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Synthesis and Photophysics of novel 4-aryl-polyhydroacridinodiones: Fluorescence confinement effect

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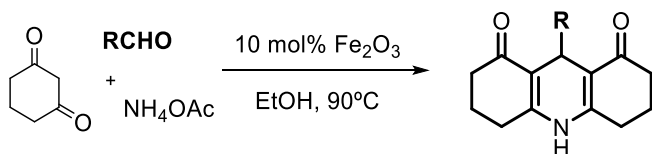
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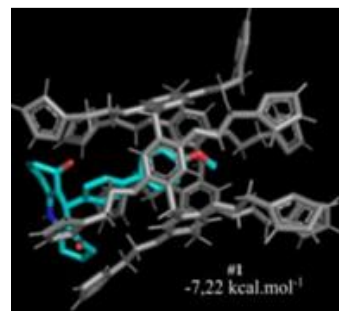
Keywords: Polyhydroacridinodiones, Multicomponent Reaction, Pillararenes, Substrate-receptor, Fluorescence

ABSTRACT

Polyhydroacridinodiones (PHA) are compounds derived from 1,4-dihydropyridines, an important class of bioactive molecules with wide applicability in medicinal chemistry. Pillararenes are a recent class of macrocycles that allow complexation with other molecules through the substrate-receptor system, resulting in a series of applications. We have successfully synthesized new PHA derivatives by Hantzsch multicomponent reaction using maghemite ($\gamma\text{-Fe}_2\text{O}_3$) as a catalyst, with yields between 40 and 91%. Optimized geometries of products and intermediates were calculated by DFT. Photophysical study of PHA in ethanol was also carried out in the presence of the macrocycle pillar[5]arene imidazole (**P[5]Im**), which indicated the possibility of formation of an inclusion complex with structure **2a'**. All compounds are fluorescent in the blue region (~420 nm) and the presence of the macrocycle selectively increased the fluorescence emission intensity of the biphenyl derivative. The interaction was evidenced by NOESY NMR analysis, and a plausible structure was achieved by molecular docking.



1a' - R = 2,3,5-trimethoxyphenyl	40%
2a' - R = 4-methoxybiphenyl	91%
3a' - R = 3-trifluoromethoxyphenyl	56%
4a' - R = 4-methoxyphenyl	78%



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INCT Catalysis, UFSC, CNPq, Capes and FAPESC.

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