Supporting Information for "Vapor-liquid equilibrium simulations of hydrocarbons using molecular dynamics with long-range Lennard-Jones interactions"

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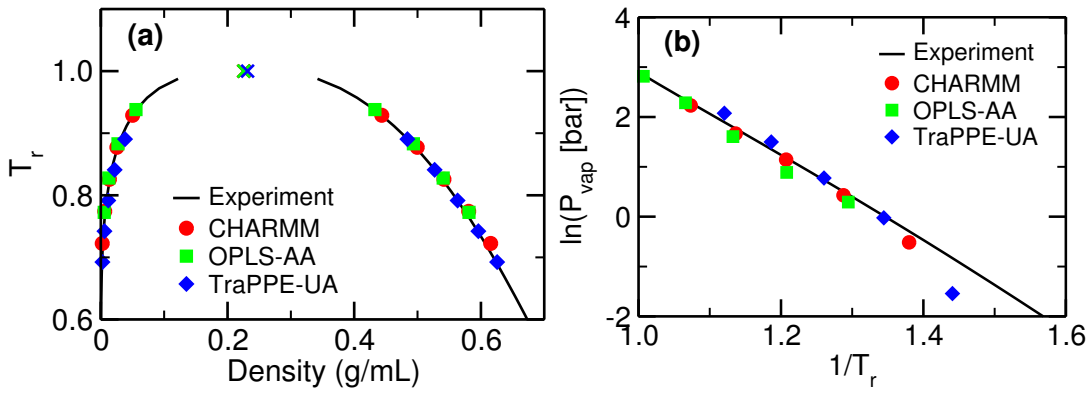

Figure S1: Vapor-liquid coexistence curves **(a)** and vapor pressures **(b)** for *n*-dodecane obtained using CHARMM, OPLS-AA, and TraPPE-UA. Experimental data obtained from the NIST webbook.[1] T_r is the temperature normalized by the corresponding T_c.

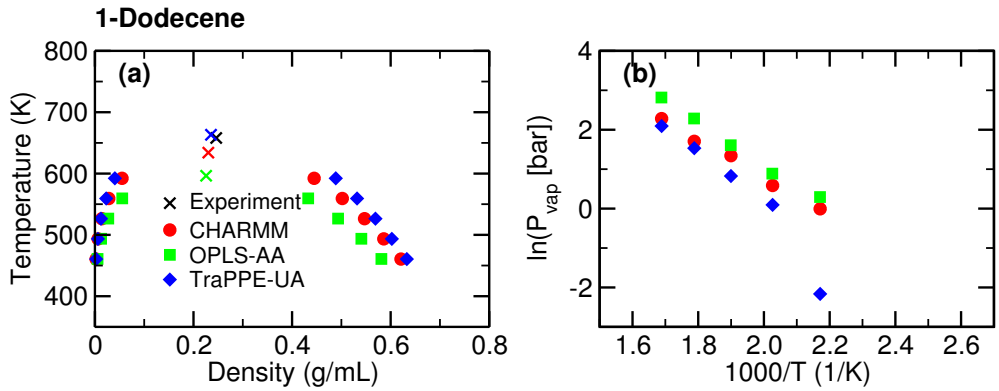

Figure S2: Vapor-liquid coexistence curves **(a)** and vapor pressures **(b)** for 1-dodecene obtained using CHARMM, OPLS-AA, and TraPPE-UA. Experimental data obtained from the NIST webbook.[1]

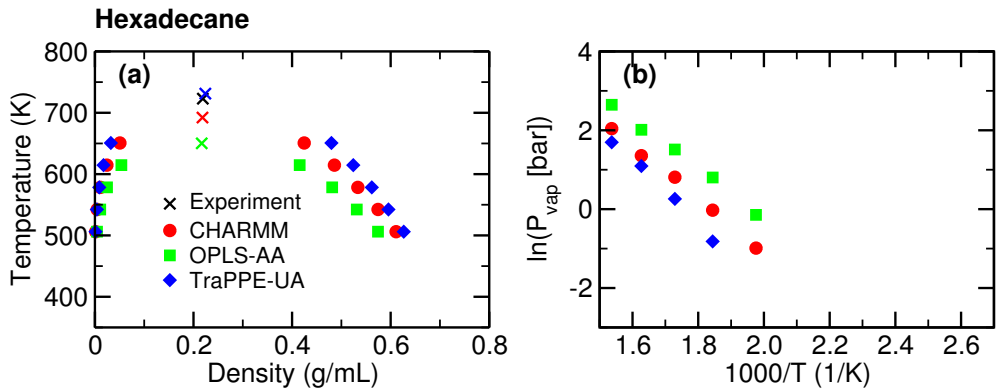

Figure S3: Vapor-liquid coexistence curves **(a)** and vapor pressures **(b)** for *n*-hexadecane obtained using CHARMM, OPLS-AA, and TraPPE-UA. Experimental data obtained from the NIST webbook.[1]

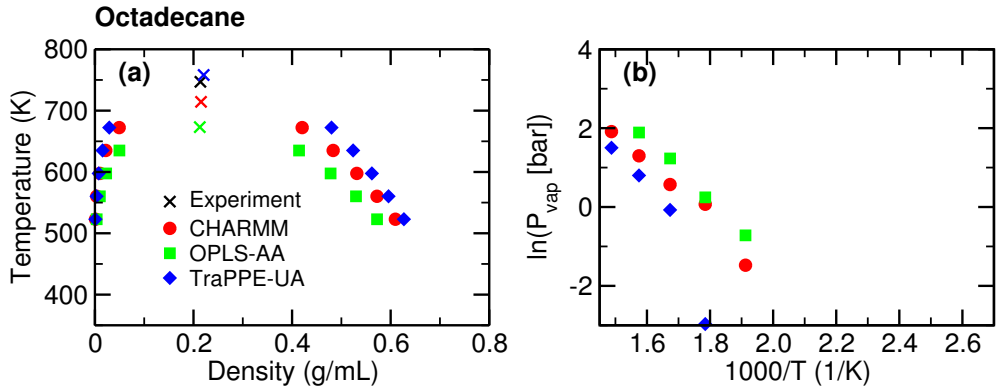

Figure S4: Vapor-liquid coexistence curves **(a)** and vapor pressures **(b)** for *n*-octadecane obtained using CHARMM, OPLS-AA, and TraPPE-UA. Experimental data obtained from the NIST webbook.[1]

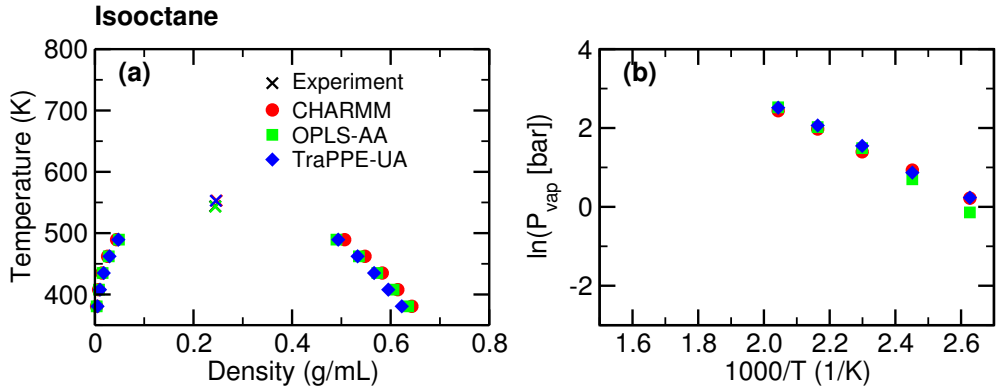

Figure S5: Vapor-liquid coexistence curves **(a)** and vapor pressures **(b)** for isooctane obtained using CHARMM, OPLS-AA, and TraPPE-UA. Experimental data obtained from the NIST webbook.[1]

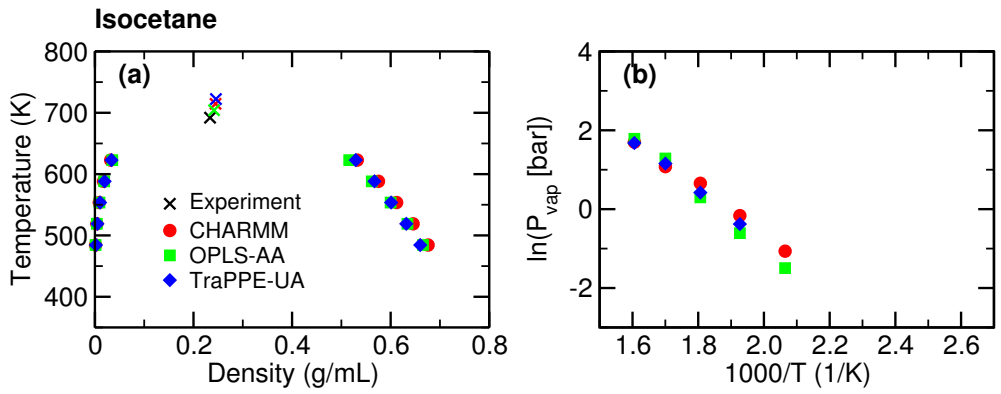

Figure S6: Vapor-liquid coexistence curves **(a)** and vapor pressures **(b)** for isocetane obtained using CHARMM, OPLS-AA, and TraPPE-UA. Experimental data obtained from the NIST webbook.[1]

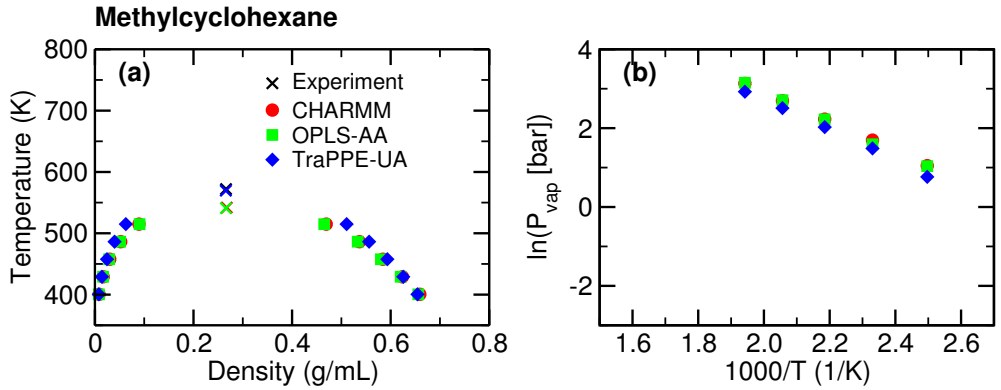

Figure S7: Vapor-liquid coexistence curves **(a)** and vapor pressures **(b)** for methylcyclohexane obtained using CHARMM, OPLS-AA, and TraPPE-UA. Experimental data obtained from the NIST webbook.[1]

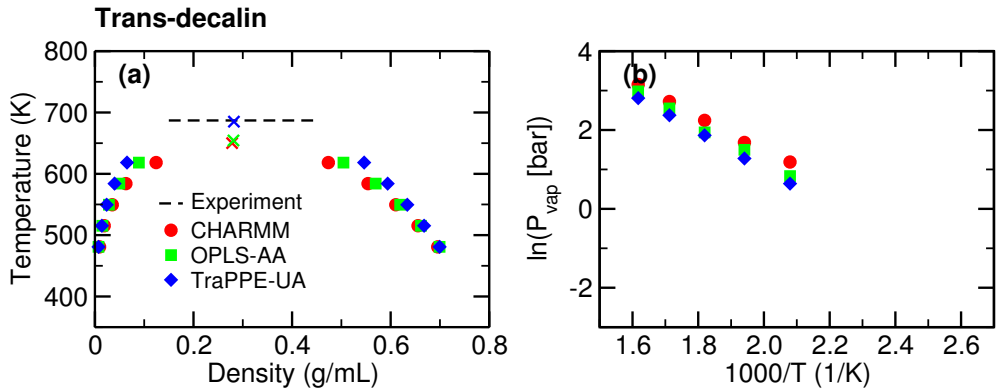

Figure S8: Vapor-liquid coexistence curves **(a)** and vapor pressures **(b)** for trans-decalin obtained using CHARMM, OPLS-AA, and TraPPE-UA. Experimental data obtained from the NIST webbook.[1]

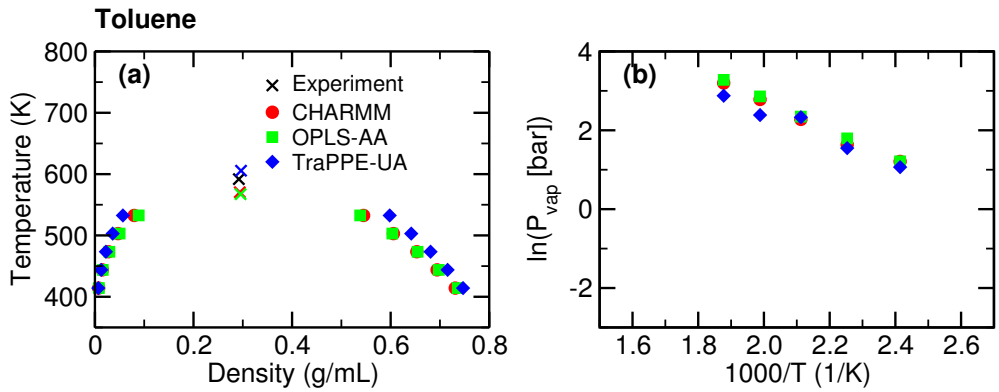

Figure S9: Vapor-liquid coexistence curves **(a)** and vapor pressures **(b)** for toluene obtained using CHARMM, OPLS-AA, and TraPPE-UA. Experimental data obtained from the NIST webbook.[1]

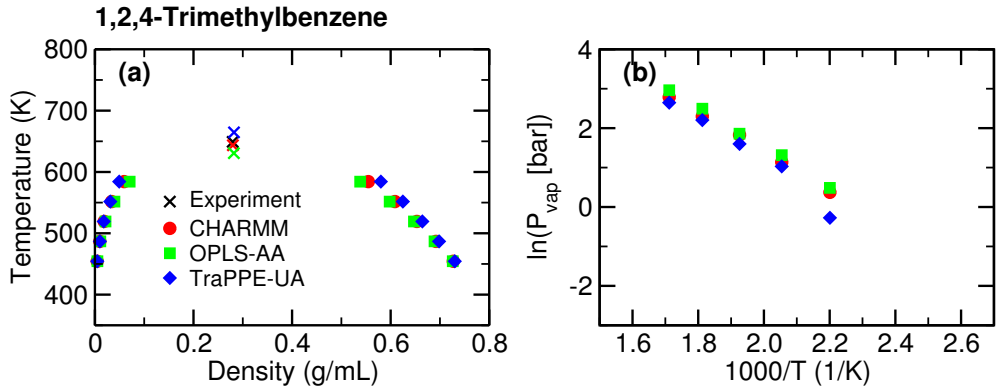

Figure S10: Vapor-liquid coexistence curves **(a)** and vapor pressures **(b)** for 1,2,4-trimethylbenzene obtained using CHARMM, OPLS-AA, and TraPPE-UA. Experimental data obtained from the NIST webbook.[1]

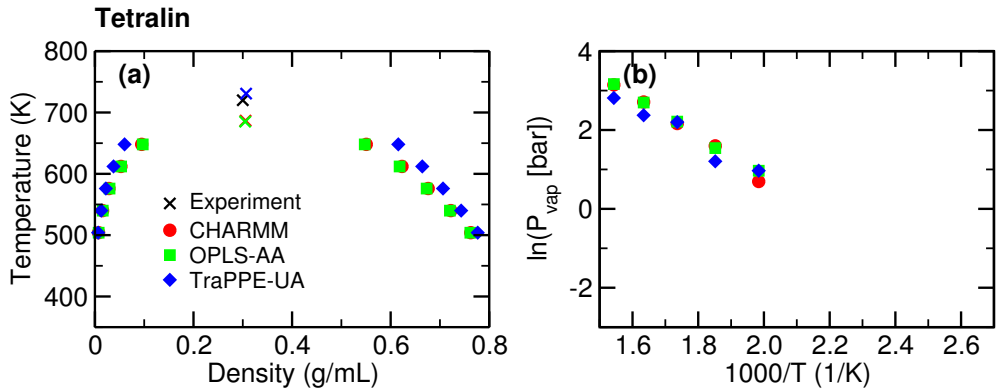

Figure S11: Vapor-liquid coexistence curves **(a)** and vapor pressures **(b)** for tetralin obtained using CHARMM, OPLS-AA, and TraPPE-UA. Experimental data obtained from the NIST webbook.[1]

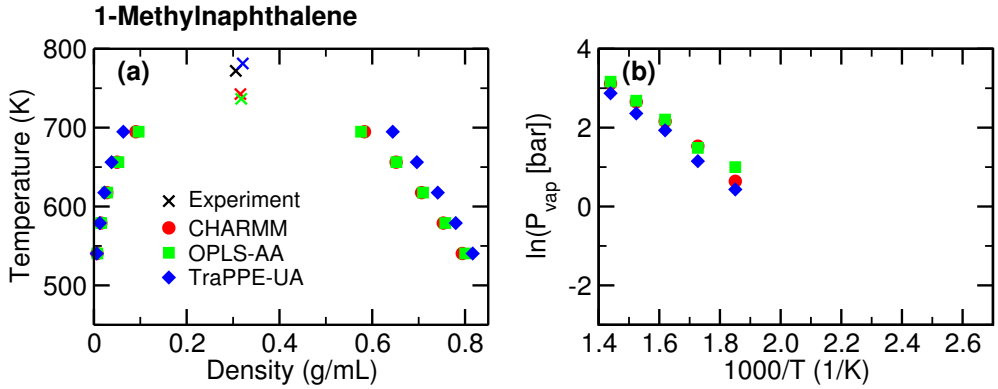

Figure S12: Vapor-liquid coexistence curves **(a)** and vapor pressures **(b)** for 1-methylnaphthalene obtained using CHARMM, OPLS-AA, and TraPPE-UA. Experimental data obtained from the NIST webbook.[1]

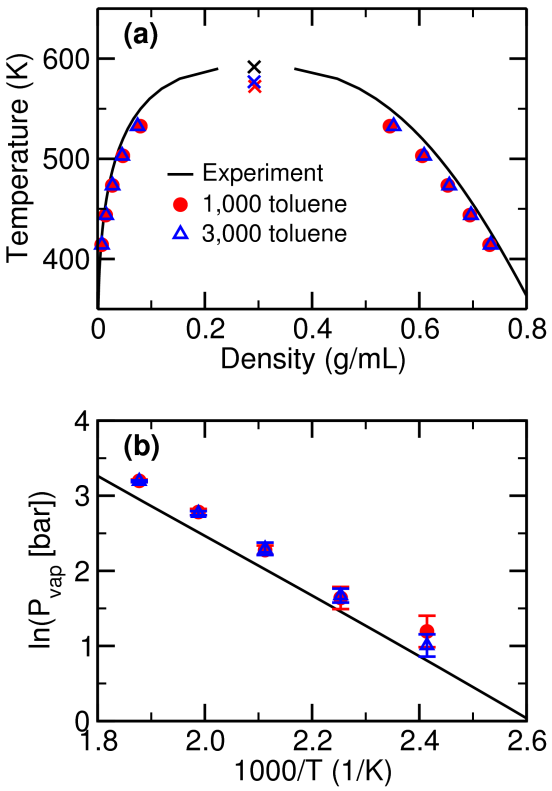

Figure S13: Vapor-liquid coexistence curves **(a)** and vapor pressures **(b)** for toluene simulated using CHARMM. The 3,000 molecule systems were generated by tripling both the thickness of the initial slab as well as the length of the z-axis.

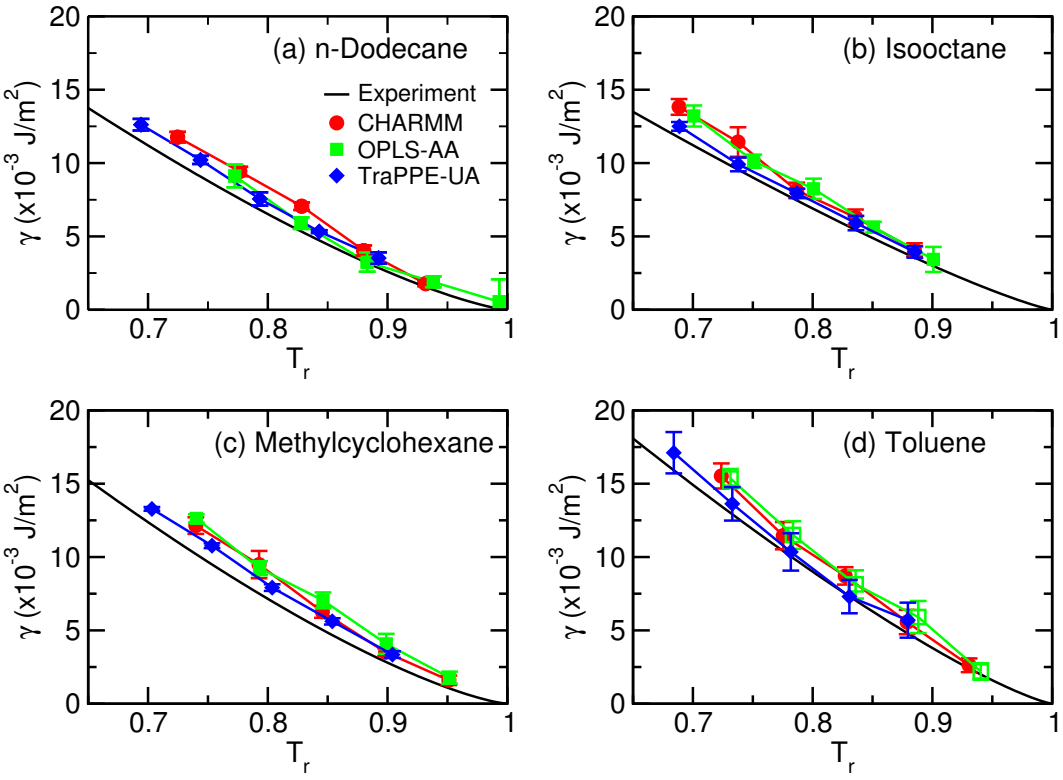

Figure S14: Surface tension, γ, of n-dodecane **(a)**, isooctane **(b)**, methylcyclohexane **(c)**, and toluene **(d)** as a function of reduced temperature, T_r. T_r is the temperature normalized by the corresponding T_c. Experimental data plotted using Eqn. 7 from the main text, with constants obtained from Ref. 2.

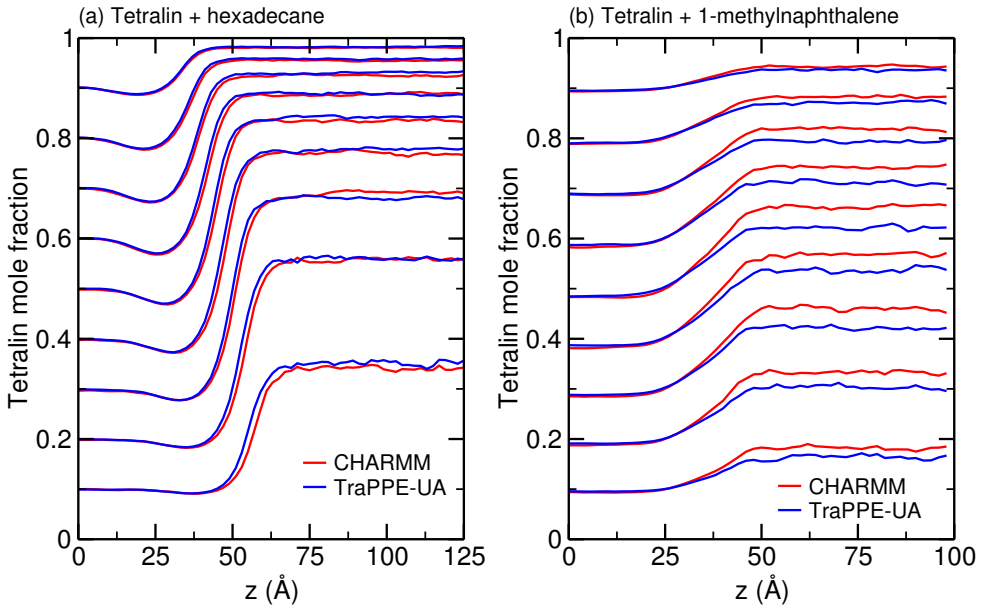

Figure S15: Tetralin mole fraction as a function of distance from liquid slab center of mass for binary mixtures of tetralin with n-hexadecane **(a)** or 1-methylnaphthalene **(b)** at 523.15 K. System compositions range from 0.1 to 0.9 mole fraction tetralin moving from bottom to top.

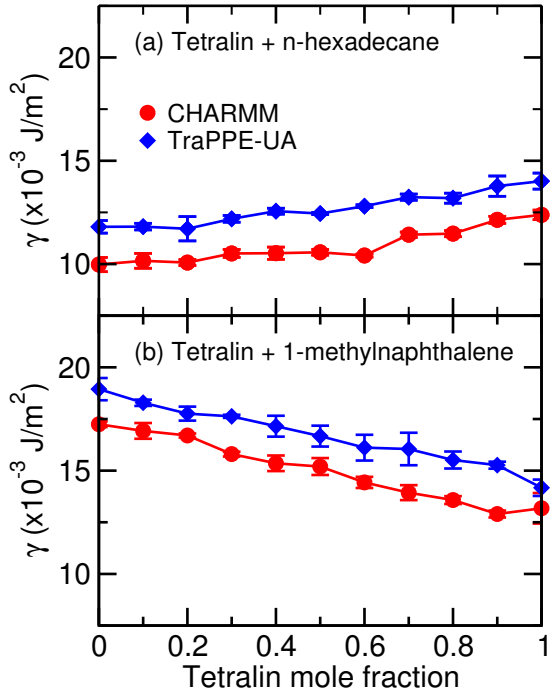

Figure S16: Surface tension γ as a function of composition for binary mixtures of tetralin with n-hexadecane **(a)** or 1-methylnaphthalene **(b)** at 523.15 K.

References

(1) https://webbook.nist.gov/chemistry/.

(2) Yaws, C. L. *Yaws' Handbook of Thermodynamic and Physical Properties of Chemical Compounds*; Knovel: Norwich, NY, 2003.