Supporting information for "SAMPL9 blind predictions for toluene/water partition coefficients using nonequilibrium alchemical approaches"

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	water		1-octanol		toluene				
	ΔG_s	A^2	ΔG_s	A^2	ΔG_s	A^2	LogP_{ow}	Exp	LogP_{tw}
01	-10.46 ± 0.42	0.50	-18.12 ± 0.67	0.41	-18.42 ± 0.20	0.26	5.58 ± 0.57	2.7	5.81 ± 0.34
02	-2.61 ± 0.30	0.54	-11.63 ± 0.80	0.46	-12.49 ± 0.20	0.28	6.58 ± 0.62	3.1	7.21 ± 0.26
03	-3.30 ± 0.44	0.23	-13.40 ± 0.49	0.22	-14.39 ± 0.24	0.30	7.37 ± 0.48	4.92	8.09 ± 0.37
04	-5.15 ± 0.28	0.50	-15.74 ± 0.55	0.30	-17.39 ± 0.24	0.39	7.73 ± 0.45	4.77	8.93 ± 0.27
05	-0.88 ± 0.35	0.29	-12.66 ± 0.67	0.52	-13.56 ± 0.24	0.16	8.60 ± 0.55	3.38	9.26 ± 0.31
06	-10.35 ± 0.32	0.15	-11.46 ± 0.53	0.27	-10.57 ± 0.14	0.45	0.81 ± 0.45	-1.37	0.16 ± 0.25
07	-8.52 ± 0.72	0.72	-20.50 ± 1.01	0.57	-22.21 ± 0.36	0.24	8.74 ± 0.91	4.36	9.99 ± 0.59
08	-28.19 ± 0.52	1.77	-38.59 ± 4.16	0.28	-32.18 ± 0.50	1.24	7.59 ± 3.06	3.75	2.91 ± 0.53
09	-4.72 ± 0.36	0.41	-14.37 ± 0.65	0.65	-15.56 ± 0.21	0.27	7.04 ± 0.54	4.8	7.91 ± 0.30
10	-10.17 ± 0.34	0.70	-13.99 ± 0.34	0.58	-14.73 ± 0.23	0.39	2.79 ± 0.35	3.13	3.33 ± 0.30
11	-8.97 ± 0.30	0.61	-15.02 ± 0.85	0.59	-14.72 ± 0.18	0.26	4.41 ± 0.66	1.59	4.20 ± 0.25
12	-13.09 ± 0.22	0.22	-14.41 ± 0.86	0.47	-11.84 ± 0.16	0.26	0.96 ± 0.65	0.91	-0.91 ± 0.20
13	-7.60 ± 0.33	0.31	-14.21 ± 0.71	0.49	-14.70 ± 0.20	0.26	4.82 ± 0.57	1.75	5.18 ± 0.28
14	-6.83 ± 0.58	0.53	-17.03 ± 0.45	0.52	-17.61 ± 0.26	0.22	7.44 ± 0.54	3.44	7.87 ± 0.47
15	-19.11 ± 0.30	0.41	-24.72 ± 1.28	0.18	-21.96 ± 0.24	0.26	4.09 ± 0.96	0.89	2.08 ± 0.28
16	-15.43 ± 0.57	0.17	-25.05 ± 1.38	0.52	-23.96 ± 0.26	0.43	7.02 ± 1.09	2.68	6.22 ± 0.46

TABLE S1. Calculated solvation free energies, ΔG_s (kcal/mol), A^2 (Anderson Darling test of normality), octanol/water (LogP_{ow}) and toluene/water (LogP_{tw}) partition coefficients for the compounds in Figure 1 of the main paper. Atomic charges are of the AM1-BCC type. The entry marked "Exp." are the experimental LogP_{ow}.

	water		1-octanol		toluene				
	ΔG_s	A^2	ΔG_s	A^2	ΔG_s	A^2	LogP_{ow}	Exp.	LogP_{tw}
01	-14.26 ± 0.70	0.49	-19.42 ± 0.88	0.26	-19.21 ± 0.20	0.19	3.77 ± 0.82	2.7	3.61 ± 0.53
02	-7.50 ± 0.55	0.33	-12.47 ± 0.50	0.23	-12.89 ± 0.20	0.19	3.63 ± 0.54	3.1	3.94 ± 0.42
03	-3.07 ± 0.52	0.44	-13.45 ± 0.48	0.56	-14.15 ± 0.24	0.19	7.58 ± 0.51	4.92	8.09 ± 0.40
04	-9.08 ± 0.25	0.36	-17.86 ± 1.02	0.50	-18.26 ± 0.24	0.26	6.41 ± 0.77	4.77	6.70 ± 0.26
05	-2.66 ± 0.33	0.21	-12.37 ± 0.37	0.41	-14.14 ± 0.24	0.20	7.09 ± 0.36	3.38	8.38 ± 0.28
06	-15.81 ± 0.59	0.46	-13.85 ± 0.72	0.43	-11.74 ± 0.14	0.19	-1.43 ± 0.68	-1.37	-2.97 ± 0.45
07	-14.23 ± 1.39	0.28	-24.25 ± 1.13	0.40	-22.22 ± 0.36	0.34	7.32 ± 1.31	4.36	5.83 ± 1.05
08	-35.73 ± 0.59	1.70	-44.63 ± 0.96	0.60	-36.33 ± 0.50	0.95	6.50 ± 0.82	3.75	0.44 ± 0.82
09	-2.85 ± 0.36	0.39	-13.88 ± 0.36	0.36	-15.56 ± 0.21	0.28	8.06 ± 0.37	4.8	9.28 ± 0.33
10	-11.80 ± 0.28	0.41	-16.33 ± 0.85	0.57	-14.96 ± 0.23	0.19	3.30 ± 0.65	3.13	2.30 ± 0.24
11	-13.54 ± 0.24	0.35	-18.97 ± 1.76	0.48	-17.20 ± 0.18	0.20	3.97 ± 1.29	1.59	2.68 ± 0.23
12	-14.47 ± 0.23	0.52	-15.49 ± 0.88	0.49	-11.58 ± 0.16	0.14	0.74 ± 0.66	0.91	-2.11 ± 0.20
13	-10.04 ± 0.49	0.26	-16.30 ± 1.12	0.23	-15.14 ± 0.20	0.24	4.57 ± 0.90	1.75	3.73 ± 0.40
14	-12.05 ± 1.17	0.42	-18.45 ± 1.02	0.29	-19.03 ± 0.26	0.24	4.67 ± 1.13	3.44	5.10 ± 0.87
15	-20.87 ± 0.54	0.30	-24.33 ± 1.35	0.16	-21.67 ± 0.24	0.28	2.52 ± 1.06	0.89	0.58 ± 0.44
16	-13.62 ± 0.91	0.52	-23.68 ± 1.19	0.22	-23.78 ± 0.26	0.27	7.34 ± 1.09	2.68	7.41 ± 0.69

TABLE S2. Calculated solvation free energies, ΔG_s (kcal/mol), A^2 (Anderson Darling test of normality), octanol/water (LogP_{ow}) and toluene/water (LogP_{tw}) partition coefficients for the compounds in Figure 1 of the main paper. Atomic charges are computed ate the HF/6-31Gd level of theory. The entry marked "Exp." are the experimental LogP_{ow}.

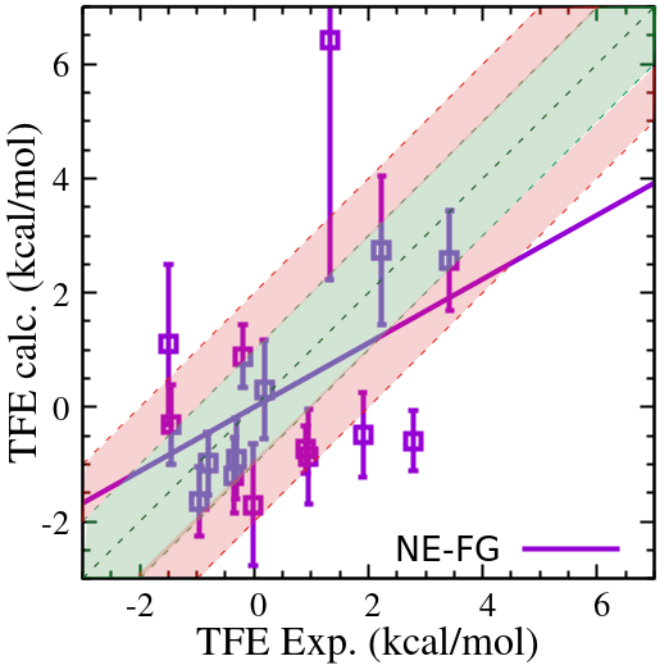

FIG. S1. Experimental and calculated (NE-FG) 1-octanol to toluene transfer free energy (TFE). The experimental value of the TFE from 1-octanol to toluene has been derived from the experimental values of the LogP_{ow} and LogP_{tw} as $\mathrm{TFE}(o \to t) = RT\ln(10)(\mathrm{LogP}_{tw} - \mathrm{LogP}_{p})$

Submission	MAE	R	τ	CCC	Method	Ranked
tran-lser-ufz	0.74	0.92	0.78	0.90	Emp.	T
tran-lser	0.91	0.91	0.77	0.88	Emp.	T
prediction-TN-KL	0.92	0.93	0.80	0.88	QM	T
Pitt-JWang	0.95	0.89	0.72	0.85	Emp.	T
NE-FG	1.12	0.83	0.58	0.82	MD	T
predictions-VoelzLab	1.26	0.90	0.72	0.82	MD	T
3DS	1.28	0.91	0.65	0.86	QM	T
ECRISM-1	1.40	0.89	0.68	0.79	QM	T
SAMPL9-Beckstein-Iorga-GAFF-TIP3P	1.50	0.79	0.61	0.75	MD	F
QM	1.56	0.87	0.64	0.77	QM	T
SAMPL9-Beckstein-Iorga-OPLS-AA-M24	1.72	0.88	0.63	0.73	MD	T
oxford	1.78	0.44	0.20	0.42	MD	T
SAMPL9-Beckstein-Iorga-OPLS-AA-TIP4P	1.88	0.91	0.70	0.72	MD	F
ECRISM-2	2.29	0.87	0.63	0.62	QM	F
Mixed	2.36	0.21	0.22	0.19	QM/MD	F
MD(Patel)	2.63	0.25	0.13	0.21	MD	F
paluch-sm8-basis	2.92	0.63	0.53	0.38	QM	F
paluch-sm8	2.92	0.63	0.53	0.38	QM	T
Sprick	3.03	0.66	0.63	0.47	MD	F

TABLE S3. Assessment metrics for LogP_{tw} SAMPL9 challenge for all predictions (ranked or not ranked). Entries in the "Method column": Emp. (empirical, knowledge-based); QM (quantum chemical calculation; implicit/solvent) MD (molecular dynamics, FEP or NE); QM/MD (mixed QM and MD)