In silico design of light propelled molecular machines for the scrutiny and control of biological processes

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Language Spanish

Description:

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

Light-driven molecular machines afford the monitoring and manipulation of biological and biochemical processes within the same spatial and temporal scales of nature, contributing to their understanding and to the identification of potential dysfunctions. The aim of the present activity is to scrutinize the working mechanism of azo-based BODIPY photoswitches, as prototypes for turn-on hypoxia fluorescent probes, and only-photon unidirectional hemithioindigo molecular motors, employing full dimensional molecular dynamics simulations, and state of the art electronic structure approaches. These results are intended to establish structural-photophysical relationships that might serve as a basis for the rational design of novel biomarkers and molecular motors with improved absorbing properties, efficiency and sensitivity.

Web:

Links
[1] https://www.uam.es/uam/inicio [2] https://www.res.es/