

REPORT

From bioinformatics analysis of genomes to computational structural biology and applications

AKTION project number: 95p4

Basic data: Beginning of the project FebruJanuary 1, 2023
Completion of the project November 30, 2023

Project partners:

Prof. Mgr. Václav Brázda, Ph.D., Brno University of Technology, Faculty of Chemistry, Institute of Food Science and Biotechnology

Assoc. Prof. Dr. Pedro A. Sánchez Murcia, Medical University of Graz, Otto-Lewi Research Center, Division of Medicinal Chemistry

Course of the project and student stays:

11. 4. – 14. 4. 2023 – Workshop in Brno, lead: Prof. Václav Brázda (20 participants)

Participants from Graz: researchers: Prof. Pedro A. Sanchez Murcia, Christoph Nusshold
students: Spela Mandl, Bruno Di Geronimo, Juan Toledo, Daniel Platero-Rochart, Gibu George, Javier Ortin, Carmen Barambio

Program:

In this first workshop, the students were trained theoretically in the analysis of the genome and the local structure of nucleic acids (NA), in multifilament structures of NA as well as in their biochemical characterization. Students learned about the functions and use of genomic databases and online tools such as G4 hunter or Palindrom analyzer. Furthermore, the students were introduced to PCR technique, which they also practically tried out and in the last part of the seminar they looked at Python programming. An important part of the stay in Brno was a visit to the Mendel's Museum, as the father of Genetic Science, and also collaborative activities.

The public lectures in the course were attended by 58 and 45 participants mostly from the chemistry faculty of the BUT (Photo documentation and lists of participants are attached in Annex 1 (*A-1_95p4-foto-lists.pdf*)).

11. 9.-14. 9. 2023 - Workshop in Graz, lead: Prof. Pedro Sánchez Murcia

Participants from Brno: researchers: Prof. Václav Brázda, Julie Hoová

students: Lucia Dzurická, Lucie Šislerová, Michaela Dobrovolná, Libuše Kratochvilová

Program:

The focus of the second workshop was the study of computational structural biology. First, the students learned about databases, prediction of structure in proteins and nucleic acid and free energy calculations in theoretical lessons. The next day they had their first practical lessons where they tried Molecular Dynamics simulations and on the last day, they tried also free energy calculations to compute ligant-macromolecule interaction. Of course, the stay in Graz also included excursions to discover the beauties of this historical city.

Student stays:

31. 5. – 30. 6. 2023 Brno University of Technology, Spela Mandl

Stays program:

The stay was focused on learning various laboratory techniques such as: isothermal titration calorimetry (ITC), atomic force microscopy (AFM), including sample preparation and image processing.

Furthermore, the stay included working with mammalian cells, yeast cultures, isolating plasmid DNA from bacterial cultures and using this DNA for AFM.

11.9. - 9.10.2023 Medical University Graz, Lucie Šislerová

Stays program:

The aim of the residency was Molecular Dynamics simulation of the secondary structure of DNA, specifically the G quadruplex and simulation of the interaction with various natural ligands such as gallic acid, epicatechin or brucine. All the work was purely computational but these results will be connected to the experimental outputs.

Overview of the use of the approved funding: All sources were spent according to the AKTION rules as expected, all expenses are given in detail in the *Annex 2 (A-2_účetní sestava_2023Brazda.pdf)*.

Project evaluation:

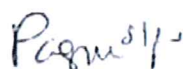
The project was very positively evaluated by both students and scientific prospectors. The workshops enabled effective acquaintance of both Czech and Austrian participants with the methods and issues being addressed at the individual sites. The mutual use of experimental and computational methods brings many benefits for both parties involved. The exchange visits were also very positively evaluated, where one student from the Czech and Austrian side had the opportunity to use the acquired knowledge in depth. In addition to the scientific benefits, the participants also appreciated the possibility of mutual cultural and social enrichment in the context of getting to know the cities of Brno and Graz. Due to the mutual satisfaction, a follow-up project was submitted so that other students could be involved in these exchange activities.

Brno Dec 13, 2024



Prof. Mgr. Václav Brázda, Ph.D.

Brno University of Technology, Faculty of Chemistry



Assoc. Prof. Dr. Pedro A. Sánchez Murcia

Medical University of Graz, Otto-Lewi Research Center

Annexes:

Annex 1 (A-1_95p4-foto-lists.pdf) – Photo documentation and list of participants

Annex 2 (A-2_účetní sestava_2023Brazda.pdf) - Accounting report