Universitas Esa Unggul

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PENGANTAR BIOINFORMATIKA
IBT 431

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Meeting 14

Hands On Protein Modelling

Sasaran Perkuliahan

- Mahasiswa daoat menentukan anotasi gen pada sekuen DNA menggunukan SnapGene
- Mahasiswa dapat menentukan struktur 3D protein dengan menggunakan **SWISS**- **MODEL** dan **PyMOL**

Hands on

Prediksi Struktur 3D protein dan permodelannya menggunakan SWISS_MODEL dan PyMOl

Protein modeling will be carried out using 5 *tools*

1. SWISS-MODEL https://swissmodel.expasy.org/ by **automated mode**
2. SWISS-MODEL https://swissmodel.expasy.org/ by **user template**
3. I-TASSER https://zhanglab.ccmb.med.umich.edu/I-TASSER/
4. QUARK https://zhanglab.ccmb.med.umich.edu/QUARK/
5. Phyre2 http://www.sbg.bio.ic.ac.uk/phyre2/html/page.cgi?id=index by **normal mode**

Use the query amino acid below under the name of **MTGase**

Three urgents to do today

1. Register on I-TASSER web on your first day the 17th April. If possible run, the analysis on the first day
2. Register on QUARK web on your first day the 17th April. If possible run, the analysis on the first day
3. Register on PyMOL web on your first day the 17th April, use institutional email only

SWISS-MODEL automated mode

1. Access https://swissmodel.expasy.org/
2. Make sure you are at “User Template”
3. Paste your query (.FASTA) on the box
4. Click “Search for Templates” to find your templates
5. Chose the best template and then hit “Build Model”
6. Save the .pdb file of the automated model
7. Rename if necessary

SWISS-MODEL user-template mode

1. Access https://swissmodel.expasy.org/
2. Input directly your query sequence .FASTA to the provided query box
3. Upload your template .pdf file “**3le2**” at “Template File”
4. Hit “Build Model”
5. Save the .pdb file of the user-template model
6. Rename if necessary

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I-TASSER automated mode

Register on I-TASSER web on your first day the 17th April
If possible run, the analysis on the first day

1. Access https://zhanglab.ccmb.med.umich.edu/I-TASSER/
2. Input directly your query sequence .FASTA to the provided query box
3. Put your institutional email ONLY (you will have your password by the confirmation sent by I-TASSER after registration)
4. Keep the parameters "default" – change nothing
5. Run I-TASSER
6. **The analysis will run for 60 to 100 hours (be patient)**

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QUARK automated mode

Register on QUARK web on your first day the 17th April
If possible run, the analysis on the first day

1. Access https://zhanglab.ccmb.med.umich.edu/QUARK/
2. Input directly your query sequence .FASTA to the provided query box
3. Put your institutional email ONLY (you will have your password by the confirmation sent by QUARK after registration)
4. **Remember: passwords from I-TASSER and QUARK are different**
5. Keep the parameters “default” – change nothing
6. Run I-TASSER
7. **The analysis will run for 36 to 100 hours (be patient)**

Phyre2 normal-mode

1. Access Phyre2 at http://www.sbg.bio.ic.ac.uk/phyre2/html/page.cgi?id=index
2. Input directly your query sequence .FASTA to the provided query box
3. Select modeling mode at “normal”
4. Hit “Phyre2 Search”
5. Download all result in .tar.gz
6. Rename if necessary
7. Take a look at the result and do **Phyre2 investigator on the best model**

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PyMOL registration

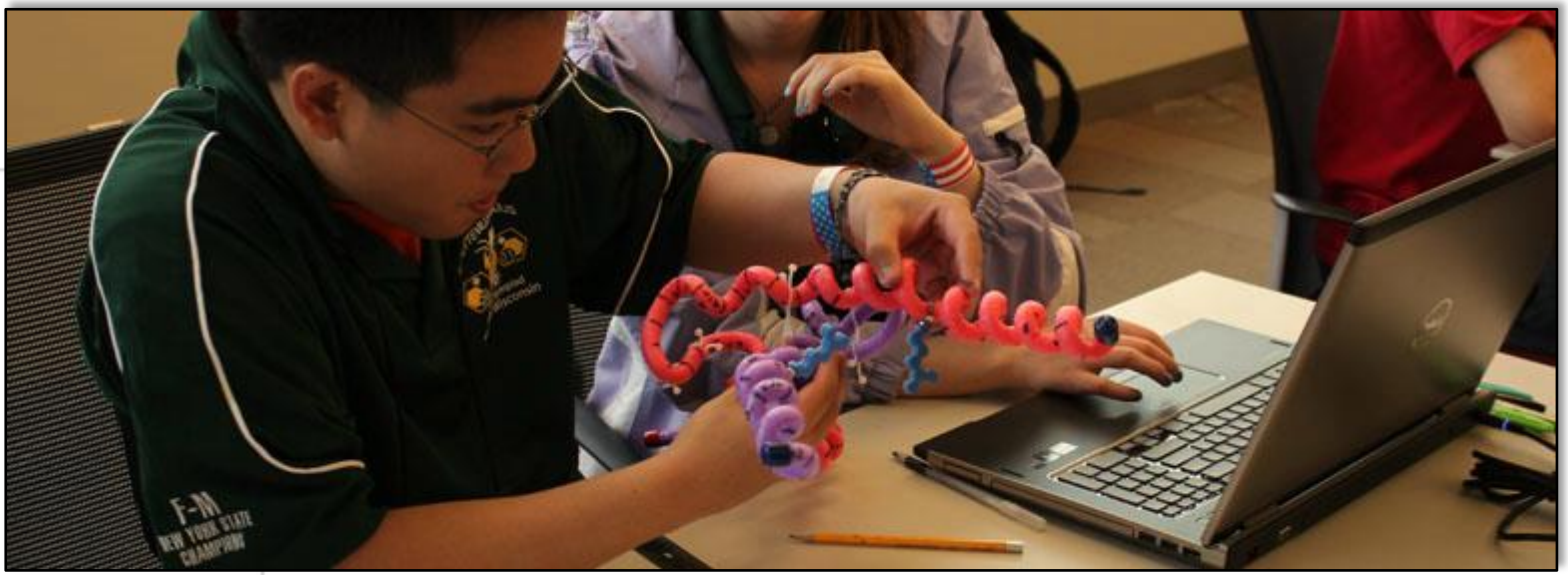
Register on PyMOL web on your first day the 17th April

1. Register first https://pymol.org/edu/?q=educational/
2. Fill everything and pretend that you are a teacher going to teach in a class
3. Wait for the email for password and link to **license code** and **software**
4. Install the software – **suggestion: PyMOL 2.0 if you can**
5. For 32-bit Windows computer use the version “PyMOL 1.3r1 edu” at the Google Drive
6. For Linux and Mac, use the file resided in Google Drive

PyMOL visualization and superimposition

1. Open your PyMOL software
2. Upload by "**Open**" every .pdf file of every models from SWISS-MODEL auto, SWISS-MODEL user template, I-TASSER, QUARK, Phyre2
3. Click on one model, go to "Action", select "Align", select "all to this (*/CA)"
4. You will have superimposition for all models
5. **Which one is distinctly different from the others?**

Thank you modeling!




THANK YOU
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