Exercise 1 (1)

1. Search for “Green Fluorescent Protein” at RCSB.
2. Because you will get too many results, search again with PDB ID “1GFL.”
3. Download its data in the PDB format and save it on Desktop.
4. Open it in Chimera.
5. Choose “Select”→“Chain”→“B” to select chain B. Then, Choose “Actions”→“Atoms/Bonds”→“delete” to delete chain B.
6. Choose “Actions”→“Focus” to fit the structure image to the window.

Exercise 1 (2)

This protein emits green fluorescence when it is excited with UV light. The chromophore is formed by spontaneous cyclization of Ser65-Tyr66-Gly67.

7. Choose “Tools”→“Sequence”→ “Sequence” to display sequence and select Ser65, Tyr66, and Gly67.
8. Choose “Actions”→“Atoms/Bonds”→“show” to display these residues.
9. Choose “Actions”→“Ribbon”→“hide” to hide the ribbon. Confirm that these residues form a cyclic structure.
10. Clear the selection. Choose “File”→“Save Image” to save the image.

Exercise 2

1. Display kadai.fasta at the web page of this lecture. Search for the protein structure with this amino-acid sequence.
2. Find the PDB ID of the protein with the highest sequence identity. Search PDB at RCSB for the entry with this ID.
   - Find the protein name and the structure determination method.
3. Open the PDB file in Chimera.
4. Create an image of the whole structure of the biological assembly and save the image in the PNG format.
   - If the PDB file contains multiple chains, indicate which chain corresponds to the sequence.

Submitting your paper

- Create a PowerPoint file with two slides. Insert the image of Exercise 1 into the first slide. Circle the chromophore in red.
- Insert the image of Exercise 2 into the second slide. Write the PDB ID, the protein name, and the structure determination method.
- Send the PowerPoint file as an attachment to email.
  - Put “Structural bioinformatics exercise” in the Subject field of the email.
  - Be sure to put your name, registration ID (e.g. 18001), and ID card number (if you are a student) in the body of the email.
  - Send the email to Prof. Tohru Terada (tterada@iu.a.u-tokyo.ac.jp).
  - Use web mail service at https://sr.iu.a.u-tokyo.ac.jp/mail_en/.