



National Institute of Chemistry, Ljubljana, Slovenia
Department of Computational Biochemistry and Drug Design (D01)

announces an open Young Researcher (PhD student) position



COMPUTATIONAL ENZYMOLOGY: A TOOL FOR THE UNDERSTANDING AND CONTROL OF NEURODEGENERATIVE DISEASES

RESEARCH FIELD. Computational enzymology in the context of pharmacology of the central nervous system / metabolism of neurotransmitters and other (biogenic or synthetic) monoamines / monoamine oxidase enzymes / neurodegeneration.

RESEARCH METHODS. Molecular (computer) simulation of chemical reactions, mainly Empirical Valence Bond (EVB) methodology and quantum chemistry. Extension to experimental research possible in collaboration with partner research groups.

SUMMARY. Molecular simulation has evolved into an established tool for the prediction of structure, functionality and various physical and chemical properties of matter, representing an important support (or even substitute) for experimental techniques. The research will include investigation of chemical reactions in the central nervous system that contribute to the development of neurodegenerative diseases such as Parkinson and Alzheimer disease. Neurodegeneration is critically influenced by oxidative decomposition of neurotransmitters (dopamine, serotonin) catalyzed by monoamine oxidase (MAO) enzymes. Importantly, due to genome variations, individuals can have slightly different sequence of MAO enzymes, therefore performance of MAO can vary between individuals, leading to different tendency towards neurodegenerative diseases. Since the presently used simulation methods can accurately predict the activity of MAO as function of point mutation, the challenge of the present work is to improve precision medicine by linking molecular simulation and neurological sciences. The research will include elucidation of reactions mechanisms catalyzed by MAO enzymes and investigation of the factors governing the performance of MAO (e.g., point mutations). Various state-of-the-art computational techniques will be used, including EVB methodology. The proposed research will significantly improve the understanding of neurodegenerative diseases and provide new perspectives for neuroscience and precision medicine. Computational research in this field is highly interdisciplinary and unconventional.

REQUIREMENTS & EXPECTED COMPETENCES:

- An undergraduate degree (BSc or Masters) in the field of natural sciences, particularly (bio)chemistry, pharmacy, physics, medicine, mathematics, computer sciences or related disciplines.
- Age 28 years or less.
- Passion for science, curiosity, proactivity.

Experience in any of the related fields and techniques (computational chemistry, pharmacology, Linux/Unix operating system) is welcome but not required.

The research program will be supervised by senior research associate dr. Jernej Stare and will start in October 2017 as a full, 4-year term employment.

ENVIRONMENT. The host institution is located in Ljubljana, the capital of Slovenia. One of the smallest, yet at the same time one of the most diverse European countries, Slovenia excels with spectacular landscape, calm, clean and safe environment, affordable tourism and high quality of living.

For more information please contact the host supervisor: jernej.stare@ki.si; phone: +386 1 476 0379.

All applications welcome! / <http://www.ki.si>