Universitat de les Illes Balears

METHODLODOGY			
General keyword	**Details in topic**	**Researchers involved**	**Insitiute (Group Acronym)**
Molecular Dynamics Simulations	Atomistic MD		
	Coarse-grained MD		
	Markov State Models		
	Metadynamics		

Enhanced sampling & free energy methods in molecular dynamics simulations	Umbrella Sampling	Juan Frau Munar, Joaquín Ortega Castro, Rodrigo Casasnovas Perera	ReacMOL
	Steered Molecular Dynamics		
	Replica Exchange Molecular Dynamics		
Molecular mechanics methods	MM		
Monte Carlo methods	MC		
Quantum Chemistry methods	HF & post-HF methods		
	DFT		
	Conceptual DFT		

Ab Initio & QM/MM MD	Born-Oppenheimer MD			
APPLICATIONS				
Systems	**Property**	**Methods**	**Researchers involved**	**Insitiute (Group Acronym)**
Globular Proteins & Instrinsic Disordered Proteins (IDPs)	Structure	Molecular Dynamics Simulations, Enhanced sampling & free energy methods in molecular dynamics simulations, Drug-discovery methods	Juan Frau	
	Dynamics			
	Aggregation propensity			
	Folding			

	Ligand binding		Munar, Joaquín Ortega Castro, Rodrigo Casasnovas Perera	ReacMOL
Materials, Semiconductors , Surfaces	Thermodynamics properties	Quantum Chemistry Methods, Ab Initio, MM and MC		
	Mechanical properties			
	Bands, DOS, PDOS, Optical Properties in solid			
	Adsorption on surface			