OS-B-MON-03-03

Photodegradation in the infrared region of indocyanine green in aqueous solution

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14:50–15:10 / Room 3

Indocyanine green (ICG) is a water soluble anionic tricarbocyanine dye which has been widely used for biological applications. The photodegradation and aggregation of ICG were studied in aqueous solution by absorbance spectrum measurements. Two excitation wavelengths were used, 780 and 808 nm. The photodegradation analysis was performed based on the number of absorbed photons and rate equations of the electronic excited states. The aggregation effect is influenced by the diluent medium and also a third emission band at 640 nm, associated with PBS solution, could be observed. This new emission band is associated to a trimeric band, when ICG is diluted in PBS. The degradation of the solution with aggregated forms does not follow the Beer-Lambert law. The exposure to light increases the degradation rates. The photodegradation rates were distinct between the two excitation wavelengths.

OS-B-MON-03-04

Computational models for light-tissue interactions: recent advances

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15:10–15:30 / Room 3

Computational simulations could be used as a tool to better understand how biochemical changes translate into structural changes that generate pathological states. By computational calculations, it is possible to obtain the vibrational spectrum of molecules and macromolecules. It is possible to verify which atoms or molecules contribute to the existence of each characteristic vibrational mode, identify and interpret the interactions between these modes, and associate these pieces of information to the pathological processes. In this work we will present recent advances from our group by using density functional theory (DFT) to model normal, inflammatory, and tumoral tissues in a minimalist way (100 atoms). Comparison with experimental data (vibrational spectroscopy data) will also be presented. Perspectives on using molecular dynamics on large models (> 60,000 atoms) will also be discussed.