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rational design, is the inventive process of finding new medications based on the knowledge of a biological target. The drug is most commonly an organic small molecule that activates or inhibits the function of a biomolecule such as a protein, which in turn results

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in a therapeutic benefit to the patient. In the most basic sense, drug design involves the design of molecules that are complementary in shape and charge to the biomolec

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Rational Drug Design: It begins with a hypothesis that modulation of a specific biological target may have therapeutic value compared to traditional design that relies in trial-and-error. Computer-Assisted Drug Design: This methodology uses computational chemistry to

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and related biologically active
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arylquinoline derivatives was
designed retaining significant

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pharmacophoric features and three dimensional geometry of bedaquiline. In silico ADME study was performed to assess drug likeness and toxicity profiles of the designed molecules.

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several aspects of rational drug
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bioactive drugs; development and
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