PROCEDIMENT DE SELECCIÓ DE PERSONAL INVESTIGADOR POSTDOCTORAL CONTRACTAT A CÀRREC DE FINANÇAMENT FINALISTA EXTERN O A CÀRREC DE FINANÇAMENT DE POLÍTIQUES DE LA UNIVERSITAT DE BARCELONA (PROCEDIMENT ORDINARI)

ANNEX DE LES BASES DE LA CONVOCATÒRIA	
DADES GENERALS	
Objecte	The spectroscopy and photophysics of biological systems are intimately related to the underlying structure of both the light-absorbing molecules (chromophores) participating in the process and the macromolecular entity, e.g. a protein, that hosts them. Understanding the subtle interplay between photophysics and structure, however, is rather complex, and constitutes an important challenge in two areas of growing interest in the research community: the light harvesting mechanisms of photosynthesis, which serve as inspiration for the design of next generation photovoltaic devices, and the emergence of dynamic structural biology as a key field in biomedicine, which underscores the importance of dynamics in order to achieve a complete understanding of how structure determines function. The project will focus on the development and application of multiscale QM/MM computational tools to improve the description of the spectroscopy and Förster resonance energy transfer (FRET) properties of biosystems, as well as the use of molecular dynamics simulations either based on classical, multiscale or machine learning approaches to study the impact of structural changes on excited state properties. These computational techniques will be applied to tackle the properties of different systems, like photosynthetic antennae, disordered proteins, or protein-ligand complexes.
Funcions	We are seeking a postdoctoral researcher willing to pursue an academic career in the study of the photophysics and biophysics of biological systems with computational methods. The work of the selected candidate will involve the following tasks: • Reviewing the current literature and state-of-the-art in the research topics addressed. • Planning, executing, and analyzing multiscale QM/MM simulations aimed at studying the interrelation between FRET/excited state properties and underlying structure in biosystems. • Planning, executing, and analyzing physics and machine learning-based calculations aimed at generating plausible protein-protein and protein-ligand complexes, and analyzing their conformational properties using Molecular Dynamics simulations. • The candidate will work on the research topic, including the possibility to supervise early-stage researchers; contribute to the writing of publications from research results; and present the results at national or international conferences.

Tipus de finançament i òrgan finançador	CEX2021-001202-M («Unidades de Excelencia María de Maeztu» 2021) amb Finançament a càrrec M2RN002499. MCIN/AEI/10.13039/501100011033
Destinació	Institut de Química Teòrica i Computacional (IQTC). Facultat de Farmàcia i Ciències de l'Alimentació. Departament de Farmàcia i Tecnologia Farmacèutica, i Fisicoquímica.
Durada del contracte	1 year extendable for 1 year
Possibilitat de pròrroga	No
Data d'incorporació i termini màxim per incorporar-se	1 January 2024
Dedicació	Full time
Retribució anual bruta (sou sense quota patronal)	23.660,04€
Termini de presentació de sol·licituds	10 days Des de l'endemà de la publicació a la seu electrònica.
Termini per acceptar l'oferta de treball	10 days
Web o adreça de correu electrònic on formalitzar la sol·licitud	https://www.ub.edu/eadministracio/IG.html
Fonts de reclutament	Seu electrònica de la UB i Euraxess. https://seu.ub.edu/ https://euraxess.ec.europa.eu/
REQUISITS DELS ASPIRANTS	

Requisits	- PhD degree in the field of Theoretical and Computational Chemistry. - Excellent English oral and writing skills. - Experience in the study of excited states and absorption/emission processes using time-dependent density functional theory and continuum and multiscale solvation models. - Expertise in Molecular Dynamics simulations and programming with Python or other languages is desirable.
Documentació requerida	- CV - Motivation Letter - Short Research Summary - At least 1 Reference Letter
PROCÉS DE SELECCIÓ	
Criteris de selecció i barems (criteris que es tindran en compte a l'hora d'avaluar els aspirants, així com quin pes es donarà a cada criteri en una escala de 100).	• Adequacy of the CV (max 50 points) - Specialized PhD (10 points), generic PhD (5 points) - Publications and dissemination activities (20 points) - Expertise in computational methods relevant to the project (10 points) - Complementary skills, management skills and autonomy (10 points) • Research Summary (max 20 points) • Motivation letter (max 20 points) • Experience in the field (max 10 points) - Experience >2 years (10 points), < 2 years (5 points)
Puntuació mínima per superar el procés de selecció	60 points