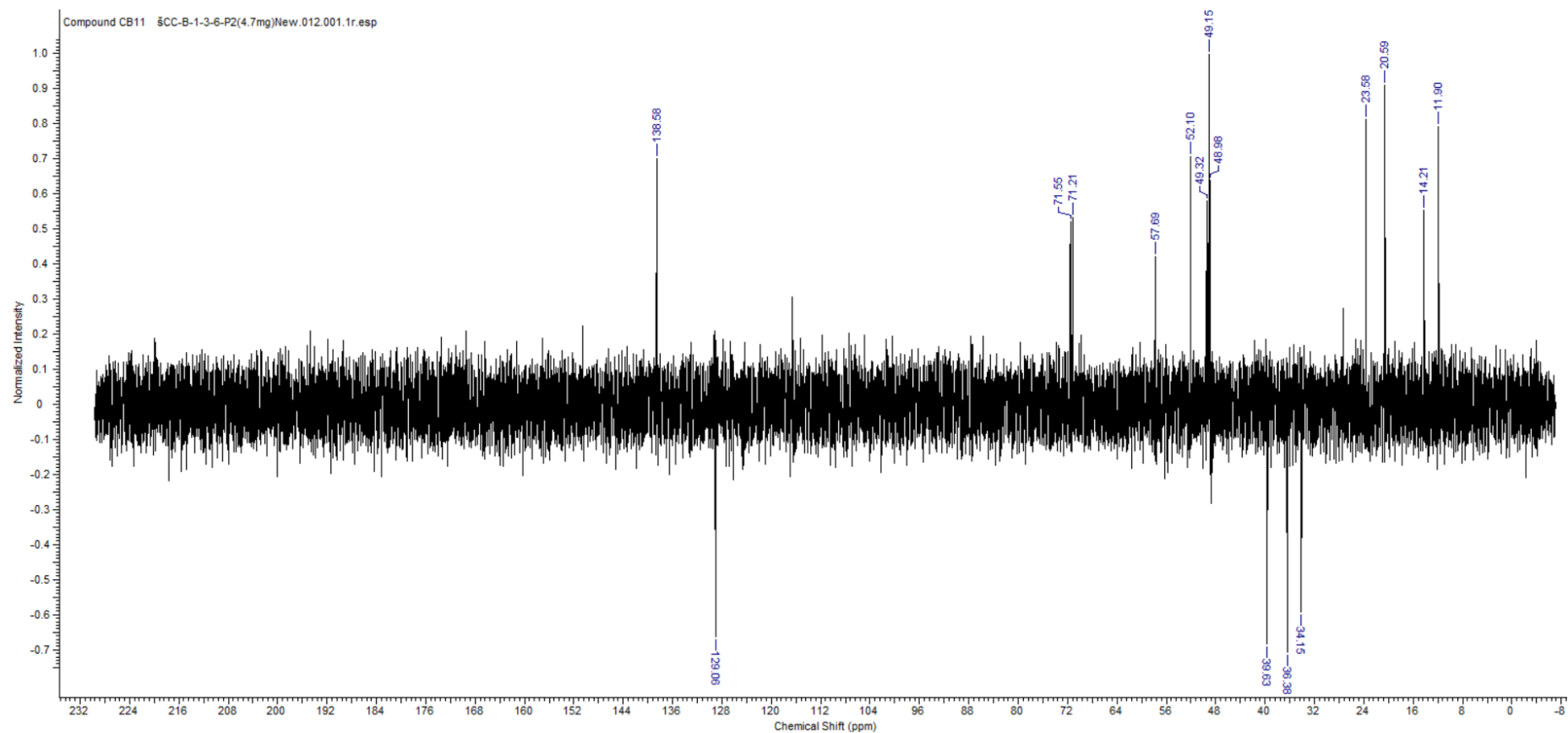


Figure S23. ^{13}C DEPT135 NMR spectrum of **3** in MeOD (125 MHz)

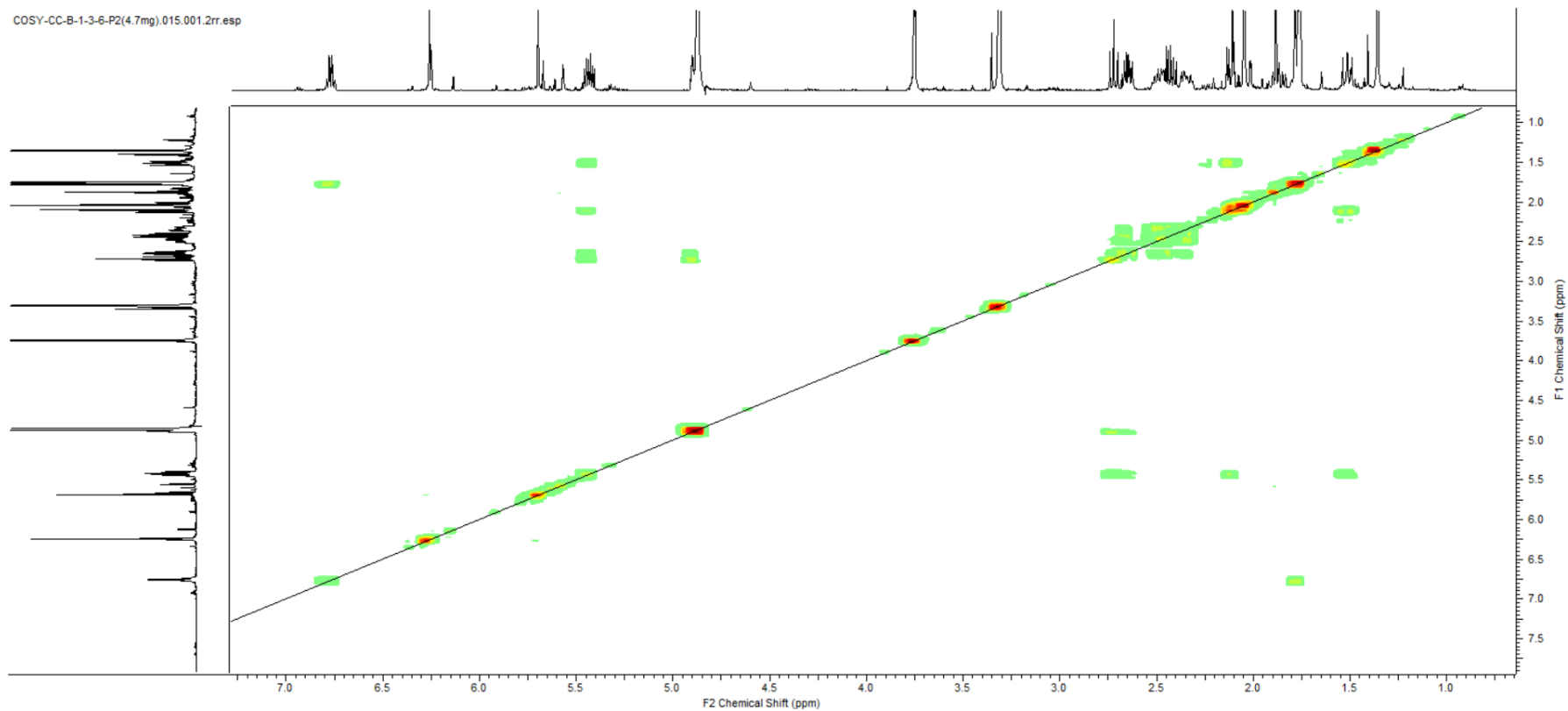


Figure S24. ^1H - ^1H COSY spectrum of **3** in MeOD (500 MHz)

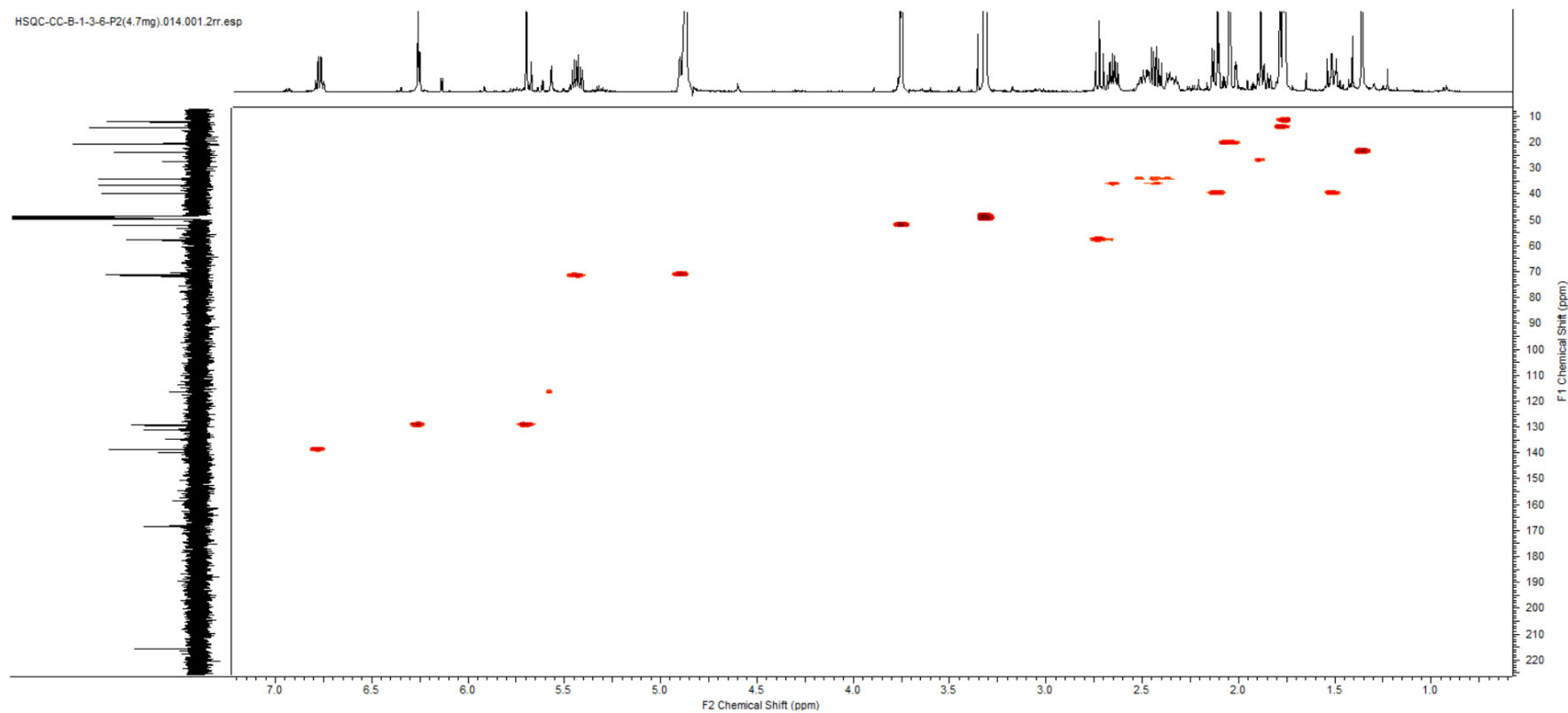


Figure S25. HSQC spectrum of **3** in MeOD (500 MHz)

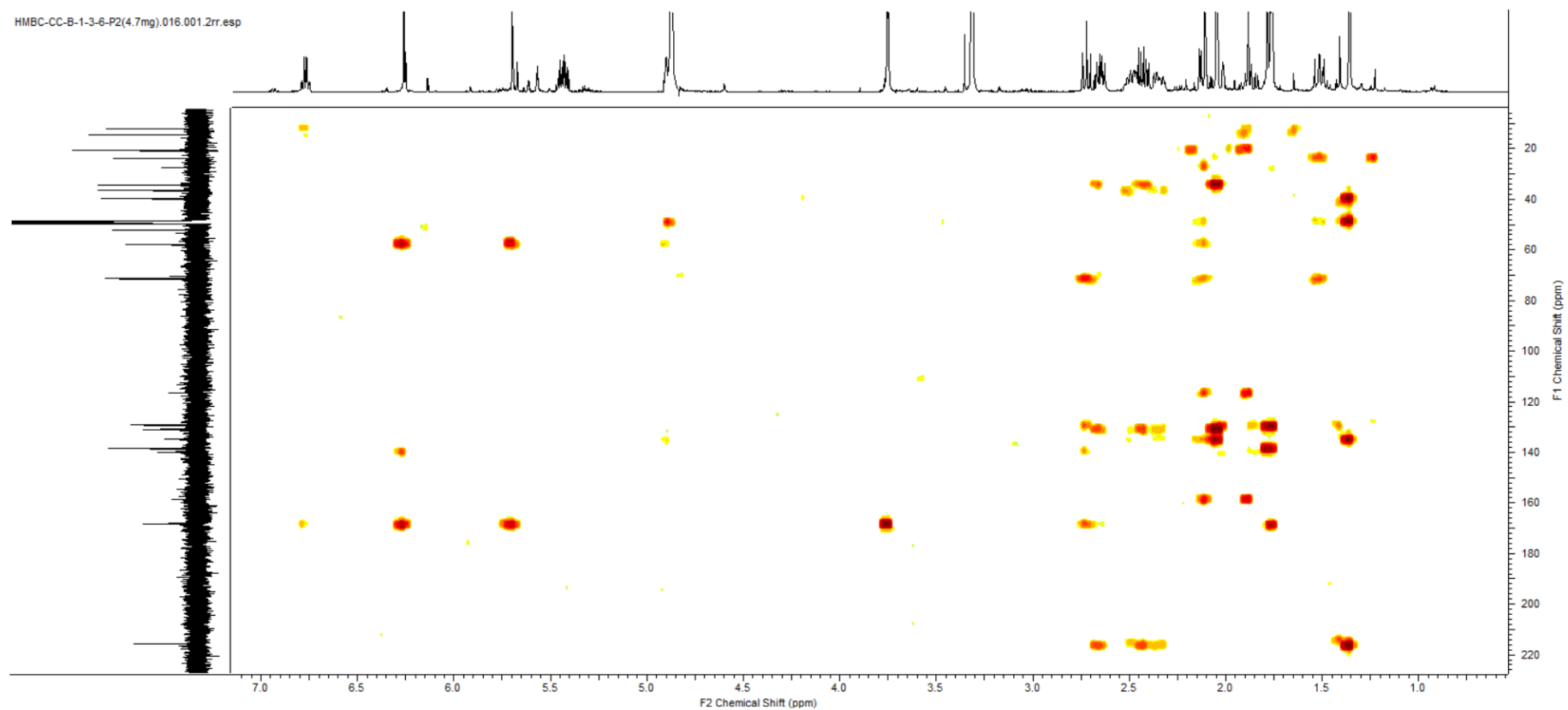


Figure S26. HMBC spectrum of **3** in MeOD (500 MHz)

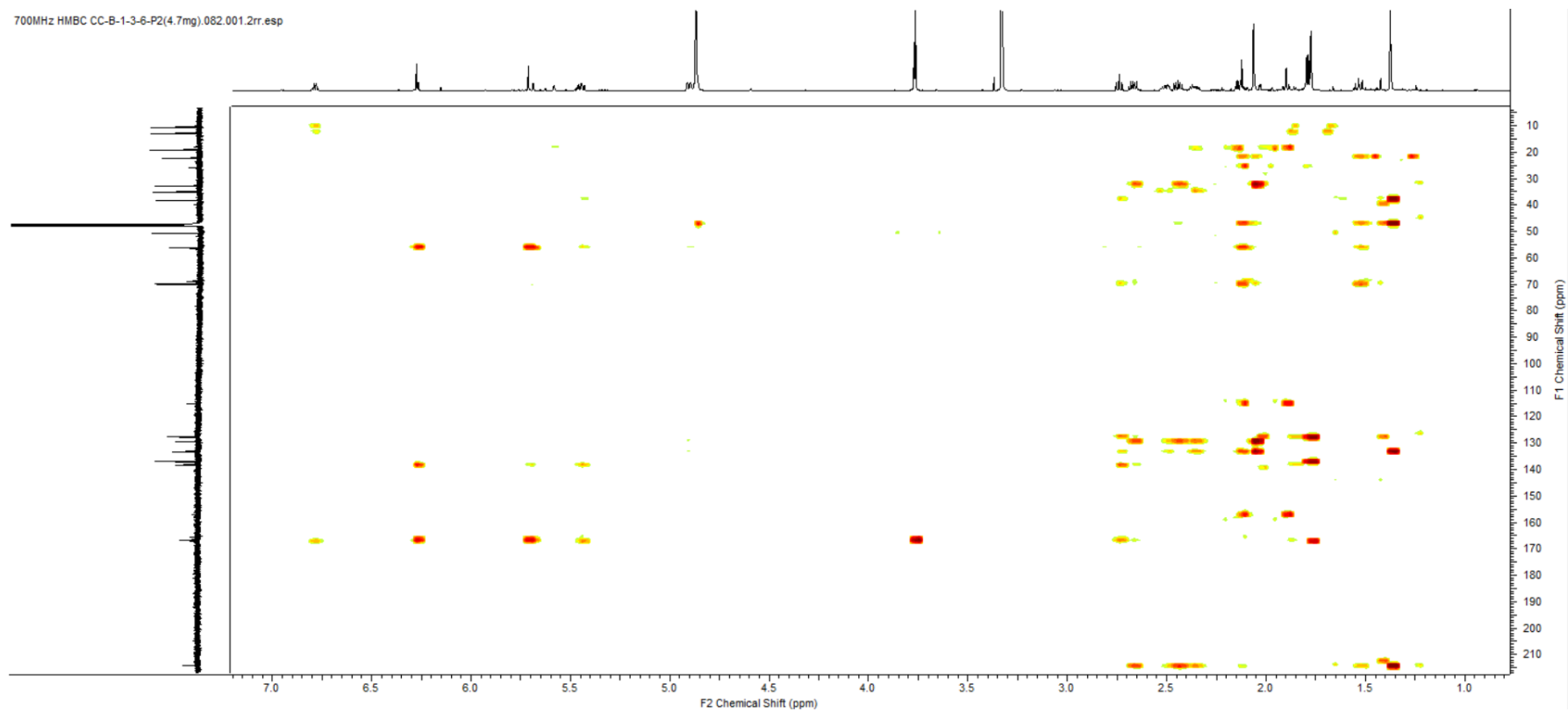


Figure S27. HMBC spectrum of **3** in MeOD (700 MHz)

NOESY-CC-B-1-3-6-P2(4.7mg)-NOESY.011.001.2rr.esp

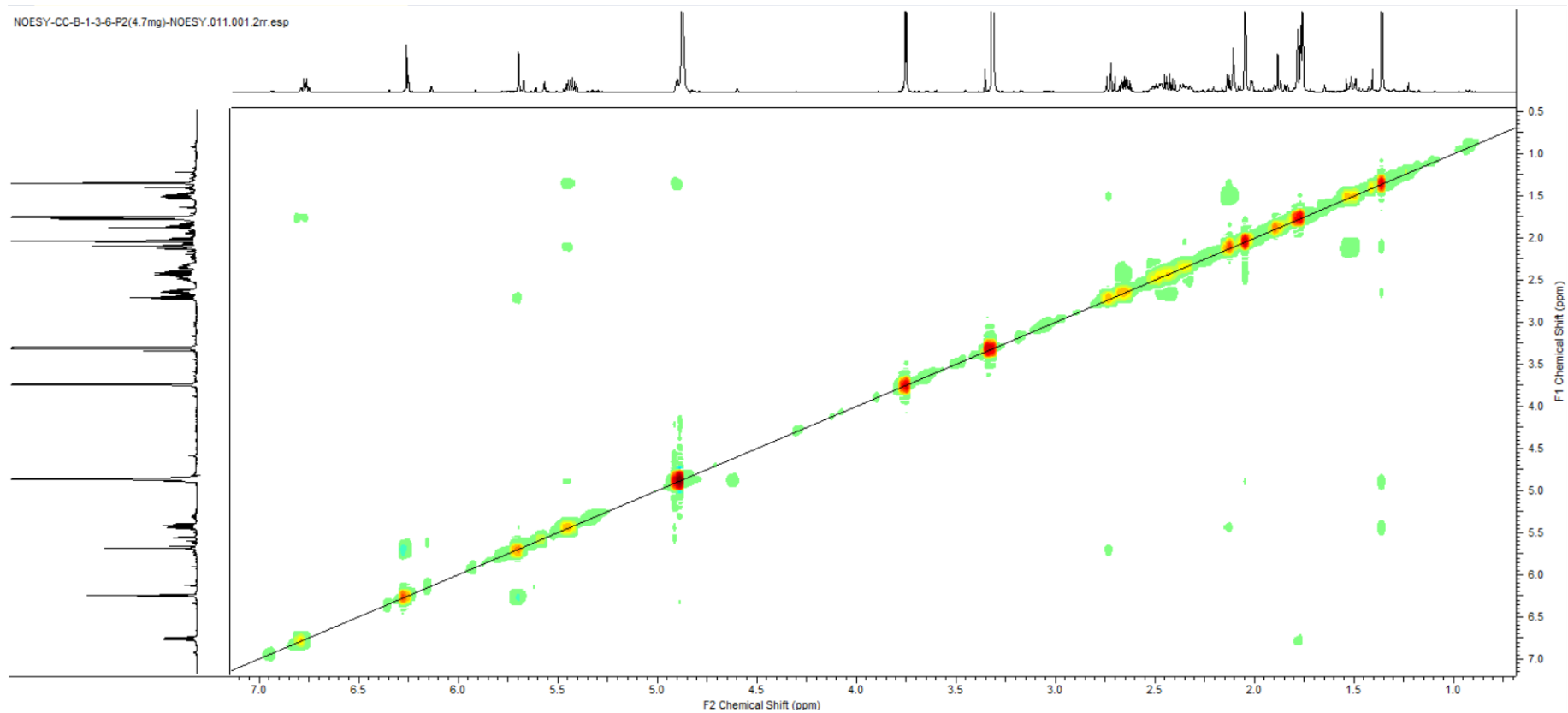


Figure S28. PS-NOESY spectrum of **3** in MeOD (500 MHz)

CC-B-1-3-6 P2 + #7 RT: 0.08 AV: 1 NL: 3.12E6
 F: FTMS + p ESI Full ms [100.00-2000.00]

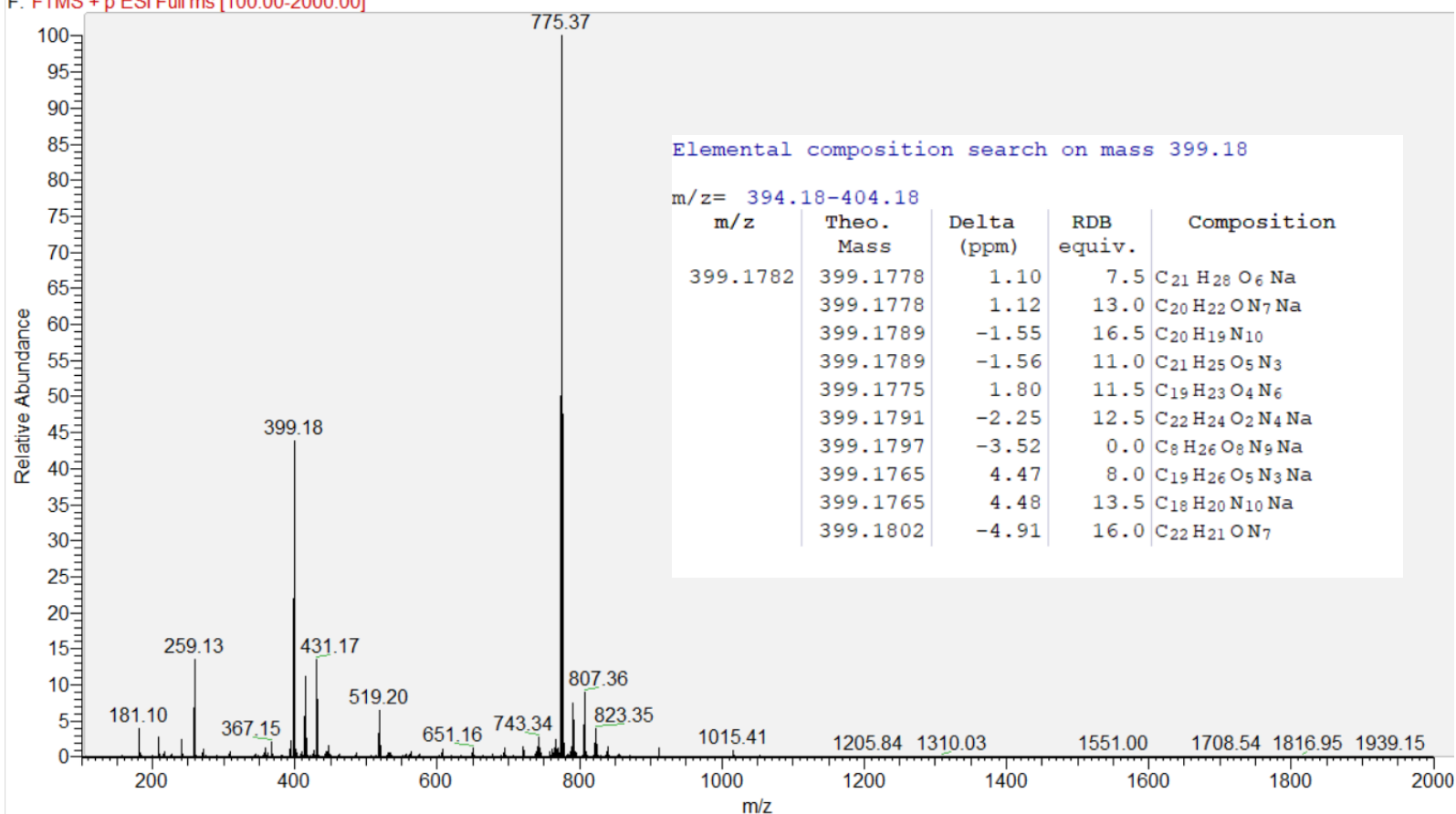


Figure S29. HR-ESI-MS spectrum of **3**

CC-B-1-3-6 P2 + #11 RT: 0.13 AV: 1 NL: 5.25E4
F: ITMS + c ESI d Full ms2 399.18@cid35.00 [95.00-410.00]

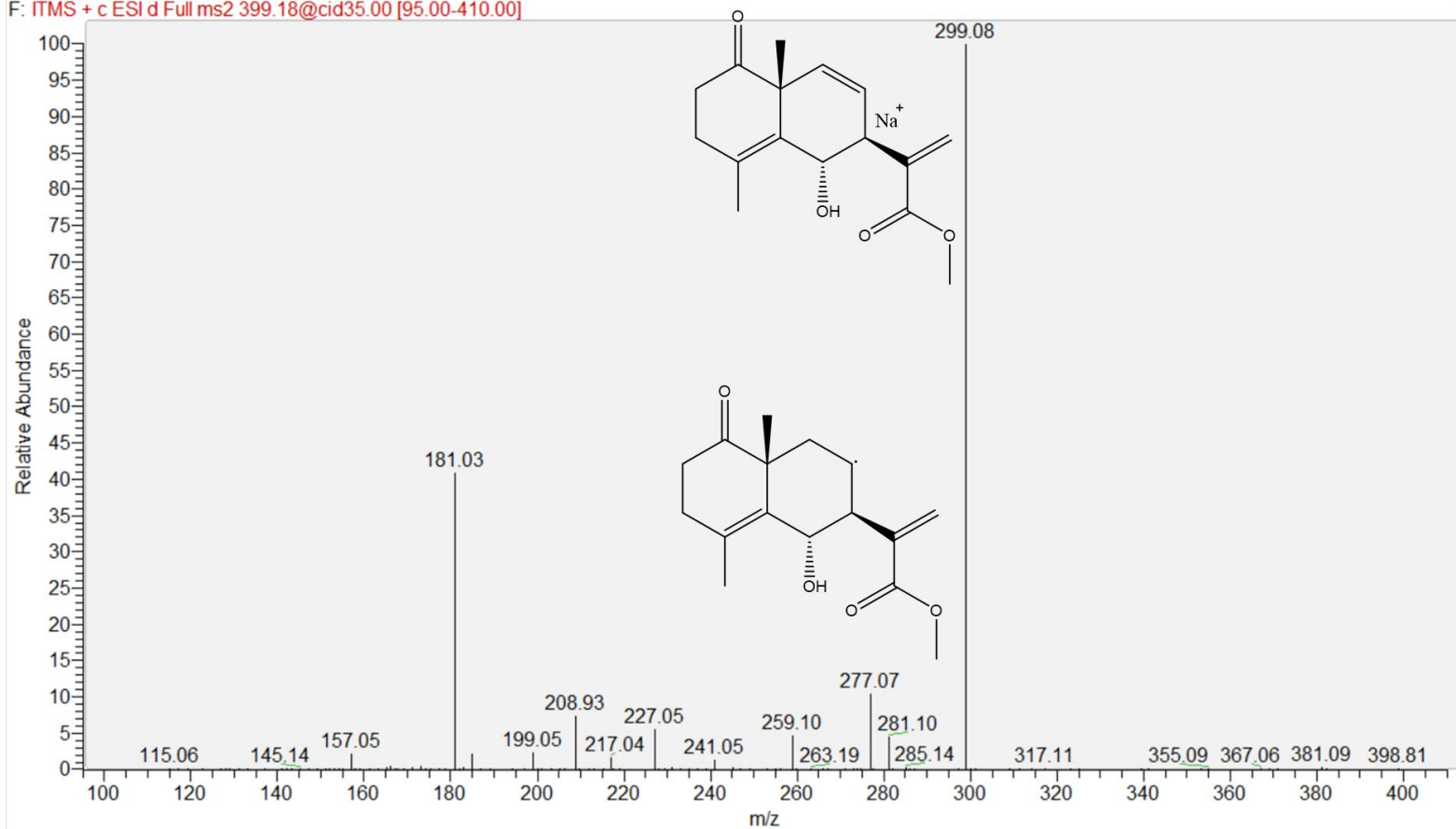


Figure S30. ESI-MS/MS spectrum of 3

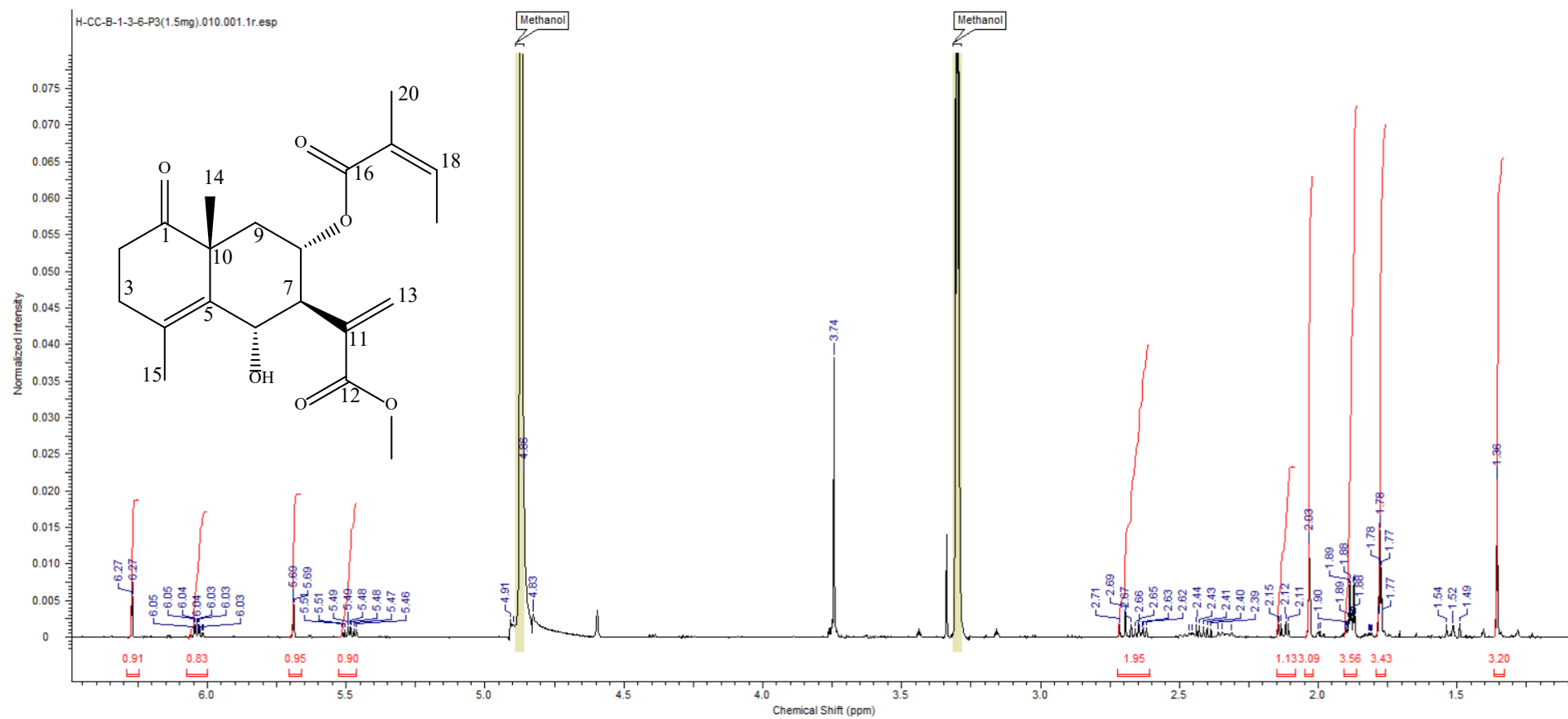


Figure S31. ^1H -NMR spectrum of 4 in MeOD (500 MHz)

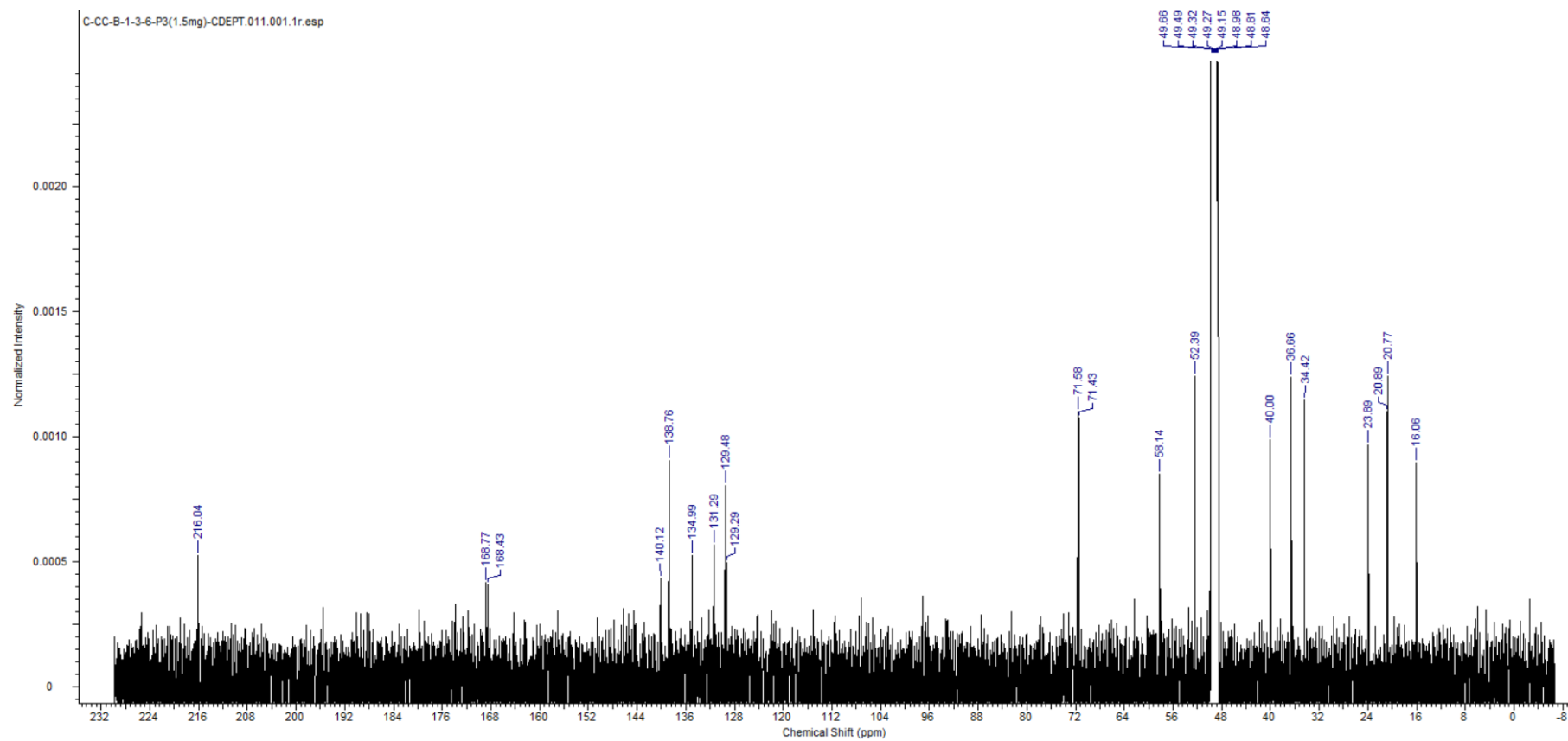


Figure S32. ^{13}C -NMR spectrum of **4** in MeOD (125 MHz)

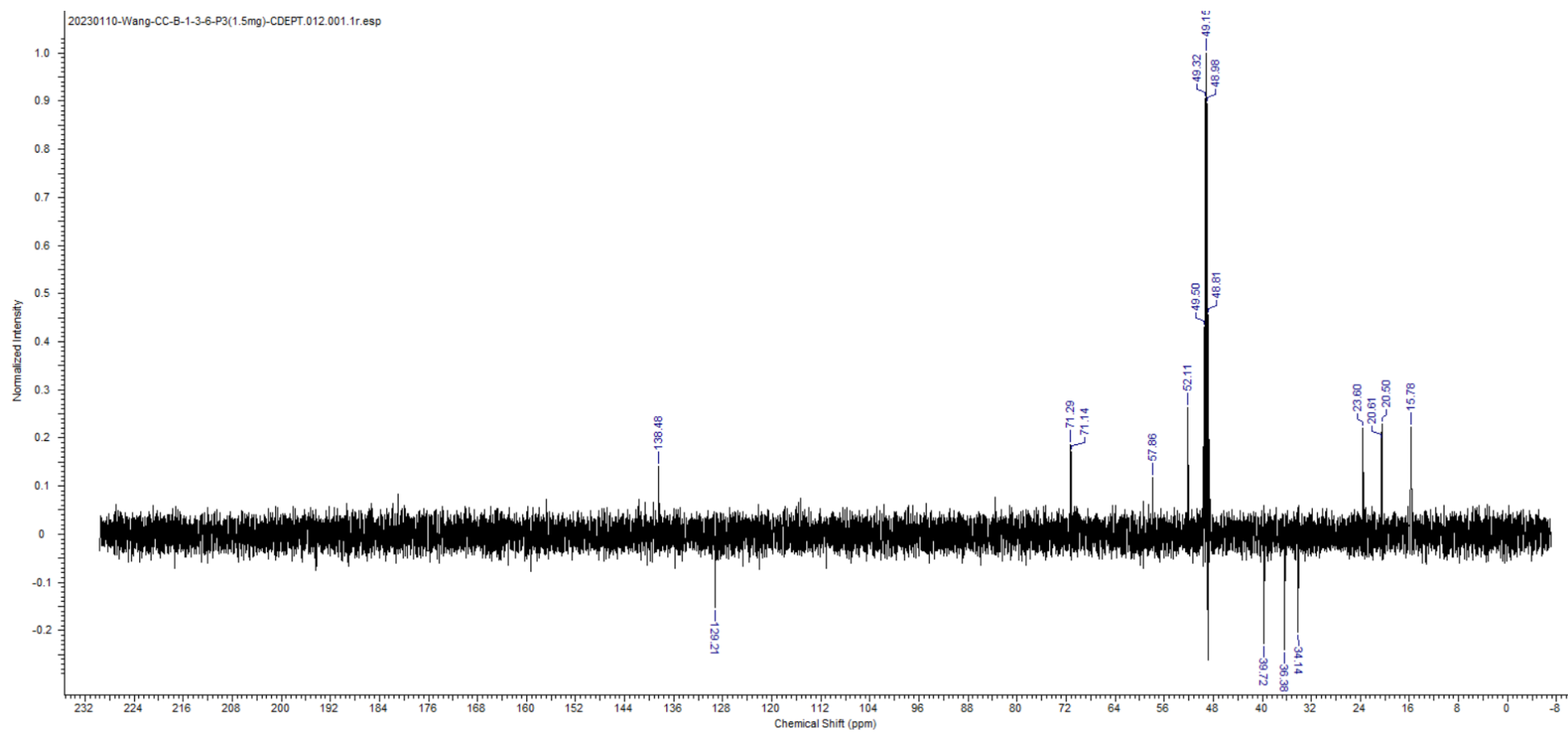


Figure S33. ^{13}C DEPT135 NMR spectrum of **4** in MeOD (125 MHz)

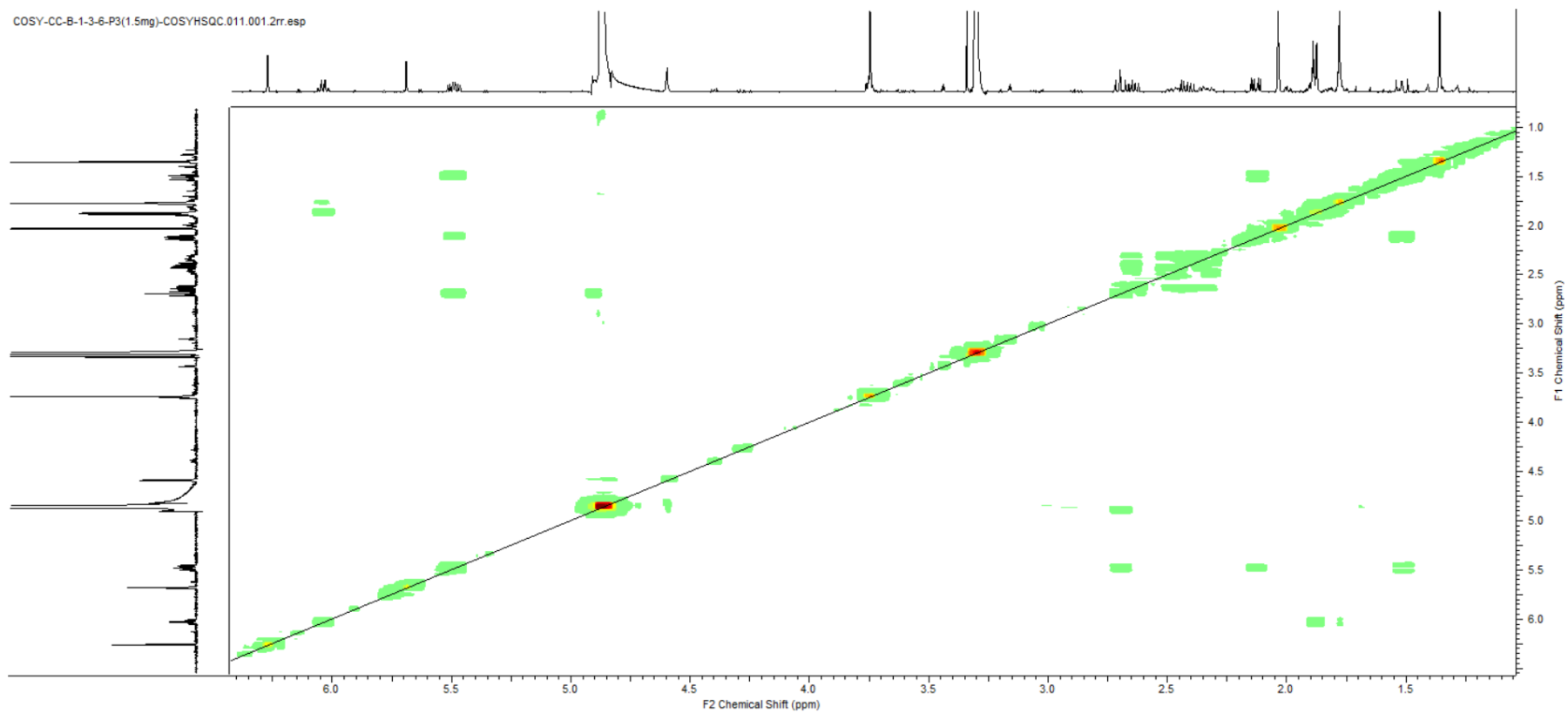


Figure S34. ¹H-¹H COSY spectrum of **4** in MeOD (500 MHz)

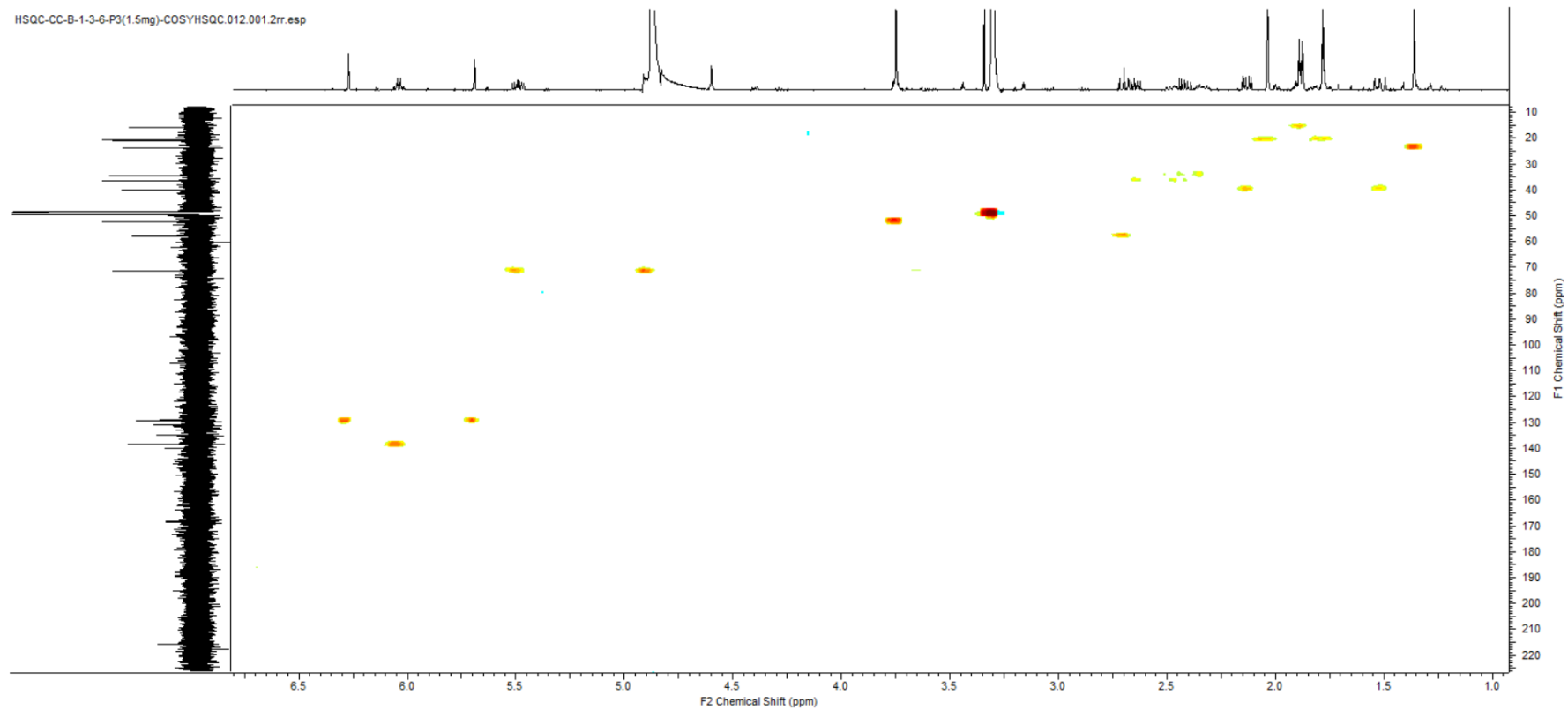


Figure S35. HSQC spectrum of **4** in MeOD (500 MHz)

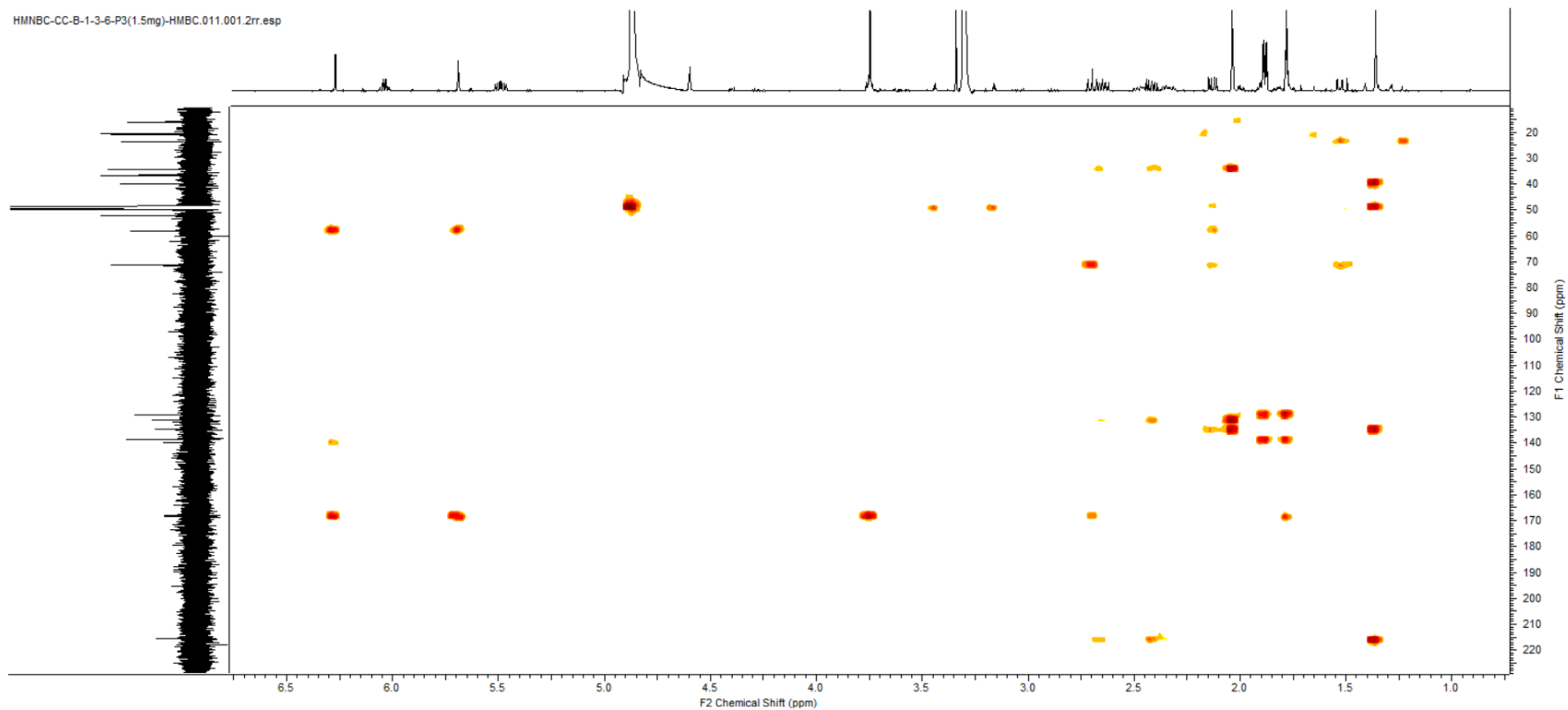


Figure S36. HMBC spectrum of **4** in MeOD (500 MHz)

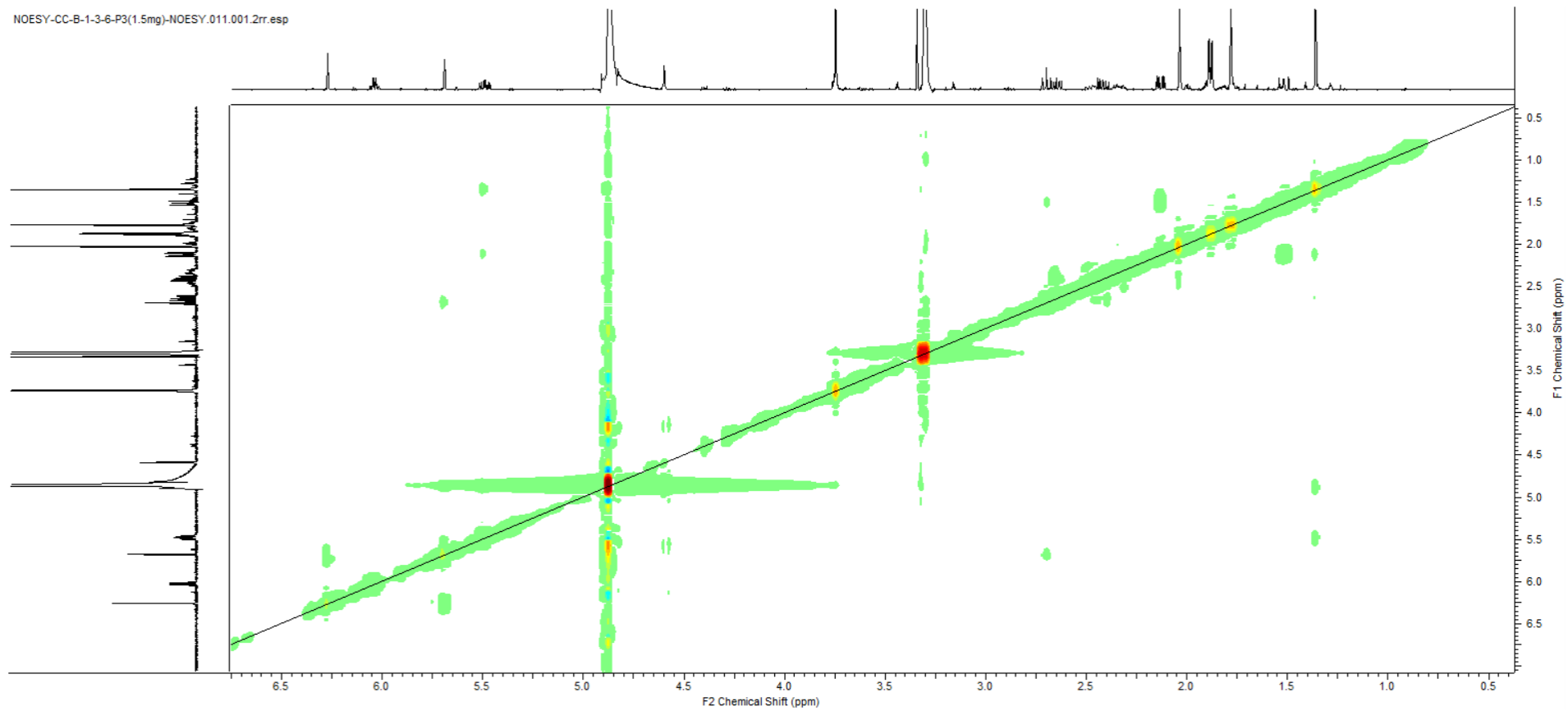


Figure S37. PS-NOESY spectrum of **4** in MeOD (500 MHz)

CC-B-1-3-6 P3 + #7 RT: 0.08 AV: 1 NL: 1.82E6
F: FTMS + p ESI Full ms [100.00-2000.00]

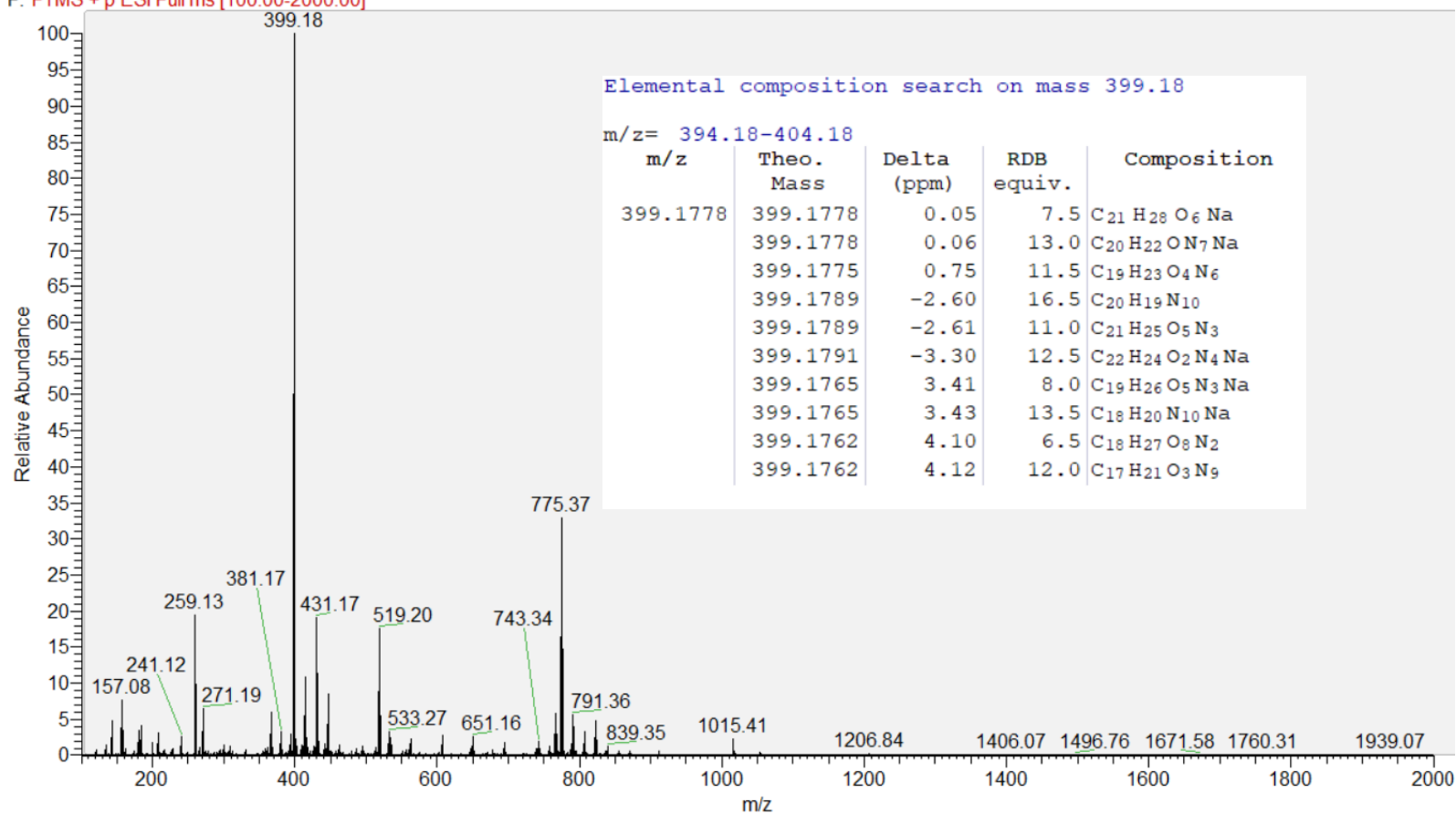


Figure S38. HR-ESI-MS spectrum of 4

CC-B-1-3-6 P3 + #8 RT: 0.09 AV: 1 NL: 2.52E4
F: ITMS + c ESI d Full ms2 399.18@cid35.00 [95.00-410.00]

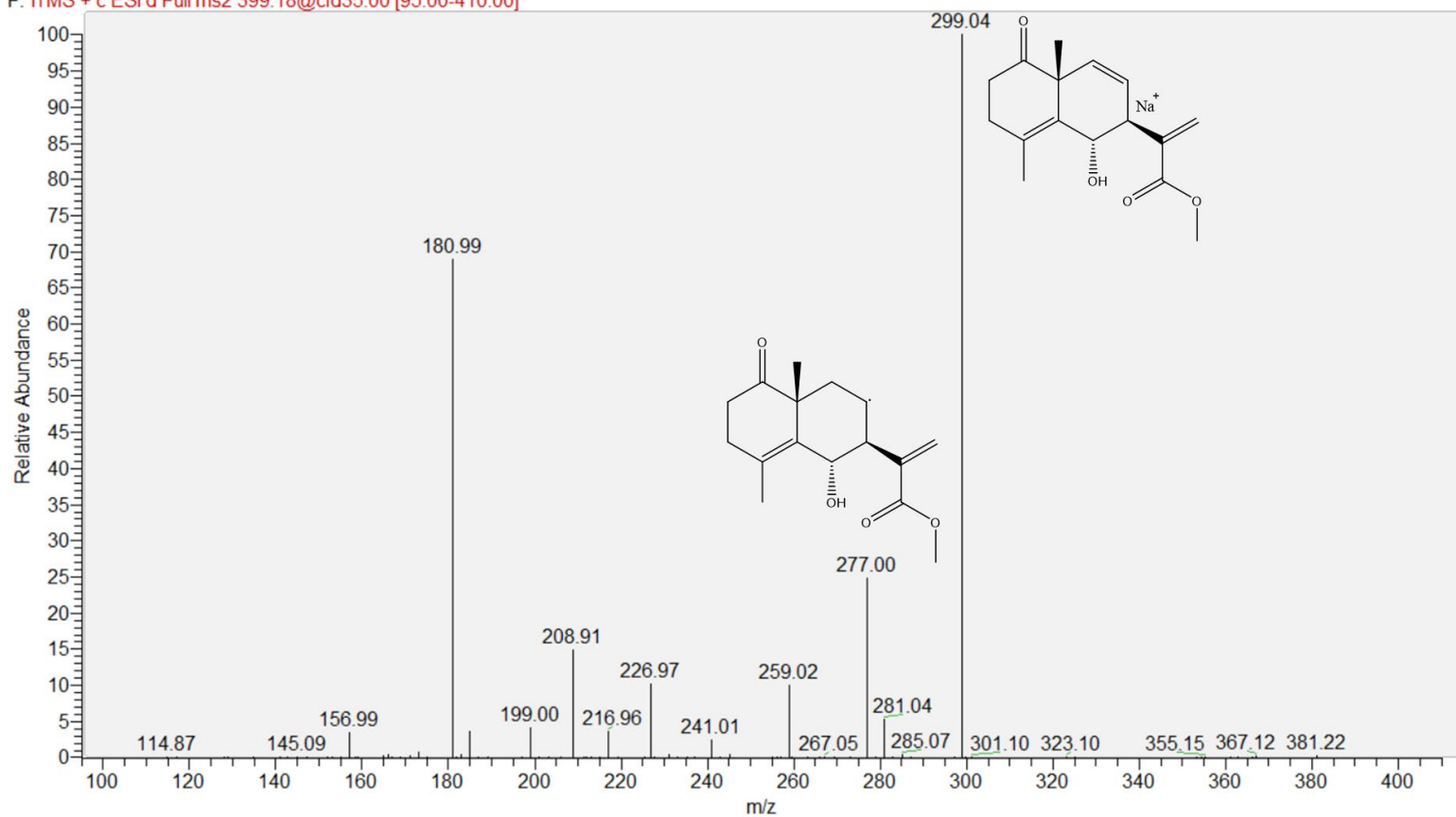


Figure S39. ESI-MS/MS spectrum of 4

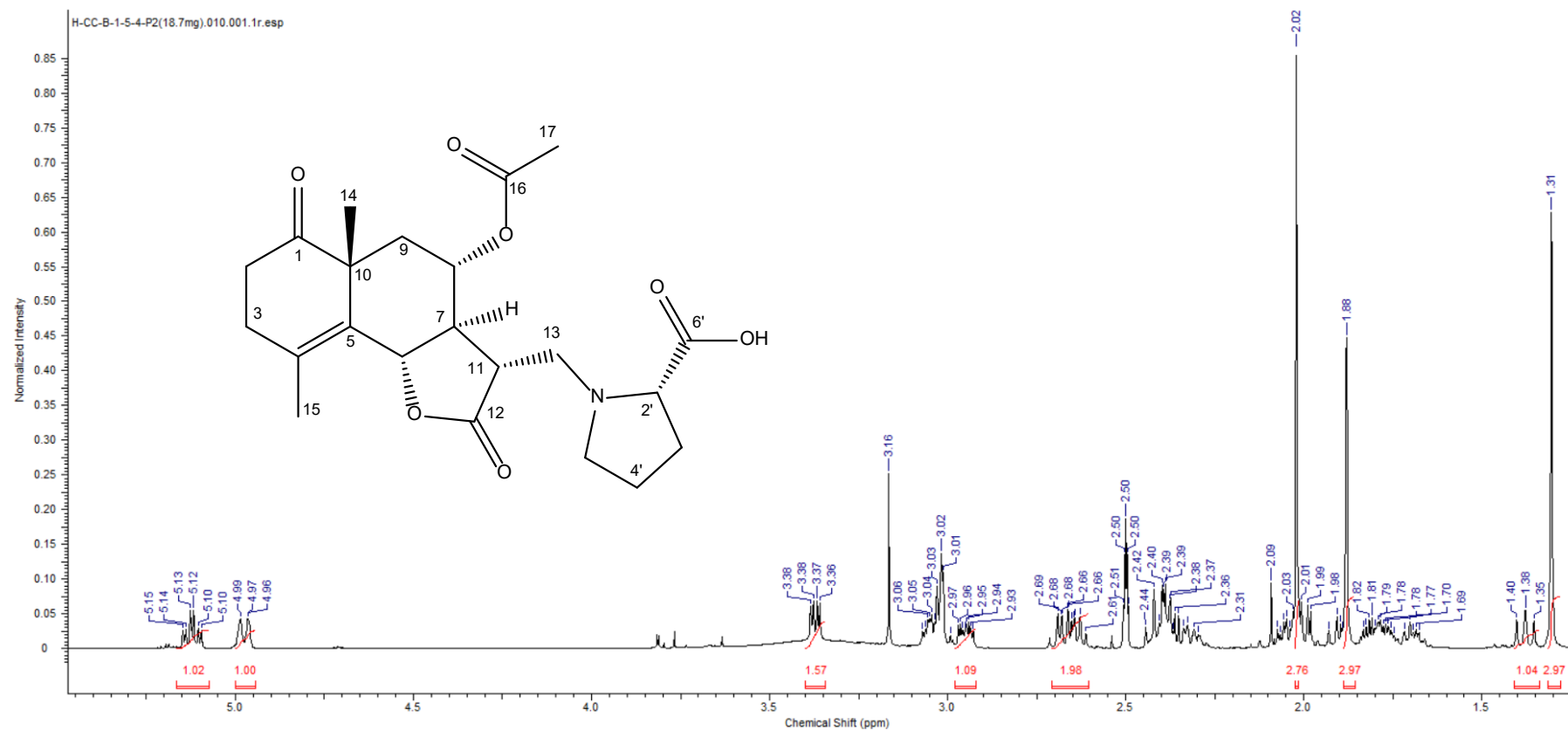


Figure S40. ^1H -NMR spectrum of **5** in $\text{DMSO}-d_6$ (500 MHz)

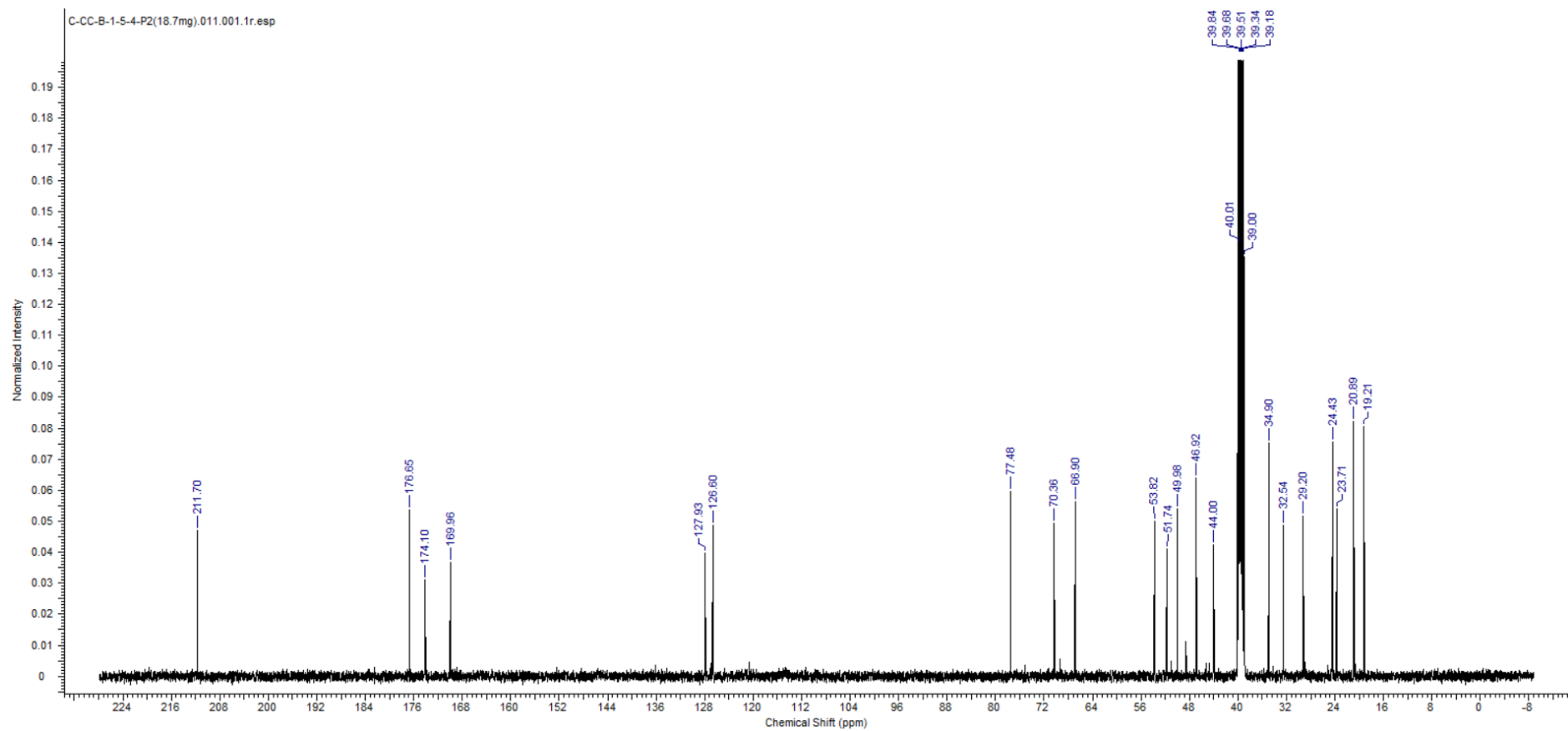


Figure S41. ^{13}C -NMR spectrum of **5** in $\text{DMSO-}d_6$ (125 MHz)

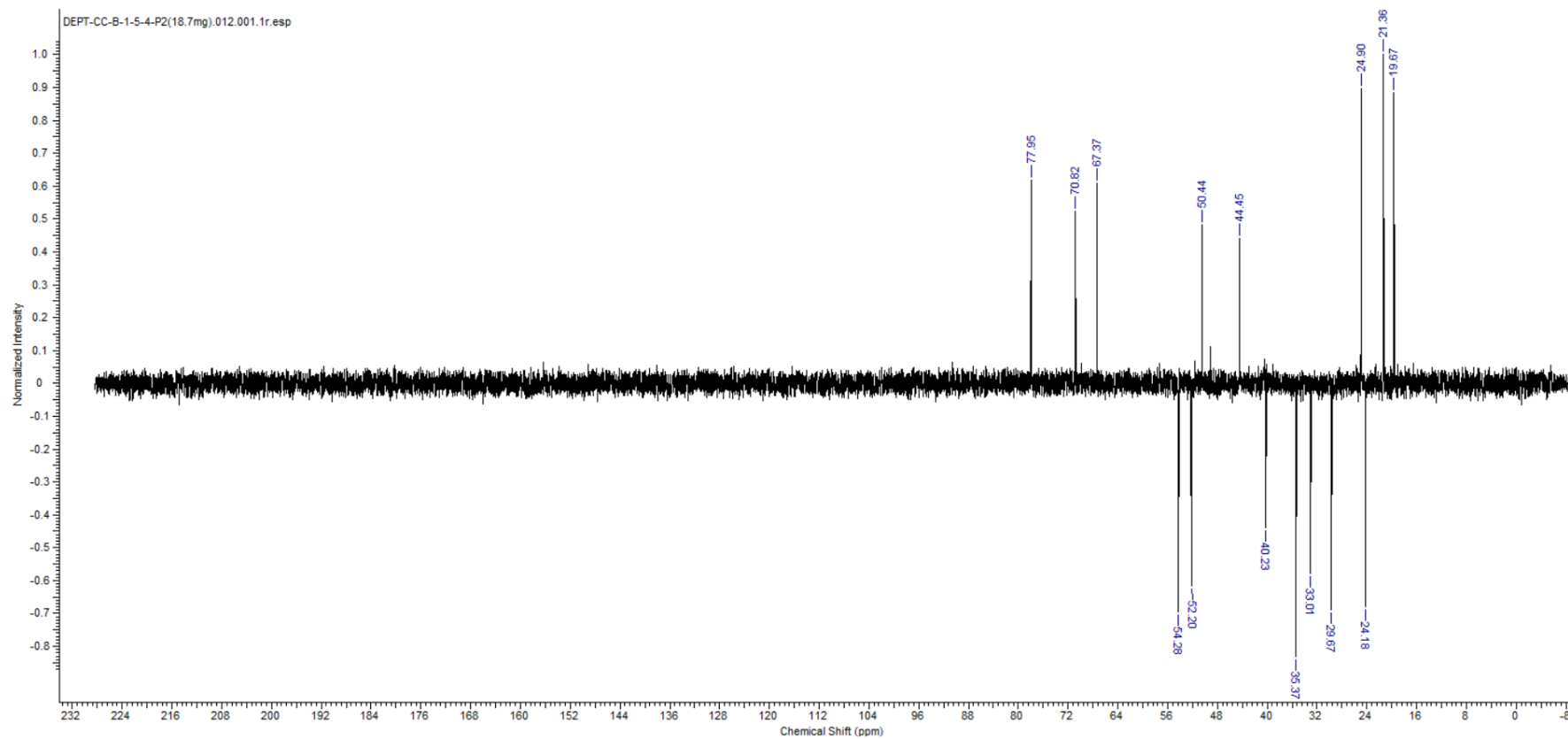


Figure S42. ^{13}C DEPT135 NMR spectrum of **5** in $\text{DMSO}-d_6$ (125 MHz)

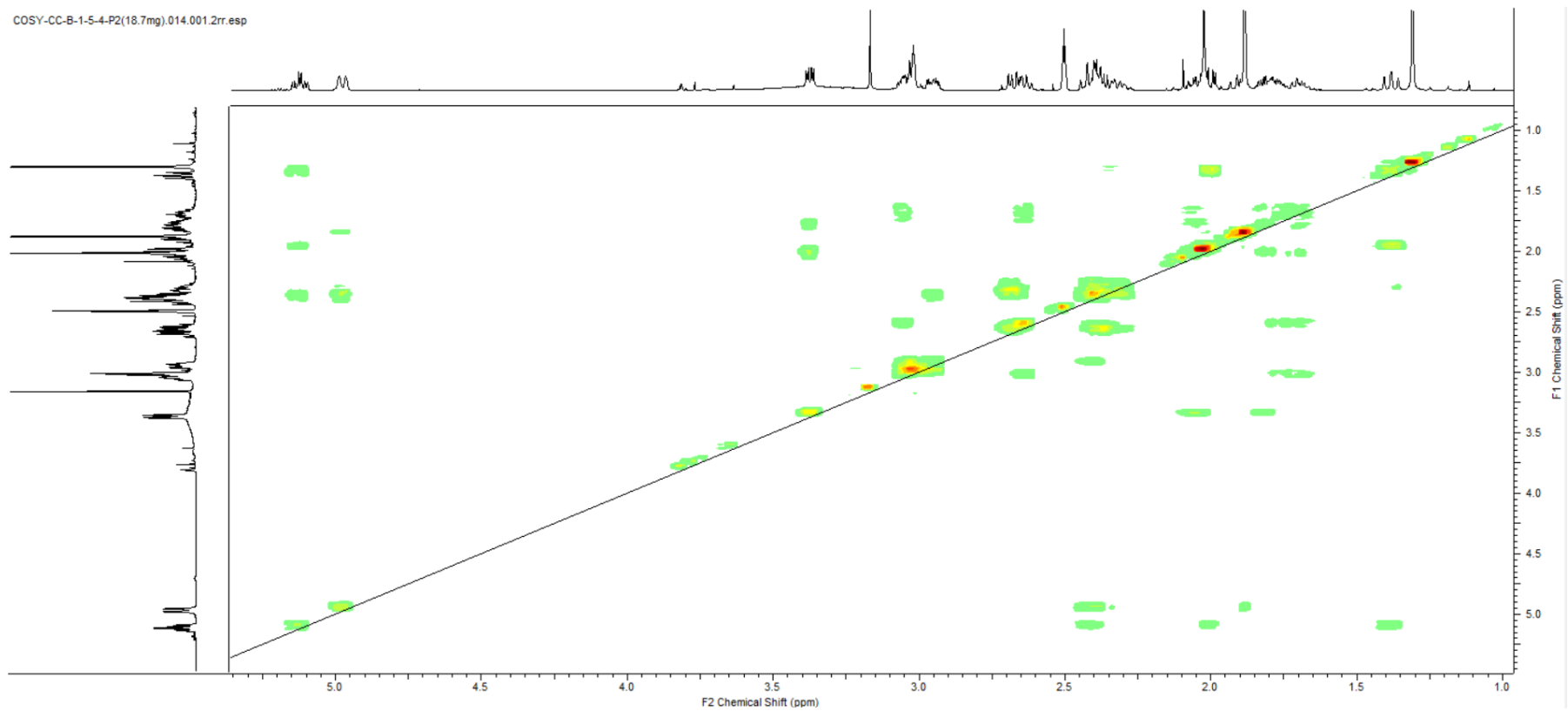


Figure S43. ^1H - ^1H COSY spectrum of **5** in $\text{DMSO}-d_6$ (500 MHz)

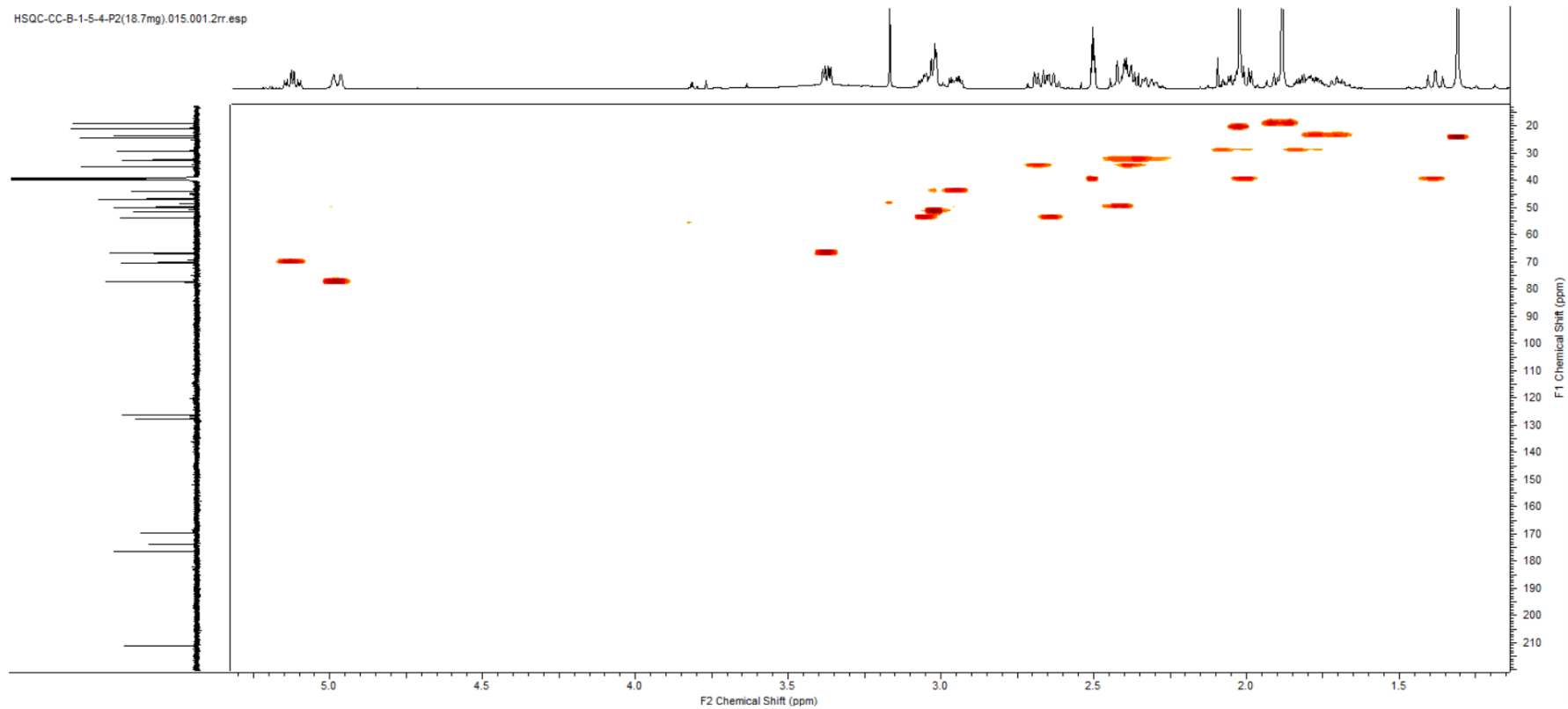


Figure S44. HSQC spectrum of **5** in DMSO- d_6 (500 MHz)

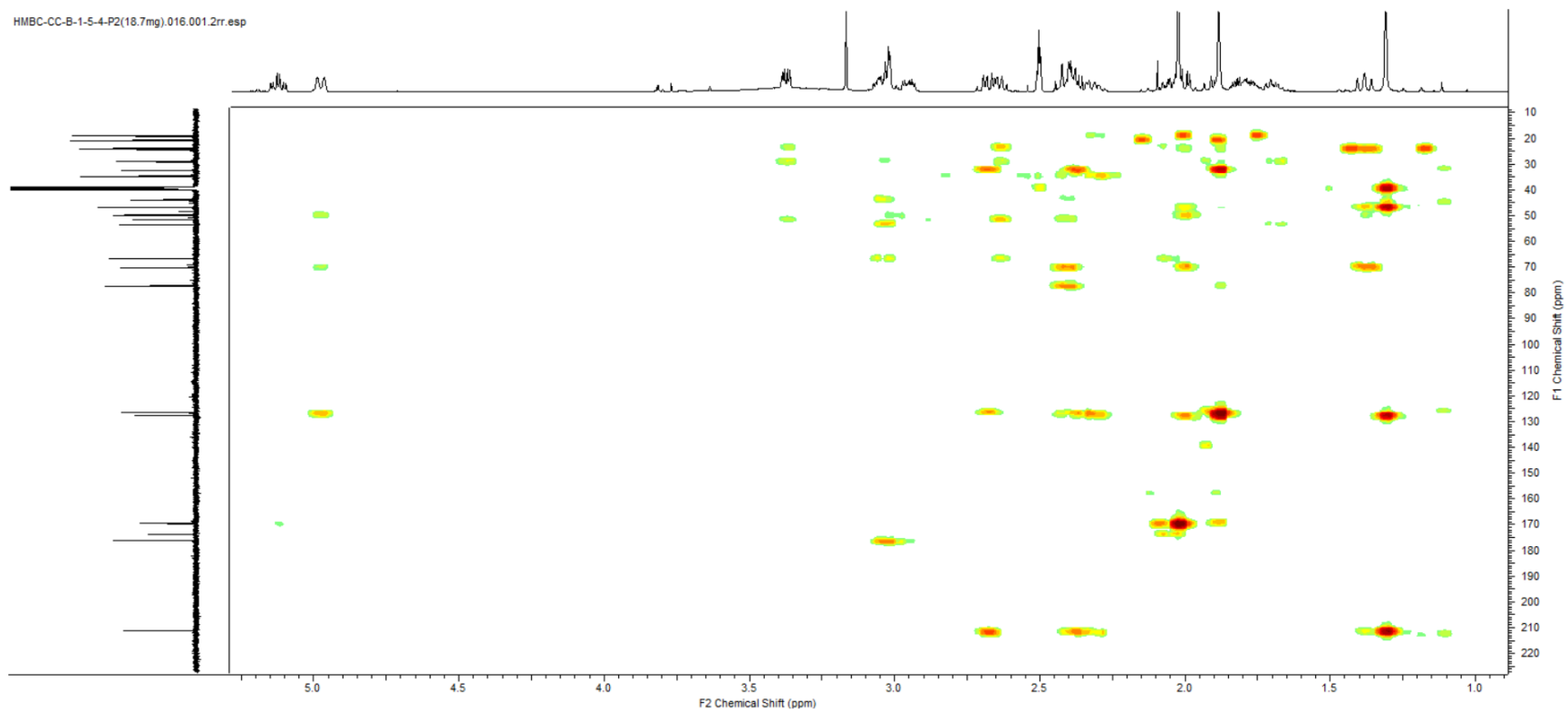


Figure S45. HMBC spectrum of **5** in DMSO- d_6 (500 MHz)

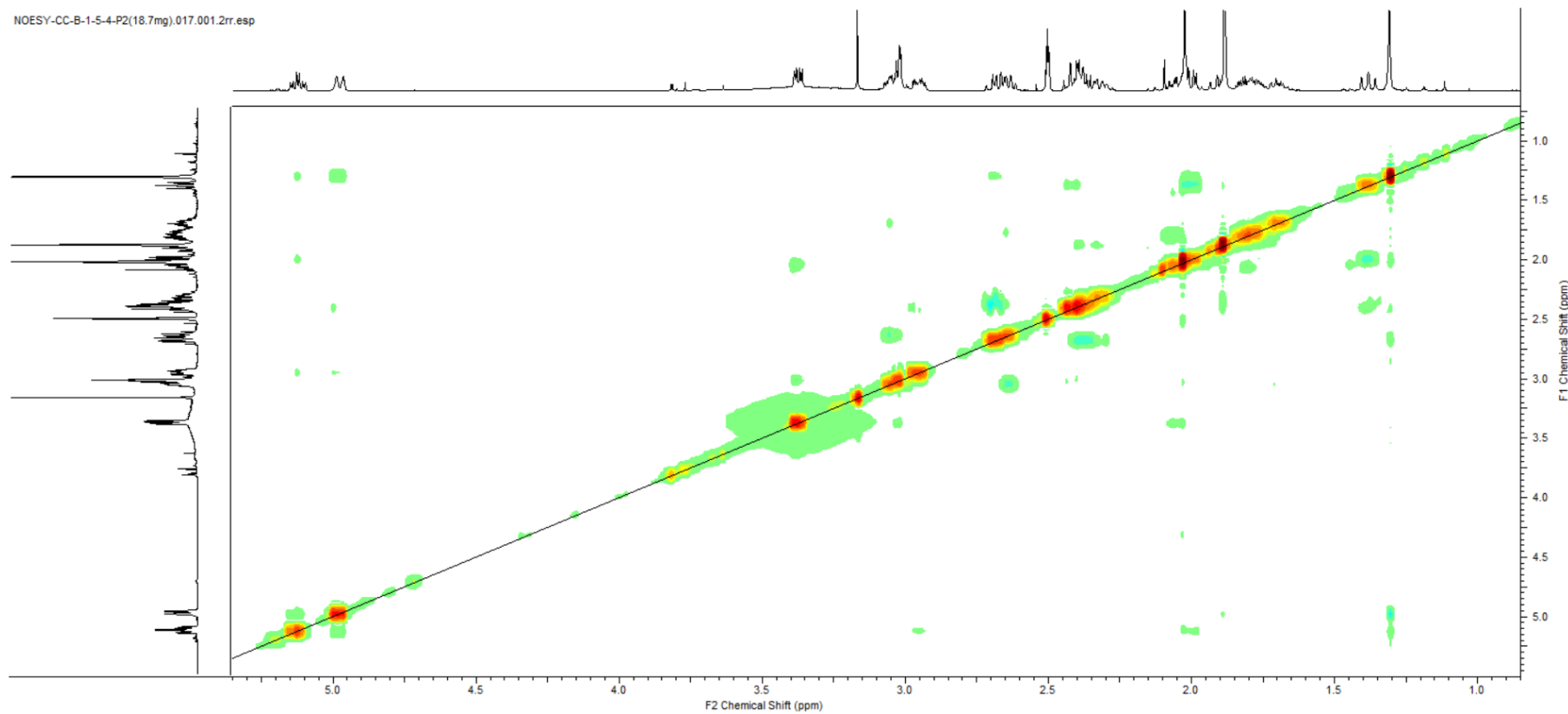


Figure S46. PS-NOESY spectrum of **5** in DMSO- d_6 (500 MHz)

CC-B-1-5-4-P2 + #7 RT: 0.08 AV: 1 NL: 1.84E6
 F: FTMS + p ESI Full ms [100.00-2000.00]

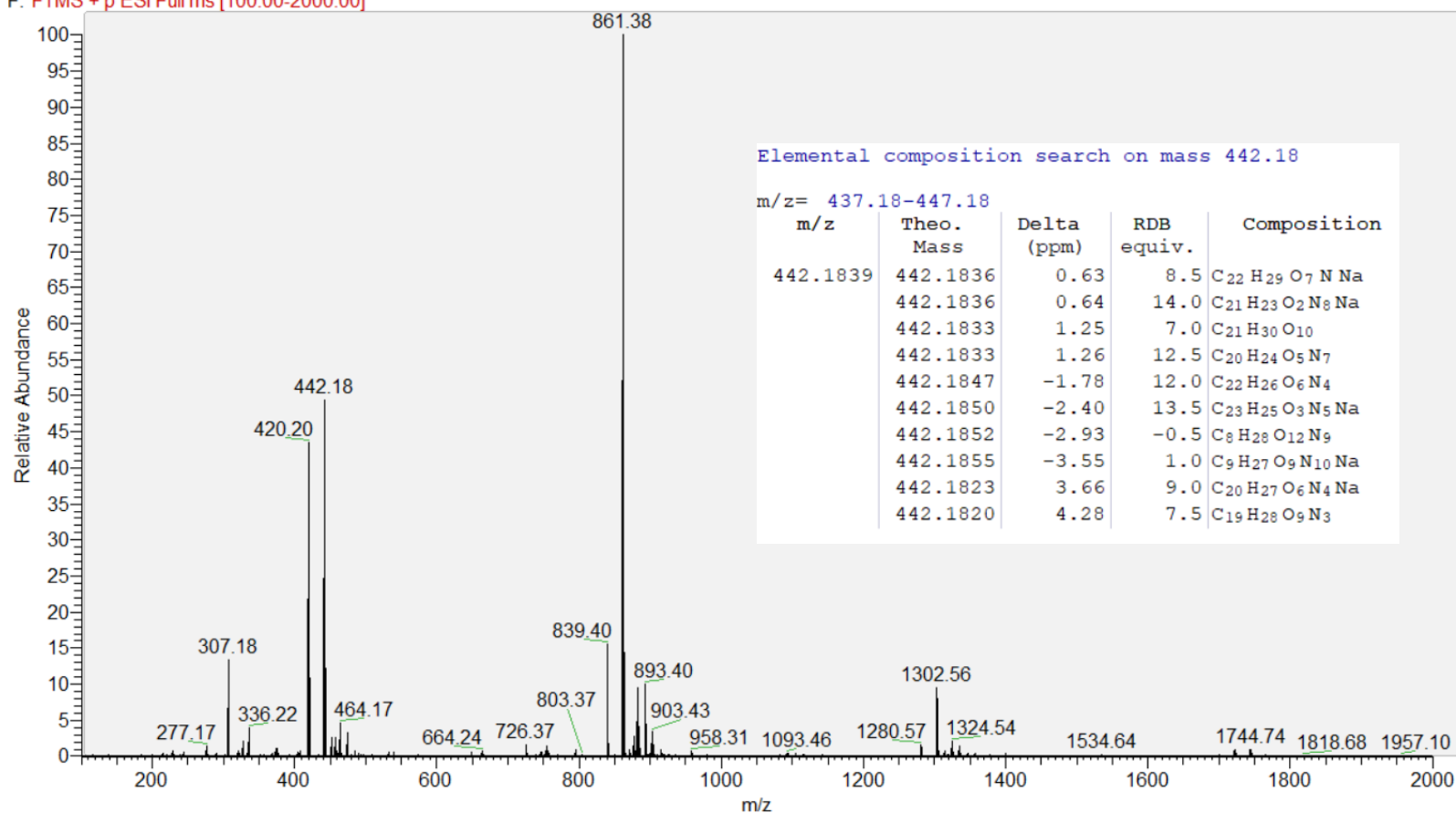


Figure S47. HR-ESI-MS spectrum of **5**

CC-B-1-5-4-P2 + #5 RT: 0.06 AV: 1 NL: 3.10E3
F: ITMS + c ESI d Full ms2 442.18@cid35.00 [110.00-455.00]

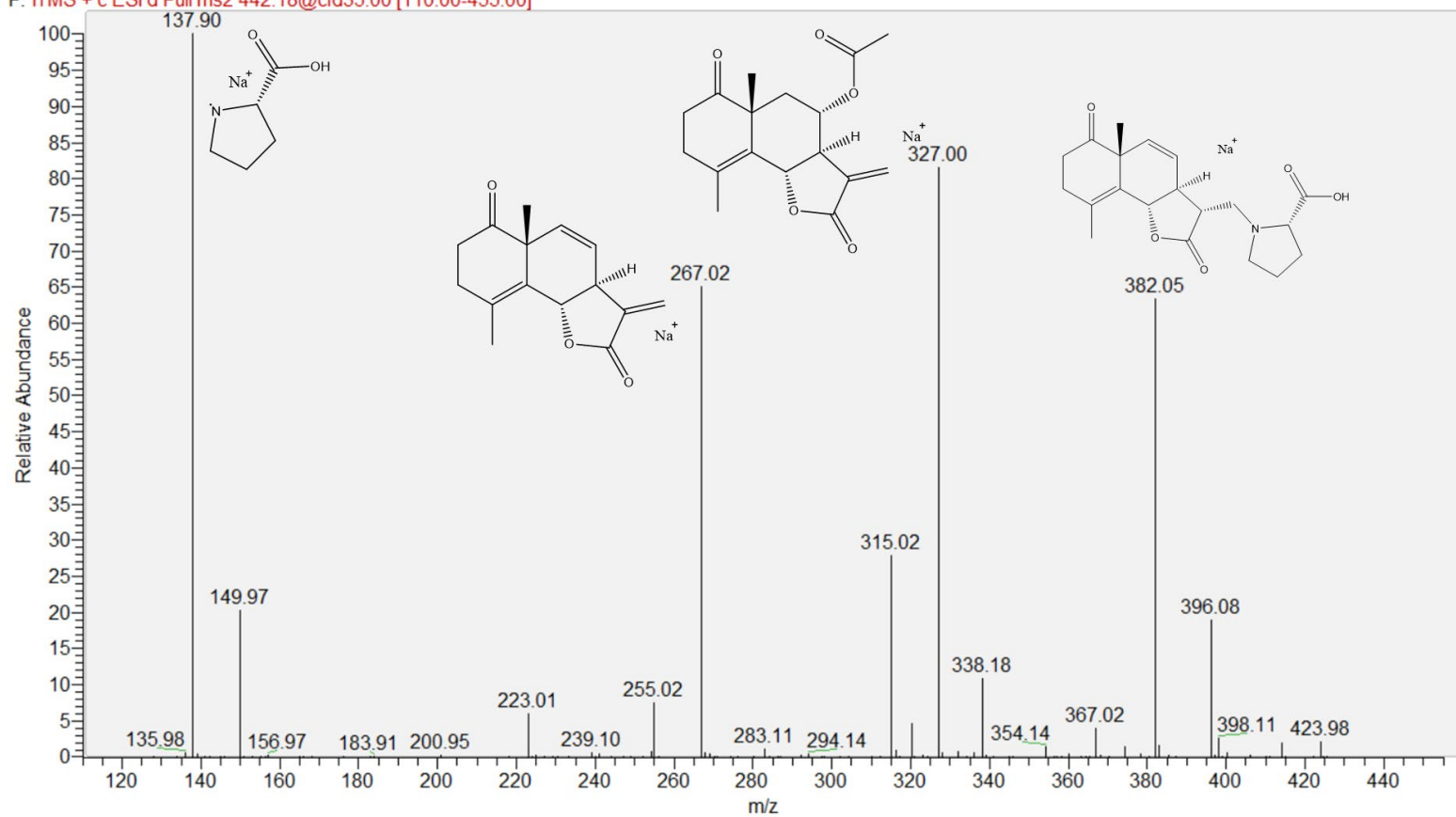


Figure S48. ESI-MS/MS spectrum of 5

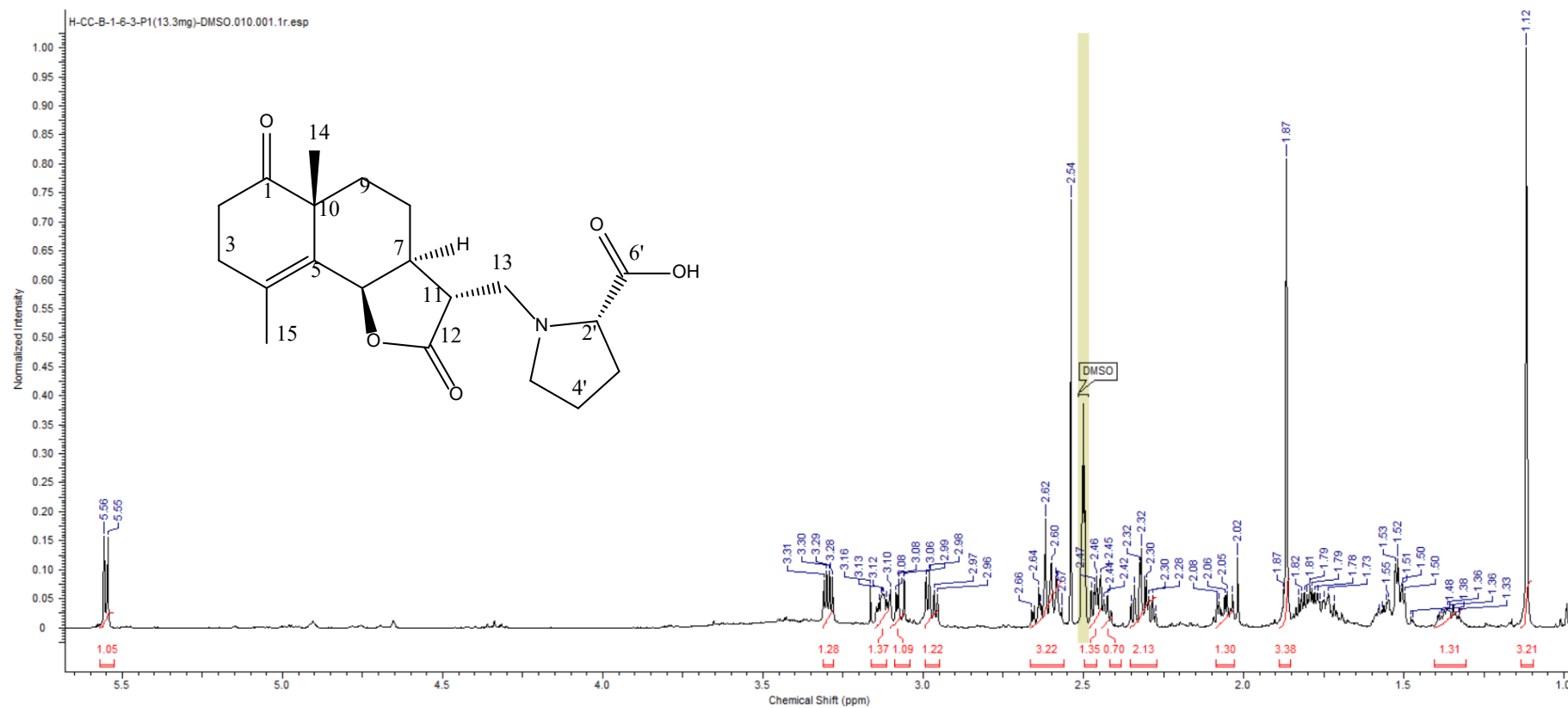


Figure S49. ^1H -NMR spectrum of **6** in $\text{DMSO}-d_6$ (500 MHz)

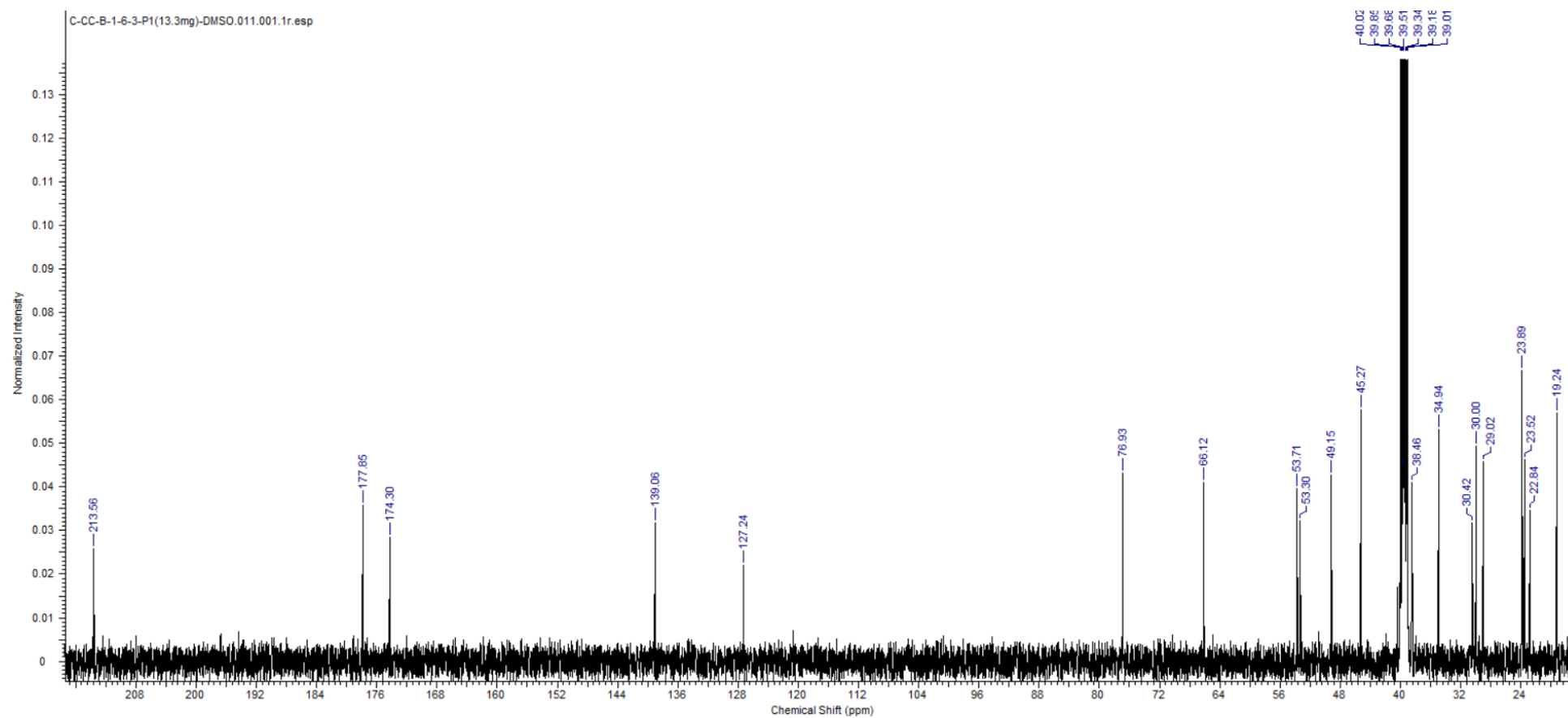


Figure S50. ^{13}C -NMR spectrum of **6** in $\text{DMSO}-d_6$ (125 MHz)

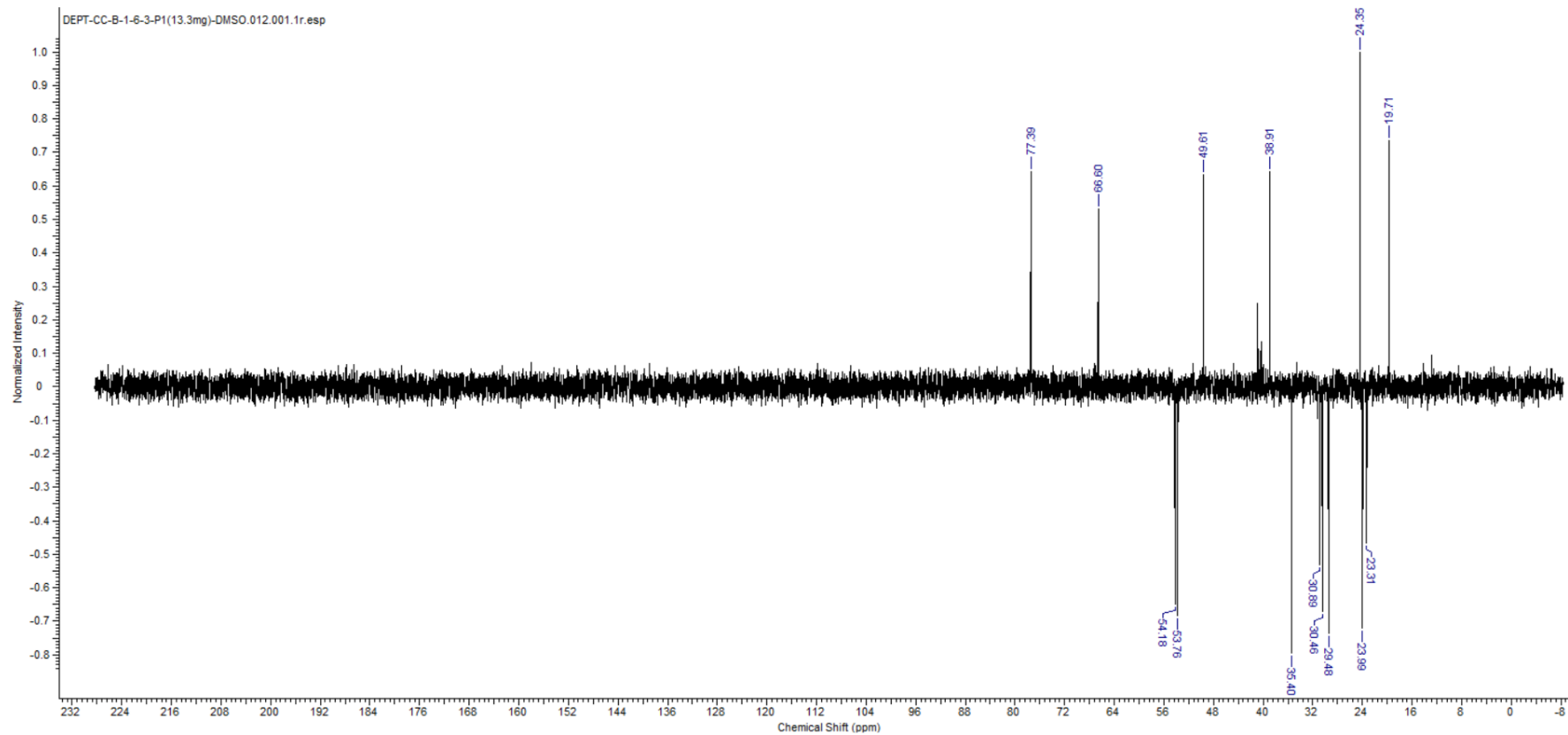


Figure S51. ^{13}C DEPT135 NMR spectrum of **6** in $\text{DMSO-}d_6$ (125 MHz)

COSY-CC-B-1-6-3-P1(13.3mg)-DMSO.014.001.2rr.esp

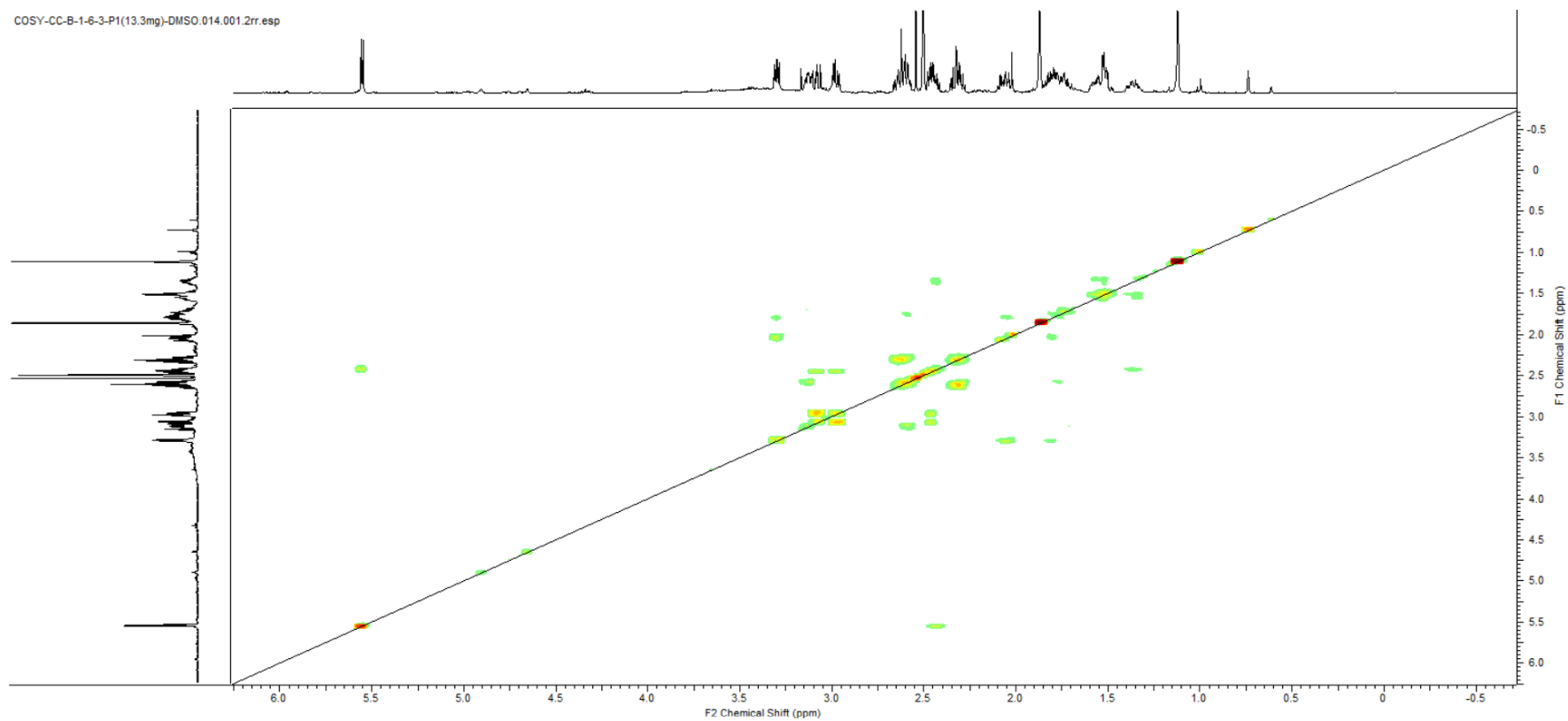


Figure S52. ¹H-¹H COSY spectrum of **6** in DMSO-*d*₆ (500 MHz)

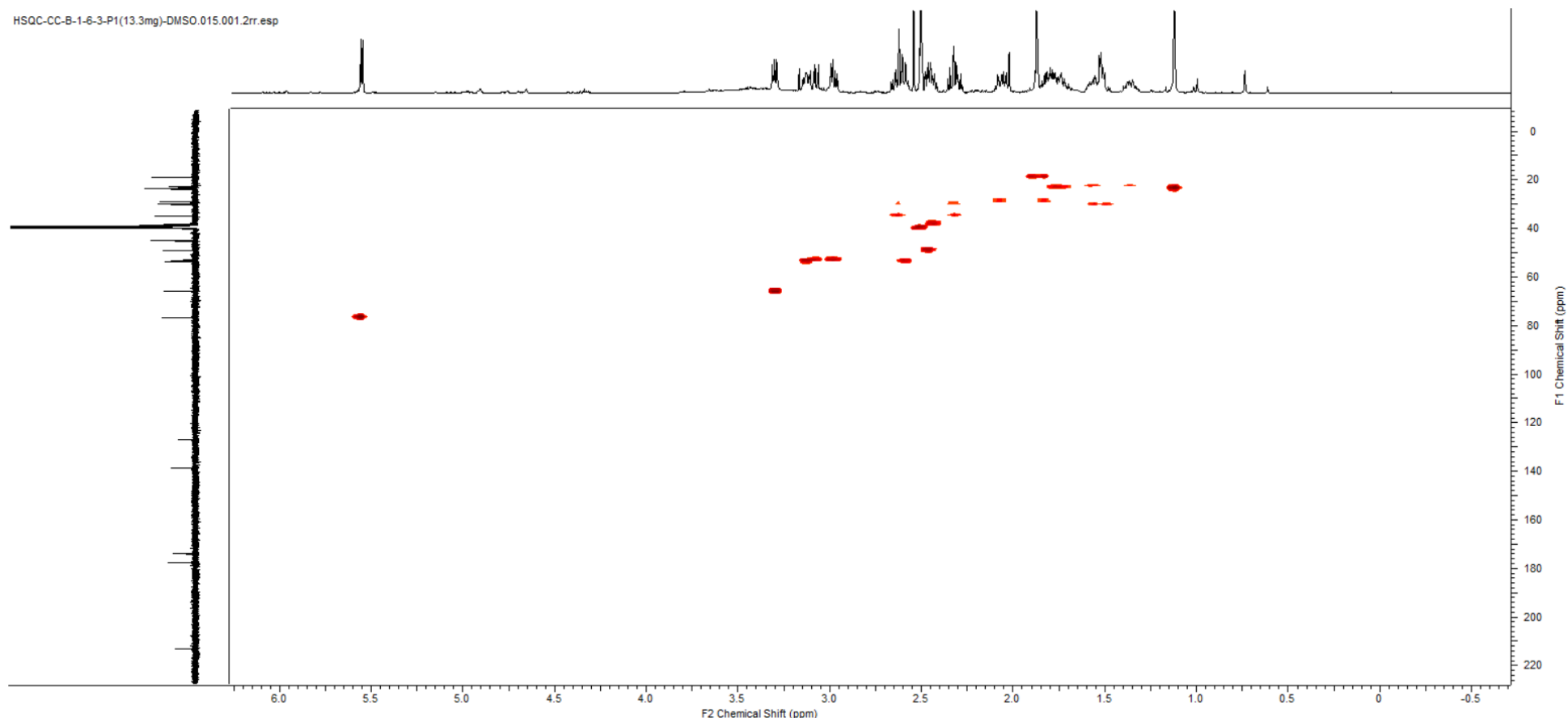


Figure S53. HSQC spectrum of **6** in DMSO-*d*₆ (500 MHz)

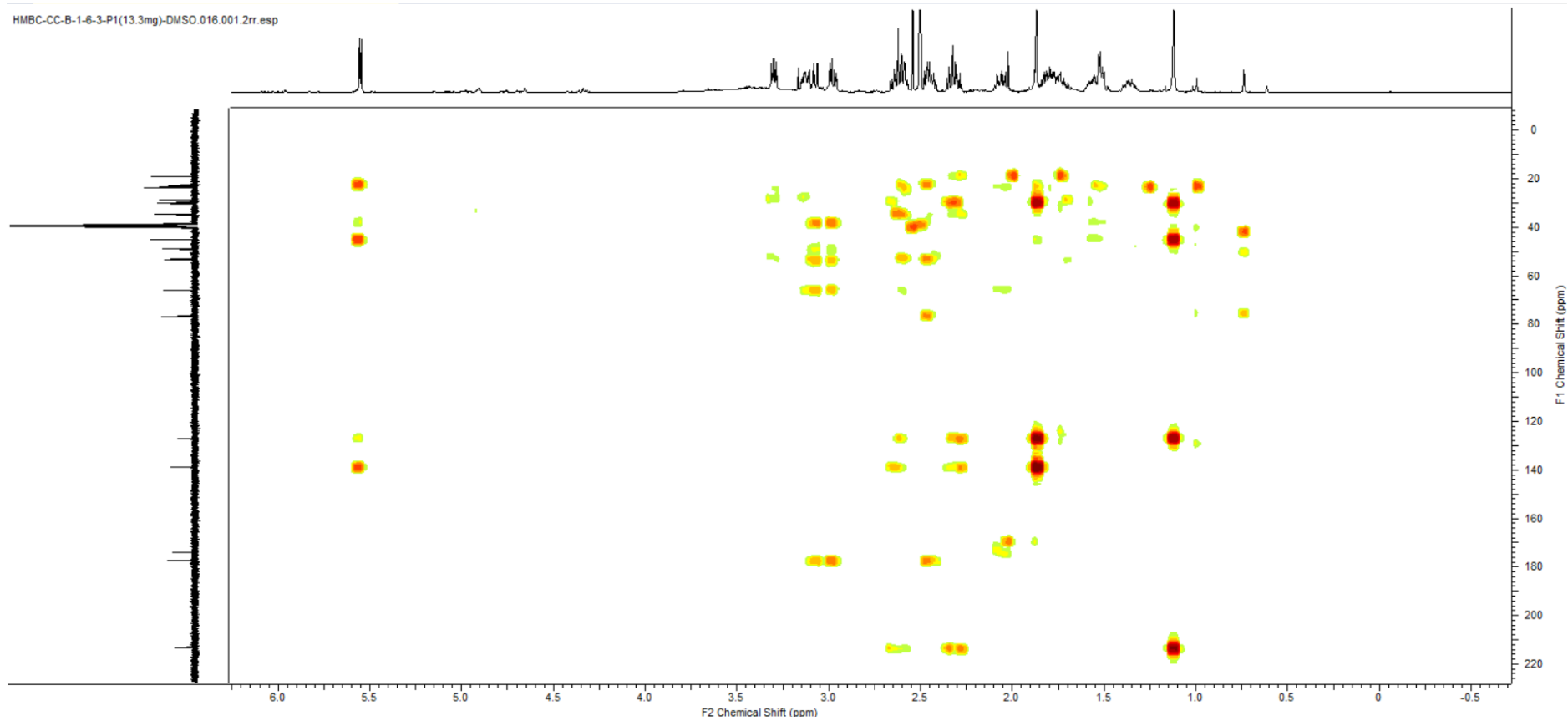


Figure S54. HMBC spectrum of **6** in DMSO-*d*₆ (500 MHz)

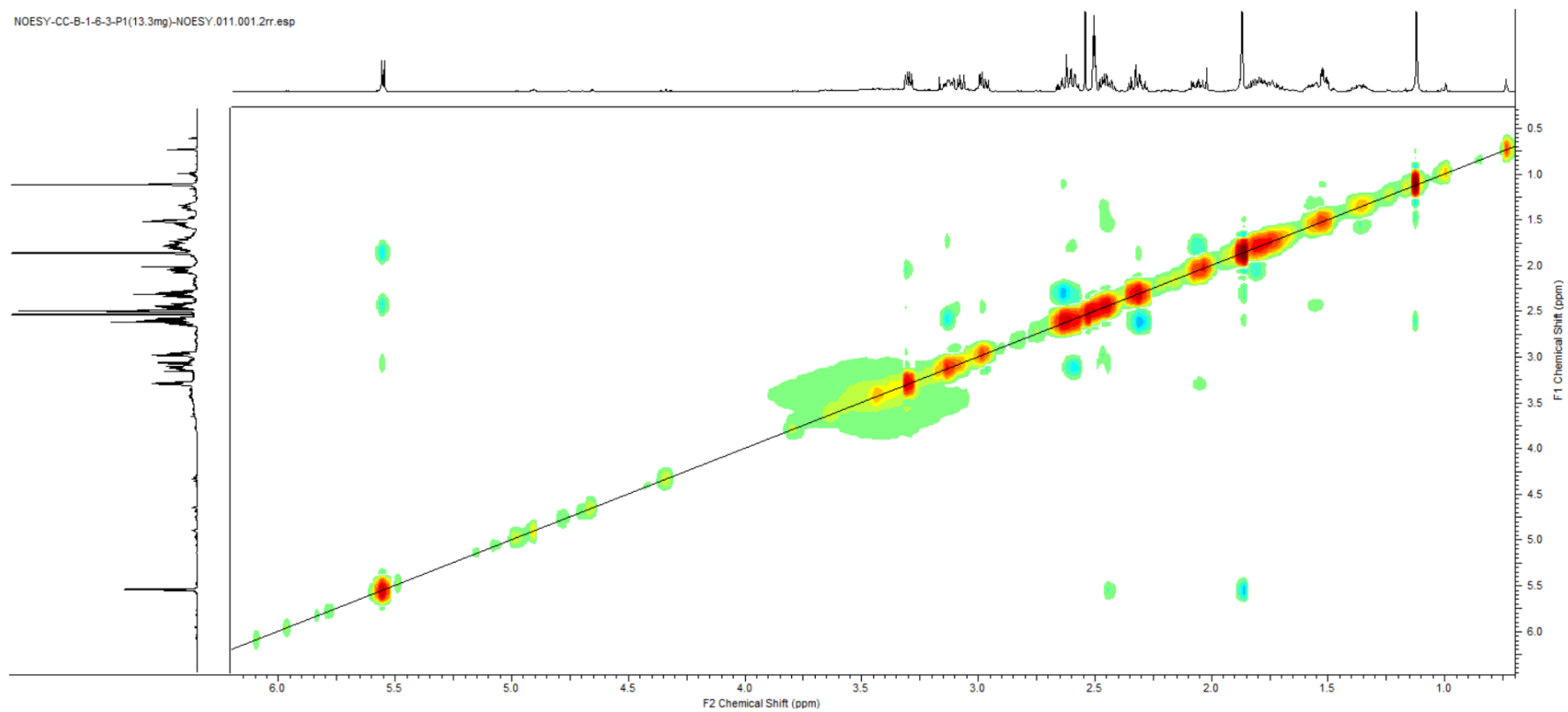


Figure S55. PS-NOESY spectrum of **6** in $\text{DMSO}-d_6$ (500 MHz)

CC-B-1-6-3-P1 + #10 RT: 0.13 AV: 1 NL: 1.19E6
F: FTMS + p ESI Full ms [100.00-2000.00]

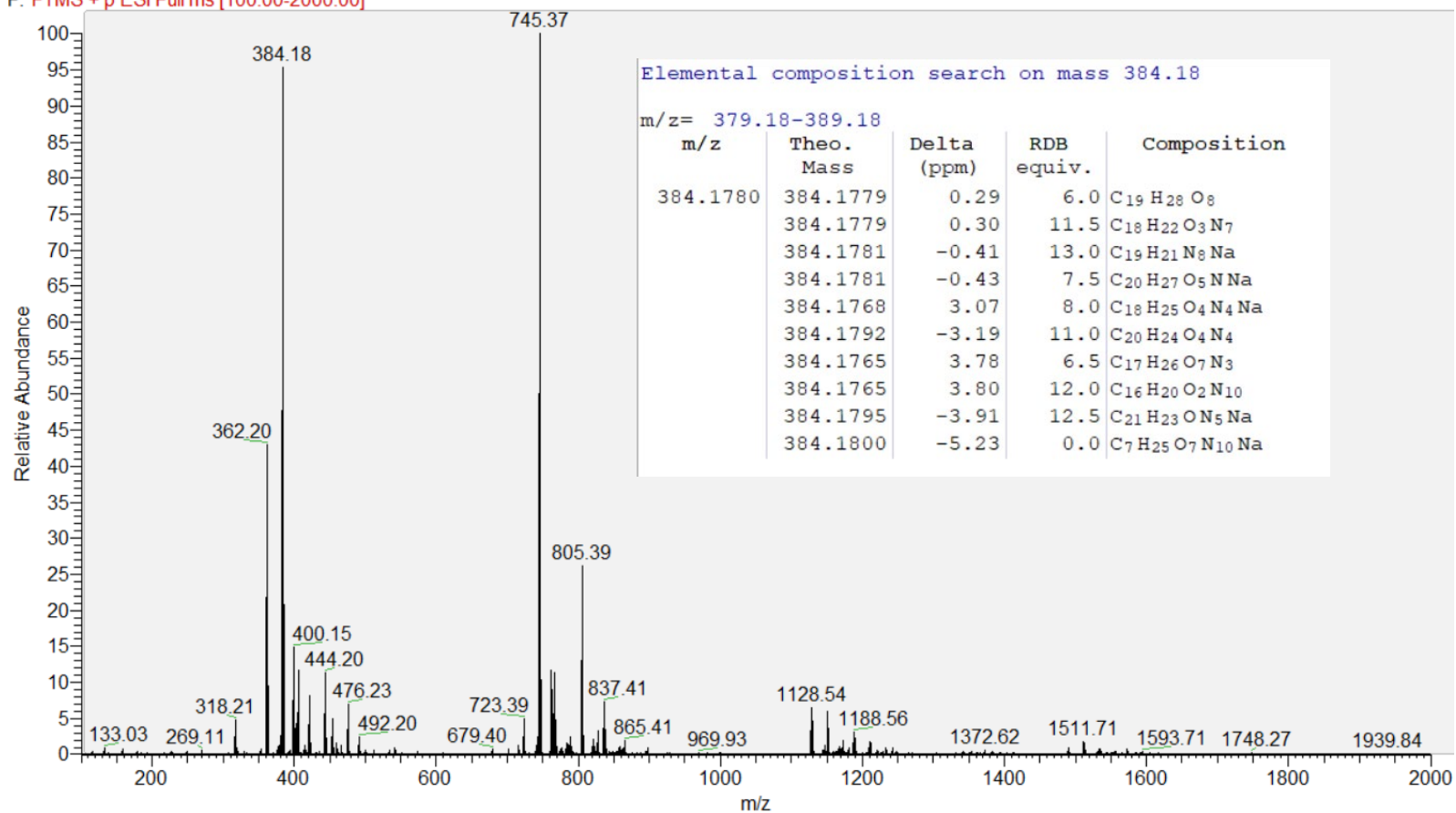


Figure S56. HR-ESI-MS spectrum of **6**

CC-B-1-6-3-P1 + #11 RT: 0.14 AV: 1 NL: 6.52E3
F: ITMS + c ESI d Full ms2 384.18@cid35.00 [95.00-395.00]

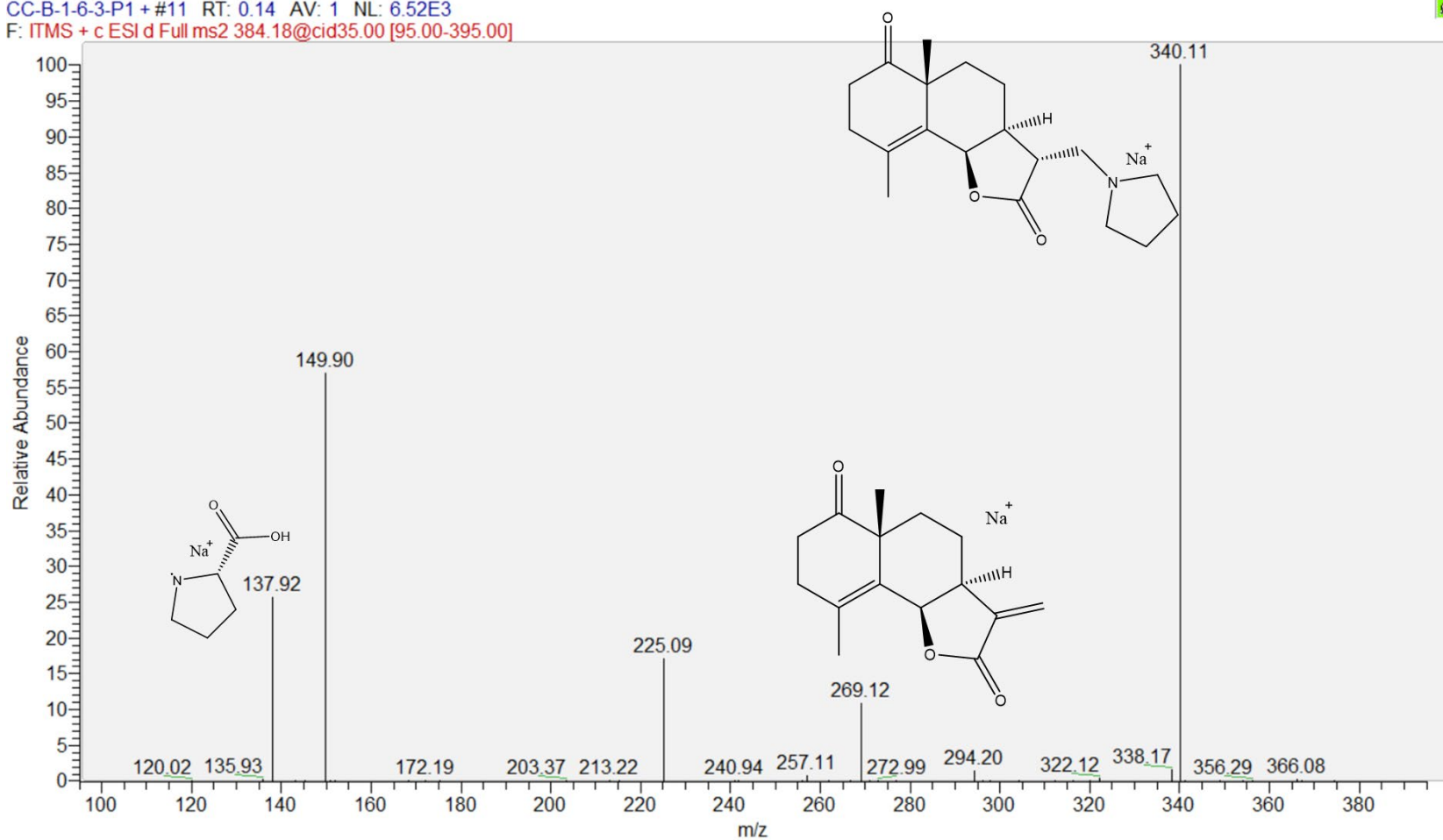


Figure S57. ESI-MS/MS spectrum of 6

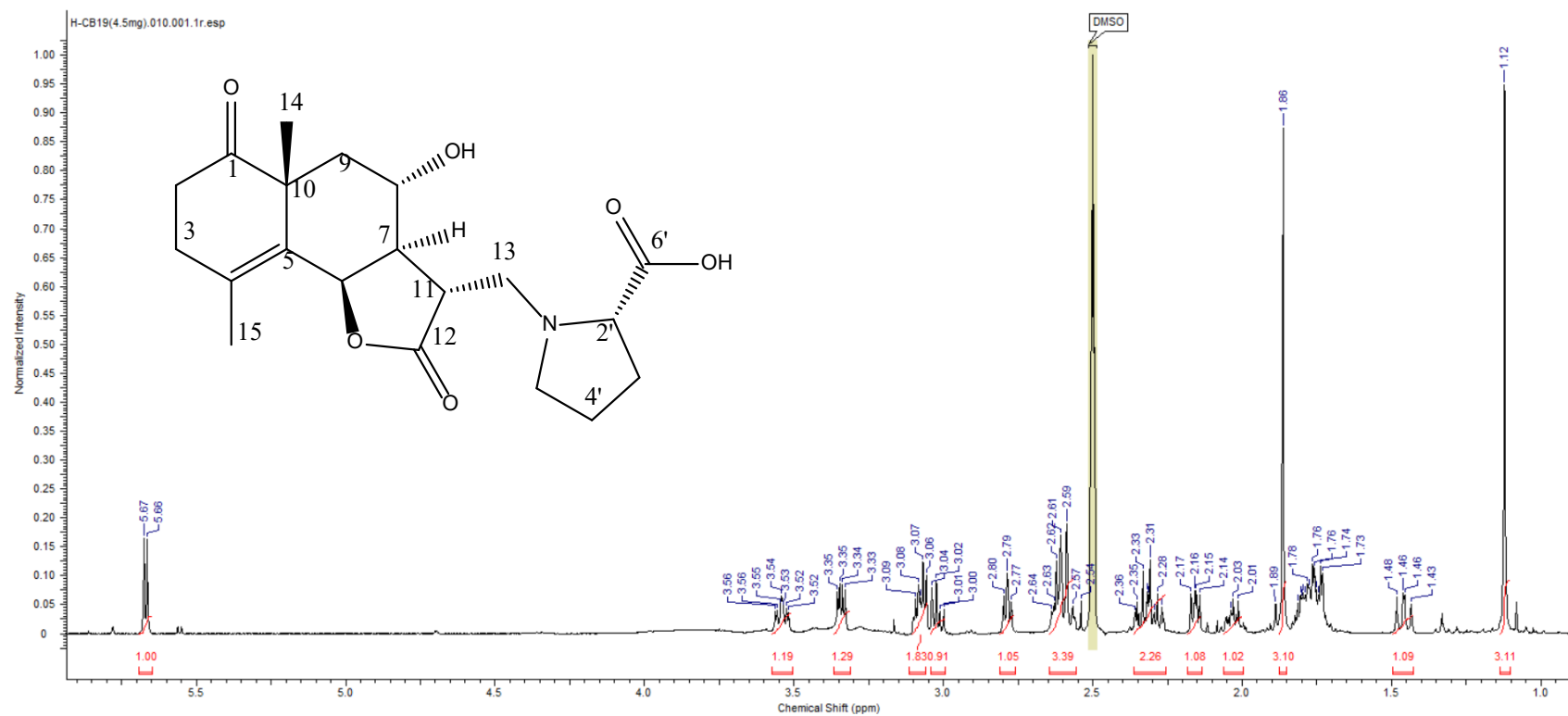


Figure S58. ^1H -NMR spectrum of **7** in $\text{DMSO}-d_6$ (500 MHz)

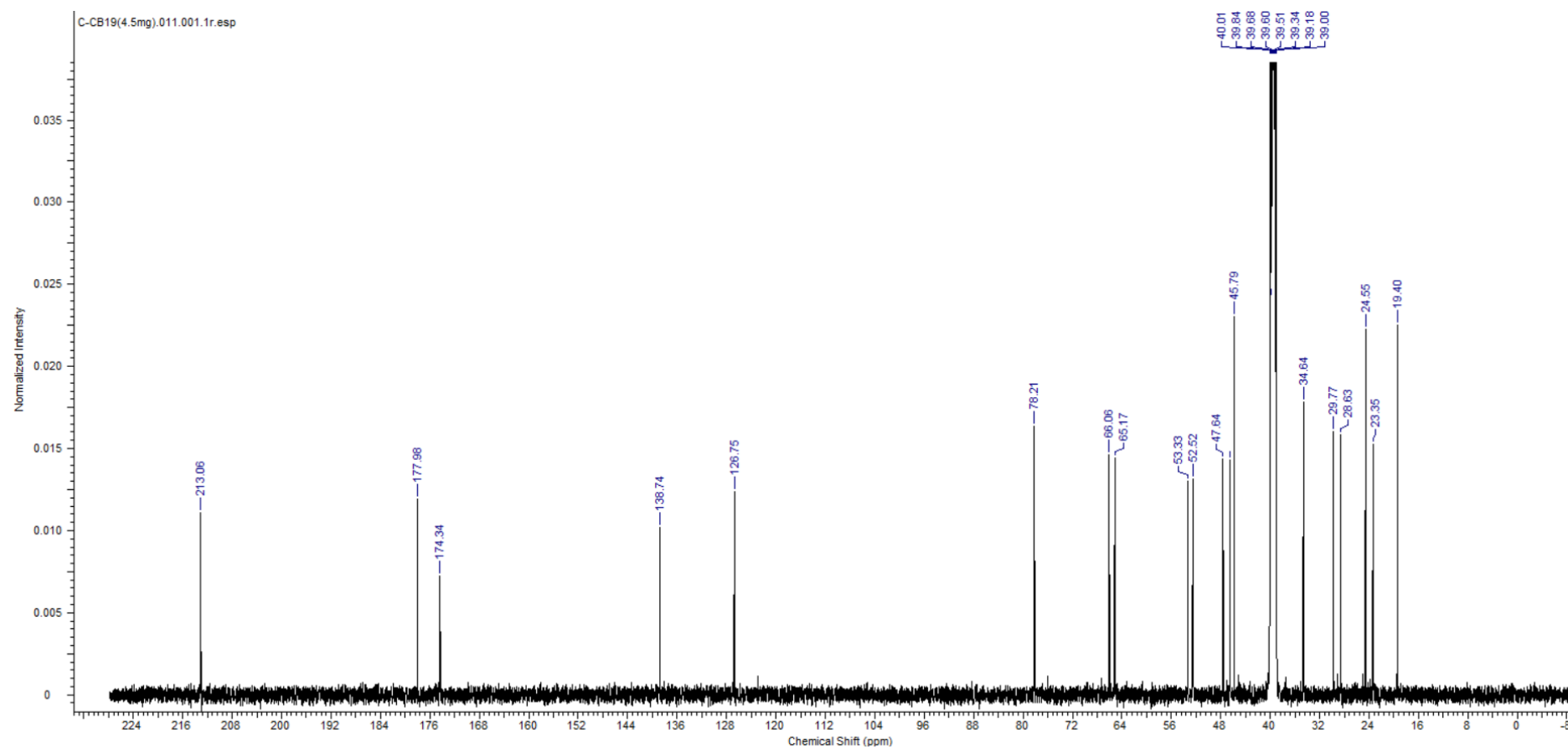


Figure S59. ^{13}C -NMR spectrum of **7** in $\text{DMSO}-d_6$ (125 MHz)

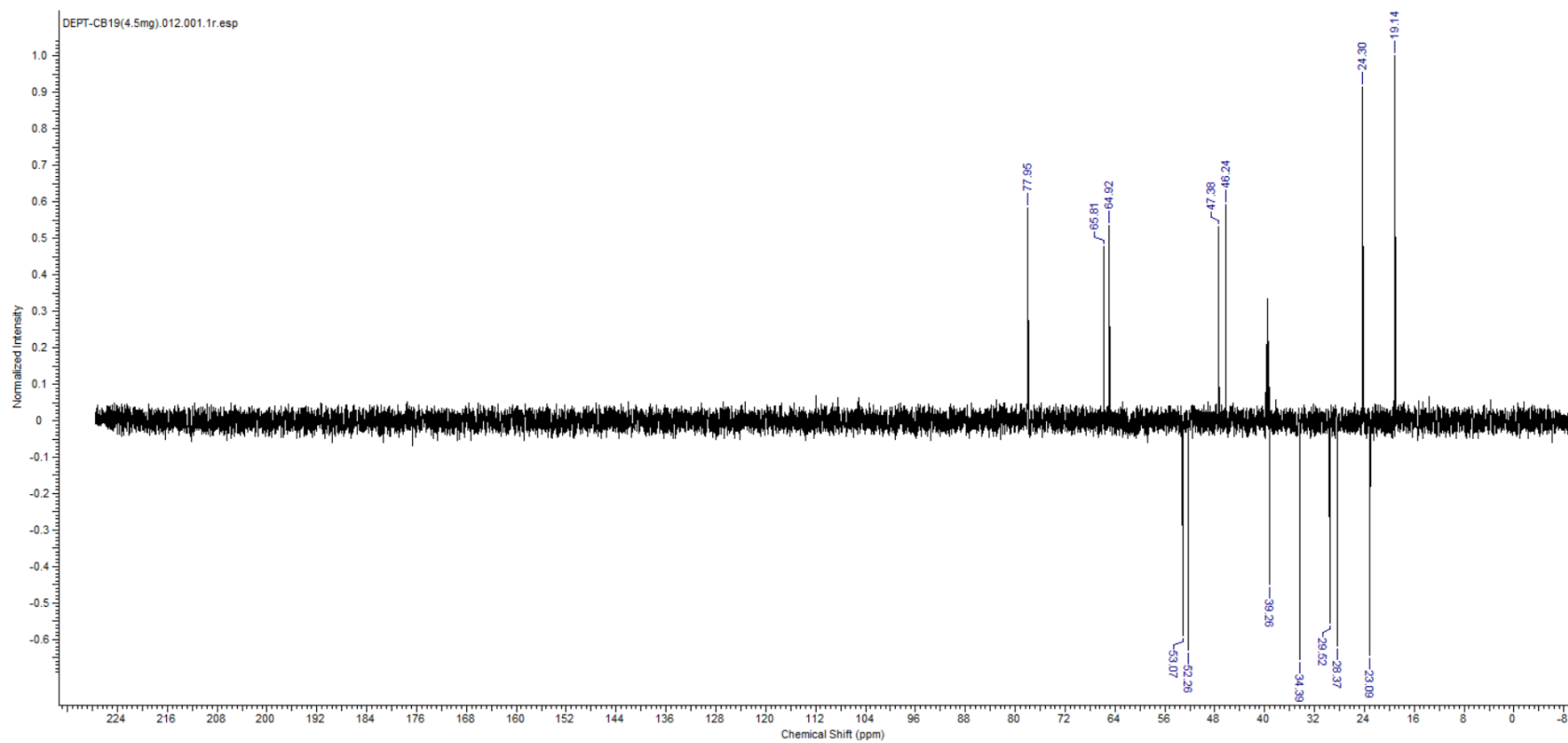


Figure S60. ^{13}C DEPT135 NMR spectrum of **7** in $\text{DMSO-}d_6$ (125 MHz)

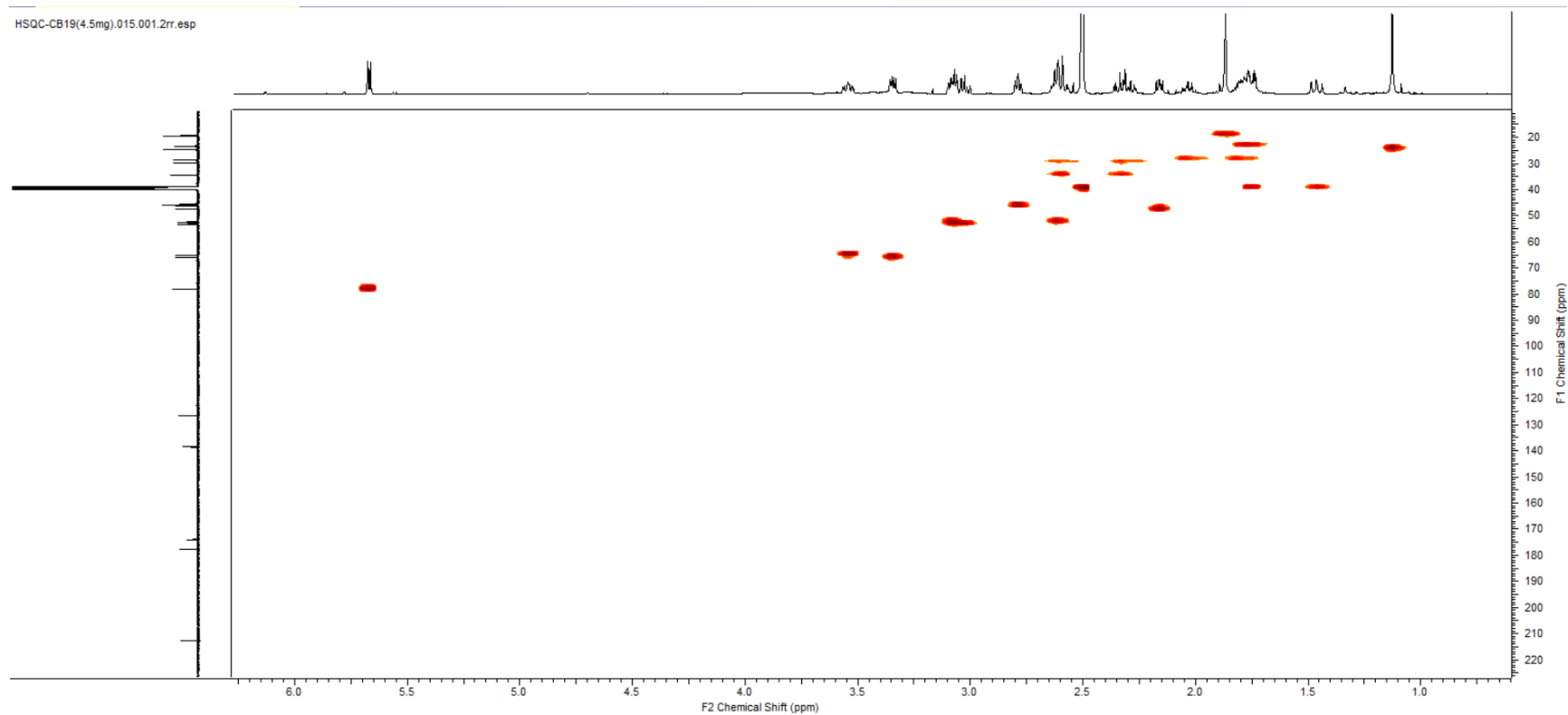


Figure S62. HSQC spectrum of **7** in DMSO-*d*₆ (500 MHz)

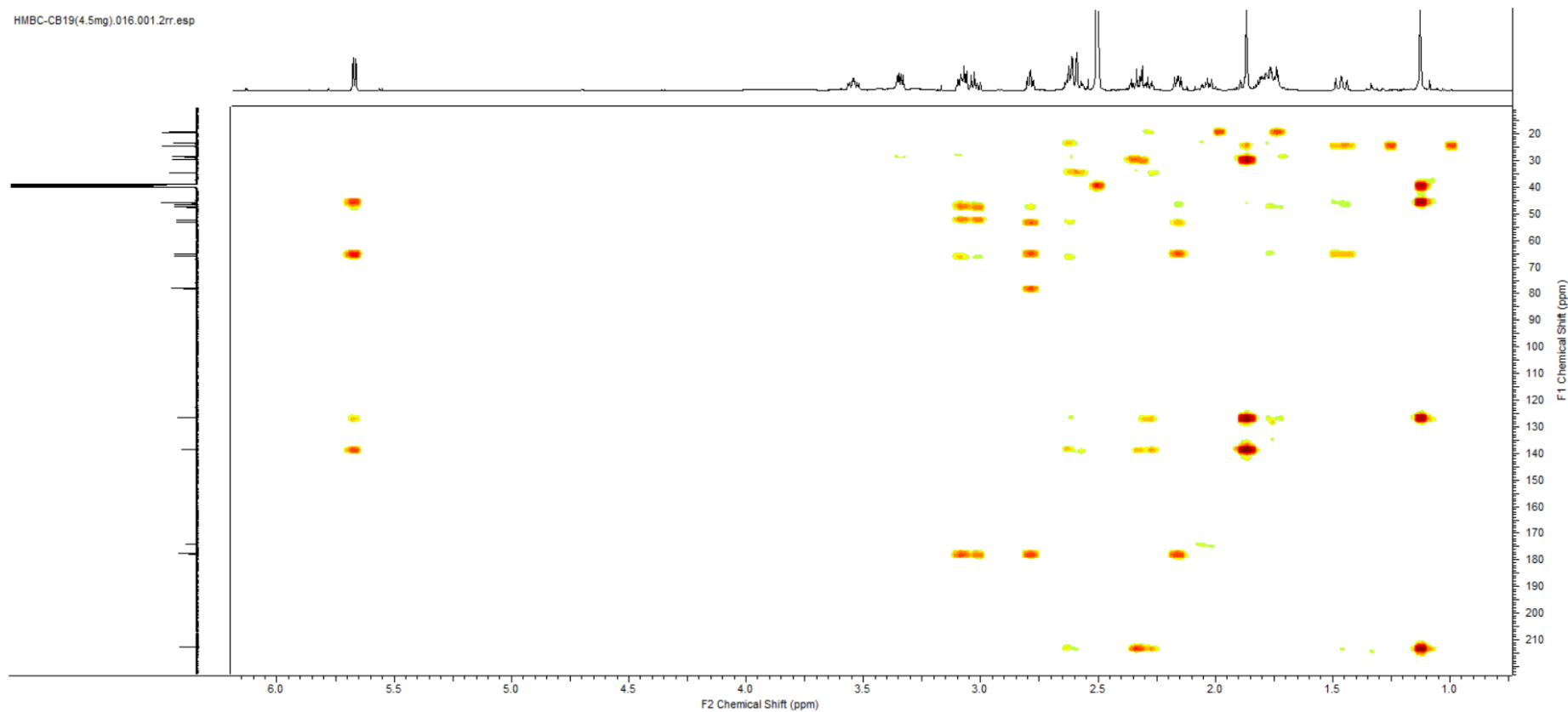


Figure S63. HMBC spectrum of **7** in DMSO-*d*₆ (500 MHz)

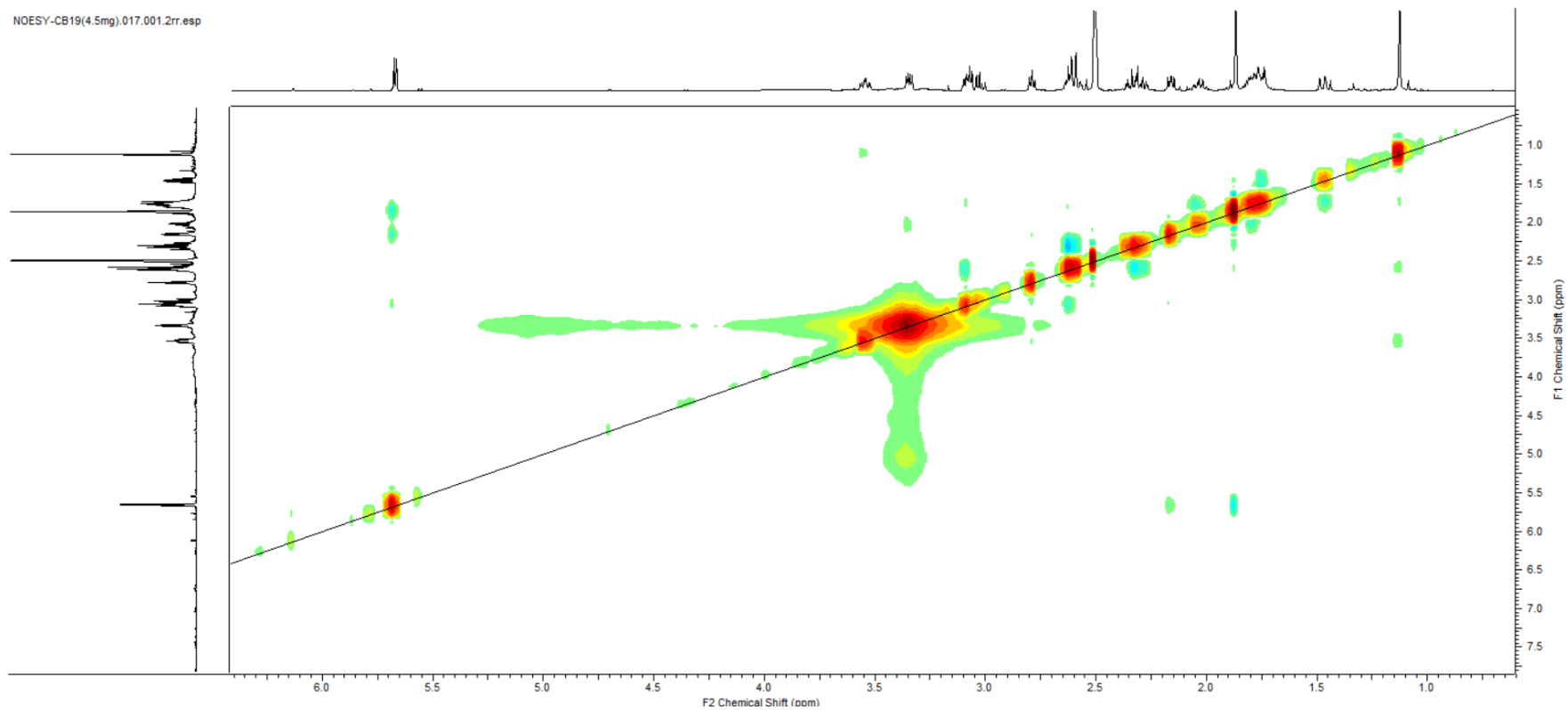


Figure S64. PS-NOESY spectrum of **7** in DMSO-*d*₆ (500 MHz)

CC-B-1-5-3-P1 + #7 RT: 0.08 AV: 1 NL: 7.81E5
 F: FTMS + p ESI Full ms [100.00-2000.00]

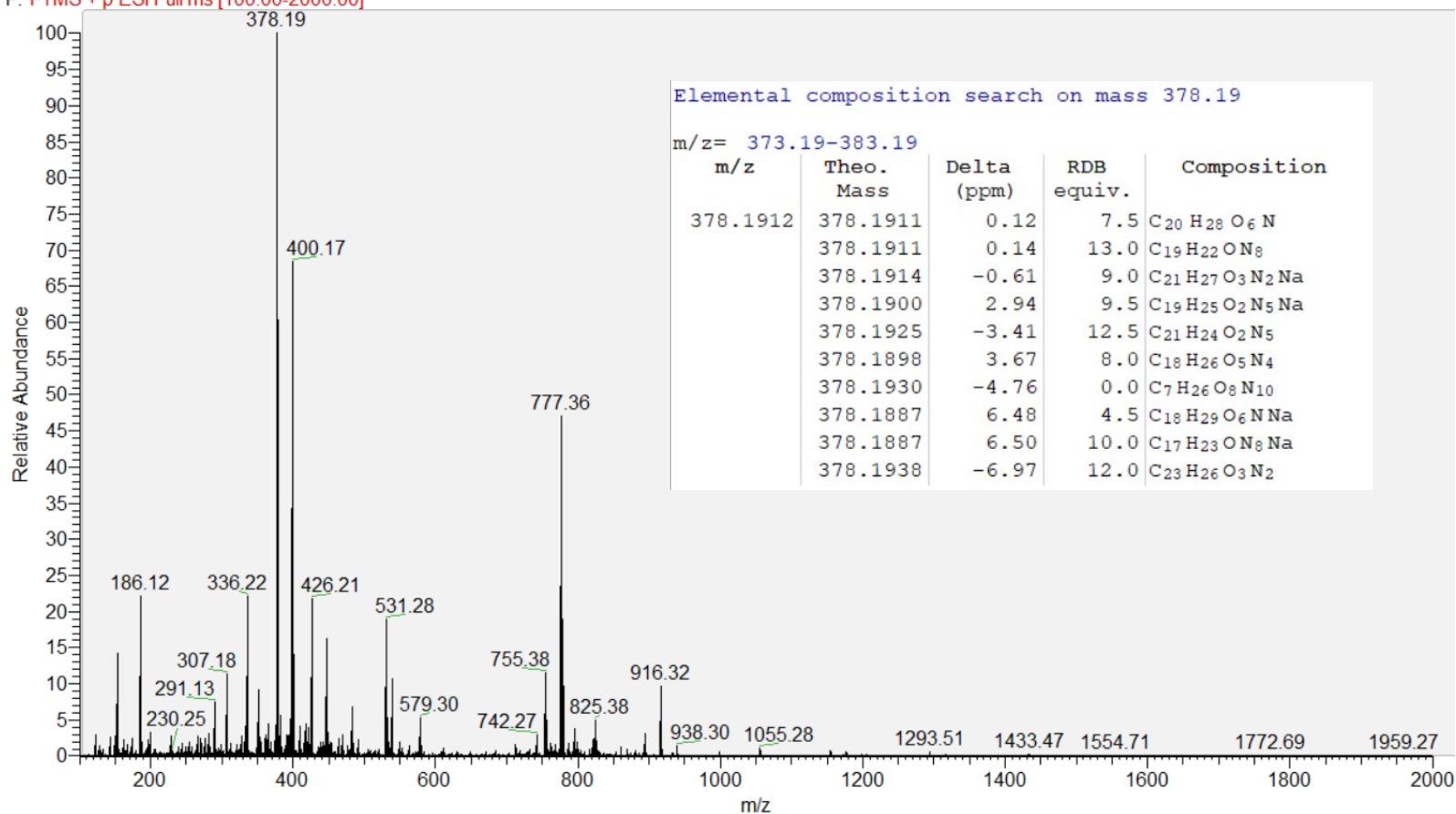


Figure S65. HR-ESI-MS spectrum of 7

CC-B-1-5-3-P1 + #8 RT: 0.09 AV: 1 NL: 2.49E4
F: ITMS + c ESI d Full ms2 378.19@cid35.00 [90.00-390.00]

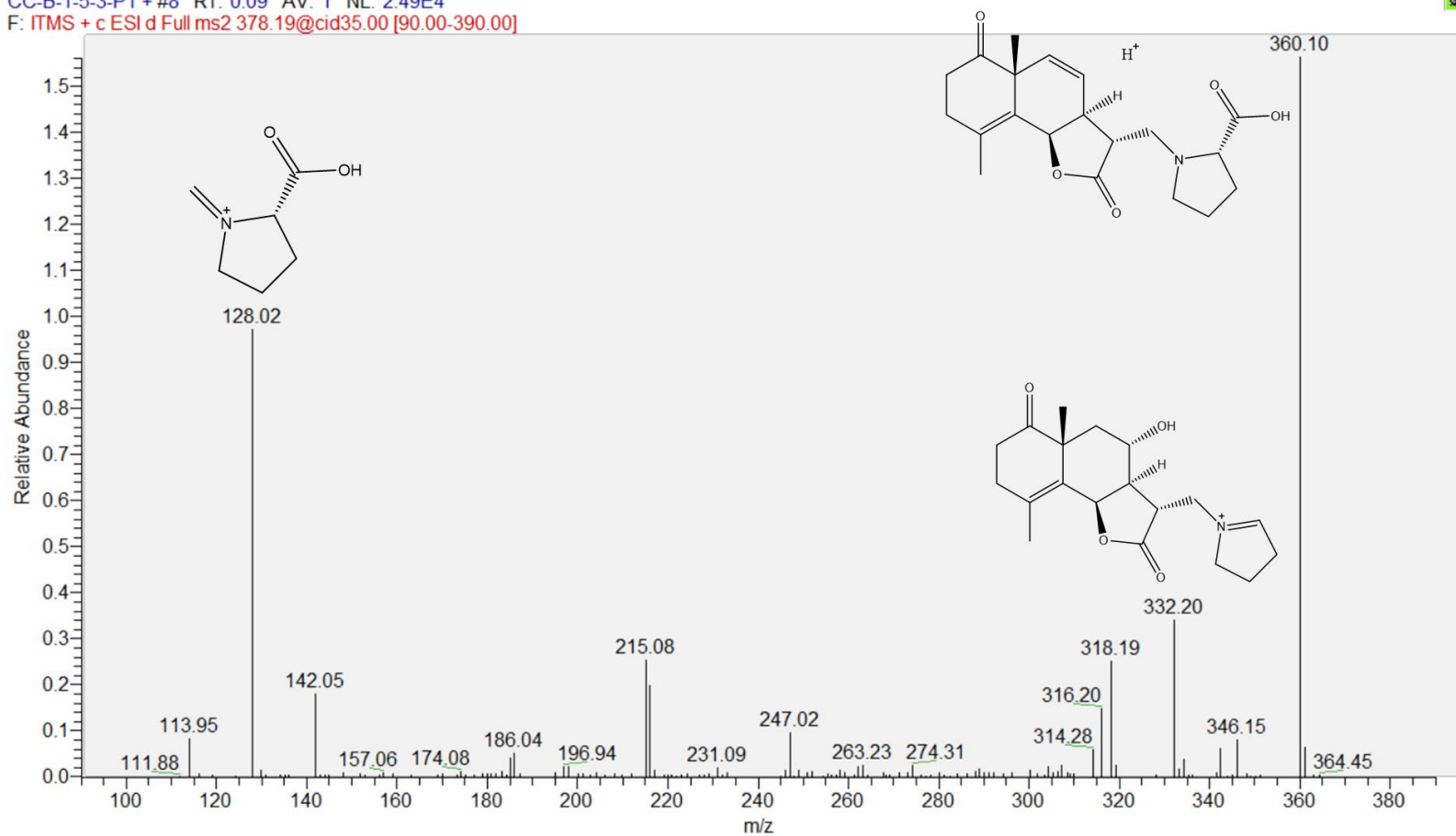


Figure S66. ESI-MS/MS spectrum of 7

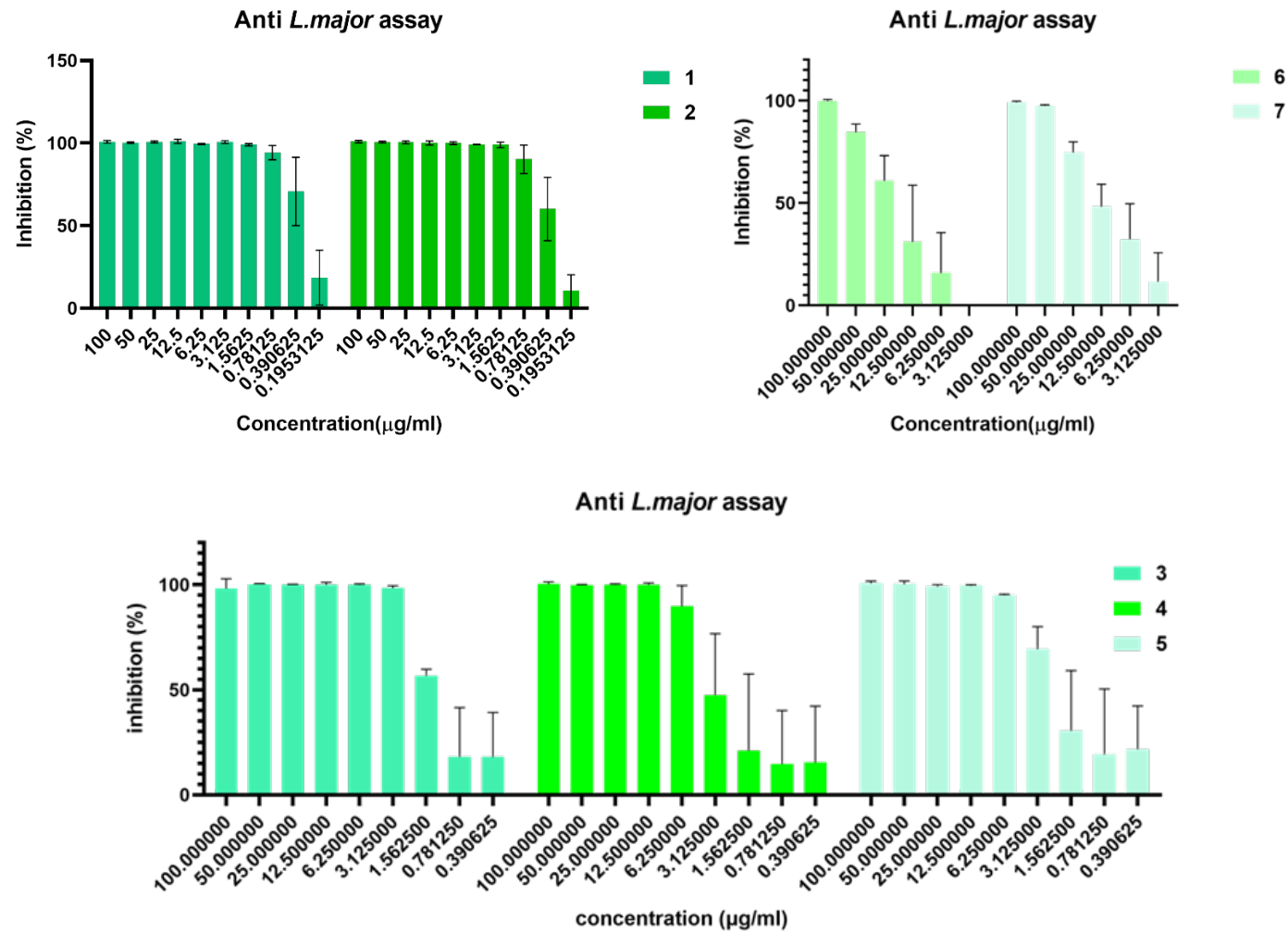


Figure S67. Anti-*L. major* data of 1-7

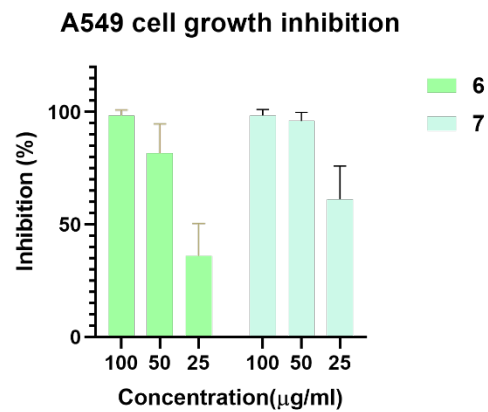
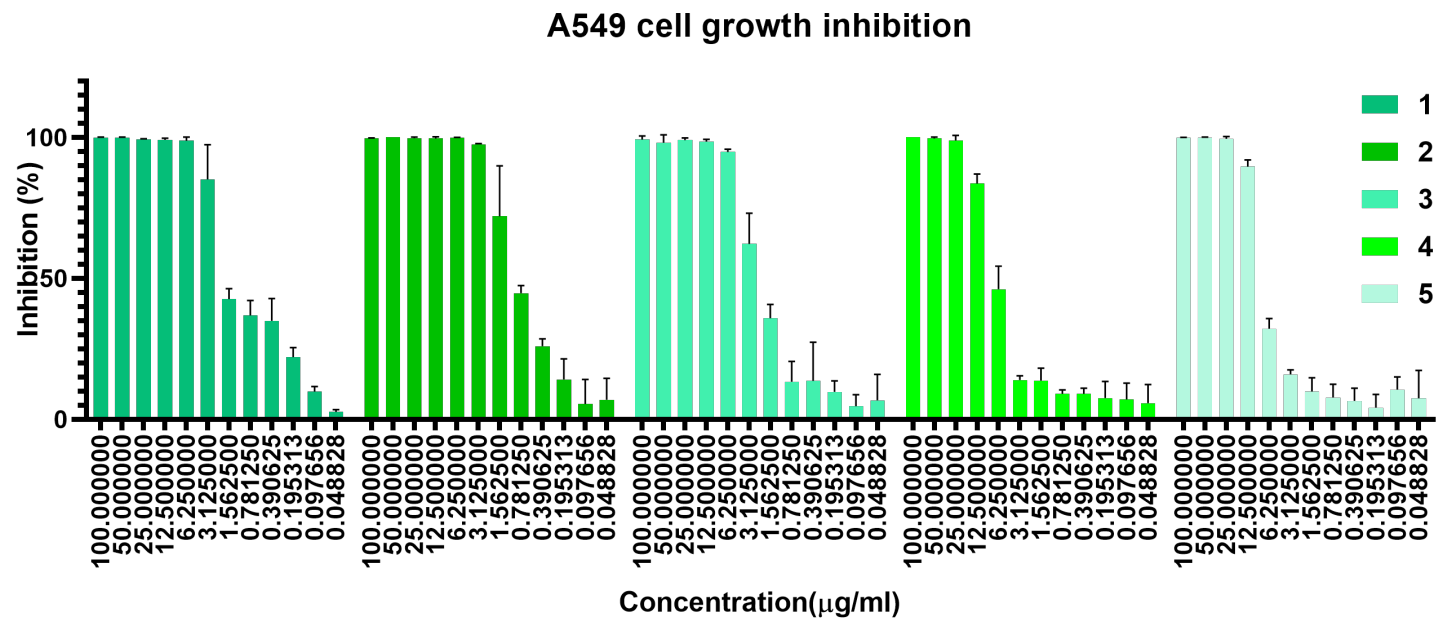


Figure S68. Anti-A549 data of 1-7

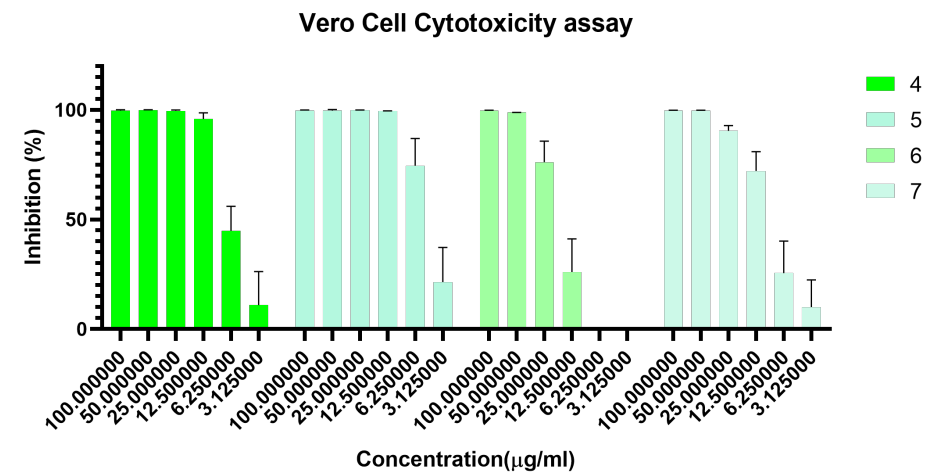
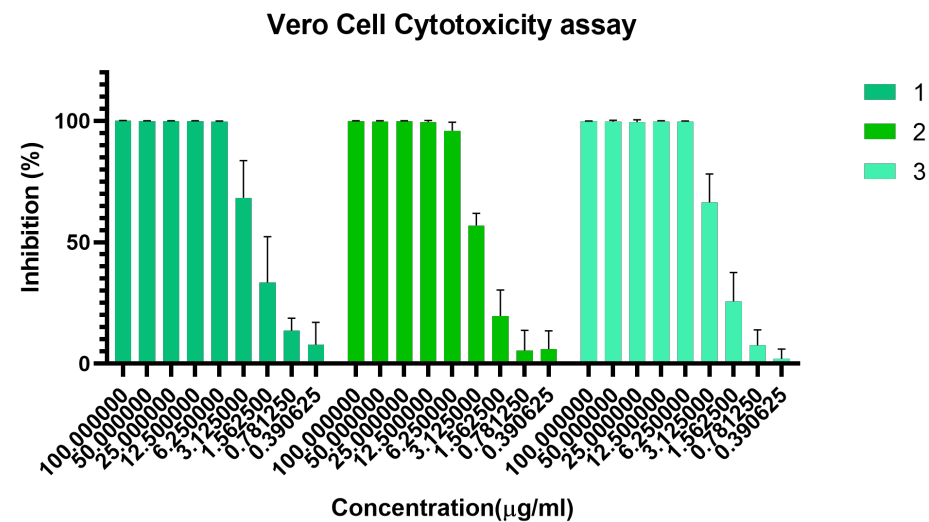


Figure S69. Vero cell cytotoxicity data of **1-7**