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In vitro, *in vivo* and *in silico* inhibitory activities and lead optimization of organic compounds

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Abstract

Nowadays, drug development process is conducted in various sequential phases such as in vitro, in vivo and in silico for their initial inhibitory potential and selection of lead candidate for clinical trials. Due to rapid and large scale synthesis of organic compounds and their derivatives, it's very important to screen in short time for their pharmacological potency, therefore in vitro enzyme inhibition (Urease, Tyrosinase, α-glucosidase, α-amaylase, Acetylcholine esterase, Elastase, Carbonic anhydrase etc) assays proved to be less expensive, accurate and valuable methods. After that chemo-informatics and computational chemistry plays vital role in initial drug examination such as molecular docking and molecular dynamic simulation has recently established as a powerful technique for high through put screenings. Molecular docking study defines the 'best-fit' positioning of a compound that interacts with the target protein and online tools used for determination of physiological and biochemical parameters of leading molecules such as absorption, distribution, metabolism, excretion or toxicity (ADMET).

Biography

Dr. Qamar Abbas, has his expertise in Physiology and Medicinal chemistry (In vitro, in vivo and in silico). He is presently Assistant Professor at University of Sindh, Jamshoro, Pakistan. He is author of 46 research articles in the field of Pharmacology and Medicinal chemistry. He is actively engage with various research groups of medicinal chemistry and nanomedicines for testing of newly developed molecules.

Publications

- Methoxy-Substituted Tyramine Derivatives Synthesis, Computational Studies and Tyrosinase Inhibitory Kinetics
- Enzyme Inhibitory Kinetics and Molecular Docking Studies of Halo-Substituted Mixed Ester/Amide-Based Derivatives as Jack Bean Urease Inhibitors
- Identification of novel C-2 symmetric Bis-Azo-Azamethine molecules as competitive inhibitors of mushroom tyrosinase and free radical scavengers: synthesis, kinetics, and molecular docking studies
- Synthesis, spectroscopic characterization, X-ray crystal structure, antimicrobial, DNA-binding, alkaline phosphatase and insulin-mimetic studies of oxidovanadium(IV) complexes of azomethine precursors
- Understanding the enzymatic inhibition of intestinal alkaline phosphatase by aminophenazone-derived aryl thioureas with aided computational molecular dynamics simulations: synthesis, characterization, SAR and kinetic profiling

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