

METHODOLOGY			
General keyword	Details in topic	Researchers involved	
Molecular thermodynamics	Calculation of Thermodynamic magnitudes of peptides in water solution through Molecular Dynamics simulations	Adolfo Bastida Pascual	
		José Zúñiga Román	
Theoretical description of molecules of atmospheric or interstellar interest	Calculation of the rovibrational spectrum of small molecules through extensive variational calculations	Adolfo Bastida Pascual	
		José Zúñiga Román	
APPLICATIONS			
Systems	Property	Methods	Researchers involved
Peptides in water solution	Folding thermodynamic magnitudes during conformational changes	Molecular Dynamics simulations	Adolfo Bastida Pascual
			José Zúñiga Román
Molecules of atmospheric or interstellar interest	Rovibrational energy levels and eigenfunctions	Extensive quantum variational calculations	José Zúñiga Román