ENCAPSULATION OF PRODAN IN A BETA-CYCLODEXTRIN ENVIRONMENT: AN EXPERIMENTAL AND THEORETICAL STUDY VIA ELECTRONIC SPECTROSCOPY AND MOLECULAR MECHANICS

ANWESHA BANERJEE, BIDISA SENGUPTA[a], SUDIP CHAUDHURI and PRADEEP K. SENGUPTA,
Biophysics Division, Saha Institute of Nuclear Physics, 1/AF, Bidhannagar, Kolkata 700064, India.

The naphthalene based fluorescence probe 6-propionyl-2- (dimethylamino)-napthalene (Prodan) finds widespread applications in biophysical studies due to its remarkable spectroscopic and physico-chemical properties. In particular, the exquisitely sensitive dependence of its fluorescence emission maximum to the microenvironment, high emission yield, as well as significant solubility in a wide range of media of different polarities makes it an attractive choice as an optical probe for studying the structure, function and dynamics of proteins, biomembranes and membrane mimicking organized assemblies. In the present study we have examined the electronic absorption and fluorescence spectroscopic characteristics of Prodan incorporated in succinyl-2-hydroxypropyl beta-cyclodextrin (SHP CD), a cyclic oligosaccharide with attractive potential as a drug delivery system. We report that upon increase in the concentration of SHP CD from 0 to 10 mM the emission maximum of Prodan undergoes a pronounced blue shift of 31 nm (from 523 nm (in water) to 492 nm (in 10mM SHP CD)), accompanied by increase in the emission yield, fluorescence anisotropy and lifetime values as well as changes in the emission and excitation spectral profiles. Detailed analyses of the fluorescence along with relevant absorption spectroscopic data indicate that Prodan readily enters the doughnut-shaped hydrophobic cavity of SHP CD and forms a 1:1 inclusion complex. Furthermore, docking studies performed via molecular mechanics methods (MM+) reveal that upon encapsulation, the dimethylamino group of Prodan is most likely to be oriented towards the wider rim of the cyclodextrin cavity. The binding characteristics of the Prodan-SHP CD complex have been compared with that of the unsubstituted CD in relation to its potential advantages as a prospective drug carrier.

[a]present address: Department of Applied Physics, Chalmers University of Technology, 412 96 Götenborg, Sweden