Computational Approaches In Cheminformatics And Bioinformatics

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Computational Approaches In Cheminformatics And
Computational chemistry is a branch of chemistry that uses computer simulation to assist in solving chemical problems. It uses methods of theoretical chemistry, incorporated into computer programs, to calculate the structures and properties of molecules, groups of molecules, and solids.It is essential because, apart from relatively recent results concerning the hydrogen molecular ion ...

Computational chemistry - Wikipedia
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Computational science, also known as scientific computing or scientific computation (SC), is a field in mathematics that uses advanced computing capabilities to understand and solve complex problems. It is an area of science that spans many disciplines [which?], but at its core, it involves the development of models and simulations to understand natural systems.

Computational science - Wikipedia
Dr. Lobanov has deep expertise across chemistry, cheminformatics, computational chemistry, machine learning and clinical trial operations, leading the delivery of innovative solutions for drug ...

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Molecular docking computationally predicts the conformation of a small molecule when binding to a receptor. Scoring functions are a vital piece of any molecular docking pipeline as they determine the fitness of sampled poses. Here we describe and evaluate the 1.0 release of the Gnina docking software, which utilizes an ensemble of convolutional neural networks (CNNs) as a scoring function. We ...

GNINA 1.0: molecular docking with deep learning | Journal of ...
Some computational peptide structure prediction methods have been developed to model cyclic peptides, such as PEP-FOLD [27,28,29], Peplook , and PEPstrMOD . These methods can generate a certain number of peptide conformations, which can be used for docking [13,14,15, 32]. However, the prediction accuracy of these algorithms is still not ...

Efficient 3D conformer generation of cyclic peptides formed by a ...
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