



Erasmus+

Learning Agreement

Student Mobility for Traineeships

Higher Education:
Learning Agreement form
Bálint DUDÁS
Academic Year 2017/2018

Trainee	Last name(s)	First name(s)	Date of birth	Nationality ¹	Sex [M/F]	Study cycle ²	Field of education ³
	Bálint	Dudás	4/6/1994	Hungarian	M	EQF level 7	0710
Sending Institution	Name	Faculty/ Department	Erasmus code ⁴ (if applicable)	Address	Country	Contact person name ⁵ ; email; phone	
	Pázmány Péter Catholic University	Information Technology and Bionics	HU BUDAPEST12	1083 Budapest Práter utca 50/a	Hungary	Henrietta Novák novak.henrietta@itk.ppke.hu +361 8864706	
Receiving Organisation /Enterprise	Name	Department	Address; website	Country	Size	Contact person ⁶ name; position; e-mail; phone	Mentor ⁷ name; position; e-mail; phone
	King's College London	Department of Chemistry	www.kcl.ac.uk	UK	☐ < 250 employees ☒ > 250 employees	Leigh Aldous Dept. Erasmus Coordinator leigh.alldous@kcl.ac.uk +44(0)207 848 1748	Edina Rosta Senior Lecturer edina.rosta@kcl.ac.uk +44(0)207 848 7334

After the Mobility

Table D - Traineeship Certificate by the Receiving Organisation/Enterprise
Name of the trainee: Bálint DUDÁS
Name of the Receiving Organisation: Department of Chemistry, King's College London
Sector of the Receiving Organisation: Higher education and research
Address of the Receiving Organisation/Enterprise 7 Trinity St, SE1 1DB London, UK; 020 7848 7517; https://www.kcl.ac.uk/nms/depts/chemistry/index.aspx
Start date and end date of traineeship: from [day/month/year] 1/6/2018 to [day/month/year] 5/8/2018
Traineeship title: QM/MM study on the Mycobacterium tuberculosis D-alanine:D-alanine ligase (DDL) reaction mechanism
Detailed programme of the traineeship period including tasks carried out by the trainee: Literature research Building the system of DDL Molecular dynamics simulations using CHARMM Defining QM region for simulations QM/MM minimisations on the system QM/MM reaction path mapping QM/MM finite temperature string calculations of the reaction mechanism Defining activation barriers Deducing reaction pathway Analysis of the obtained results, future prospective
Knowledge, skills (intellectual and practical) and competences acquired (achieved Learning Outcomes): Biology of DDL working principles General QM/MM method principles Applying QM/MM on a specific problem Learning about and applying finite temperature string free energy calculations Independent problem solving
Evaluation of the trainee: Bálint has made excellent progress during his Erasmus+ stay at King's College London. He has performed QM/MM minimisations and advanced finite temperature string free energy calculations of a key phosphate catalytic enzyme, D-Ala:D-Ala ligase. His simulations identified a novel proton transfer pathway via which the catalytic reaction can proceed, which was not available before he joined the group. These calculations will form the basis of a manuscript that we are currently writing based on mostly his results, and some previous results exploring alternative mechanisms. Despite his short stay, he was also involved in other projects. He helped to set up and test QM/MM protocols using NAMD and ORCA/MOPAC. Furthermore, he performed bioinformatics analyses of a key problem we are currently working on, to identify and compare the evolutionary background of phosphate catalytic enzymes.
Date: 6/8/2018
Name and signature of the Supervisor at the Receiving Organisation/Enterprise: Dr. Edina ROSTA 