Supporting Information

Grassystatins D–F, Potent Aspartic Protease Inhibitors from Marine Cyanobacteria as Potential Antimetastatic Agents Targeting Invasive Breast Cancer

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ROESY Spectrum of Grassystatin F (**3**) in DMSO-d_6 S22

TOCSY Spectrum of Grassystatin F (**3**) in DMSO-d_6 S23

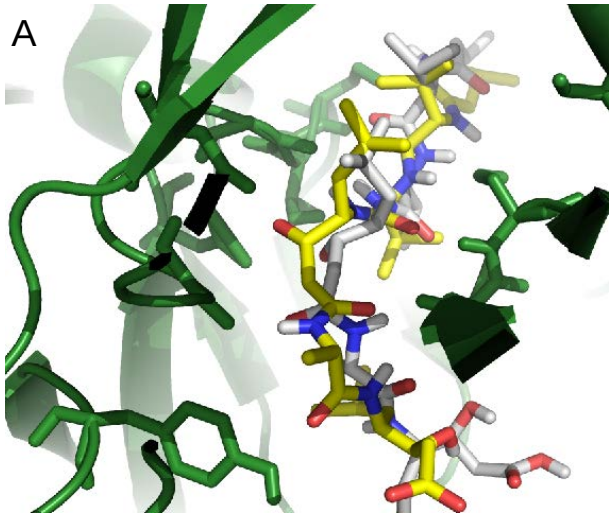
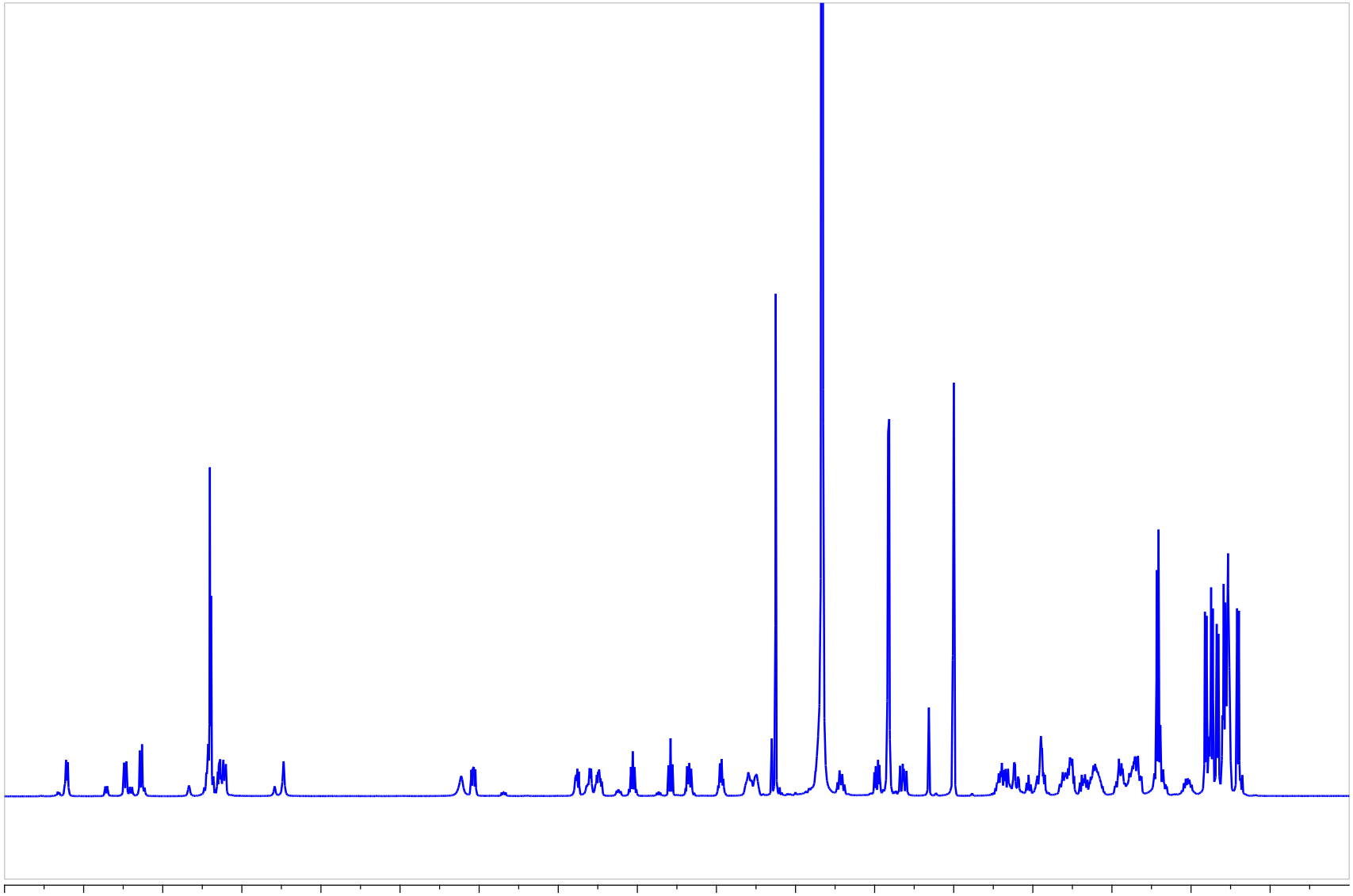
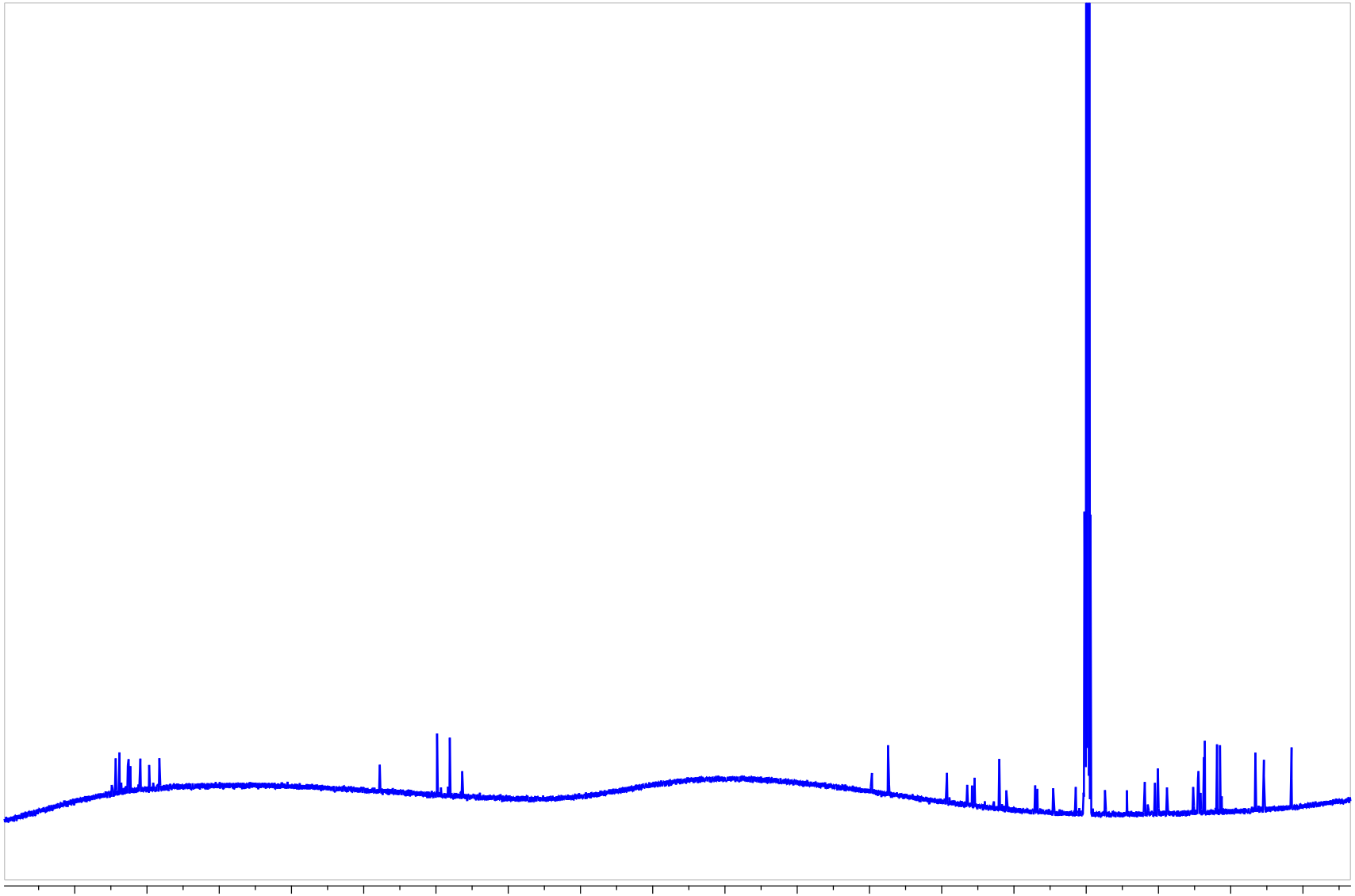


Figure S1. Overlay of docked structures of pepstatin A (**6**) (white) with previously published docked structure (yellow) in cathepsin D (1LYB) (green).

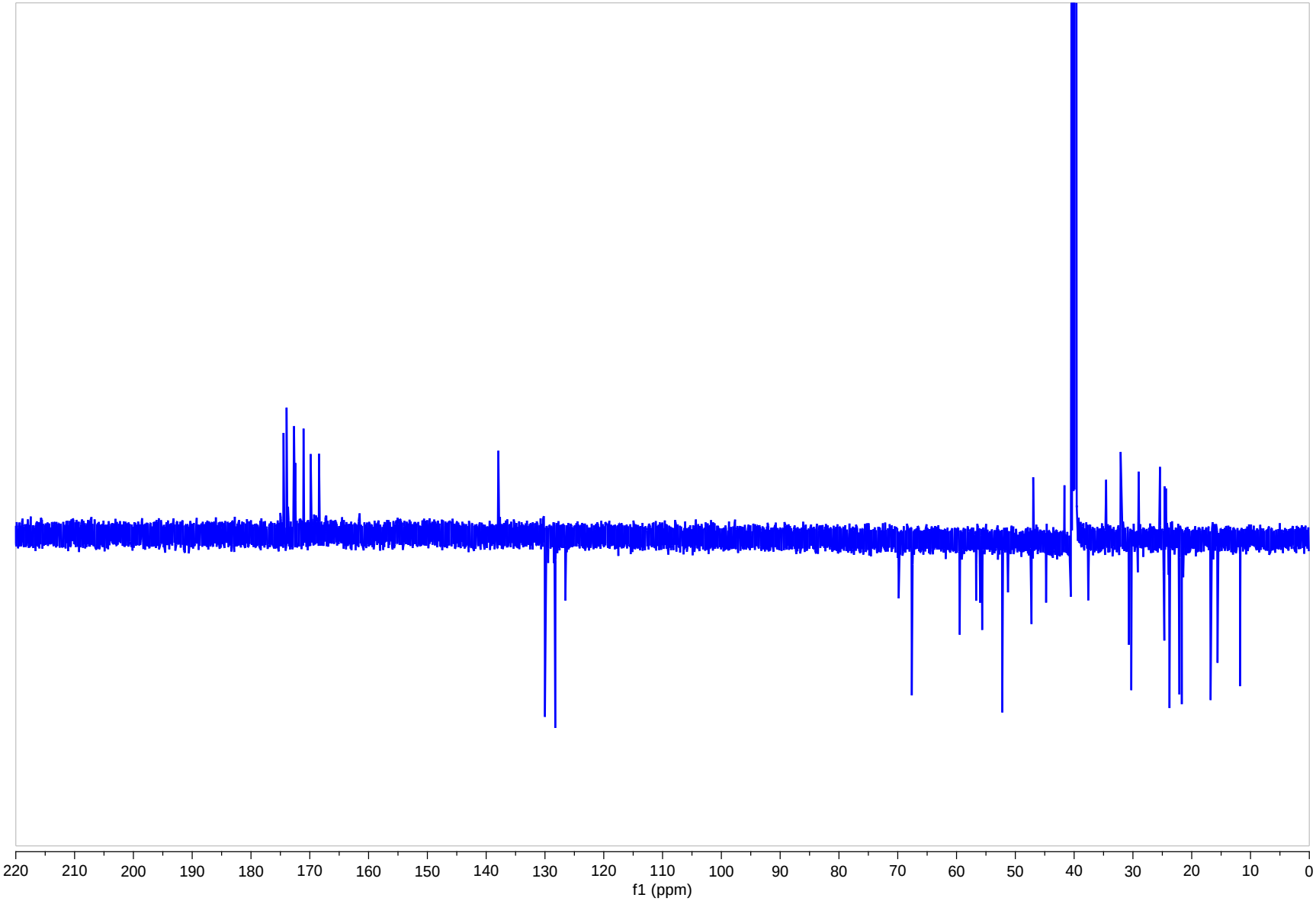
^{1}H NMR Spectrum of Grassystatin D (**1**) in DMSO-d_6, 600 MHz



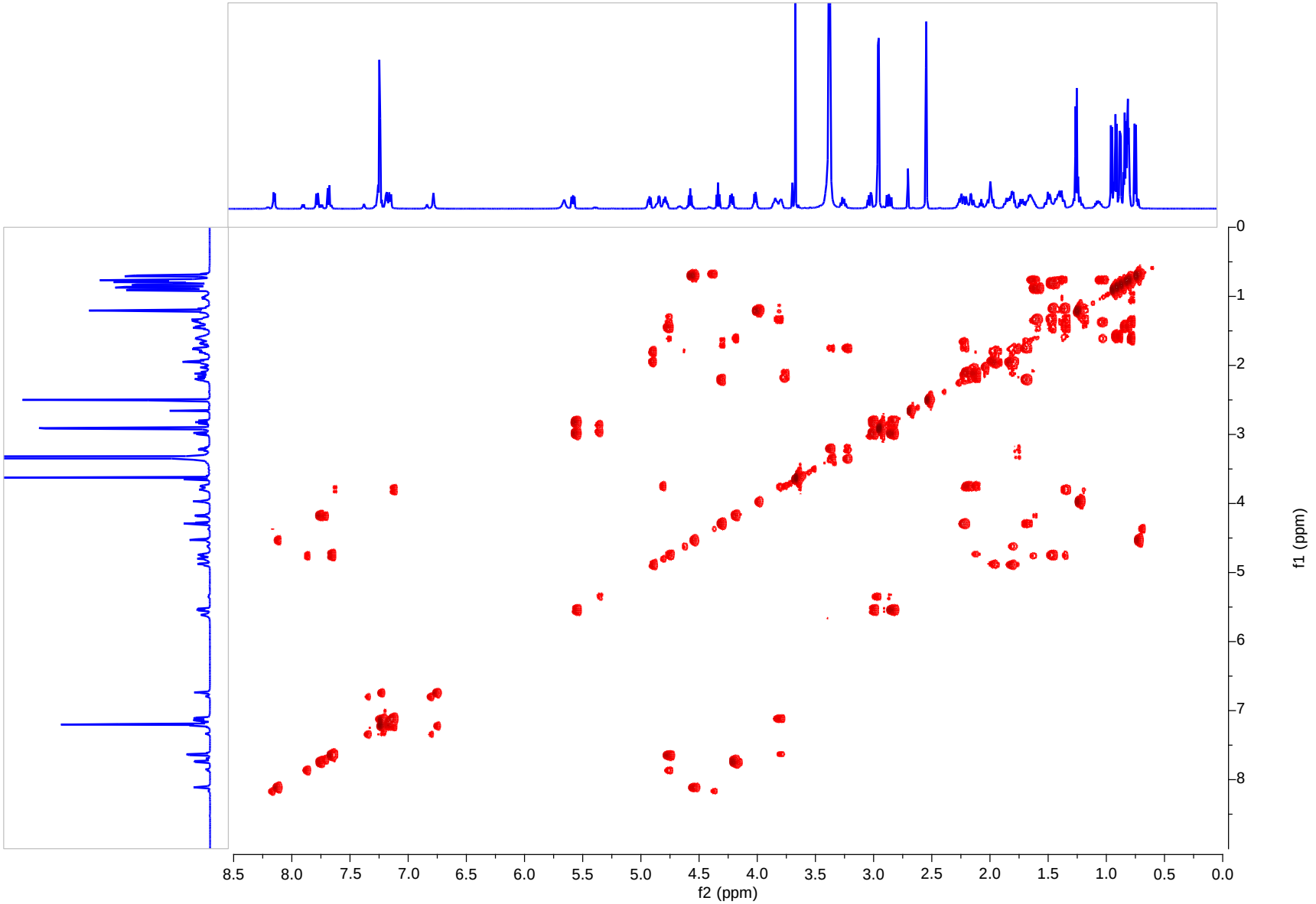
^{13}C Spectrum of Grassystatin D (**1**) in DMSO-d_6, 150 MHz



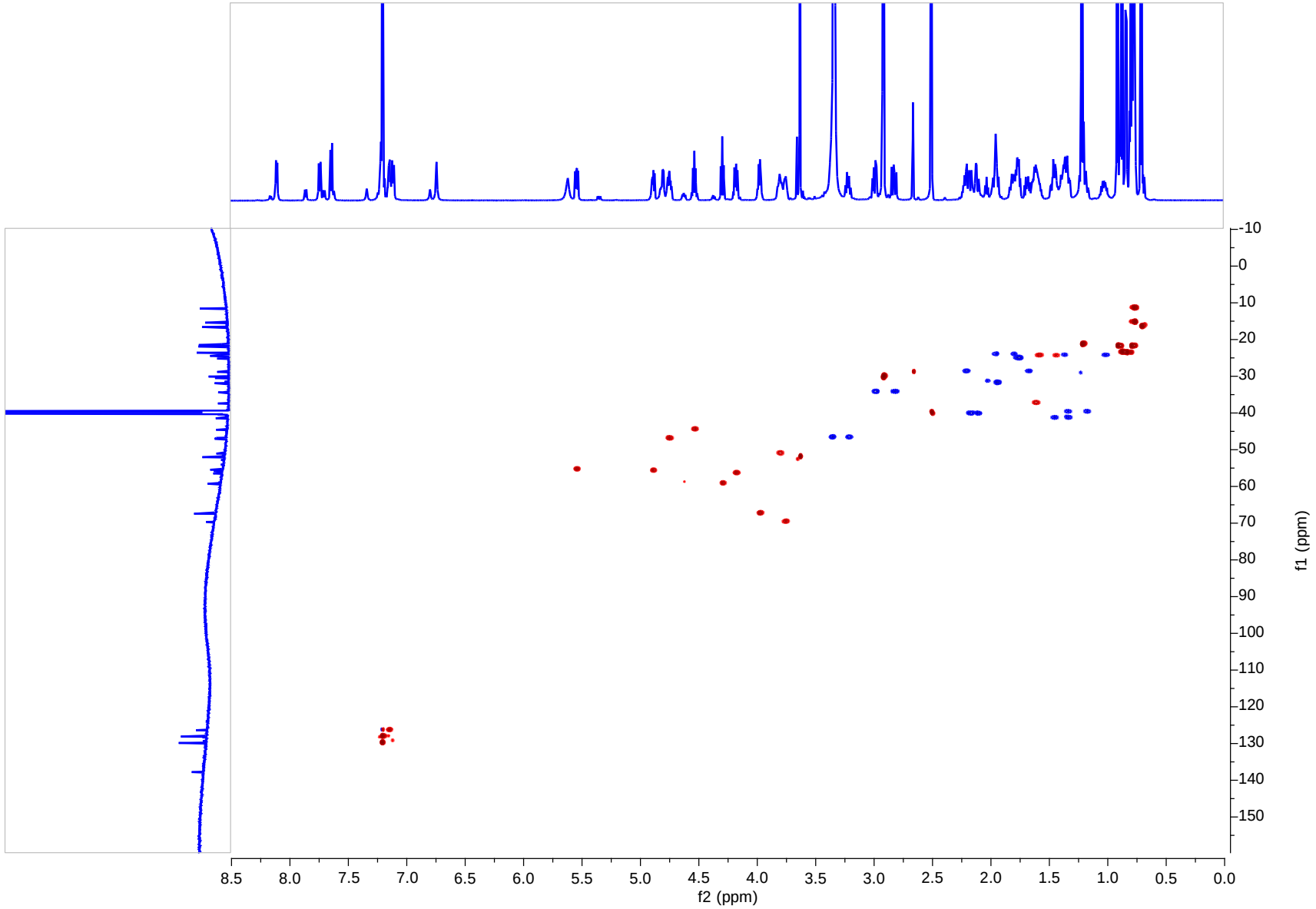
APT Spectrum of Grassystatin D (**1**) in DMSO-d_6, 150 MHz



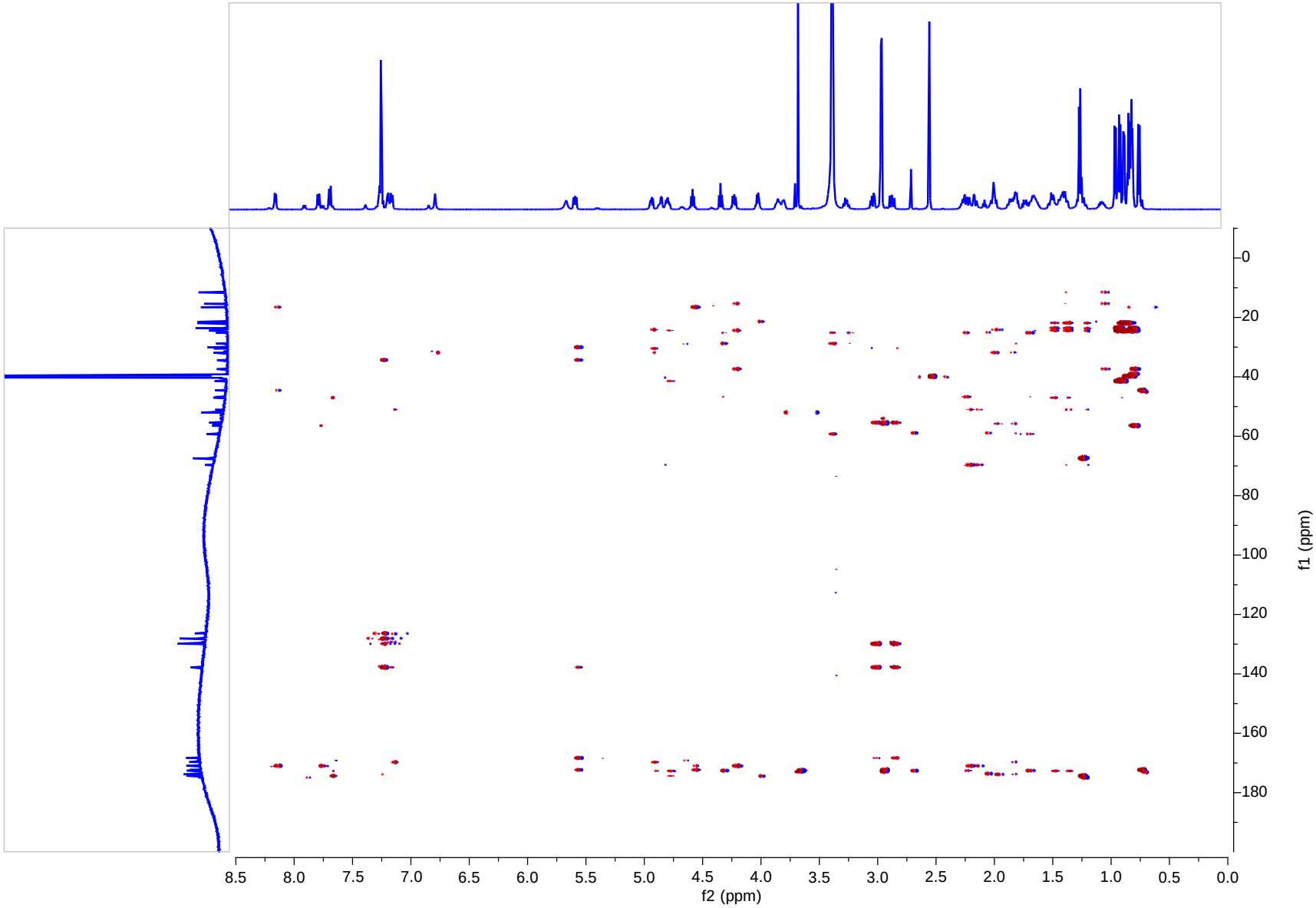
COSY Spectrum of Grassystatin D (**1**) in DMSO-d_6, 600 MHz



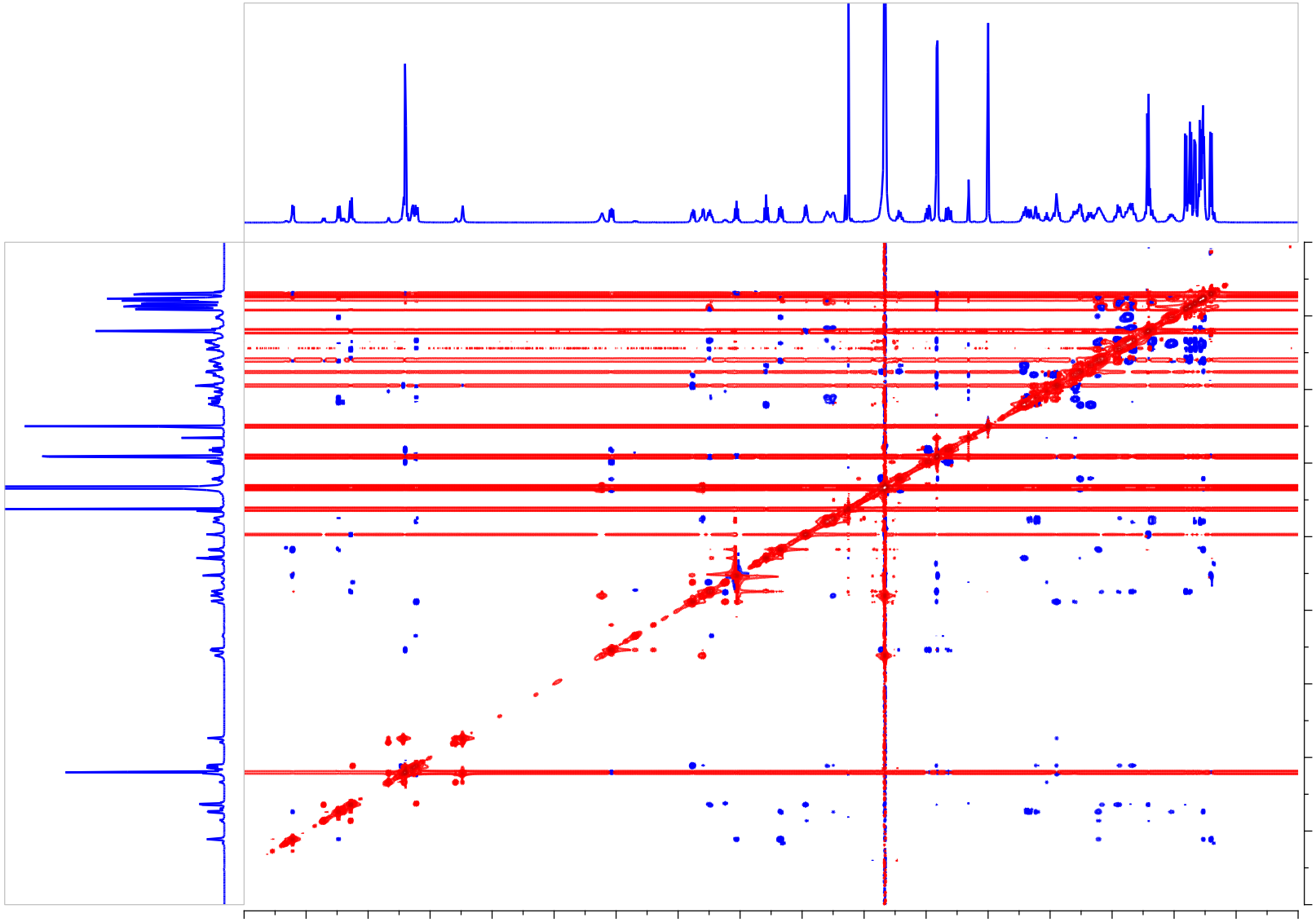
HSQC Spectrum of Grassystatin D (**1**) in DMSO-d_6, 600 MHz



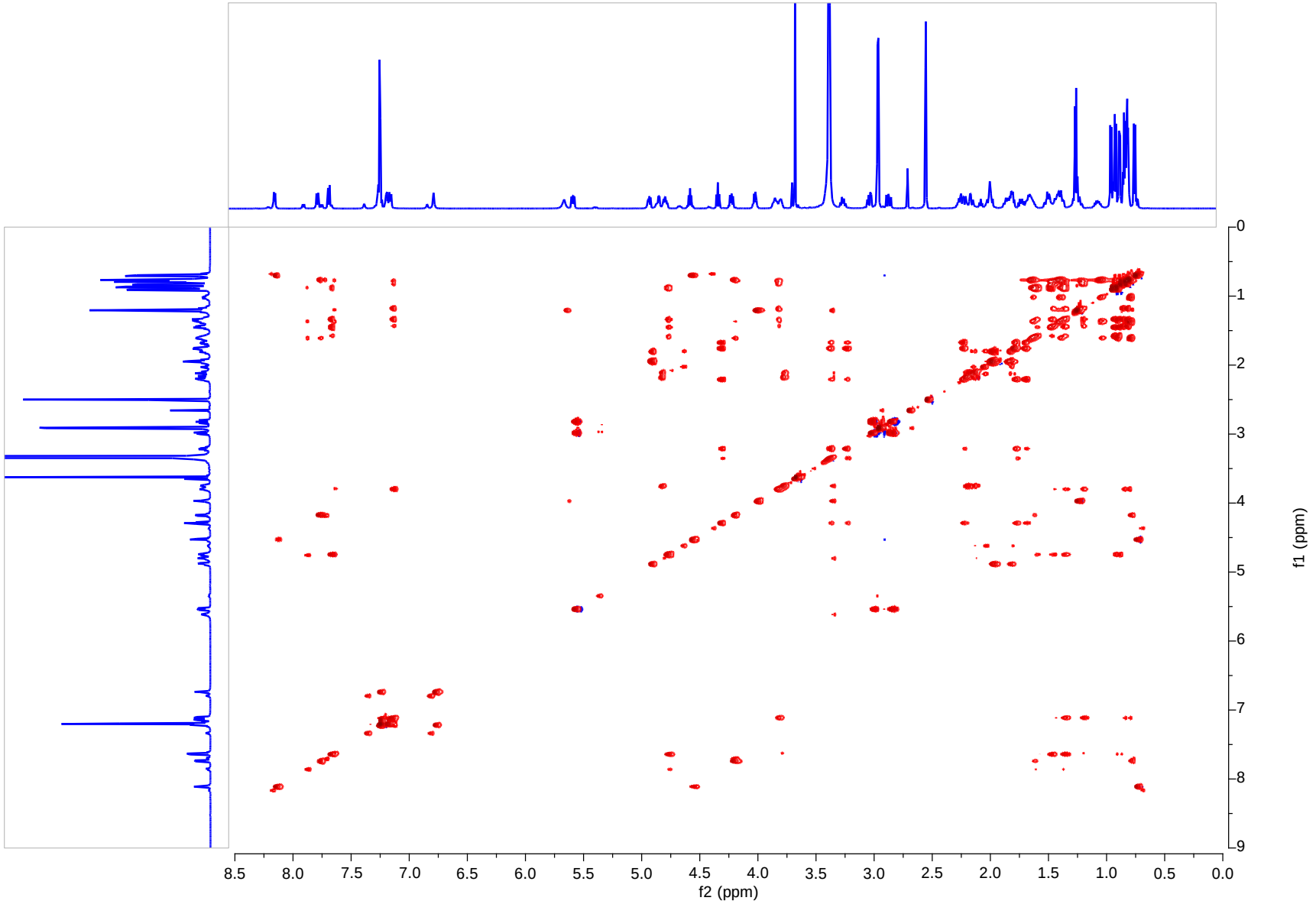
HMBC Spectrum of Grassystatin D (**1**) in DMSO-d_6, 600 MHz



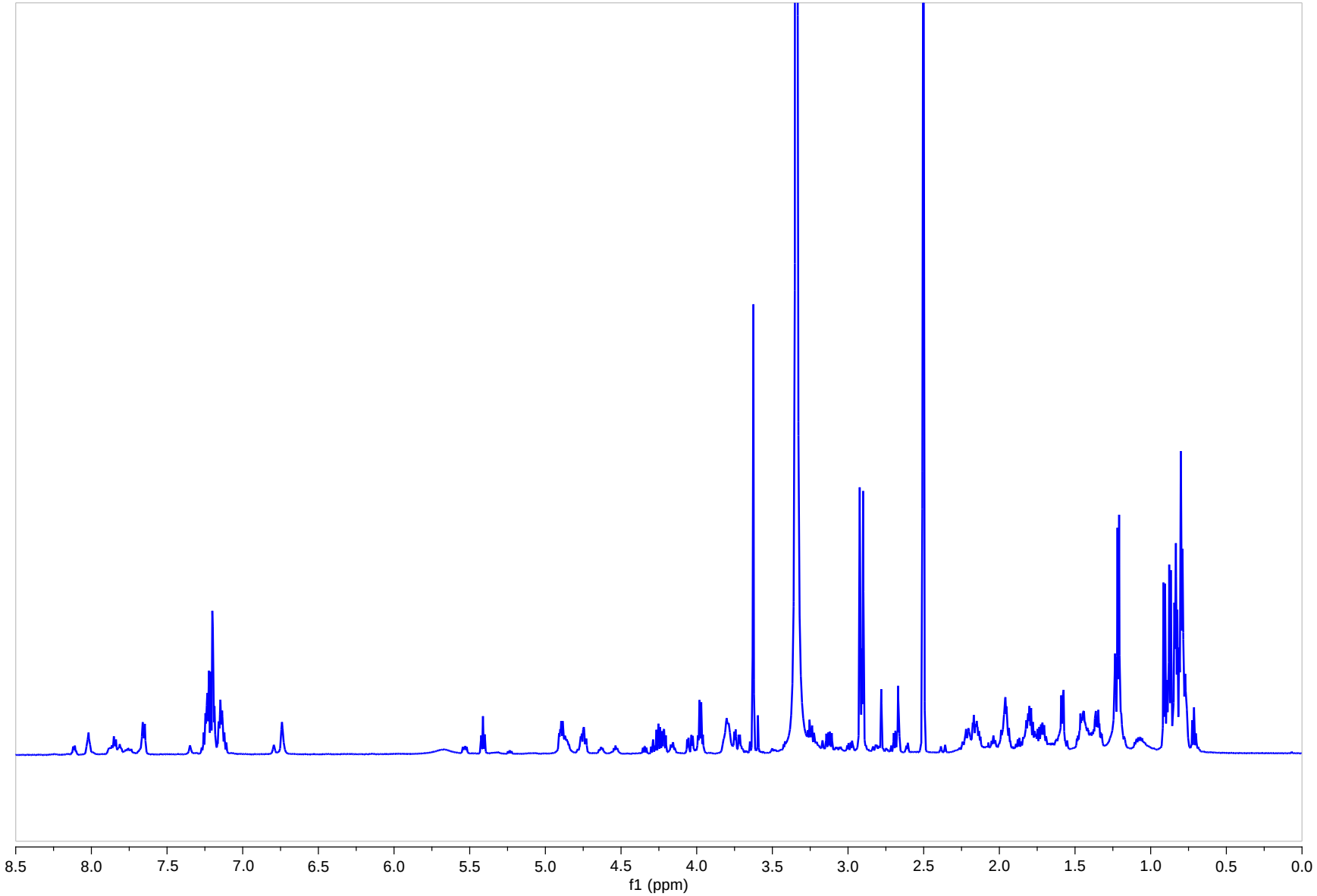
ROESY Spectrum of Grassystatin D (**1**) in DMSO-d_6, 600 MHz



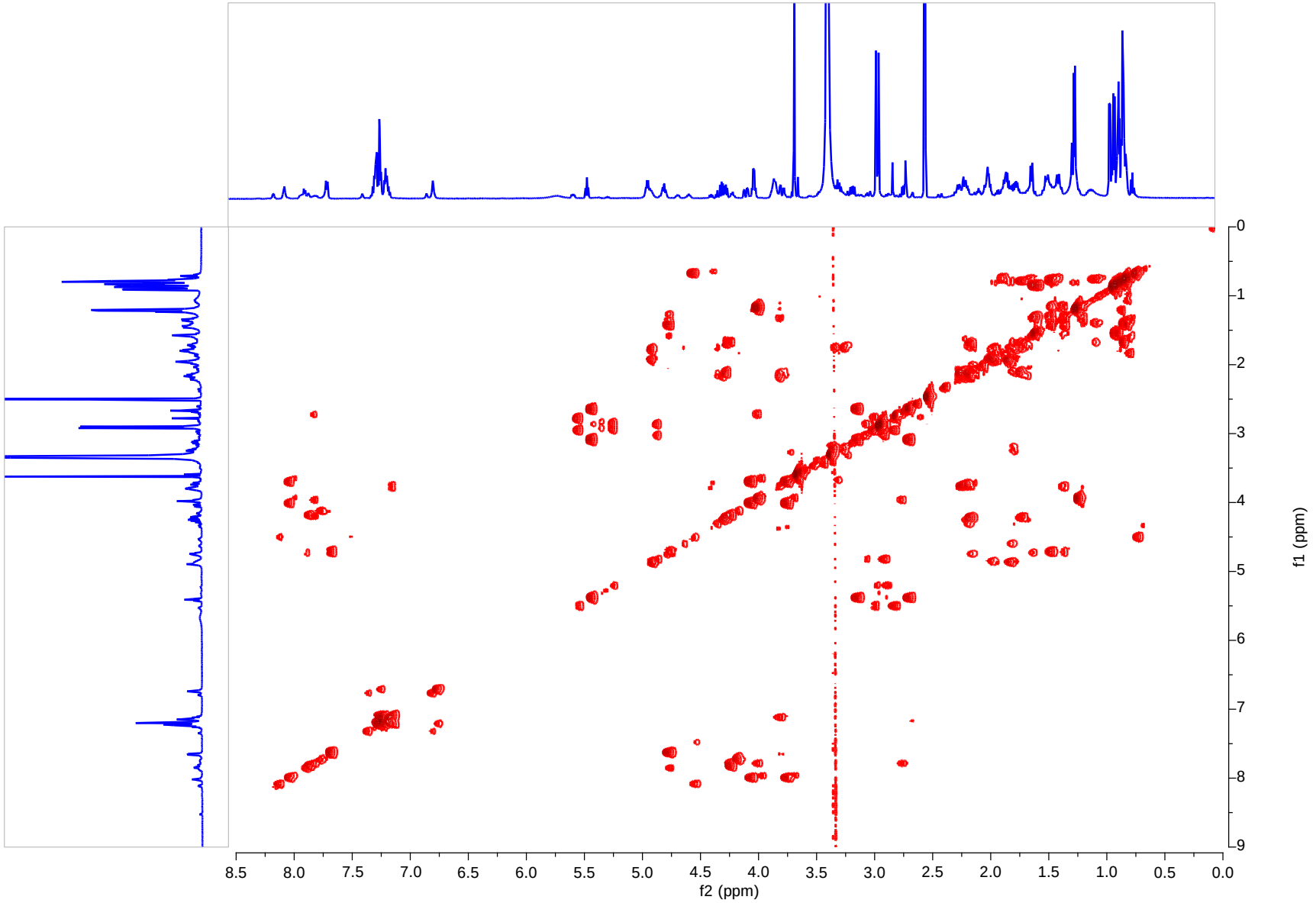
TOCSY Spectrum of Grassystatin D (**1**) in DMSO-d_6, 600 MHz



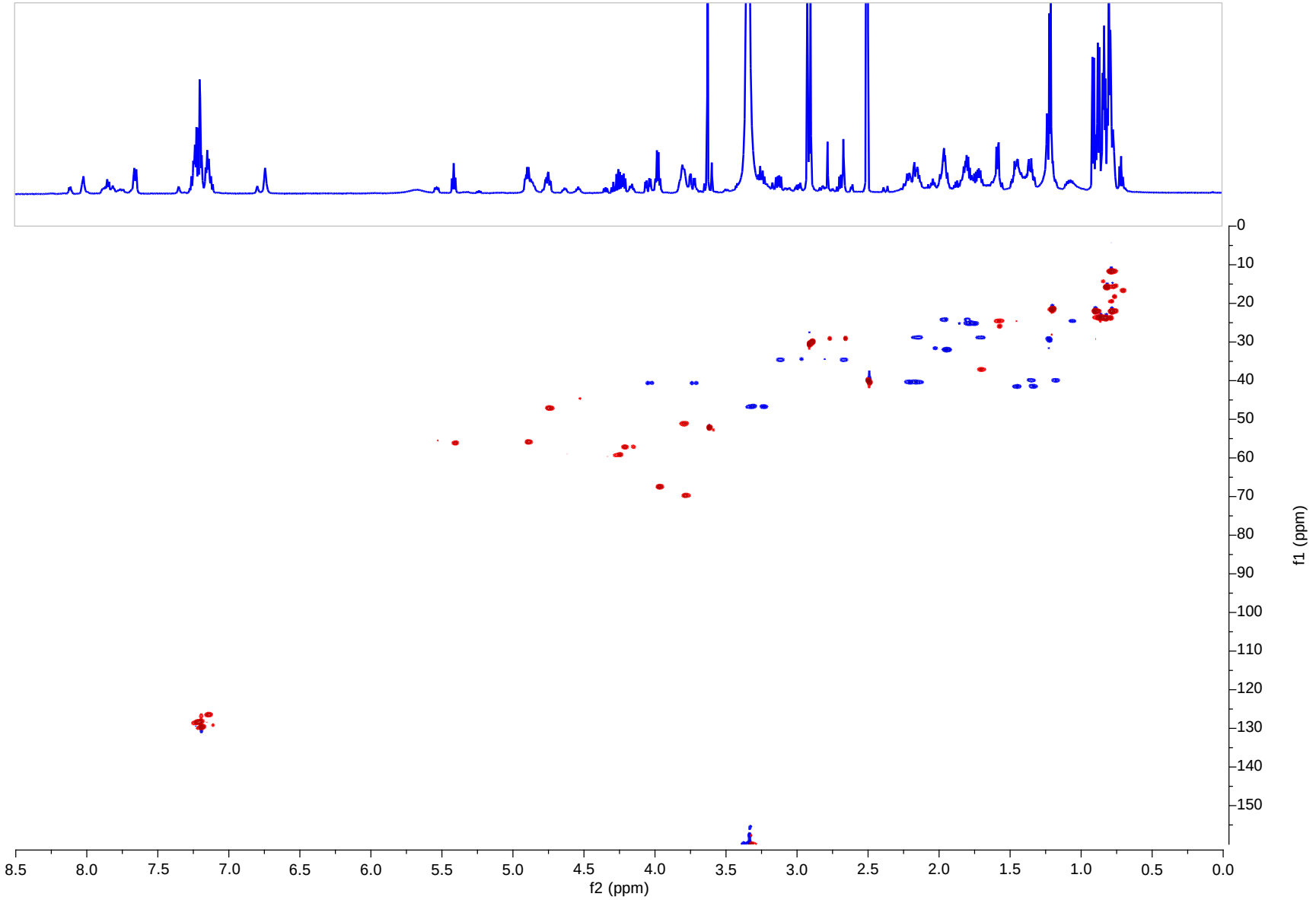
^{1}H NMR Spectrum of Grassystatin E (**2**) in DMSO-d_6, 600 MHz



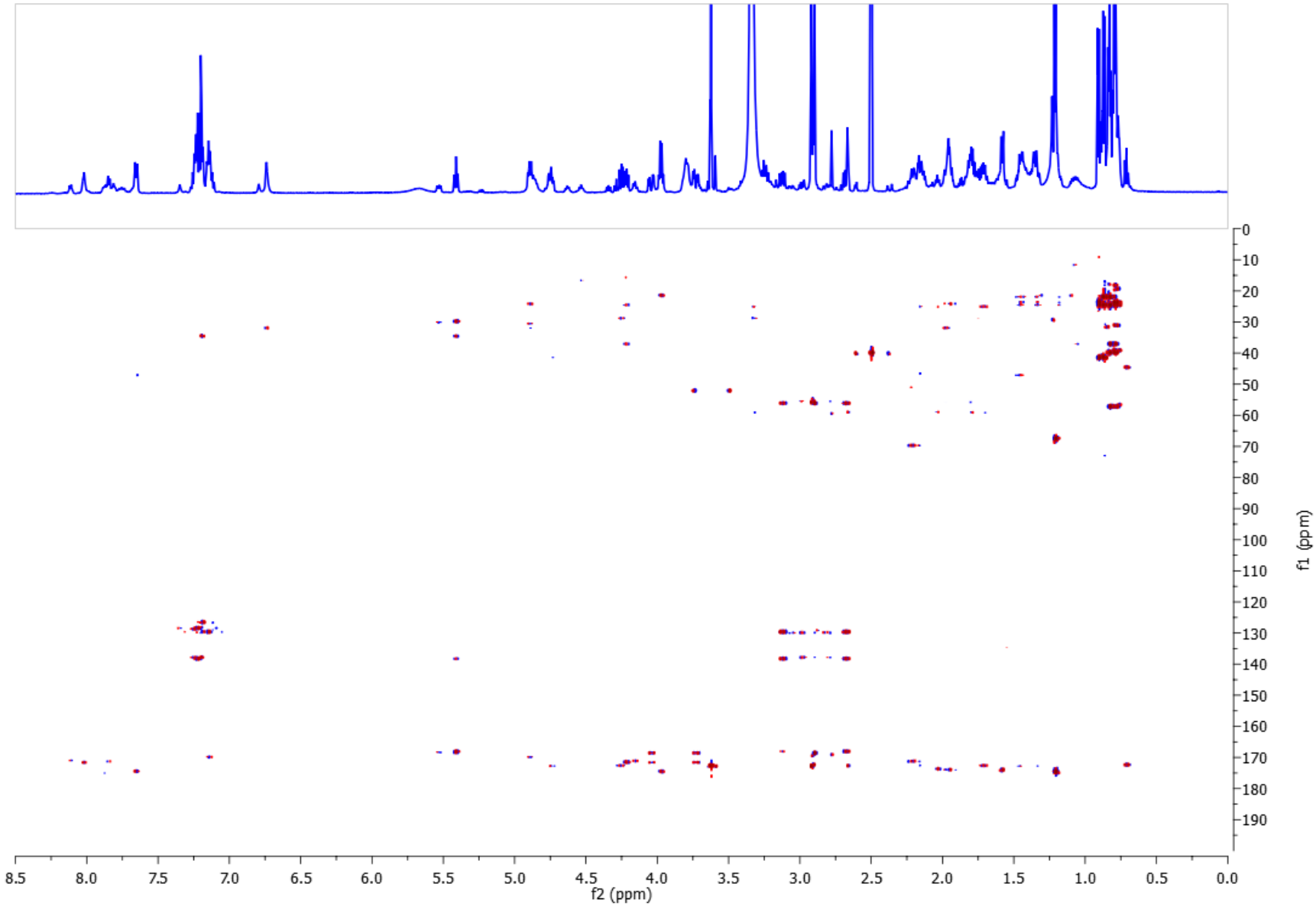
COSY Spectrum of Grassystatin E (**2**) in DMSO-d_6, 600 MHz



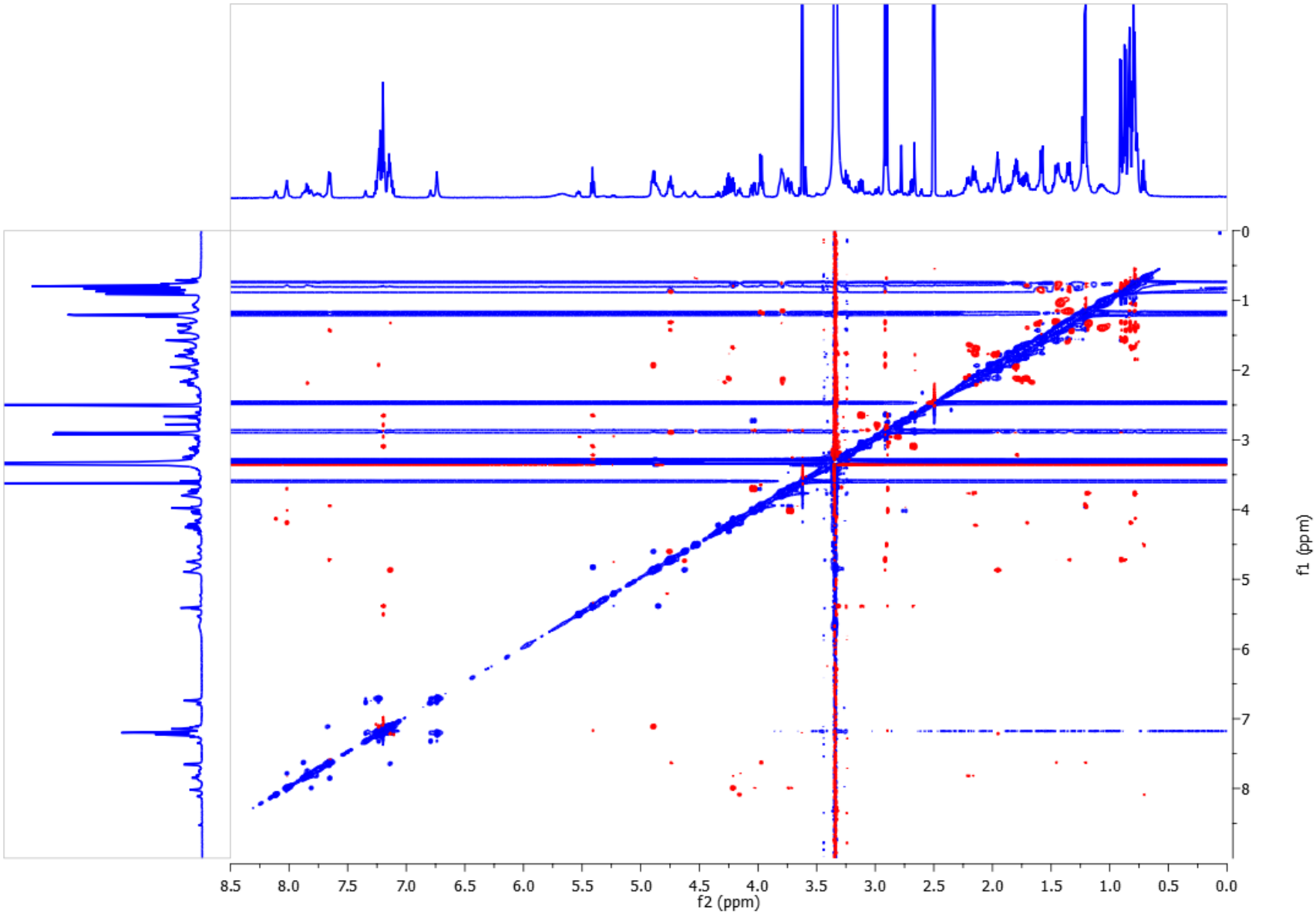
HSQC Spectrum of Grassystatin E (**2**) in DMSO-d_6, 600 MHz



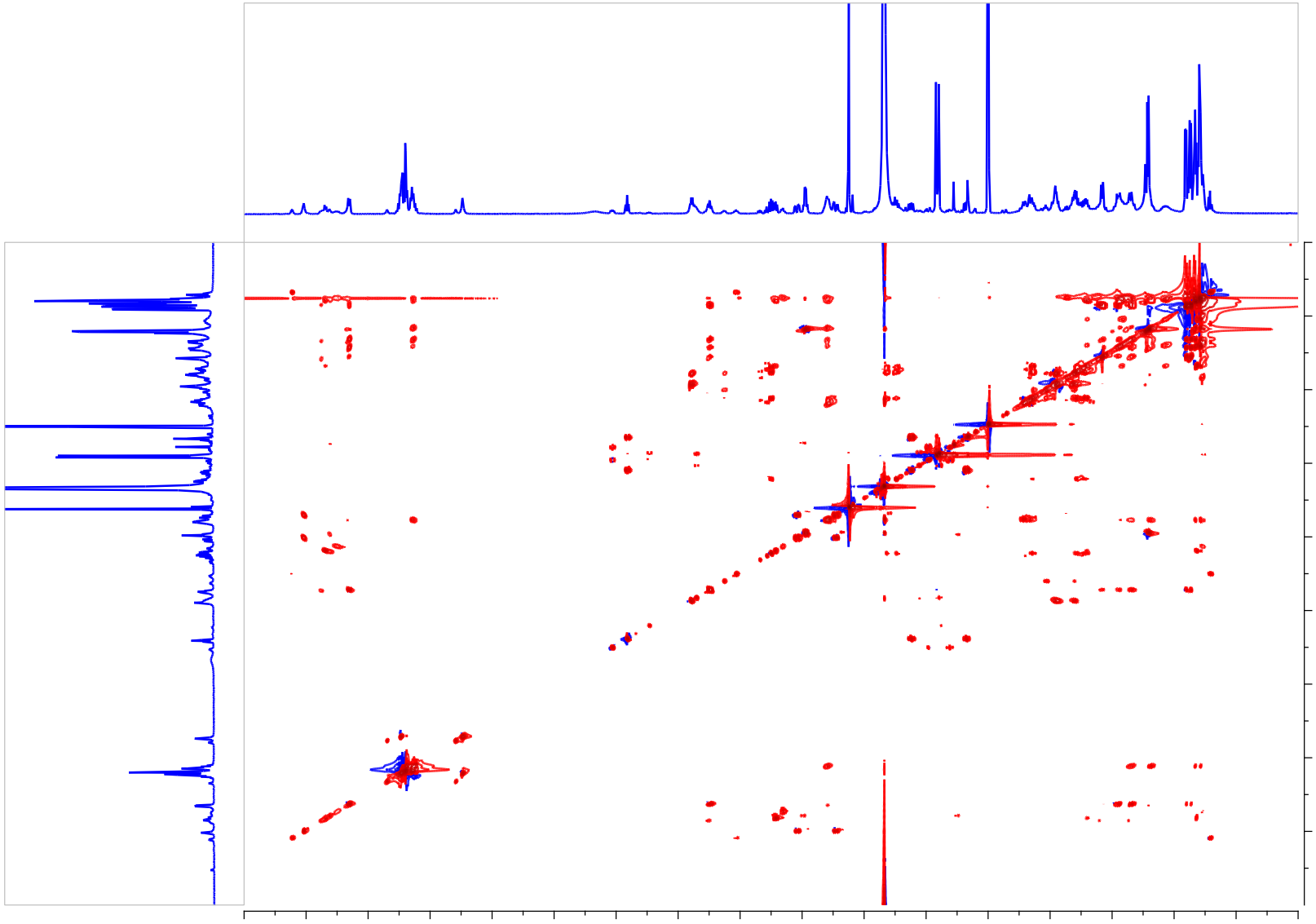
HMBC Spectrum of Grassystatin E (**2**) in DMSO-d_6, 600 MHz



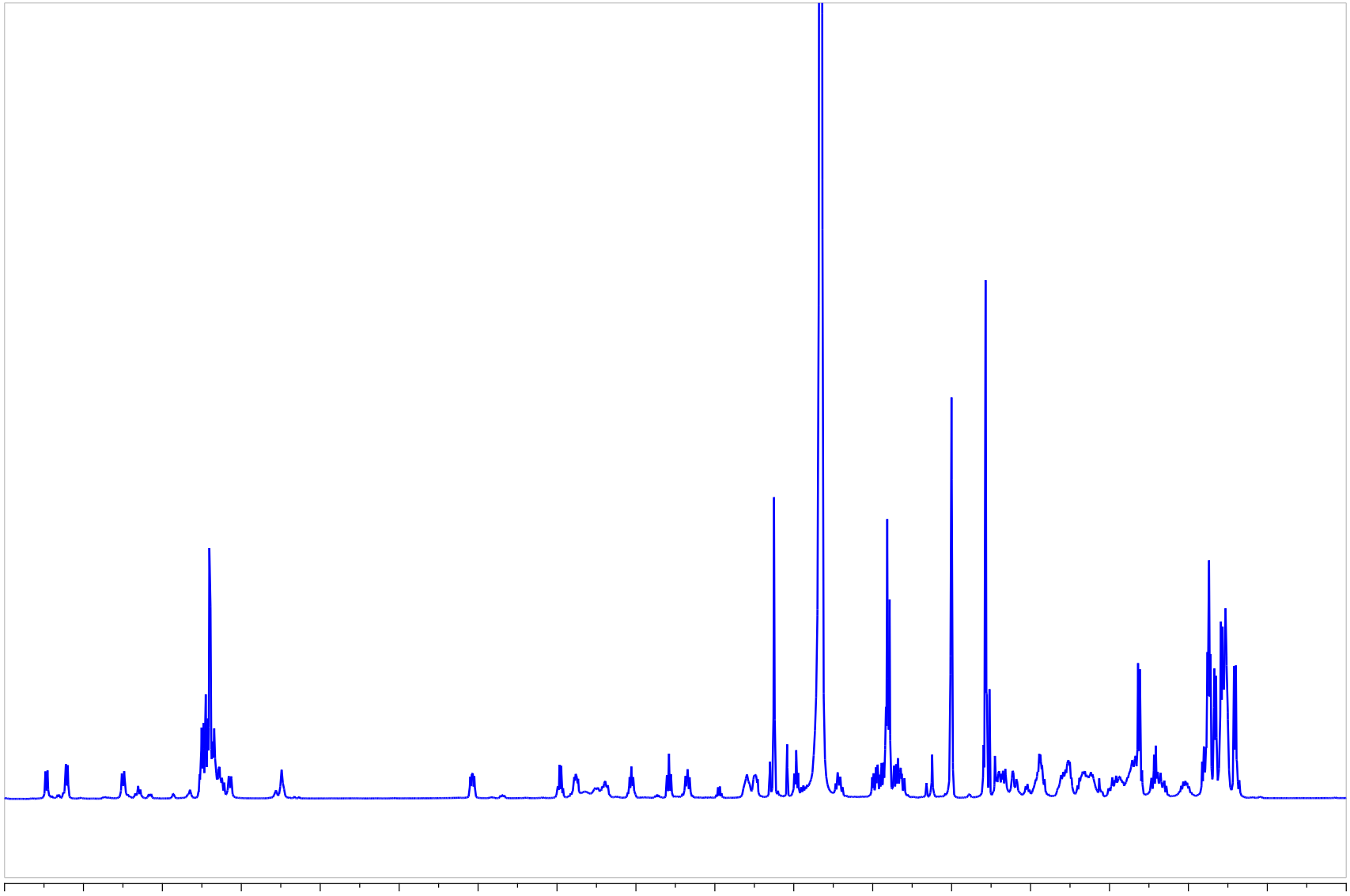
ROESY Spectrum of Grassystatin E (**2**) in DMSO-d_6, 600 MHz



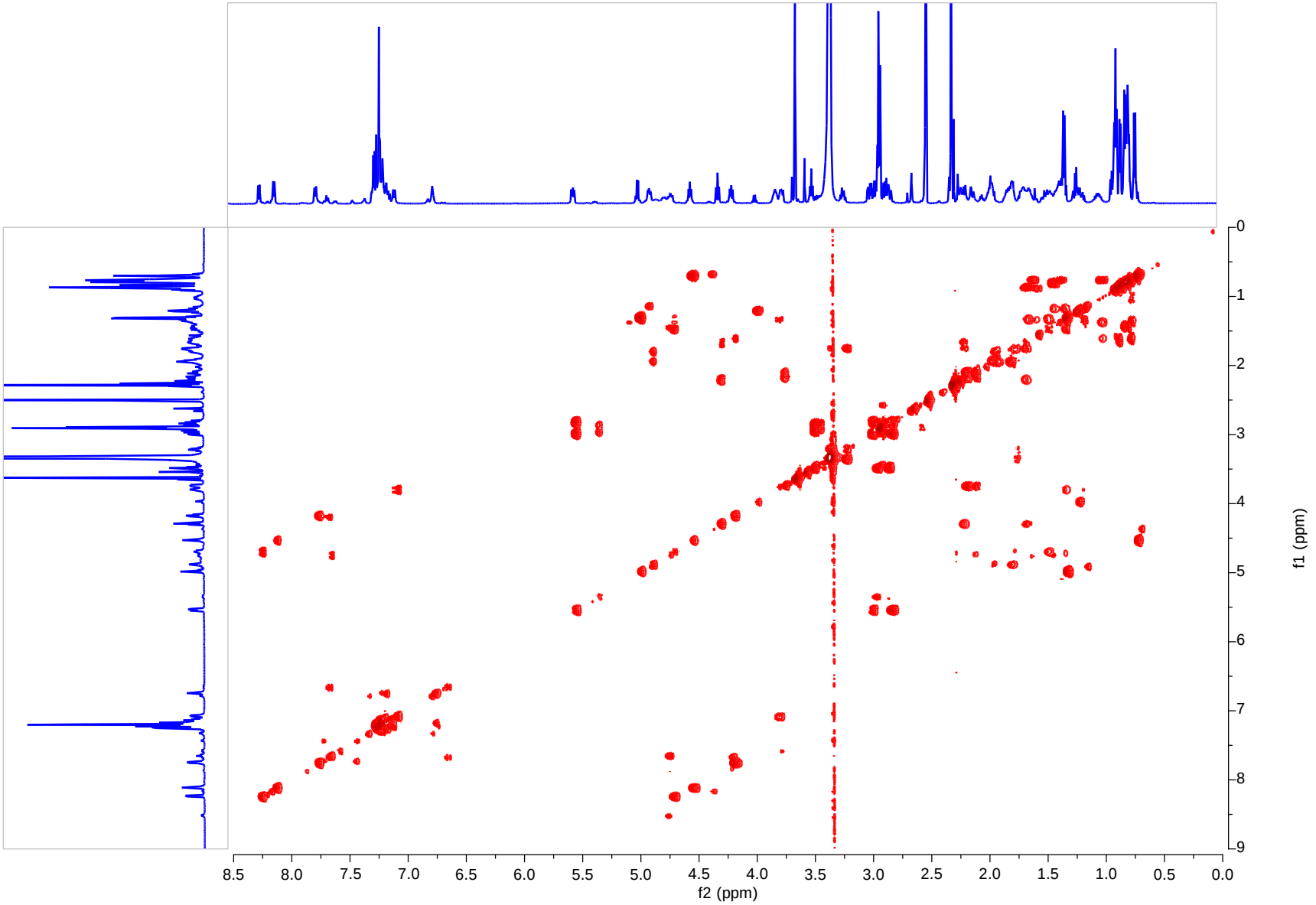
TOCSY Spectrum of Grassystatin E (**2**) in DMSO-d_6, 600 MHz



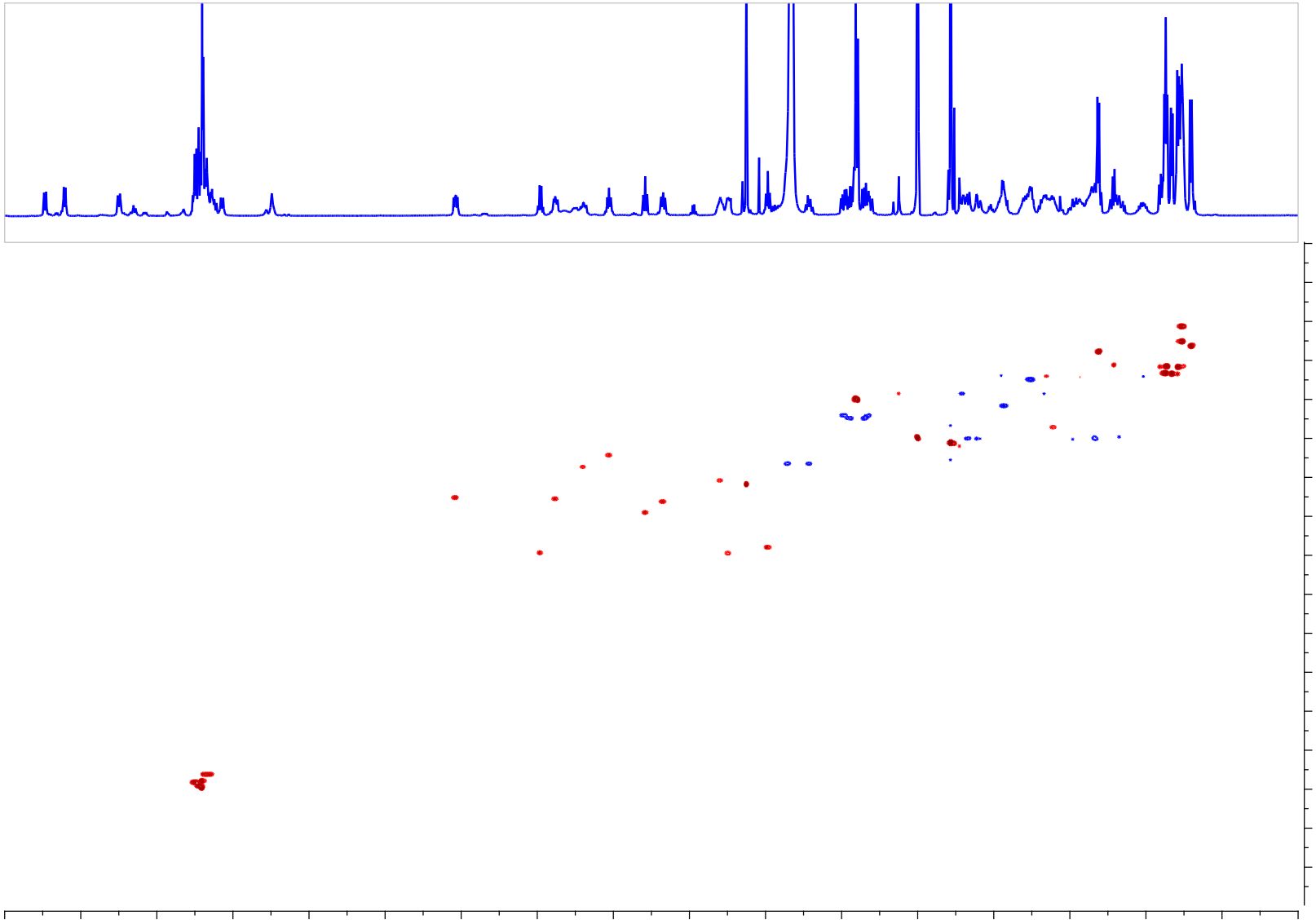
^{1}H NMR Spectrum of Grassystatin F (**3**) in DMSO-d_6, 600 MHz



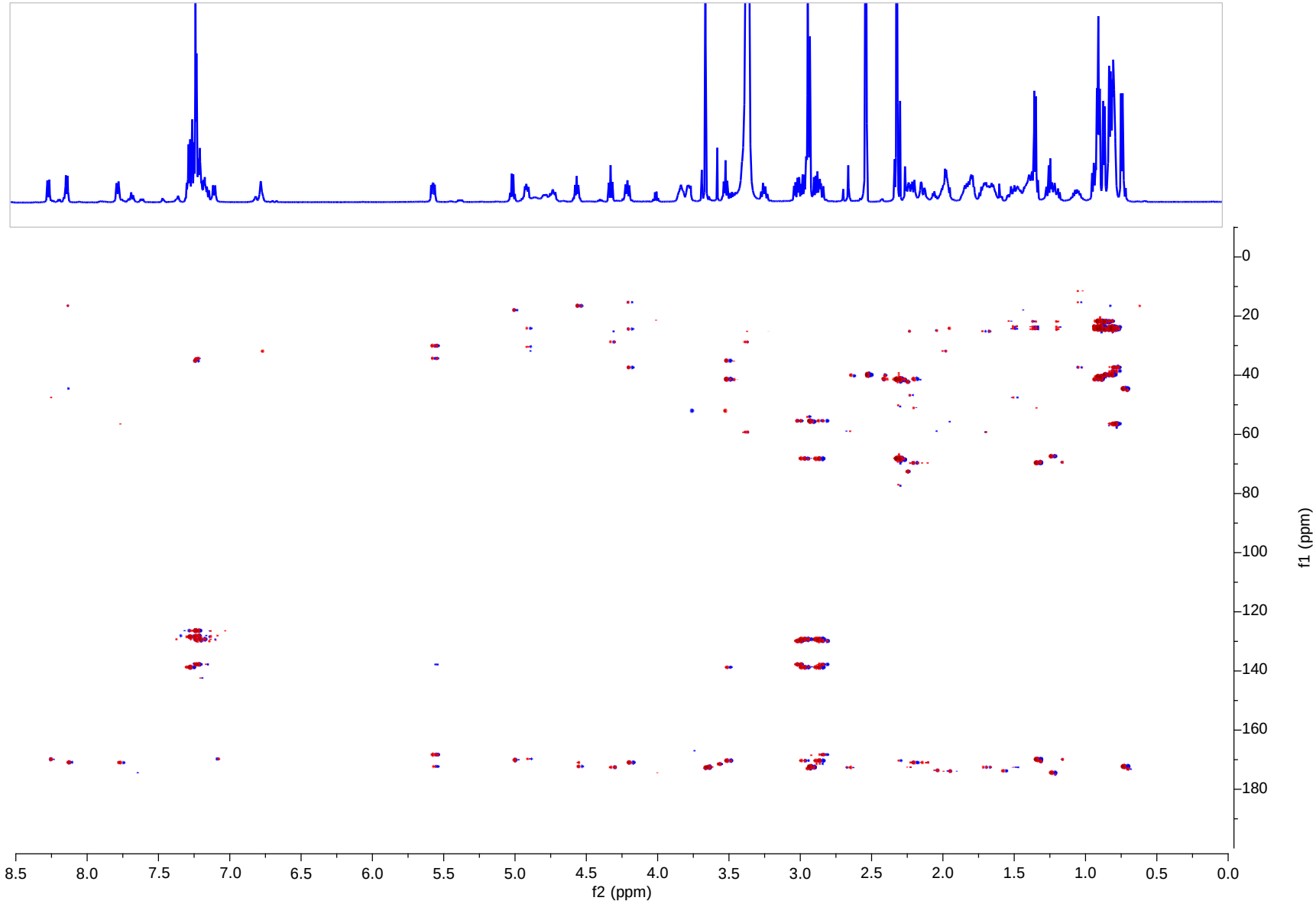
COSY Spectrum of Grassystatin F (**3**) in DMSO-d_6, 600 MHz



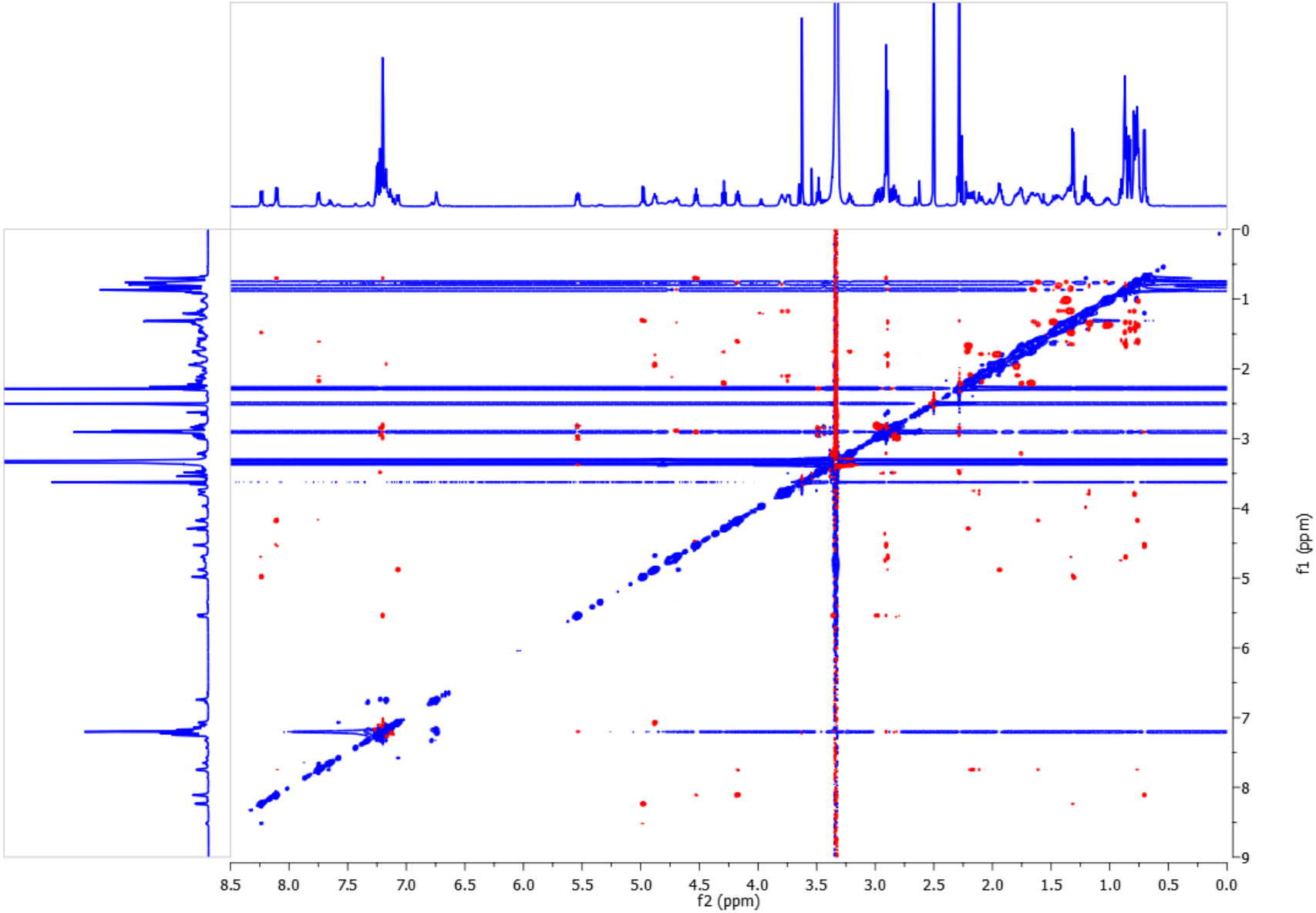
HSQC Spectrum of Grassystatin F (**3**) in DMSO-d_6, 600 MHz



HMBC Spectrum of Grassystatin F (**3**) in DMSO-d_6, 600 MHz



ROESY Spectrum of Grassystatin F (**3**) in DMSO-d_6, 600 MHz



TOCSY Spectrum of Grassystatin F (**3**) in DMSO-d_6, 600 MHz