pH Tunable and Divalent Metal Ion Tolerant Polymer Lipid Nanodiscs

*Thirupathi Ravula,[†] Nathaniel Z. Hardin,[†] Sudheer Kumar Ramadugu and Ayyalusamy Ramamoorthy**

Biophysics Program and Department of Chemistry, The University of Michigan, Ann Arbor, MI 48109-1055, USA.

Electronic supplementary information

Fourier-Transform Infrared (FT-IR) Spectroscopy:

The FT-IR spectra from 4000 cm^{-1} to 800 cm^{-1} were recorded using a Thermos scientific ATR-FTIR instrument. Water was removed by lyophilization from each of the samples before recording the spectrum.

^{31}P CSA: As shown in the main text, the parallel edge at 25.5 ppm and the perpendicular edge at -26.43 ppm to result in a CSA span for the ^{31}P powder patter to be ~50 ppm (Figure 3E in the main text, pH 6.0). On the other hand, the sample prepared at pH=8.5 exhibited the parallel edge at 27.2 ppm and the perpendicular edge at -21.4 ppm to result in a similar CSA span for the ^{31}P powder patter to be ~50 ppm (Figure 3F in the main text, pH=8.5).

Dynamic Light Scattering (DLS): All DLS experiments were performed using Wyatt Technology® DynaPro® NanoStar® using a 1 µL quartz MicroCuvette.

Transmission Electron Microscopy (TEM): All TEM micrographs were obtained using a Technai® T-20® machine (FEI®, Netherlands) with a 80 kV operating voltage. A dilute solution was dropped on the carbon-coated copper grid and dried overnight at room temperature in a desiccator before using in the experiments.

Measuring the effect of divalent metal ions on SMA-EA nanodiscs: Nanodiscs were titrated using 3.3 M $CaCl_2$ or 5 M $MgCl_2$ in 10 mM citric acid buffer or 10 mM HEPES in low or high pH condition, respectively.

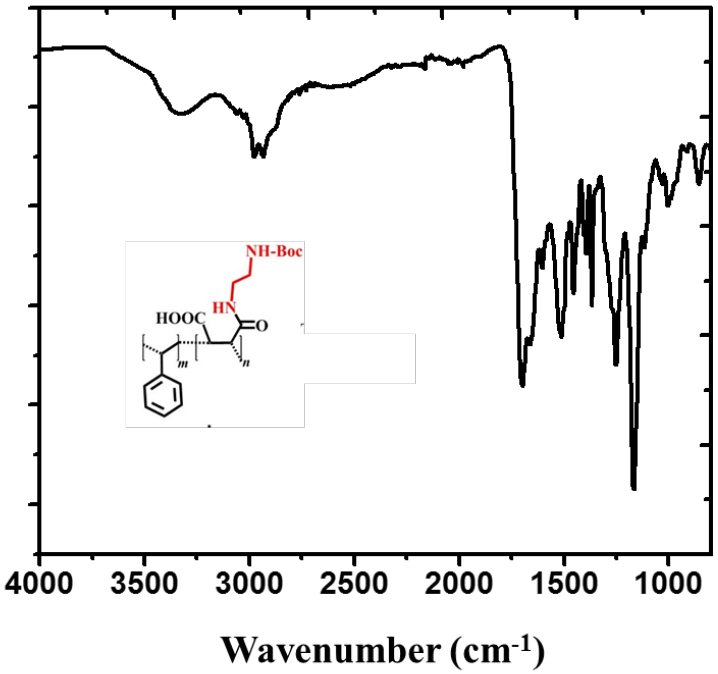

Figure S1: FTIR spectrum of **N-Boc-SMA-ED**.

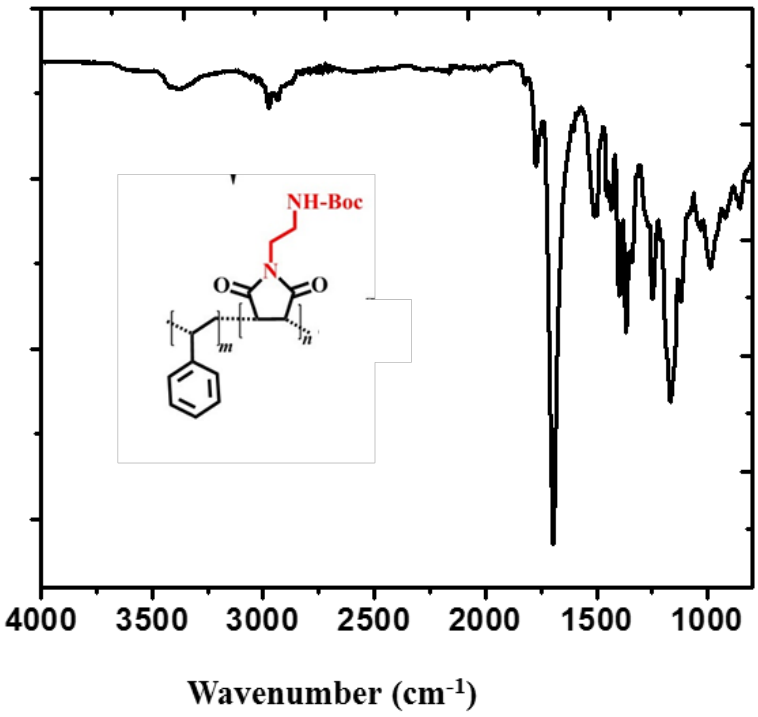

Figure S2: FTIR spectrum of **N-Boc-SMAd-A**.

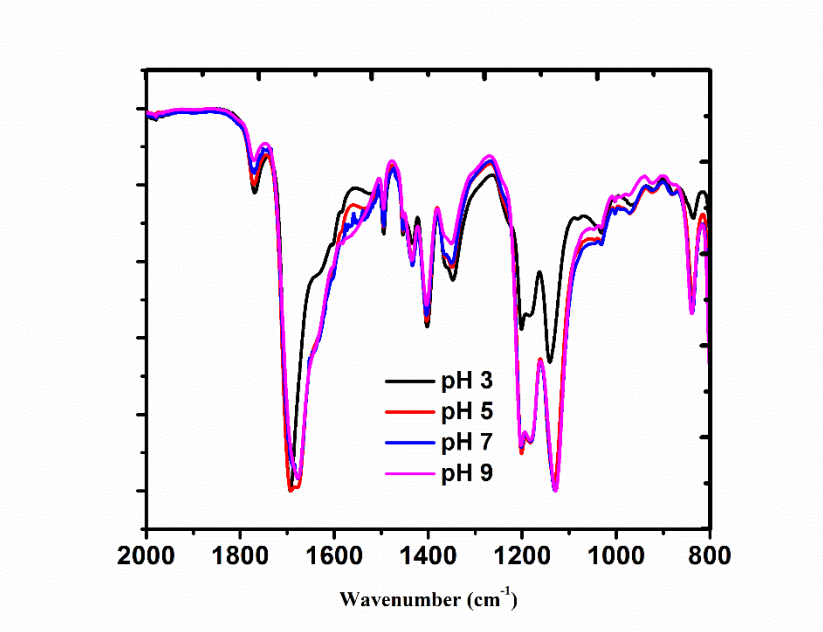

Figure S3: FT-IR spectra of SMAd-A at different pH showing the absence of carboxylate peak under basic pH. This observation confirms the successful formation of the maleimide group.

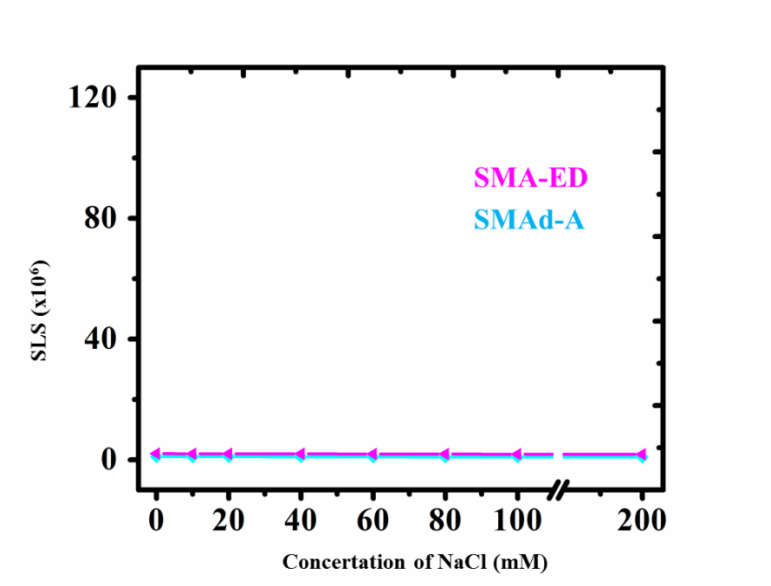

Figure S4: SLS profiles of nanodiscs made up of SMA-ED or SMAd-A showing stability in the presence of indicated NaCl concentration.