



GUI-CANDIY (gooey candy)

Chemical Algorithms for Network based Decisions
on Interactions for modeling reactivity

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GUI – Computational Analytics based Docking

Building a GUI for CANDIY using Avogadro

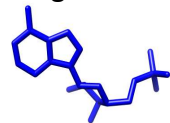
Structure

Protein processing

Fragmentation

Reaction

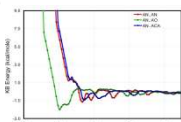
Input ligand structure



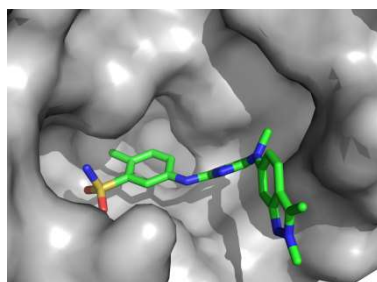
Ligand processing



Fragmentation



Statistical potential functions



Flexible docking

PURDUE
UNIVERSITY

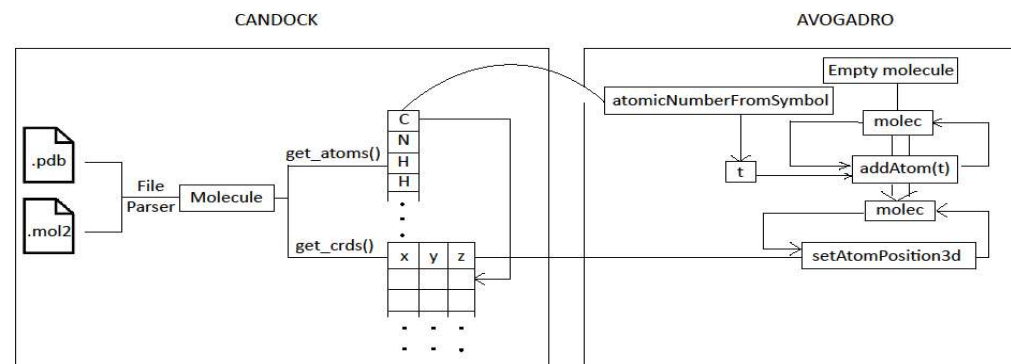


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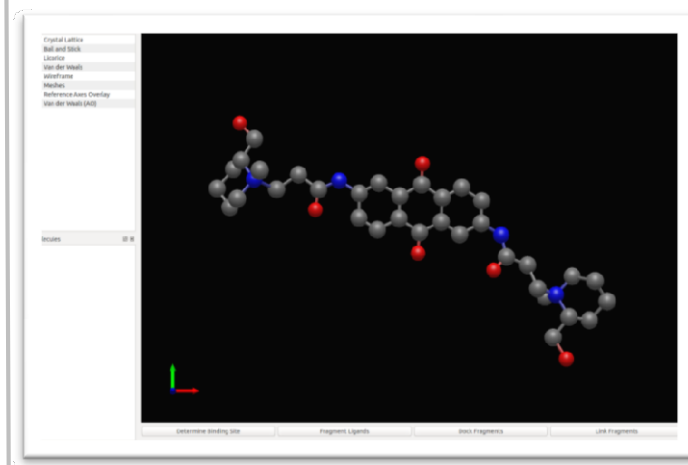


Approach

- Molecule representation: connect CANDOCK and Avogadro



Key Results



PURE