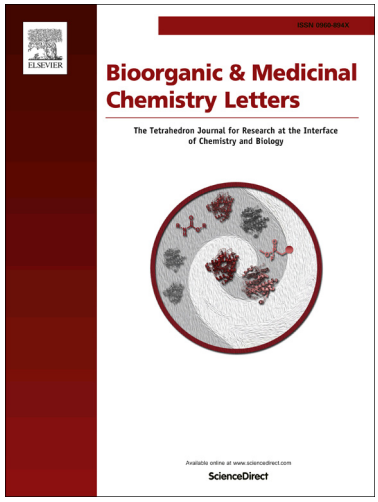

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Synthesis of Novel Derivatives of Oxindole, their Urease Inhibition and Molecular Docking Studies

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Abstract: We synthesized a series of novel **5-24** derivatives of oxindole**.** The synthesis started from 5-chlorooxindole, which was condensed with methyl 4-carboxybezoate and result in the formation of benzolyester derivatives of oxindole which was then treated with hydrazine hydrate. The oxindole benzoylhydrazide was treated with aryl acetophenones and aldehydes to get target compounds **5-24**. The synthesized compounds were evaluated for urease inhibition; the compound **5** (IC_{50} = 13.00 ± 0.35 μM) and **11** (IC_{50} = 19.20 ± 0.50 μM) showed potent activity as compared to the standard drug thiourea (IC_{50} = 21.00 ± 0.01 μ M). Other compounds showed moderate to weak activity. All synthetic compounds were characterized by different spectroscopic techniques including ^{1}H-NMR, ^{13}C-NMR, IR and EI MS. The molecular interactions of the active compounds within the binding site of Urease enzyme were studied through molecular docking simulations.

Keywords: Oxindole, urease activity, docking studies, novel derivatives

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