Supporting information for

Unfolding the Antibacterial Activity and Acetylcholinesterase Inhibition Potential of Benzofuran-Triazole Hybrids: Synthesis, Antibacterial, Acetylcholinesterase Inhibition, and Molecular Docking Studies

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^{1}H and ^{13}C NMR spectra of compound **10a-e**

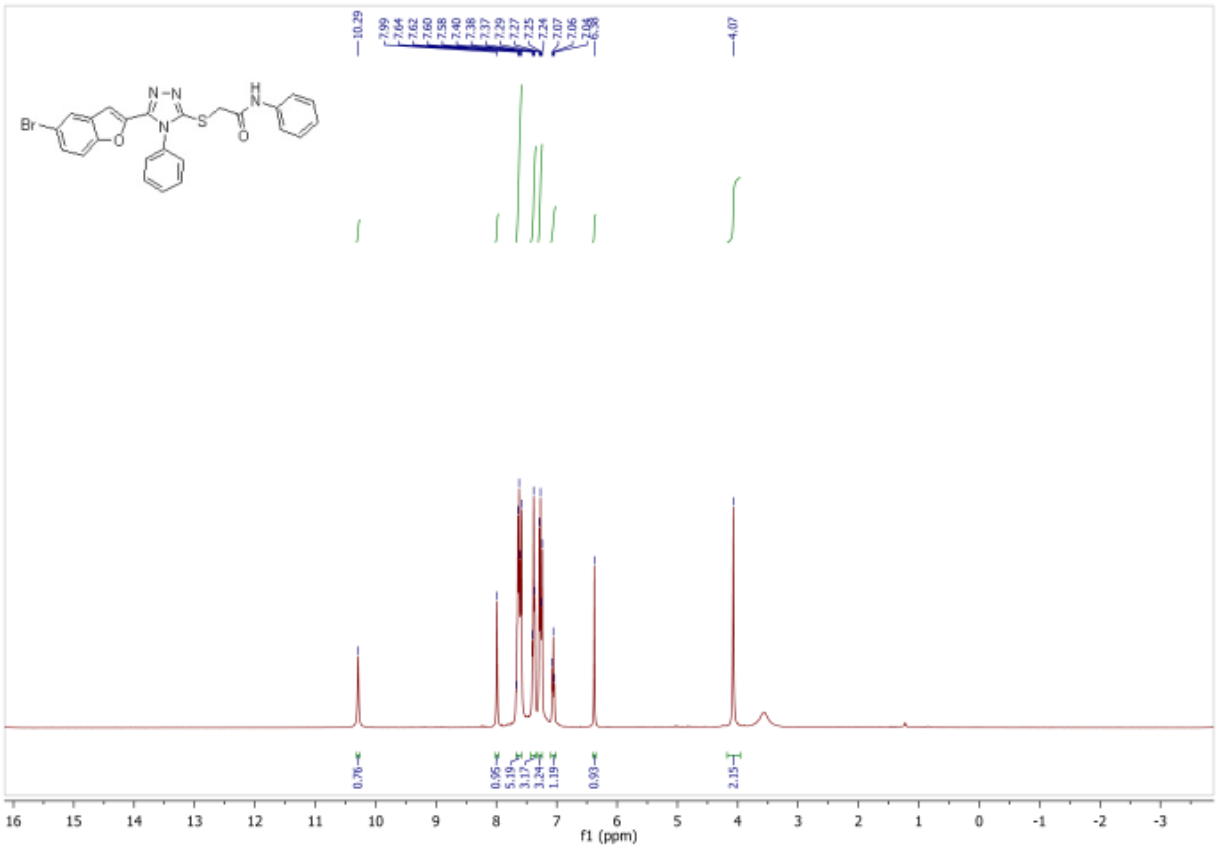

Figure S1: ^{1}H NMR spectrum of 2-((5-(5-bromobenzofuran-2-yl)-4-phenyl-4*H*-1,2,4-triazol-3-yl)thio)-*N*-phenylacetamide (**10a**).

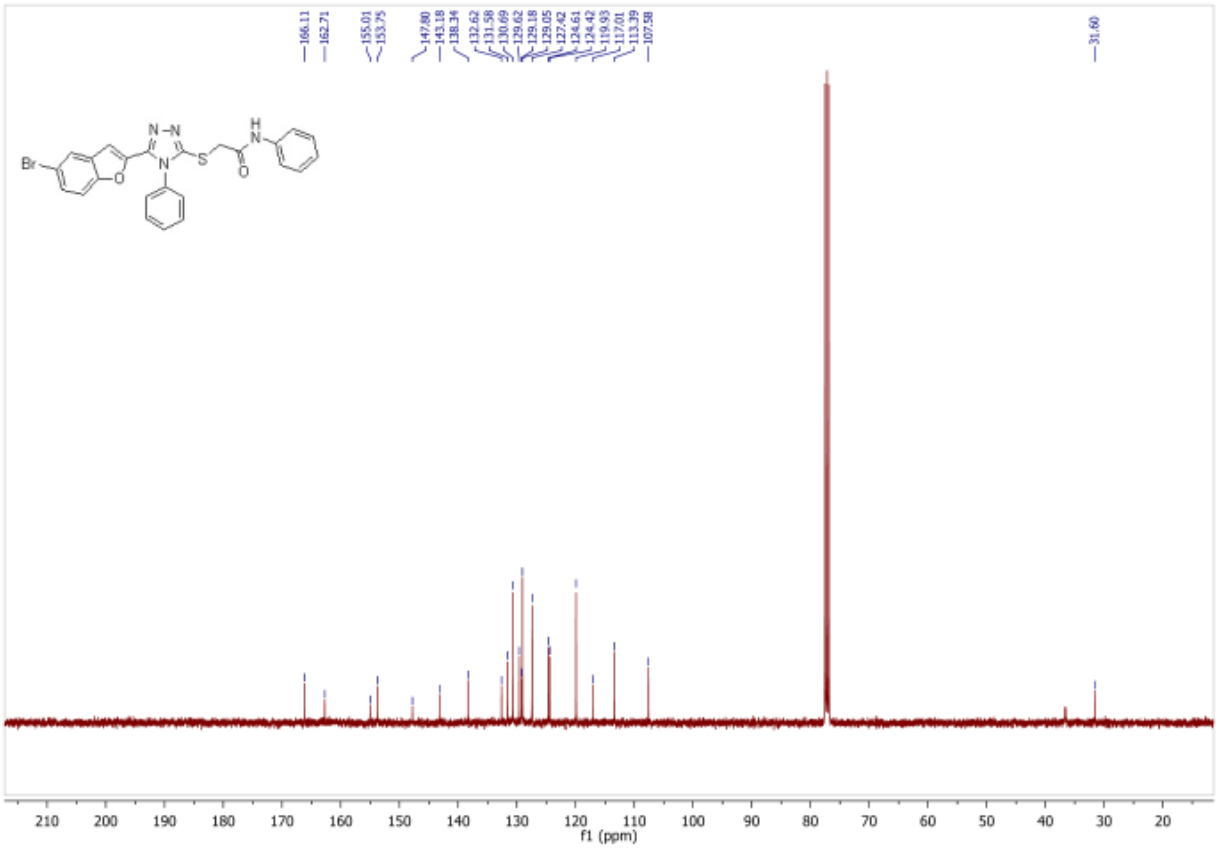

Figure S2: ^{13}C NMR spectrum of 2-((5-(5-bromobenzofuran-2-yl)-4-phenyl-4*H*-1,2,4-triazol-3-yl)thio)-*N*-phenylacetamide (**10a**).

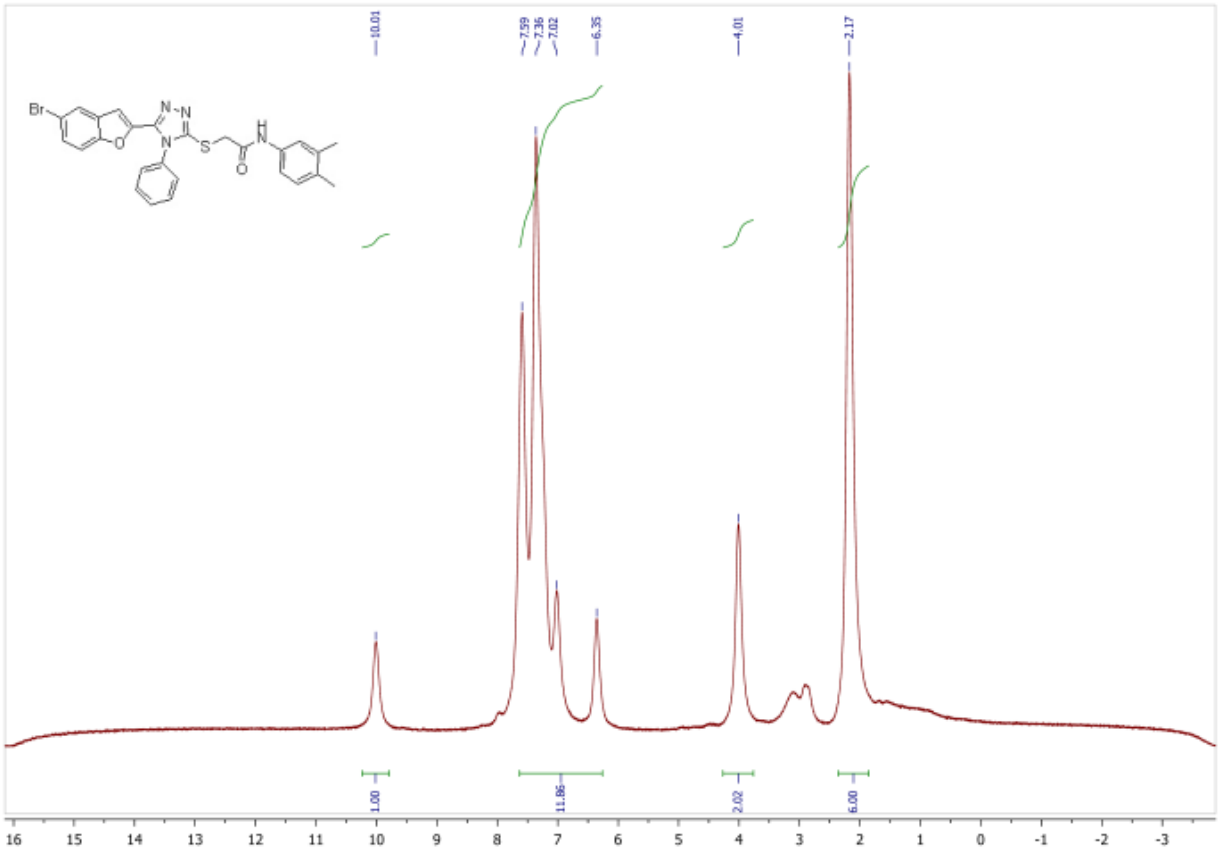

Figure S3: ^{1}H NMR spectrum of 2-((5-(5-bromobenzofuran-2-yl)-4-phenyl-4*H*-1,2,4-triazol-3-yl)thio)-*N*-(3,4-dimethylphenyl)acetamide (**10b**).

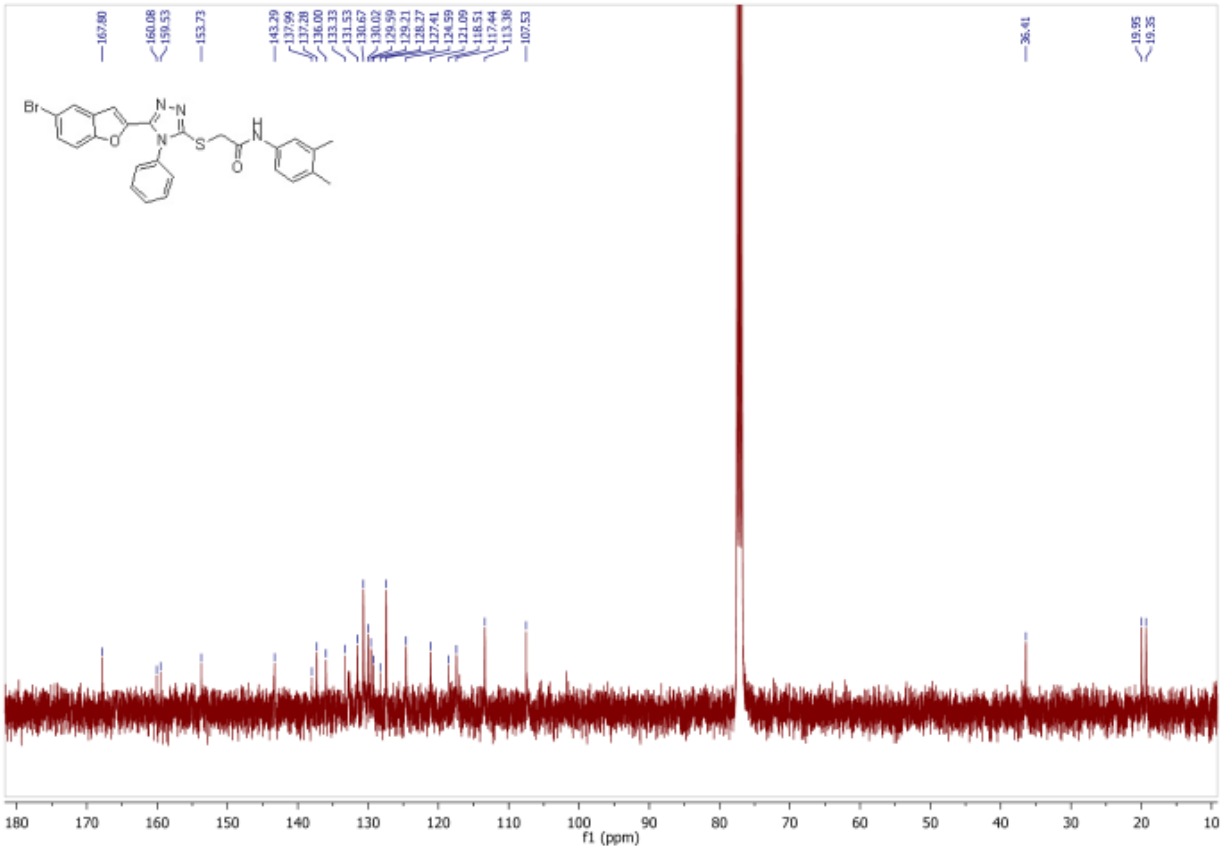

Figure S4: ^{13}C NMR spectrum of 2-((5-(5-bromobenzofuran-2-yl)-4-phenyl-4*H*-1,2,4-triazol-3-yl)thio)-*N*-(3,4-dimethylphenyl)acetamide (**10b**).

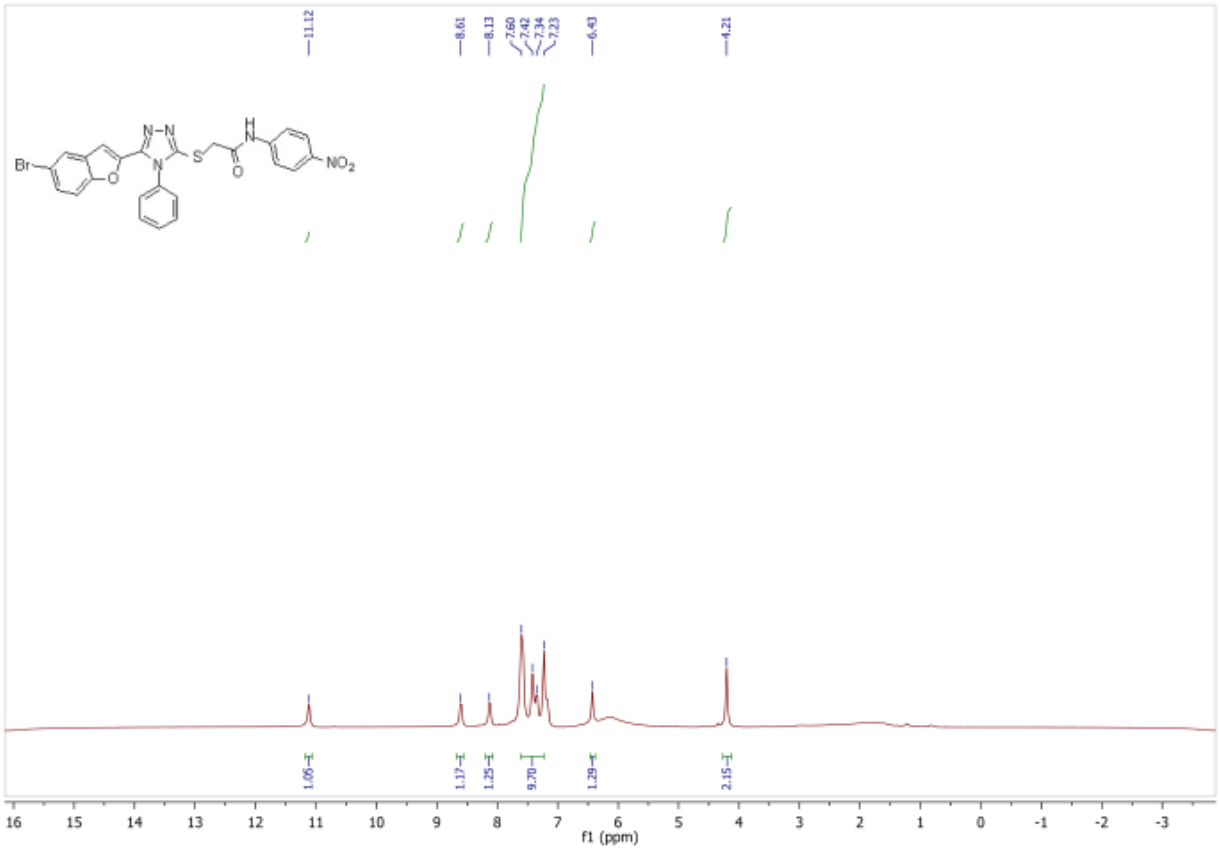

Figure S5: ^{1}H NMR spectrum of 2-((5-(5-bromobenzofuran-2-yl)-4-phenyl-4*H*-1,2,4-triazol-3-yl)thio)-*N*-(4-nitrophenyl)acetamide (**10c**).

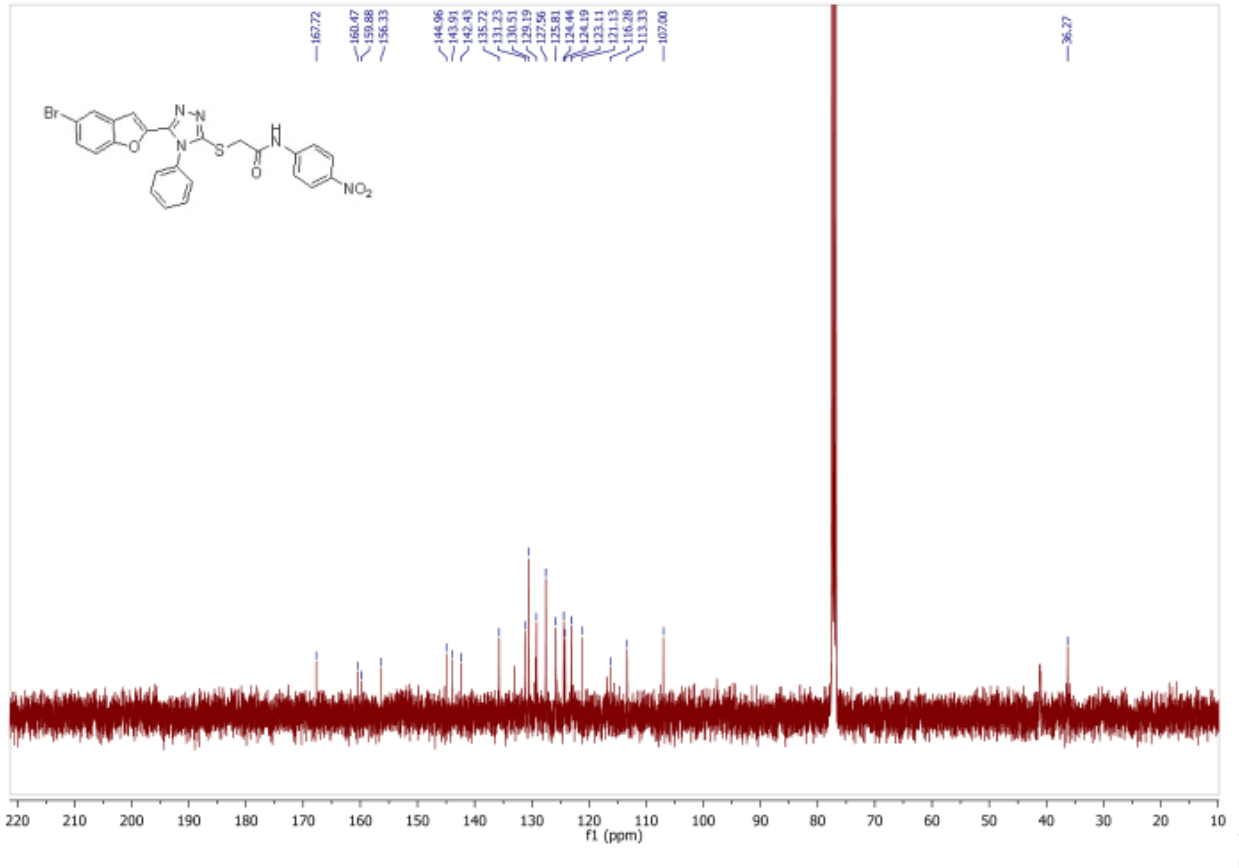

Figure S6: ^{13}C NMR spectrum of 2-((5-(5-bromobenzofuran-2-yl)-4-phenyl-4*H*-1,2,4-triazol-3-yl)thio)-*N*-(4-nitrophenyl)acetamide (**10c**).

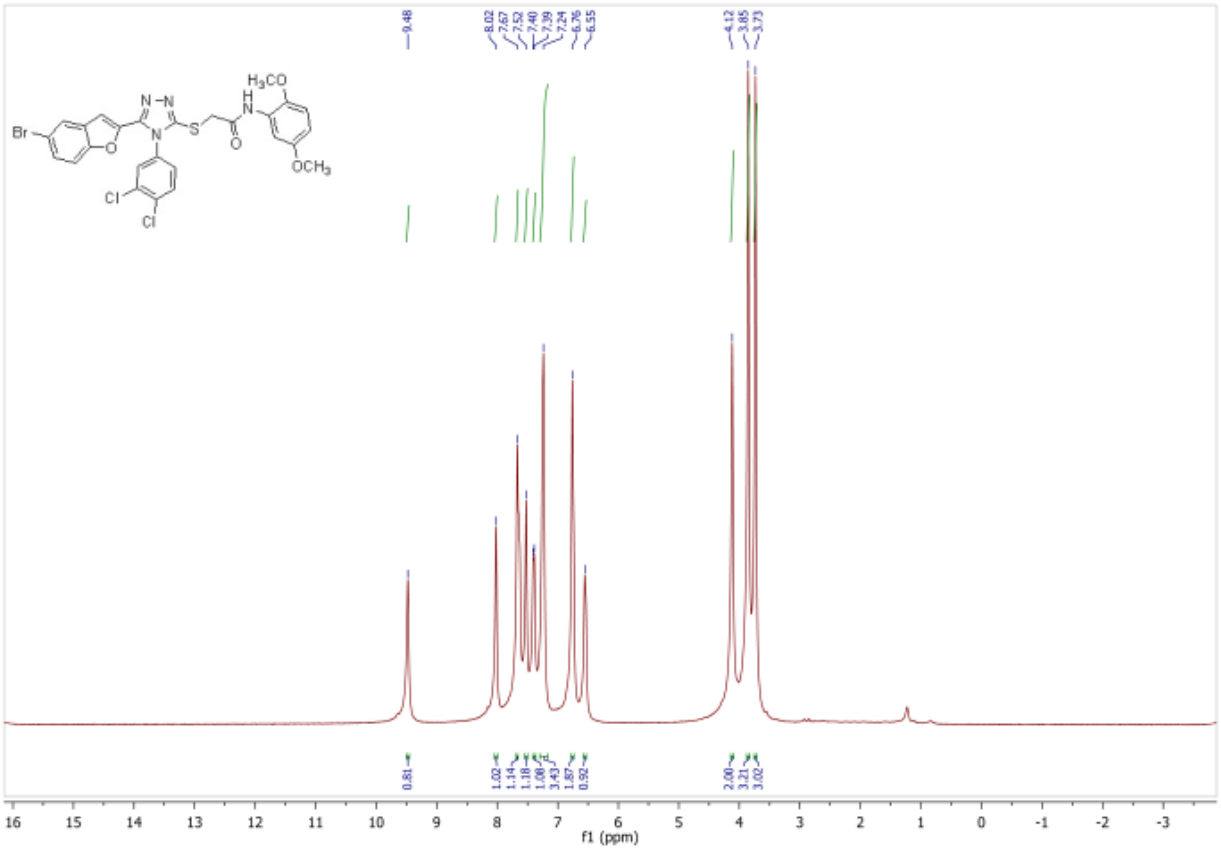

Figure S7: ^{1}H NMR spectrum of 2-((5-(5-bromobenzofuran-2-yl)-4-(3,4-dichlorophenyl)-4*H*-1,2,4-triazol-3-yl)thio)-*N*-(2,5-dimethoxyphenyl)acetamide (**10d**).

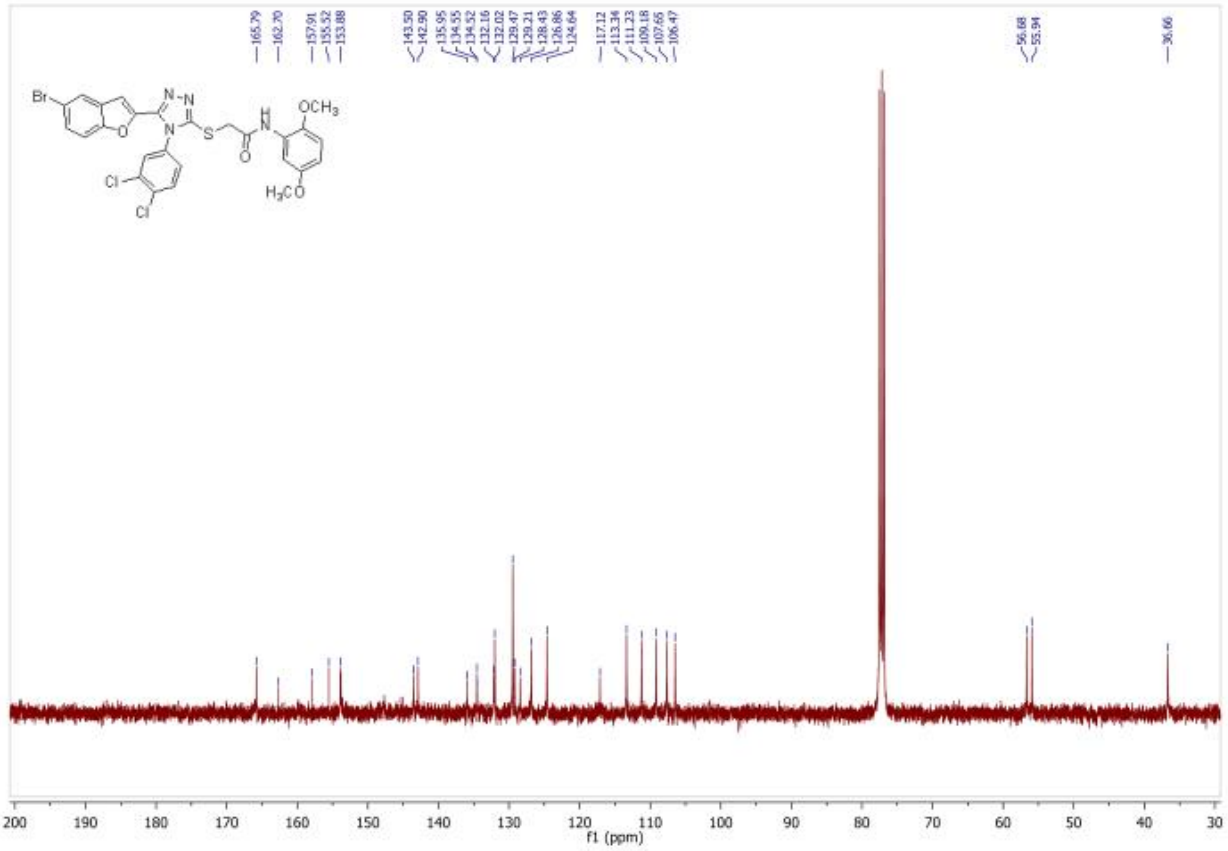

Figure S8: ^{13}C NMR spectrum of 2-((5-(5-bromobenzofuran-2-yl)-4-(3,4-dichlorophenyl)-4*H*-1,2,4-triazol-3-yl)thio)-*N*-(2,5-dimethoxyphenyl)acetamide (**10d**).

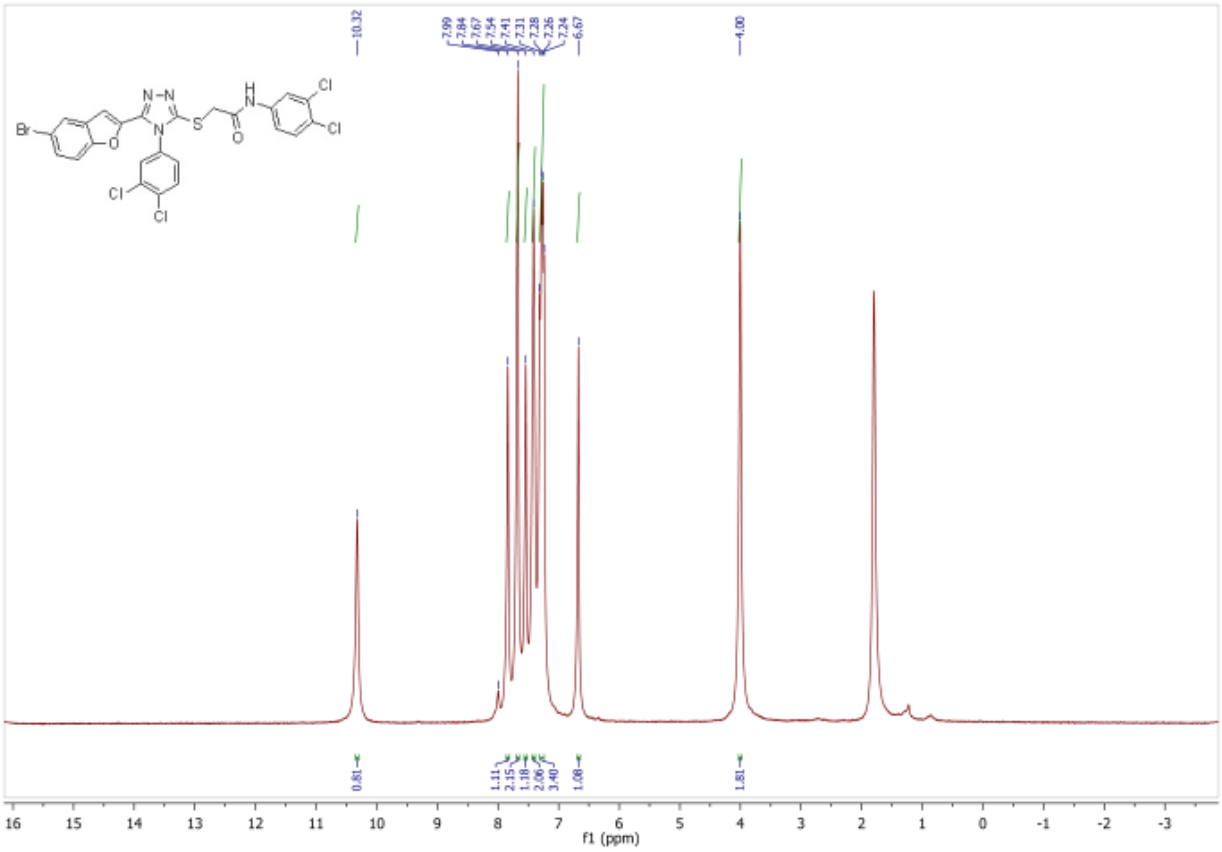

Figure S9: ^{1}H NMR spectrum of 2-((5-(5-bromobenzofuran-2-yl)-4-(3,4-dichlorophenyl)-4*H*-1,2,4-triazol-3-yl)thio)-*N*-(3,4-dichlorophenyl)acetamide (**10e**).

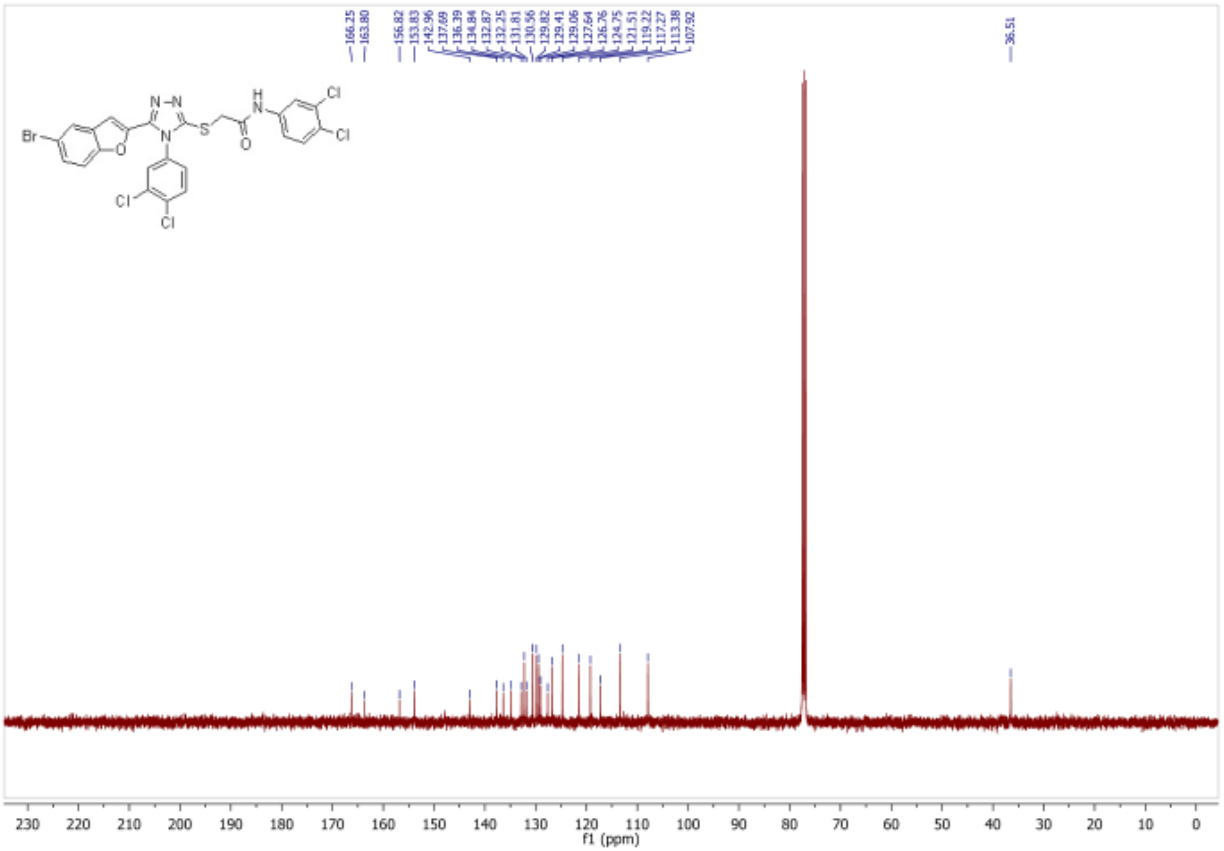

Figure S10: ^{13}C NMR spectrum of 2-((5-(5-bromobenzofuran-2-yl)-4-(3,4-dichlorophenyl)-4*H*-1,2,4-triazol-3-yl)thio)-*N*-(3,4-dichlorophenyl)acetamide (**10e**).

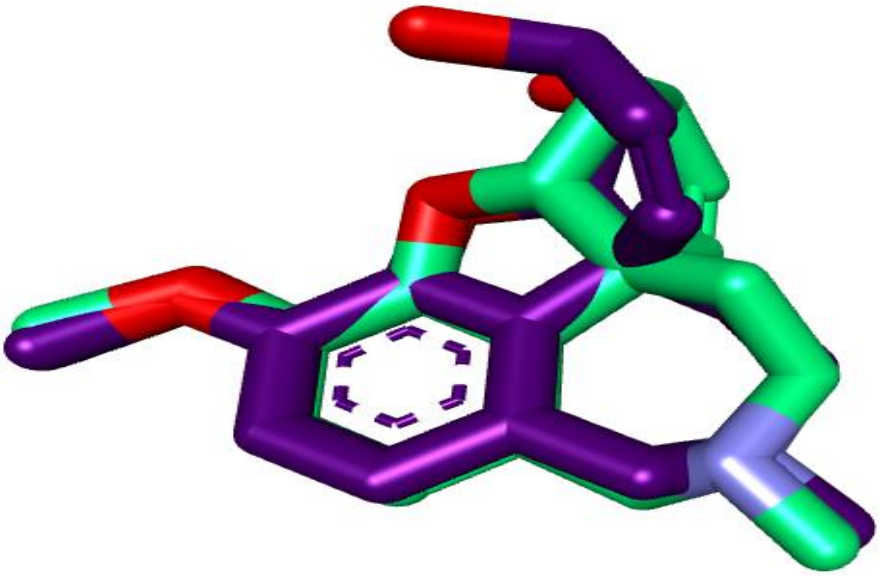

Figure S11. Cognate re-docking of co-crystalized ligand of AChE (4EY6) to validate IFD protocol; Co-crystalized apo-conformation (green) of native ligand aligned against its re-docked conformation reproduced by IFD protocol.