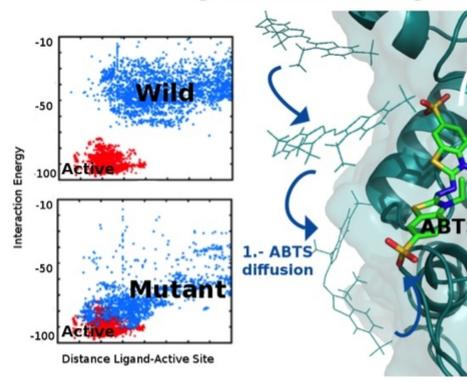
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PELE-e project selected for CaixaImpulse programme

The objective of this initiative by the Obra Social de la Caixa and Caixa Capital Risc is to drive a transformation of scientific knowledge in companies.

Manganese Peroxidase redisign usi



PELE-e aims to perfect the PELE simulation program and make it suitable for use in the optimisation of enzymes for therapeutic purposes.

The project will create a platform that will provide highly relevant information on the mutations to be applied to an enzyme to improve its properties such as catalytic activity, stability and specificity.

<u>PELE-e</u>, a project developed by the <u>Electronic and Atomic Protein Modelling team</u> at BSC, was one of the 20 selected for this year's <u>CaixaImpulse</u> programme. This means that the project will receive financial support of up to 70,000 euros as well as a comprehensive programme of training and expert advice.

The main objective of the CaixaImpulse programme is to drive the transformation of scientific knowledge in businesses and of products in the field of health and life sciences that generate social value. Robert Soliva, project leader, confirms that "for BSC, Caixaimpulse is therefore a unique opportunity to bring PELE-e closer to the market."

This is the second time that a BSC-led project has been awarded funding from the CaixaImpulse programme, with SMUFIN having been selected in 2015.

PELE-e and enzyme optimisation for therapeutic purposes

There is a large number of congenital diseases that affect one or more enzymes in the human body. In the majority of cases, either no treatment exists or approved treatments based on Enzyme Replacement Therapy (ERT) are not sufficiently effective. There is therefore a significant medical need for progress in this area. *In silico* simulation techniques have reached a level of maturity which allows them to complement effectively estimations achieved from experimentation.

PELE-e is a project aiming to perfect the PELE simulation system and make it suitable for use in the optimisation of enzymes for therapeutic purposes. Robert Soliva explains that "the progress made in the project will make available a platform which is both reliable and has a controlled computational cost. The platform will provide highly relevant information on the one-time mutations that must be applied to an enzyme so as to improve its properties such as catalytic activity, stability and specificity." The competitive advantage that PELE-e holds is chiefly based on "the correct modelling of the enzyme's flexibility, a key point on which the majority of currently available *in silico* estimations fall down," he adds.

Support from CaixaImpulse "will allow us to finish developing the PELE program and find one or more Proof of Concept (PoC) use cases in which to test the platform alongside biotech companies specialising in this niche market. It will also allow us to determine the best commercial exploitation strategy," concludes Soliva.

About CaixaImpulse

According to the Innovation Union Scoreboard 2016 (IUS) report, Spain has cutting-edge infrastructure and first-rate research centres and professionals. Nevertheless, it is ranked 21st in the European Union (EU) for innovation. In order to help change this reality, Obra Social "la Caixa" and Caixa Capital Risc launched CaixaImpulse, the first comprehensive programme in Spain for the creation of biotechnology companies. B oth institutions use their expertise in the fields of research and the creation, development and investment in early-stage companies for a common aim: the transfer of research results to society.

Read the CaixaImpulse press release here.

Nota de prensa en castellano (pdf)

Barcelona Supercomputing Center - Centro Nacional de Supercomputación

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