REPORT

From bioinformatics analysis of genomes to computational structural biology and applications

AKTION project number: 98p10

Basic data: Beginning of the project FebruJanuary 1, 2024

Completion of the project November 30, 2024

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:

23. 4. – 26. 4. 2024 – Workshop in Brno, lead: Prof. Václav Brázda (20 participants)

Participants from Graz: researchers: Prof. Pedro A. Sanchez Murcia, Christoph Nusshold students: Spela Mandl, Aleksandra Ptaczek, Juan Toledo, Daniel Platero-Rochart, Manuel Sanchez, Alvaro de la Cruz, Dilara Balci.

Program:

In this worksho p, 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 museum of anatomy and collaborative activities.

The public lecture in the course were attended by 60 participants mostly from the chemistry faculty of the BUT (Photo documentation and lists of participants are attached in Annex 1 (***A-1_ 98p10-foto-lists.pdf)***.

24. 9.-26. 9. 2024 - Workshop organized by MedUni Graz in Obertraun, lead: Prof. Pedro

Sánchez Murcia

Participants from Brno: researchers: Prof. Václav Brázda, Lucia Dzurická

students: Lucie Šislerová, Michaela Dobrovolná, Libuše Kratochvilová, Kristína Trebulová

Program:

The focus of the workshop in Austria 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. The stay in Obertaun also included excursions.

Student stays:

14. 9. – 14. 10. 2024 Brno University of Technology, Aleksandra Ptaczek 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 bioinformatical tools for analyses non-B DNA structures in various sequences and genomes.

1. 9. - 30. 9. 2024 Medical University Graz, Michaela Dobrovolná

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 and also with p53 protein. 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_2024Brazda.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 16, 2024

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Medical University of Graz, Otto-Lewi Research Center

Annexes:

Annex 1 (A-1_ 98p10 -foto-lists.pdf) – Photo documentation and list of participants

Annex 2 (A-2_účetní sestava_2024Brazda.pdf) - Accounting report