



The objectives of FragNet are to (a) train a cohort of ESRs across FBLD methods and (b) develop individual skills in research into either new methods in FBLD or to apply FBLD to interrogate biological systems.

We are looking for highly motivated and talented students with a MSc degree who are interested in an ambitious multidisciplinary project on Fragment-Based Lead Discovery (FBLD).

At this moment we have 15 vacancies



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ESR9: Fragment evolution platform - chemical navigation.

Host: University of Barcelona, Spain

Academic supervisor: Prof. Xavier Barril (University of Barcelona)

Industrial supervisor: Dr. Ulf Bremberg (Beactica)

Synopsis

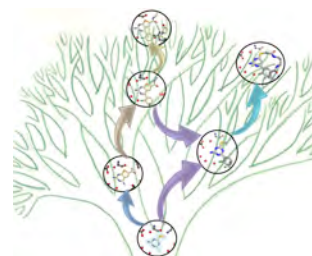
Computer-aided drug design (CADD) approaches are able to generate accurate molecular models that integrate available structural data with biochemical and biophysical data. In this project, a computational platform will be established that will help to guide efficient fragment hit evolution.

Objectives

1. Assemble the necessary cheminformatic infrastructure to generate, store and navigate chemical collections. Docking software will be an integral part of the system in order to exploit structural information, when available.
2. Identify chemical transformations in published fragment evolution programmes, assessing frequency and potency gain.
3. Create an algorithm capable of identifying an optimal list of evolved fragments for testing, given a fragment hit and optional additional information (e.g. list of compounds tested, structural information).
4. Use the platform in prospective FBDD projects, in collaboration with other ESRs.

Approach

Starting from existing software and computational methods developed in our lab, the ESR will develop a computational platform capable of suggesting an optimal set of molecules to test experimentally. The platform will accept as input a list of active and inactive fragments and, optionally, three-dimensional structures of the target. The ESR will generate robust and adaptable pipelines, combining computational packages in the fields of statistics, chemoinformatics, computational chemistry and others. This work will be carried out in close collaboration with the rest of the FRAGNET consortium to ensure that the final tool offers a practical solution in the majority of fragment-based scenarios. The ESR will also provide training to early adopters and apply the software to existing FBLD projects within FRAGNET.



Qualifications

Required diploma: MSc Bioinformatics or related degree and a background in chemistry, mathematics, pharmaceutical sciences or molecular life sciences.

Required expertise: Strong programming and scripting skills. Experience with molecular modelling, chemoinformatics tools, databases, statistical analysis and web interfaces.

Recommended expertise: Synthetic chemistry, structural biology, biophysical methods and analysis of screening data would be an advantage. Experience with network analysis or machine learning methods would also be highly valued. An interest in computer-aided drug design and strong interpersonal skills are essential to establish fruitful collaborations within the consortium.



Key publications

1. Radusky *et al.* Database (Oxford). **2014**, 2014(0), bau035.
2. Ruiz-Carmona *et al.* PLOS Computational Biology **2014**, 10(4):e1003571
3. Schmidtke *et al.* Bioinformatics, **2011**, 27(23), 3276-3285
4. Schmidtke *et al.* J. Med. Chem. **2010**, 53(15), 5858–5867



FragNet offers:

- Generously funded positions (duration 36 months) for 15 Early stage researchers (ESRs)
- High profile research projects in an Innovative European Training Network Program
- Excellent facilities for research and education
- Research training in both academic and industrial settings
- Training in state-of-the-art scientific and transferable skills
- Intensive contacts with international collaborators & secondments in other research laboratories

FragNet is looking for candidates that:

- are highly motivated and talented
- are able to work in a multidisciplinary team
- are keen on intra-European mobility to perform PhD research abroad
- have good communication skills

Selection criteria of the candidate:

- fulfil the eligibility criteria (ESR, international mobility) for Marie Skłodowska-Curie Innovative Training Networks (Horizon 2020)
- have a MSc degree in Life Sciences or obtain a MSc degree by September 2016
- have completed a research internship with relevant expertise
- have obtained high grades during his/her studies
- be fluent in English

Application procedure:

1. Send your application mentioning the **ESR number** in the subject line to hrm@fragnet.eu.
2. **Deadline for applications: 31 January 2016.**
3. Please send all the necessary information as **one pdf file** to hrm@fragnet.eu.
 - Detailed **CV** (include information on your BSc and MSc studies, languages, achievements, expertise)
 - **Motivation letter**, addressed to the FragNet selection committee, explaining your motivation why you apply with us. You have to indicate which FragNet ESR project(s) you are interested in (please motivate your selection and indicate which has your preference).
 - Provide contact details of at least 2 references (names, addresses, emails).
 - **Reference letter** from one of the enlisted references
 - Copies of your key educational certificates
 - **Transcript of Records** (i.e. documents enlisting your performance as BSc and MSc student over time by listing the course units or modules taken, credits gained and the grades awarded). If you have not completed your MSc degree yet include all grades obtained so far.
4. You may apply to more than one ESR position. If you do, submit a separate and dedicated application file for each position.
5. If applicable provide a language certificate Application is OPEN 3. The applications will be assessed by the FragNet selection committee, in which all group leaders are represented. Candidates are in particular evaluated on creativity, originality, intellectual capacity and quality of CV and motivation letter. The selection committee also takes into account interdisciplinary and gender balance.
6. Potential (Skype) interviews will be arranged with the group leaders associated with the ESR projects.
7. The ultimate starting date for the ESR projects is: **1st September 2016**, as the complete Fragnet ESR cohort will participate in the first Fragnet workshop that will be organized in York, UK in September 2016.

For other FragNet related questions please contact: info@fragnet.eu

Eligibility criteria

Eligibility criteria of Marie Curie Initial Training Networks apply. Only applicants who comply to the following conditions will be considered:

Conditions of experience (ESR)

Candidates must be, at the time of recruitment by the host organisation, in the first four years (full-time equivalent) of their research careers and have not yet been awarded a doctoral degree. This is measured from the date when they obtained the MSc degree which would formally entitle them to embark on a doctorate.

Conditions of international mobility

Eligible candidates may be of any nationality but must not, at the time of recruitment have resided or carried out their main activity (work, studies, etc.) in the country of their host organisation for more than 12 months in the 3 last years immediately prior to the reference date.



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