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Synthesis and *in-silico* analysis of some 4-bromophenyl enones

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Abstract. Nine substituted styryl 4-bromophenyl ketones were synthesized by potassium hydrogen phthalate ($KHC_6H_4O_4$) assisted crossed-aldol condensation of 4-bromoacetophenone and benzaldehydes in stirring method. This method yields more than 80 % product. In this condensation, the effect of solvents was studied. The purities of these enones were analyzed by their data reported earlier in literature. The molecular structure of 4-bromophenyl chalcones was investigated using Density Functional Theory (DFT) at the B3LYP/6-311G(d,p) level of theory. The simulations provide insights into total energy, frontier molecular orbitals (HOMO and LUMO), and molecular electrostatic potential (MEP) surfaces. Molecular docking analysis of 4-bromophenyl chalcones against D-glutamate ligase (PDB ID:1UAG) bacterial protein that gives highest binding affinity value -6.63 with the compound **1c.** ADMET results support the further development of pharmacologically active drugs. The enzyme target prediction ligand-based method demonstrates 4-bromophenyl chalcone derivatives (**1a-i**) effective inhibitors of oxidoreductase, kinases, and proteases enzymes. These findings revealed 4-bromophenyl chalcone derivatives as potential candidates for therapeutic applications.

***Keywords*:** potassium hydrogen phthalate; crossed-aldol condensation; 4-bromophenyl chalcone; DFT; molecular docking; ADMET studies.

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