Supporting Information

S-nitrosated polypropylene sulfide nanoparticles for thiol-dependent transnitrosation and toxicity against adult female filarial worms

*Alex Schudel, Timothy Kassis, J. Brandon Dixon, and Susan N. Thomas**

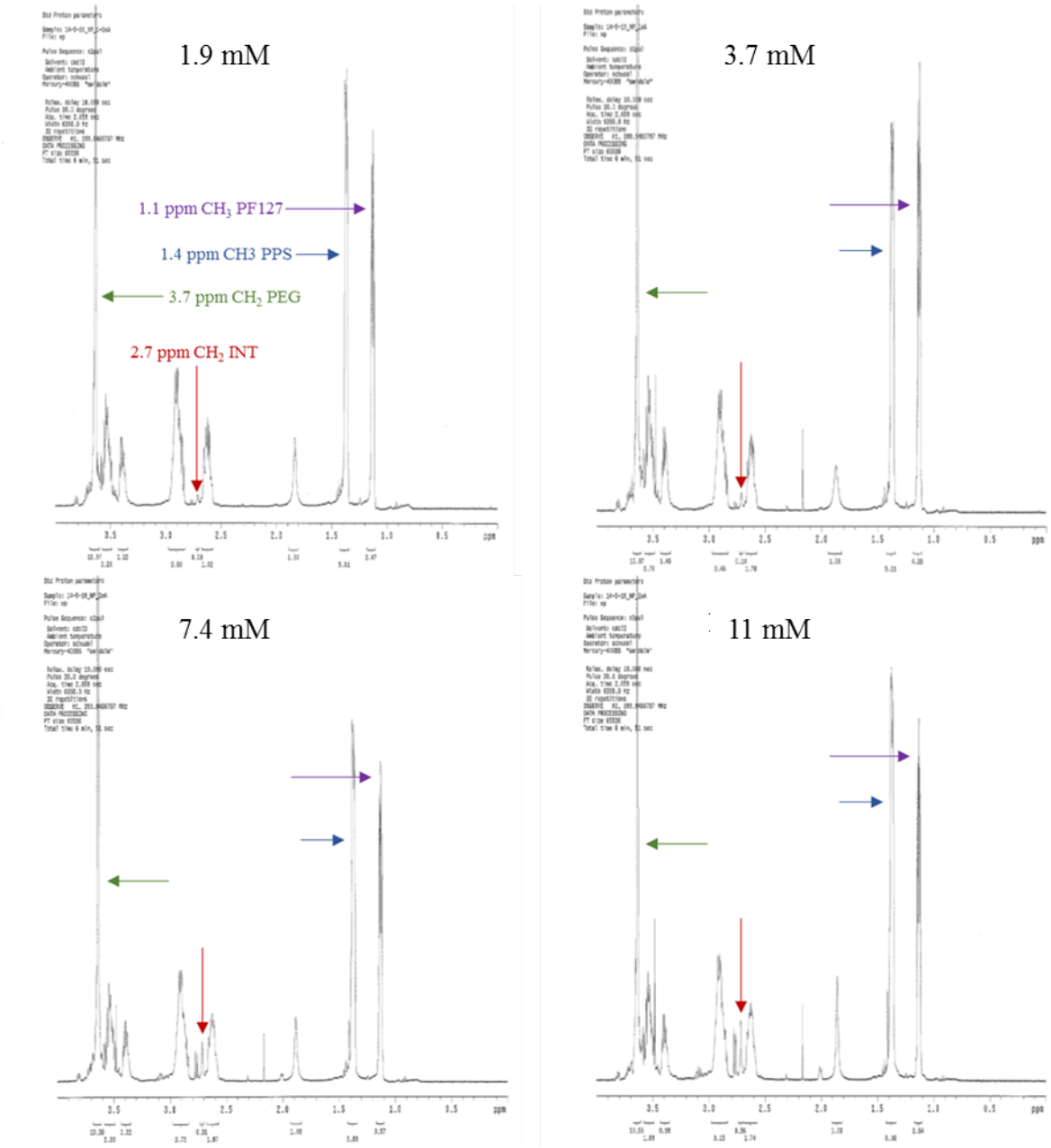

Figure S1. ^{1}H NMR data of lyophilized NP solution. The following have been assigned according to van der Vlies et al. as the functional group peaks: 1.1 ppm – CH_3 Pluronic (-CH_2-$CH(CH_3)$-O-), 1.4 ppm – CH_3 poly(propylene sulfide) (-CH_2-$CH(CH_3)$-S-), 2.7 ppm – CH_2 initiator (-C-CH_2-S-), and 3.7 ppm – CH_2 PEG (-CH_2-CH_2-O-).[1] The integral of each peak is displayed under the axis. Normalizing each integral to the number of H atoms (3, 3, 2, and 4 respectively) and multiplying by the weight of the functional group allows for the mass

percentage of NP solution and degree of polymerization to be determined. Pluronic is taken as the combination of the $–CH_2-CH(CH_3)-O-$ and $–CH_2-CH_2-O-$ fragments.

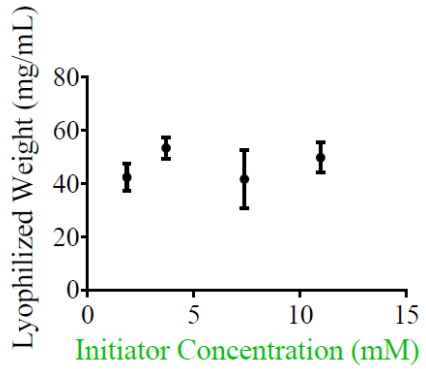

Figure S2. Lyophilization data showing that the total NP polymer weight/mL is unaffected by initiator concentration. 100 uL samples of NP solution synthesized under different initiator concentrations were lyophilized and the weight percent of polymer was determined.

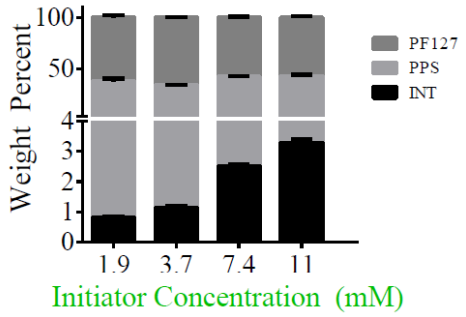

Figure S3. Increasing initiator concentration during polymerization results in increasing the weight percent of initiator incorporated into the NP solution. NP were synthesized under different initiator concentrations and lyophilized. The weight percent of each constituent component, Pluronic F127, poly(propylene sulfide), and initiator were determined using ^{1}H NMR (Figure S1).

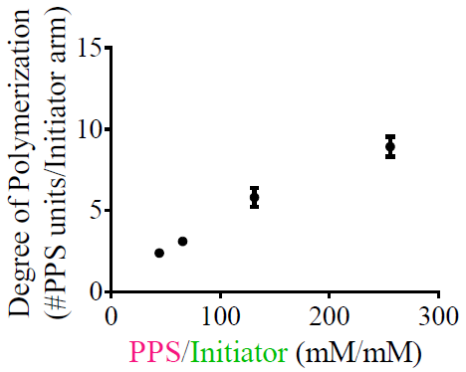

Figure S4. Degree of polymerization of propylene sulfide increases as molar ratio of propylene sulfide to initiator is increased. NP were synthesized with different initiator concentrations, lyophilized, and analyzed via ^{1}H NMR (Figure S1). Using specific peak assignments and normalizing each peak to the number of hydrogen atoms per repeat group, the total number of poly(propylene sulfide) groups and initiator groups were determined.

Taking the ratio of poly(propylene sulfide) groups to initiator groups and dividing by the number of arms per initiators (four), the number of poly(propylene sulfide) repeats per initiator and the degree of polymerization were determined.

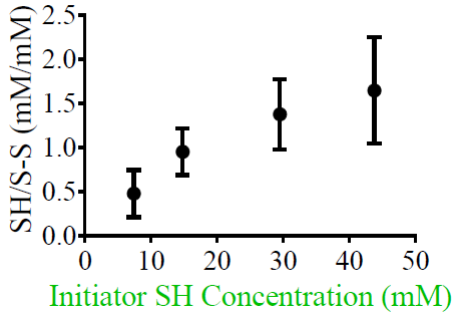

Figure S5. The ratio of thiol to calculated disulfide bond concentration increases with increasing initiator thiol concentration. NP were synthesized with different initiator concentrations. Assuming no initiator loss, the ratio between the measured final free thiol concentration and remaining disulfides as determined by the added amount of initiator thiols was determined.

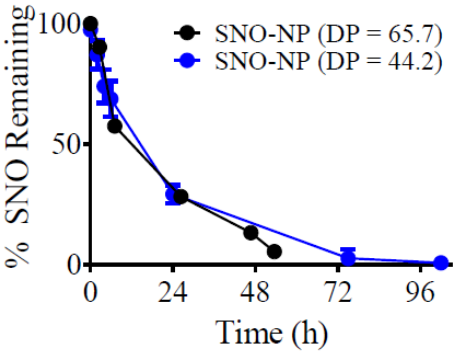

Figure S6. Degradation of SNO-NP at 37°C is unaffected by degree of polymerization. SNO-NP synthesized with 7.4 and 11 mM initiator, corresponding to degrees of polymerization (DP) of 65.7 and 44.2, respectively, showed similar rates of NO release at 37°C.

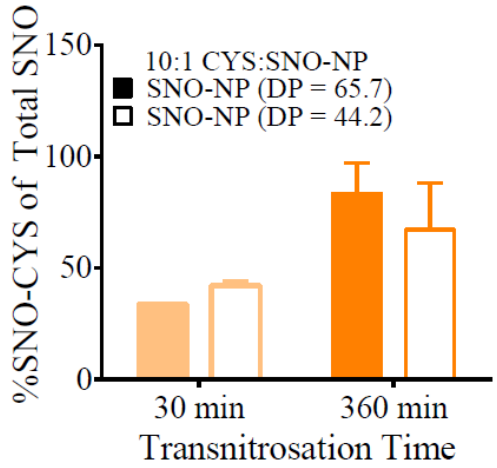

Figure S7. The extent of transnitrosation of SNO-NP to CYS at 37°C is unaffected by degree of polymerization. SNO-NP synthesized with 7.4 and 11 mM initiator, corresponding to

degrees of polymerization (DP) of 65.7 and 44.2, respectively, showed similar extents of transnitrosation to CYS over time at 37^{o}C.

References

[1] A. J. van der Vlies, C. P. O'Neil, U. Hasegawa, N. Hammond, J. A. Hubbell, *Bioconjugate. Chem.* **2010**, *21*, 653.