

Supplementary Information

Rational Design of New Biocompatible Near-Infrared Conjugated Polymer Nanoparticles for Biomedical Applications

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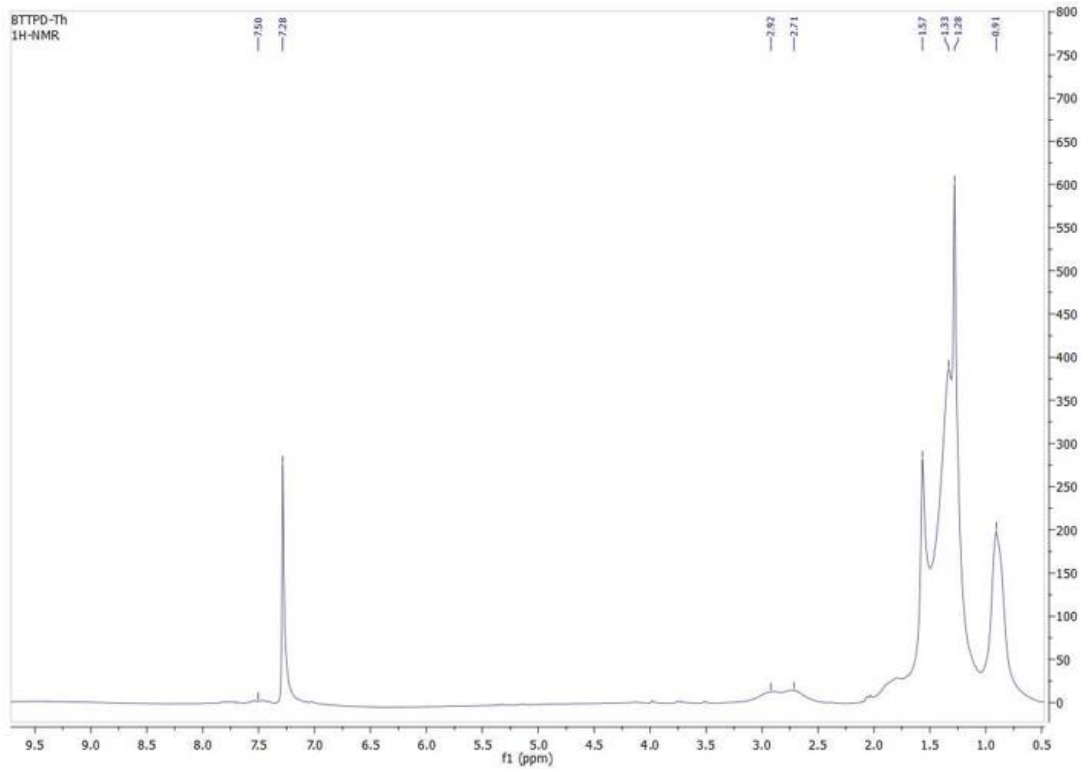
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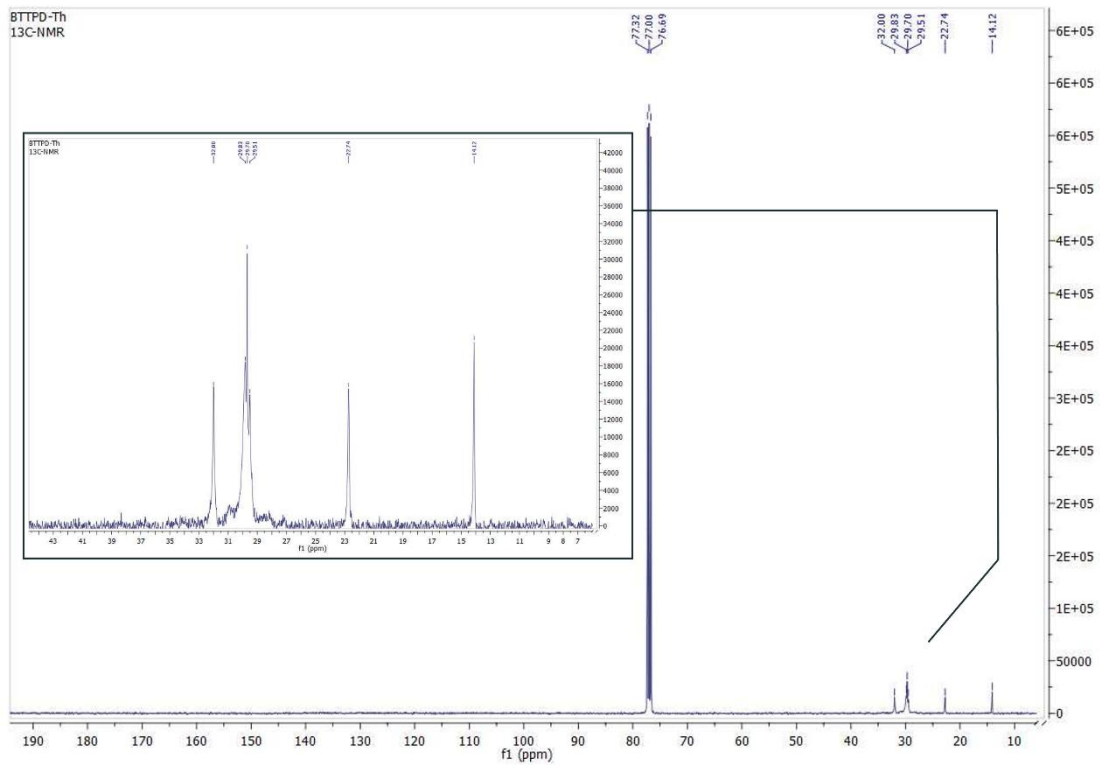
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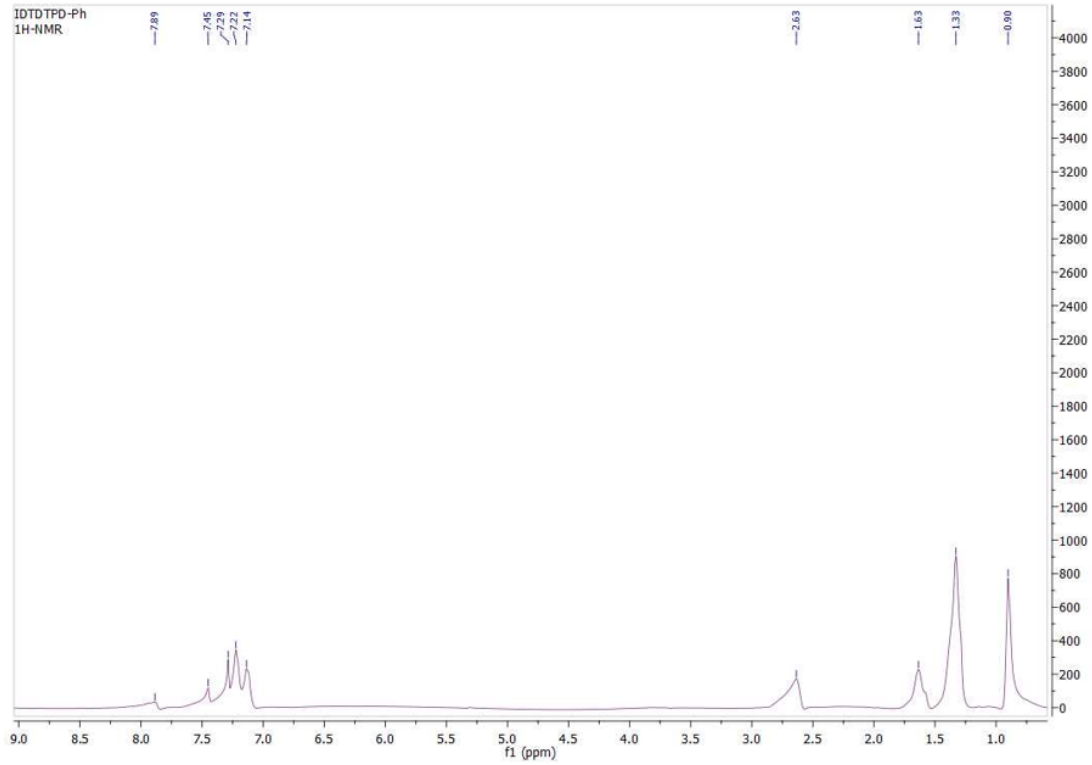
Corresponding author email address: chochos@eie.gr



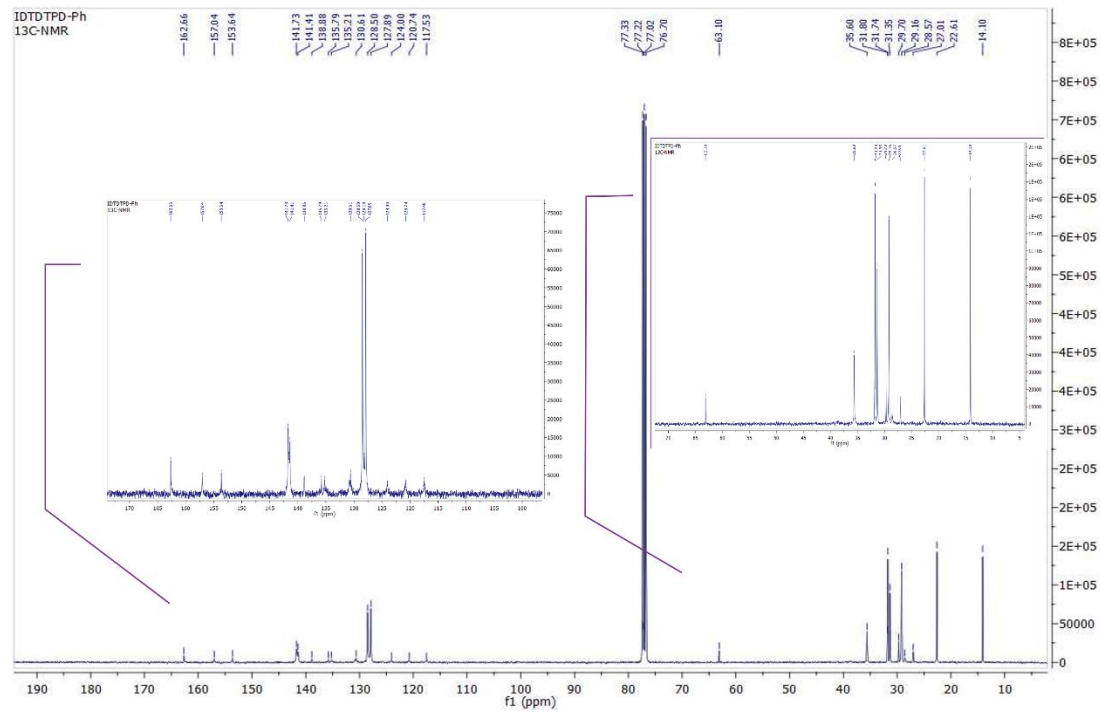
S2: $^1\text{H-NMR}$ of CP1 in CDCl_3



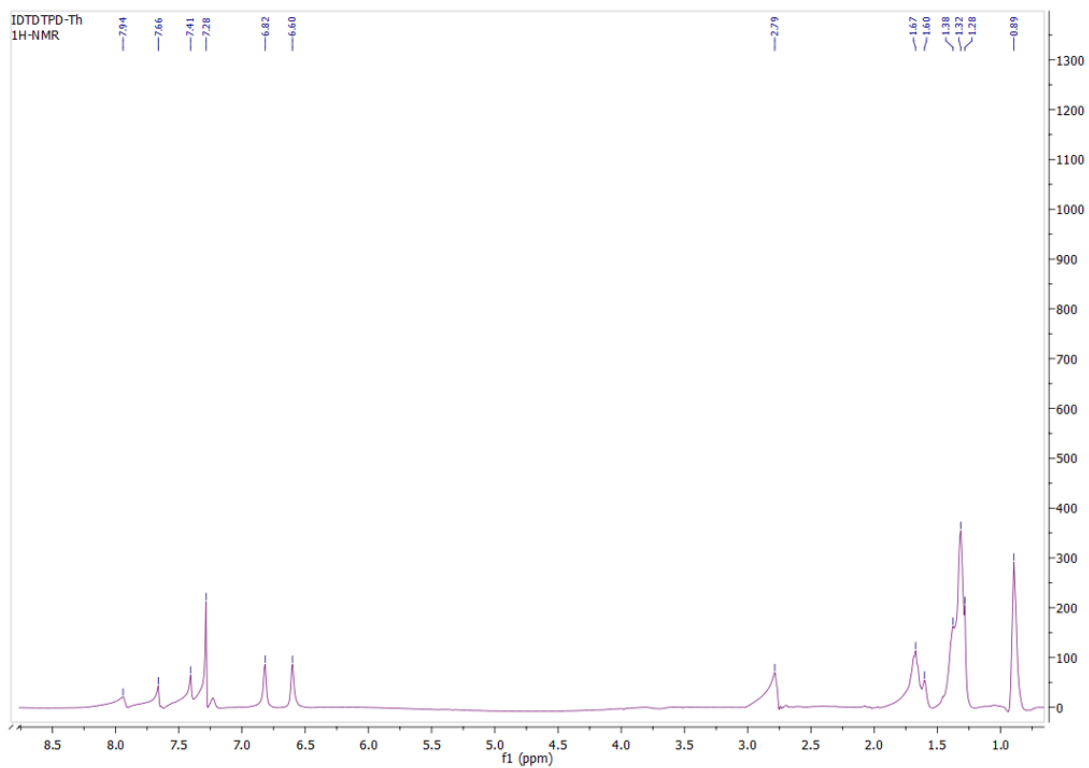
S3: $^{13}\text{C-NMR}$ of CP1 in CDCl_3



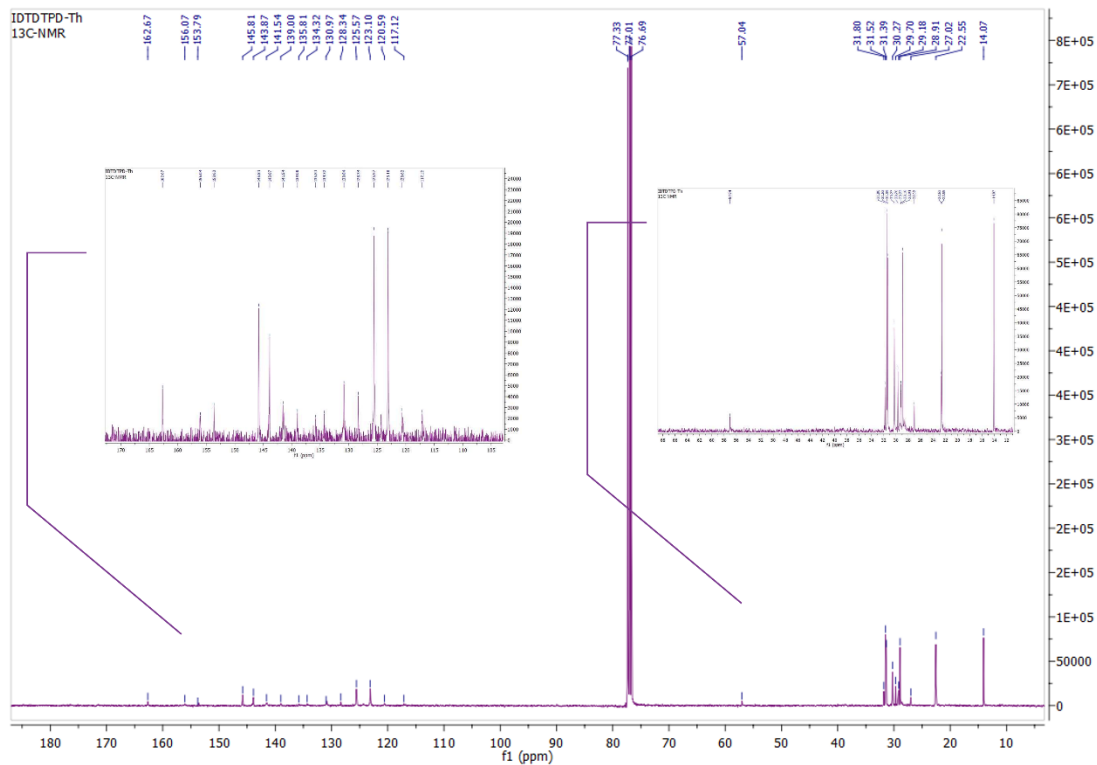
S4: $^1\text{H-NMR}$ of CP2 in CDCl_3



S5: $^{13}\text{C-NMR}$ of CP2 in CDCl_3

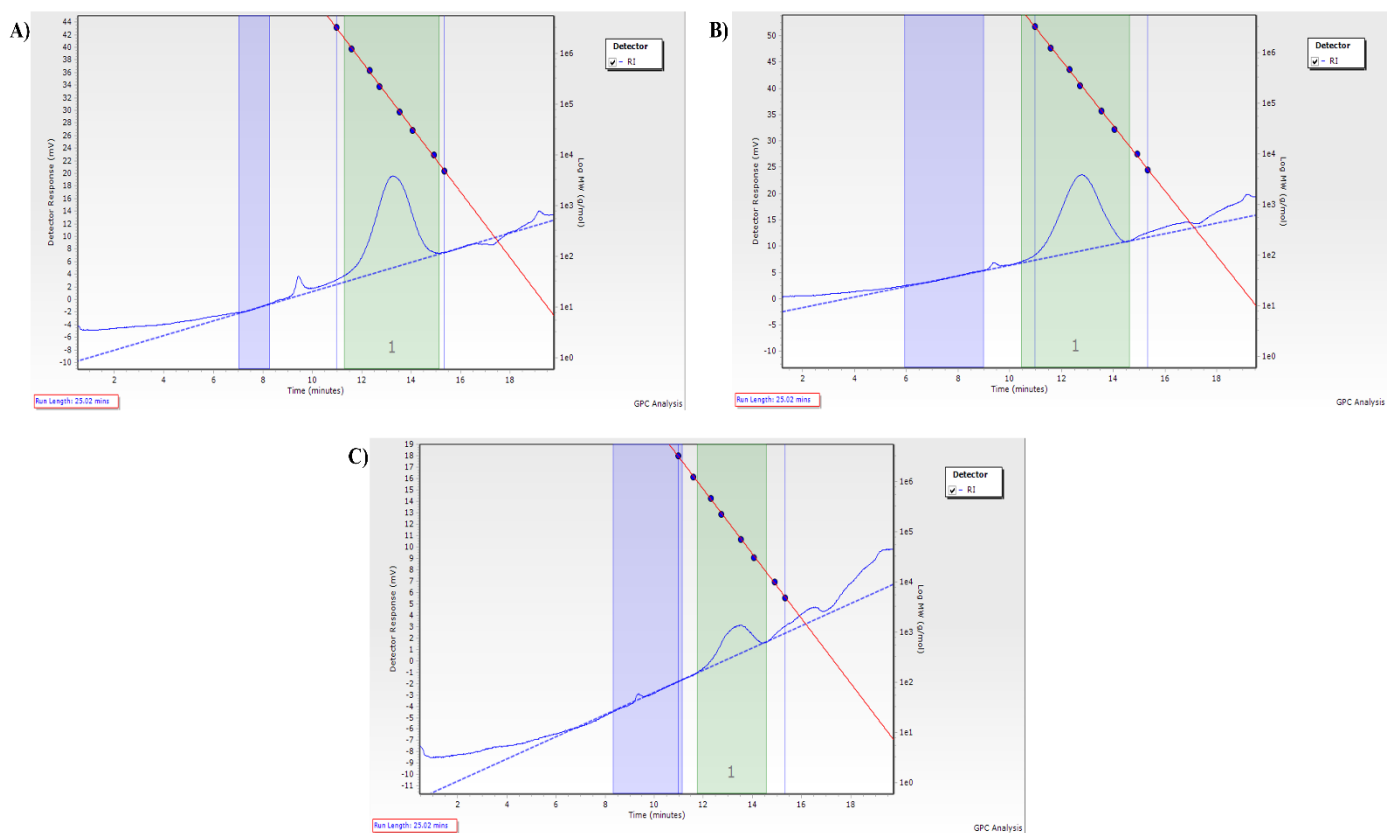


S6: ¹H-NMR of CP3 in CDCl₃

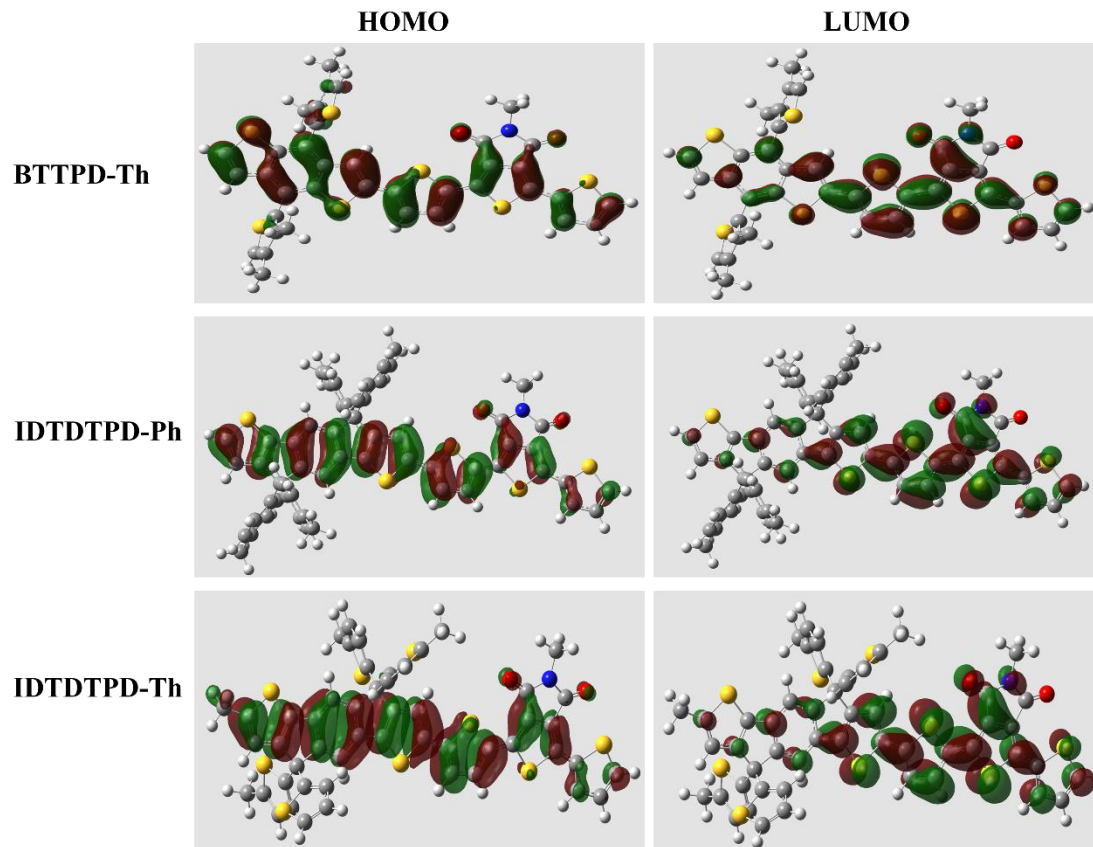


S7: ¹³C-NMR of CP3 in CDCl₃

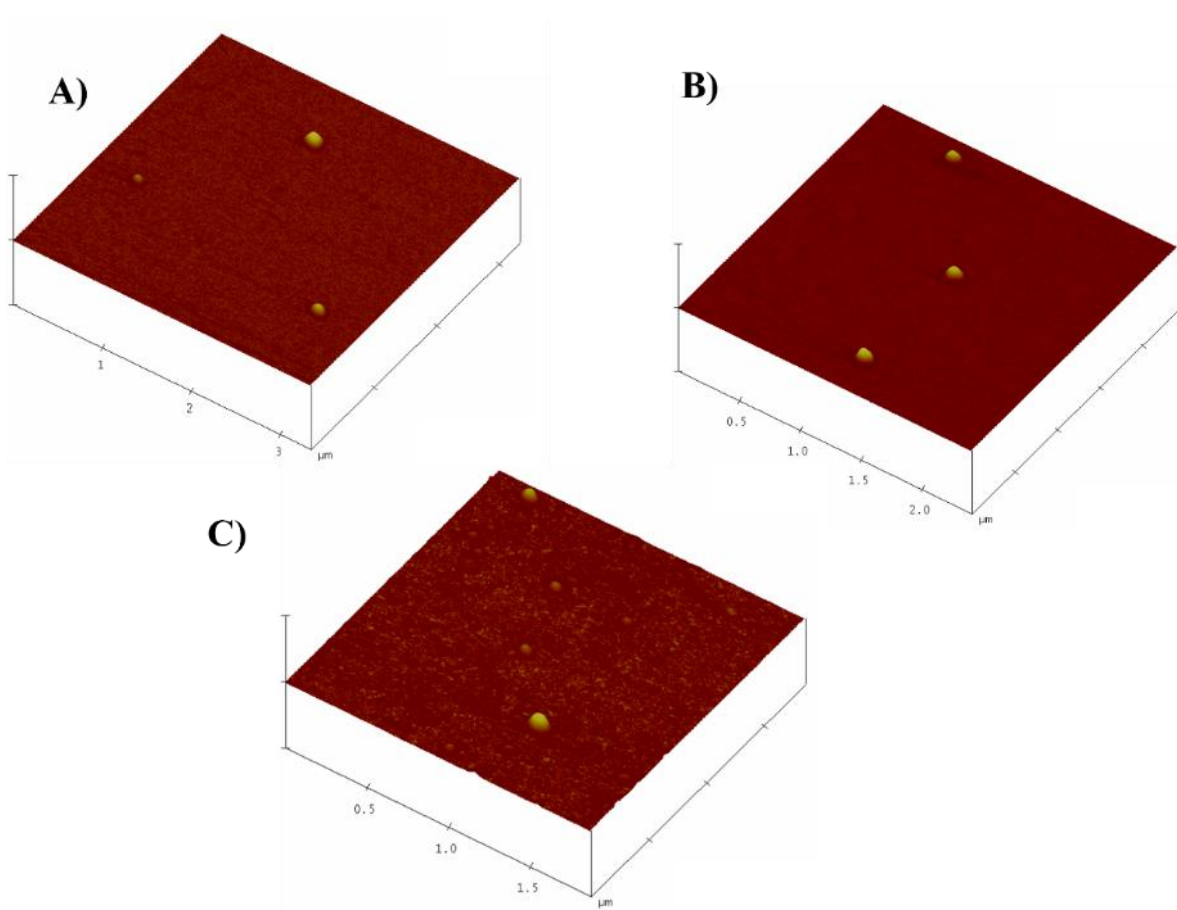
Concerning the $^1\text{H-NMR}$ spectra presented in Figures S4 and S6 for polymers CP2 and CP3, we made several efforts to optimize the shimming process. However, the improvement was not as significant as anticipated. We believe that this limitation arises from the low quality of field homogenization, which is likely influenced by the high molecular weight of the polymers. The latter may promote partial aggregation of the polymer chains in chloroform solution, thereby affecting the magnetic field homogeneity during measurement. In addition, the referencing was done with the known CDCl_3 peak position (7.26 ppm).



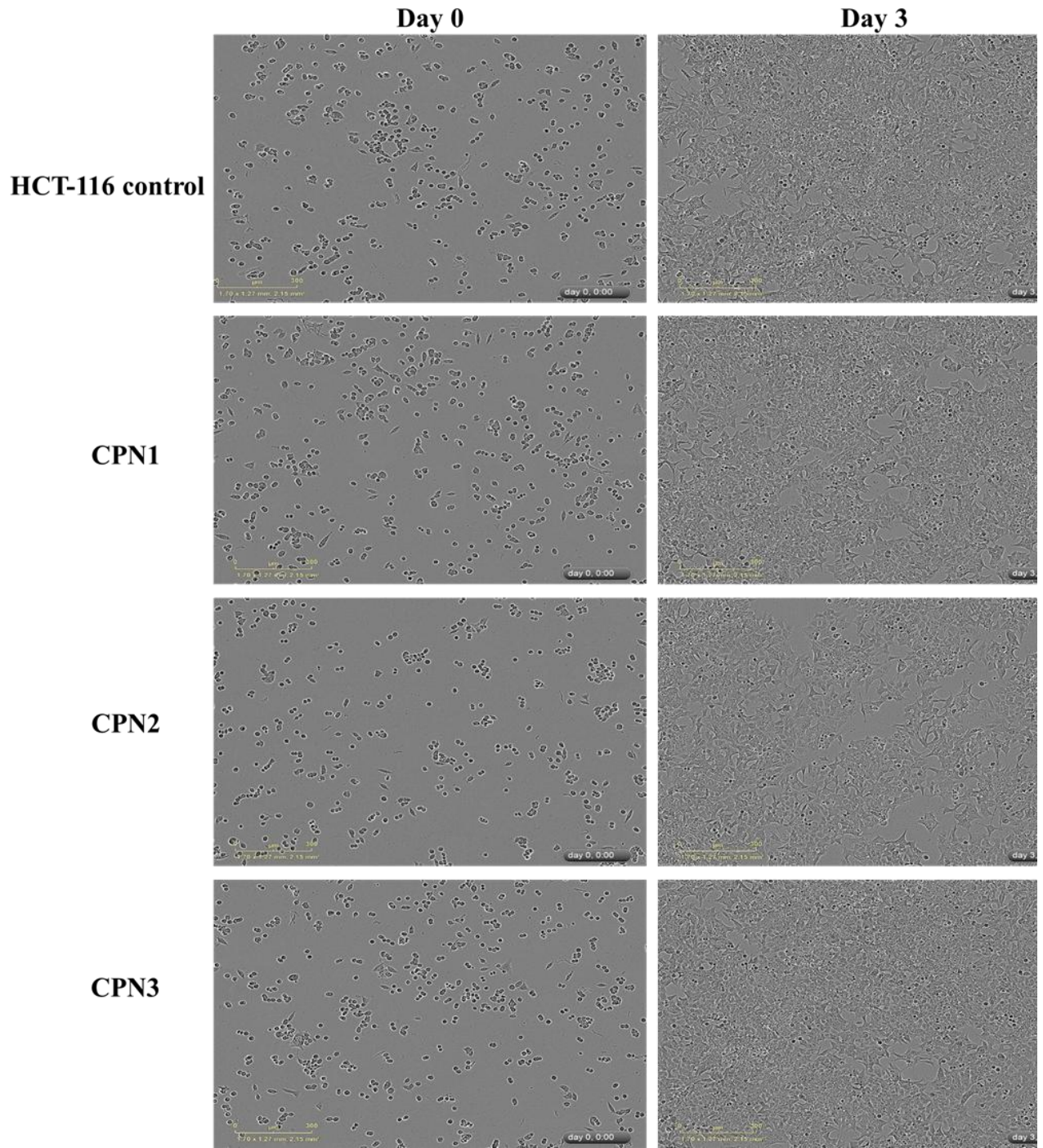
S8: Gel Permeation Chromatographs of **A)** CP1, **B)** CP2 and **C)** CP3.



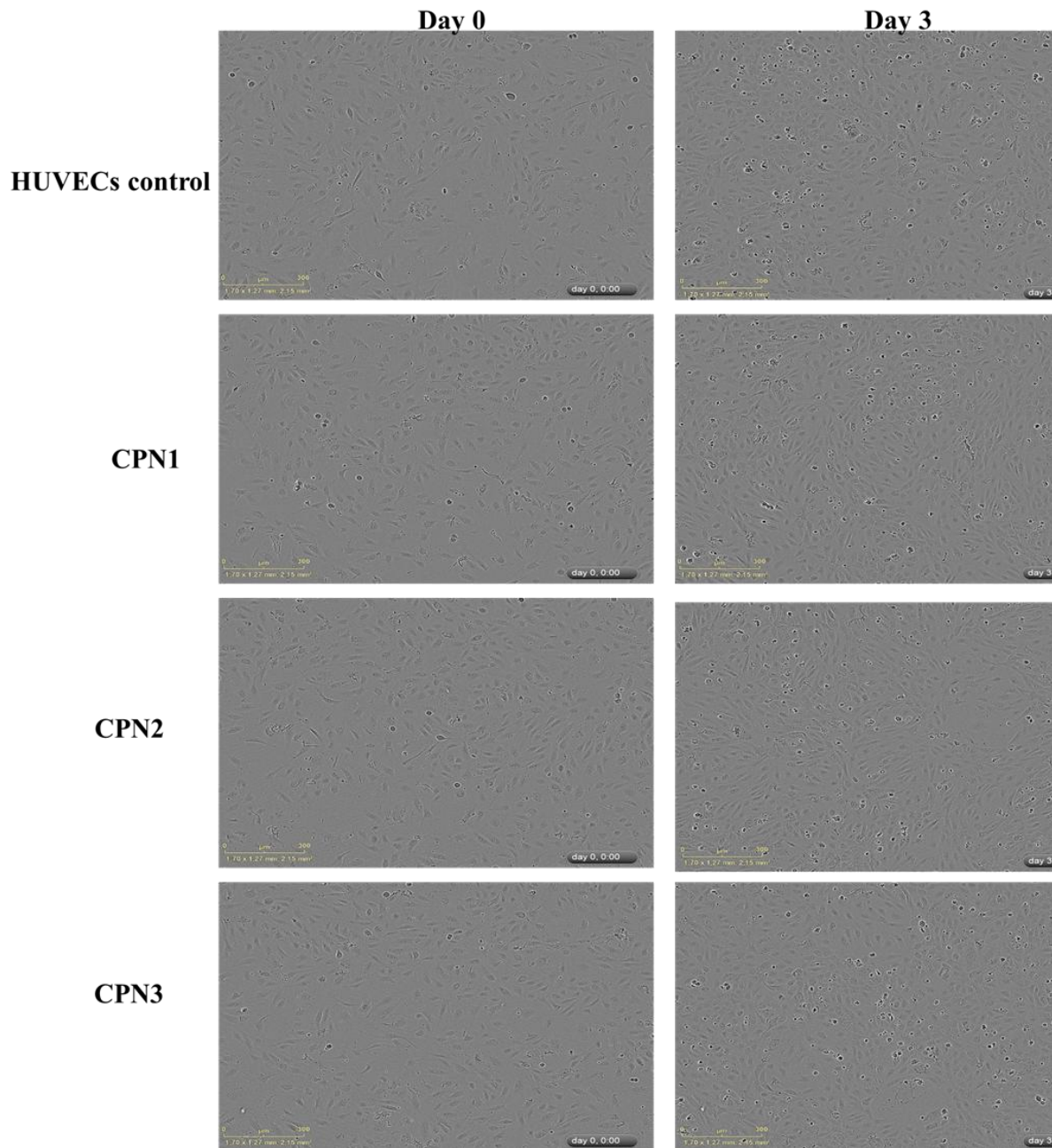
S9: HOMO-LUMO of each polymeric structure calculated by TD-DFT-B3LYP/6-31+G in Gaussian 09W.



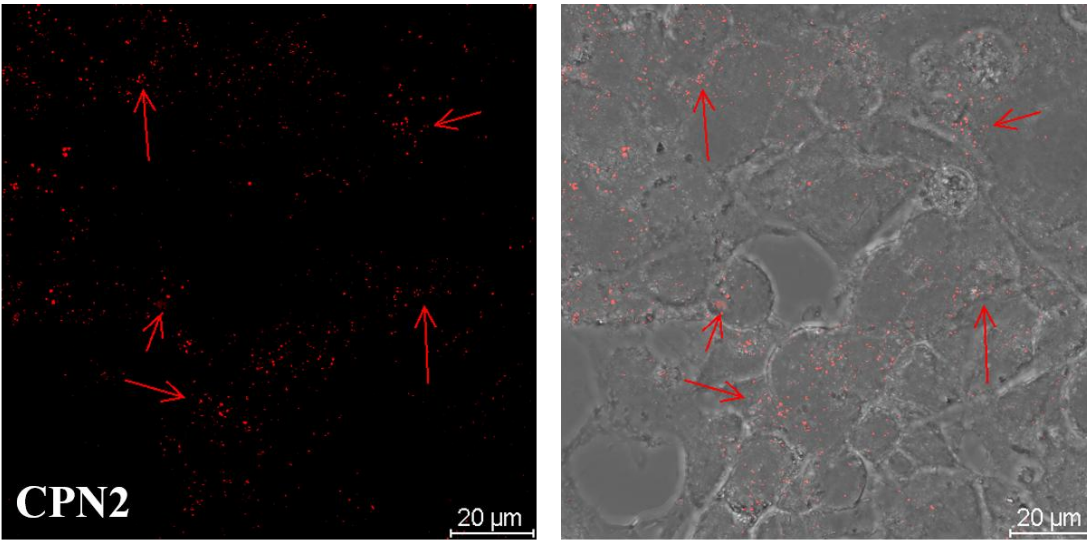
S10. AFM 3D morphology of A) CPN1, B) CPN2 and C) CPN3.



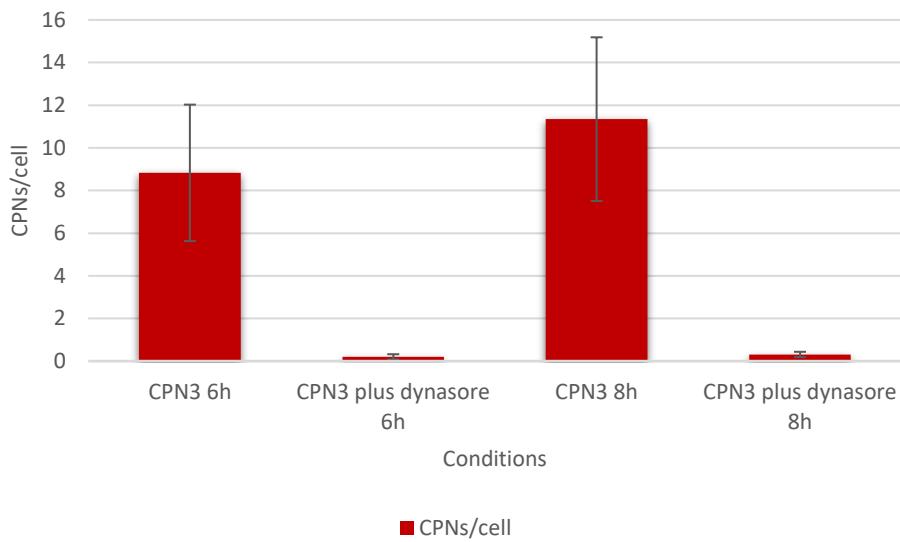
S11: IncuCyte photos of HCT-116 cells on day 0 and 3 incubated with CPNs at a concentration of 0.5µg/ml.



S12: IncuCyte photos of HUVEC cells on day 0 and day 3 incubated with CPNs at a concentration of 0.5μg/ml.



S13: Confocal fluorescence microscopy images in maximum projection pictures from 24h incubation of CPN2 in HCT-116 cells exhibited a tendency to accumulate at areas of cell-cell contact and on top of the cells. Representative images after confocal microscopy are presented (n=3). Scale bar: 20μm



S14: Quantification of NPs (CPN3) per cell when incubated with and without dynasore for 6 and 8h for determination of the dynamin inhibition. (n=3)