

## Supplementary Materials

# Application of Cyclized Polyacrylonitrile for Ultrafiltration Membrane Fouling Mitigation

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**Table S1.** Calculated enthalpies, entropies, and Gibbs free energies (in Hartree) for optimized equilibrium model structures (H, S, and G, respectively).

Model Structure	H	G	S
PAI	0.319999	0.218247	214.155
m-PAN	0.445113	0.371262	155.434
A	0.752333	0.594360	332.484
B	0.751947	0.598635	322.672
C	0.748442	0.593602	325.889
D	0.738990	0.588033	317.716