Ultrasonic-Assisted Synthesis of Benzofuran Appended Oxadiazole Molecules as Tyrosinase Inhibitors: Mechanistic Approach through Enzyme Inhibition, Molecular Docking, Chemoinformatics, ADMET and Drug-Likeness Studies

Ali Irfan [1], Ameer Fawad Zahoor [1,*], Shagufta Kamal [2], Mubashir Hassan [3] and Andrzej Kloczkowski[3,4,*]

SUPPLEMENTARY INFORMATION

Spectral analysis of compounds 5a-5j

2-((5-(5-Bromobenzofuran-2-yl)-1,3,4-oxadiazol-2-yl)thio)-N-(2-fluorophenyl)acetamide (5a)

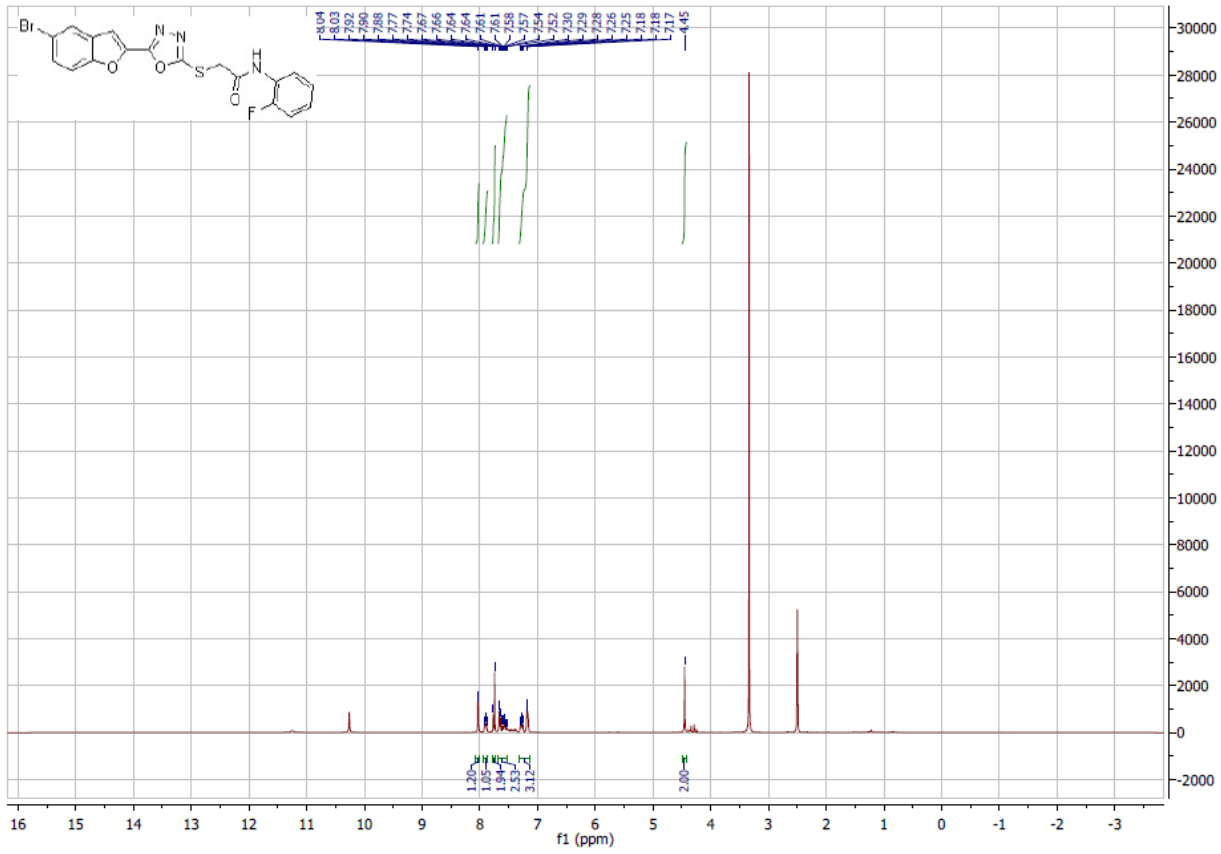

Figure S1.[1]H NMR spectrum of compound **5a**

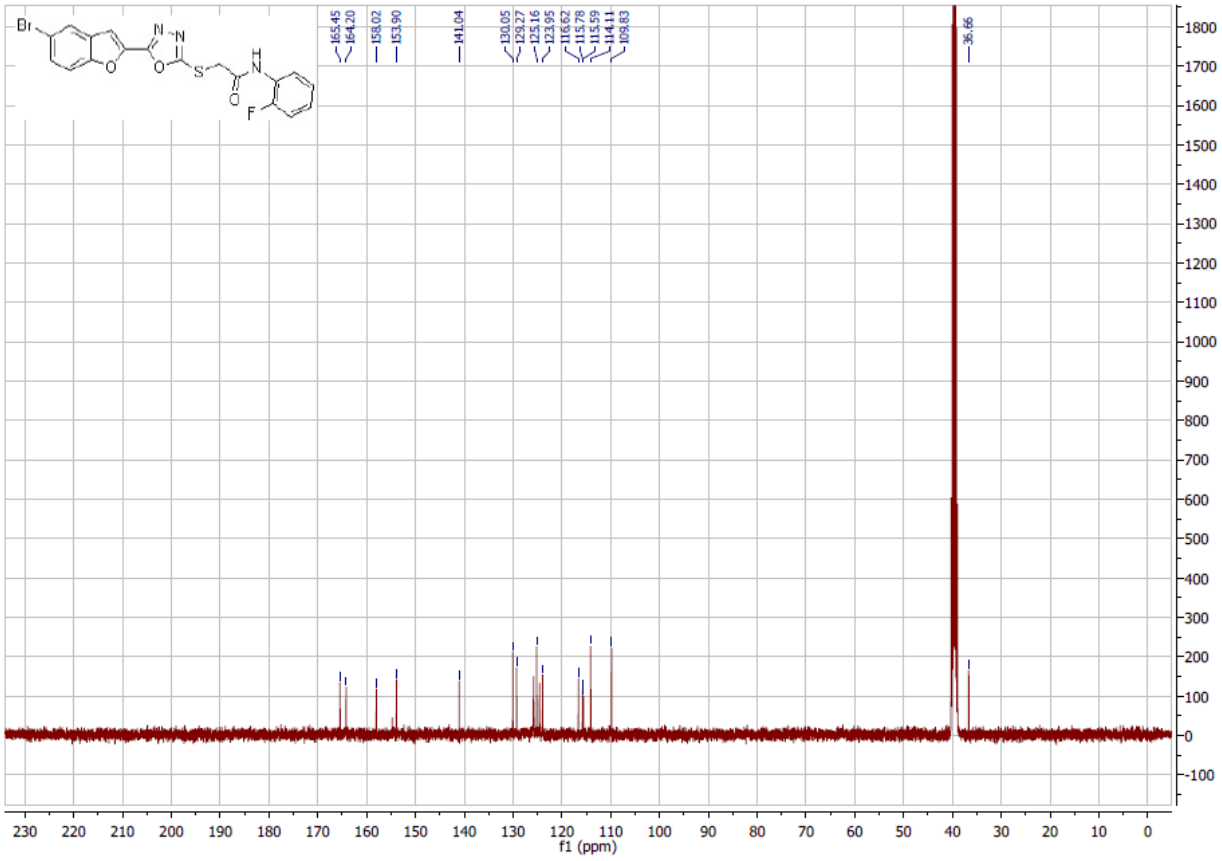

Figure S2. ^{13}C NMR spectrum of compound **5a**

2-((5-(5-Bromobenzofuran-2-yl)-1,3,4-oxadiazol-2-yl)thio)-N-(2-chlorophenyl)acetamide (5b)

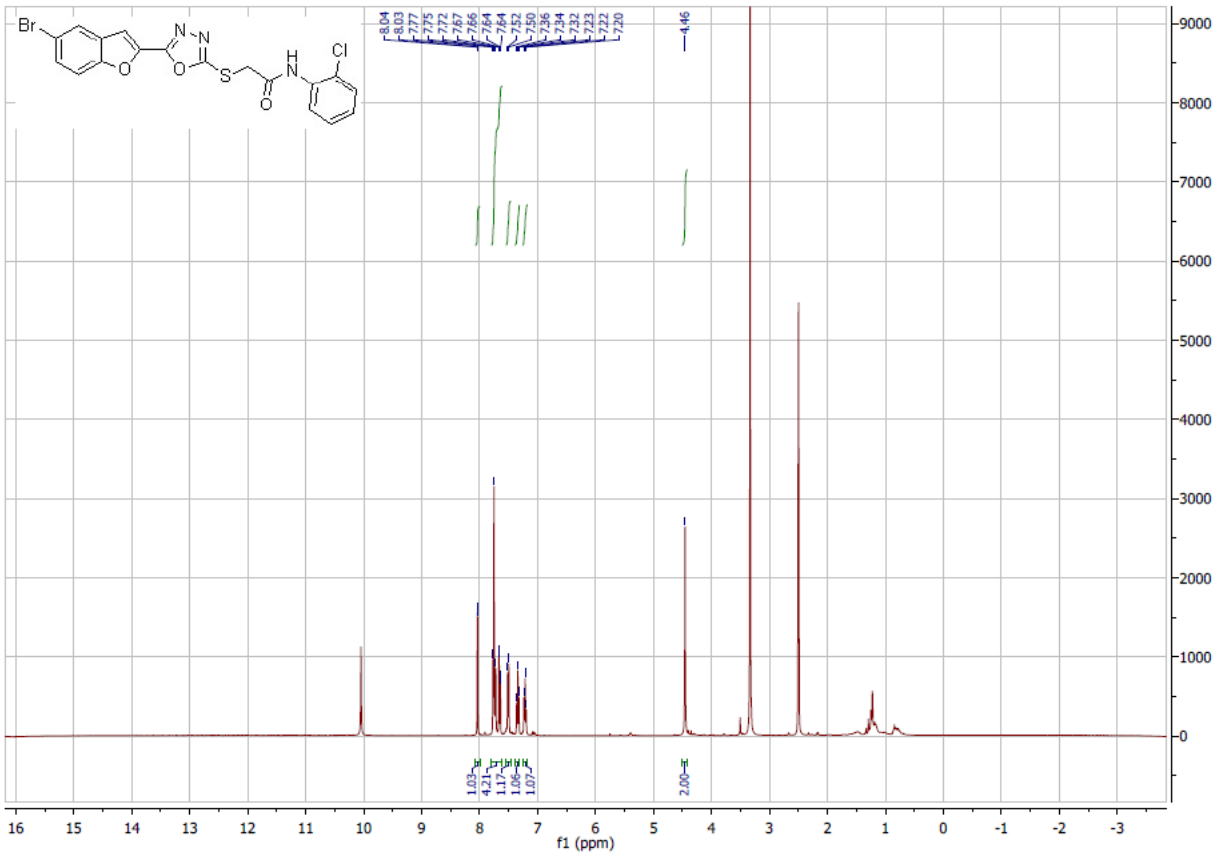

Figure S3.[1]H NMR spectrum of compound **5b**

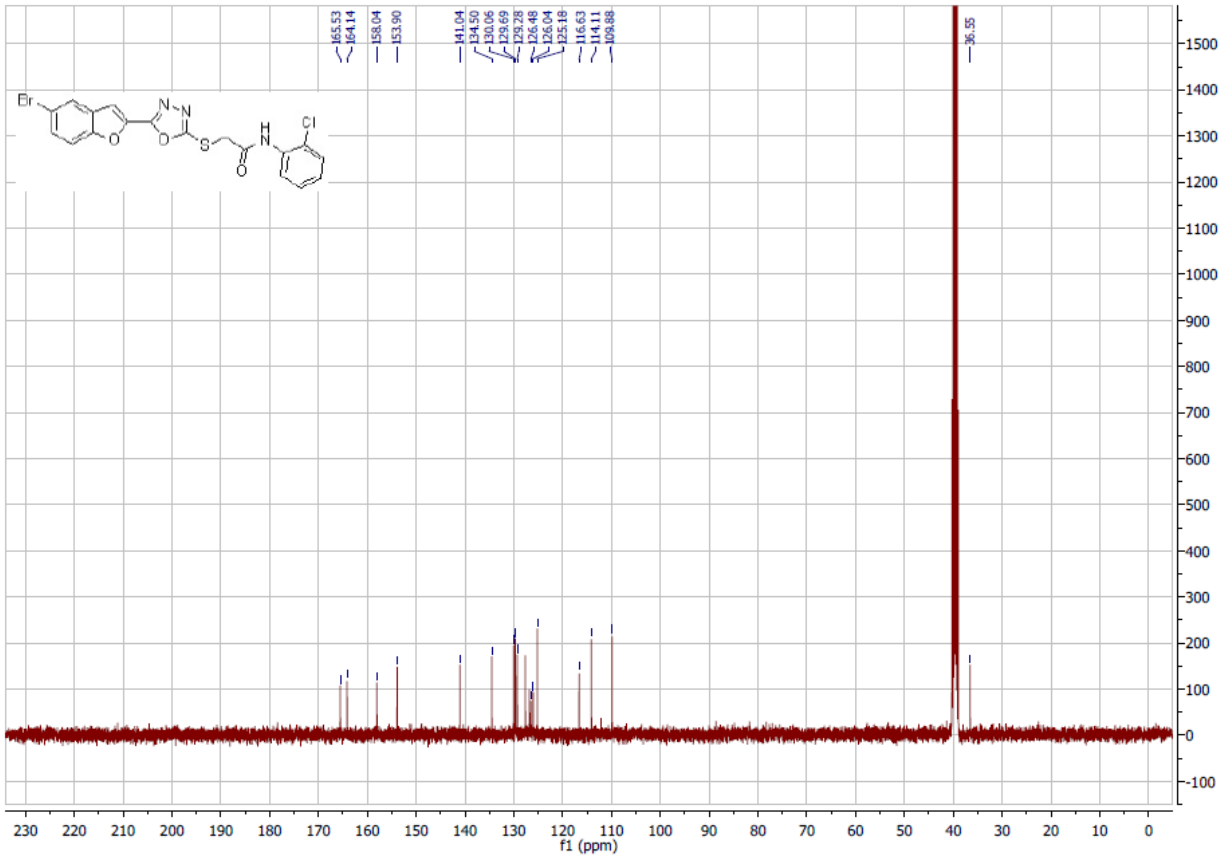

Figure S4. ^{13}C NMR spectrum of compound **5b**

2-((5-(5-Bromobenzofuran-2-yl)-1,3,4-oxadiazol-2-yl)thio)-*N*-(3,4-dichlorophenyl)acetamide (5c)

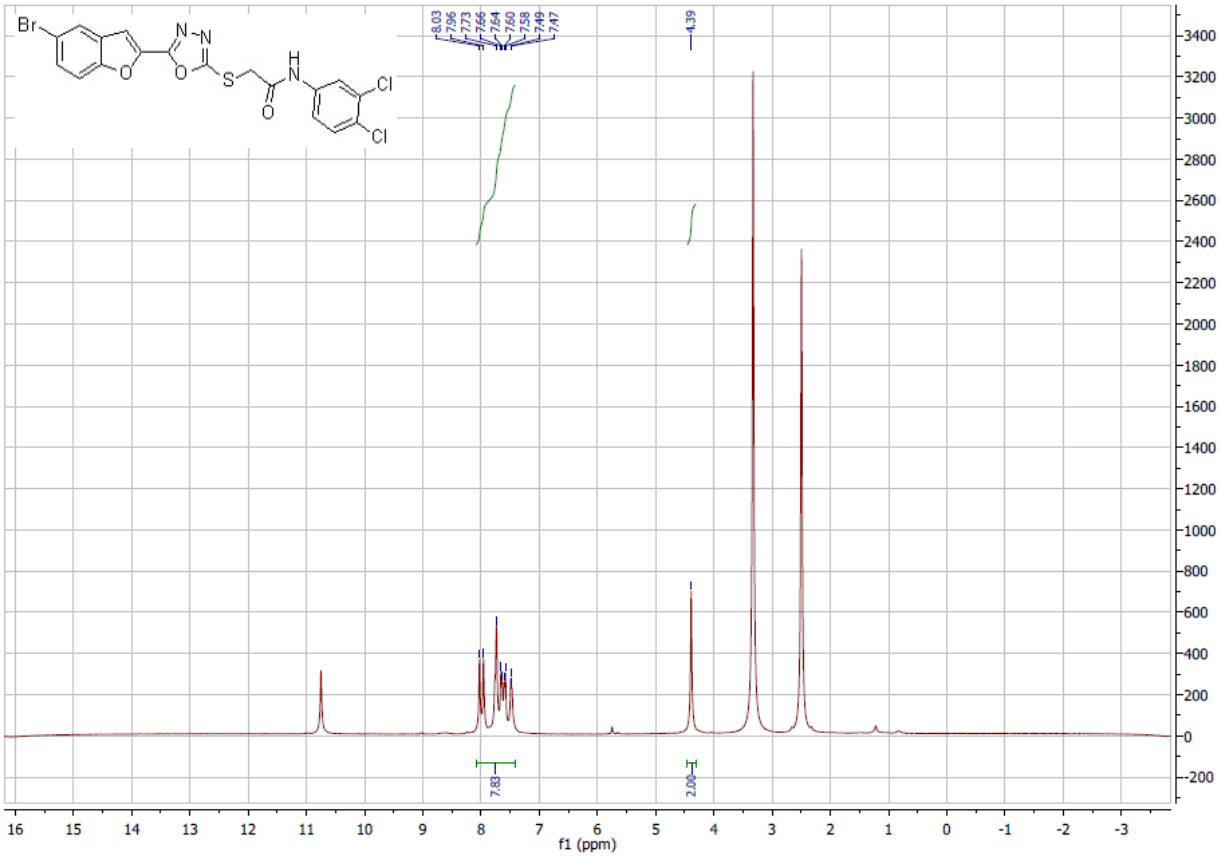

Figure S5.[1]H NMR spectrum of compound **5c**

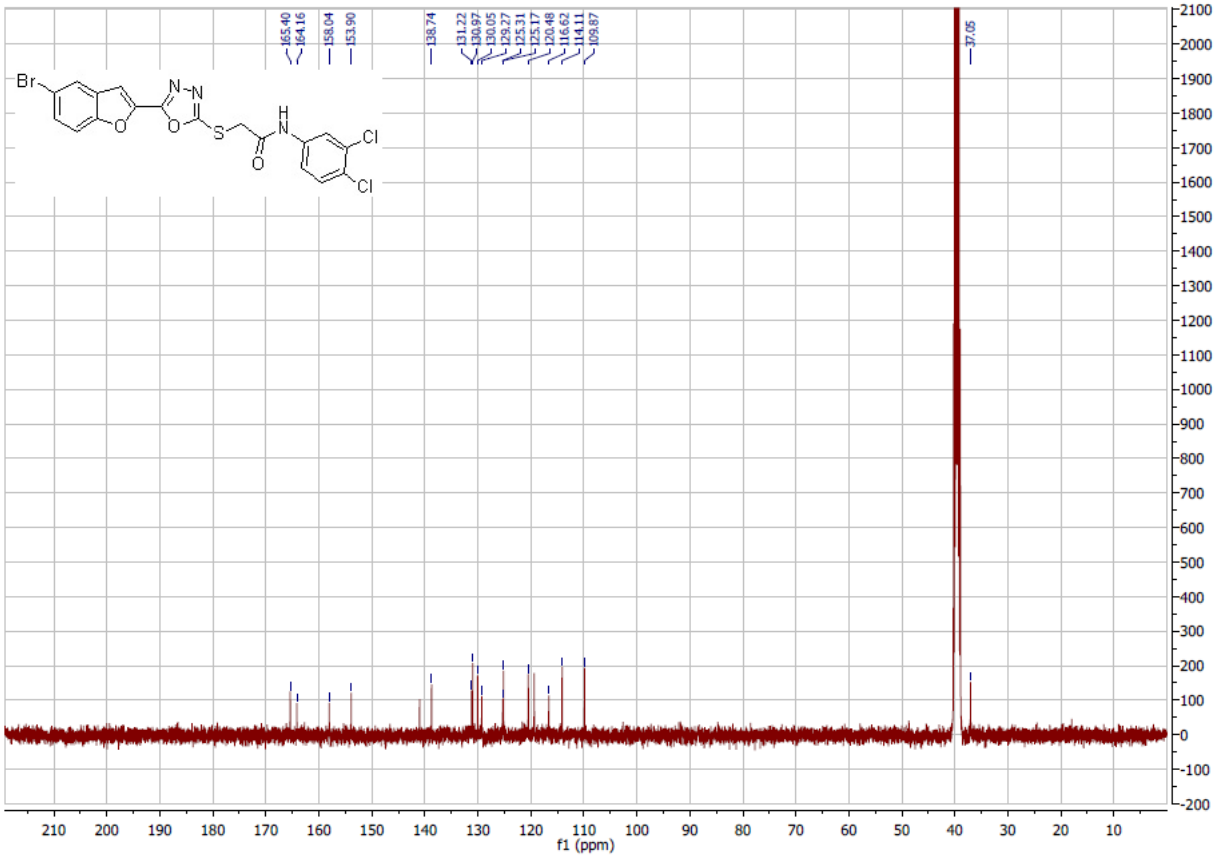

Figure S6. ^{13}C NMR spectrum of compound **5c**

2-((5-(5-bromobenzofuran-2-yl)-1,3,4-oxadiazol-2-yl)thio)-N-(4-fluorophenyl)acetamide (5d)

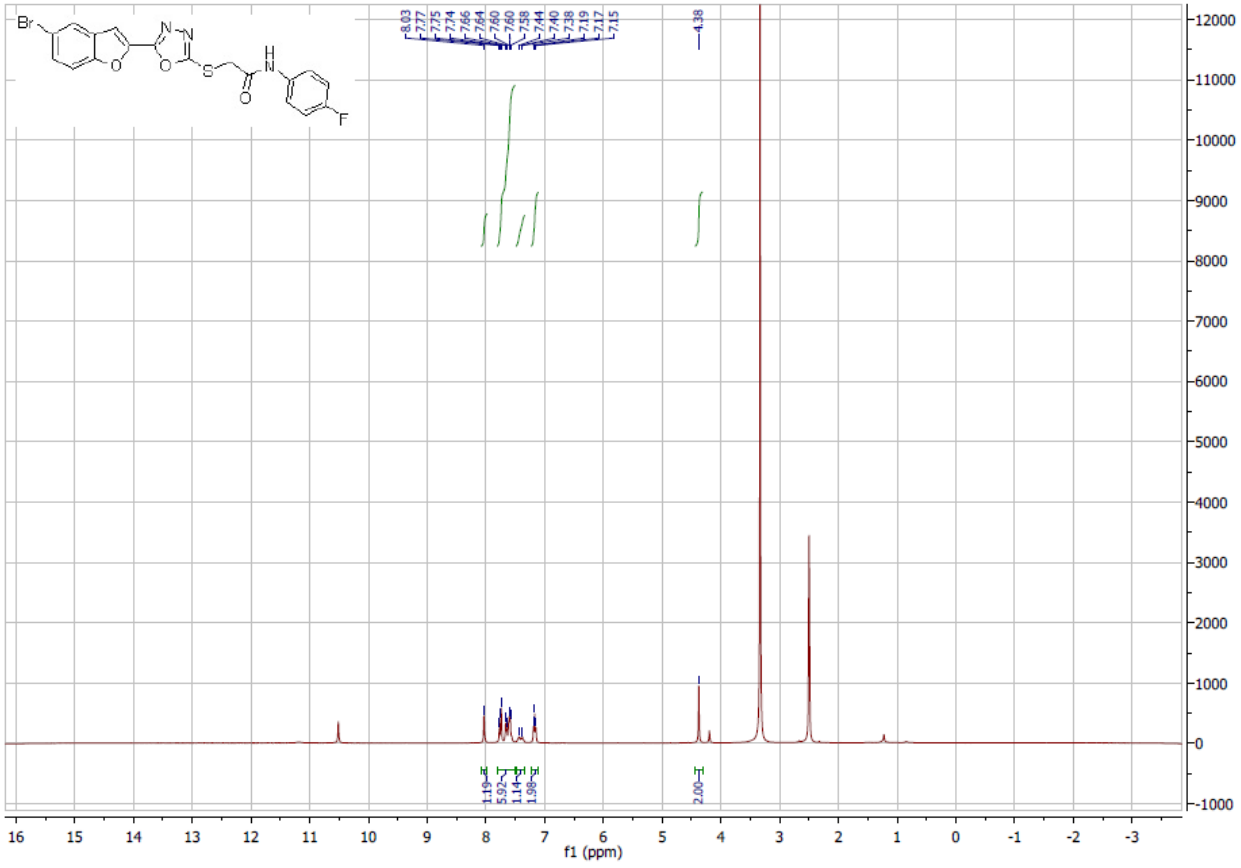

Figure S7.[1]H NMR spectrum of compound **5d**

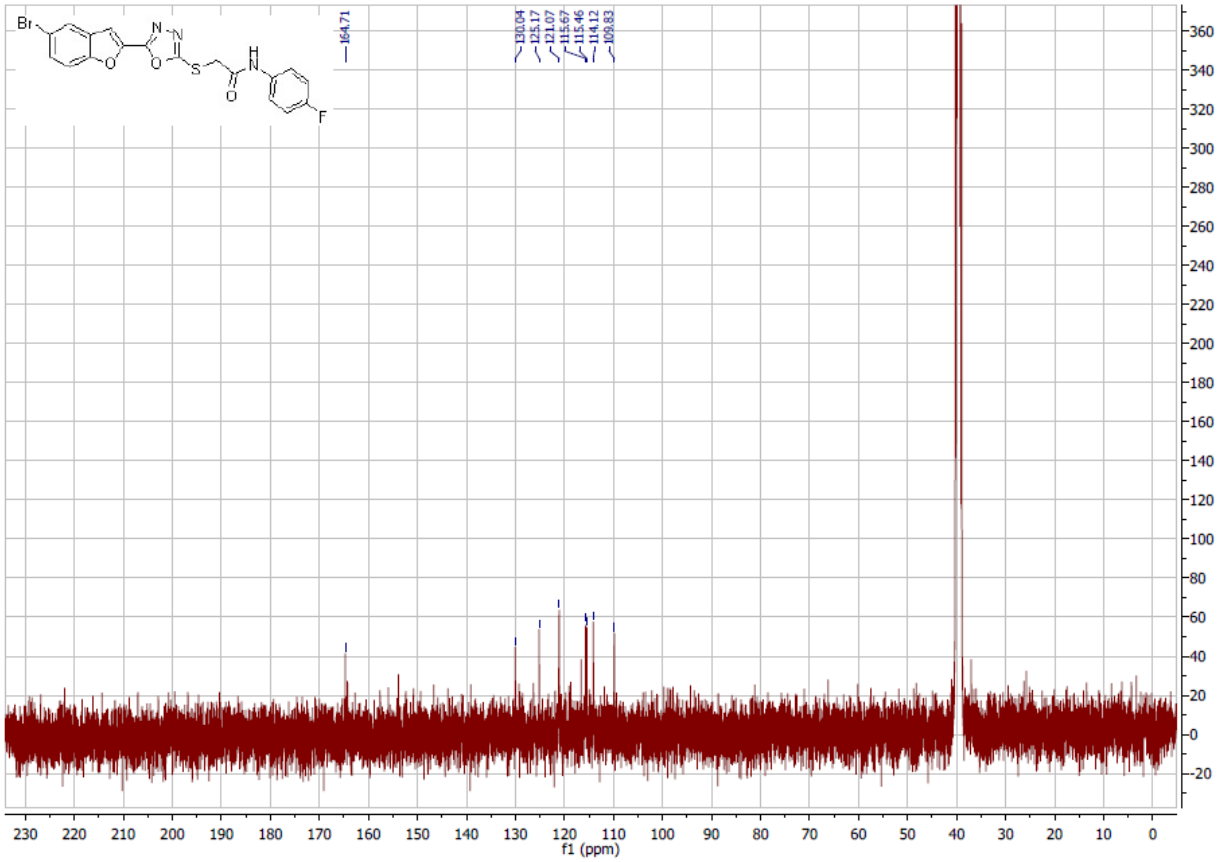

Figure S8. ^{13}C NMR spectrum of compound **5d**

2-((5-(5-bromobenzofuran-2-yl)-1,3,4-oxadiazol-2-yl)thio)-N-(3,4-dimethylphenyl)acetamide (5e)

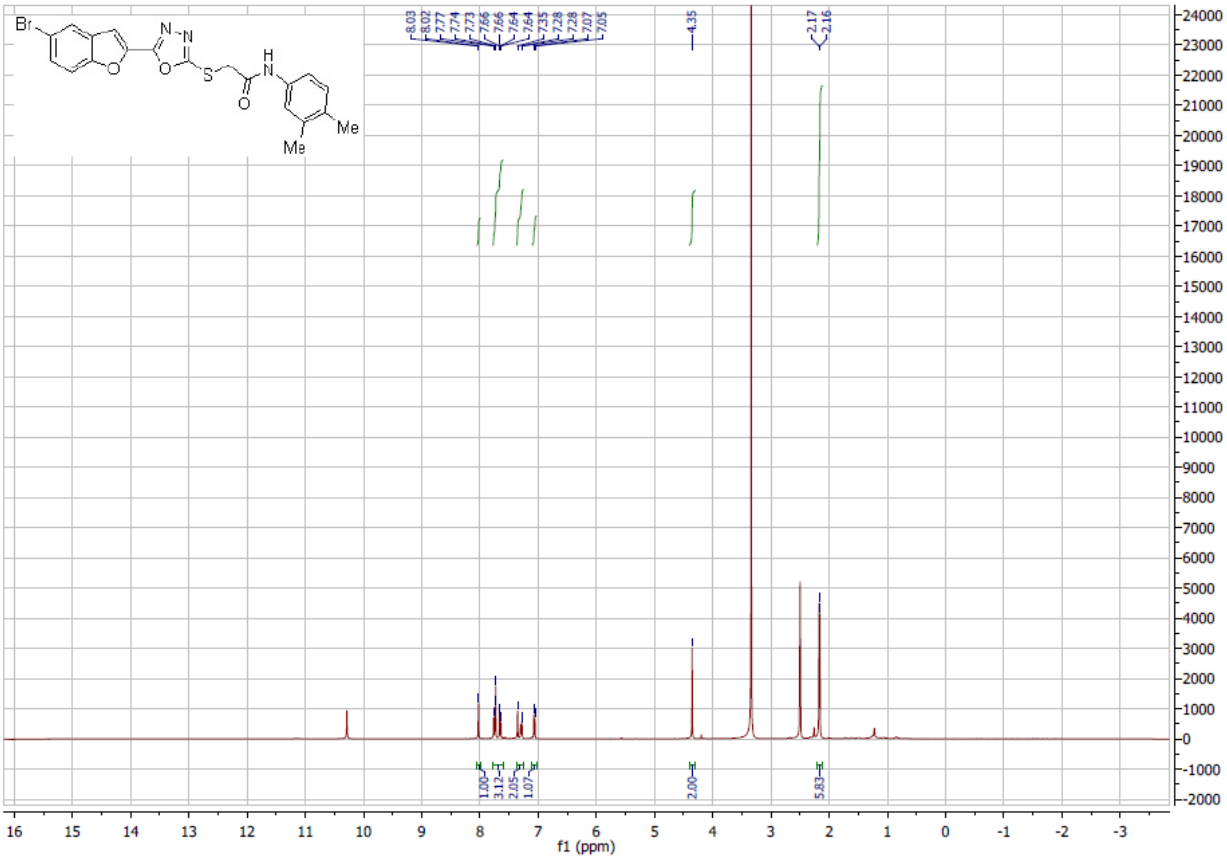

Figure S9.[1]H NMR spectrum of compound **5e**

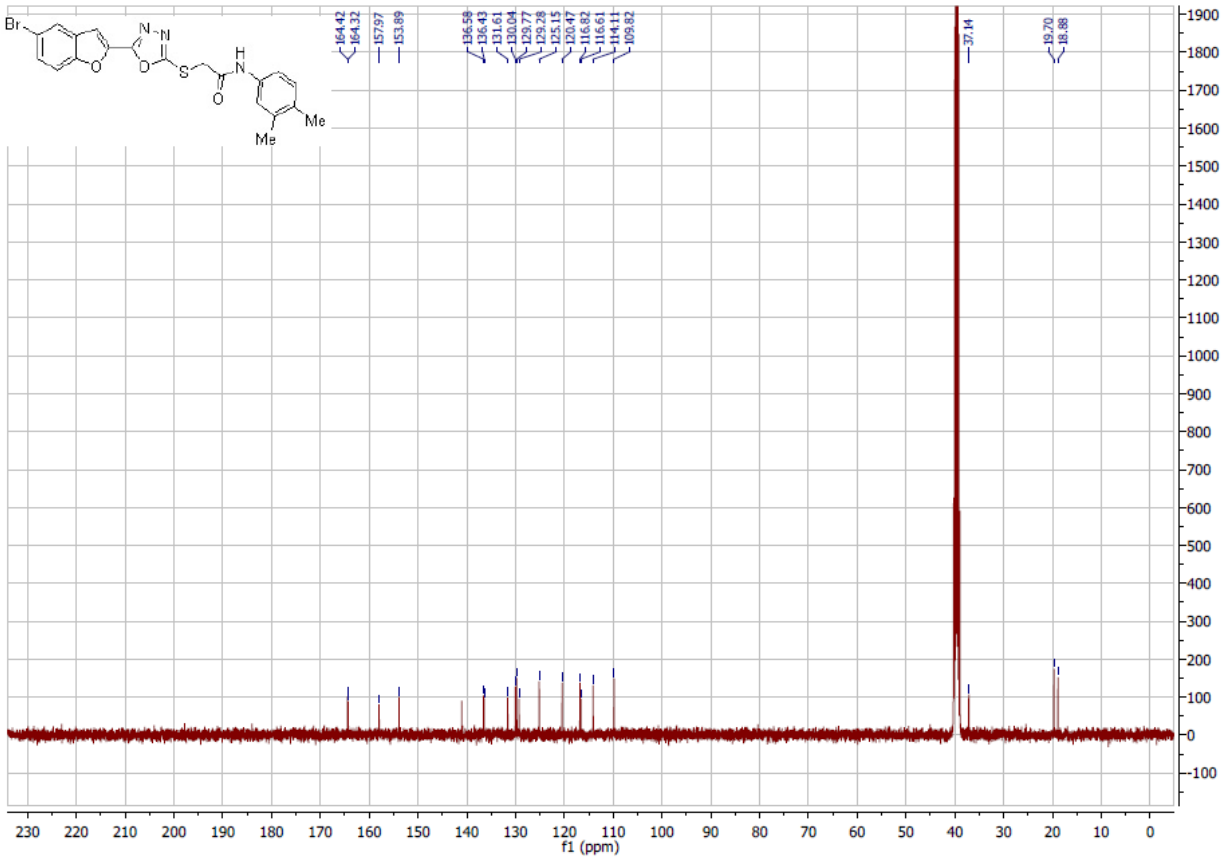

Figure S10. ^{13}C NMR spectrum of compound **5e**

2-((5-(5-Bromobenzofuran-2-yl)-1,3,4-oxadiazol-2-yl)thio)-N-(2-methoxyphenyl)acetamide (5f)

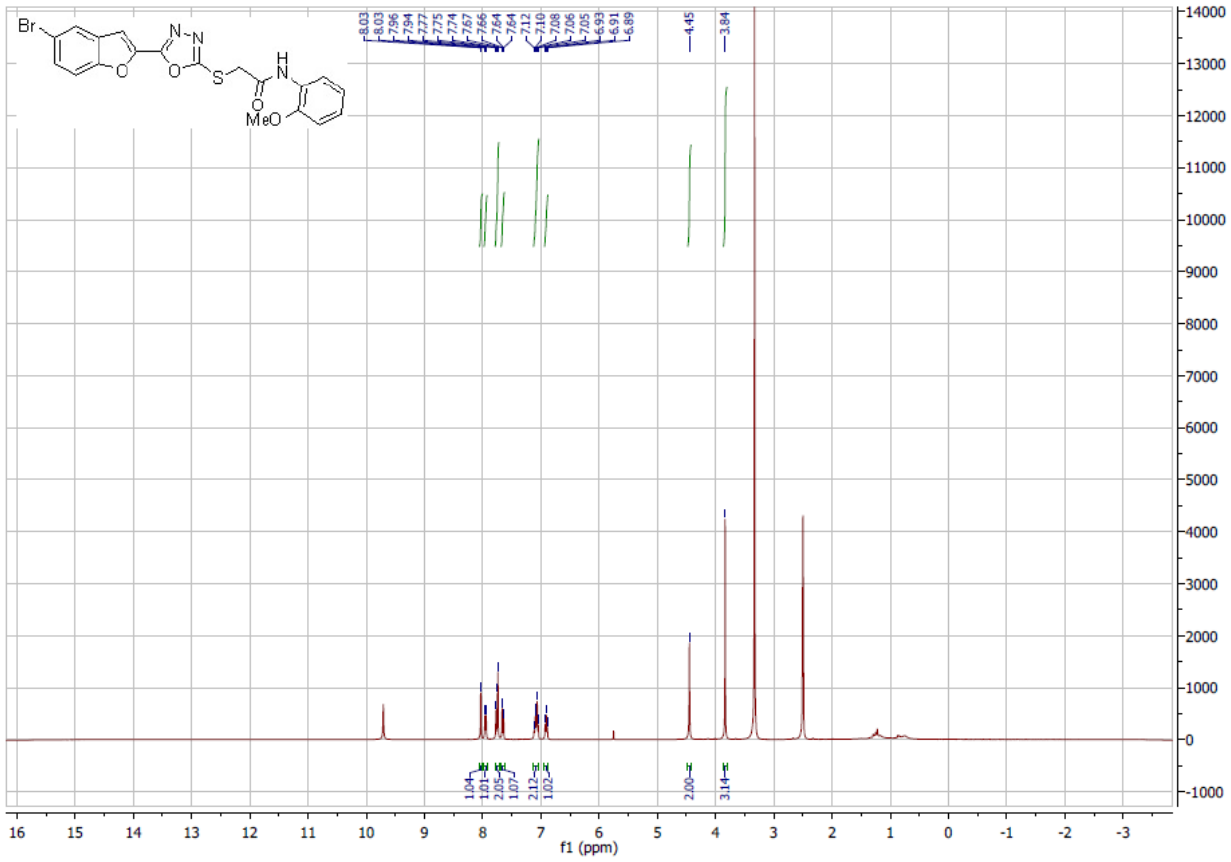

Figure S11^{1}H NMR spectrum of compound **5f**

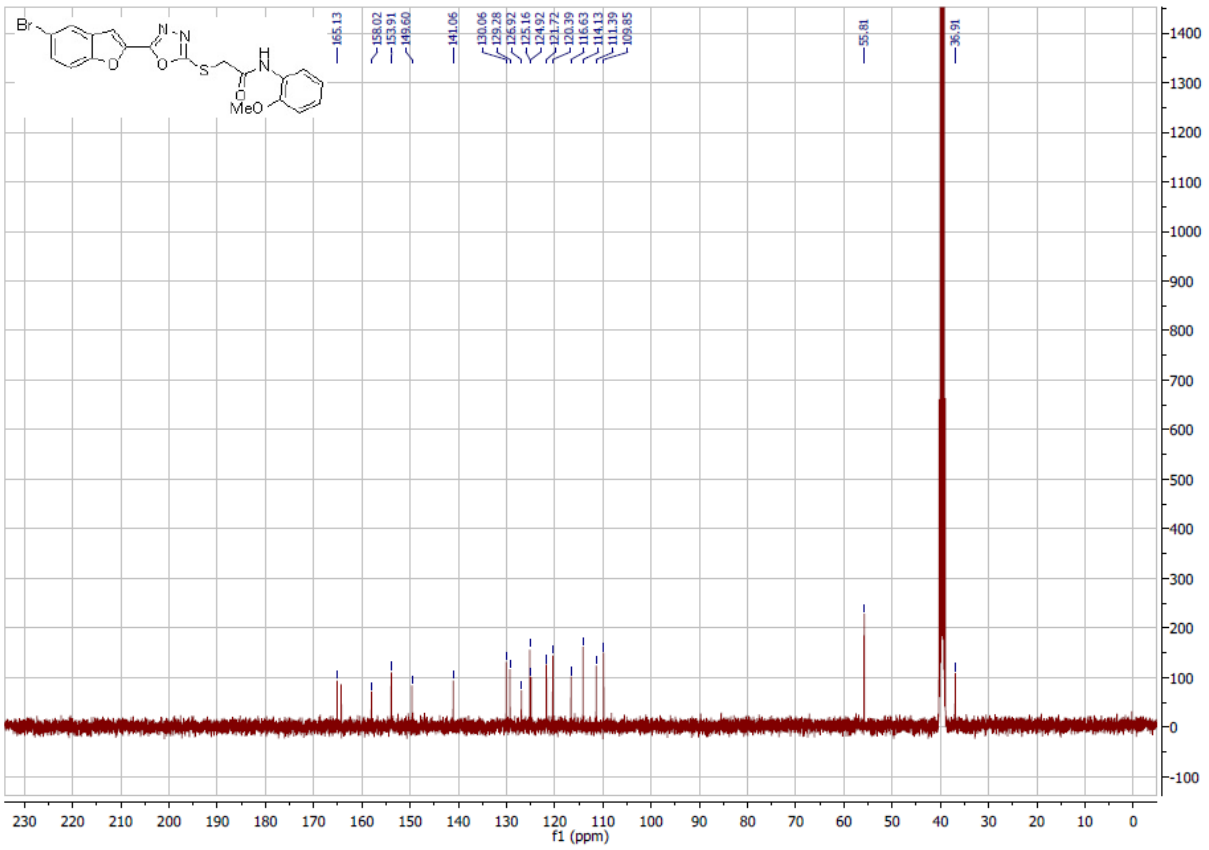

Figure S12. ^{13}C NMR spectrum of compound **5f**

2-((5-(5-Bromobenzofuran-2-yl)-1,3,4-oxadiazol-2-yl)thio)-*N*-phenylacetamide (5g)

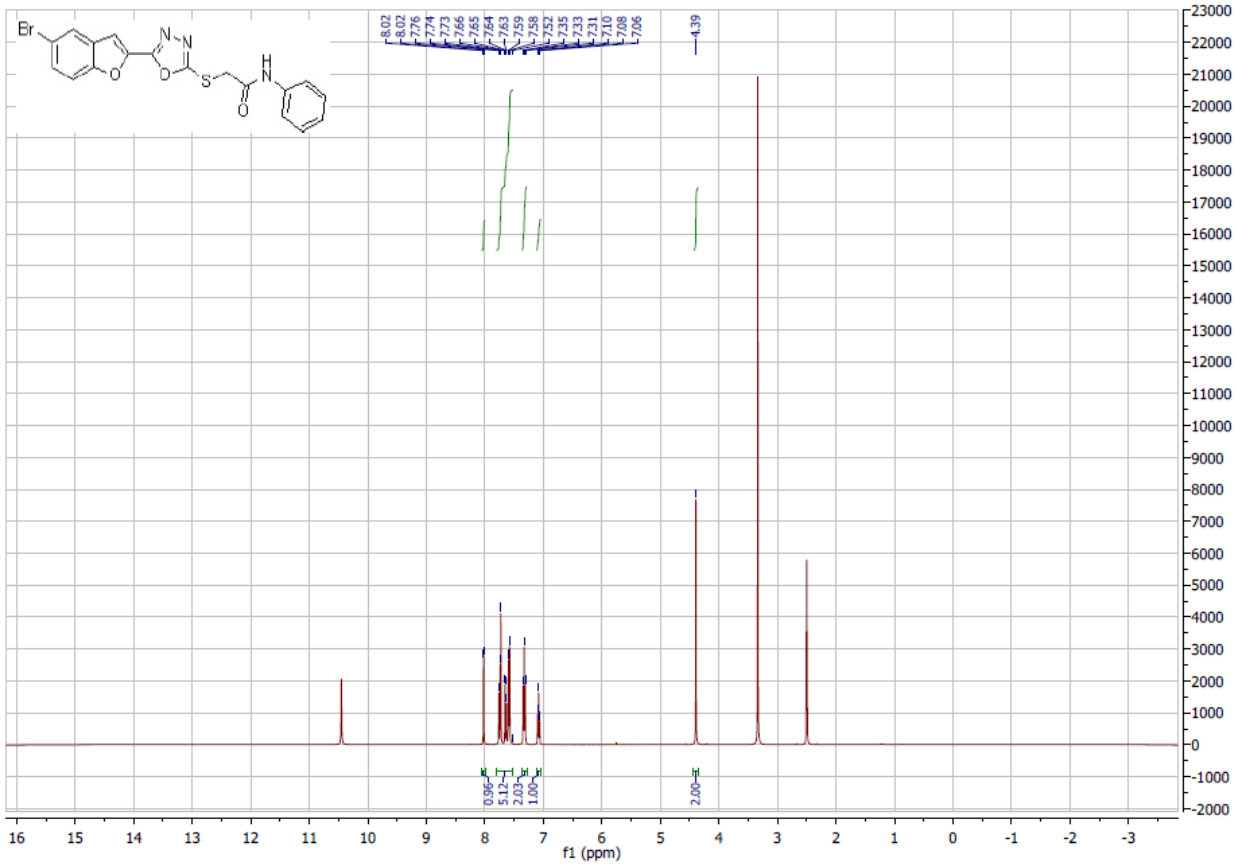

Figure S13. ^{1}H NMR spectrum of compound **5g**

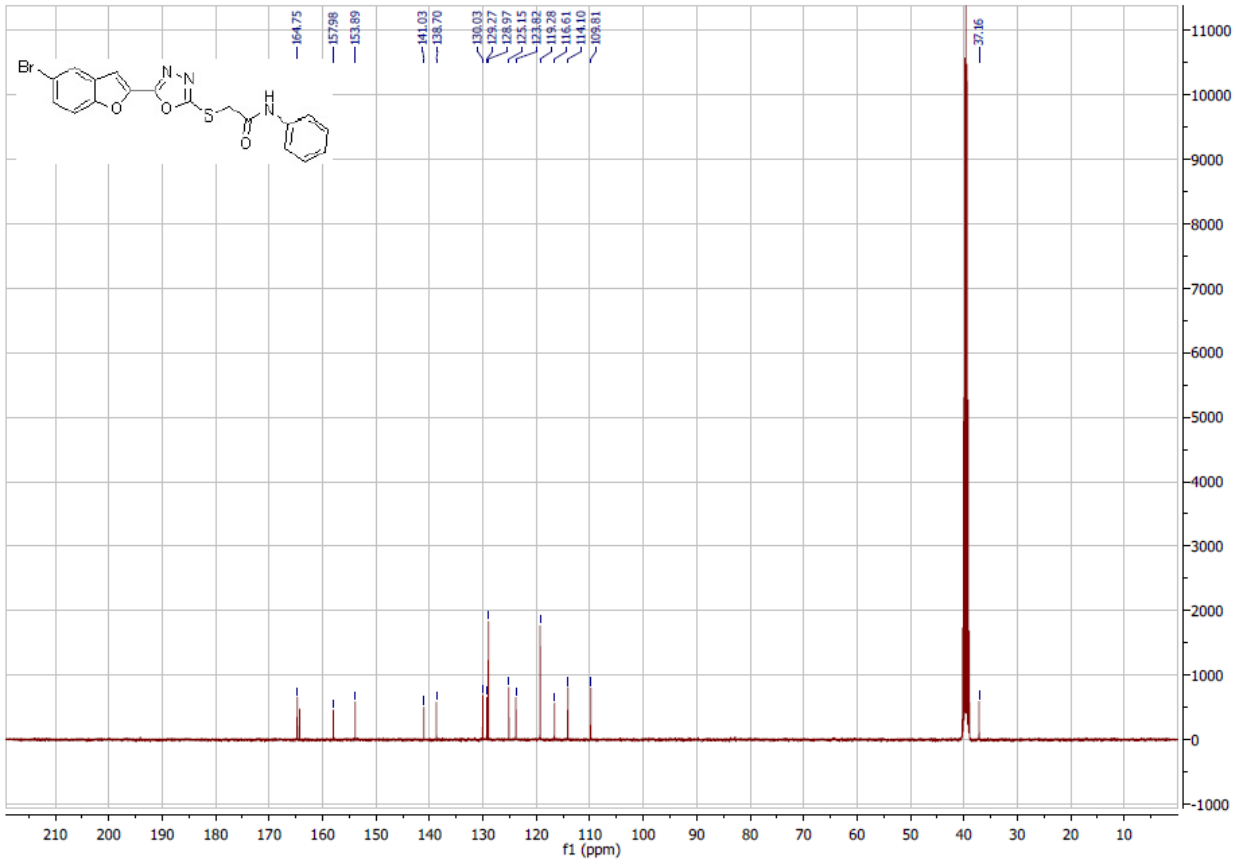

Figure S14. ^{13}C NMR spectrum of compound **5g**

2-((5-(5-Bromobenzofuran-2-yl)-1,3,4-oxadiazol-2-yl)thio)-*N*-(2,4-dimethylphenyl)acetamide (5h)

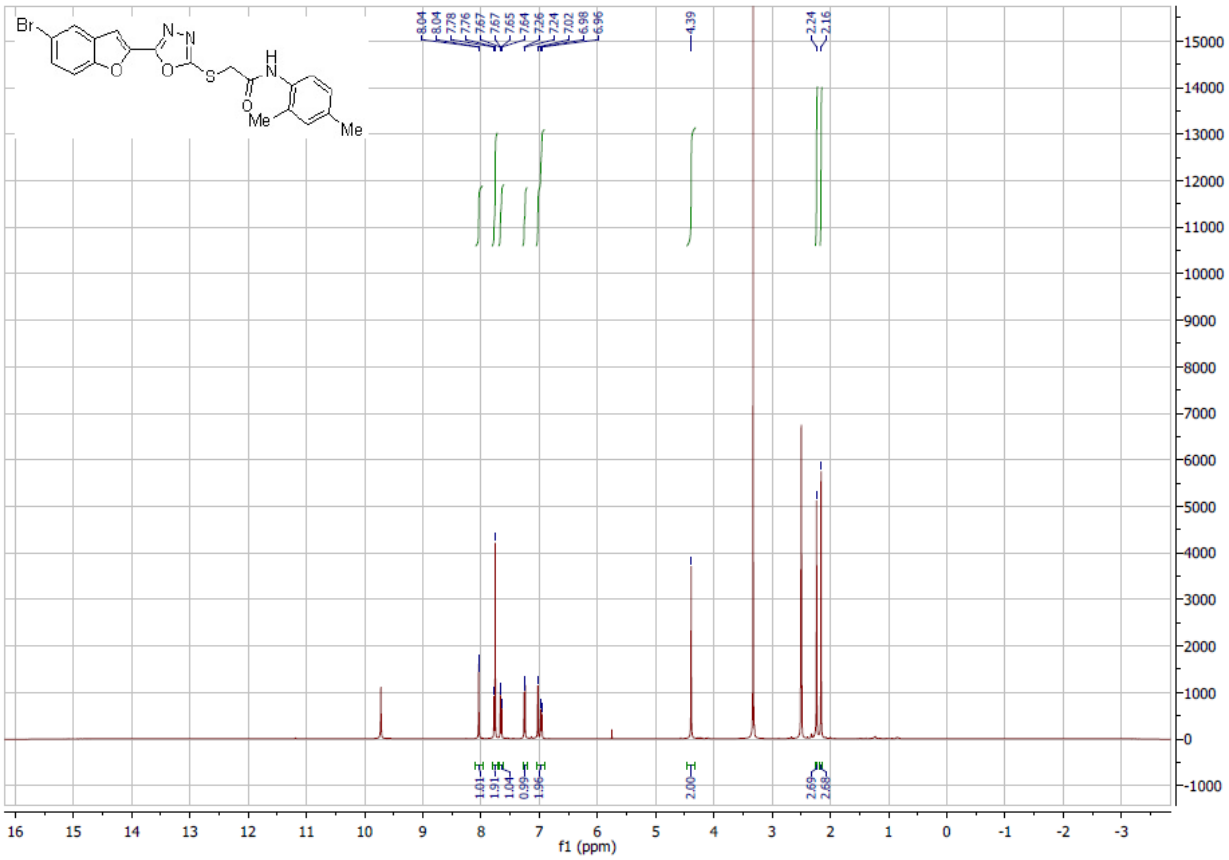

Figure S15. ^{1}H NMR spectrum of compound **5h**

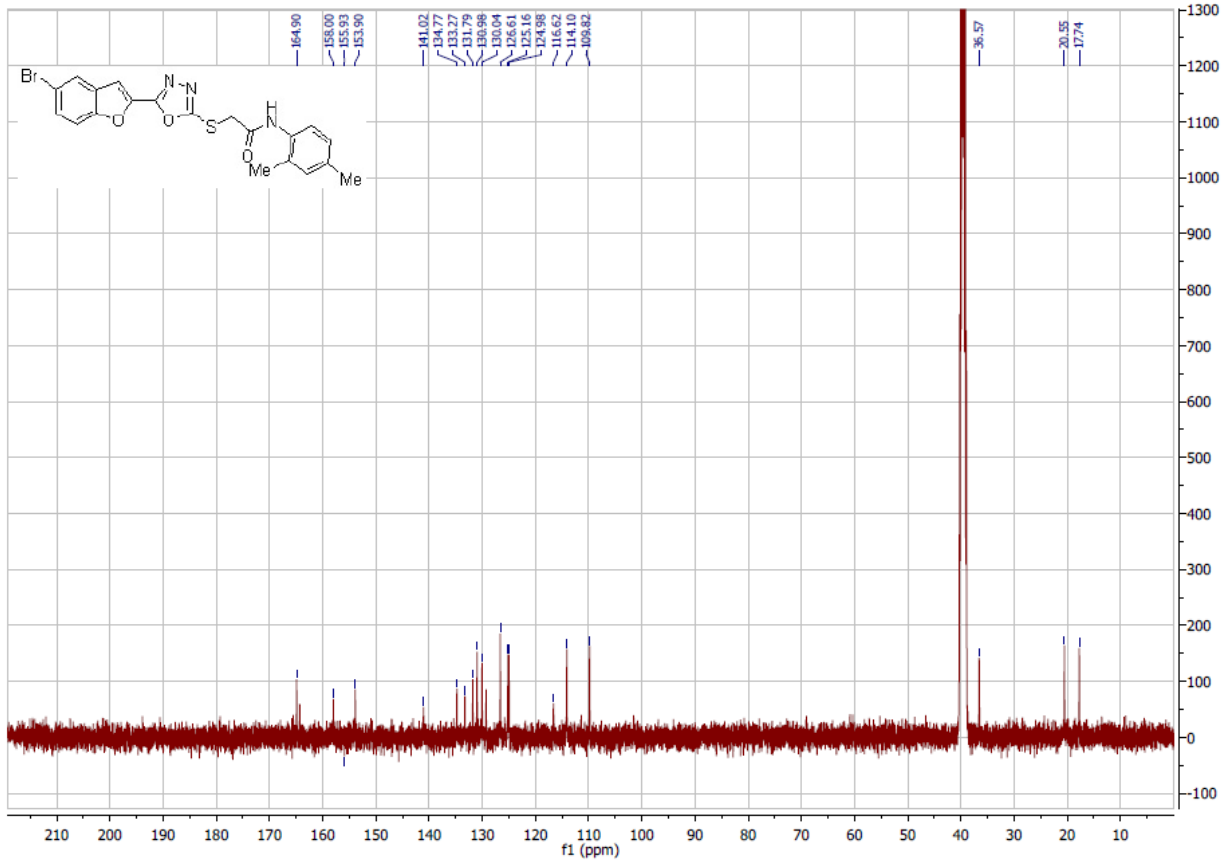

Figure S16. ^{13}C NMR spectrum of compound **5h**

2-((5-(5-Bromobenzofuran-2-yl)-1,3,4-oxadiazol-2-yl)thio)-N-(2,5-dimethoxyphenyl)acetamide (5i)

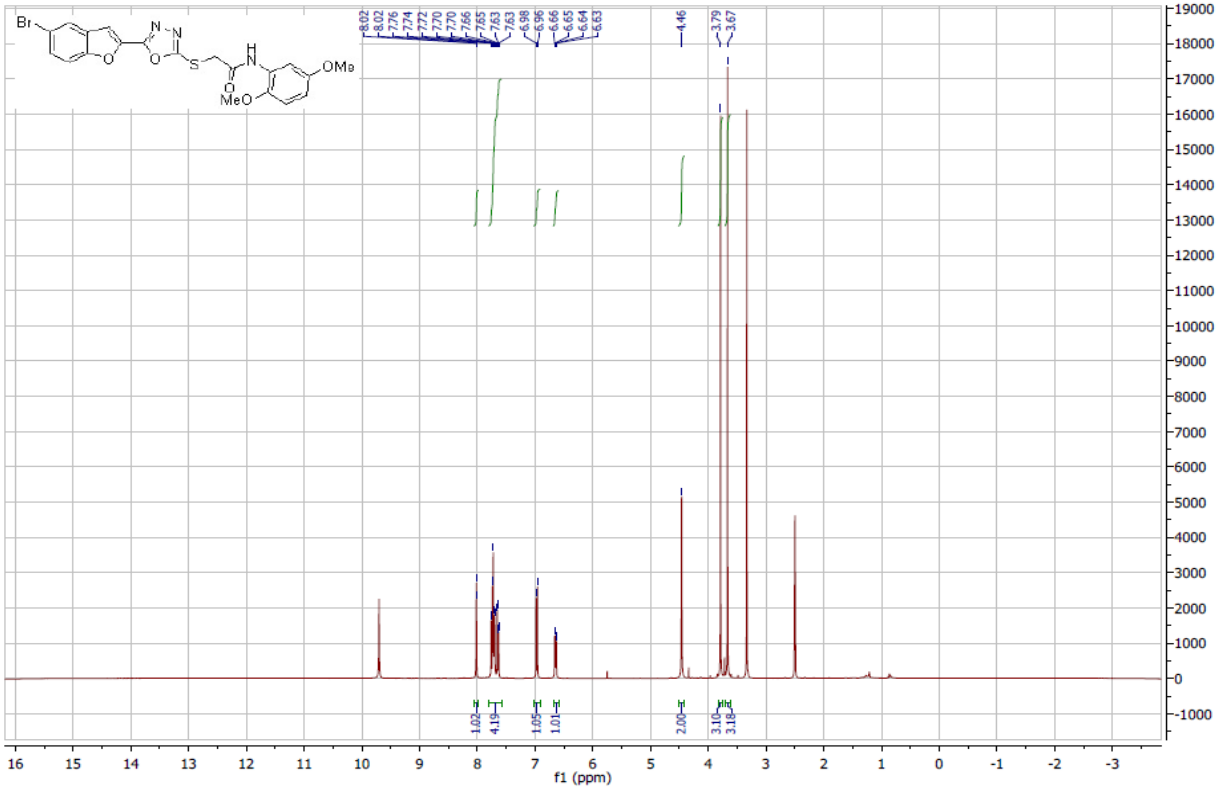

Figure S17.[1]H NMR spectrum of compound **5i**

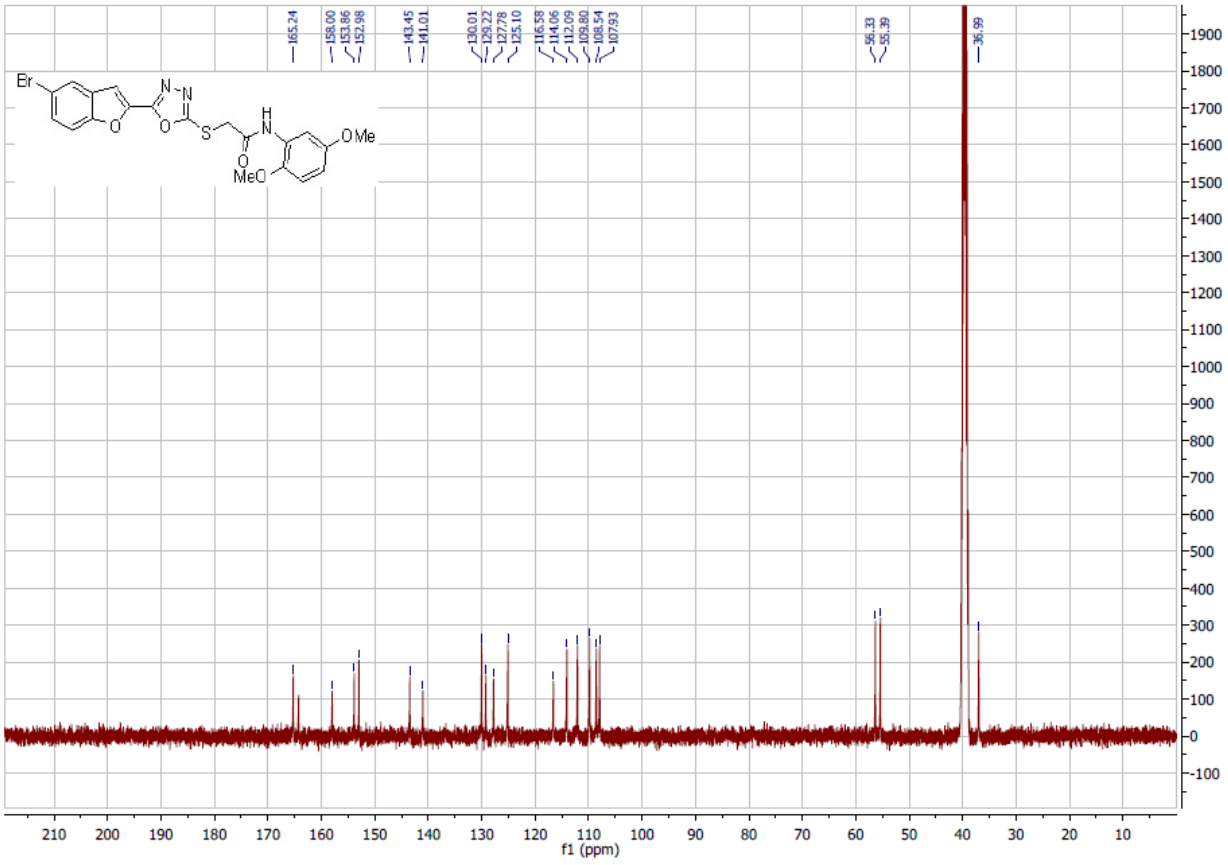

Figure S18. ^{13}C NMR spectrum of compound **5i**

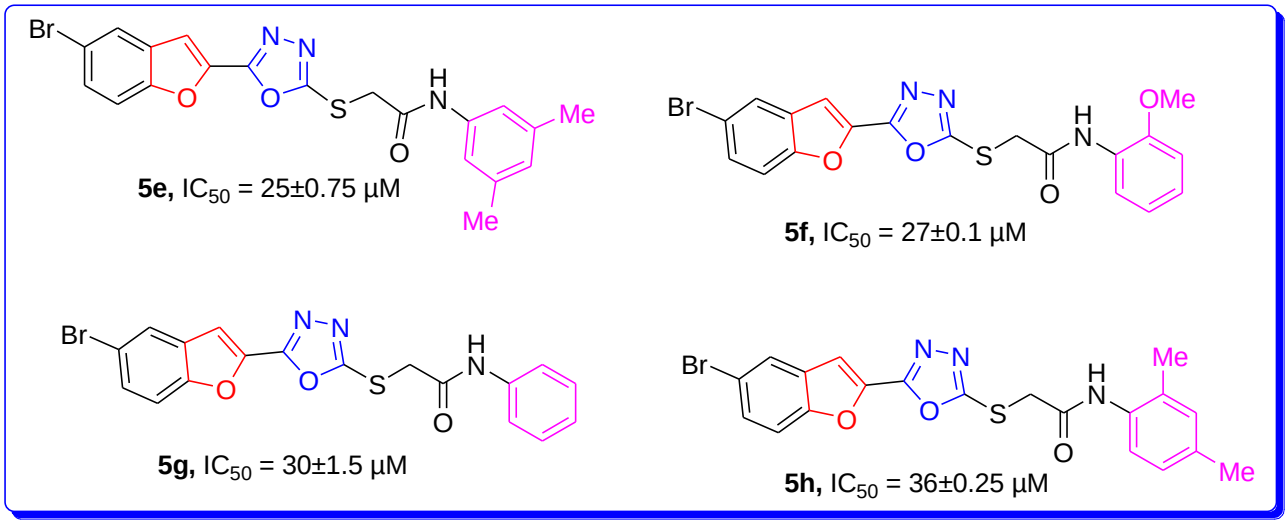

Figure S19. The moderate biologically active oxadiazole based furan derivatives **5e**- **5h** as tyrosinase inhibitors

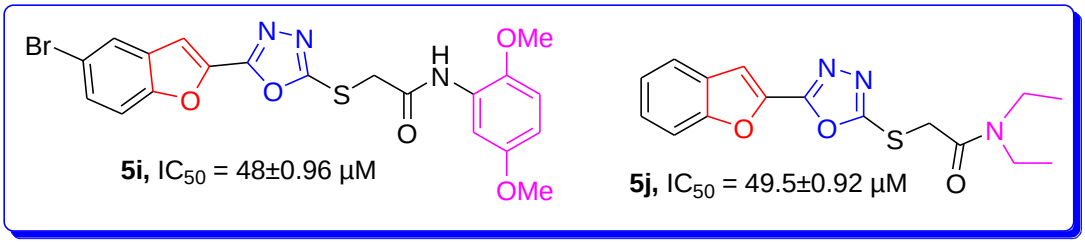

Figure S20. The least biologically active oxadiazole based furan derivatives **5i**- **5j** as tyrosinase inhibitors