

(54) Title of the invention : A NEW ALTERNATIVE SYNTHESIS OF POTENTIAL ANTI-COAGULANT DRUG RIVAROXABAN: MOLECULAR DYNAMICS SIMULATIONS, DENSITY FUNCTIONAL THEORY, MOLECULAR DOCKING, AND ADMET STUDIES

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(57) Abstract :

The current invention provides a new and alternative synthesis of an anti-coagulant drug rivaroxaban, molecular dynamics simulations, density functional theory, molecular docking, and ADMET studies. We developed the synthesis with an overall yield of 24%, and diminished reaction times. A new alternative and inexpensive chemical urea, which formed oxazolidinone ring in a cost-efficient method have been developed. This synthetic protocol offers an economic, cost-effective, eco-friendly, high yielding, non-tedious, by-product-free, and impurity-free synthesis of rivaroxaban which enables direct isolation of API.

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