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Triethylamine-based ionic liquids as anticancer agent: Synthesis, characterization, *in silico* and DFT studies

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The present study has focused on investigating the potential of triethylamine-based compounds tagged with 1,3-benzodioxole motif ionic liquids as inhibitors of tubulin proteins and anti-cancer therapeutics. Molecular docking analysis has been used to determine their binding capabilities with molecular targets and their impact on anti-cancer drug efficacy. *In silico* studies have found that N-(benzo[d][1,3] dioxol-5-ylmethyl)-N,N-diethylethanaminium iodide (Compound 1) has the highest binding affinity to the tubulin protein. DFT studies have also been performed and various parameters recorded for compound 1. So, compound 1 has been synthesized using *meta*-synthesis methods and characterized using NMR techniques. Based on these findings, compound 1 has proven its potential as an anticancer agent with high potential for further studies.

Keywords: Anticancer drug, 1,3-Benzodioxole, Molecular Docking, Ionic Liquids, Tubulin