Electronic Supplementary Information (ESI)

Experimental Section

Materials and methods: 4-(Dimethylamino)benzaldehyde, dodecane-1,12-diamine, $NaBH_4$, and the solvents employed were used as supplied without further purification. Cucurbit[8]uril was synthesized according to a literature method.[6b] ^1H NMR spectra were recorded at 20 °C on a Varian INOVA-400 spectrometer. Absorption spectra of the host–guest complexes were recorded on an Agilent 8453 spectrophotometer at room temperature. Fluorescence spectra were recorded on a Varian RF-540 fluorescence spectrophotometer.

N,N'-Bis(4-dimethylaminobenzyl)dodecane-1,12-diamine chloride (C_{12}DA): A solution of 4-(dimethylamino)benzaldehyde (30 mmol) in ethanol (20 mL) was added to a stirred solution of dodecane-1,12-diamine (15 mmol) in ethanol (20 mL), and the mixture was allowed to react at room temperature for 3 h. Thereafter, the solvent was removed by evaporation, and the solid material was redissolved in methanol (30 mL). The resulting solution was cooled in an ice bath and a solution of $NaBH_4$ (30 mmol) in methanol (20 mL) was added dropwise with stirring. On completion of the addition, the mixture was refluxed for 4 h. Some precipitate appeared, which was collected by filtration; concentrated HCl (10 mL) was then added to the filter mass. The chloride salt was precipitated from acetone, collected by filtration, washed with diethyl ether, and dried in air.

Q[8]·C_{12}DA: C_{12}DA (0.12 g, 0.20 mmol) and $ZnCl_2$ (0.027 g, 0.20 mmol) were dissolved in H_2O (50 mL), and to this solution Q[8] (0.27 g, 0.20 mmol) was added. The mixture was heated to dissolve the host and guest and then filtered. Slow evaporation of the H_2O from the filtrate over a period of four weeks provided rod-shaped colorless crystals.

Single-crystal X-ray crystallography: Diffraction data for Q[8]·C_{12}DA were collected at 173 K with a Bruker SMART Apex-II CCD diffractometer using graphite-monochromated Mo-K_α radiation (λ = 0.71073 Å). The structure was solved by direct methods and refined using full-matrix least-squares on F^2 (SHELXTL, Bruker, 2000). Crystal data for Q[8]·C_{12}DA: $C_{312}H_{554}Cl_{52}N_{144}O_{135}Zn_{12}$, M = 11110.83, monoclinic, a = 21.4729(10) Å, b = 35.6109(17) Å, c = 31.4762(15) Å, β = 95.867(3)°, U = 23943(2) Å^3, space group $P2_1/n$, Z = 2, Dc = 1.538 g cm^{-3}, $F(000)$ = 11476, GoF = 1.017, R_{int} = 0.0624, R_1 = 0.0883, wR_2 = 0.2329. CCDC-751114 (Q8C12DA) contains the supplementary crystallographic data for this paper. These data can be obtained free of charge from The Cambridge Crystallographic Data Centre via www.ccdc.cam.ac.uk/data_request/cif.