

# Exercise 1

---

1. Download new\_data.xls from the web site of this lecture and calculate the secondary structure propensities,  $P_{s,a}$ , of amino acids.
2. What are the two strongest formers and the two strongest breakers of  $\alpha$  helix,  $\beta$  sheet, and coil?
3. Calculate secondary structure propensity scores of residues 42–55 (EWTYDDATKTFTVT) using  $P_{s,a}$  calculated above and seq\_score.xlsx. Which secondary structure has the best score for this sequence?

# Exercise 2

---

1. Perform sequence and structure alignments between chain B (c-Raf-1 RBD) of 1GUA and chain A of 1PGA with blast2seq and jCE, respectively. What are the E-value, Z-score, and RMSD obtained from these analyses?
2. Which class, fold, superfamily, and family does 1PGA belong to in the SCOP classification?
3. Compare them with those of 1UBQ and c-Raf-1 RBD of 1GUA. Up to which level is 1PGA classified into the same categories as 1UBQ and chain B (c-Raf-1 RBD) of 1GUA?

# Submitting your paper

---

- Send the Excel file containing the table of  $P_{s,a}$  as an attachment to email.
- Put the answers to questions 2 and 3 of Exercise 1 and all the answers to the questions of Exercise 2 in the body of the email.
- Put “Structural bioinformatics exercises” 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. Terada ([tterada@iu.a.u-tokyo.ac.jp](mailto:tterada@iu.a.u-tokyo.ac.jp)).

# Web mail server

- Access to [https://sr.iu.a.u-tokyo.ac.jp/mail\\_en/](https://sr.iu.a.u-tokyo.ac.jp/mail_en/)
- You can submit your papers using this page.

**Send E-mail(1/2)**

Send to:

Subject:

Name:

Affiliation:

ID card number:

E-mail:   Send Cc to me

Body:

Number of attachments:  (Give the file names of attachments in the next step)