

CHARLES UNIVERSITY

is proud to announce our guest SIEGERIED SCHWARZ

Professor of Pathophysiology at Biocenter of Medical University Innsbruck, Austria who is going to introduce here a novel lecture topic as well as the lecture format.

We would like to welcome undergraduate students of Medicine as well as Biology, from the 3rd semester onwards. You are kindly invited to attend a 3-day interactive and interdisciplinary course, learn molecular modelling methods, perform your individual homework and give a final 10-minutes presentation in English. Successful participants receive 4 credit points.

PROGRAMME:

November 16th, 10:00 - 18:00

at IMG ASCR, Vídeňská 1083, Praha 4, ground floor seminar room (https://goo.gl/maps/G957SiyWTwE2)

10:00 – 12:00 Siegfried Schwarz: Opening lecture I:

Crucial importance of understanding proteins for understanding diseases in general, the example DIABETES INSIPIDUS and other endocrine diseases

14:00 – 16:00 Karel Drbal: Lecture II: Innate immunity structures and diseases

16:00 – 18:00 Jiří Hatina: Lecture III: HLA and diseases

November 17th, 10:00 – 16:00, November 18th 10:00 – 16:00 at Faculty of Science, CUNI, Viničná 7, Praha 2, seminar room B311 (https://goo.gl/maps/4896ARK4NPC2)

Practical training days in the PC room for introduction to molecular modelling software and how to use PDB and OMIM databases-computers provided, your personal comps allowed.

It includes an assignment of a single disease case report to each student for your homework on linking the protein structure to the underlying molecular pathophysiology.

<u>December 9th, at 10:00 – 17:00 (proposed term)</u>, room B311 Presentation of students' homework and discussion. Receipt of credits.

Consensual decision on the date of final case report presentations of your homework will be taken on Nov, 16th.

No admissions fees. Limited number of 25 students allowed. Sign-in by enrolling in SIS: course EA0103031 or email to: Jiri.Hatina@lfp.cuni.cz



MEDIZINISCHE UNIVERSITÄT

This course gives you a general overview on our understanding of the normal as well as abnormal protein structures originating from particular gene mutations and/ or allosteric effector function in health as well as in a diseased state. Introduction provides couple of examples of structure-function relationships in human medicine.

Next day we follow with a hands-on course in a computer room where attendees receive a detailed step-by-step description how to perform practical molecular modelling on PC using appropriate open-source software (PyMol).

Having the X/Y/Z coordinates of atoms, as deposited in the Brookhaven Protein Data Bank (PDB), students can visualize and manipulate 3D structures of crystallized proteins, alone or after interaction with small or large ligands such as their substrates, drugs, DNA or other proteins. Attendees will learn also how to use the OMIM (Online Inheritance in Men) Data Bank from where they can retrieve the published mutations and a corresponding disease pathology. Thereby, various structural characteristics can be recognized: domains of certain structure or charge, hydrophobicity or shape and other properties, which can serve e.g. as a ligand-binding domain, a DNA-binding domain, a drug-metabolizing pocket or as a domain for any other biological function. The real power of molecular modelling resides in its informative value displaying the molecular structure, in total or in portions thereof, in different formats such as wireframe, protein backbone, atoms, overall surface etc. It is possible to turn the molecule in all directions and to see in real time various aspects of its structure. Most importantly, points of mutation, as documented in the OMIM and other databases, can be mapped into a structural model in order to understand which function of the protein would thus be altered and whether this change in structure would result in loss-of-function or gain-offunction showing recessive or dominant effect. Link between arginine vasopressin precursor (AVP) and Diabetes insipidus serves as an illustrative and informative example.

In the second part of this course, students will get assigned an individual mutated protein and a corresponding disease pathology that they have to elaborate as a homework according to the demo example they have seen in the course. Each student should prepare a short (10 minutes) lecture in Power Point or alternative and discuss her/his observations, published data and clinical outcomes.

On the last day of the course (after at least 2 weeks), students are going to present their homework in front of all attending colleagues including teachers. As such, everybody learns from the others - kind of a multiplication effect.

The course is based on a textbook published by Siegfried Schwarz: MOLECULES OF LIFE & MUTATIONS (Karger, Basel 2002, ISBN: 978-3-8055-7395-5), in which structures of 150 most important molecules are displayed.

http://www.karger.com/Book/Home/227359

MOLECULES OF LIFE & MUTATIONS

A practical computer course: molecular modelling and disease explanation

November 16th, 17th and 18th 2016

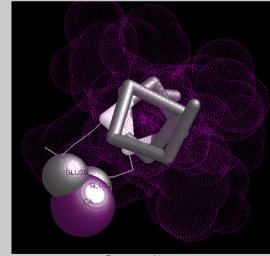
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Prof. Siegfried Schwarz, Medical University Innsbruck, Austria

and

Assoc. Prof. Jiří Hatina, Faculty of Medicine in Pilsen, Charles University in Prague, Czech Republic

Dr. Karel Drbal, Faculty of Science, Charles University in Prague, Czech Republic



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