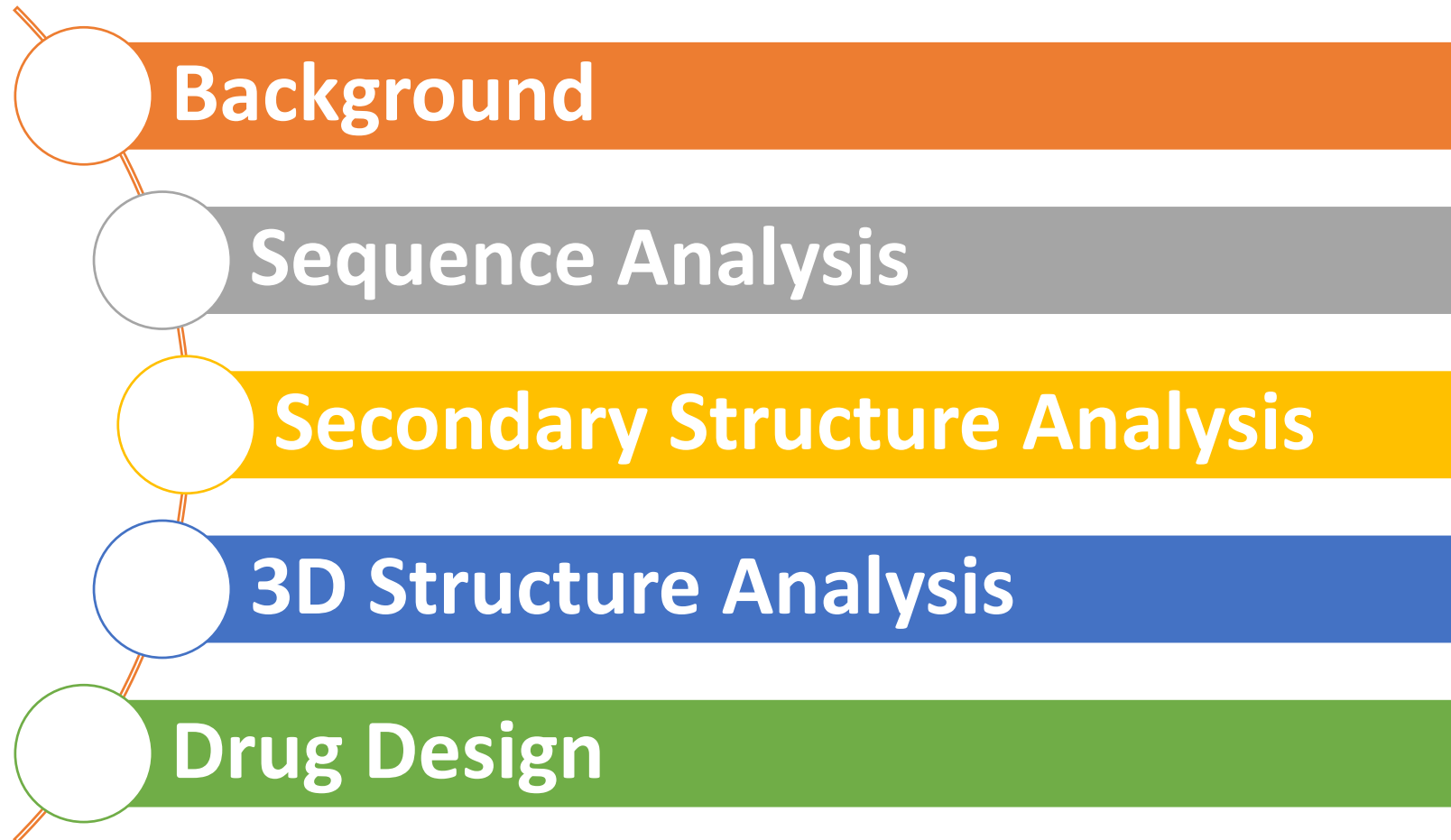# Bioinformatics Analysis of Cryptochrome
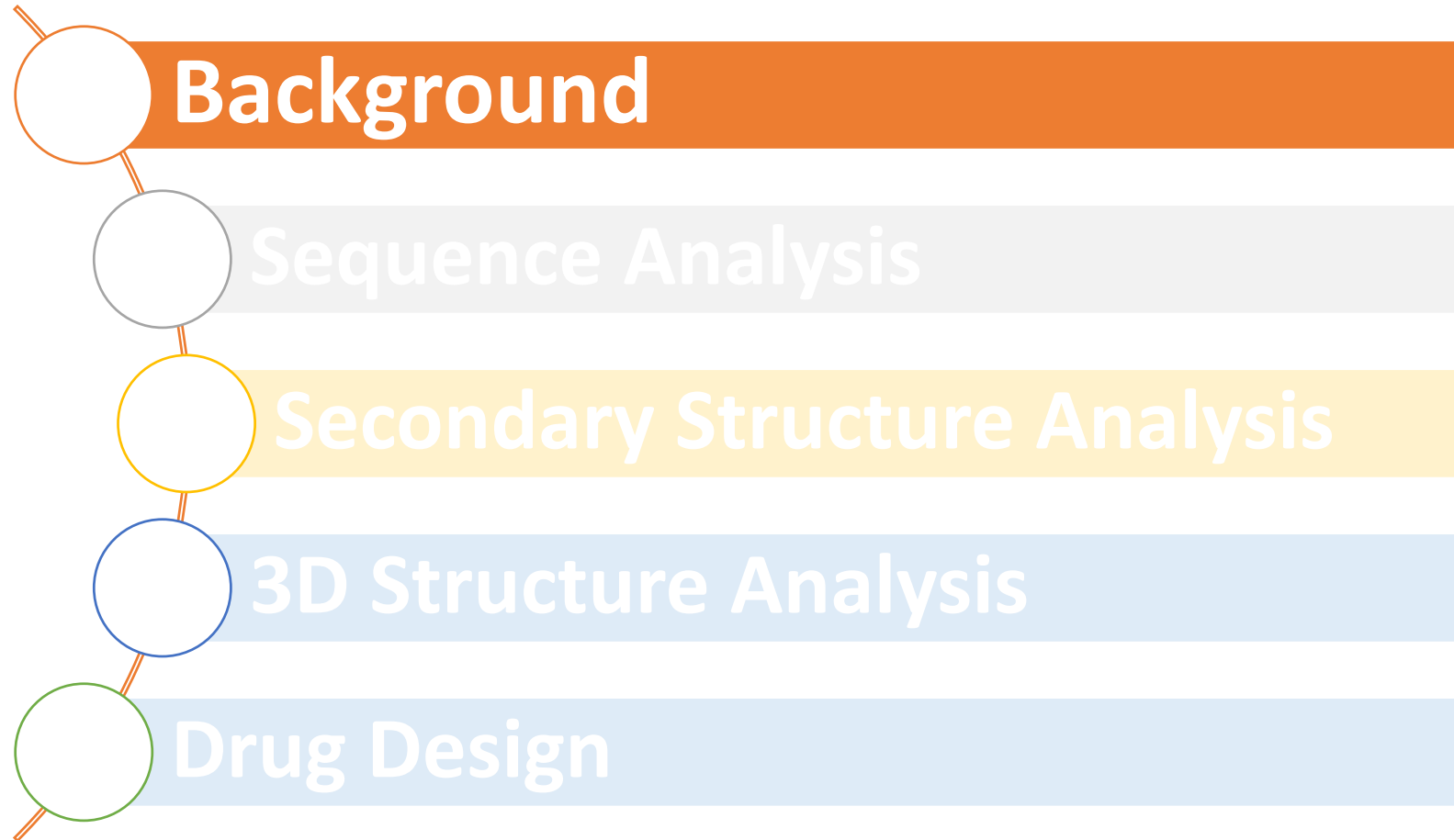
白秀珍 杨喆 徐优俊 解晓雯

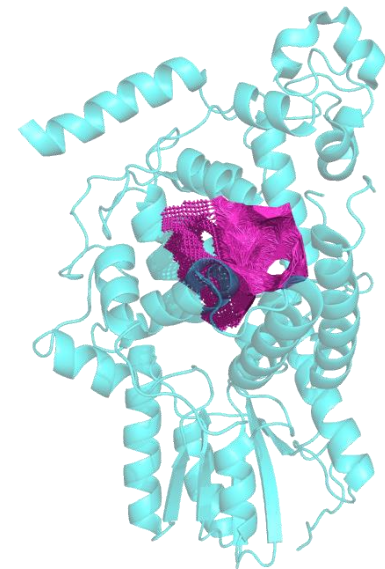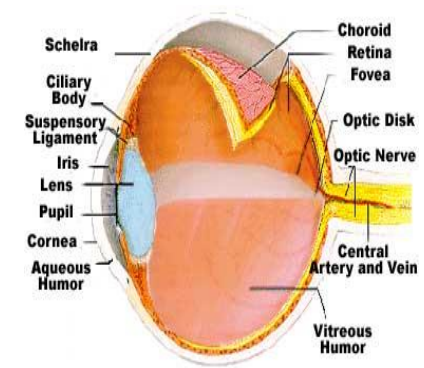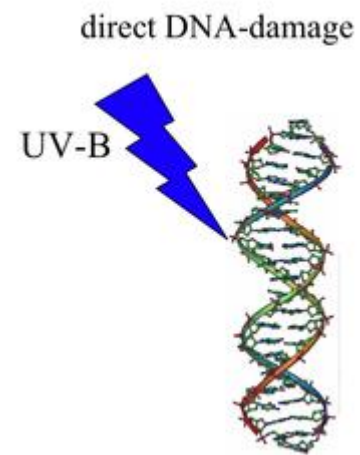**2015.06.27**

Outline

Background

Sequence Analysis

Secondary Structure Analysis

3D Structure Analysis

Drug Design
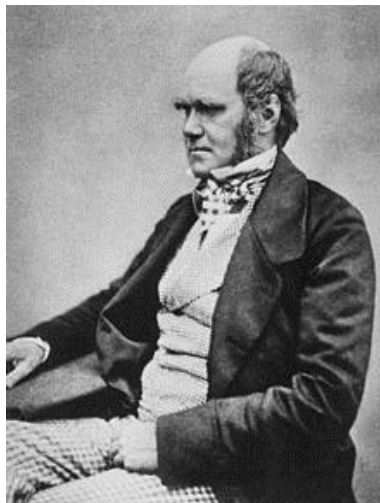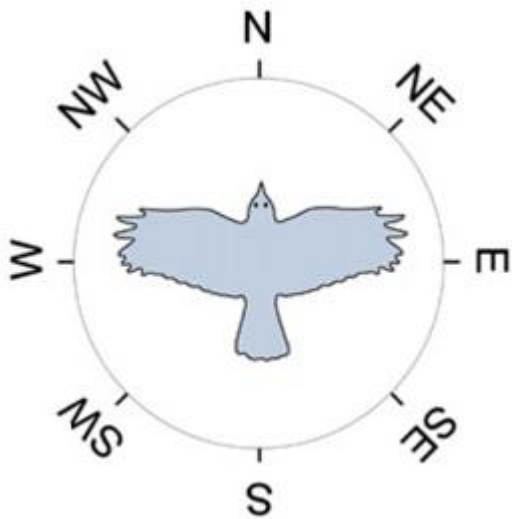
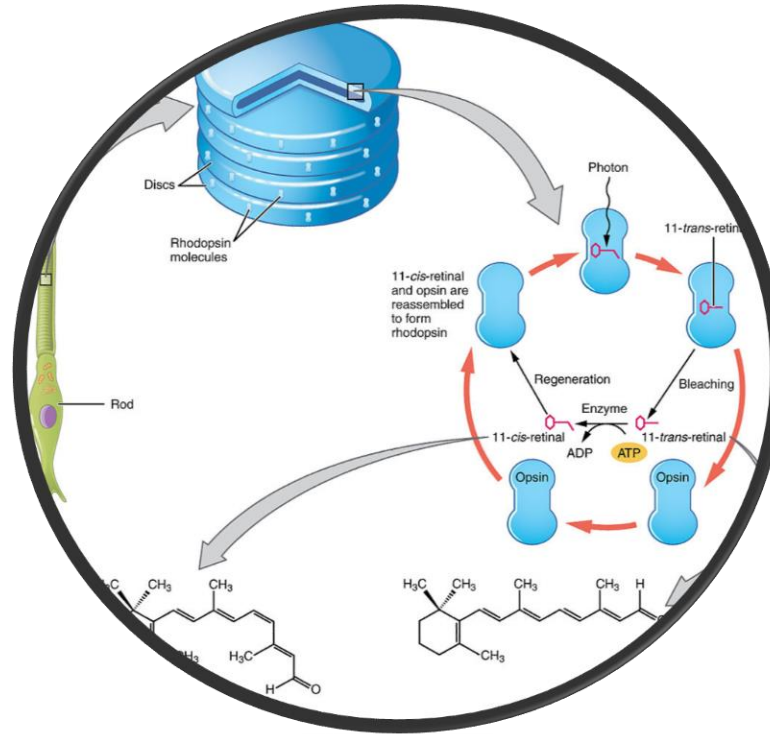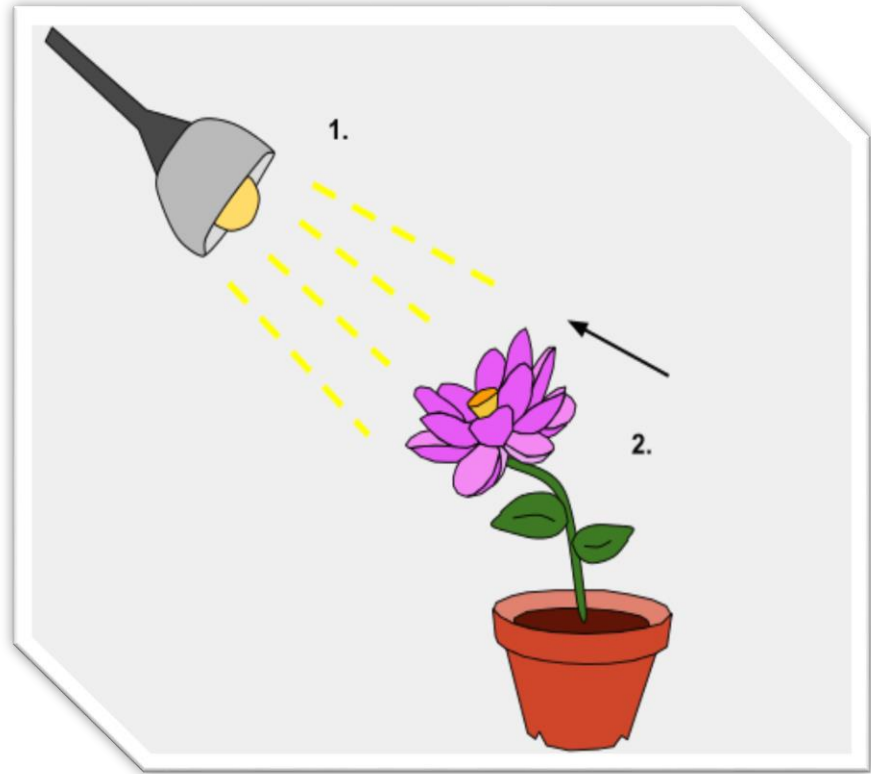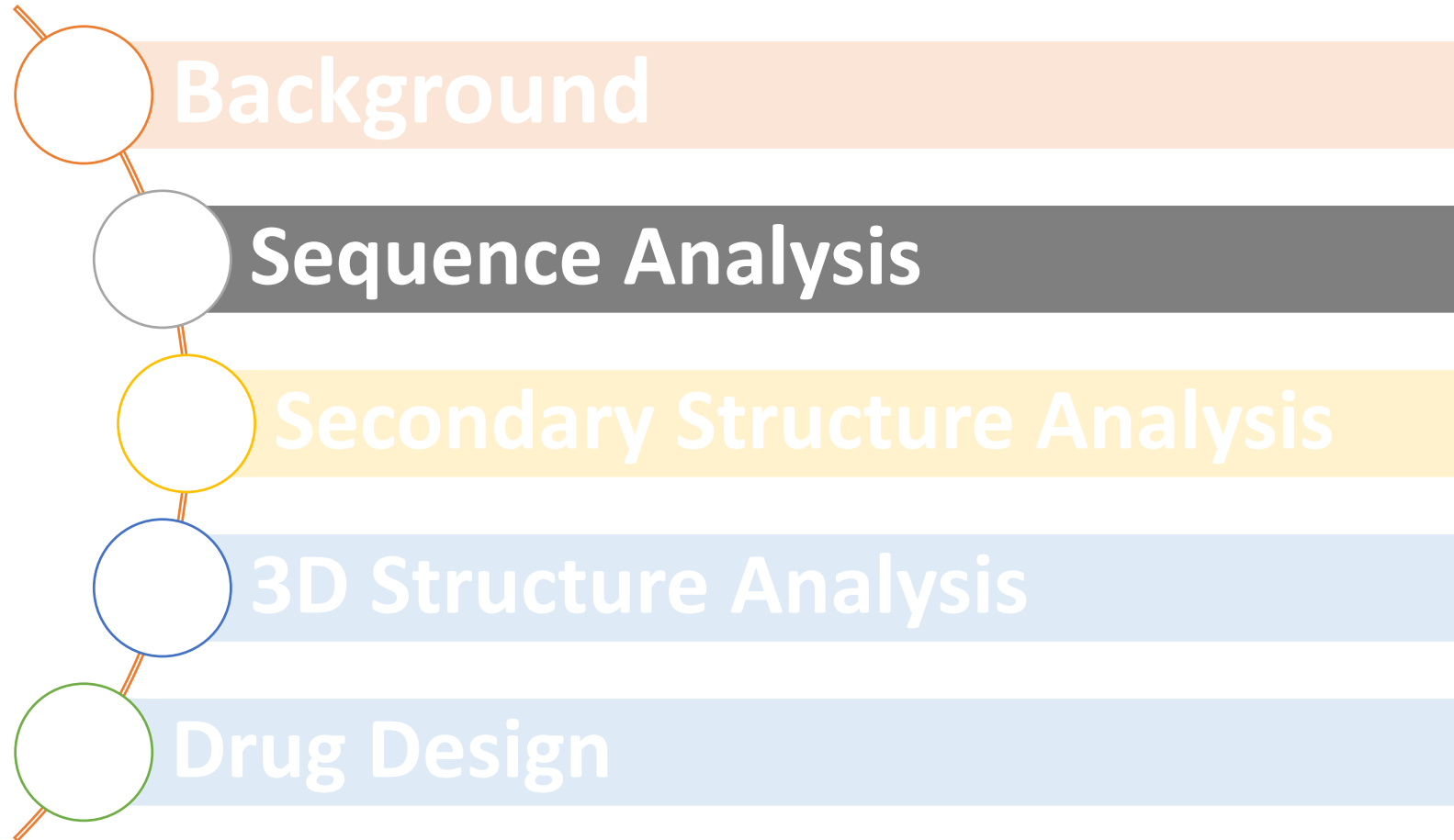# Outline

Background

Background

The absorption of light leads to an isomeric change in the retinal molecule.
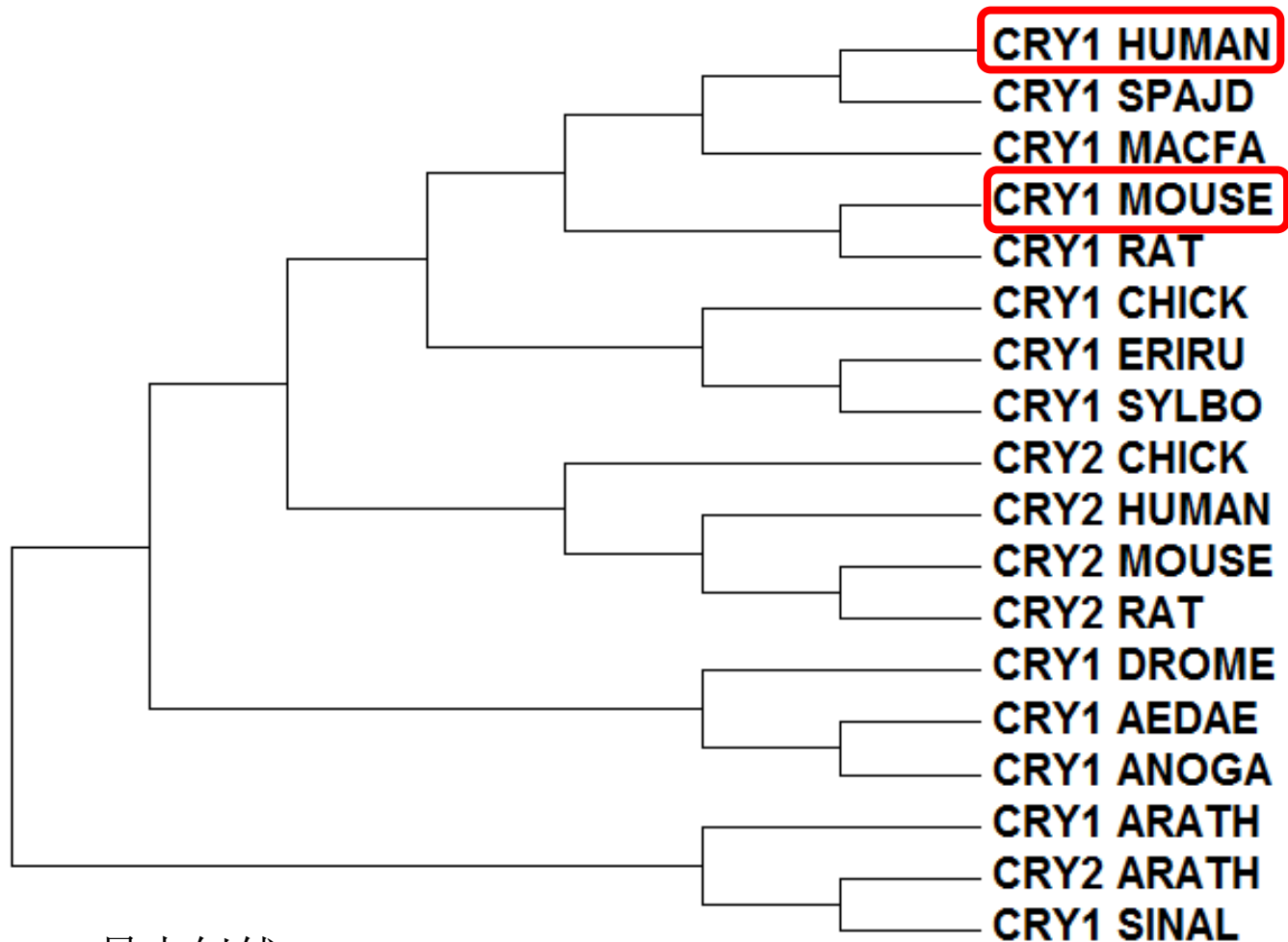
Outline

- Background
- Sequence Analysis
- Secondary Structure Analysis
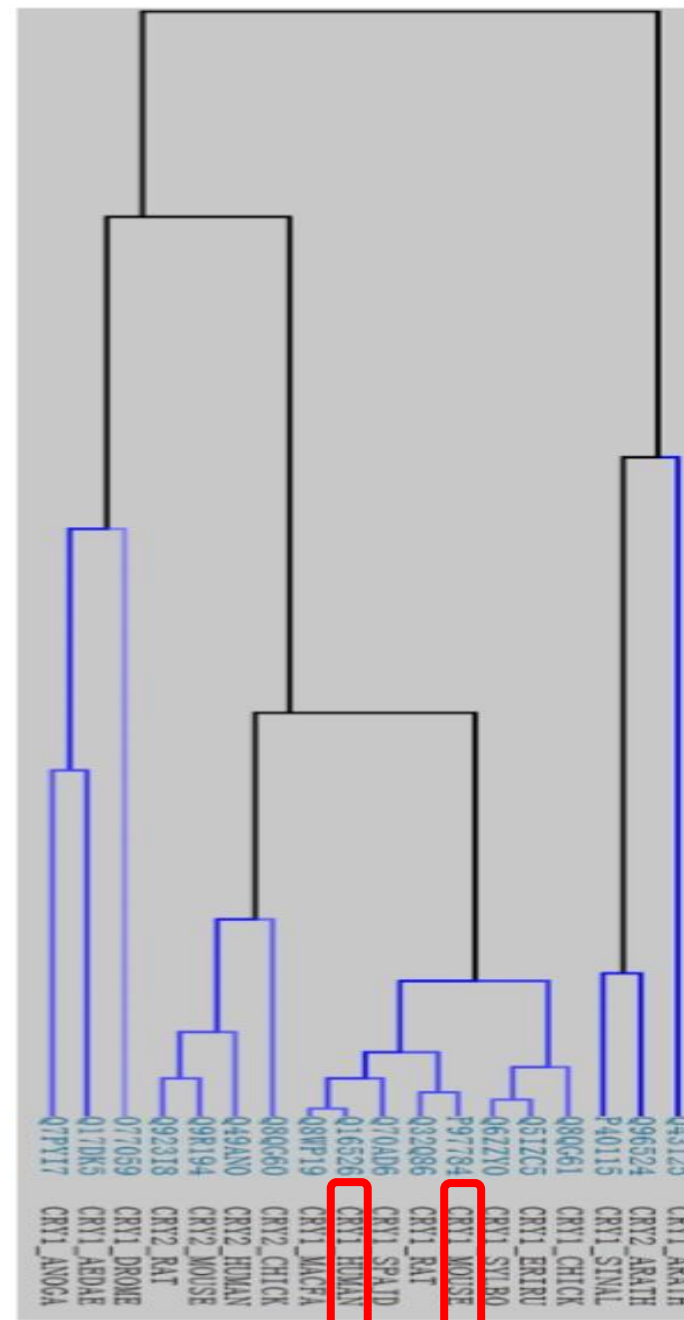- 3D Structure Analysis
- Drug Design

最大似然 bootstrap=1000

CRY1_HUMAN: CRY1_MACFA >
CRY1_SPAJD > CRY1_RAT =
CRY1_MOUSE

全序列比对

By Mega 6.0

By Uniprot

CRY1_HUMAN: Identity
CRY1_MACFA: 97.785%
CRY1_SPAJD: 99.317%
CRY1_MOUSE: 93.324%
CRY1_RAT: 95.748%
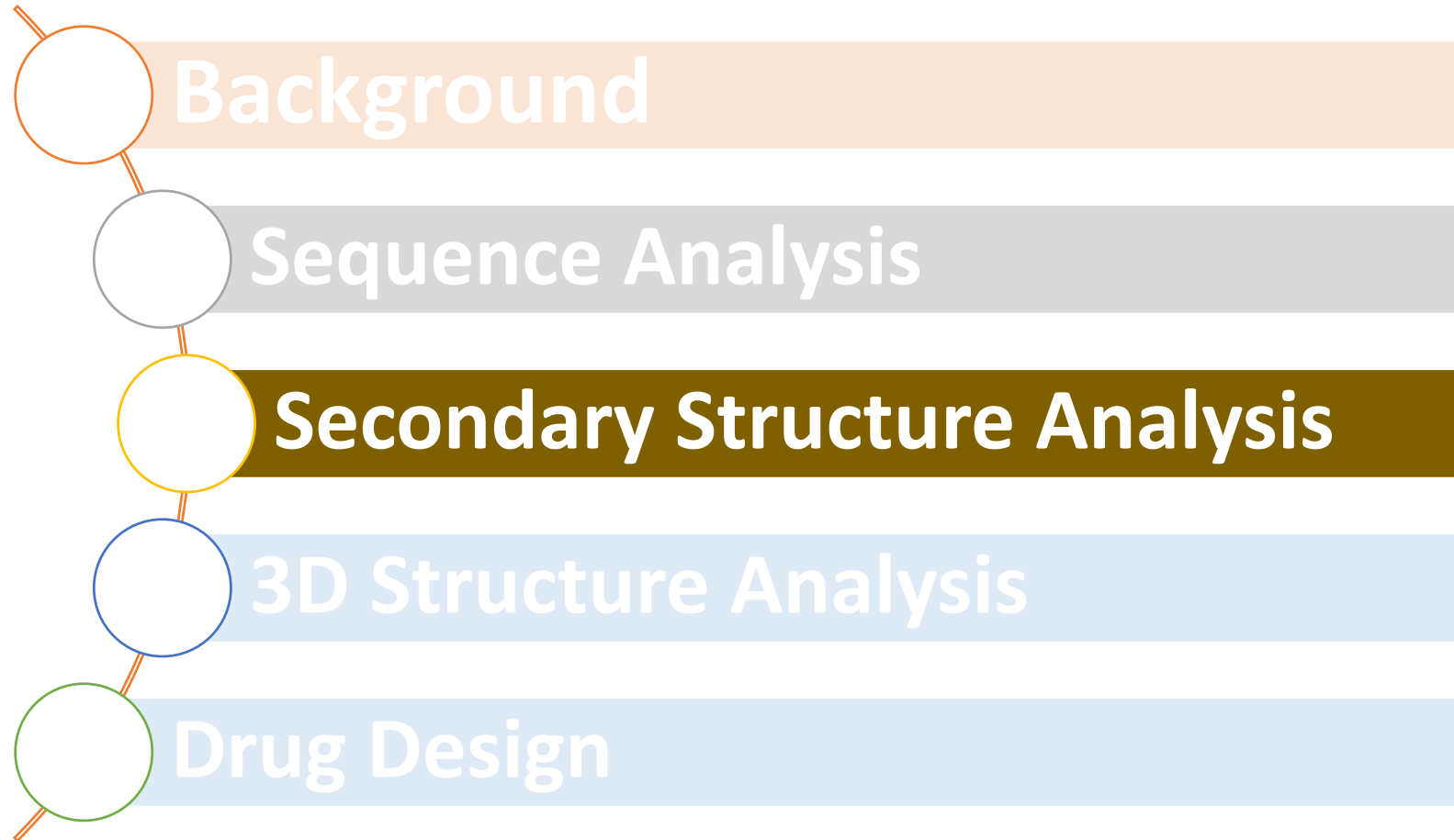
emma(v6.0.1) - Multiple alignment program - interface to ClustalW program

Outline

- Background
- Sequence Analysis
- **Secondary Structure Analysis**
- 3D Structure Analysis
- Drug Design

Tandem Sequence Repeats Analysis

Protein
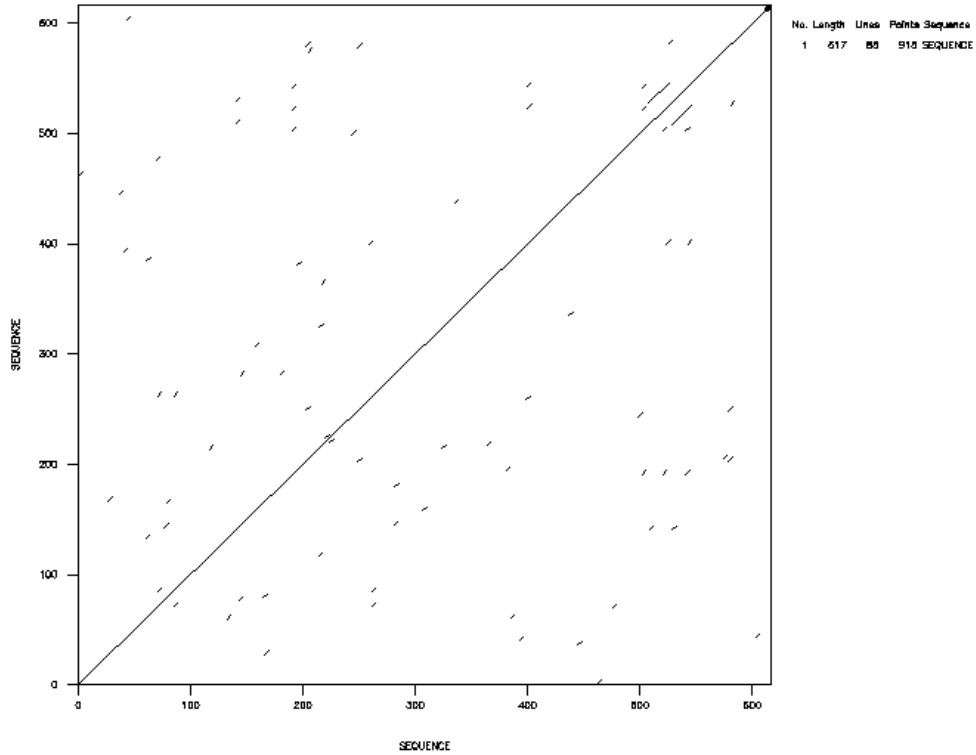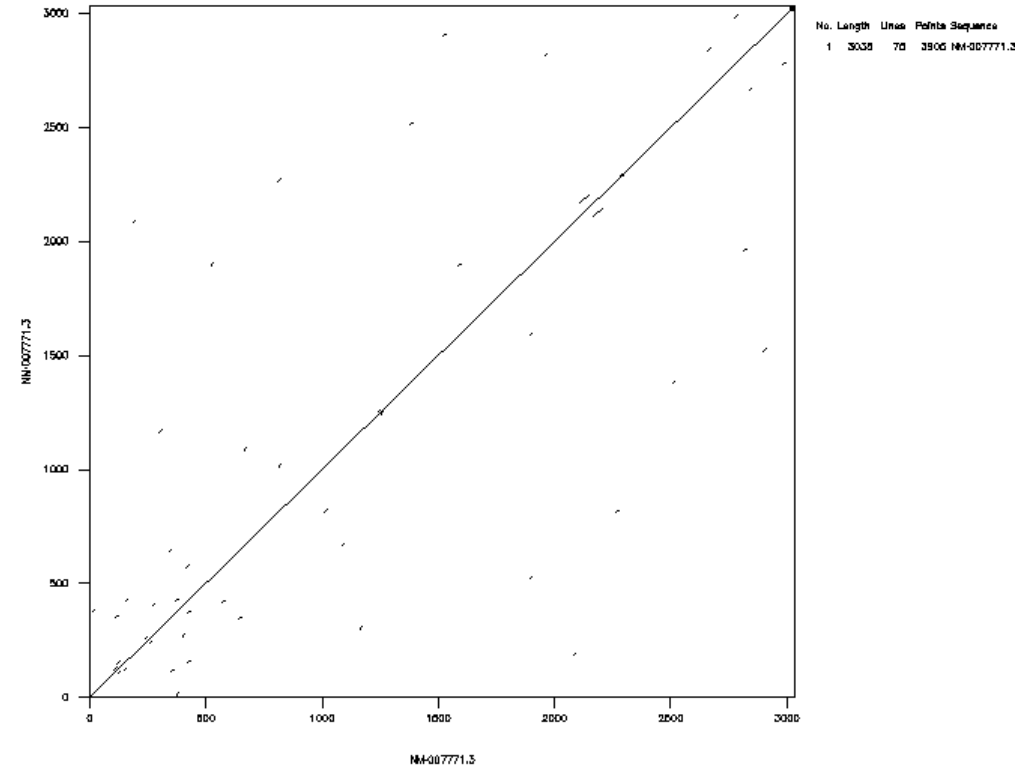
Word size = 3

mRNA

Word size = 9

Hydrophilic and Hydrophobic Analysis
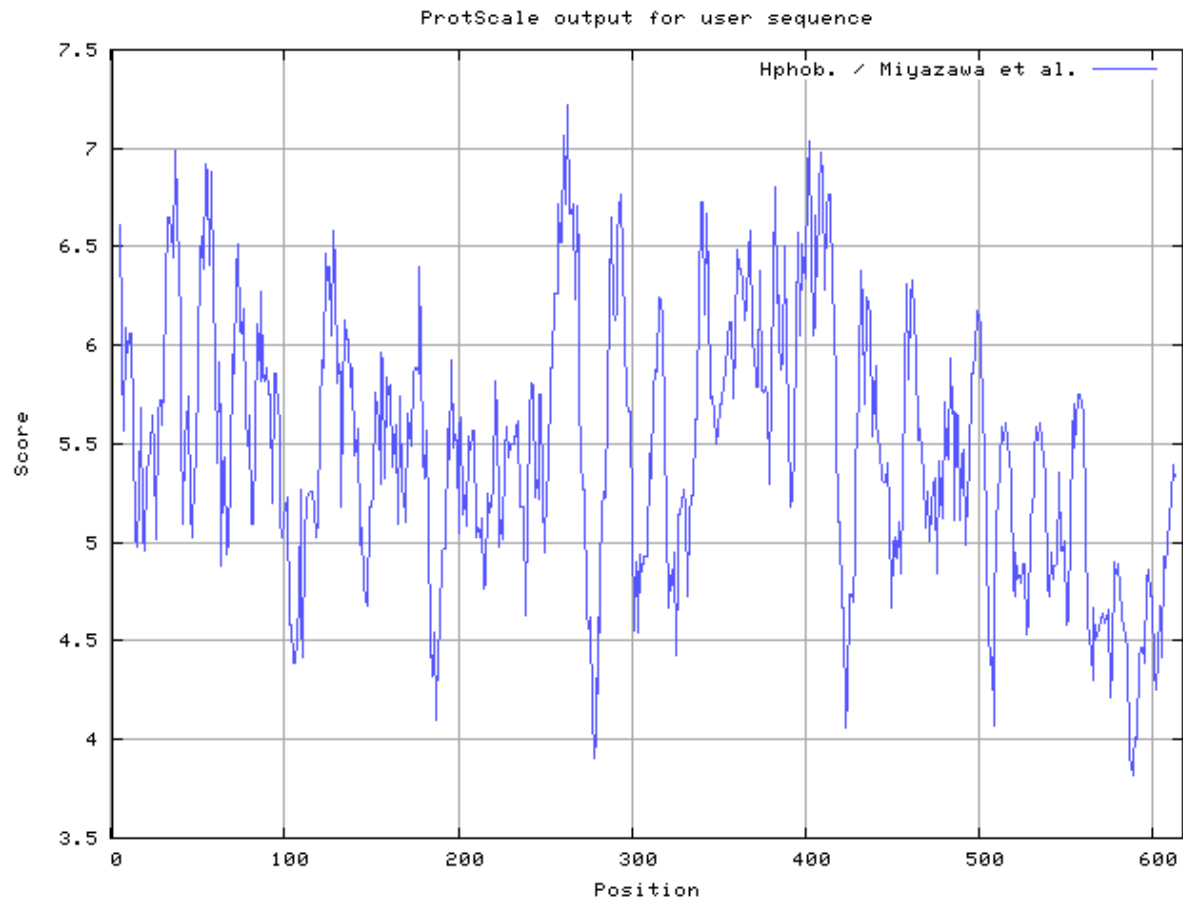
Average Flexibility

Alpha-helix
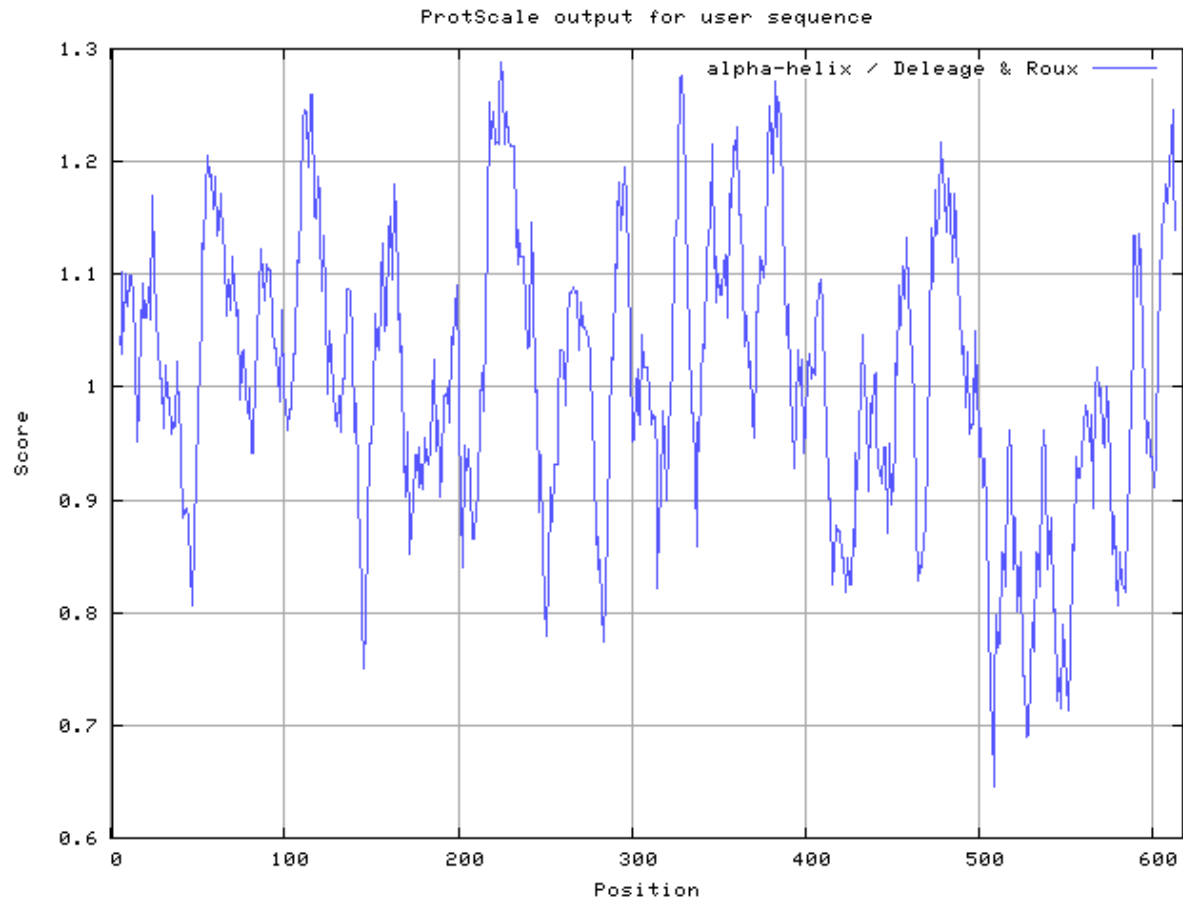
Coil
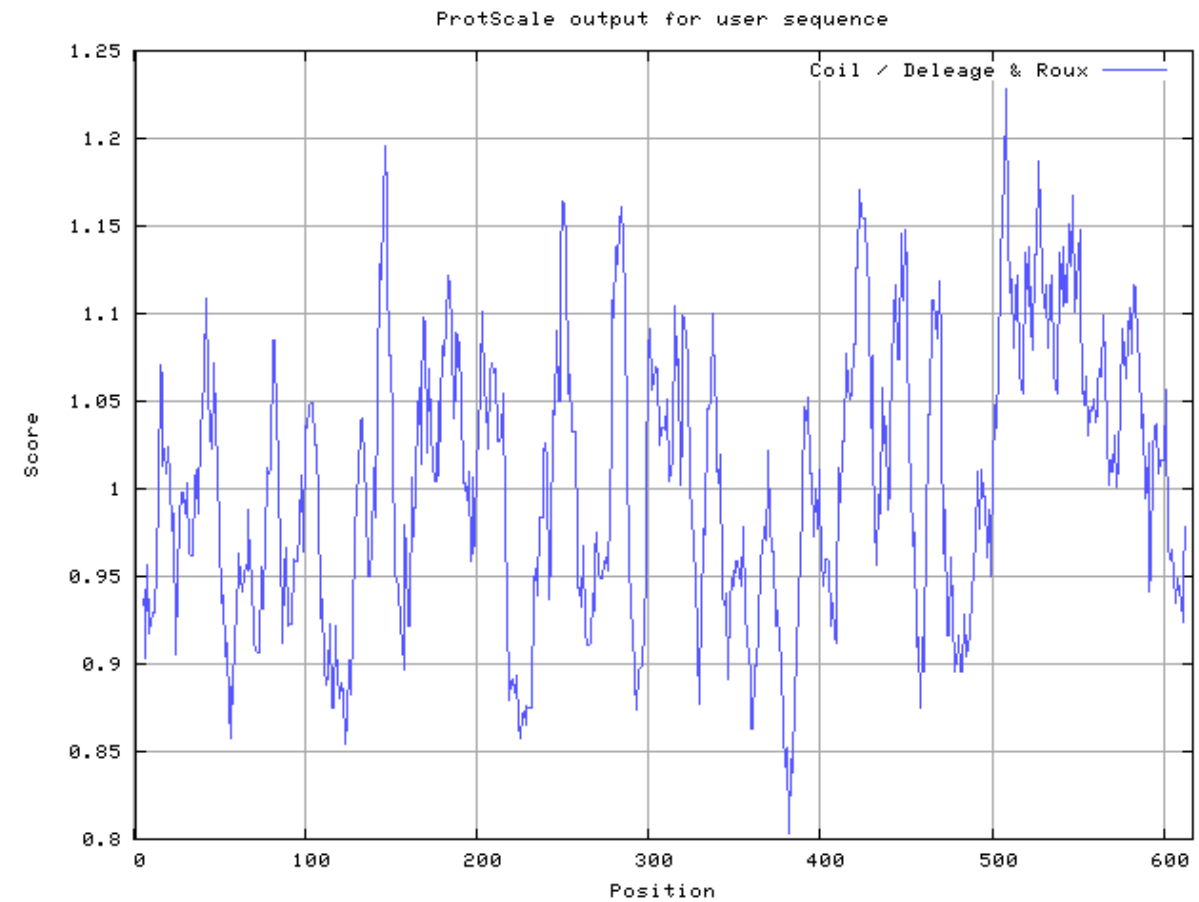
Transmembrane Tendency

Tmap
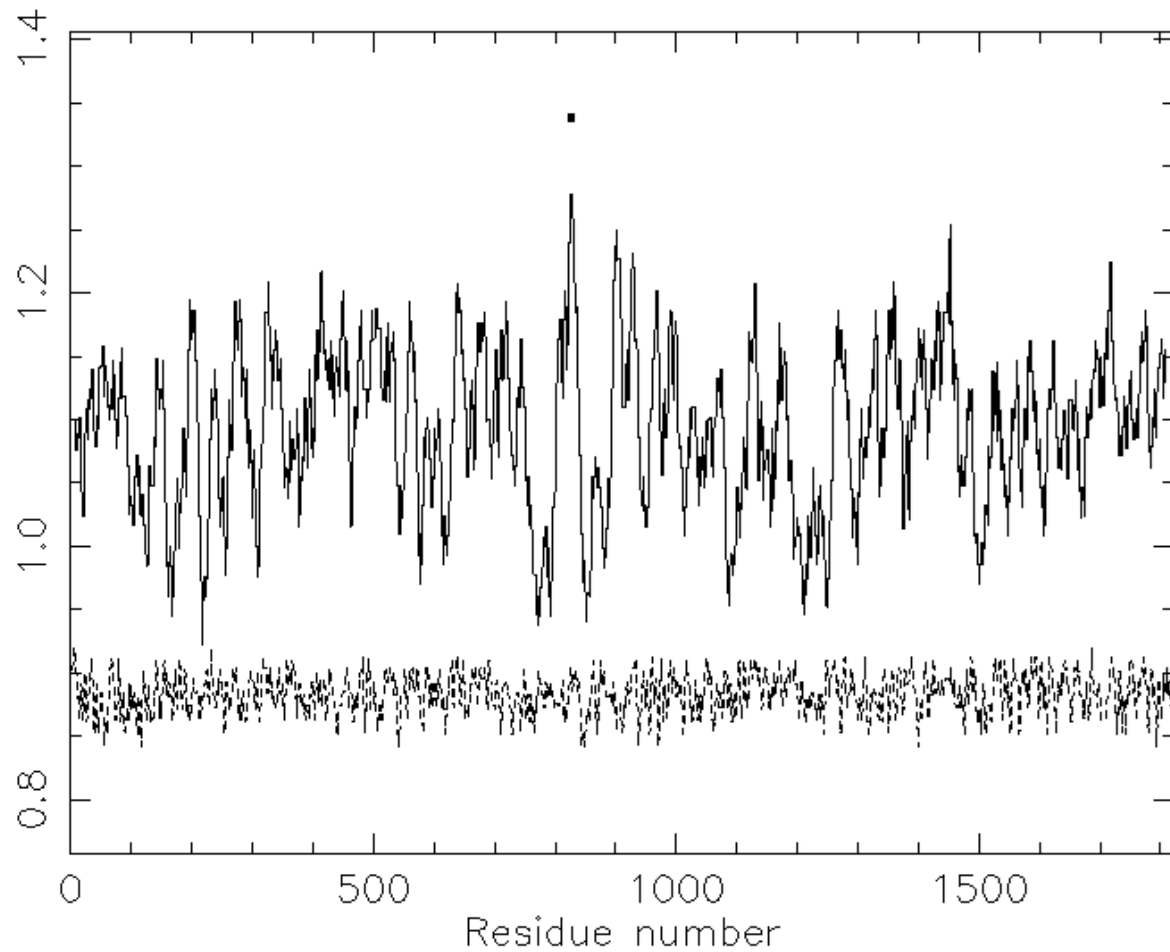
Signal Protein

SignalP-4.1 prediction (euk networks): 4K0R_A_PDBID_CHAIN_SEQUENCE

# Measure	Position	Value	Cutoff	signal peptide?
max. C	31	0.116		
max. Y	11	0.134		
max. S	1	0.201		
mean S	1-10	0.131		
D	1-10	0.133	0.450	NO

Secondary Structure and Disorder Prediction
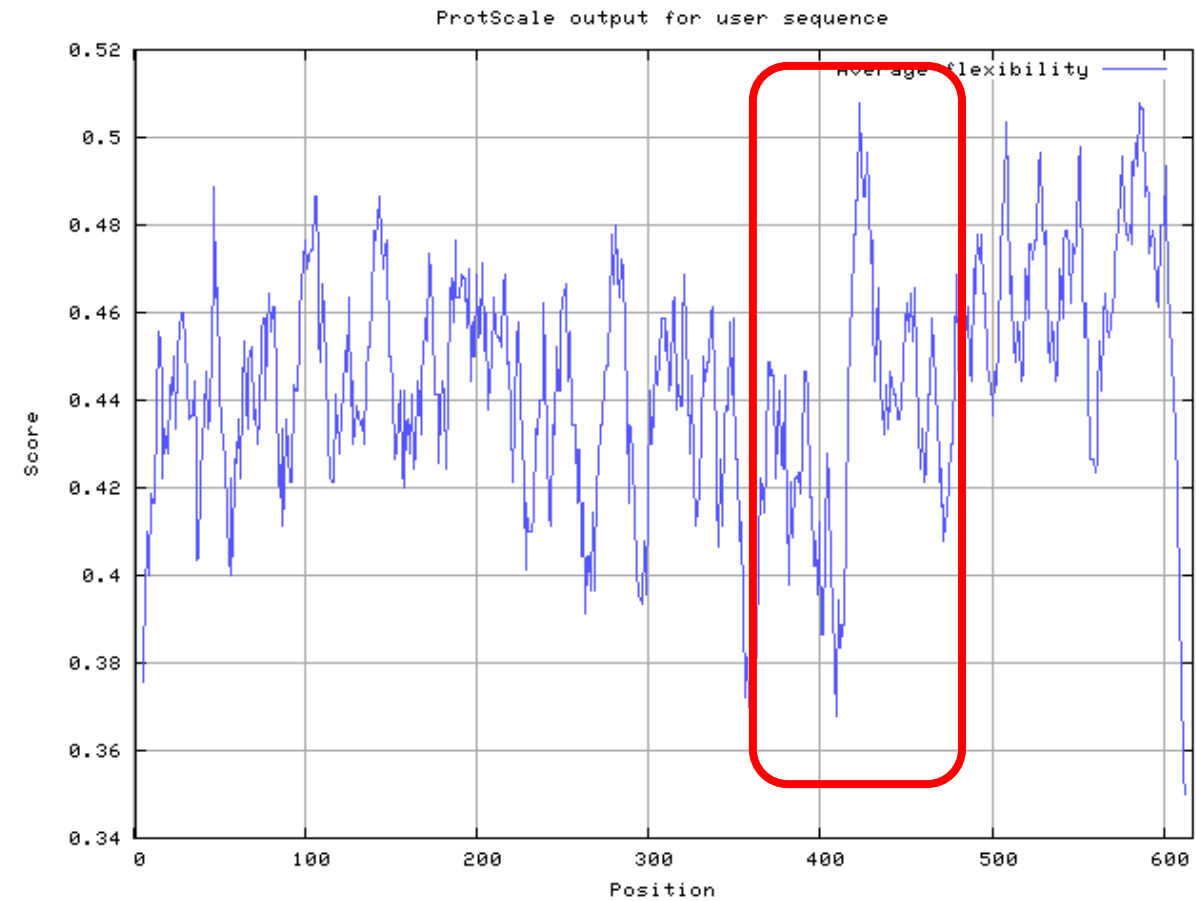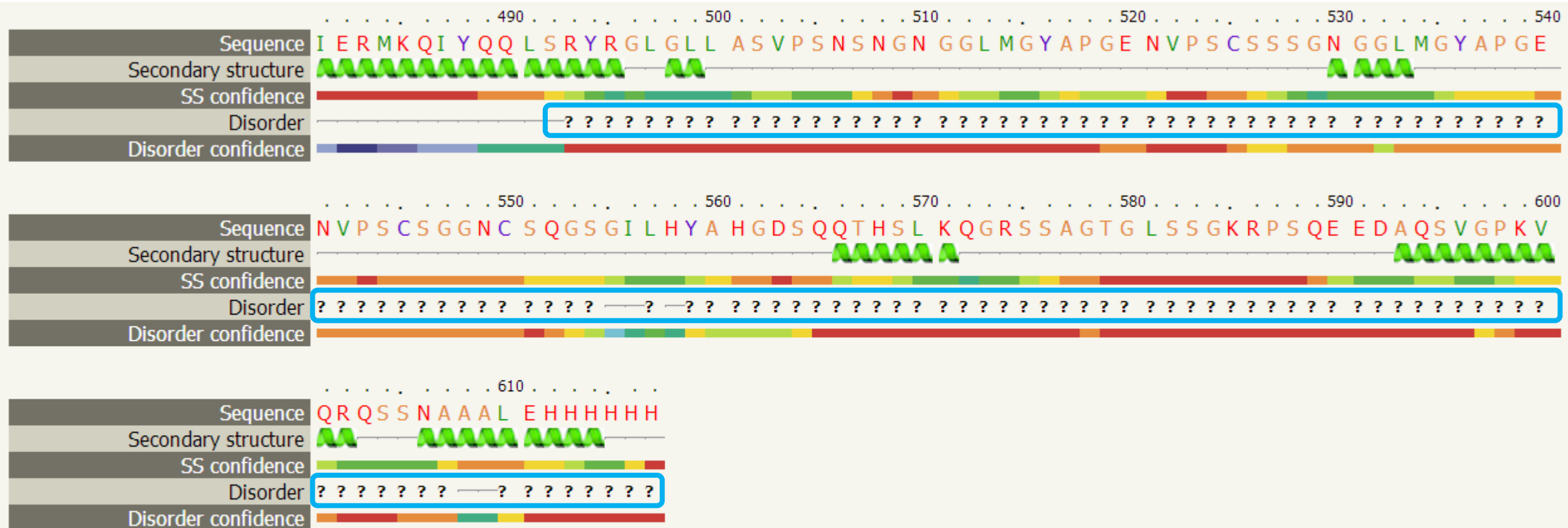
Outline

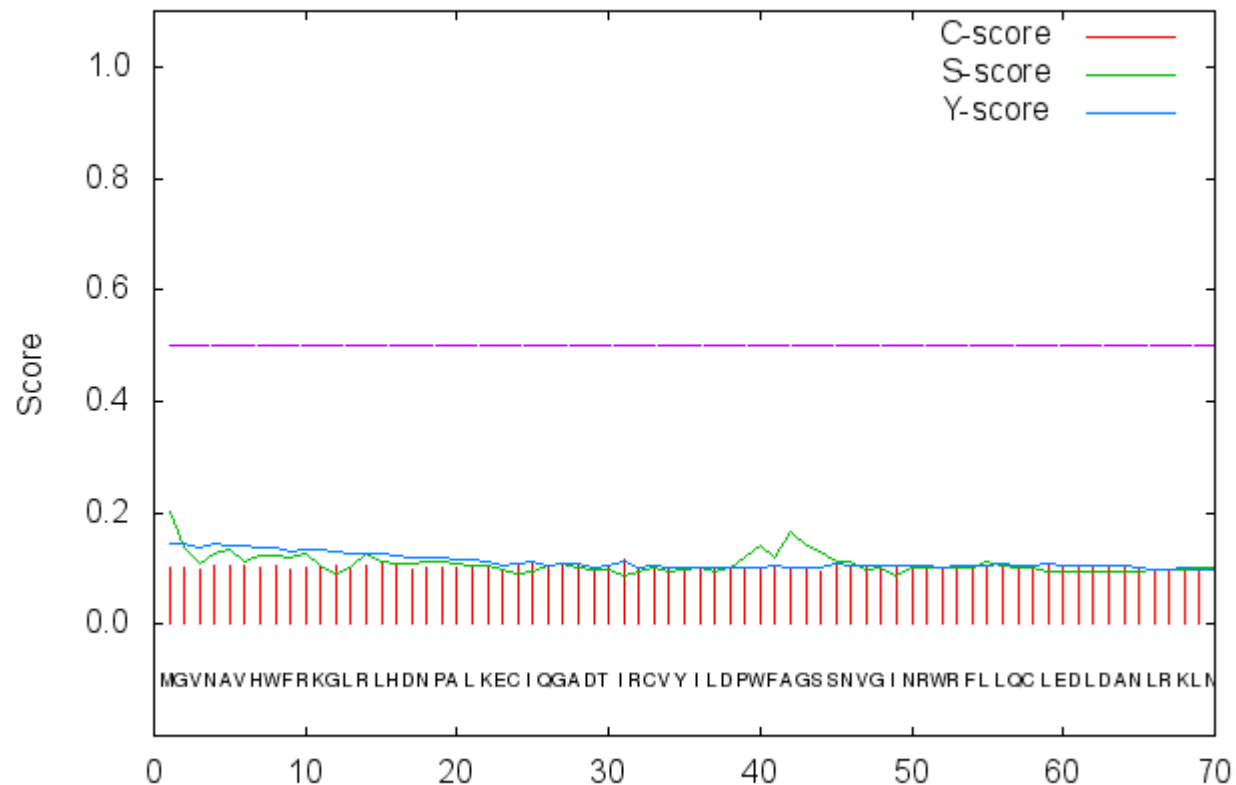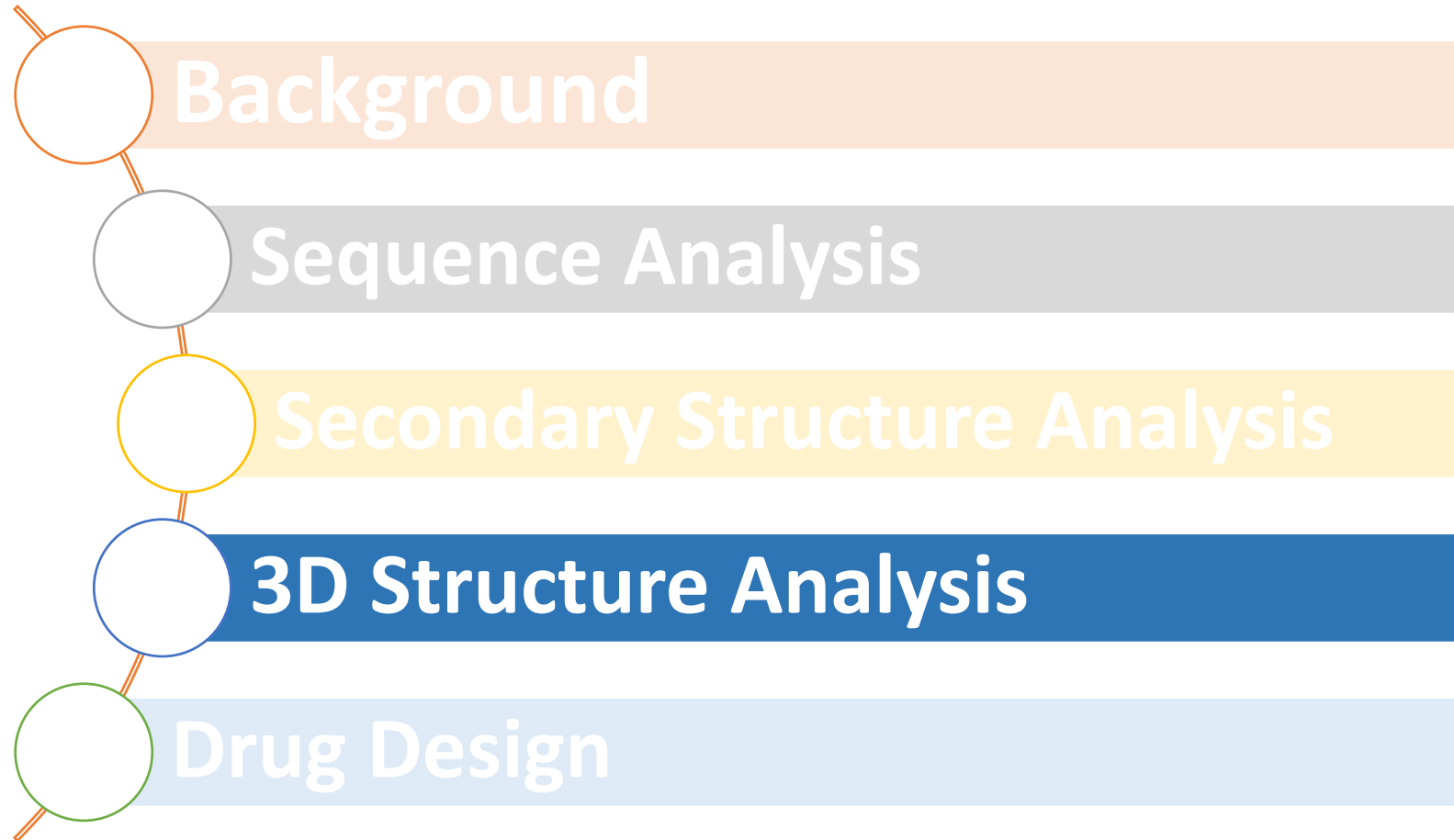Background

Sequence Analysis

Secondary Structure Analysis

3D Structure Analysis

Drug Design

3D structure of Cryptochrome(4I6G)

FAD

Cry2 monomer with FAD ligand

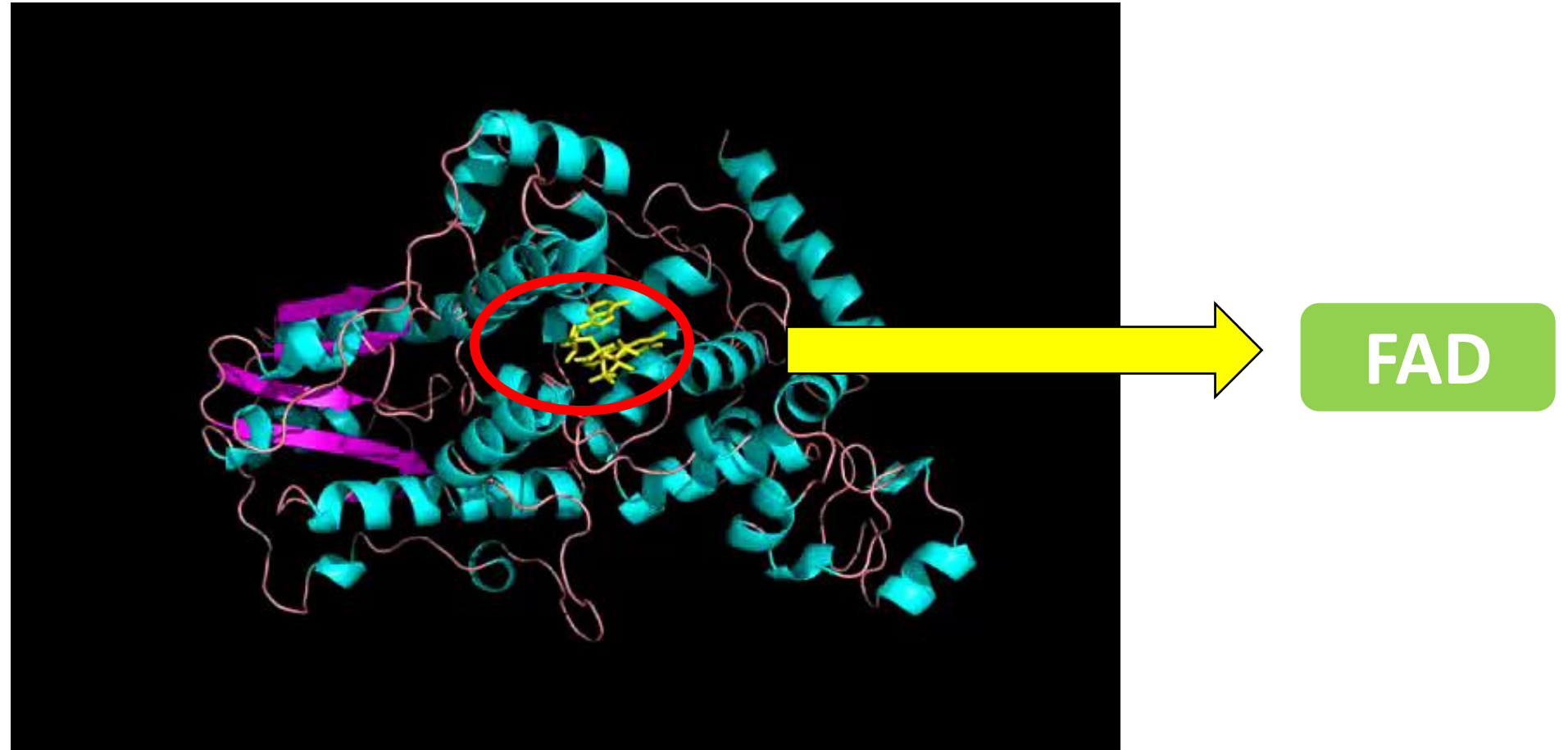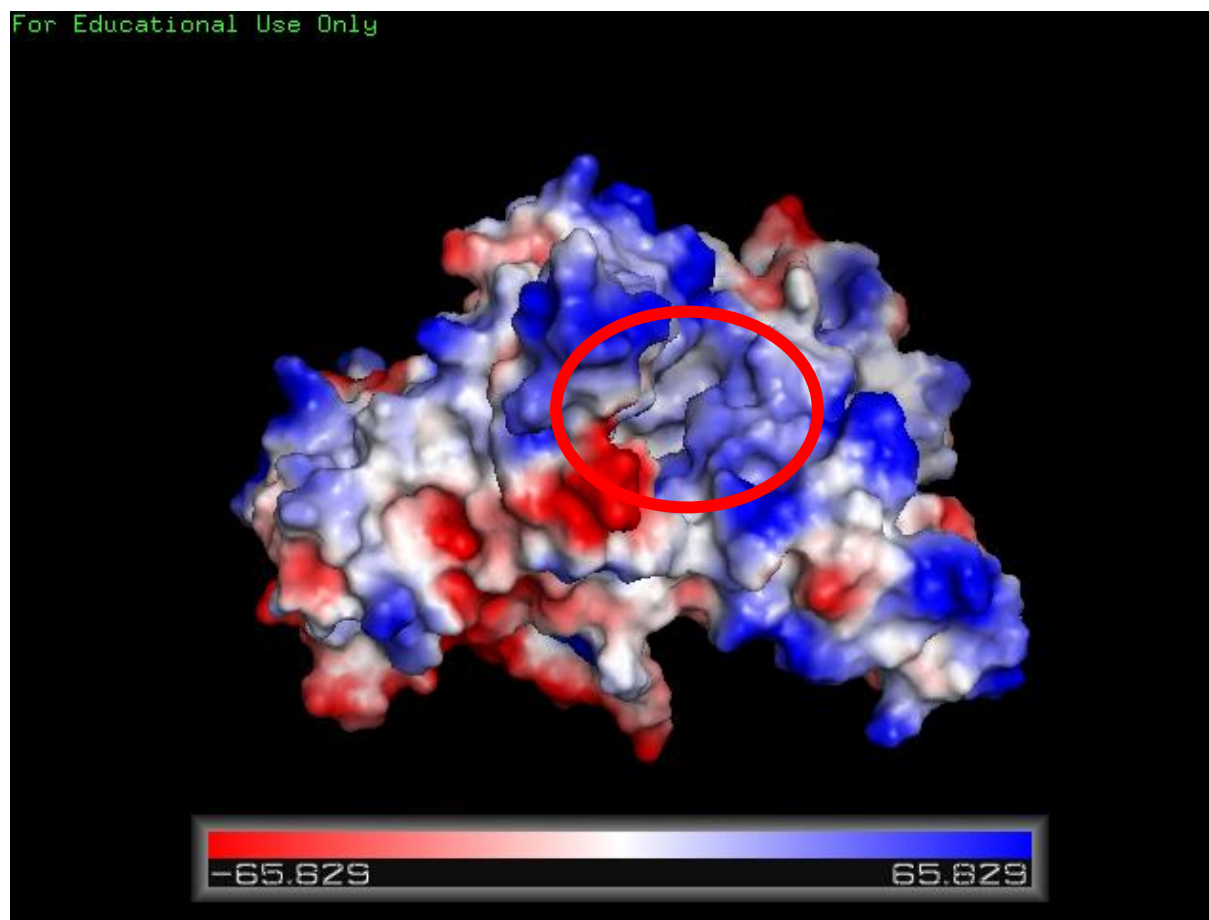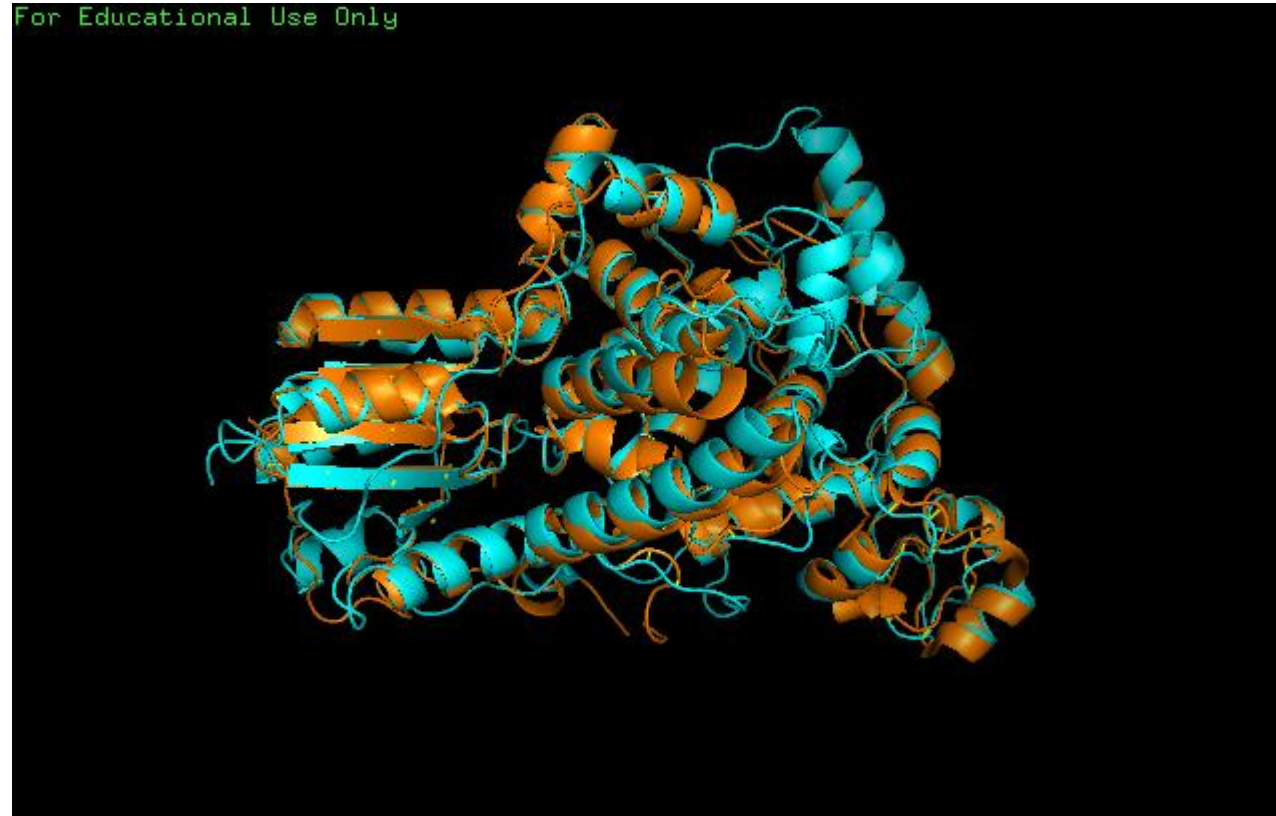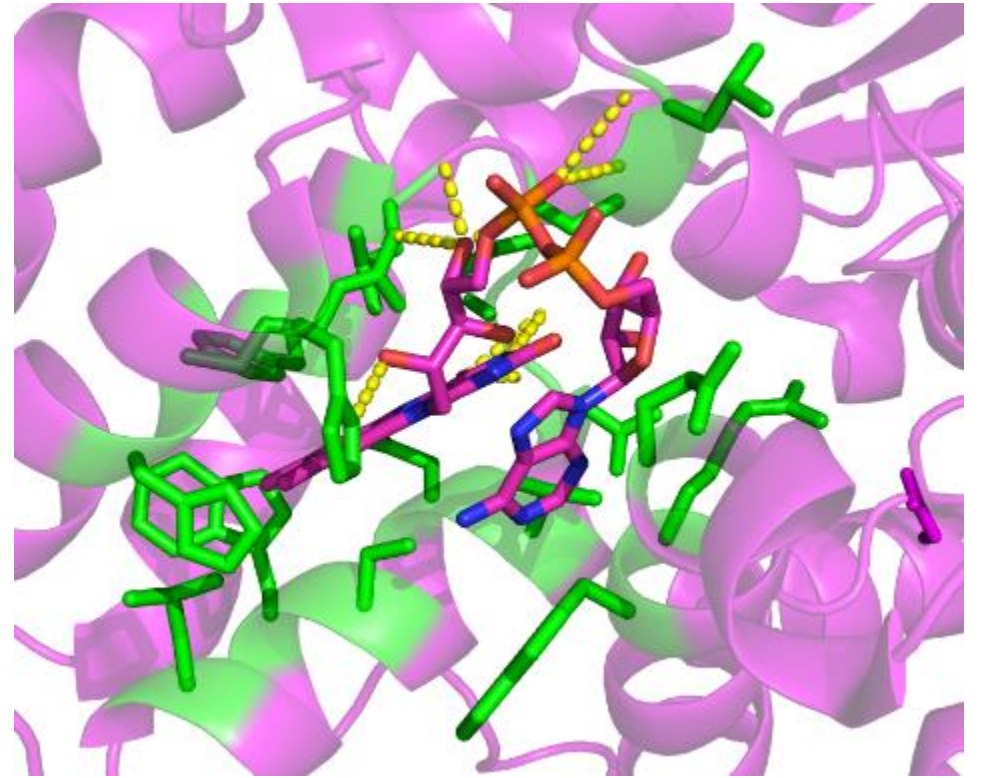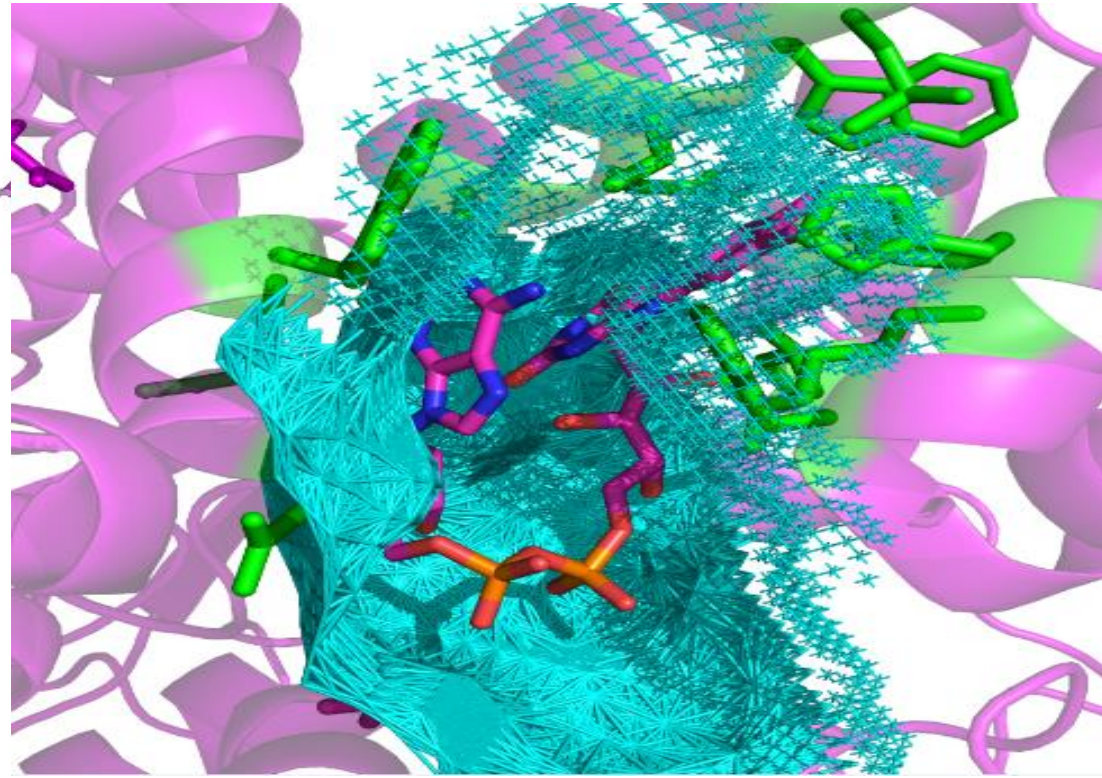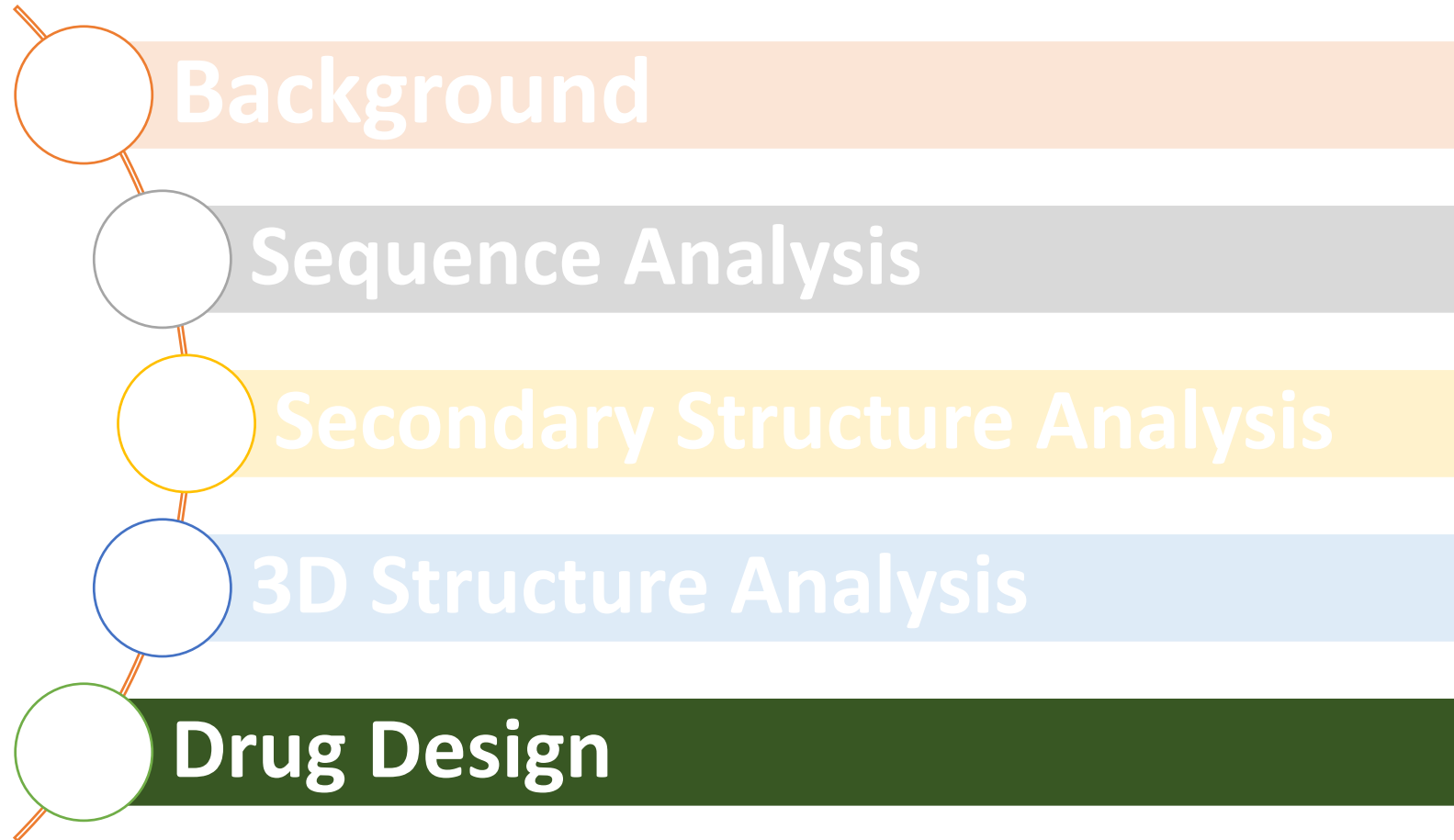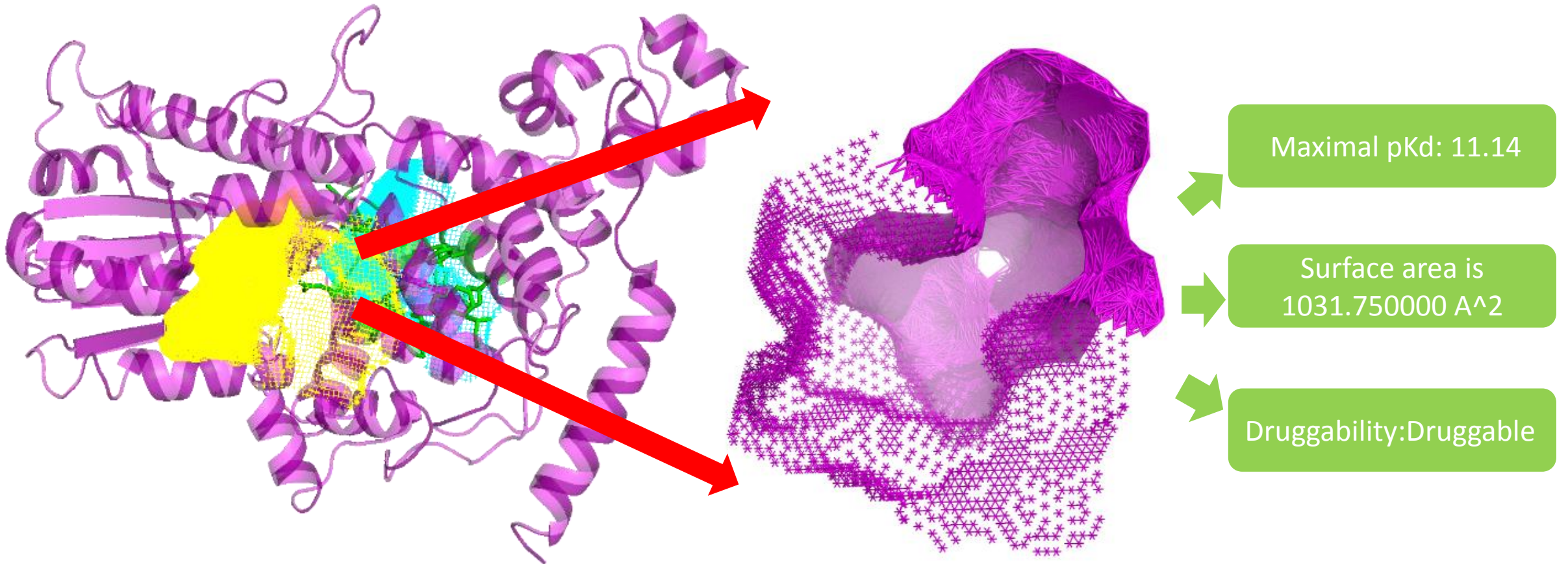# Vacuum Electrostatics (4I6G)

Align Cry1_mouse with Cry1_Droso

FAD Binding Site Analysis

Outline

- Background
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- 3D Structure Analysis
- Drug Design

Another Druggable Pocket by *CAVITY*
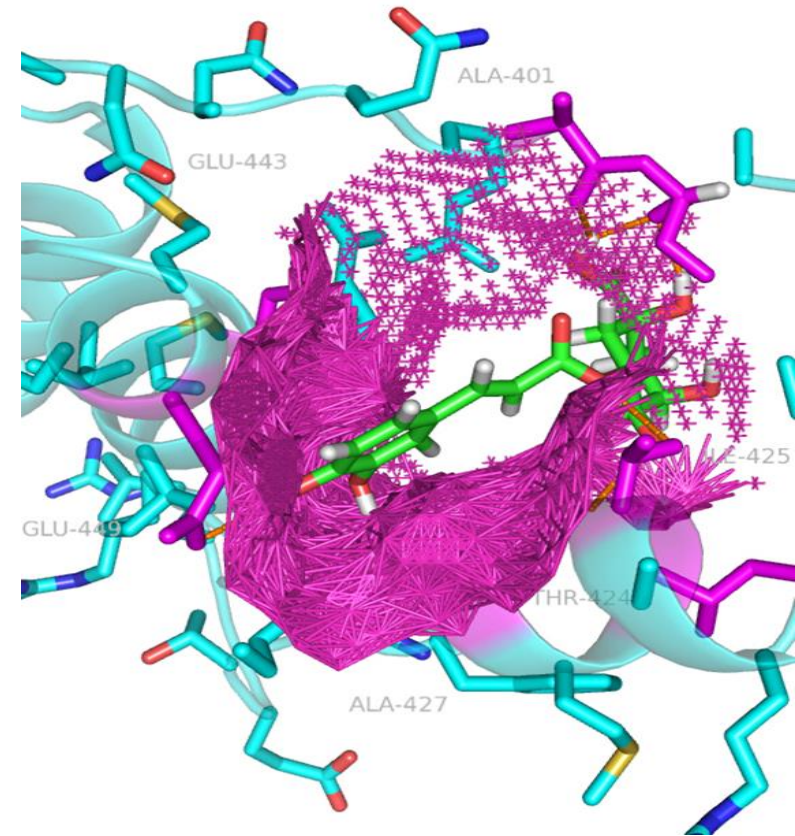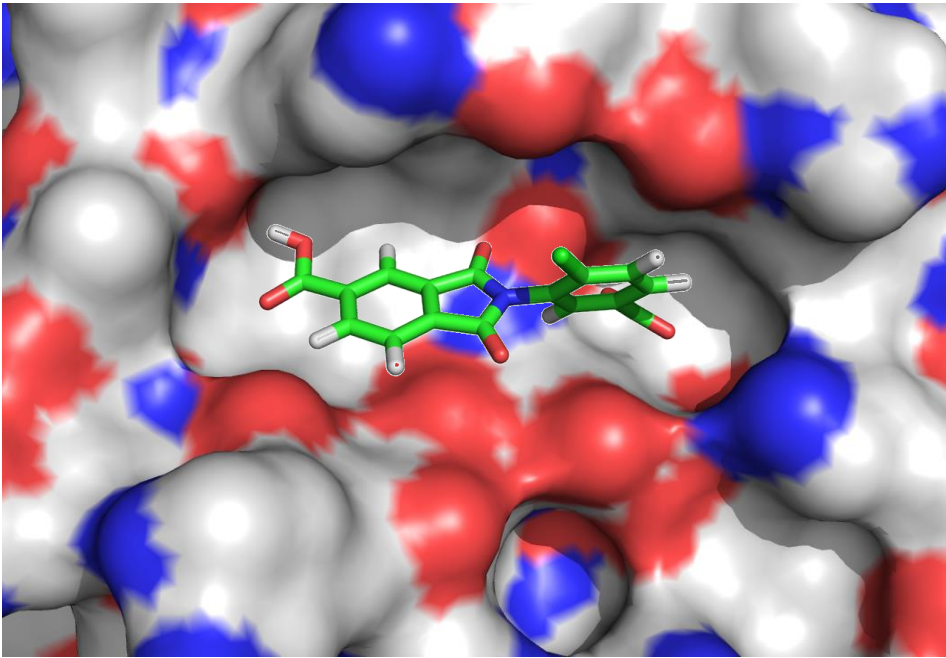

Maximal pKd: 11.14

Surface area is 1031.750000 A^2

Druggability:Druggable

Future work

Acknowledgement

Prof. Jingchu Luo
Prof. Luhua Lai
Xiuzhen Bai
Zhe Yang
Youjun Xu

THANK YOU