

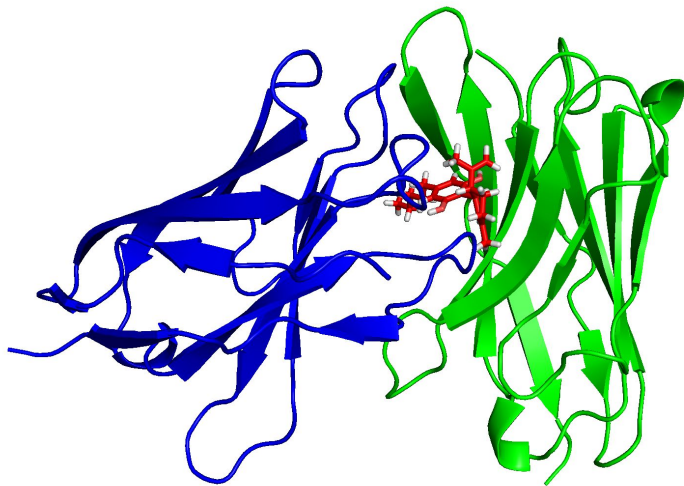
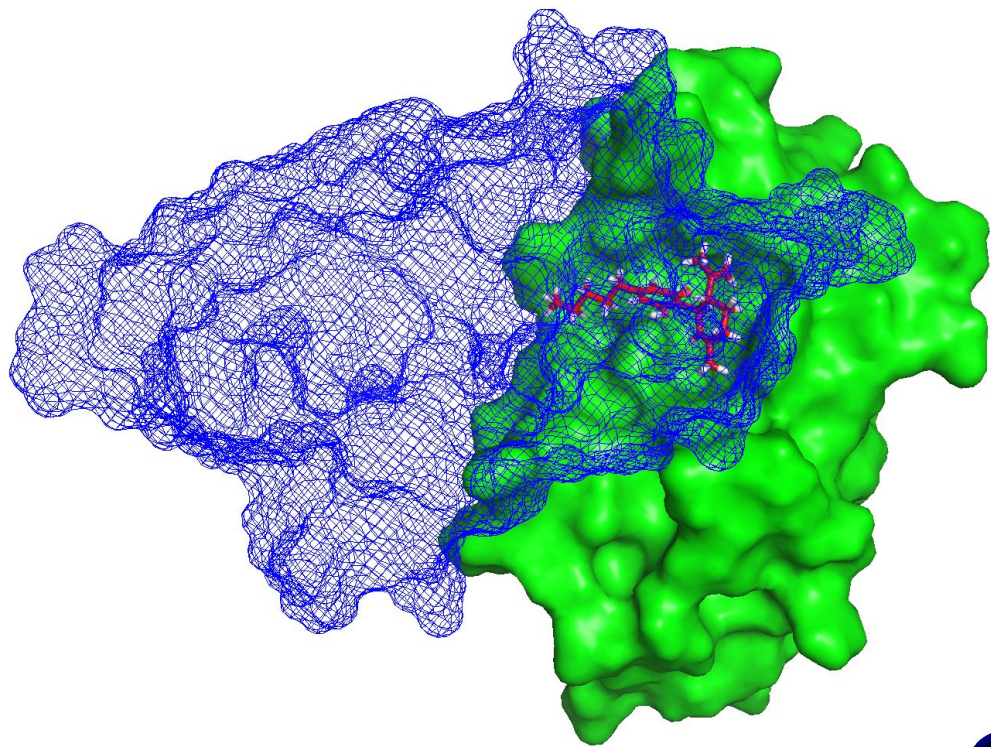
Intro to Rosetta

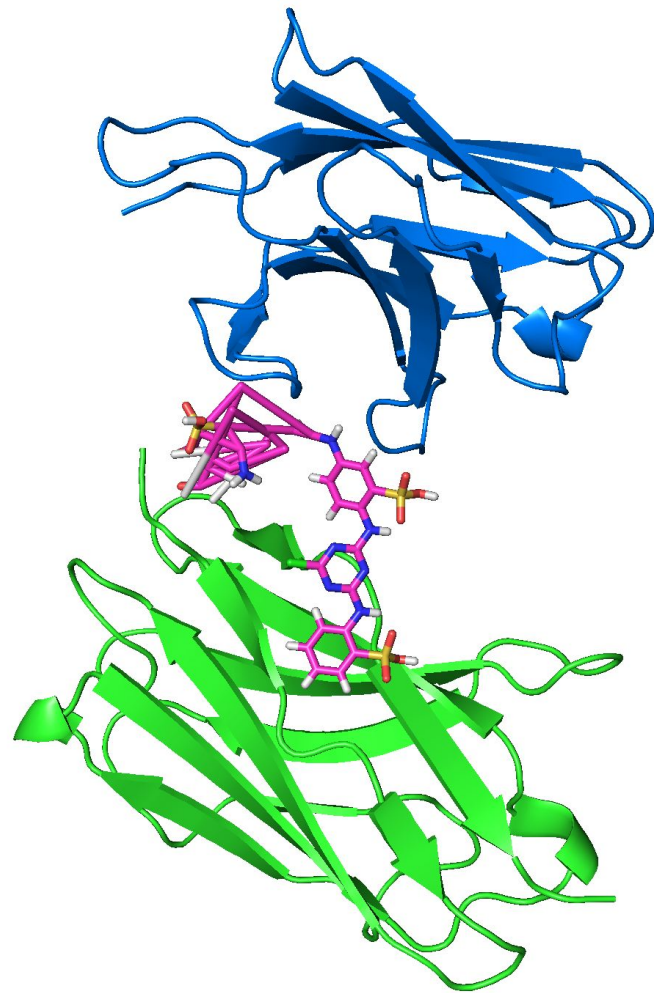
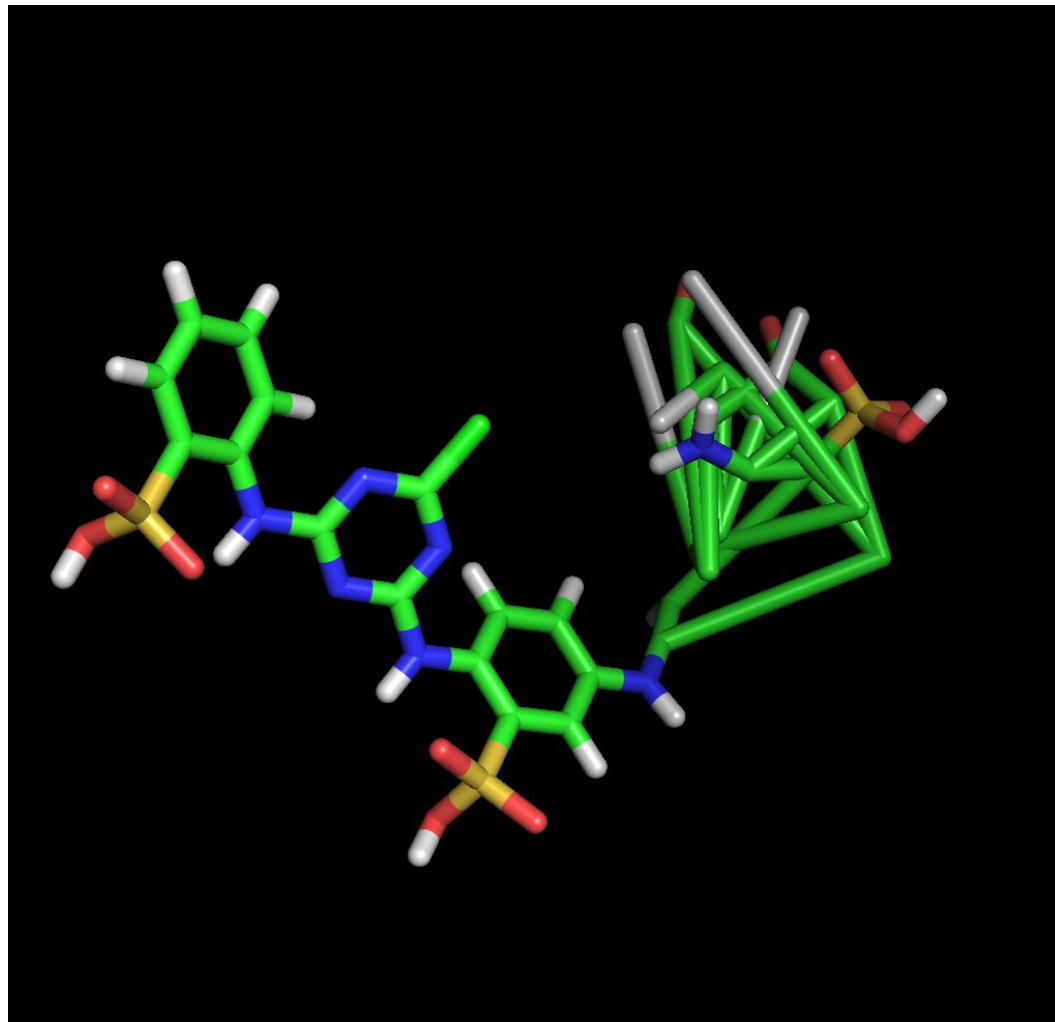
Ed van Bruggen

Week 5

May 2 2019

Attendance
tinyurl.com/y33jhcxr





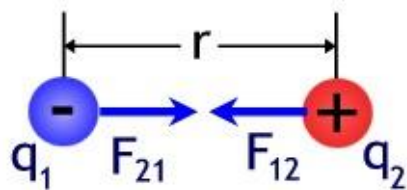


Rosetta Commons

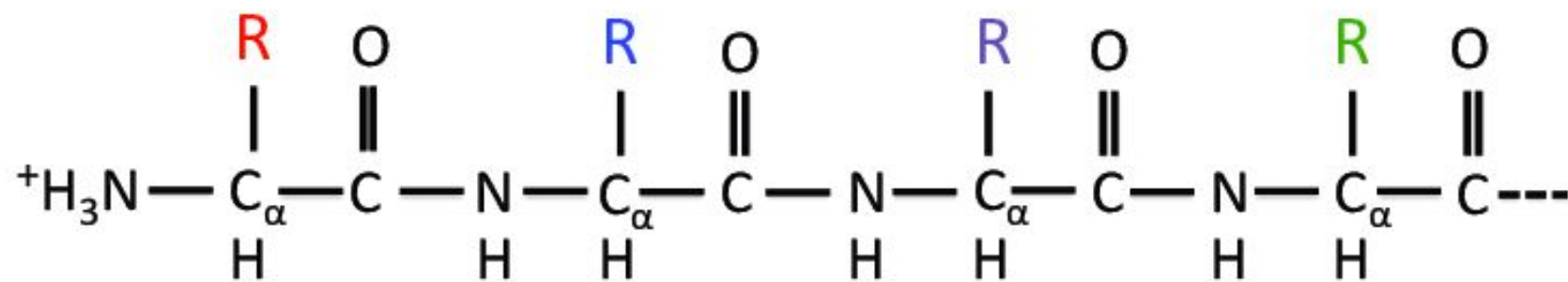
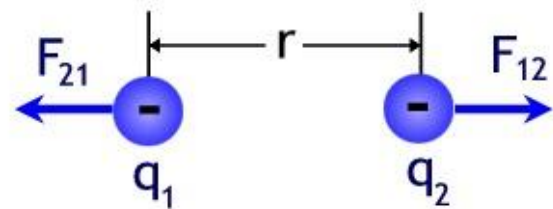
- Protein modeling suite
 - 7GB of source code
 - Hundreds of different modules and functions
 - Many different applications and uses
- Developed by Dr Baker at the Institution of Protein Design here at UW
- Written mainly in C++
- Skills
 - Command line, bash scripting, XML, editing text files
- Do not try to buy, can get free license through UW

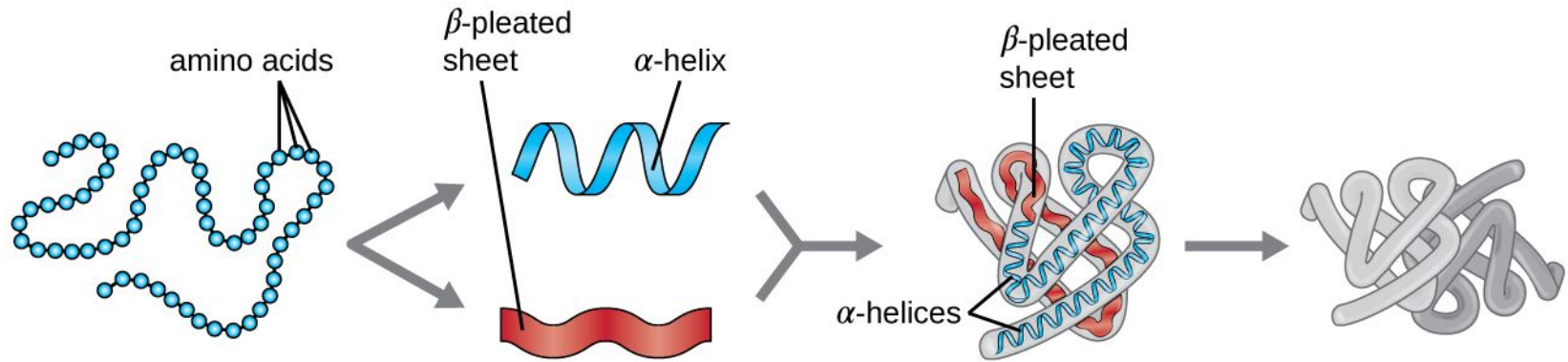


- Protein structure is very important
 - Structure dictates function
 - Hard to experimentally measure structure
- Rosetta can be used to predict a protein's structure based on amino acid sequence
 - De novo
 - Homology
- Used to model interactions
 - Ligand docking
 - Protein to protein docking



$$F = k \frac{q_1 q_2}{r^2}$$





Primary Protein Structure

Sequence of a chain of amino acids

Secondary Protein Structure

Local folding of the polypeptide chain into helices or sheets

Tertiary Protein Structure

three-dimensional folding pattern of a protein due to side chain interactions

Quaternary Protein Structure

protein consisting of more than one amino acid chain

Protein Data Bank



- Database of thousands of known proteins
 - Many have experimentally measured 3D structures found through crystallography
 - If we know anything about a protein, it's probably here
- Rosetta's Bionumbers
- Use BLAST to find similar proteins for homology modeling
- Protein structures are stored in PDB files (.pdb)

.fasta – Protein's amino acid sequence

.pdb – Proteins 3D structure

.clustal_num – 2 proteins aligned

.grishin – Rosetta alignment format

.xml – Rosetta config

.frags – Amino acid shorthand fragments

.sh – Bash script

PyMOL



- Protein visualization tool
 - Reads and displays PDB files generated by Rosetta
- Written in Python
- Used as visual confirmation
- Place ligands near predicted activation site
- Make pictures and animations
- Can also get for free

Weekly Assignment

- Download and compile Rosetta
 - Takes long time to download
 - Takes even longer time to compile
 - Do not leave to last minute
 - Leave laptop running overnight