Supporting Information for

Solvent-Mediated Contaminant Removal from Plastic Waste Using Thermodynamic Modeling

Panzheng Zhou[1,#], *Ugochukwu M. Ikegwu*[1,#], *Elizaveta Radkevich*[1], *Euncheol Ra*[1], *Hadeia Liburd*[2],

George W. Huber[1], *Victor M. Zavala*[1], *and Reid C. Van Lehn*[1,3,]*

[1]Department of Chemical and Biological Engineering, University of Wisconsin – Madison, Madison, WI, 53706, United States.
[2]Department of Chemical Engineering, Howard University, Washington, DC, 20059, United States.
[3]Department of Chemistry, University of Wisconsin – Madison, Madison, WI, 53706, United States.

*send correspondence to: vanlehn@wisc.edu
[#]These authors contributed equally.

Polymer and Solvent Modeling

In previous work,[1, 2] we developed a computational approach to compute temperature-dependent polymer solubilities that comprises three main steps: (1) performing molecular dynamics (MD) simulations of representative oligomers of each polymer in dilute solution to sample a wide range of chain conformations, (2) selecting a representative subset of conformations and computing screening charge densities using density functional theory (DFT) calculations, and (3) using average σ-profiles from these calculations with a reference experimentally determined solubility for the desired polymer to perform solubility calculations using COSMO-RS. The polymer σ-profiles obtained using this approach were also used in this study to compute contaminant log P values; here, we provide details on this previous methodology.

Polymers were modeled as oligomers and simulated in dilute solution. All-atom MD simulations were performed in the isothermal–isobaric (*NPT*) ensemble using GROMACS 2016. Solvents were selected based on literature reports of good solvents for each polymer: PE, PP, and PS were simulated in toluene, whereas PVC and PET were simulated in dichloromethane. All molecules were modeled using the Generalized AMBER Force Field (GAFF). Systems were initialized in cubic simulation boxes containing a single polymer chain, solvated, energy minimized, and equilibrated for 2 ns in the NPT ensemble at 300 K and 1 bar. Production simulations of 10 ns were subsequently performed under NPT conditions. Representative oligomer conformations (hereafter referred to as conformers) were extracted from the production trajectories based on two structural descriptors: the radius of gyration (R_g) and the solvent-accessible surface area (SASA). To ensure broad conformational coverage, a two-dimensional R_g–SASA scatter plot was partitioned using a square grid, and conformers closest to grid intersection points were selected. The selected conformers were used as initial configurations for DFT calculations to generate COSMO files containing screening charge densities. For these calculations, geometry optimization was performed using the conductor-like polarizable continuum model (CPCM), followed by single-point calculations in the infinite dielectric constant limit. All DFT calculations were carried out using Gaussian 16 at the BVP86/TZVP/DGA1 level of theory. Precomputed COSMO files for solvents were obtained from the COSMObase-1901-BP-TZVP database. Oligomer COSMO files were used as input for COSMO-RS solubility calculations by averaging σ-profiles for all oligomer conformers, with terminal groups deactivated to approximate polymer behavior, to represent the corresponding polymer. These profiles were used to compute polymer chemical potentials and predict solubility via a solid–liquid equilibrium calculation requiring the polymer melting temperature and an experimentally measured reference solubility. The same average σ-profiles were used to represent the polymer phase for the log P calculations performed in the main text using COSMOtherm 19 with the BP_TZVP_19 parameterization. Complete details on this methodology are included in our prior work.[1, 2]

Summary of Experimental Methods for Brominated Flame Retardant (BFR) Extraction

For the BFR removal case study (Case Study 1) reported in the main text, molecular modeling predictions were validated against experimentally reported data from two prior studies that investigated the solvent-based extraction of polybrominated diphenyl ethers (PBDEs)[3] and other selected BFRs (hexabromocyclododecane, decabromodiphenylether, and TBBPA-bis-2,3-dibromopropylether).[4] Here, we briefly summarize the experimental methods used in these studies.

In the first study by Singla et al, standard solution mixtures containing 2,4,4′-tribromodiphenyl ether (tri-PBDE) at varying concentrations were prepared. Four types of plastics (PET, LDPE, PP, and PS) were used. These materials were originally sourced from food-contact products (*e.g.,* water bottles and straws) and mechanically reduced to particle sizes ranging from 4 to 700 µm; particles of approximately 500 µm were used for the extraction experiments. A known mass of plastic was submerged in the prepared tri-PBDE solution, heated to 40°C under agitation for 2 hours, and subsequently allowed to stand at room temperature for 24 hours. The solution was then filtered, and the recovered plastics containing sorbed tri-PBDE were dried at room temperature. For the extraction step, the contaminated microplastics were immersed in various organic solvents and left undisturbed for 48 hours. The organic phase was then analyzed to determine extraction efficiencies for the different solvents. We refer to the cited literature for a more detailed description of the experimental and analytical techniques.[3]

In the second study by Altwaiq et al, PS was obtained from discarded television and personal computer housings and ground to an average particle size of approximately 1000 µm. For solvent-based BFR removal, 0.2g of the polymer material was added to 20 mL of the selected solvent and stirred 60 °C for 2 hours. After cooling to room temperature, the mixture was filtered, and the solvent phase was analyzed to quantify bromine concentration as a measure of BFR extraction efficiency. We refer to the cited literature for a more detailed description of the experimental and analytical techniques.[4]

Table S1. Summary of log *P* values for all four BFRs studied in this work, their miscibility, and PS polymer solubilities in 32 common solvents. The log *P* and BFR miscibility calculations are performed at room temperature (25°C) with PS as the polymer phase. The remark column of “yes” indicates that the solvent satisfies all leaching criteria and “no” if it does not satisfy all criteria. For this analysis, a maximum RT solubility of 6 wt% is used as part of the leaching criteria to reflect the maximum predicted solubility value that was associated with high experimental extraction efficiency in Table 1 of the main text; this threshold is higher than the threshold for precipitation during STRAP to account for the preference for slight swelling during leaching without excessive polymer dissolution.

Solvents	**Th (ºC)**	**log *P* values in each solvent at (RT)**				**Miscibility in each solvent at (RT)**				**Polymer Solubility (%)**		**Remark**
		Tri-PBDE	**HBCD**	**DECA**	**TBBPA-dbp**	**Tri-PBDE**	**HBCD**	**DECA**	**TBBPA-dbp**	**RT (ºC)**	**Th (ºC)**	
methanol	63.6	-0.1	1.0	-1.5	0.3	Yes	Yes	No	Yes	0.0	0.0	No
dichloromethane	39.0	0.9	1.7	1.0	2.1	Yes	Yes	Yes	Yes	4.6	8.5	Yes
ethylene glycol	120.0	-1.2	-0.2	-3.5	-1.6	No	Yes	No	No	0.0	0.0	No
Acetone	55.0	1.5	3.1	0.5	3.7	Yes	Yes	Yes	Yes	9.2	21.3	No
Isopropanol	81.3	-0.3	0.3	-1.6	-0.3	Yes	Yes	No	Yes	0.0	1.2	No
1-propanol	96.2	-0.3	0.3	-1.6	-0.4	Yes	Yes	No	Yes	0.0	2.8	No
toluene	109.6	0.8	0.9	1.1	1.2	Yes	Yes	Yes	Yes	3.6	41.0	Yes
chloroform	60.1	0.8	1.2	1.1	1.6	Yes	Yes	Yes	Yes	2.3	9.8	Yes
tetrahydrofuran	64.0	1.4	2.7	0.2	3.2	Yes	Yes	Yes	Yes	14.0	31.3	No
tetrahydropyran	87.0	1.0	1.9	-0.2	2.1	Yes	Yes	Yes	Yes	7.2	33.7	No
cyclohexane	79.7	-0.6	-1.3	-1.3	-2.2	Yes	No	No	No	0.2	4.6	No
heptane	97.5	-0.8	-1.5	-1.5	-2.4	Yes	No	No	No	0.1	5.2	No
triethylamine	88.0	0.5	1.7	-0.8	1.6	Yes	Yes	No	Yes	0.8	12.9	No
1,2-propanediol	120.0	-0.9	-0.1	-2.9	-1.2	No	Yes	No	No	0.0	0.3	No
dimethyl sulfoxide	120.0	1.7	3.8	0.1	4.4	Yes	Yes	Yes	Yes	1.5	18.2	Yes
hexane	67.7	-0.7	-1.4	-1.3	-2.3	Yes	No	No	No	0.1	1.9	No
acetylacetone	120.0	0.9	2.3	-0.4	2.5	Yes	Yes	Yes	Yes	0.5	23.0	No
tert-butanol	81.4	-0.3	0.1	-1.7	-0.5	Yes	Yes	No	Yes	0.0	2.0	No
ethyl acetate	76.1	1.2	2.4	0.2	2.8	Yes	Yes	Yes	Yes	5.4	24.9	Yes
isopropylamine	30.7	0.8	2.1	-0.8	2.3	Yes	Yes	No	Yes	1.8	2.7	No
diphenyl ether	120.0	0.7	0.9	1.0	1.2	Yes	Yes	Yes	Yes	0.8	25.3	Yes
dodecane	120.0	-1.1	-1.9	-2.0	-3.0	No	No	No	No	0.0	4.1	No
N,N-dimethylformamide	120.0	1.9	3.8	0.6	4.6	Yes	Yes	Yes	Yes	7.4	47.9	No
2,3-dihydropyran	85.0	0.8	1.3	0.3	1.6	Yes	Yes	Yes	Yes	5.1	31.2	Yes
methylacetate	55.8	1.3	2.7	0.4	3.2	Yes	Yes	Yes	Yes	4.9	14.9	Yes
ethanol	77.2	-0.1	0.7	-1.4	0.2	Yes	Yes	No	Yes	0.0	0.7	No
cyclohexanol	120.0	-0.5	-0.3	-2.1	-1.1	Yes	Yes	No	No	0.0	8.4	No
2-butanone	78.5	1.2	2.5	0.1	2.9	Yes	Yes	Yes	Yes	6.9	30.9	No
water	99.0	-6.2	-5.3	-10.5	-10.3	No	No	No	No	0.0	0.0	No
benzene	79.0	1.0	1.3	1.5	1.8	Yes	Yes	Yes	Yes	5.3	29.3	Yes
acetic acid	116.9	-0.1	1.1	-1.5	0.6	Yes	Yes	No	Yes	0.0	0.6	No
o-xylene	120.0	0.6	0.6	0.8	0.8	Yes	Yes	Yes	Yes	2.4	41.5	Yes

Table S2. Summary of log *P* for all four BFRs studied in this work, their miscibility, and PET polymer solubilities in 32 common solvents. The log *P* and BFR miscibility calculations are performed at room temperature (25°C) with PET as the polymer phase. The remark column of "yes" indicates that the solvent satisfies all leaching criteria and "no" if it does not satisfy all criteria. For this analysis, a maximum RT solubility of 6 wt% is used as part of the leaching criteria to reflect the maximum predicted solubility value that was associated with high experimental extraction efficiency in Table 1 of the main text; this threshold is higher than the threshold for precipitation during STRAP to account for the preference for slight swelling during leaching without excessive polymer dissolution.

Solvents	**Th (ºC)**	**log *P* values in each solvent at (RT)**				**Miscibility in each solvent at (RT)**				**Polymer Solubility (%)**		**Remark**
		Tri-PBDE	**HBCD**	**DECA**	**TBBPA-dbp**	**Tri-PBDE**	**HBCD**	**DECA**	**TBBPA-dbp**	**RT (ºC)**	**Th (ºC)**	
methanol	63.6	-0.6	-0.1	-1.6	-1.1	Yes	Yes	No	Yes	0.0	0.0	No
dichloromethane	39.0	0.5	0.5	0.9	0.7	Yes	Yes	Yes	Yes	0.3	0.8	Yes
ethylene glycol	120.0	-1.6	-1.3	-3.6	-3.0	No	Yes	No	No	0.0	0.0	No
Acetone	55.0	1.1	2.0	0.4	2.3	Yes	Yes	Yes	Yes	0.1	0.7	Yes
Isopropanol	81.3	-0.7	-0.8	-1.7	-1.7	Yes	Yes	No	Yes	0.0	0.0	No
1-propanol	96.2	-0.7	-0.9	-1.7	-1.8	Yes	Yes	No	Yes	0.0	0.1	No
toluene	109.6	0.3	-0.3	1.0	-0.2	Yes	Yes	Yes	Yes	0.0	2.5	No
chloroform	60.1	0.3	0.0	1.0	0.2	Yes	Yes	Yes	Yes	0.2	1.0	No
tetrahydrofuran	64.0	1.0	1.5	0.1	1.8	Yes	Yes	Yes	Yes	0.0	0.8	Yes
tetrahydropyran	87.0	0.5	0.8	-0.3	0.7	Yes	Yes	Yes	Yes	0.0	0.8	No
cyclohexane	79.7	-1.0	-2.5	-1.4	-3.6	Yes	No	No	No	0.0	0.0	No
heptane	97.5	-1.2	-2.7	-1.6	-3.8	Yes	No	No	No	0.0	0.0	No
triethylamine	88.0	0.1	0.6	-0.9	0.2	Yes	Yes	No	Yes	0.0	0.0	No
1,2-propanediol	120.0	-1.3	-1.2	-3.0	-2.6	No	Yes	No	No	0.0	0.0	No
dimethyl sulfoxide	120.0	1.3	2.6	0.0	3.0	Yes	Yes	Yes	Yes	0.0	8.3	No
hexane	67.7	-1.1	-2.6	-1.4	-3.6	Yes	No	No	No	0.0	0.0	No
acetylacetone	120.0	0.4	1.1	-0.5	1.1	Yes	Yes	Yes	Yes	0.0	2.0	No
tert-butanol	81.4	-0.7	-1.0	-1.8	-1.9	Yes	Yes	No	Yes	0.0	0.0	No
ethyl acetate	76.1	0.8	1.3	0.1	1.4	Yes	Yes	Yes	Yes	0.0	0.5	Yes
isopropylamine	30.7	0.4	1.0	-0.9	0.9	Yes	Yes	No	Yes	0.0	0.0	No
diphenyl ether	120.0	0.3	-0.2	0.9	-0.2	Yes	Yes	Yes	Yes	0.0	1.4	No
dodecane	120.0	-1.5	-3.1	-2.1	-4.4	No	No	No	No	0.0	0.0	No
N,N-dimethylformamide	120.0	1.4	2.7	0.6	3.2	Yes	Yes	Yes	Yes	0.2	18.4	Yes
2,3-dihydropyran	85.0	0.4	0.2	0.2	0.2	Yes	Yes	Yes	Yes	0.0	0.7	Yes
methylacetate	55.8	0.9	1.6	0.3	1.8	Yes	Yes	Yes	Yes	0.0	0.2	Yes
ethanol	77.2	-0.5	-0.4	-1.5	-1.2	Yes	Yes	No	Yes	0.0	0.0	No
cyclohexanol	120.0	-1.0	-1.4	-2.2	-2.5	Yes	Yes	No	No	0.0	0.3	No
2-butanone	78.5	0.8	1.4	0.0	1.5	Yes	Yes	Yes	Yes	0.0	1.4	No
water	99.0	-6.6	-6.4	-10.5	-11.7	No	No	No	No	0.0	0.0	No
benzene	79.0	0.6	0.2	1.5	0.4	Yes	Yes	Yes	Yes	0.0	0.9	Yes
acetic acid	116.9	-0.5	-0.1	-1.5	-0.8	Yes	Yes	No	Yes	0.0	0.1	No
o-xylene	120.0	0.2	-0.5	0.7	-0.6	Yes	Yes	Yes	Yes	0.0	2.5	No

Table S3. Summary of log *P* for all four BFRs studied in this work, their miscibility, and PE polymer solubilities in 32 common solvents. The log *P* and BFR miscibility calculations are performed at room temperature (25°C) with PE as the polymer phase. The remark column of "yes" indicates that the solvent satisfies all leaching criteria and "no" if it does not satisfy all criteria. For this analysis, a maximum RT solubility of 6 wt% is used as part of the leaching criteria to reflect the maximum predicted solubility value that was associated with high experimental extraction efficiency in Table 1 of the main text; this threshold is higher than the threshold for precipitation during STRAP to account for the preference for slight swelling during leaching without excessive polymer dissolution.

Solvents	**Th (ºC)**	**log *P* values in each solvent at (RT)**				**Miscibility in each solvent at (RT)**				**Polymer Solubility (%)**		**Remark**
		Tri-PBDE	**HBCD**	**DECA**	**TBBPA-dbp**	**Tri-PBDE**	**HBCD**	**DECA**	**TBBPA-dbp**	**RT (ºC)**	**Th (ºC)**	
methanol	63.6	0.6	2.5	-0.2	2.6	Yes	Yes	No	Yes	0.0	0.1	No
dichloromethane	39.0	1.6	3.1	2.4	4.5	Yes	Yes	Yes	Yes	0.0	0.1	Yes
ethylene glycol	120.0	-0.5	1.3	-2.1	0.7	No	Yes	No	No	0.0	0.9	No
Acetone	55.0	2.3	4.6	1.8	6.0	Yes	Yes	Yes	Yes	0.0	0.3	Yes
Isopropanol	81.3	0.5	1.8	-0.3	2.0	Yes	Yes	No	Yes	0.0	1.6	No
1-propanol	96.2	0.5	1.8	-0.3	2.0	Yes	Yes	No	Yes	0.0	4.2	No
toluene	109.6	1.5	2.3	2.4	3.5	Yes	Yes	Yes	Yes	0.1	22.6	Yes
chloroform	60.1	1.5	2.6	2.4	3.9	Yes	Yes	Yes	Yes	0.0	0.6	Yes
tetrahydrofuran	64.0	2.1	4.2	1.5	5.5	Yes	Yes	Yes	Yes	0.1	1.7	Yes
tetrahydropyran	87.0	1.7	3.4	1.1	4.5	Yes	Yes	Yes	Yes	0.1	7.3	Yes
cyclohexane	79.7	0.1	0.1	0.0	0.1	Yes	No	No	No	0.1	6.9	No
heptane	97.5	0.0	-0.1	-0.1	-0.1	Yes	No	No	No	0.1	15.3	No
triethylamine	88.0	1.2	3.2	0.6	3.9	Yes	Yes	No	Yes	0.1	8.7	No
1,2-propanediol	120.0	-0.2	1.4	-1.6	1.1	No	Yes	No	No	0.0	3.2	No
dimethyl sulfoxide	120.0	2.5	5.3	1.5	6.7	Yes	Yes	Yes	Yes	0.0	5.3	Yes
hexane	67.7	0.1	0.1	0.1	0.1	Yes	No	No	No	0.1	3.1	No
acetylacetone	120.0	1.6	3.8	1.0	4.8	Yes	Yes	Yes	Yes	0.0	8.2	Yes
tert-butanol	81.4	0.4	1.6	-0.3	1.8	Yes	Yes	No	Yes	0.0	2.1	No
ethyl acetate	76.1	1.9	3.9	1.6	5.1	Yes	Yes	Yes	Yes	0.0	1.6	Yes
isopropylamine	30.7	1.5	3.6	0.5	4.6	Yes	Yes	No	Yes	0.1	0.1	No
diphenyl ether	120.0	1.4	2.4	2.3	3.6	Yes	Yes	Yes	Yes	0.0	18.5	Yes
dodecane	120.0	-0.4	-0.4	-0.7	-0.7	No	No	No	No	0.1	32.5	No
N,N-dimethylformamide	120.0	2.6	5.3	2.0	6.9	Yes	Yes	Yes	Yes	0.0	16.2	Yes
2,3-dihydropyran	85.0	1.5	2.8	1.7	3.9	Yes	Yes	Yes	Yes	0.1	5.0	Yes
methylacetate	55.8	2.1	4.2	1.8	5.6	Yes	Yes	Yes	Yes	0.0	0.3	Yes
ethanol	77.2	0.6	2.2	-0.1	2.5	Yes	Yes	No	Yes	0.0	0.9	No
cyclohexanol	120.0	0.2	1.2	-0.7	1.2	Yes	Yes	No	No	0.0	22.1	No
2-butanone	78.5	1.9	4.0	1.5	5.3	Yes	Yes	Yes	Yes	0.0	2.3	Yes
water	99.0	-5.4	-3.8	-9.1	-8.0	No	No	No	No	0.0	0.0	No
benzene	79.0	1.8	2.8	2.9	4.1	Yes	Yes	Yes	Yes	0.0	3.1	Yes
acetic acid	116.9	0.6	2.6	-0.1	2.9	Yes	Yes	No	Yes	0.0	2.0	No
o-xylene	120.0	1.3	2.1	2.1	3.1	Yes	Yes	Yes	Yes	0.1	37.8	Yes

Table S4. Summary of log *P* for all four BFRs studied in this work, their miscibility, and PP polymer solubilities in 32 common solvents. The log *P* and BFR miscibility calculations are performed at room temperature (25°C) with PP as the polymer phase. The remark column of "yes" indicates that the solvent satisfies all leaching criteria and "no" if it does not satisfy all criteria. For this analysis, a maximum RT solubility of 6 wt% is used as part of the leaching criteria to reflect the maximum predicted solubility value that was associated with high experimental extraction efficiency in Table 1 of the main text; this threshold is higher than the threshold for precipitation during STRAP to account for the preference for slight swelling during leaching without excessive polymer dissolution.

Solvents	**Th (ºC)**	**log *P* values in each solvent at (RT)**				**Miscibility in each solvent at (RT)**				**Polymer Solubility (%)**		**Remark**
		Tri-PBDE	**HBCD**	**DECA**	**TBBPA-dbp**	**Tri-PBDE**	**HBCD**	**DECA**	**TBBPA-dbp**	**RT (ºC)**	**Th (ºC)**	
methanol	63.6	0.8	2.6	0.1	2.8	Yes	Yes	No	Yes	0.0	0.1	No
dichloromethane	39.0	1.8	3.3	2.6	4.7	Yes	Yes	Yes	Yes	0.2	0.5	Yes
ethylene glycol	120.0	-0.3	1.5	-1.9	1.0	No	Yes	No	No	0.0	0.1	No
Acetone	55.0	2.4	4.8	2.0	6.3	Yes	Yes	Yes	Yes	0.3	1.4	Yes
Isopropanol	81.3	0.6	2.0	0.0	2.2	Yes	Yes	No	Yes	0.1	2.3	No
1-propanol	96.2	0.6	1.9	-0.1	2.2	Yes	Yes	No	Yes	0.1	4.1	No
toluene	109.6	1.7	2.5	2.6	3.7	Yes	Yes	Yes	Yes	1.1	30.9	Yes
chloroform	60.1	1.7	2.8	2.7	4.1	Yes	Yes	Yes	Yes	0.5	3.1	Yes
tetrahydrofuran	64.0	2.3	4.3	1.8	5.7	Yes	Yes	Yes	Yes	2.0	10.1	Yes
tetrahydropyran	87.0	1.9	3.6	1.3	4.7	Yes	Yes	Yes	Yes	2.0	20.9	Yes
cyclohexane	79.7	0.3	0.3	0.3	0.4	Yes	No	No	No	4.0	24.0	No
heptane	97.5	0.1	0.1	0.1	0.1	Yes	No	No	No	2.9	29.3	No
triethylamine	88.0	1.4	3.3	0.8	4.2	Yes	Yes	No	Yes	2.8	23.2	No
1,2-propanediol	120.0	0.0	1.6	-1.3	1.3	No	Yes	No	No	0.0	0.6	No
dimethyl sulfoxide	120.0	2.6	5.4	1.7	7.0	Yes	Yes	Yes	Yes	0.0	1.7	Yes
hexane	67.7	0.2	0.2	0.3	0.3	Yes	No	No	No	3.6	16.2	No
acetylacetone	120.0	1.8	3.9	1.2	5.0	Yes	Yes	Yes	Yes	0.0	3.0	Yes
tert-butanol	81.4	0.6	1.8	-0.1	2.0	Yes	Yes	No	Yes	0.3	3.8	No
ethyl acetate	76.1	2.1	4.0	1.8	5.3	Yes	Yes	Yes	Yes	0.4	4.3	Yes
isopropylamine	30.7	1.7	3.8	0.7	4.8	Yes	Yes	No	Yes	0.8	1.1	No
diphenyl ether	120.0	1.6	2.6	2.6	3.8	Yes	Yes	Yes	Yes	0.2	13.0	Yes
dodecane	120.0	-0.2	-0.3	-0.5	-0.5	No	No	No	No	1.4	31.1	No
N,N-dimethylformamide	120.0	2.8	5.5	2.2	7.1	Yes	Yes	Yes	Yes	0.2	9.0	Yes
2,3-dihydropyran	85.0	1.7	3.0	1.9	4.1	Yes	Yes	Yes	Yes	1.0	14.4	Yes
methylacetate	55.8	2.2	4.4	2.0	5.8	Yes	Yes	Yes	Yes	0.2	1.0	Yes
ethanol	77.2	0.8	2.4	0.1	2.7	Yes	Yes	No	Yes	0.1	1.0	No
cyclohexanol	120.0	0.4	1.4	-0.5	1.4	Yes	Yes	No	No	0.2	14.7	No
2-butanone	78.5	2.1	4.2	1.7	5.5	Yes	Yes	Yes	Yes	0.5	5.7	Yes
water	99.0	-5.3	-3.6	-8.9	-7.7	No	No	No	No	0.0	0.0	No
benzene	79.0	1.9	3.0	3.1	4.3	Yes	Yes	Yes	Yes	0.7	9.6	Yes
acetic acid	116.9	0.8	2.7	0.1	3.1	Yes	Yes	No	Yes	0.0	0.3	No
o-xylene	120.0	1.5	2.3	2.3	3.3	Yes	Yes	Yes	Yes	1.1	37.2	Yes

Table S5. Phthalates considered in this work and their applications in plastic products.[5]

ID	Phthalates	Usage
P1	BBP butyl benzyl phthalate	Vinyl tiles, food conveyor belts, artificial leather, automotive trim, traffic cones
P2	DBP di-n-butyl phthalate	PVC plastics, latex adhesives, cosmetics (most common phthalate added to nail polish), personal care products, cellulose plastics, solvent for dyes
P3	DEHP di-(2-ethylhexyl) phthalate	Building products (wallpaper, wire and cable insulation), car products (vinyl upholstery, car seats), clothing (footwear, raincoats), food packaging, children's products (toys, grip bumpers), medical devices, most widely added phthalate to PVC to make products flexible
P4	DEP diethyl phthalate	Personal care products, most common phthalate added to enhance fragrance, cosmetics.
P5	DiDP di-isodecyl phthalate	PVC plastics, covering on wires and cables, artificial leather, toys, carpet backing, pool liners
P6	DiNP di-isononyl phthalate	Garden hoses, pool liners, flooring tiles, tarps, toys (most common phthalate added as a softener in the manufacture of toys and childcare products - bath toys, drinking straws, and rubber ducks)
P7	DnHP di-n-hexyl phthalate	Dipmolded products, tool handles, dish-washer baskets, flooring, vinyl gloves, flea collars, conveyer belts used in food processing
P8	DnOP di-n-octyl phthalate	Garden hoses, pool liners, flooring tiles, tarps, seam cements, bottle cap liners, conveyor belts

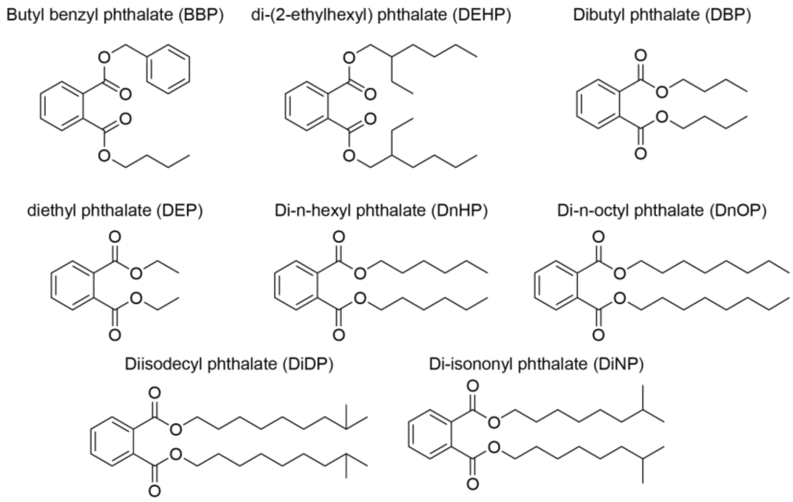

Figure S1. Chemical structures of the eight phthalates considered in this work.

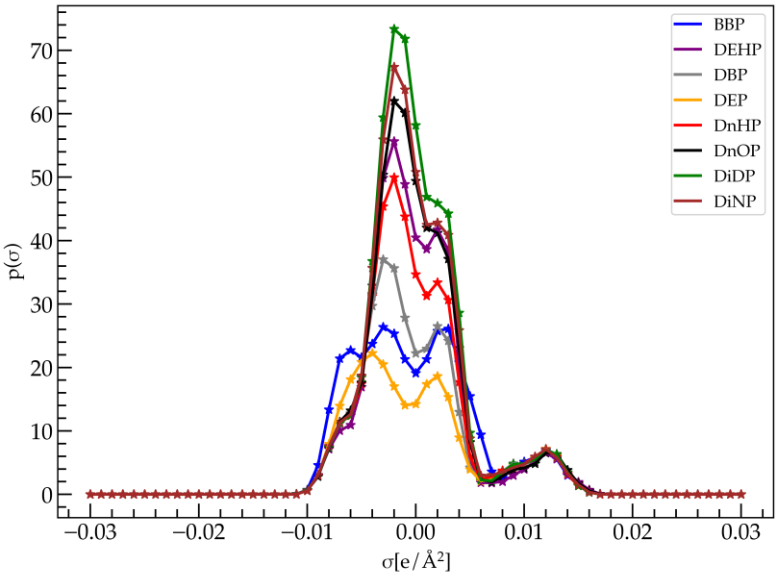

Figure S2. σ-profiles for the eight phthalates considered in this work. Abbreviations are reported in Figure S1.

Table S6. Summary of log *P* calculations for all eight phthalates in 32 common solvents. All calculations were performed at room temperature (25°C) with PVC as the polymer phase. Positive log *P* values (indicating partitioning into the solvent) are in green. The “all>0” reports if all eight phthalates have positive log *P* values in the given solvent, and “mean” reports the average log *P* value for that solvent across all eight phthalates.

Solvent	log *P* values for each phthalate in the selected solvent								all>0	mean
	P1	**P2**	**P3**	**P4**	**P5**	**P6**	**P7**	**P8**		
methanol	-0.50	-0.61	-0.83	-0.31	-1.34	-1.23	-0.88	-1.09	no	-0.88
dichloromethane	1.64	1.57	1.77	1.48	1.83	1.78	1.64	1.75	yes	1.70
ethylene glycol	-1.33	-1.45	-2.19	-0.84	-3.03	-2.77	-2.01	-2.51	no	-2.12
Acetone	1.09	0.69	0.84	0.70	0.91	0.88	0.76	0.83	yes	0.81
Isopropanol	-0.33	-0.24	-0.10	-0.26	-0.21	-0.22	-0.24	-0.19	no	-0.19
1-propanol	-0.32	-0.24	-0.11	-0.24	-0.23	-0.24	-0.25	-0.20	no	-0.19
toluene	0.44	0.43	0.81	0.24	1.00	0.90	0.63	0.83	yes	0.72
chloroform	1.57	1.67	2.08	1.45	2.20	2.10	1.82	2.08	yes	1.94
tetrahydrofuran	1.01	0.83	1.30	0.60	1.64	1.50	1.11	1.38	yes	1.21
tetrahydropyran	0.65	0.59	1.08	0.32	1.43	1.29	0.88	1.17	yes	0.99
cyclohexane	-0.81	-0.39	0.27	-0.82	0.65	0.47	-0.02	0.34	no	0.11
heptane	-1.01	-0.59	0.02	-0.98	0.35	0.19	-0.25	0.07	no	-0.14
triethylamine	-0.26	-0.06	0.51	-0.40	0.86	0.70	0.26	0.58	no	0.38
1,2-propanediol	-0.88	-0.91	-1.27	-0.57	-1.78	-1.64	-1.22	-1.48	no	-1.27
dimethyl sulfoxide	0.86	0.31	0.21	0.52	0.03	0.07	0.21	0.12	no	0.23
hexane	-0.93	-0.50	0.12	-0.92	0.47	0.30	-0.16	0.18	no	-0.04
acetylacetone	0.45	0.07	-0.08	0.26	-0.24	-0.18	-0.03	-0.15	no	-0.05
tert-butanol	-0.30	-0.18	0.05	-0.26	0.05	0.00	-0.10	0.01	no	-0.04
ethyl acetate	0.79	0.54	0.76	0.47	0.88	0.82	0.66	0.77	yes	0.71
isopropylamine	0.60	0.54	0.86	0.40	1.05	0.95	0.71	0.89	yes	0.78
diphenyl ether	0.26	0.19	0.33	0.14	0.34	0.31	0.24	0.30	yes	0.29
dodecane	-1.28	-0.84	-0.31	-1.20	-0.01	-0.16	-0.54	-0.25	no	-0.45
N,N-dimethylformamide	1.11	0.63	0.71	0.69	0.76	0.73	0.67	0.71	yes	0.71
2,3-dihydropyran	0.65	0.59	0.97	0.39	1.20	1.09	0.80	1.01	yes	0.88
methylacetate	0.89	0.54	0.65	0.57	0.67	0.65	0.58	0.62	yes	0.62
ethanol	-0.27	-0.27	-0.25	-0.18	-0.48	-0.45	-0.36	-0.39	no	-0.32
cyclohexanol	-0.50	-0.31	-0.08	-0.41	-0.07	-0.12	-0.23	-0.11	no	-0.17
2-butanone	0.87	0.60	0.83	0.53	0.98	0.91	0.73	0.85	yes	0.79
water	-5.54	-5.48	-8.21	-3.33	-11.3	-10.3	-7.54	-9.41	no	-8.02
benzene	0.66	0.57	0.87	0.44	0.99	0.92	0.71	0.86	yes	0.80
acetic acid	-0.07	-0.33	-0.77	0.12	-1.49	-1.31	-0.77	-1.06	no	-0.77
o-xylene	0.28	0.31	0.70	0.09	0.91	0.81	0.52	0.73	yes	0.61

Table S7. List of all 26 PFAS and their groups based on structural features.

ID	PFAS Compound	CASRN	Group
1	Perfluorobutanoic acid (PFBA)	375-22-4	1
2	Perfluoropentanoic acid (PFPA)	2706-90-3	1
3	Perfluorohexanoic acid (PFHxA)	307-24-4	1
4	Perfluoroheptanoic acid (PFHA)	375-85-9	1
5	Perfluorooctanoic acid (PFOA)	335-67-1	1
6	Perfluorononanoic acid (PFNA)	375-95-1	1
7	Perfluorodecanoic acid (PFDA)	335-76-2	1
8	2,3,3,3-Tetrafluoro-2-(heptafluoropropoxy)propanoic acid (TFPA)	13252-13-6	1
9	Perfluorotridecanoic acid (PFTriDA)	72629-94-8	1
10	Perfluoroundecanoic acid (PFUnDA)	2058-94-8	1
11	Perfluorododecanoic acid (PFDoDA)	307-55-1	1
12	Perfluorotetradecanoic acid (PFTetraDA)	376-06-7	1
13	Perfluorobutanesulfonic acid (PFBS)	375-73-5	2
14	Perfluoropentanesulfonic acid (PFPS)	2706-91-4	2
15	Perfluorohexanesulfonic acid (PFHxS)	355-46-4	2
16	Perfluoroheptanesulfonic acid (PFHS)	375-92-8	2
17	Perfluorooctanesulfonic acid (PFOS)	1763-23-1	2
18	Perfluoroundecanesulfonic acid (PFUnDS)	749786-16-1	2
19	Perfluorotridecanesulfonic acid (PFTriDS)	791563-89-8	2
20	Perfluorodecanesulfonic acid (PFDS)	335-77-3	2
21	Perfluorododecanesulfonic acid (PFDoDS)	79780-39-5	2
22	Potassium 9-chlorohexadecafluoro-3-oxanonane-1-sulfonate (KClHxDFS)	73606-19-6	2
23	Perfluorononanesulfonate (PFNS)	474511-07-4	2
24	Sodium dodecafluoro-3H-4, 8-dioxanonanoate (NaDoDFNt)	2250081-67-3	3
25	Ammonium 2,3,3,3-tetrafluoro-2-(heptafluoropropoxy)propanoate (NH4TetraFPt)	62037-80-3	3
26	Ammonium 4,8-dioxa-3H-perfluorononanoate (NH4PFNt)	958445-44-8	3

Group 1

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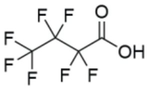

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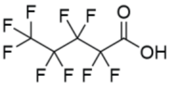

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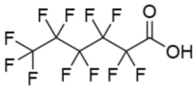

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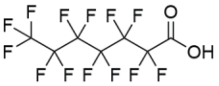

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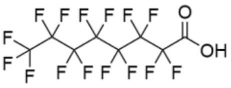

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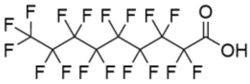

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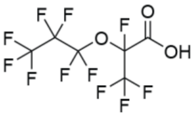

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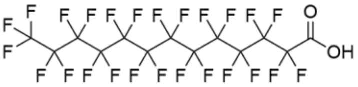

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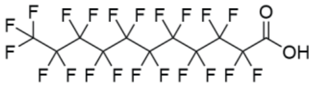

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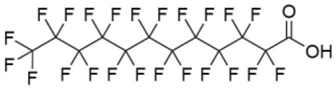

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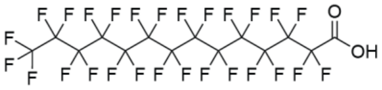

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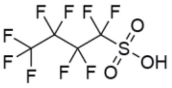

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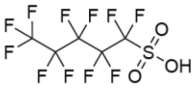

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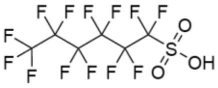

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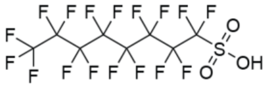

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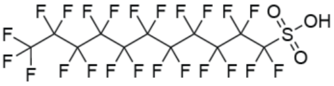

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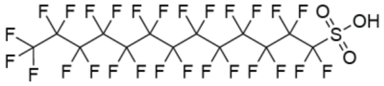

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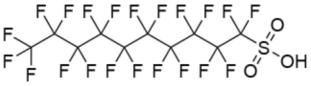

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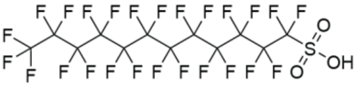

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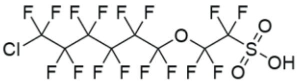

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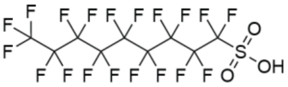

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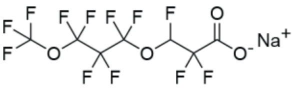

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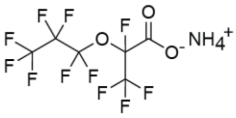

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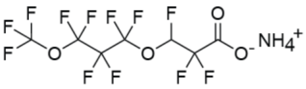

Figure S3. Chemical structures of all twenty-six (26) PFAS studied in this work and divided into four groups based on their chemical structures. Each structure is labeled with a number corresponding to an entry in Table S7.

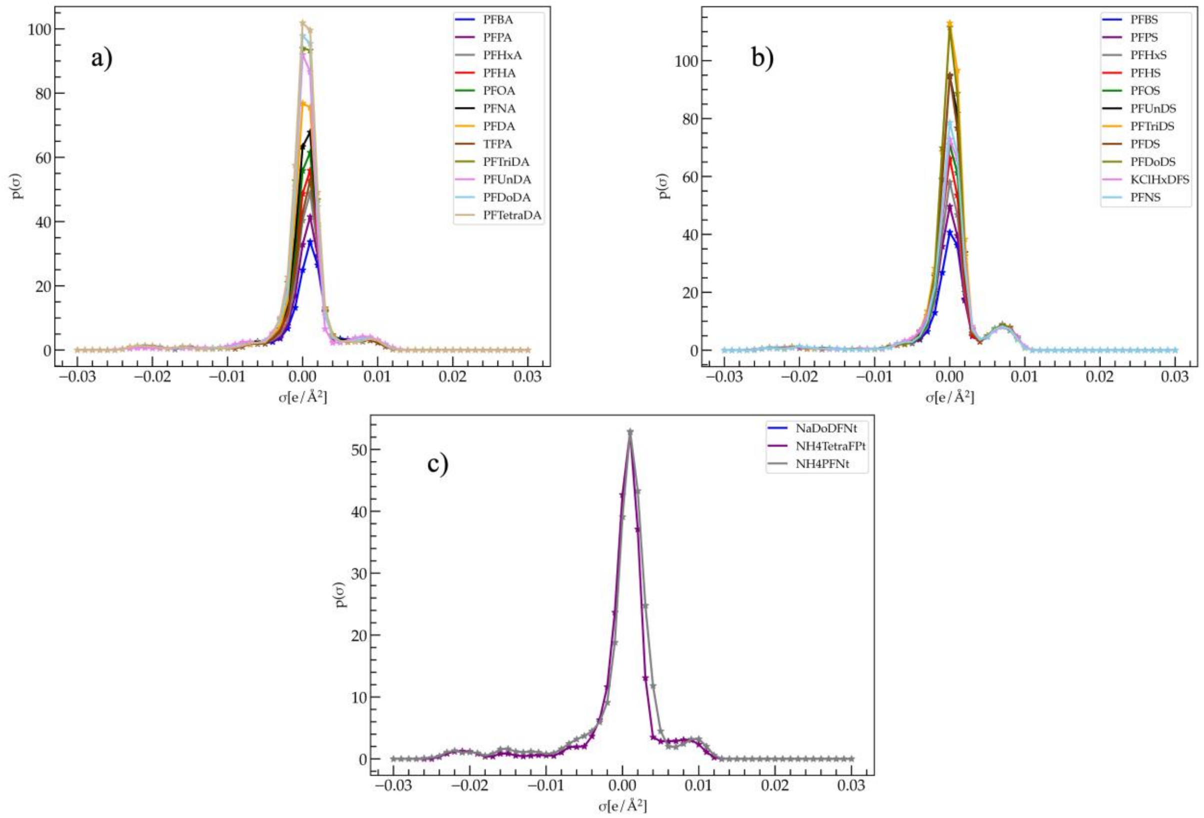

Figure S4. σ-profiles for all twenty-six PFAS studied in this work. PFAS are grouped based on their structures (shown in Figure S3). Similar structures lead to similar σ-profiles as expected.

Effect of Dissolved Contaminants on Partitioning

Case Study 1 of the main text analyzed the partitioning of four BFRs and Case Study 2 experimentally validated the modeling framework through the extraction of BBP from PVC. In these and other case studies, the partitioning of each contaminant was considered independently, but partitioning behavior could change if mixtures of multiple contaminants were considered. We thus sought to analyze the impact of mixtures of contaminants. We assume that the selected solvent initially contains a known concentration of contaminant *A* and is subsequently used to extract a different contaminant *B* from a polymer matrix. Since xylenes were experimentally employed to extract BBP from PVC (**Figure 6** of the main text), we consider a scenario in which the resulting spent xylenes are reused to extract BFRs from PS, PET, PE, and PP polymers, which are commonly reported to contain such BFRs.[3, 6] Accordingly, we predict log *P* values for tri-PBDE, DECA, HBCD, and TBBPA-dbP between a polymer phase and a solvent phase consisting of o-xylene with a known concentration of BBP. From **Figure 6**, at an elevated temperature of 130 °C, the experimental extraction efficiency of BBP from PVC using xylenes was approximately 100%, corresponding to complete removal of 0.3 g of BBP using 75 g of solvent based on the BBP–PVC blend mass ratio. Under these conditions, the resulting spent solvent would contain ~0.4 wt% BBP. In contrast, at room temperature, where only about 50% of the 0.3 g BBP was removed in a single wash, the spent xylene would contain ~0.2 wt% BBP. We thus compared log *P* values computed for both conditions and compared to values computed without assuming any dissolved BBP, with results summarized in Tables S8 and S9.

Table S8. Predicted log *P* values for BFRs in four different systems containing different polymers and spent o-xylene with a BBP concentration of 0.2 wt% at room temperature.

Polymer	Tri-PBDE		DECA		HBCD		TBBPA-dbP	
	0 wt% BBP	0.2 wt% BBP	0 wt% BBP	0.2 wt% BBP	0 wt% BBP	0.2 wt% BBP	0 wt% BBP	0.2 wt% BBP
PS	0.6	0.6	0.8	0.8	0.6	0.6	0.8	0.8
PET	0.2	0.2	0.7	0.7	-0.5	-0.5	-0.6	-0.6
PE	1.3	1.3	2.1	2.1	2.1	2.1	3.1	3.1
PP	1.5	1.5	2.3	2.3	2.3	2.3	3.3	3.3

Table S9. Predicted log *P* values for BFRs in four different systems containing different polymers and spent o-xylene with a BBP concentration of 0.4 wt% at 130°C. Values in bold indicate differences associated with the 0.4 wt% fraction.

Polymer	Tri-PBDE		DECA		HBCD		TBBPA-dbP	
	0 wt% BBP	0.4 wt% BBP	0 wt% BBP	0.4 wt% BBP	0 wt% BBP	0.4 wt% BBP	0 wt% BBP	0.4 wt% BBP
PS	0.6	0.6	0.8	0.8	0.6	0.6	0.8	0.8
PET	0.4	0.4	0.7	0.7	0.0	0.0	0.1	0.1
PE	0.9	0.9	1.5	1.5	1.4	1.4	2.1	2.1
PP	1.1	1.1	1.7	1.7	1.6	1.6	2.3	2.3

The predicted log *P* values in both Tables S8 and S9 indicate that, at a given temperature, the predicted partitioning of each BFR is not affected by the presence of dissolved BBP in the solvent phase. There are observed temperature-dependent variations in log *P*, chiefly for BFR removal from PET, but these do not depend upon the BBP concentration. We also note that we chose BBP removal as a worst-case scenario because of the high amount of phthalate present in the PVC case study. In practical conditions, typical concentrations of BFRs and phthalates in polymer-solvent systems are on the order of ppm,[7, 8] which is substantially more dilute than the concentration considered here. Consequently, we believe it is unlikely that the presence of contaminants at typical dilute conditions will impact predicted partitioning behavior.

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(1) Zhou, P.; Sánchez-Rivera, K. L.; Huber, G. W.; Van Lehn, R. C. Computational approach for rapidly predicting temperature-dependent polymer solubilities using molecular-scale models. *ChemSusChem* **2021**, *14* (19), 4307–4316.

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