

METHODOLOGY			
General keyword	Details in topic	Researchers involved	Institute (Group)
Development of methods to study chemical reaction mechanisms	Automated search of transition states	Antonio Fernández and Emilio Martínez	
	Conformational search and thermochemistry	Antonio Fernández and Emilio Martínez	
APPLICATIONS			
Systems	Property	Methods	Researchers involved
Degradation of organic pollutants	Reaction mechanisms and kinetics	AutoMeKin (https://rxnkin.usc.es/index.php/AutoMeKin) Pilgrim (https://github.com/cathedralpkg)	Antonio Fernández and Emilio Martínez
Combustion of biofuels	Reaction mechanisms and kinetics		Antonio Fernández and
Small peptides	Molecular flexibility	TorsiFlex (https://github.com/cathedralpkg)	Antonio Fernández and
Polymers	UV and ECD spectra	DFT and TD-DFT	Berta Fernández Rodríguez
Intermolecular complexes	Interaction energies and spectroscopic properties	Ab initio, DFT and TD-DFT	Berta Fernández Rodríguez