Supporting Information

Separation of antioxidants from trace fraction of *Ribes himalense* via chromatographic strategy and their antioxidant activity supported by molecular simulations

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Figure S1. Apparatus diagrams

The actual polyamide-MPLC system (A) and the schematic diagram of online HPLC-DPPH screening system (B).

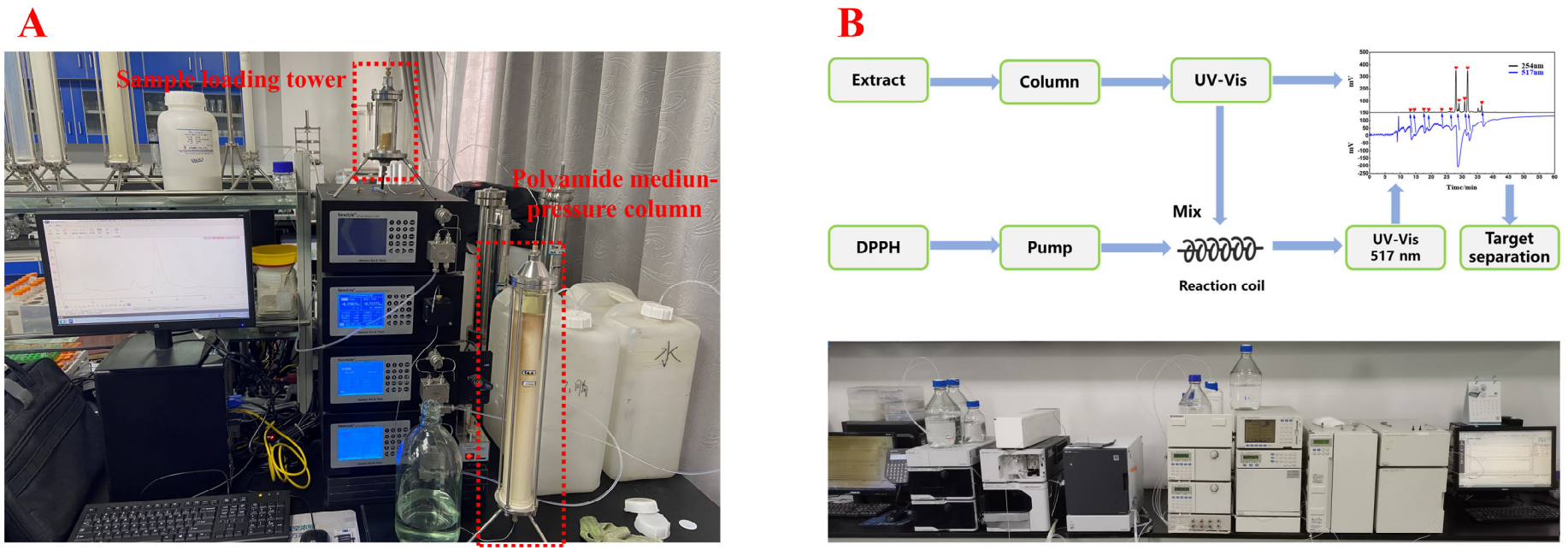

Figure S2. Schematic diagram of substance extraction process

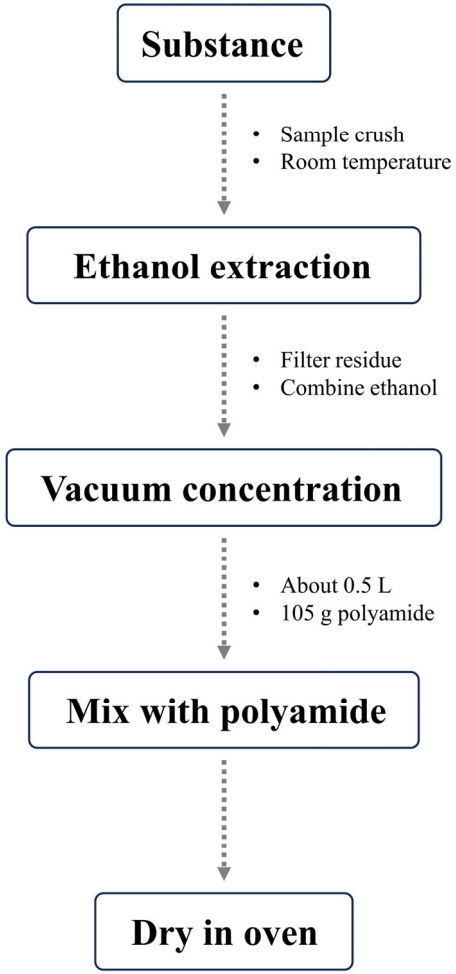

Figure S3. ESI-MS data of Fr4-1-1

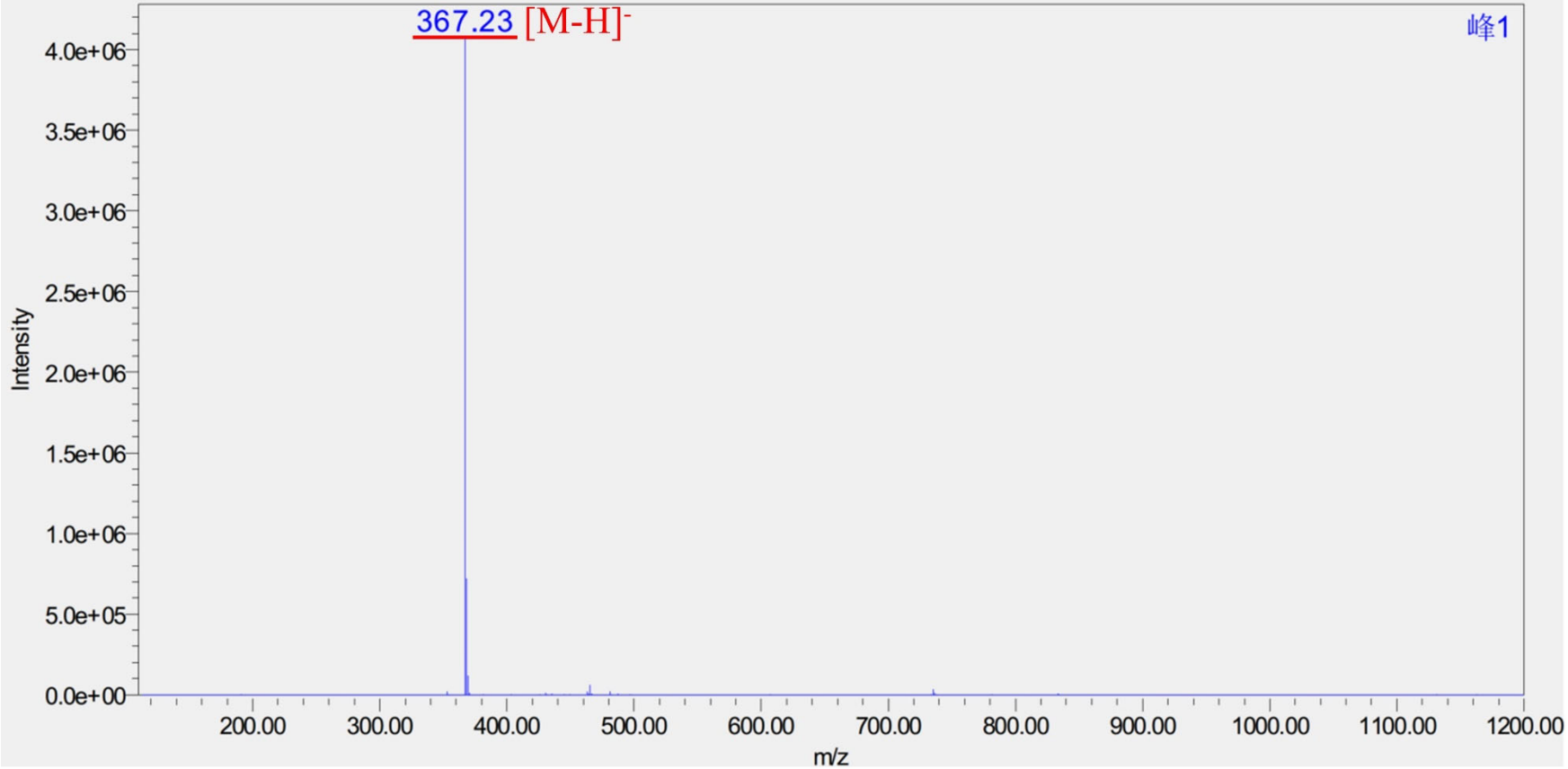

Figure S4. ^{1}H NMR (600 MHz) data of Fr4-1-1 (in DMSO-d_6)

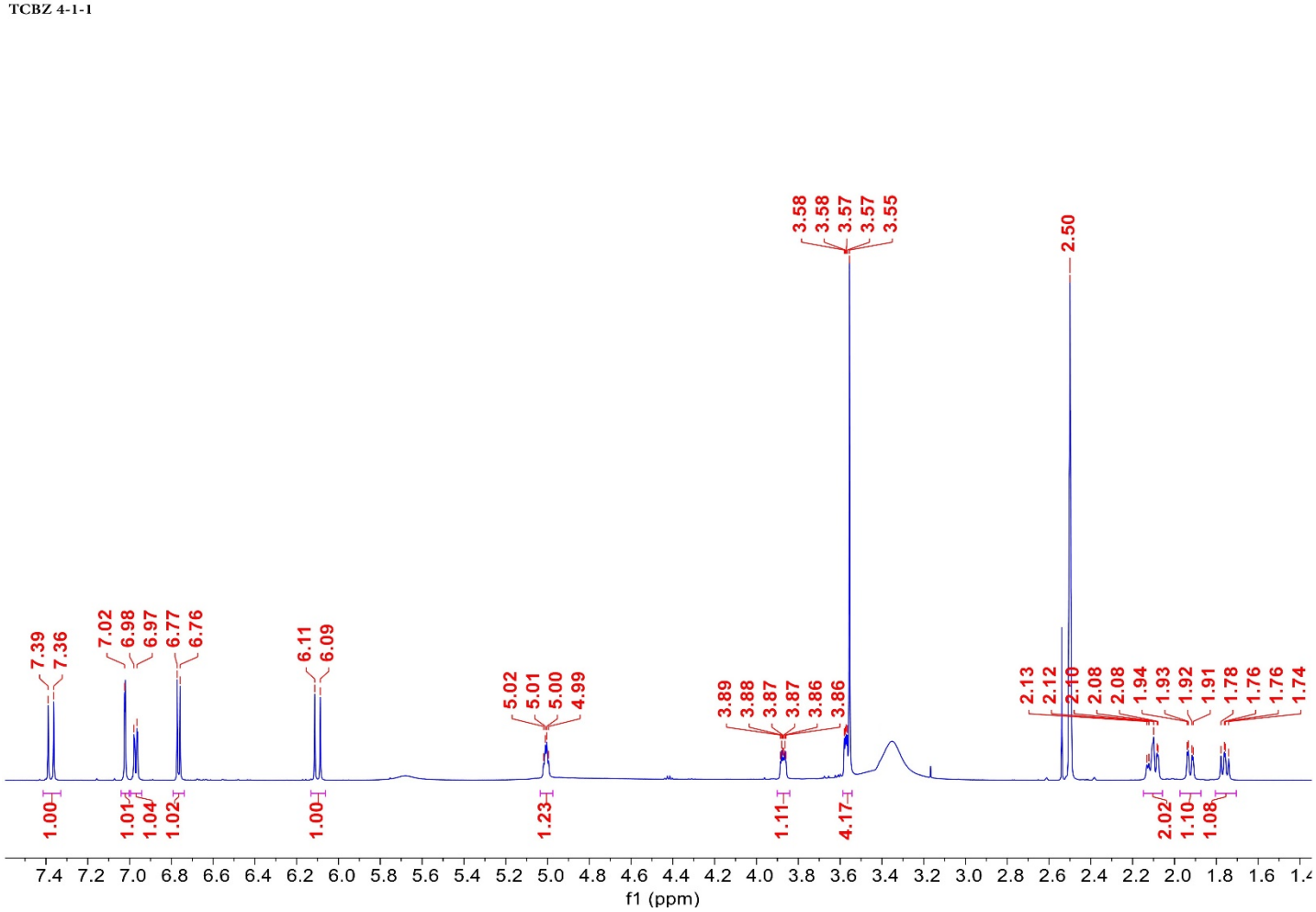

Figure S5. ^{13}C NMR (151 MHz) data of Fr4-1-1 (in DMSO-d_6)

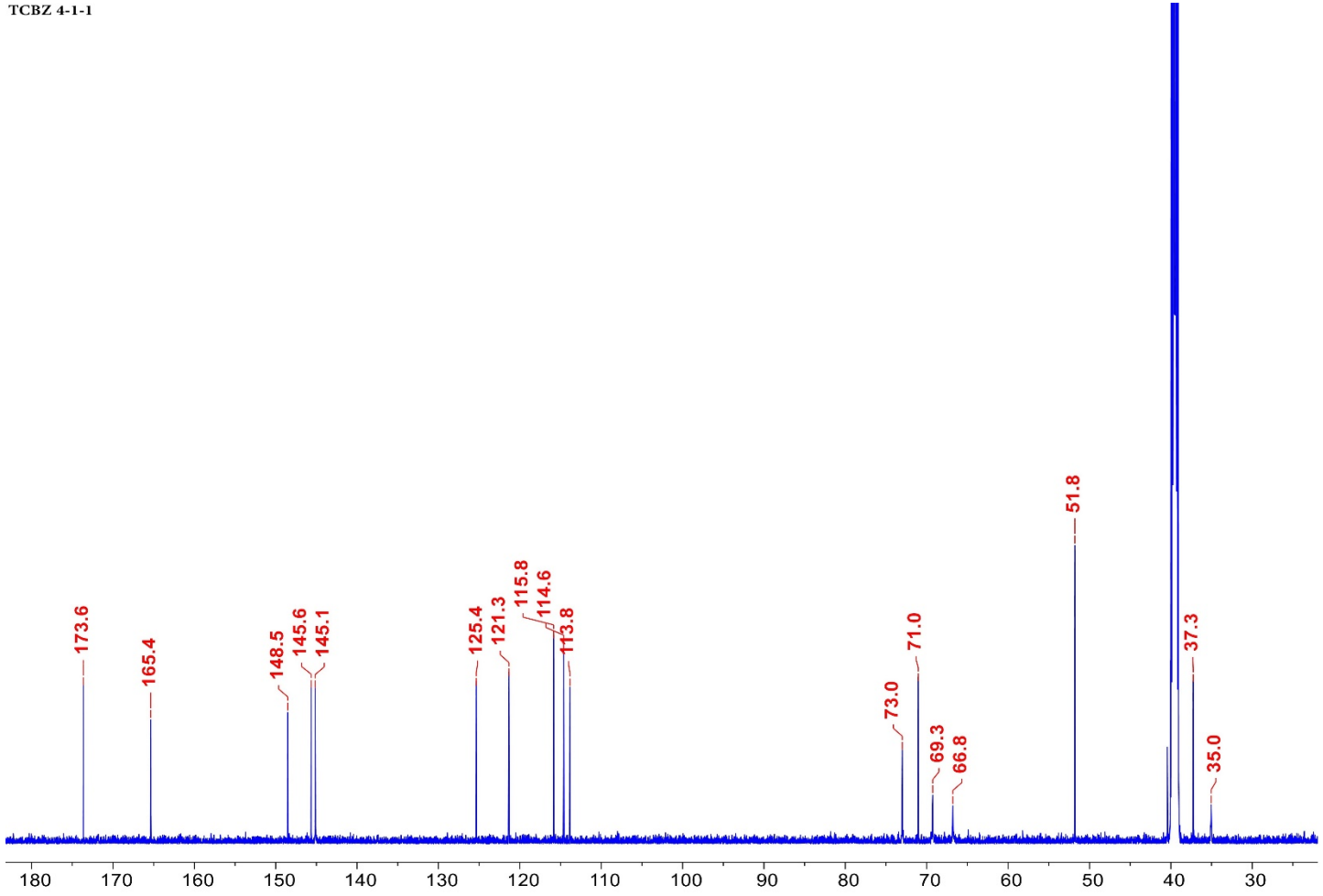

Figure S6. HR-ESI-MS data of Fr4-1-2

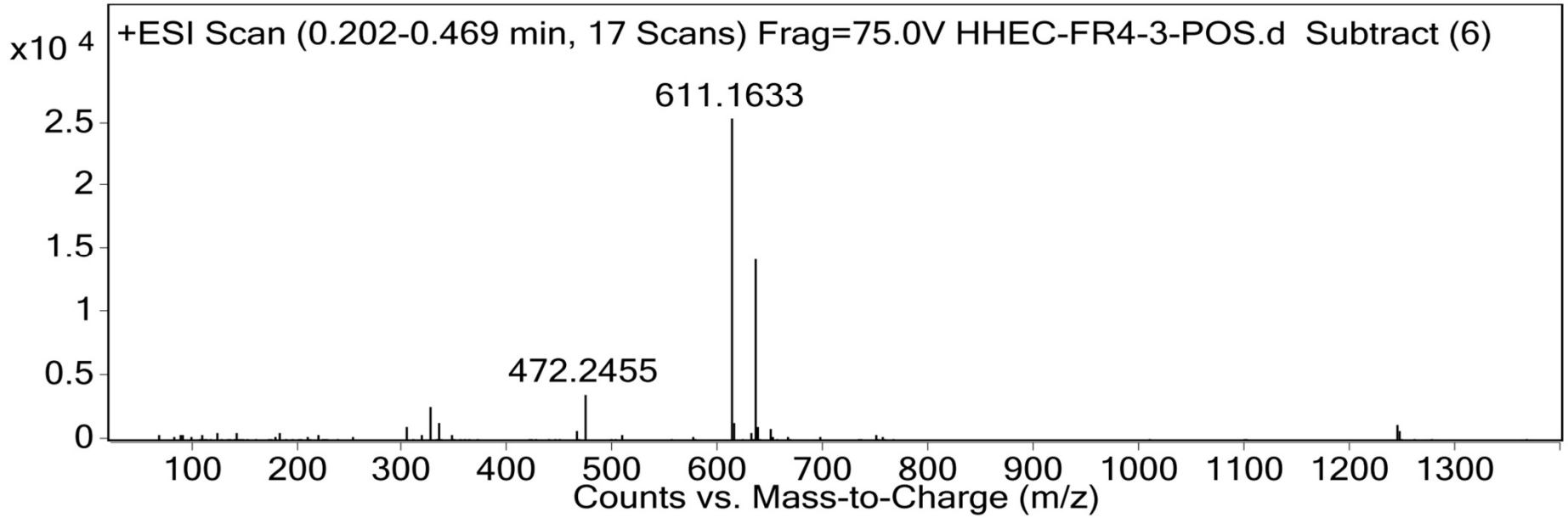

Figure S7. ^{1}H NMR (600 MHz) data of Fr4-1-2 (in MeOH-d_4)

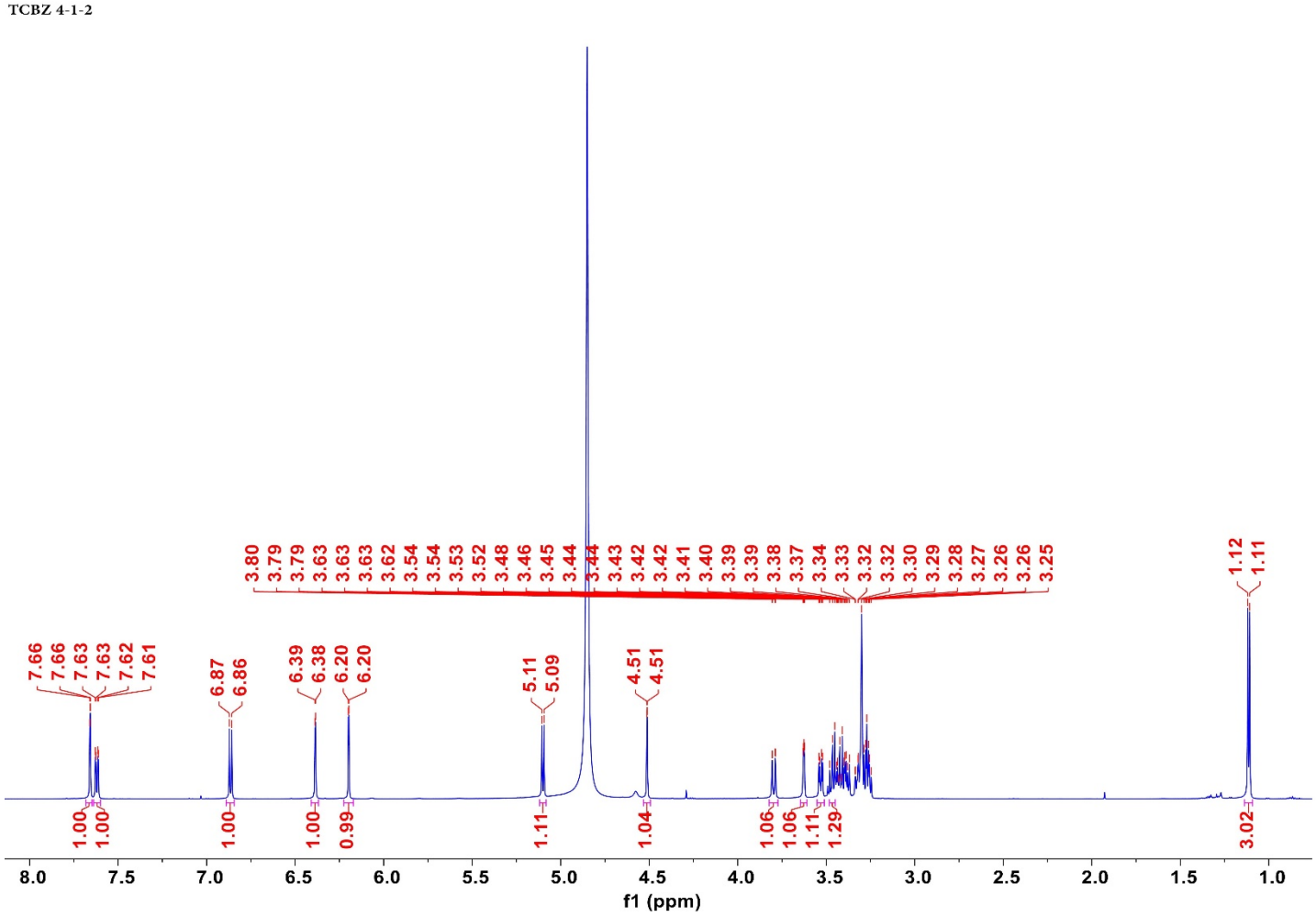

Figure S8. ^{13}C NMR (151 MHz) data of Fr4-1-2 (in MeOH-d_4)

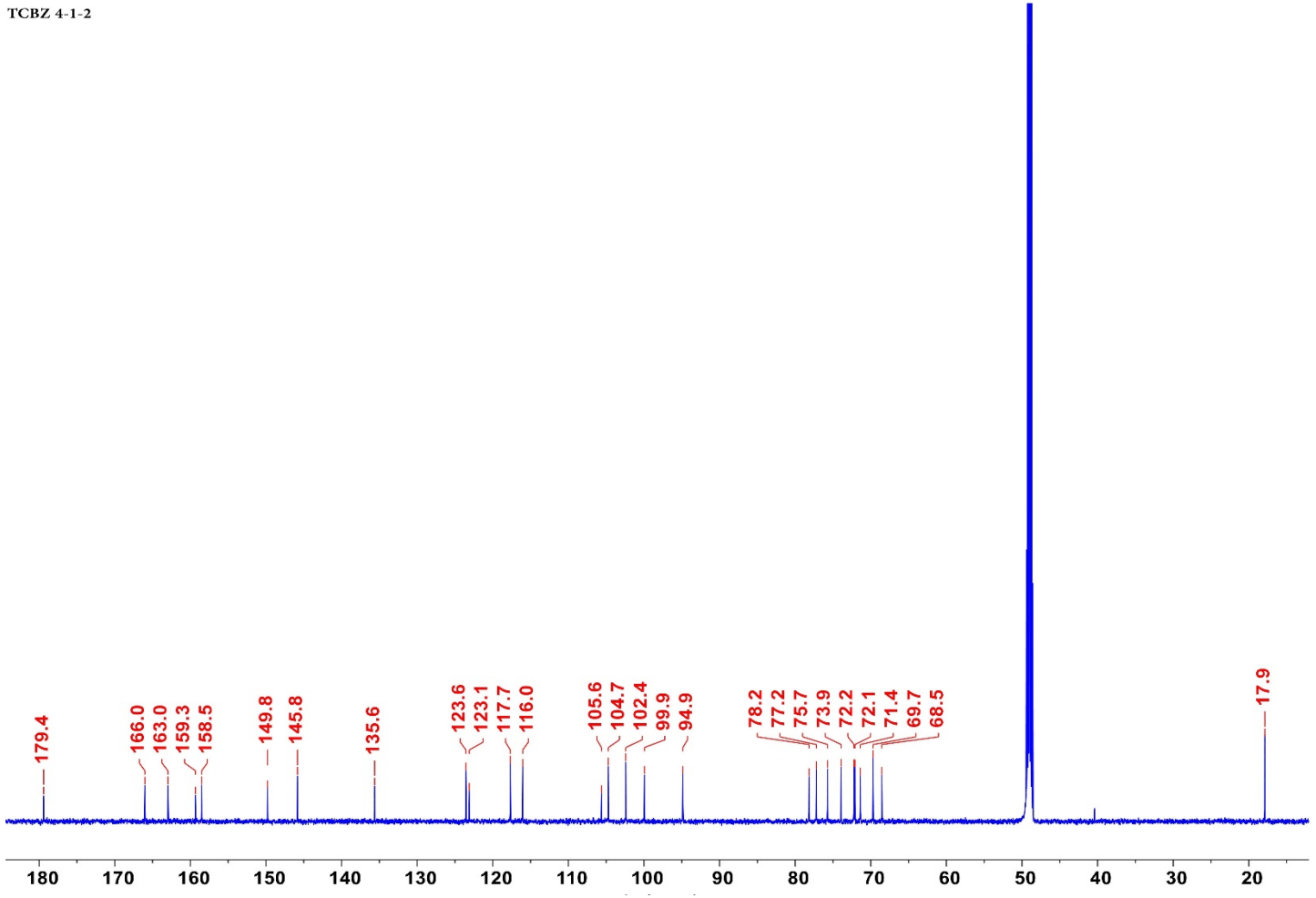

Figure S9. HMBC data of Fr4-1-2 (in MeOH-d_4)

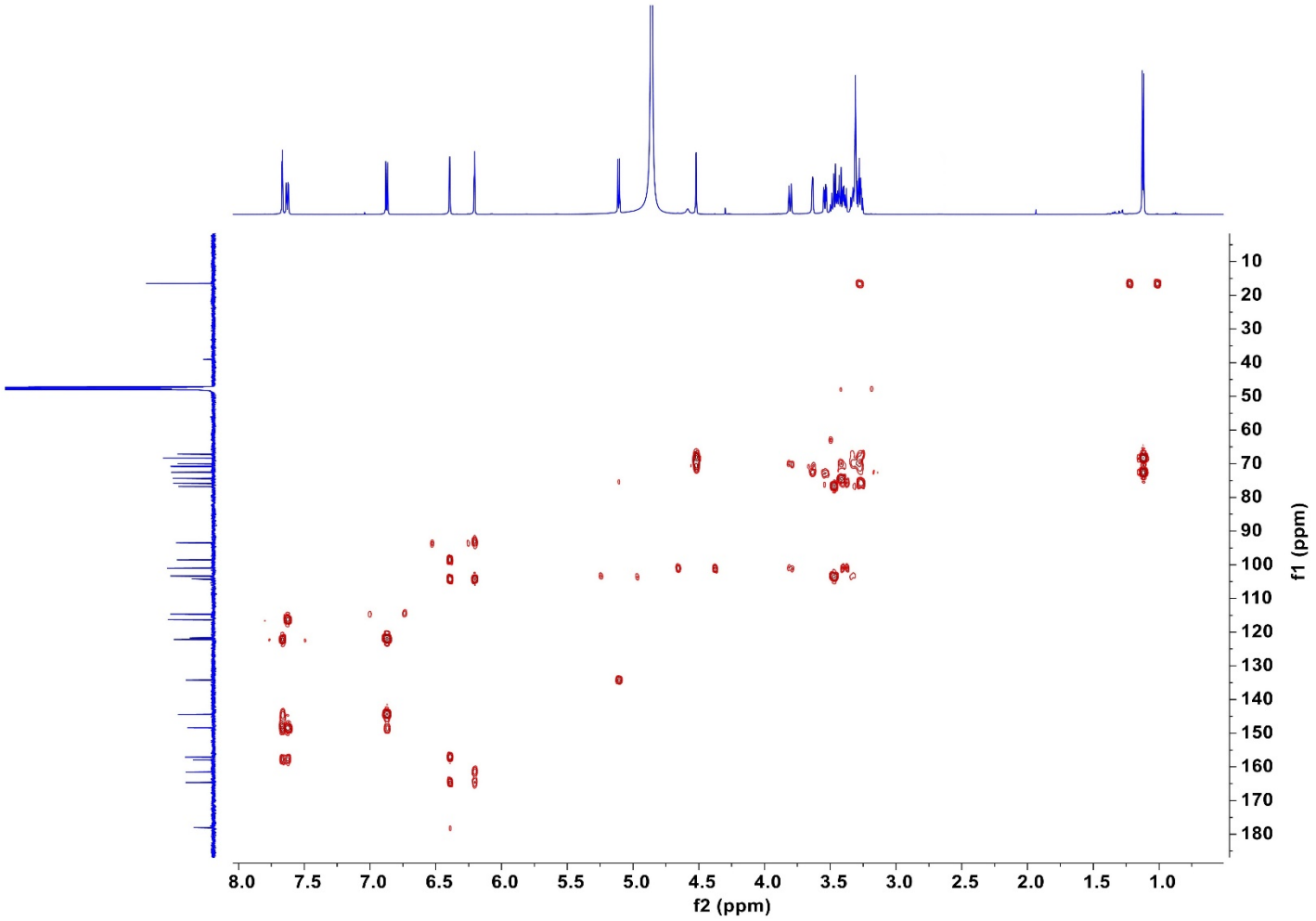

Figure S10. ESI-MS data of Fr4-2

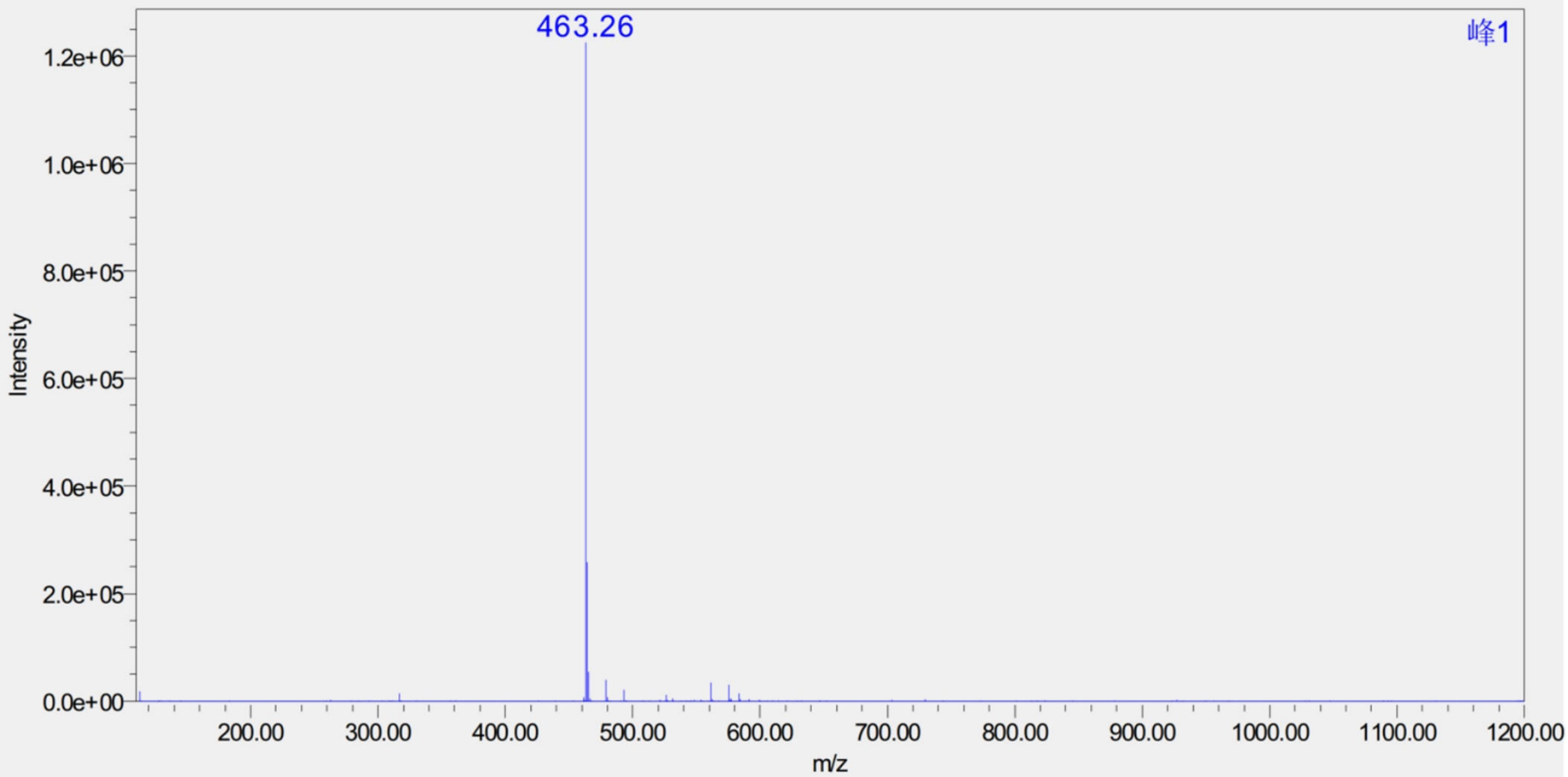

Figure S11. ^{1}H NMR (600 MHz) data of Fr4-2 (in DMSO-d_6)

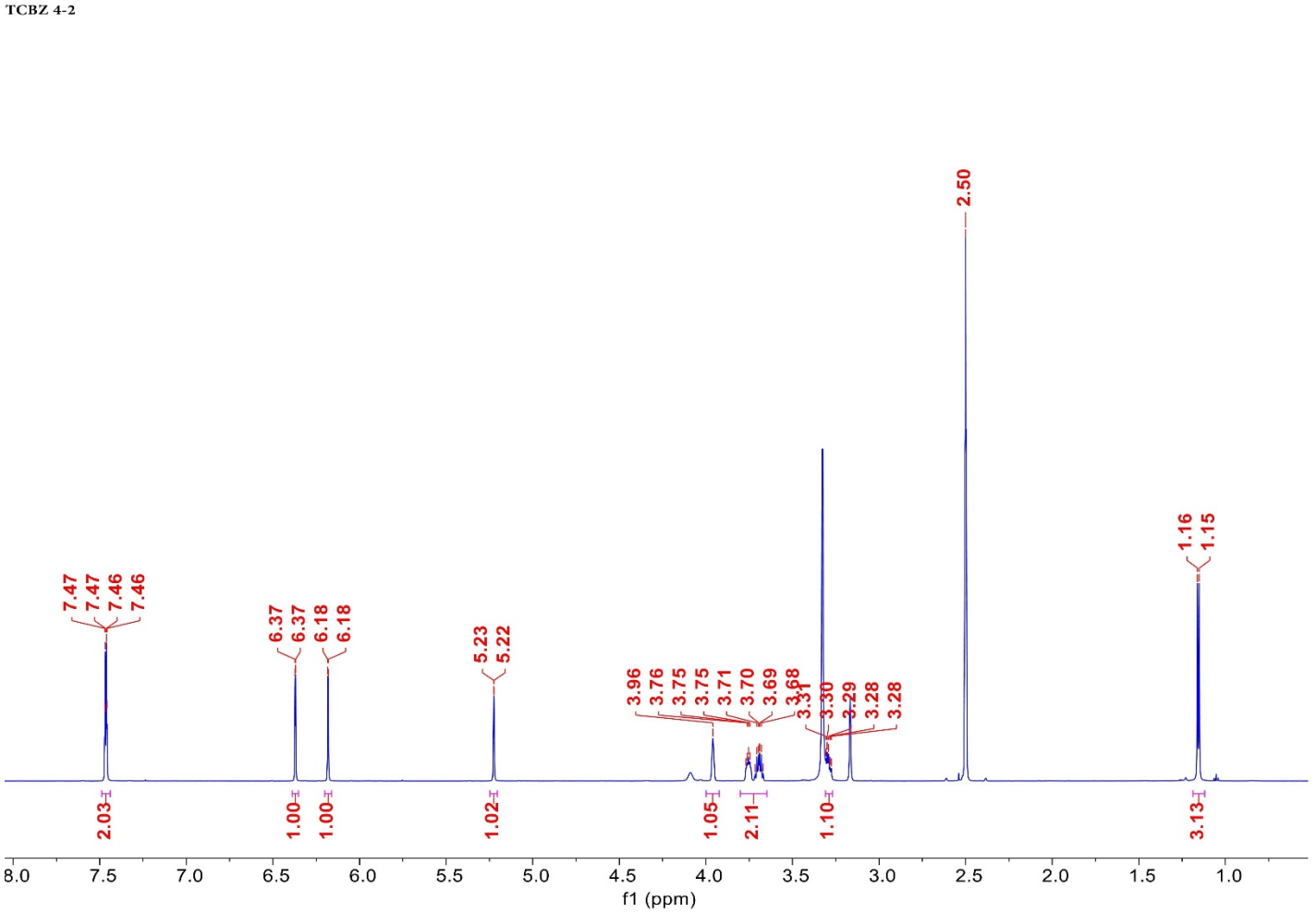

Figure S12. ^{13}C NMR (151 MHz) data of Fr4-2 (in DMSO-d_6)

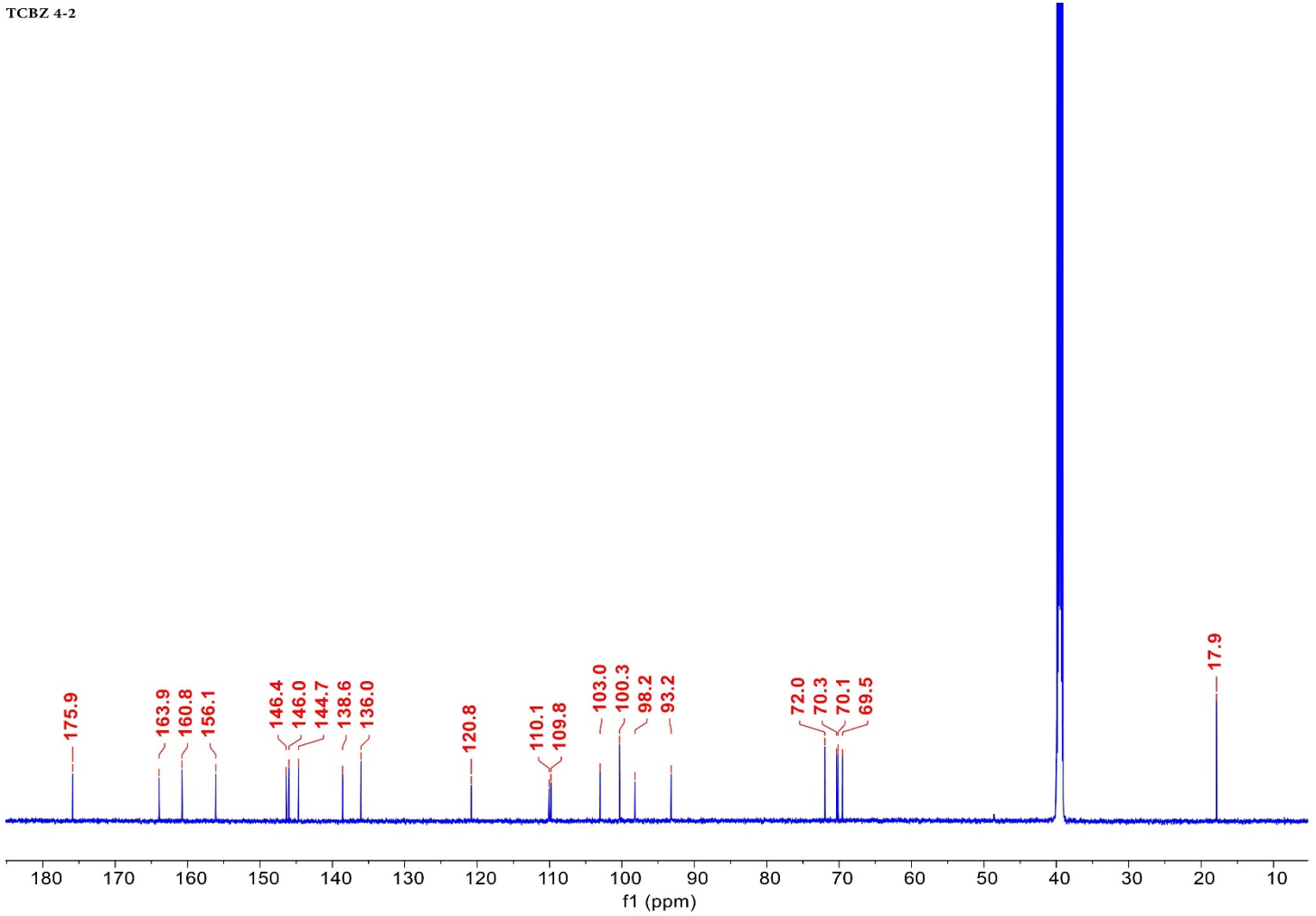

Figure S13. Docking results of antioxidants with target proteins

2D-interaction diagram between HO-1 and Fr4-1-1 (A); 2D-interaction diagram between HO-1 and Fr4-1-2 (B); 2D-interaction diagram between HO-1 and Fr4-2 (C); 2D-interaction diagram between Nrf2 and Fr4-1-1 (D); 2D-interaction diagram between Nrf2 and Fr4-1-2 (E); 2D-interaction diagram between Nrf2 and Fr4-2 (F); 2D-interaction diagram between iNOS and Fr4-1-1 (G); 2D-interaction diagram between iNOS and Fr4-1-2 (H); 2D-interaction diagram between HO-1 and Fr4-2 (I).

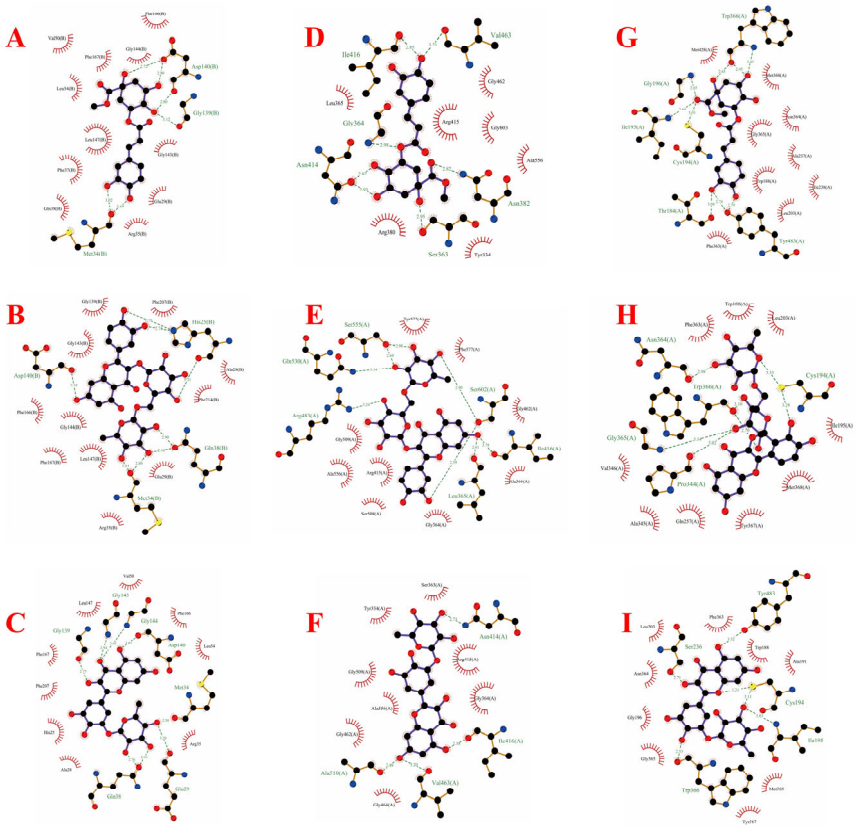

Figure S14. Histogram of all docking results

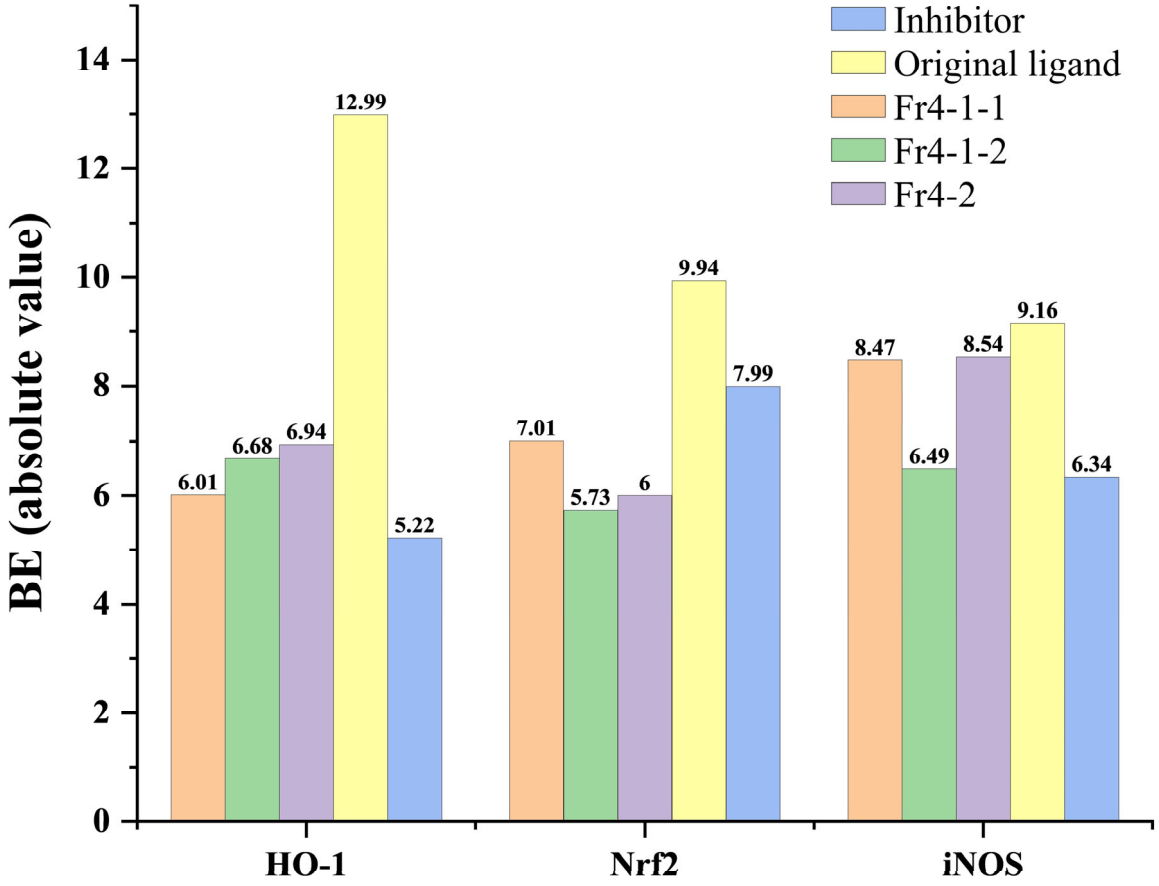

Figure S15. The binding sites of small molecule ligands and target proteins

2D-interaction diagram between HO-1 and Heme Oxygenase-1-IN-1 (A); 2D-interaction diagram between Nrf2 and ML385 (B); 2D-interaction diagram between iNOS and Isoquercetin (C); 2D-interaction diagram between HO-1 and HEM (D); 2D-interaction diagram between Nrf2 and IQK (E); 2D-interaction diagram between iNOS and 228 (F).