

After the Mobility

Table D - Traineeship Certificate by the Receiving Organisation/Enterprise

Name of the trainee: Bálint DUDÁS
Name of the Receiving Organisation/Enterprise: Ecole Normale Supérieure de Cachan
Sector of the Receiving Organisation/Enterprise: Laboratoire de Biologie et Pharmacologie Appliquée
Address of the Receiving Organisation/Enterprise [street, city, country, phone, e-mail address], website: 61 Avenue du Président Wilson, Cachan 94230, France aurore.patey@ens-cachan.fr, + 33 1 47 40 24 76
Start date and end date of traineeship: from [day/month/year] 01/06/16 to [day/month/year] 01/08/16
Traineeship title: Mapping allosteric binding pockets of the oncogenic human KRAS protein
Detailed programme of the traineeship period including tasks carried out by the trainee: Building the systems of KRAS wild type in GDP and GTP bound states Energy minimising all systems using CHARMM. Finding best start conformation for method MDeNM Heating all systems using CHARMM Running simulations at constant pressure and temperature with constant amount of molecules in NAMD Finding best structure to carry out Normal Modes analysis Combining MD and NM with the help of recently developed method by the group of David Perahia. Adapt method to this particular protein Develop method to fit for the purpose Searching for optimal parameters for MDeNM MDeNM for both wild GDP and GTP bound proteins Processing results by filtering Searching for nature related conformations MD simulations on chosen structures Conclusions and prospective
Knowledge, skills (intellectual and practical) and competences acquired (achieved Learning Outcomes): Programming in CHARMM Programming in NAMD Applying the new method MDeNM Developing and adapting simulation methods Independent problem solving
Evaluation of the trainee: Balint Dudas achieved an excellent work during his internship in our laboratory. He applied different simulation methods (molecular dynamics, normal modes and a new method developed here) and acquired multiple skills how to simulate the KRAS with GDP and GTP and analyze the results. The goal was to characterize the conformational characteristics and the stable structures adopted by the terminal tail in this protein which could explain its role in the activity of this protein in the presence of GDP or GTP. The results he obtained was extremely insightful and in accord with many experimental indications. He was very efficient in his work and very active in defining new strategies how to orient the work for its full achievement. He took many initiatives to fulfill the work and make advance the ideas. He was confronted to both technical developments of the simulation methods, and their applications to a biological problem. The developments to which he took part will certainly be useful for other applications. The results on KRAS will also certainly conduct to increase our understandings on this protein and lead to new ideas how to inhibit its function. Balint Dudas showed the qualities of an excellent researcher
Date: 02/08/16
Name and signature of the Supervisor at the Receiving Organisation/Enterprise: David PERAHIA 
