Supplementary Data

N-Arylation of protected & unprotected 5-bromo 2-amino benzoimidazole as Organic material: Non-linear optical (NLO) properties and structural feature determination through computational approach

Mubeen Mumtaz [1], Nasir Rasool [1,*], Gulraiz Ahmad [1], Naveen Kosar [2,3], Umer Rashid [4,*]

[1] Department of Chemistry, Government College University, Faisalabad 38000, Pakistan

[2] Department of Chemistry, University of Management and Technology (UMT), C11, Johar Town Lahore, Pakistan

[3] Department of Chemistry, COMSATS University Islamabad, Abbottabad Campus, Abbottabad, Pakistan

[4] Institute of Advanced Technology, University Putra Malaysia, 43400 UPM Serdang, Selangor, Malaysia

* Corresponding authors E-mail addresses:

Nasir Rasool Email: nasirrasool@gcuf.edu.pk

Umer Rashid Email:umer.rashid@upm.edu.my

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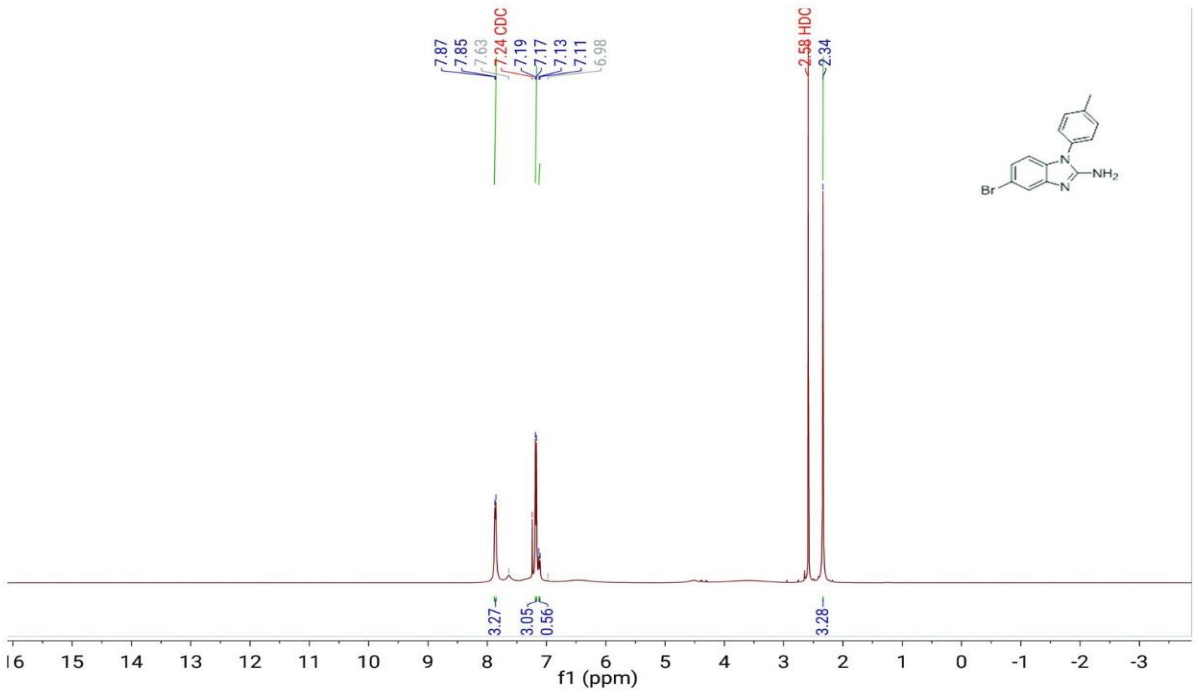

Figure S1. ^{1}H NMR (400 MHz, $CDCl_3$) of compound **1a**.

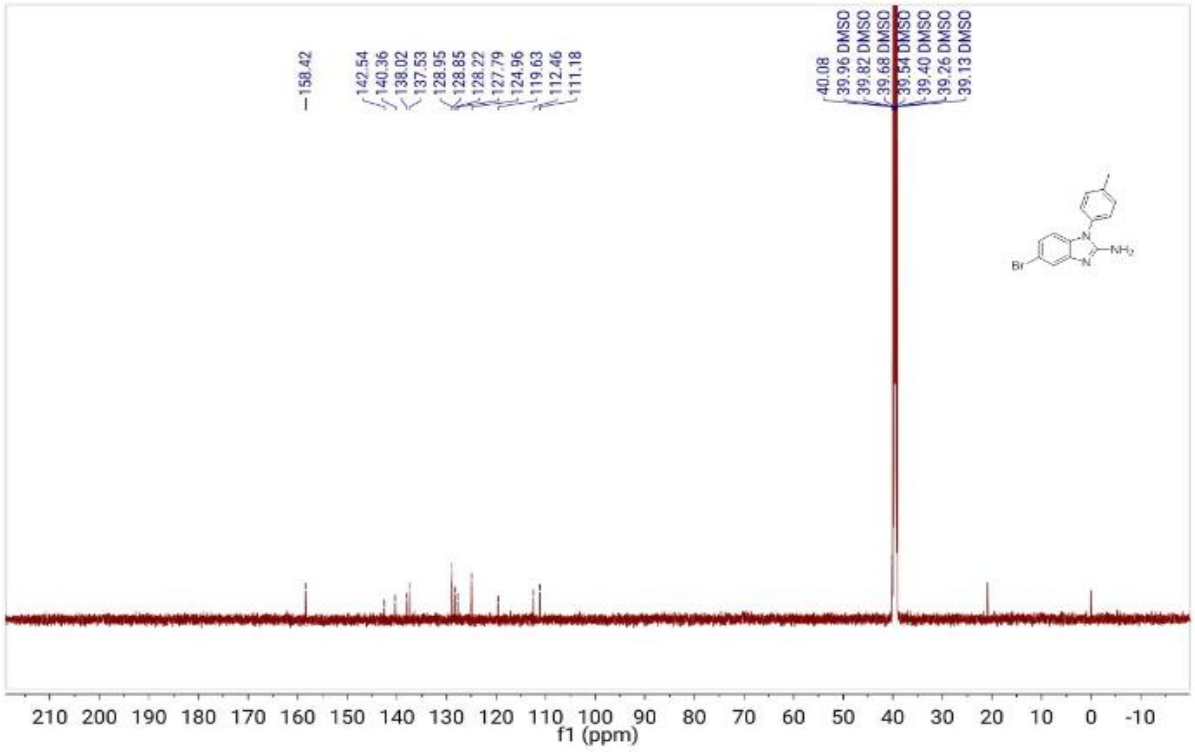

Figure S2. ^{13}C NMR (125 MHz, DMSO-d_6) of compound **1a**.

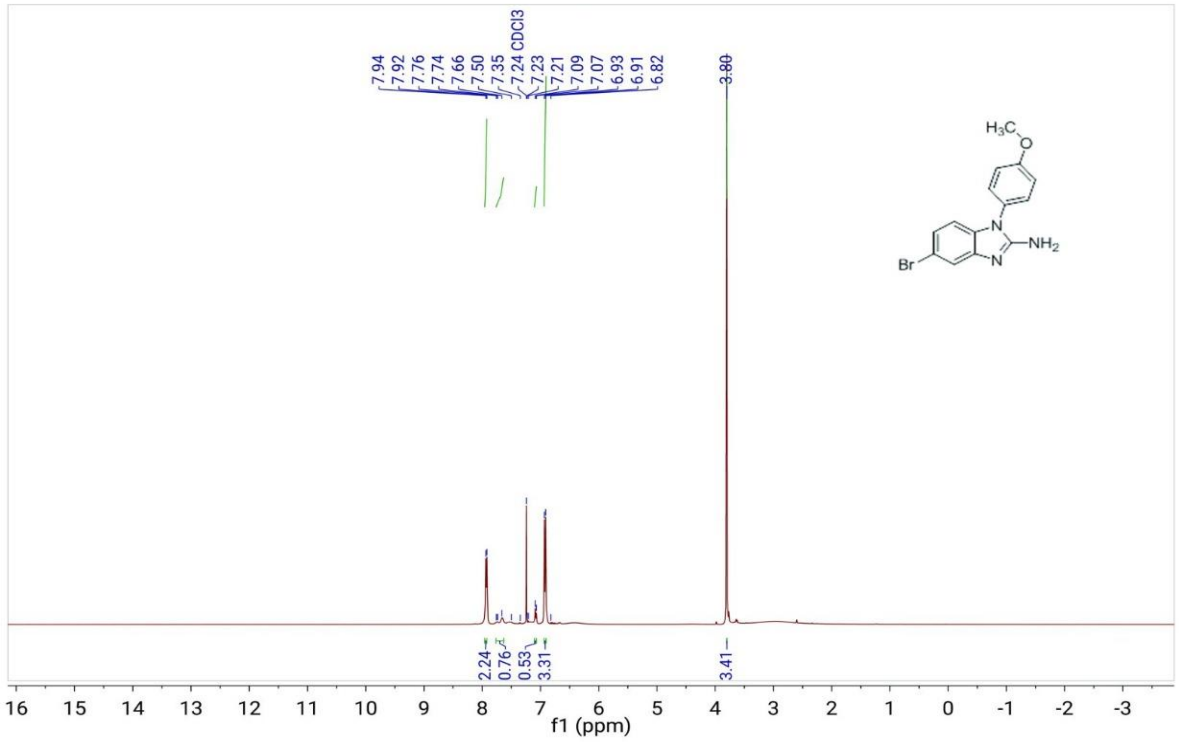

Figure S3. ^{1}H NMR (400 MHz, $CDCl_3$) of compound **1b**.

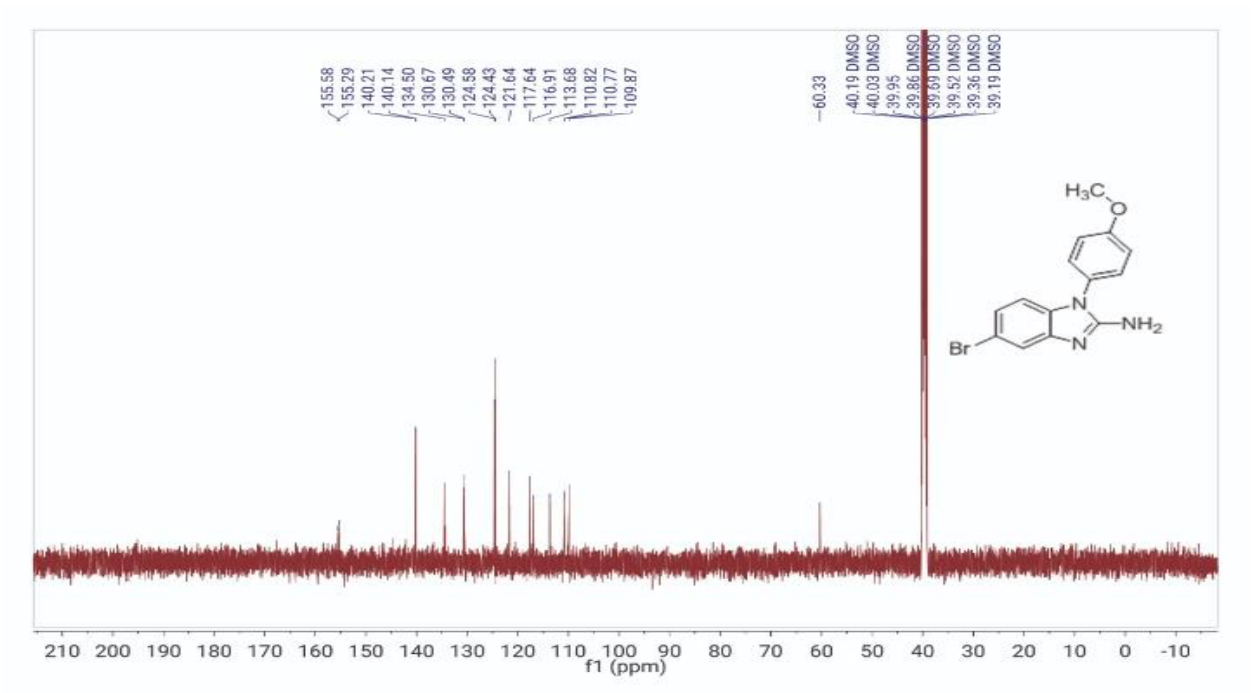

Figure S4. ^{13}C NMR (125 MHz, DMSO-d_6) of compound **1b**.

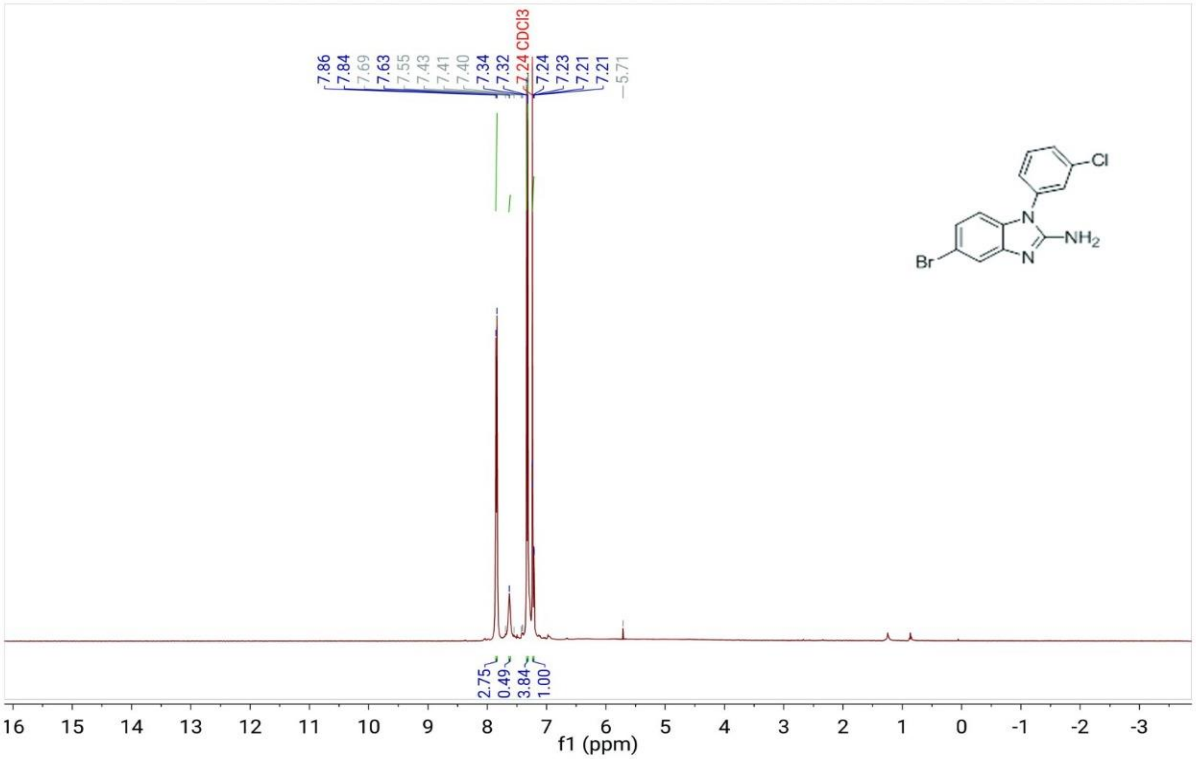

Figure S5. ^{1}H NMR (400 MHz, $CDCl_3$) of compound **1c**.

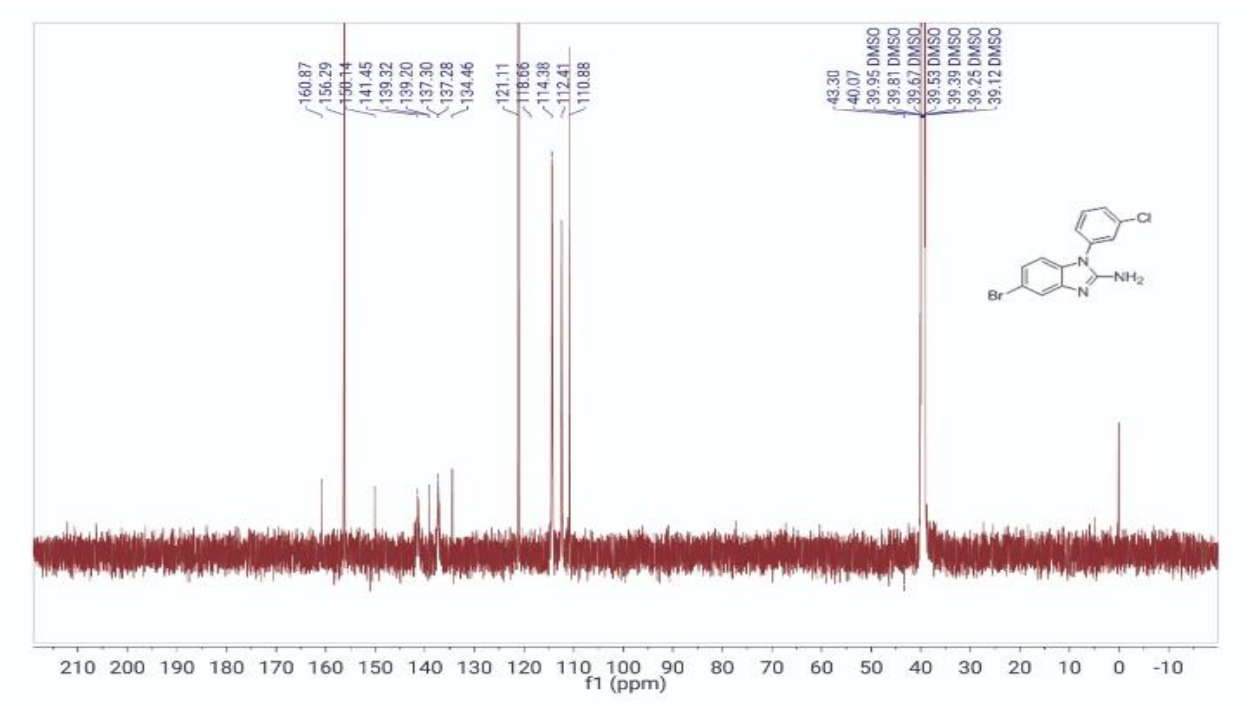

Figure S6. ^{13}C NMR (125 MHz, DMSO-d_6) of compound **1c**.

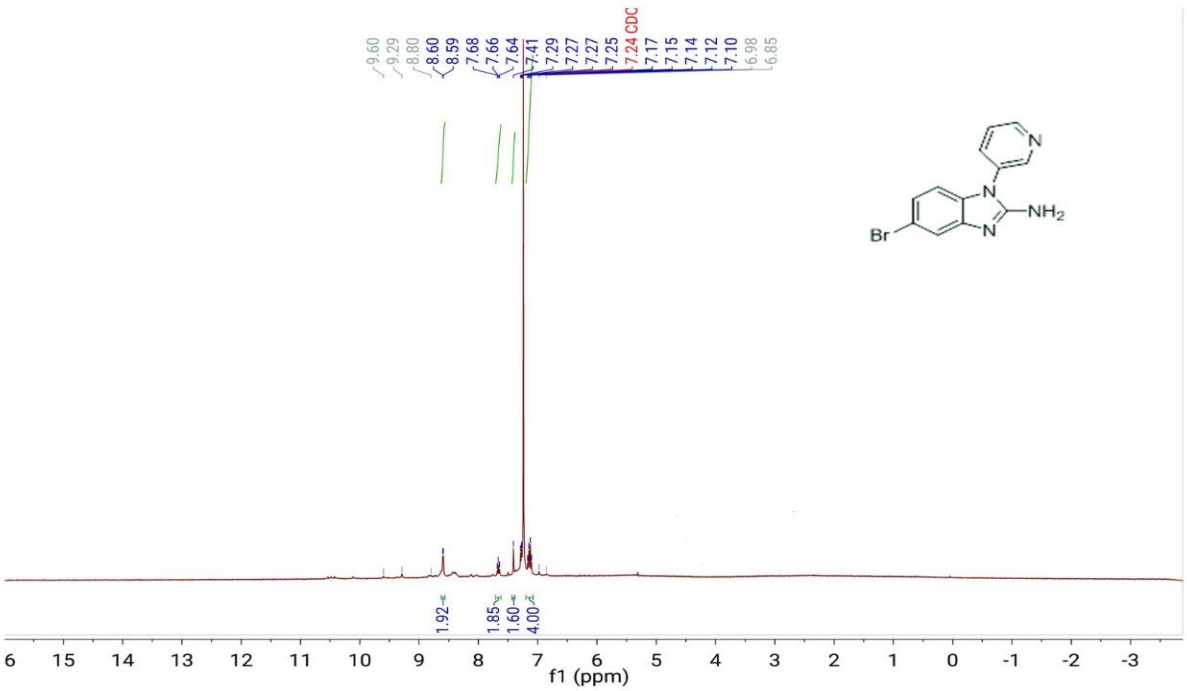

Figure S7. ^{1}H NMR (400 MHz, $CDCl_3$) of compound **1d**.

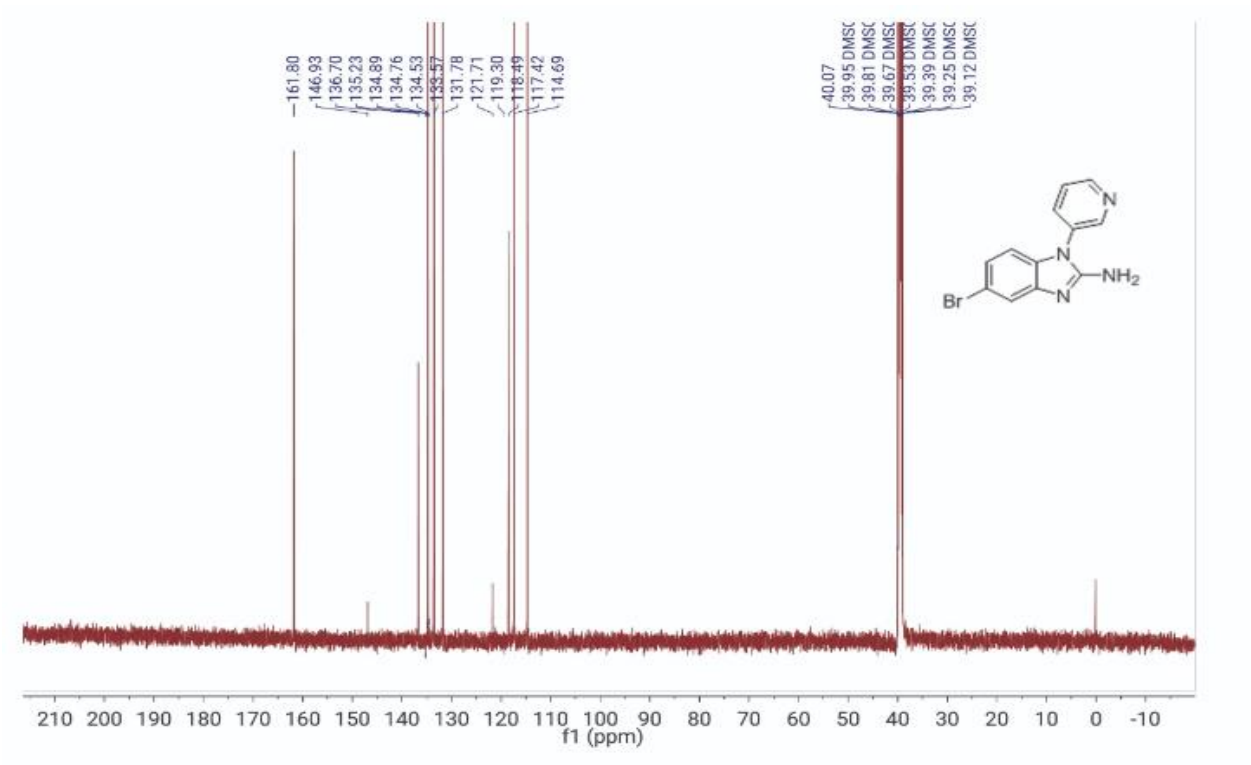

Figure S8. ^{13}C NMR (125 MHz, DMSO-d_6) of compound **1d**.

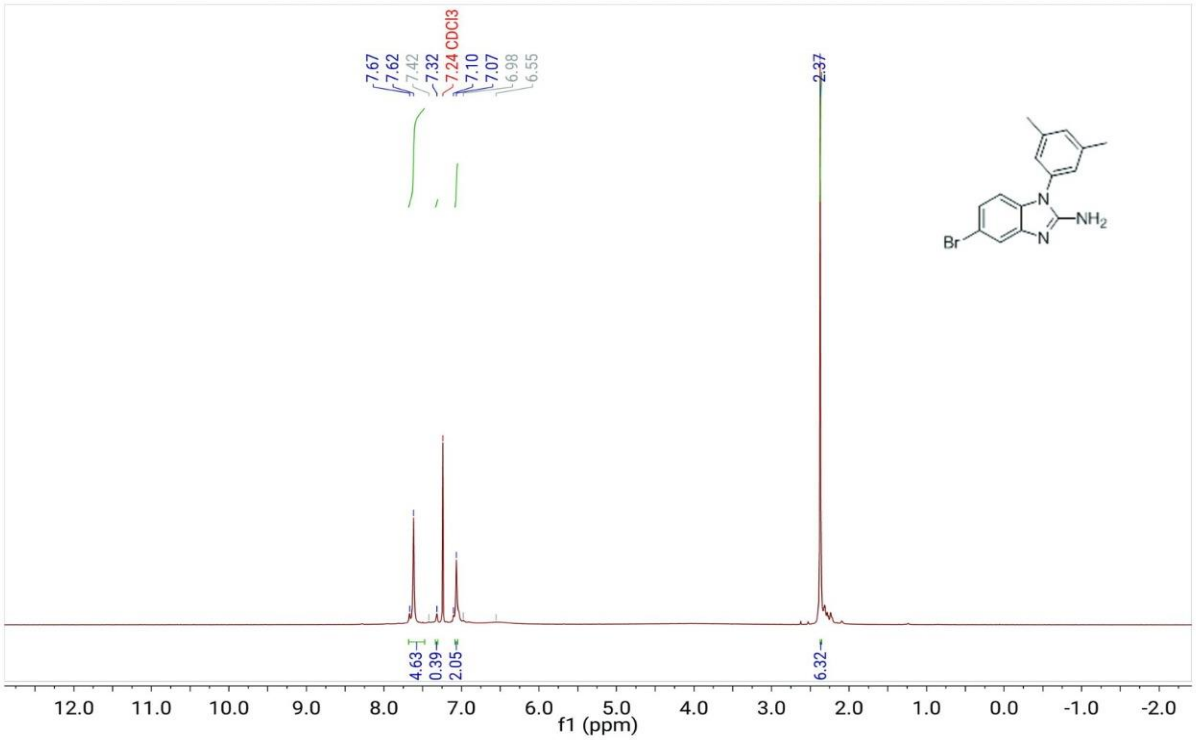

Figure S9. ^{1}H NMR (400 MHz, $CDCl_3$) of compound **1e**.

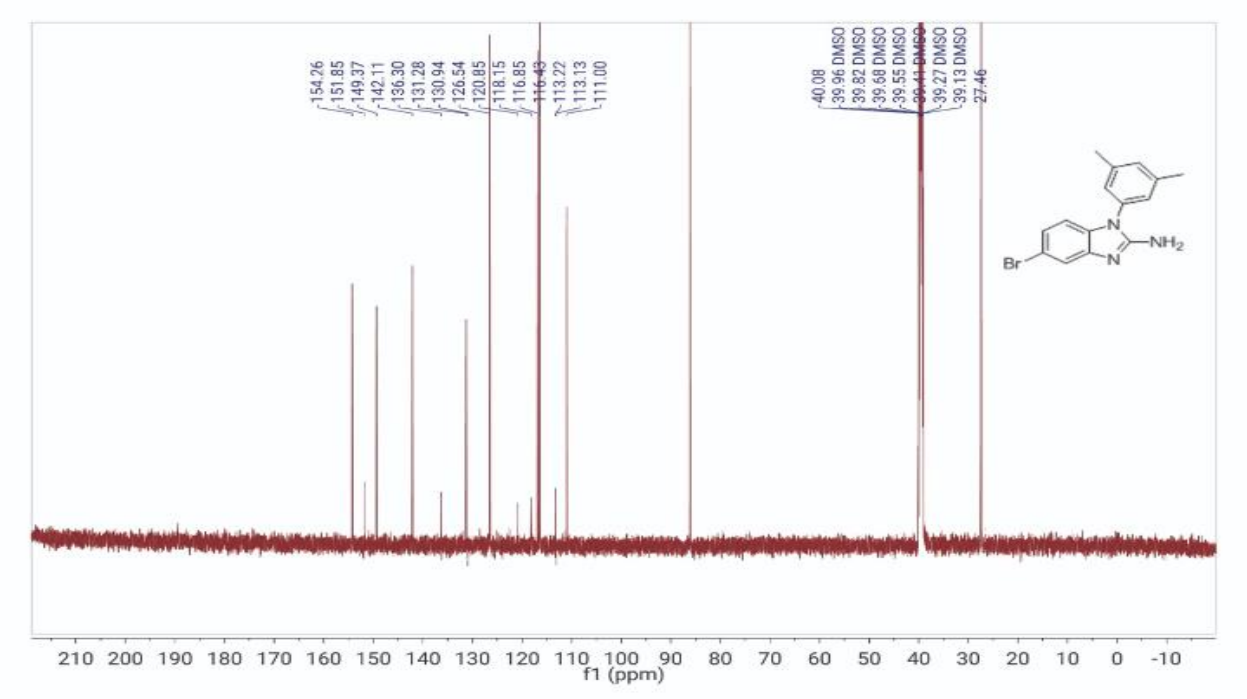

Figure S10. ^{13}C NMR (125 MHz, DMSO-d_6) of compound **1e**.

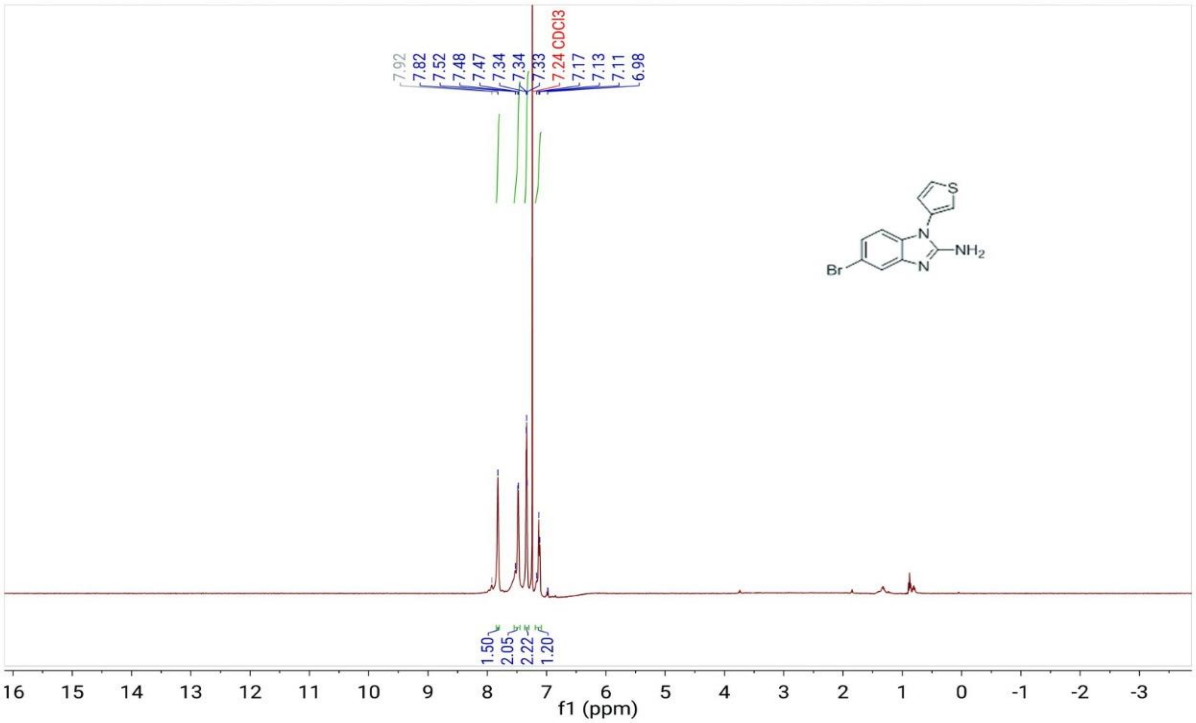

Figure S11. ^{1}H NMR (400 MHz, $CDCl_3$) of compound **1f**.

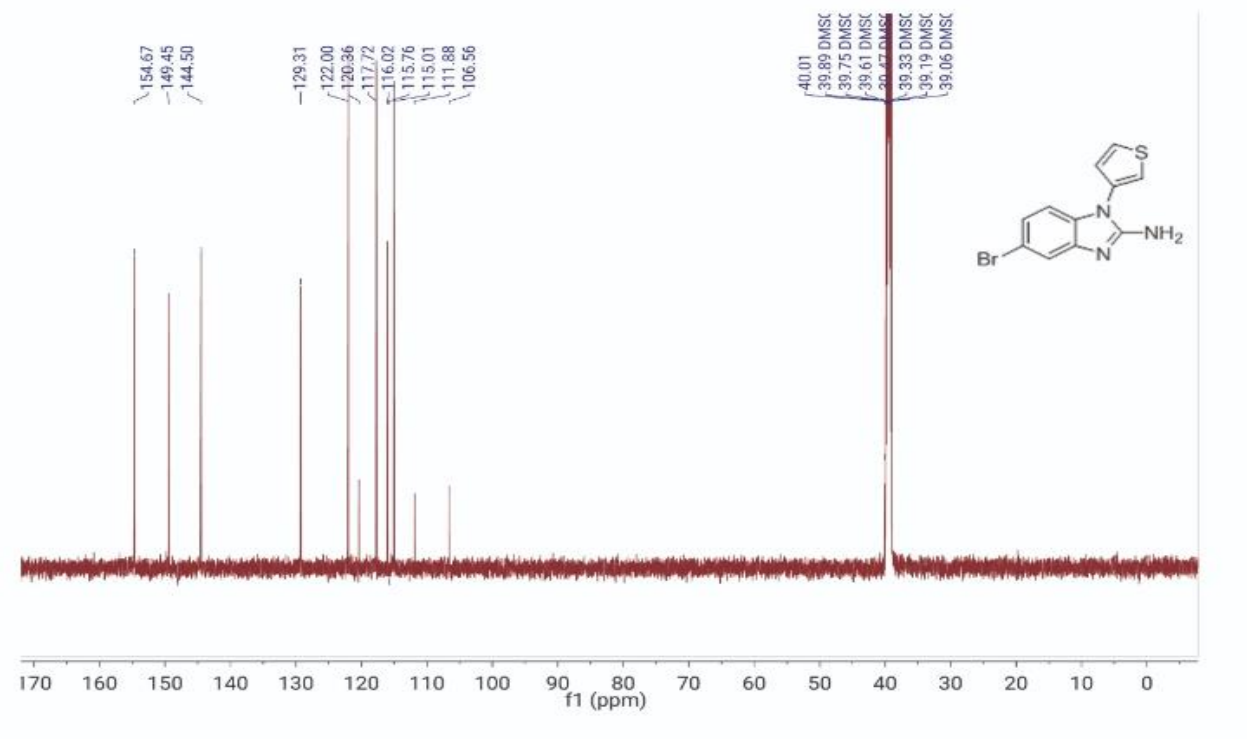

Figure S12. ^{13}C NMR (125 MHz, DMSO-d_6) of compound **1f**.

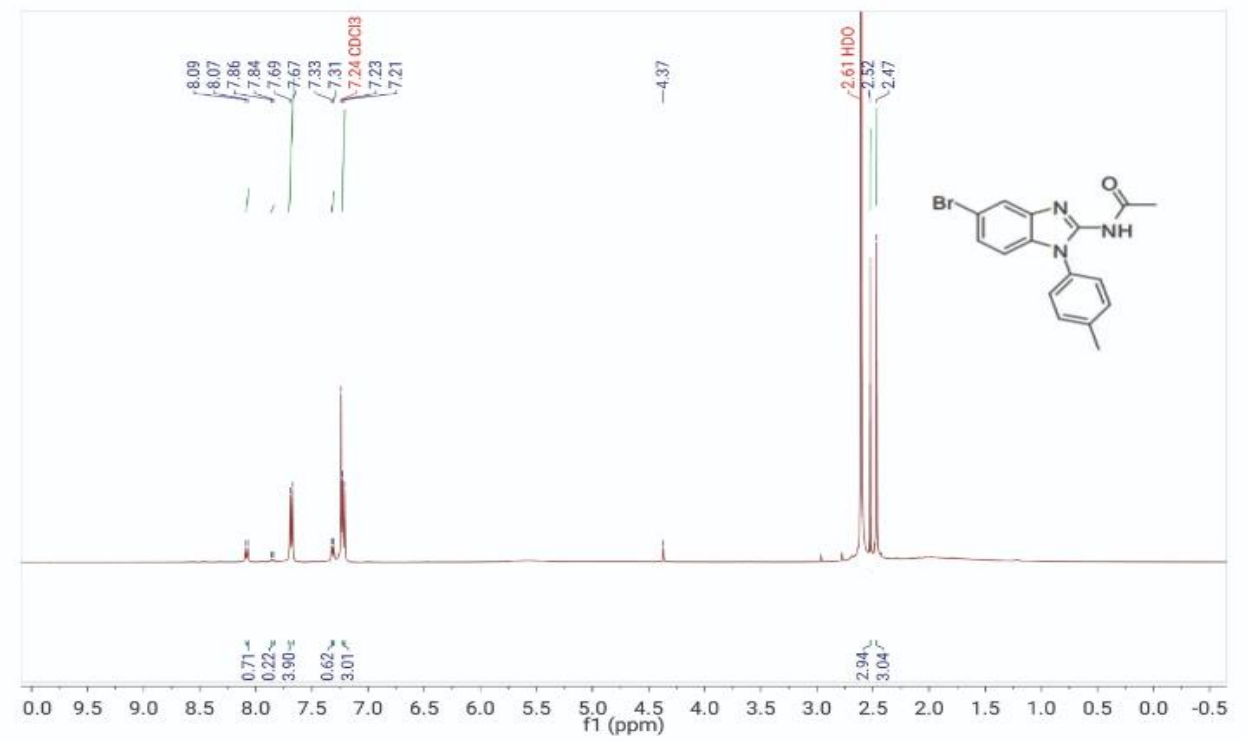

Figure S13. ^{1}H NMR (400 MHz, $CDCl_3$) of compound **2a**.

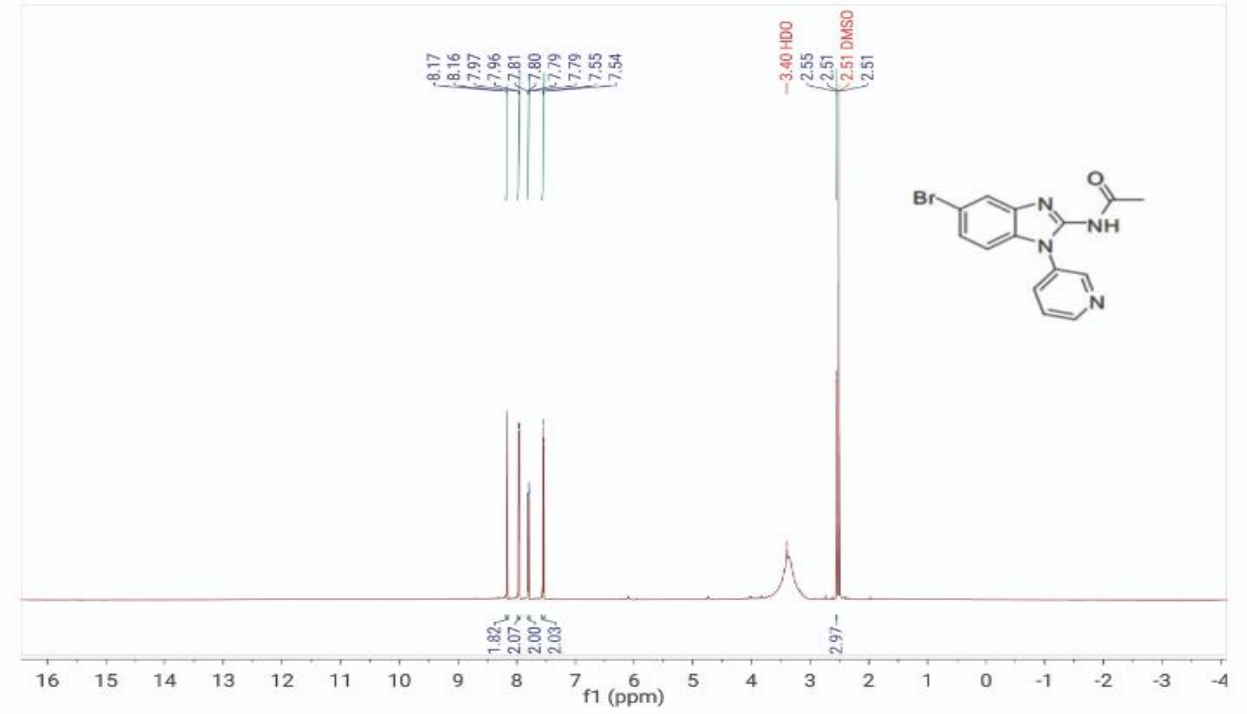

Figure S14. ^{1}H NMR (400 MHz, DMSO-d_6) of compound **2d**.

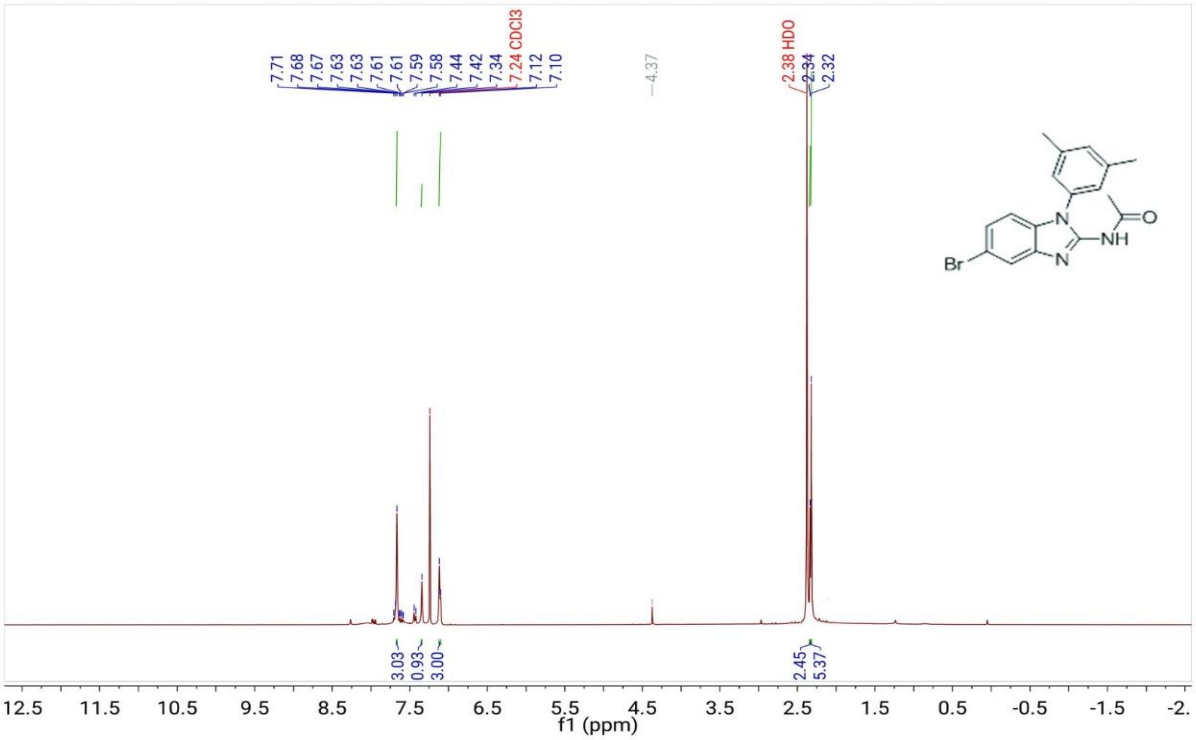

Figure S15. ^{1}H NMR (400 MHz, $CDCl_3$) of compound **2e**.

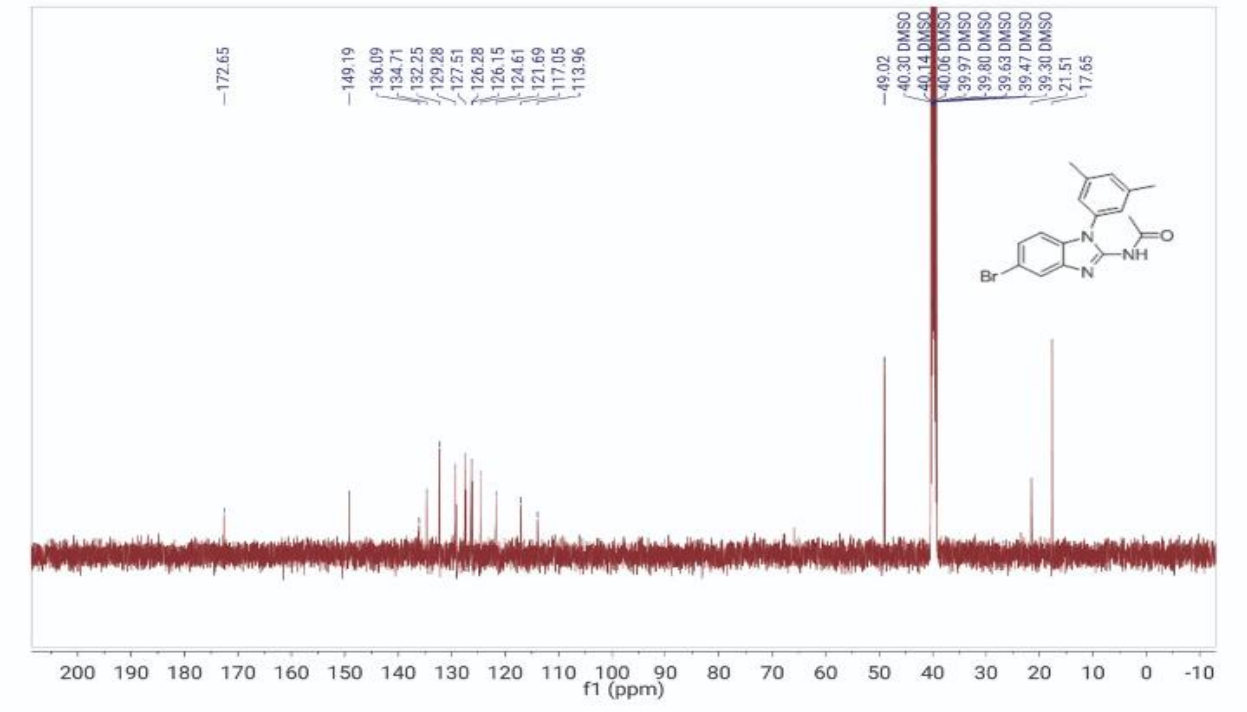

Figure S16. ^{13}C NMR (125 MHz, DMSO-d_6) of compound **2e**.

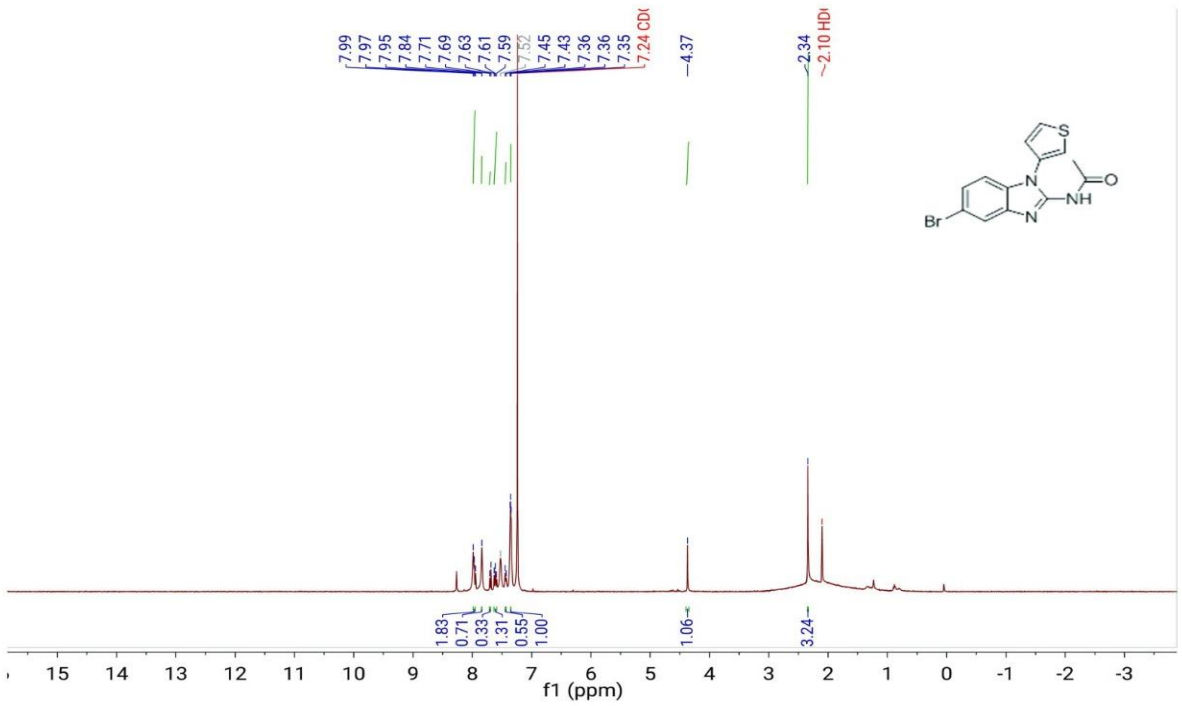

Figure S17. ^{1}H NMR (400 MHz, $CDCl_3$) of compound **2f**.

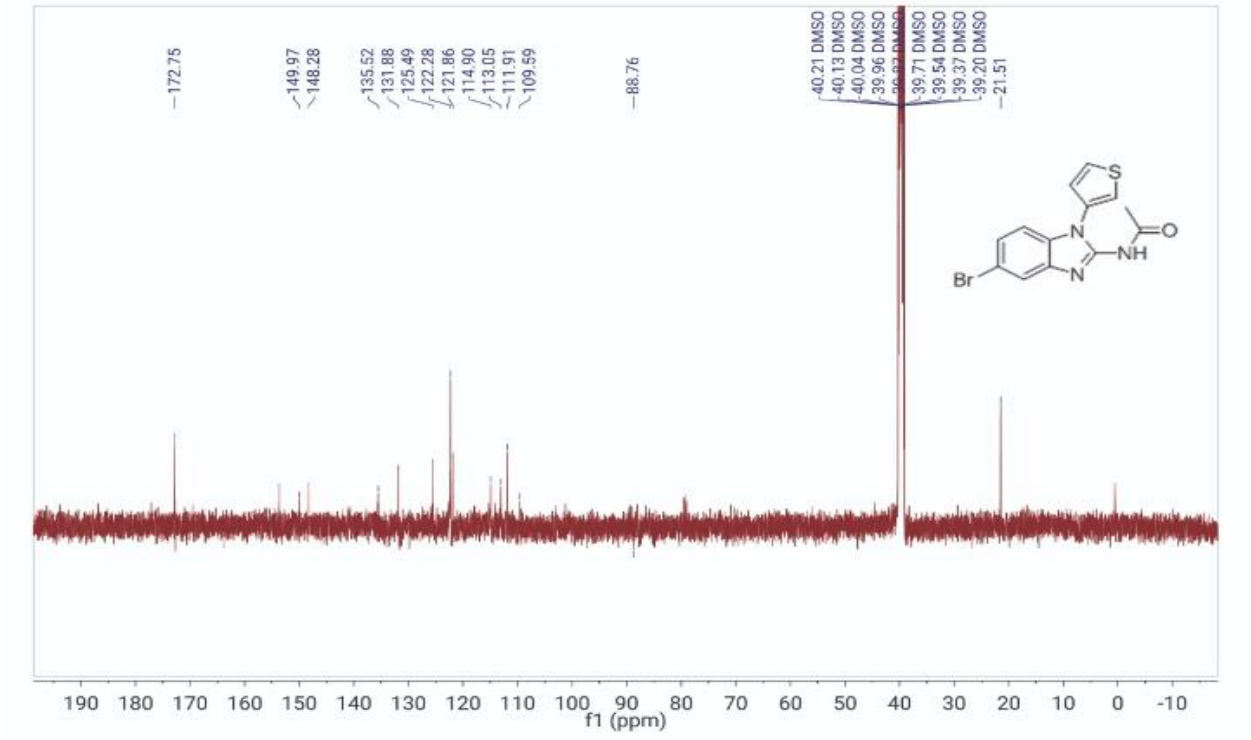

Figure S18. ^{13}C NMR (125 MHz, DMSO-d_6) of compound **24**.

Table S1. Polarizability (α_o, in au) and hyperpolarizability (β_o, in au) of compounds**1a-1f** and **2a-2f** at LC-BLYP, and ωB97XD.

Compounds	LC-BLYP		ωB97XD	
	α_o	β_o	α_o	β_o
1a	220	3.69×10^{-30}	227	4.40×10^{-30}
1b	208	5.63×10^{-30}	215	5.31×10^{-30}
1c	203	3.83×10^{-30}	210	3.53×10^{-30}
1d	183	3.89×10^{-30}	189	4.17×10^{-30}
1e	214	3.82×10^{-30}	221	3.70×10^{-30}
1f	182	3.98×10^{-30}	188	3.99×10^{-30}
2a	228	1.81×10^{-30}	235	1.93×10^{-30}
2b	232	3.82×10^{-30}	239	3.44×10^{-30}
2c	228	1.89×10^{-30}	236	1.90×10^{-30}
2d	208	1.80×10^{-30}	215	2.27×10^{-30}
2e	239	1.73×10^{-30}	246	1.95×10^{-30}
2f	208	1.98×10^{-30}	214	2.44×10^{-30}