**Supplementary Materials**

for

# Molecular Solvation Theory Studies of Liquid Oleyl Alcohol and Molecular Partitioning in Water-Oleyl Alcohol Mixture

Dipankar Roy[1], Andriy Kovalenko[1,2,3,*]

[1]Department of Mechanical Engineering, University of Alberta, 10-203 Donadeo Innovation Centre for Engineering, 9211-116 Street NW, Edmonton, Alberta T6G 1H9, Canada

[2]Departments of Biological Sciences, University of Alberta, CW 405, Biological Sciences Bldg., Edmonton, Alberta T6G 2E9, Canada

[3]Nanotechnology Research Centre, National Research Council of Canada, 11421 Saskatchewan Drive, Edmonton, Alberta T6G 2M9, Canada

e-Mail: andriy.kovalenko@ualberta.ca

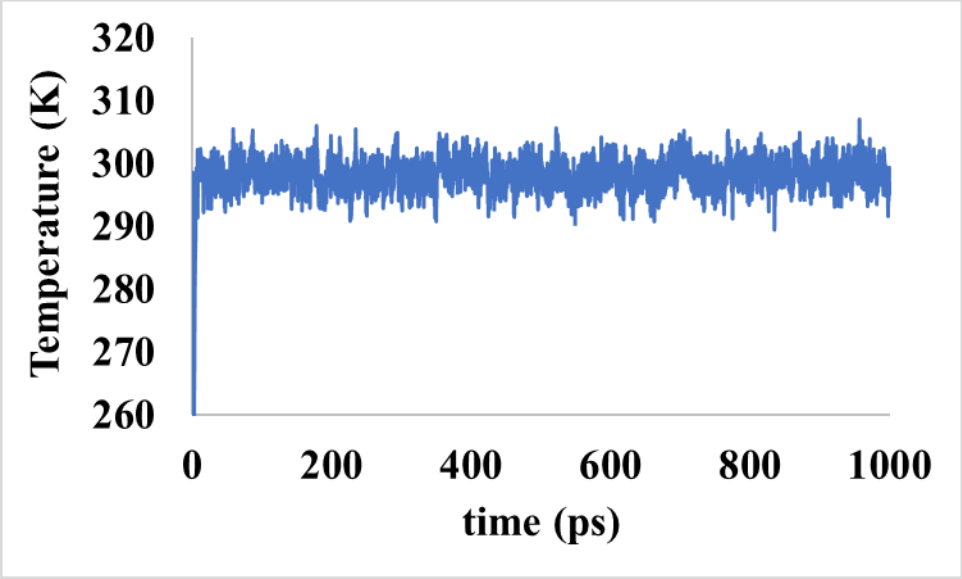


**Figure S1**. Temperature profile from the NVT equilibration run.

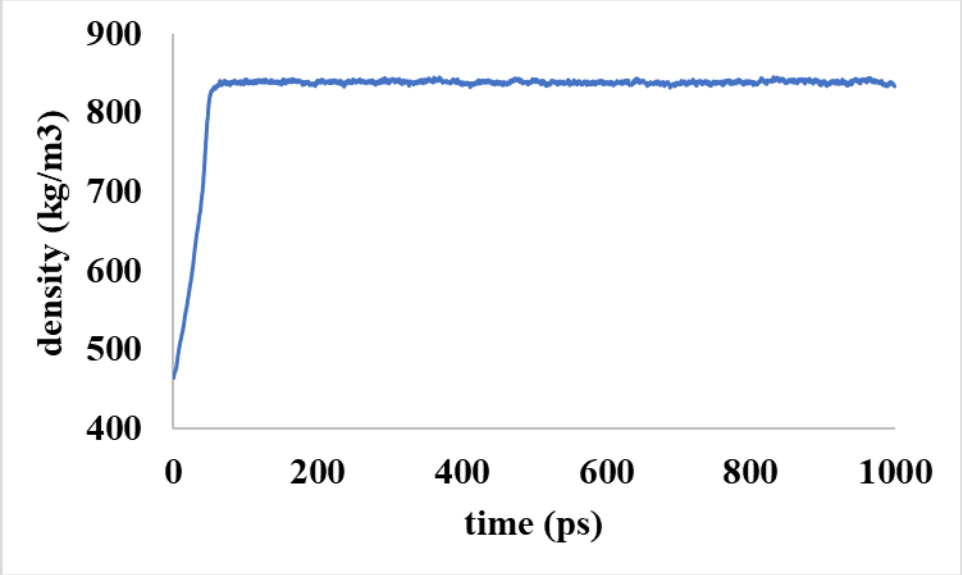


**Figure S2**. Density profile from the NVT equilibration run.

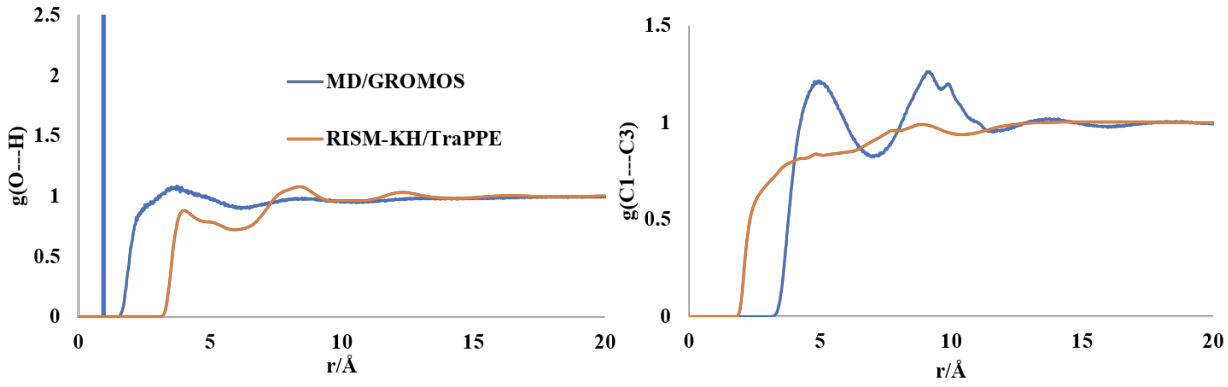


**Figure S3**. Radial distribution functions obtained from the MD simulation of oleyl alcohol with the GROMOS96 force field.

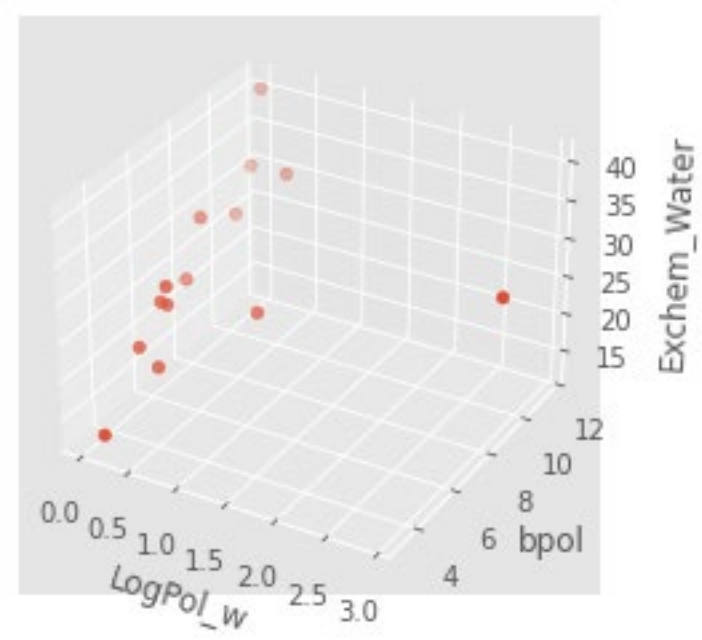


**Figure S4**. Correlation plot of the oleyl alcohol-water partition coefficient ($LogP_{Ol\text{-}W}$) with the 3D-RISM-KH computed excess chemical potential in water and 2D-molecular descriptor of polarity (bpol).

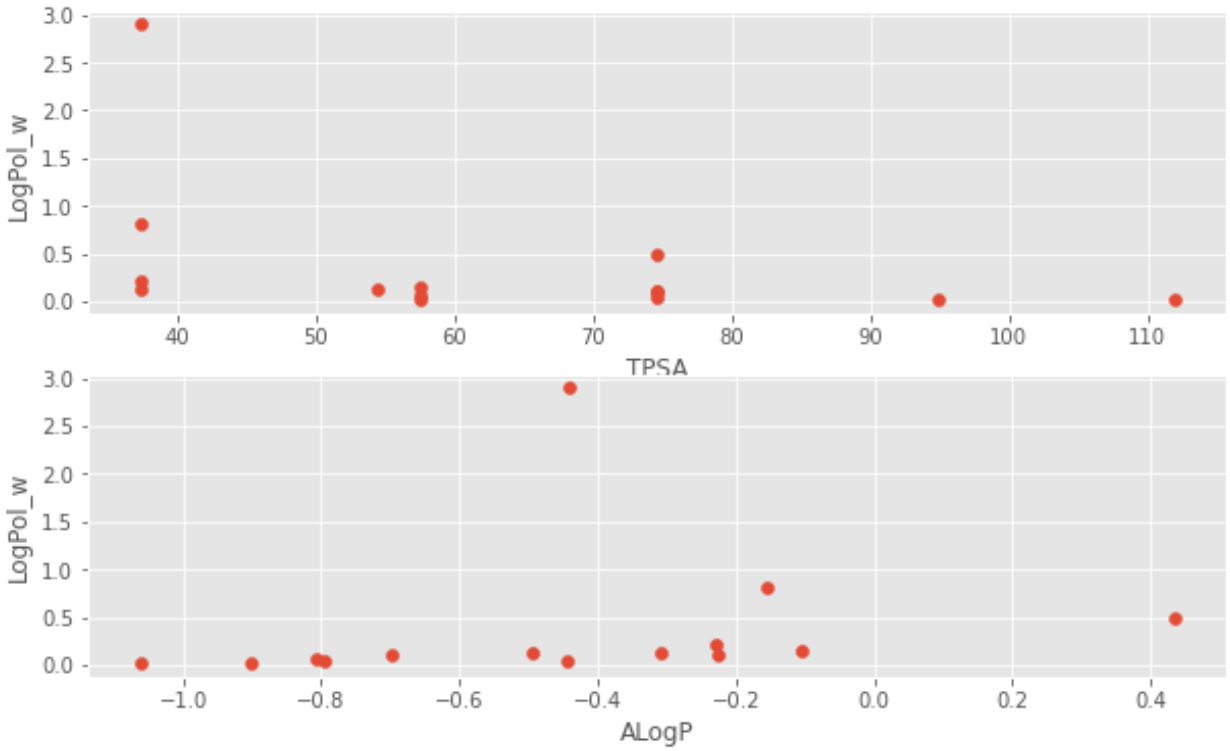


**Figure S5**. Correlation plot of the oleyl alcohol-water partition coefficient ($LogP_{Ol\text{-}W}$) with the topological polar surface area (TPSA) descriptor and Octanol-Water permeability calculated using the ALogP algorithm.

**Table S1**. Molecular descriptors used for the QSAR modeling of the oleyl alcohol/water partition function.

| Name | ALogP | *Bpol* | nHBAcc (Lipinski)[a] | TopoPSA | MW[b] |
|---|---|---|---|---|---|
| Acetic acid | -0.23 | 5.33 | 2 | 37.3 | 60.02 |
| Butyric acid | -0.44 | 9.70 | 2 | 37.3 | 88.05 |
| Dimethylmalonic acid | 0.43 | 10.66 | 4 | 74.6 | 132.04 |
| Formic acid | -0.31 | 3.14 | 2 | 37.3 | 46.01 |
| Glutaric acid | -0.70 | 10.66 | 4 | 74.6 | 132.04 |
| Glycolic acid | -0.90 | 5.33 | 3 | 57.53 | 76.02 |
| Lactic acid | -0.81 | 7.52 | 3 | 57.53 | 90.03 |
| Maleic acid | -0.23 | 6.29 | 4 | 74.6 | 116.01 |
| Malic acid | -1.06 | 8.48 | 5 | 94.83 | 134.02 |
| Malonic acid | -0.44 | 6.29 | 4 | 74.6 | 104.01 |
| 2-hydroxyisobutyric acid | -0.11 | 9.70 | 3 | 57.53 | 104.05 |
| Propionic acid | -0.15 | 7.52 | 2 | 37.3 | 74.04 |
| Pyruvic acid | -0.49 | 6.29 | 3 | 54.37 | 88.02 |
| Tricarbalylic acid | -0.79 | 11.62 | 6 | 111.9 | 176.03 |

[a]Number of H-bond acceptor as per Lipinski convention. [b]Molecular Weight.

**Table S2**. 3D-RISM-KH computed excess chemical potentials ($\mu^{GF}$) of the solutes in oleyl alcohol (Ol) with the UFF and GAFF parameters, and in water (W) with the GAFF parameters.

| Name | $\mu^{GF}_{Ol}$/UFF | $\mu^{GF}_{W}$ | $\mu^{GF}_{Ol}$/GAFF |
|---|---|---|---|
| Acetic acid | 3.434 | 17.266 | 1.061 |
| Butyric acid | 4.365 | 26.910 | 2.923 |
| Dimethylmalonic acid | 8.717 | 32.710 | 4.245 |
| Formic acid | 3.267 | 12.904 | 0.160 |
| Glutaric acid | 5.682 | 32.549 | 1.521 |
| Glycolic acid | 4.109 | 19.176 | -0.452 |
| Lactic acid | 5.034 | 23.649 | 1.109 |
| Maleic acid | 6.364 | 25.507 | 1.208 |
| Malic acid | 6.559 | 29.719 | -0.220 |
| Malonic acid | 4.906 | 23.243 | -0.194 |
| 2-hydroxyisobutyric acid | 6.438 | 28.139 | 2.910 |
| Propionic acid | 3.930 | 21.939 | 2.171 |
| Pyruvic acid | 4.624 | 23.125 | 0.859 |
| Tricarbalylic acid | 11.129 | 40.639 | 4.215 |