Electronic Supplementary Information

Multi-responsible Chameleon Molecule with Chiral Naphthyl and Azobenzene Moieties

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Characterization data

Chemical structures and purities of NCA2M and its intermediates were confirmed by thin layer chromatography (TLC), 1H NMR, and 13C NMR in deuterated chloroform (CDCl3). All the chemical compounds synthesized in this research were purified by recrystallization and/or column chromatography using the silica gel. Chemical shifts were quoted in part per million (ppm) with a reference of tetramethylsilane (TMS).

Chemical structure of compound 4-(4-pentylphenylazo)phenol (1) was identified by increased integration of protons at azobenzene groups (7.76-6.92 ppm, 8H). The protons of ether (-O-CH2-, 2H) in compound 4-(6-bromohexyloxy)phenyl-(4-pentylphenyl)diazene (2) appeared at 4.04 ppm. Chemical structure of compound 3,5-bis[6-(4-(4-pentylphenylazo)phenoxy)hexyloxy]benzoic acid ethyl ester (3) was identified by new peak at 7.16 ppm (-C-CH-C-, 2H), 6.64 ppm (-C-CH-C-, 1H) and 3.89 ppm (-O-CH3, 3H) as a singlet from methyl benzoate. Chemical structure of compound 3,5-bis[6-(4-(4-pentylphenylazo)phenoxy)hexyloxy]benzoic acid (4) was confirmed from the disappearance of methyl group in ester adjacent to the benzoate. Chemical structure of NCA2M was identified by increased integration of protons and a new peak at around 1.84 ppm (-CH-CH3, 3H) corresponding to the chiral naphthyl group.
Fig. S1 $^1$H NMR spectrum of compound 1

Fig. S2 $^1$H NMR spectrum of compound 2
Fig. S3 $^1$H NMR spectrum of compound 3

Fig. S4 $^1$H NMR spectrum of compound 4
Fig. S5 $^1$H NMR spectrum of compound NCA$_2$M

Fig. S6 $^{13}$C NMR spectrum of compound NCA$_2$M
Fig. S7 MALDI-ToF MS spectrum of compound NCA₂M

Fig. S8 Elemental analysis of compound NCA₂M
Fig. S9. The first-order plots of the trans-cis (a) and cis-trans photo-isomerization (b) of NCA$_2$M in chloroform solution

Fig. S10. Energy-minimized geometric dimensions of NCA$_2$M