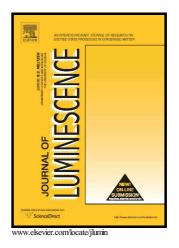
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ACCEPTED MANUSCRIPT

An efficient molecular probe for visual detection of adenosine triphosphate in aqueous medium

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A naphthalimide-anthracene linked molecular dyad, **5** has been designed, synthesized and evaluated for ionic and biomolecular recognition. It has been observed that the synthesized molecular dyad can efficiently recognise adenosine triphosphate (ATP) in the presence of closely related adenosine diphosphate (ADP), adenosine monophosphate (AMP), guanosine triphosphate (GTP) and guanosine diphosphate (GDP). The recognition event is unique for ATP as there is no interference of other biologically important anions (acetate, dihydrogen phosphate, chloride, hydrogen sulphate, fluoride, bromide and sulphocyanide) and amino acids (Cys, Lys, Val, Ala, Leu, Ile, Tyr, Trp, His, Pro). The binding stoichiometry of the dyad **5** and ATP has been found to be 1:2 as calculated from Job's plot and Benesi-Hildebrand mole ratio evaluation through fluorescence titrations. The nature of interaction has been studied through infrared spectroscopy, NMR and fluorescence decay profiling as well as geometry optimization through density functional calculations.

Graphical Abstract

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