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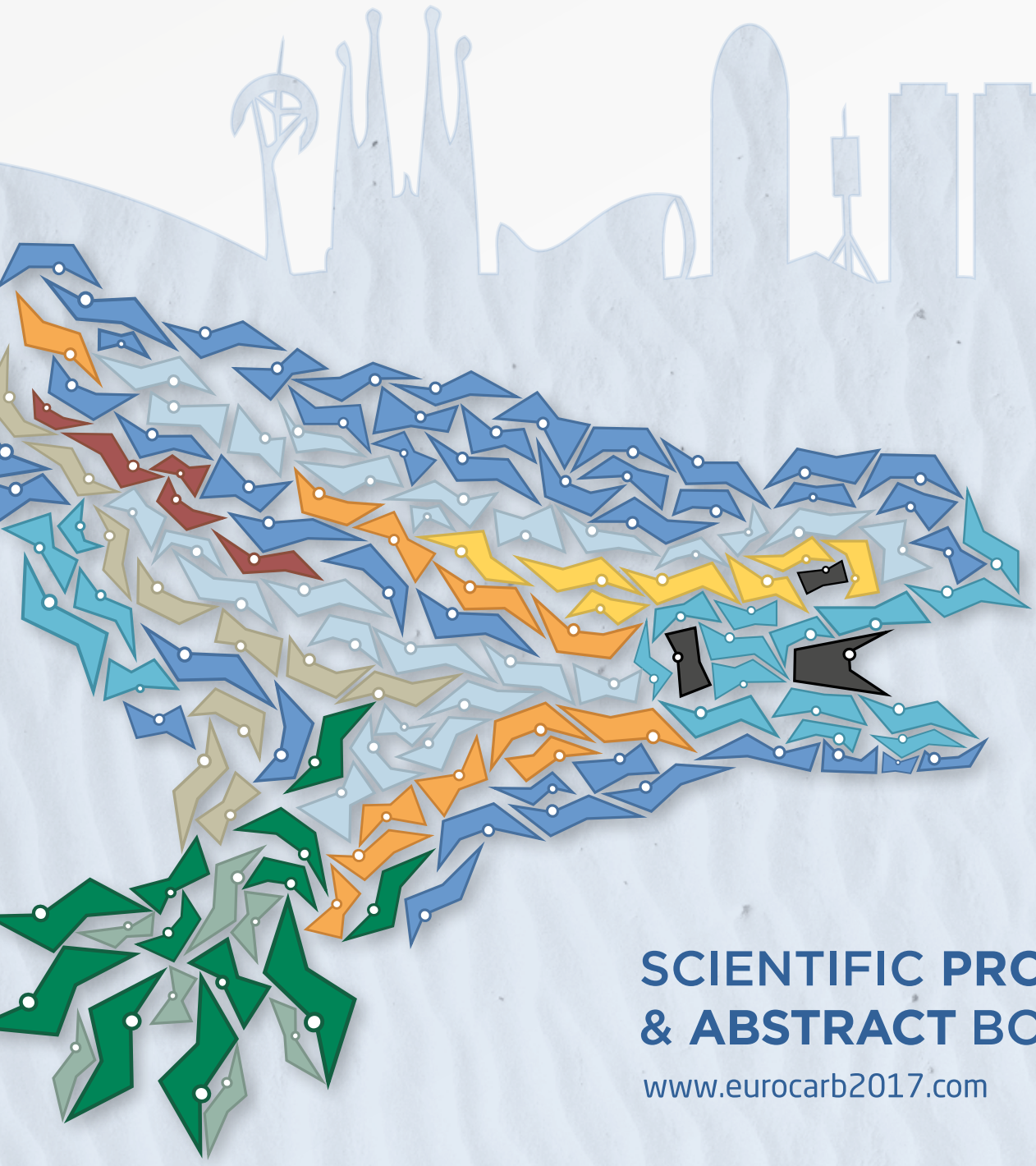

SCIENTIFIC PROGRAM & ABSTRACT BOOK

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A DYNAMIC COMBINATORIAL CHEMISTRY APPROACH TO QUANTIFY THE CONTRIBUTION OF ELECTROSTATICS TO THE STABILITY OF CH/π BONDS IN WATER

Laura Montalvillo-Jiménez,[1] Ester Jiménez-Moreno,[1] Ana M. Gómez,[1] Agatha Bastida,[1] Francisco Corzana,[2] Gonzalo Jiménez-Oses,[2] Jesús Jiménez-Barbero,[3] and Juan Luis Asensio[1]

[1]Departamento de Química Bio-orgánica, Instituto de Química Orgánica General (CSIC). Madrid. Spain.
[2]Departamento de Química, Universidad de la Rioja. Logroño (La Rioja). Spain.
[3]CICbioGUNE, Parque Tecnológico de Bizkaia. Derio- Bizkaia. Spain.
Email: lmontalvillo@iqog.csic.es

Nowadays it has become clear that CH/π interactions play a key role in a variety of molecular recognition processes including conformation stabilization, crystal packing, formation of gas phase clusters, or chiral discrimination. Nevertheless, there are still aspects of these interactions that remain poorly understood.

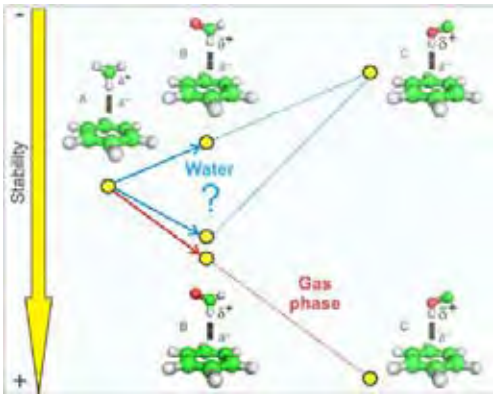

Figure 1. Effect of *CH* polarization (A and B) on the stability of *CH*/π complexes in gas phase, together with those expected in water. The influence of water solvation on the stability of OH/π complexes (C) is also represented for comparison.

Thus, electrostatic and charge-transfer contributions to *CH*/π complexes can be modulated by the attachment of electron-withdrawing substituents to the carbon atom leading to a stabilization of the complex in gas phase. Intriguingly, the outcome of this simple chemical modification in water is more difficult to predict. In fact, exposed R-OH/π contacts are usually highly destabilized in water due to the competence provided by the stronger and ubiquitous ROH/H_2O conventional hydrogen bonds. Following a similar reasoning, the polarization of a particular *CH* could also enhance its own polar interactions with the solvent, thus leading to a minor stabilization, a null effect, or even a significant destabilization of the *CH*/π bonds. However, to the best of our knowledge, no unambiguous experimental evidences have been presented so far to support the stabilizing role of *CH* polarization in water. These questions have evident implications in the molecular recognition and drug design fields.
Our work provides an unambiguous and quantitative answer to this question employing a simple strategy based on dynamic combinatorial chemistry that is of general relevance for different fields of chemistry and biology. [1]

[1] Jiménez-Moreno, E.; Gómez, A. M.; Bastida, A.; Corzana, F.; Jiménez-Oses, G.; Jiménez-Barbero, J.; Asensio, J. L. Angew. Chem. Int. Ed., **2015**, *54*, 4344.

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