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An Overview to 3D QSAR and Molecular Docking

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Abstract

3D-QSAR has emerged as a natural extension to the classical Hansch and Free-Wilson approaches which exploits the three-dimensional properties of the ligands to predict their biological activities using robust chemometric techniques such as PLS, G/PLS, ANN etc. The integration of computational and experimental strategies has been of great value in the identification and development of novel promising compounds. Broadly used in modern drug design, molecular docking methods explore the ligand conformations adopted within the binding sites of macromolecular targets. Molecular docking and 3D QSAR model are the two potent methods in drug discovery process. Today, a variety of docking algorithms are available, so an understanding of the advantages and limitations of each method is of fundamental importance in the development of effective strategies and the generation of

relevant results. In this review, we outline recent advances in development and applications of 3D QSAR and protein–ligand docking approaches, as well as combined approaches for conventional organic compounds and for nanostructured materials, such as fullerenes and carbon nanotubes.

Keywords: 3D QSAR, Molecular Docking, Chemometric techniques, Steric property, Statistical model.