

Supplementary Materials

Cyclic Tetrapeptides with Synergistic Antifungal Activity from the Fungus *Aspergillus westerdijkiae* Using LC-MS/MS-Based Molecular Networking

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Table S1. Culture media with different compositions and conditions for *A. westerdijkiae*.

		Medium compositions	Conditions	
1	Rice medium	80 g rice/60 mL distilled wate	25°C	3 weeks
2	wheat medium	80 g wheat/60 mL distilled wate	25°C	3 weeks
3	Aspergillus Minimal Medium (AMM)	MgSO ₄ 0.24g; NaNO ₃ 6g; KCl 0.52g; KH ₂ PO ₄ 0.815; K ₂ HPO ₄ 1.05g; FeSO ₄ ·7H ₂ O 5mg; EDTA 0.05g; ZnSO ₄ ·7H ₂ O 22mg; H ₃ BO ₃ 11mg; MnCl ₂ ·7H ₂ O 5mg; CuSO ₄ ·5H ₂ O 1.6mg; (NH ₄) ₆ MO ₇ O ₂₄ ·7H ₂ O 1.1mg; Dextrose 1g	25°C 180 rpm	2 weeks
4	PDB	Potato Dextrose Broth 24 g in 1L distilled water	25°C 180 rpm	2 weeks

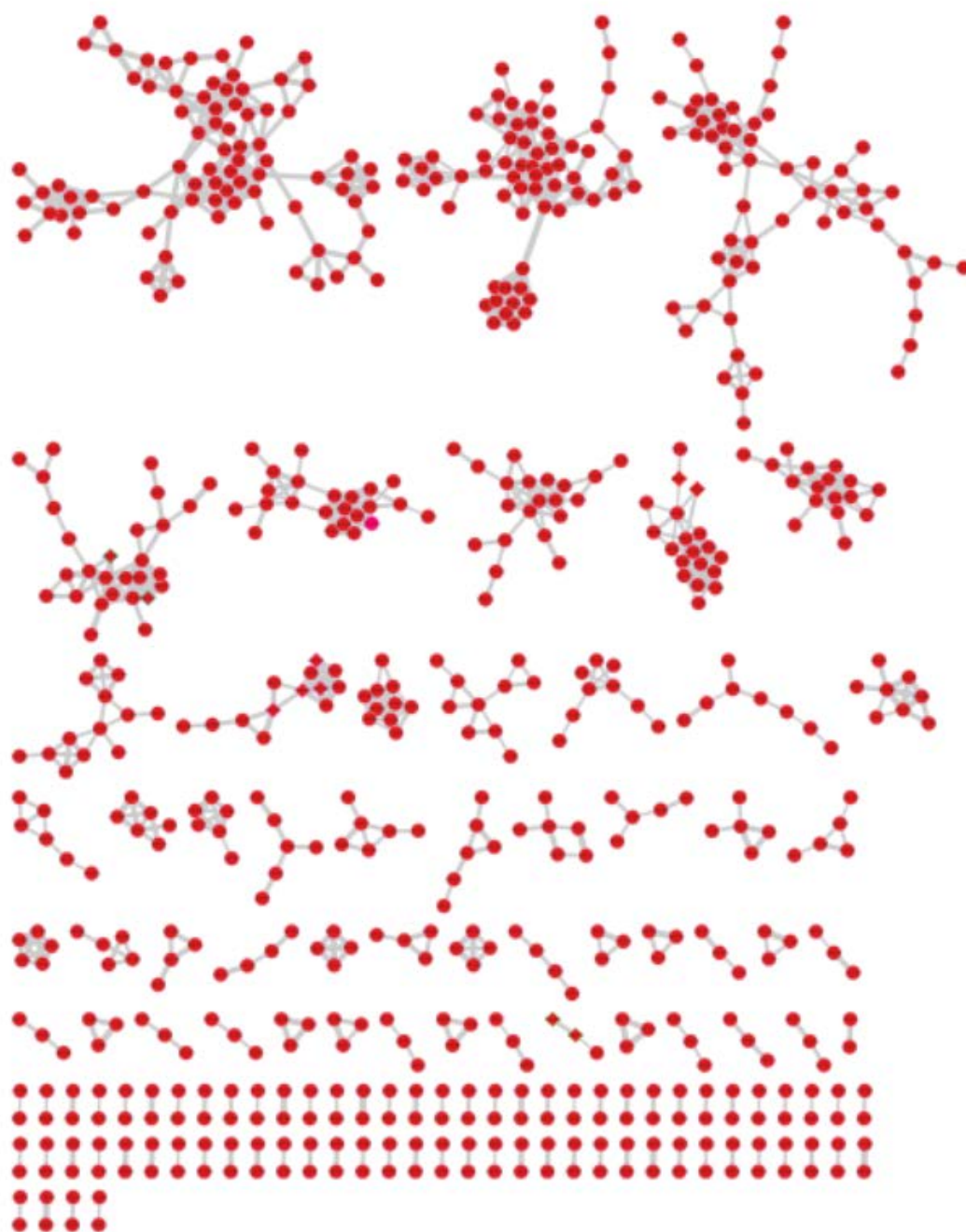
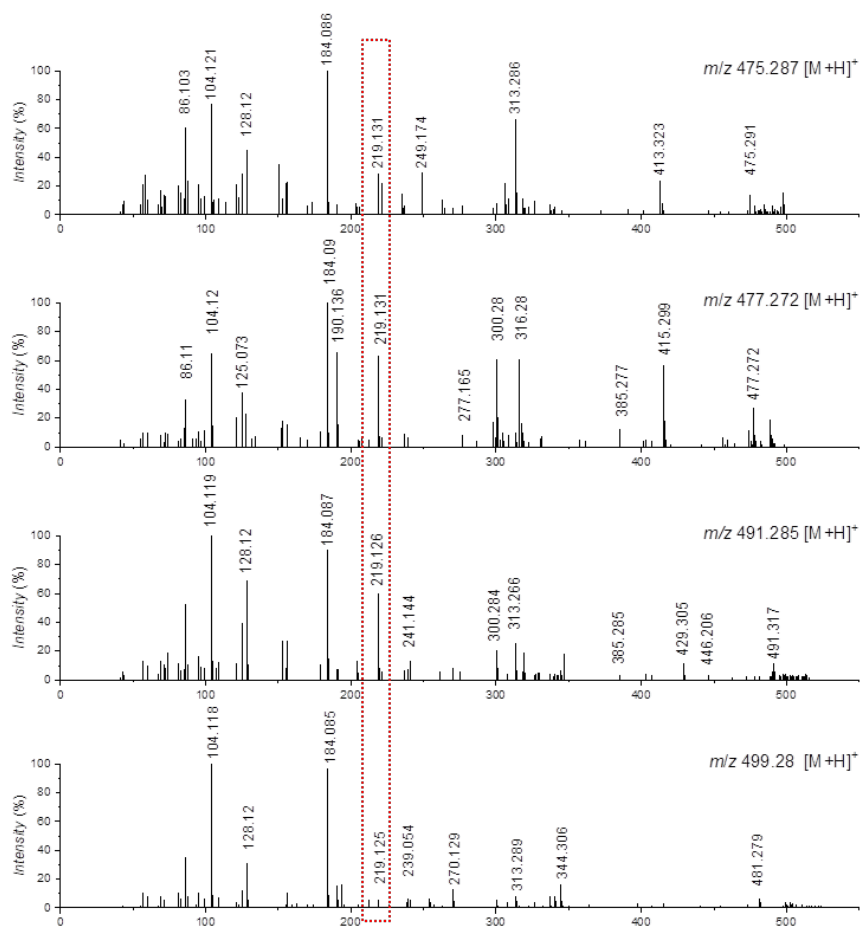
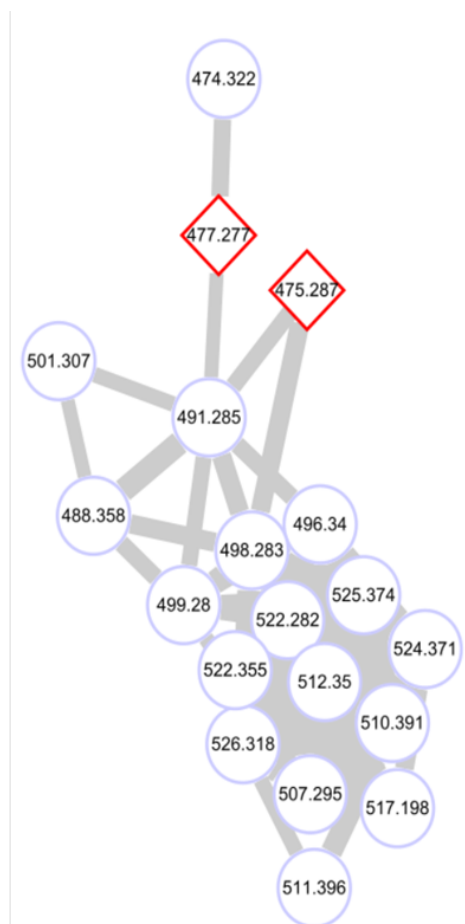
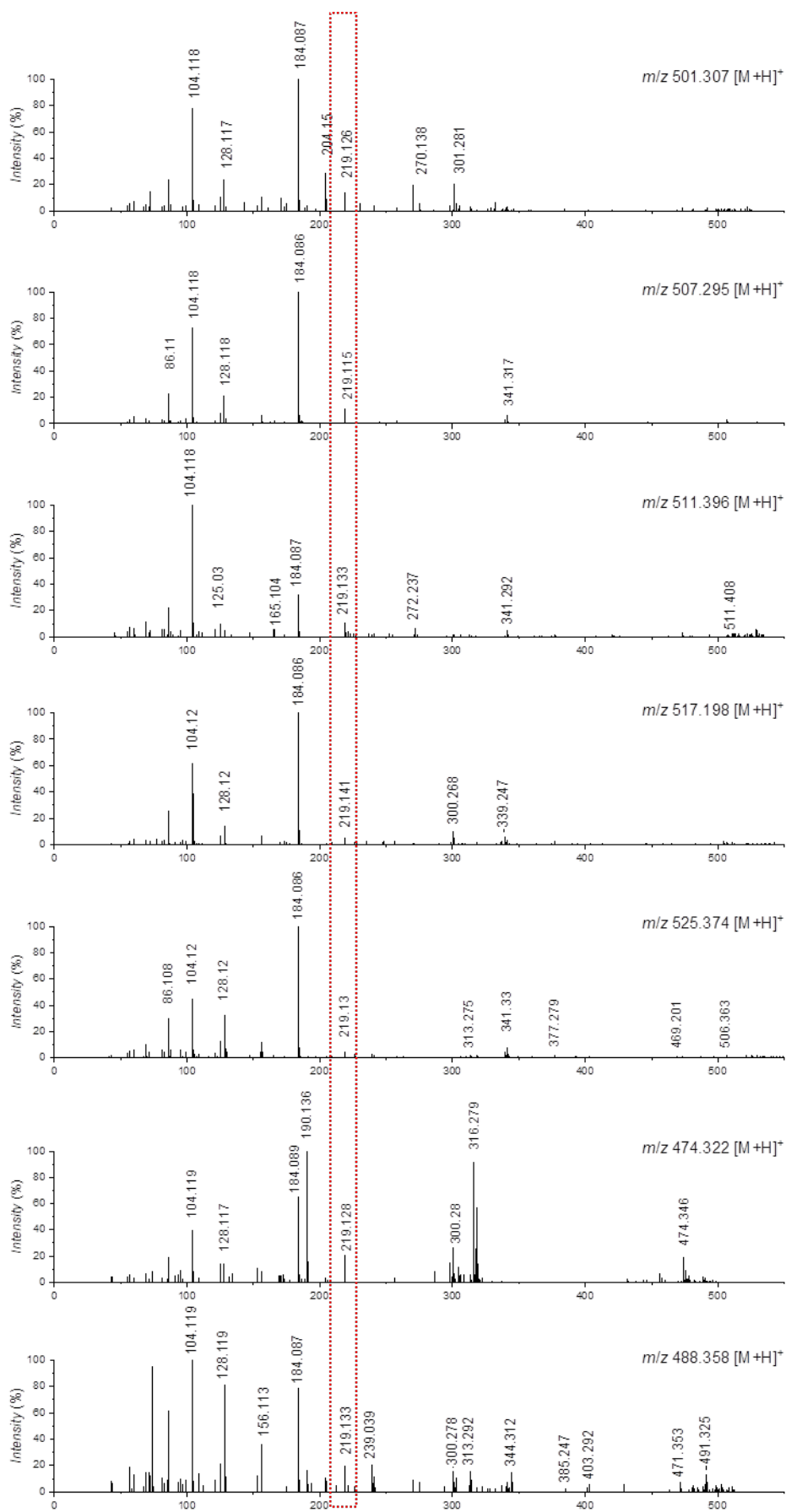


Figure S1. The molecular network obtained by combining the LC-MS/MS analyses of rice fermentation extract extracts from *A. Westerdijkiae* L1295





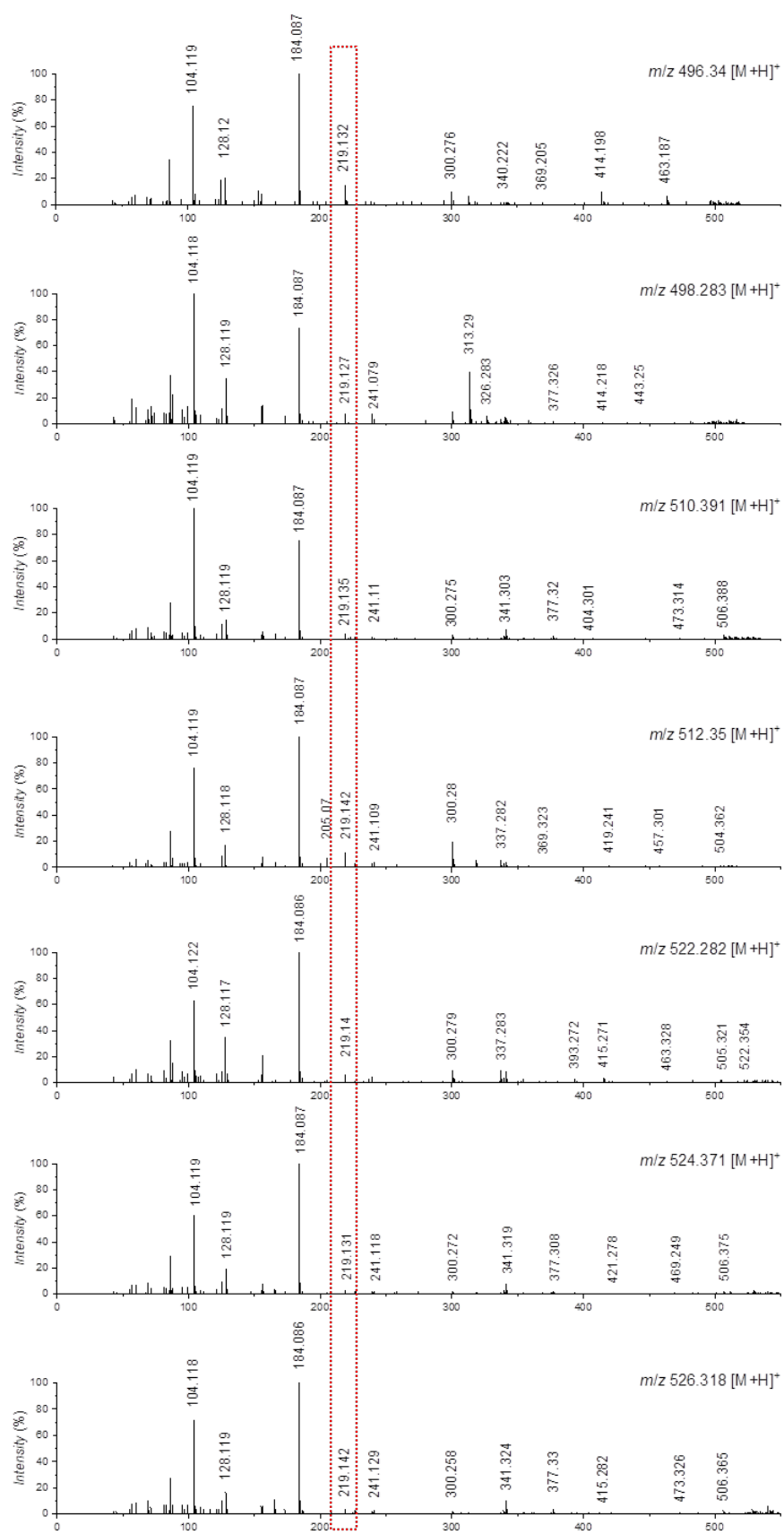


Figure S2. Cyclotetrapeptides -cluster and the MS/MS spectrum of each node

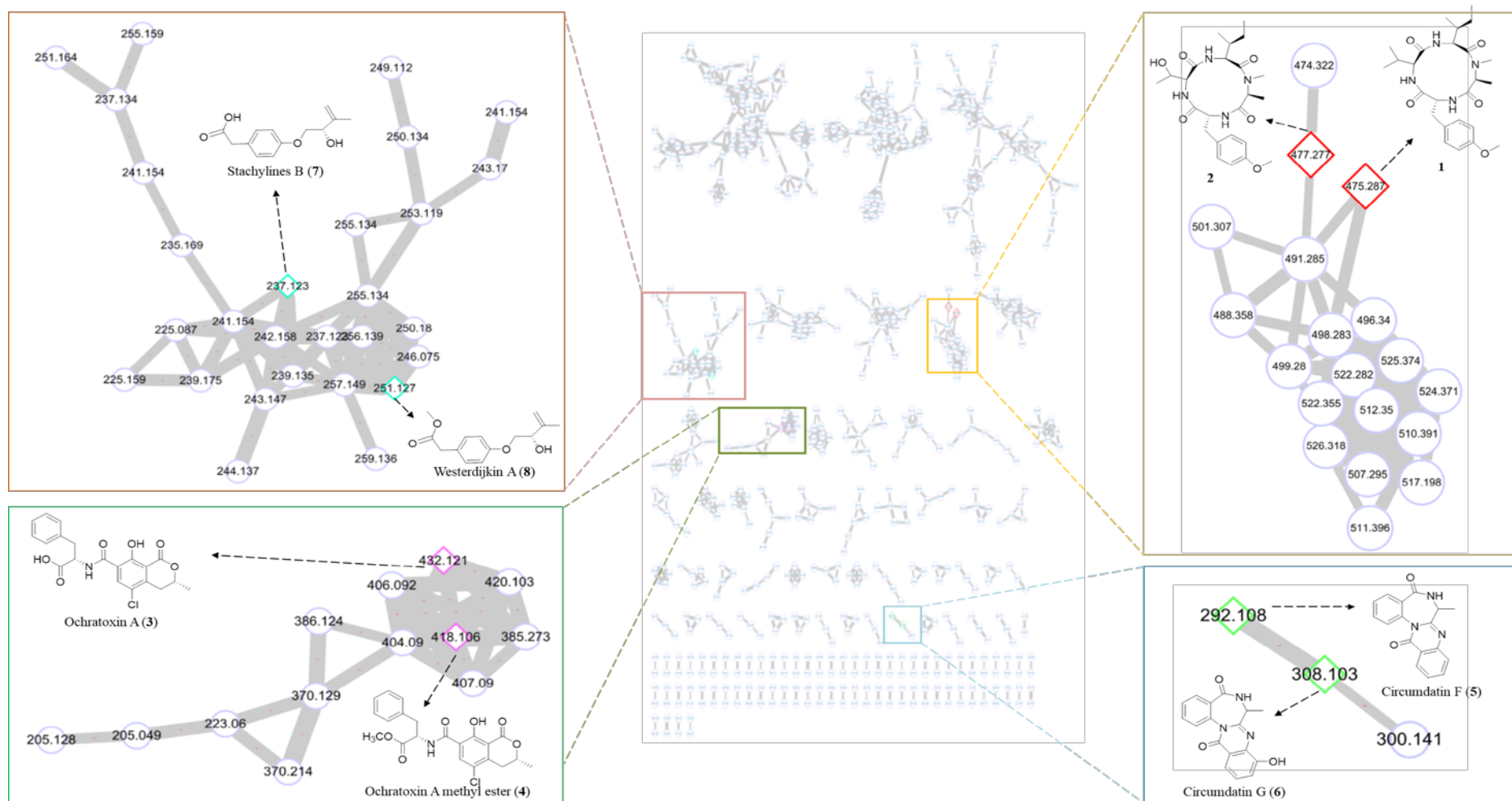


Figure S3. The cluster corresponding to compounds observed in the molecular networking

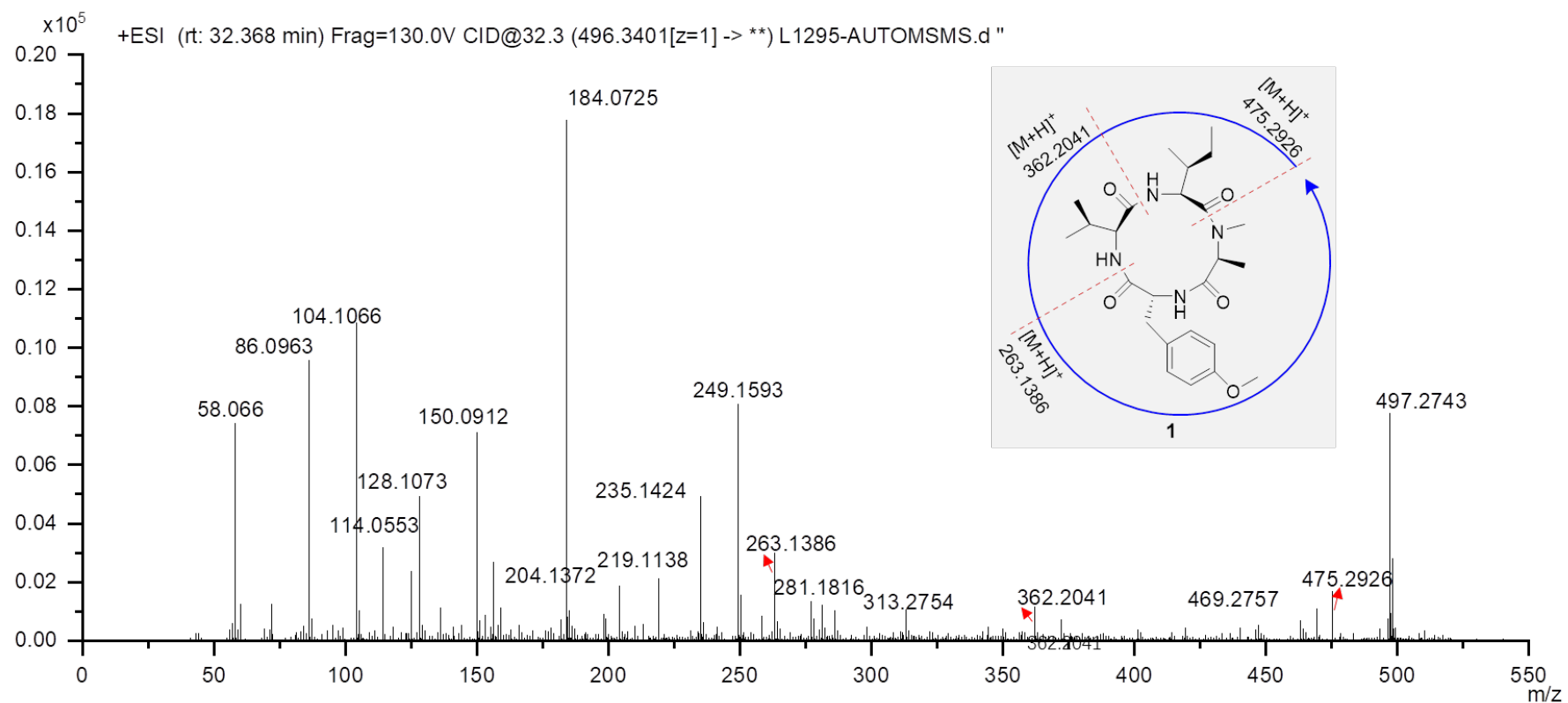


Figure S4. The ESI-MS/MS spectrum of **1**.

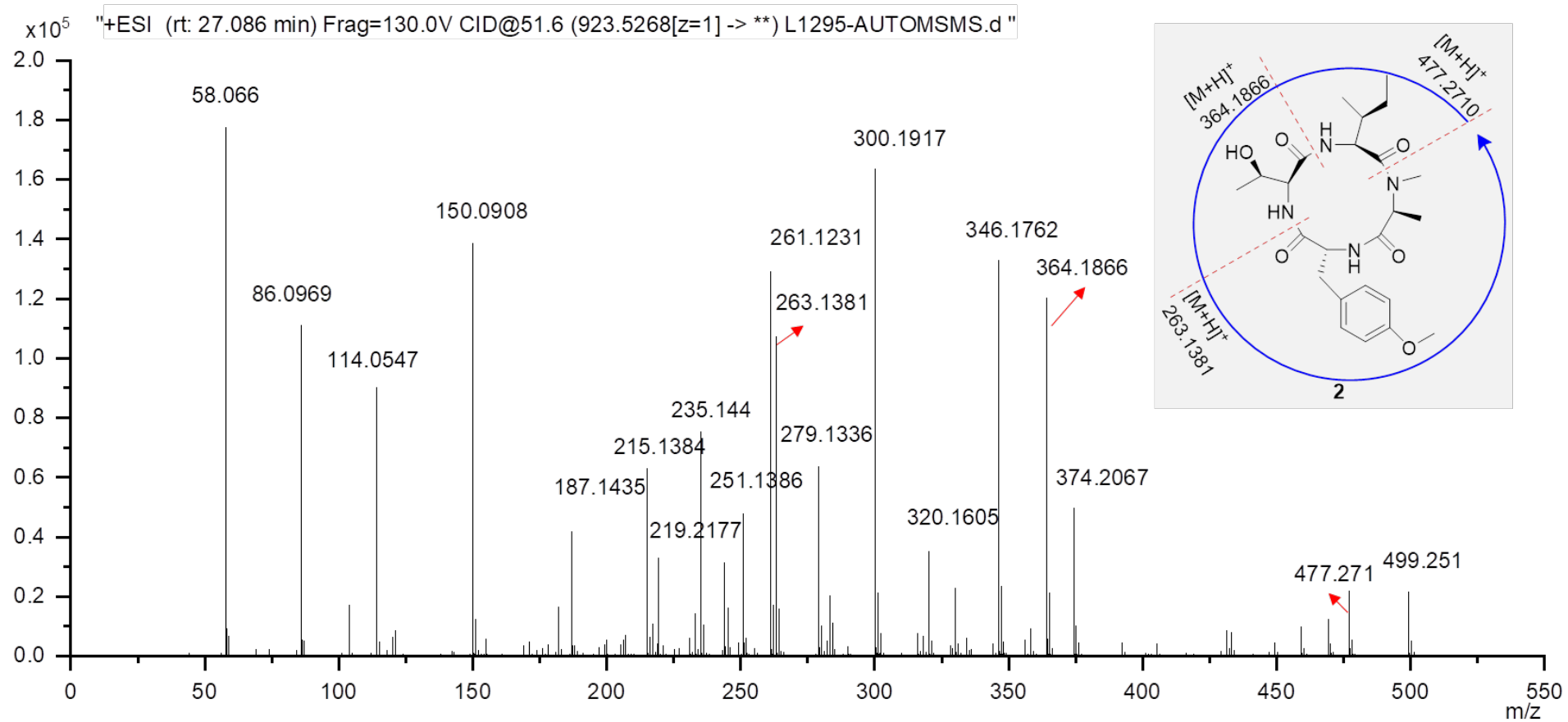


Figure S5. The ESI-MS/MS spectrum of 2.

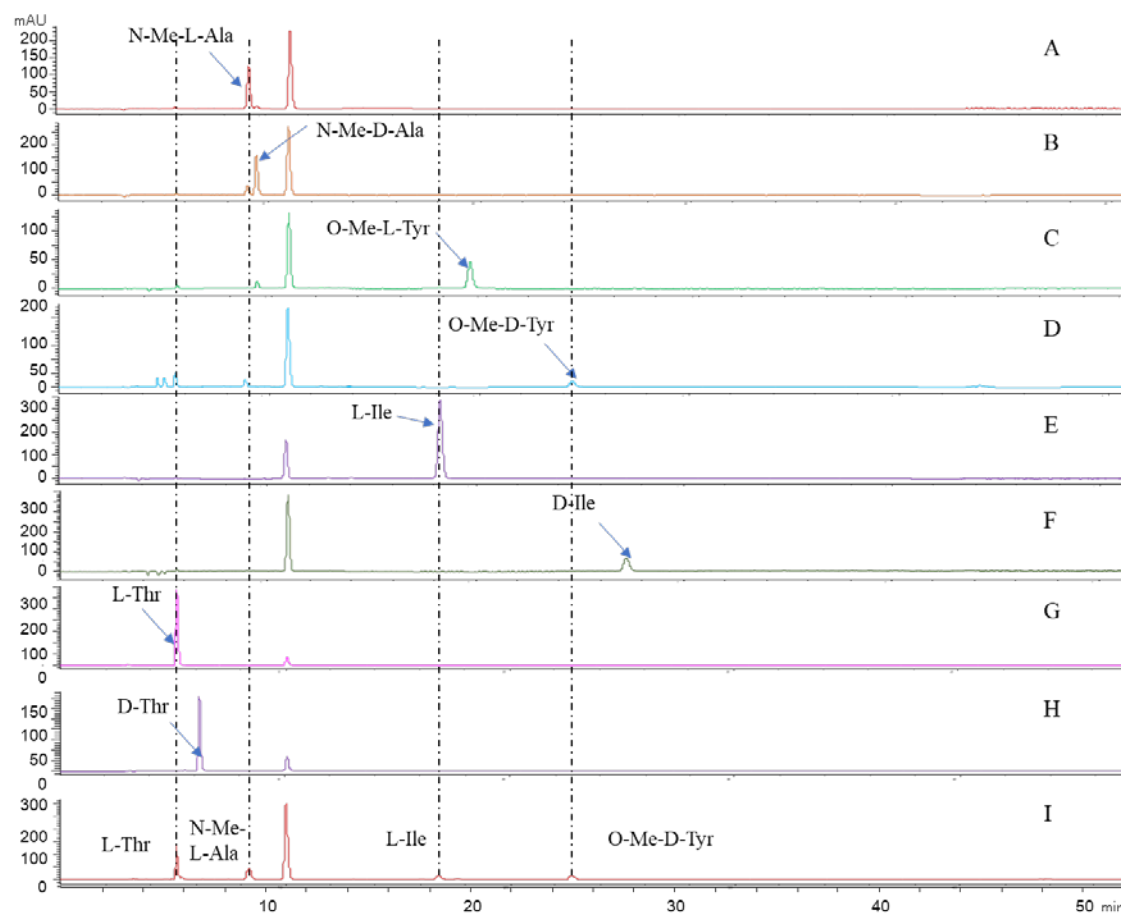


Figure S6. Advanced Marfey's analysis of compound **2**. (A-H): The retention times for the FDAA derivatives of *N*-Me-L-Ala, *N*-Me-D-Ala, *O*-Me-L-Tyr, *O*-Me-D-Tyr, L-Ile, D-Ile, L-Thr, and D-Thr, respectively. (I): The FDAA derivatives of the hydrolysate of **2**. The derivatives of the acid hydrolysate and the standard amino acids were subjected to RP HPLC analysis (Kromasil C18 column; 5 μ m, 4.6 \times 250mm; 1.0 mL/min; UV detection at 340 nm) with a linear gradient of acetonitrile (35%-45%) in water (TFA, 0.01%) over 40 min.

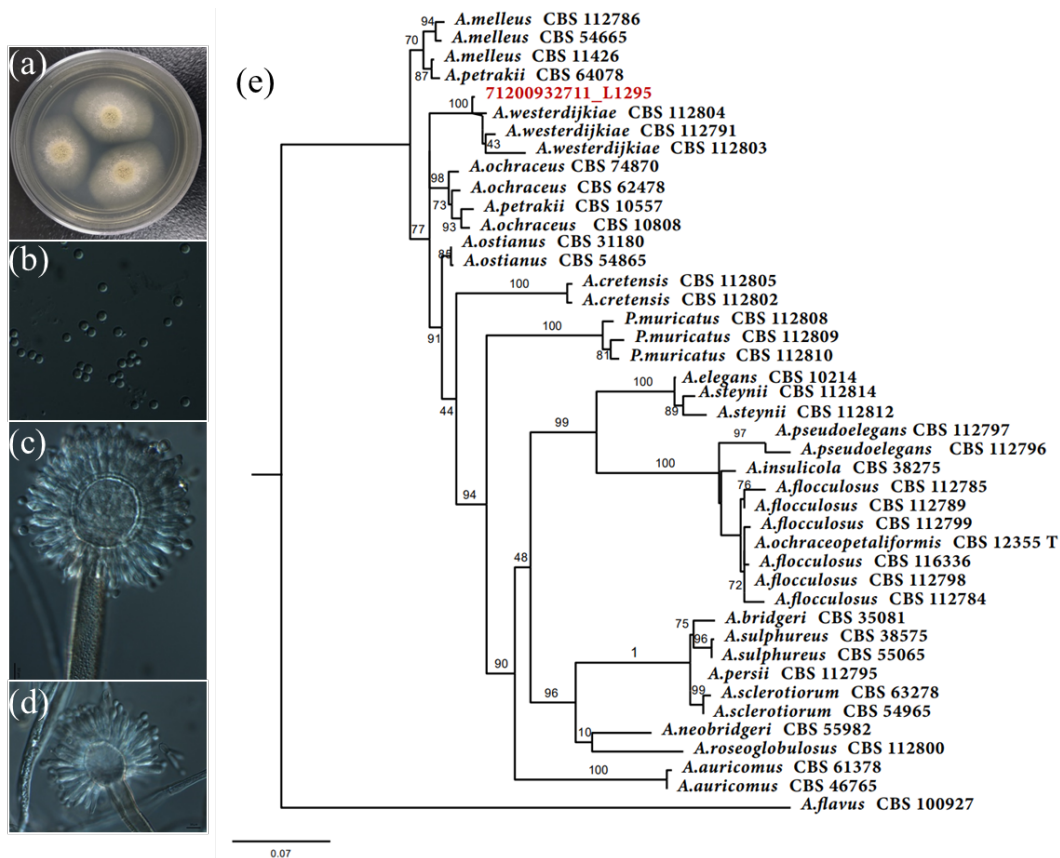


Figure S7. Phylogenetic analysis and morphological characters of *Aspergillus westerdijkiae* (a): Colonies on PDA after 7 d; (b): Conidiophores; (c-d): Conidia. Scale bars: b–d = 10 μ m; (e). Phylogenetic analysis of *A. westerdijkiae* based on β -tubulin dataset.

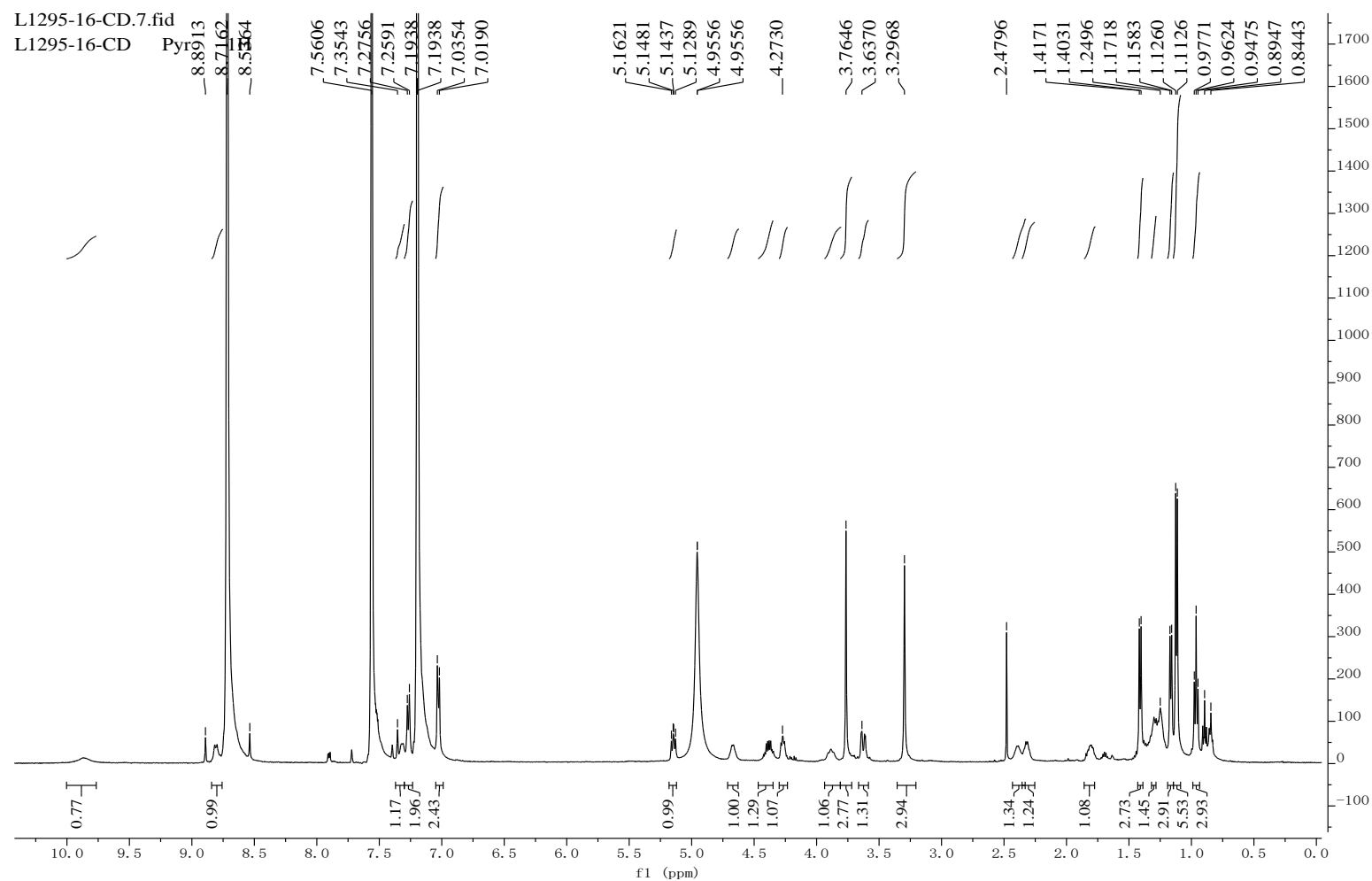


Figure S8. ^1H NMR spectrum of westertide A (**1**) in Pyridine- d_5 (500 MHz)

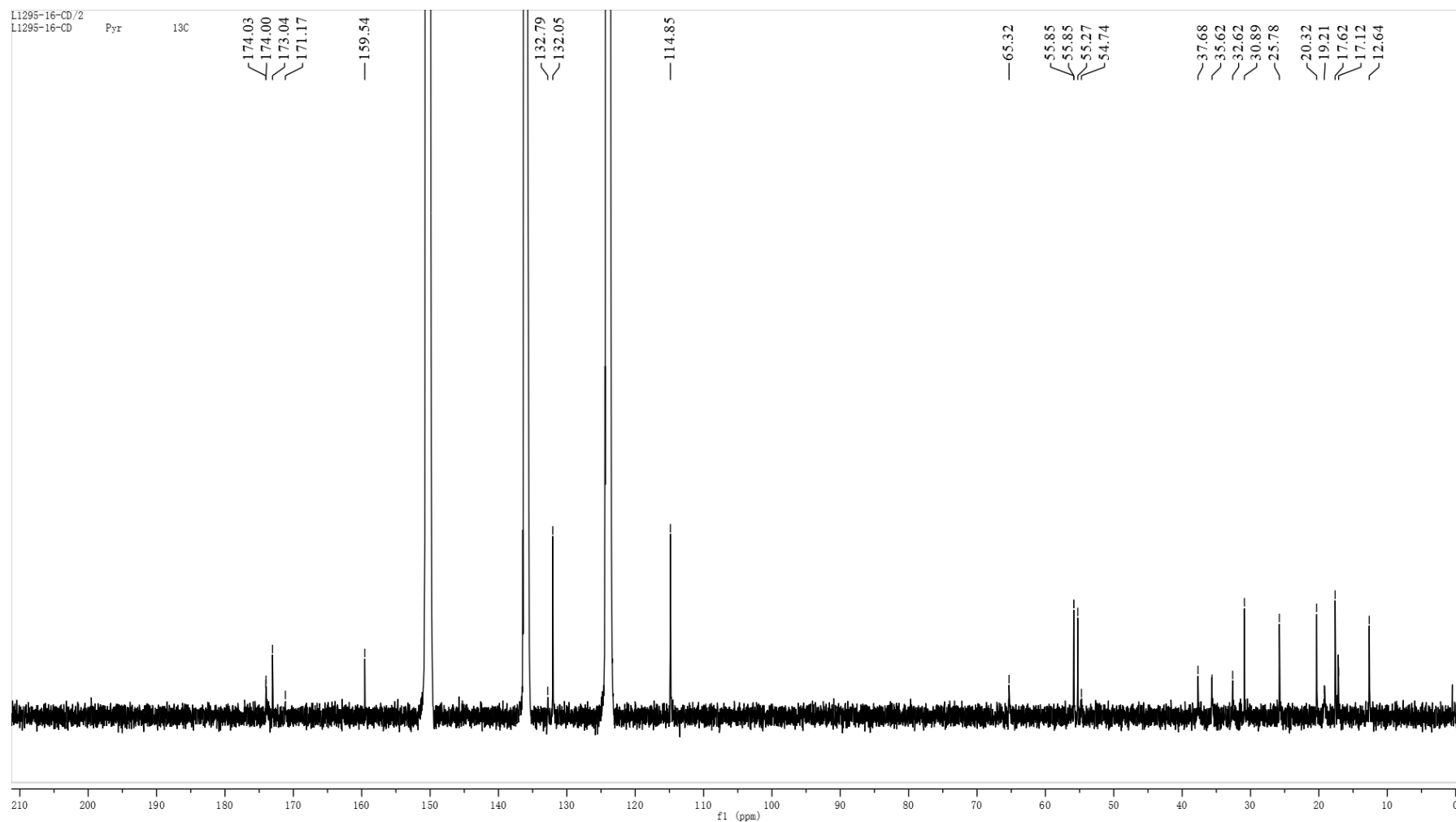


Figure S9. ^{13}C NMR spectrum of westertide A (**1**) in Pyridine- d_5 (125 MHz)

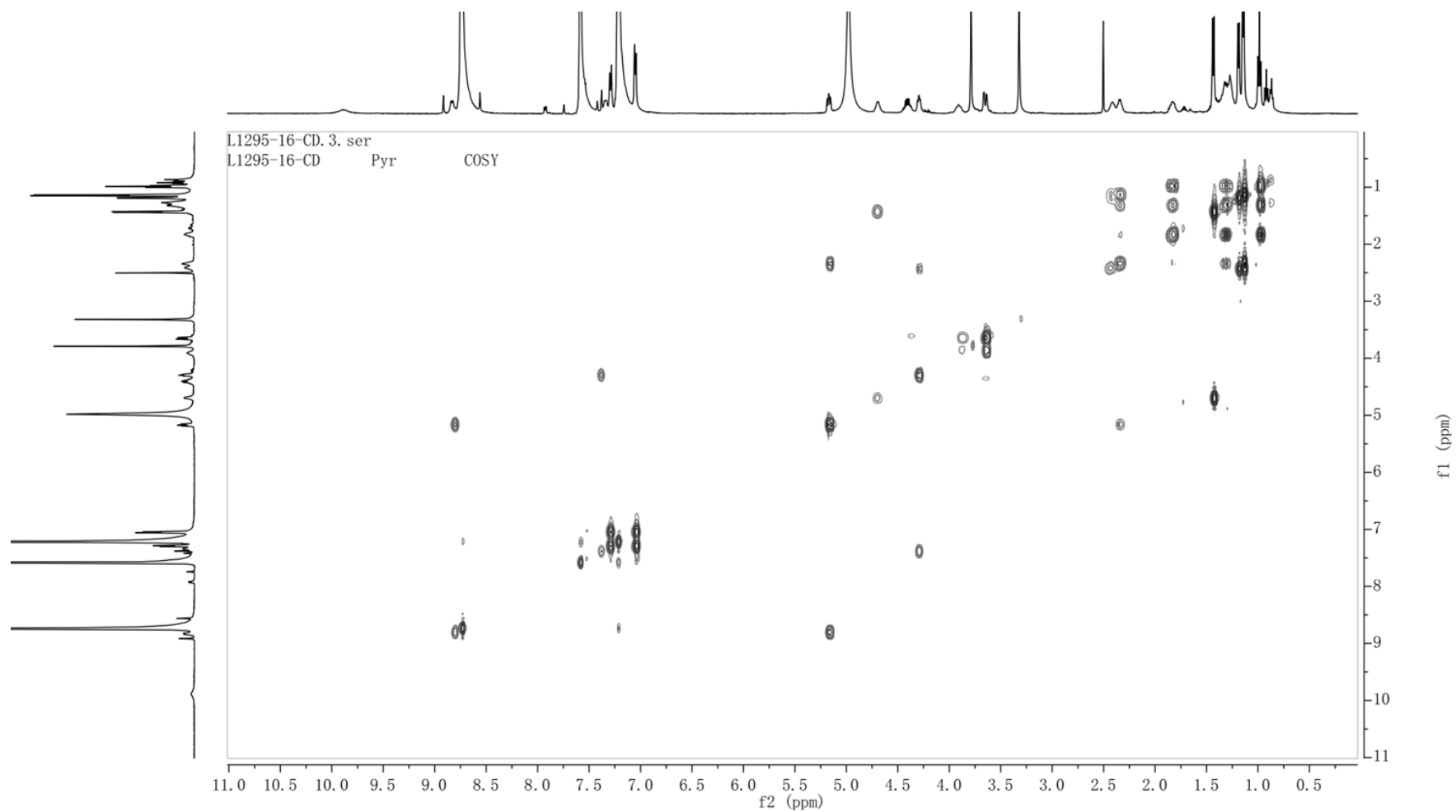


Figure S10. ^1H - ^1H COSY spectrum of westertide A (**1**) in Pyridine- d_5

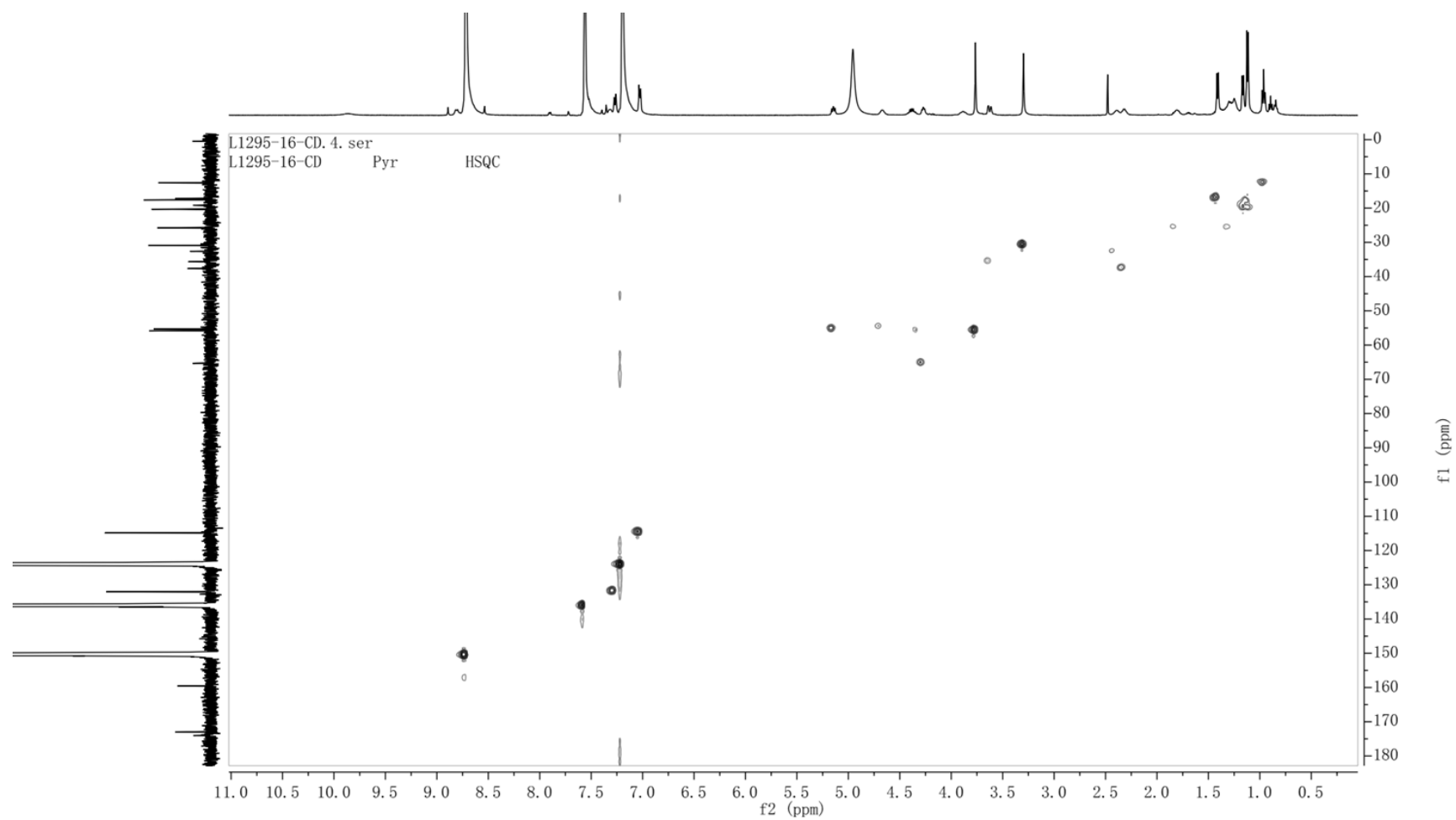


Figure S11. HSQC spectrum of westertide A (**1**) in Pyridine- d_5

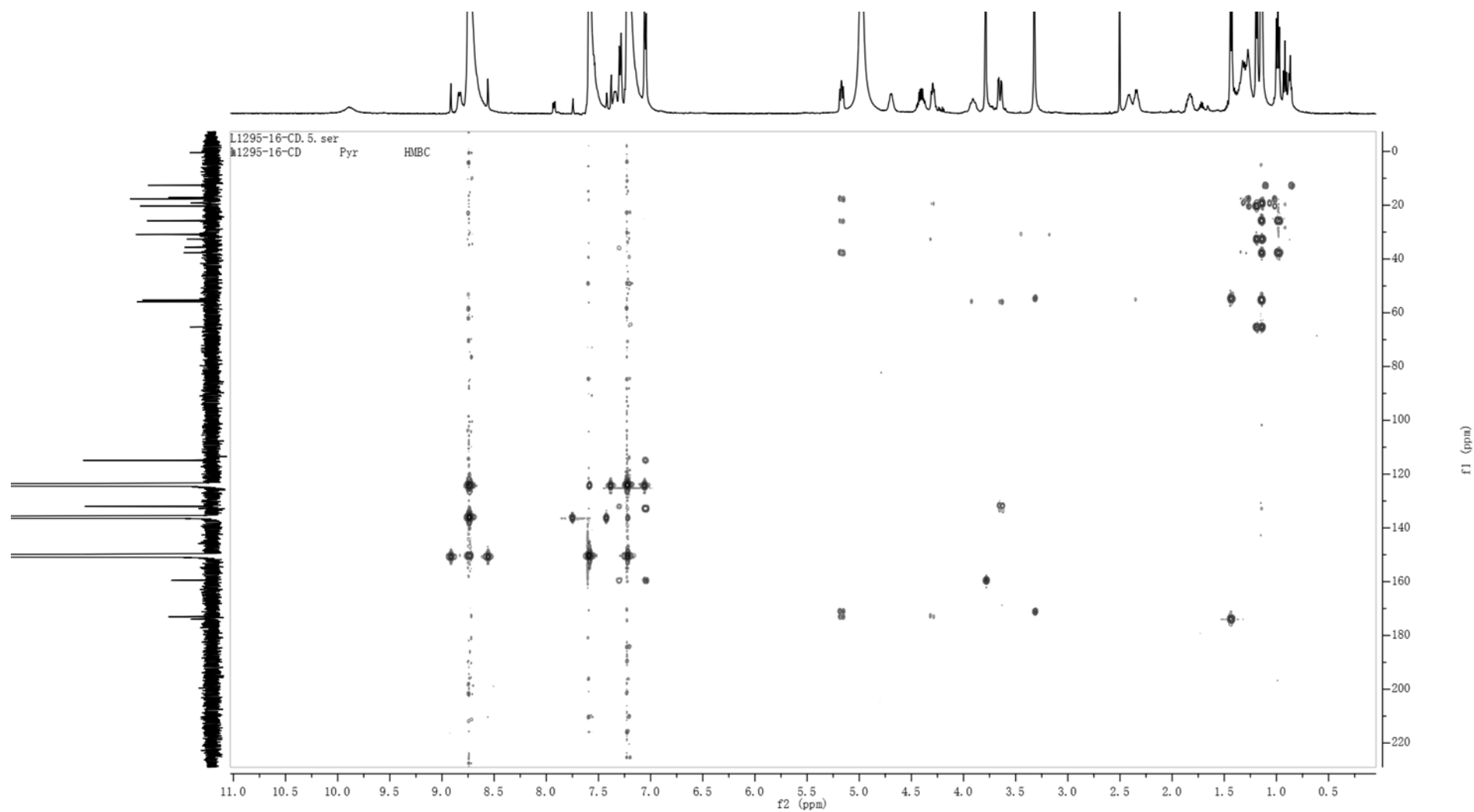


Figure S12. HMBC spectrum of westertide A (**1**) in Pyridine- d_5

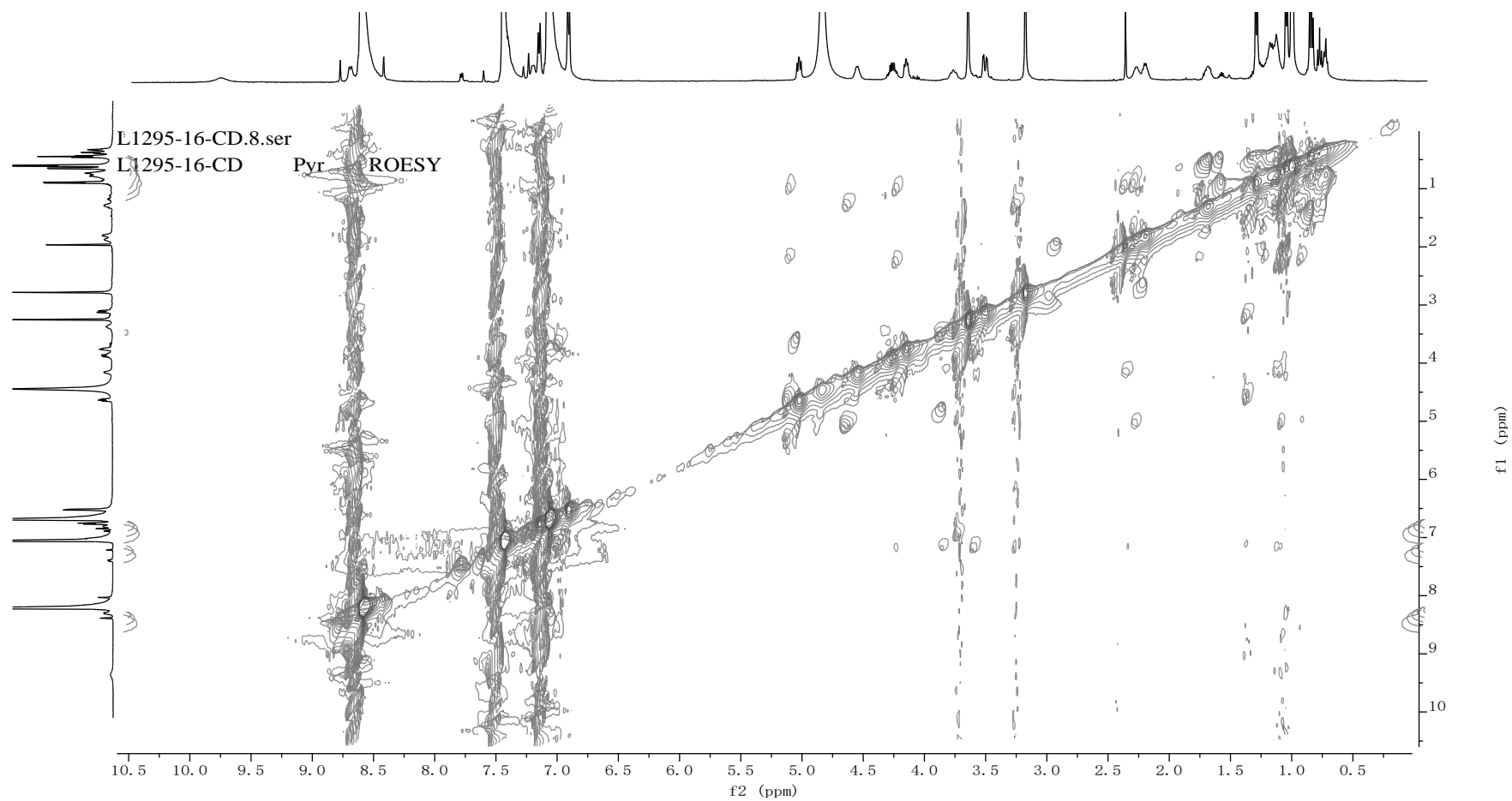


Figure S13. NOESY spectrum of westertide A (**1**) in Pyridine- d_5

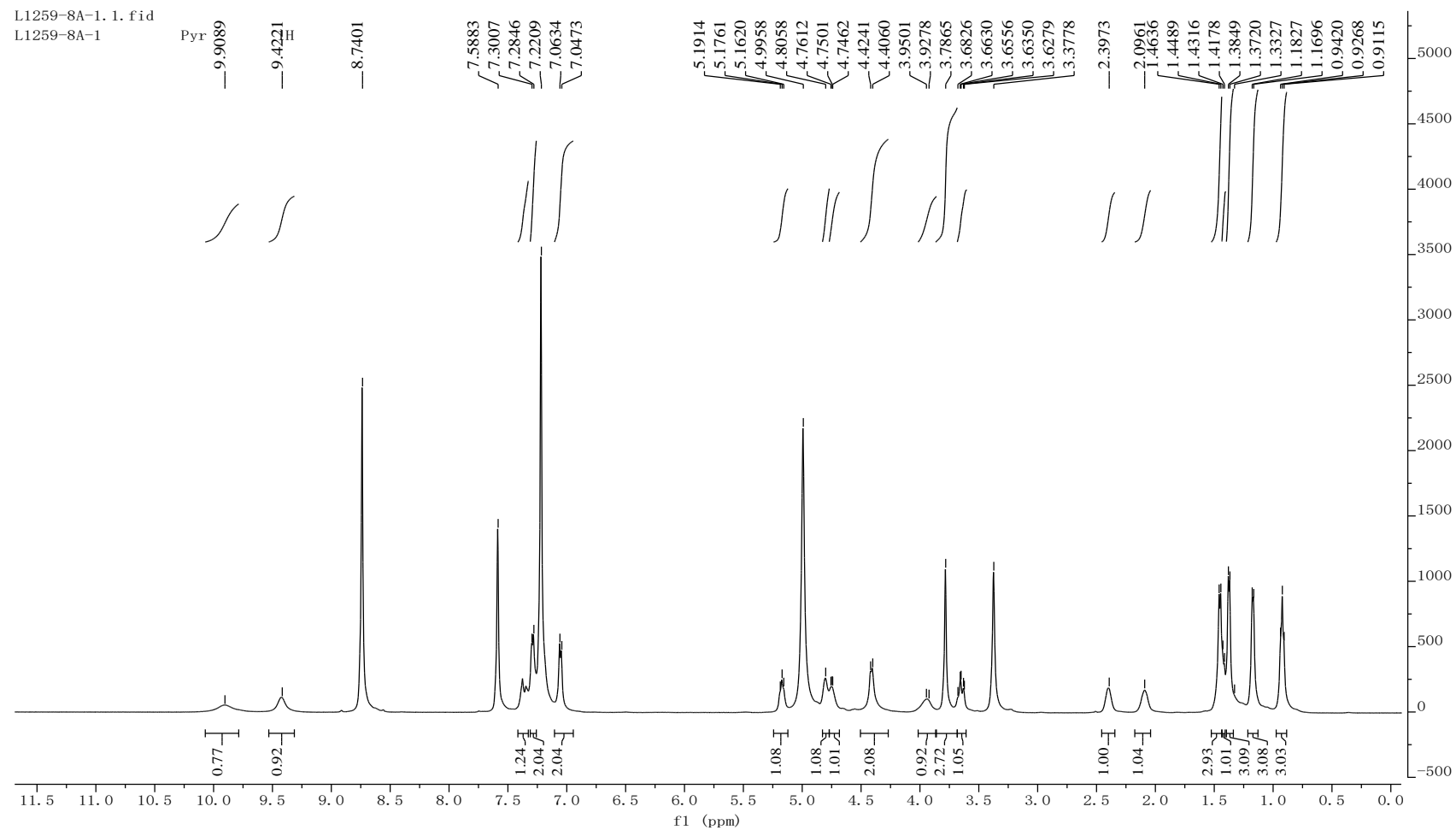


Figure S14. ^1H NMR spectrum of westertide B (**2**) in Pyridine- d_5 (500 MHz)

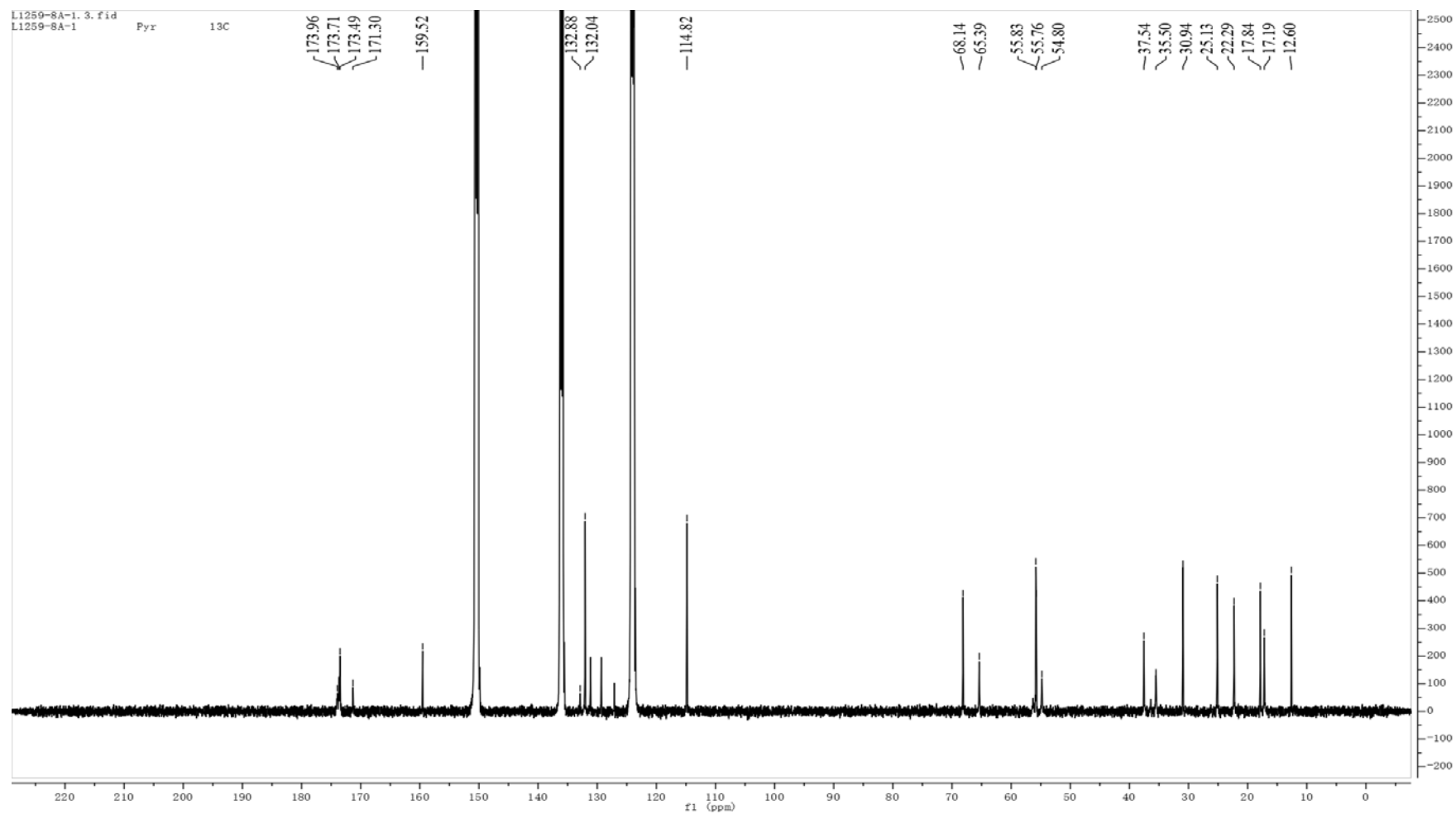


Figure S15. ^{13}C NMR spectrum of westertide B (**2**) in Pyridine- d_5 (125 MHz)

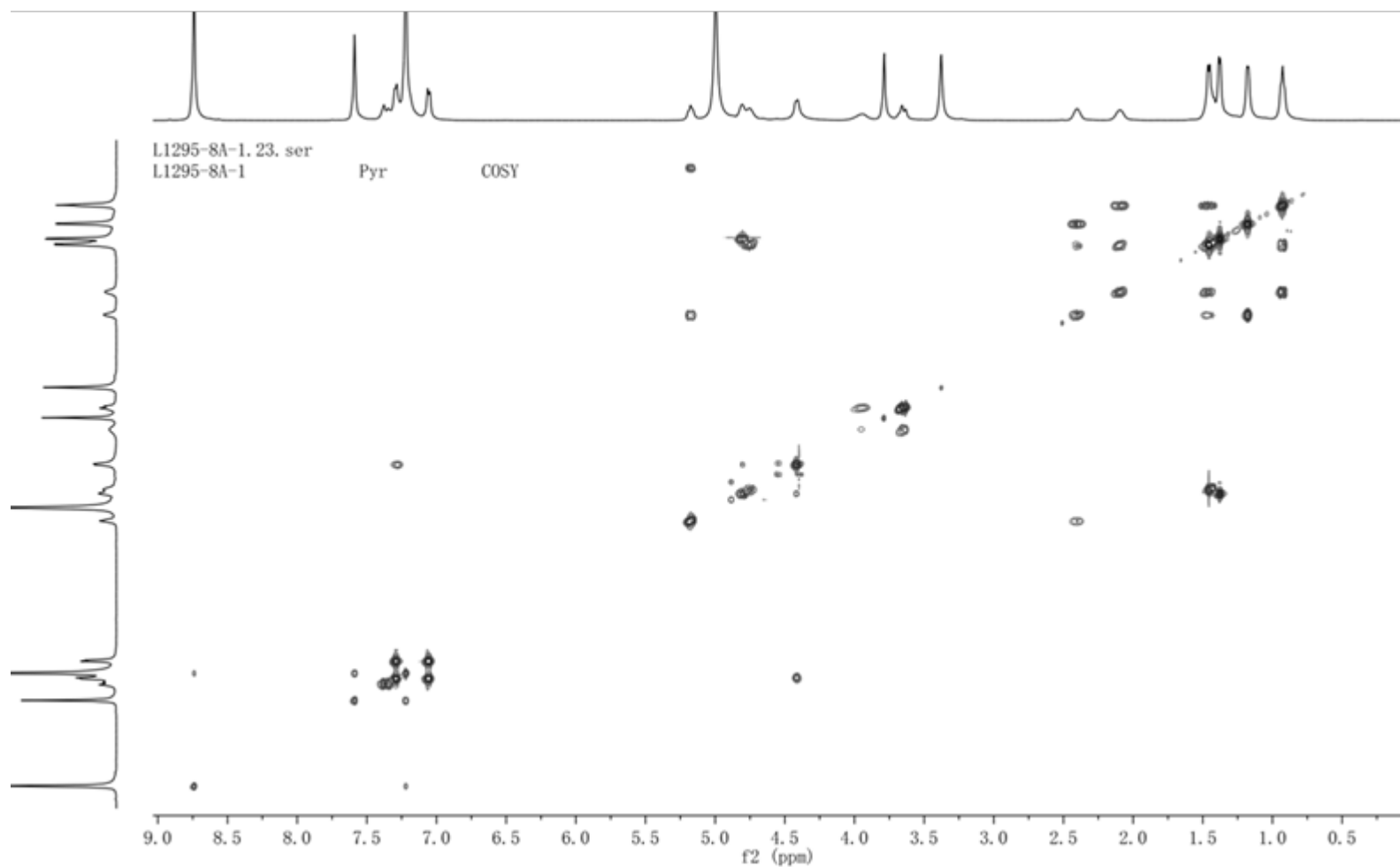


Figure S16. ^1H - ^1H COSY spectrum of westertide B (**2**) in Pyridine- d_5

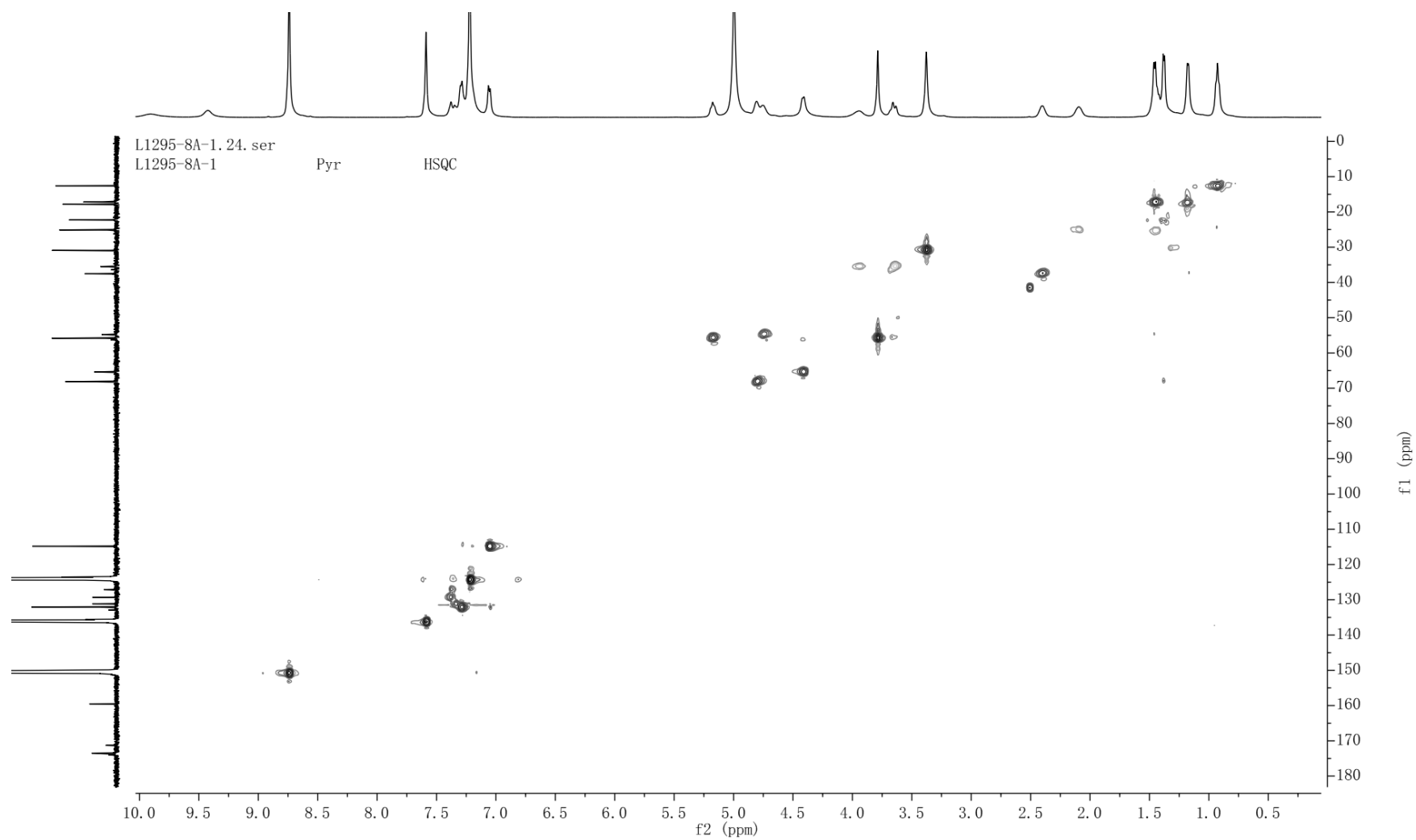


Figure S17. HSQC spectrum of westertide B (**2**) in Pyridine-*d*₅

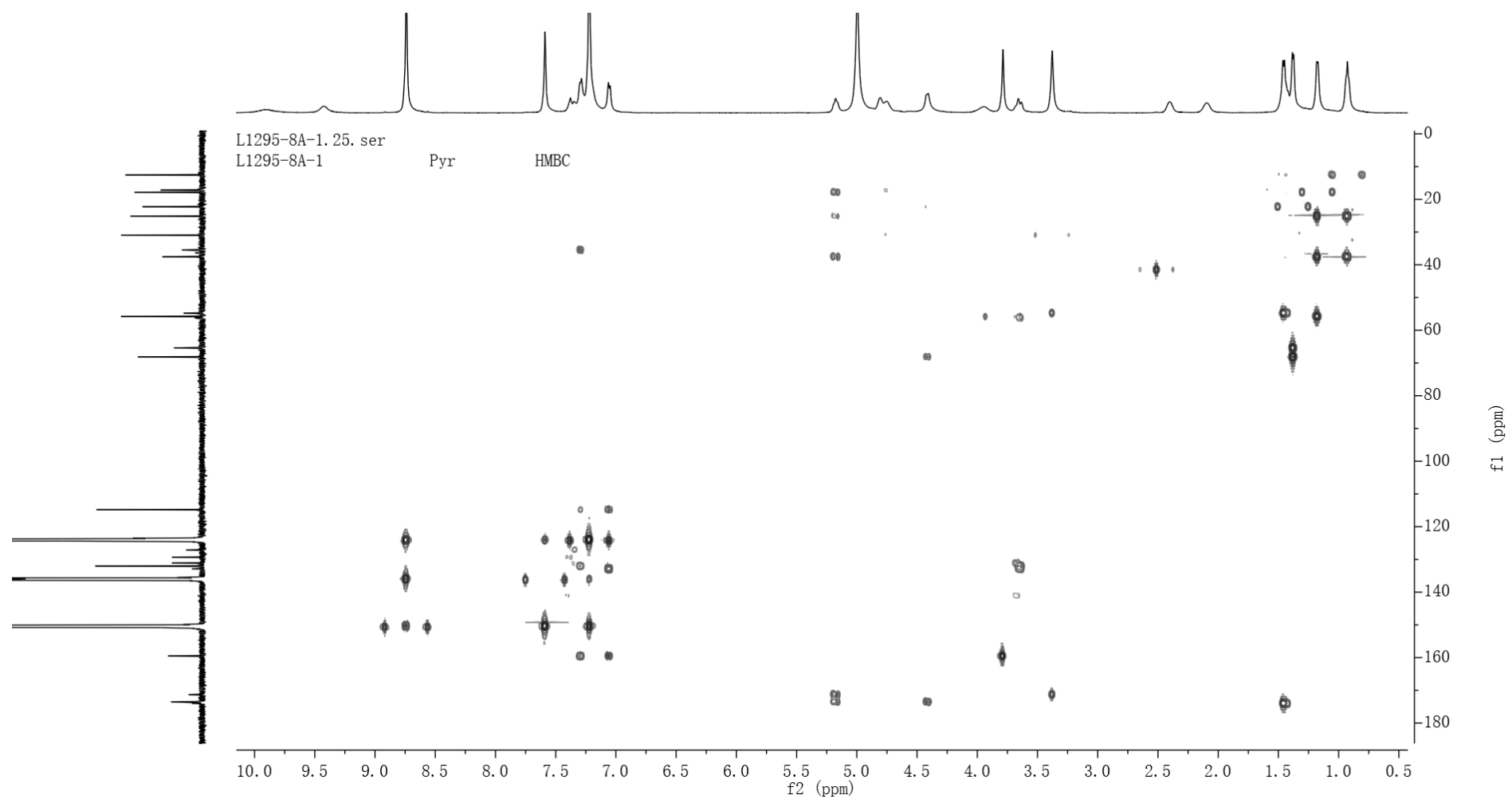


Figure S18. HMBC spectrum of westertide B (**2**) in Pyridine-*d*₅

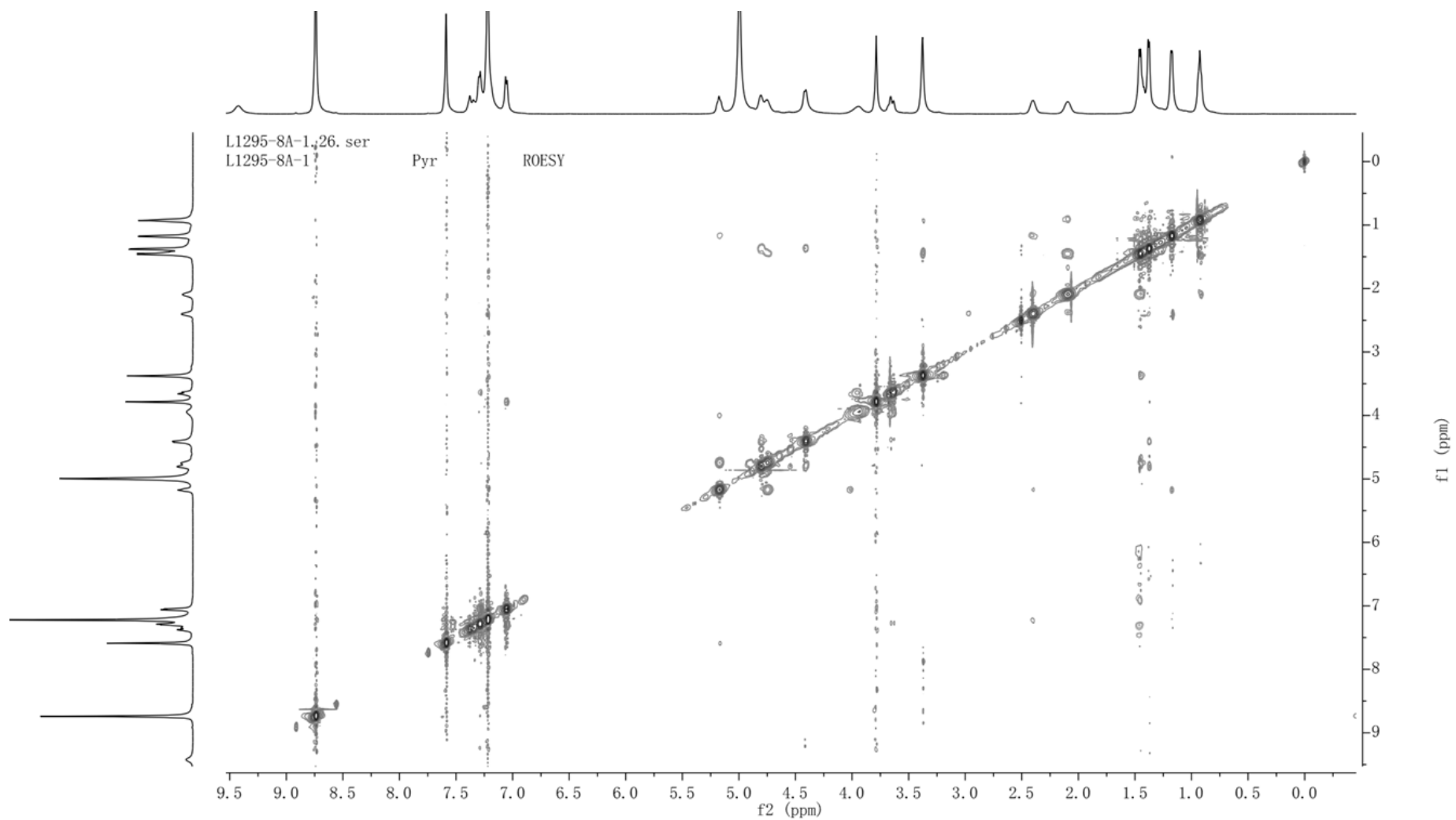


Figure S19. NOESY spectrum of westertide B (**2**) in Pyridine- d_5