Eidgenössische Technische Hochschule Zürich
Ecole polytechnique fédérale de Zurich
Politecnico federale di Zurigo
Swiss Federal Institute of Technology Zurich

Institute of Theoretical Computer Science
Lecturer: Prof. Jack Snoeyink
Assistant: Yves Brise

March 21, 2007

Geometric Computations in Molecular Biology SS07
Exercise Set 1

Course Webpage: `http://www.ti.inf.ethz.ch/ew/courses/GCMB07/`

Due date: see below

Molecule of the week: presentation assignment

This assignment aims to give you some familiarity with the protein databank, molecular visualization tools, and how to read a biochemistry paper. You are to choose a molecular structure that you will present in class; this is broken into subtasks with individual deadlines.

Part A

- Select a molecule. There are many proteins behind diseases or drugs in the news, so you may already have a favorite (like Alcohol Dehydrogenase) or least favorite (like Rhinovirus). I recommend looking at David Goodsell's well-drawn series of Molecule of the Month pages:
  `www.rcsb.org/pdb/static.do?p=education_discussion/molecule_of_the_month/index.html`
- Take a look at Myoglobin, the first protein whose structure was determined, and at Cytochrome P450, which is a recent structure. Many of these proteins have interesting stories, such as the Ribosome, F1 ATP-ase, Designer Proteins, Actin/Myosin, GroEL/GroES, Calmodulin, G proteins, TATA-Binding Protein,...

Deadline: As soon as possible
Send an email to Yves Brise `<ybrise@inf.ethz.ch>` to reserve your favorite molecule; he will keep an online list of the molecules that have been reserved and will arbitrate on race conditions.

Part B

- Obtain the structure from the protein databank (PDB file) `www.rcsb.org/pdb`.

  Goodsell's articles link directly to the PDB structures, or you can search to find a molecule's structure (usually several, coming from different species or with different engineered mutations).

- Display your molecule.

  Turn in two pictures of your chosen molecule using with two different visual models (e.g., van der Wals spheres, ball-stick, ribbon/cartoon, backbone trace) that you have gener-

ated from a molecular visualization system (e.g., pymol, KiNG, rasmol/protein explorer, VMD).

Deadline: March 28
Send an email containing the pictures and some explanation to Yves, or hand in print-outs in the lecture.

Part C

- Find the original paper where they determined the structure of the molecule, usually by crystallography or NMR and answer the following questions: What motivated the determination of the structure of this molecule? By what technology was the structure determined? What is the resolution? How has knowledge of the structure helped elucidate its function, or suggested new experiments?
- You should meet with Jack Snoeyink at least once before you do your presentation. Schedule a time to meet with Jack `<snoeyink@cs.unc.edu>`, and to present your molecule in class or exercise session.

Deadline: April 4

Part D

- Present your molecule in a class or exercise session. A 12-15 minute presentation should be sufficient to tell the story of your structure at a high level and answer the questions from part C.
- For those who present after April 18, run your structure through MolProbity and comment on its quality.

How to read a biochemistry paper

The format of a biochemistry paper may seem strange if you are accustomed to the mathematical or computational literature. A common order is Introduction, Results, Discussion, Methods (in small type) – where CS places the greatest emphasis on the Methods, biochemistry places the least.

The key to reading is to do the following steps: first, read and mostly understand the abstract, which should summarize everything the authors believe is important in the paper. Second, read and understand the figure captions, skimming the text where the figure caption does not tell enough of the story (usually it does). After this, you will know the story of this paper, and can decide how much additional detail from the text you need.

The key to presenting is to use the figures, and maybe some of your own, Goodsell's, or animations from the internet to present the story of your molecule.