

Supplementary data

Asperindoles A-D and *p*-Terphenyl Derivative from the Ascidian-Derived Fungus *Aspergillus candidus* Link KMM 4676

Elena V. Ivanets¹, Anton N. Yurchenko¹, Olga F. Smetanina¹, Anton B. Rasin¹, Olesya I. Zhuravleva^{1,2}, Mikhail V. Pivkin¹, Roman S. Popov¹, Gunhild von Amsberg³, Shamil Sh. Afiyatullof¹ and Sergey A. Dyshlovoy^{1,2,3}

¹ G.B. Elyakov Pacific Institute of Bioorganic Chemistry, Far Eastern Branch of the Russian Academy of Sciences, Prospect 100-letiya Vladivostoka, 159, Vladivostok 690022, Russia; ev.ivanets@yandex.ru (E.I.), yurchant@ya.ru (A.Y.); smetof@rambler.ru (O.S.); abrus__54@mail.ru (A.R.); oid27@mail.ru (M.P.); prs_90@mail.ru (R.P.); afiyat@piboc.dvo.ru (S.A.)

² School of Natural Science, Far Eastern Federal University, Sukhanova St., 8, Vladivostok 690000, Russia;

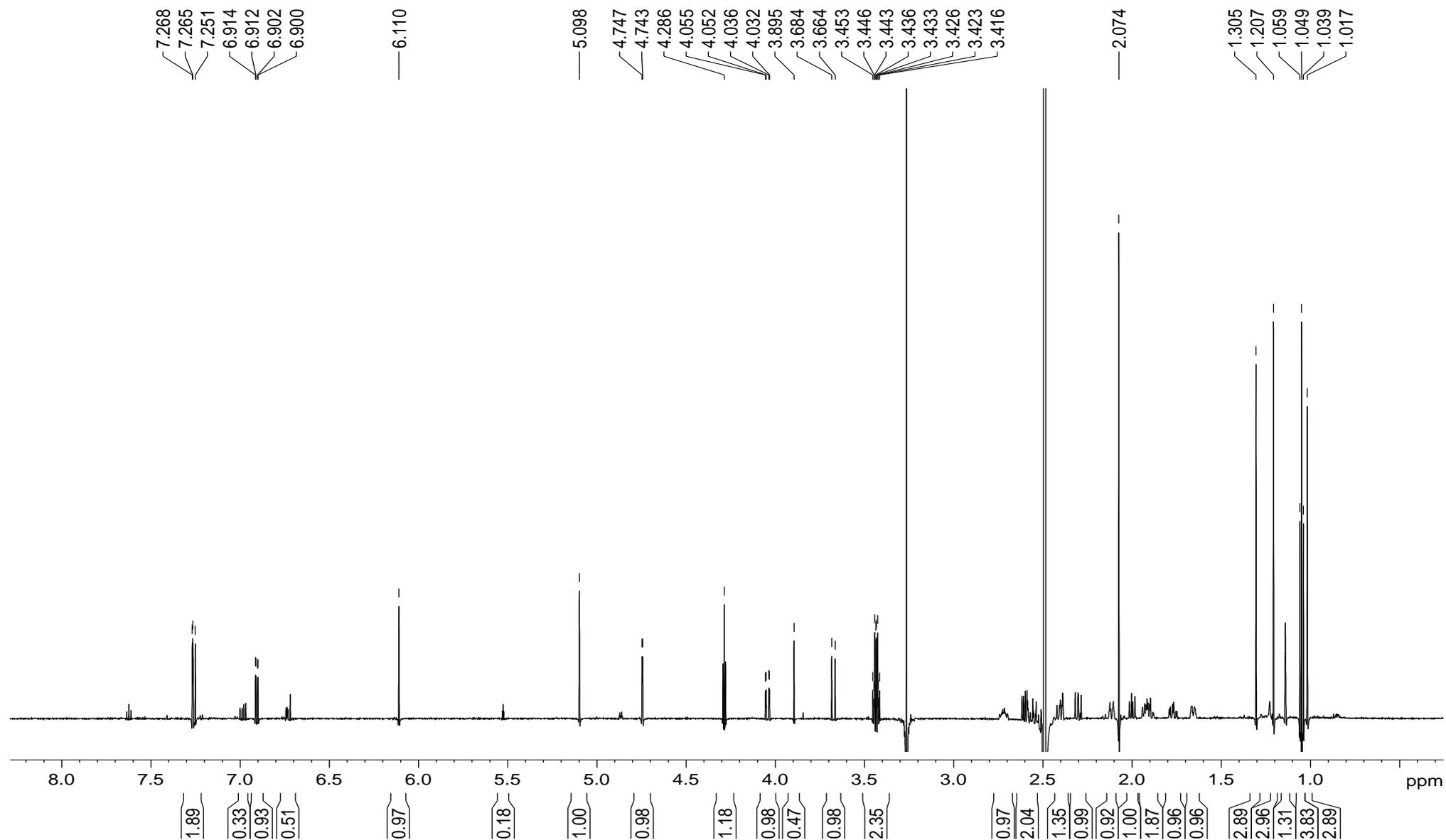
³ Laboratory of Experimental Oncology, Department of Oncology, Hematology and Bone Marrow Transplantation with Section Pneumology, Hubertus Wald-Tumorzentrum, University Medical Center Hamburg-Eppendorf, Hamburg 20246, Germany; cbokemeyer@uke.de (C.B.); g.von-amsberg@uke.de (G.A.); dyshlovoy@gmail.com (S.D.)

* Correspondence: yurchant@ya.ru; Tel.: +7-423-231-1168

Content

Figure S1. ^1H NMR (700 MHz, DMSO- d_6) spectrum of asperindole A (1).....	3
Figure S2. ^{13}C NMR (125 MHz, DMSO- d_6) spectrum of asperindole A (1)	5
Figure S3. DEPT-135 (125 MHz, DMSO- d_6) spectrum of asperindole A (1)	6
Figure S4. HSQC (700 MHz, DMSO- d_6) spectrum of asperindole A (1).....	7
Figure S5. HMBC (700 MHz, DMSO- d_6) spectrum of asperindole A (1).....	8
Figure S6. ROESY (700 MHz, DMSO- d_6) spectrum of asperindole A (1)	9
Figure S7. ^1H NMR (500 MHz, DMSO- d_6) spectrum of asperindole B (2).....	10
Figure S8. ^{13}C NMR (125 MHz, DMSO- d_6) spectrum of asperindole B (2).....	12
Figure S9. DEPT-135 (125 MHz, DMSO- d_6) spectrum of asperindole B (2)	13
Figure S10. ^1H - ^1H COSY (500 MHz, DMSO- d_6) spectrum of asperindole B (2).....	14
Figure S11. HSQC (500 MHz, DMSO- d_6) spectrum of asperindole B (2)	15
Figure S12. HMBC (500 MHz, DMSO- d_6) spectrum of asperindole B (2).....	16
Figure S13. ROESY (500 MHz, DMSO- d_6) spectrum of asperindole B (2).....	17
Figure S14. ^1H NMR (500 MHz, DMSO- d_6) spectrum of asperindole C (3)	18
Figure S15. ^{13}C NMR (125 MHz, DMSO- d_6) spectrum of asperindole C (3).....	20
Figure S16. DEPT-135 (125 MHz, DMSO- d_6) spectrum of asperindole C (3)	21
Figure S17. ^1H - ^1H COSY (500 MHz, DMSO- d_6) spectrum of asperindole C (3).....	22
Figure S18. HSQC (500 MHz, DMSO- d_6) spectrum of asperindole C (3)	23
Figure S19. HMBC (500 MHz, DMSO- d_6) spectrum of asperindole C (3).....	24
Figure S20. ROESY (500 MHz, DMSO- d_6) spectrum of asperindole C (3).....	25
Figure S21. ^1H NMR (500 MHz, DMSO- d_6) spectrum of asperindole D (4)	26
Figure S22. ^{13}C NMR (125 MHz, DMSO- d_6) spectrum of asperindole D (4)	27
Figure S23. ^1H NMR (700 MHz, acetone- d_6) spectrum of 3''-hydroxyterphenyllin (5).....	28
Figure S24. ^{13}C NMR (125 MHz, acetone- d_6) spectrum of 3''-hydroxyterphenyllin (5)	29
Figure S25. DEPT-135 (125 MHz, acetone- d_6) spectrum of 3''-hydroxyterphenyllin (5)	30
Figure S26. HSQC (700 MHz, acetone- d_6) spectrum of 3''-hydroxyterphenyllin (5).....	31
Figure S27. HMBC (700 MHz, acetone- d_6) spectrum of 3''-hydroxyterphenyllin (5).....	32
Figure S28. ROESY (700 MHz, acetone- d_6) spectrum of 3''-hydroxyterphenyllin (5)	33

Figure S1. ^1H NMR (700 MHz, DMSO-d_6) spectrum of asperindole A (**1**)



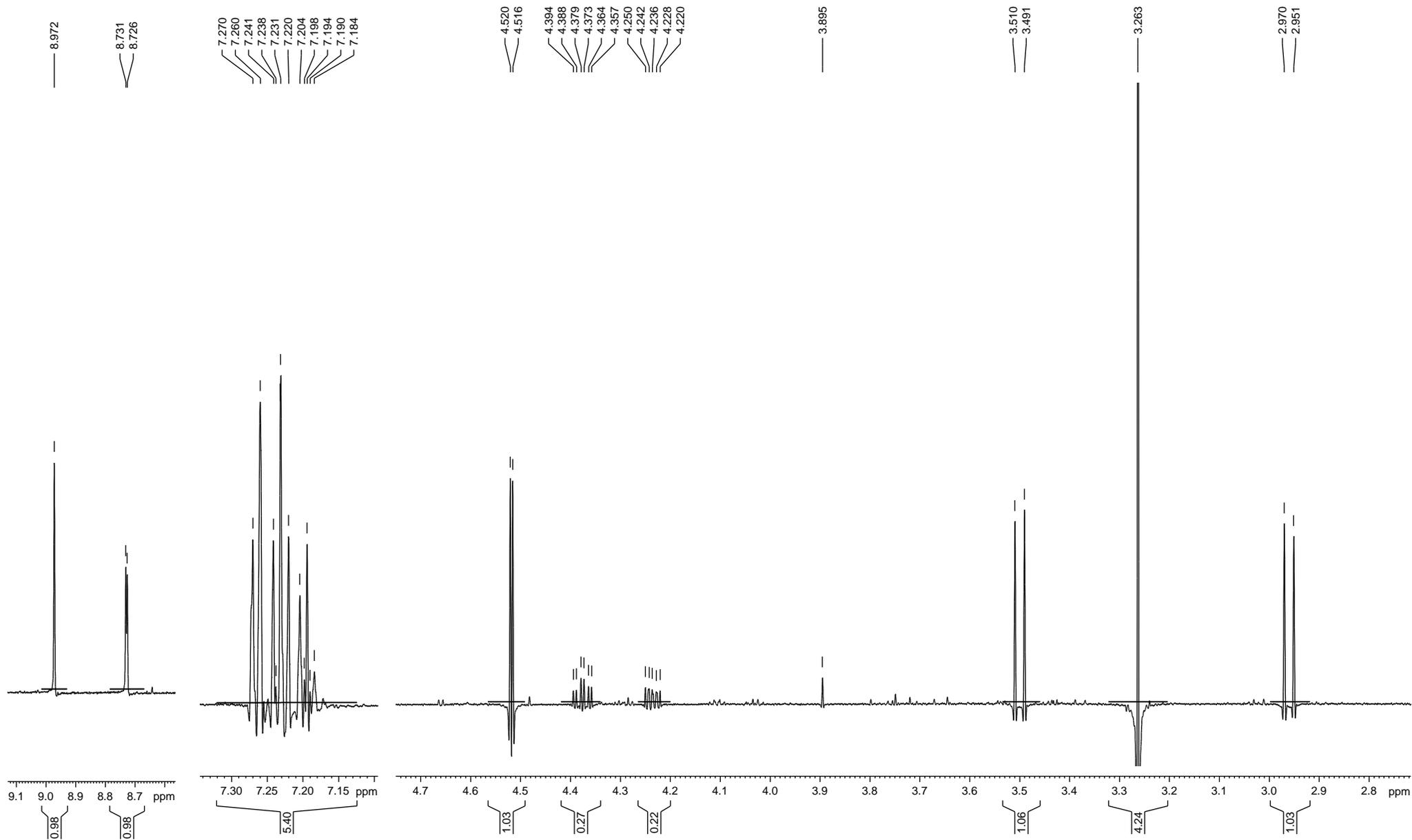


Figure S2. ^{13}C NMR (125 MHz, DMSO- d_6) spectrum of asperindole A (**1**)

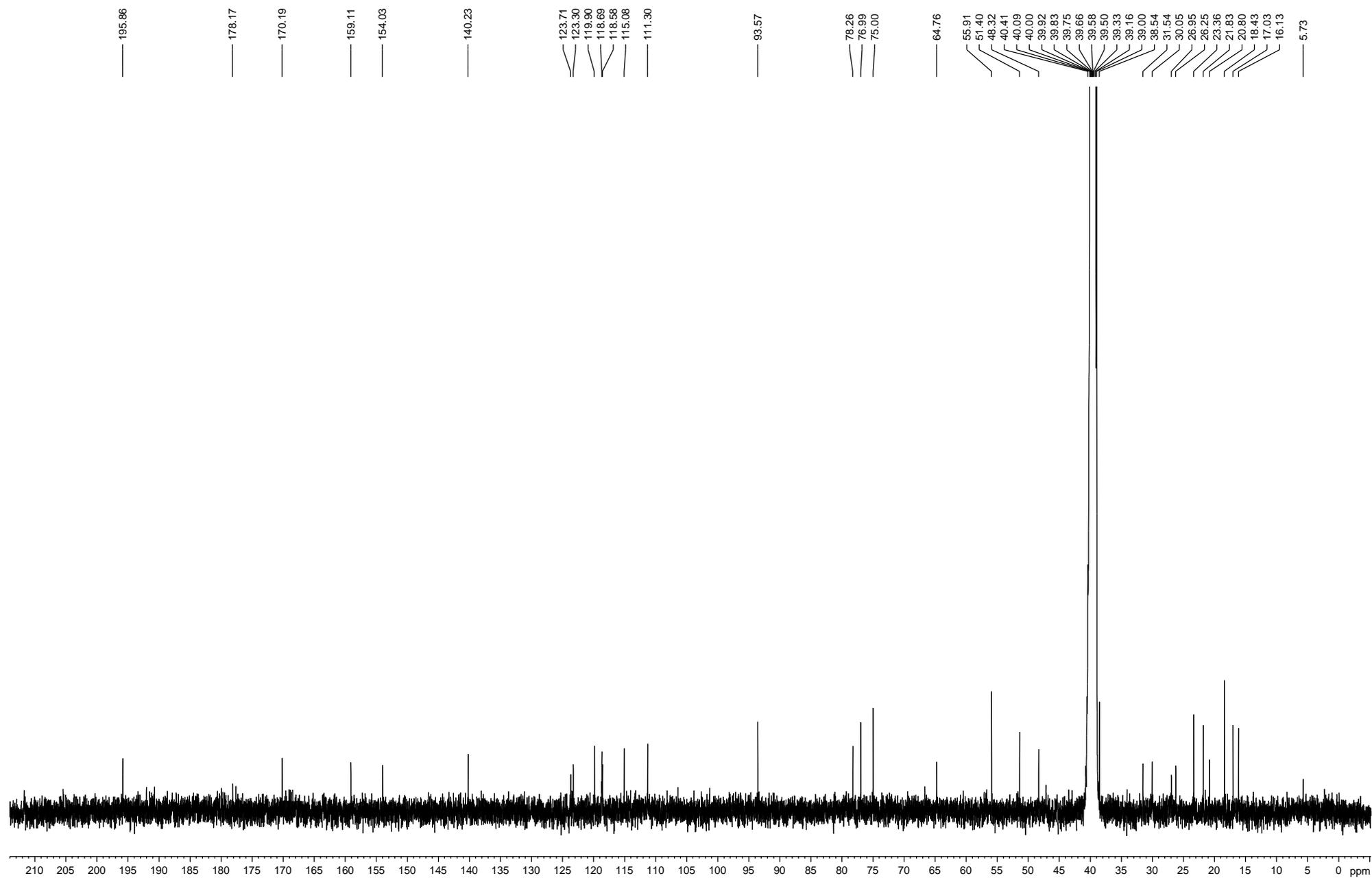


Figure S3. DEPT-135 (125 MHz, DMSO-d₆) spectrum of asperindole A (**1**)

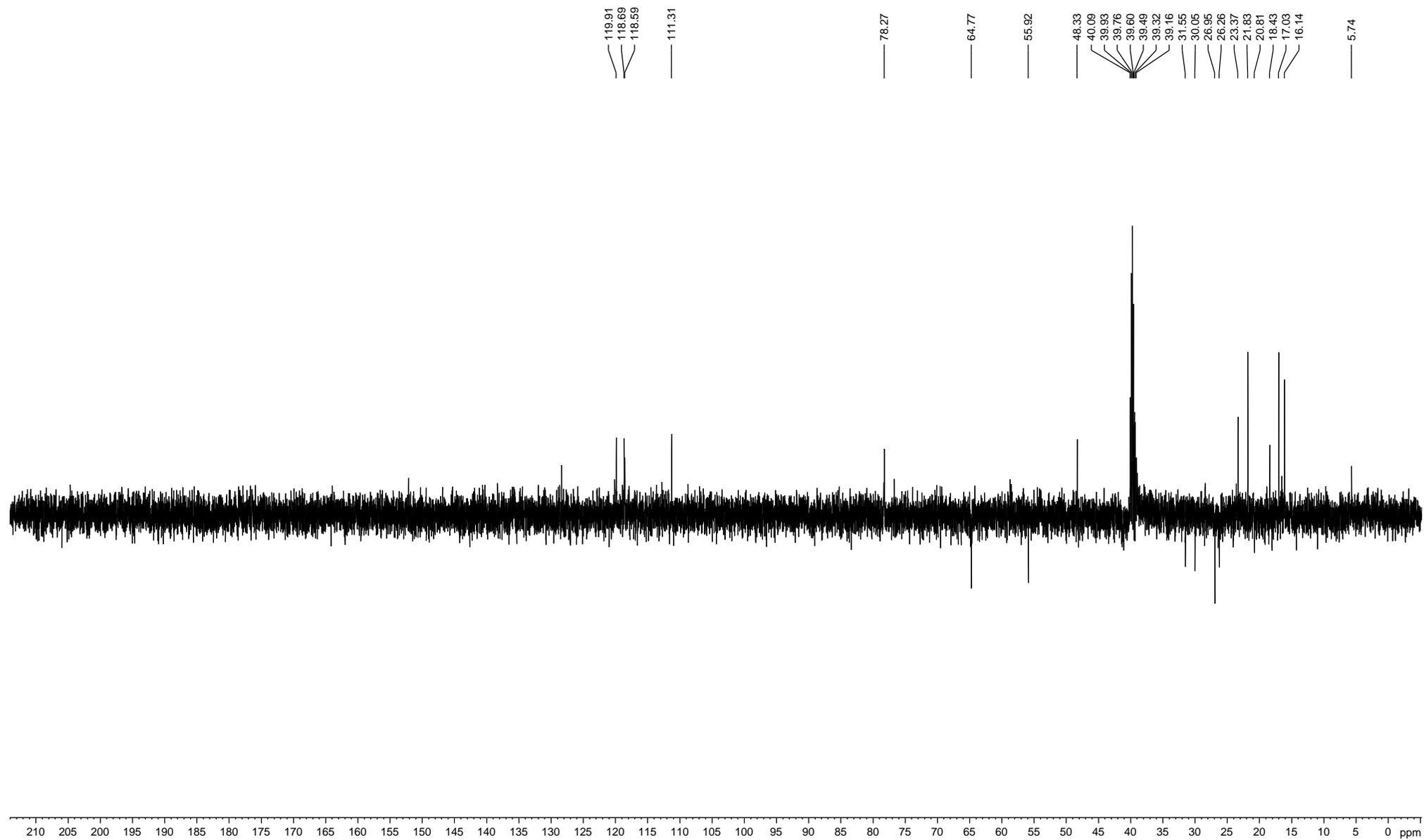


Figure S4. HSQC (700 MHz, DMSO-d₆) spectrum of asperindole A (1)

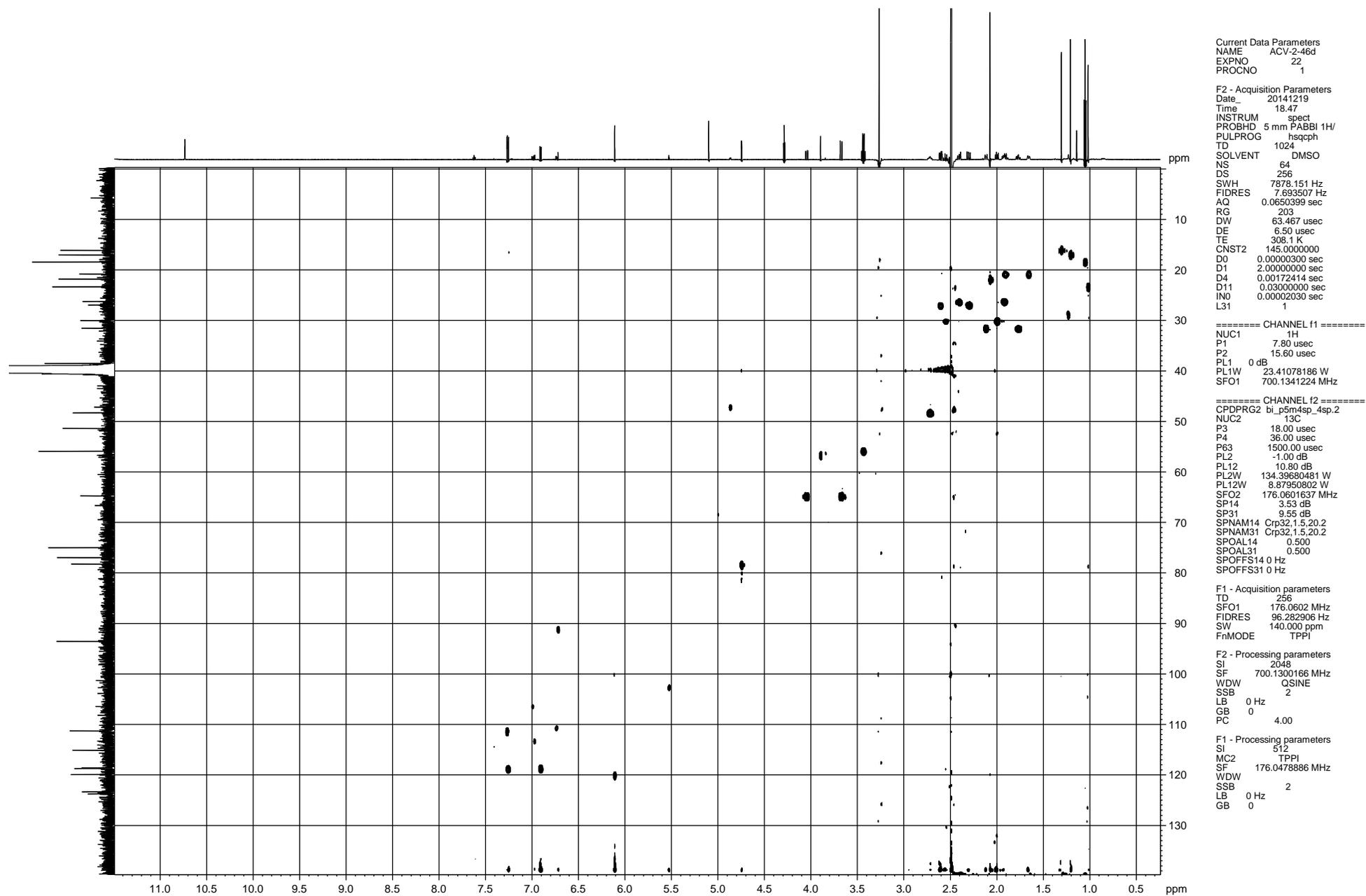


Figure S5. HMBC (700 MHz, DMSO-d₆) spectrum of asperindole A (1)

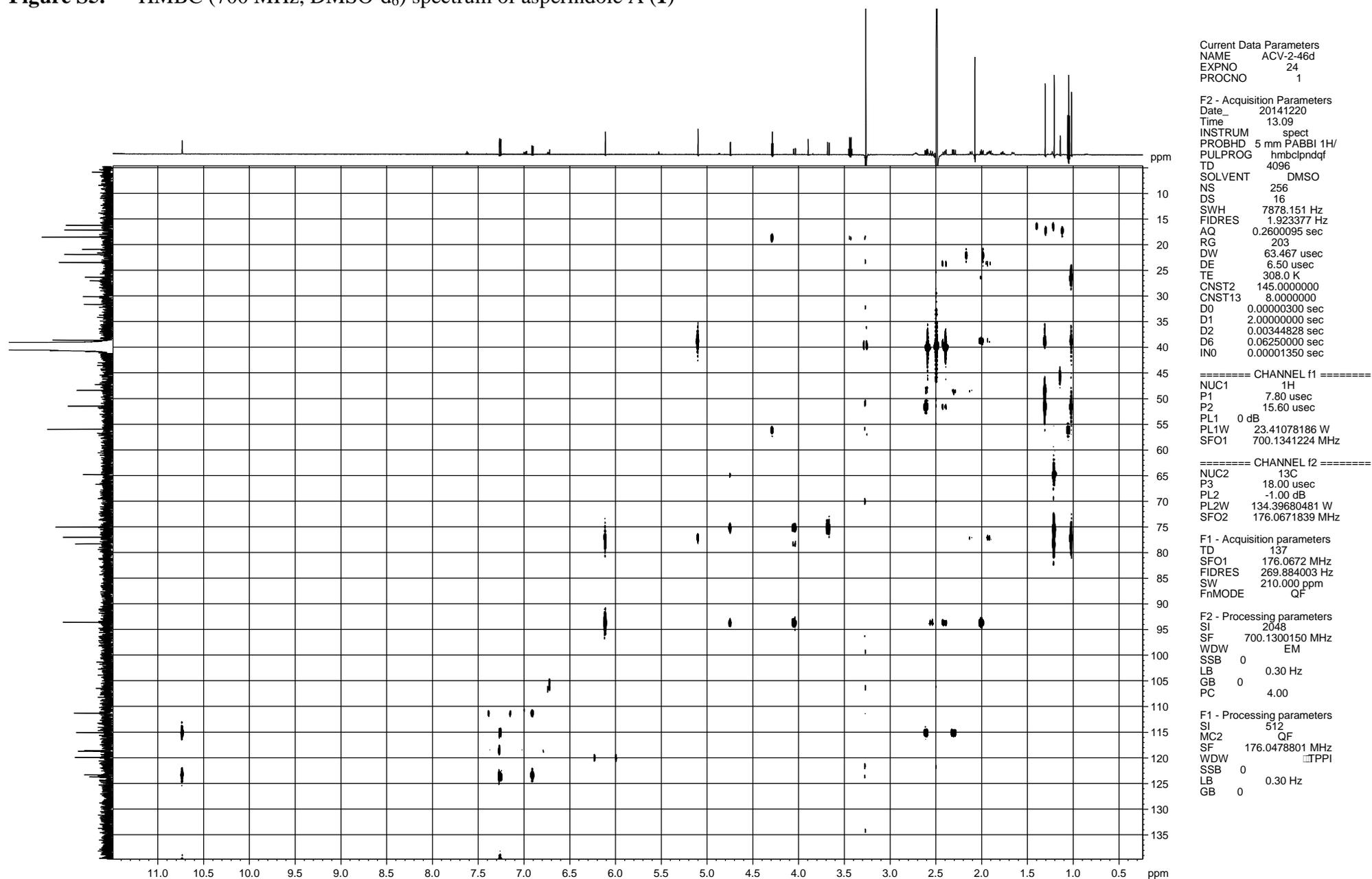


Figure S6. ROESY (700 MHz, DMSO-d₆) spectrum of asperindole A (1)

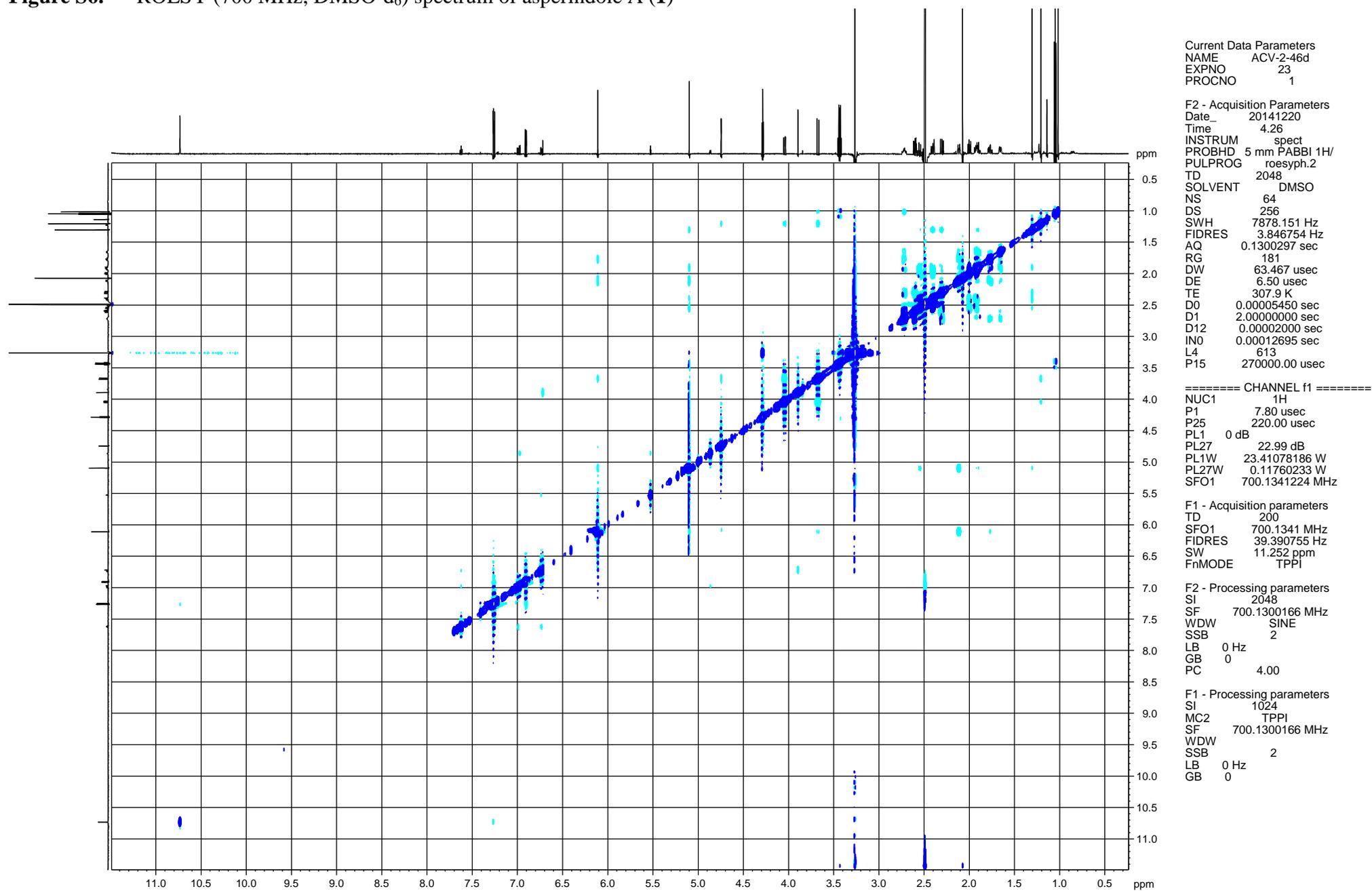
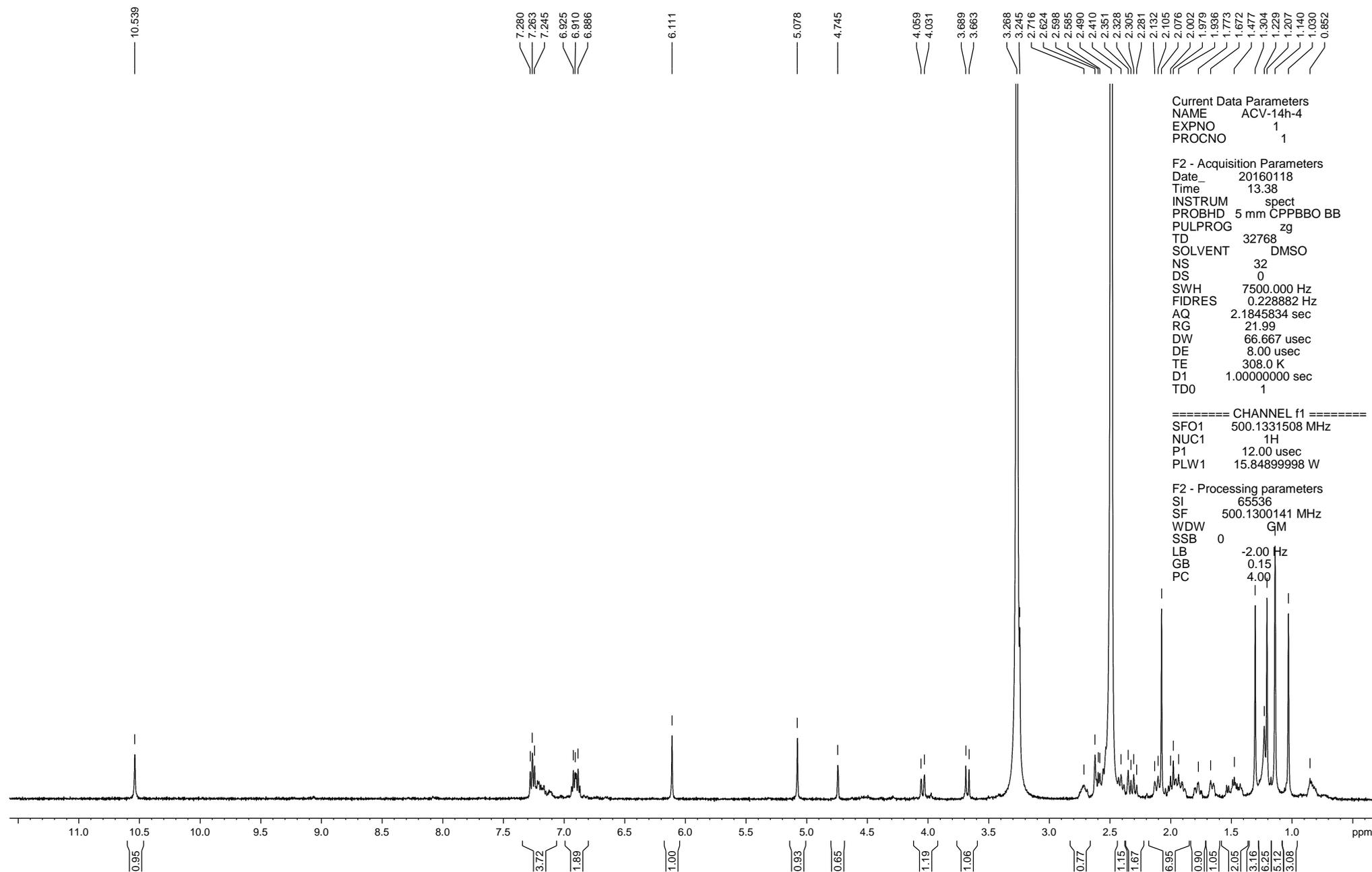


Figure S7. ^1H NMR (500 MHz, DMSO- d_6) spectrum of asperindole B (**2**)



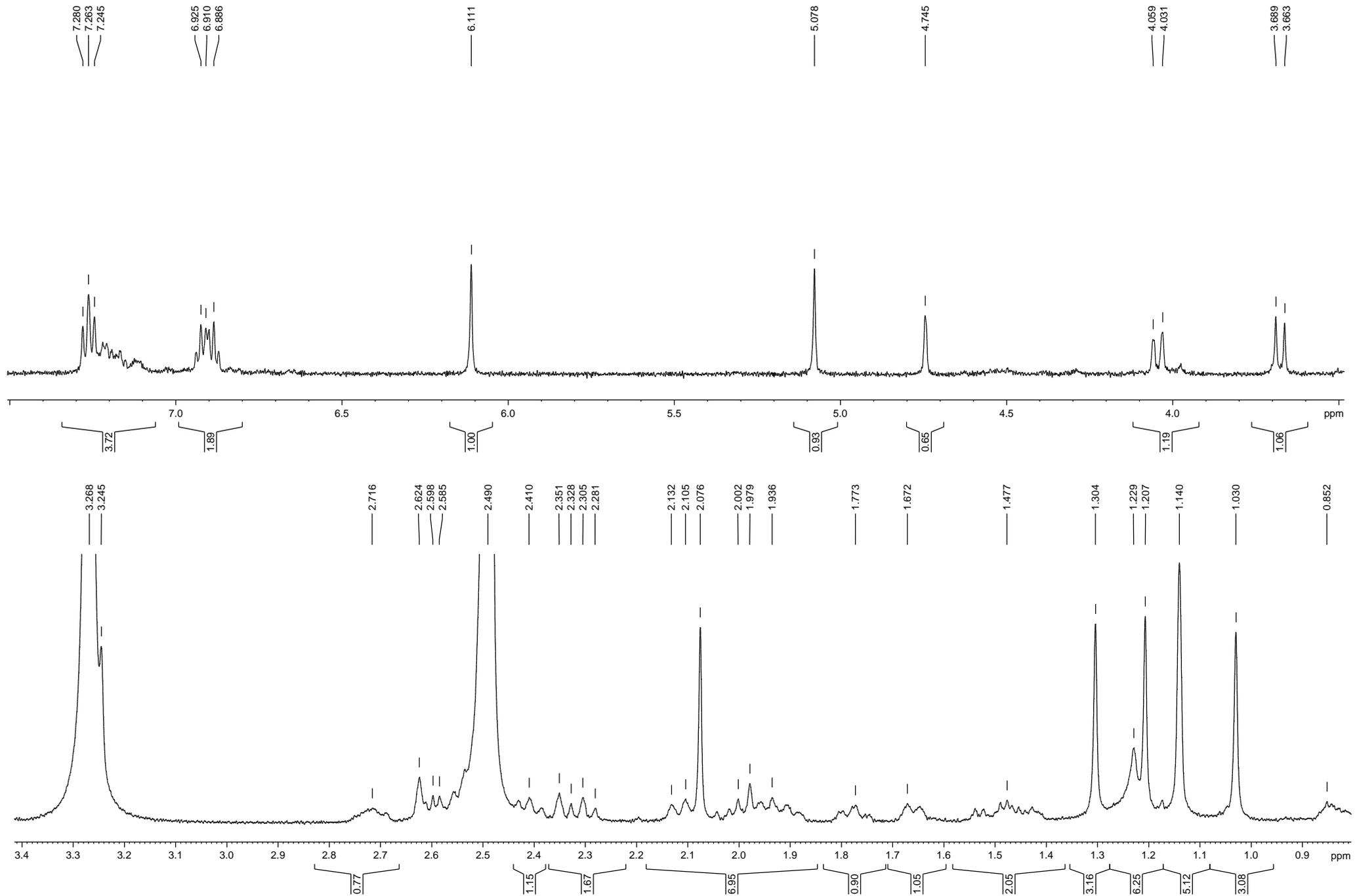


Figure S8. ^{13}C NMR (125 MHz, DMSO-d_6) spectra of asperindole B (**2**)

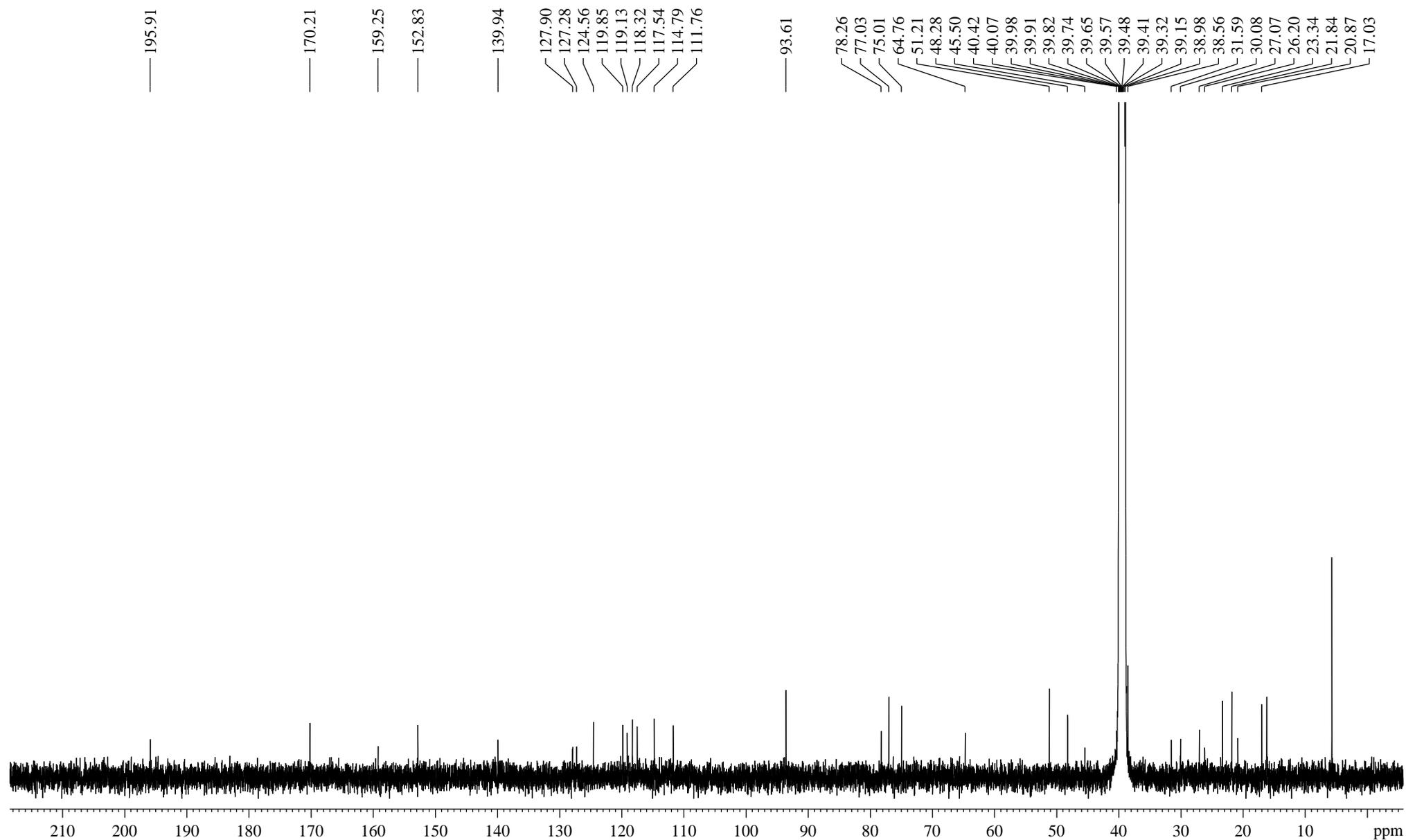


Figure S9. DEPT-135 (125 MHz, DMSO-d₆) spectrum of asperindole B (2)

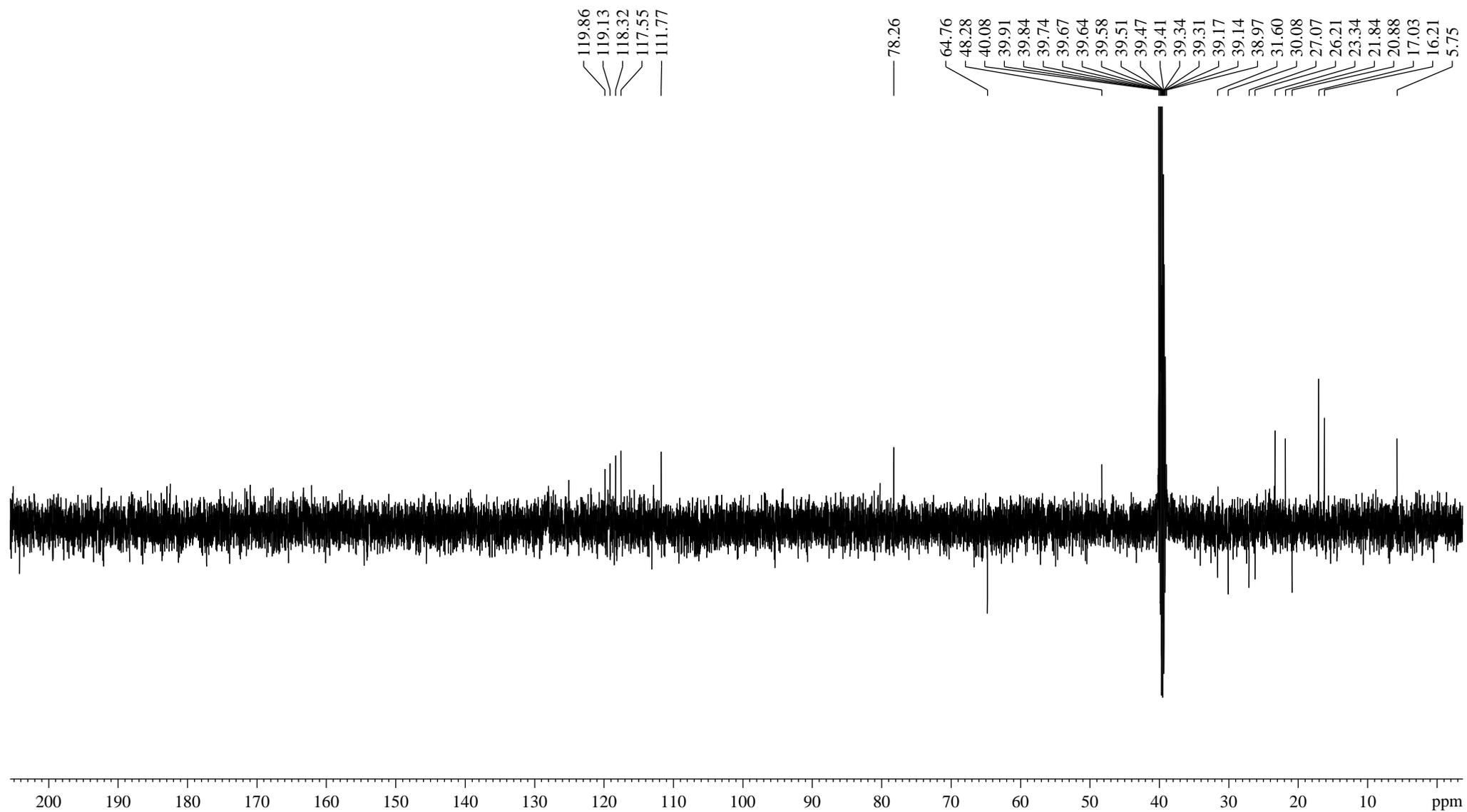


Figure S10. ^1H - ^1H COSY (500 MHz, DMSO- d_6) spectrum of asperindole B (2)

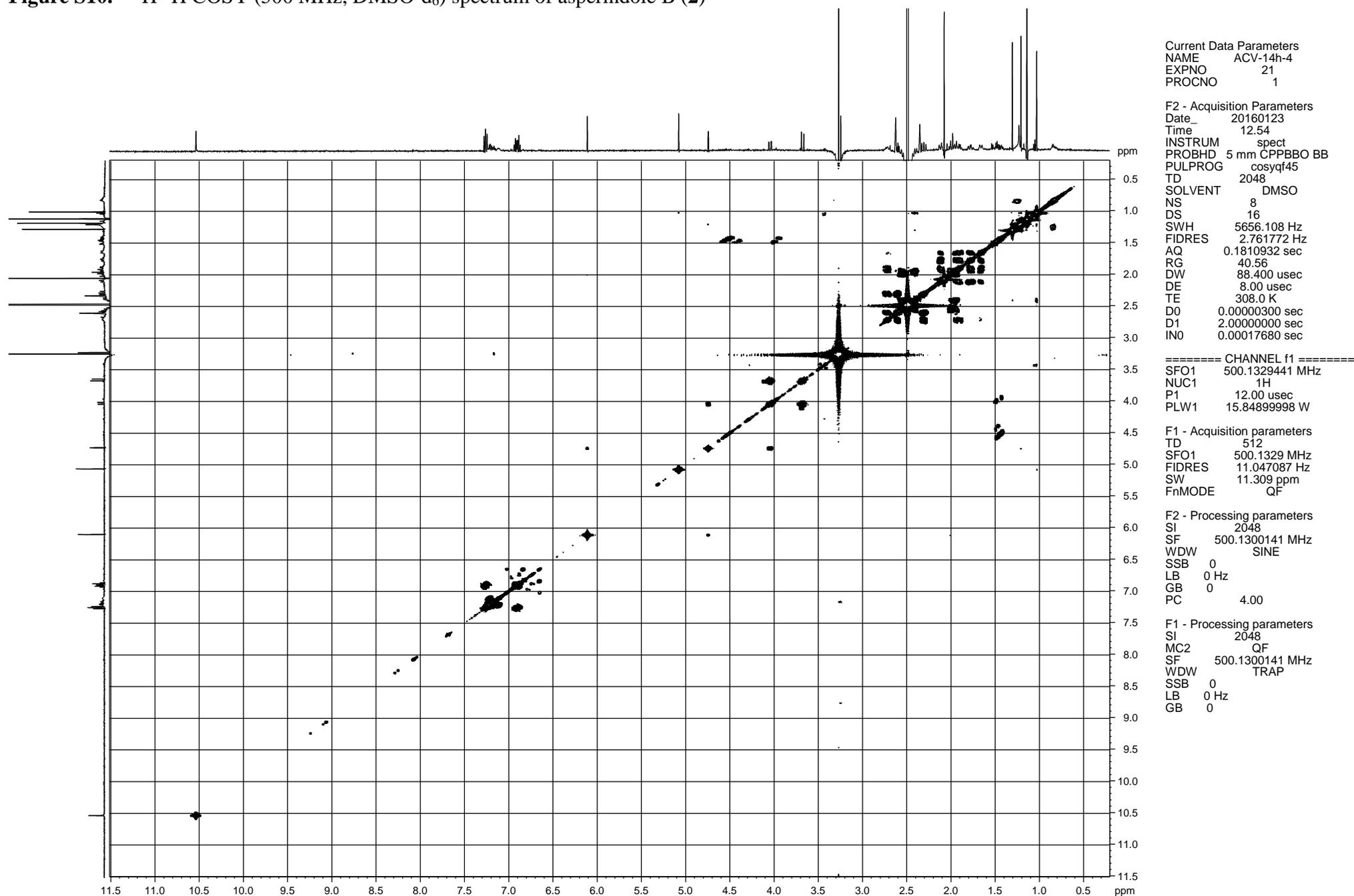


Figure S11. HSQC (500 MHz, DMSO-d₆) spectrum of asperindole B (2)

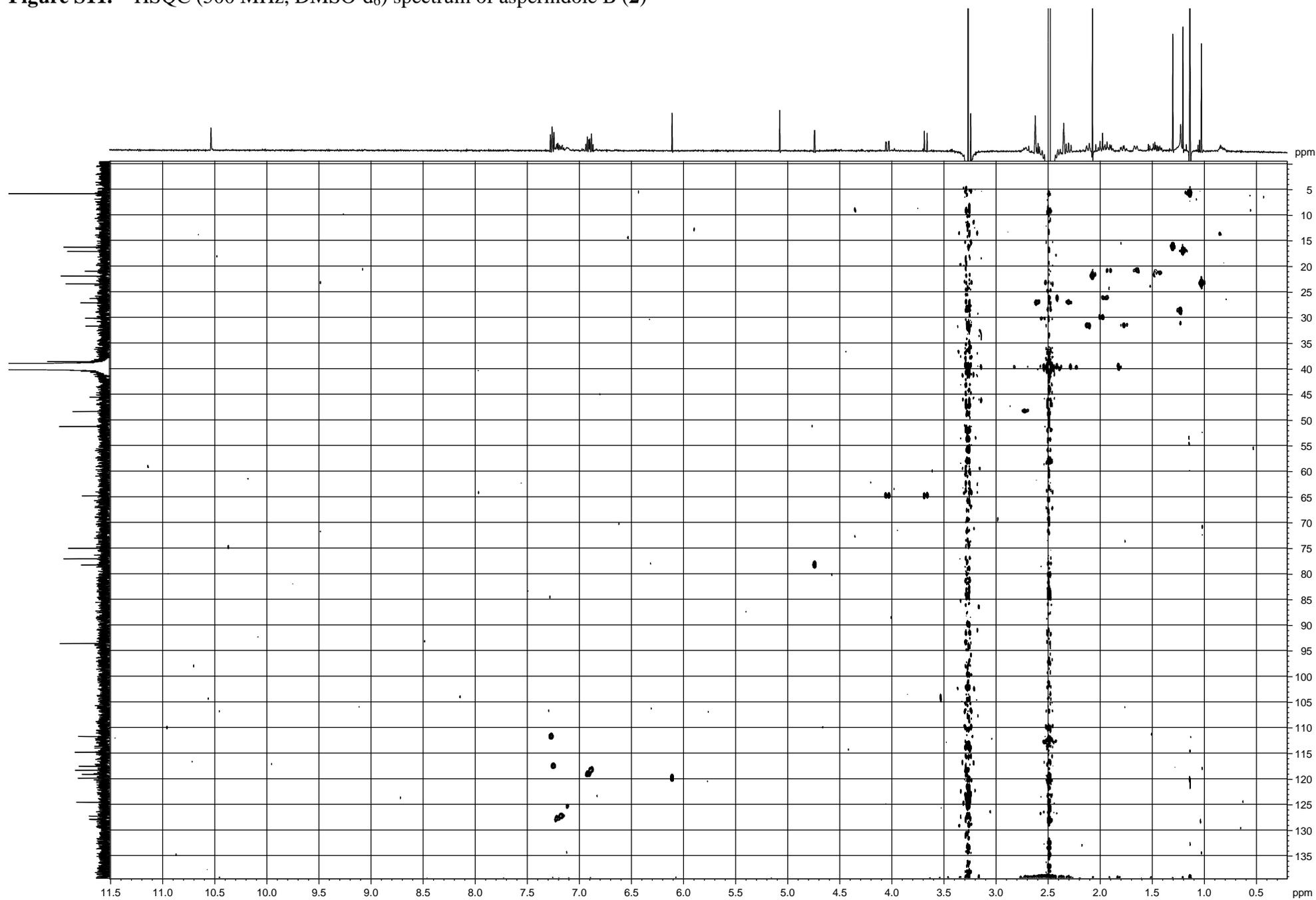


Figure S12. HMBC (500 MHz, DMSO-d₆) spectrum of asperindole B (2)

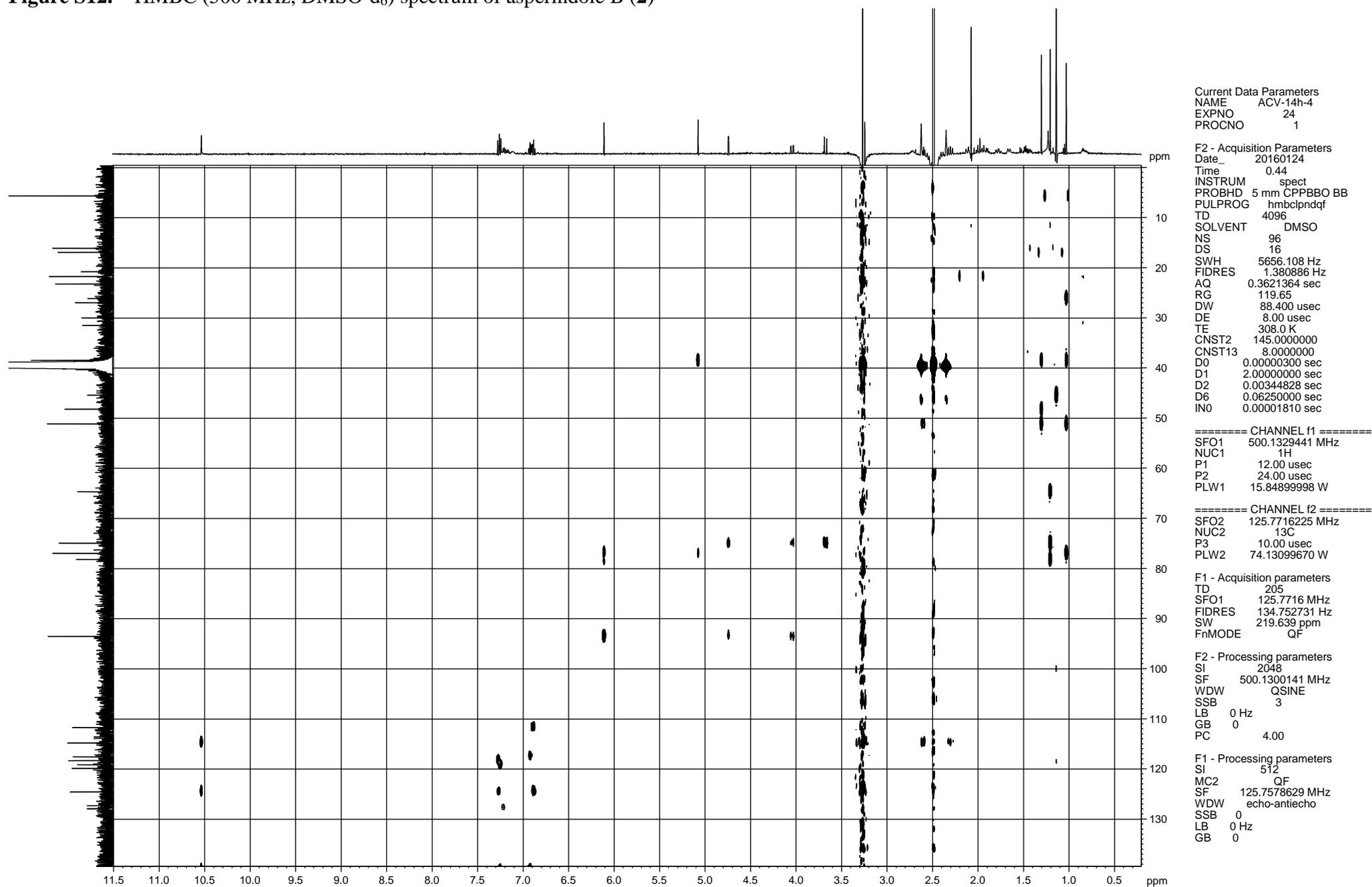


Figure S13. ROESY (500 MHz, DMSO-d₆) spectrum of asperindole B (2)

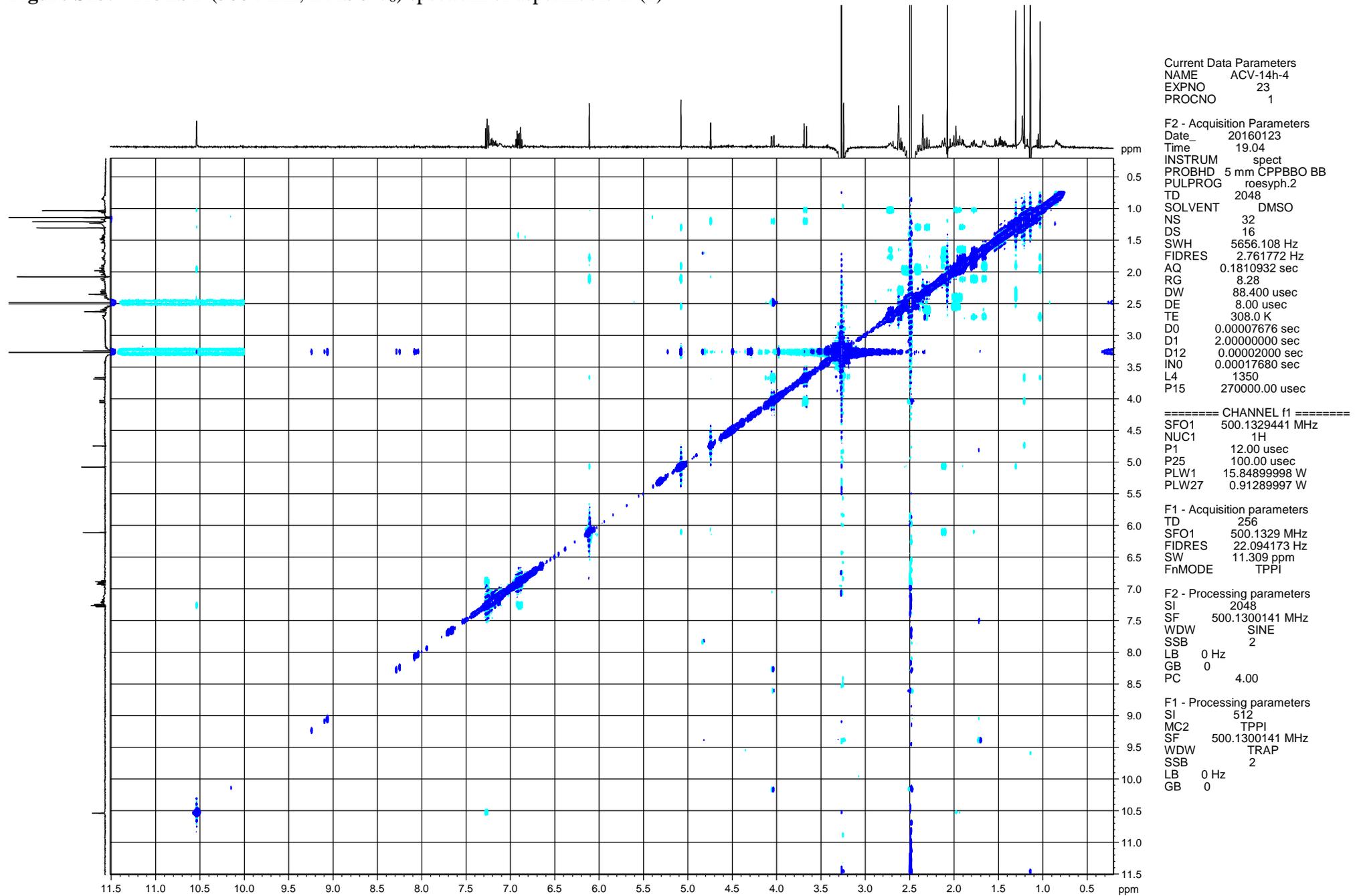
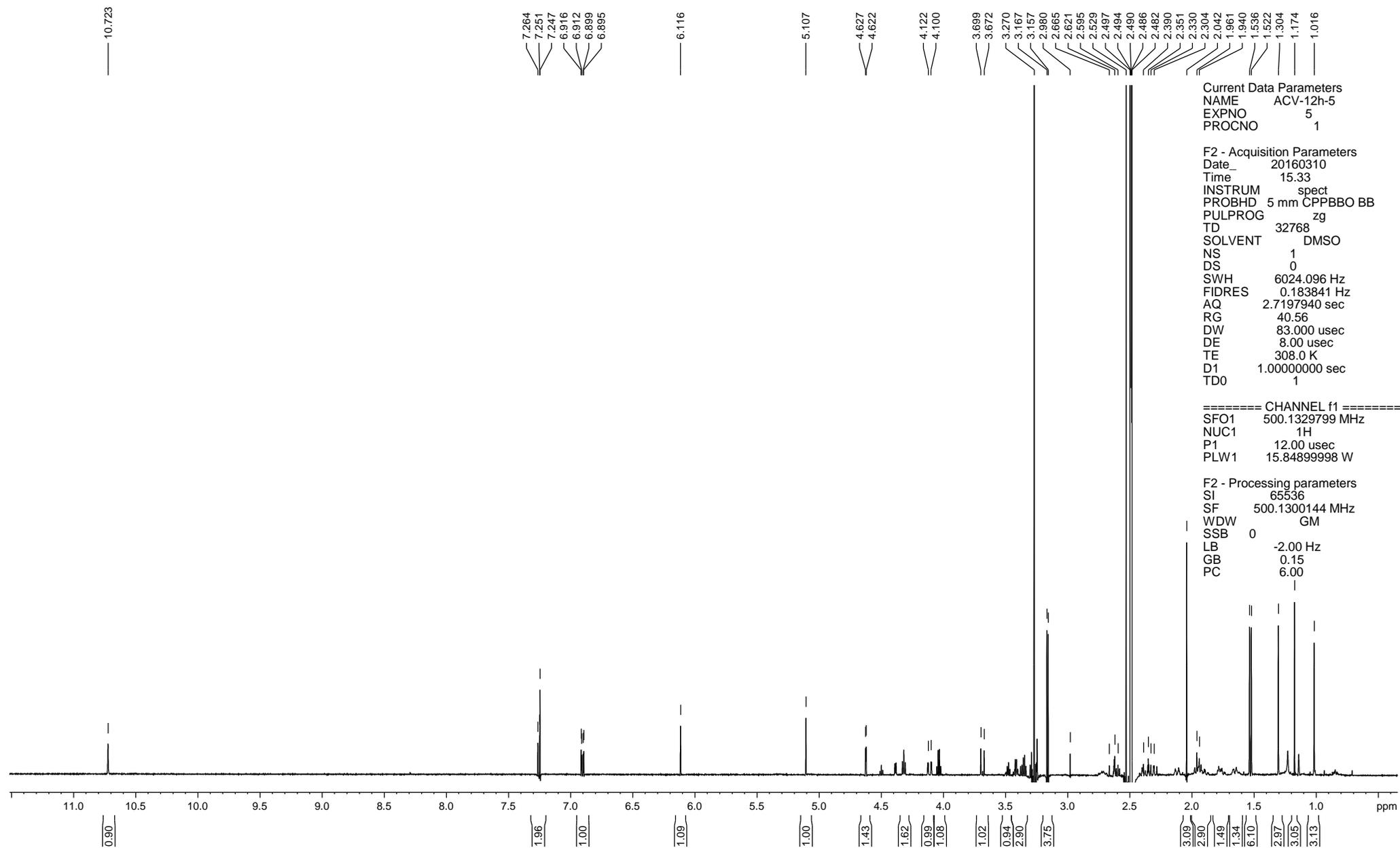


Figure S14. ^1H NMR (500 MHz, DMSO-d₆) spectrum of asperindole C (**3**)



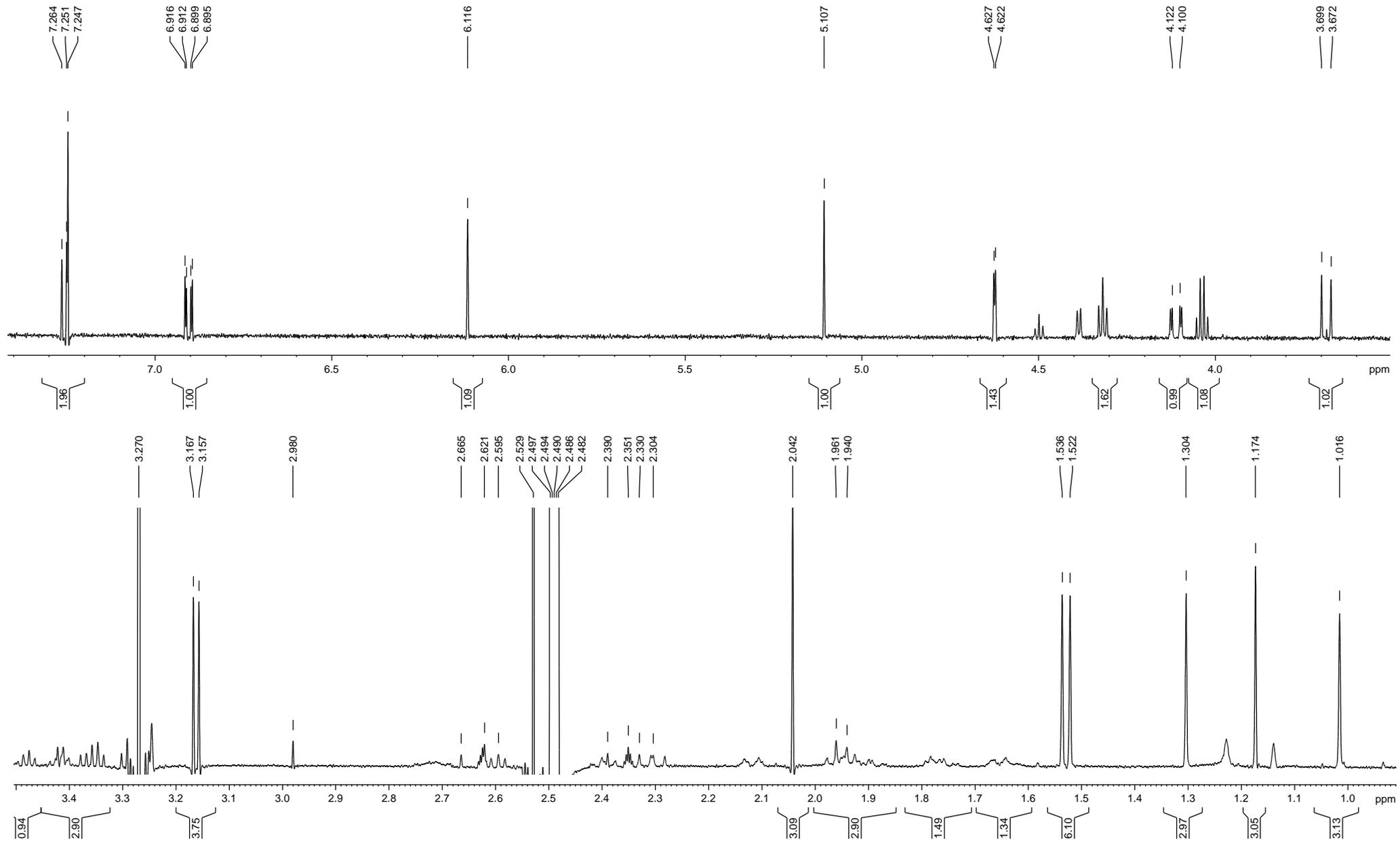


Figure S15. ^{13}C NMR (125 MHz, DMSO-d₆) spectra of asperindole C (**3**)

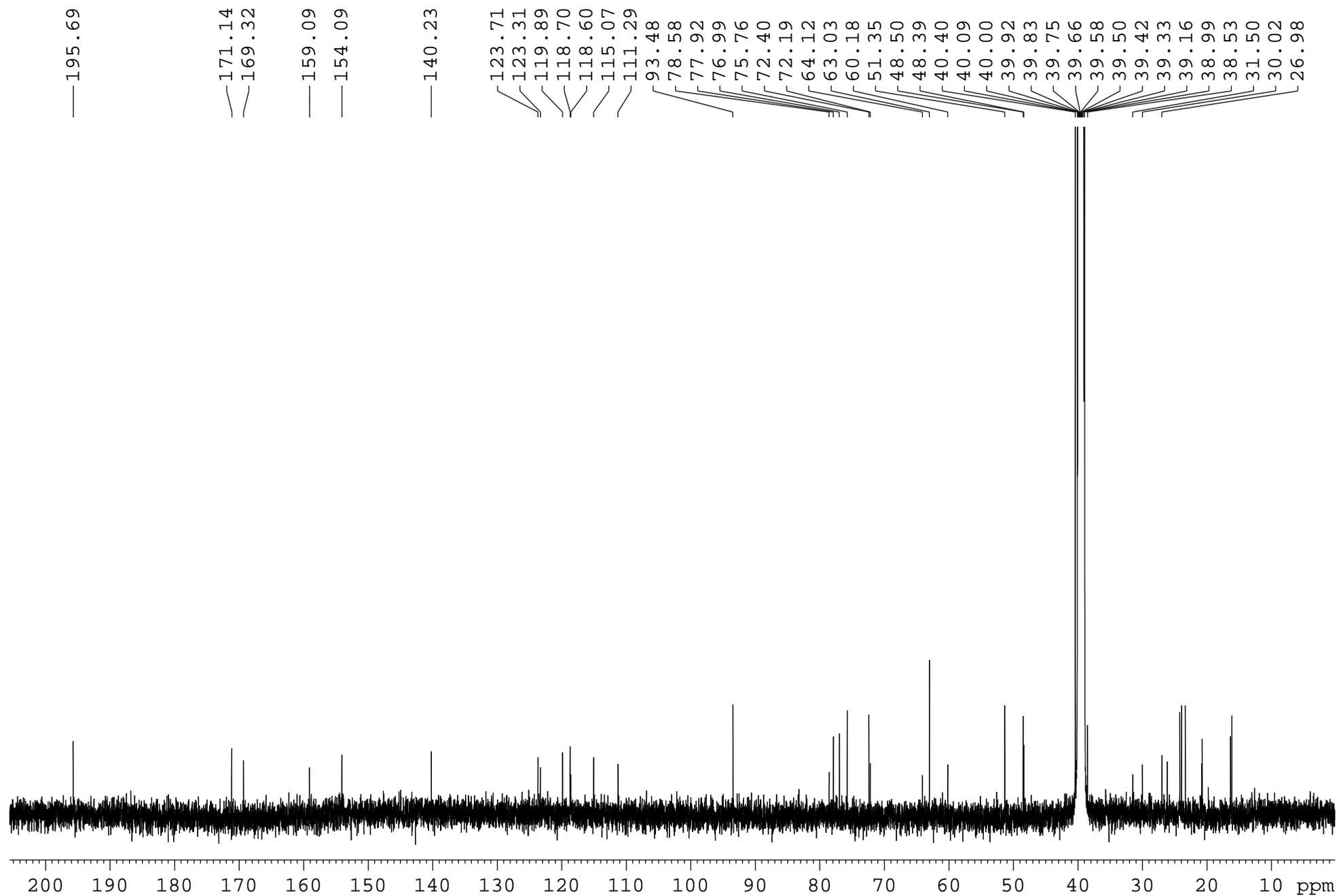


Figure S16. DEPT-135 (125 MHz, DMSO-d₆) spectrum of asperindole C (**3**)

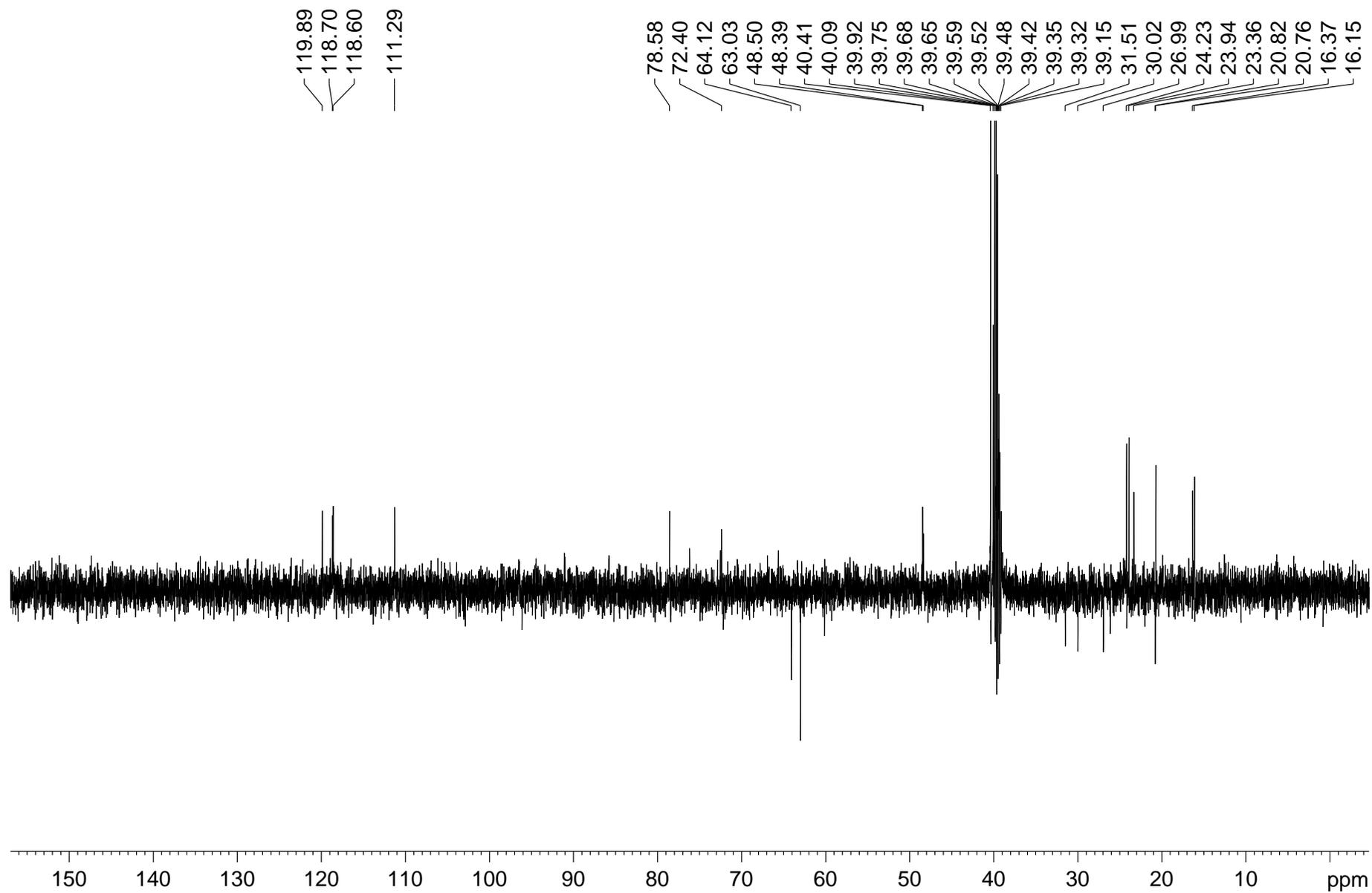


Figure S17. ^1H - ^1H COSY (500 MHz, DMSO-d₆) spectrum of asperindole C (3)

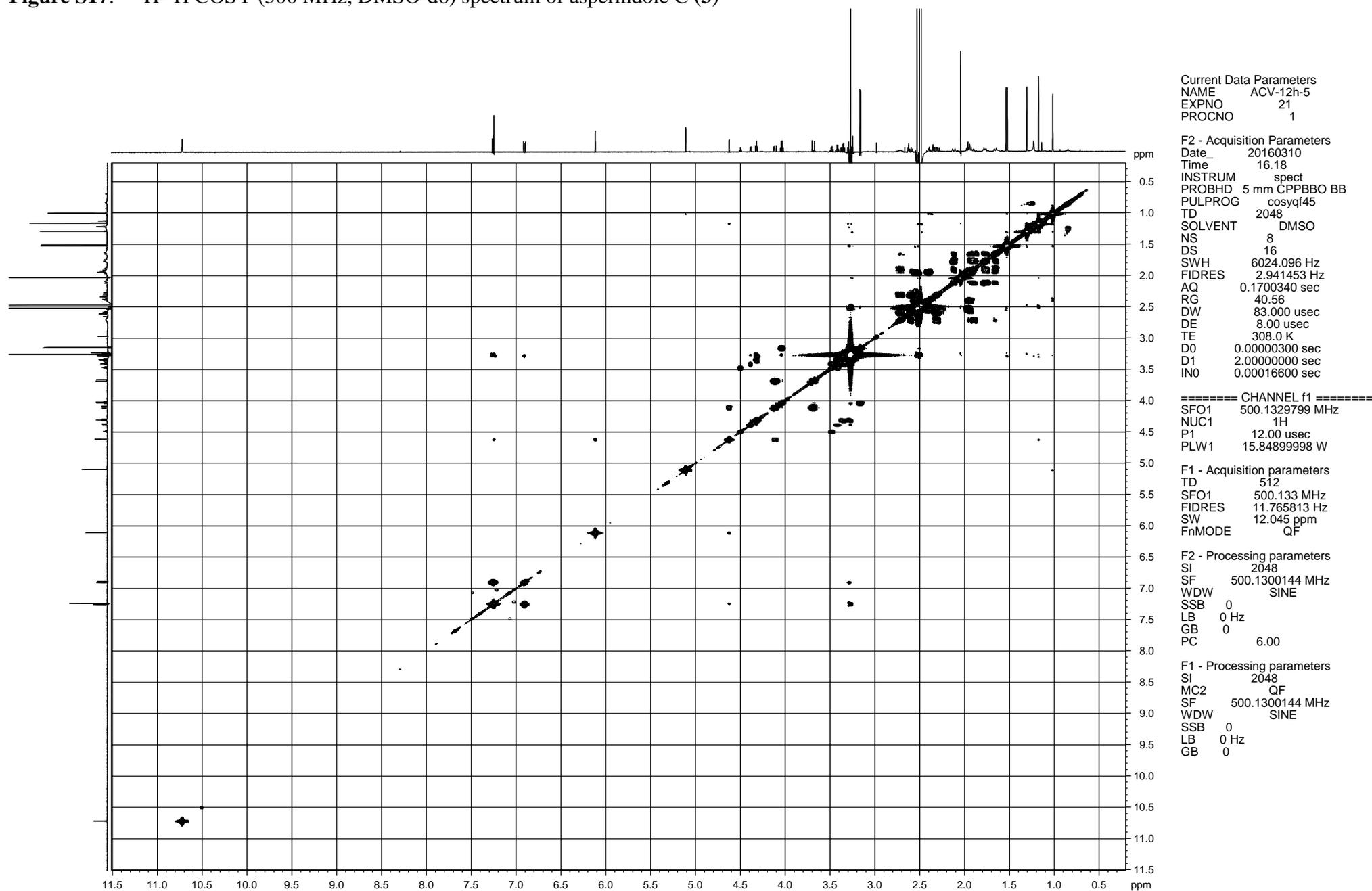


Figure S18. HSQC (500 MHz, DMSO-d6) spectrum of asperindole C (3)

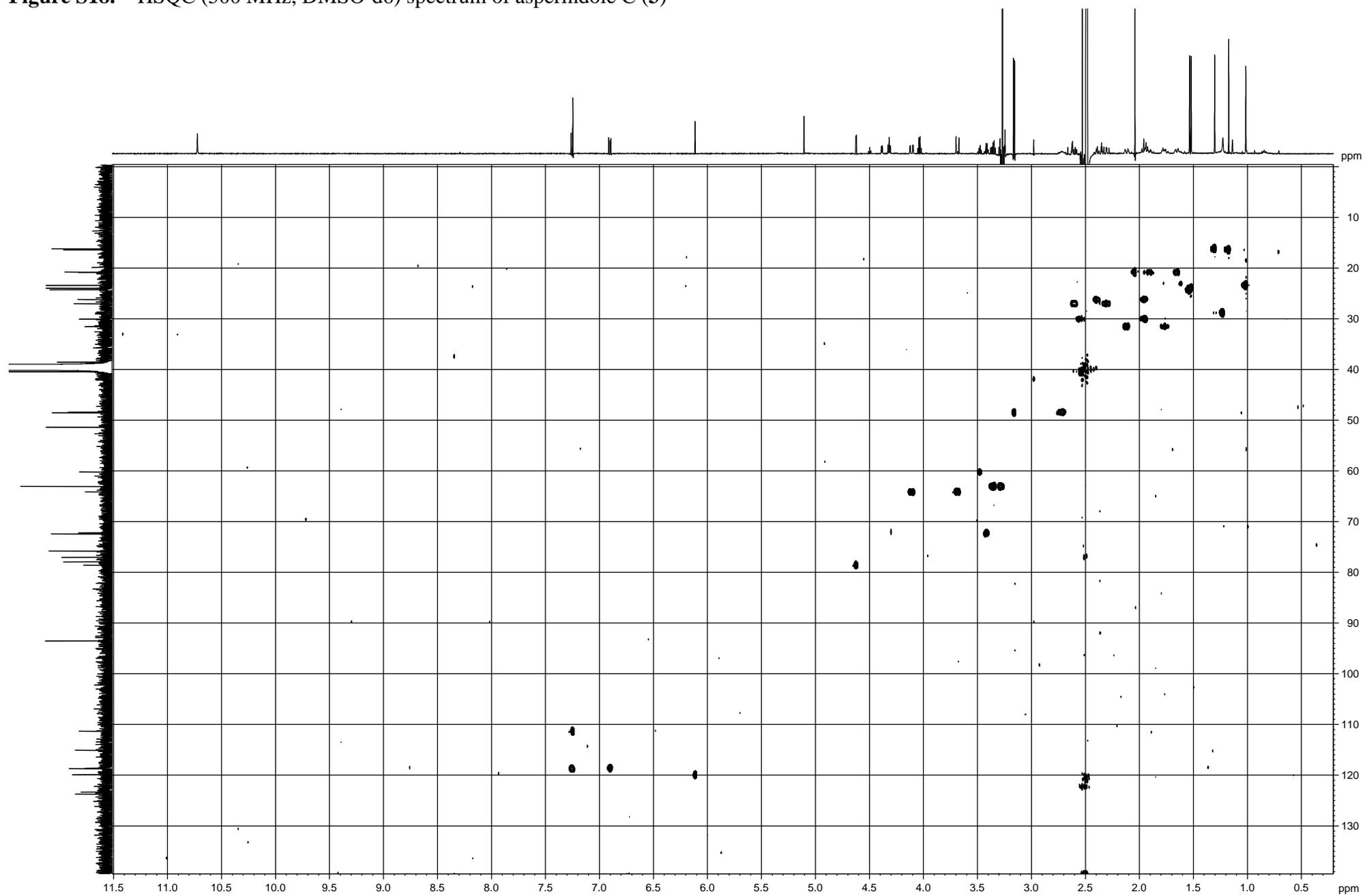


Figure S19. HMBC (500 MHz, DMSO-d₆) spectrum of asperindole C (3)

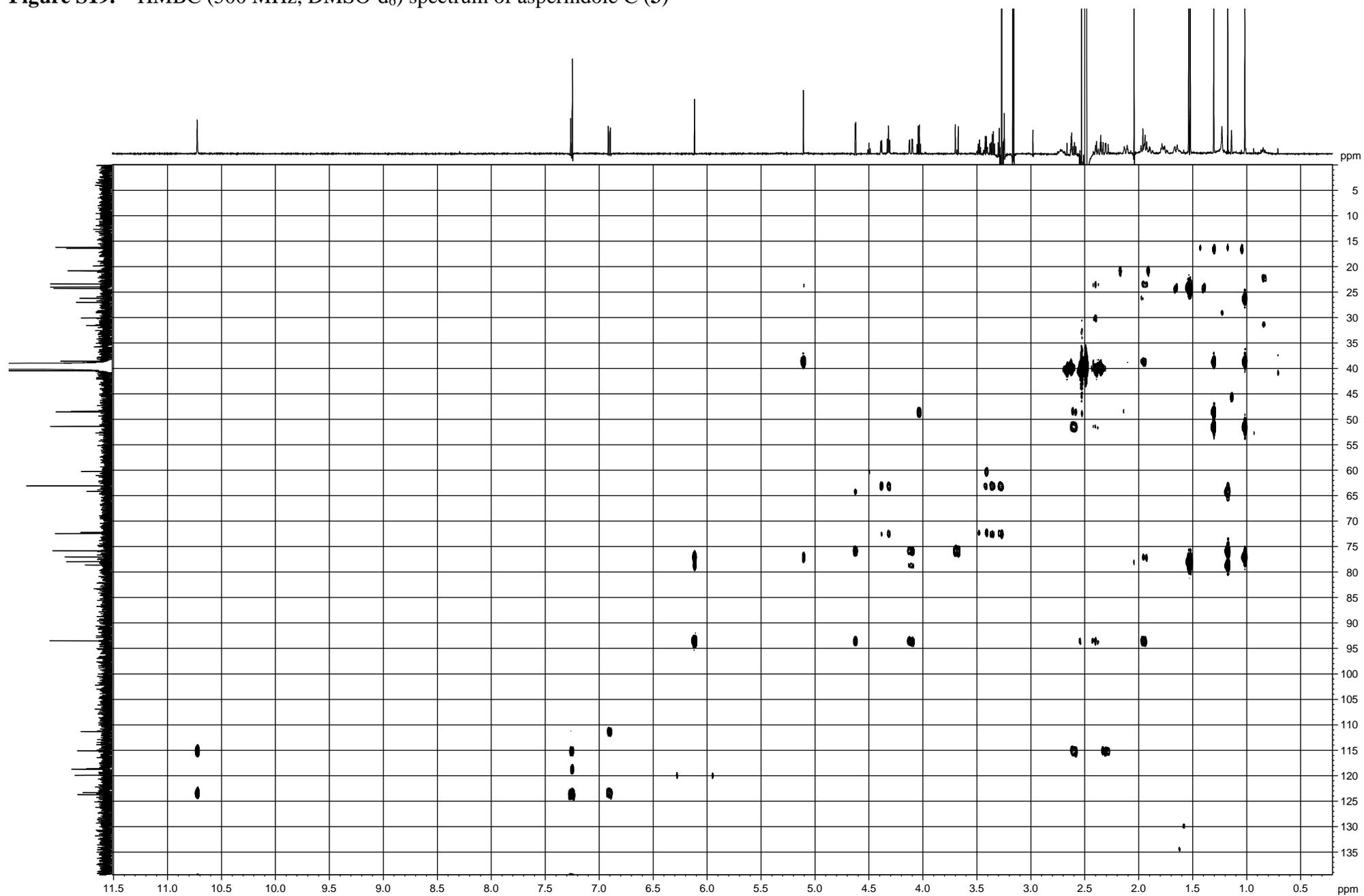


Figure S20. ROESY (500 MHz, DMSO-d₆) spectrum of asperindole C (3)

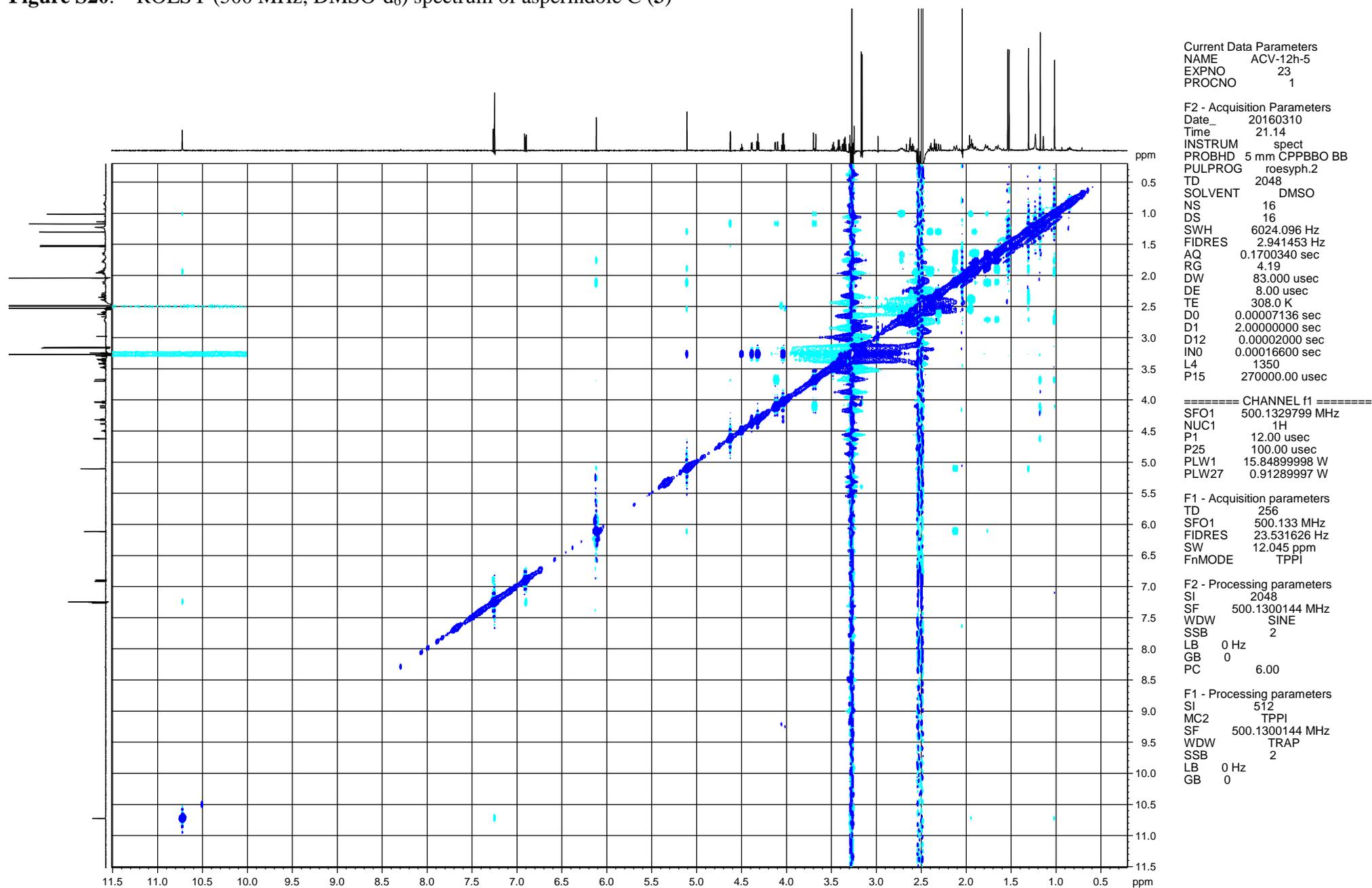


Figure S21. ^1H NMR (500 MHz, DMSO-d_6) spectrum of asperindole D (**4**)

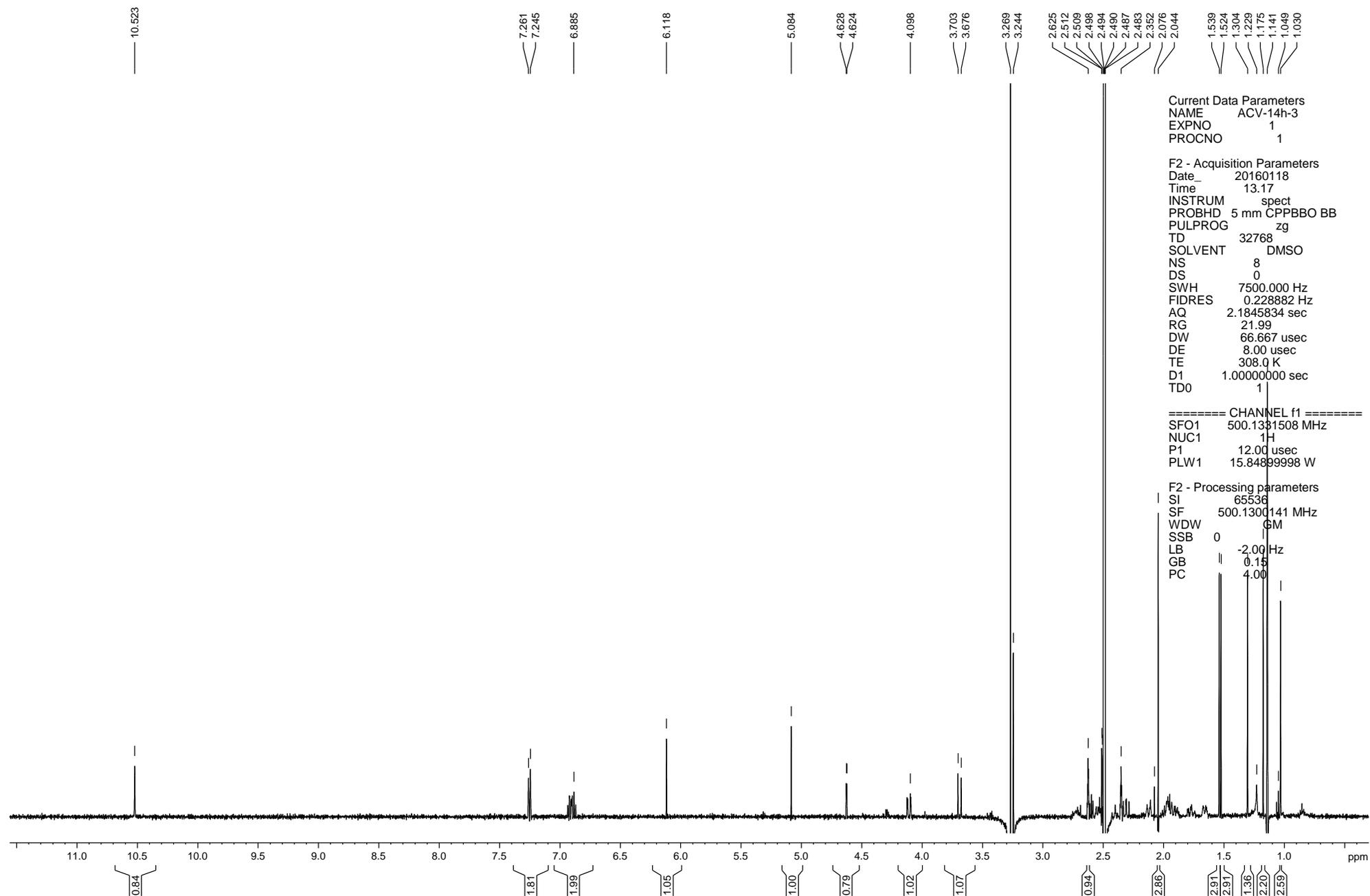


Figure S22. ^{13}C NMR (125 MHz, DMSO- d_6) spectra of asperindole D (4)

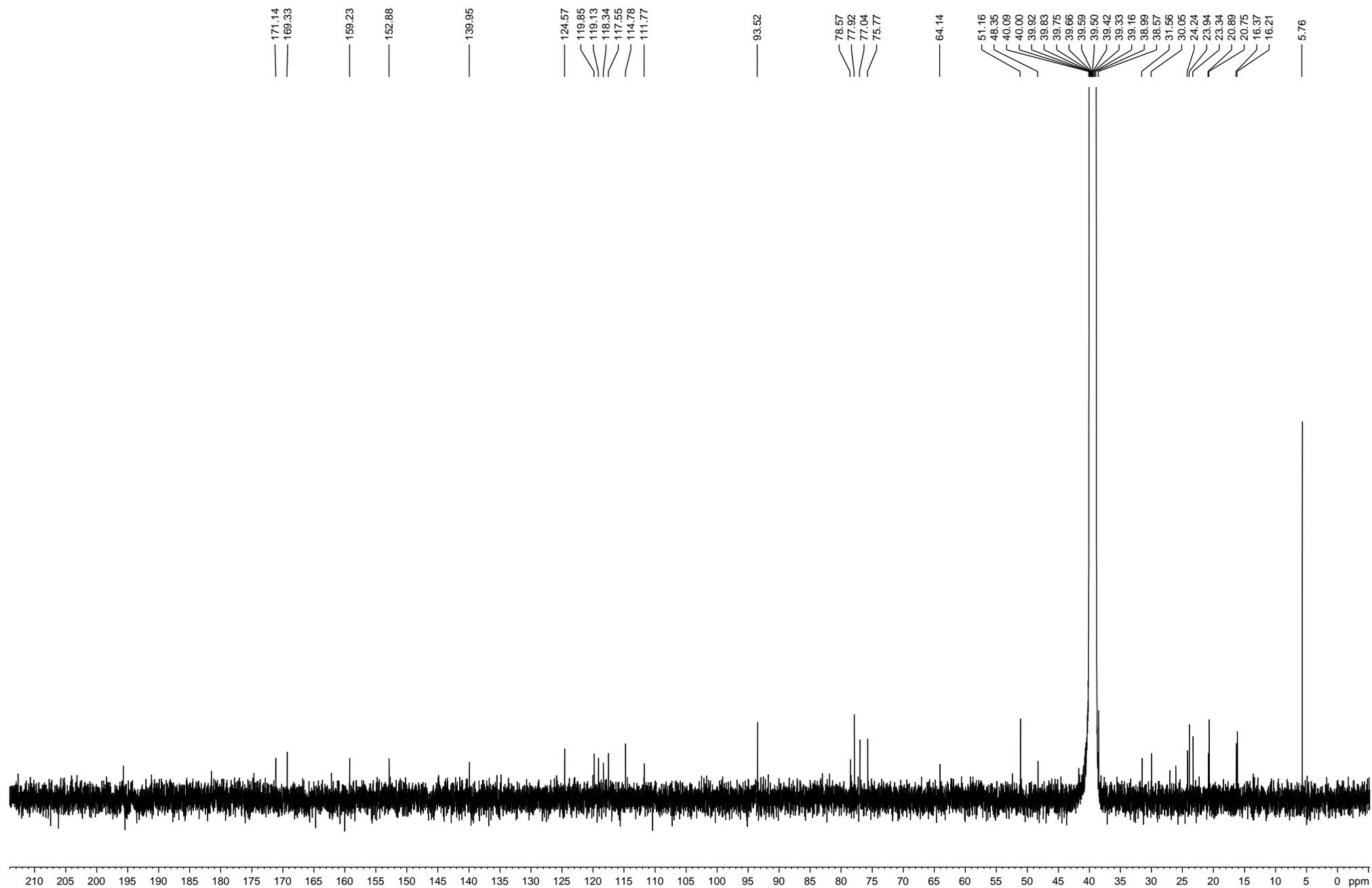


Figure S23. ^1H NMR (700 MHz, acetone- d_6) spectrum of 3''-hydroxyterphenyllin (**5**)

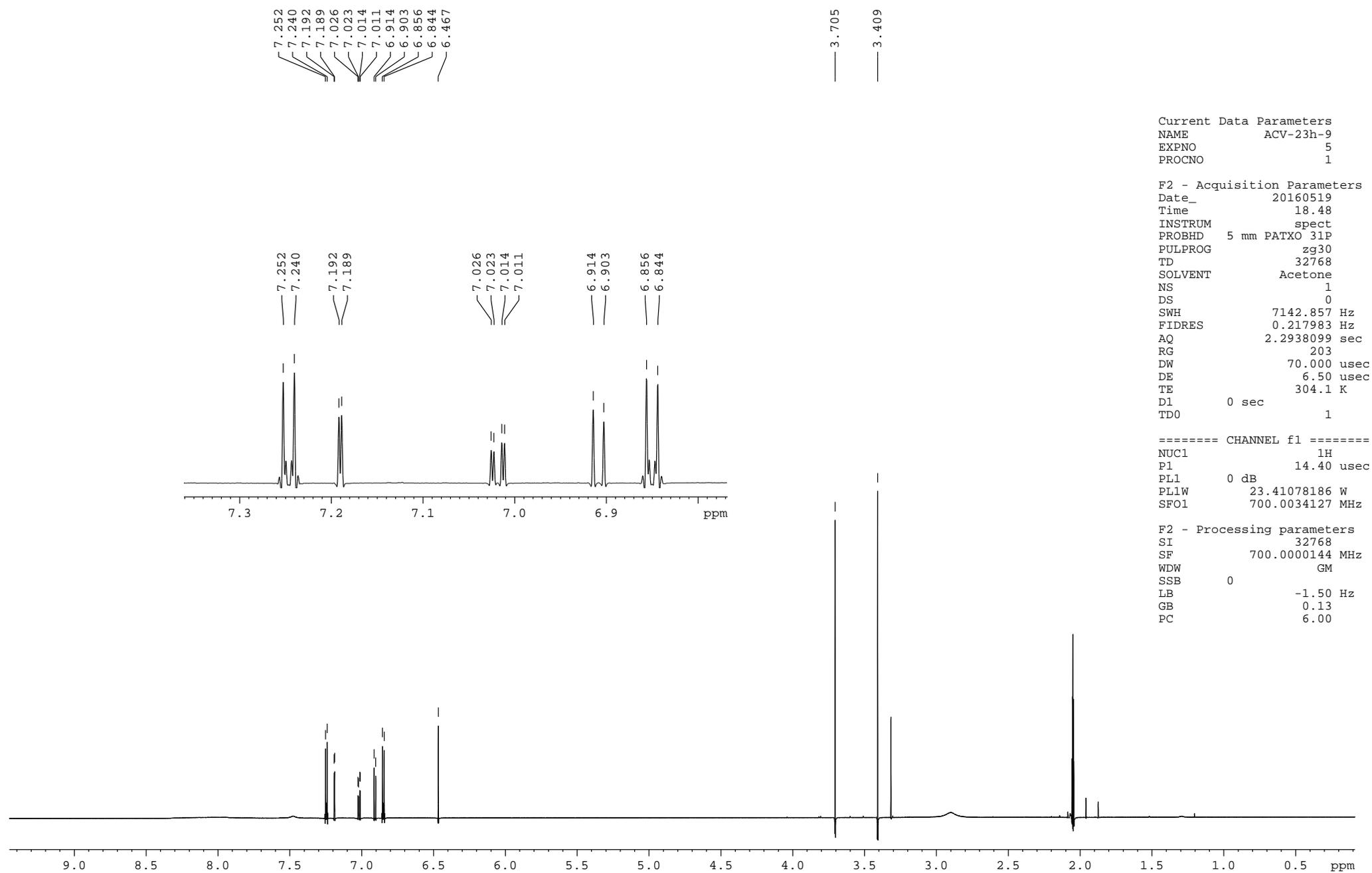


Figure S24. ^{13}C NMR (125 MHz, acetone- d_6) spectrum of 3''-hydroxyterphenyllin (**5**)

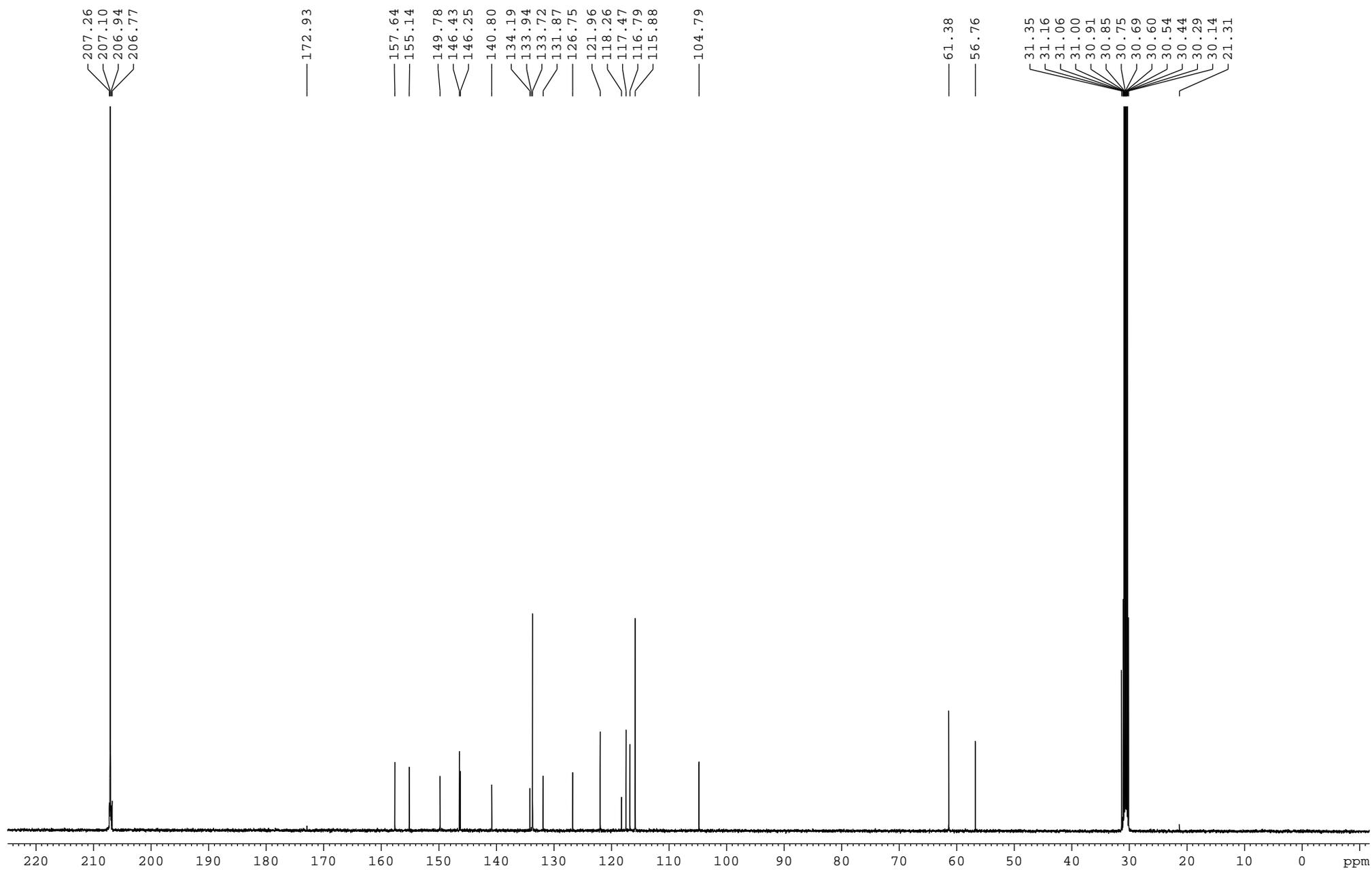


Figure S25. DEPT-135 (125 MHz, acetone-d₆) spectrum of 3''-hydroxyterphenyllin (**5**)

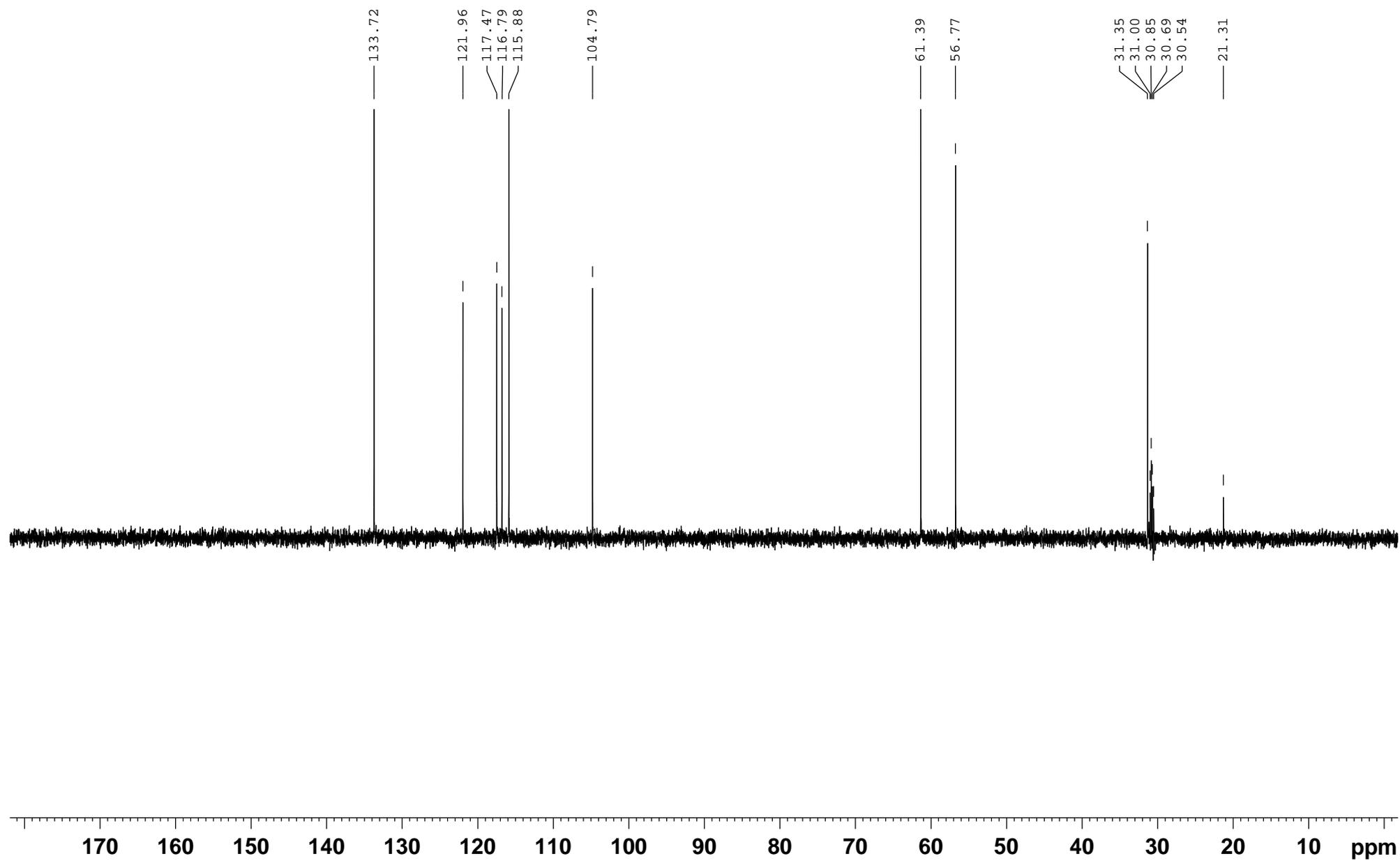


Figure S26. HSQC (700 MHz, acetone-d₆) spectrum of 3''-hydroxyterphenyllin (**5**)

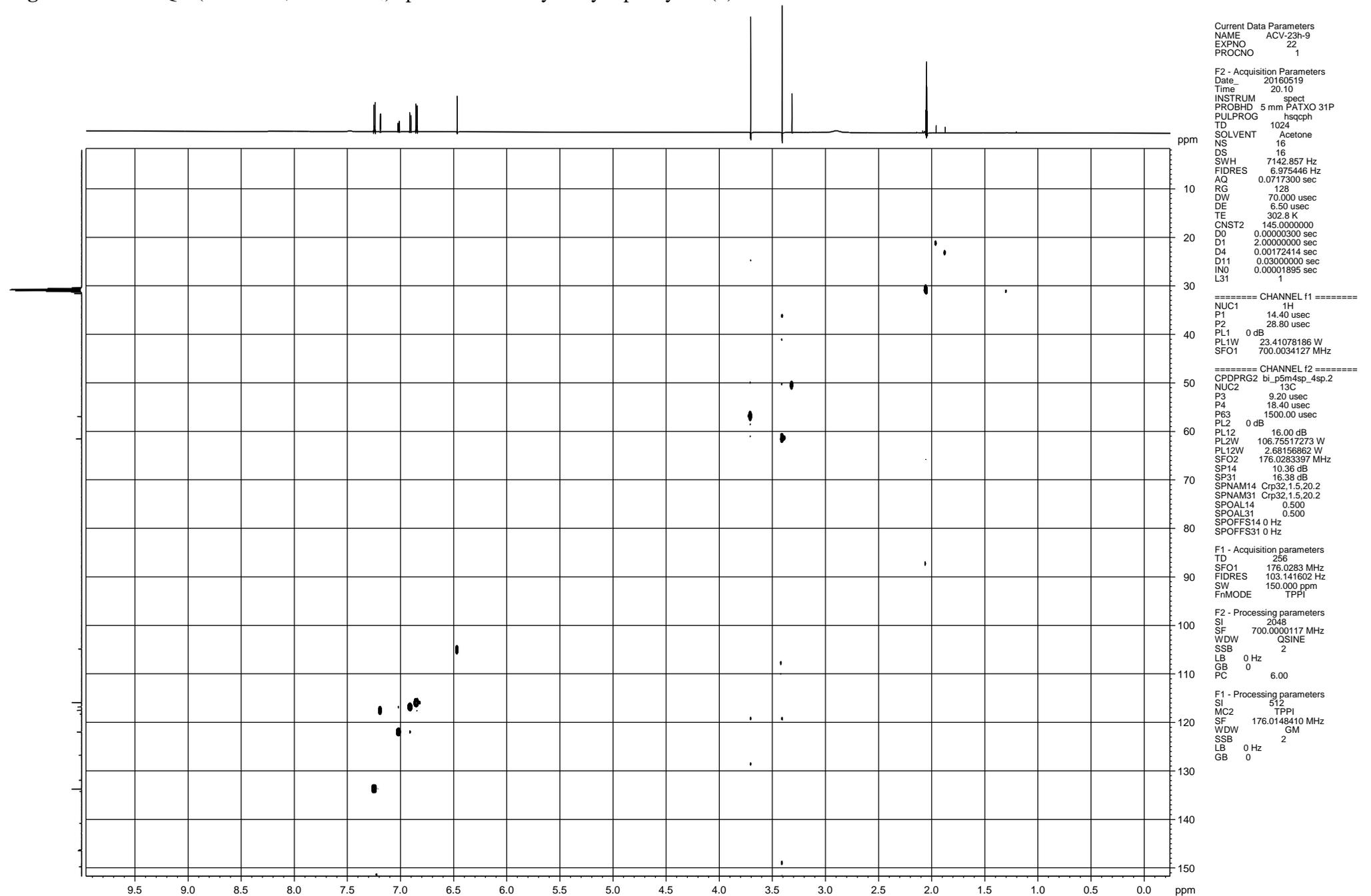


Figure S27. HMBC (700 MHz, acetone-d₆) spectrum of 3''-hydroxyterphenyllin (5)

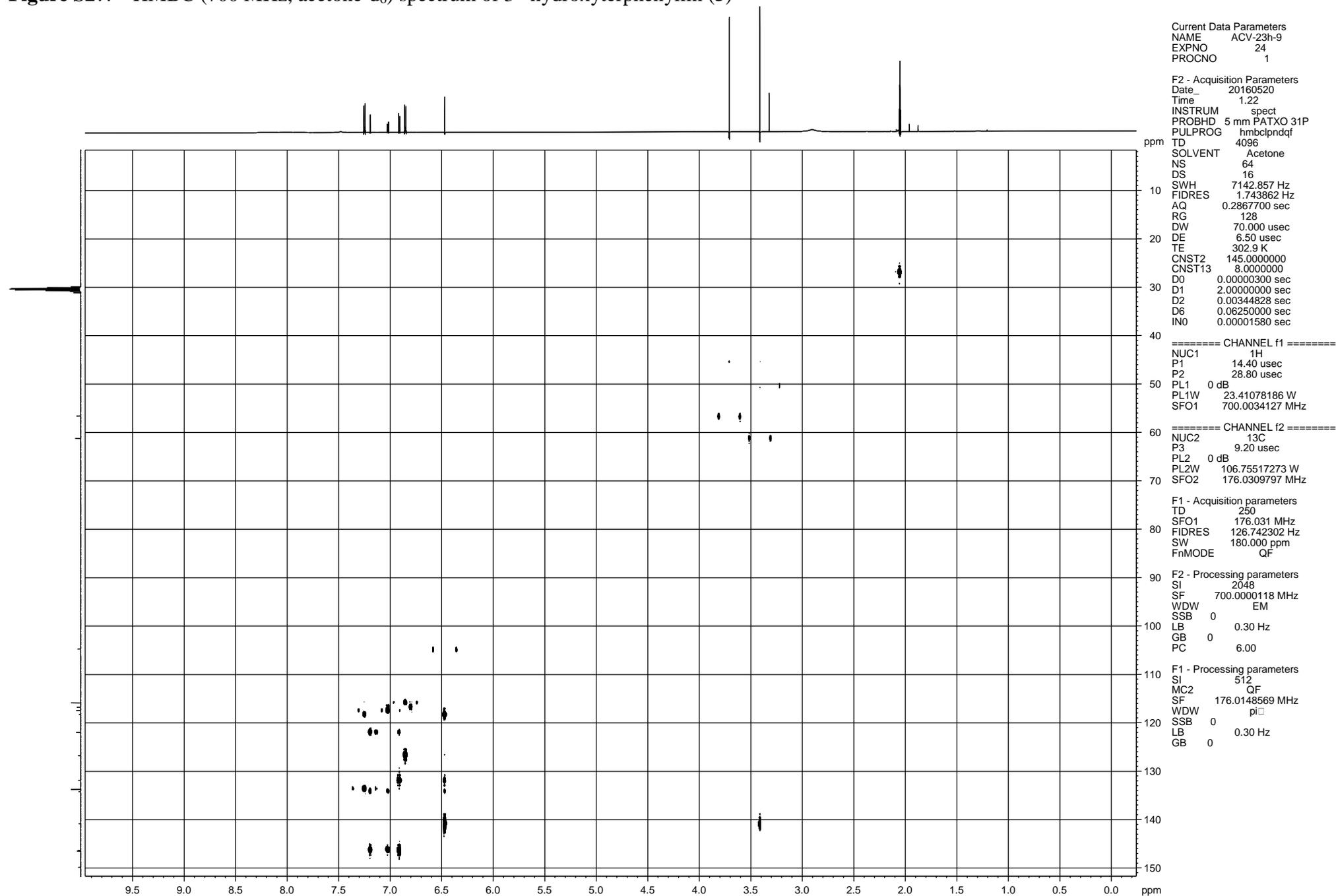


Figure S28. ROESY (700 MHz, acetone-d₆) spectrum of 3''-hydroxyterphenyllin (**5**)

