Special Issue

Molecular Docking in Drug Discovery: Methods and Applications

Message from the Guest Editor

Molecular docking has been a useful tool to aid drug discovery. It helps to find new hits from compound libraries, to optimize drug leads, to suggest docking poses to rationalize experimental data or to give insights into new synthesis. Molecular docking can do these better now with new methodologies and new computer technologies. Machine learning has been used to refine scoring functions, to post-process docking results to improve predictions, and to speedup virtual screening. Some models now account for receptor flexibility. Web servers are available to help users perform docking. GPU-computing is leveraged to screen large compound libraries. Nevertheless, many gaps remain. This special issue invites contributions that further improve or evaluate molecular docking for drug discovery. Insightful applications are also welcomed.

Guest Editor

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