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Design, synthesis, and characterization of Zn(II)porphyrin as a contrast agent for photoacoustic imaging

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Development of molecular photoacoustic (PA) contrast agents places significant challenges in the next generation biomedical imaging technics. This paper demonstrates a general protocol to design small molecules to exhibit large PA coefficients by molecular structure engineering. We hypothesize that a major fraction of the excited electron energy could be converted into phonons through the judicious placing of functional groups of higher vibrational energies near to the higher order unoccupied molecular orbitals. Using Zn(II)porphyrins as a model system and employing the state of the art DFT, we have designed four molecules (RJ-Cn-MYm, where n=12 or 8 and m=1–4) with systematic variation in the vibrational energies of C-H functional groups placed near higher order unoccupied molecular orbitals (which appeared in the 0.36–0.42eV region in this case). The absorption coefficients of C-H vibrational modes decrease in the order of RJ-C12-MY1>RJ-C12-MY2>RJ-C12-MY3>RJ-C8-MY4, therefore, a similar variation in the PA signals is predicted. The four molecules are synthesized in good yields by acid-catalyzed oxidation, Knoevenagel condensation, MacDonald (2+2) condensation, bromination, metalation, deprotection, and Sonogashira coupling reactions. The theoretical predictions are validated by PA coefficients measurements and PA tomography. The PA coefficients and tomographic intensities decreased in the order RJ-C12-MY1>RJ-C12-MY2>RJ-C12-MY3>RJ-C8-MY4, as predicted by DFT. Large PA coefficients are observed for the RJ-C12-AY1, which is superior to that of the existing small molecules.

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