

Useful properties of DTE:CB8 supramolecular switches in aqueous medium

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The development of drug delivery devices or advanced molecular machines demands a profound knowledge of its potential building blocks. Therefore, it is imperative to have highly advantageous capabilities available in such components. Our work is focused on photoswitchable host-guest systems in water. They are based on the synthetic macrocyclic host cucurbit[8]uril (CB8) and guests belonging to the dithienylethene family (DTE). The photochemical properties of these guests allow control over the complexation affinity and kinetics with red or near infrared light, converting the colored ring-closed isomers into their fluorescent open forms [1]. The association constants of these 1:1 complexes range from micro to picomolar affinity, being higher for the closed isomers (up to 10000-fold) [2]. Therefore, they can be applied to catch and release biologically relevant guests through competitive binding (figure 1). In addition to their response to light stimulus, these complexes are also responsive to other stimuli, such as ionic strength and pH. We also show that the presence of two negatively charged side arms in the DTE act as an electrostatic kinetic barrier for the inclusion of the guest, slowing down the inclusion kinetics. This allowed the emergence of out-of-equilibrium complexes in unusual three-dimensional arrangements that otherwise could not be observed [3].

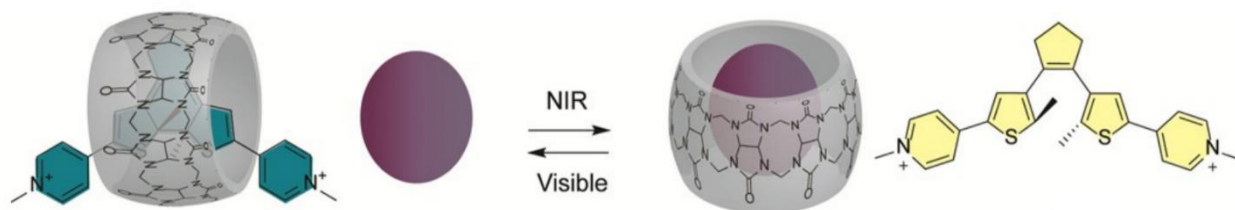


Figure 1 – Light induced catch and release of drugs through DTE:CB8 complexes [1].

[1] Ferreira, P. et al. (2019) *Chem.Eur.J.*, 25, 3477-3482;

[2] Máximo, P. et al. (2022) *Org. Chem. Front.*, DOI: 10.1039/d2qo00423b;

[3] Colaço, M. et al. (2021) *Chem. Eur. J.*, 27, 9550-9555.

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