Supramolecular exo-functionalized palladium cages: fluorescent properties and biological activity

Metallosupramolecular systems are promising new tools for pharmaceutical applications. Thus, novel self-assembled Pd(ii) coordination cages were synthesized which were exo-functionalized with naphthalene or anthracene groups with the aim to image their fate in cells. The cages were also investigated for their anticancer properties in human lung and ovarian cancer cell lines in vitro. While the observed cytotoxic effects hold promise and the cages resulted to be more effective than cisplatin in both cell lines, fluorescence emission properties were scarce. Therefore, using TD-DFT calculations, fluorescence quenching observed in the naphthalene-based system could be ascribed to a lower probability of a HOMO-LUMO excitation and an emission wavelength outside the visible region. Overall, the reported Pd2L4 cages provide new insights into the chemical-physical properties of this family of supramolecular coordination complexes whose understanding is necessary to achieve their applications in various fields.