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Computation of Molecular Properties and Drug Likeness for Polymethoxy Chalcone

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ABSTRACT: The chalcones derived from 1-(2,4,6-trimethoxy-3-(3-methylbut-2-enyl)phenyl) ethanone with 4-substitued and 2-substituted benzaldehyde were selected for the calculation of molecular properties drug likeness using molinspiration software. Twenty compounds were designed to predict molecular properties, drug likeness score on the basis of Lipinski's rule, and bioactivity prediction through molinspiration software. MilogP of these compounds were found above 5 that means these shows poor permeability across cell membranes. TPSA below 160Å^2, n violations=1, it means compound easily binds to receptor, molecular mass < 500, nrotb > 5, No. of hydrogen bond donors ≤ 5, No. of hydrogen acceptor ≤ 10. Compounds 1-20 were taken further calculation of the bioactivity score by calculating the activity score of GPCR ligand, ion channel modulator, nuclear receptor ligand, kinase inhibitor, protease inhibitor. Compound 1-20 showed a good drug likeness score and bioactivity score.

KEYWORDS: Molecular properties; Drug molecule; Bioactivity score; Chalcones**;** Lipinski rules.