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Screening and Toxicity Risk Assessment of Selected Compounds to Target Cancer using QSAR and Pharmacophore Modelling

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Abstract : To target TGFβ type I receptor, around 63 compounds have been identified from the binding database and3D-QSAR study was carried out using PHASE of Schrodinger software. Through thorough validation, a best pharmacophore model screened 4000 compounds from National Cancer Institute(NCI) and Zinc database. Further docking studies around 4000 molecules were docked by targeting the protein TGFβ type I (PDB**ID**: **1VJY**). Based on docking or Glide score 25best compounds were identified. In addition to these, QikProp module 7 lead compounds were screened and their toxicity parameters evaluated using OSIRIS property explorer and Molinspiration and ToxTree software.
The molecular parameters like clogS, clogP and Molecular weight were calculated using Molinspiration software as well as the drug-likeness and drug score using the OSIRIS property explorer. Their toxicity parameters like mutagenic, tumorigenic, irritant and reproductive effective were calculated using data warrior. The teratogenicity of the compounds was calculated using *insilico* first software and its toxicity to *S.typhimurium* TA100 mutagen, eye irritation as well as corrosion, skin sensitation alerts, negative for genotoxic carcinogenicity and non genotoxic carcinogenicity. From the results the compound 7 (Zinc-69489055) was found to be safe to use as a drug. Hence, the compound could be further redesigned, synthesized to target cancer.
Keywords: 3D-QSAR, pharmacophore modelling, NCI and Zinc database, TGF-β type I receptor, QikProp, ToxTree, OSIRIS, Data warrior and Molinspiration.

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