CONFERENCE ABSTRACT

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IN SILICO IDENTIFICATION AND EVALUATION OF HITS AS A TOPOISOMERASE II INHIBITORS VIA LIGAND BASED PHARMACOPHORE MAPPING AND VIRTUAL SCREENING

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ABSTRACT:

The hunt for the hits as anti-cancer candidates is fascinating nowadays. At this instant, computational technology has emerged as a trending tool to improve the domain of computer aided drug designing. The present study reports a ligand based pharmacophore model generation that elucidates vital pharmacophoric features helpful for the inhibition of topoisomerase II activity. A six featured pharmacophore model of topoisomerase II has been generated via 10 training sets of reported topoisomerase II inhibitors in Molecular Operating Environment 2009.10. pharmacophore constructing tool. The generated pharmacophore model was then validated by the 24 test set database of the reported naphthoquinone topoisomerase II inhibitors. In a while the validated pharmacophore model was then used to virtual screening of the possible hits from the ZINC drug database by using ZINCpharmer tool. The virtually screened hits were filtered by Lipinski's rule of five and further assessed through molecular docking and ADMET studies. The results of docking and interaction studies were validated through binding score analysis. Seven hits (ZINC ID's: 00000903, 02570830, 02012726, 00001402, 02040199, 01481831, and 00006923) of different scaffolds having interactions with important active site residues of topoisomerase II were predicted. In future, these pharmacophore models will assist to discover the new anticancer compounds and these screened hits could serve as strong and potential drug candidates in the development of potent topoisomerase II inhibitors against cancer. The findings will be useful as they provide insight into the effectiveness of the drug before its manufacturing and testing on a pilot scale in the pharmaceutical industry (for *in vivo* drug design and development).

KEY WORDS: Drug Design, Anti cancer, Docking.

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