Quantum chemical elucidation of the turn-on luminescence mechanism in two new Schiff bases as selective chemosensors of Zn2+: Synthesis, theory and bioimaging applications

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We report the synthesis and characterization of two new selective zinc sensors (S,E)-11-amino-8-((2,4-di-tert-butyl-1-hydroxybenzylidene) amino)-11-oxopentanoic acid (A) and (S,E)-11-amino-8-((8-hydroxybenzylidene)amino)-11-oxopentanoic acid (B) based on a Schiff base and an amino acid. The fluorescent probes, after binding to Zn2+ ions, presented an enhancement in fluorescent emission intensity up to 30 times (? = A 50.10 and B 18.14%). The estimated LOD for compounds A and B was 1.17 and 1.20 ?M respectively (mixture of acetonitrile?:?water 1?:?1). Theoretical research has enabled us to rationalize the behaviours of the two selective sensors to Zn2+ synthesized in this work. Our results showed that in the free sensors, PET and ESIPT are responsible for the quenching of the luminescence and that the turn-on of luminescence upon coordination to Zn2+ is mainly induced by the elimination of the PET, which is deeply analysed through EDA, NOCV, molecular structures, excited states and electronic transitions via TD-DFT computations. Confocal fluorescence microscopy experiments demonstrate that compound A could be used as a fluorescent probe for Zn2+ in living cells. © The Royal Society of Chemistry.