Supporting Information

Sugar Mimics and their Probable Binding Site: Design and Synthesis of Thiazole Linked Coumarin-Piperazine Hybrids as Galectin-1 Inhibitors

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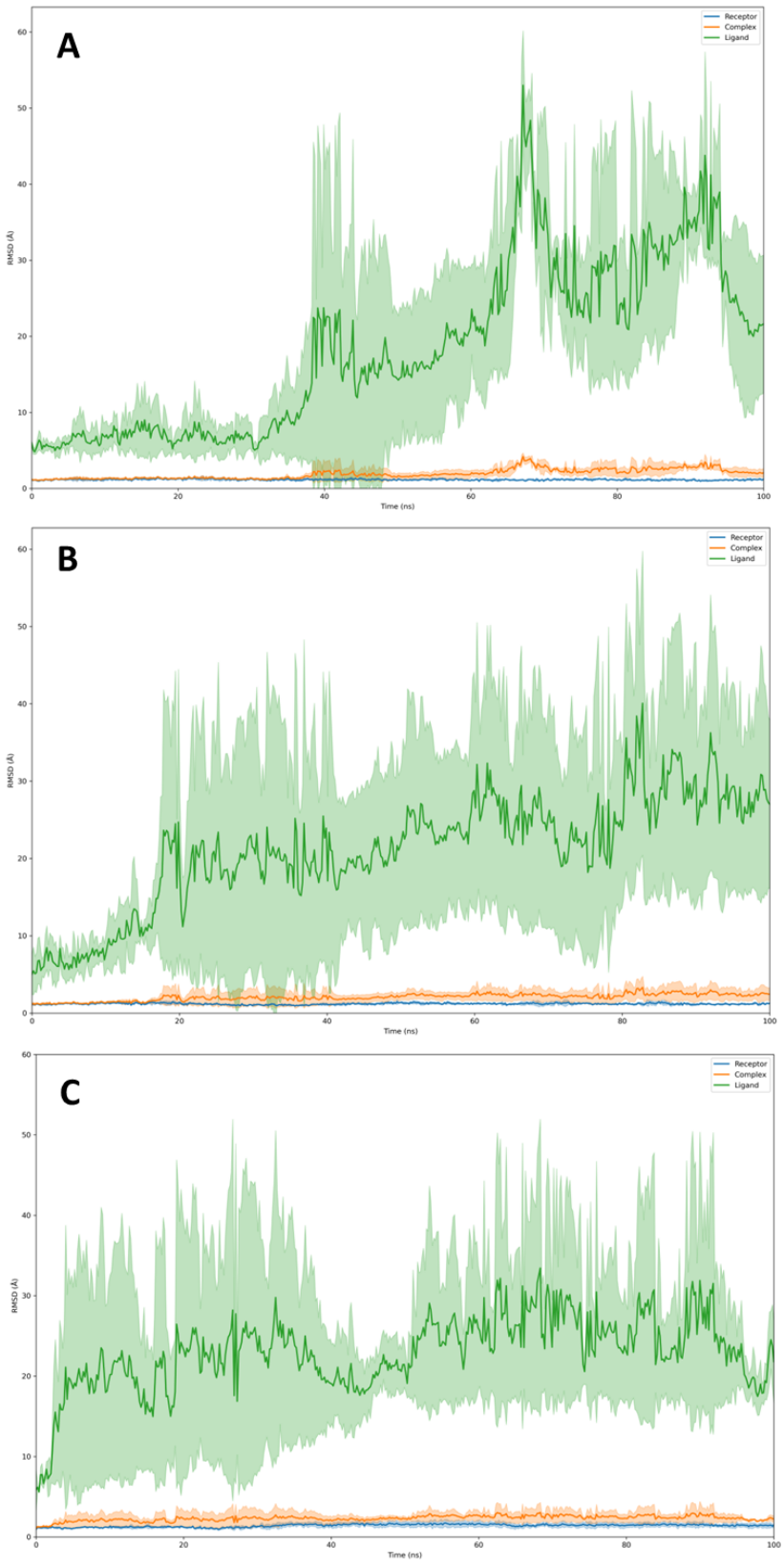


Figure S1 RMSD of ligand i.e. compound 10g (green), complex (orange) and the receptor (blue) for Pose 1 (A), pose 3 (B) and pose 15 (C) over the course of the simulation. The shaded regions represent the standard deviation of the RMSD values.

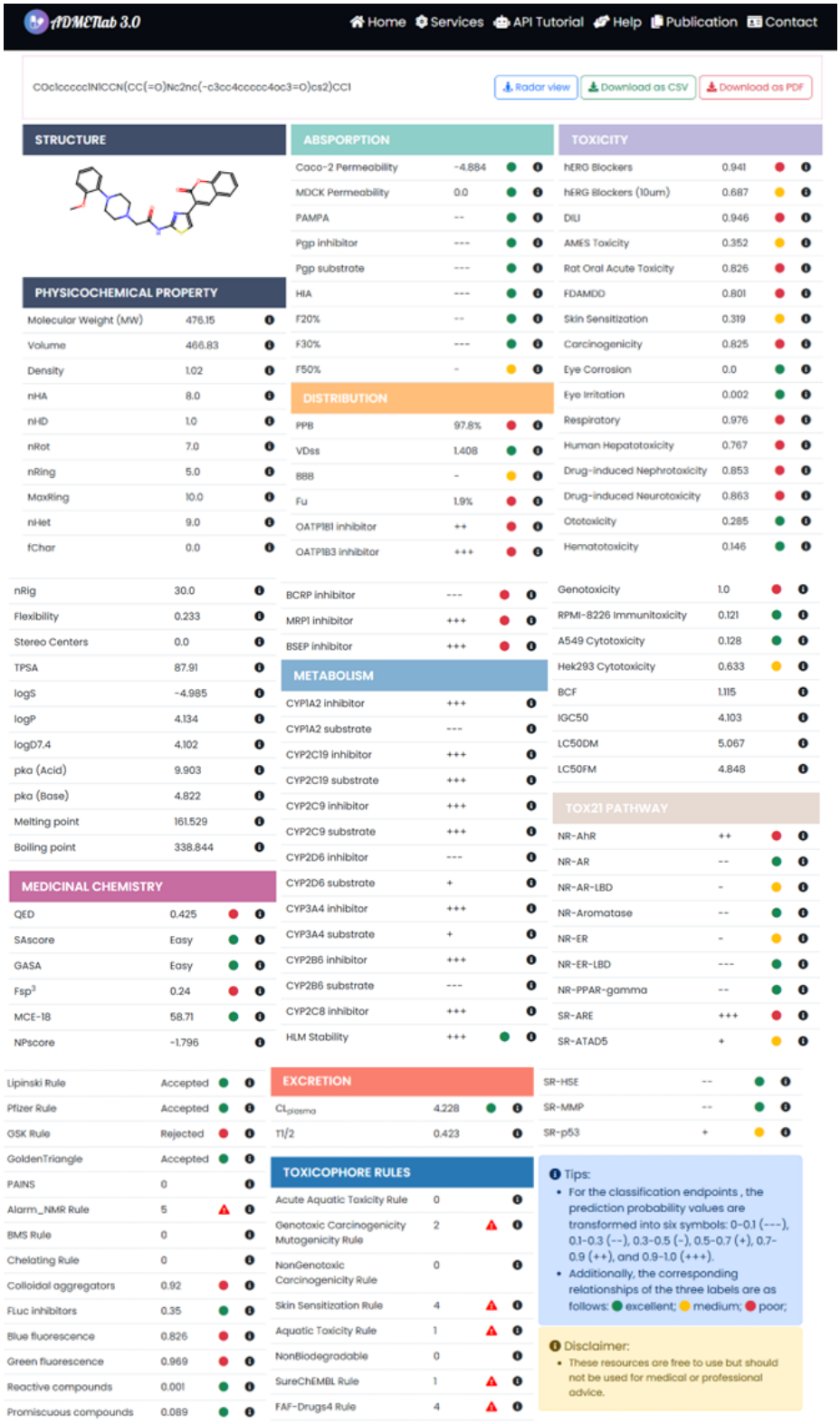


Figure S2 Predicted ADMET values for compound 10g using ADMETlab 3.0.

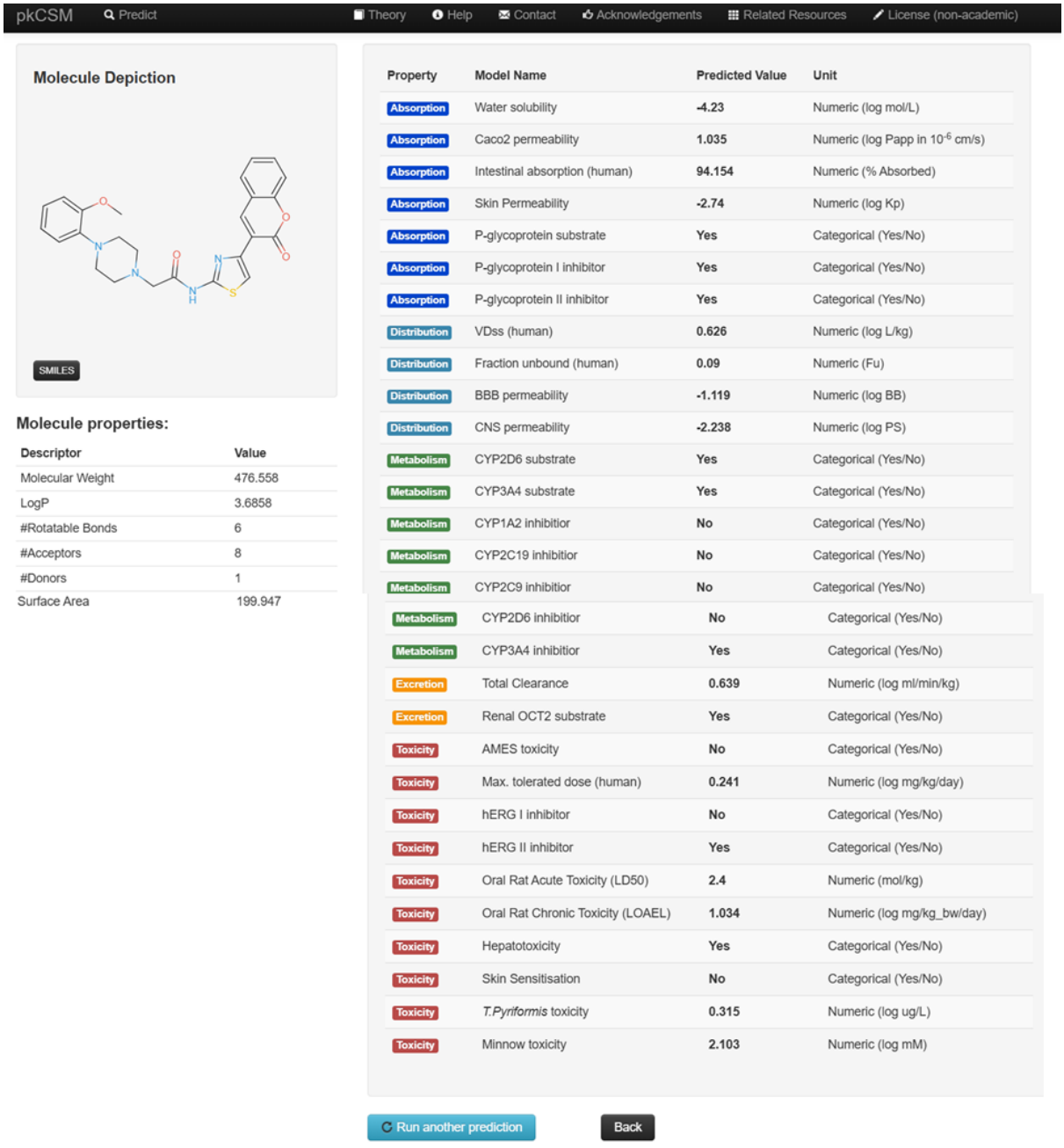
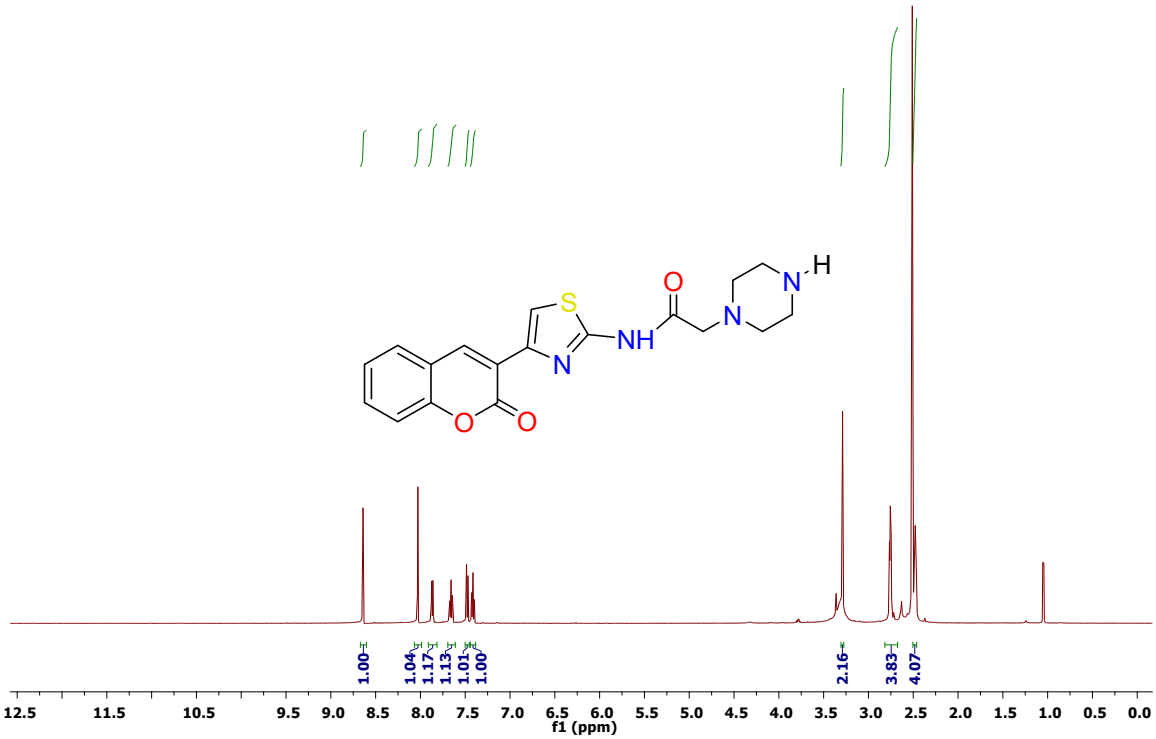
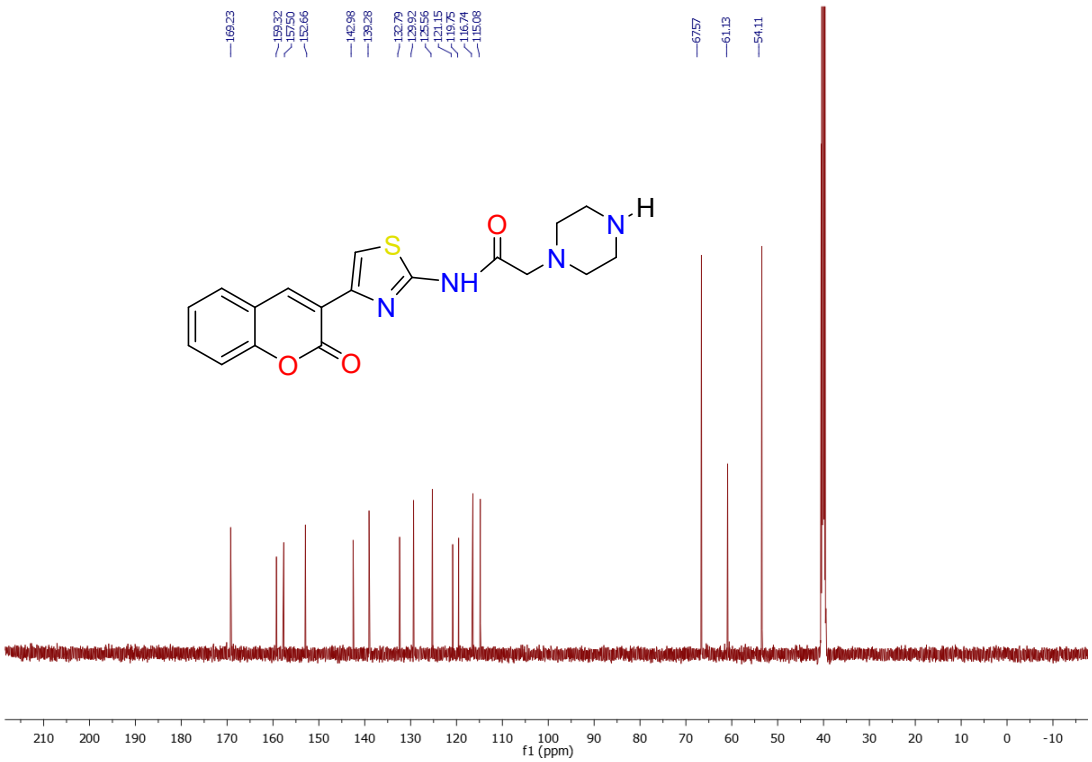


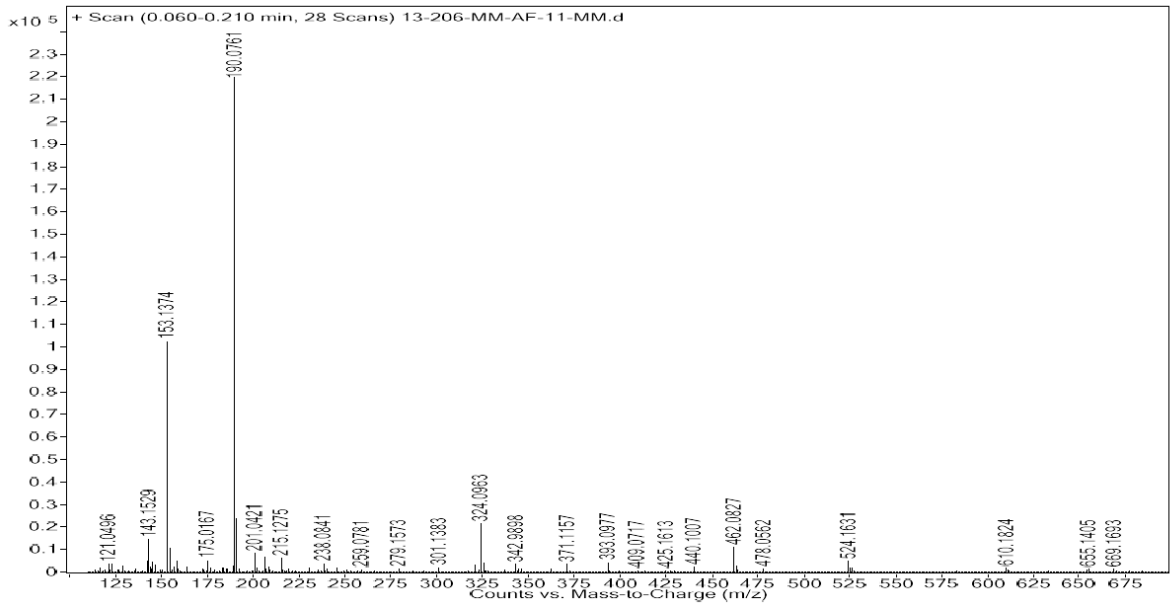
Figure S3 Predicted ADMET values for compound 10g using pkCSM.



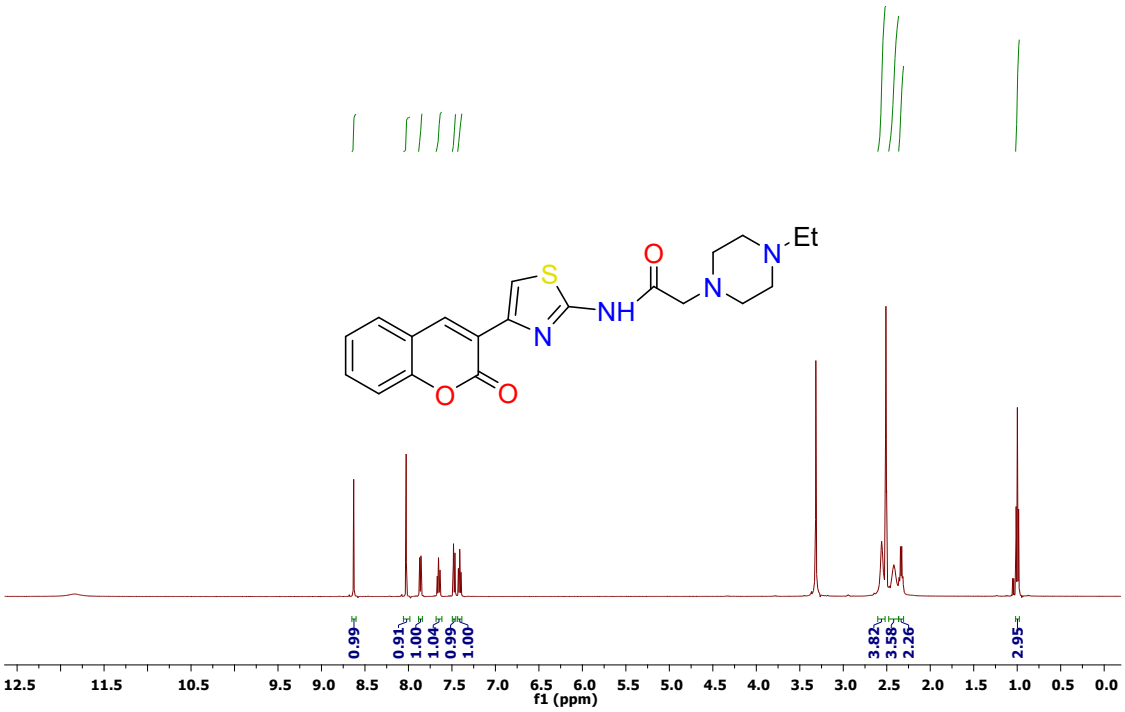
^{1}H NMR (500 MHz, DMSO-d_6) spectrum of compound **10a**



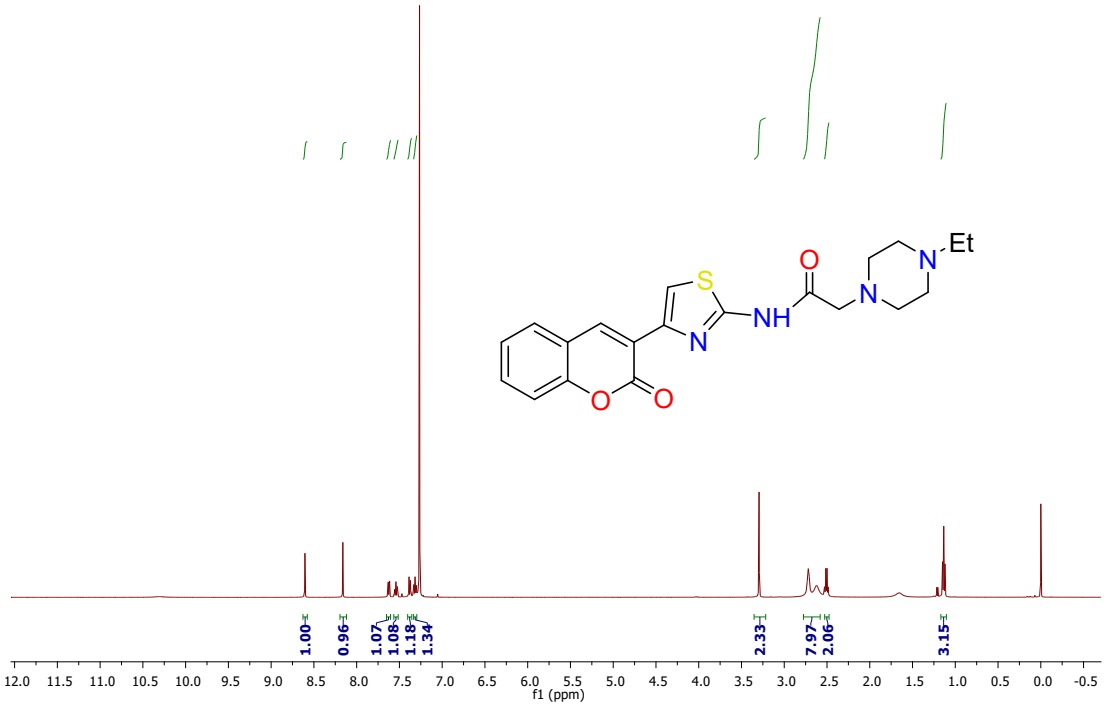
^{13}C NMR (125 MHz, DMSO-d_6) spectrum of compound **10a**



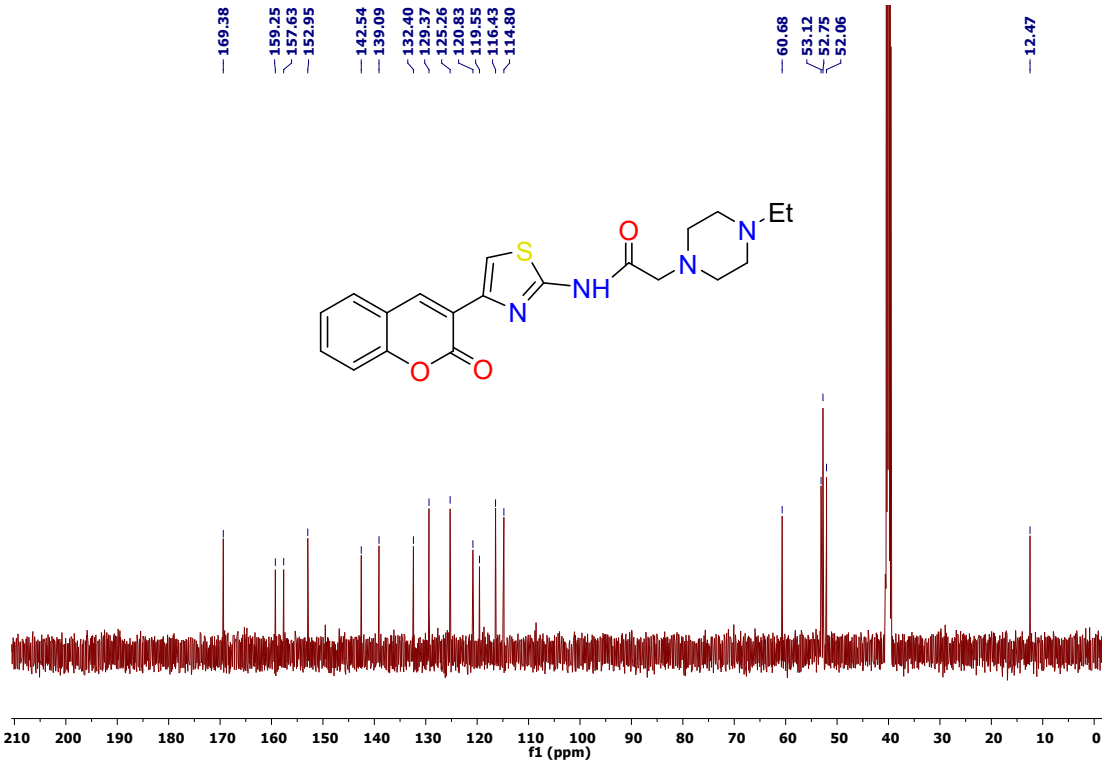
HRMS of compound **10a**



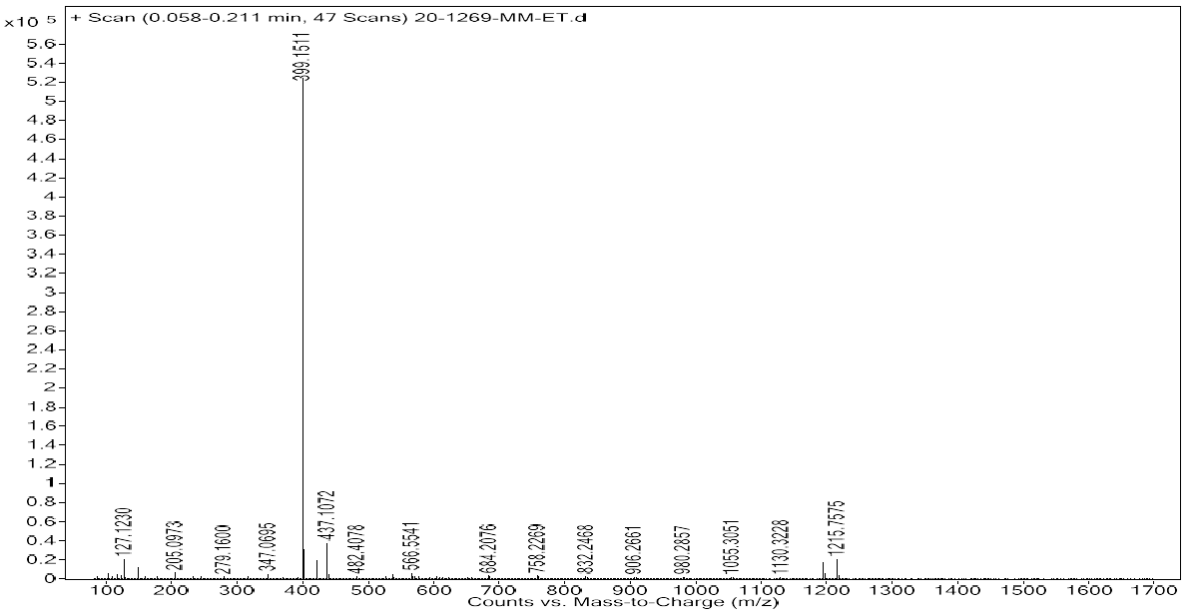
^{1}H NMR (500 MHz, DMSO-d_6) spectrum of compound **10b**



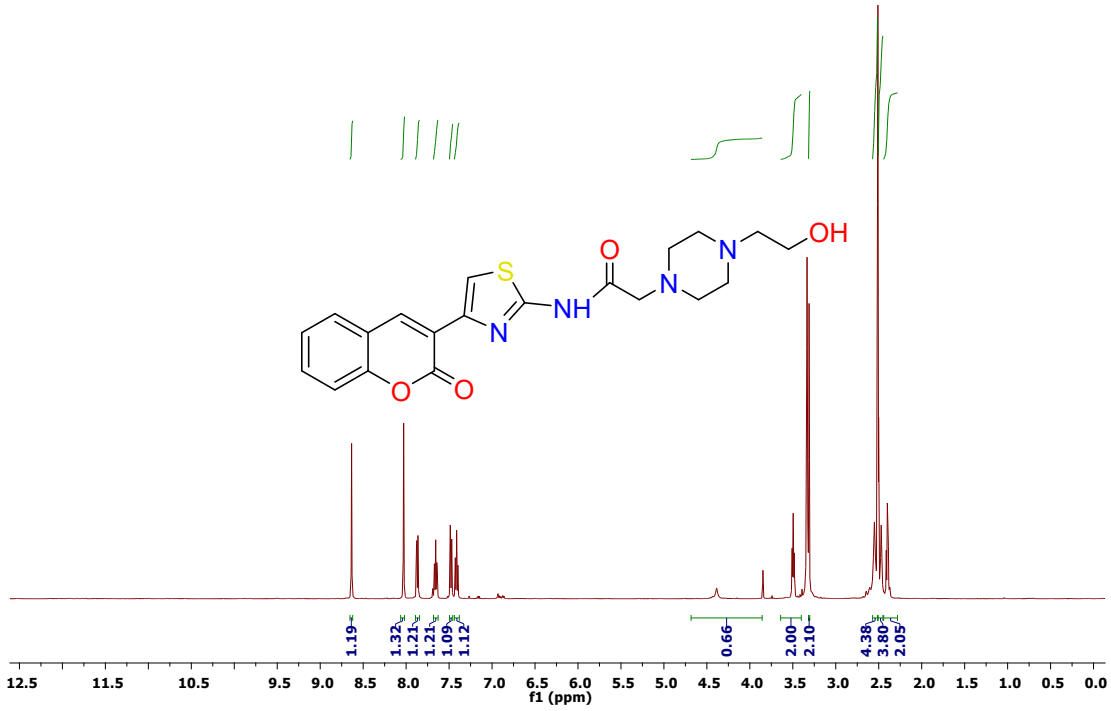
^{1}H NMR (500 MHz, $CDCl_3$) spectrum of compound **10b** - Carried out to identify missing CH_2 protons which had overlapped with moisture peak (δ 3.33) in DMSO solvent



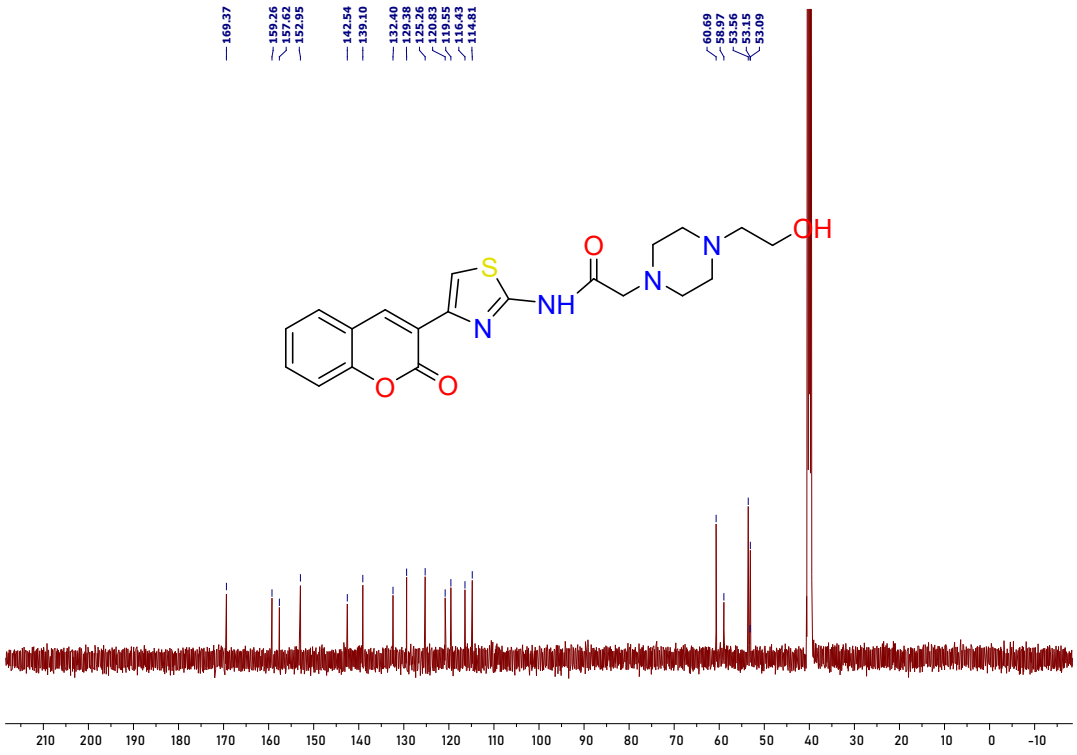
^{13}C NMR (125 MHz, DMSO-d_6) spectrum of compound **10b**



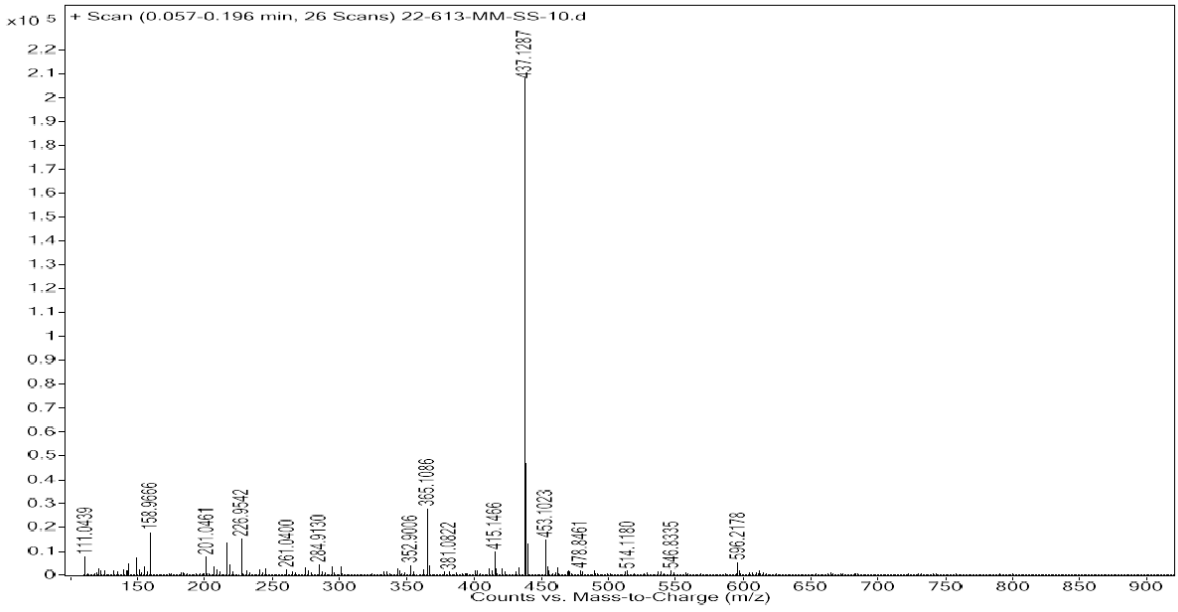
HRMS of compound **10b**



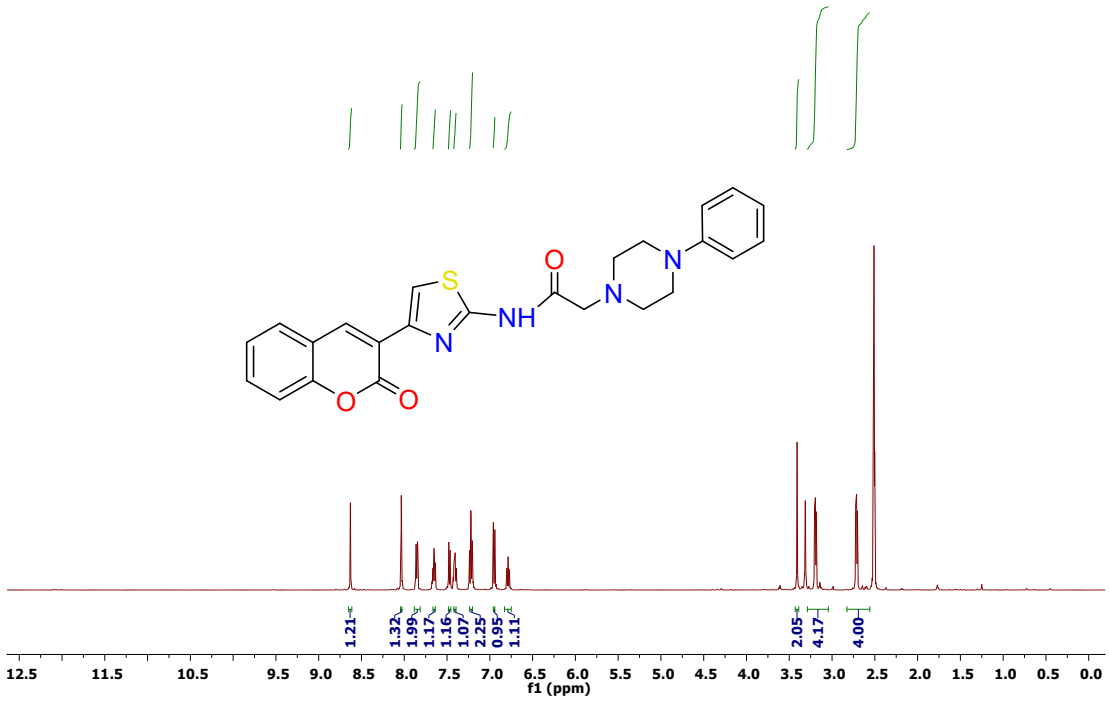
^{1}H NMR (500 MHz, DMSO-d_6) spectrum of compound **10c**



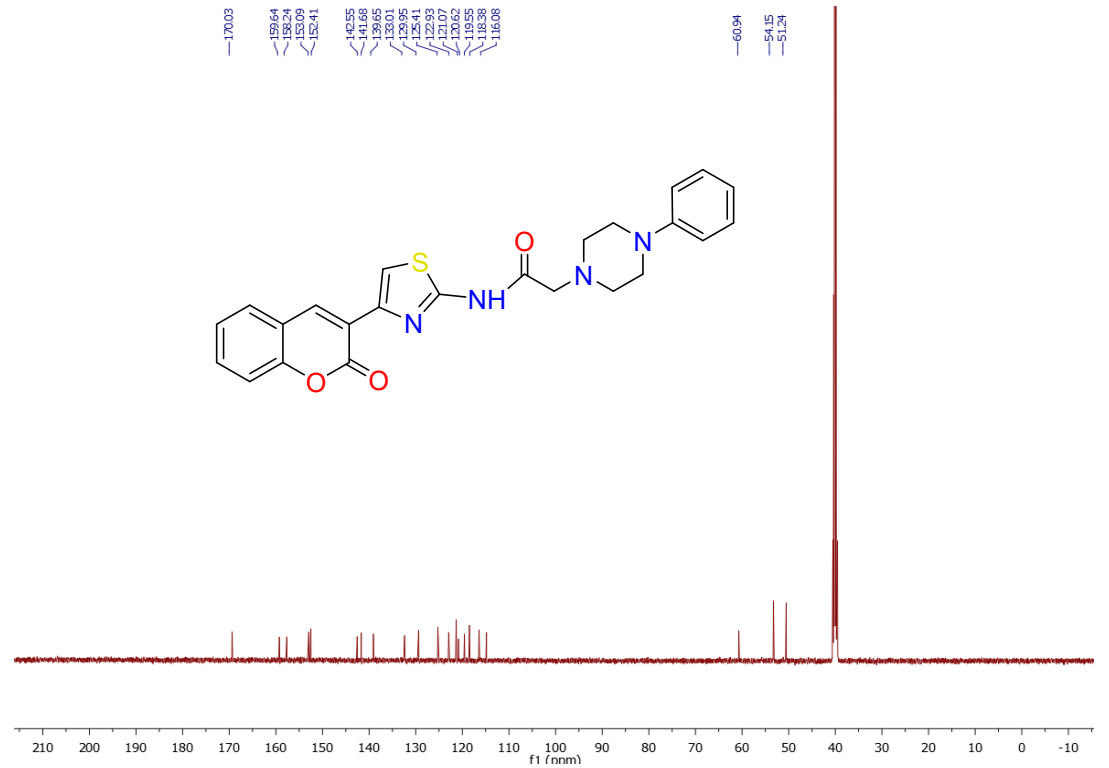
^{13}C NMR (125 MHz, DMSO-d_6) spectrum of compound **10c**



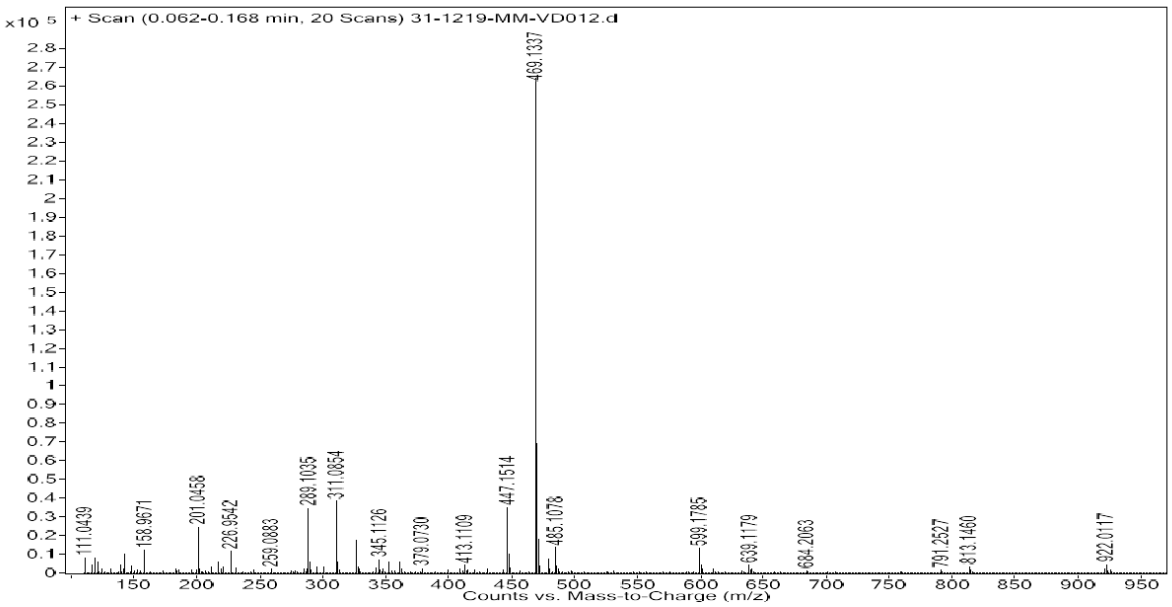
HRMS of compound **10c**



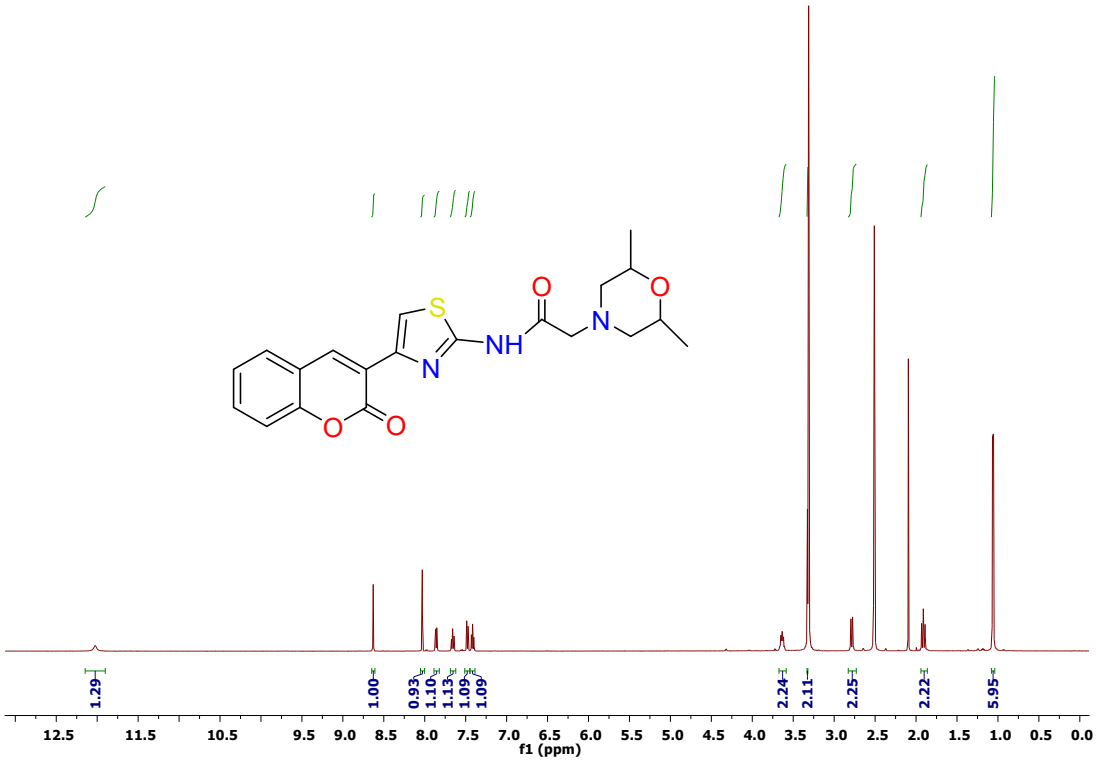
^{1}H NMR (500 MHz, DMSO-d_6) spectrum of compound **10d**



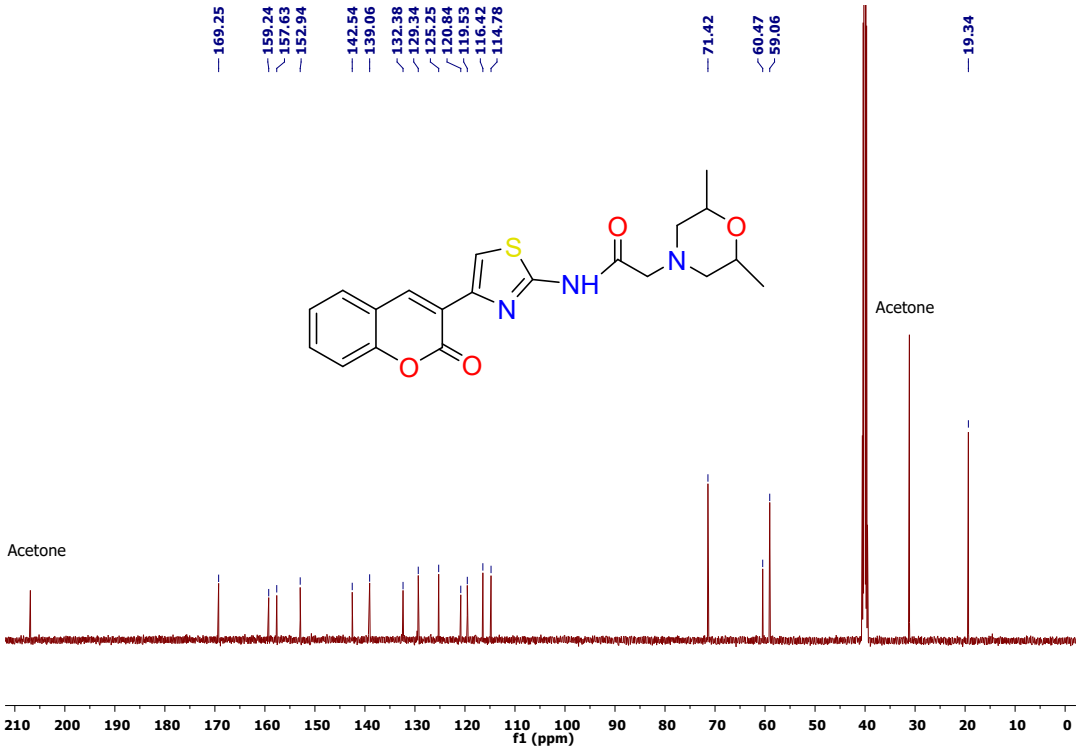
^{13}C NMR (125 MHz, DMSO-d_6) spectrum of compound **10d**



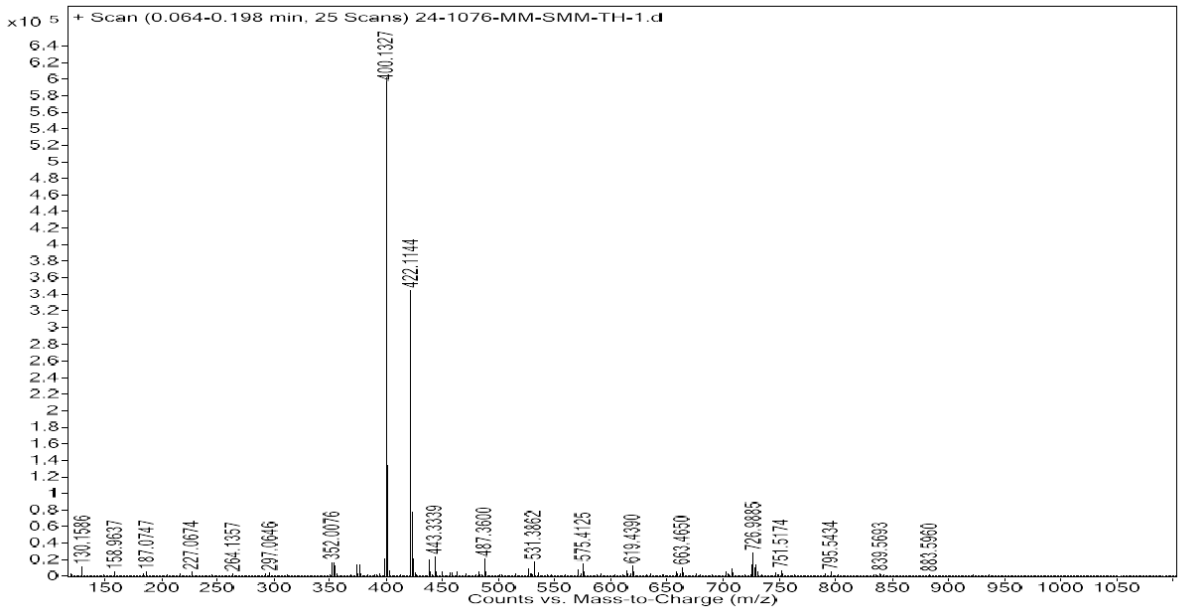
HRMS of compound **10d**



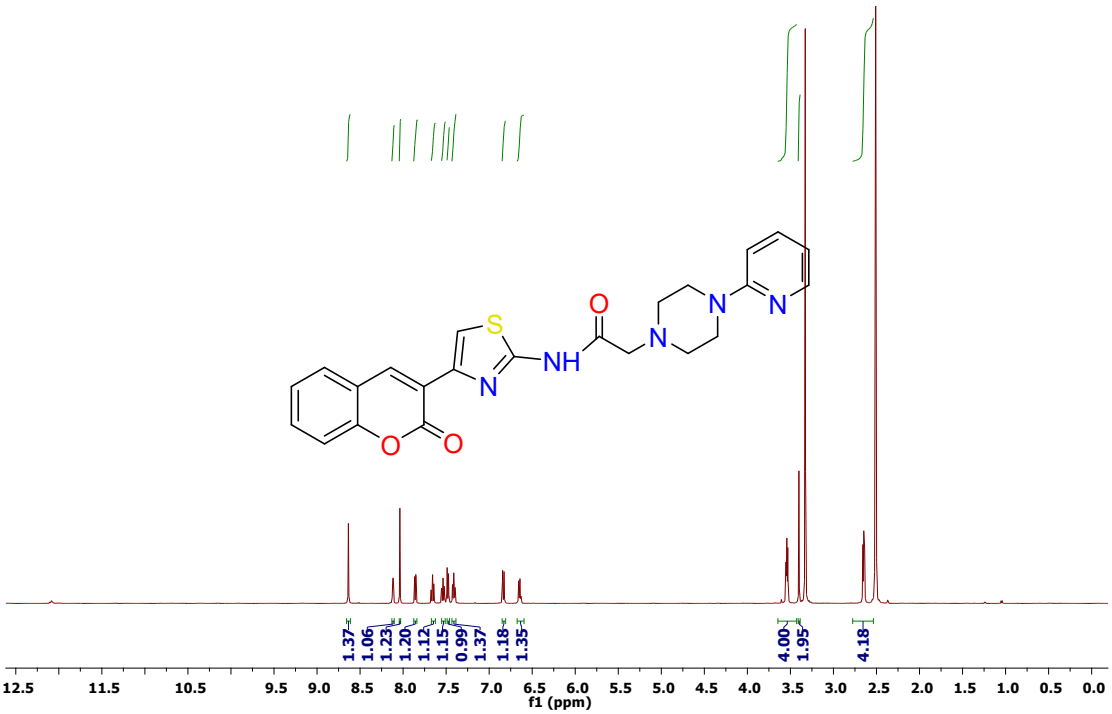
^{1}H NMR (500 MHz, DMSO-d_6) spectrum of compound **10e**



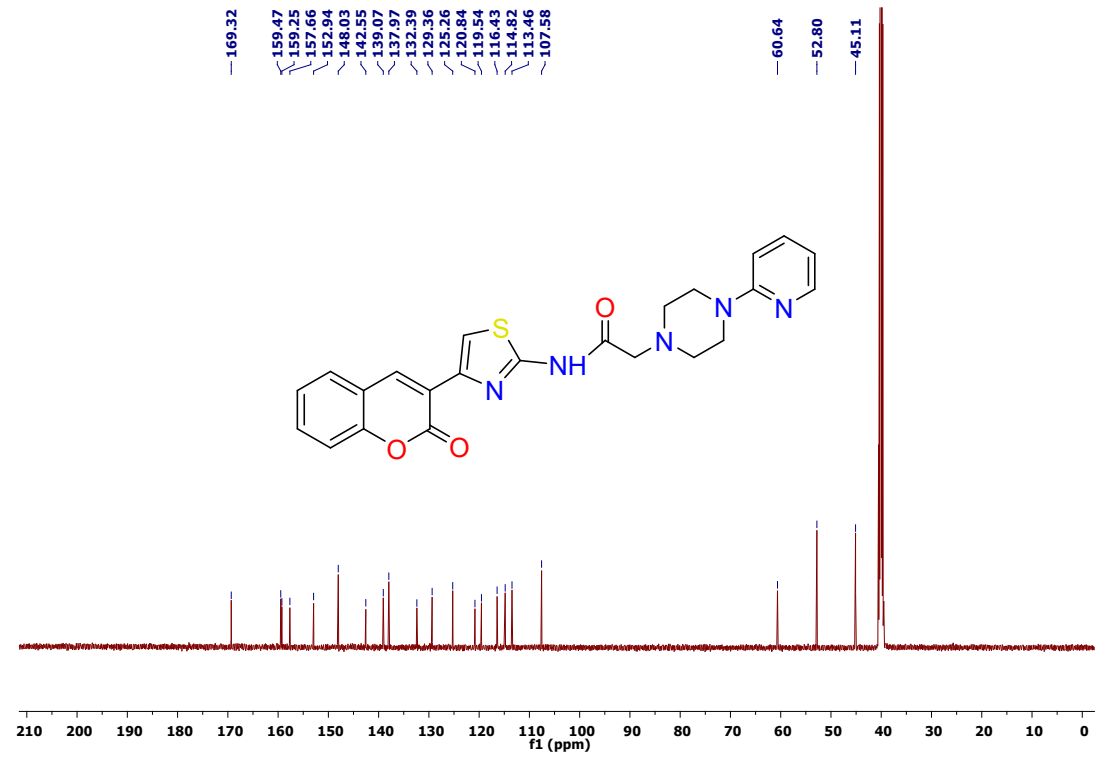
^{13}C NMR (125 MHz, DMSO-d_6) spectrum of compound **10e**



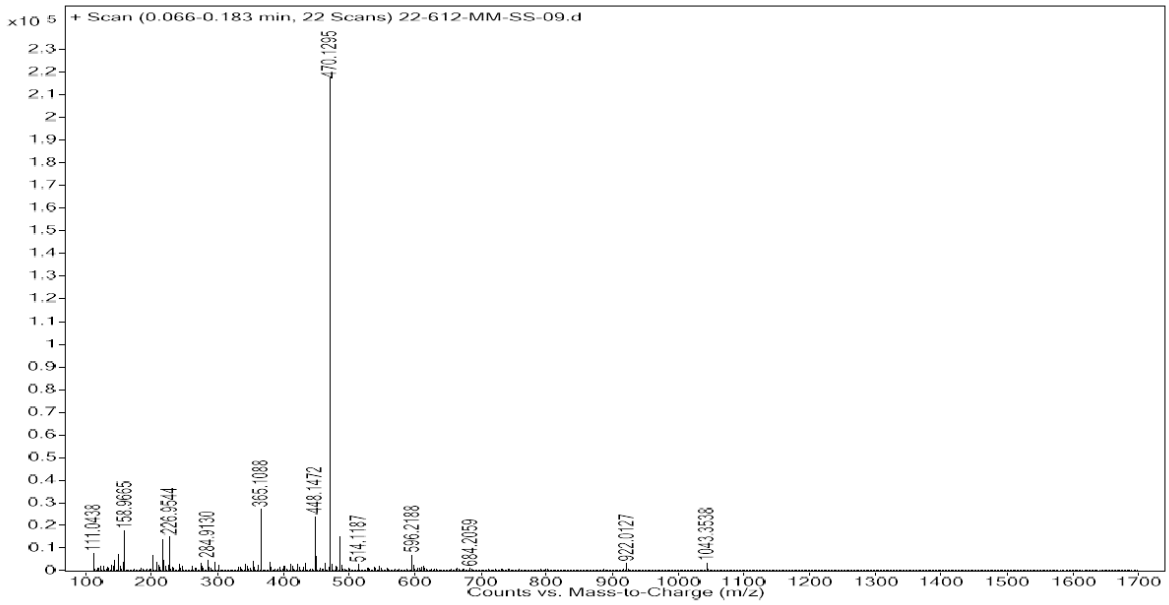
HRMS of compound **10e**



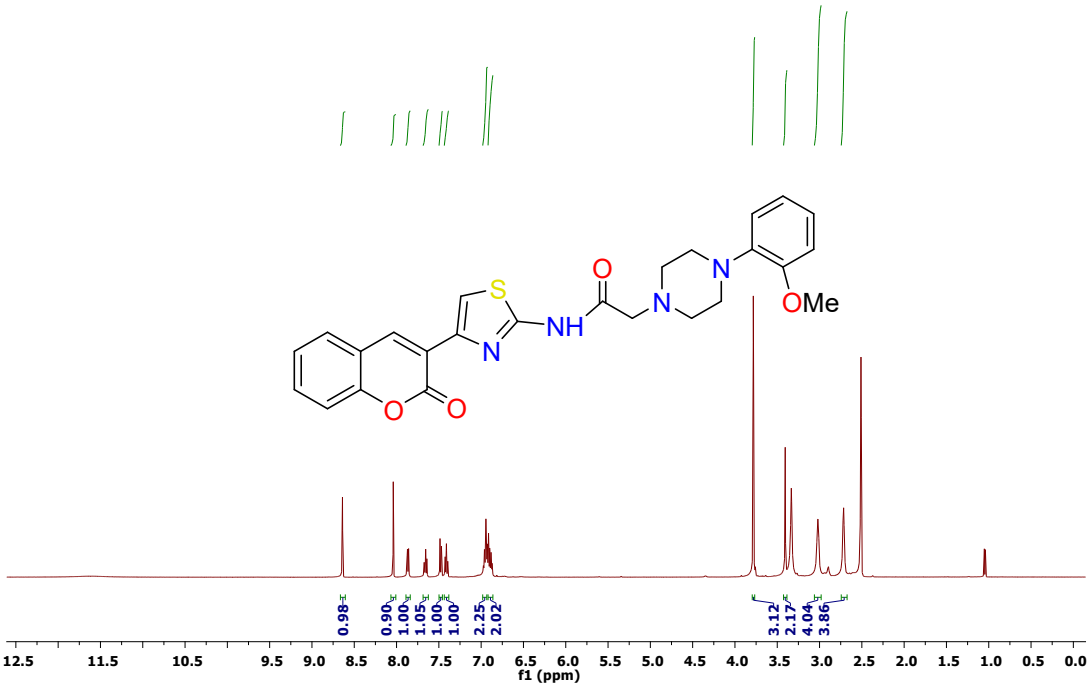
^{1}H NMR (500 MHz, DMSO-d_6) spectrum of compound **10f**



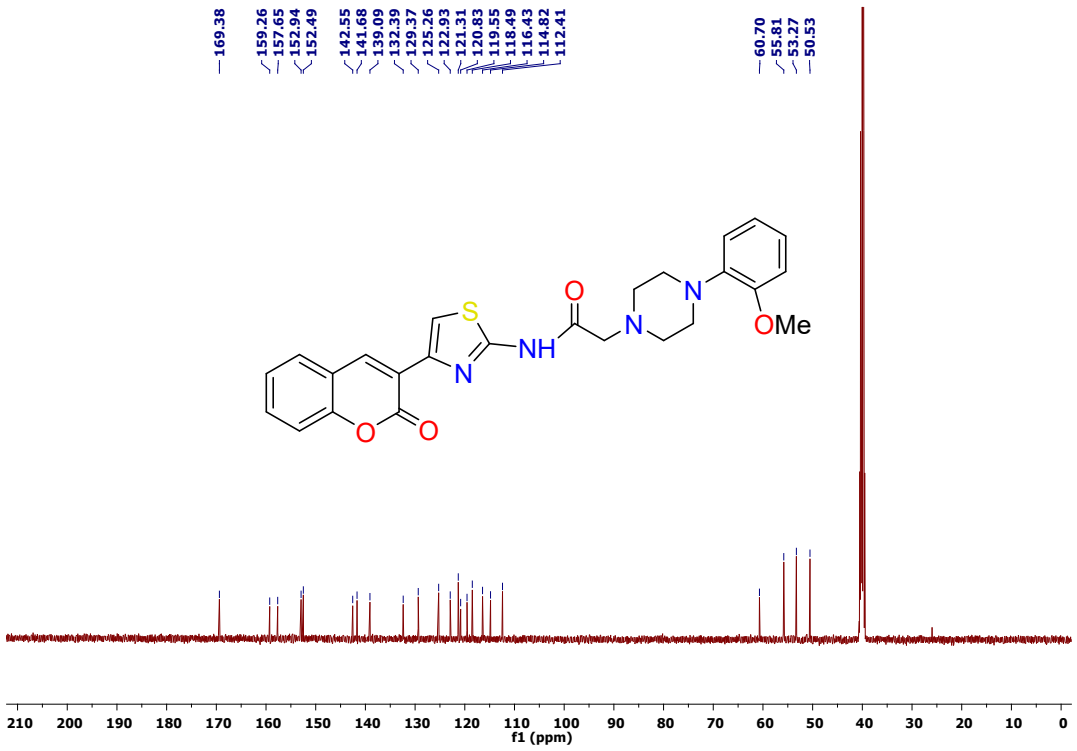
^{13}C NMR (125 MHz, DMSO-d_6) spectrum of compound **10f**



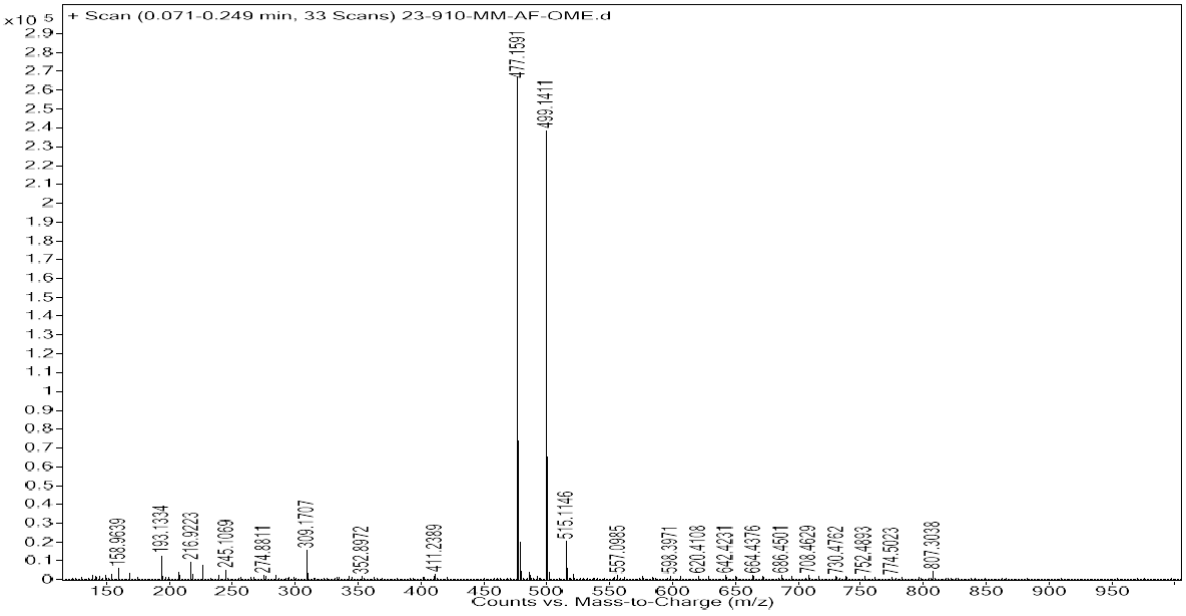
HRMS of compound **10f**



^{1}H NMR (500 MHz, DMSO-d_6) spectrum of compound **10g**



^{13}C NMR (125 MHz, DMSO-d_6) spectrum of compound **10g**



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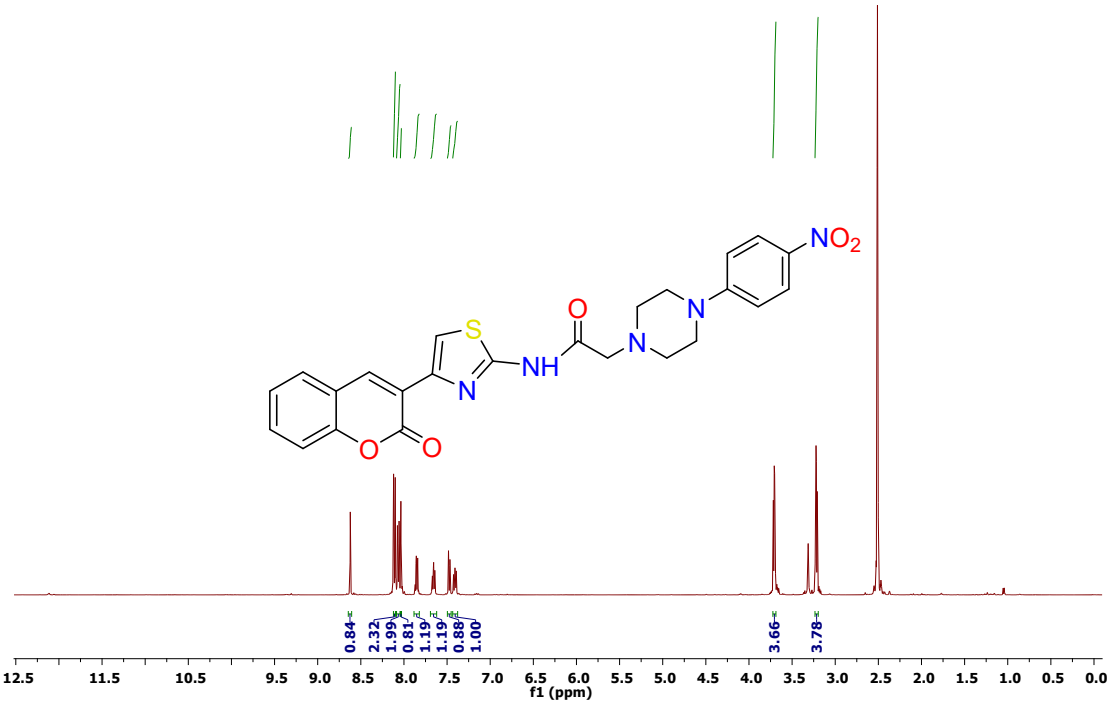
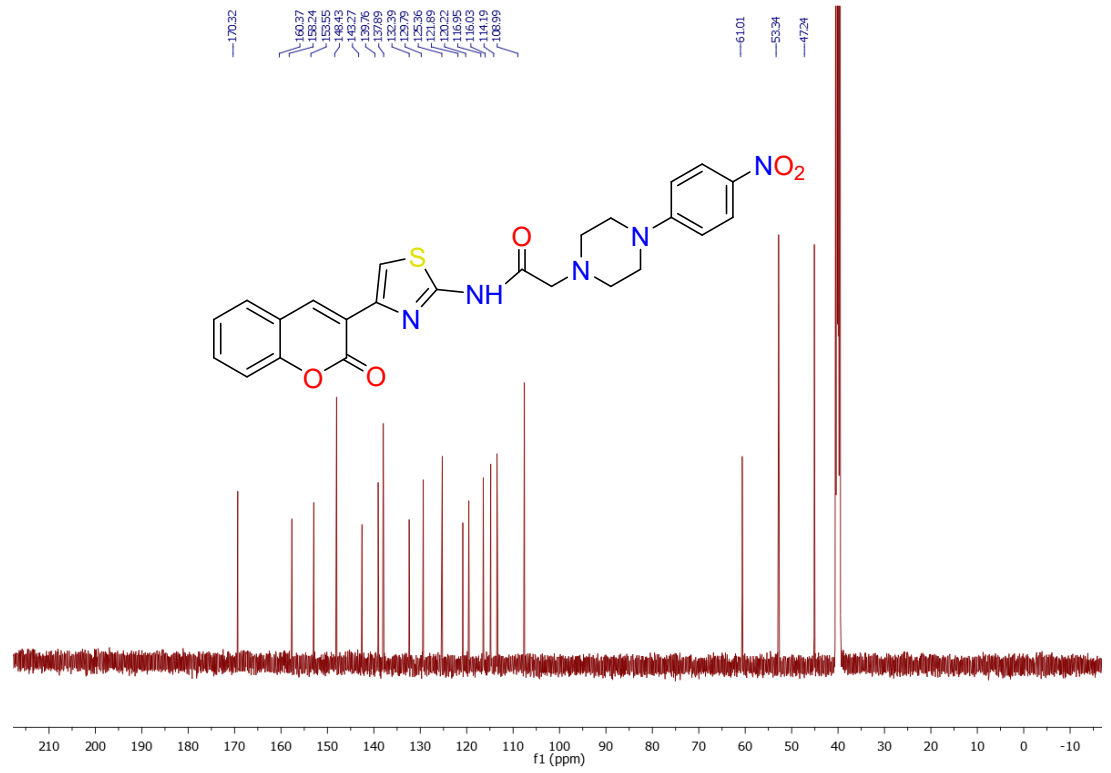
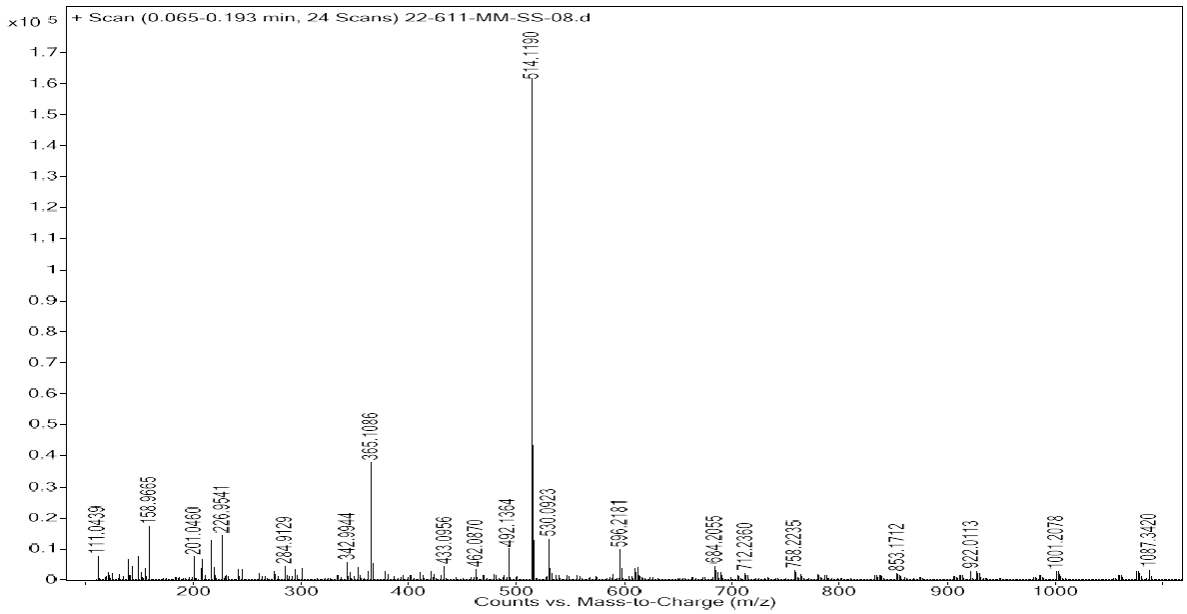


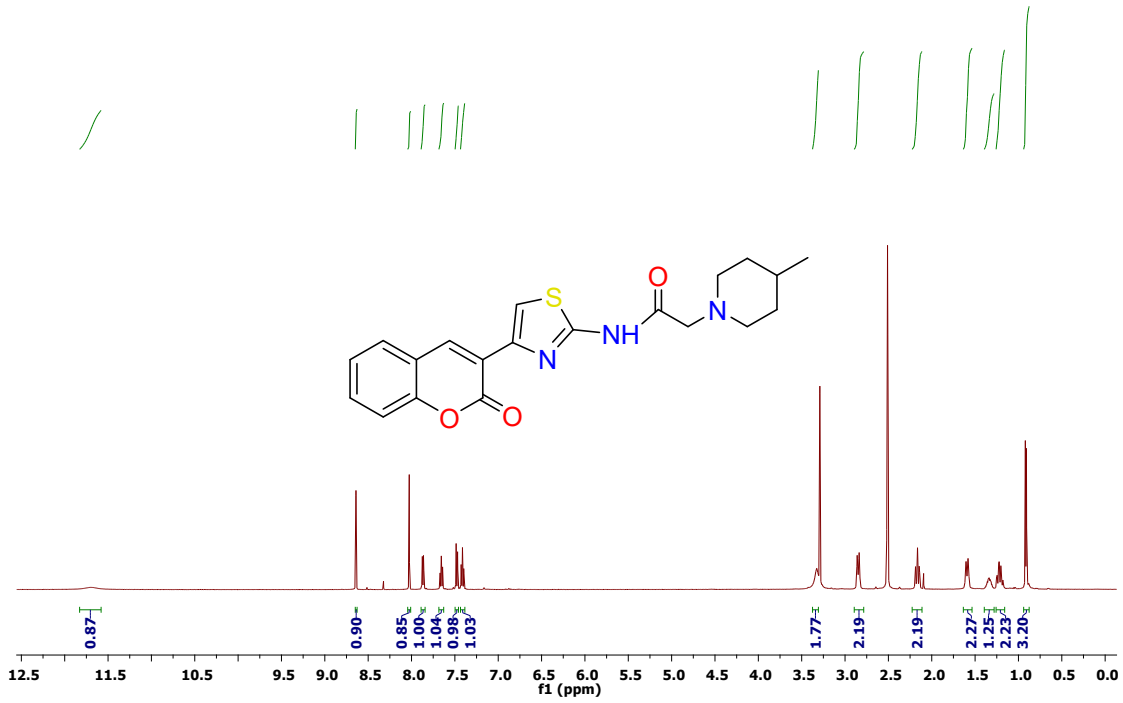
^{1}H NMR (500 MHz, DMSO-d_6) spectrum of compound **10h**



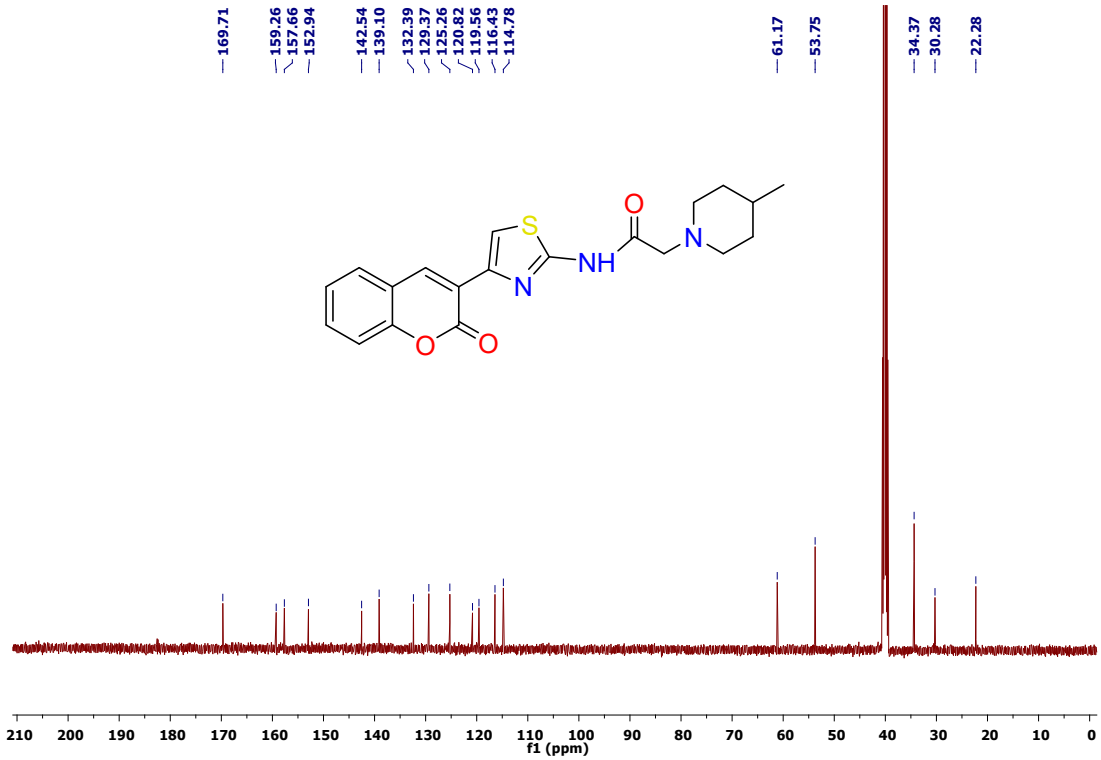
^{13}C NMR (125 MHz, DMSO-d_6) spectrum of compound **10h**



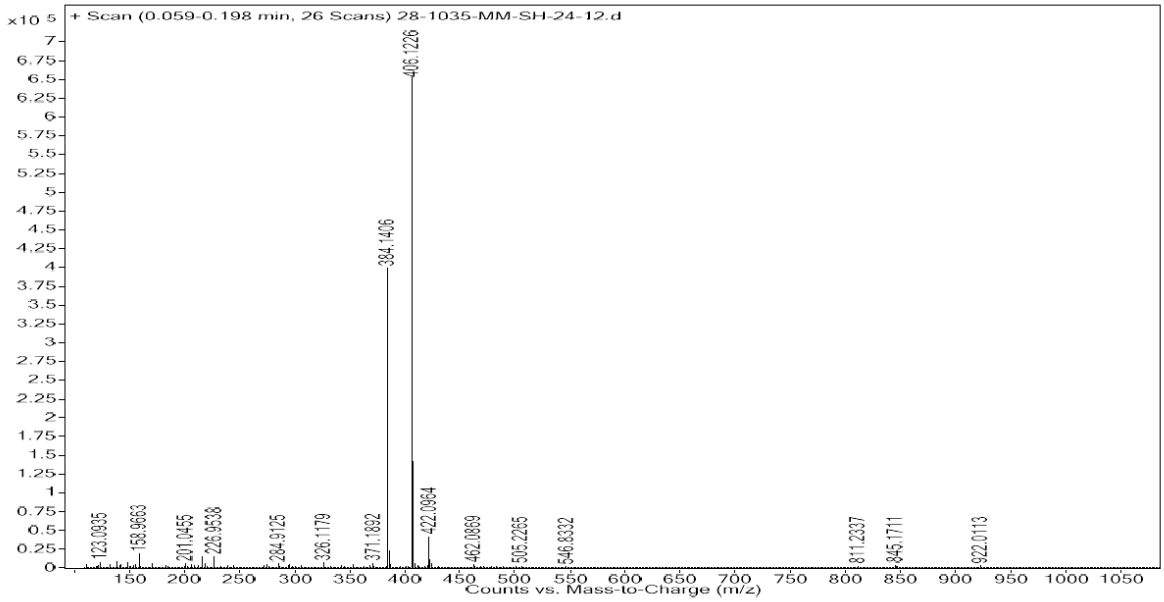
HRMS of compound **10h**



^{1}H NMR (500 MHz, DMSO-d_6) spectrum of compound **10i**



^{13}C NMR (125 MHz, DMSO-d_6) spectrum of compound **10i**



HRMS of compound **10i**