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Detection of resorcinol by supramolecular host guest recognition

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Benzene-1,3-diol (resorcinol) is a reagent in manufacturing industries like rubber, plastics, pharmaceuticals, dyes and cosmetics. Effluents from these industries are sources of resorcinol which are of environmental concern. Biological hazards of resorcinol like suppression of thyroid hormone in human, induction of chromatid ruptures in Chinese hamster ovary cells, carcinogenesis in the upper digestive tract, haematological abnormalities due to life time exposure and even fatal cases of resorcinol poisoning are reported for human fetus. Despite these established disadvantages, literatures are found to be insignificant on guest specific receptors for resorcinol. Here we report 1,6-bis(2,6-bis(benzothiazol-2-yl)pyridine-4-yloxy)hexane as the first specific ditopic receptor which selectively recognizes resorcinol among its structurally identical benzene metabolites like phenol, hydroquinone and catechol. A photoluminescence based detection technique has been devised for easy detection of resorcinol. The exact mechanism of supramolecular host guest recognition have been characterized with the experimental evidences from simple spectroscopic techniques (UV–visible and NMR spectroscopy), which are again in agreement with the details of photoluminescence studies.

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X-ray crystallographic and biochemical studies provide the structual basis for substrate specificity of *Helicobacter pylori* aminopeptidase

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The standard H. pylori eradication therapy has lost its efficacy, with an eradication rate dropping to as low as 60% in Western Europe. Aiming to develop an alternative therapy, we have performed initial characterisation of H. pylori M17 aminopeptidase (HpM17AP). To address the structural basis of catalysis and inhibition of this enzyme, we have established its specificity towards an N-terminal amino acid of the substrate and determined the crystal structures of HpM17AP and its complex with the inhibitor bestatin. We have analysed the diffraction data sets for HpM17AP and its bestatin complex. HpM17AP activity was screened against a fluorogenic substrate library containing both natural and unnatural amino acids. The position of phenylalanine moiety of the inhibitor with respect to the active-site residues and with respect to other M17 aminopeptidases suggested that it represents the S1 subsite. In contrast to most characterized M17 aminopeptidases, HpM17AP displays preference to L-Arg over L-Leu. A close similarity between the structures of HpM17AP and its homologues from other bacteria has allowed the structural features that determine differences in their substrate specificity to be analysed. The results have interesting implications for metabolic utilisaton of arginine for the production of primary amines, and cysteine scavenging through degradation of mucosal glutathione.

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