Feasibility of using 2,3,3,3-tetrafluoropropene (R1234yf) as a solvent for solidliquid extraction of biopharmaceuticals

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Electronic Supporting Information

1. Energy graphs

Table S1 shows the data used in the plot of the energy graphs, Figure 4.

(kcal/mol)	E misfit	E H-bonding	E VdW	H total	μ mix	In Y
tetrafluoroethane	3.19186	-0.85635	-10.00739	-7.67183	-5.13526	-2.29601555
propanone	5.66174	-0.08433	-12.29371	-6.71622	-4.06840	-0.46366906
tetrafluoropropene	3.19456	-0.42565	-10.44859	-7.67962	-3.69730	0.17369733
toluene	3.89751	0.00000	-12.72758	-8.83001	-3.50890	0.49728391
water	4.36574	-4.55268	-10.40504	-10.59193	0.95658	8.16678235

Table S1. Data for energy graphs

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