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Docking moléculaire & valorisation du potentiel bioactif

Combining Computational Chemistry and In Silico Methods for Predictive Insights into Biochemical Systems!

Code C9

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At the Dawn of this 21st century, In Silico methods, including computational chemistry, Molecular Modeling, QSAR models, Molecular Docking and ADMET, are fast emerging areas which are used for the modeling and simulation of small chemical and biological systems in order to understand and predict their behavior at the molecular level [2]. In Silico methods are based on recognizing the relationship between a structure and its molecular properties. The increasing availability of fast computers with the support of Machine Learning toolkits and the Databases, a wide variety of suitable chemical drawing and modelling programs at relatively low cost now allow access to computational modeling covering a wide range of applications in materials and life sciences [2].

Considering the importance of this new “PARADGIM”, we aim to give a comprehensive overview of in silico methods with survey results from literature and perspectives on many of these topics. Of particular interest, Due to its high impact on medicine, and its potential to interest a wide audience, Computed-Aided Drug Design (CADD) is an emerging tool devoted to design and discovery of new drugs, providing a rare opportunity to introduce several concepts in computational sciences, e.g., Bioinformatics & Cheminformatics, combined QM/MM for proteins, computational enzymology...etc.

In fact, with the help of CADD, millions of drug molecules (virtual screening) and drug targets (protein receptors, enzymes, kinases, signaling proteins, etc..) have been evidenced [3].

Keywords: *In Silico methods, Computational Modeling, Chemical & Biomolecular systems.*

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