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Molecular docking with Python in Jupyter Notebooks: Towards the development of accessible docking procedures

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Molecular docking is a computational technique used to predict ligand binding potential, conformation, and location for a given receptor, and is regarded as an attractive method to use in drug design due to its relatively low computational and monetary cost. However, molecular docking programs tend not to be accessible to novice users. To increase general access to molecular docking, basil_dock utilizes a series of easy-to-use Jupyter notebooks that do not assume familiarity with molecular docking procedures and concepts, requiring little command-line usage and software installation. The notebooks, divided based on the different steps in the molecular docking process, focus on user customization and flexibility as well as teaching users the basis behind molecular docking. The first version of basil_dock allows users to choose from receptors uploaded to the Protein Data Bank and to add additional ligands as desired. Users can then select between the Vina and Smina docking engines and change ligand functional groups to see how the substitution of atom groups affects binding affinity and ligand conformation. Machine learning algorithms can then be utilized to determine residues in the receptor and atom groups in the ligand that are likely to be integral to forming the ligand-protein complex and to discern which ligands are likely to be orally bioactive based on Lipinski's Rule of Five.

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