SIMICA

THERAPEUTIC SITE-SELECTIVE
PROTEIN-MODIFICATION CHEMISTRIES

Newsletter VIII

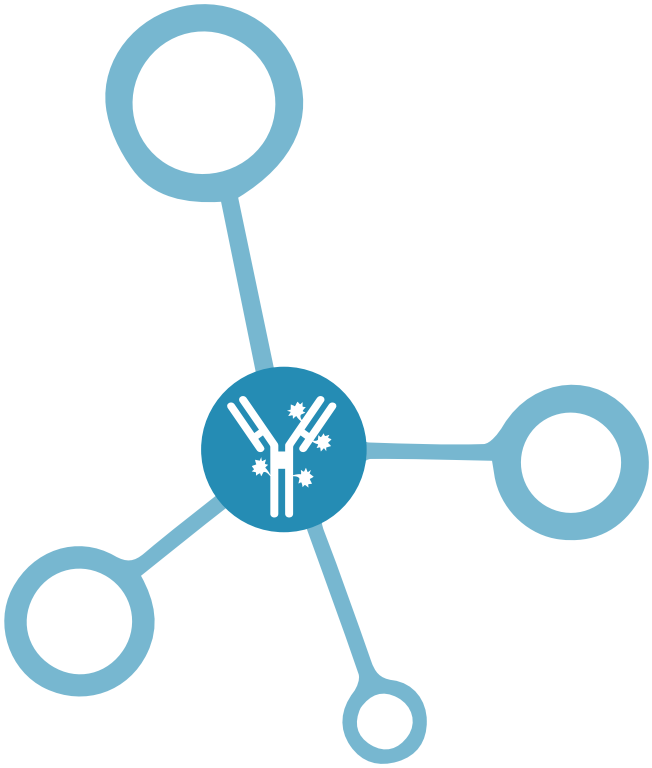
Aug 2022

SIMICA

THERAPEUTIC SITE-SELECTIVE PROTEIN-MODIFICATION CHEMISTRIES

OVERVIEW OF THE PROJECT

The SIMICA Project intends to place the Instituto de Medicina Molecular João Lobo Antunes within the core of a European network of laboratories that seeks to produce cutting-edge research in the field of site-selective protein modification.



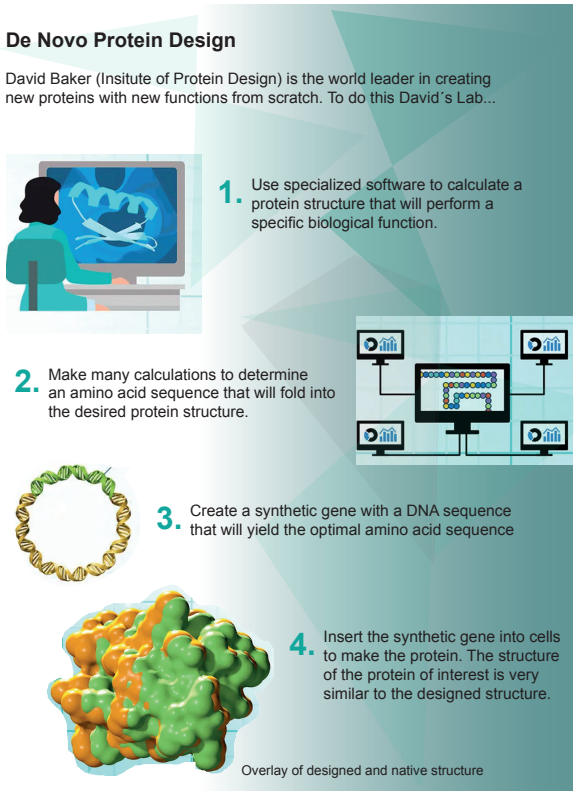
Did you know that:

Constructing proteins de novo is ultimately about choosing amino acid sequences that fold into structures with desired shapes and properties.

De novo protein design:

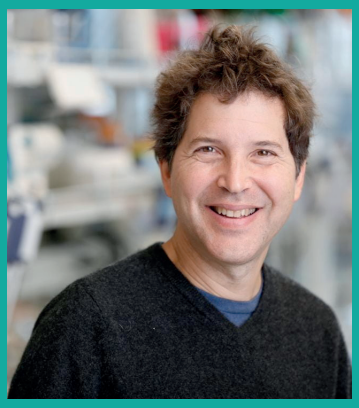
Proteins have a remarkable ability to carry out complex molecular processes with high efficiency and precision, characteristics that make them ideal for use in medicine. Protein engineering involves modifying a protein sequence by altering nucleotides in the encoding genes to achieve desired functions or specific properties. This approach mostly involves the amendment of existing protein sequences/structures to achieve desired/improved functions.

Advances in structural bioinformatics, new protein design algorithms, and increased information on 3D protein structure have ushered in the use of computational approaches for the design of new proteins. More recently, machine learning models and in silico screening processes have been recruited to improve this process (Nature 2016;537(7620):320-7).



Meet the SIMICA Collaborators

David Baker is the director of the Institute for Protein Design, a Howard Hughes Medical Institute Investigator, the Henrietta and Aubrey Davis Endowed Professor in Biochemistry, and an adjunct professor of genome sciences, bioengineering, chemical engineering, computer science, and physics at the University of Washington. His research group is focused on the design of macromolecular structures and functions. He received his Ph.D. in biochemistry with Randy Schekman at the University of California, Berkeley, and did postdoctoral work in biophysics with David Agard at UCSF. David Baker has published over 550 research papers, been granted over 100 patents, and co-founded 17 companies.



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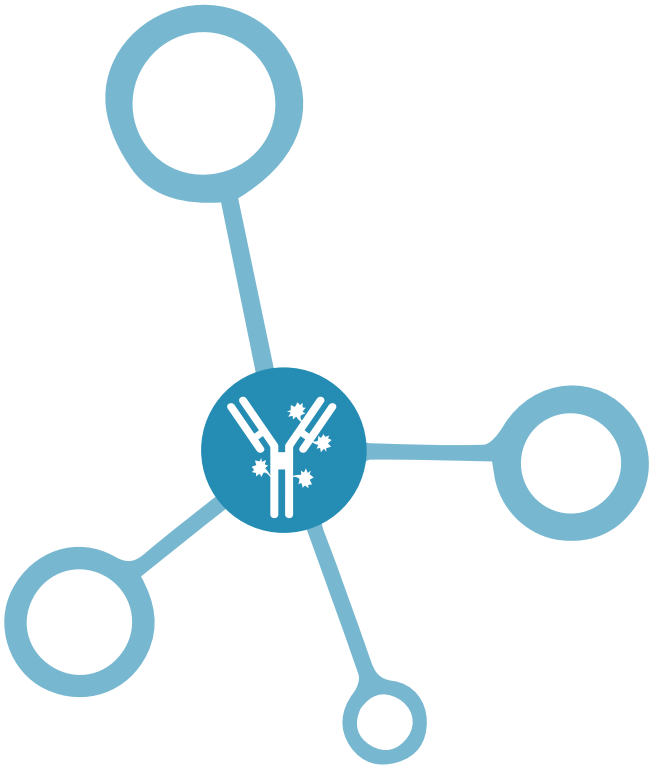
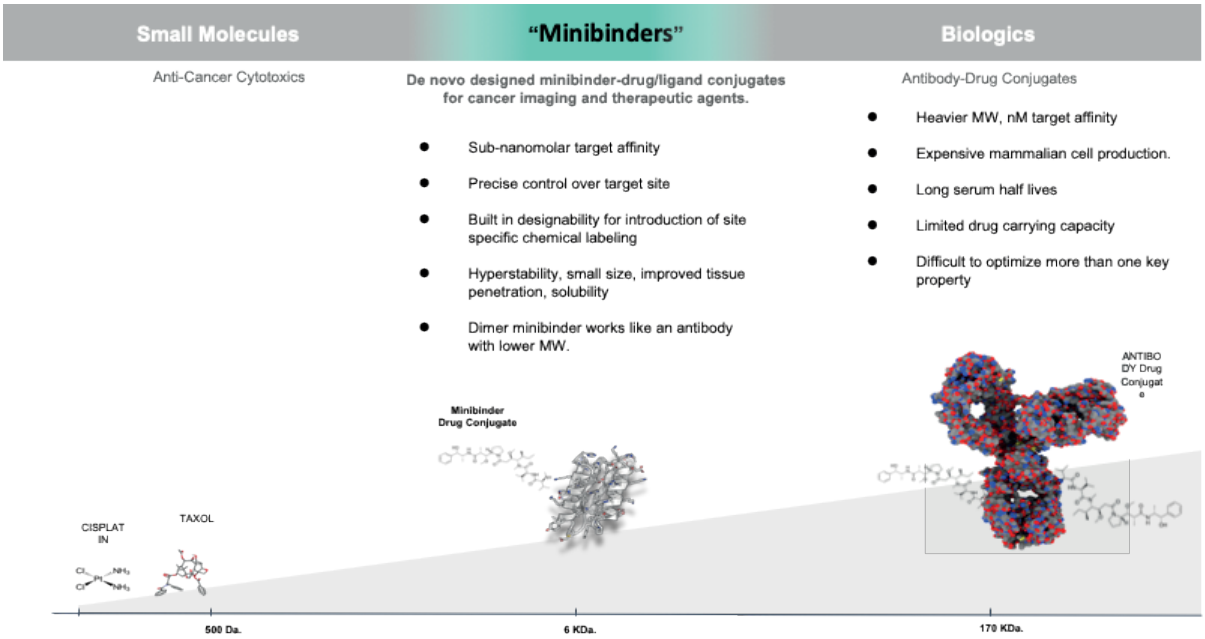


De novo protein design explores the full sequence space, guided by the physical principles that underlie protein folding. Computational methodology has advanced to the point that a wide range of structures can be designed from scratch with atomic-level accuracy. With this novel technology it is possible to design new functional proteins that have a completely different sequence when compared with the naturally occurring proteins. David´s Baker Lab is pioneering the development of such methods to design miniproteins targeting receptors overexpressed in tumors.
In a collaborative work with David´s lab, SIMICA is using chemical methods for protein modification to conjugate to the miniproteins toxic drugs for cancer therapy and fluorophores for imaging. We are exploring these miniprotein-drug conjugates as a new class of bioactive drugs which might have improved efficacy compared to ADCs due to their increased tumor penetration.



SIMICA news:

- Gonçalo Bernardes from @ChemCambridge was promoted to Full Professor at the University of Cambridge.
- SIMICA Knowledge Transfer Zone held on June 28 with the participation of UCAM and PERC Partners.
- SIMICA established a research protocol with the Portuguese biopharma company BASI.
- Bruno Oliveira was awarded with a FCT individual grant for scientific employment (grant N° 2022.03265.CEECIND, title - A molecular imaging approach for screening chemo-immunotherapeutics against PD-L1 expressing tumors) in collaboration with Gonçalo Bernardes and David Baker.