



Evaluation of Antioxidant Activities of Novel Tetralone-Derived Triazoles Derivatives: Synthesis and *in silico* Studies

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In present study, twelve novel tetralone-linked triazole derivatives (**6a-l**) were synthesised and structurally characterised using ¹H NMR, ¹³C NMR and mass spectrometric techniques. The antioxidant potential of the synthesised compounds was evaluated through 2,2-diphenyl-1-picrylhydrazyl (DPPH) radical scavenging and lipid peroxidation (LPO) inhibition assays. Among the tested derivatives, compounds **6e**, **6h**, **6d** and **6i** consistently exhibited the strongest antioxidant activities. In the DPPH assay, compound **6e** demonstrated the highest radical-scavenging capacity with 79.9% inhibition at 120 µM, followed by **6h** (64.3%), **6d** (56.18%) and **6i** (51.8%), reflecting a clear dose-dependent response. These findings were further supported by the LPO assay, where the same four derivatives showed significant protection against oxidative damage to lipid membranes. At 120 µM, compound **6e** displayed the most potent activity with showing 79.9% inhibition, while **6h**, **6d** and **6i** exhibited 64.3%, 60.1% and 52.12% inhibition, respectively. The corresponding IC₅₀ values (24-30 µM) further confirmed their strong ability to suppress the chain-propagation phase of lipid peroxidation. Moreover, the molecular docking studies were performed to investigate the interactions of the synthesised derivatives with the oxidoreductase protein (PDB ID: 3NM8) and their pharmacokinetic profiles were predicted using *in silico* absorption, distribution, metabolism, excretion and toxicity (ADMET) analysis.

Keywords: Tetralone-linked triazole derivatives, Antioxidant activity, Molecular docking, ADMET analysis.