# Supporting Information

# The Challenges of Using COSMO-RS To Describe Polymer Solution Behavior

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## S.1 – σ-profiles of PEG400 conformers and comparison to PPG400 conformer

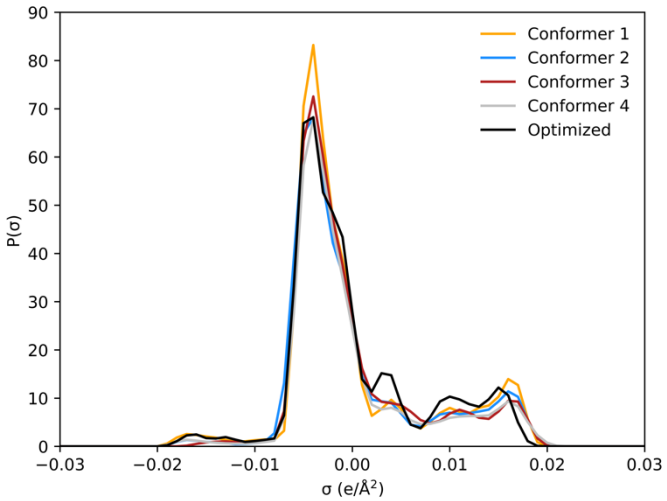


**Figure S1** – σ-profiles of the conformers used in the COSMO-RS calculations shown in Figure 2 of the article. Conformers 1-4 were obtained from MD simulations and the optimized conformer corresponds to the minimum energy at the BP86/def-TZVP level of theory.

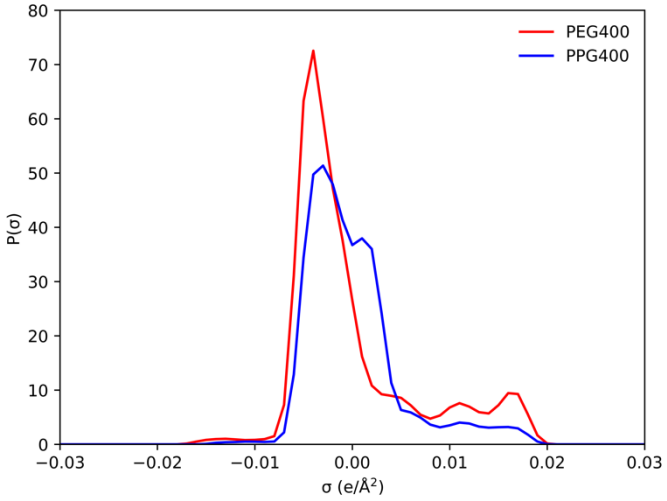


**Figure S2** – σ-profiles of PEG 400 and PPG 400 used in the calculations shown in Figure 6 of the article. The two conformers represent the most probable Rg and SASA values.

## S.2 – Equations

$$\textbf{Eq. S1: } \ln(x_i\gamma_i) = \frac{\Delta_m H_i}{R}\left(\frac{1}{T_{m,i}} - \frac{1}{T}\right)$$

Where $x_i$is the mole fraction of compound $i$, $\gamma_i$ the activity coefficient, $\Delta_m H_i$ the enthalpy of melting, $T_{m,i}$ the melting temperature and T the absolute temperature.