

Prof. Jean-Didier Maréchal
InSiliChem, Universitat Autònoma de Barcelona



Biosketch:

Professor Jean-Didier Maréchal is a computational chemist expert in modeling the interactions and activation of small molecules by biomolecular systems.

He graduated from the Ecole Normale Supérieure de Paris in 1996, from where he moved to the Universitat Autònoma of Barcelona to do his double Ph.D. on the modeling by quantum mechanics of the oxygen binding mechanism to heme and non-heme proteins. From 2002 to 2006, he pursued several post-docs in the UK and France. He was trained in approaches based on classical physics, like docking and molecular dynamics, and worked on the modeling of the metabolism of xenobiotics by cytochromes P450 and a series of drug design projects on cancer and HIV-1.

In 2006, he was recruited as a lecturer back at the UAB, where he set up his independent laboratory. He was promoted to full professor in 2024. The group's activity is centered on developing and applying computational methods, including multiscale approaches that combine statistical approaches, quantum-based calculations, and molecular mechanics. The group is renowned for its contributions to the study of biometallic systems, including the study and design of natural and artificial metalloenzymes, the development of Metal-based medicines, and a series of software filling gaps in today's modeling toolbox.