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| Title: | Structure Correlated Study on C10-(H) Arylated N-(pyren-1-yl) Picolinamide towards Multiple Metal Cation Sensing |
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| Keywords: | C10-(H)<br>Cation Sensing |
| Issue Date: | 28-Jul-2021 |
| Publisher: | IISERM |
| Abstract: | Photophysical characterisation and computational studies were conducted on a set of C(10)-H arylated N-(pyren-1yl) picolinamides. Based on the important photophysical parameters few among them were chosen to investigate metal cation recognition property. The project attempts to correlate the observed sensing behaviour with molecular structure of C(10)-H arylated N-(pyren-1-yl) picolinamide through spectroscopic techniques. Additionally, to gather a better understanding on structure-property relationship, a comparison study with C-10 unsubstituted N-(pyren-1-yl) picolinamide was also conducted. Based on the functional group present at C-10 position of pyrenyl picolinamide, the compounds under consideration were classified into two series I) methoxy group at para- and meta- position of phenyl ring II) methyl group at para- and meta- position of phenyl ring. Irrespective of functionalisation difference, all compounds exhibited characteristic absorption and emission response towards Cu 2+ and Fe 3+ . While methoxy containing pyrenyl picolinamides along with reference compound displayed a fluorescence turn-off behaviour, methyl containing pyrenyl picolinamides proceeds through excimer formation ~ 550 nm, in the presence of Cu 2+ and Fe 3+ . Detailed sensing studies were carried out to quantify the metal cation binding by each compound. The resuslts indicate that the C-10 unsubstituted pyrenyl picolinamide has the highest binding affinity towards metal cations among all the five compounds. This could be because less crowding around the binding pocket compared to others. Temperature dependent fluorescence emission and fluorescence excitation studies were carried out to distinguish the type of excimers produced by metal cations. The observations indicate that the association of 10b-Fe 3+ and 10e-Cu 2+ leads to the formation of static excimers. On the other hand, 10b-Cu 2+ complexation give rise to dynamic excimer. |
| URI: | http://hdl.handle.net/123456789/3938 |
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