

Supplementary Information (SI-1) NMR Spectra

2-Benzylidenebenzofuran-3(2H)-ones as a New Class of Alkaline Phosphatase Inhibitors: Synthesis, SAR Analysis, Enzyme Inhibitory Kinetics and Computational Studies

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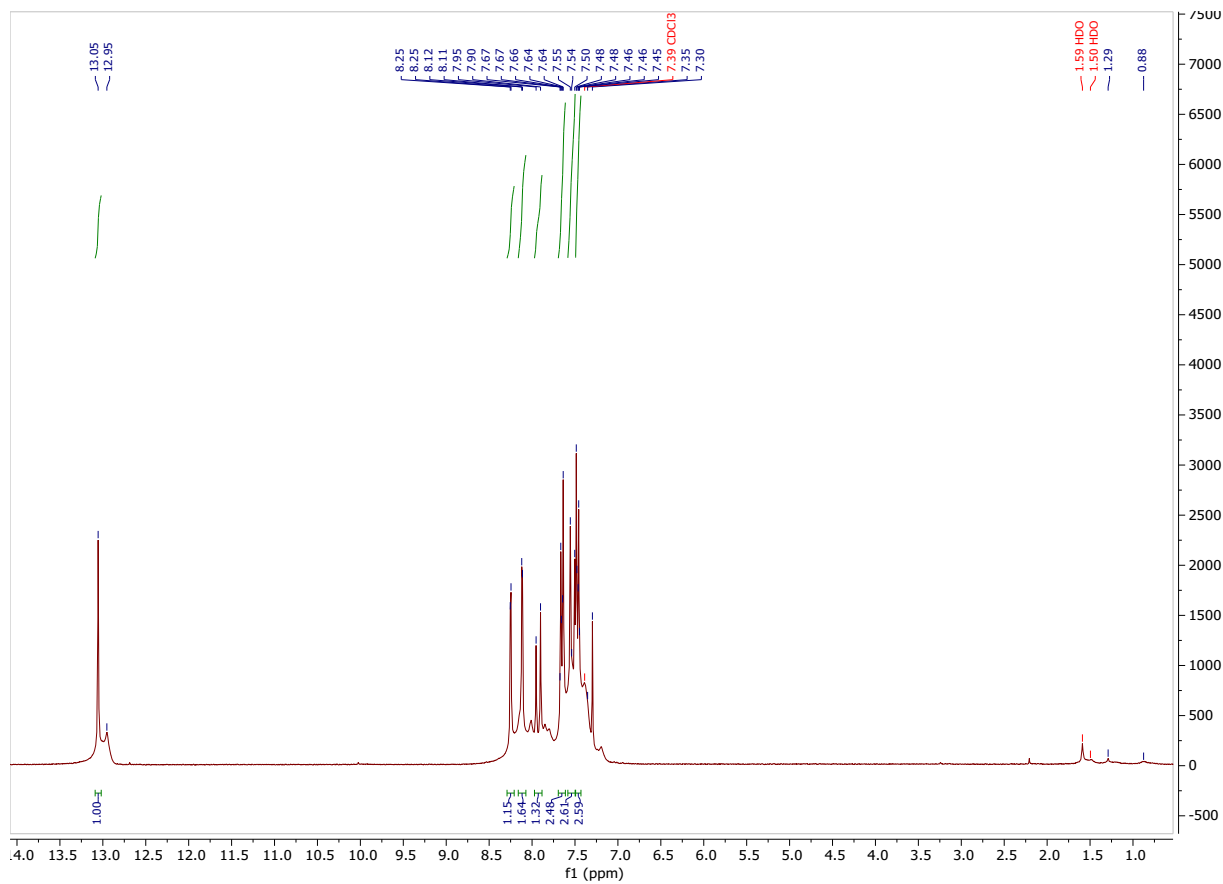
^k*Department of Chemistry, Faculty of Applied Science, Umm Al-Qura University, 21955 Makkah Saudi Arabia*

^l*Chemistry Department, Faculty of Science, Assiut University, 71516 Assiut, Egypt*

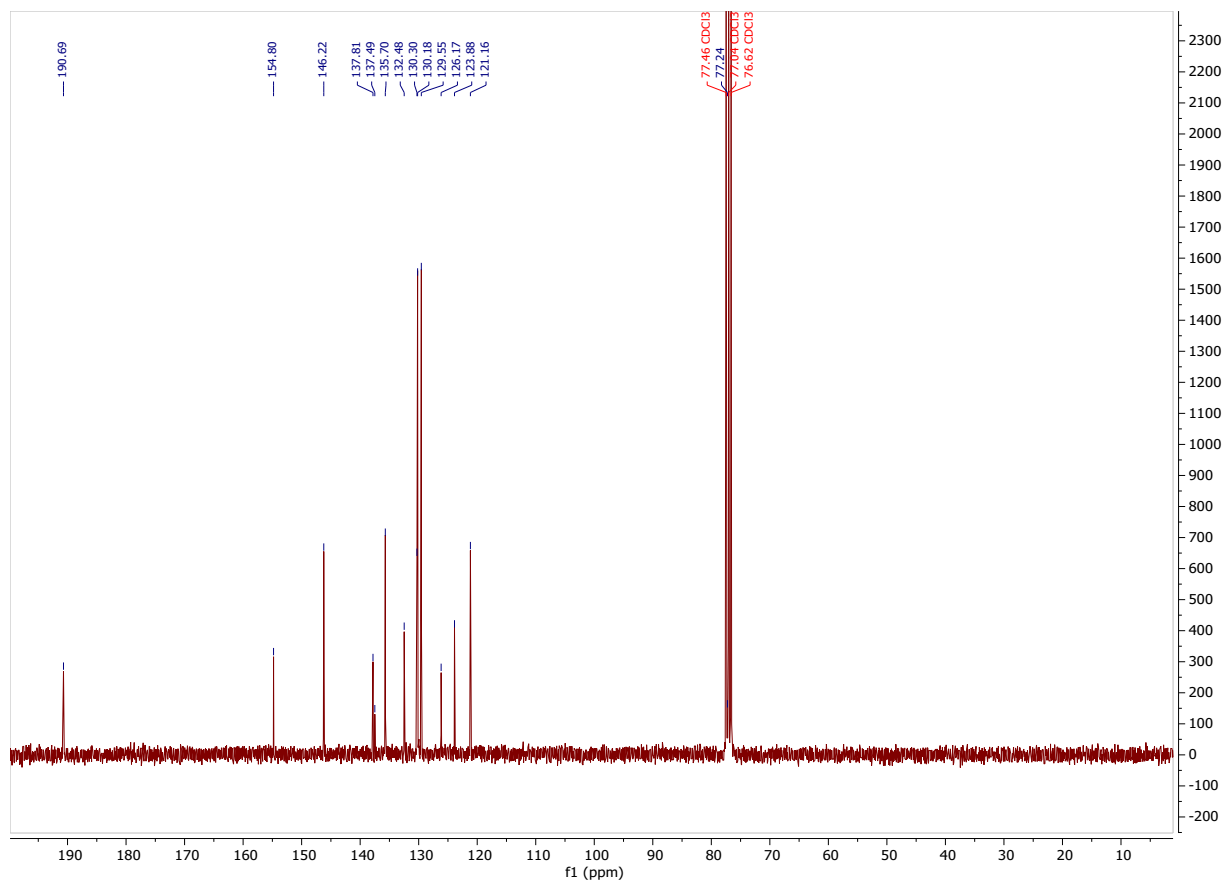
NMR Spectra of all the Newly Synthesized Compounds

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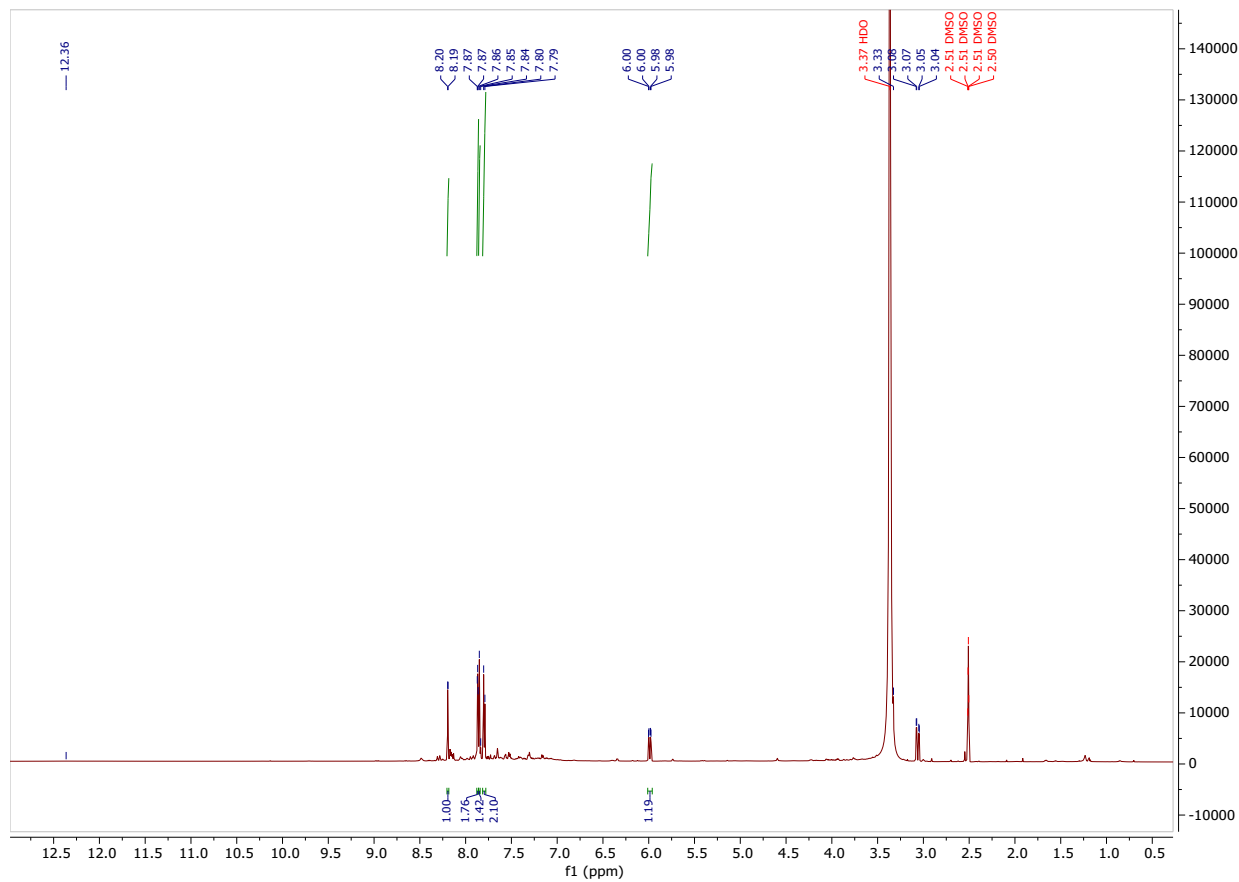
¹H-NMR (300 MHz, CDCl₃) Spectrum of Compound 2



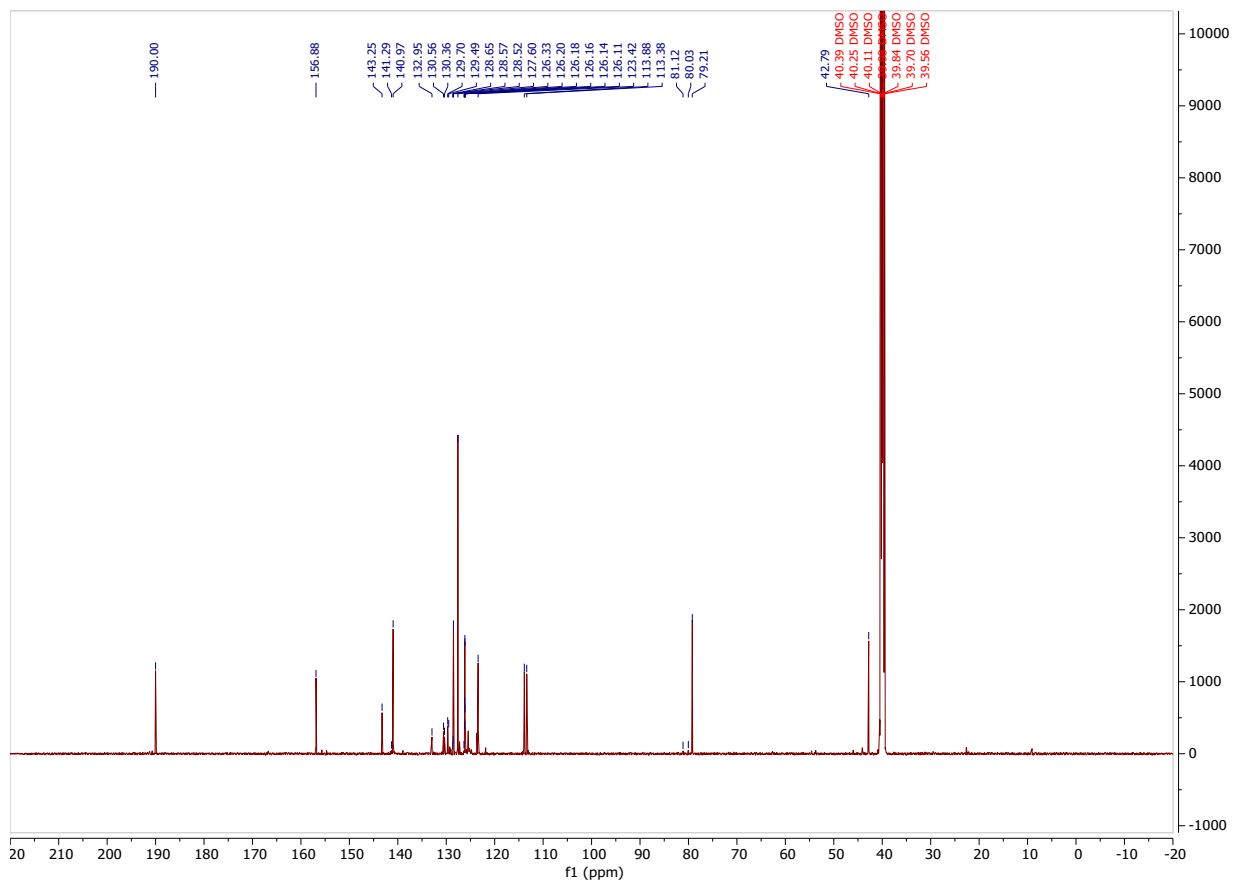
¹³C-NMR (75 MHz, CDCl₃) Spectrum of Compound 2



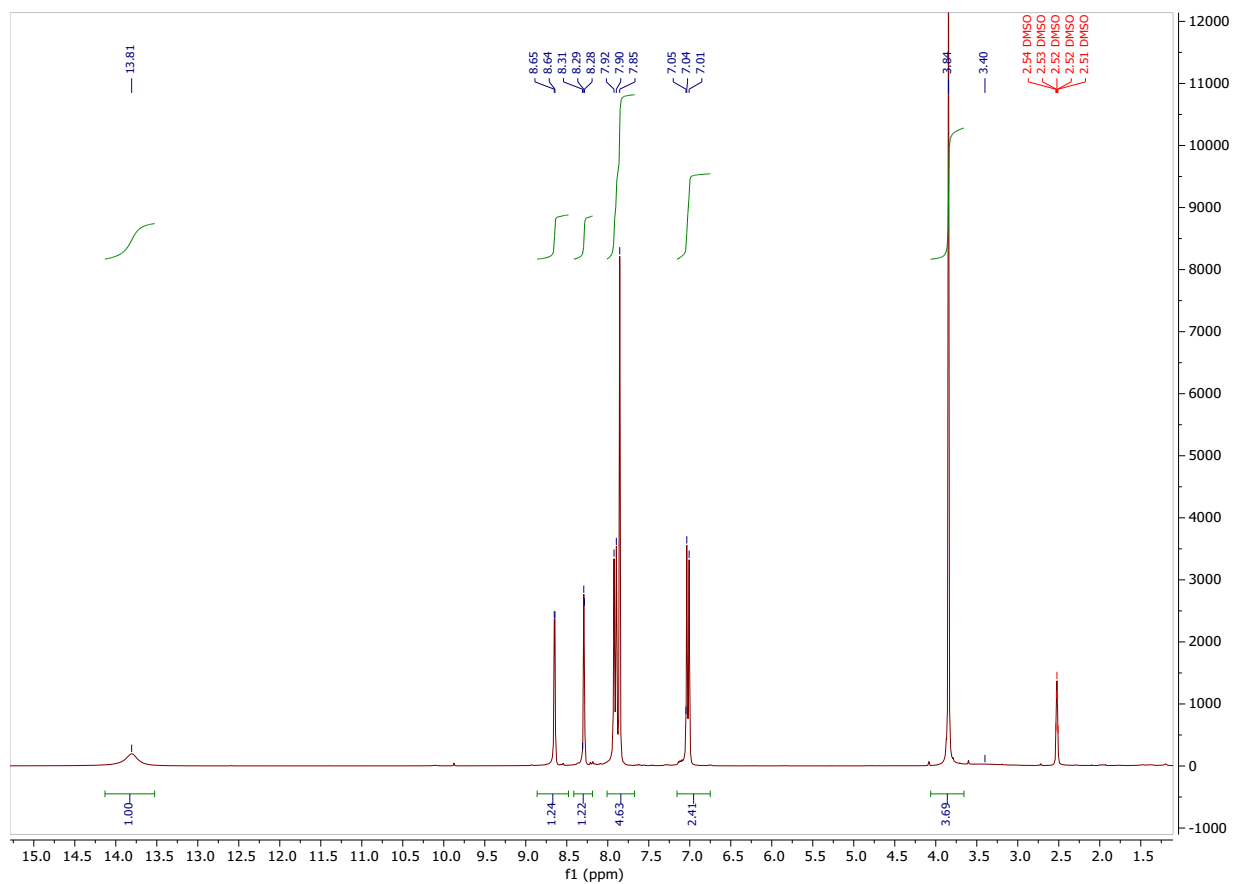
¹H-NMR (600 MHz, DMSO-d₆) Spectrum of Compound 3



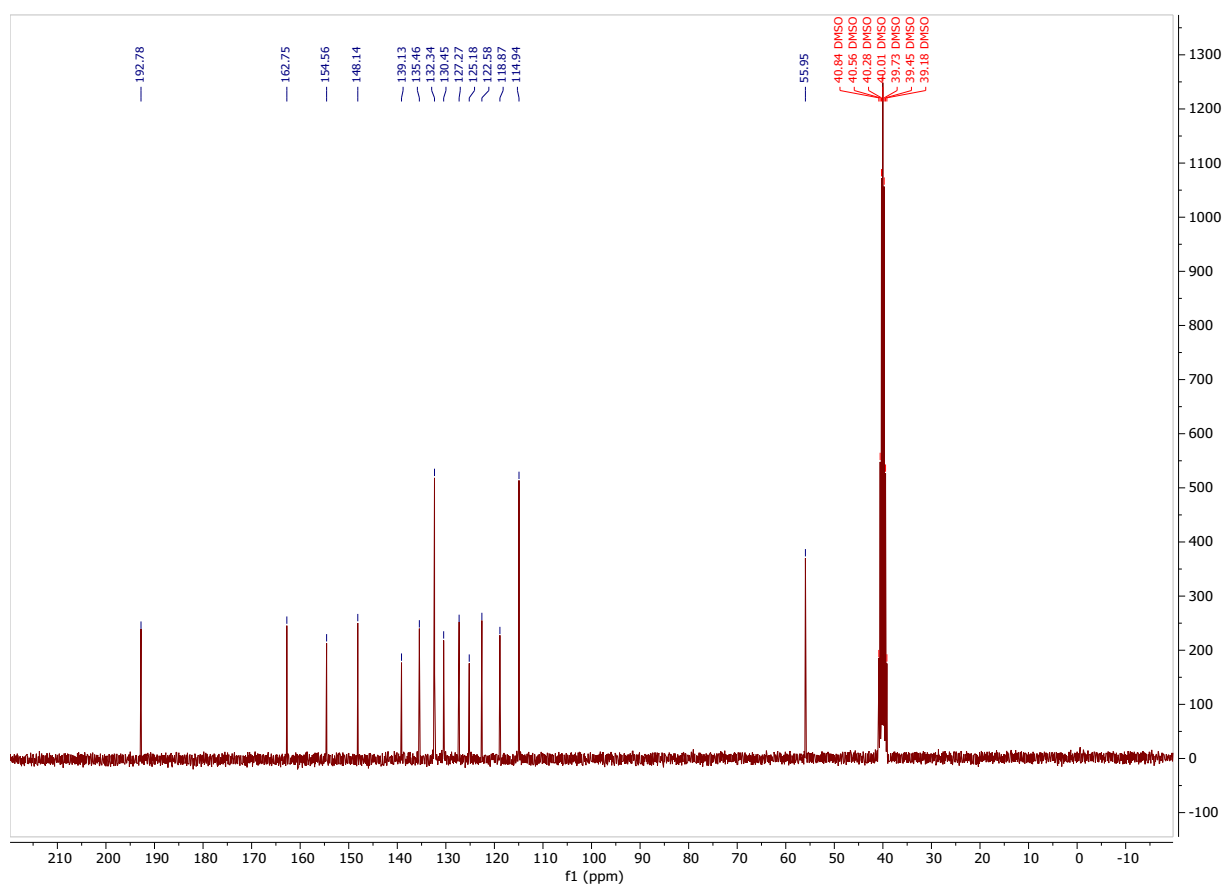
^{13}C -NMR (151 MHz, DMSO- d_6) Spectrum of Compound 3



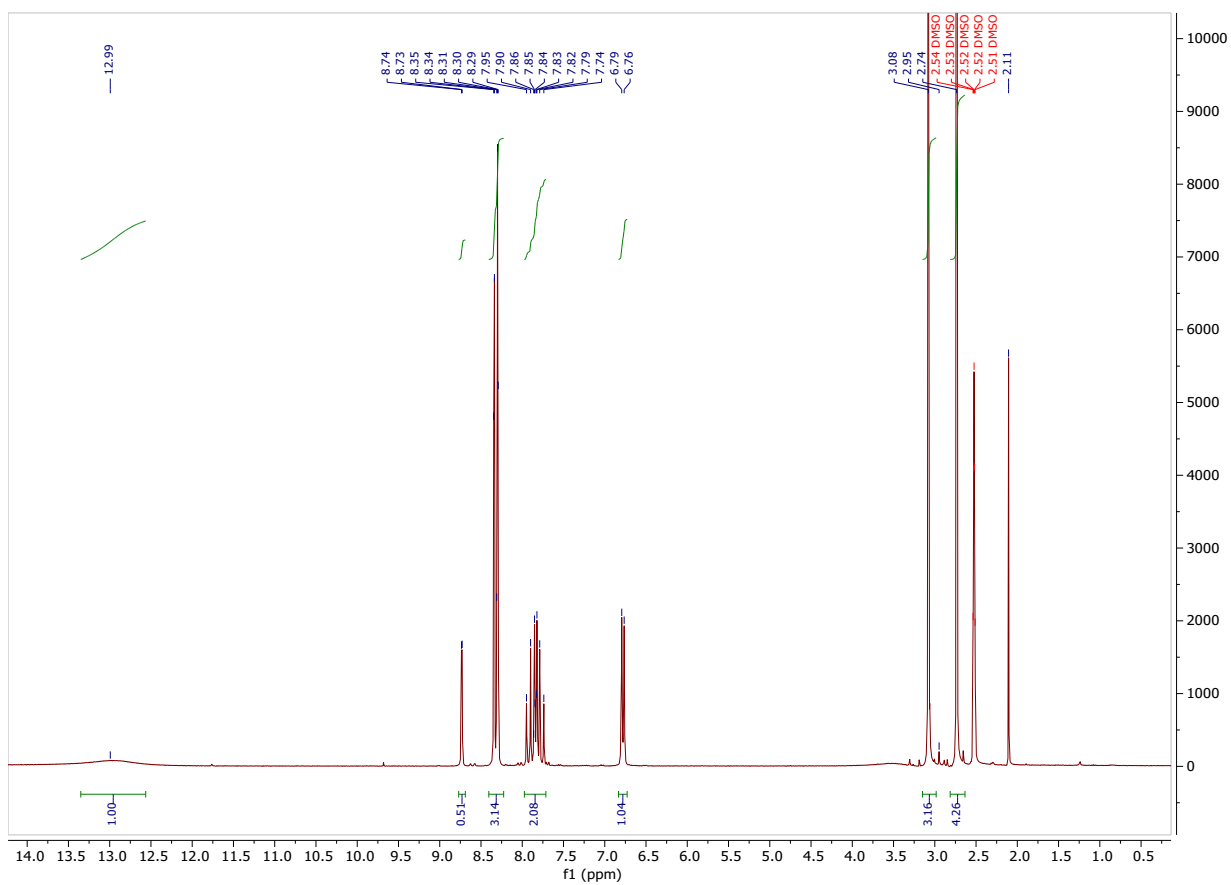
¹H-NMR (300 MHz, DMSO-d₆) Spectrum of Compound 4



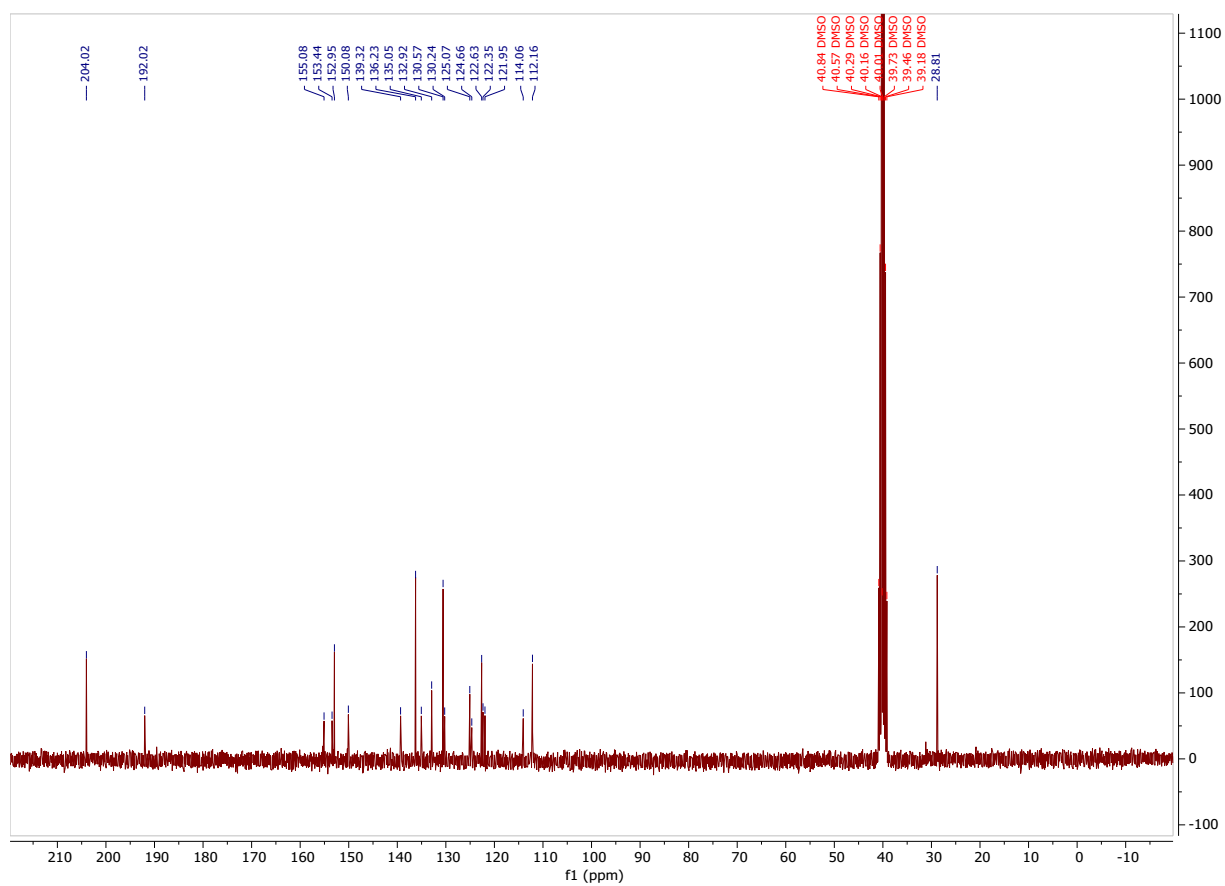
^{13}C -NMR (75 MHz, DMSO- d_6) Spectrum of Compound 4



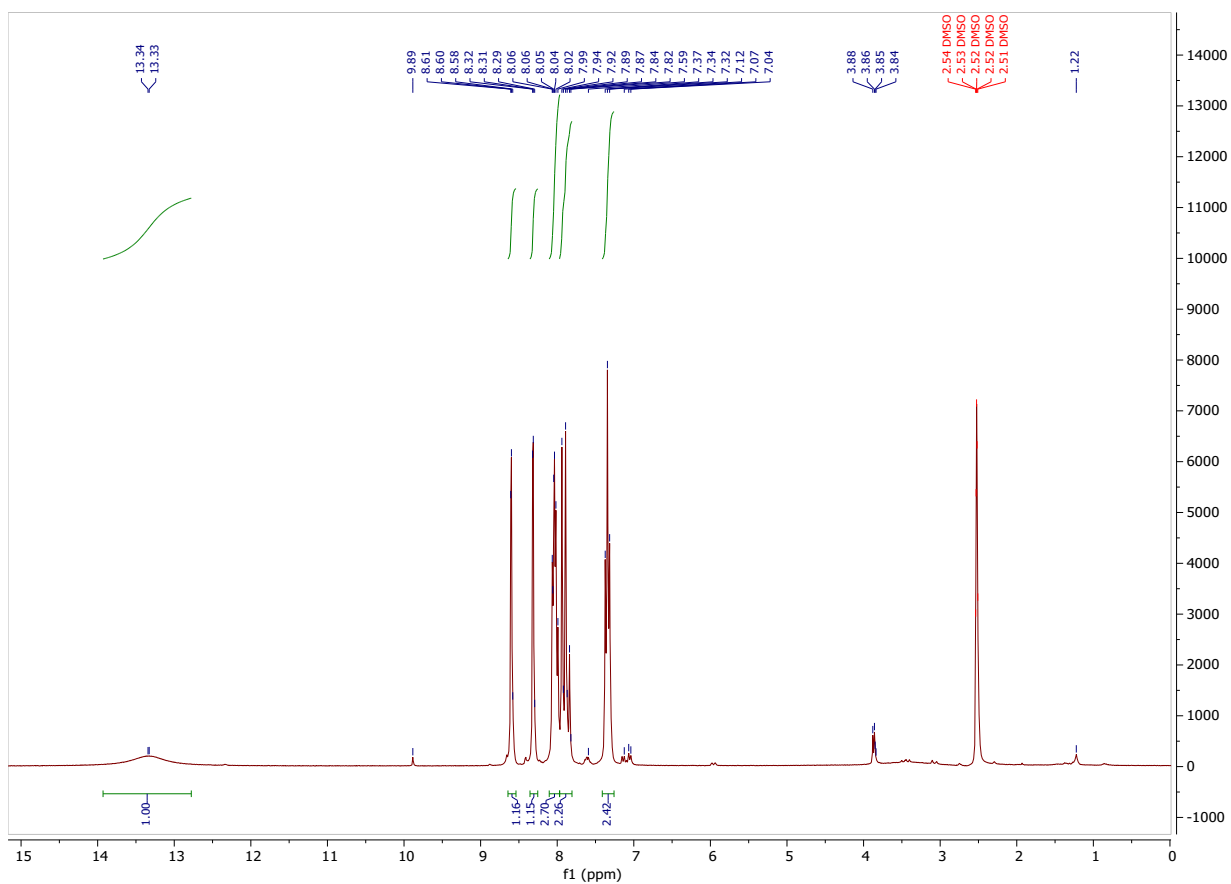
¹H-NMR (300 MHz, DMSO-d₆) Spectrum of Compound 6



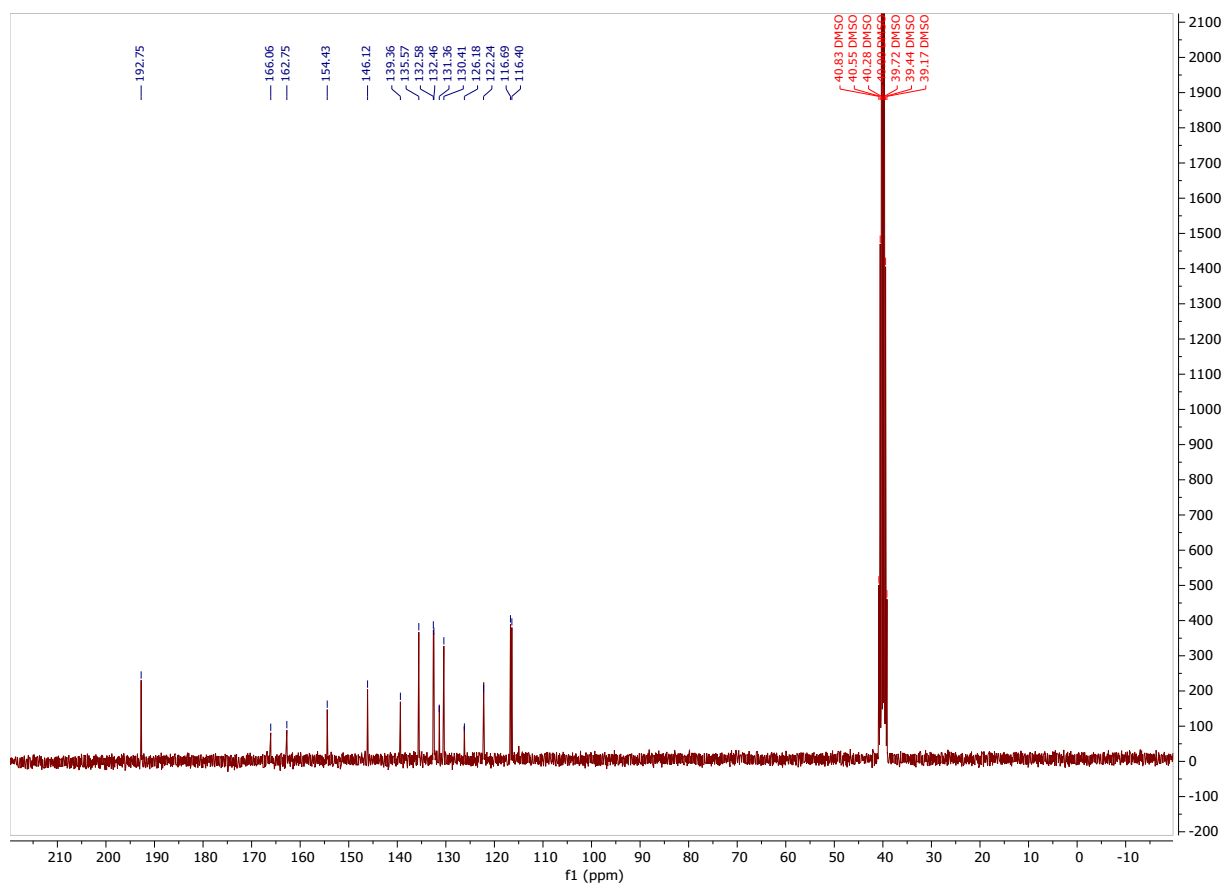
^{13}C -NMR (75 MHz, DMSO- d_6) Spectrum of Compound 6



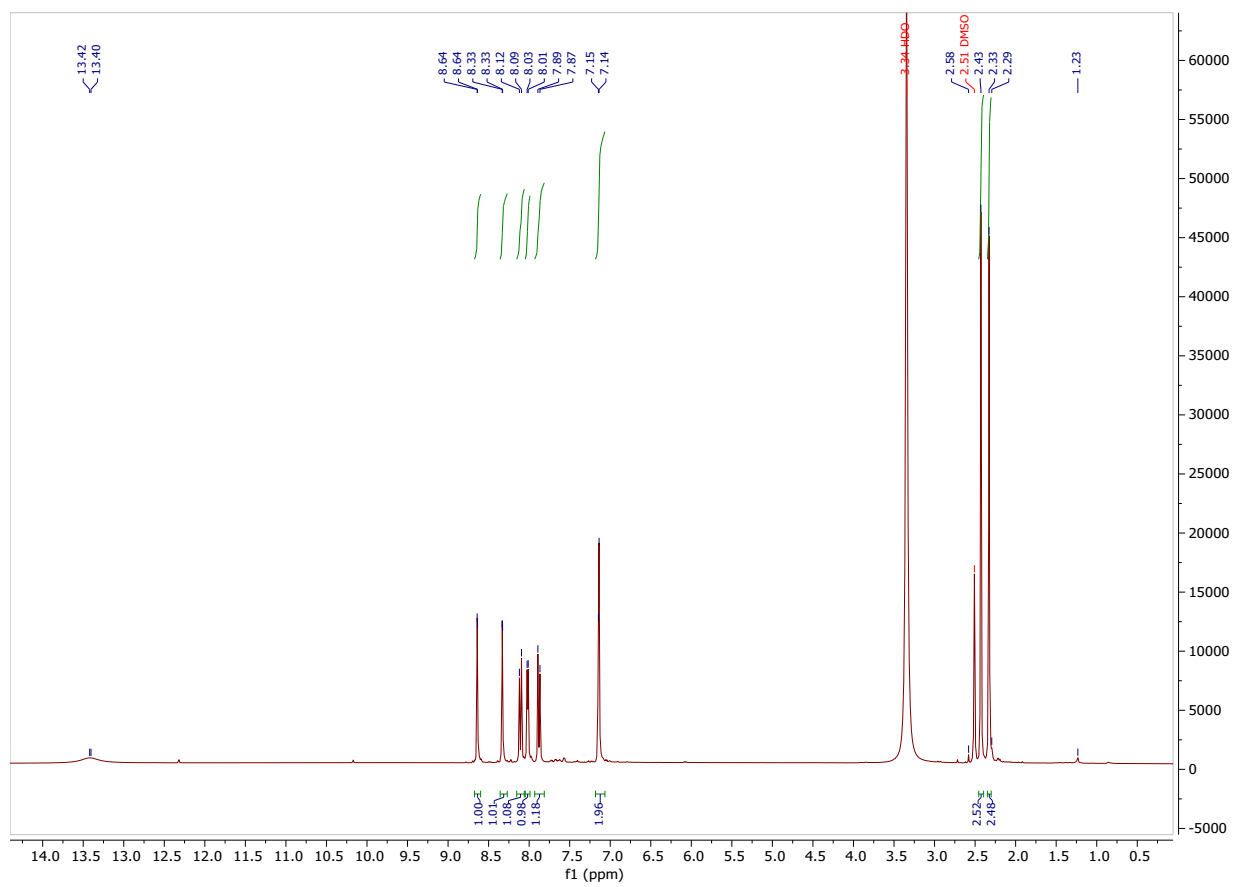
¹H-NMR (300 MHz, DMSO-d₆) Spectrum of Compound 7



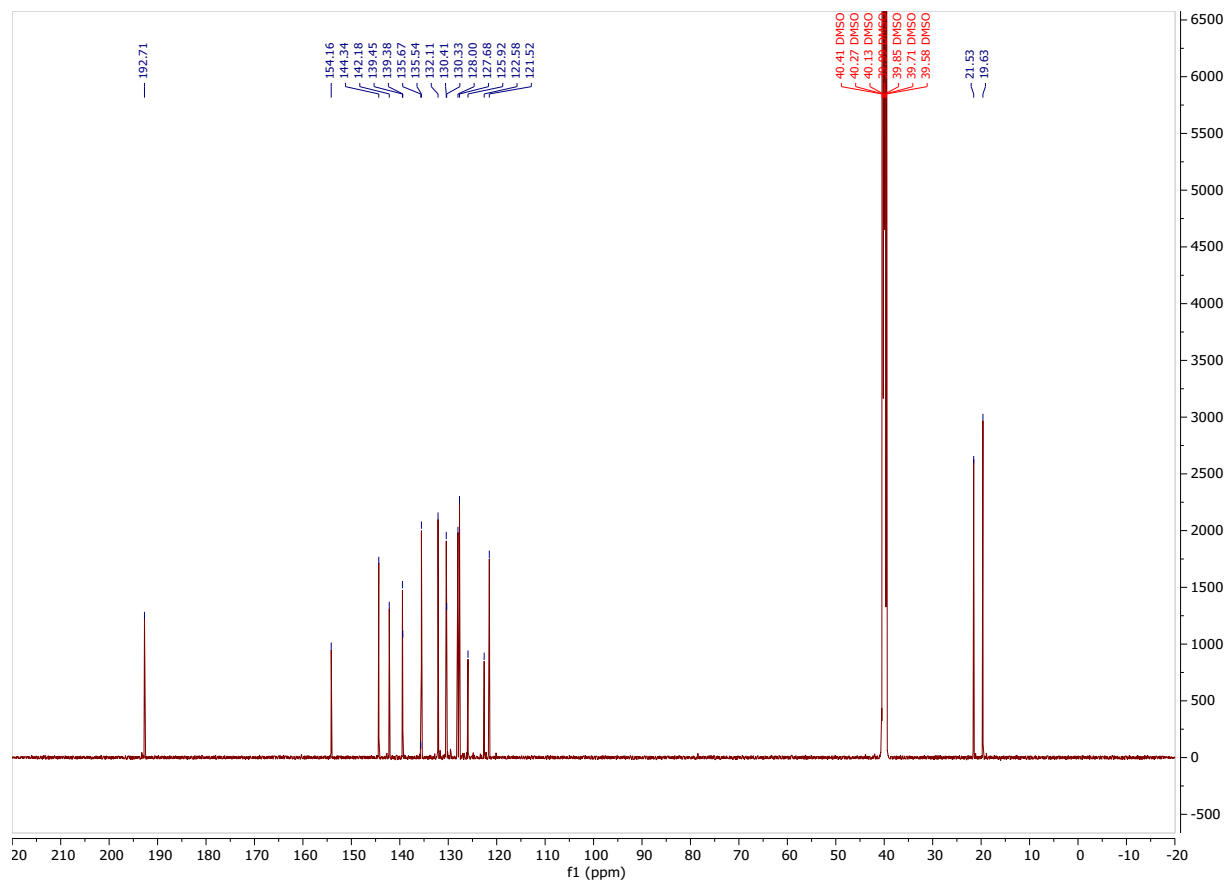
^{13}C -NMR (75 MHz, DMSO- d_6) Spectrum of Compound 7



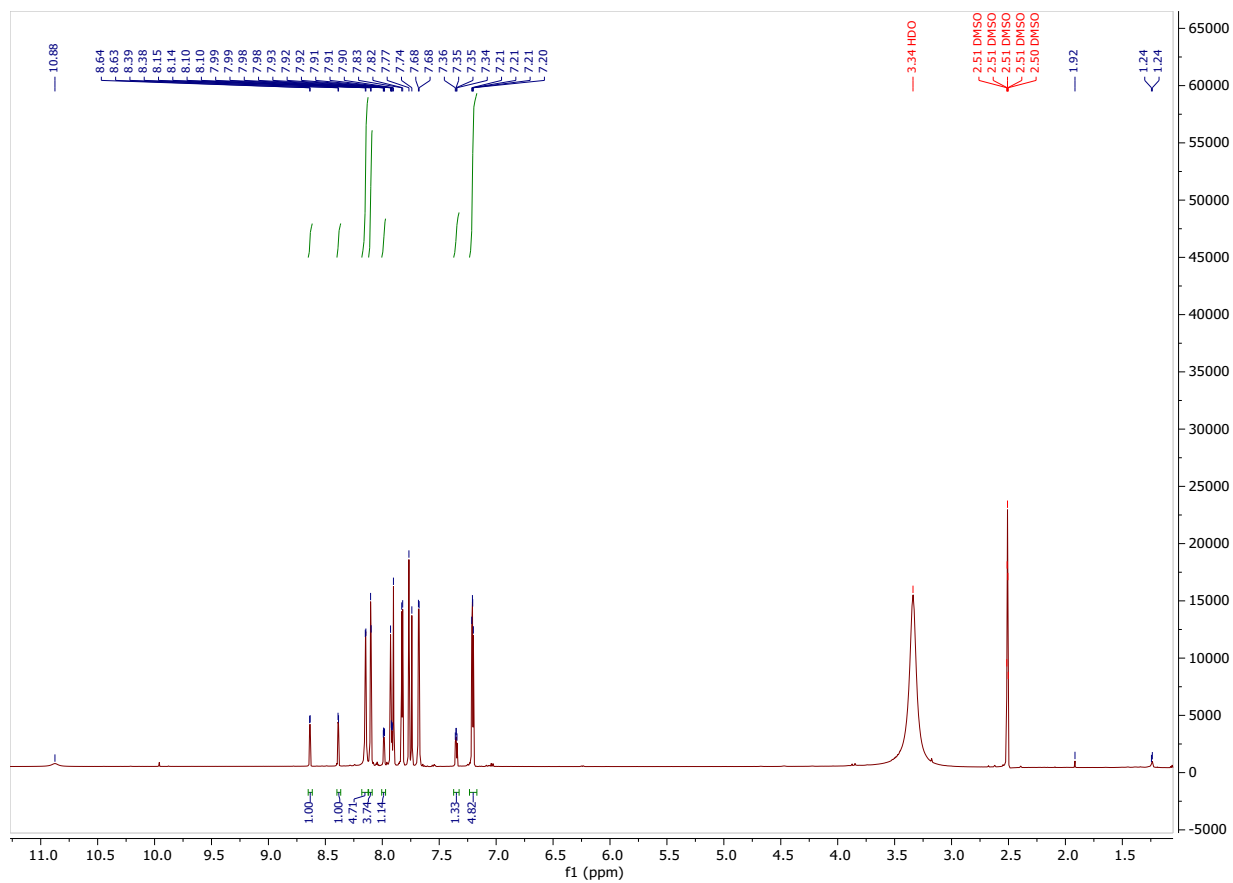
¹H-NMR (600 MHz, DMSO-d₆) Spectrum of Compound 8



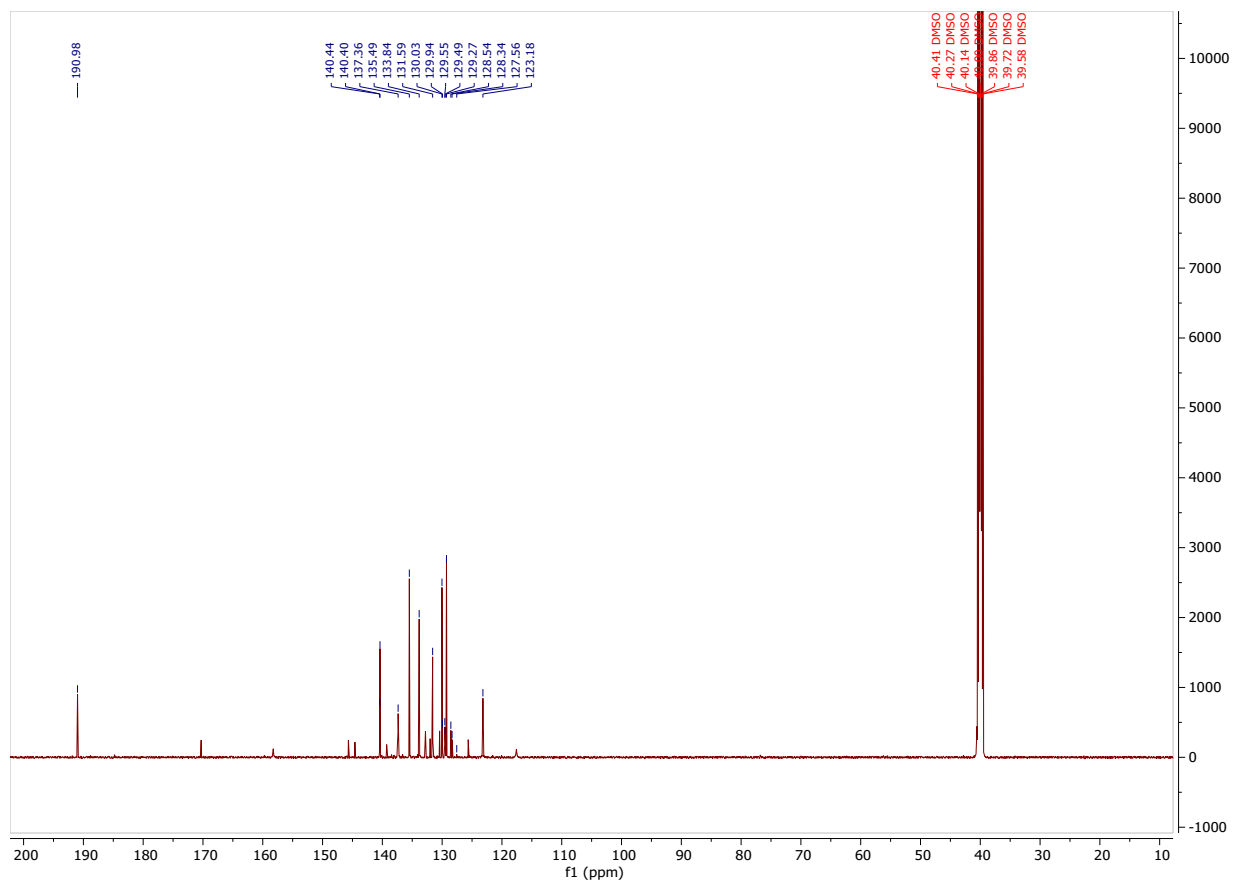
^{13}C -NMR (151 MHz, DMSO- d_6) Spectrum of Compound 8



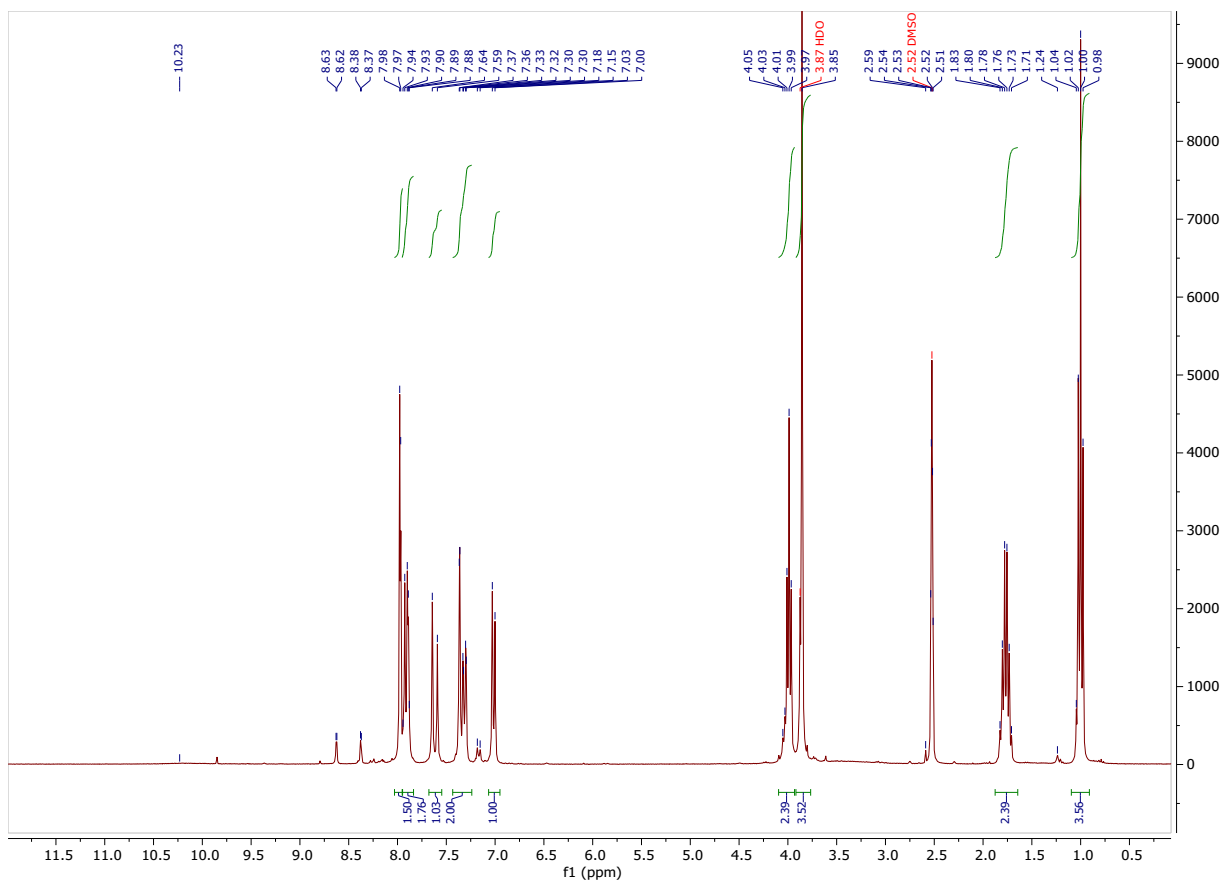
¹H-NMR (600 MHz, DMSO-d₆) Spectrum of Compound 9



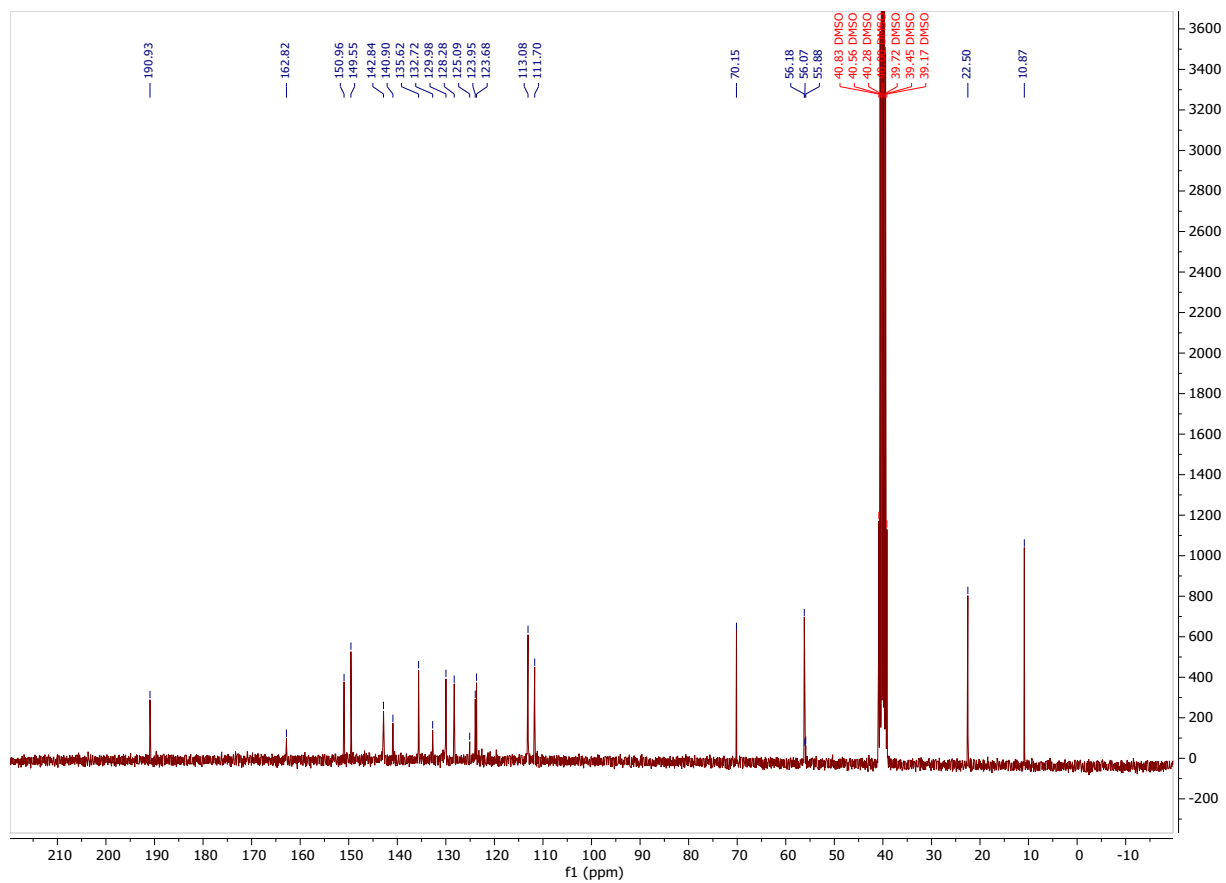
¹³C-NMR (151 MHz, DMSO-d₆) Spectrum of Compound 9



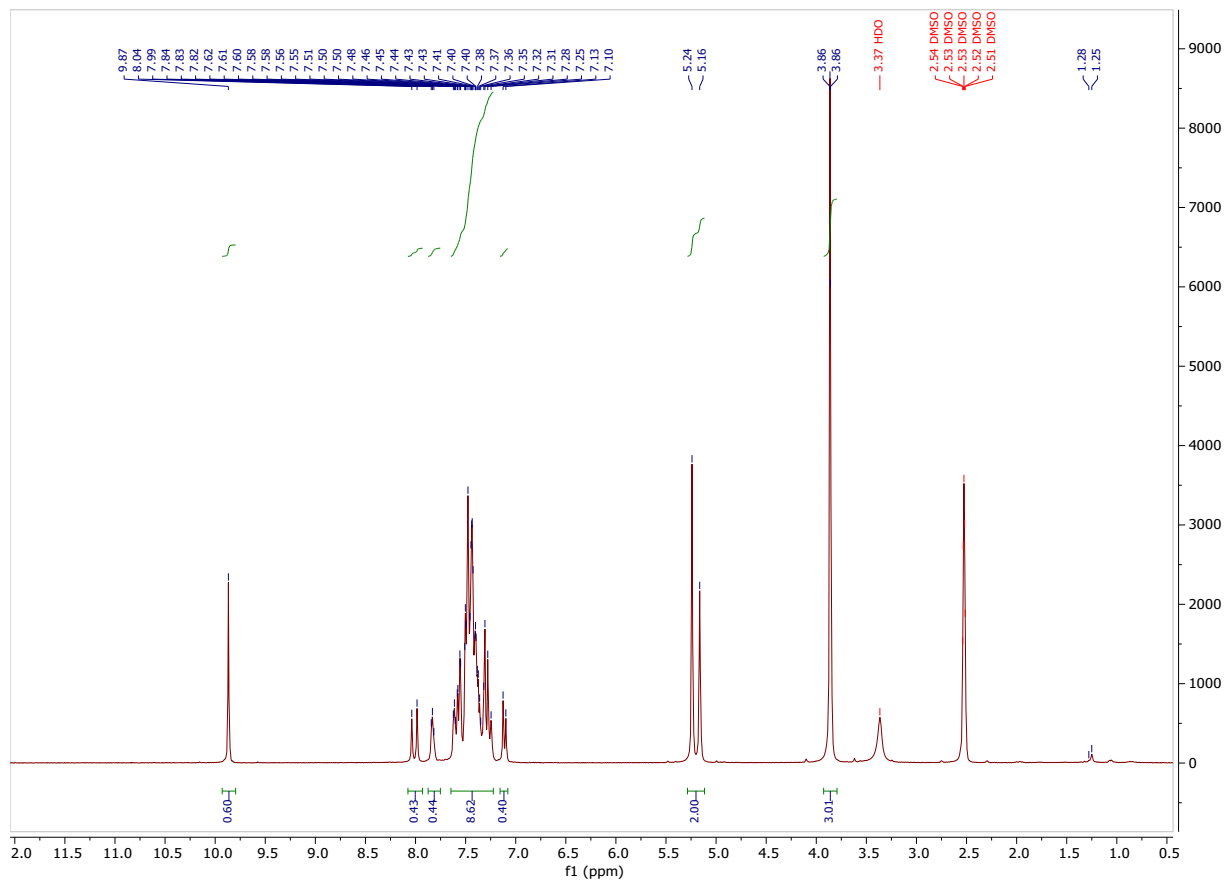
¹H-NMR (300 MHz, DMSO-d₆) Spectrum of Compound 10



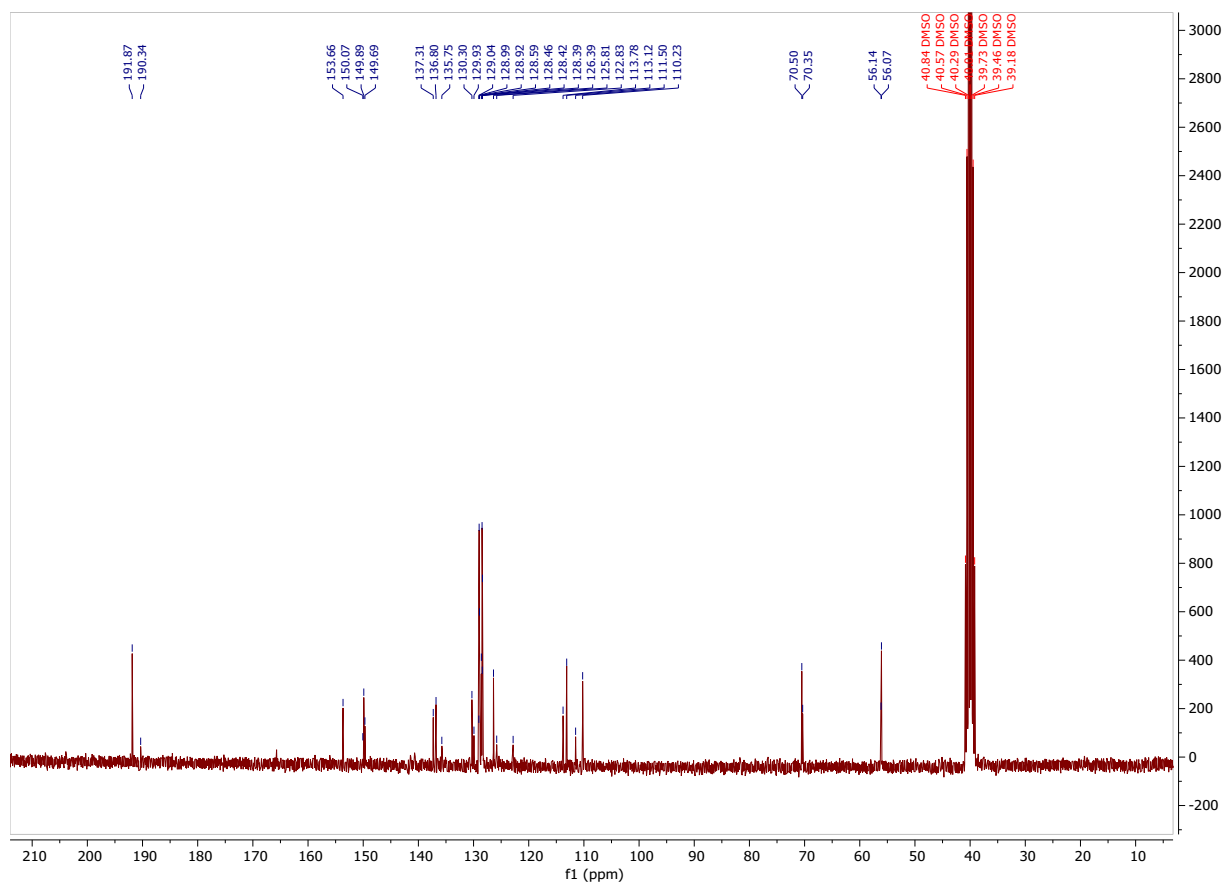
^{13}C -NMR (75 MHz, DMSO- d_6) Spectrum of Compound 10



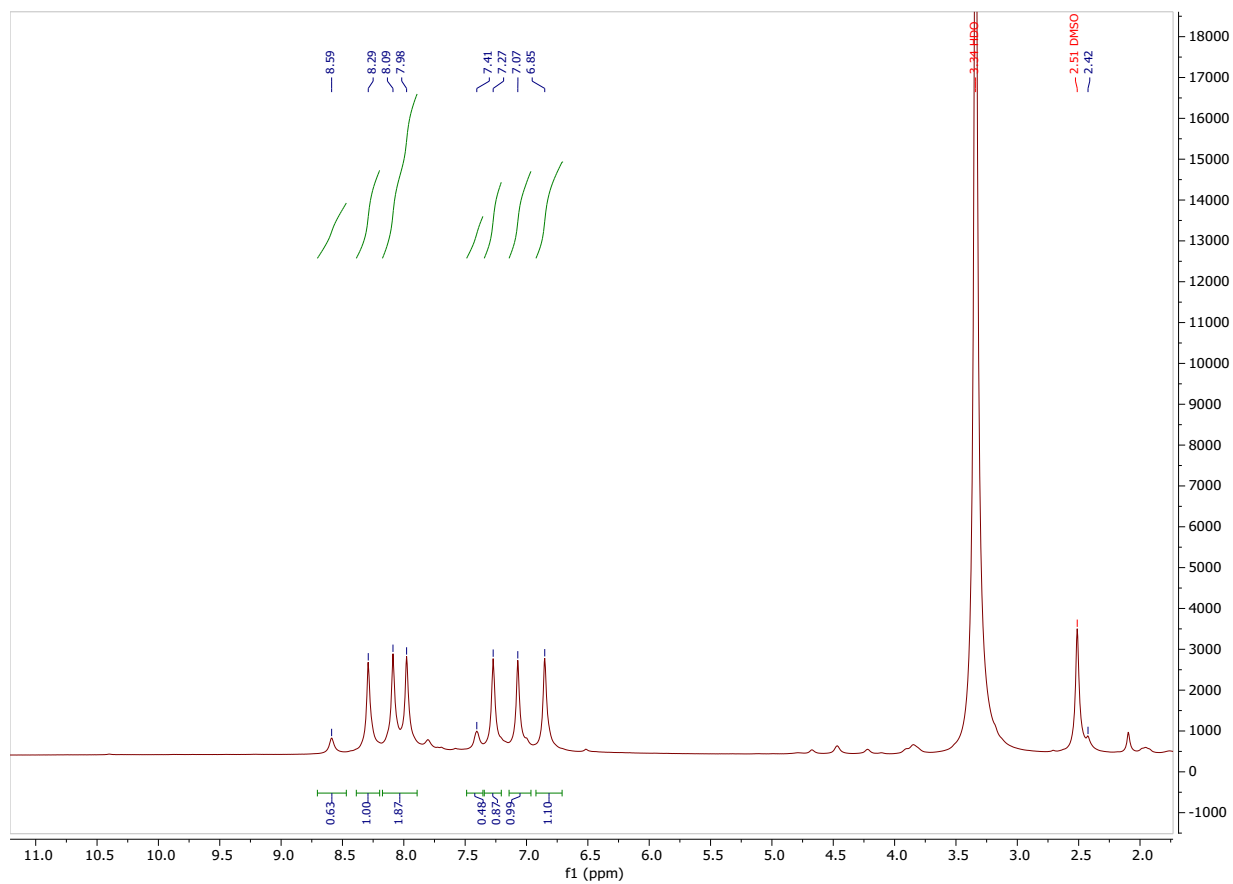
¹H-NMR (300 MHz, DMSO-d₆) Spectrum of Compound 11



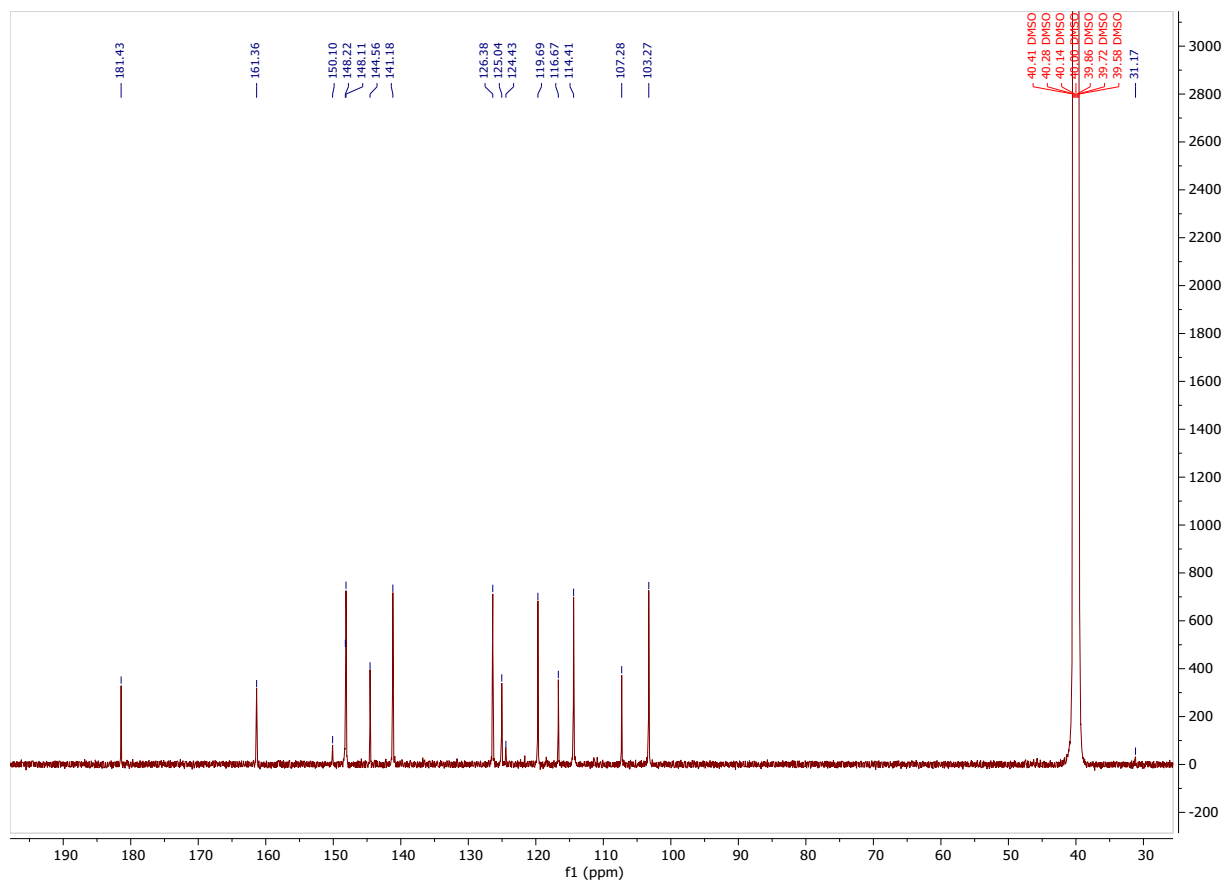
^{13}C -NMR (75 MHz, DMSO- d_6) Spectrum of Compound 11



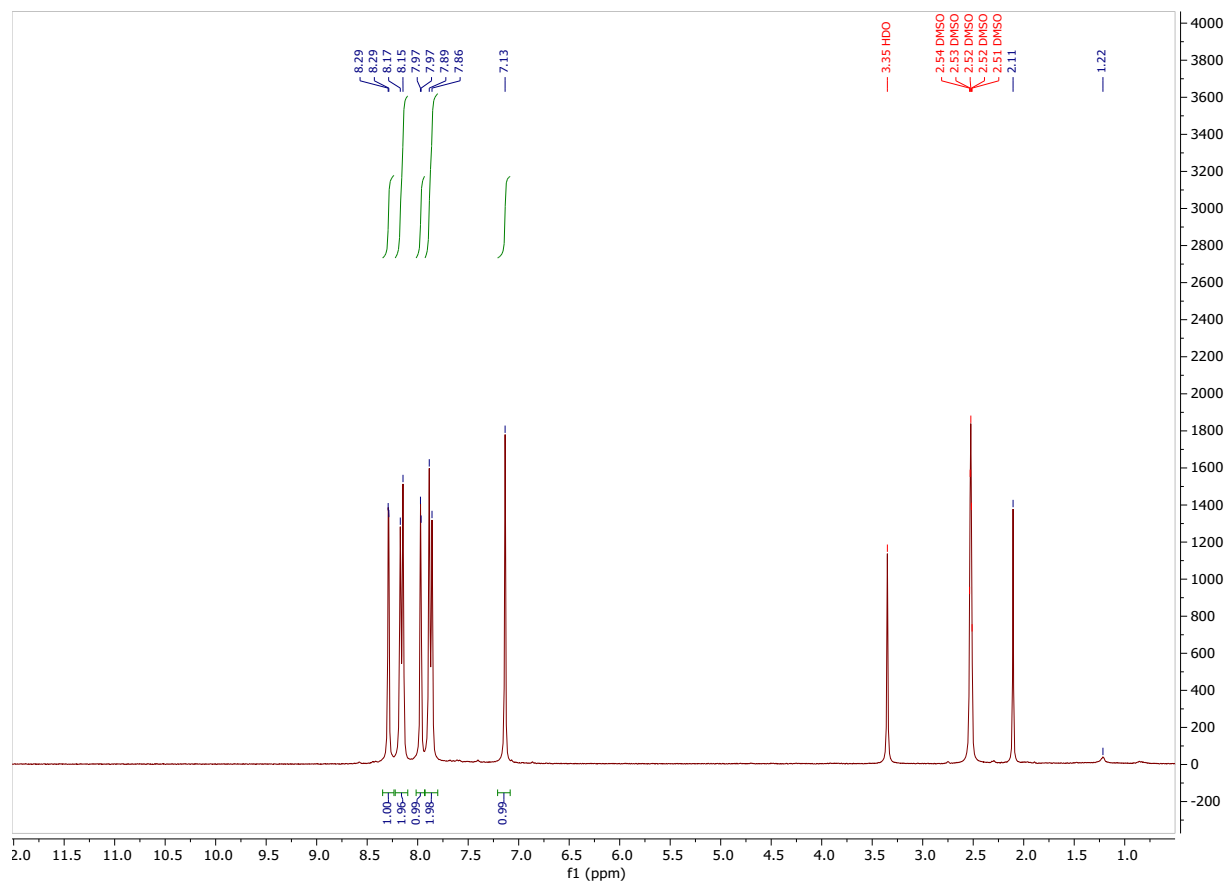
¹H-NMR (600 MHz, DMSO-d₆) Spectrum of Compound 12



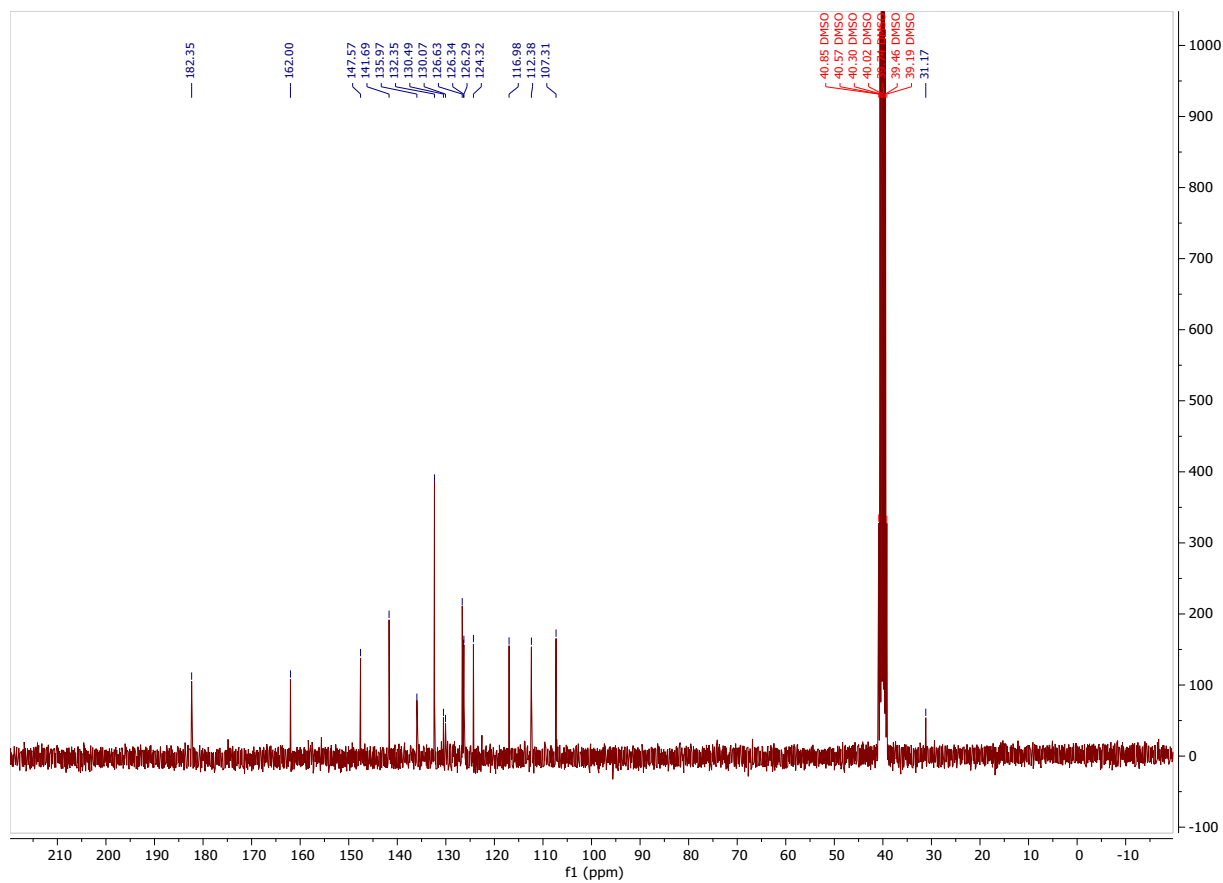
¹³C-NMR (151 MHz, DMSO-d₆) Spectrum of Compound 12



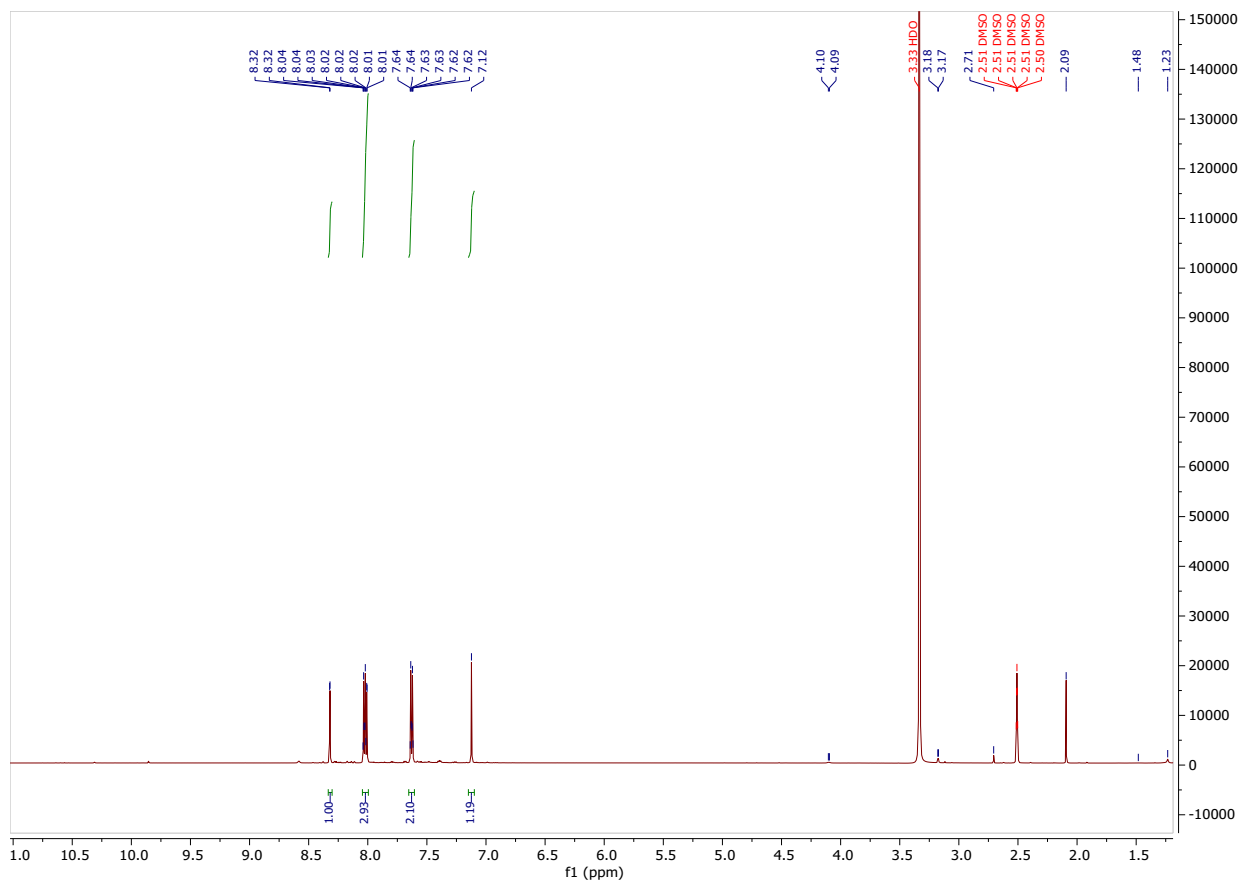
¹H-NMR (300 MHz, DMSO-d₆) Spectrum of Compound 13



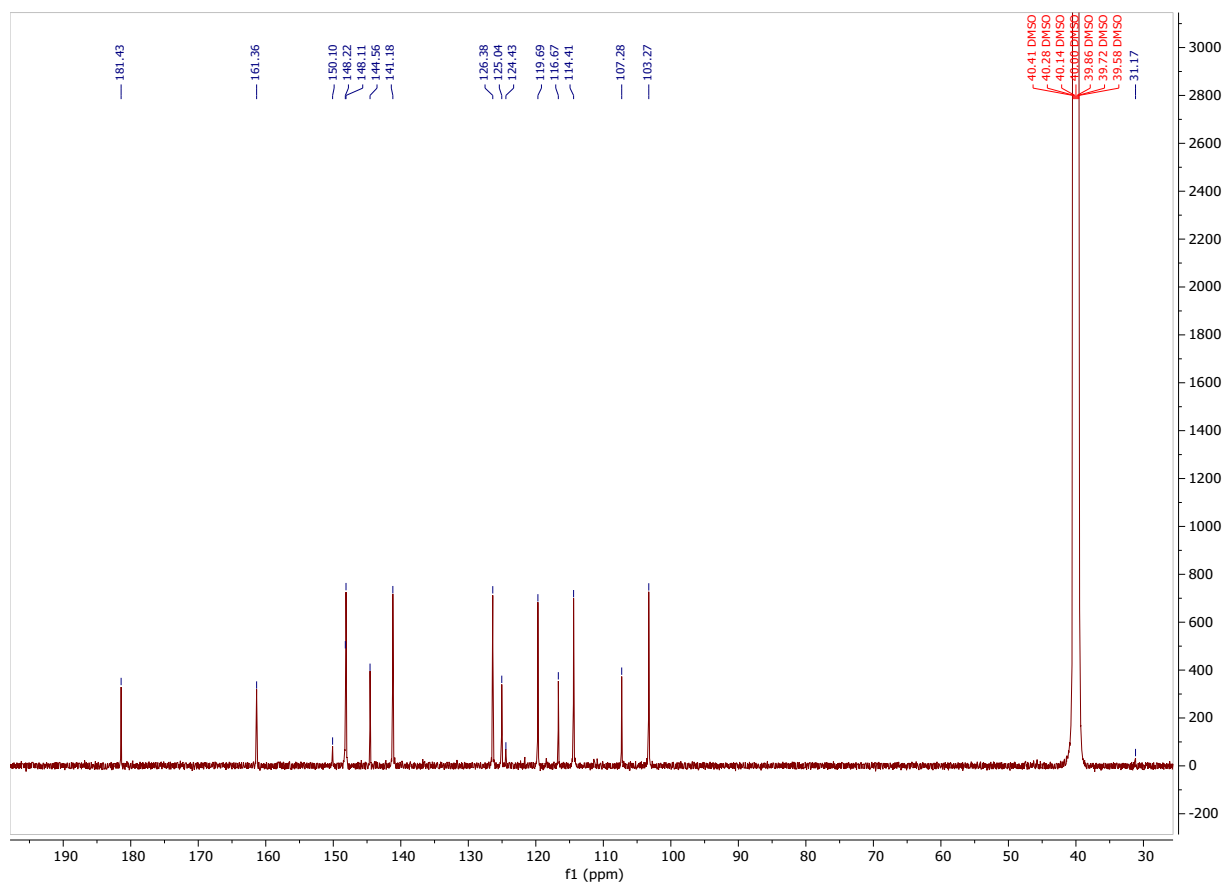
^{13}C -NMR (75 MHz, DMSO- d_6) Spectrum of Compound 13



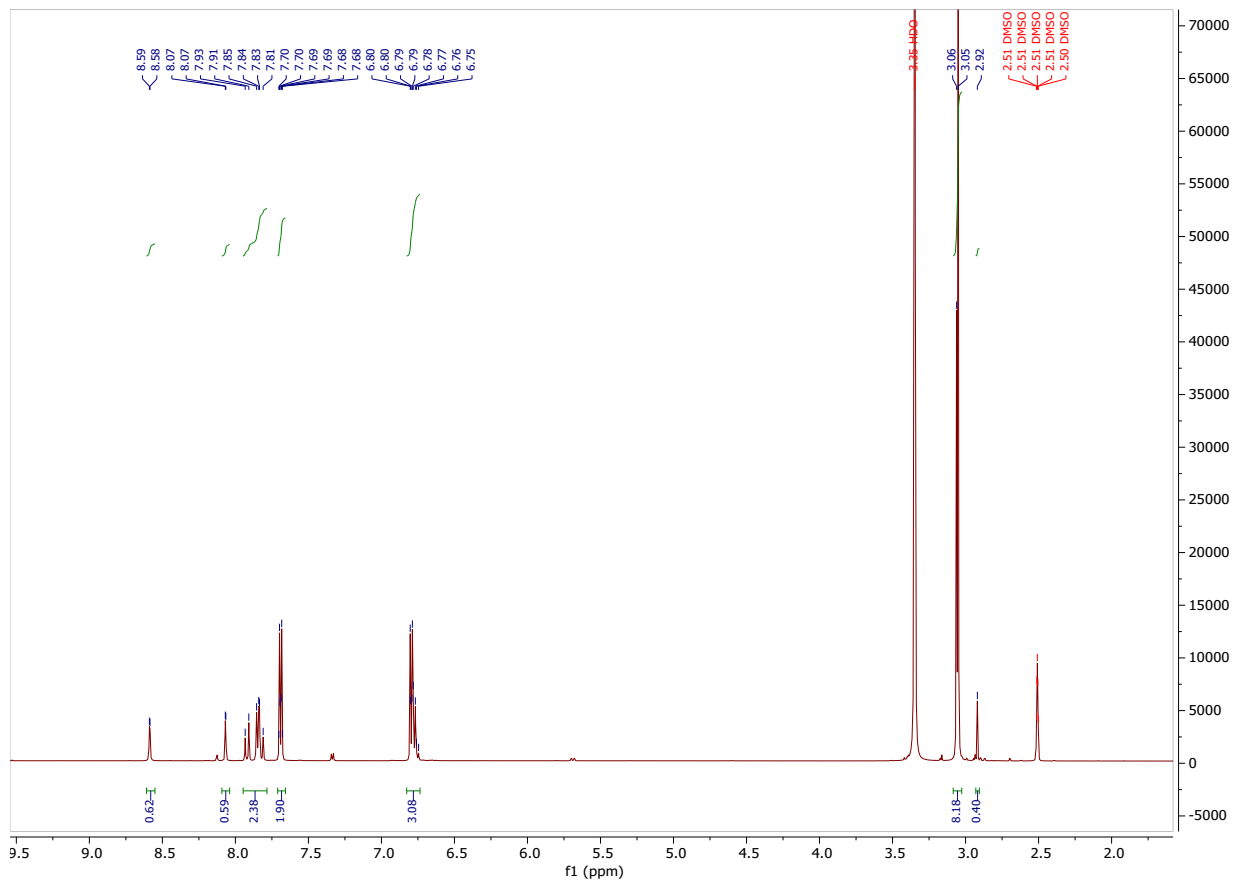
¹H-NMR (600 MHz, DMSO-d₆) Spectrum of Compound 14



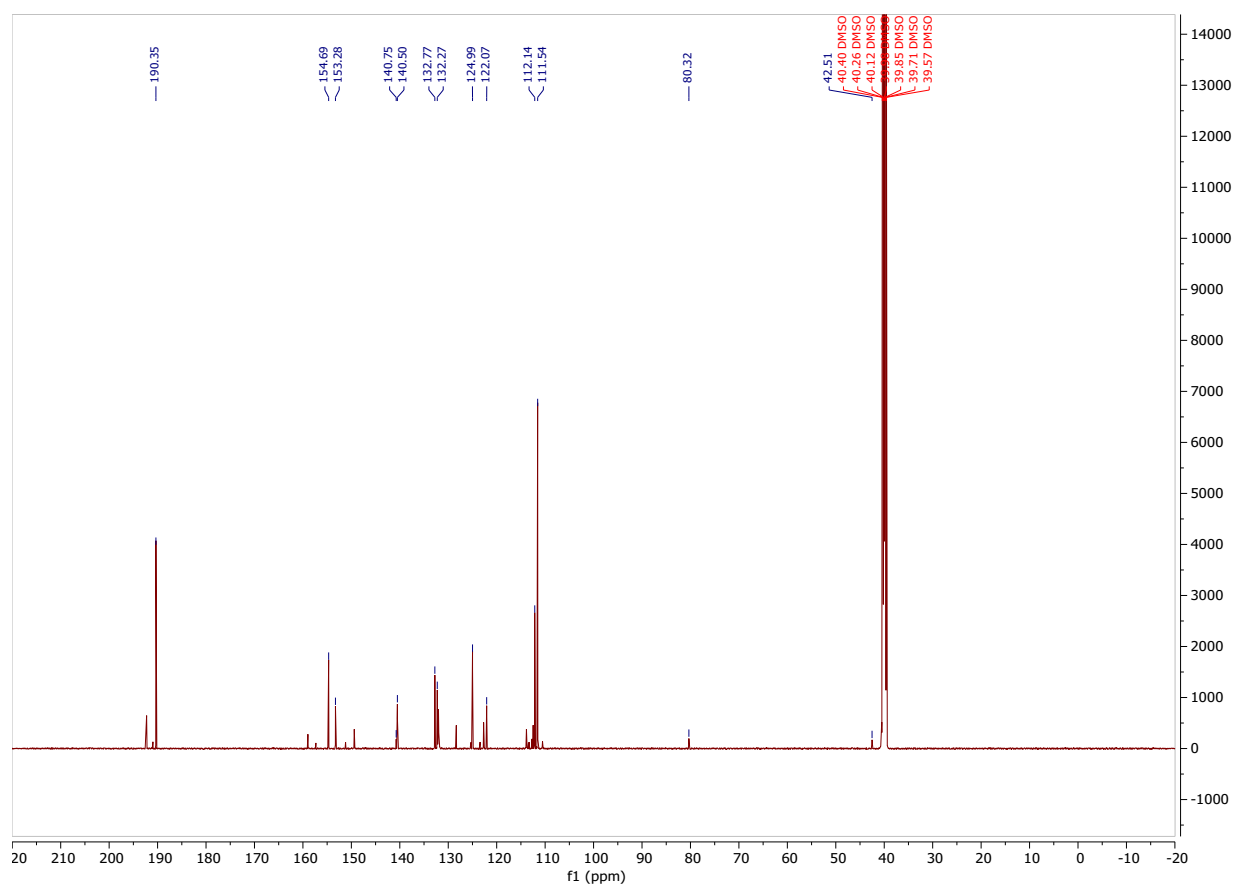
^{13}C -NMR (151 MHz, DMSO- d_6) Spectrum of Compound 14



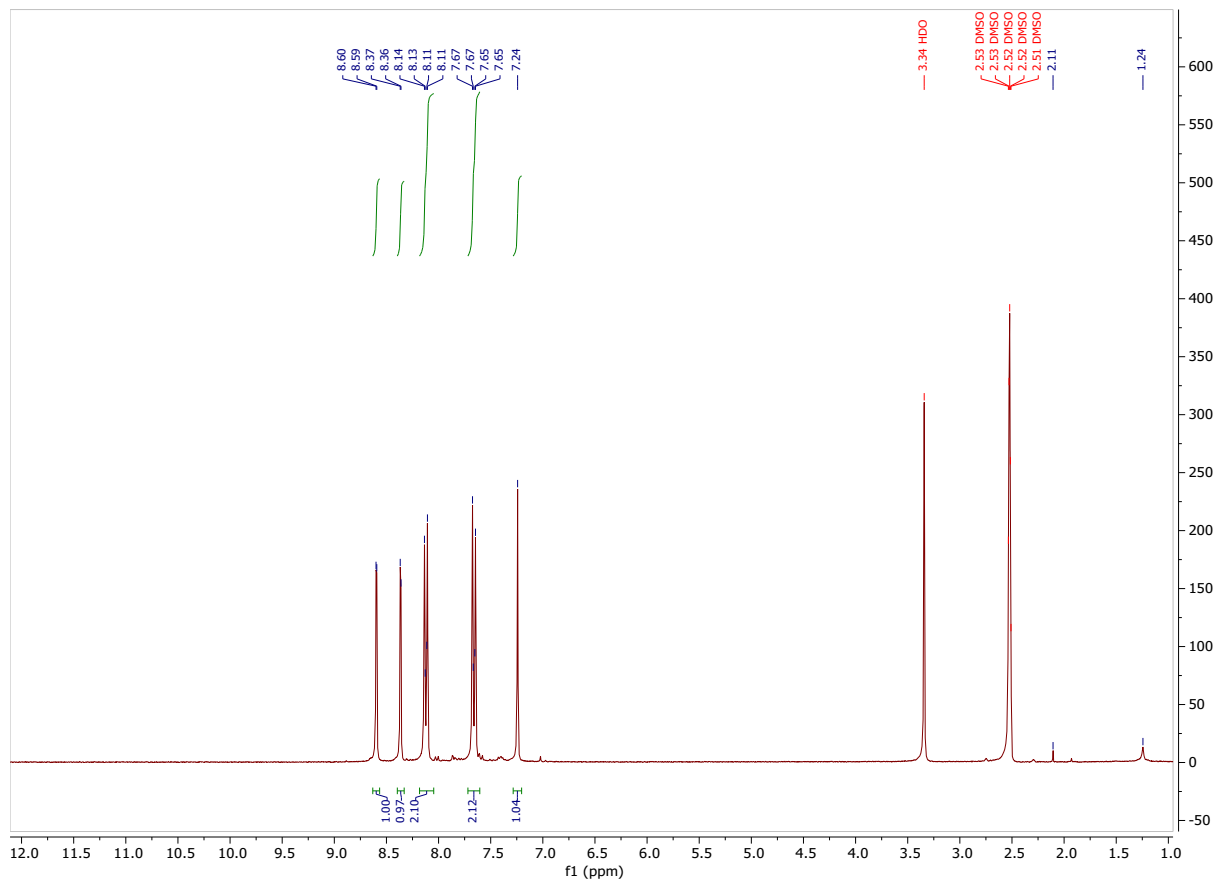
¹H-NMR (600 MHz, DMSO-d₆) Spectrum of Compound 15



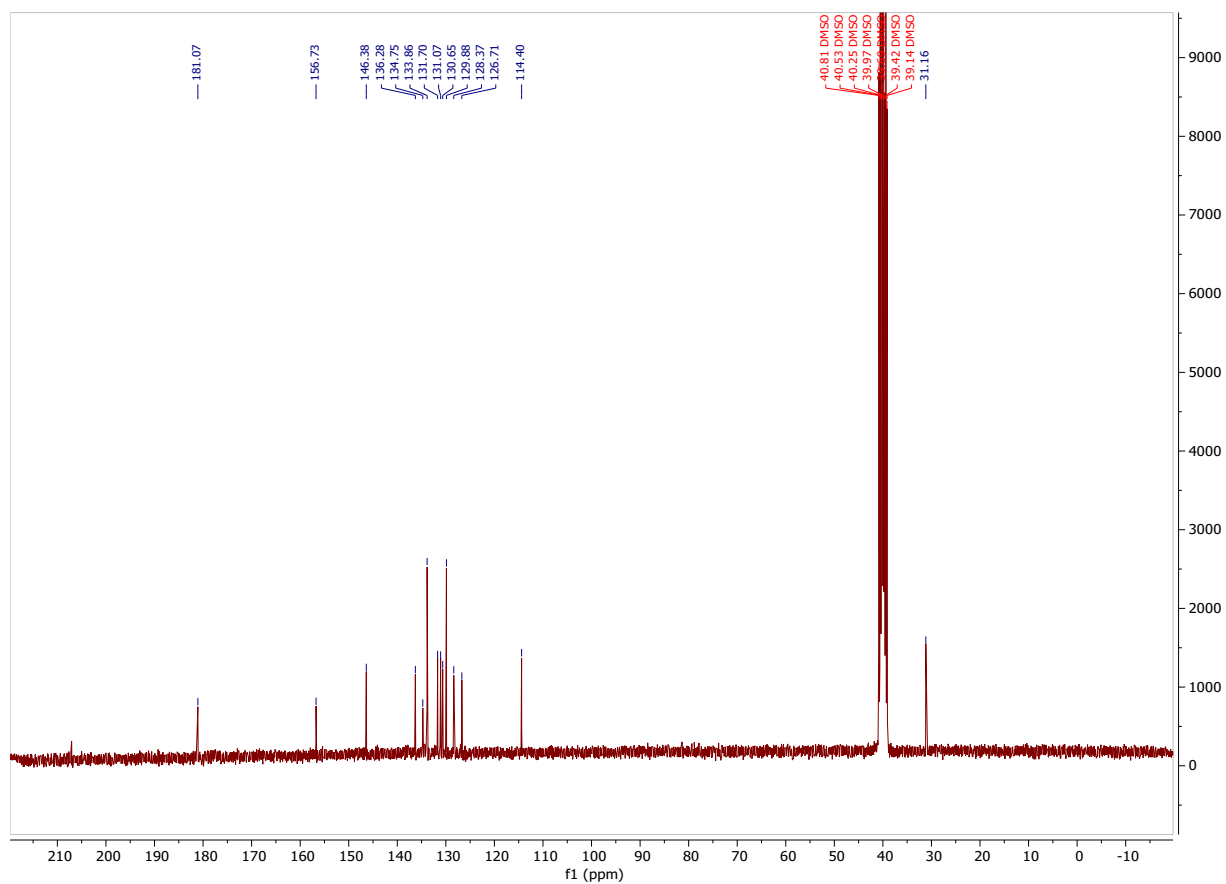
^{13}C -NMR (151 MHz, DMSO- d_6) Spectrum of Compound 15



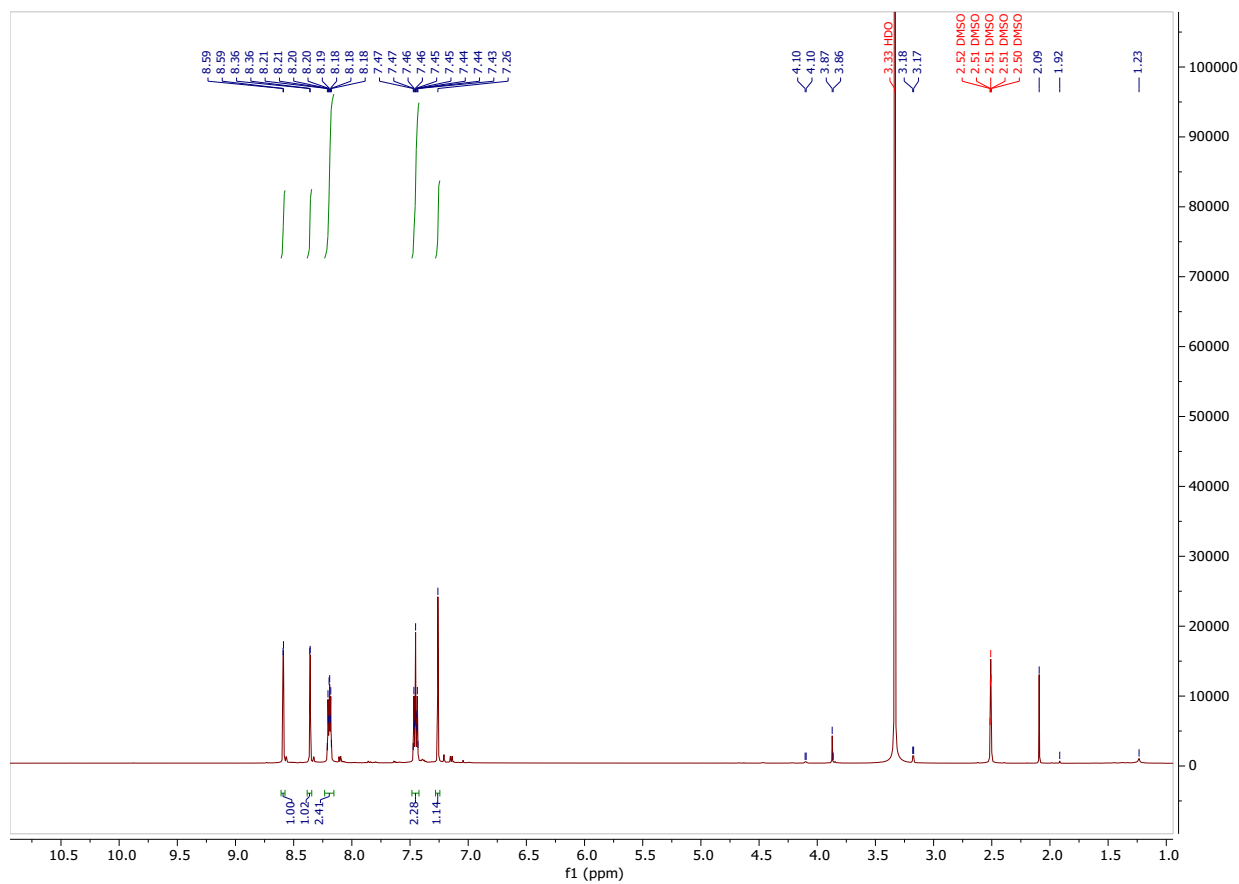
¹H-NMR (300 MHz, DMSO-d₆) Spectrum of Compound 16



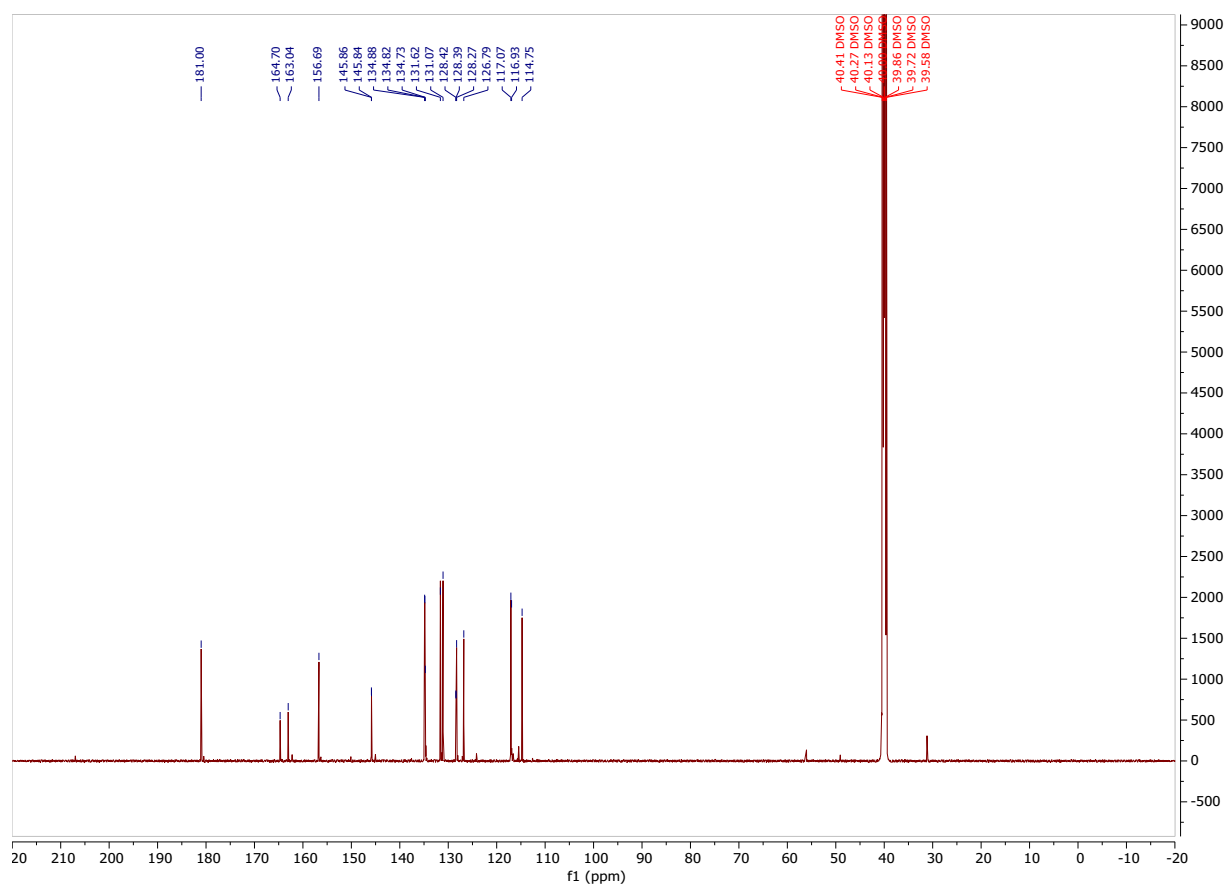
¹³C-NMR (75 MHz, DMSO-d₆) Spectrum of Compound 16



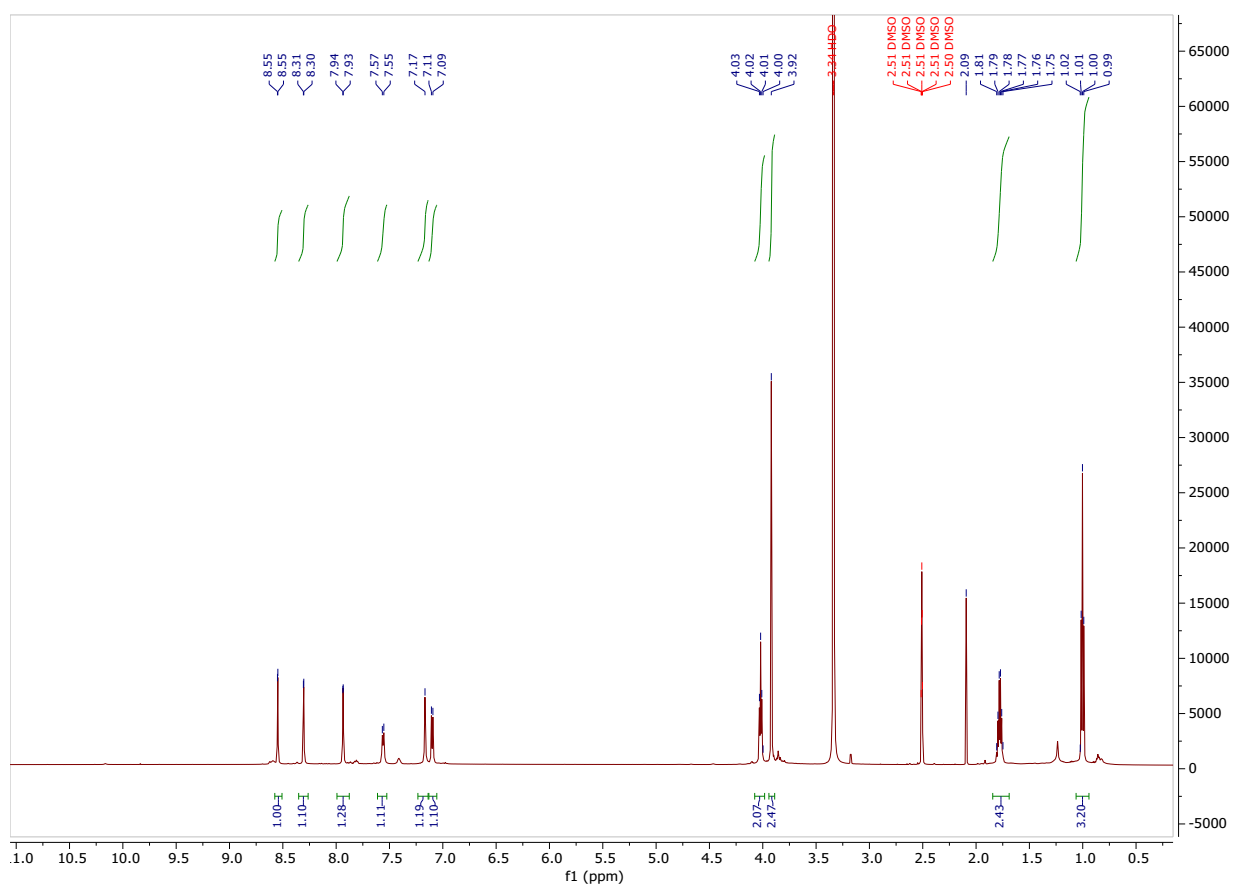
¹H-NMR (600 MHz, DMSO-d₆) Spectrum of Compound 17



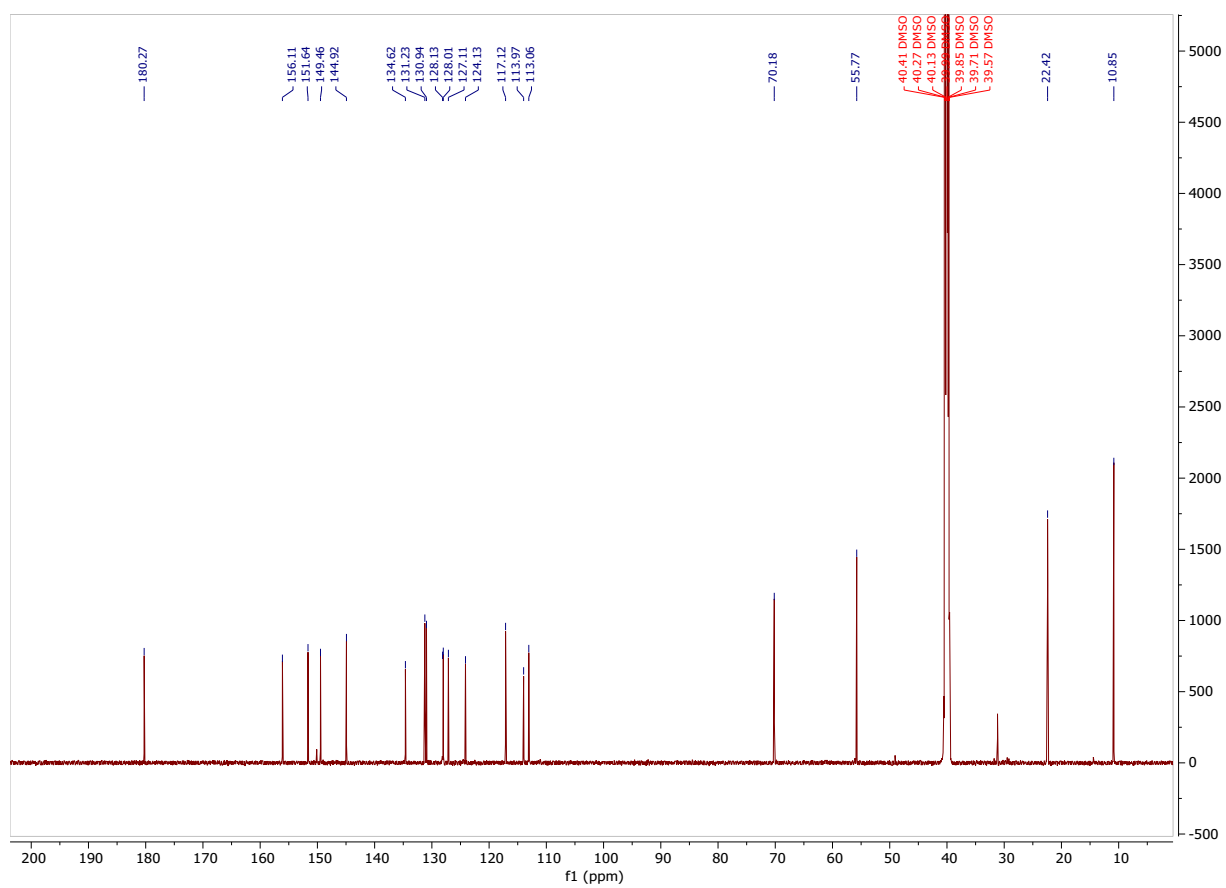
^{13}C -NMR (151 MHz, DMSO- d_6) Spectrum of Compound 17



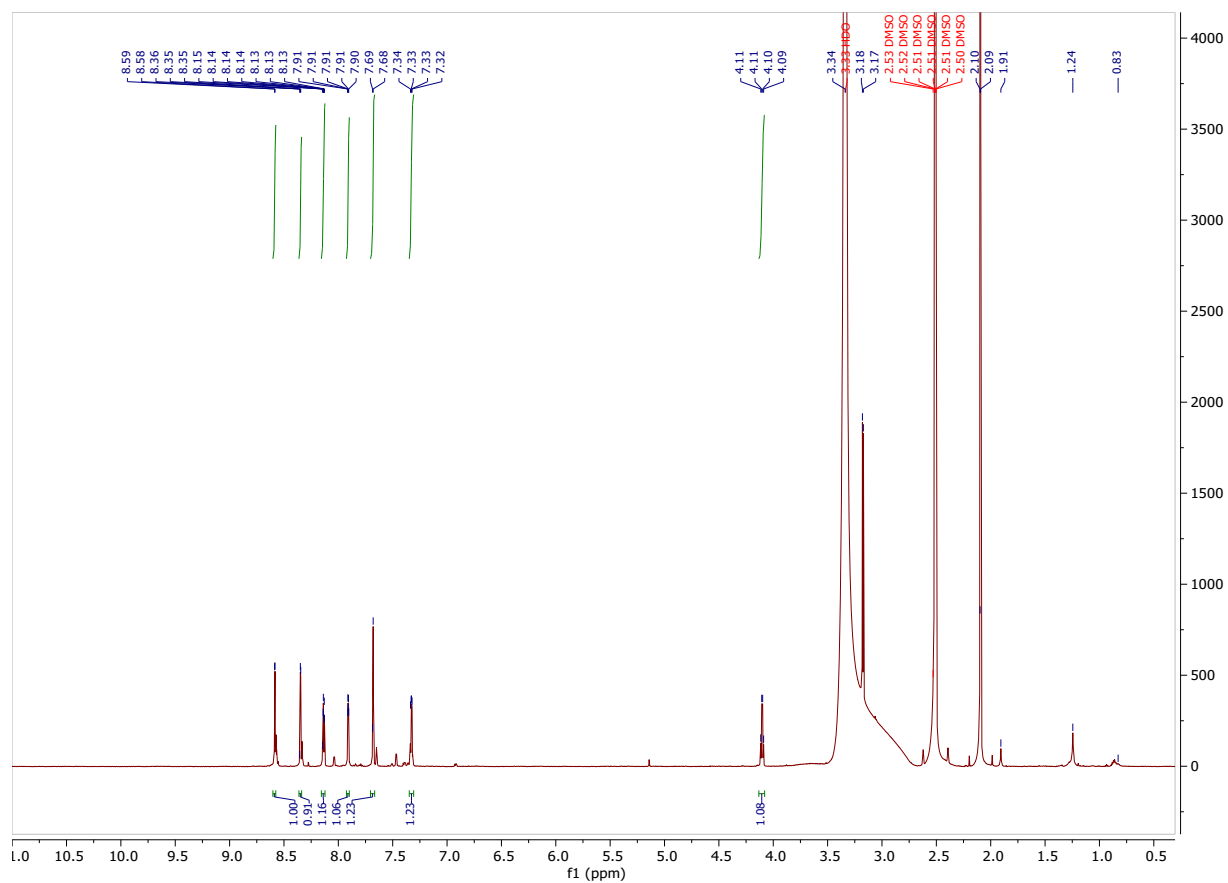
¹H-NMR (300 MHz, DMSO-d₆) Spectrum of Compound 18



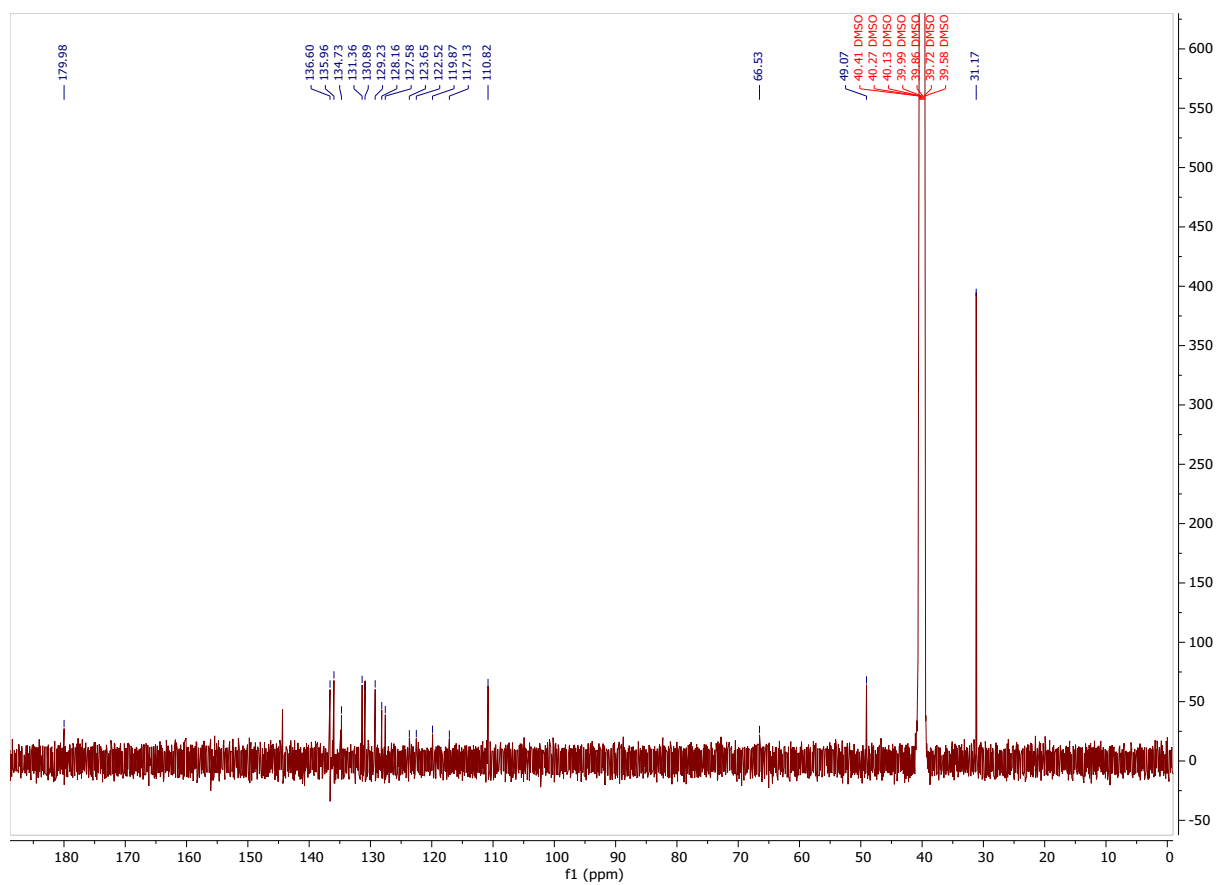
¹³C-NMR (75 MHz, DMSO-d₆) Spectrum of Compound 18



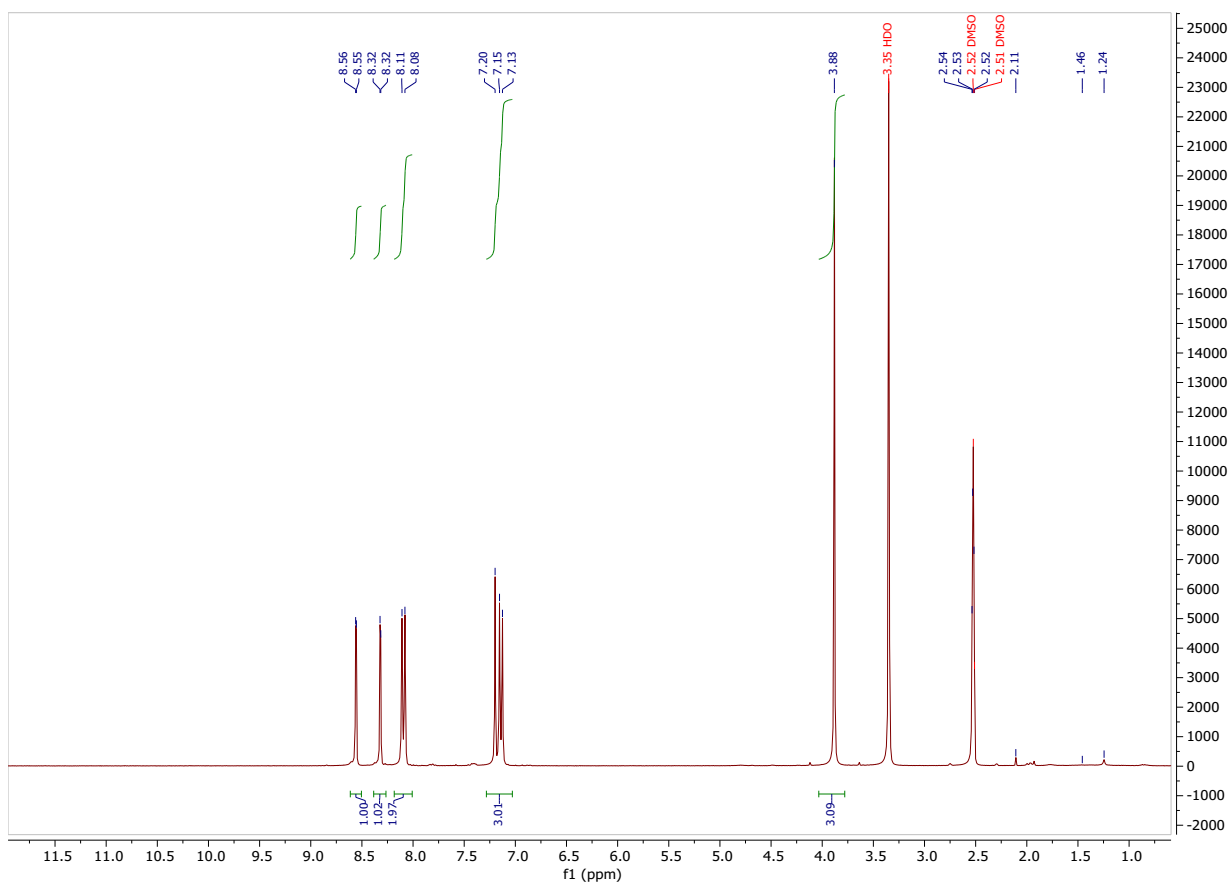
¹H-NMR (600 MHz, DMSO-d₆) Spectrum of Compound 19



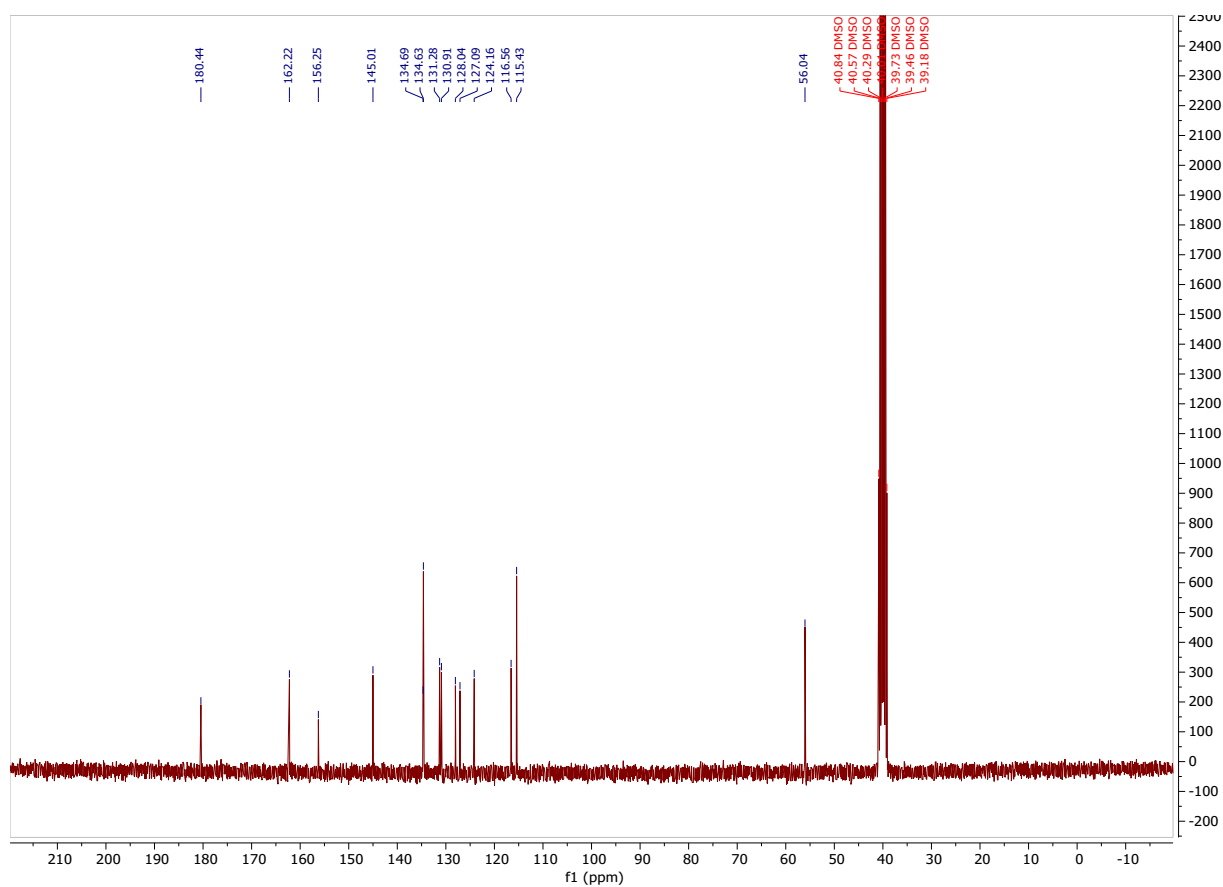
^{13}C -NMR (151 MHz, DMSO- d_6) Spectrum of Compound 19



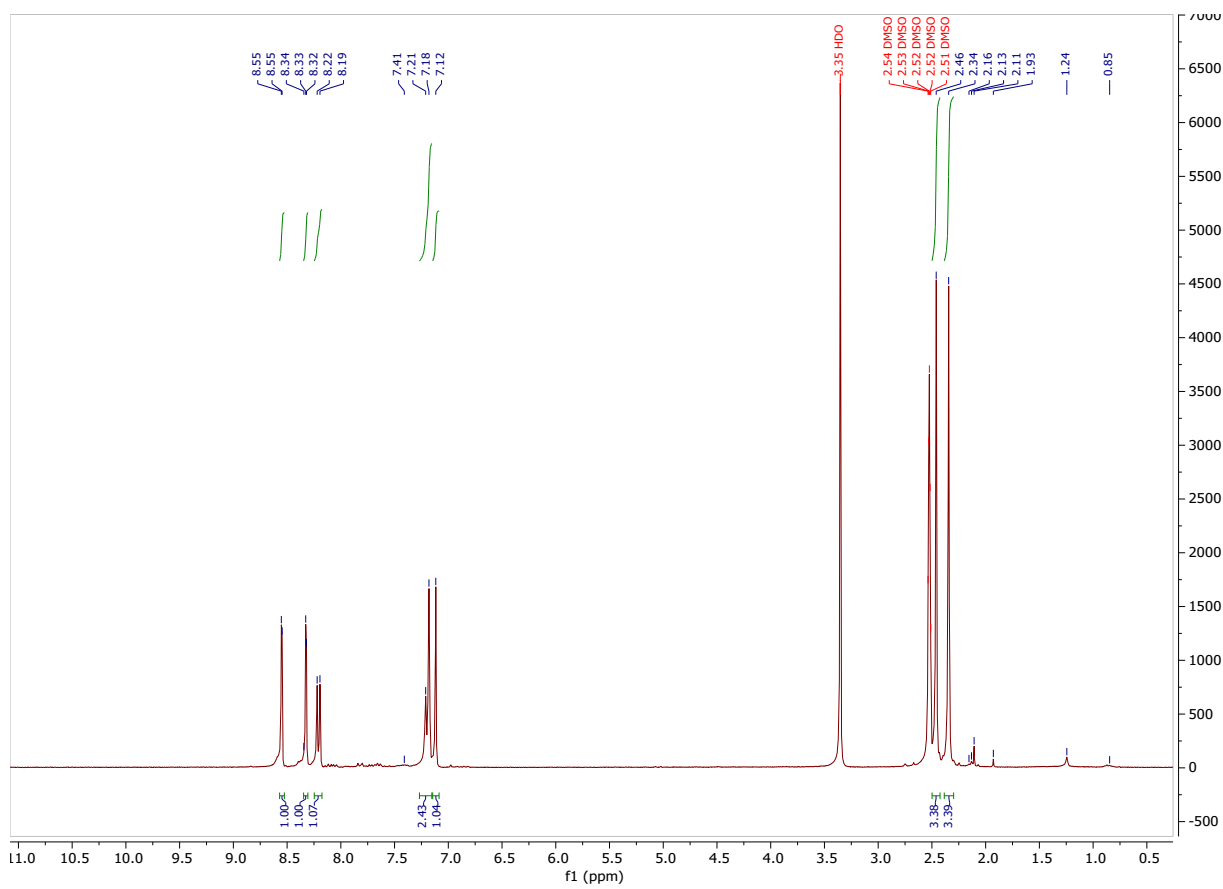
¹H-NMR (300 MHz, DMSO-d₆) Spectrum of Compound 20



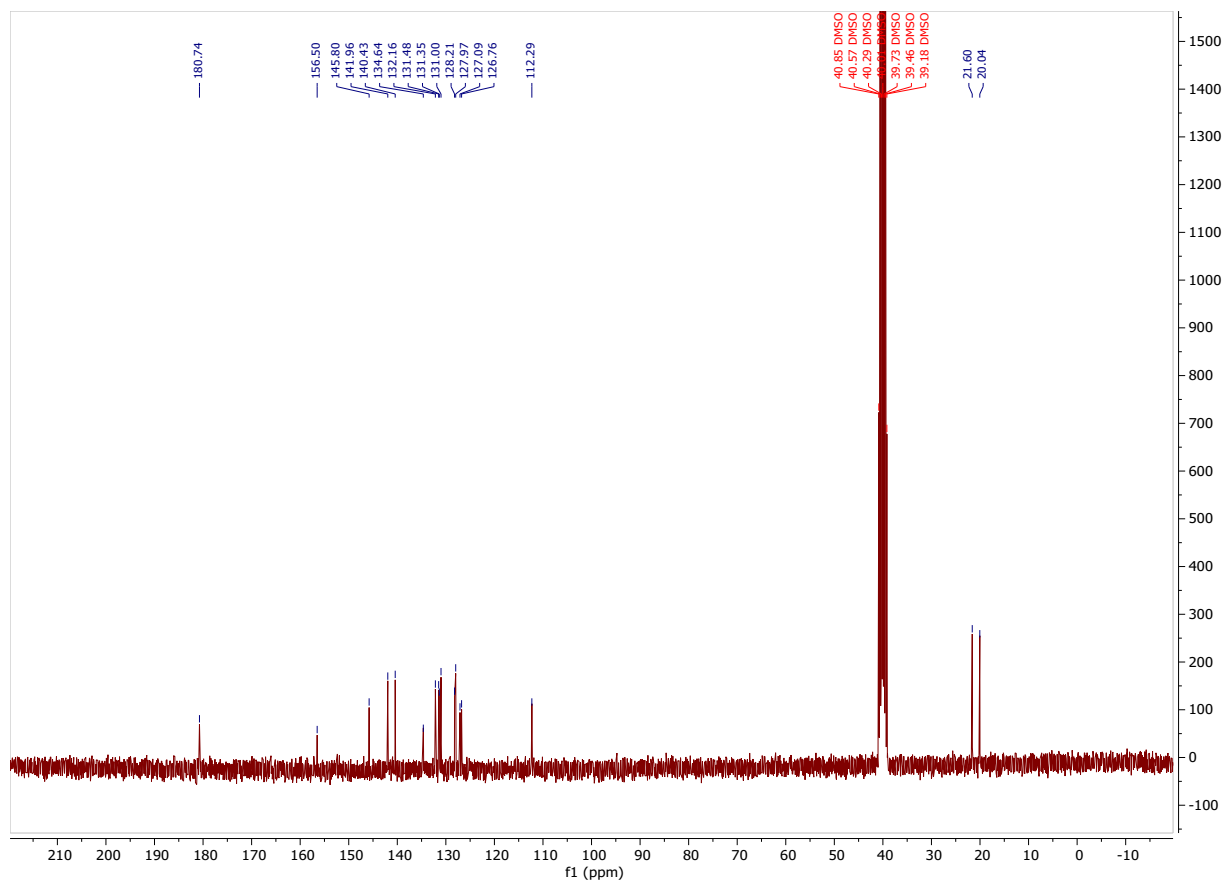
^{13}C -NMR (75 MHz, DMSO- d_6) Spectrum of Compound 20



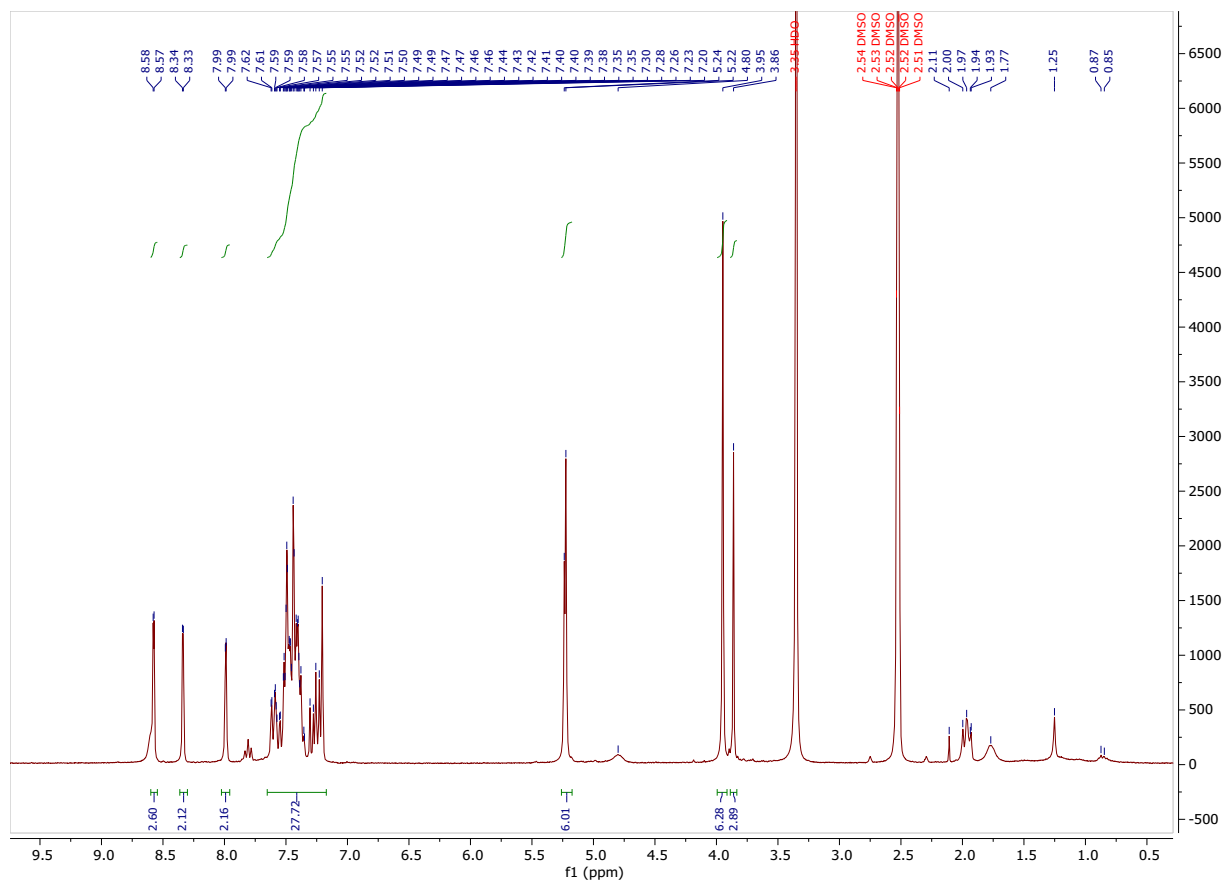
¹H-NMR (600 MHz, DMSO-d₆) Spectrum of Compound 21



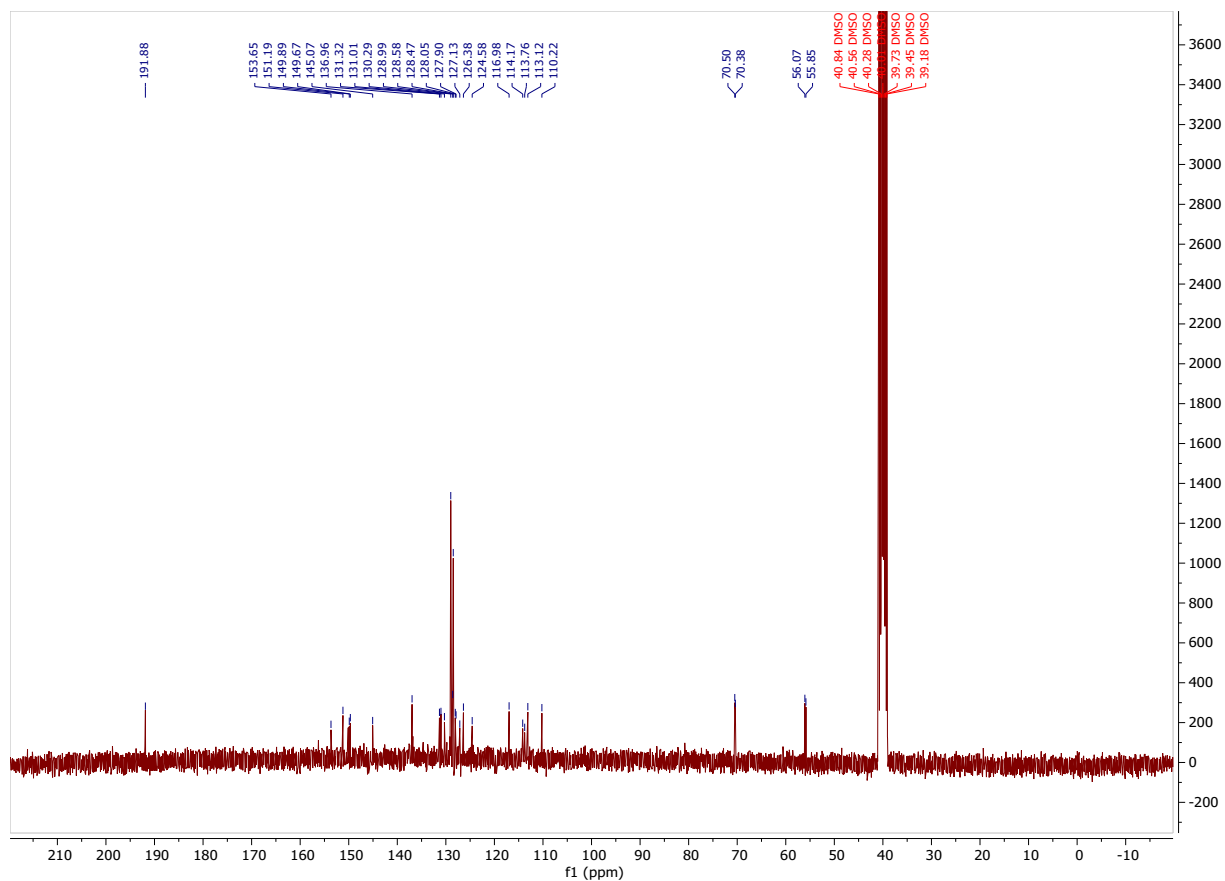
^{13}C -NMR (151 MHz, DMSO- d_6) Spectrum of Compound 21



$^1\text{H-NMR}$ (300 MHz, DMSO-d_6) Spectrum of Compound 22



¹³C-NMR (75 MHz, DMSO-d₆) Spectrum of Compound 22



Supplementary Information (SI-2) Docking Images

2-Benzylidenebenzofuran-3(2H)-ones as a New Class of Alkaline Phosphatase Inhibitors: Synthesis, SAR Analysis, Enzyme Inhibitory Kinetics and Computational Studies

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^gDepartment of Chemistry, Quaid-i-Azam University, Islamabad-45320, Pakistan

^hDepartment of Chemistry, COMSATS University Islamabad, Abbottabad, Pakistan

ⁱDepartment of Chemistry, Faculty of Science, Ferdowsi University of Mashhad, Mashhad, 9177948974, Iran

^jDepartment of Chemistry, Faculty of Science, Farhangian University, Tehran, Iran

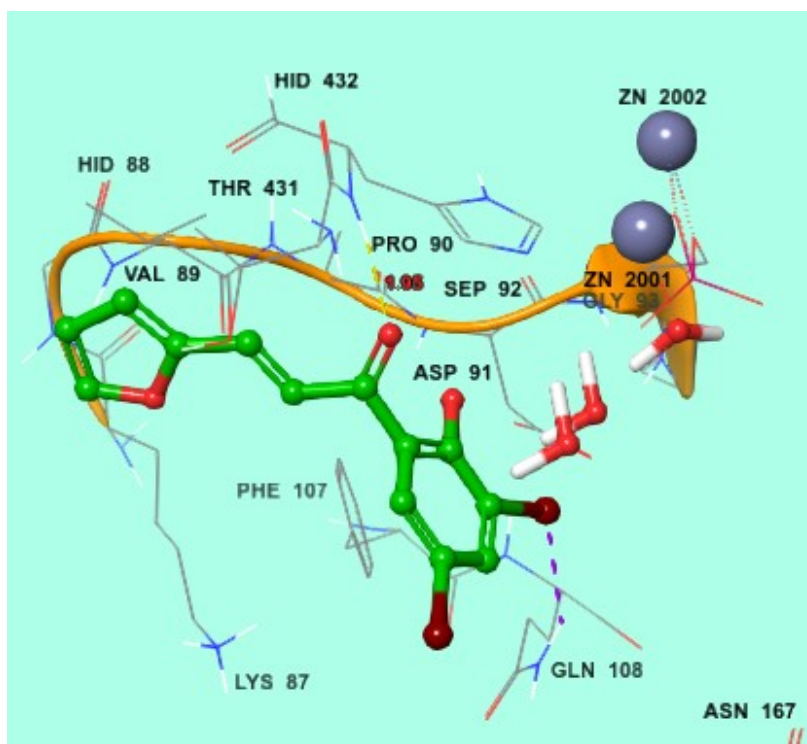
^kDepartment of Chemistry, Faculty of Applied Science, Umm Al-Qura University, 21955 Makkah Saudi Arabia

^lChemistry Department, Faculty of Science, Assiut University, 71516 Assiut, Egypt

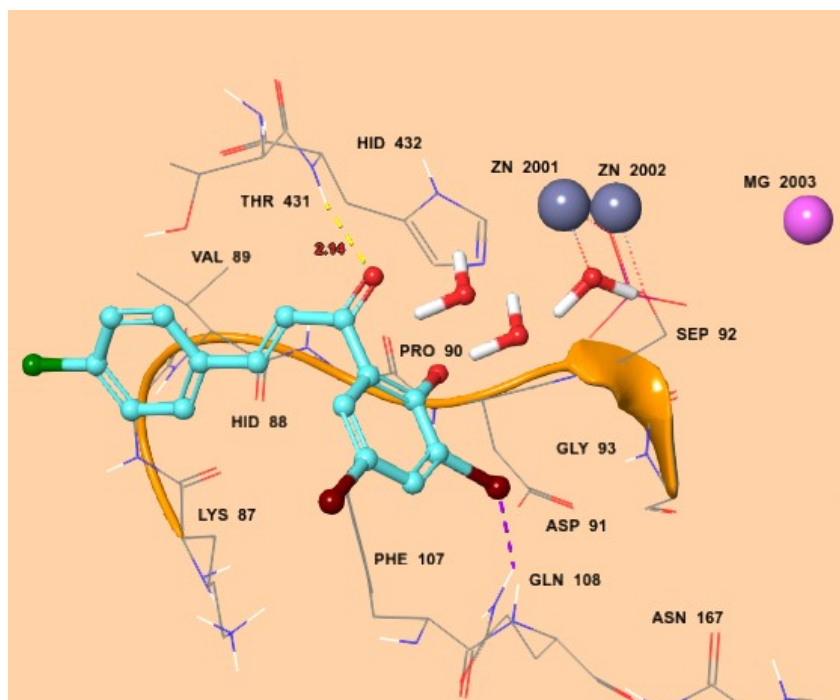
Representative Docking Images of All the Synthesized Compounds

Compound-1

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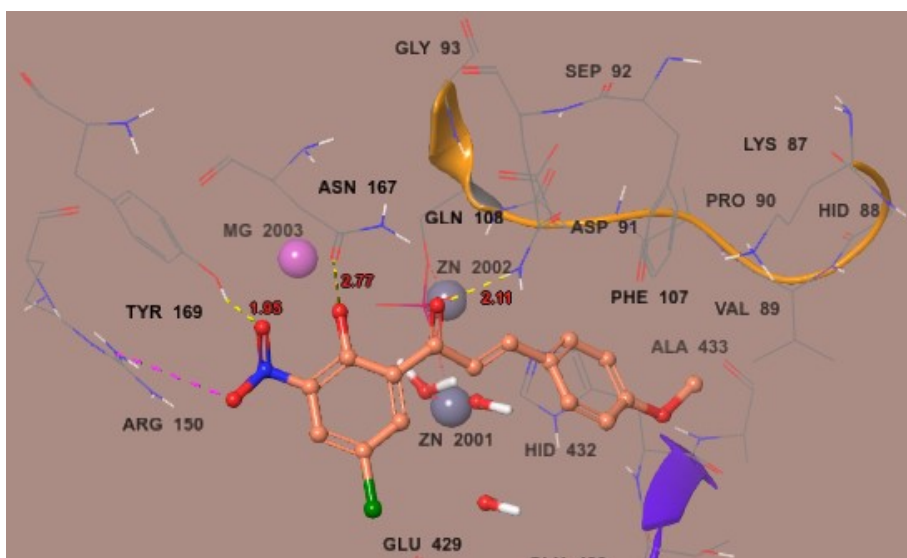
Compound-2



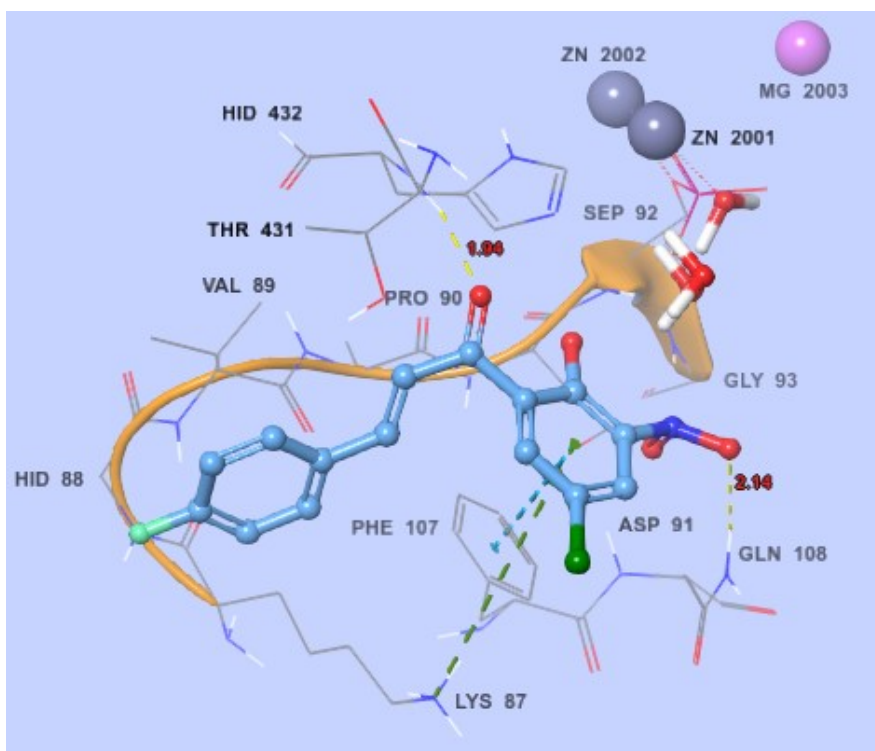
Compound-3



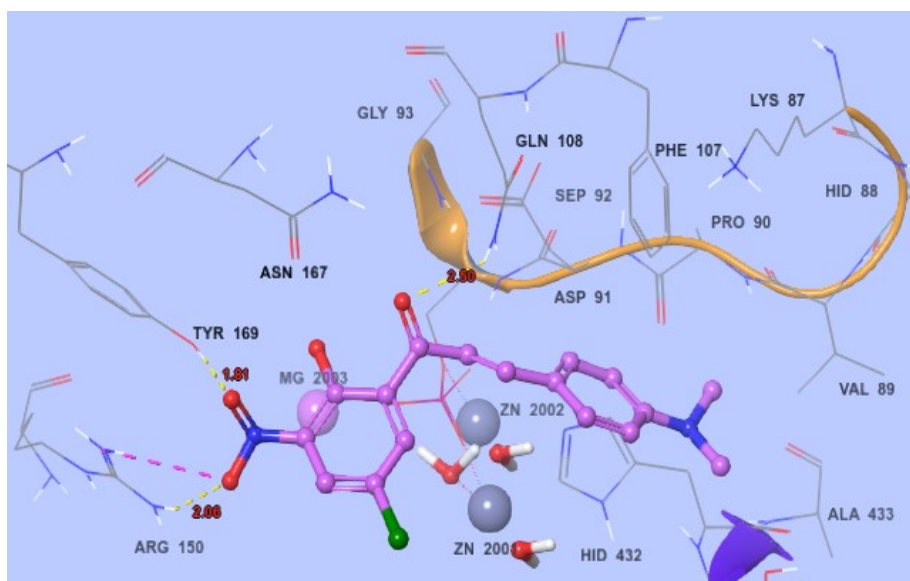
Compound-4



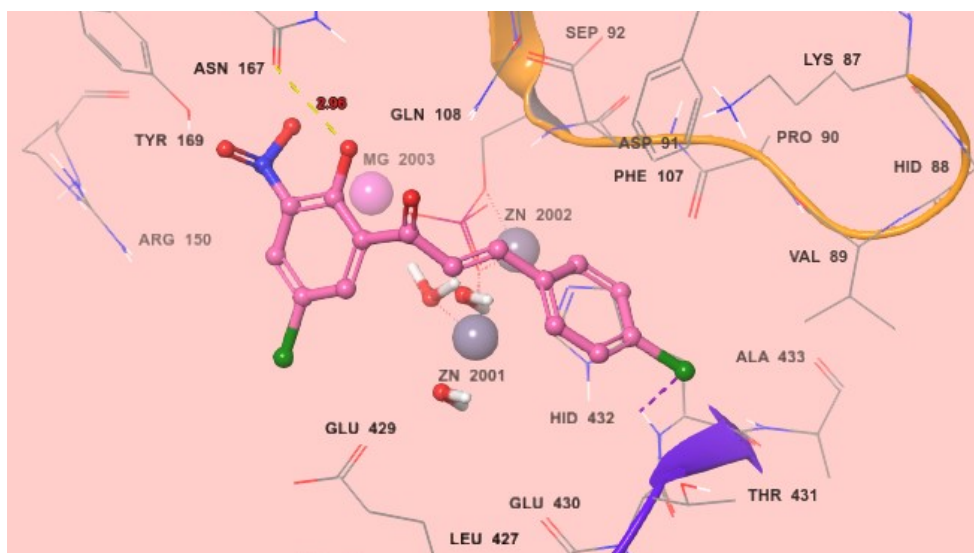
Compound-5



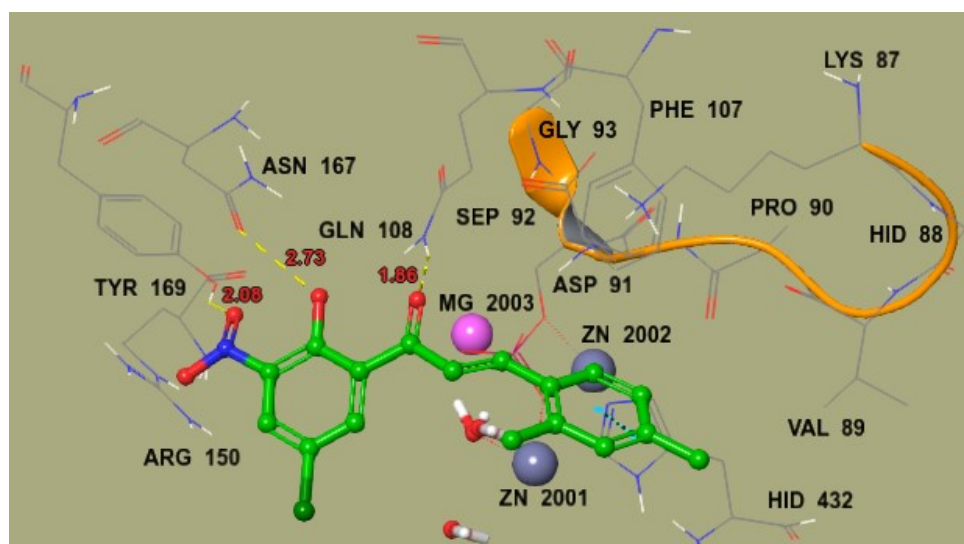
Compound-6



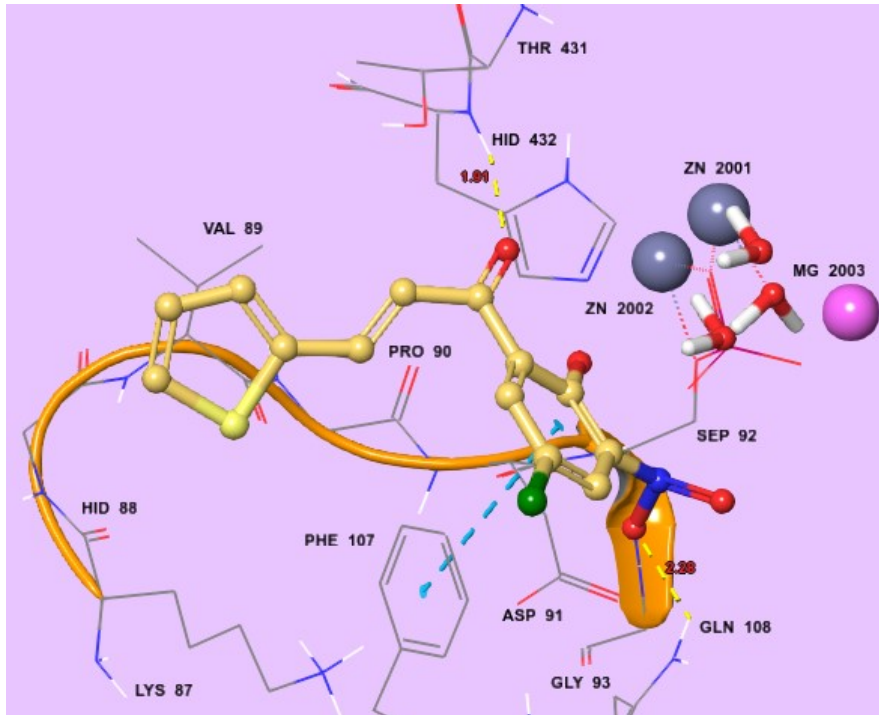
Compound-7



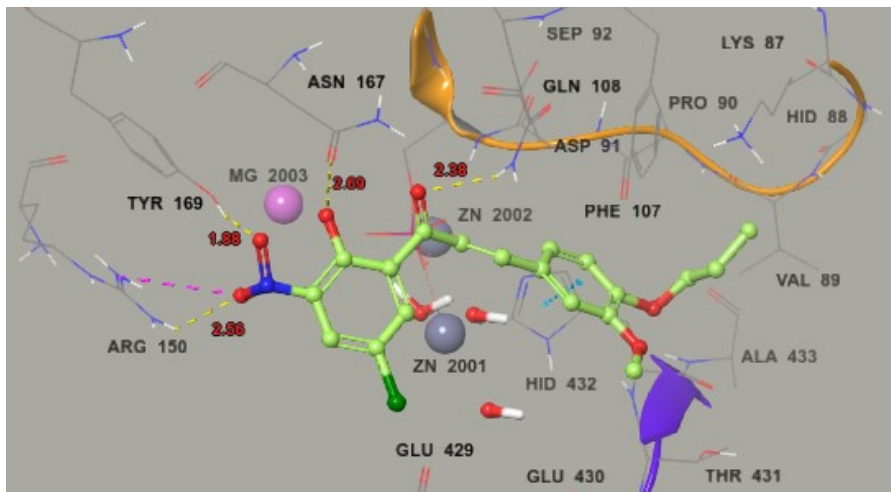
Compound-8



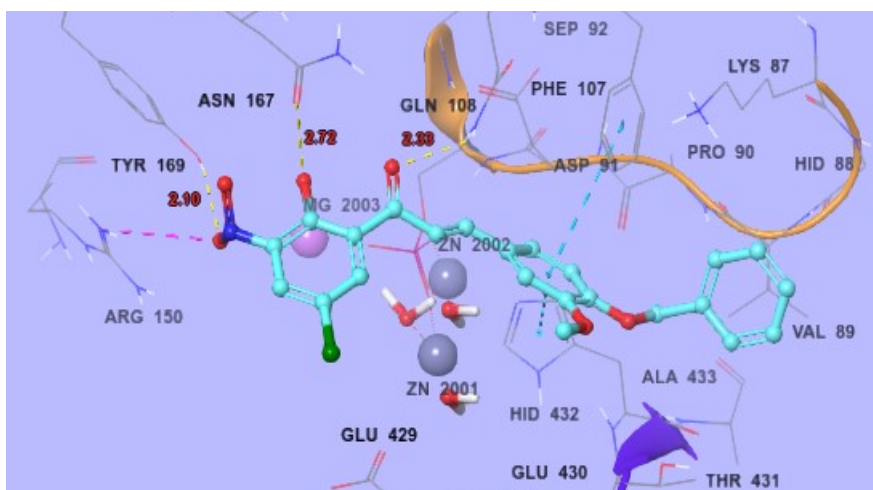
Compound-9



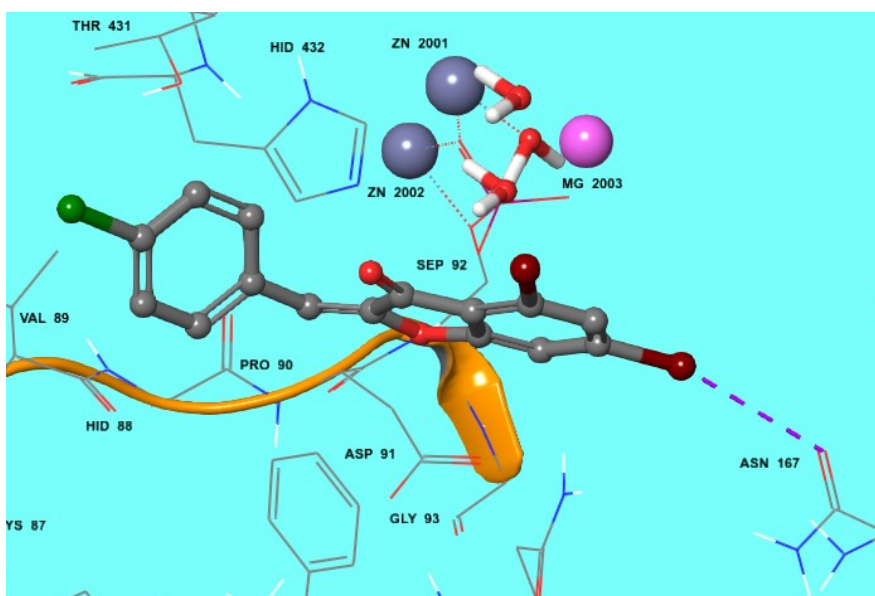
Compound-10



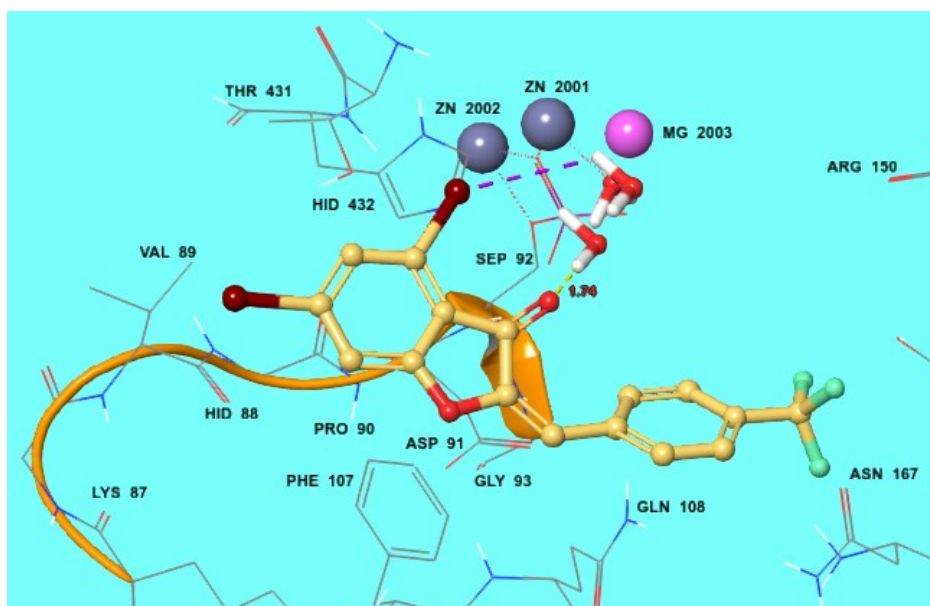
Compound-11



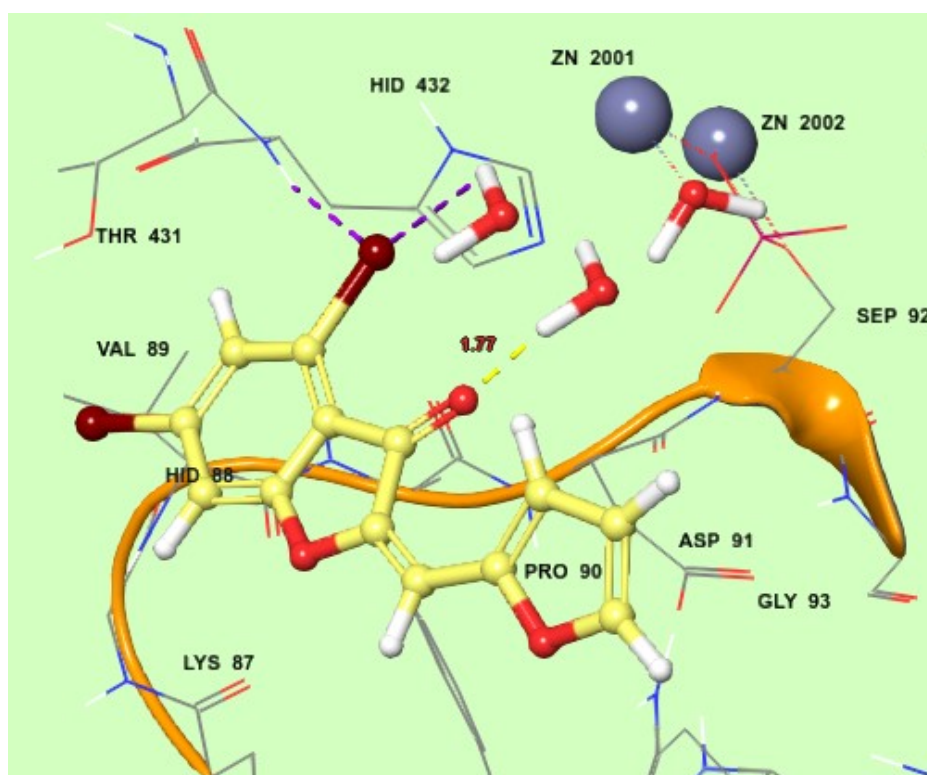
Compound-12



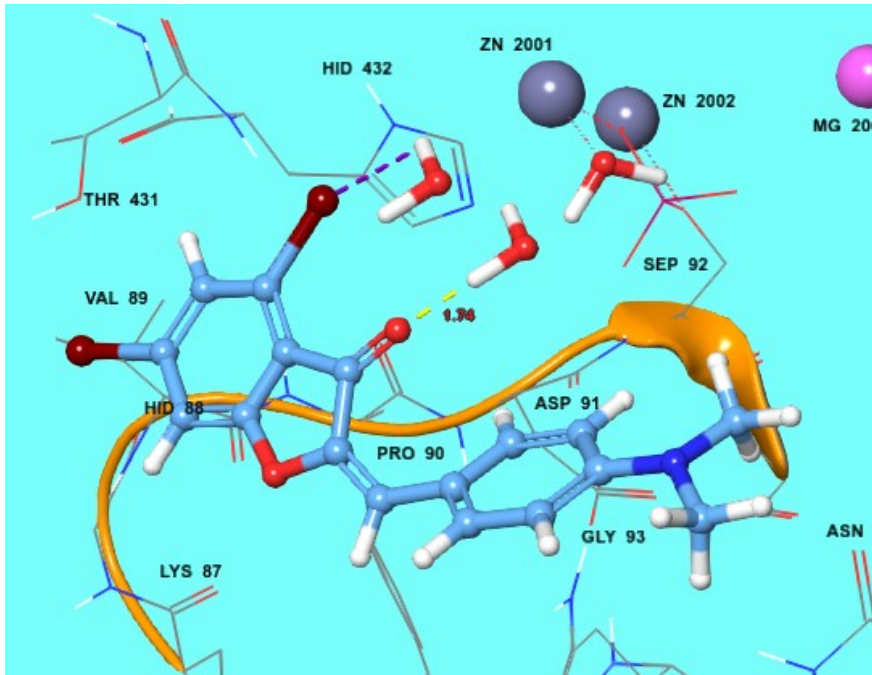
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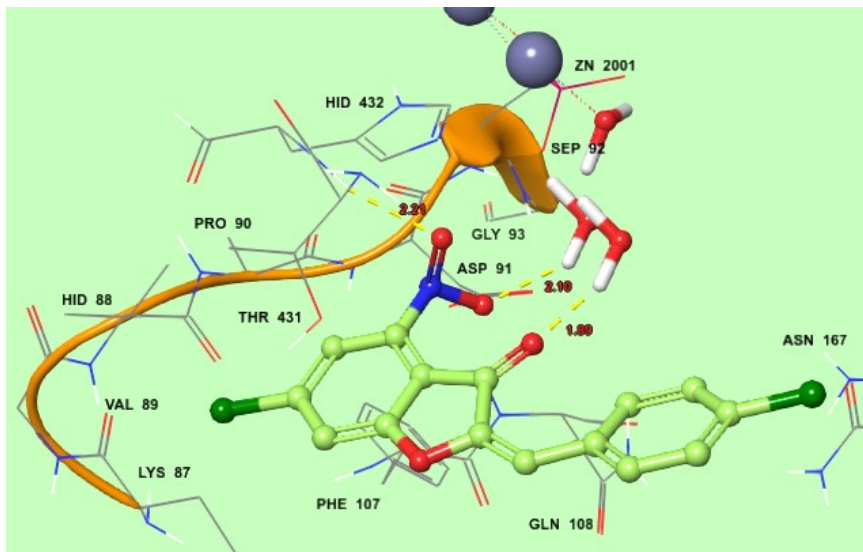
Compound-14



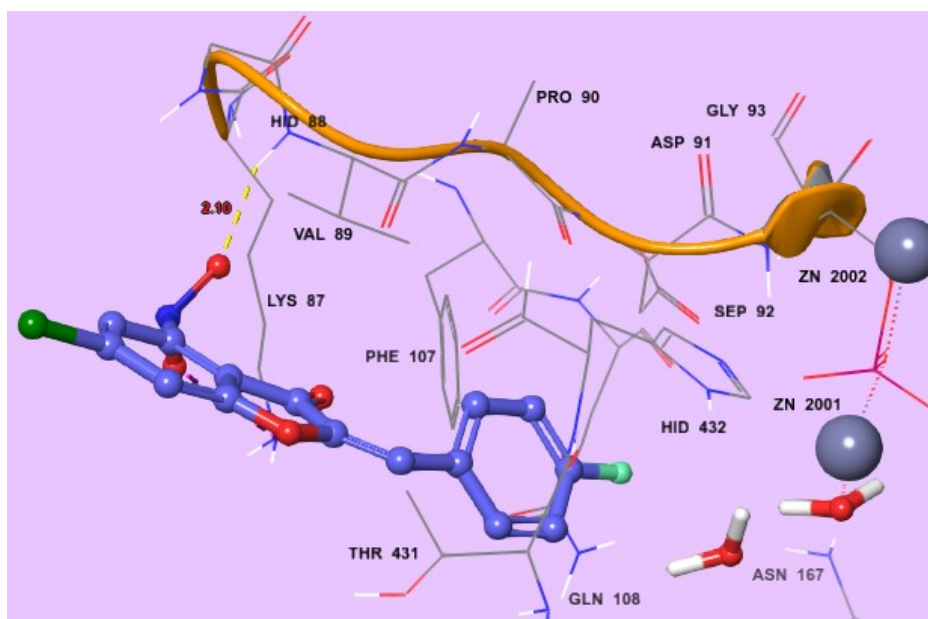
Compound-15



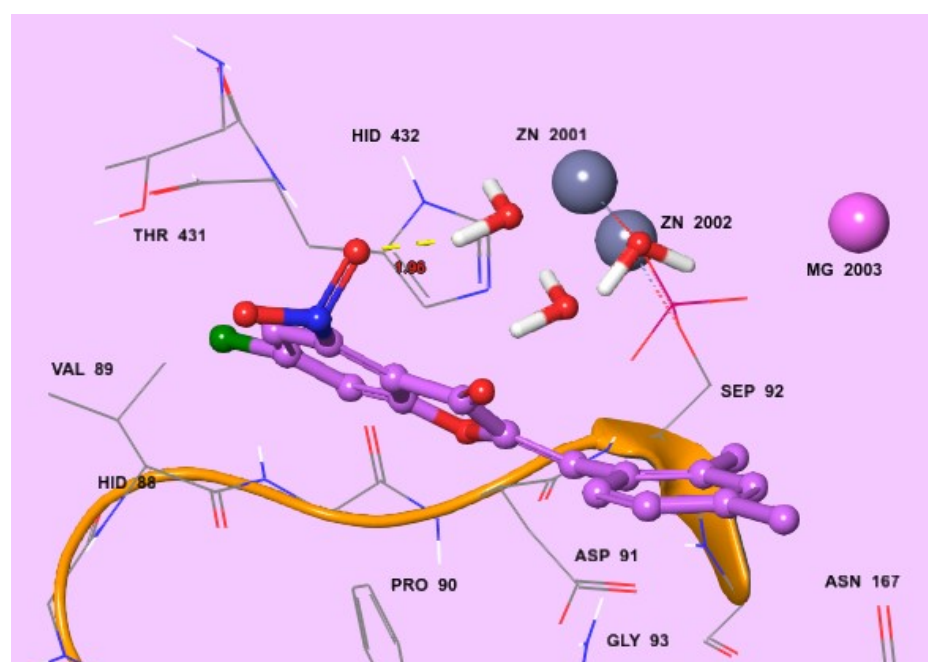
Compound-16



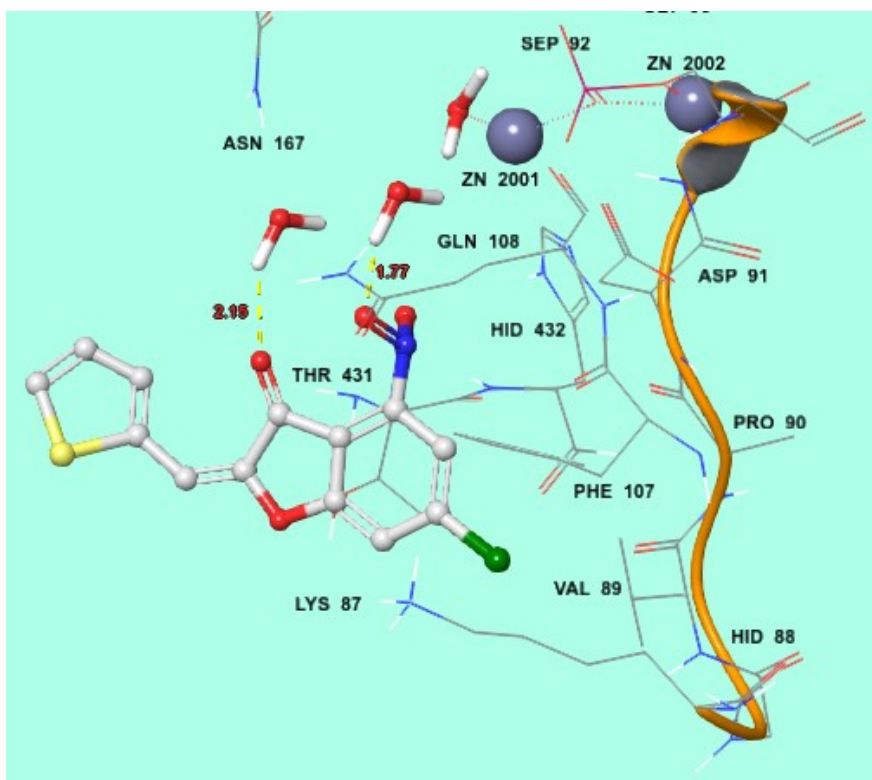
Compound-17



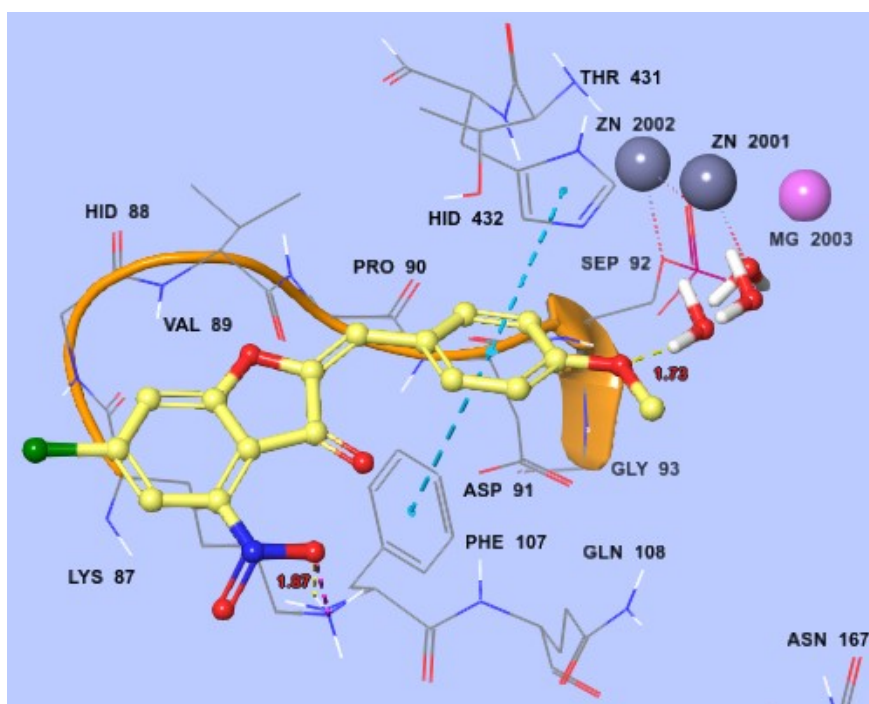
Compound-18



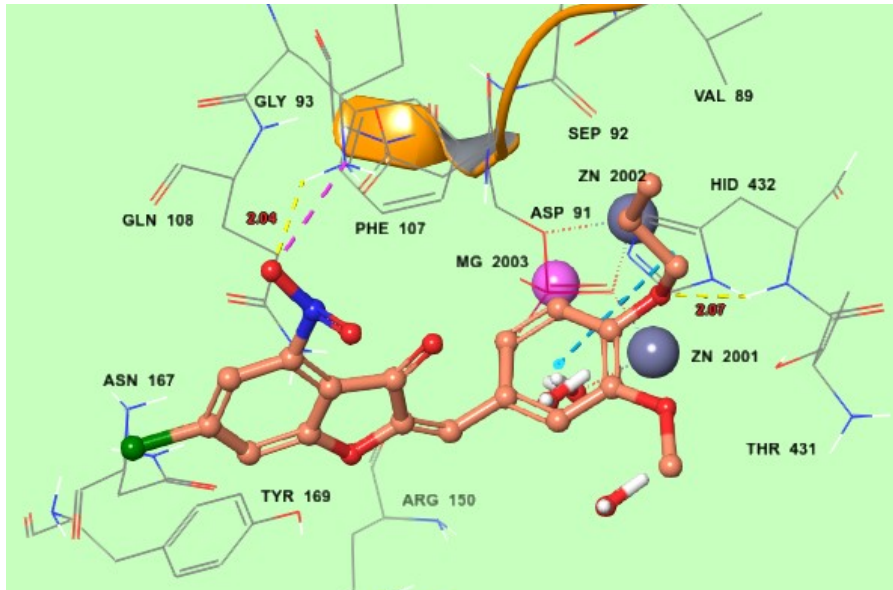
Compound-19



Compound-20



Compound-21



Compound-22

