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Comparative Analysis of Molecular Docking, In Silico Modeling, and Experimental Genotoxicity and Cytotoxicity Assay

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Abstract: This study compares molecular docking, in silico analysis, and experimental genotoxicity and cytotoxicity assays to evaluate their effectiveness in predicting molecular interactions and toxicity. First computational methods, such as molecular docking and in silico tools, were used to predict binding affinities and toxicity profiles whether they might be harmful or not. These methods provide quick and cost effective way for evaulating chemicals before conducting Laboratory tests. Then experimental assays, including genotoxicity (DNA damage) and cytotoxicity (Cell death), provided validation. Results show that computational approaches are efficient for initial screening but require experimental validation for accuracy. The integration of these methods improves the reliability of toxicity assessment and molecular interaction studies. This work highlights the importance of combining computational and experimental techniques to advance research in molecular biology and biotechnology. By combining these methods, researchers can improve **drug development, chemical safety testing, and biotechnology research,** leading to safer and more effective scientific advancements.

Keywords: Molecular docking, in silico analysis, genotoxicity, cytotoxicity, Biotechnology