

Receptors for organochlorine pesticides based on calixarenes

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Abstract:

The water soluble 4-sulfocalix[n]arenes (with $n=4,6,8$) have been investigated as potential synthetic receptors for cyclodiene organochlorine pesticides. Steady state fluorescence experiments in ethanol solution have shown that only the cavitands with n equal to 6 and 8 form complexes, of comparable stability, with heptachlor. Electrochemical data, obtained in water solution, confirmed the ability of 4-sulfocalix[6]arene to bind the heptachlor, unlike the smaller calixarene. Moreover, a significant increase in the stability constant is observed in water solutions. This stability is caused by the sterical hindrance of pesticides with respect to the cavity dimension of the calixarene. This results in a selective interaction of this molecule with other organochlorine pesticides. Binding experiments, carried out with endosulfan have shown that, despite of chemical similarity, 4-sulfocalix[6]arene and 4-sulfocalix[8]arene behave in a very different way: the former is unable to bind this pesticide, while the latter shows a binding constant of 4.7×10^5 with endosulfan. To investigate the molecular features of the interactions, molecular dynamic simulations of 4-sulfocalix[6]arene in presence of heptachlor in water solution have been performed. These simulations show that different configurations of heptachlor inside the calixarene cavity are equally populated and easily interconverting, suggesting that a non specific hydrophobic interaction plays a key role in the complex stability. These studies have permitted to individuate versatile synthetic receptors for organochlorine pesticides.

Keywords Chemoreceptor . Organochlorine pesticide . Sulfocalixarene . Molecular dynamics simulation