

EXPLORING THE CONFORMATIONAL LANDSCAPE OF BIOACTIVE MOLECULES BY CHIRPED PULSE MICROWAVE SPECTROSCOPY AND LASER VAPORIZATION

OTGER CREHUET I VILADELBOSCH, *Physical Chemistry, University of the Basque Country (UPV/EHU), Bilbao, Spain*; PABLO PINACHO, *Physical Chemistry, University of the Basque Country, Leioa Bilbao, Spain*; EMILIO J. COCINERO, *Departamento de Química Física, Universidad del País Vasco (UPV-EHU), Bilbao, Spain*; MAIDER PARRA-SANTAMARIA, *Physical Chemistry, University of the Basque Country (UPV/EHU), Bilbao, Spain*.

The study of bioactive molecules is an important field if we want to understand how living organisms work, in this contribution we present three molecules: indole-3-carbinol (I3C), picaridin and DEET.

By a combination of quantum-chemical calculations and microwave spectroscopy all molecules were interrogated. I3C was vaporized by ultrafast UV laser radiation and 1 conformers were detected. In addition, the structure could be determined by minor isotopologues species[1]. Picaridin and DEET were examined in the pulse-chirped spectrometer [2][3] and 2 and 4 species were observed respectively. Studies are in progress and higher energy conformers will be investigated and hydrated species will be analysed.

References

[1] E. J. Cocinero, A. Lesarri, P. Écija, J. Grabow, J. A. Fernández, F. Castaño. *Angew. Chem. Int. Ed.* 2012, 51, 3119–3124 [2] E. J. Cocinero, A. Lesarri, P. Écija, J. Grabow, J. A. Fernández, F. Castaño. *Phys. Chem. Chem. Phys.*, 2010, 12, 12486-12493. [3] I. Uriarte, C. Pérez, E. Cballero-Mancebo, F. J. Basterretxea, A. Lesarri, J. A. Fernández, E. J. Cocinero, *Chem. Eur. J.* 2017, 23, 7238–7244.