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Abstract

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, β-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). Initially, for in vivo trails of drugs mouse, rats and rabbits were used but recently zebrafish arise as good human disease animal model such as human pathologies, acquired diseases, genetic disorders, and many physiological processes are extremely conserved throughout the vertebrate evolution. The advantages of the zebrafish comprise its production of visually clear embryos, fecundity and its size. In conclusion, in vitro enzyme inhibition assay, in silico molecular docking, molecular dynamic simulations and ADMET properties and in vivo zebrafish assays. Together, all these methods provide the way forward to pharmaceutical and academic researchers for drug development.

Key words: - In vitro, In Silico, Lead optimization, synthesis, enzyme inhibition

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 40 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.

Publication of speakers:

1. Qamar Abbas, et al., Recent progress of the development of dipeptidyl peptidase-4 inhibitors for the treatment of type 2 diabetes mellitus; J of Pharmaceutical sciences & Drug Development; 151 (2018), pp. 145-157

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