Supporting Information

Contents

Synthesis and DNA Binding Studies of Novel Triazine-isatin Hybrids: Experimental and Computational Insights

Alia Mushtaq, Muhammad Moazzam Naseer*

Department of Chemistry, Quaid-i-Azam University, Islamabad 45320, Pakistan

*Corresponding author: moazzam@qau.edu.pk (M. M. Naseer)

Instrumentation and Materials

The melting points of the products were determined in open-end capillary tubes, by using Gallenkamp apparatus. Infrared spectra were recorded on Bruker Tensor II spectrophotometer (Germany) for functional group analysis. ^{1}H and ^{13}C NMR spectra were recorded on Bruker Avance 300 MHz NMR spectrophotometer (Switzerland) using deuterated solvents and the chemical shifts were calibrated relative to the residual solvent signal. *In vacuo* removal of solvents was performed using the Buchi rotary evaporator.

All the chemicals were obtained from Sigma Aldrich (Germany) and used as received. The solvents were distilled as per requirement using standard protocols. To monitor the progress of the reaction, Thin Layer Chromatography (TLC) was performed by using pre-coated silica plates (Kieselgel-60 F_{254}, Merck, Germany). For product purification, flash chromatography was performed on silica gel (70-230 mesh).

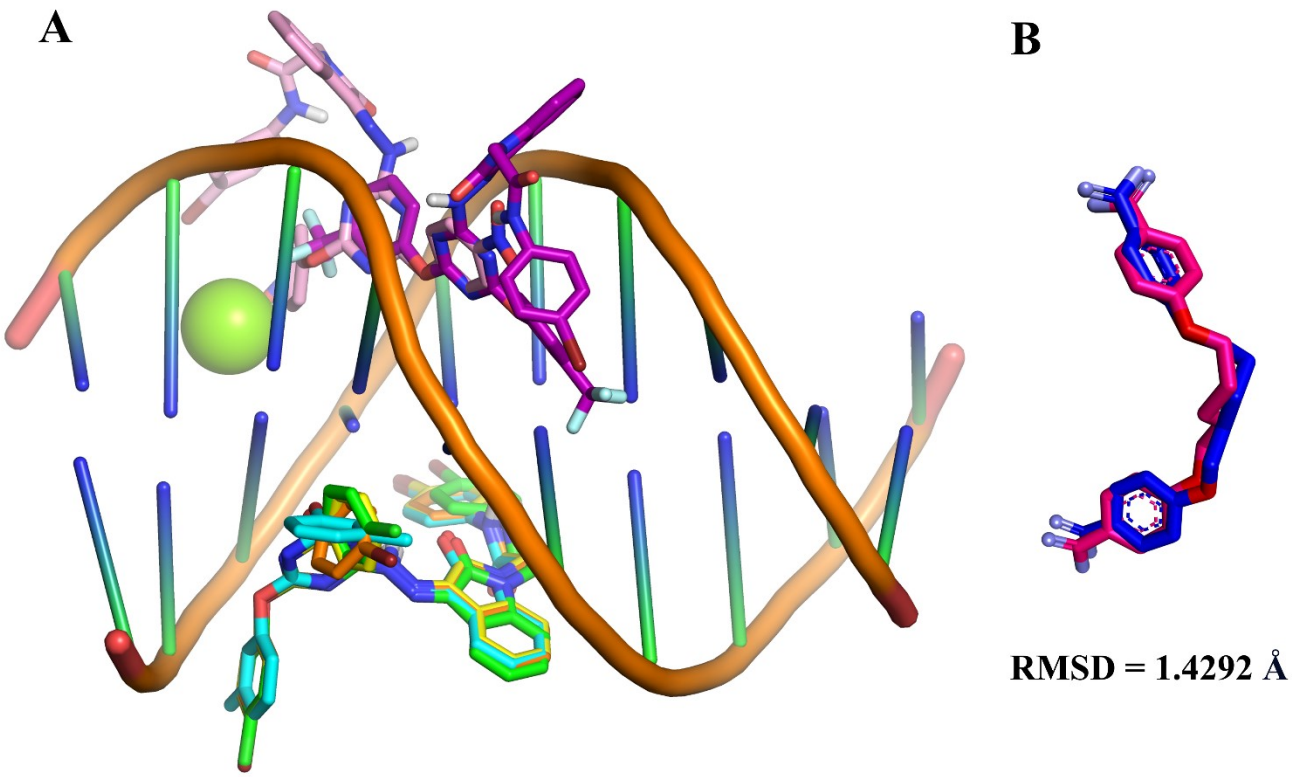
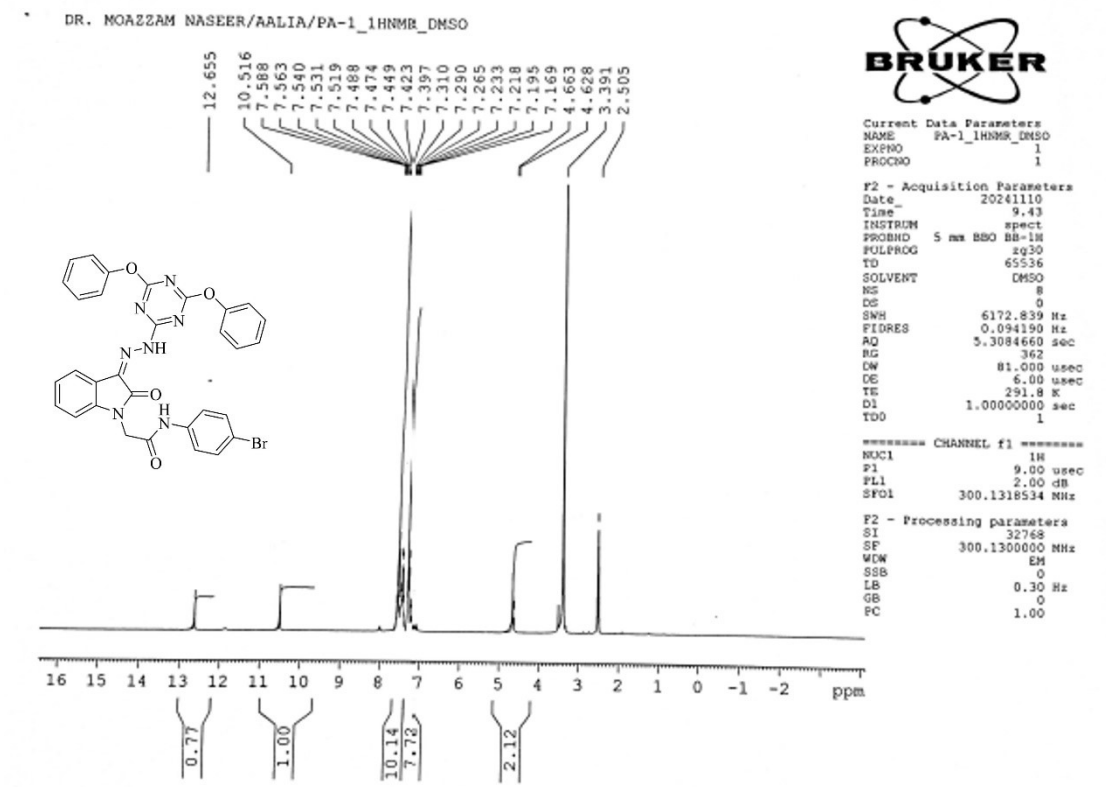


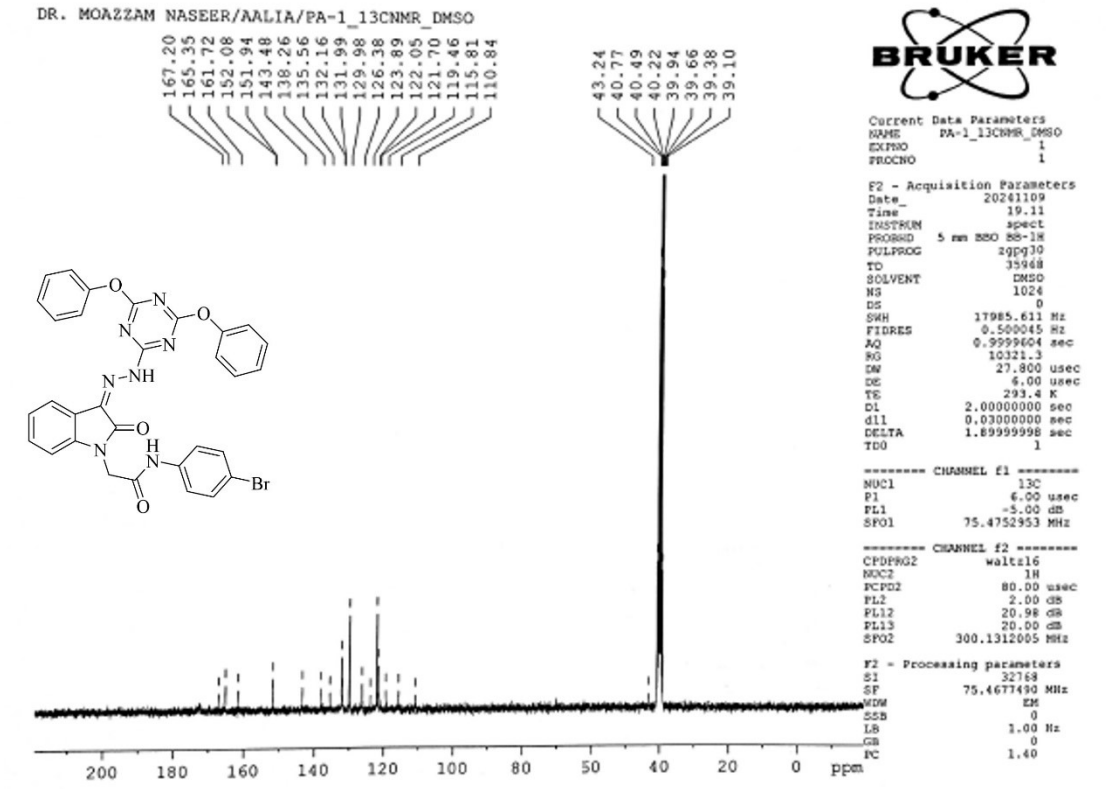
Figure S1: (A) Overlay of docked compounds 7a (yellow), 7b (orange), 7c (green), 7d (pink), 7e (cyan) and 7f (purple). (B) DNA (3EY0) validation with the docked structure (magenta) superimposed on the cocrystallized ligand (blue).

Copies of NMR Spectras

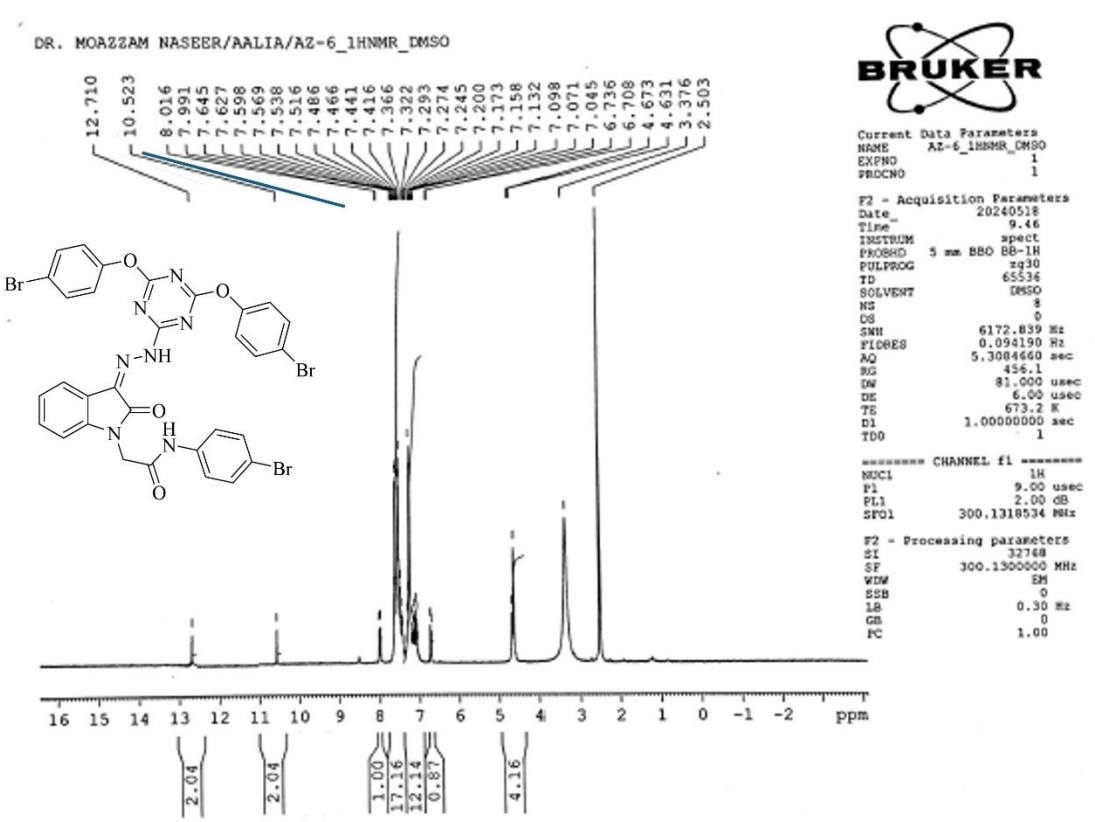
^{1}H NMR spectrum of compound 7a



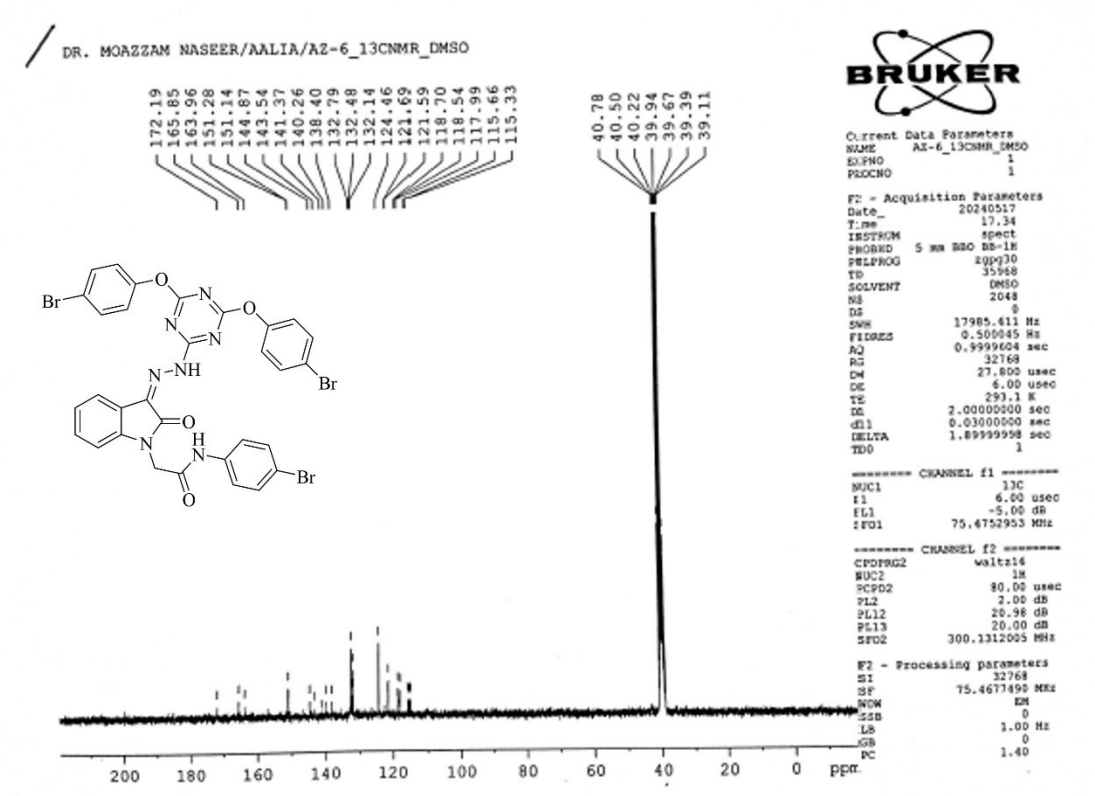
^{13}C NMR spectrum of compound 7a



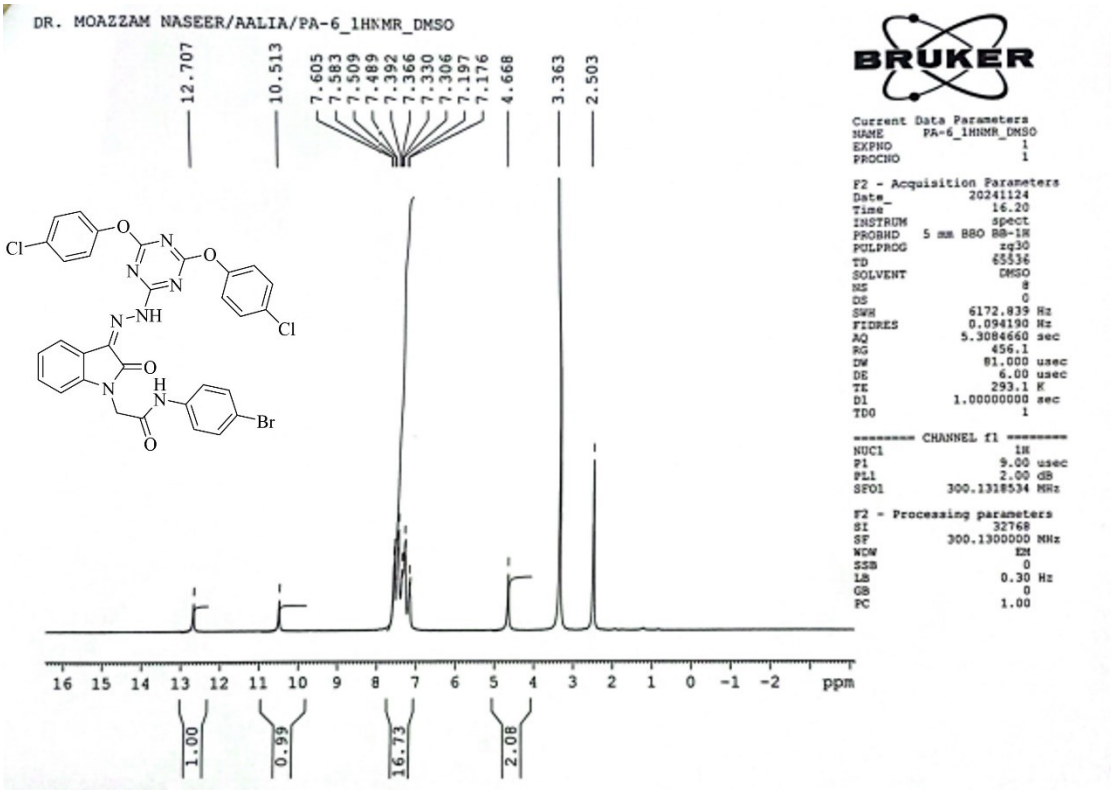
^{1}H NMR spectrum of compound 7b



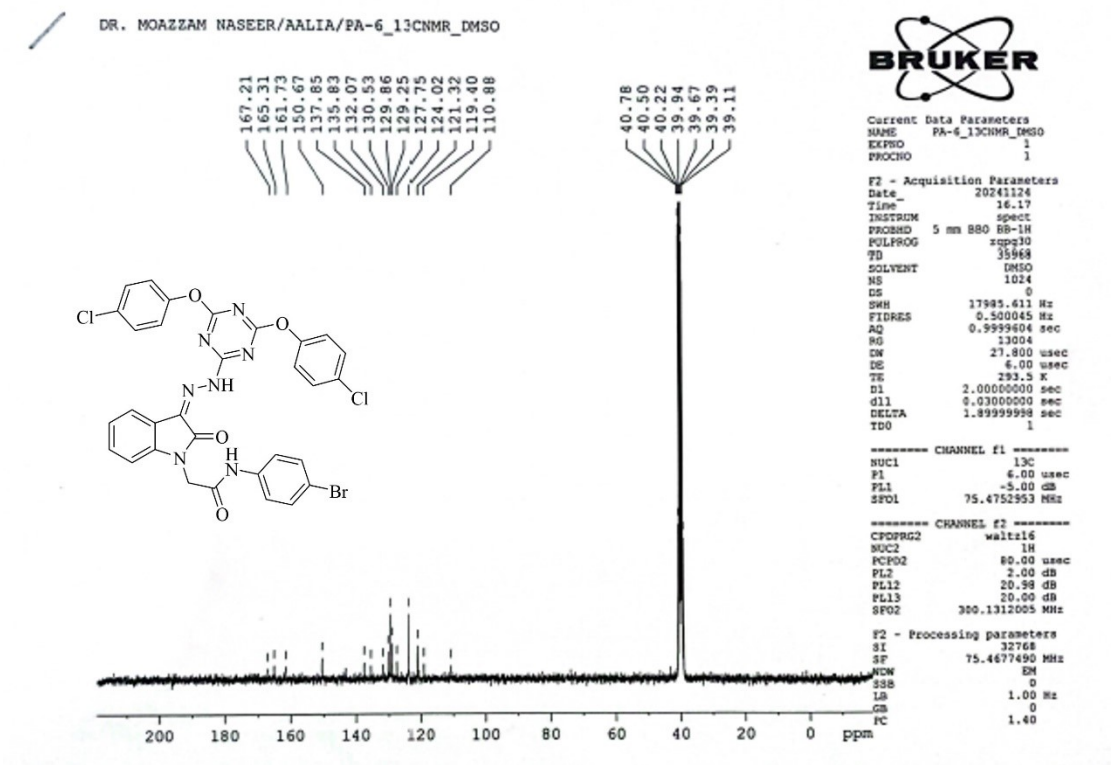
^{13}C NMR spectrum of compound 7b



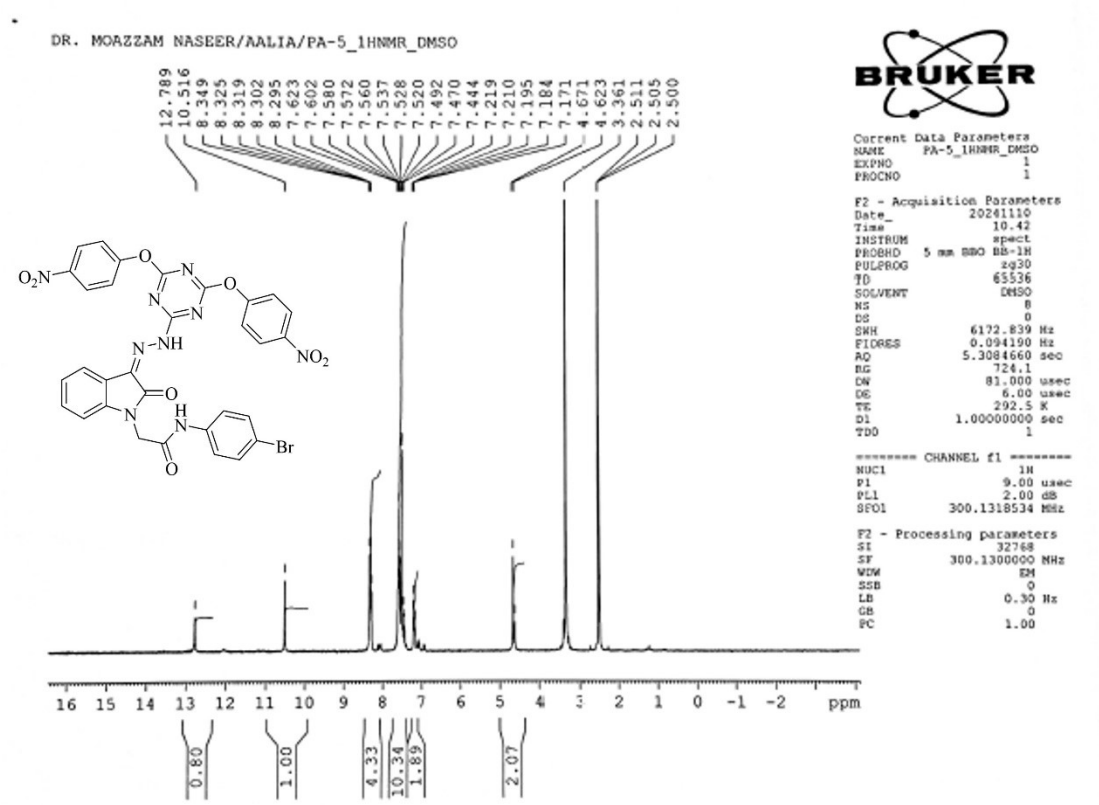
^{1}H NMR spectrum of compound 7c



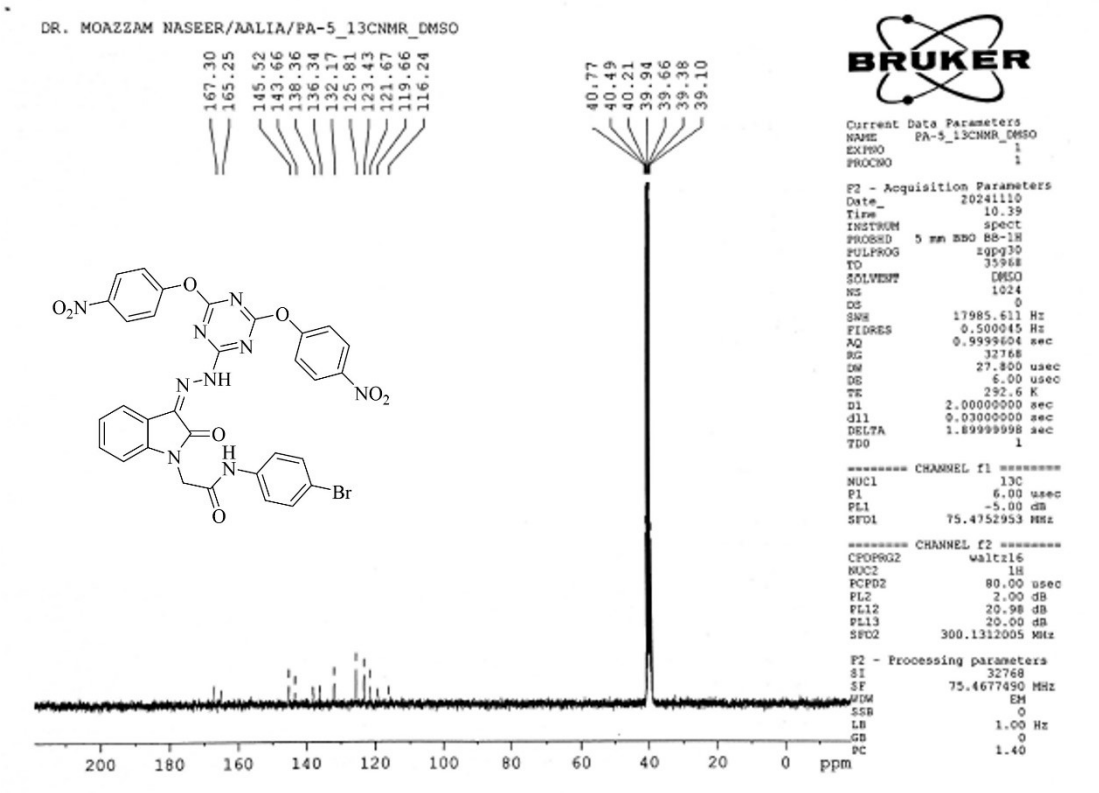
^{13}C NMR spectrum of compound 7c



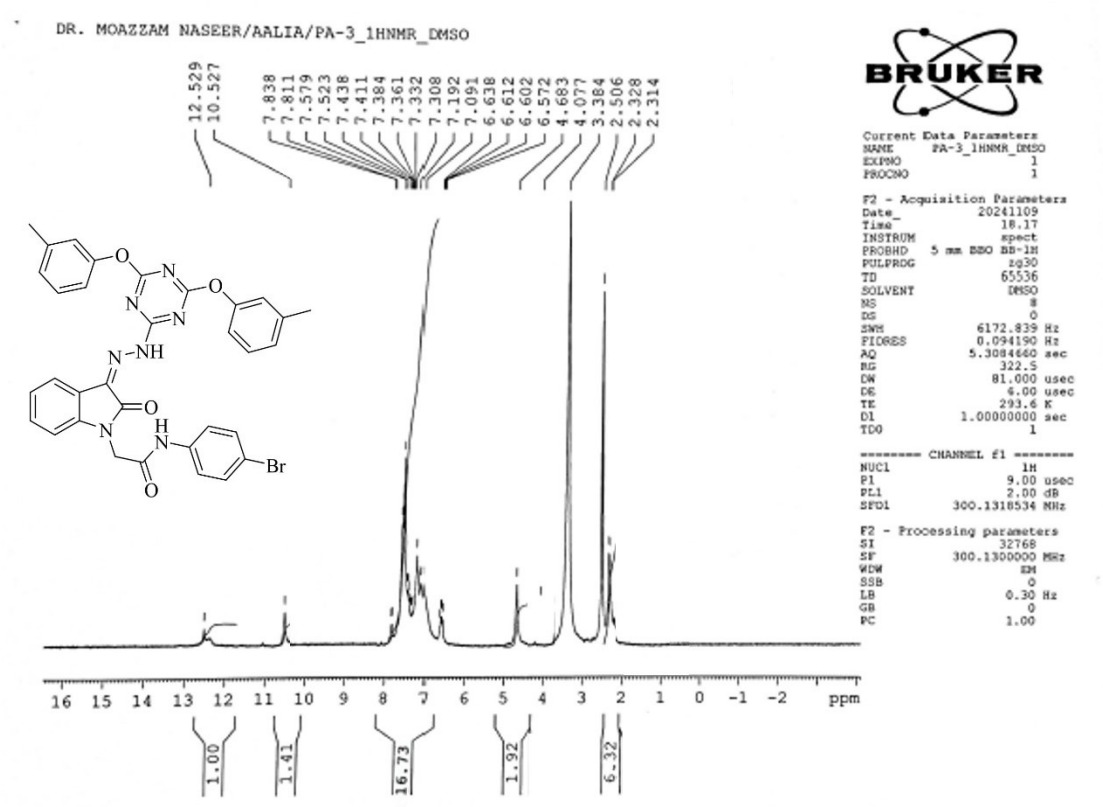
^{1}H NMR spectrum of compound 7d



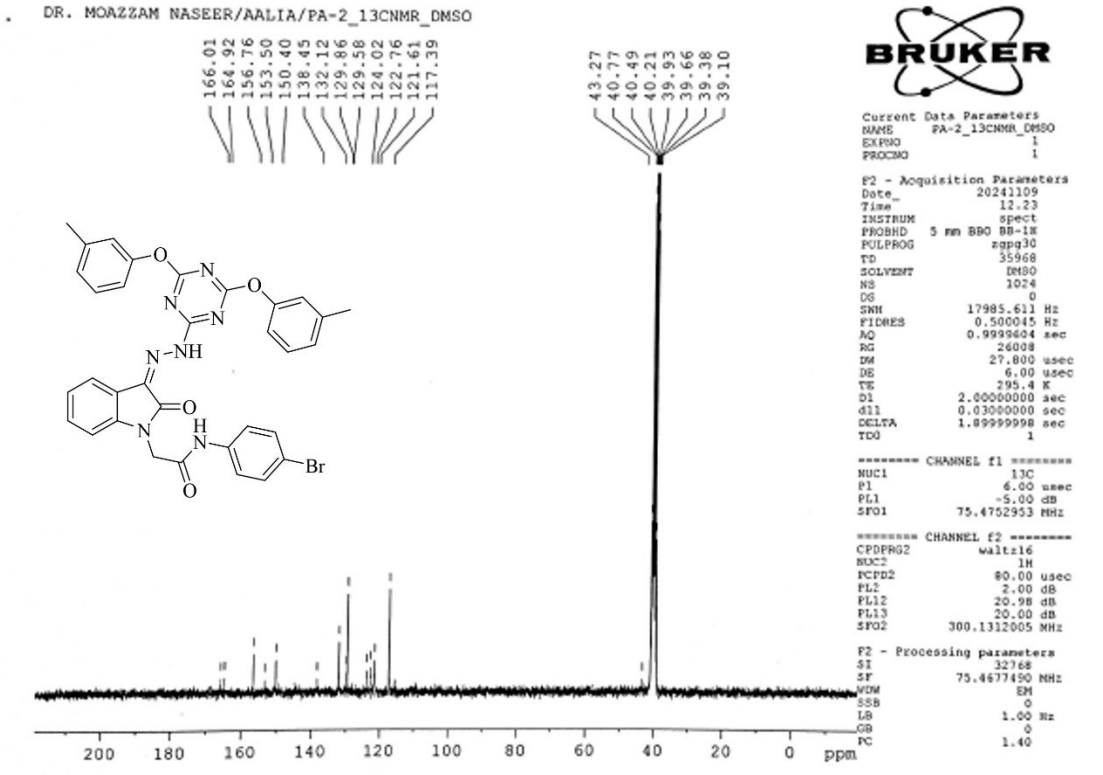
^{13}C NMR spectrum of compound 7d



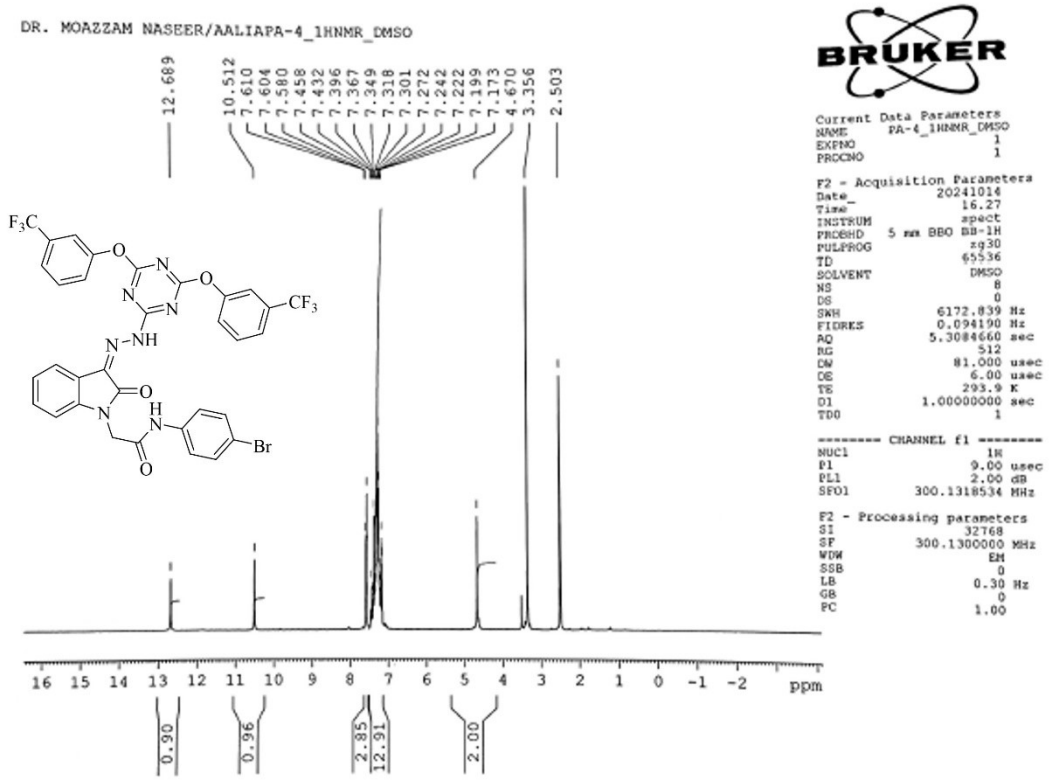
^{1}H NMR spectrum of compound 7e



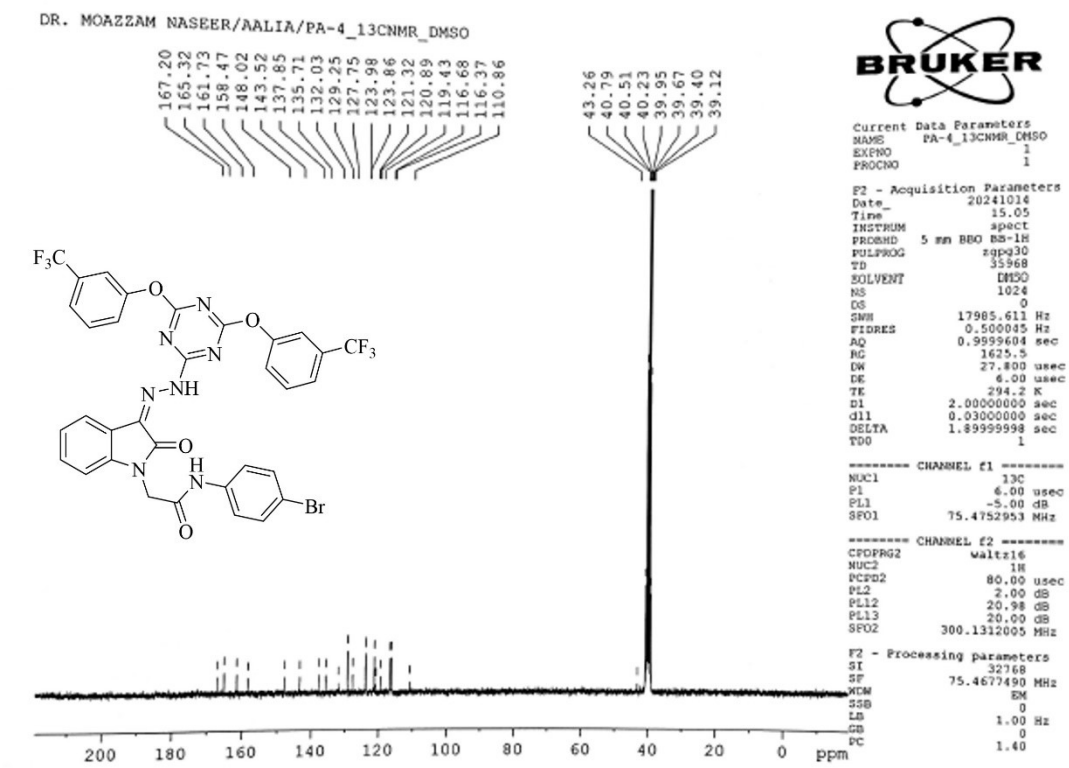
^{13}C NMR spectrum of compound 7e



^{1}H NMR spectrum of compound 7f

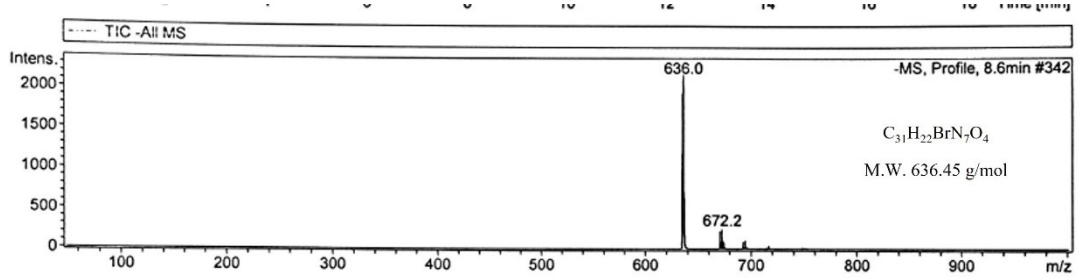


^{13}C NMR spectrum of compound 7f

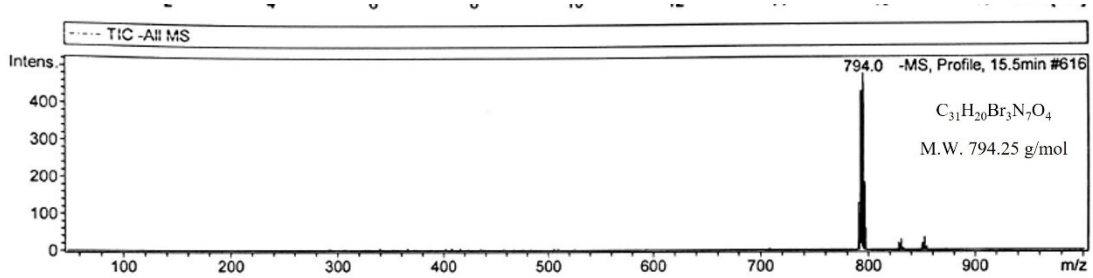


Copies of LCMS Spectras

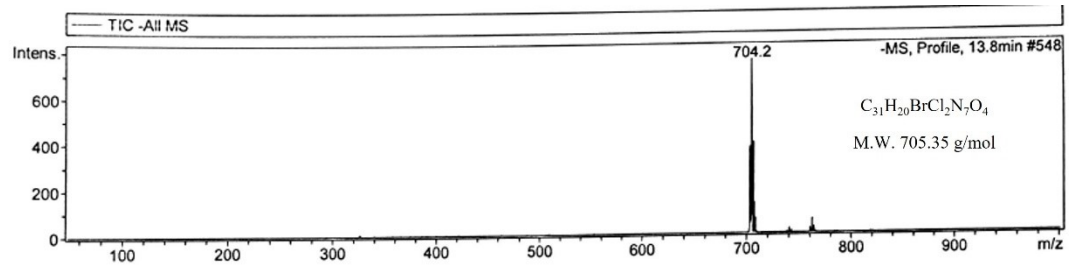
LCMS spectrum of compound 7a



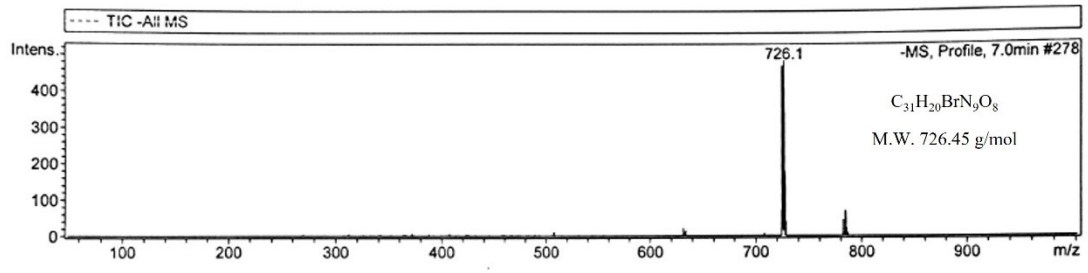
LCMS spectrum of compound 7b



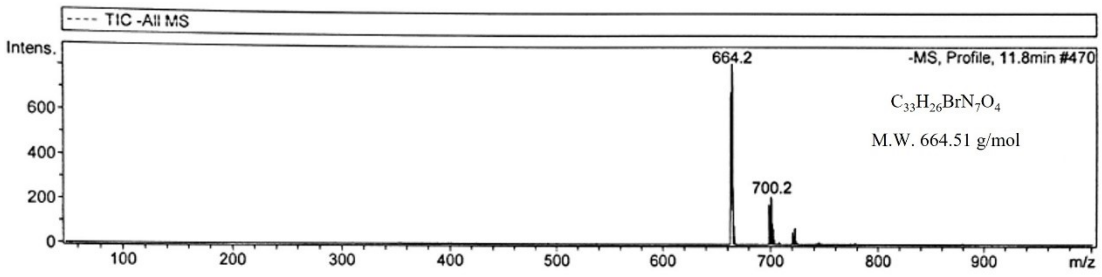
LCMS spectrum of compound 7c



LCMS spectrum of compound 7d



LCMS spectrum of compound 7e


TIC -All MS
Intens.
664.2
-MS, Profile, 11.8min #470
C33H26BrN7O4
M.W. 664.51 g/mol
700.2
600
400
200
0
100
200
300
400
500
600
700
800
900
m/z