
Atomistic Simulations to Investigate Phosphocholine Micelle Self-assembly and Degradation

Researchers:

- Christian Lorenz (I.P.). [King's College London](#) [1].

Language Undefined

Description:

Proyecto asignado a través de la [Red Española de Supercomputación](#) [2].

A large number of small molecules currently under development as drug candidates are hydrophobic, and as a result many of these drugs may not make it to market because of problems encountered due to poor water solubility. The therapeutic effects of many drugs already on the market could also be enhanced by developing drug delivery vehicles which increase their solubility. This work is a multiscale analysis of the formation and degradation of self-assembling phospholipid micelles for their potential application in the delivery of these hydrophobic drug molecules by encapsulating them within the hydrophobic core of the micelle and then degrading to release the hydrophobic drugs at the target site.

Source

URL:<https://web.computaex.es/en/proyectos/atomistic-simulations-investigate-phosphocholine-micelle-self-assembly-and-degradation>

Links

[1] <https://www.kcl.ac.uk/> [2] <https://www.res.es/>