Supplementary Material (ESI) for Journal of Materials Chemistry

Supporting Information For:

The Self-assembly and Photophysical Characterization of Tri(cyclopenta[def]phenanthrene)-derived Nanoparticles: A Template Free Synthesis of Hollow Colloidosomes.

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Table S1. Electronic absorption properties of oligo-MCPPs calculated using Gaussian 03 at the B3LYP/6-31G* level.

Molecule	**Major Transitions**		
	Transition	**Energy (eV)**	**Oscillator strength(f)**
MCPP	**HOMO-0→LUMO+0(+70%)**, HOMO-1→LUMO+1(20%)	4.24	0.0734
	HOMO-0→LUMO+1 (51%), HOMO-1→LUMO+0 (26%)	4.94	0.3083
	HOMO-2→LUMO+1(45%), HOMO-0→LUMO+3(30%)	6.05	0.3068
	HOMO-4→LUMO+0(+43%), HOMO-2→LUMO+2(27%)	6.61	0.2324
di-MCPP	**HOMO-0→LUMO+0(+51%)**, HOMO-0→LUMO+2(+18%), HOMO-2→LUMO+0(+13%), HOMO-2→LUMO+2(12%)	3.74	0.0676
	HOMO-0→LUMO+2(+45%), HOMO-0→LUMO+0(28%), HOMO-2→LUMO+0(+13%), HOMO-1→LUMO+1(5%)	3.93	0.3427
	HOMO-1→LUMO+1(+66%), HOMO-0→LUMO+2(+9%), HOMO-2→LUMO+0(6%)	4.34	1.1705
tri-MCPP	**HOMO-0→LUMO+0(+80%)**	3.63	1.1425
	HOMO-3→LUMO+1(+22%), HOMO-1→LUMO+2(+13%), HOMO-4→LUMO+1(+12%), HOMO-3→LUMO+2(+9%) HOMO-2→LUMO+3(+9%), HOMO-3→LUMO+4(+6%) HOMO-1→LUMO+3(6%), HOMO-2→LUMO+2(+6%)	4.25	0.4711
	HOMO-3→LUMO+1(+42%), HOMO-4→LUMO+1(26%)	4.26	1.21
	HOMO-3→LUMO+4(+31%), HOMO-4→LUMO+4(+23%)	4.78	0.5087

	HOMO-0→LUMO+6(20%),HOMO-0→LUMO+5(6%)		
tetra-MCPP	**HOMO-0→LUMO+0(+89%)**,	3.5	2.13
	HOMO-5→LUMO+1(+32%), HOMO-4→LUMO+2(+27%)	4.22	1.5455
penta-MCPP	**HOMO-0→LUMO+0(+87%)**	3.94	2.9182
	HOMO-1→LUMO+4(+10%), HOMO-4→LUMO+0(+10%) HOMO-7→LUMO+3(9%), HOMO-2→LUMO+0(+7%) HOMO-5→LUMO+1(+7%), HOMO-5→LUMO+2(+6%) HOMO-7→LUMO+1(+6%)	4.21	1.7773
	HOMO-1→LUMO+6(+33%), HOMO-0→LUMO+7(16%) HOMO-4→LUMO+0(+14%)	4.22	0.93

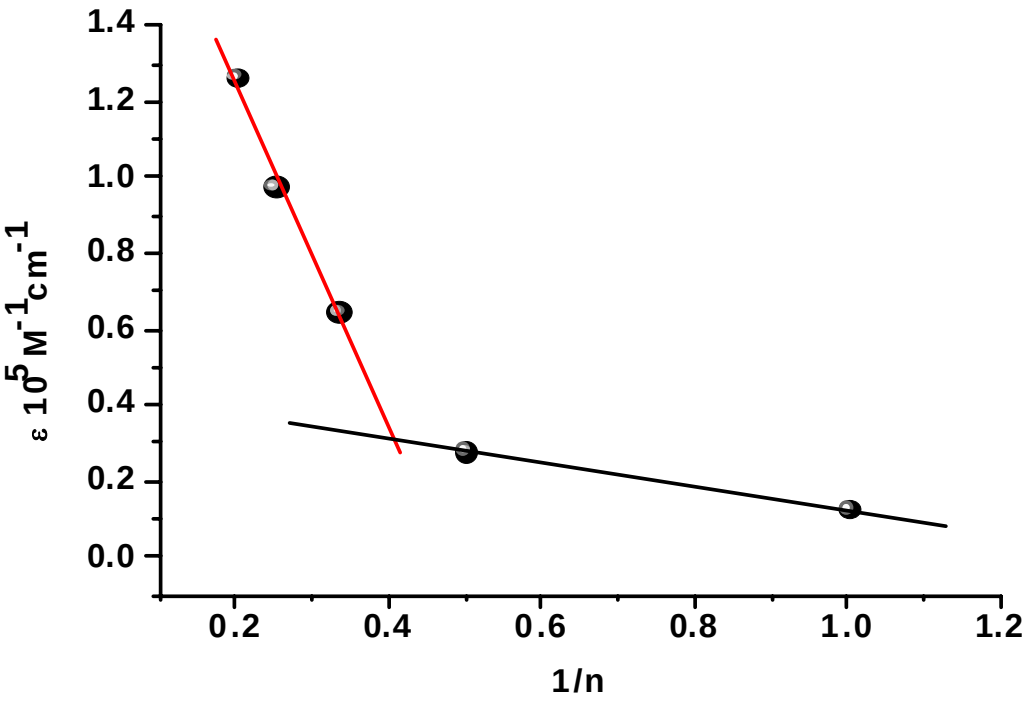
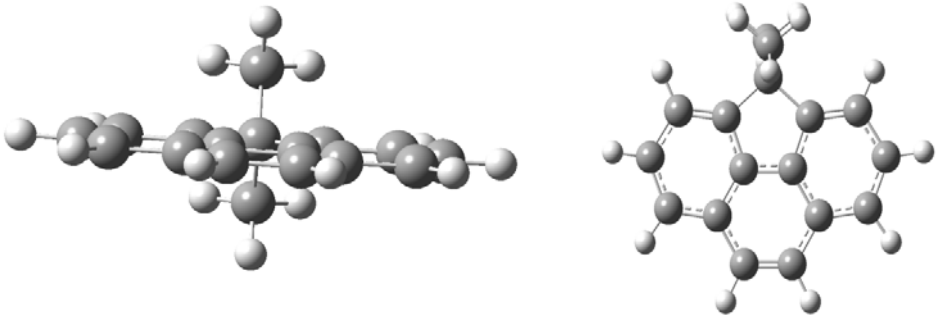


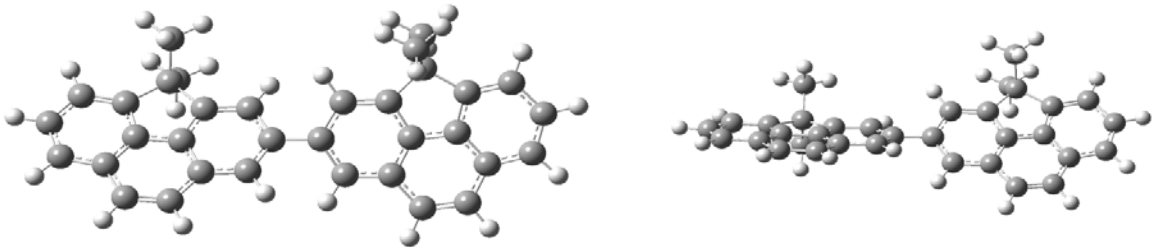
Figure S1. Plot of molar absorptivity at the low-energy absorption maximum vs. the inverse of the number of monomeric subunits.

Optimized Geometries

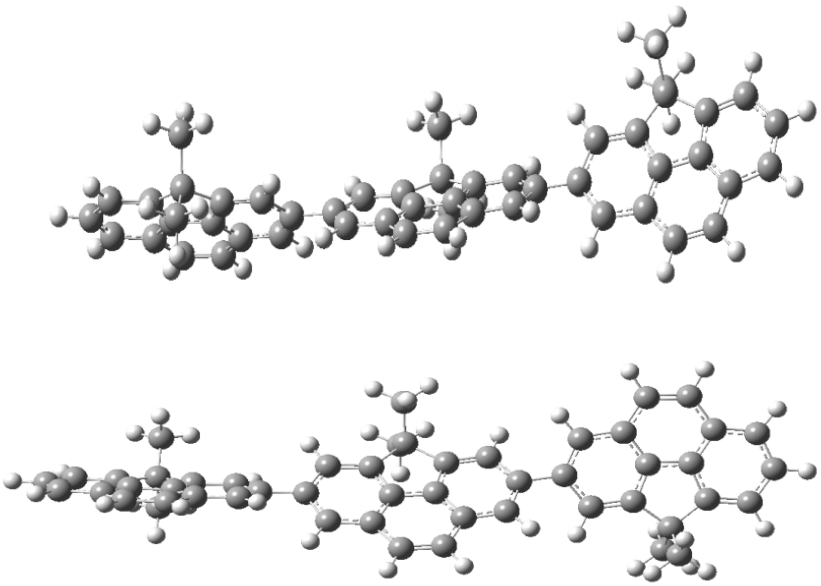
MCPP



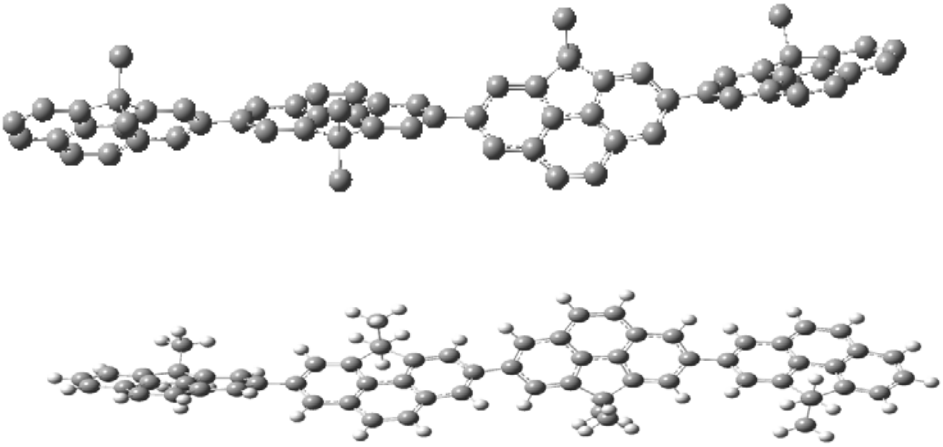
di-MCPP



tri-MCPP



tetra-MCPP



penta-MCPP

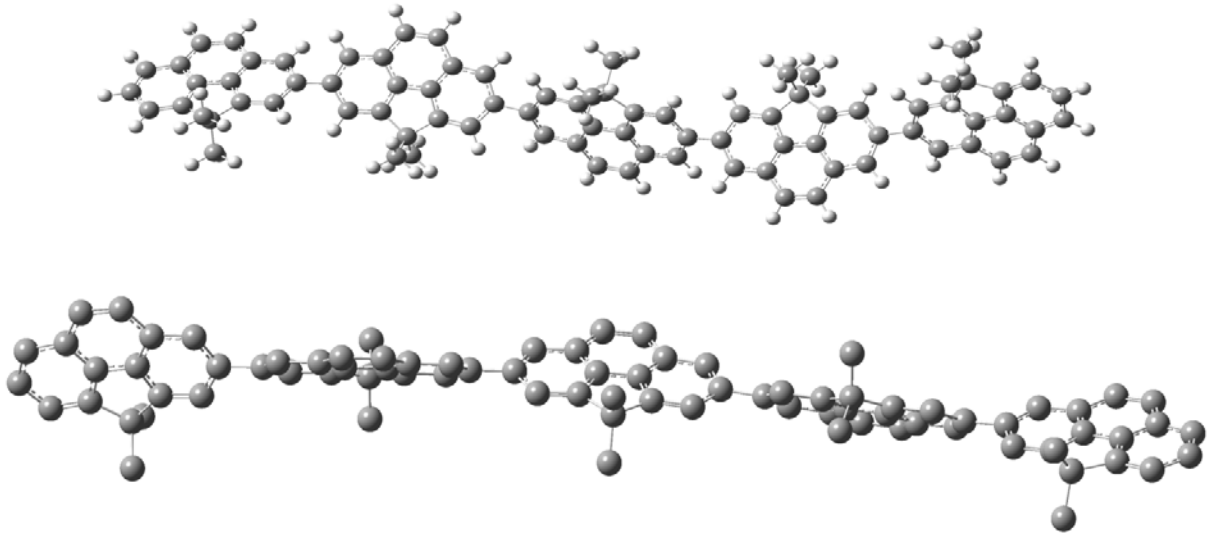


Figure S2. Optimized geometries (calculated at the B3LYP/6-31G* level) of the **MCPP** oligomers considered in this study.

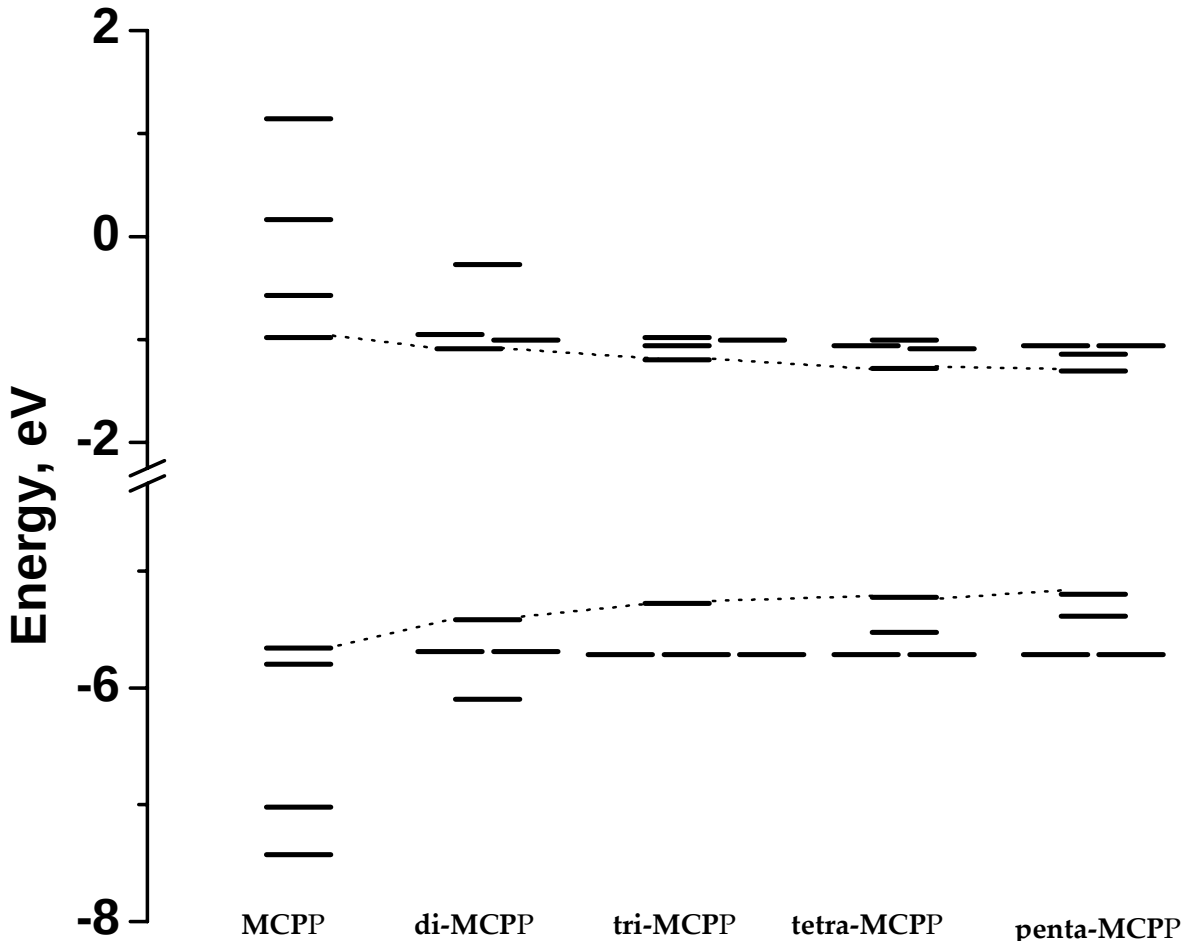


Figure S3. MO energy levels of the oligomers of this study calculated using Gaussian 03 at the B3LYP/6-31G* level

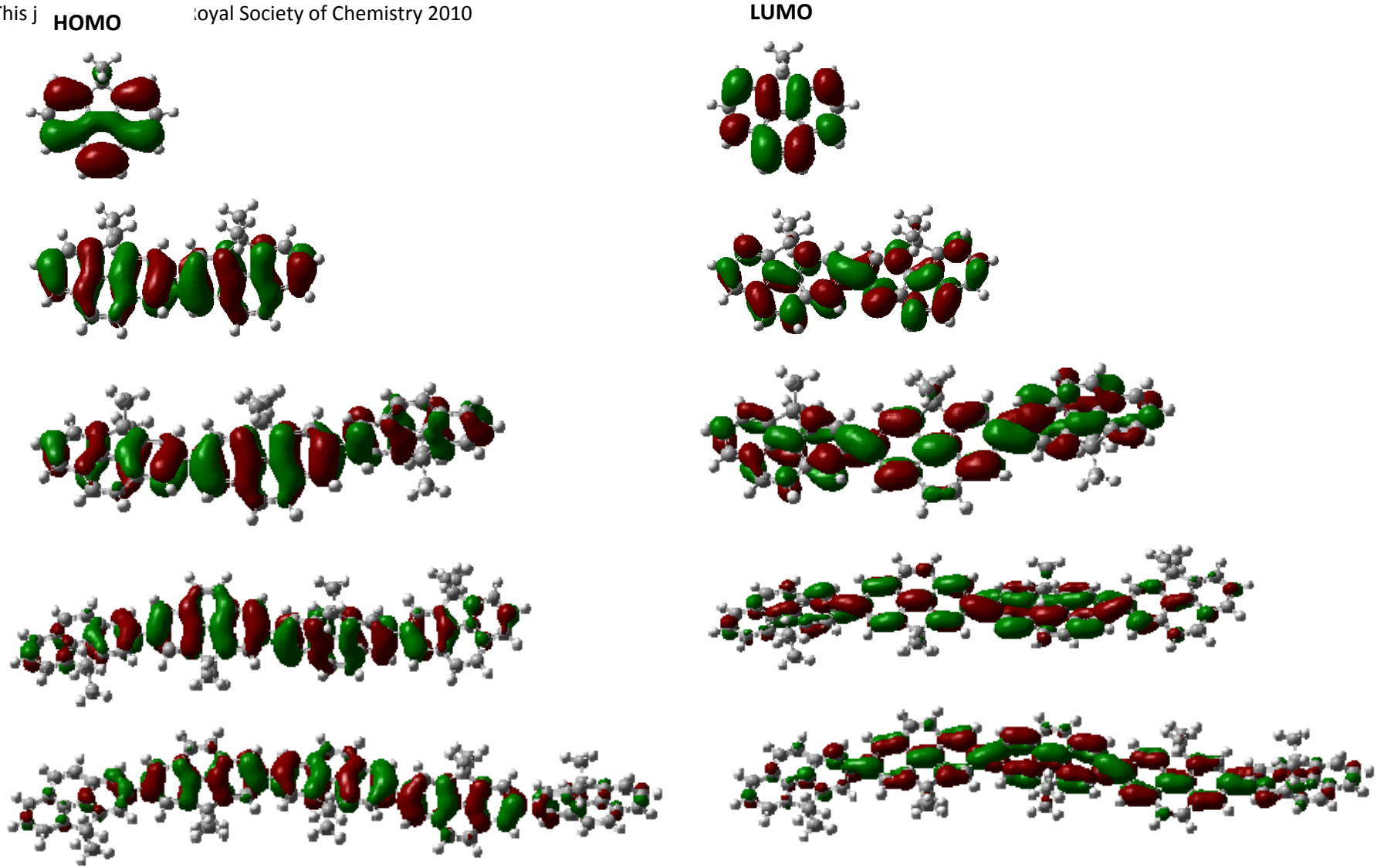


Figure S4. MO diagrams of the oligomers of this study calculated using Gaussian 03 at the B3LYP/6-31G* level.

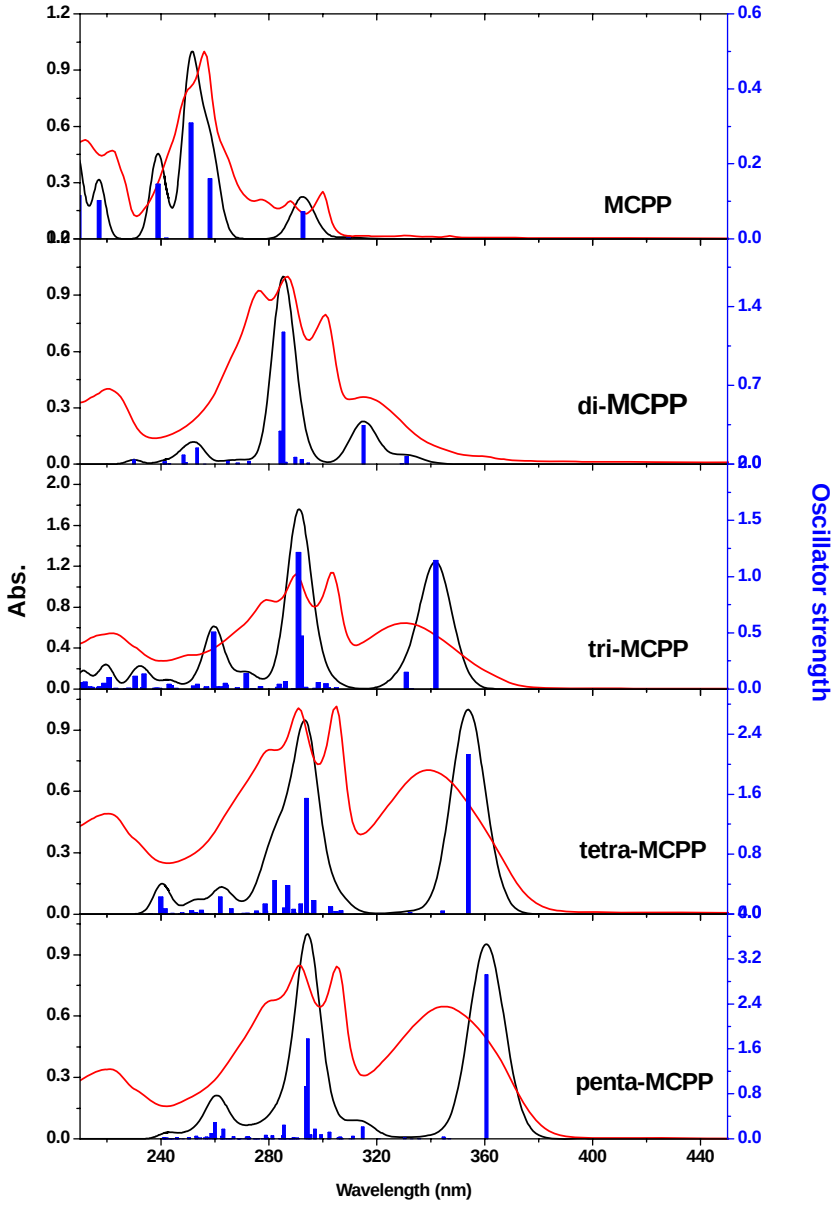


Figure S5. Simulated absorption (black)) and the electronic transitions (blue) of various oligo-MCPPs obtained using Gaussian 03 at the B3LYP/6-31G* level. Absorption spectra of the oligo-MCPPs (black) are given for comparison.

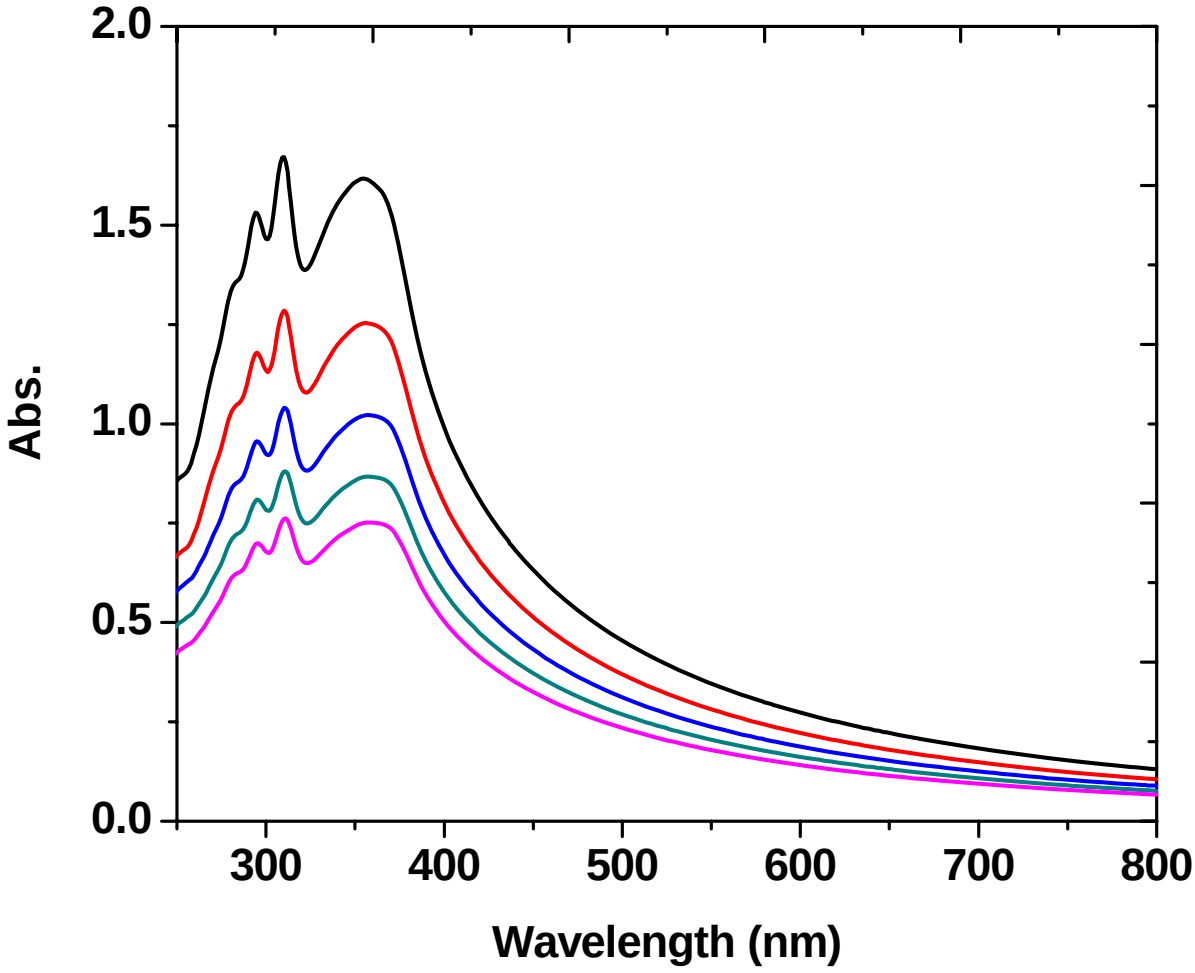


Figure S6. Change in the absorption spectra of **tri-MCPP-N2** observed upon dilution with water

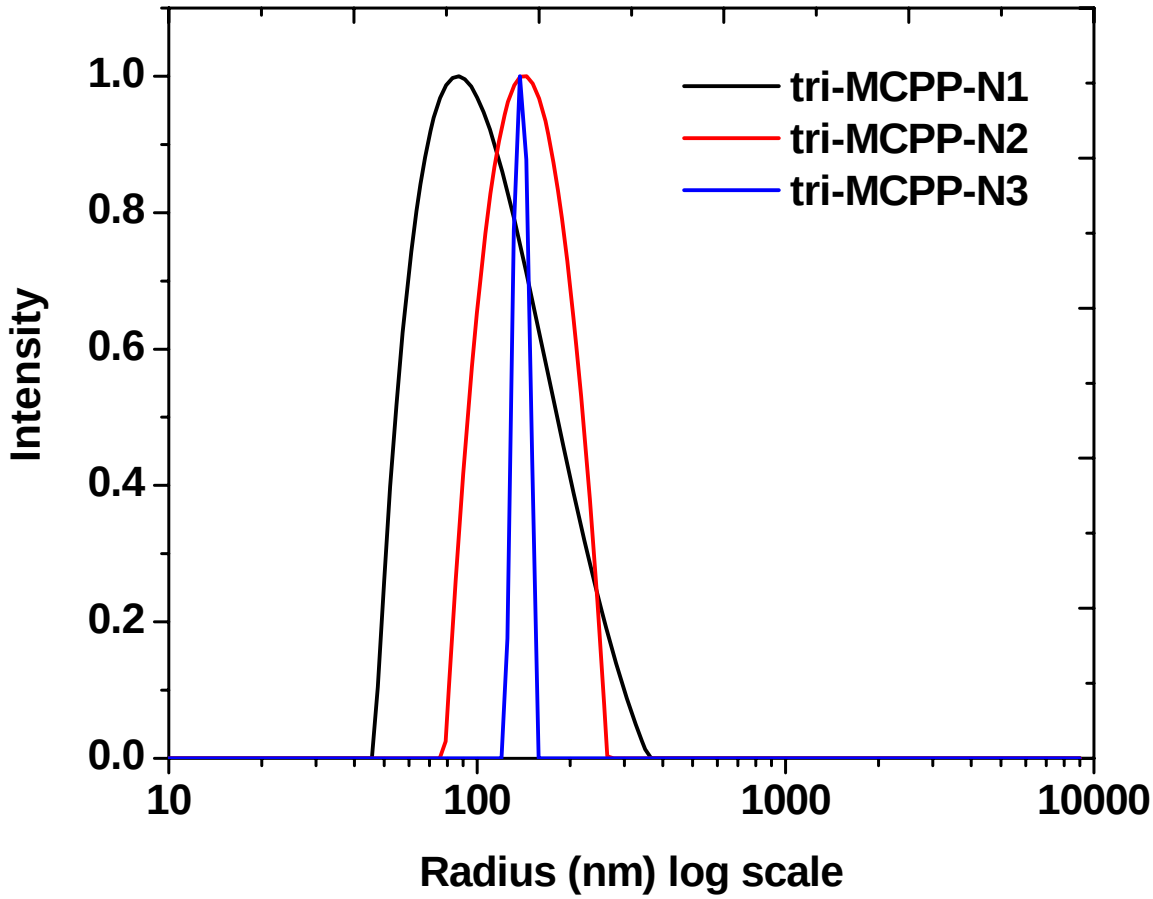


Figure S7. Dynamic light scattering spectra of nanostructures generated from **tri-MCPP** by using different water/THF ratios by volume

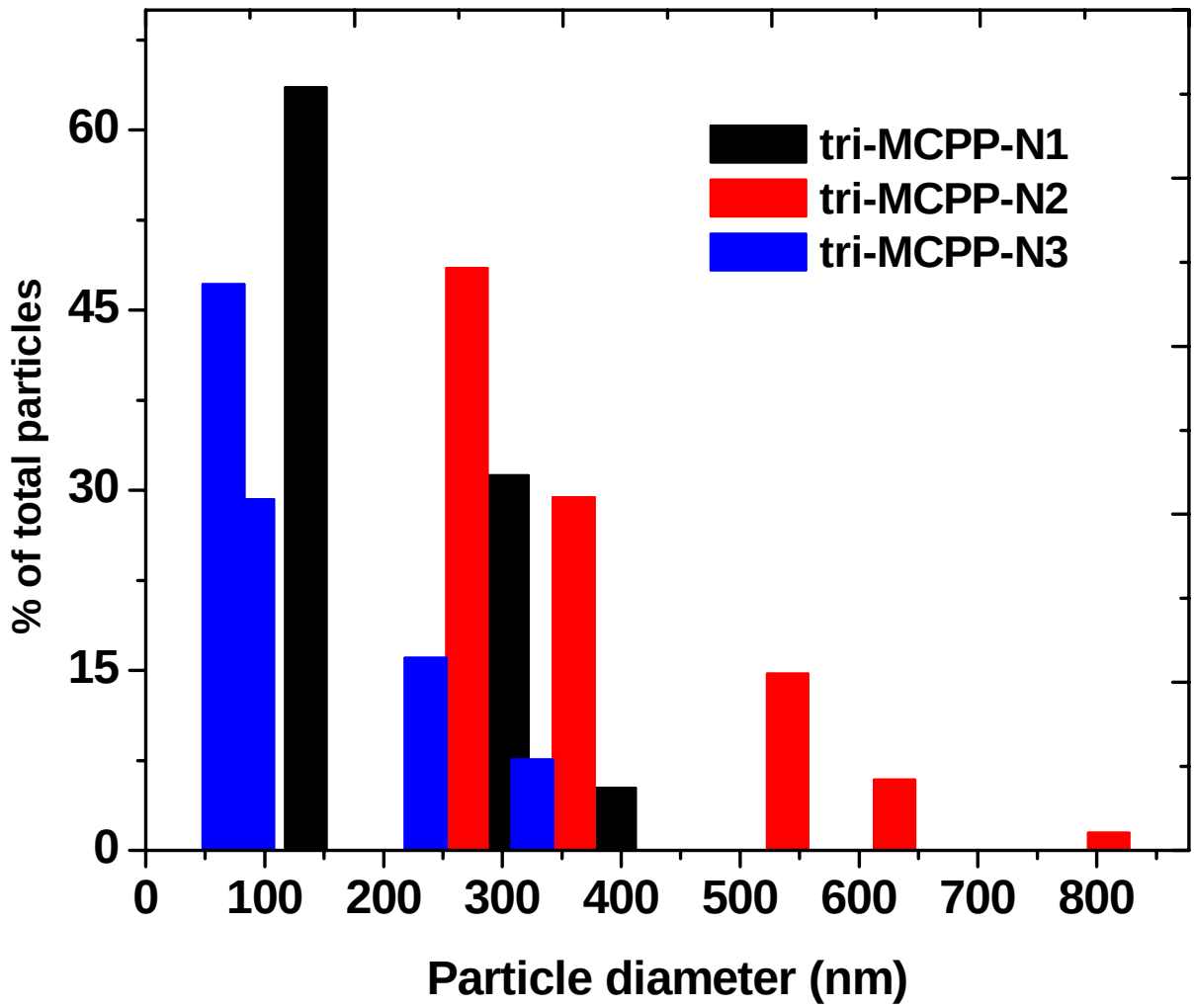


Figure S8. Particle size distribution determined from SEM images recorded using drop casted films of nanostructures formed from **tri-MCPP** by using different water/THF ratios by volume

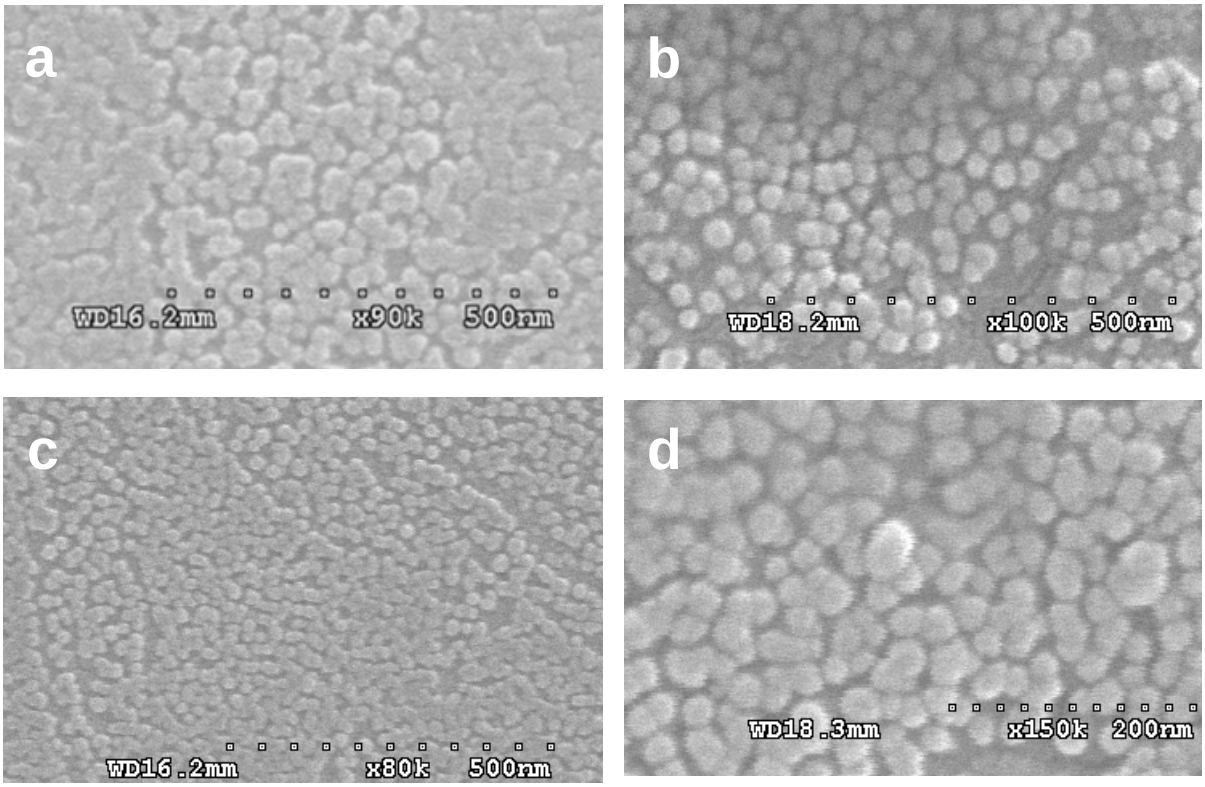


Figure S9. Representative SEM images of the aggregates formed from phenanthrene oligomers a) **MCPP**, b) **di-MCPP**, c) **tetra-MCPP** and d) **penta-MCPP** when subject to reprecipitation at 90%-10% water/THF ratios by volume

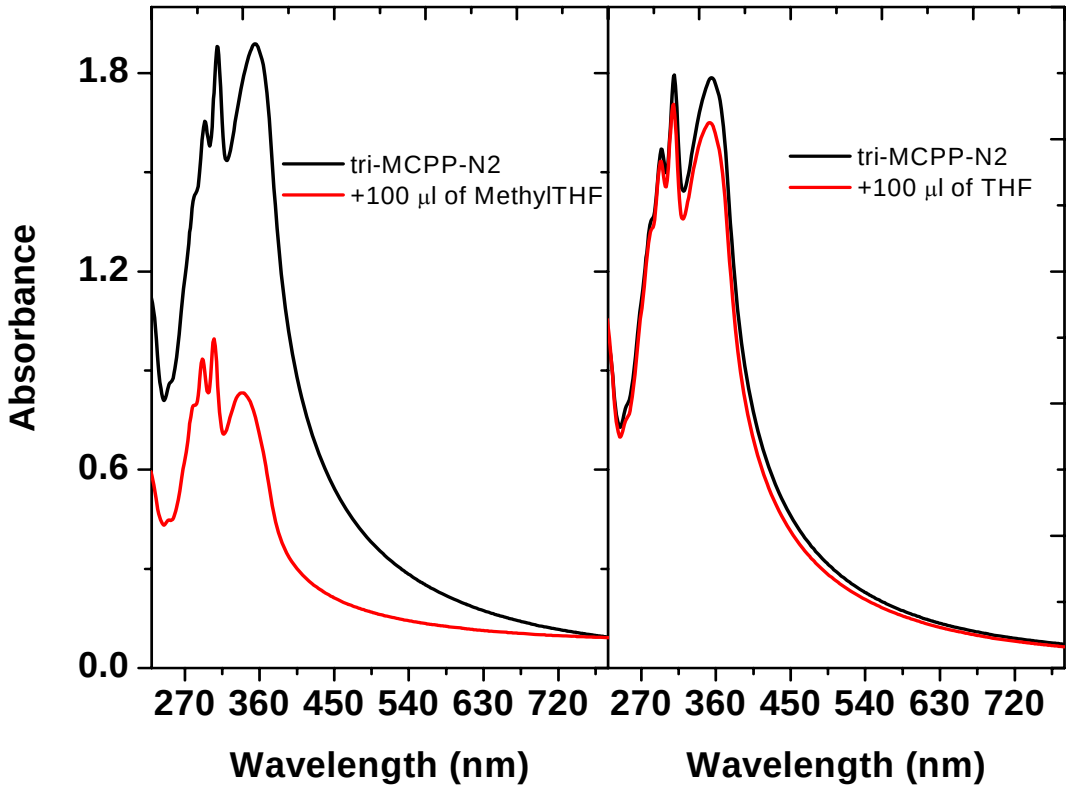


Figure S10. UV-visible absorption spectrum of **tri-MCPP-N2** recorded at a concentration of ~5×10^{-5} M^{-1} in a water/THF solvent mixture, 80:20 by volume