

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 α helix, β 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. 19001), 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).

Web mail server

- Access to https://sr.iu.a.u-tokyo.ac.jp/mail_en/
- You can submit your papers using this page.

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