STudent REseArch Mobility Programme (STREAM)

Host University:
Utrecht University

Field:
Natural sciences, mathematics and statistics

Specified field, subject:
Computational Structural Biology

Research project title:
How do biomolecules get in touch?

Possible starting month(s):

Sep	Oct	Nov	Dec	Jan	Fev	Mar	Apr	May	Jun	Jul	Aug
☒	☒	☒	☒	☒	☒	☒	☒	☒	☐	☐	☐

Possible duration in months:

1	2	3	4	5	6	7	8	9	10	11	12
☐	☐	☒	☒	☒	☒	☒	☒	☒	☒	☒	☒

Suitable for students in: ☒ Bachelor level ☒ Master level

Prerequisites:
Knowledge of structural biology / biomolecules
Some degree of familiarity with molecular modeling software and Linux is a plus

Description:
The fact that an entire genome can nowadays be sequenced for less than $5000 led to a boom in genetic information, which in turn attracted particular attention to biomolecular interactions. It is estimated that a human cell is regulated by over 300000 protein interactions, but only a small fraction of these have been structurally characterized by experimental methods such as x-ray crystallography or NMR. Other biochemical and biophysical methods can provide partial structural information on these interactions, while bioinformatics analysis can also contribute important evolutionary data. Combining these with computational methods for structure prediction of interactions – docking – allows the generation of atomic structural models.

All docking methods share three common elements: first, three-dimensional (3D) structural models of the individual components must be available; second, they must explore the conformational landscape of the interaction and generate candidate structural models of the complex, what is called sampling; finally, they must assess the generated models and select those that are more likely to be representatives of the native complex, what is called scoring. We have developed for this purpose an integrative, information-driven docking approach called HADDOCK (http://www.haddocking.org). It currently one of the best docking method in the world as assessed in a blind international competition. Nevertheless, there are still many challenges open related to describing larger and more complex systems, improving our scoring functions

and assessing the impact of a variety of data and energy functions on the prediction performance.

We are thus looking for motivated students to help us further develop HADDOCK and expand/improve its modelling capabilities.

Reference

J.P.G.L.M Rodrigues and A.M.J.J. Bonvin. Integrative computational modeling of protein interactions. *FEBS J.*, *281*, 1988-2003 (2014).

Faculty and/or Department:

Faculty of Science / Chemistry / Computational Structural Biology Group
http://bonvinlab.org

Contact person:

Please contact your own university for application procedure

Deadline for nomination to reach host university:

Ongoing

Notification of admission given by the end of:

Three weeks after application