



**A European training network for the discovery of neurotrophins small molecule mimetics as candidate therapeutic agents for neurodegeneration and neuroinflammation (EuroNeurotrophin)**

This project has received funding from the European Union's Horizon 2020 research and innovation programme under the Marie Skłodowska-Curie grant agreement No 765704



**PhD student - Early Stage Researcher (ESR3)  
Computer-aided molecular design**

**EuroNeurotrophin Overview**

**EuroNeurotrophin** will be the first European consortium to study small molecule neurotrophin mimetics (synthetic or natural) in depth, use them as molecular probes to interrogate neurotrophins, and emphasise their clinical translation.

**Neurodegenerative diseases (ND)**, like Alzheimer's disease, Parkinson's disease, Multiple Sclerosis and motor neuron disease, are on the rise worldwide. Preclinical studies point to the therapeutic potential of neurotrophins in preventing or slowing the progression of ND. The key idea behind this project is to address the major limitations of neurotrophins by developing novel **small molecule, neurotrophin mimetics** with favourable profiles of stability, tissue penetration and targeted biological actions.

**EuroNeurotrophin** meets the emerging need for training young researchers in drug discovery and development with a focus on the design, synthesis and isolation of new neuroprotective small molecule neurotrophin mimetics and their assessment using multimodal approaches, as well as their use towards market applications.

**Host Institution**

Heidelberg Institute for Theoretical Studies, HITS ([www.h-its.org/en/](http://www.h-its.org/en/)) is a private, non-profit research institute carrying out multidisciplinary research in the computational sciences. The Molecular and Cellular Modeling group at HITS is led by Prof. Rebecca Wade. It is an interdisciplinary group of ca. 12 researchers with expertise in computational structural biology, molecular modeling and simulation, structure-based drug design, bioinformatics and structural systems biology. The focus of the group is on the development and application of computer-aided methods to predict and simulate protein interactions. The computational approaches are mostly based on the 3D structures of macromolecules. Techniques cover a wide spectrum from interactive, web-based visualization tools to molecular and Brownian dynamics simulations.

Prof. Rebecca Wade is a Full Professor of "Computational Structural Biology" at Heidelberg University and Leader of the Molecular and Cellular Modelling Group at HITS. She has 28 years research experience, she is a member of the faculty of two Heidelberg university graduate schools [HBIGS (biology) and HGS (scientific computing)]. She is author of over 200 publications, and software and

web servers developed by her group are used worldwide.

### Description of tasks for the position

The aim of this project will be to design and optimize small molecule mimetics and potentiators of neurotrophins using a combination of ligand-based and receptor-based drug design approaches. The project will include the modelling of proteins and protein-protein complexes, the analysis of protein binding properties, and the computational docking and design of compounds. Methods used will include the PIPSA ([pipsa.h-its.org](http://pipsa.h-its.org)) and TRAPP ([trapp.h-its.org](http://trapp.h-its.org)) software tools developed by the host research group. Tasks will include: 1) Modelling and analysis of target receptors, 2) Docking of known neurotrophin modulators and compounds identified in the compound library screen by UNICAEN, 3) Design, docking and optimization of compounds for binding and ADMET properties, 4) Iteration of design based on experimental feedback.

### Requirements

- Applicants must hold a MSc or equivalent in bioinformatics, chemoinformatics, biochemistry, medicinal chemistry, pharmacy, molecular biotechnology, or a related discipline. Candidates should have a strong theoretical background, experience in biomolecular modelling and simulation, programming skills, and a genuine interest in interdisciplinary research.
- Applicants can be of any nationality.
- Applicants must have a very good knowledge (written and oral) of the English language.
- **H2020 MSCA Mobility Rule:** researchers must not have resided or carried out their main activity (work, studies, etc.) in the country of the host organisation for more than 12 months in the 3 years immediately before the recruitment date. Compulsory national service, short stays such as holidays, and time spent as part of a procedure for obtaining refugee status are not taken into account.
- **H2020 MSCA eligibility criteria:** Early Stage Researchers (ESRs) must, at the date of recruitment by the host organisation, be in the first four years (full-time equivalent research experience) of their research careers and have not been awarded a doctoral degree. Full-Time Equivalent Research Experience is measured from the date when the researcher obtained the degree entitling him/her to embark on a doctorate (either in the country in which the degree was obtained or in the country in which the researcher is recruited, even if a doctorate was never started or envisaged).

### Benefits

- ✓ The position is full-time with a 12 month duration renewable to 36 months.
- ✓ A very attractive salary plus allowances package according to the allowance amounts defined in the rules for Early Stage Researchers (ESRs) EU Marie Skłodowska-Curie Actions Innovative Training Networks (ITN) ([http://ec.europa.eu/research/participants/data/ref/h2020/wp/2016\\_2017/main/h2020-wp1617-msca\\_en.pdf](http://ec.europa.eu/research/participants/data/ref/h2020/wp/2016_2017/main/h2020-wp1617-msca_en.pdf))
- ✓ Network-wide specialised training and training in transferable/technical skills.
- ✓ Local specialist training provided by the host institution.
- ✓ Intersectoral and interdisciplinary secondments within the EuroNeurotrophin network.

✓ International exposure through participation in scientific conferences.

#### **Application**

The application form can be downloaded from our website ([www.euroneurotrophin.eu](http://www.euroneurotrophin.eu)). Interested candidates for the position should submit the completed application form along with their cv, motivation letter, copies of publications and/or thesis (if available) and scans of transcripts at the link given for this opening on <https://www.h-its.org/en/jobs/> and by email to [info@euroneurotrophin.eu](mailto:info@euroneurotrophin.eu)  
**IMPORTANT:** Please also arrange for two recommendation letters to be submitted at the link given for this opening on <https://www.h-its.org/en/jobs/> and sent by email to [info@euroneurotrophin.eu](mailto:info@euroneurotrophin.eu)

#### **Additional Information**

For additional information about the research project and this individual position, please contact: Professor Rebecca Wade. Email: [rebecca.wade@h-its.org](mailto:rebecca.wade@h-its.org)