

Predicting Ligand Binding Sites with UOBPRM and Machine Learning

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Introduction to Ligand Binding

Ligand Binding process

- A ligand (drug) binds to a specific pocket on a protein
- Stable reaction between atoms of both ligand and protein

Application

• Analyzing the efficiency of drug molecules, by how they bind to proteins (enzymes) in the body.

Problem

• Given a ligand and protein, predict ligand binding sites on the protein surface.



Motion Planning

Given an environment: robot, obstacles, start and goal configurations, find a valid collision-free path between start and goal configuration

Application to ligand binding

- Robot: ligand (linkage)
- Obstacle: protein (rigid body)
- Certain metrics: whether a path exists to a configuration



UOBPRM (Uniform Obstacle-Based Probabilistic Roadmap)

- Generates samples uniformly around the obstacle
- Desirable because binding pockets are on protein surface

Generating 1000 samples around an obstacle using UOBPRM



Machine Learning

"A computer program is said to learn from experience E with respect to some task T and some performance measure P, if its performance on T, as measured by P, improves with experience E." -- Tom Mitchell, Carnegie Mellon University

- E: proteins and ligands with known binding sites
- T: predicting binding sites on a new protein for which real sites are unknown
- P: accuracy of prediction based on metrics



-0.0000084171298 0

-0.0000000151420 0

-0.0000004566106 1

41.920 51.208

54.944

15

. . .

-0.000000

0.000000 1

1.8482726 0

