XXIX RSEQ Biennial Meeting in Organic Chemistry

Santa Cruz de Tenerife, June 26-28, 2024

ABSTRACT BOOK

ORAL COMMUNICATION

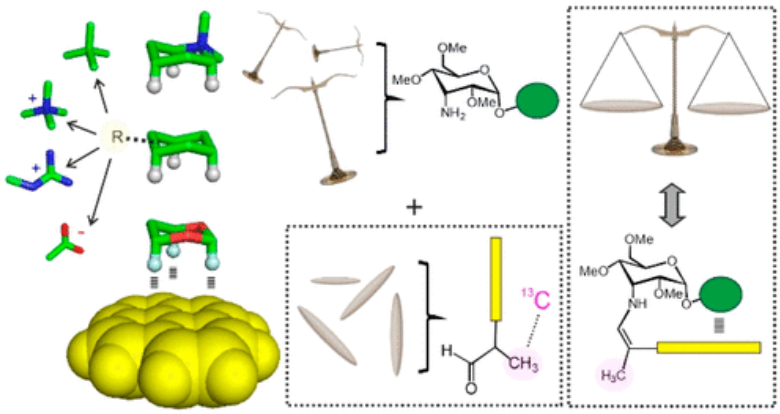
Illuminating a Solvent-Dependent Hierarchy for Aromatic CH/π Complexes with Dynamic Covalent Glyco-Balances

Laura Díaz-Casado,[a] Alejandro Villacampa,[a] Francisco Corzana,[b] Jesús Jiménez-Barbero,[c] Ana M. Gómez,[a] **Andrés G. Santana**,[d] Juan Luis Asensio[a]*

[a]Instituto de Química Orgánica General (IQOG-CSIC). Madrid - 28006
[b]Dpto. Química, Univ. de la Rioja. Logroño – 26006
[c]CIC Biogune. Derio – 48170
[d]Instituto de Productos Naturales y Agrobiología (IPNA-CSIC). La Laguna – 38206

andres.g.santana@csic.es

CH/π interactions are prevalent among aromatic complexes and represent invaluable tools for stabilizing well-defined molecular architectures. Typically, their energy contributions are exceptionally sensitive to structural and environmental factors, resulting in a context-dependent nature that has led to conflicting findings in the scientific literature. Consequently, a universally accepted hierarchy for aromatic CH/π interactions has remained elusive. Herein, we present a comprehensive experimental investigation of aromatic CH/π complexes, employing a novel approach that involves isotopically labeled glyco-balances generated *in situ*. This innovative strategy allows us to uncover both thermodynamic and kinetic information. Our analyses yielded more than 180 new free energy values while considering key factors such as solvent properties, the interaction geometry, and the presence and nature of accompanying counterions. Remarkably, our results challenge conventional wisdom regarding the stability order of common aromatic complexes and provide valuable guidelines for the selection of optimal interacting partners in every chemical environment, allowing the design of tailored aromatic complexes with applications in supramolecular chemistry, organocatalysis, and/or material sciences.[1]



Acknowledgments: This investigation was supported by research grants PID2019-107476GB-I00 and PID2022-141085NB-I00, funded by MCIN/AEI/10.13039/501100011033 and by ERDF *A way of making Europe*. A.G.S. is grateful for grant RYC2021-031704-I funded by MCIN/AEI/10.13039/501100011033 and by European Union NextGeneration EU/PRTR.

References:

1. Díaz-Casado, L.; Villacampa, A.; Corzana, F.; Jiménez-Barbero, J.; Gómez, A.M.; Santana, A.G., Asensio, J. L. *JACS Au* **2024**, *4*, 476.