



## GUI-CANDIY (gooey candy)

Chemical Algorithms for Network based Decisions on Interactions for modeling reactivity

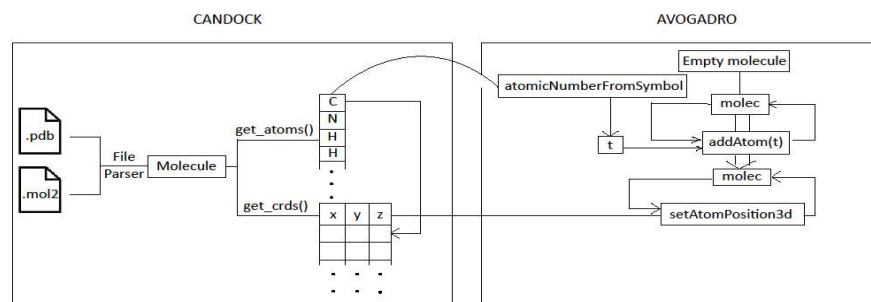
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## Approach

- Molecule representation: connect CANDOCK and Avogadro

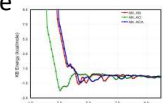
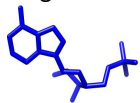
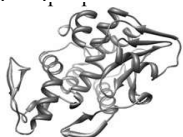


## Research

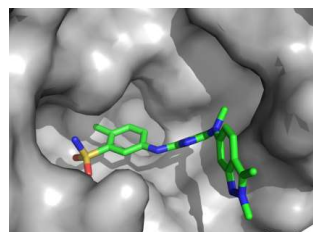
- CANDOCK – Computational Analytics based Docking
- Developing a GUI for CANDIY using Avogadro

Input protein structure

Input ligand structure



Statistical potential functions



Flexible docking

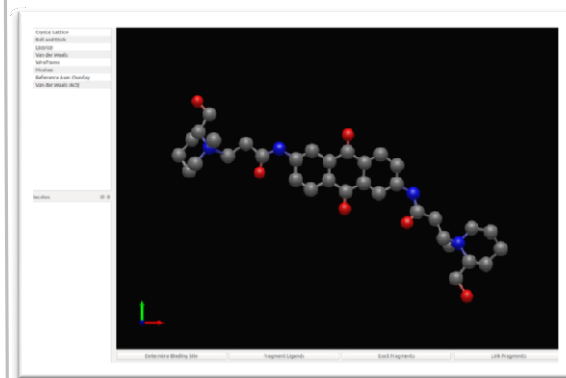
Protein processing

Ligand processing

Binding site identification

Fragmentation

## Key Results



Binding Site Identification | Ligand Fragmenting | Scoring Function | Fragment Docking | Residue Field | Fragment Linking

Minimum Z score of ligands to consider in clustering: 2.00  
 Minimum number of points required to form a cluster: 10  
 Cluster radius for predicted ligands: 3.00  
 Cluster radius for centroid series: 3.00  
 Only allow ligands that are in the similar regions:   
 Number of binding sites to predict or read in: 3

Read binding site library from file: biblib.biblib.net  
 Directory with ligand name: biblib\data\ligandnames  
 Directory with Probbis ligands database: biblib\data\libo  
 SIF File Name: probbis.sif  
 NCI2 formatted alignments output: probbis.nci2  
 Jmol formatted Probbis alignments output: probbis.jmol  
 Binding Site Z-Scores file: z\_scores.pdf  
 Jmol formatted alignment with transparent ligands: probbis\_with\_ligands.jmol  
 Ligand clusters found by Probbis: ligand\_clusters.pdf  
 Final verbose binding site output: site.out

Feature Defaults

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