COMPUTATIONAL SELECTION OF FUNCTIONAL MONOMERS FOR THE SYNTHESIS OF MOLECULARLY IMPRINTED POLYMERS SPECIFIC FOR CAFFEINE.

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One of the challenging steps in the design of molecularly imprinted polymers (MIPs) is the selection of functional monomers, as these are responsible for interacting with the target and leading to molecular recognition. Our study is centred on the evaluation of the best computational methods for the screening of potential functional monomers able to form a stable complex with caffeine. This work is part of a project for the development of new sensors based on the molecular imprinting technology, for the evaluation of different components in coffee. In this work the target compound is caffeine (see fig. 1A), one of the key components in the coffee beverage and a molecule that has interesting biological properties.

The first part of the project focused on the validation of the methodology. This fundamental step was achieved by testing different computational methods, to identify the one that could reproduce more closely the experimental data related to the interactions that caffeine molecules can form. From the crystallographic structure of anhydrous caffeine[1], the interaction occurring between two caffeine molecules was extrapolated (see fig. 1B). This structure was reproduced using different methodologies, both based on molecular mechanics and quantum mechanics theory. The DFT calculations using gaussian wavefunction and planewave functions, were found to be in good agreement with the experimental data (see fig. 1C and fig 1D).

A library of fluorescent monomers characterized by different spectroscopic properties was designed. Particular emphasis was given to monomers that were able to form π-π stacking interaction and H-bonds, with caffeine.

The interaction between functional monomers and caffeine was evaluated in 1:1 complexes. Results on the studies of the interaction between the different functional monomers and the target will be presented.

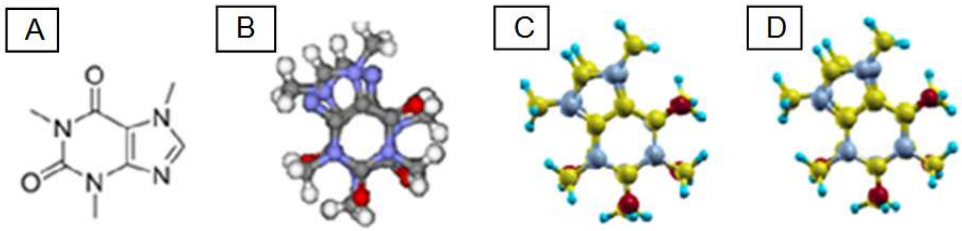

Figure. 1. A: Caffeine molecule. B: The interaction between two caffeine molecules occurring in caffeine crystal. C: The interaction between two caffeine molecules reproduced using the B3LYP 6-31G* simulation. D: The interaction between two caffeine molecules reproduced using planewaves functions.

References

[1] Lehmann C W, Stowasser F (2007) The Crystal Structure of Anhydrous β-Caffeine as Determined from X-ray Powder-Diffraction Data. *Chemistry A European Journal* 13: 2908-2911.