Organic nanocrystals of [2.2]paracyclophanes achieved via sonochemistry: enhanced red-shifted emission involving edge-to-face chromophores

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Supporting Information

Materials: pCp was purchased from Carbosynth (Compton, Berkshire, UK). SDS was purchased from Sigma Aldrich Chemical Company (St. Louis, MO, USA). N.N-dimethylformamide, toluene, and ethanol were purchased from Fisher Scientific Company (Pittsburgh, PA, USA). tpcp was prepared as reported. All chemicals were used without further purification.

Methods: PXRD data was collected using a Bruker D-5000 diffractometer equipped with a Bruker SOL-X energy-sensitive detector using CuK_α radiation (λ = 1.54056 Å). Particle size measurements were determined by a Zetasizer Nano ZS (Malvern, Southborough, MA) instrument at 25°C. SEM images were obtained using a Hitachi S-48000 with an accelerating voltage range of 2-5 kV. SEM samples were prepared by depositing each sample on a Si wafer. Absorption and emission measurements were obtained using a HORIBA Jobin Yvon FluoroMax-4 (Edison, NJ, USA). All measurements were made on the as-prepared suspensions with a scan rate of 5 mm sec^{-1} and both slit widths set to 2 nm. Solution-based measurements were obtained using N,N-dimethylformamide as solvent. Micrometer-sized and Nanometer-sized particles were measured as suspensions in water and 0.021 M $SDS_{(aq)}$. The suspension measurements were conducted using an aliquot of the suspension after re-precipitation (micro) and/or after sonication (nano).

PXRDs

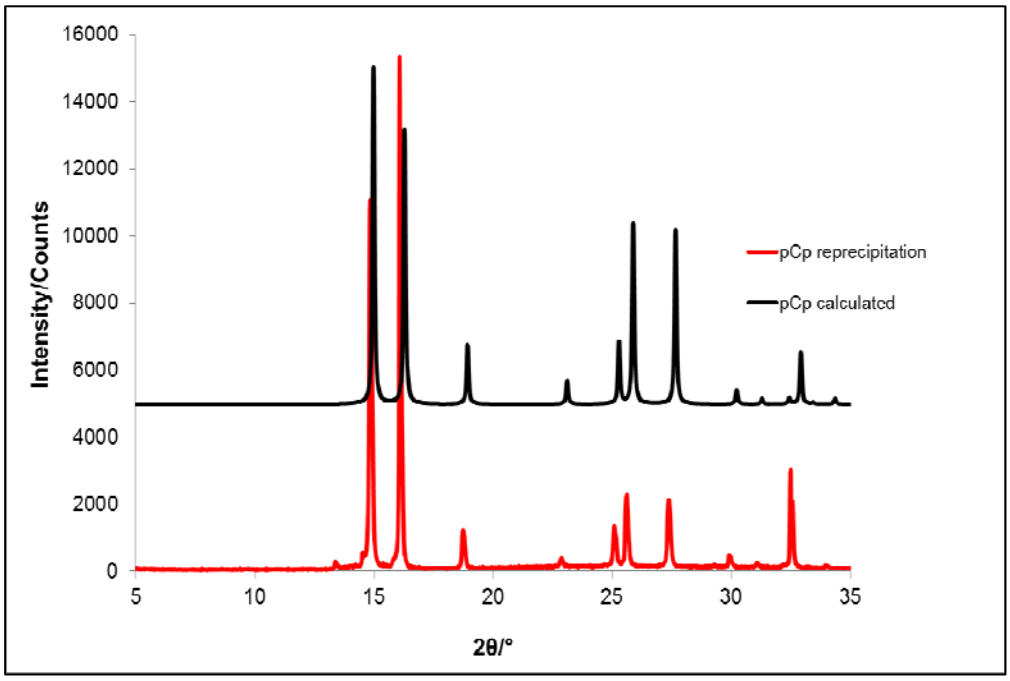

Figure S-1: PXRD diffractogram of a sample obtained during reprecipitation of pCp compared to the calculated pattern.

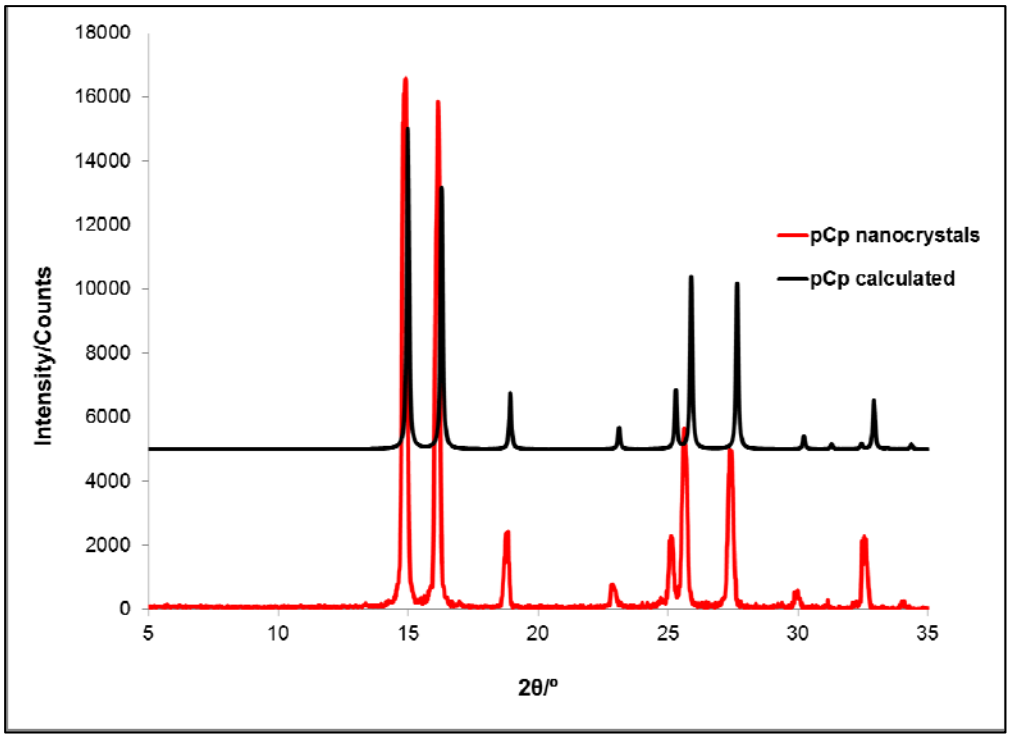

Figure S-2: PXRD diffractogram of pCp nanocrystals compared to the calculated pattern.

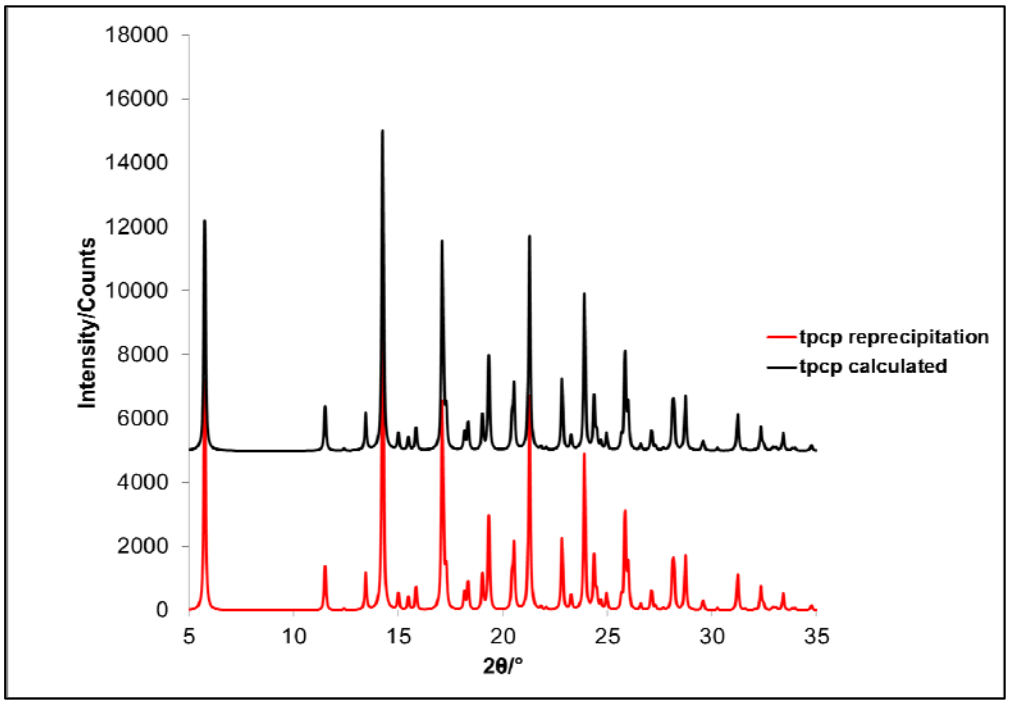

Figure S-3: PXRD diffractogram of a sample obtained during reprecipitation of tpcp compared to the calculated pattern.

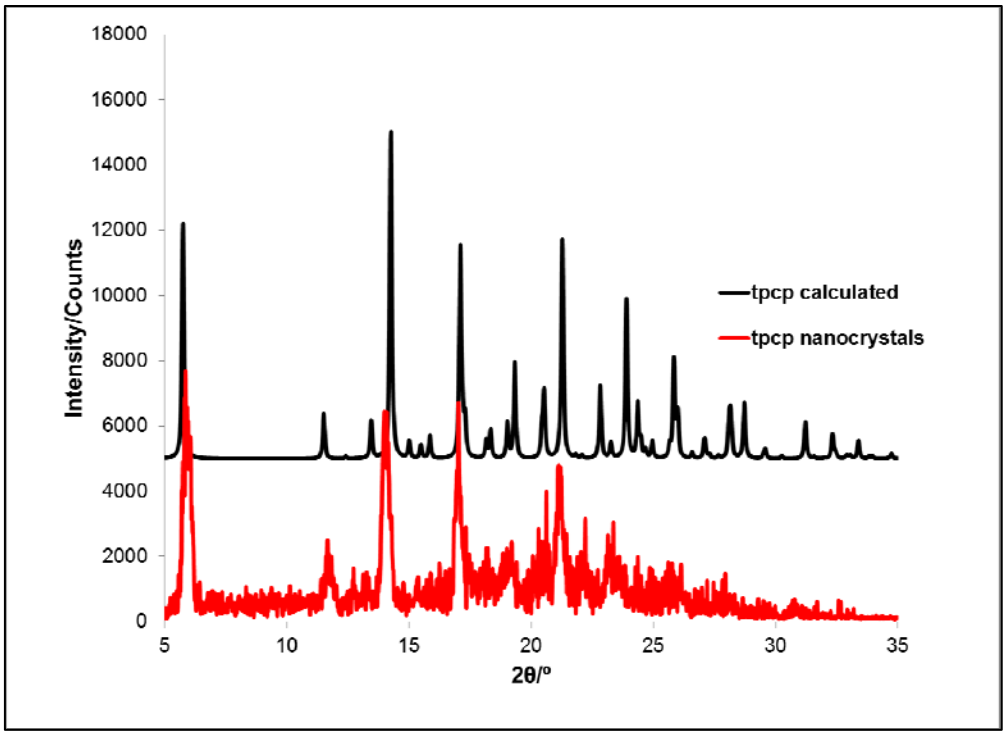

Figure S-4: PXRD diffractogram of tpcp nanocrystals compared to the calculated pattern.

Spectroscopic Data

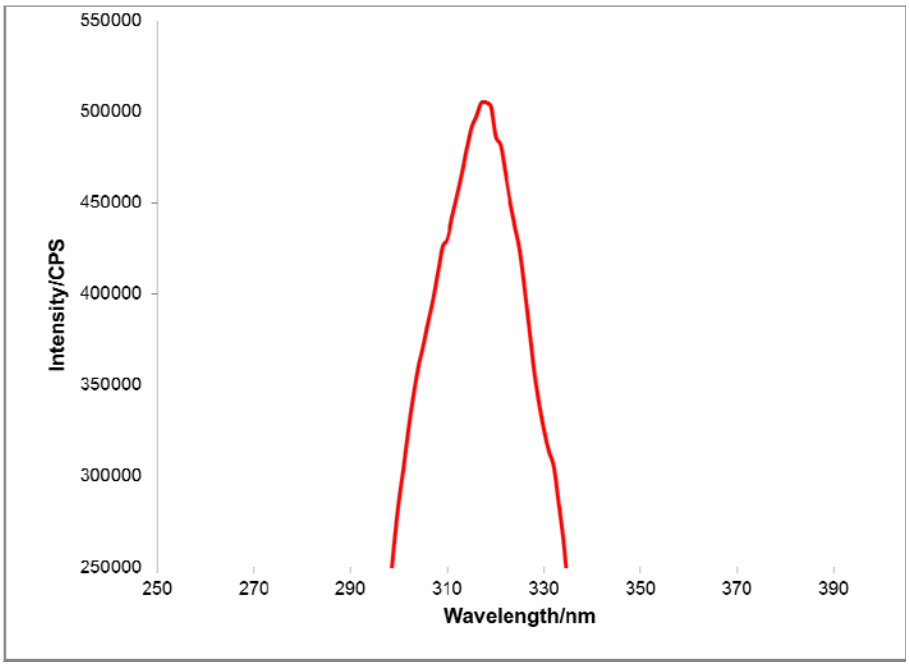

Figure S-5: Excitation spectrum of pCp in DMF.

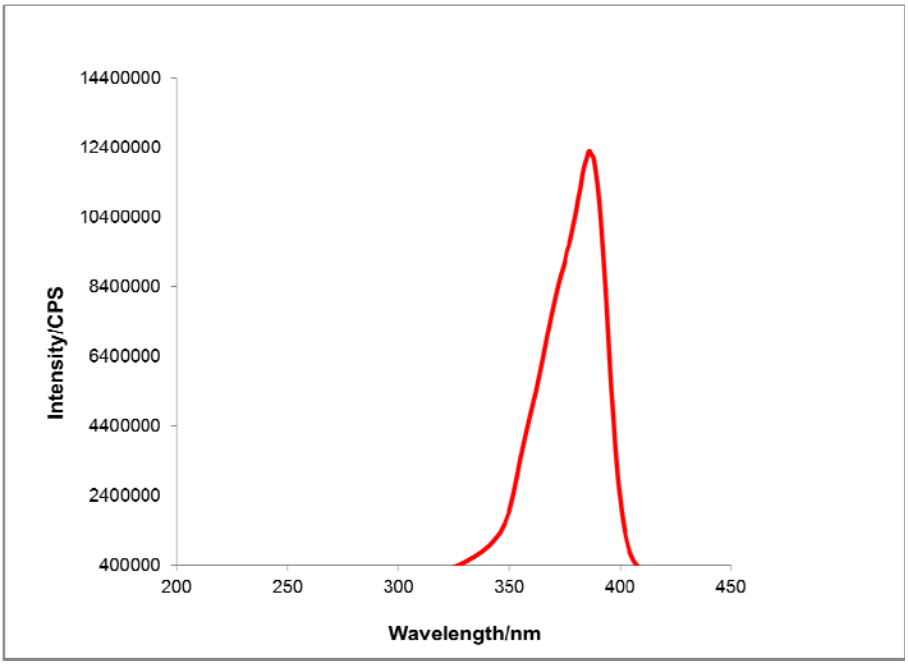

Figure S-6: Excitation spectrum of tpcp in DMF.

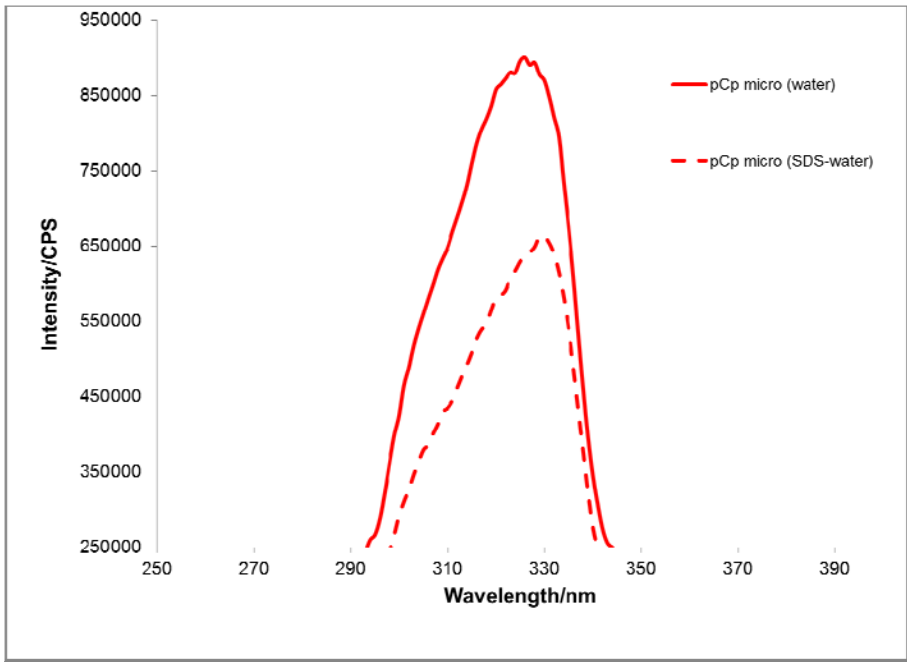

Figure S-7: Excitation spectra of pCp microcrystalline suspensions.

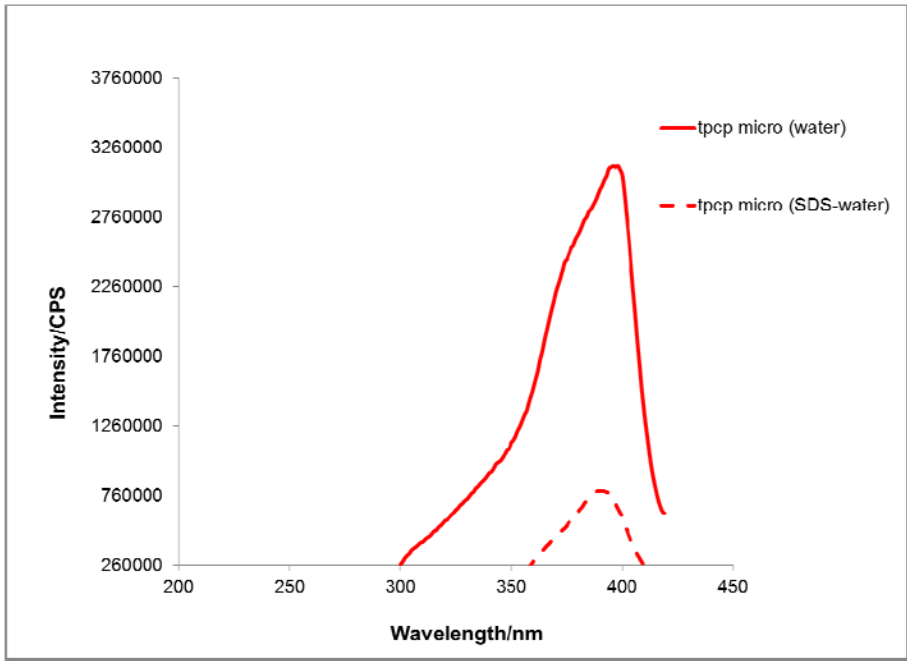

Figure S-8: Excitation spectra of tpcp microcrystalline suspensions.

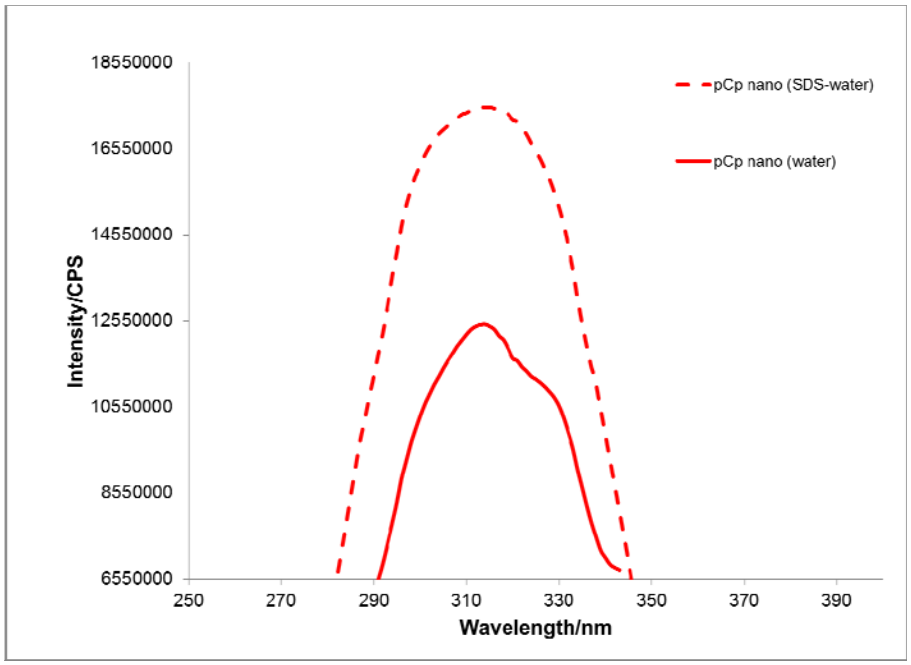

Figure S-9: Excitation spectra of pCp nanocrystalline suspensions.

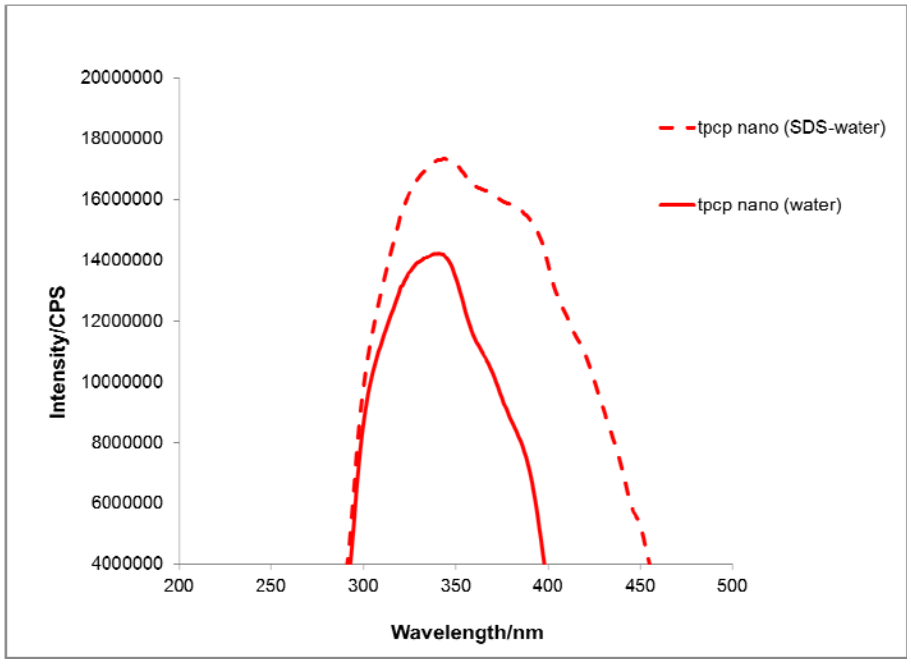

Figure S-10: Excitation spectra of tpcp nanocrystalline suspensions.

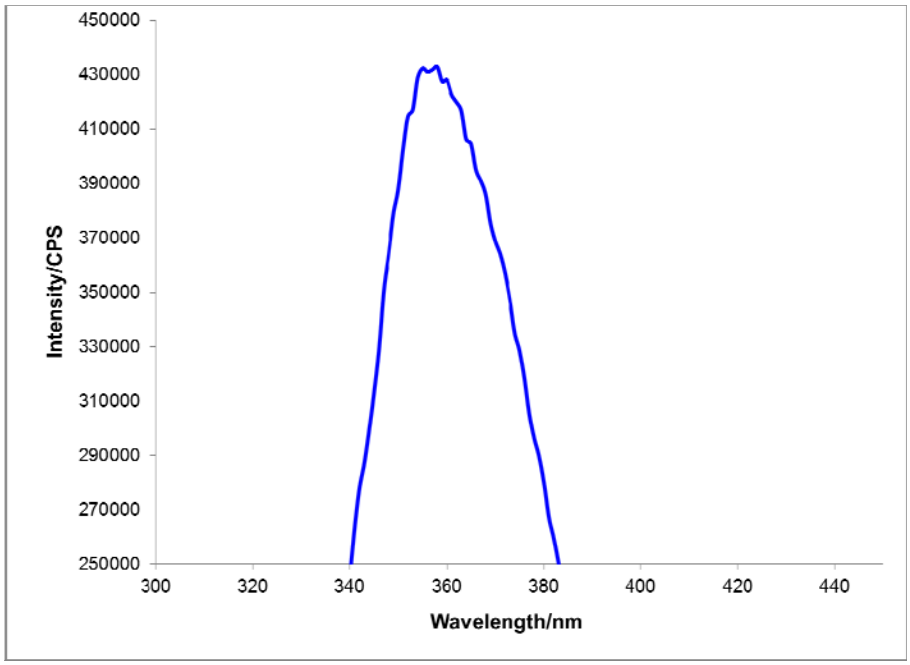

Figure S-11: Emission spectrum of pCp in solution.

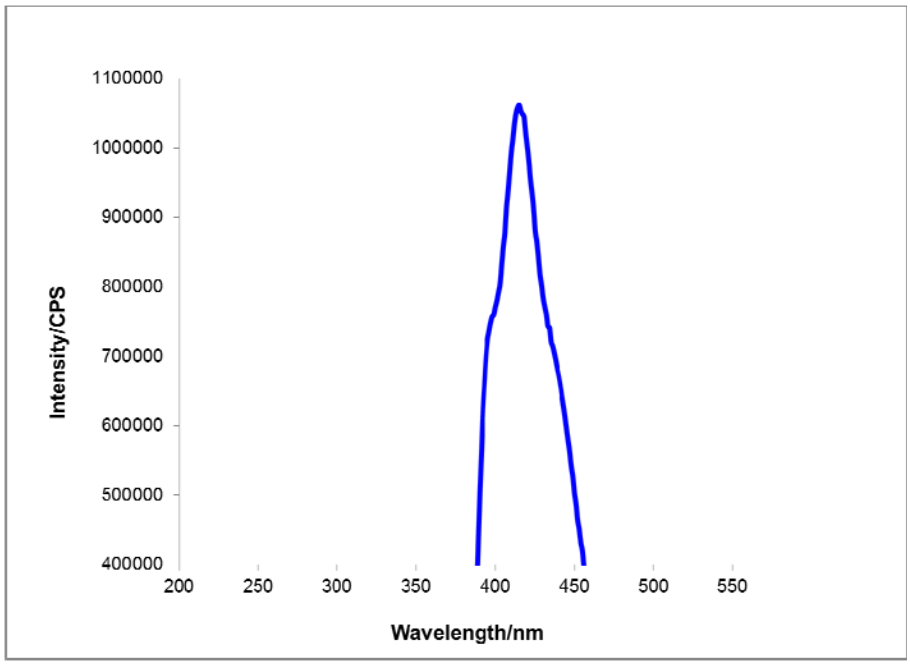

Figure S-12: Emission spectrum of tpcp in solution.

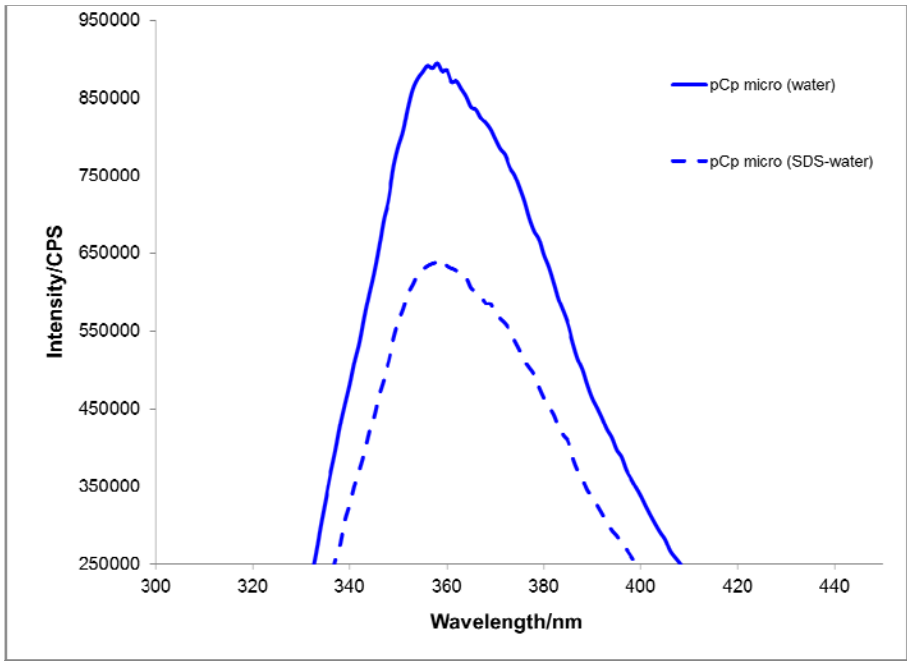

Figure S-13: Emission spectra of pCp microcrystalline suspensions.

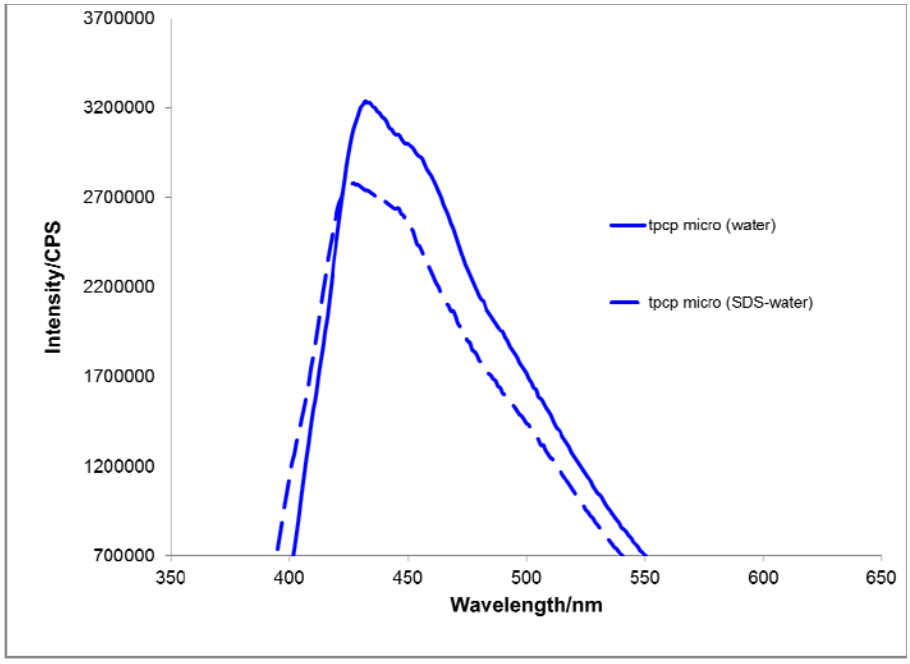

Figure S-14: Emission spectra of tpcp microcrystalline suspensions.

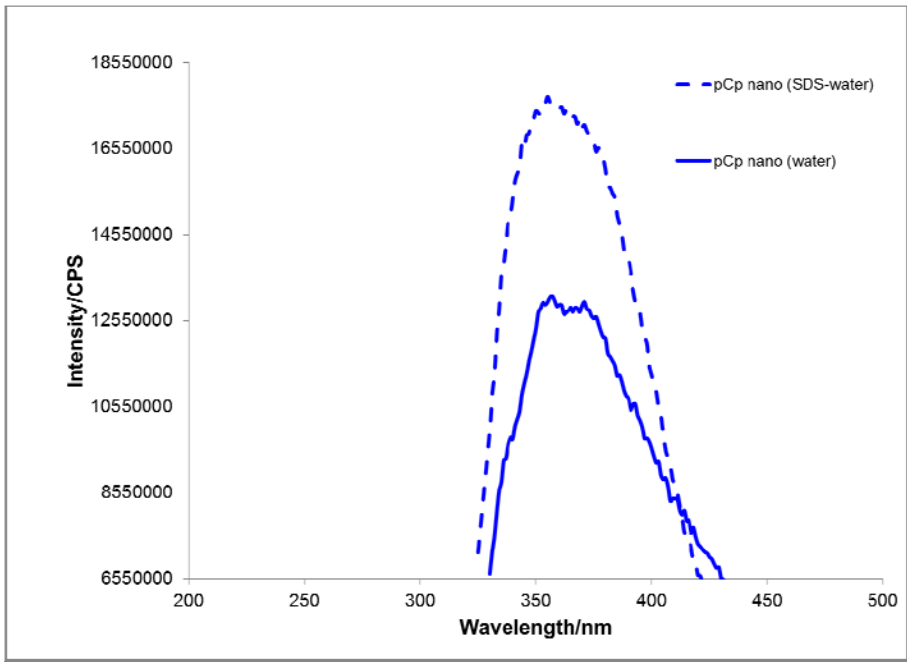

Figure S-15: Emission spectra of pCp nanocrystalline suspensions.

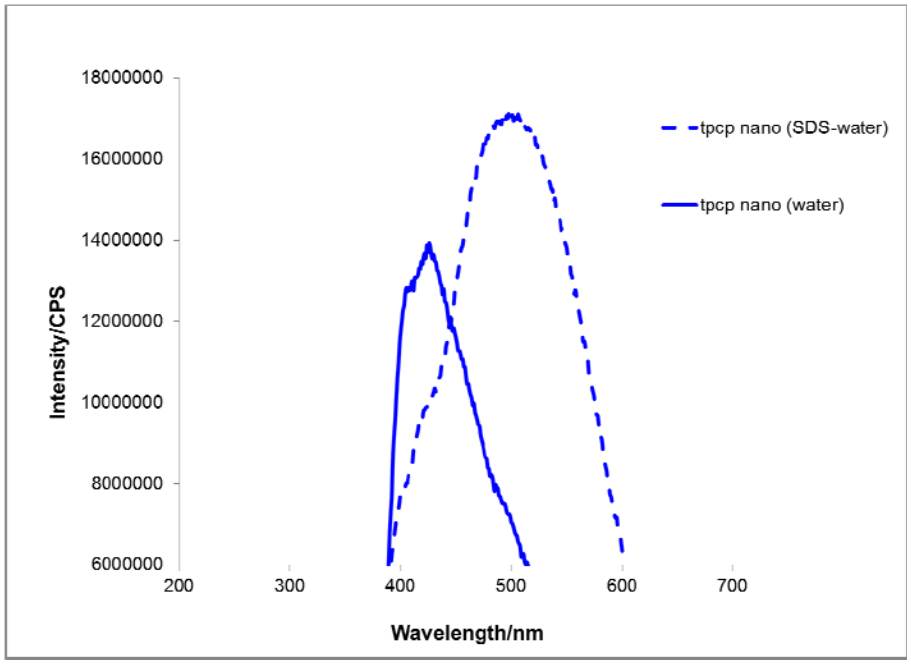

Figure S-16: Emission spectra of tpcp nanocrystalline suspensions.

Comparison of Emission Profiles

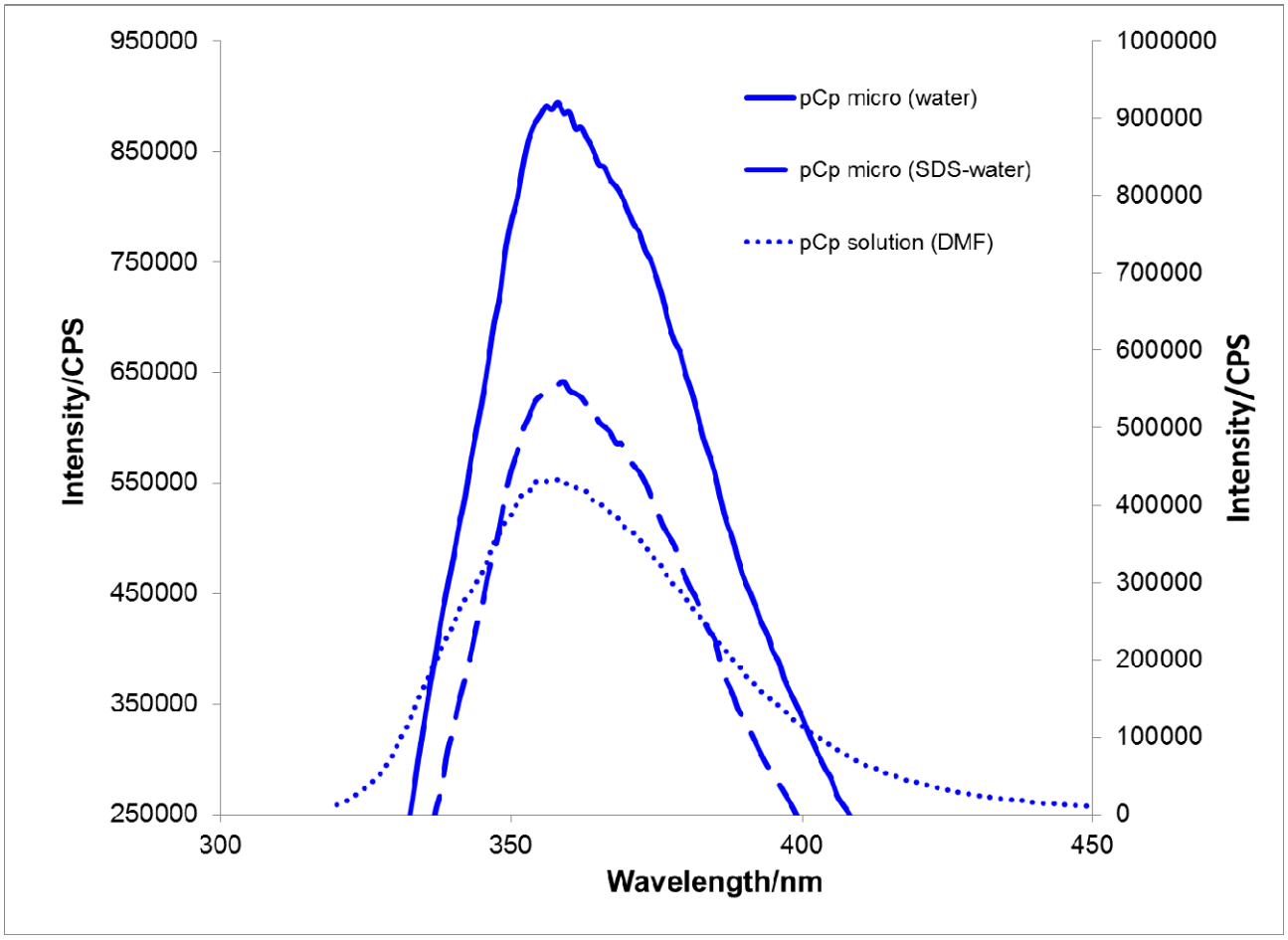

Figure S-17: Emission spectra of pCp microcrystalline suspensions compared to pCp in solution (solution result is plotted on the secondary axis).

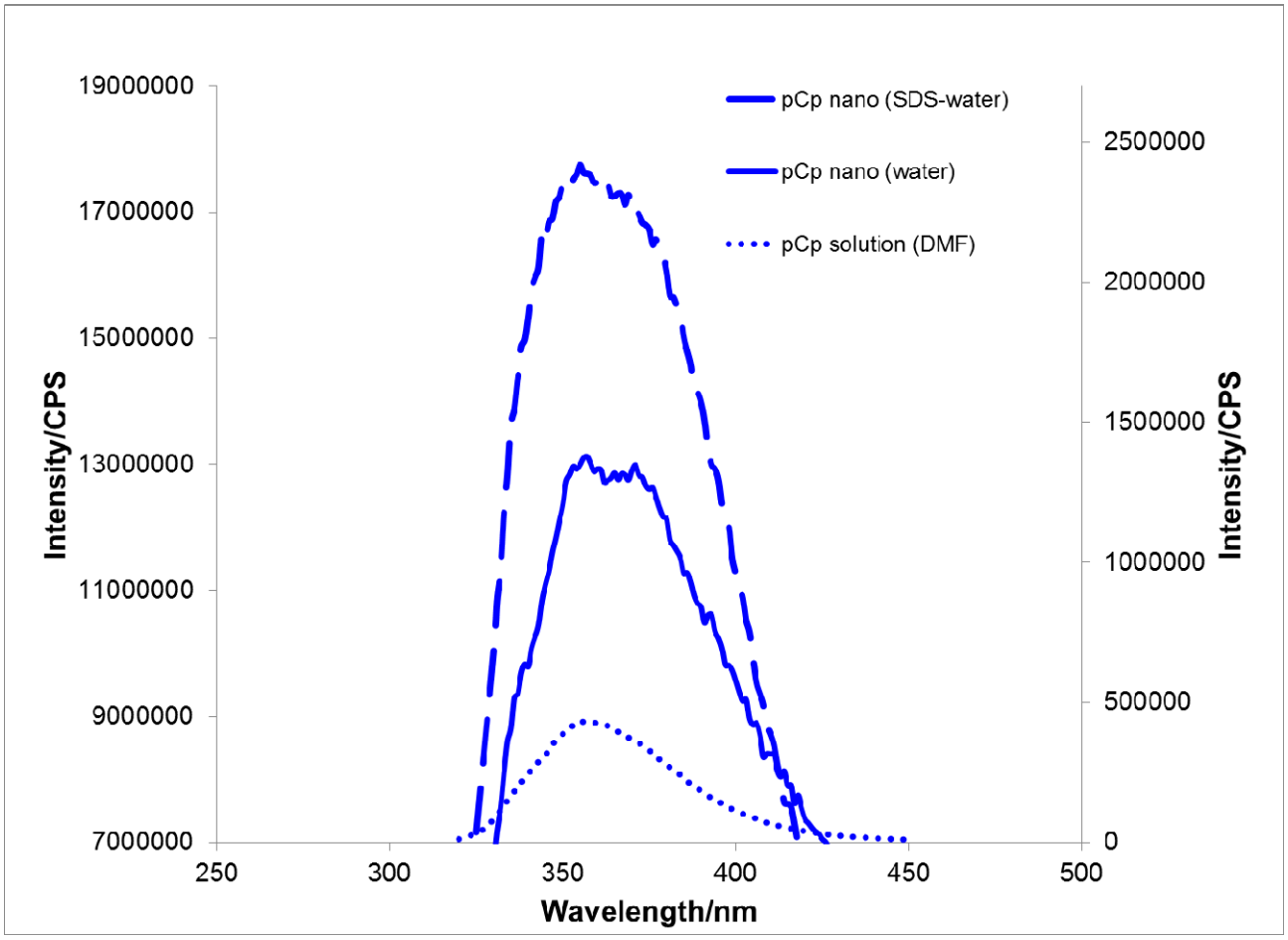

Figure S-18: Emission spectra of pCp nanocrystalline suspensions compared to pCp in solution (solution result is plotted on the secondary axis).

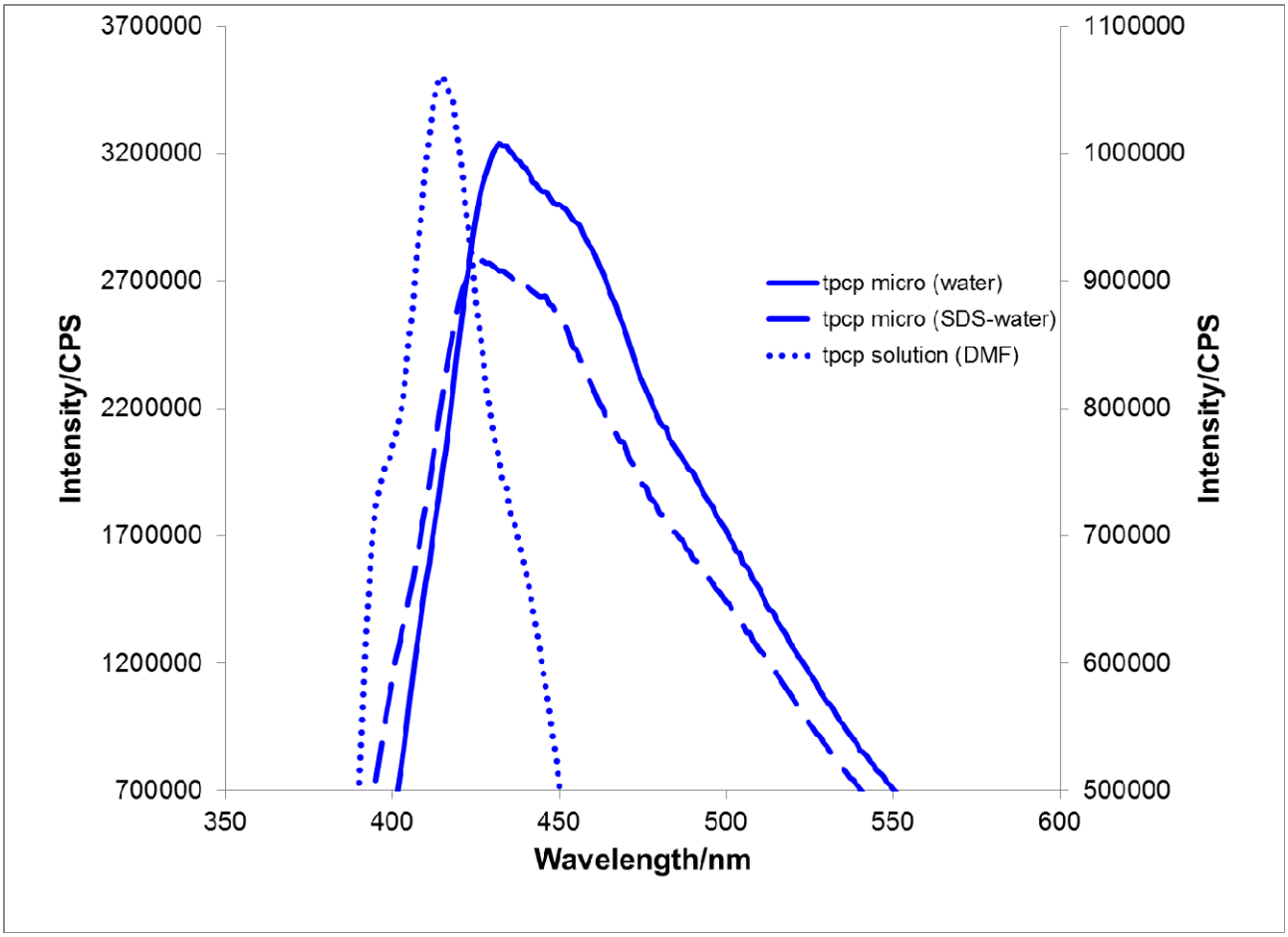

Figure S-19: Emission spectra of tpcp microcrystalline suspensions compared to tpcp in solution (solution result is plotted on the secondary axis).

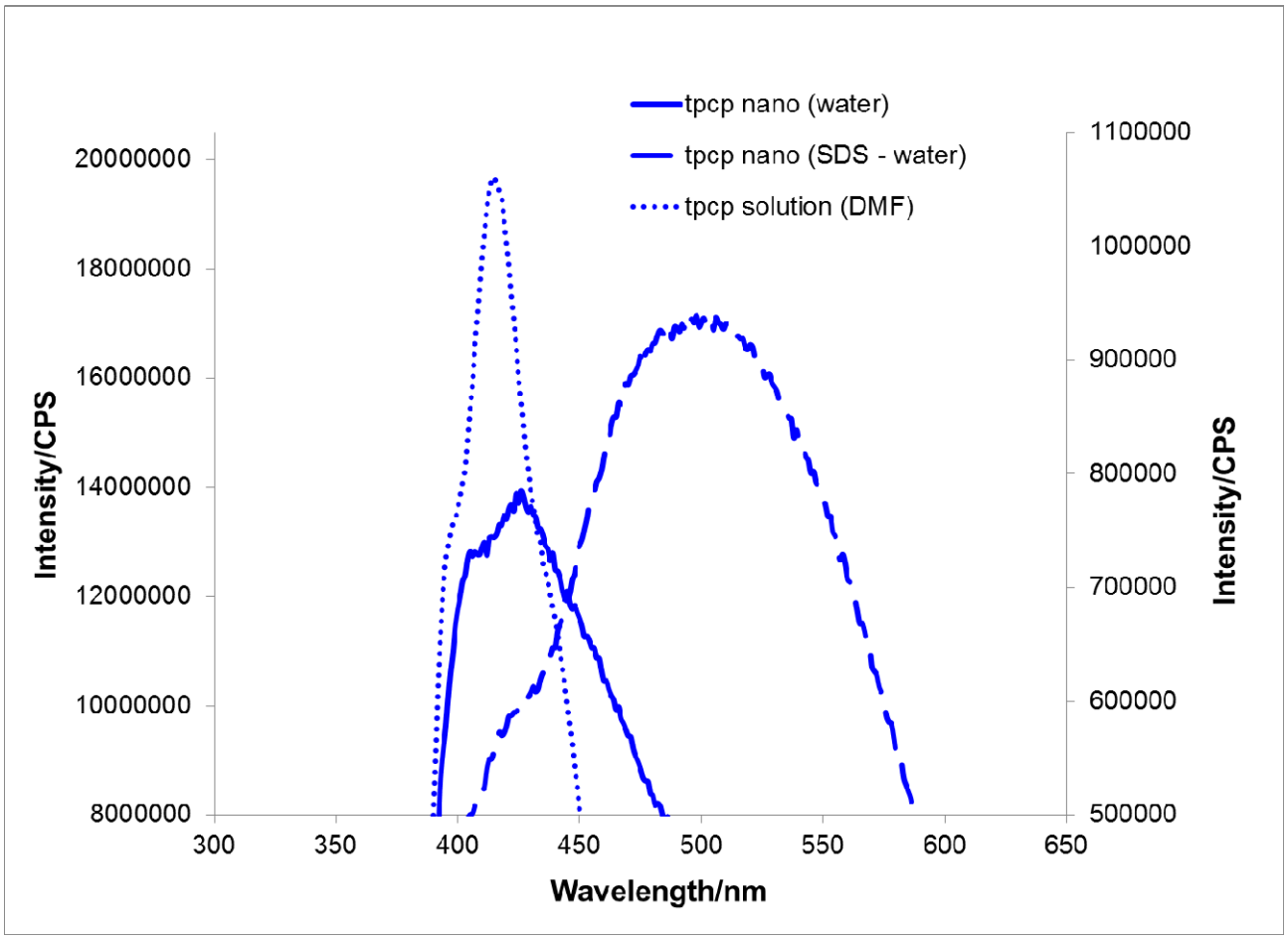

Figure S-20: Emission spectra of tpcp nanocrystalline suspensions compared to tpcp in solution (solution result is plotted on the secondary axis).

SEM Micrographs:

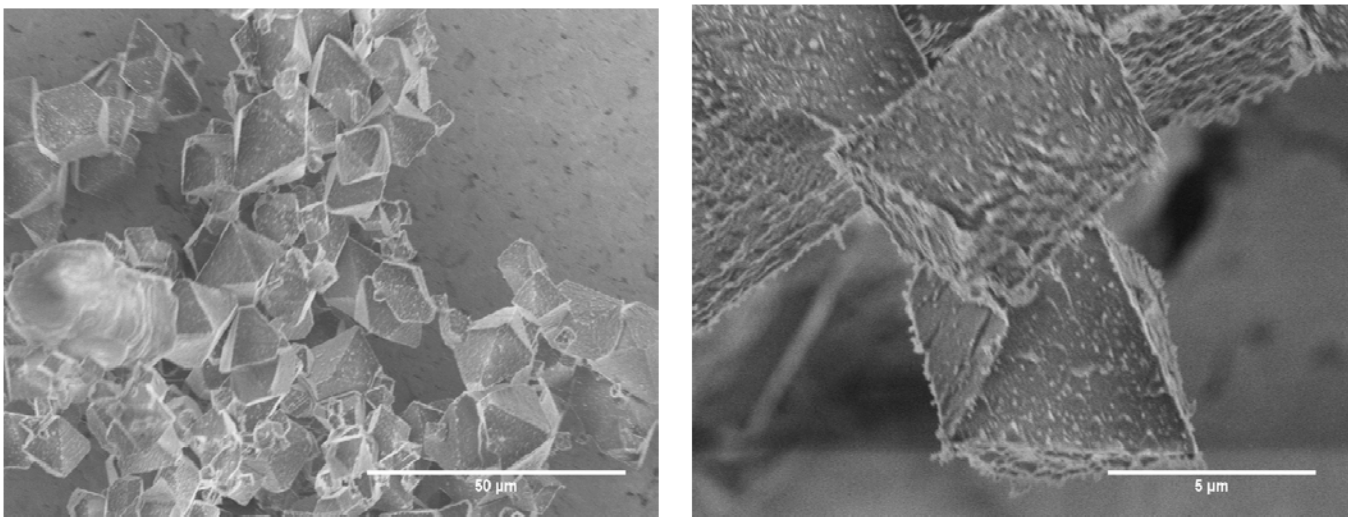

Figure S-21: SEM micrographs of pCp microcrystals from reprecipitation.

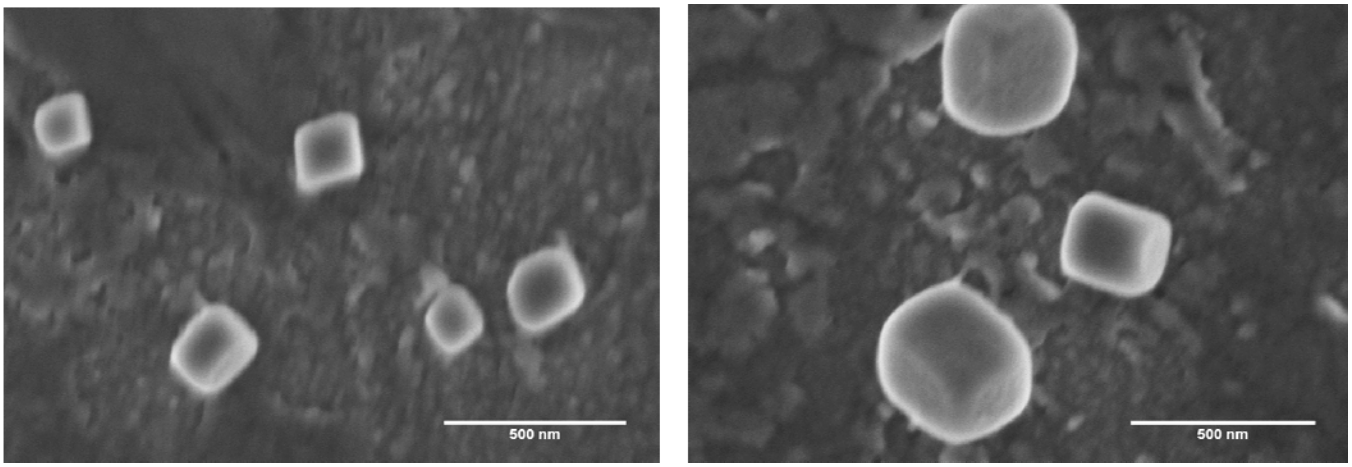

Figure S-22: SEM micrographs of pCp nanocrystals generated using sonochemistry.

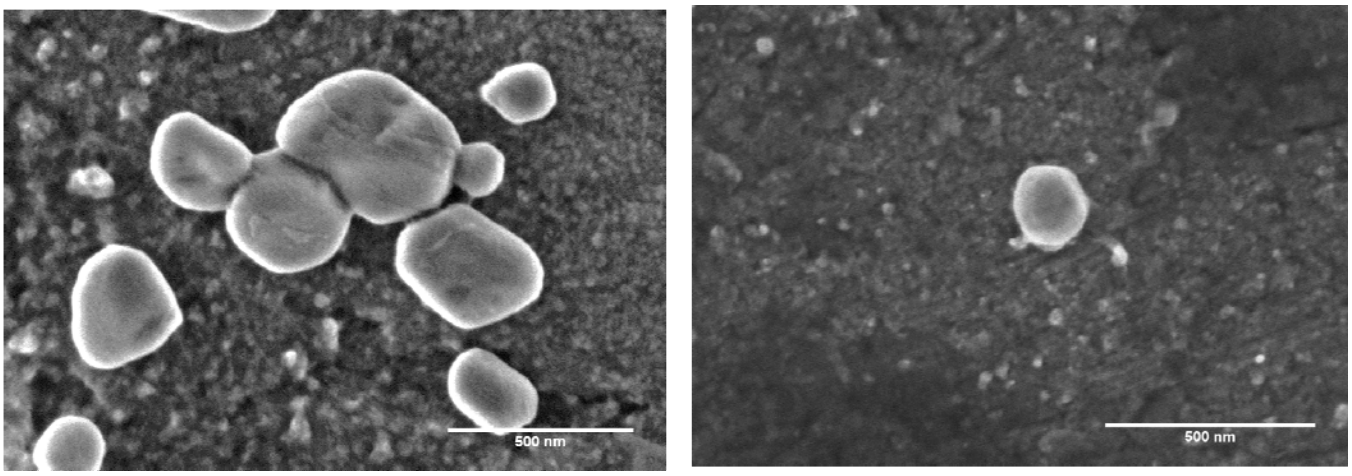

Figure S-23: SEM micrographs of pCp nanocrystals generated using sonochemistry with the addition of SDS.

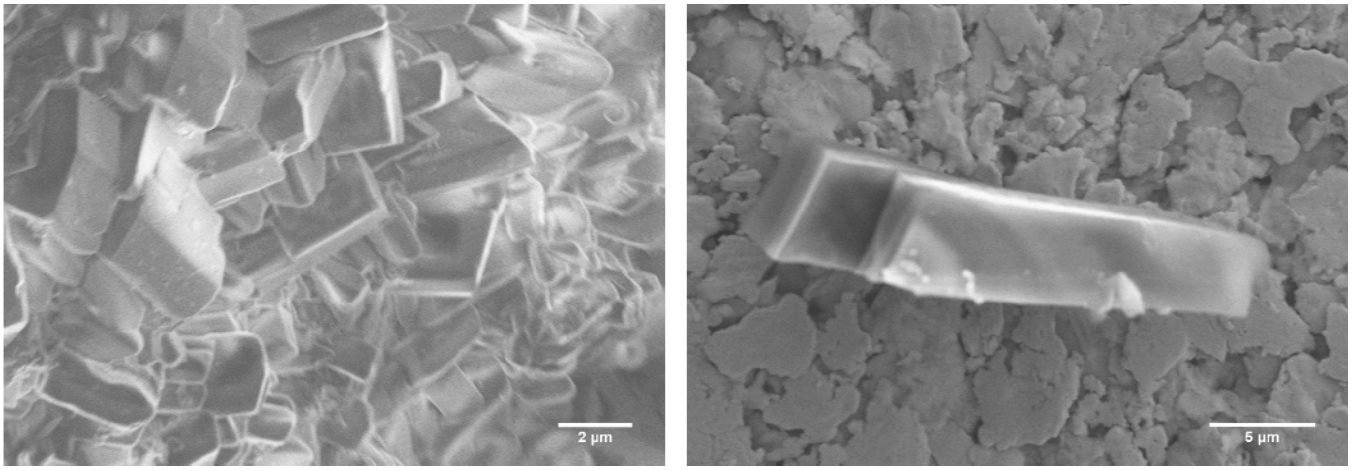

Figure S-24: SEM micrographs of tpcp microcrystals from reprecipitation.

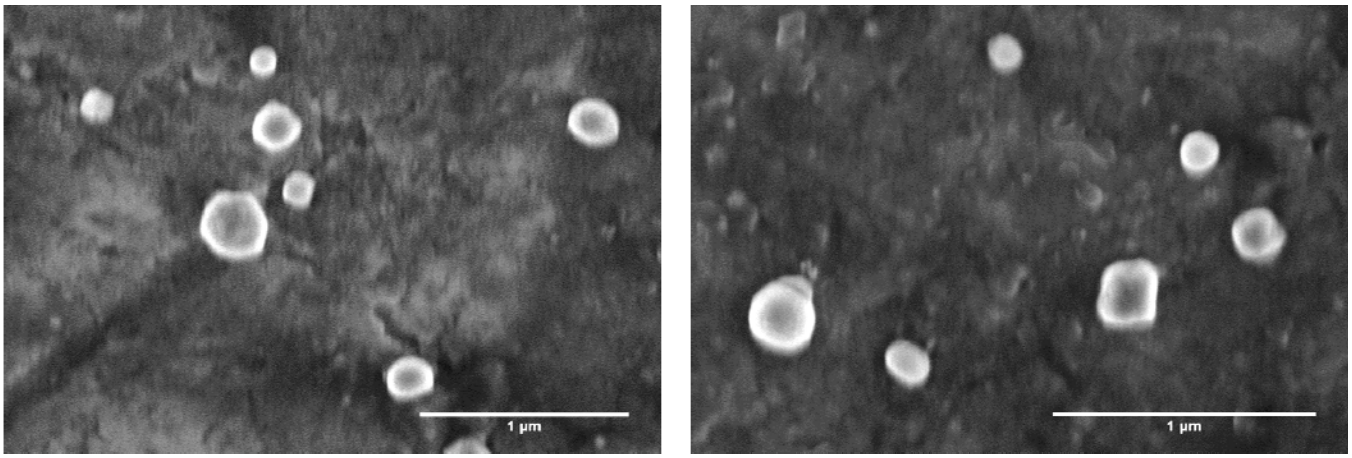

Figure S-25: SEM micrographs of tpcp nanocrystals generated using sonochemistry.

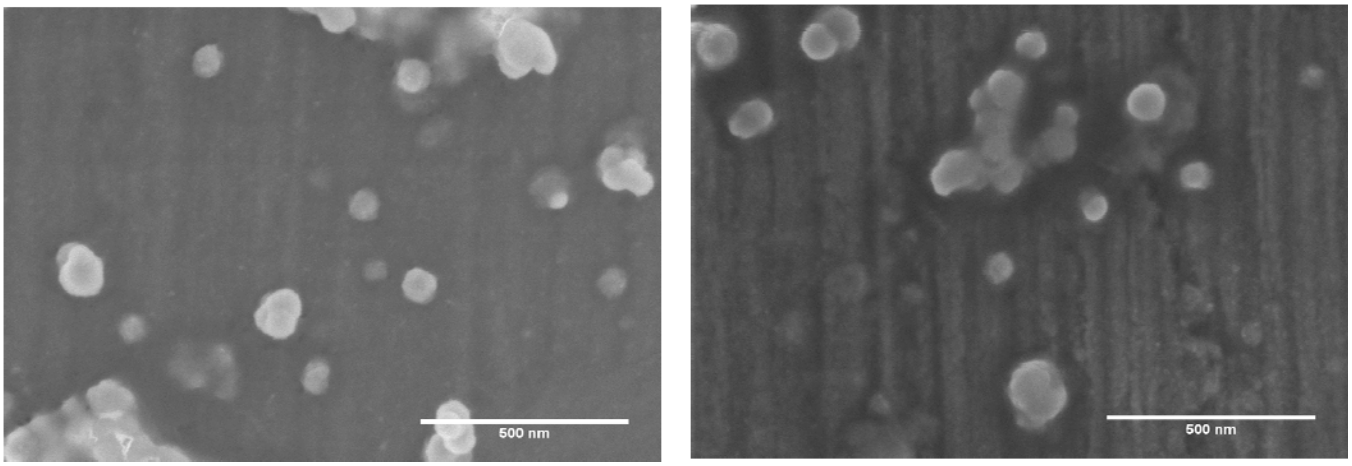

Figure S-26: SEM micrographs of tpcp nanocrystals generated using sonochemistry with the addition of SDS.