Electronic Supplementary Information for

Aggregation-Induced Chiral Symmetry Breaking of A Naphthalimide−Cyanostilbene Dyad

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Supplementary Figures

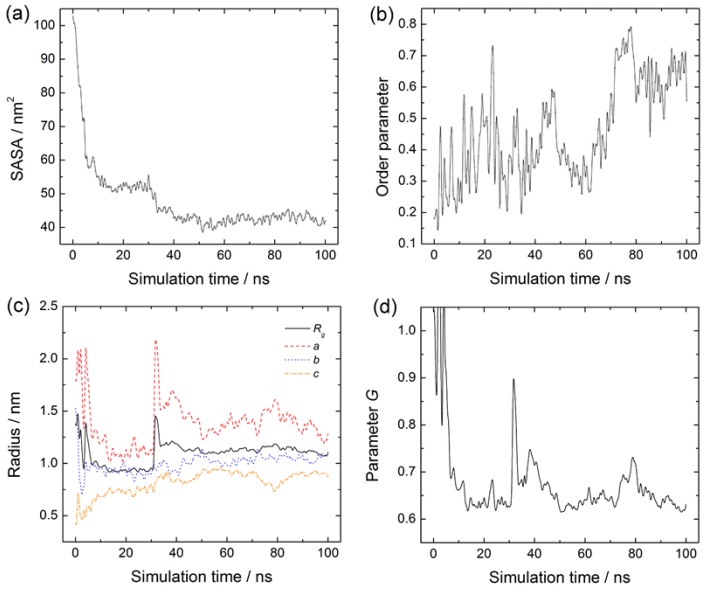

Figure S1. (a) Solvent accessible surface area (SASA) of the self-assemblies of the naphthalimide-cyanostilbene dyad in DMSO/H_2O (1:9) solution. (b) Order parameter of cyanostilbene and naphthalimide subunits in the self-assemblies of the naphthalimide-cyanostilbene dyad. (c) Radius of gyration R_g and the three effective radii a, b and c along the principal axes of the self-assembly. (d) The triaxial ellipsoid shape parameter G determined by a, b and c.

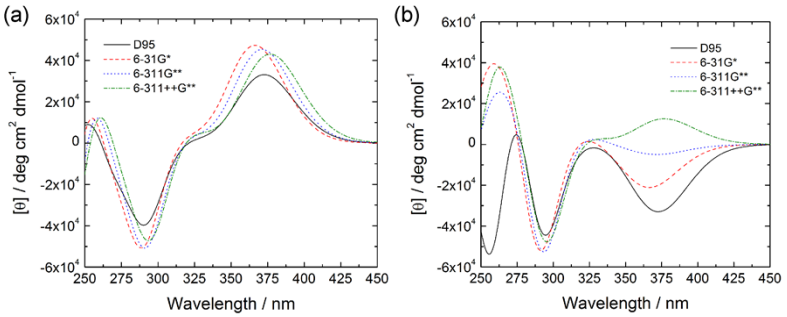

Figure S2. Basis set benchmark for (a) the dipole-velocity and (b) the dipole-length formula for CD spectrum, computed at a snapshot of the "**N**" unit using the hybrid PBE0 functional and different basis sets.

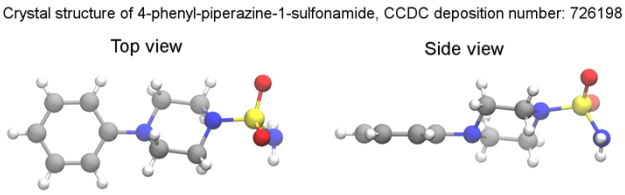

Figure S3. Crystal structure of an *N*-arylpiperazine derivative showing tetrahedral configuration of aryl nitrogen atom.

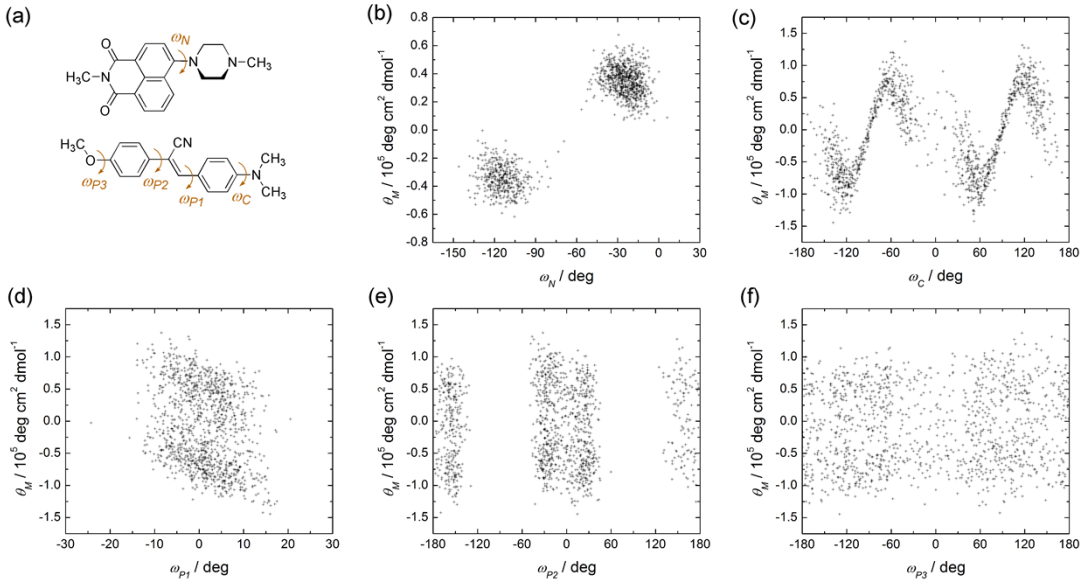

Figure S4. (a) Dihedral angles of the two chromophores. (b) Dependence of θ_M on dihedral angle ω_N. (c−f) Dependence of θ_M on dihedral angles (c) ω_C, (d) ω_{P1}, (e) ω_{P2}, and (f) ω_{P3}.

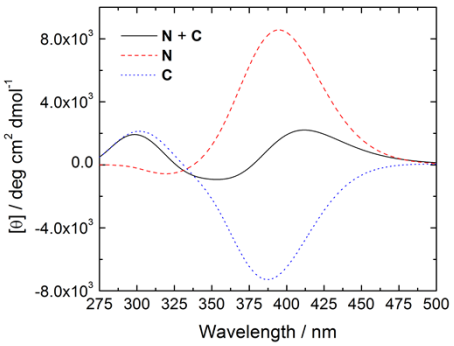

Figure S5. Averaged CD spectrum of the monomers: the "N" unit, the "C" unit, and their sum "N+C".

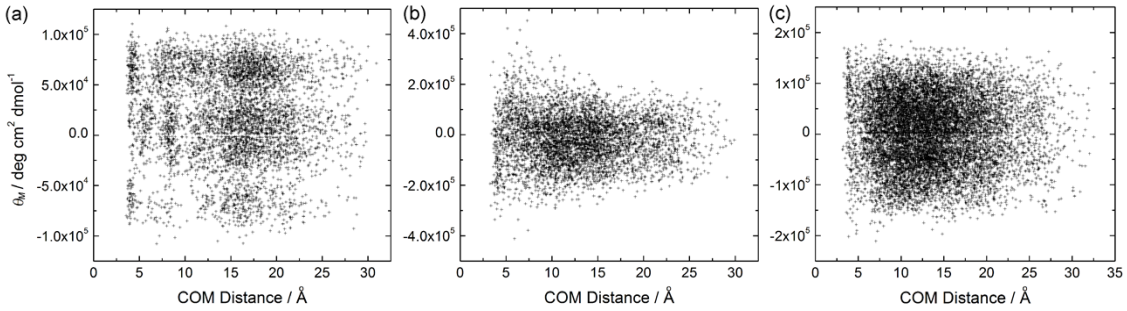

Figure S6. Dependence of maximal molar ellipticity θ_M of dimers on the center-of-mass (COM) distance between the two units for (left) the "N-N" dimer, (middle) the "C-C" dimer, and (right) the "N-C" dimer.

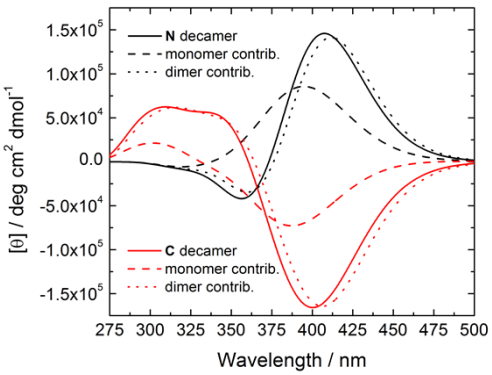

Figure S7. CD spectra computed by the exciton-coupled matrix method for the "N" decamer and the "C" decamer, together with their corresponding monomer and dimer contributions.