GUI-CANDIY (gooey candy)

Chemical Algorithms for Network based Decisions on Interactions for modeling reactivity

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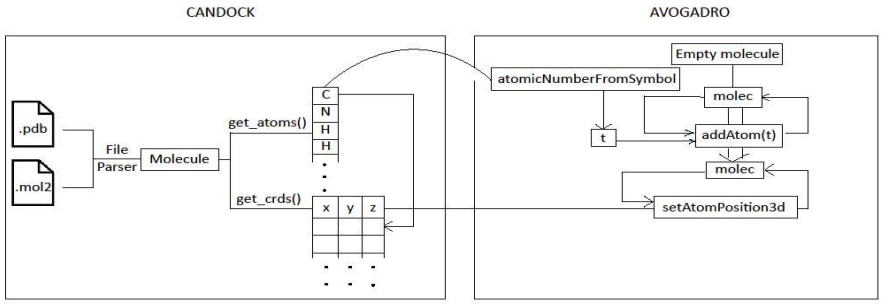
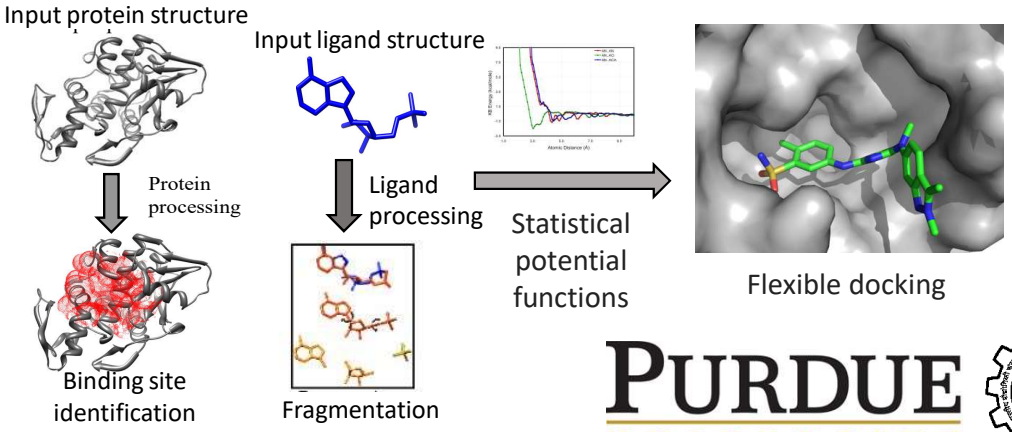
Approach

- Molecule representation: connect CANDOCK and Avogadro

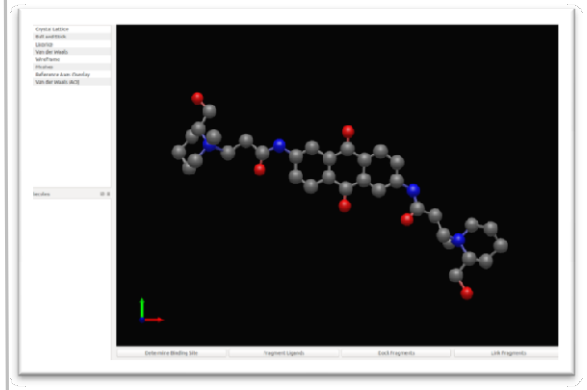


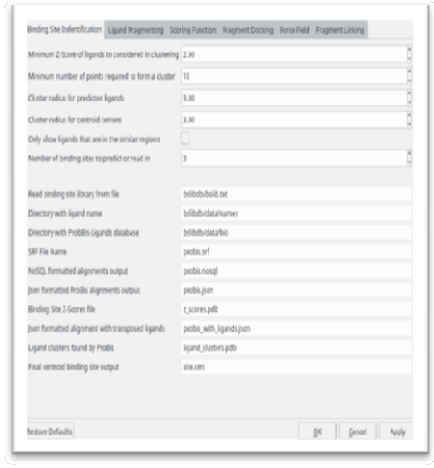
Research

- CANDOCK – Computational Analytics based Docking
- Developing a GUI for CANDIY using Avogadro



Key Results





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