Adv. Pharmacol. Toxicol. Vol. 12 (2) 2011, 85-94
ISSN - 0973-2381

INSILICO DESIGN AND QSAR ANALYSIS OF 2, 5-DIHYDROXY-3-UNDECYL-1, 4-BENZOQUINONE SCAFFOLD

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The knowledge of a pharmacophore, or the 3D arrangement of features in the biologically active molecule that is responsible for its pharmacological activity, can help in the search and design of new or better drug action on the same or related target. The present study consists of the non – steroidal phytochemical scaffold 2,5-Dihydroxy-3-undecyl-1,4-benzoquinone for its contraception activity. Applying the concept of SAR study and combinatorial chemistry a library of 97 analogs are generated and 17 scaffold analogs of 2,5-Dihydroxy-3-undecyl-1,4-benzoquinone are identified which are biologically active drugs and having a desired ic50 value with their indigenous receptor site. Both the sets are submitted to binding analysis with HSP 90 receptor protein, giving a desire output as compared to gamendazole. 633 active descriptors are calculated from the biological active drugs using the concept of combine qsar model. Applying the regression analysis on the best 37 docked complex of the 97 combinatorial set molecules in combine prediction method a predicted biological value is calculated. Overall submitting data to analysis 1841 physiochemical descriptors are identified from their inter and intra interaction, correlating these descriptors with the biological activity to evaluate a better model. Applying the training and test condition iterative approaches of QSAR methodology identified a better and potential lead with better q2 (goodness of prediction) and r2 (goodness of fit) value.

INTRODUCTION

Advancement in the accurate prediction in lead generation may significantly impact the intended goals of modern drug design and developmental approaches to enable faster, less expensive and more predictable drug development. Thus, the ability to identify ligands (inhibitors) for clinically significant transporters is essential to improve lead profiling. Most commonly utilized ligand-based methods are quantitative structure activity relationship (QSAR) and pharmacophore modeling. Summation the features of SAR, binding analysis and Pharmacophoric point's descriptors identified to generate a QSAR model. The concept of a pharmacophore is widely used in modern drug design and it is generally defined as the 3D arrangement of certain features in the ligand that are responsible for its activity against a

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