

Chem 437/737 Syllabus Applications of Molecular Modeling

Dr. Gund – Spring 2018

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Office Hours T 2:30-3:30; Th 11:30-12:30
Other times by appointment

Topics To Be Covered

- 1: Introduction to Molecular Modeling. Nicotinic/Muscarinic/
2. Sybyl 2.1- Hands on tutorial on use of Sybyl
Alchemy and spartan
3. Project 1. Receptor Agonists-Antagonists
Molecule Building, energy calculations, optimization
4. Conformational Analysis of receptor agonists
5. Finding bioactive conformation of agonist/antagonists
Superposition of Agonists/antagonists
6. Molecular mechanics- Force Fields
7. Charge Calculations – Mopac and other programs- Contour mapping- density and electrostatic surfaces – Read structures into Spartan
8. Lecture on Computational Methods
Molecular Mechanics, SemiEmpirical, Density Functional and ab Initio Methods
9. Other topics in Modeling, Docking, QSAR
10. Reports on Projects- Presentations

Course Requirements: Must do projects. At the end hand in a report the form of a paper for publication including introduction, results, discussion, findings and diagrams.

One exam may be given during the duration of the course.

Grade will be computed on the basis of 75 % report and 25 % presentation.