Electronic Supplementary Material (ESI) for Physical Chemistry Chemical Physics.

Figure S1. Simulated absorption and emission spectra for [n]CPP (n=12,15,16) at 300K and 10K with separated contributions of different excited states to the absorption spectrum.

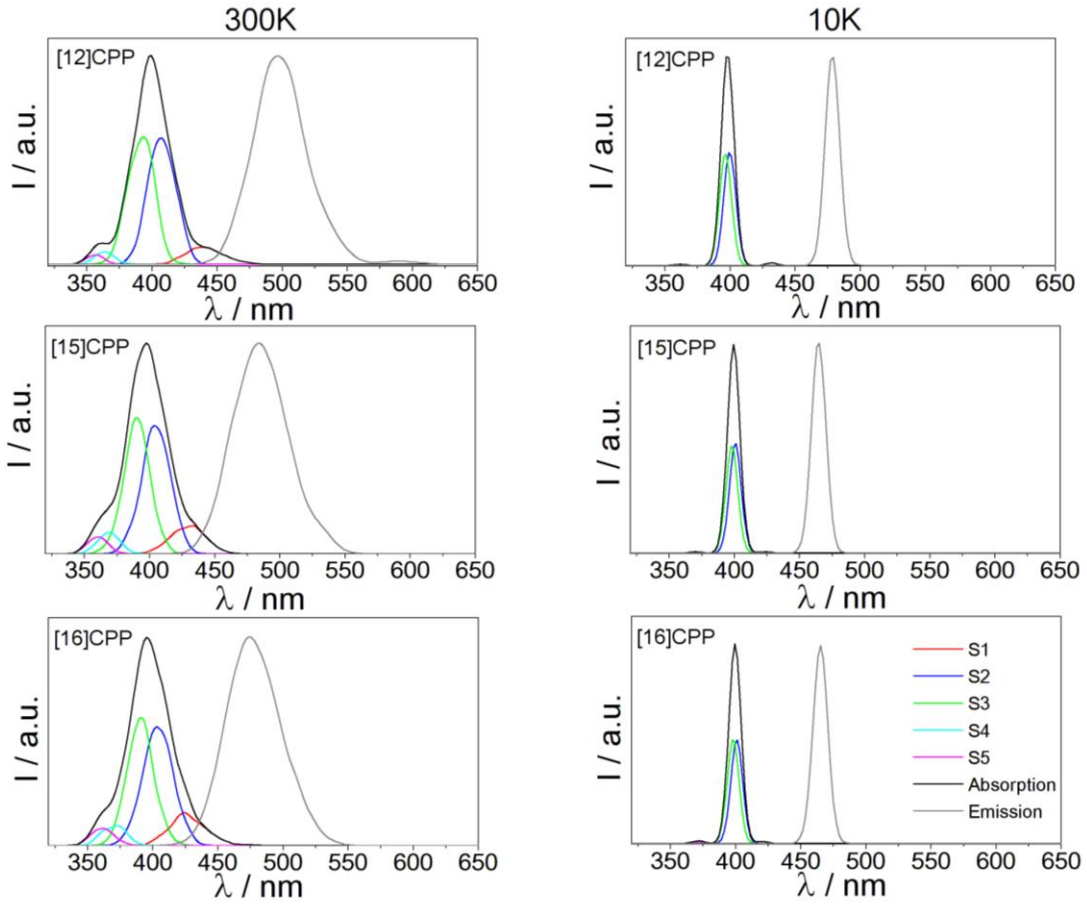

Figure S2. Dihedral angle distributions at the initial ground state configurations spectra for [n]CPP (n=12,15,16)at 300K and 10K.

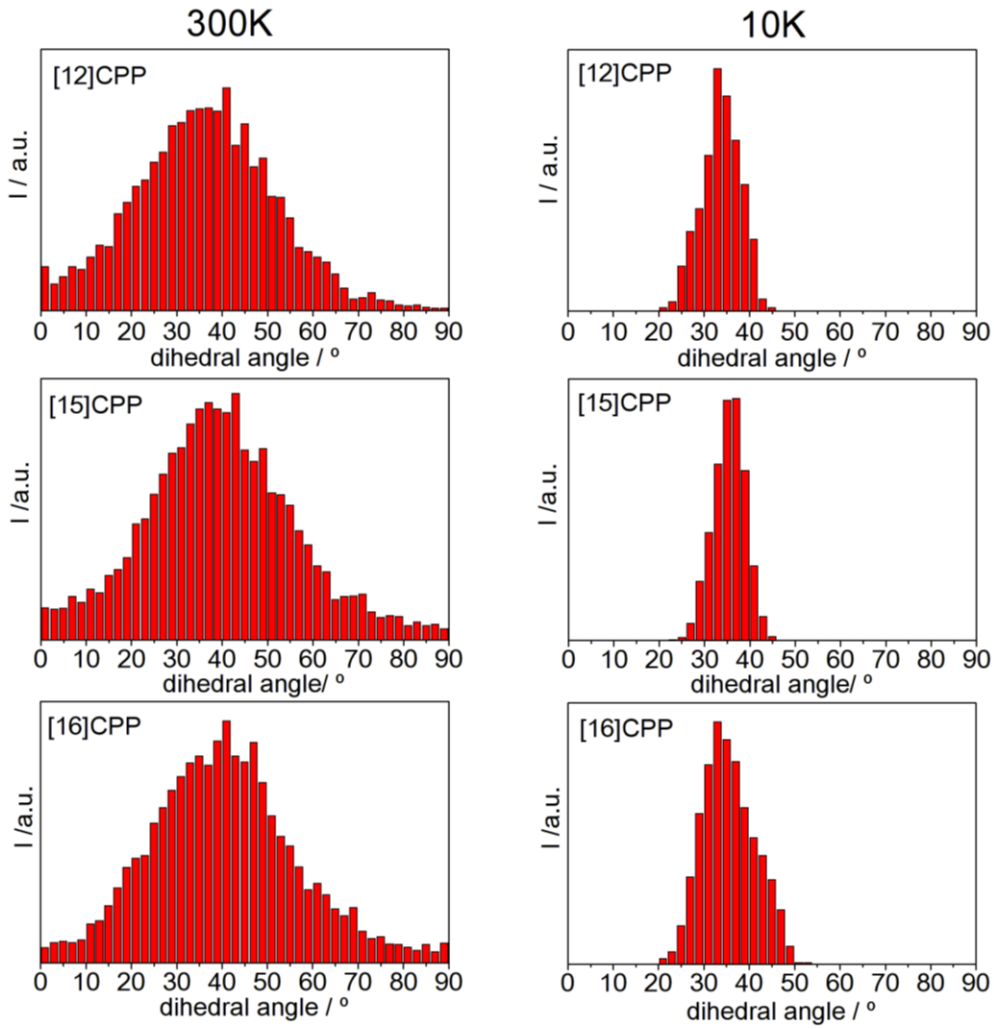

Figure S3. Variation in time of the dihedral angle distribution during the NEX-MD simulations at 300K and 10K for [n]CPP (n=12,15,16).

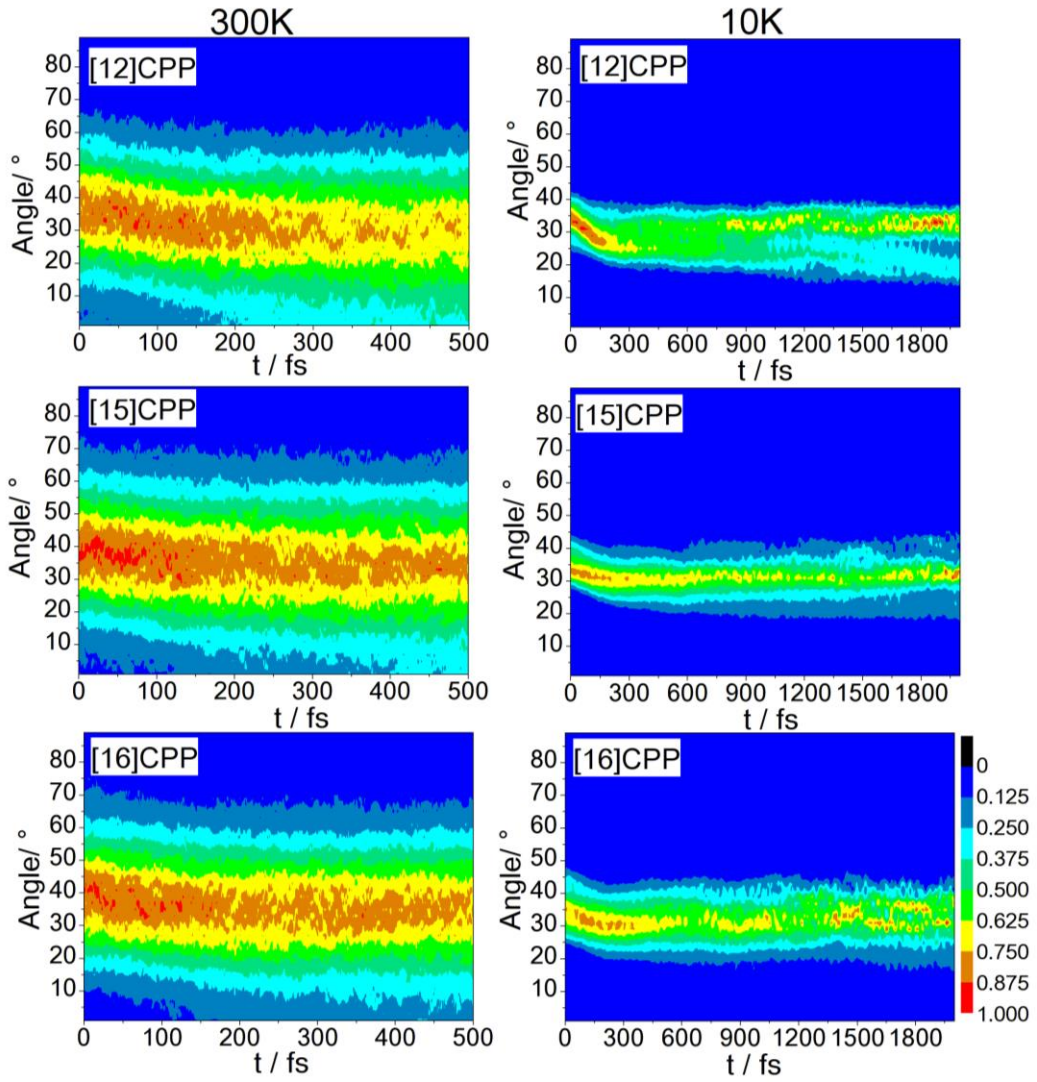

Figure S4. Variation in time of the relative probability for each ring to retain a significant contribution to total electronic transition density for [n]CPP(n=12,14,15,16) calculated during NEX-MD simulations at 300K

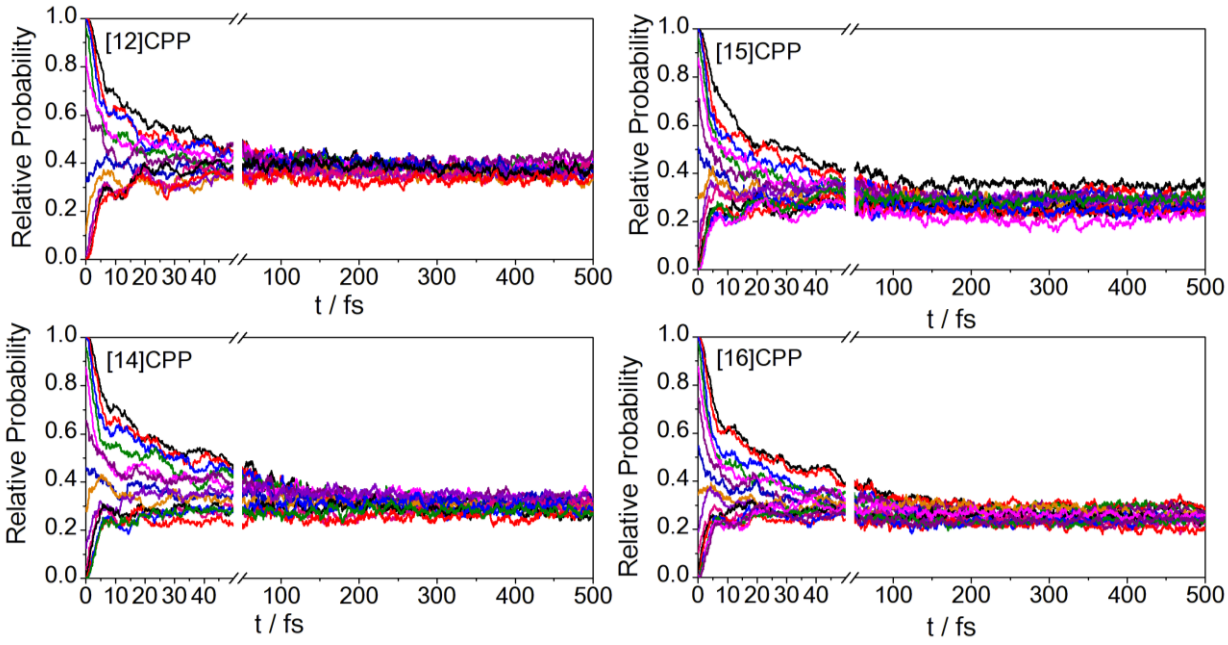

Figure S5. Variation in time of the relative probability for each ring to retain a significant contribution to total electronic transition density for [n]CPP(n=12,14,15,16)calculated duringadiabatic molecular dynamics on S1 state at 300K and 10K.