

Applied protein structure bioinformatics Educational subject description sheet

Basic information

Study programme		Didactic cycle	
Biotechnologia		2024/25	
Speciality -		Subject code 01BTS.22JO.15679.24	
Organizational unit Faculty of Biology		Lecture languages English	
Study level Second-cycle programme		Course type Elective	
Study form Full-time		Block foreign languages	
Education profile General academic			
Subject coordinator	Jan Brezovsky		
Lecturer	Jan Brezovsky		
Period Semester 2	Activities and hours Lecture: 15, Graded credit 		Number of ECTS points 1

Goals

Code	Goal
C1	Reinforce the knowledge of protein structure and its major components.
C2	Learn about fundamental characteristics of common methods for protein structure determination and prediction.
С3	Learn how to select appropriate protein structures from relevant databases.
C4	Get overview of possible errors in protein structures and methods for their identification.
C5	Learn about biophysical origins of the structure, function and dynamics of proteins.
C6	Learn about methods to analyze protein structures and their complexes to obtain information about their function, dynamics and stability.
C7	Get familiar with principles of primary methods in structural bioinformatics.
C8	Learn about elementary mechanisms behind the effects of deleterious as well as beneficial mutations.
С9	Learn about understand principles of computational mutagenesis and data-driven protein engineering.
C10	Learn about approaches to predict binding poses of small molecules and evaluate their relevance as inhibitors or substrates of enzymes.
C11	Evaluate the key benefits and limitations of applications of structural bioinformatics methods in protein biotechnologies.

Subject learning outcomes

Code	Outcomes in terms of	Learning outcomes	Examination methods
Knowledge - Student:			
W1	is able to describe the structures of proteins and knows the general principles of the methods for their determination and predictions	BTE_K2_W01, BTE_K2_W02, BTE_K2_W05, BTE_K2_W06	Test
W2	understands the biophysical origins of structure, function and dynamics of proteins	BTE_K2_W01	Test
W3	knows key structural bioinformatics methods to analyze the structures of proteins and their complexes to obtain information about their function, dynamics and stability	BTE_K2_W05	Test
W4	knows principles of data-driven protein engineering strategies	BTE_K2_W03, BTE_K2_W05, BTE_K2_W06	Test
W5	knows methods for identification of putative inhibitors and substrates of enzymes	BTE_K2_W05	Test
W6	understands the most prevalent mechanism behind the effects of deleterious and beneficial mutations	BTE_K2_W01, BTE_K2_W03, BTE_K2_W06	Test
W7	knows the key benefits and limitations of applications of structural bioinformatics methods	BTE_K2_W05	Test
Skills - Student:			

Code	Outcomes in terms of	Learning outcomes	Examination methods
U1	is able to select appropriate protein structures from relevant databases, being aware of possible errors in these structures	BTE_K2_U02, BTE_K2_U08	Test

Study content

No.	Course content	Subject learning outcomes	Activities
1.	Basic physical principles of protein structure and its hierarchy.	W1, W2	Lecture
2.	Experimental and computatioanl sources of protein structures.	W1	Lecture
3.	Structure quality control.	U1	Lecture
4.	Structure visualization.	W1, W3	Lecture
5.	Analysis of protein structures.	W2, W3, W7	Lecture
6.	Common molecular foundations of the effects of mutation.	W6	Lecture
7.	Protein engineering objectives and targets.	W2, W4	Lecture
8.	Computer-guided semi-rational protein design.	W3, W4, W6	Lecture
9.	Rational protein design.	W3, W4	Lecture
10.	Mutant structure prediction.	W2, W3, W6	Lecture
11.	Protein stabilization approaches.	W3, W4, W6, W7	Lecture
12.	Stability-solubility trade-off.	W2, W3, W4, W6	Lecture
13.	Predicting inhibitors and substrates of enzymes with molecular docking methods.	W3, W5, W7	Lecture

Additional information

Activities	Teaching and learning methods and activities
Lecture	Lecture with a multimedia presentation of selected issues, Discussion

Activities	Credit conditions
Lecture	25 questions with multiple choices, each worth 1 point. Partial positive and negative points can be awarded within a single question. The overall grading scheme: 22+ points = 5.0 20.00-21.99 points = 4.5 17.00-19.99 points = 4.0 14.00-16.99 points = 3.5 11.00-13.99 points = 3.0 0.00-10.99 points = 2.0

Literature

Obligatory

- 1. Ng PC & Henikoff S (2006). Predicting the effects of amino acid substitutions on protein function. Annual Review of Genomics and Human Genetics 7: 61-80.
- 2. Bendl J et al. (2016). HotSpotWizard 2.0: automated design of site-specific mutations and smart libraries in protein engineering. Nucleic Acids Res. 44: W479-487.
- 3. Wijma HJ, Floor RJ & Janssen DB (2013). Structure-and sequence-analysis inspired engineering of proteins for enhanced thermostability. Current Opinion Structural Biology 23: 588–594.
- 4. Lutz S (2010). Beyond directed evolution: semi-rational protein engineering and design. Current Opinion in Biotechnology 21: 734-V743.
- 5. Daniel L et al. (2015) Mechanism-Based Discovery of Novel Substrates of Haloalkane Dehalogenases using in Silico Screening. Journal of Chemical Information and Modeling 55:54-62.
- Wang Z et al. (2016) Comprehensive evaluation of ten docking programs on a diverse set of protein-ligand complexes: the prediction accuracy of sampling power and scoring power. Physical Chemistry Chemical Physics 18: 12964-12975.

Optional

- 1. Liljas A et al. (2009). Textbook Of Structural Biology, World Scientific Publishing Company, Singapore.
- 2. Schwede T & Peitsch MC (2008). Computational Structural Biology: Methods and Applications, World Scientific Publishing Company, Singapore.
- 3. Broom A et al. (2017). Computational tools help improve protein stability but with a solubility tradeoff. The journal of biological chemistry. 292: 14349-14361.
- 4. Bendl J et al. (2014). PredictSNP: Robust and accurate consensus classifier for prediction of disease-related mutations. PLOS Computational Biology10: e1003440.
- 5. Potapov V et al.(2009). Assessing computational methods for predicting protein stability upon mutation: good on average but not in the details. Protein Engineering, Design & Selection 22: 553-560.
- 6. Gu J. & Bourne P. E. : Structural Bioinformatics, 2nd Edition, Wiley-Blackwell, Hoboken, New Jersey, 2009

Calculation of ECTS points

Activities	Activity hours*
Lecture	15
Reading the indicated literature	10
Preparation for the exam	5
Student workload	Hours 30
Number of ECTS points	ECTS 1

* academic hour = 45 minutes

Efekty uczenia się dla kierunku

Kod	Treść
BTE_K2_U02	The graduate can krytycznie analizować, selekcjonować i wykorzystywać wiedzę specjalistyczną z zakresu nauk przyrodniczych w celu rozwiązania problemu badawczego
BTE_K2_U08	The graduate can posługiwać się językiem angielskim w zakresie nauk przyrodniczych zgodne z wymaganiami określonymi dla poziomu B2+
BTE_K2_W01	The graduate knows and understands mechanizmy funkcjonowania organizmów w aspektach: molekularnym, komórkowym i fizjologicznym
BTE_K2_W02	The graduate knows and understands problemy badawcze z pogranicza nauk biologicznych, które wymagają zastosowania zaawansowanych narzędzi nauk ścisłych
BTE_K2_W03	The graduate knows and understands wykorzystanie modeli badawczych oraz zasady projektowania i modyfikacji materiału genetycznego
BTE_K2_W05	The graduate knows and understands zaawansowane narzędzia bioinformatyki i statystyki niezbędne do realizacji eksperymentów oraz interpretacji wyników
BTE_K2_W06	The graduate knows and understands techniki modyfikacji i analizy materiału biologicznego aktualnie stosowane w biotechnologii