Nanociencia y Nanotecnología: lo pequeño es diferente

Nanoscience and Nanotechnology: small is different

seminar

Tuesday April 29th

c/ Faraday, 9
Sala de Conferencias, Hall
Imdea Nanociencia
Ciudad Universitaria de Cantoblanco

12.00h

Computing natural compounds for an atomistic-scale understanding

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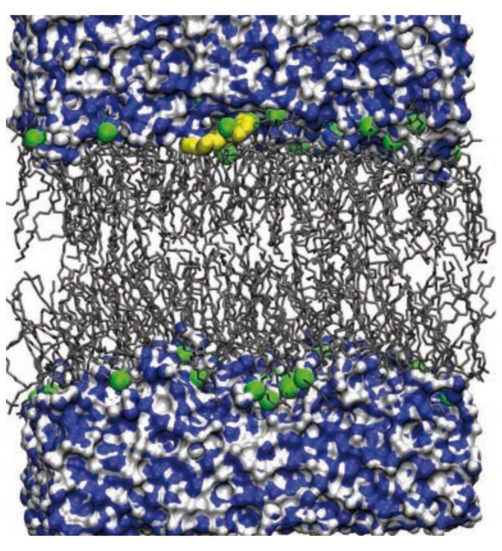
Quantum calculations (mainly DFT) and molecular dynamics are increasingly effective tools to evaluate the physico-chemical properties of natural and bio-inspired compounds.

Free Radical Scavenging Capacity.[1-13] Thermodynamic parameters (mainly bond dissociation enthalpies -BDEof the O-H phenolic bond) allowed an accurate prediction of the antioxidant capacities of natural compounds. Based on the Transition State and the Marcus Theories (for atom- and electron-transfers, respectively), kinetics was also evaluated providing a better prediction of the antioxidant behaviour in solution or in the organism.

Interaction with Lipid Bilayer Membranes.[14-15] Over the past years, building models to figure out drug-membrane interaction has deserved a major interest. Membrane penetration / accumulation / crossing / positioning play a crucial role in drug delivery and metabolism in the human body. Molecular dynamics is a much promising tool, complementary to experimental measurements, to get into this knowledge. Such theoretical simulations have been performed to provide an accurate picture of the interaction between natural compounds (polyphenols and other π-conjugated derivatives of pharmaceutical interest) and lipid bilayer membranes, predicting their location and orientation.

Pigmentation and Optical Properties.[16-19] TD-DFT is a very effective tool to reproduce the capacity of natural polyphenols to absorb UV/Vis. light. The accurate prediction of spectroscopic shifts and modulation of oscillator strength helps understanding of pigmentation and copigmentation (mainly driven by π-stacking interaction). The quantum tool is much promising for practical applications, mainly in wine chemistry to tune pigmentation.

Conformational analysis of supramolecular assemblies.[20] Molecular modelling methods may provide accurate description of the conformational space, accounting for non-covalent interactions (H-bonding and π-stacking). As an example, we have elucidated the stereochemistry of skyllamycin, a non-ribosomally synthesized cyclic depsipeptide from Streptomyces sp. Acta 2897, employing a combination of data from NOESY-NMR spectroscopy, simulated annealing and free molecular dynamics simulations. A similar conformational analysis has also been performed on plantazolicin, a new antimicrobial compound, belonging to the thiazole/oxazole-modified microcin (TOMM) family. Here we show the important role of non-covalent interactions, mainly π-stacking.



Drug penetration in lipidbilayer membranes

References

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