

# The CAMD approach for the developing of new materials

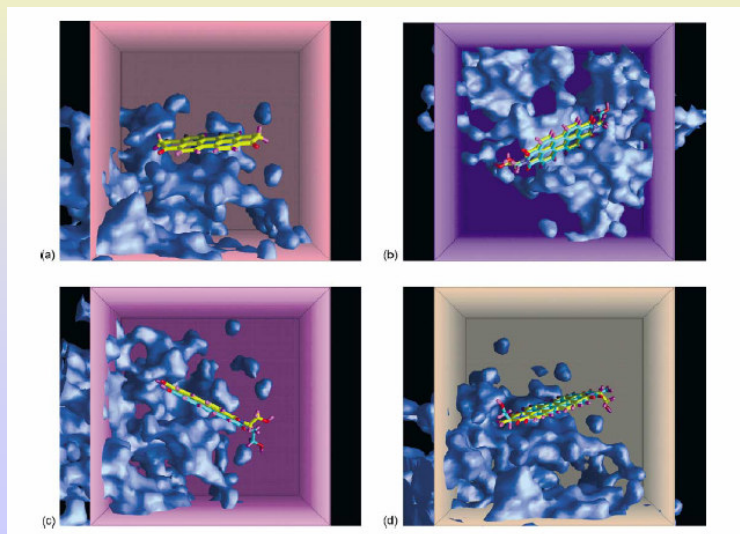
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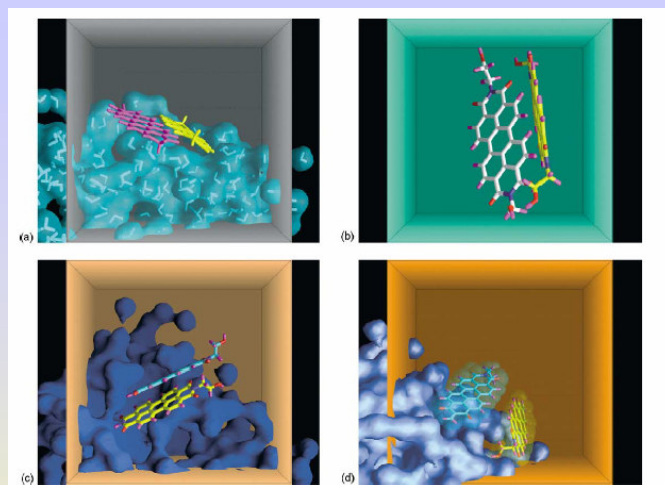


The application of computer-assisted molecular design (CAMD) approach to the development of new materials is being actively explored. This considerable interest arises from the enormous gain in design efficiency that is possible from its use. Our group started by dealing with X-ray crystallography, contributing to the generation of extensive structural data that has been the “launching pad” for computing simulations. The next step was developing expertise in understanding the underlying factors responsible for molecular recognition which is fundamental for reliable biopharmaceutical agents design. The computational techniques we used to carry out the investigations range from mimicking the original binding ligand in terms of shape or electrostatic distribution, through *docking* algorithms to fit new ligands into the active site of enzymes. The extension of CAMD approach in material science was a natural progression and we undertake the task of using this methodology to study the arrangement of imide perylene derivatives as they form a monolayer on a water surface, giving special attention to the spatial arrangement of a deposited perylene molecule and the orientation of a second one. The technological interest appears when Langmuir-Blodgett or another kind of films are produced with perylene derivatives. The substituents attached to the ends of the chromophore do not affect directly the properties of the molecules but they can interact strongly with the water layer under the film, lifting the molecules in some degree with respect to the aqueous plane.

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*Perylene derivative orientations with respect to the water layer: (a) molecule 1; (b) molecule 2; (c) molecule 3; (d) molecule 4.*



*Perylene derivative orientations with respect to the receptor constituted by a water layer plus first part orientation: (a) molecule 1; (b) molecule 2; (c) molecule 3; (d) molecule 4.*

## Acknowledgements:

