Supporting Information

Org. Commun. **16:4 (2023) 175-186**

Water extract of onion: chemoselective synthesis of 2-substituted benzimidazole derivatives

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S1: Preparation and Standardization of Onion Extract[1]

Two gram of cut pieces of onion were taken into 100 mL clean beaker. To this 10 mL of Milli-Q water was added and stirred for half an hour. The stirred suspension was allowed to stand for 10 min. followed by filtration. The filtrate was used as a catalyst and stored in refrigerator. The strength of the onion extract is 0.0034 N, which is determined by using acid-base titrations and the pH of the catalyst is 3.6. The strength and pH of the catalyst were examined periodically over the month and found to be consistent.

The main constituent of onion is 1-propenylcysteine sulfoxide (isoalliin, an alkylated cysteine sulfoxide) (Figure 1), when cutting the onion, isoalliin undergoes a series of rapid reactions. The enzyme Alliinase, catalyzes the conversion of (E)-(prop-1-en-1-ylsulfinyl)alanine to (E)-1-propenesulfenic acid, which is then rearranged to the volatile and highly reactive lachrymatory factor (LF) (Z)- propanethial S-oxide,[65,66] which on treatment with water to produce acetaldehyde, sulphuric acid and hydrogen sulfide.[67,68]

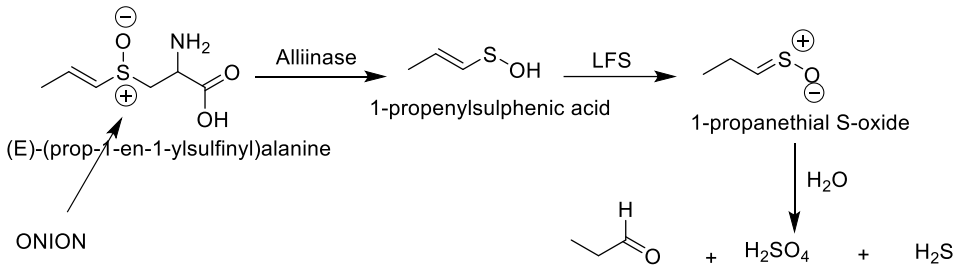

Figure S1: Metabolic pathway of onion

References

[1] Prabakaran, K.; Sivakumar, M.; Perumal, M. S. A Simple, Efficient Green Protocol for the Synthesis of β-Enaminone and Enamino Ester Derivatives by Using Onion Extract as Green Catalyst. *ChemistrySelect.* **2017**, *2*, 2363-2372.

[2] Thomson, S. J.; Rippon, P.; Butts, C.; Olsen, S.; Shaw, M.; Joyce, N. I.; Eady, C. C. Inhibition of platelet activation by lachrymatory factor synthase (LFS)-silenced (tearless) onion juice. *J. Agric. Food. Chem*. **2013**, *61*, 10574-10581.

[3] Imai, S.; Tsuge, N.; Tomotake, M.; Nagatome, Y.; Sawada, H.; Nagata, T.; Kumagai, H. An onion enzyme that makes the eyes water. *Nature* **2002**, *419*, 685-985.

[4] Paolo, A.; Angelo, A. Can onions be engineered for not tearing? *IUBMB Life*, **2003**, *55*, 49-50.

[5] Eric B. The chemistry of garlic and onions. *Sci Am*, **1985**, 252, 114-118.

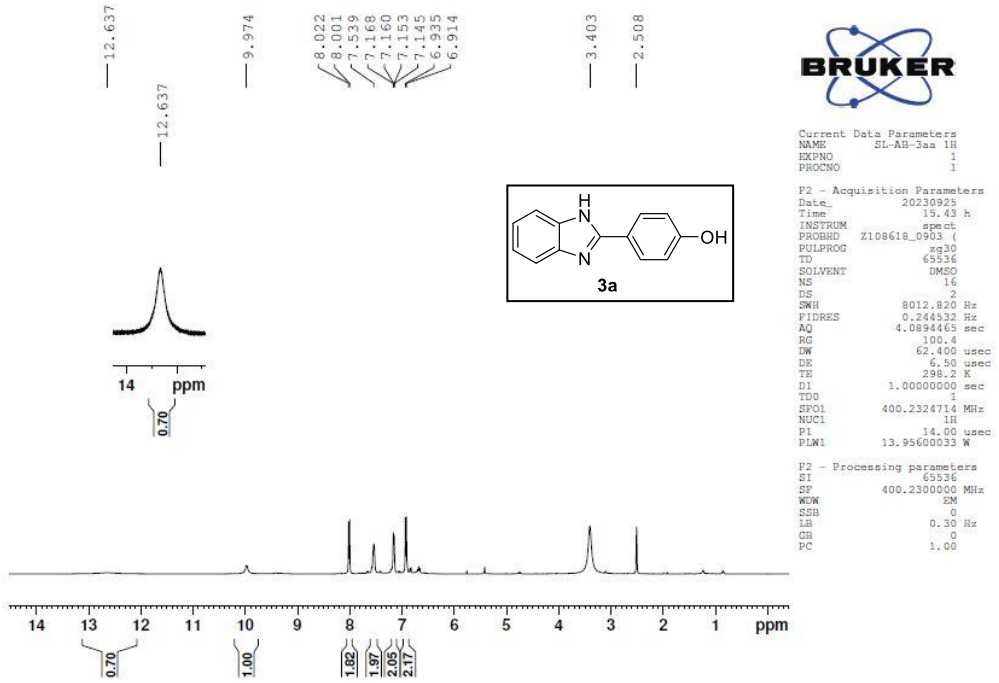

Figure S2: ^{1}H NMR (400 MHz, DMSO-d_6) Spectrum of compound **3a**

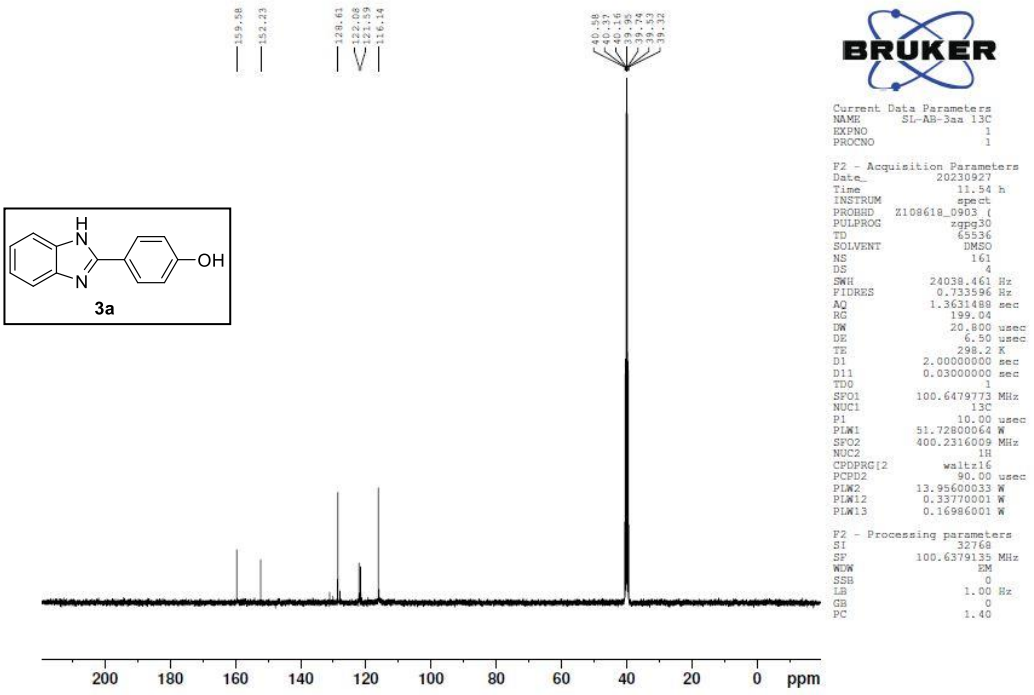

Figure S3: ^{13}C NMR (100 MHz, DMSO-d_6) Spectrum of compound **3a**

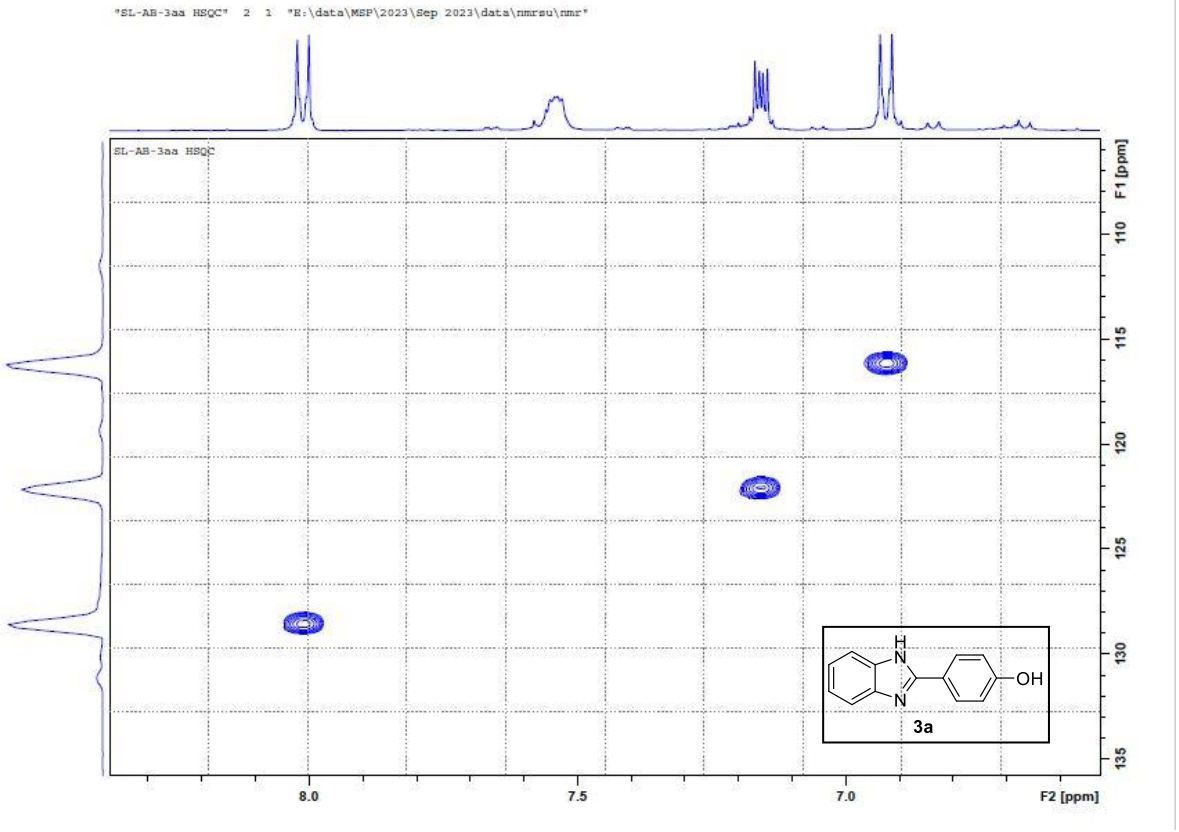

Figure S4: HSQC Spectrum of compound **3a**

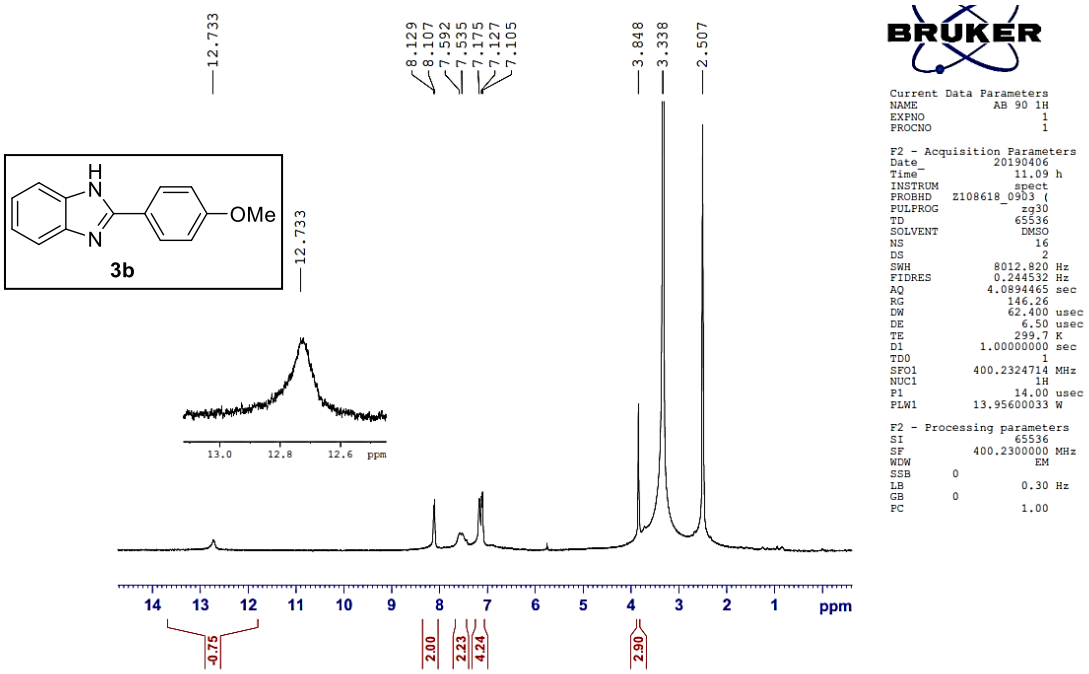

Figure S5: ^{1}H NMR (400 MHz, DMSO-d_6) Spectrum of compound **3b**

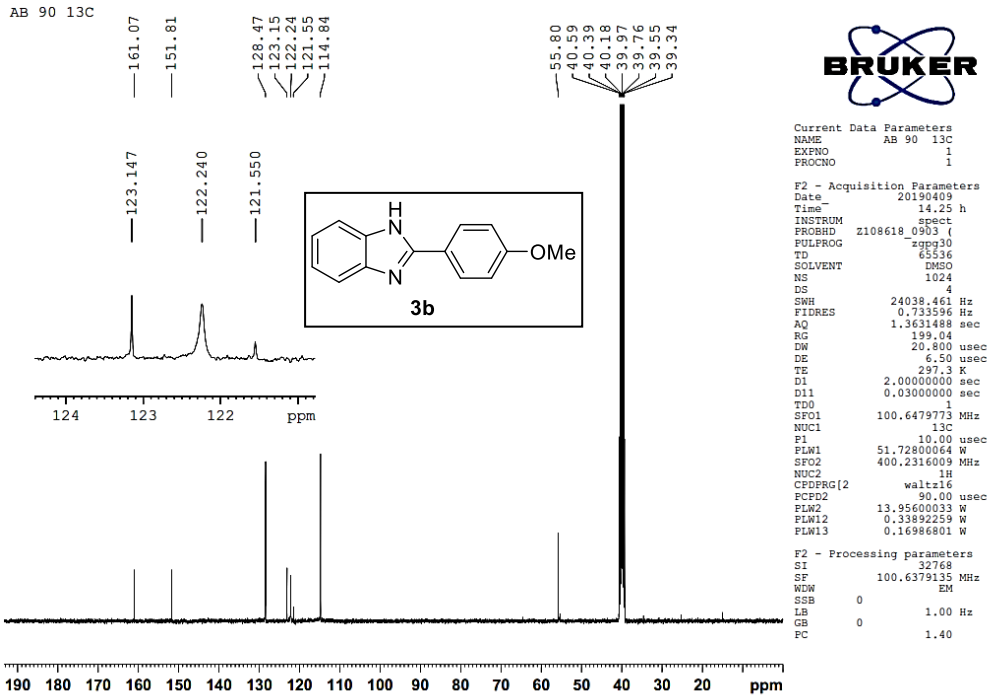

Figure S6: ^{13}C NMR (100 MHz, DMSO-d_6) Spectrum of compound **3b**

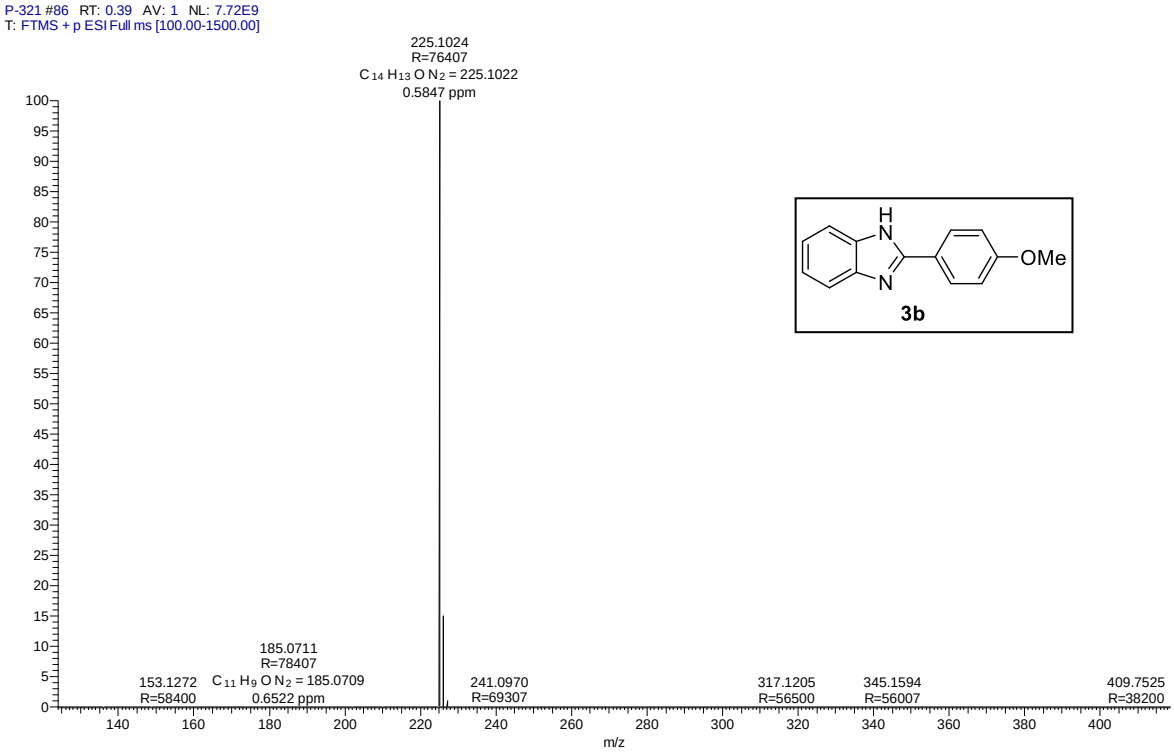

Figure S7: Mass Spectrum of compound **3b**

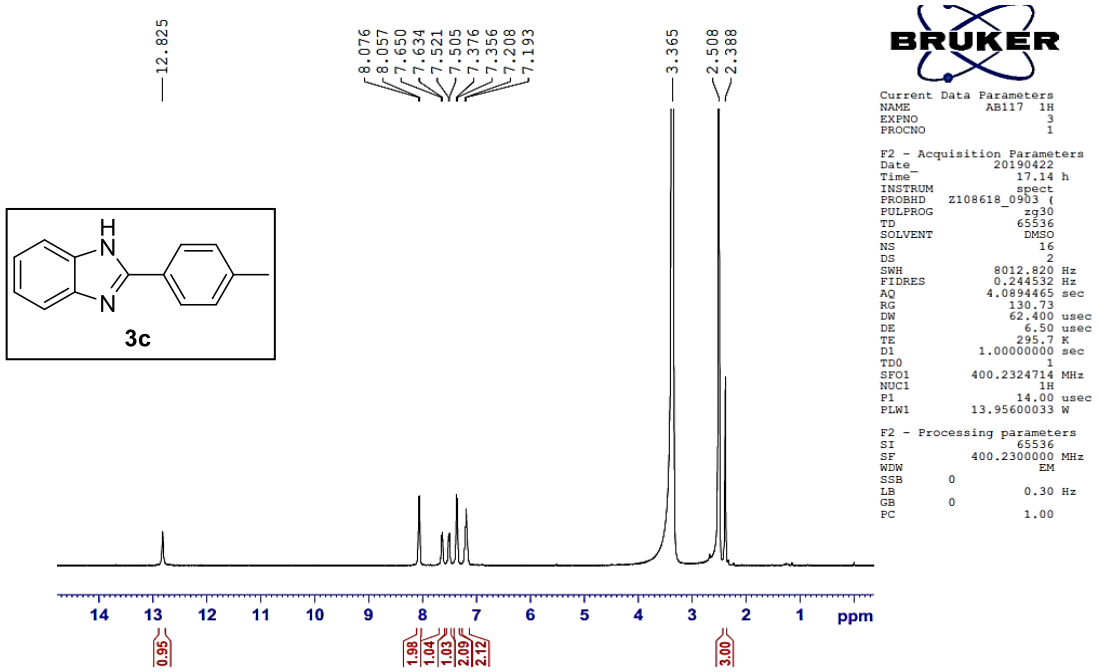

Figure S8: ^{1}H NMR (400 MHz, DMSO-d_6) Spectrum of compound **3c**

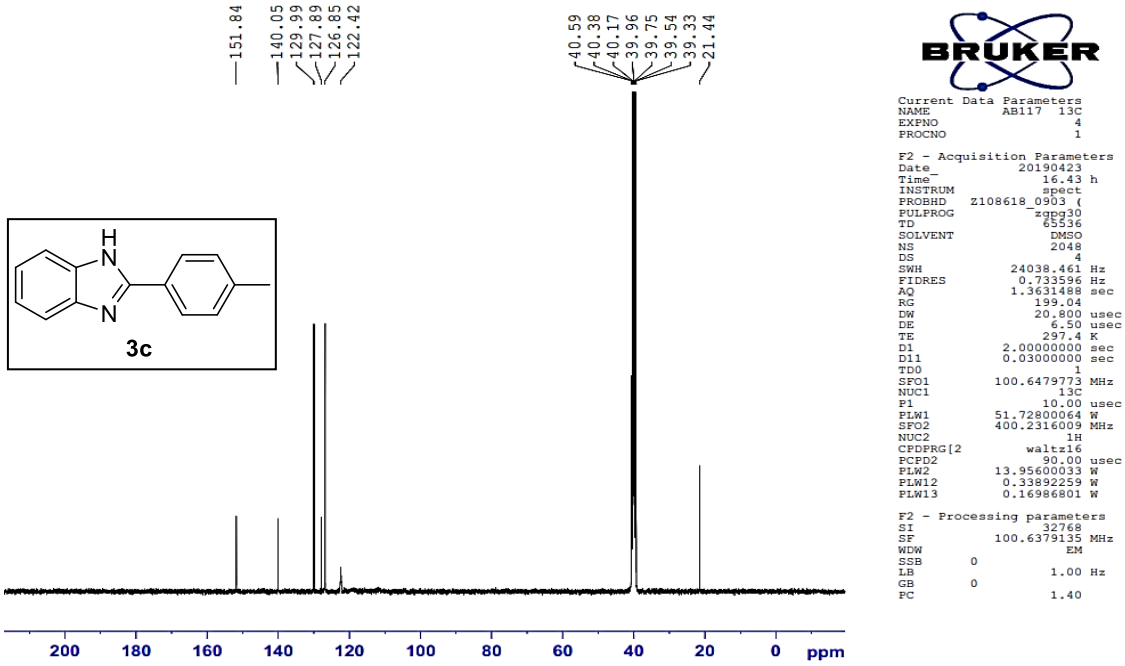

Figure S9: ^{13}C NMR (100 MHz, DMSO-d_6) Spectrum of compound **3c**

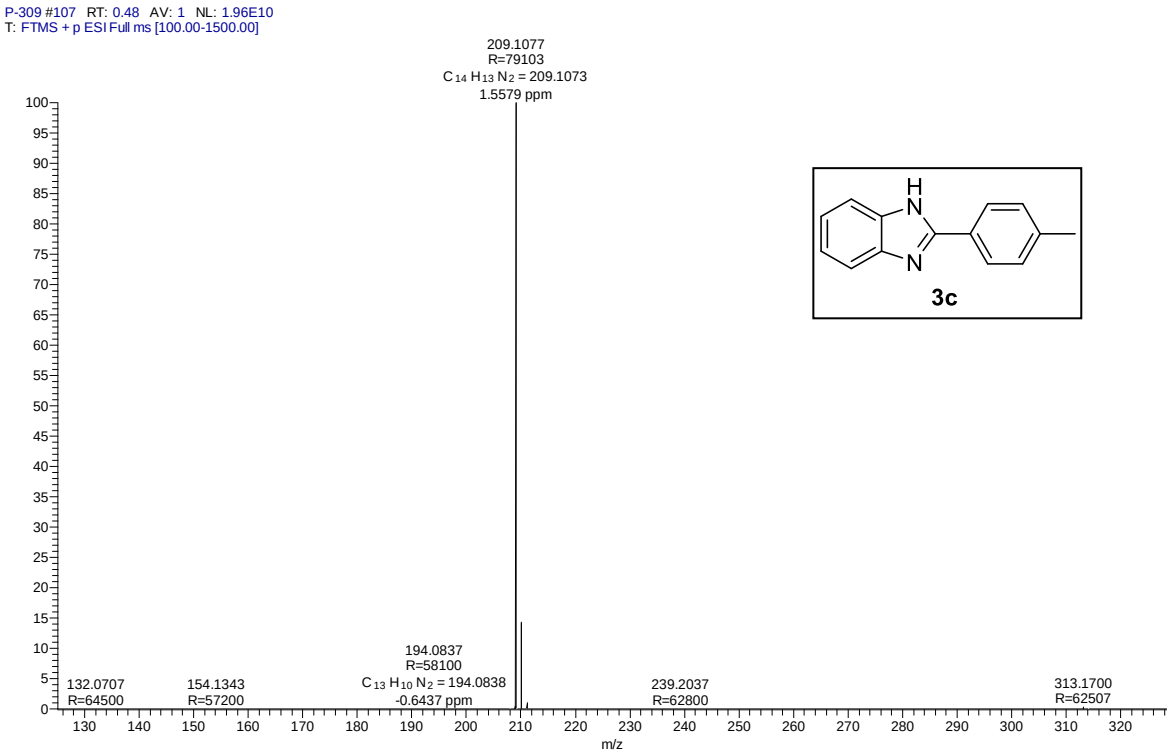

Figure S10: Mass Spectrum of compound **3c**

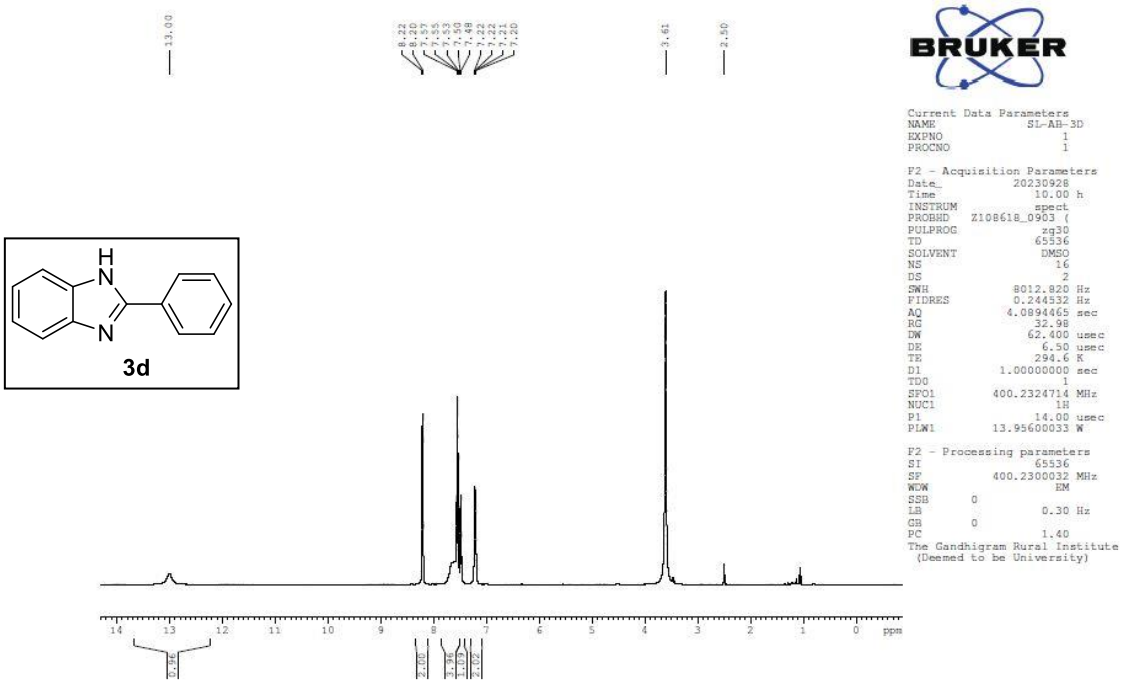

Figure S11: ^{1}H NMR (400 MHz, DMSO-d_6) Spectrum of compound **3d**

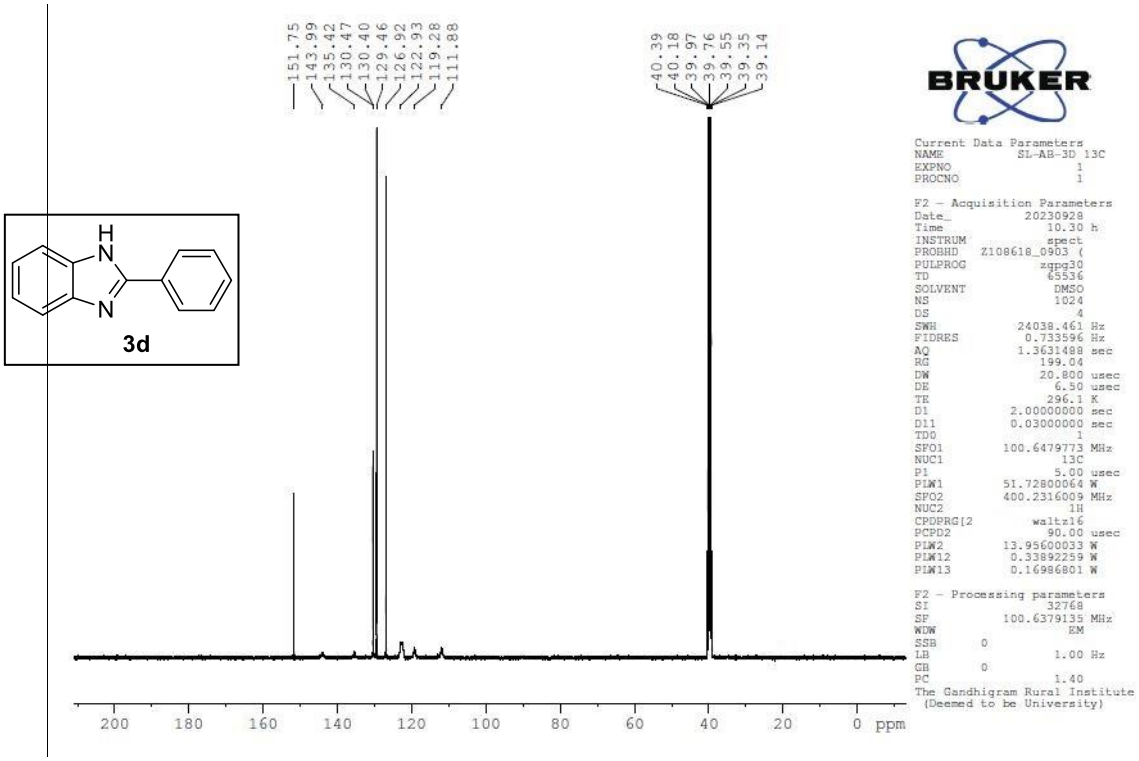

Figure S12: ^{13}C NMR (100 MHz, DMSO-d_6) Spectrum of compound **3d**

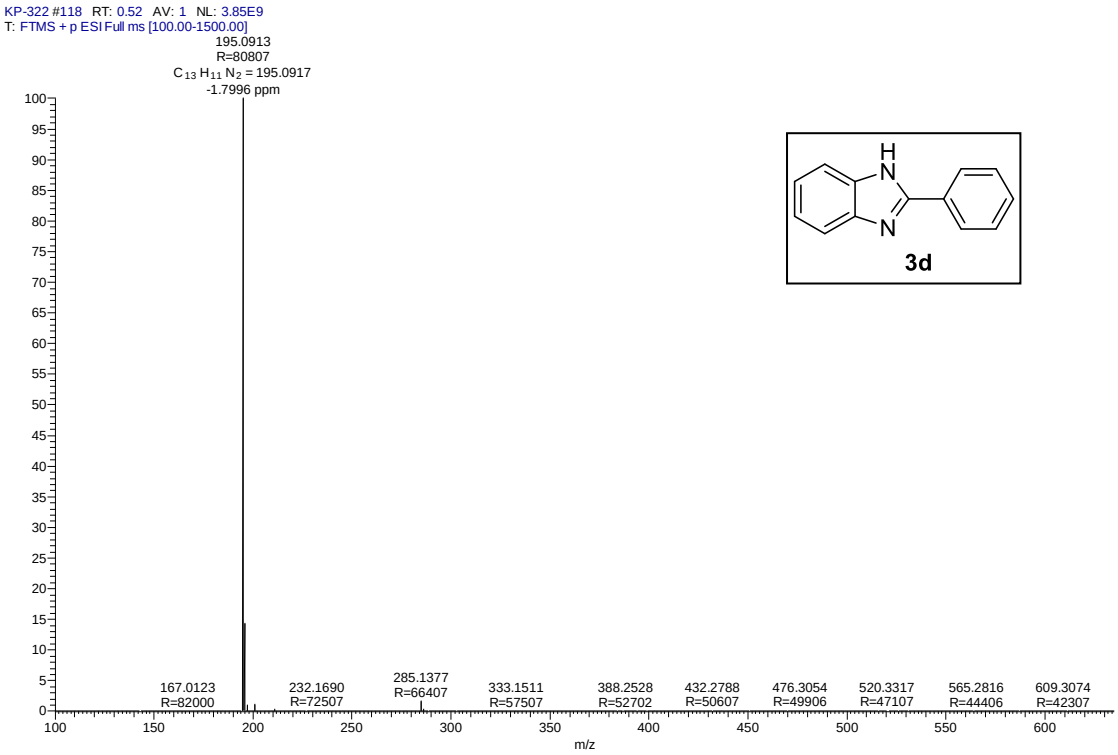

Figure S13: Mass Spectrum of compound **3d**

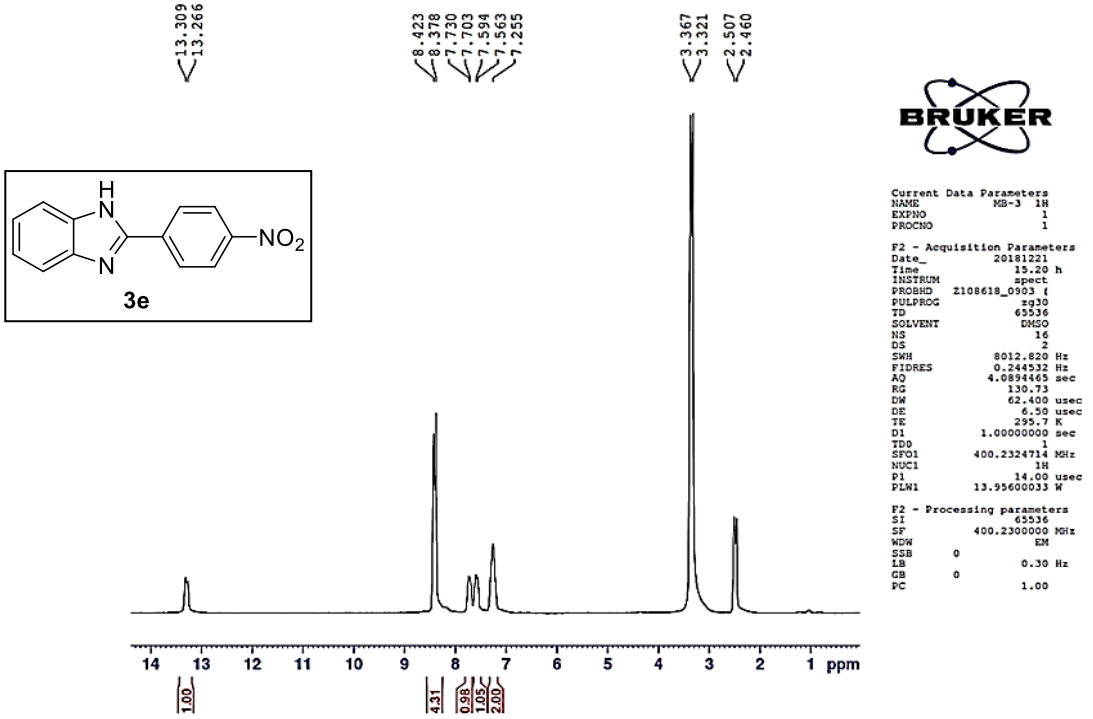

Figure S14: ^{1}H NMR (400 MHz, DMSO-d_6) Spectrum of compound **3e**

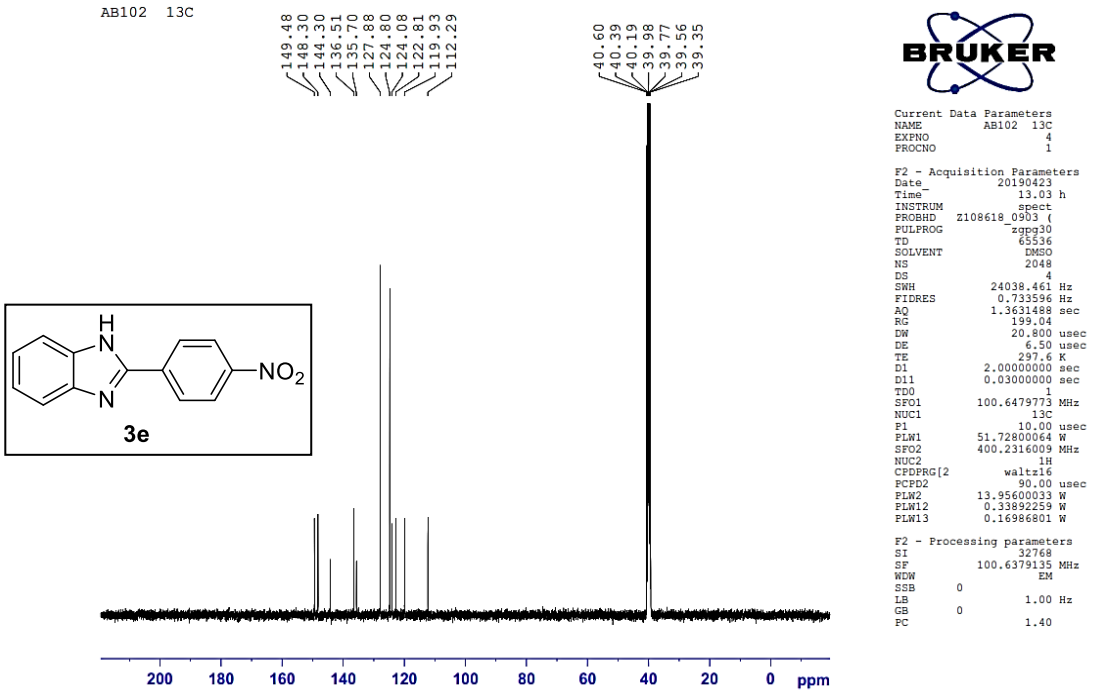

Figure S15: ^{13}C NMR (100 MHz, DMSO-d_6) Spectrum of compound **3e**

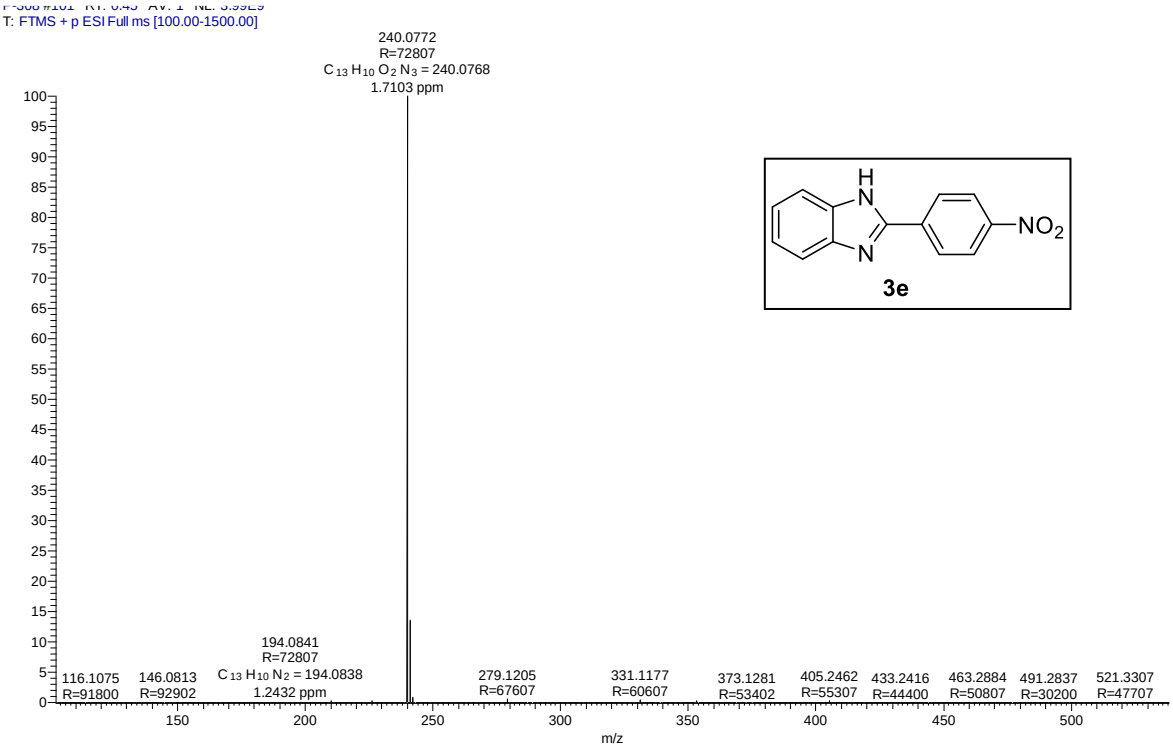

Figure S16: Mass Spectrum of compound **3e**

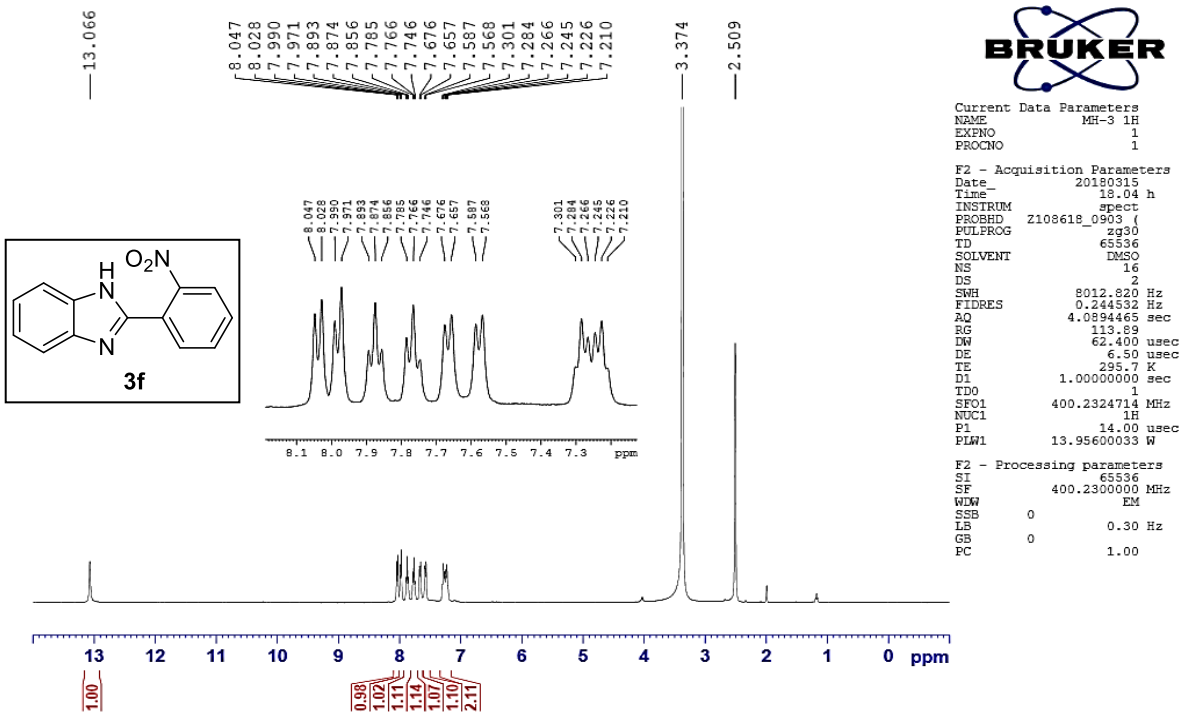

Figure S17: ^{1}H NMR (400 MHz, DMSO-d_6) Spectrum of compound **3f**

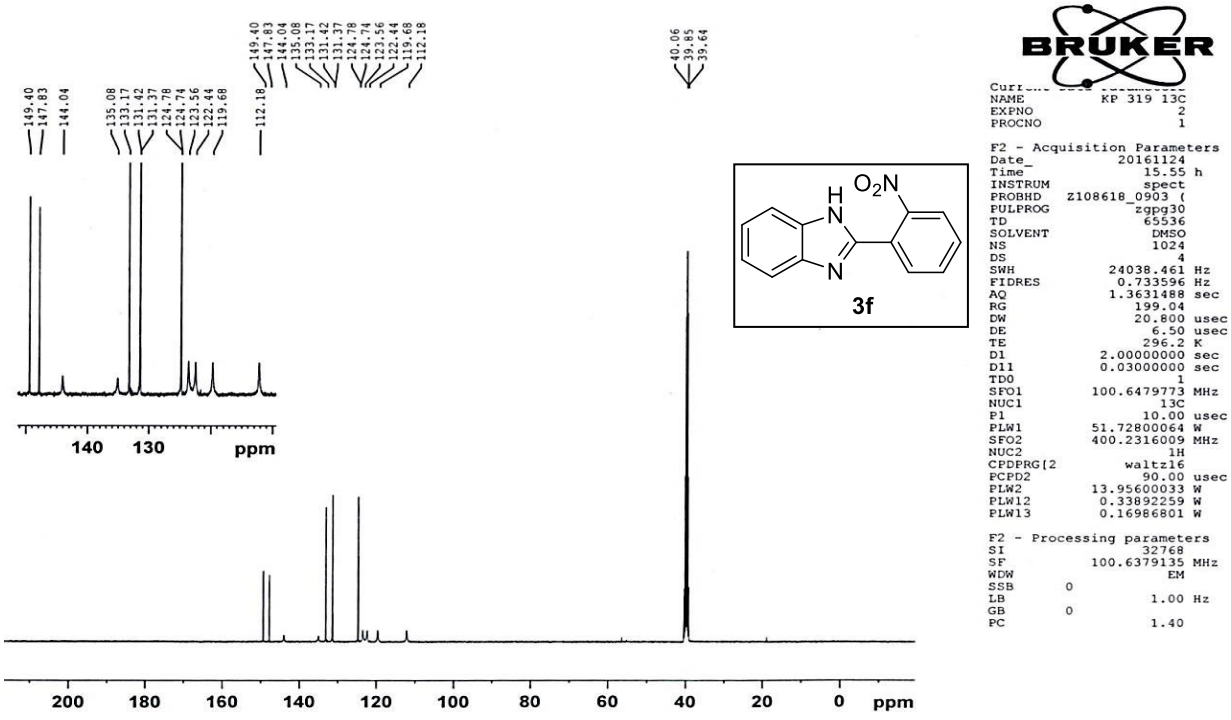

Figure S18: ^{13}C NMR (100 MHz, DMSO-d_6) Spectrum of compound **3f**

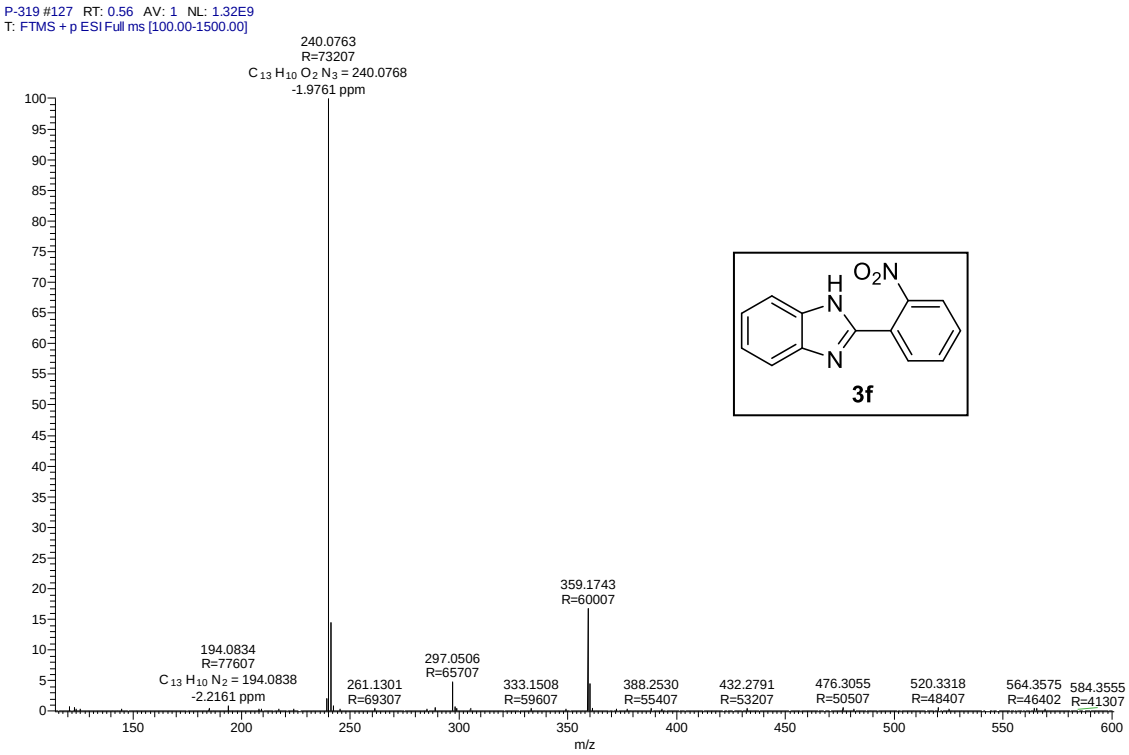

Figure S19: Mass Spectrum of compound **3f**

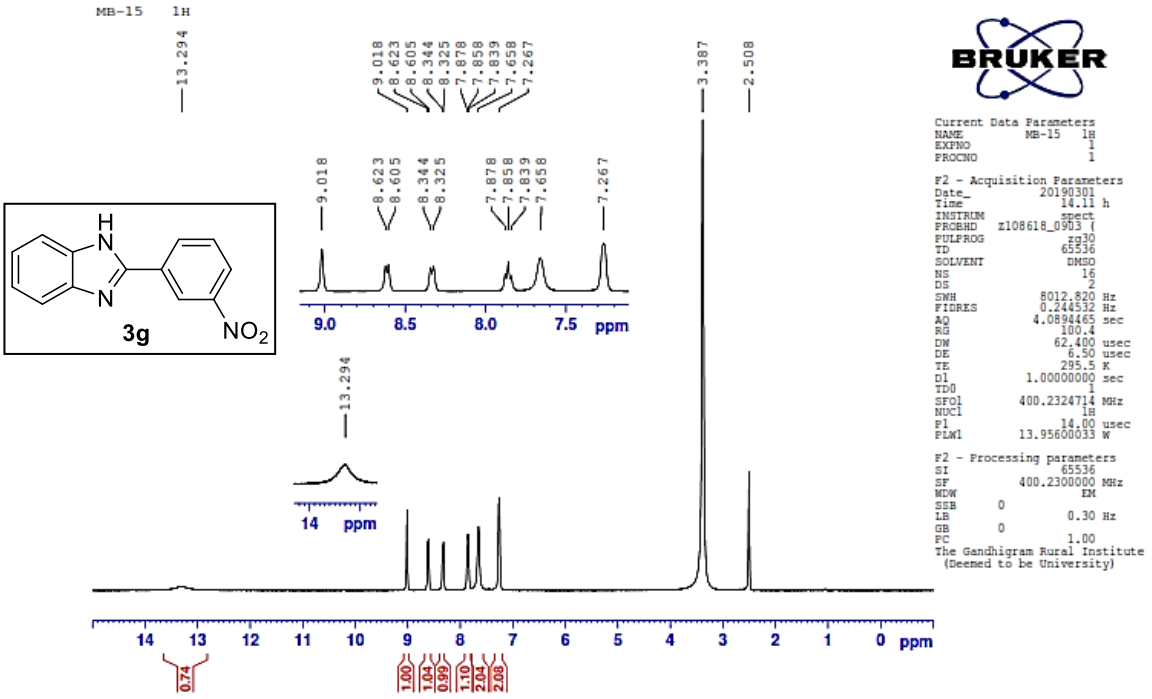

Figure S20: ^{1}H NMR (400 MHz, DMSO-d_6) Spectrum of compound **3g**

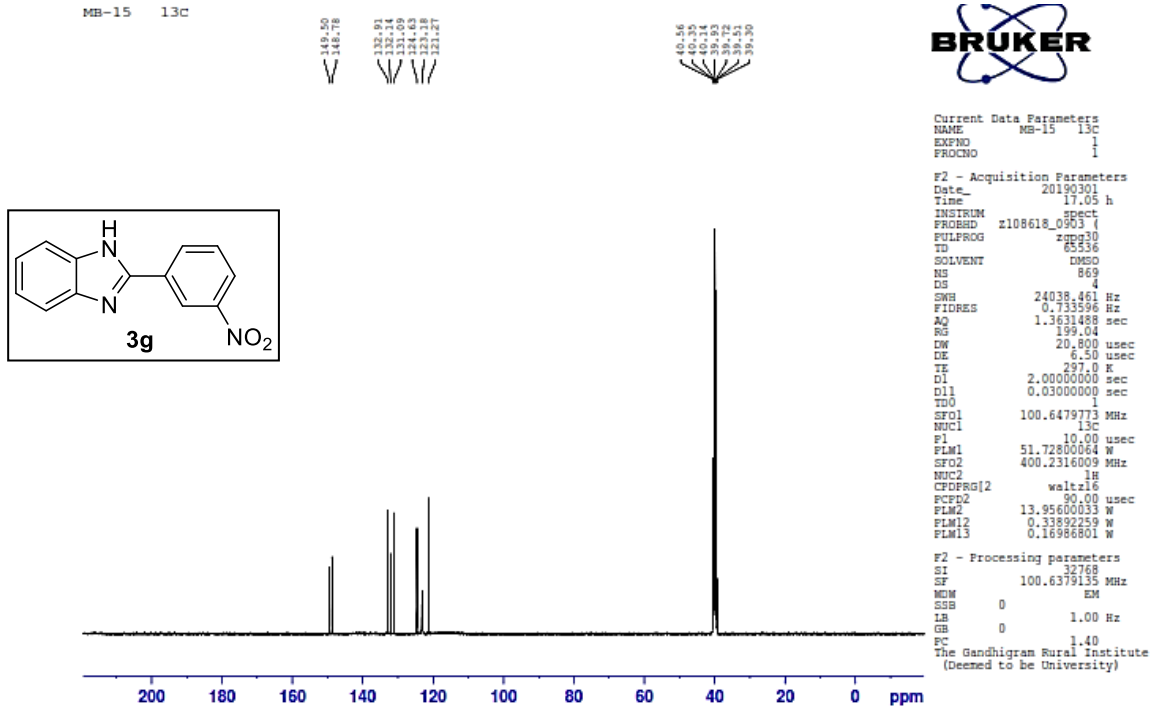

Figure S21: ^{13}C NMR (100 MHz, DMSO-d_6) Spectrum of compound **3g**

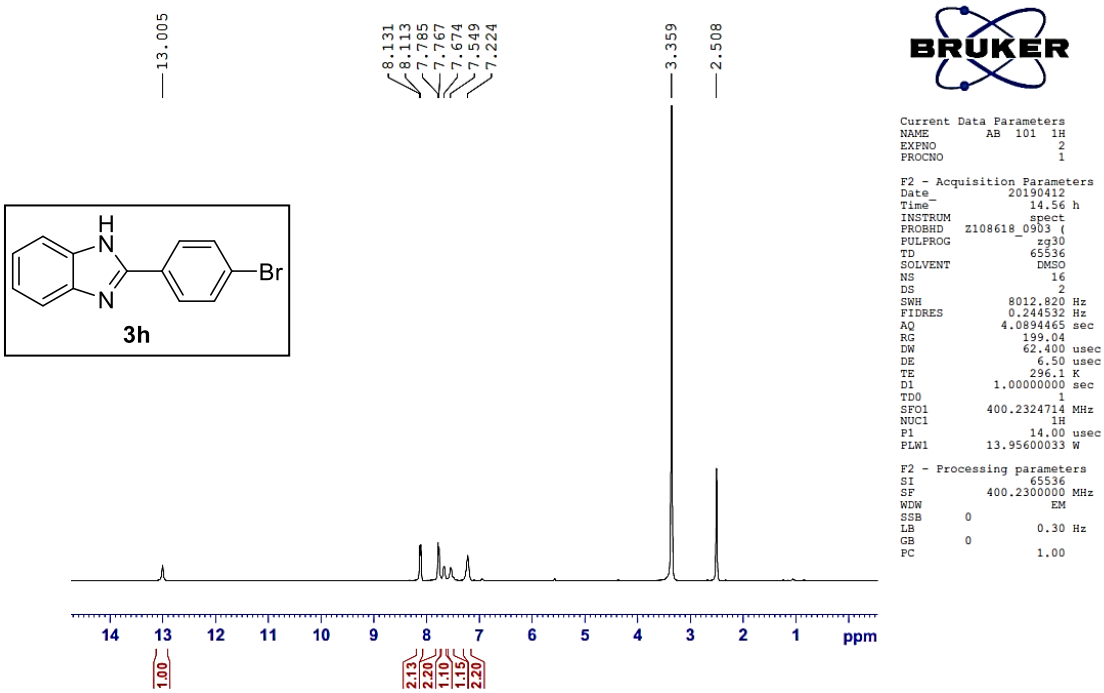

Figure S22: ^{1}H NMR (400 MHz, DMSO-d_6) Spectrum of compound **3h**

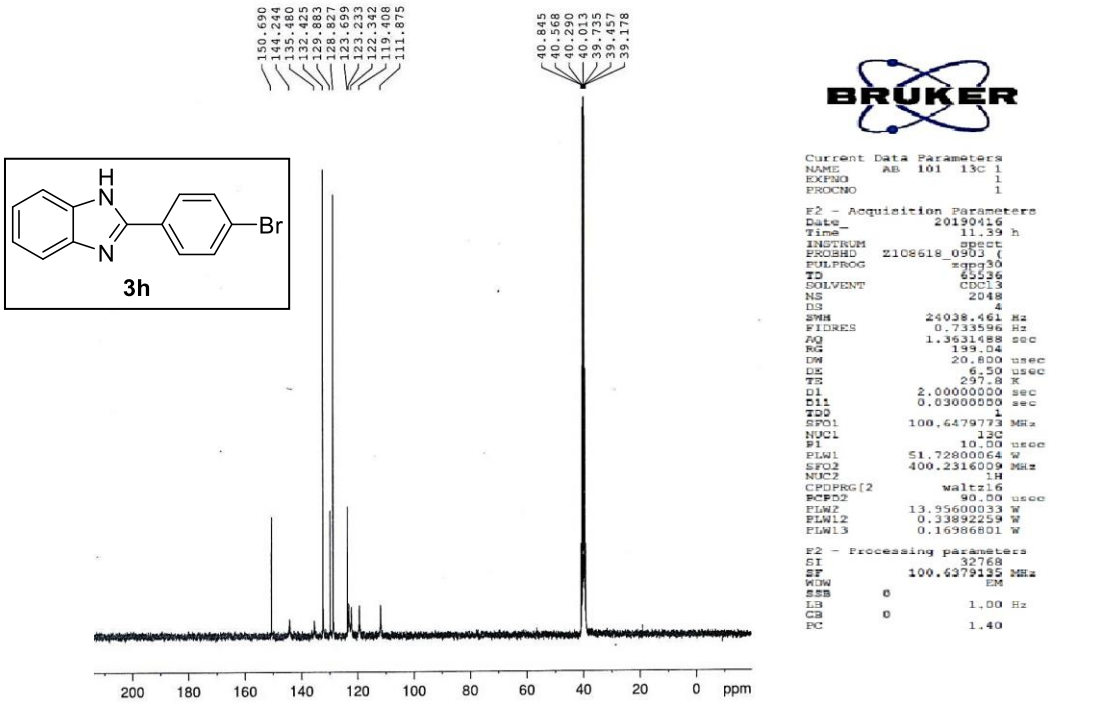

Figure S23: ^{13}C NMR (100 MHz, DMSO-d_6) Spectrum of compound **3h**

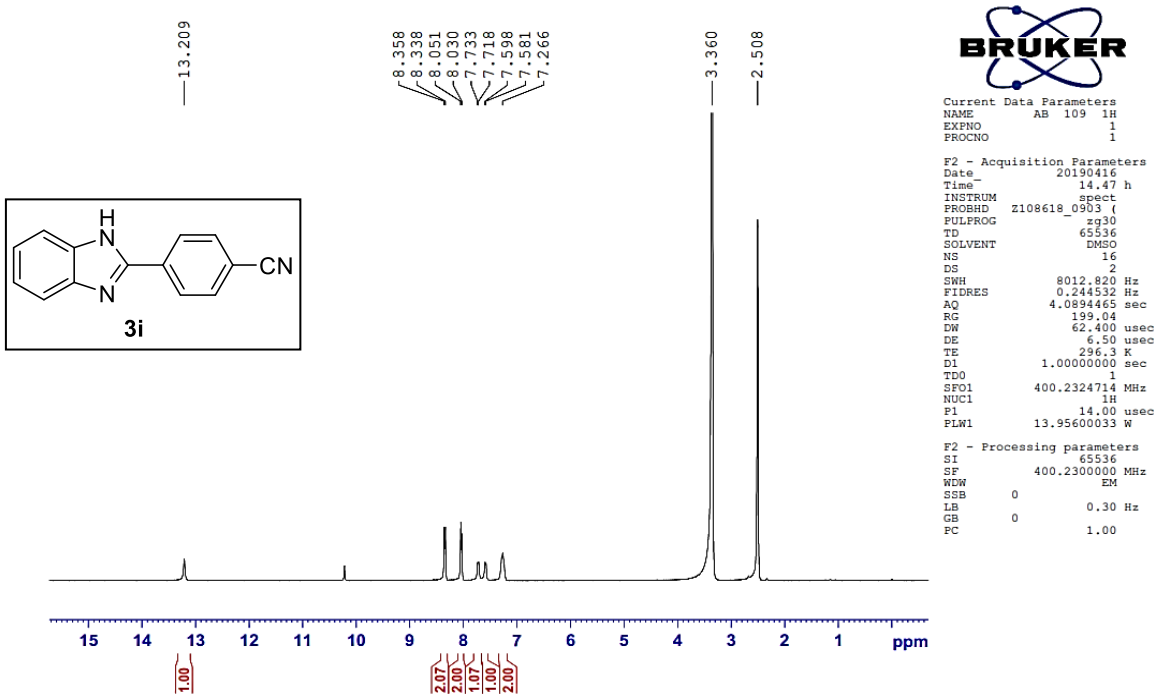

Figure S24: ^{1}H NMR (400 MHz, DMSO-d_6) Spectrum of compound **3i**

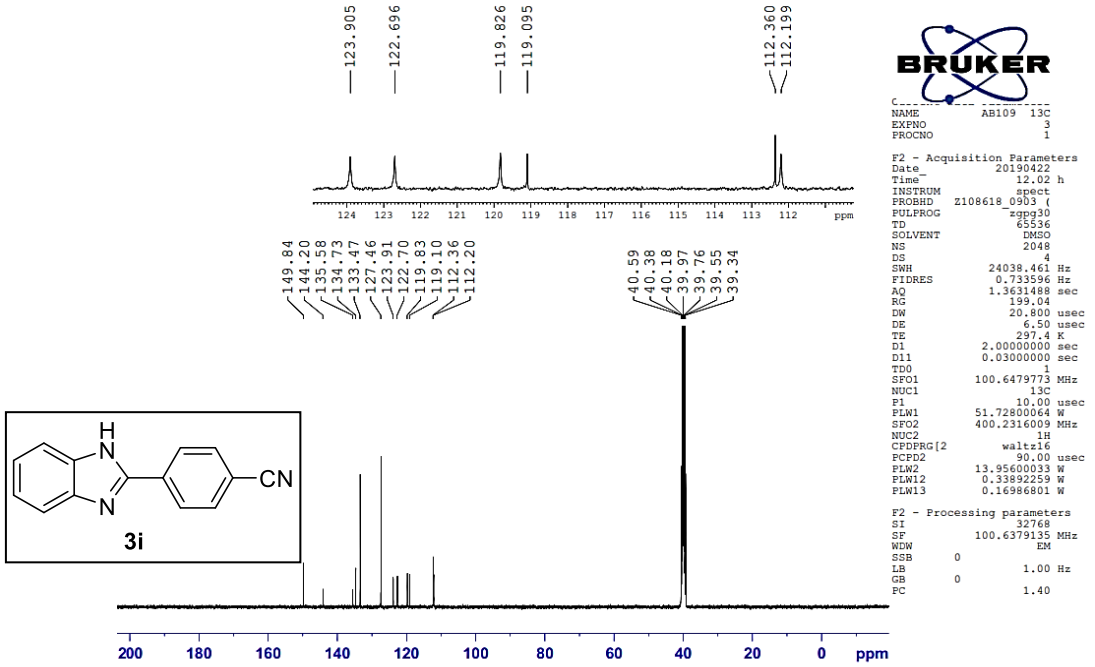

Figure S25: ^{13}C NMR (100 MHz, DMSO-d_6) Spectrum of compound **3i**

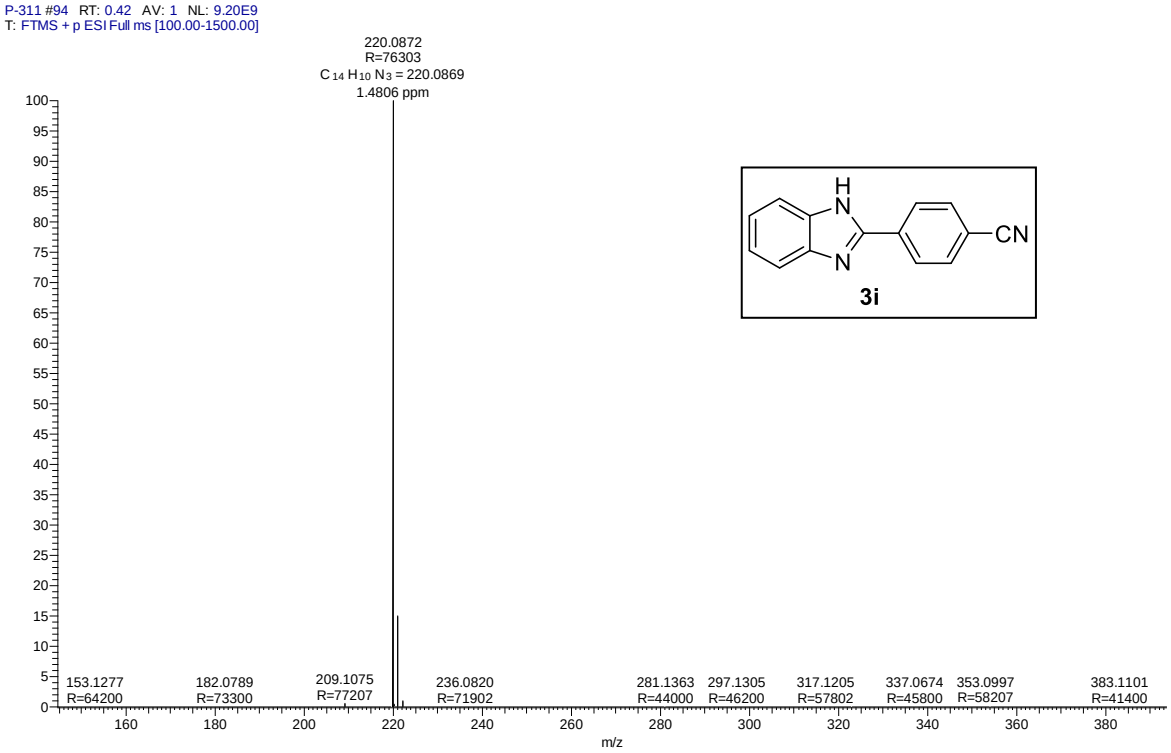

Figure S26: Mass Spectrum of compound **3i**

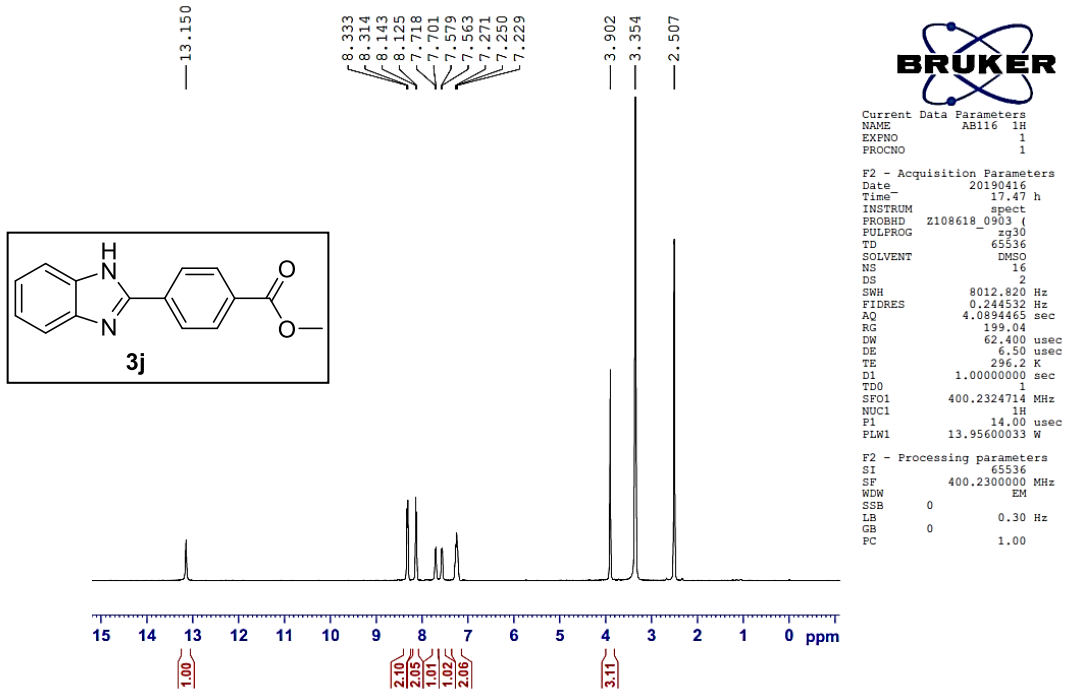

Figure S27: ^{1}H NMR (400 MHz, DMSO-d_6) Spectrum of compound **3j**

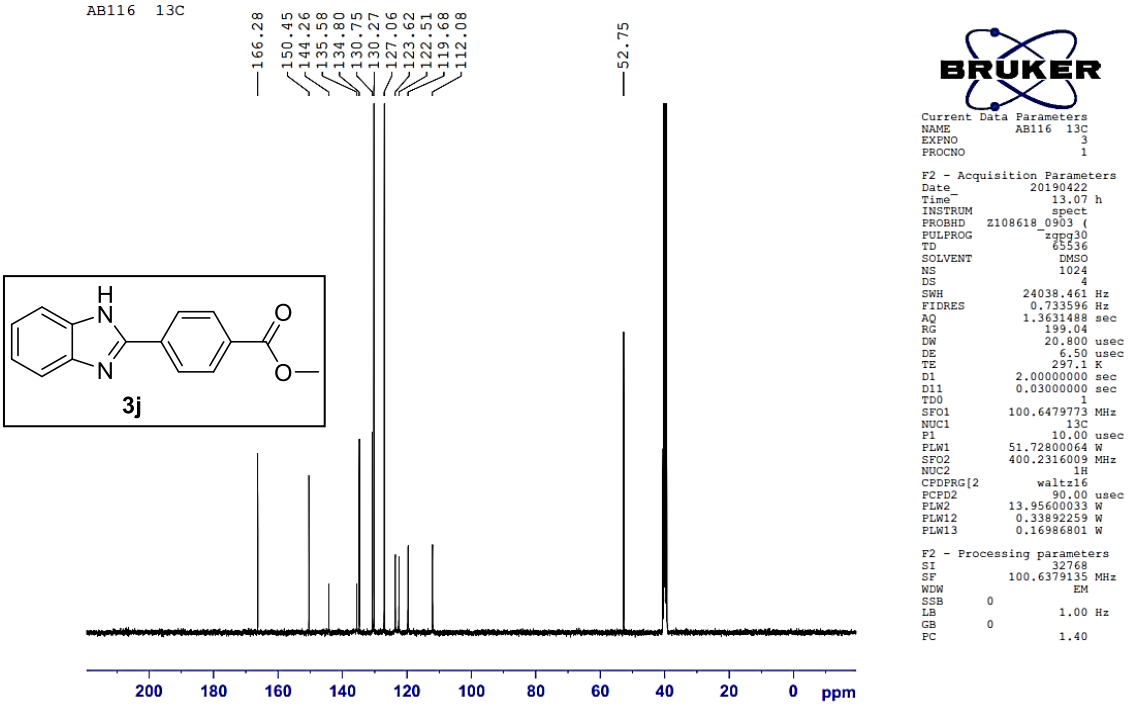

Figure S28: ^{13}C NMR (100 MHz, DMSO-d_6) Spectrum of compound **3j**

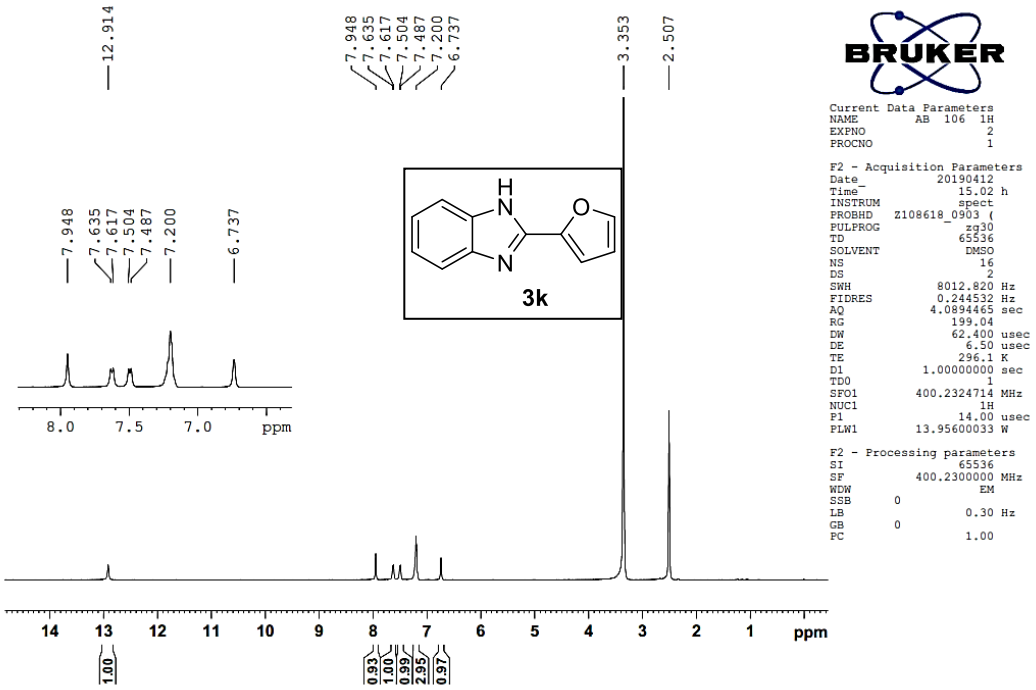

Figure S29: ^{1}H NMR (400 MHz, DMSO-d_6) Spectrum of compound **3k**

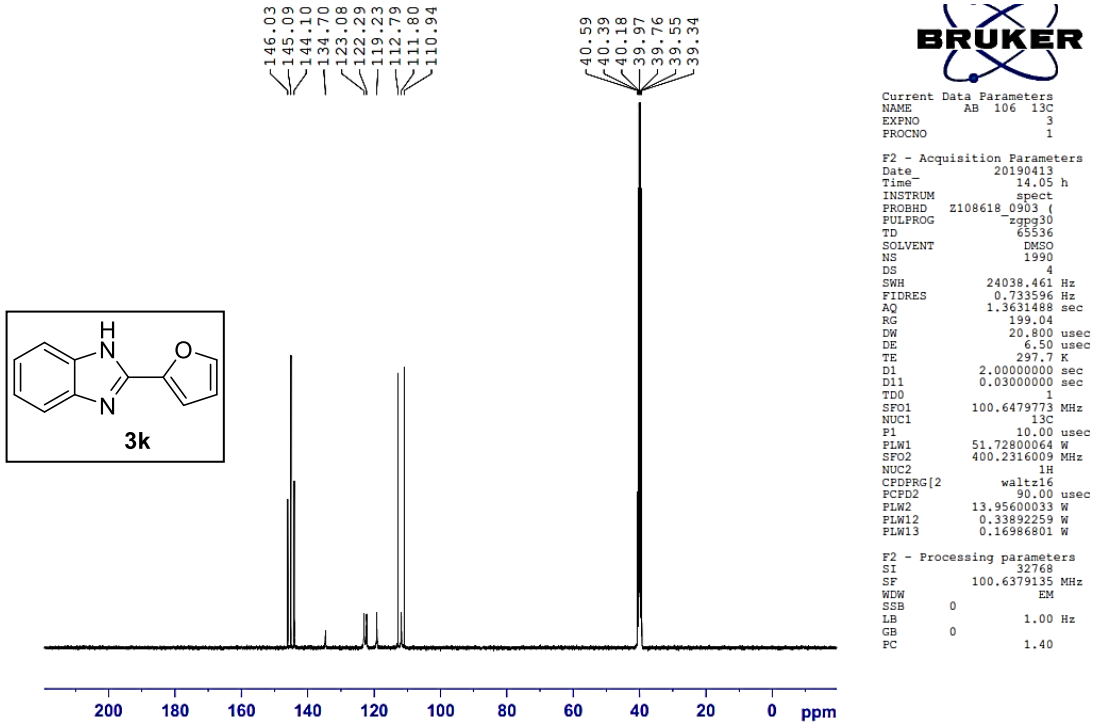

Figure S30: ^{13}C NMR (100 MHz, DMSO-d_6) Spectrum of compound **3k**

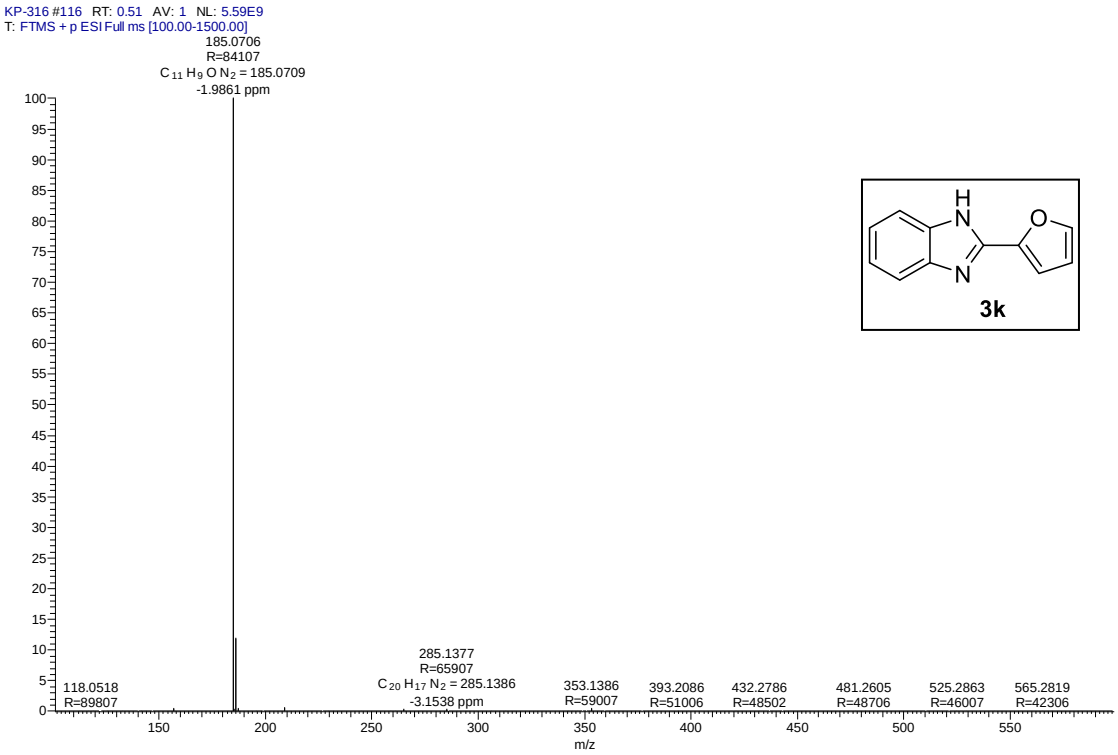

Figure S31: Mass Spectrum of compound **3k**

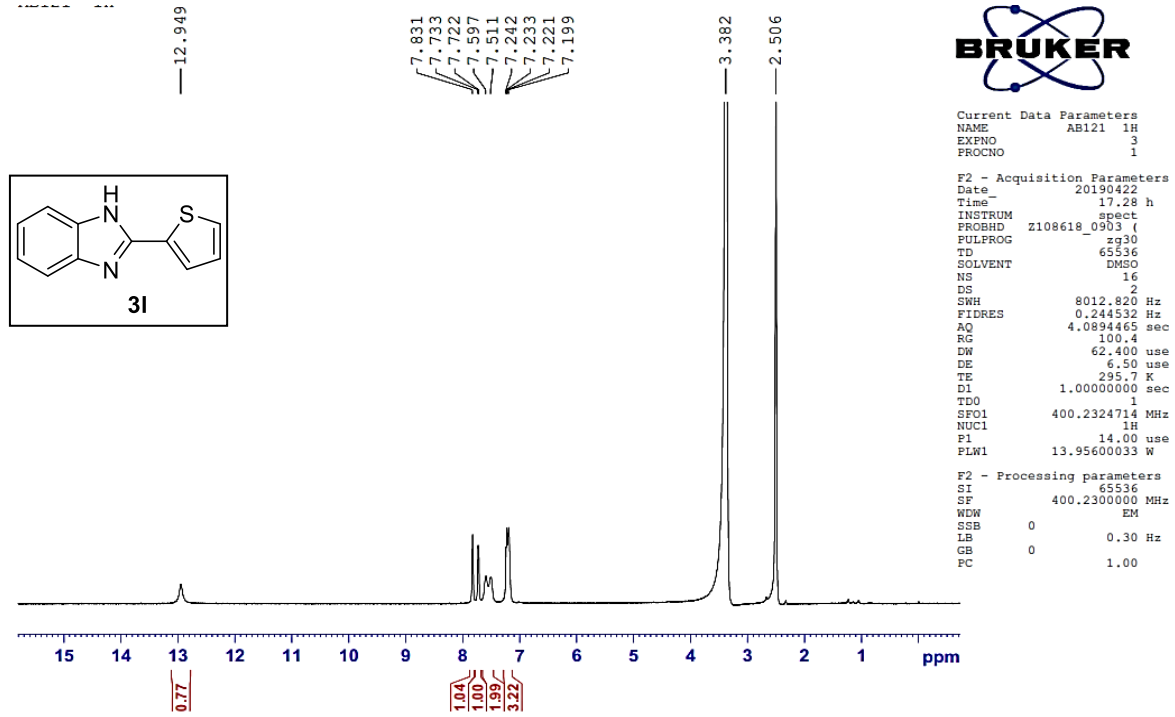

Figure S32: ^{1}H NMR (400 MHz, DMSO-d_6) Spectrum of compound **3l**

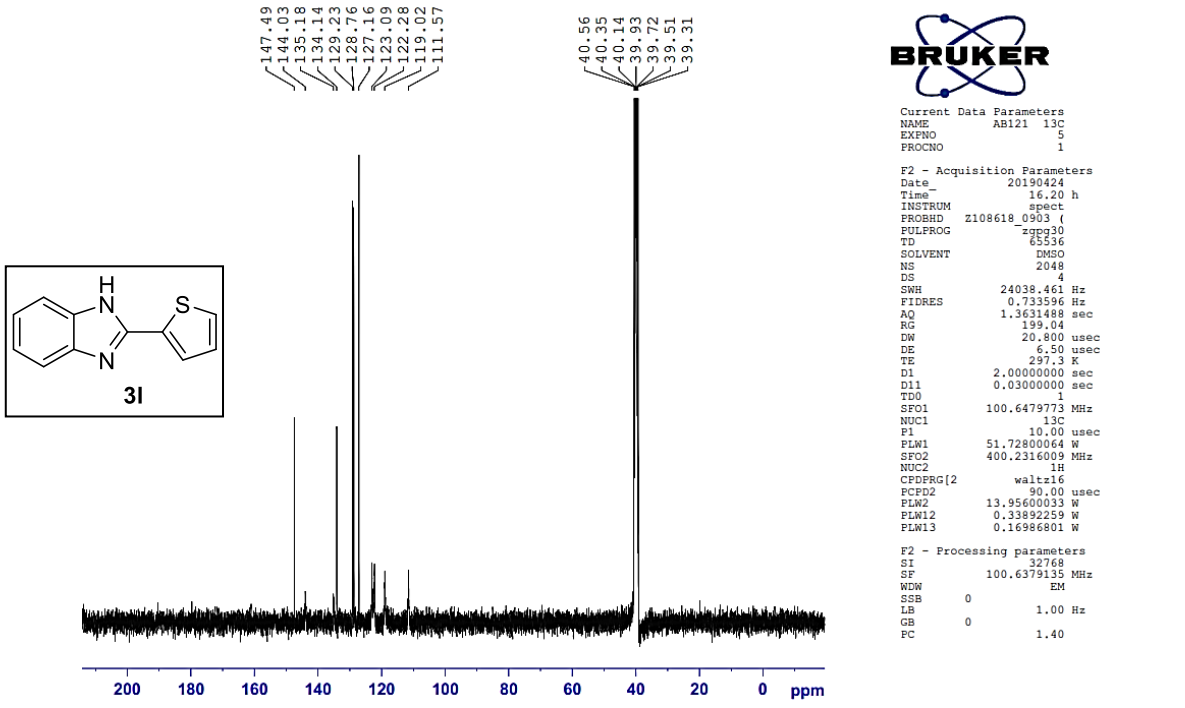

Figure S33: ^{13}C NMR (100 MHz, DMSO-d_6) Spectrum of compound **3l**

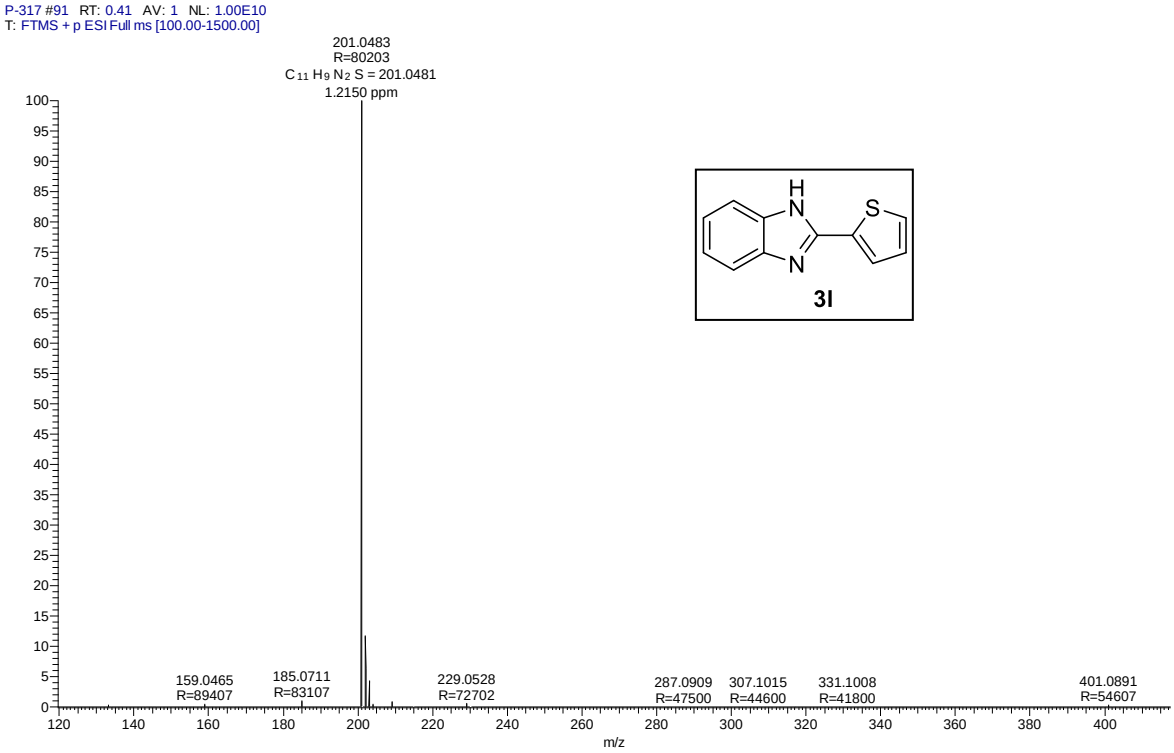

Figure S34: Mass Spectrum of compound **3l**

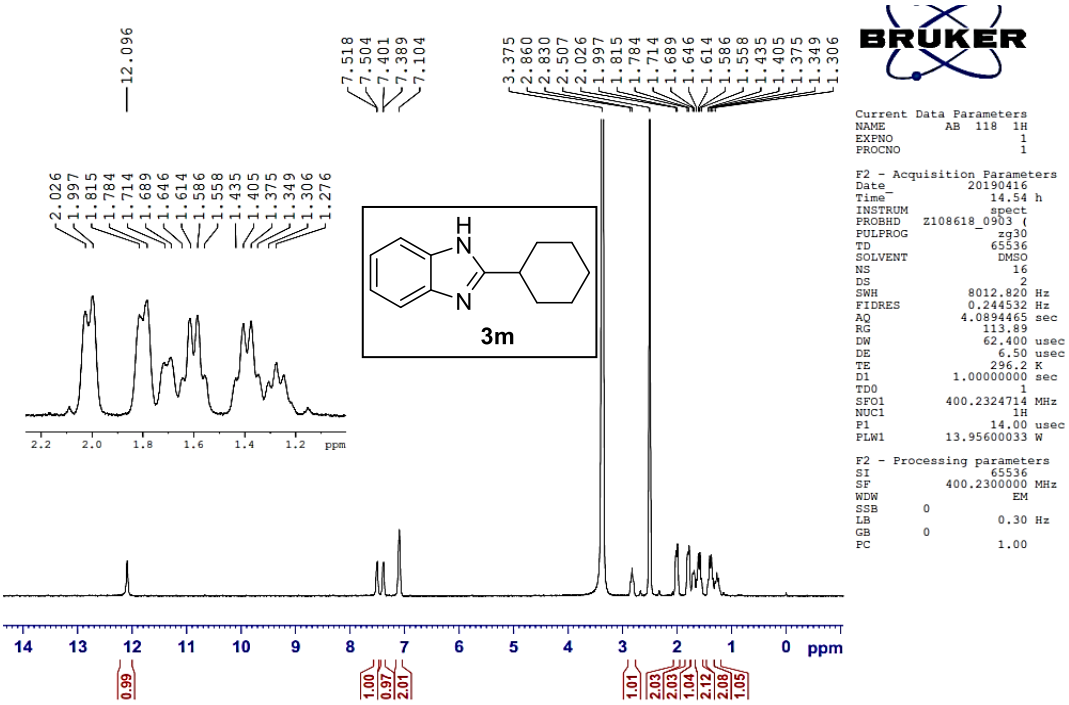

Figure S35: ^{1}H NMR (400 MHz, DMSO-d_6) Spectrum of compound **3m**

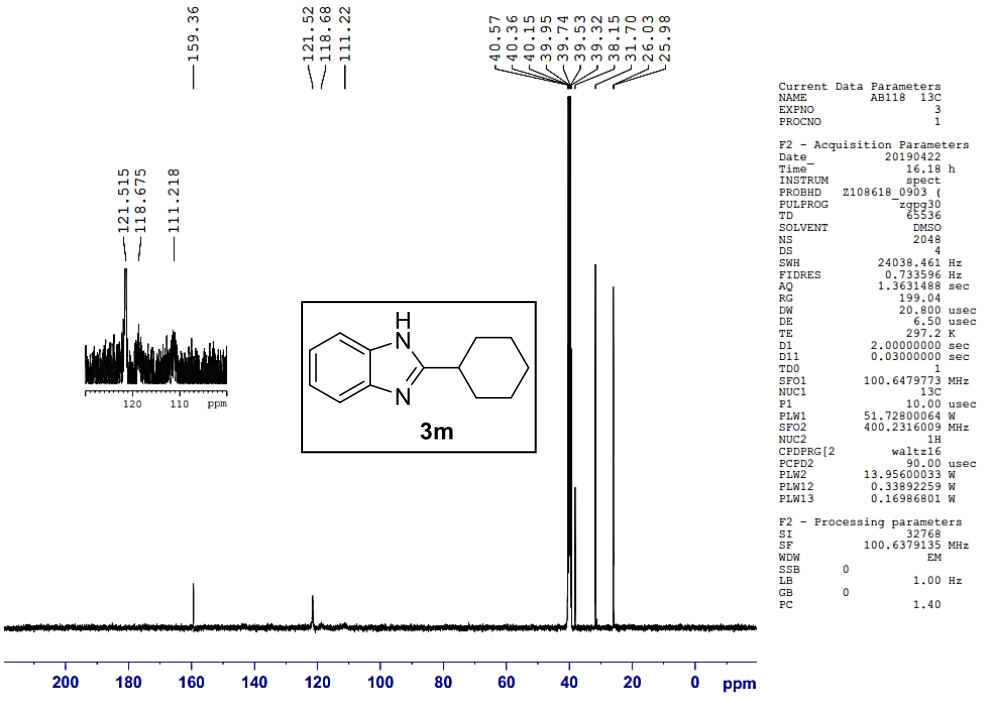

Figure S36: ^{13}C NMR (100 MHz, DMSO-d_6) Spectrum of compound **3m**

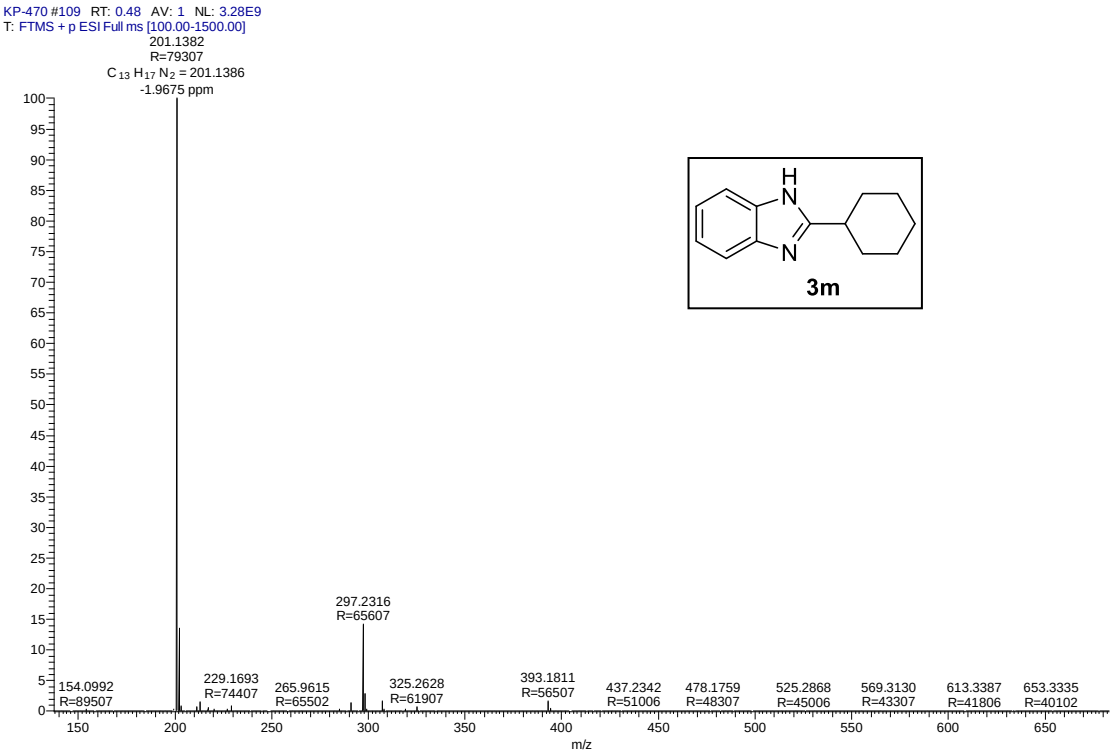

Figure S37: Mass Spectrum of compound **3m**

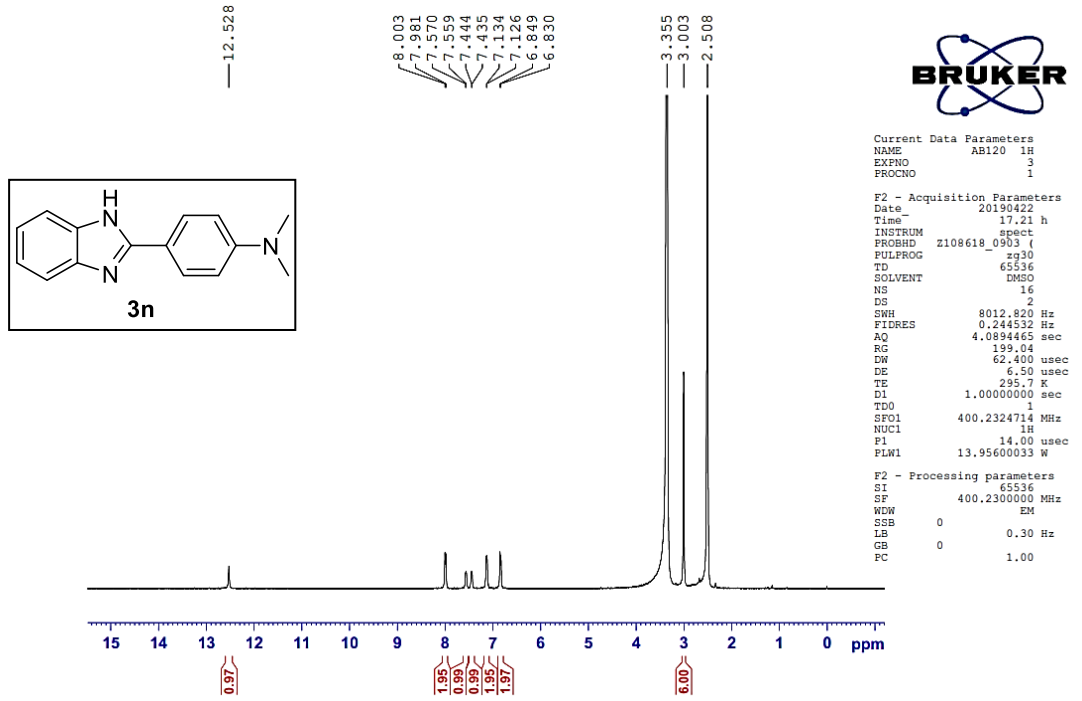

Figure S38: ^{1}H NMR (400 MHz, DMSO-d_6) Spectrum of compound **3n**

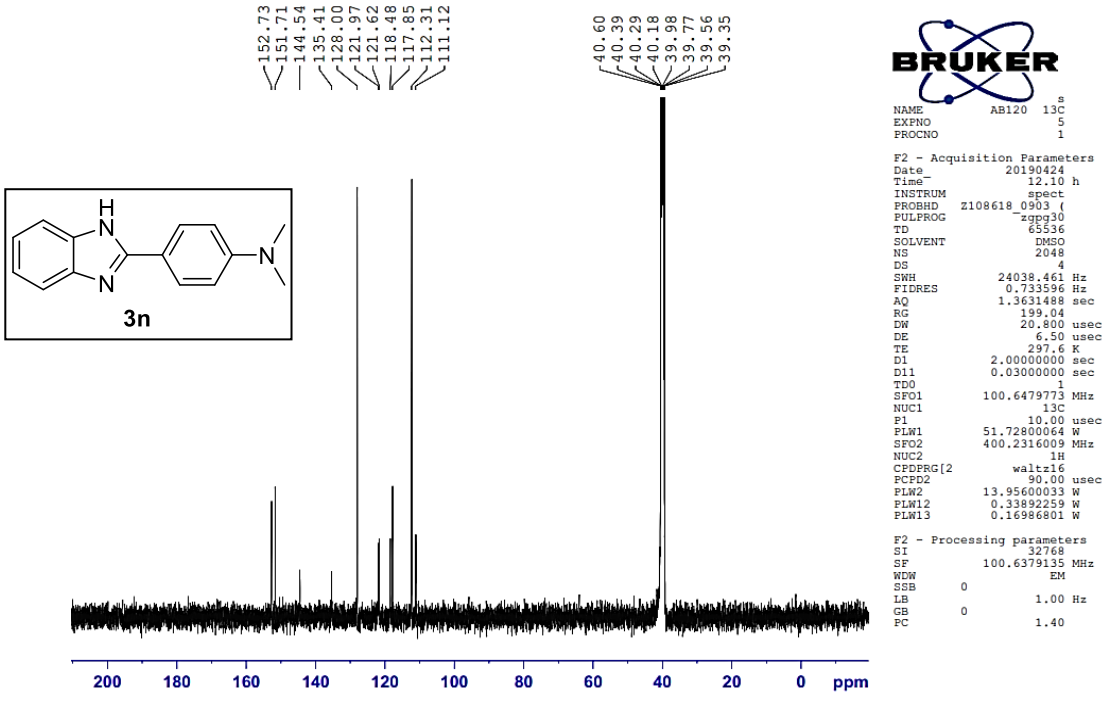

Figure S39: ^{13}C NMR (100 MHz, DMSO-d_6) Spectrum of compound **3n**

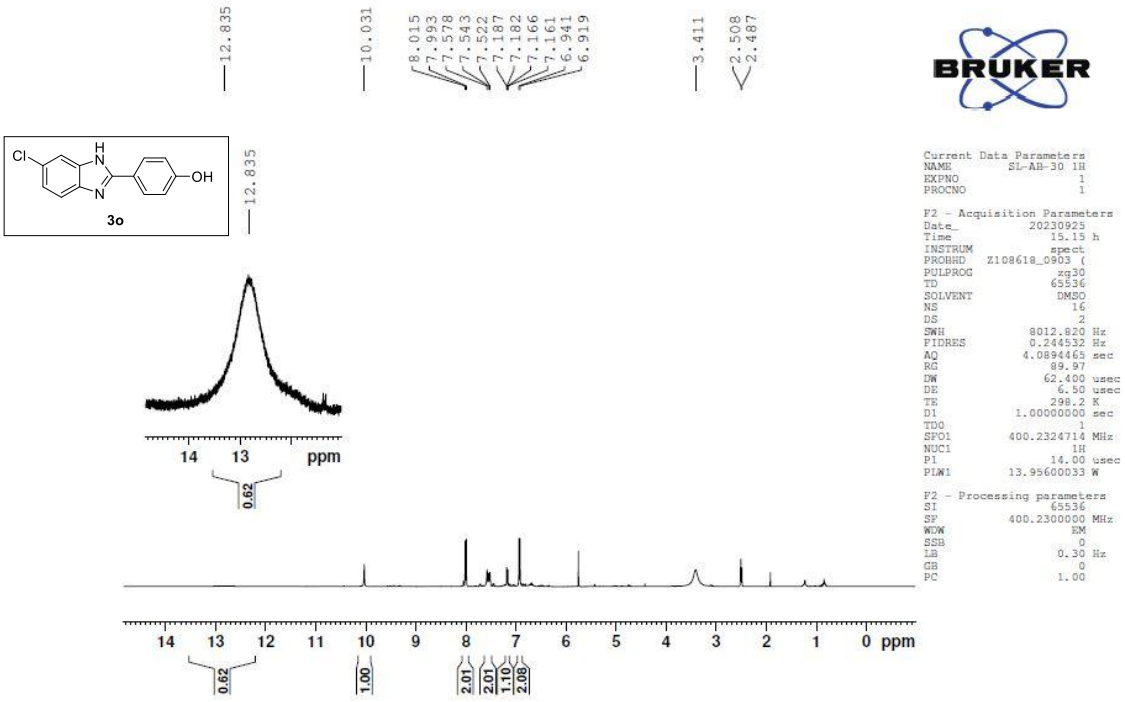

Figure S40: ^{1}H NMR (400 MHz, DMSO-d_6) Spectrum of compound **3o**

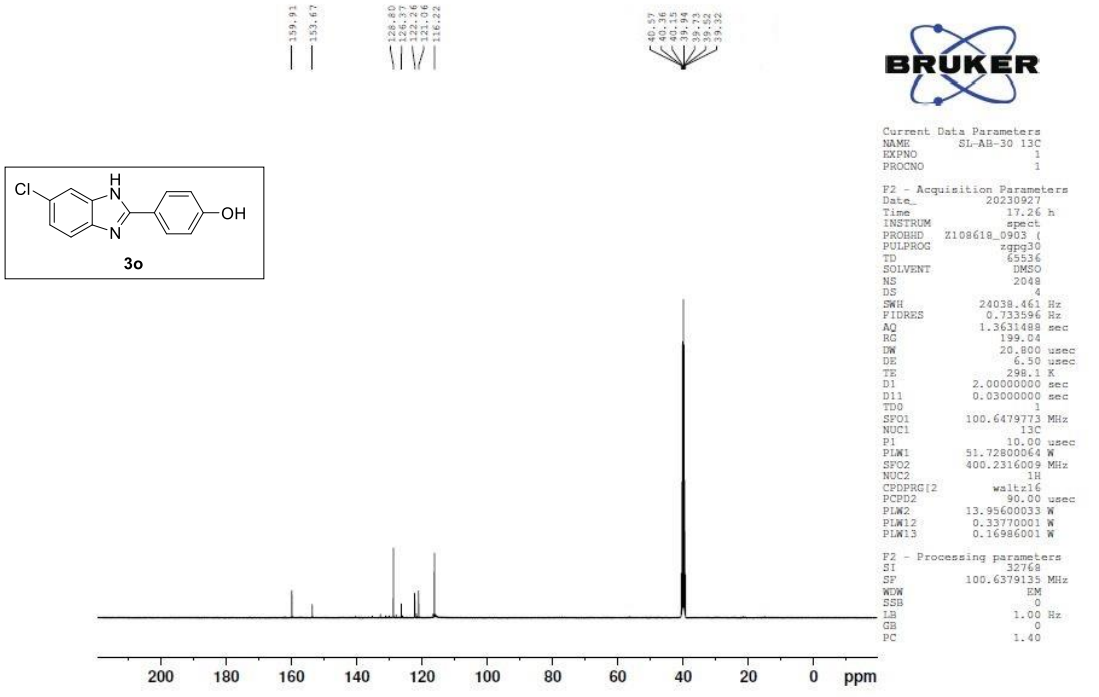

Figure S41: ^{13}C NMR (100 MHz, DMSO-d_6) Spectrum of compound **3o**