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In-silico Analysis of Plumbagin against Cancer Receptors

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Abstract : Cancer is an uncontrolled growth of abnormal cells in the body. It is one of the most serious diseases on which extensive research work has been going on all over the world. Structure-based drug designing is a computational approach which helps in the identification of potential leads that can be used for the development of a drug. Plumbagin is a naphthoquinone derivative from Plumbago zeylanica roots and belongs to one of the largest and diverse groups of plant metabolites. Anticancer and antiproliferative activities of plumbagin have been observed in animal models as well as in cell cultures. Plumbagin shows inhibitory effects on multiple cancer-signaling proteins; however, the binding mode and the molecular interactions have not yet been elucidated for most of these protein targets. In this investigation, an attempt to provide structural insights into the binding mode of plumbagin against four cancer receptors using molecular docking was performed. Plumbagin showed minimal energy against targeted cancer receptors, therefore suggested its stability and potential towards different cancers. The least binding energies of plumbagin with COX-2, TACE, and CDK6 are -5.39, -4.93, - and 4.81 kcal/mol, respectively. Comparison studies of plumbagin with different receptors showed that it is a promising compound for cancer treatment. It was also found that plumbagin obeys the Lipinski's Rule of 5 and computed ADMET properties which showed drug likeliness and improved bioavailability. Since plumbagin is from a natural source, it has reduced side effects, and these results would be useful for cancer treatment.

Keywords : cancer, receptor, plumbagin, docking
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