

Rapid Evaluation of Suitable Substrates with High Affinity to Artificial Caffeine Receptors by MS Based Techniques

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A modification of our triphenylene ketal based receptor facilitates electrospray tandem mass spectrometry investigations. Binding affinities of eleven potential substrates, *e.g.* caffeine and other xanthine alkaloids, are probed in the gas phase with collision induced dissociation. The relative stabilities of the substrate-receptor complexes are rapidly determined and the findings are correlated with the corresponding results in solution.

Key words: Supramolecular Chemistry, Mass Spectrometry, Host-Guest Complexes, Receptors