

Abstract Submitted
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Study on the Fluorescent Functionalized Fullerenes as Contrast Agents For Bio-imaging DIANA OH, RICHARD KYUNG, CRG-NJ — An adequate balance between biochemical stability and reactivity for the agents must be determined in order to effectively relax or stabilize the contrast agents used in the detection of tumor cells in the body. Due to the lack of stability and the potential of toxicity of iodine and gadolinium chelates, even though they are less toxic than the gadolinium element itself, fluorescent functionalized fullerenes are studied in this paper to see if they stabilize or reduce the LD50 value despite the increase of reactivity. Other than the functionalized fullerenes with various functional groups attached, transition metal oxide nanoparticles and nanoscale metal-organic frameworks could also significantly contribute to the medical field with relatively high stability and effective transportation method for delivering significant amounts of paramagnetic metal centers, respectively. This paper found that the PC61BA-(Gd-DO3A) is the most thermodynamically stable, amongst tested functionalized fullerenes, with the lowest optimization energy of 13894.8 KJ/mol. Even though TiO₂ is relatively stable, it is difficult to certainly claim that one molecular compound is the best contrasting agent.

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