Formation of Binaphthyl-based Micelles Capable of Encapsulating Metallodyes

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BINOL (1,1'-binaphthyl-2,2'-diol) is an excellent, chiral aromatic compound due to its characteristic axial chirality, versatile functionality, and synthetic accessibility in supramolecular chemistry. Although various BINOL-based macrocyclic and cage-like compounds generate chiral cavities, their host functions have been largely limited so far, owing to the open and rigid frameworks.

Here we report novel chiral aromatic micelles bearing BINOL frameworks and their ability of efficient chirality transfer to metallodyes. Three types of bent amphiphiles *s*/*r***BAM**, *s***BAP**, and *s***BA** were designed using different substituents at the 6,6'-positions of the BINOL framework. The bent amphiphiles were synthesized in 4-5 steps including Negishi or Suzuki-Miyaura coupling. Amphiphile *s***BAM** having mesityl groups quantitatively formed a chiral aromatic micelle in water (Fig. a, right), as confirmed by NMR, PL, UV-visible, and CD analyses. The DLS and molecular modeling studies revealed a spherical structure composed of 12•*s***BAM** with a diameter of ~3 nm (Fig. b,c). Aromatic micelle (*s***BAM**)$_n$ efficiently encapsulated Zn-porphyrin **ZnTP** *via* grinding method (Fig. a, left). The CD spectra of the resulting host-guest composite (*s*/*r***BAM**)$_n$•(**ZnTP**)$_m$ displayed mirror CD bands at 390-450 nm (Fig. e), attributed to chirality transfer from the host to the bound guests, with absorption dissymmetry factors (|g_{abs}|) being ~3 × 10^{-4}.