

PROJECTE DE DOCTORAT INDUSTRIAL EXPEDIENT 2015 DI 087

DADES DE L'EMPRESA I DE L'ENTORN ACADÈMIC

Títol del projecte

Technological developments for druggability predictions and virtual screening.

Empresa

Minoryx Therapeutics S.L.

Responsable de l'empresa

Elena Cubero Jordà

Universitat o Centre de Recerca

Universitat de Barcelona

Director/a de tesi

Xavier Barril Alonso

Treballador/a de l'empresa i doctorand/a

Guillermo Gutiérrez Teixeira

BREU DESCRIPCIÓ DEL PROJECTE DE RECERCA

Minoryx has developed the technological platform SEE-Tx (Site-directed Enzyme Enhancement Therapy). This platform allows identifying a new generation of pharmacological chaperones, which are non-competitive with the natural substrate and which have improved drug-like properties. Pharmacological chaperones are small molecules capable of rescuing the biological activity of mutant proteins and are used in the therapy of rare diseases. SEE-Tx integrates computational and experimental methods, including technology licensed from the academic partner, for the effective discovery of novel druggable sites and molecules that bind to them. At this point, we are interested in automatizing and extending the capabilities of the computational side of the SEE-Tx platform. The research project has three distinct but interrelated components: a) technological developments to increase automation, task integration and ease of use; b) application of the platform to novel targets; and c) identification of druggable cryptic pockets in proteins. The successful candidate will have excellent programming and scripting skills (python, C++, others), a chemical, biochemical or molecular biology background and will be familiar with computational chemistry methods such as molecular dynamics and docking.