

Supporting Information for "Evaluation of nine
condensed-phase force fields of the GROMOS,
CHARMM, OPLS, AMBER and OpenFF
families against experimental cross-solvation
free energies."

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S.1 Force-field comparison for individual compound pairs

For the five force fields newly considered in this work, the simulation results for all compound pairs are reported in Tab. S.1 in terms of calculated $\Delta_s G_{A:B}^{\ominus}$ values and associated statistical error bars. The reference experimental values are also given along with standard deviations σ over the available experimental estimates. This data is displayed graphically in Fig. S.1. The electrostatic and van der Waals contributions to the calculated $\Delta_s G_{A:B}^{\ominus}$ values are reported in Tab. S.2. This data is displayed graphically in Figs. S.2 and S.3. The deviations of the calculated $\Delta_s G_{A:B}^{\ominus}$ values relative to the experimental data are reported in Tab. S.3. Finally, root-mean-square errors relative to experiment for the transfer free energies $\Delta_t G_{C:A \rightarrow B}^{\ominus}$ of all solutes C between any pair of solvents A and B considering the FULL set are displayed in Fig. S.4. This figure is the analog of Main Article Fig. 6 for the FULL set. The tables analogous to Tabs. S.1 and S.2 and the figures analogous to in Figs. S.1-S.4 for the four force fields considered in our previous article¹⁶¹ are not repeated here, and can be found in Suppl. Mat. Sec. S.8 of Ref.⁴³.

Table S.1: Numerical values of the experimental and calculated cross-solvation free energies $\Delta_s G_{A:B}^{\ominus}$. The experimental values and the associated error estimates (\pm), corresponding to the standard deviation σ over available experimental values, are taken from Suppl. Mat. Tab. S.1 in Ref.⁴³ The calculated values are reported for the five force fields newly considered in this work (Main Article Tab. 1), along with their statistical error estimates (\pm) calculated using block averaging. The molecules considered and their acronyms are shown in Main Article Fig. 1. This data is displayed graphically in Fig. S.1.

Solute (A)	Solvent (B)	Experimental		GROMOS-54A7		GROMOS-ATB		OPLS-LBCC		AMBER-GAFF2		OpenFF	
		$\Delta_s G_{A:B}^{\ominus}$	\pm	$\Delta_s G_{A:B}^{\ominus}$	\pm	$\Delta_s G_{A:B}^{\ominus}$	\pm	$\Delta_s G_{A:B}^{\ominus}$	\pm	$\Delta_s G_{A:B}^{\ominus}$	\pm	$\Delta_s G_{A:B}^{\ominus}$	\pm
[kJ·mol ⁻¹]													
DAMD	DAMD	-23.32	5.0	-	-	-40.13	1.41	-33.80	0.40	-28.61	0.25	-30.37	0.33
DAMD	PPN	-26.09	-	-	-	-38.49	0.77	-33.33	0.20	-28.64	0.21	-30.66	0.19
DAMD	BTN	-24.49	-	-	-	-37.23	0.74	-32.58	0.21	-28.24	0.21	-29.84	0.18
DAMD	PYRI	-23.41	-	-	-	-38.81	1.29	-34.21	0.51	-29.62	0.26	-31.66	0.27
DAMD	H2O	-21.87	-	-	-	-34.78	1.89	-34.62	0.19	-24.96	0.20	-31.62	0.15
DAMD	C2CL2	-26.09	4.22	-	-	-38.14	0.85	-36.33	0.41	-30.25	0.26	-33.17	0.26
DAMD	EAE	-26.77	-	-	-	-37.67	0.92	-32.50	0.29	-27.65	0.21	-30.50	0.33
DAMD	PTL	-23.41	-	-	-	-36.95	1.80	-31.85	0.70	-30.83	0.60	-35.76	0.43
DAMD	MTL	-22.21	-	-	-	-38.77	0.96	-34.57	0.32	-31.34	0.31	-40.21	0.20
DAMD	ETL	-22.15	-	-	-	-38.41	1.44	-33.48	0.43	-32.61	0.35	-38.16	0.35
DAMD	BTL	-20.44	-	-	-	-36.11	1.99	-32.05	0.46	-29.80	0.90	-37.66	0.49
DAMD	2M2P	-25.81	-	-	-	-41.78	3.50	-31.90	0.55	-31.00	0.64	-36.32	0.73

Table S.1 – Continued on next page

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Solute (A)	Solvent (B)	Experimental		GROMOS-54A7		GROMOS-ATB		OPLS-LBCC		AMBER-GAFF2		OpenFF	
		$\Delta_s G_{A:B}^\ominus$	\pm	$\Delta_s G_{A:B}^\ominus$	\pm	$\Delta_s G_{A:B}^\ominus$	\pm	$\Delta_s G_{A:B}^\ominus$	\pm	$\Delta_s G_{A:B}^\ominus$	\pm	$\Delta_s G_{A:B}^\ominus$	\pm
[kJ·mol ⁻¹]													
DAMD	1PL	-22.89	-	-	-	-38.30	1.42	-32.51	0.39	-31.30	0.79	-37.72	0.28
DAMD	2PL	-23.87	-	-	-	-39.63	2.77	-32.24	0.42	-30.84	0.55	-37.26	0.43
DAMD	ANLN	-27.12	-	-	-	-46.01	1.32	-36.40	0.70	-34.11	0.86	-36.26	0.78
DAMD	DEE	-21.58	-	-	-	-34.44	0.64	-28.35	0.16	-24.57	0.11	-25.67	0.26
DAMD	CHCL3	-30.24	3.47	-	-	-44.31	1.23	-41.51	0.38	-34.92	0.31	-35.78	0.27
DAMD	DEAN	-22.1	-	-	-	-33.20	0.75	-29.92	0.21	-29.34	0.23	-28.39	0.23
DAMD	TEAN	-18.04	-	-	-	-27.80	0.79	-25.44	0.26	-21.22	0.26	-24.31	0.22
DAMD	TOL	-20.61	-	-	-	-32.85	0.88	-30.14	0.34	-26.34	0.24	-26.66	0.23
DAMD	BZN	-22.61	-	-	-	-35.77	0.90	-30.26	0.25	-27.93	0.27	-27.79	0.21
DAMD	HPE	-15.47	-	-	-	-24.79	0.65	-19.22	0.19	-18.74	0.18	-18.23	0.12
DAMD	HXE	-17.41	-	-	-	-24.69	0.59	-19.29	0.25	-19.20	0.16	-18.34	0.11
DAMD	CCL4	-19.69	-	-	-	-27.10	1.21	-	-	-21.65	0.14	-21.41	0.25
DAMD	CHE	-17.7	-	-	-	-24.26	0.64	-20.37	0.20	-19.61	0.25	-18.87	0.21
PPN	DAMD	-16.49	0.01	-	-	-19.13	1.10	-18.40	0.35	-16.80	0.22	-16.97	0.22
PPN	PPN	-17.35	0.02	-18.67	0.56	-19.37	0.60	-19.66	0.15	-17.46	0.17	-18.11	0.12
PPN	BTN	-16.7	0.02	-18.09	0.56	-19.22	0.65	-19.08	0.20	-17.08	0.18	-17.38	0.14
PPN	PYRI	-16.71	0.02	-	-	-18.49	0.96	-19.01	0.34	-17.26	0.23	-17.91	0.22
PPN	H2O	-15.95	0.08	-10.07	1.28	-14.09	1.33	-16.25	0.12	-13.53	0.15	-14.28	0.12
PPN	C2CL2	-17.67	0.2	-	-	-19.63	0.77	-21.04	0.35	-18.10	0.20	-18.82	0.17
PPN	EAE	-16.32	0.01	-18.13	0.93	-18.55	0.71	-18.56	0.26	-16.81	0.20	-16.87	0.28
PPN	PTL	-13.46	0.54	-14.28	1.25	-17.55	1.33	-17.33	0.28	-13.94	0.43	-18.39	0.39
PPN	MTL	-16.5	0.01	-15.69	0.88	-18.92	0.71	-19.18	0.16	-17.89	0.25	-21.37	0.18
PPN	ETL	-15.81	0.02	-15.43	1.01	-17.75	1.05	-19.00	0.26	-17.91	0.30	-20.26	0.29
PPN	BTL	-14.67	0.0	-14.57	0.99	-16.02	1.59	-18.12	0.34	-15.61	0.60	-18.40	0.36
PPN	2M2P	-13.76	-	-15.44	1.04	-18.18	2.55	-18.12	0.37	-16.36	0.48	-18.97	0.39
PPN	1PL	-14.27	-	-15.89	1.14	-17.37	0.97	-18.98	0.22	-16.59	0.38	-19.13	0.25
PPN	2PL	-14.45	0.2	-15.47	1.18	-17.32	1.94	-18.25	0.38	-16.68	0.53	-19.38	0.36
PPN	ANLN	-17.28	0.04	-18.92	2.49	-23.49	0.96	-20.59	0.61	-20.06	0.90	-20.02	0.56
PPN	DEE	-14.44	0.0	-15.47	0.45	-17.48	0.49	-17.27	0.16	-14.47	0.13	-14.78	0.16
PPN	CHCL3	-18.53	0.11	-18.12	0.72	-21.53	1.01	-25.48	0.27	-20.43	0.24	-20.61	0.22
PPN	DEAN	-13.3	-	-17.69	0.85	-16.78	0.57	-17.90	0.16	-17.10	0.22	-16.55	0.15
PPN	TEAN	-12.84	-	-15.13	0.57	-12.36	0.61	-14.08	0.19	-11.06	0.19	-13.50	0.17
PPN	TOL	-14.96	0.1	-16.67	0.70	-15.75	0.76	-17.39	0.18	-15.03	0.17	-15.56	0.19
PPN	BZN	-15.88	0.05	-17.13	0.64	-17.52	0.75	-17.65	0.21	-16.39	0.18	-16.00	0.20
PPN	HPE	-10.9	0.1	-12.77	0.46	-11.04	0.45	-10.24	0.13	-9.52	0.11	-9.51	0.12
PPN	HXE	-10.94	0.12	-13.11	0.45	-10.97	0.48	-10.25	0.14	-10.18	0.13	-9.96	0.09
PPN	CCL4	-13.99	0.19	-13.84	0.80	-11.15	0.89	-	-	-11.46	0.18	-11.51	0.19
PPN	CHE	-11.09	0.19	-13.50	0.51	-11.50	0.49	-10.59	0.20	-9.65	0.24	-9.68	0.23
BTN	DAMD	-18.78	0.08	-	-	-18.63	1.12	-19.82	0.38	-20.09	0.25	-19.05	0.24
BTN	PPN	-19.45	0.07	-20.95	0.57	-21.05	0.58	-21.54	0.19	-20.38	0.16	-20.34	0.15
BTN	BTN	-19.04	0.1	-20.49	0.61	-20.31	0.68	-20.99	0.23	-20.19	0.18	-19.98	0.18
BTN	PYRI	-19.46	0.1	-	-	-20.62	1.02	-20.54	0.29	-20.57	0.27	-20.17	0.19
BTN	H2O	-15.06	0.1	-9.37	1.41	-11.43	1.59	-15.54	0.16	-13.30	0.17	-13.76	0.15
BTN	C2CL2	-20.78	0.0	-	-	-21.87	0.82	-22.70	0.34	-21.44	0.20	-21.89	0.18
BTN	EAE	-18.56	0.03	-20.66	0.85	-19.71	0.80	-20.63	0.26	-19.75	0.20	-19.69	0.31
BTN	PTL	-16.27	0.0	-17.47	1.34	-18.53	1.30	-19.66	0.37	-18.20	0.54	-21.42	0.38
BTN	MTL	-19.02	0.03	-17.61	0.91	-19.39	0.74	-20.64	0.24	-20.57	0.23	-23.81	0.21
BTN	ETL	-18.04	0.01	-17.42	1.11	-18.93	1.09	-20.79	0.38	-20.96	0.36	-22.55	0.26
BTN	BTL	-17.27	0.03	-17.53	1.45	-16.87	1.62	-20.61	0.27	-17.77	0.50	-21.78	0.34
BTN	2M2P	-17.79	0.02	-18.40	1.28	-20.40	3.29	-20.48	0.36	-20.29	0.66	-22.34	0.50

Table S.1 – Continued on next page

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Solute (A)	Solvent (B)	Experimental		GROMOS-54A7		GROMOS-ATB		OPLS-LBCC		AMBER-GAFF2		OpenFF	
		$\Delta_s G_{A:B}^\ominus$	\pm	$\Delta_s G_{A:B}^\ominus$	\pm	$\Delta_s G_{A:B}^\ominus$	\pm	$\Delta_s G_{A:B}^\ominus$	\pm	$\Delta_s G_{A:B}^\ominus$	\pm	$\Delta_s G_{A:B}^\ominus$	\pm
[kJ·mol ⁻¹]													
BTN	1PL	-17.49	0.07	-17.13	1.35	-18.71	0.98	-20.83	0.34	-19.07	0.57	-22.60	0.36
BTN	2PL	-17.13	0.06	-17.45	1.25	-16.93	2.08	-19.90	0.47	-19.18	0.47	-22.23	0.32
BTN	ANLN	-20.29	0.05	-18.42	2.45	-24.35	1.05	-22.23	0.38	-22.09	1.12	-22.17	0.92
BTN	DEE	-17.3	0.0	-18.57	0.47	-18.95	0.62	-19.47	0.14	-17.97	0.15	-17.97	0.21
BTN	CHCL3	-22.61	0.23	-21.30	0.75	-23.02	0.90	-28.14	0.29	-24.53	0.24	-23.85	0.25
BTN	DEAN	-17.36	-	-20.03	0.96	-18.92	0.55	-20.16	0.24	-20.40	0.26	-18.62	0.17
BTN	TEAN	-15.6	0.32	-17.42	0.63	-14.55	0.71	-16.66	0.25	-14.44	0.17	-16.55	0.25
BTN	TOL	-17.87	0.05	-19.32	0.72	-19.04	0.75	-19.24	0.29	-18.51	0.21	-18.74	0.18
BTN	BZN	-18.66	0.01	-19.95	0.78	-19.82	0.88	-20.03	0.19	-19.61	0.23	-19.16	0.18
BTN	HPE	-14.11	0.05	-15.99	0.49	-13.51	0.57	-12.95	0.12	-13.17	0.17	-13.06	0.13
BTN	HXE	-14.49	0.12	-15.63	0.59	-14.34	0.57	-13.34	0.13	-13.68	0.16	-13.13	0.11
BTN	CCL4	-17.14	0.07	-16.71	0.92	-14.57	0.97	-	-	-15.54	0.19	-15.21	0.16
BTN	CHE	-14.46	0.19	-16.44	0.60	-14.14	0.57	-13.88	0.30	-14.02	0.28	-13.51	0.13
PYRI	DAMD	-24.69	0.6	-	-	-25.34	1.21	-28.31	0.38	-21.72	0.26	-22.73	0.17
PYRI	PPN	-22.66	-	-	-	-24.62	0.67	-27.14	0.16	-21.87	0.11	-22.39	0.18
PYRI	BTN	-22.52	0.03	-	-	-24.85	0.74	-27.11	0.20	-21.41	0.14	-22.26	0.17
PYRI	PYRI	-23.03	0.08	-	-	-25.04	1.15	-27.37	0.34	-21.24	0.26	-22.50	0.28
PYRI	H2O	-19.32	0.26	-	-	-18.14	1.38	-19.02	0.18	-11.92	0.13	-14.05	0.16
PYRI	C2CL2	-23.27	0.28	-	-	-24.60	0.77	-28.48	0.34	-22.14	0.21	-22.98	0.16
PYRI	EAE	-28.2	-	-	-	-24.97	0.82	-26.45	0.30	-21.17	0.24	-22.63	0.22
PYRI	PTL	-20.1	-	-	-	-22.88	1.32	-24.19	0.40	-18.35	0.49	-22.56	0.37
PYRI	MTL	-24.33	-	-	-	-22.98	0.80	-25.15	0.23	-19.31	0.20	-23.85	0.21
PYRI	ETL	-23.31	0.53	-	-	-22.62	1.09	-25.55	0.27	-19.93	0.22	-23.12	0.26
PYRI	BTL	-22.55	0.0	-	-	-22.19	1.38	-24.26	0.35	-18.35	0.43	-22.08	0.35
PYRI	2M2P	-21.66	0.95	-	-	-23.61	2.81	-25.47	0.34	-19.39	0.59	-22.38	0.45
PYRI	1PL	-22.78	0.01	-	-	-22.86	1.04	-25.40	0.31	-19.11	0.34	-22.85	0.28
PYRI	2PL	-22.04	0.0	-	-	-23.85	1.90	-25.22	0.35	-17.96	0.36	-23.21	0.36
PYRI	ANLN	-39.45	-	-	-	-23.97	1.08	-28.65	0.51	-22.27	1.35	-23.09	0.56
PYRI	DEE	-30.6	-	-	-	-24.26	0.60	-24.52	0.17	-19.01	0.17	-20.61	0.19
PYRI	CHCL3	-26.99	0.02	-	-	-27.36	1.00	-31.43	0.30	-23.71	0.26	-24.74	0.19
PYRI	DEAN	-19.41	-	-	-	-23.01	0.60	-25.00	0.22	-20.75	0.17	-21.77	0.21
PYRI	TEAN	-20.61	-	-	-	-21.51	0.65	-22.65	0.23	-16.87	0.16	-19.70	0.28
PYRI	TOL	-21.42	0.06	-	-	-23.61	0.72	-25.50	0.24	-19.59	0.17	-20.60	0.18
PYRI	BZN	-22.08	0.03	-	-	-25.04	0.81	-25.72	0.28	-21.41	0.22	-21.33	0.21
PYRI	HPE	-17.92	0.01	-	-	-20.10	0.66	-18.24	0.14	-15.36	0.21	-16.19	0.16
PYRI	HXE	-16.28	0.63	-	-	-19.65	0.52	-18.31	0.14	-15.54	0.11	-16.14	0.08
PYRI	CCL4	-21.08	0.24	-	-	-21.47	0.92	-	-	-17.11	0.25	-18.13	0.22
PYRI	CHE	-17.95	0.04	-	-	-19.41	0.62	-19.48	0.19	-15.65	0.19	-16.90	0.22
H2O	DAMD	-24.66	-	-	-	-19.45	0.66	-18.68	0.20	-20.18	0.18	-23.19	0.12
H2O	PPN	-14.79	-	-12.29	0.41	-15.33	0.35	-17.19	0.09	-16.95	0.09	-17.40	0.09
H2O	BTN	-10.85	-	-11.09	0.42	-13.61	0.41	-16.13	0.11	-15.51	0.13	-16.44	0.16
H2O	PYRI	-17.45	-	-	-	-15.25	0.52	-13.31	0.19	-12.54	0.12	-14.43	0.12
H2O	H2O	-26.45	0.04	-26.48	0.82	-26.33	0.85	-26.25	-	-26.40	-	-26.40	-
H2O	C2CL2	-10.28	-	-	-	-7.70	0.33	-11.07	0.12	-6.98	0.08	-6.32	0.08
H2O	EAE	-16.27	1.54	-14.81	0.52	-13.69	0.47	-14.67	0.15	-17.54	0.13	-16.23	0.17
H2O	PTL	-19.01	-	-16.88	1.81	-16.16	1.15	-17.45	0.42	-16.66	0.80	-14.78	0.34
H2O	MTL	-23.22	0.02	-22.85	0.90	-21.33	0.58	-23.52	0.11	-22.17	0.17	-20.33	0.12
H2O	ETL	-21.23	0.01	-18.74	1.07	-19.14	0.91	-22.00	0.23	-19.46	0.30	-18.13	0.19
H2O	BTL	-16.38	-	-18.19	1.27	-17.59	1.83	-19.07	0.25	-17.05	0.54	-15.72	0.38
H2O	2M2P	-34.82	-	-17.46	1.14	-17.08	2.29	-20.04	0.39	-16.77	0.66	-15.50	0.43

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Table S.1 – Continued from previous page

Solute (A)	Solvent (B)	Experimental		GROMOS-54A7		GROMOS-ATB		OPLS-LBCC		AMBER-GAFF2		OpenFF	
		$\Delta_s G_{A:B}^\ominus$	\pm	$\Delta_s G_{A:B}^\ominus$	\pm	$\Delta_s G_{A:B}^\ominus$	\pm	$\Delta_s G_{A:B}^\ominus$	\pm	$\Delta_s G_{A:B}^\ominus$	\pm	$\Delta_s G_{A:B}^\ominus$	\pm
[kJ·mol ⁻¹]													
H2O	1PL	-24.43	-	-18.51	1.49	-18.42	0.77	-20.56	0.24	-18.96	0.43	-16.85	0.27
H2O	2PL	-18.58	-	-17.41	1.37	-16.69	1.71	-19.93	0.27	-17.93	0.44	-16.35	0.30
H2O	ANLN	-14.1	-	-17.58	2.15	-17.73	0.59	-16.52	0.35	-16.89	0.99	-14.45	0.44
H2O	DEE	-4.28	-	-1.92	0.28	-7.24	0.35	-13.42	0.11	-5.29	0.10	-7.52	0.12
H2O	CHCL3	-8.61	0.09	-0.81	0.33	-5.32	0.43	-9.28	0.11	-5.74	0.12	-4.55	0.08
H2O	DEAN	-19.3	-	-14.08	0.74	-5.75	0.36	-18.44	0.18	-11.68	0.16	-16.05	0.20
H2O	TEAN	-12.33	-	-1.47	0.44	1.78	0.34	-10.69	0.16	1.26	0.11	-10.99	0.19
H2O	TOL	-7.08	0.0	-4.02	0.38	-3.46	0.37	-6.82	0.11	-4.33	0.11	-5.73	0.10
H2O	BZN	-7.13	0.01	-7.20	0.41	-5.13	0.41	-6.83	0.11	-8.09	0.11	-6.69	0.12
H2O	HPE	-1.43	1.03	3.06	0.23	3.00	0.22	2.57	0.05	3.88	0.08	3.46	0.10
H2O	HXE	-5.45	2.37	2.84	0.20	2.70	0.23	2.35	0.04	3.59	0.04	3.15	0.06
H2O	CCL4	-3.56	0.05	3.73	0.27	3.50	0.38	-	-	3.35	0.11	3.81	0.06
H2O	CHE	-1.66	0.02	3.37	0.25	2.51	0.21	3.11	0.08	4.63	0.09	4.16	0.10
C2CL2	DAMD	-21.08	0.07	-	-	-17.10	1.30	-26.19	0.55	-19.02	0.20	-19.04	0.31
C2CL2	PPN	-19.53	-	-	-	-18.37	0.64	-26.63	0.31	-19.00	0.18	-18.74	0.16
C2CL2	BTN	-20.12	0.04	-	-	-18.26	0.69	-26.17	0.30	-18.89	0.15	-18.87	0.15
C2CL2	PYRI	-16.84	-	-	-	-17.47	0.92	-25.26	0.54	-18.23	0.26	-18.05	0.16
C2CL2	H2O	-7.53	0.02	-	-	-3.46	1.51	-13.07	0.29	-2.82	0.17	-2.40	0.16
C2CL2	C2CL2	-19.87	-	-	-	-17.75	0.81	-24.43	0.57	-17.60	0.16	-17.69	0.21
C2CL2	EAE	-19.83	0.04	-	-	-17.49	0.75	-24.29	0.41	-18.90	0.26	-18.04	0.29
C2CL2	PTL	-16.33	-	-	-	-14.67	1.10	-23.20	0.58	-15.43	0.39	-15.64	0.38
C2CL2	MTL	-18.67	-	-	-	-15.41	0.67	-23.61	0.37	-14.52	0.17	-16.76	0.13
C2CL2	ETL	-17.64	-	-	-	-14.54	0.83	-24.41	0.40	-15.18	0.24	-16.67	0.24
C2CL2	BTL	-16.67	0.0	-	-	-14.44	1.14	-24.01	0.54	-15.22	0.29	-15.78	0.29
C2CL2	2M2P	-12.5	-	-	-	-15.13	2.03	-25.48	0.53	-14.93	0.61	-15.91	0.39
C2CL2	1PL	-16.79	-	-	-	-15.28	0.82	-25.20	0.35	-15.42	0.27	-16.39	0.21
C2CL2	2PL	-17.7	-	-	-	-14.81	1.24	-24.87	0.40	-14.98	0.28	-15.42	0.24
C2CL2	ANLN	-17.36	-	-	-	-17.43	1.05	-24.02	0.50	-17.66	0.93	-17.05	0.68
C2CL2	DEE	-18.61	0.0	-	-	-16.79	0.59	-23.50	0.21	-17.23	0.17	-18.04	0.17
C2CL2	CHCL3	-18.64	1.0	-	-	-18.03	0.97	-25.43	0.44	-17.60	0.21	-17.72	0.26
C2CL2	DEAN	-19.18	-	-	-	-15.77	0.60	-25.22	0.29	-17.34	0.24	-18.80	0.19
C2CL2	TEAN	-13.13	-	-	-	-14.30	0.74	-20.71	0.37	-15.13	0.19	-17.61	0.29
C2CL2	TOL	-18.33	-	-	-	-16.55	0.76	-22.96	0.39	-18.34	0.23	-17.67	0.23
C2CL2	BZN	-19.41	0.0	-	-	-17.89	0.88	-22.83	0.27	-19.23	0.22	-18.18	0.20
C2CL2	HPE	-16.98	1.51	-	-	-13.68	0.71	-14.48	0.15	-14.17	0.13	-13.60	0.16
C2CL2	HXE	-15.47	0.16	-	-	-13.75	0.59	-14.45	0.13	-14.48	0.18	-13.95	0.13
C2CL2	CCL4	-19.52	1.54	-	-	-13.97	1.05	-	-	-14.68	0.17	-14.61	0.26
C2CL2	CHE	-16.04	0.0	-	-	-13.50	0.70	-14.77	0.15	-14.46	0.31	-14.61	0.16
EAE	DAMD	-17.4	0.01	-	-	-22.94	1.35	-21.91	0.47	-20.66	0.28	-23.14	0.26
EAE	PPN	-19.75	-	-29.22	0.65	-23.06	0.71	-23.21	0.21	-21.29	0.16	-23.56	0.22
EAE	BTN	-18.82	0.02	-28.34	0.72	-22.95	0.68	-22.42	0.17	-21.03	0.21	-22.90	0.25
EAE	PYRI	-20.33	-	-	-	-23.88	1.06	-21.97	0.33	-21.43	0.26	-24.27	0.22
EAE	H2O	-12.79	0.25	-18.48	1.56	-12.57	1.63	-14.08	0.16	-14.94	0.17	-16.07	0.17
EAE	C2CL2	-20.57	0.43	-	-	-24.80	0.74	-23.34	0.34	-23.01	0.21	-25.07	0.24
EAE	EAE	-18.8	0.06	-28.75	1.09	-23.24	0.97	-22.60	0.20	-20.85	0.24	-23.54	0.23
EAE	PTL	-16.21	0.0	-27.87	2.23	-21.36	1.44	-21.49	0.29	-20.65	0.77	-24.79	0.52
EAE	MTL	-17.64	-	-27.43	1.21	-22.08	0.94	-21.61	0.25	-22.26	0.27	-26.99	0.22
EAE	ETL	-17.17	0.19	-25.69	1.73	-21.87	1.19	-21.62	0.28	-22.85	0.38	-25.98	0.27
EAE	BTL	-16.61	0.0	-26.01	1.95	-22.11	1.70	-21.52	0.42	-21.32	0.59	-25.43	0.39
EAE	2M2P	-20.55	-	-25.50	1.37	-22.04	2.34	-22.22	0.40	-22.96	0.94	-25.10	0.41

Table S.1 – Continued on next page

Table S.1 – Continued from previous page

Solute (A)	Solvent (B)	Experimental		GROMOS-54A7		GROMOS-ATB		OPLS-LBCC		AMBER-GAFF2		OpenFF	
		$\Delta_s G_{A:B}^\ominus$	\pm	$\Delta_s G_{A:B}^\ominus$	\pm	$\Delta_s G_{A:B}^\ominus$	\pm	$\Delta_s G_{A:B}^\ominus$	\pm	$\Delta_s G_{A:B}^\ominus$	\pm	$\Delta_s G_{A:B}^\ominus$	\pm
[kJ·mol ⁻¹]													
EAE	1PL	-17.24	-	-25.00	2.00	-22.98	1.00	-22.25	0.29	-21.33	0.53	-25.63	0.33
EAE	2PL	-16.73	0.2	-28.02	1.49	-21.36	2.06	-21.53	0.37	-22.00	0.66	-25.71	0.33
EAE	ANLN	-18.29	0.29	-30.57	3.36	-28.49	1.14	-24.58	0.48	-23.64	0.73	-26.54	0.78
EAE	DEE	-17.41	-	-24.72	0.56	-22.95	0.56	-21.45	0.20	-19.23	0.13	-21.79	0.17
EAE	CHCL3	-23.23	0.23	-27.96	0.86	-27.76	1.05	-28.16	0.31	-26.49	0.31	-27.81	0.26
EAE	DEAN	-16.33	-	-28.46	1.23	-22.91	0.66	-22.32	0.19	-22.47	0.27	-23.14	0.20
EAE	TEAN	-20.89	-	-23.33	0.75	-19.78	0.72	-19.41	0.23	-16.94	0.18	-20.71	0.26
EAE	TOL	-18.37	0.14	-26.53	0.85	-22.88	0.78	-22.64	0.25	-20.12	0.20	-22.82	0.19
EAE	BZN	-18.91	0.06	-27.59	0.87	-23.38	0.99	-22.99	0.23	-21.52	0.21	-23.56	0.15
EAE	HPE	-14.68	0.05	-20.33	0.69	-17.83	0.66	-15.96	0.15	-15.44	0.17	-17.52	0.22
EAE	HXE	-15.15	0.04	-19.81	0.52	-18.29	0.61	-16.16	0.16	-15.63	0.13	-17.43	0.15
EAE	CCL4	-18.29	0.27	-21.73	0.74	-19.97	1.24	-	-	-18.03	0.19	-19.96	0.21
EAE	CHE	-14.79	0.23	-21.04	0.66	-18.69	0.64	-17.26	0.29	-15.99	0.37	-17.82	0.23
PTL	DAMD	-27.86	-	-	-	-24.07	1.41	-23.44	0.58	-31.41	0.33	-29.85	0.26
PTL	PPN	-25.06	-	-29.06	0.79	-23.80	0.78	-24.46	0.18	-28.87	0.19	-27.39	0.17
PTL	BTN	-23.46	-	-28.57	0.89	-23.50	0.85	-24.21	0.26	-28.39	0.26	-27.32	0.19
PTL	PYRI	-26.83	-	-	-	-24.43	1.19	-22.80	0.49	-26.72	0.30	-26.85	0.26
PTL	H2O	-18.76	0.18	-21.59	1.68	-12.47	1.63	-18.25	0.18	-18.89	0.21	-11.98	0.19
PTL	C2CL2	-24.12	0.88	-	-	-22.13	0.86	-23.29	0.36	-24.24	0.25	-23.54	0.20
PTL	EAE	-22.64	3.0	-30.25	1.06	-23.71	1.03	-23.57	0.35	-29.99	0.34	-26.83	0.25
PTL	PTL	-29.48	2.11	-31.04	2.93	-25.70	1.65	-24.12	0.62	-28.96	0.63	-25.28	0.45
PTL	MTL	-28.14	0.01	-34.27	1.63	-25.47	0.98	-25.43	0.26	-30.30	0.31	-26.97	0.24
PTL	ETL	-28.32	-	-34.45	2.13	-25.63	1.42	-25.65	0.30	-30.64	0.45	-26.66	0.30
PTL	BTL	-28.32	0.0	-34.40	2.03	-26.30	2.13	-24.91	0.48	-30.45	0.73	-26.40	0.51
PTL	2M2P	-29.12	0.0	-31.99	1.53	-30.65	3.11	-25.41	0.64	-30.11	0.90	-26.33	0.57
PTL	1PL	-28.37	0.02	-33.48	1.94	-25.62	1.32	-25.46	0.43	-30.85	0.66	-26.37	0.24
PTL	2PL	-28.6	0.0	-34.25	1.84	-26.31	2.46	-25.86	0.55	-29.70	0.54	-26.67	0.35
PTL	ANLN	-28.32	-	-30.18	3.88	-25.29	1.11	-24.63	0.45	-27.12	1.38	-23.17	0.71
PTL	DEE	-25.52	-	-22.55	0.70	-22.20	0.68	-22.34	0.17	-22.64	0.21	-24.18	0.18
PTL	CHCL3	-24.77	0.16	-23.33	0.98	-24.00	1.03	-28.24	0.26	-26.36	0.29	-24.90	0.20
PTL	DEAN	-23.87	-	-31.27	1.32	-21.22	0.78	-24.94	0.36	-27.26	0.31	-29.47	0.27
PTL	TEAN	-23.18	-	-22.41	0.92	-17.90	0.85	-20.92	0.27	-18.56	0.21	-26.88	0.38
PTL	TOL	-21.69	0.16	-24.19	0.84	-21.35	0.88	-21.62	0.20	-22.79	0.22	-23.27	0.20
PTL	BZN	-21.34	0.01	-26.03	0.89	-22.74	1.06	-21.85	0.26	-24.84	0.24	-23.66	0.24
PTL	HPE	-17.4	0.64	-18.05	0.73	-16.83	0.67	-15.87	0.14	-16.68	0.32	-18.09	0.21
PTL	HXE	-18.48	0.38	-18.56	0.59	-17.13	0.68	-16.22	0.14	-17.24	0.17	-18.38	0.16
PTL	CCL4	-20.12	0.64	-19.84	0.89	-17.65	1.32	-	-	-19.51	0.20	-21.28	0.24
PTL	CHE	-15.53	0.94	-19.73	0.83	-17.08	0.62	-16.49	0.23	-16.30	0.29	-18.70	0.31
MTL	DAMD	-20.43	0.01	-	-	-15.05	0.76	-15.40	0.21	-17.39	0.15	-18.56	0.13
MTL	PPN	-17.29	0.01	-17.43	0.43	-13.38	0.43	-15.10	0.11	-15.49	0.13	-15.38	0.11
MTL	BTN	-16.03	0.01	-16.54	0.48	-12.73	0.54	-14.26	0.12	-14.74	0.11	-14.96	0.09
MTL	PYRI	-18.74	0.29	-	-	-12.49	0.65	-13.07	0.18	-12.15	0.17	-13.56	0.15
MTL	H2O	-21.31	0.04	-22.59	1.06	-14.90	0.97	-19.67	0.11	-17.36	0.09	-12.92	0.11
MTL	C2CL2	-10.95	0.69	-	-	-10.16	0.44	-13.34	0.19	-8.95	0.13	-9.66	0.11
MTL	EAE	-15.22	0.5	-19.28	0.67	-12.55	0.58	-13.40	0.19	-16.09	0.15	-14.67	0.14
MTL	PTL	-17.53	0.0	-23.12	1.36	-13.66	1.21	-14.75	0.42	-14.85	0.50	-12.04	0.31
MTL	MTL	-20.54	0.02	-26.09	1.23	-16.65	0.62	-18.39	0.16	-18.00	0.20	-15.36	0.12
MTL	ETL	-19.4	0.02	-24.90	1.26	-15.23	0.92	-17.50	0.23	-16.99	0.28	-14.36	0.20
MTL	BTL	-17.88	1.1	-24.71	1.37	-13.98	1.36	-15.83	0.32	-15.68	0.53	-13.25	0.23
MTL	2M2P	-19.36	0.0	-22.18	1.25	-16.40	2.86	-15.94	0.41	-15.23	0.68	-13.69	0.37

Table S.1 – Continued on next page

Table S.1 – Continued from previous page

Solute (A)	Solvent (B)	Experimental		GROMOS-54A7		GROMOS-ATB		OPLS-LBCC		AMBER-GAFF2		OpenFF	
		$\Delta_s G_{A:B}^\ominus$	\pm	$\Delta_s G_{A:B}^\ominus$	\pm	$\Delta_s G_{A:B}^\ominus$	\pm	$\Delta_s G_{A:B}^\ominus$	\pm	$\Delta_s G_{A:B}^\ominus$	\pm	$\Delta_s G_{A:B}^\ominus$	\pm
[kJ·mol ⁻¹]													
MTL	1PL	-17.97	0.01	-23.05	1.44	-15.11	0.84	-16.52	0.24	-17.13	0.48	-13.70	0.20
MTL	2PL	-19.12	0.2	-24.77	1.17	-14.84	2.00	-16.30	0.33	-16.87	0.44	-13.99	0.23
MTL	ANLN	-16.15	0.01	-25.27	2.36	-14.35	0.69	-16.00	0.42	-16.45	0.54	-13.69	0.42
MTL	DEE	-14.16	0.0	-8.99	0.39	-9.59	0.39	-12.22	0.14	-7.76	0.11	-10.72	0.13
MTL	CHCL3	-13.95	0.16	-9.30	0.50	-10.11	0.62	-15.40	0.13	-9.11	0.13	-9.75	0.16
MTL	DEAN	-14.5	-	-22.20	0.94	-8.04	0.38	-14.99	0.15	-13.01	0.21	-16.66	0.18
MTL	TEAN	-14.84	-	-9.27	0.55	-3.57	0.42	-9.76	0.18	-2.71	0.15	-13.58	0.19
MTL	TOL	-9.29	0.38	-11.51	0.53	-7.63	0.45	-9.90	0.15	-7.20	0.10	-9.47	0.10
MTL	BZN	-10.78	0.02	-13.53	0.53	-8.90	0.54	-10.10	0.13	-9.76	0.16	-10.10	0.16
MTL	HPE	-5.65	0.54	-4.55	0.35	-2.96	0.38	-3.40	0.08	-0.94	0.09	-3.85	0.10
MTL	HXE	-6.28	0.12	-4.87	0.30	-3.17	0.31	-3.58	0.09	-1.23	0.09	-4.12	0.06
MTL	CCL4	-9.27	0.32	-5.06	0.49	-3.42	0.48	-	-	-2.02	0.09	-4.62	0.15
MTL	CHE	-5.7	0.64	-5.05	0.39	-3.03	0.33	-3.22	0.11	-0.36	0.10	-3.81	0.09
ETL	DAMD	-21.89	0.33	-	-	-17.41	0.94	-17.77	0.26	-20.00	0.22	-21.50	0.16
ETL	PPN	-18.46	0.04	-19.89	0.55	-16.75	0.60	-17.67	0.13	-18.31	0.16	-18.35	0.14
ETL	BTN	-18.18	0.21	-18.88	0.56	-15.97	0.52	-16.96	0.17	-17.73	0.12	-18.04	0.14
ETL	PYRI	-21.08	0.08	-	-	-16.11	0.80	-15.54	0.30	-15.02	0.16	-17.27	0.15
ETL	H2O	-21.01	0.06	-21.76	1.20	-16.52	1.30	-20.29	0.14	-15.64	0.13	-12.93	0.13
ETL	C2CL2	-14.0	1.52	-	-	-12.63	0.61	-16.13	0.21	-12.25	0.12	-13.06	0.10
ETL	EAE	-17.29	0.25	-21.52	0.77	-16.01	0.66	-16.24	0.15	-19.06	0.21	-17.46	0.17
ETL	PTL	-19.47	0.0	-25.42	1.91	-18.41	1.30	-17.47	0.38	-17.70	0.48	-15.97	0.45
ETL	MTL	-22.2	0.01	-26.75	1.09	-20.60	0.66	-21.17	0.25	-19.68	0.18	-18.48	0.17
ETL	ETL	-21.25	0.08	-26.49	1.47	-19.73	0.97	-20.02	0.27	-19.28	0.35	-17.97	0.18
ETL	BTL	-20.5	0.29	-23.29	2.08	-19.85	1.70	-18.57	0.33	-18.45	0.60	-16.82	0.27
ETL	2M2P	-21.13	0.0	-23.32	1.63	-23.76	2.72	-18.76	0.42	-18.63	0.71	-16.98	0.48
ETL	1PL	-20.22	0.37	-26.59	1.57	-18.68	0.96	-18.96	0.24	-18.84	0.34	-16.65	0.26
ETL	2PL	-20.64	0.28	-25.71	1.55	-19.34	1.99	-19.01	0.37	-18.16	0.43	-17.20	0.33
ETL	ANLN	-18.12	0.22	-25.37	2.86	-17.08	0.77	-18.83	0.45	-17.10	0.71	-17.82	0.79
ETL	DEE	-11.31	-	-12.04	0.47	-13.27	0.51	-14.97	0.13	-11.47	0.15	-14.05	0.14
ETL	CHCL3	-16.46	0.22	-12.47	0.54	-13.18	0.81	-18.90	0.25	-13.05	0.15	-13.53	0.15
ETL	DEAN	-20.21	-	-22.66	1.02	-11.33	0.52	-17.34	0.19	-15.51	0.23	-19.03	0.16
ETL	TEAN	-17.27	0.26	-11.65	0.62	-7.11	0.54	-12.67	0.19	-6.83	0.13	-16.76	0.21
ETL	TOL	-13.69	0.5	-13.78	0.62	-11.13	0.64	-13.11	0.20	-10.84	0.17	-12.92	0.15
ETL	BZN	-14.18	0.32	-16.14	0.66	-12.32	0.68	-13.32	0.15	-12.88	0.13	-13.11	0.15
ETL	HPE	-9.07	0.13	-7.94	0.40	-6.12	0.44	-6.72	0.12	-5.27	0.11	-7.56	0.09
ETL	HXE	-10.8	0.59	-7.99	0.40	-6.68	0.38	-6.83	0.11	-5.72	0.14	-7.87	0.10
ETL	CCL4	-12.05	0.52	-8.66	0.56	-6.67	0.77	-	-	-6.62	0.16	-9.01	0.11
ETL	CHE	-10.49	0.54	-7.92	0.50	-6.54	0.43	-6.61	0.13	-5.07	0.18	-7.73	0.18
BTL	DAMD	-25.8	0.29	-	-	-24.77	1.23	-20.70	0.47	-27.97	0.26	-26.96	0.22
BTL	PPN	-23.98	-	-26.06	0.75	-23.50	0.75	-21.72	0.15	-26.02	0.19	-24.15	0.22
BTL	BTN	-23.54	0.08	-25.39	0.71	-23.42	0.72	-21.09	0.16	-25.78	0.21	-24.00	0.20
BTL	PYRI	-26.01	0.02	-	-	-24.09	0.96	-19.79	0.34	-23.64	0.24	-22.94	0.31
BTL	H2O	-19.68	0.06	-21.74	1.64	-18.58	1.75	-18.28	0.15	-20.14	0.20	-12.25	0.15
BTL	C2CL2	-20.6	0.01	-	-	-20.43	0.86	-20.65	0.37	-20.54	0.27	-19.93	0.19
BTL	EAE	-23.03	1.11	-27.23	1.00	-23.02	0.88	-20.77	0.23	-26.96	0.24	-24.17	0.25
BTL	PTL	-25.41	0.0	-29.45	2.63	-26.51	1.54	-21.48	0.47	-28.55	0.81	-22.27	0.51
BTL	MTL	-26.02	0.02	-31.99	1.40	-27.74	0.95	-23.37	0.25	-28.06	0.24	-23.86	0.18
BTL	ETL	-26.47	0.02	-31.77	1.63	-27.93	1.36	-22.85	0.37	-27.91	0.42	-23.37	0.26
BTL	BTL	-25.45	0.13	-31.83	1.80	-27.87	2.34	-22.00	0.39	-28.15	0.67	-22.96	0.52
BTL	2M2P	-26.32	0.0	-29.00	1.79	-27.48	3.55	-22.76	0.45	-28.04	0.76	-23.07	0.50

Table S.1 – Continued on next page

Table S.1 – Continued from previous page

Solute (A)	Solvent (B)	Experimental		GROMOS-54A7		GROMOS-ATB		OPLS-LBCC		AMBER-GAFF2		OpenFF	
		$\Delta_s G_{A:B}^\ominus$	\pm	$\Delta_s G_{A:B}^\ominus$	\pm	$\Delta_s G_{A:B}^\ominus$	\pm	$\Delta_s G_{A:B}^\ominus$	\pm	$\Delta_s G_{A:B}^\ominus$	\pm	$\Delta_s G_{A:B}^\ominus$	\pm
[kJ·mol ⁻¹]													
BTL	1PL	-25.51	0.02	-30.98	2.04	-27.71	1.45	-22.87	0.35	-27.66	0.75	-23.13	0.32
BTL	2PL	-25.96	0.22	-31.04	1.40	-30.12	2.09	-21.97	0.44	-27.50	0.51	-22.85	0.40
BTL	ANLN	-22.53	0.02	-32.84	3.49	-23.96	1.10	-22.16	0.48	-25.72	0.89	-20.16	0.99
BTL	DEE	-18.44	-	-18.71	0.60	-20.97	0.63	-19.81	0.20	-19.05	0.14	-20.93	0.17
BTL	CHCL3	-22.09	0.03	-20.33	0.79	-21.04	1.06	-25.02	0.23	-22.48	0.25	-21.76	0.18
BTL	DEAN	-23.01	-	-29.74	1.19	-19.25	0.72	-21.79	0.19	-24.70	0.30	-25.79	0.23
BTL	TEAN	-21.01	-	-18.61	0.80	-14.62	0.82	-17.66	0.33	-14.66	0.21	-23.47	0.34
BTL	TOL	-18.19	0.36	-20.41	0.80	-19.23	0.82	-18.58	0.25	-19.09	0.22	-19.71	0.19
BTL	BZN	-18.6	0.02	-23.04	0.85	-20.30	0.90	-18.90	0.27	-20.99	0.25	-19.75	0.18
BTL	HPE	-15.4	0.14	-14.53	0.57	-13.59	0.55	-13.22	0.14	-13.14	0.23	-14.72	0.15
BTL	HXE	-15.77	0.06	-15.00	0.52	-13.50	0.58	-13.13	0.12	-13.39	0.14	-15.04	0.10
BTL	CCL4	-17.84	0.4	-15.55	0.85	-14.05	1.05	-	-	-15.45	0.17	-17.13	0.17
BTL	CHE	-14.73	0.03	-15.55	0.68	-13.65	0.60	-13.05	0.22	-13.01	0.37	-15.26	0.27
2M2P	DAMD	-21.18	-	-	-	-28.89	1.34	-19.04	0.34	-25.55	0.30	-24.91	0.28
2M2P	PPN	-20.66	-	-19.59	0.71	-26.42	0.75	-20.69	0.16	-24.02	0.19	-22.99	0.17
2M2P	BTN	-20.23	0.27	-18.68	0.73	-25.89	0.75	-19.91	0.20	-23.64	0.17	-22.72	0.24
2M2P	PYRI	-21.82	0.3	-	-	-26.15	1.19	-19.09	0.54	-20.72	0.27	-21.52	0.22
2M2P	H2O	-18.71	0.02	-12.87	1.57	-21.74	1.58	-19.61	0.21	-16.39	0.17	-12.82	0.17
2M2P	C2CL2	-22.61	-	-	-	-22.79	0.79	-19.93	0.31	-19.06	0.25	-19.43	0.18
2M2P	EAE	-21.41	-	-19.07	1.04	-26.15	0.86	-20.00	0.24	-24.90	0.23	-22.57	0.18
2M2P	PTL	-20.95	-	-21.75	2.19	-30.81	1.49	-20.79	0.58	-24.34	0.66	-21.14	0.46
2M2P	MTL	-24.71	0.02	-22.64	1.40	-30.17	0.87	-22.76	0.32	-24.60	0.30	-23.56	0.19
2M2P	ETL	-23.45	0.01	-23.12	1.64	-31.17	1.22	-21.65	0.34	-25.48	0.31	-22.49	0.28
2M2P	BTL	-21.46	0.0	-19.25	1.94	-31.40	2.26	-21.07	0.44	-25.15	0.69	-21.89	0.47
2M2P	2M2P	-21.01	0.0	-20.37	1.60	-35.68	2.44	-21.58	0.51	-23.31	0.83	-21.30	0.43
2M2P	1PL	-22.04	-	-19.83	2.23	-29.99	1.34	-21.35	0.37	-24.38	0.68	-21.70	0.41
2M2P	2PL	-22.31	0.01	-18.61	2.08	-32.82	2.29	-21.30	0.56	-23.76	0.52	-22.09	0.35
2M2P	ANLN	-19.81	-	-22.57	3.24	-27.60	1.22	-21.52	0.56	-19.73	0.86	-20.81	0.86
2M2P	DEE	-17.47	-	-13.64	0.57	-23.55	0.78	-17.75	0.21	-17.49	0.15	-18.73	0.22
2M2P	CHCL3	-18.73	0.06	-14.55	0.80	-24.15	1.06	-24.98	0.32	-20.81	0.20	-20.58	0.23
2M2P	DEAN	-19.69	-	-19.76	1.25	-21.59	0.63	-19.39	0.22	-20.33	0.28	-22.39	0.25
2M2P	TEAN	-18.84	-	-12.82	0.79	-18.21	0.67	-15.42	0.26	-13.49	0.17	-19.50	0.36
2M2P	TOL	-15.59	0.06	-15.31	0.75	-21.84	0.83	-17.42	0.26	-16.98	0.18	-18.23	0.28
2M2P	BZN	-15.46	0.01	-16.71	0.93	-22.06	0.79	-17.80	0.23	-18.92	0.20	-18.45	0.18
2M2P	HPE	-12.7	0.08	-10.23	0.60	-16.32	0.61	-12.46	0.18	-12.25	0.14	-13.51	0.11
2M2P	HXE	-12.9	-	-10.75	0.55	-16.31	0.50	-12.47	0.13	-12.82	0.19	-13.91	0.15
2M2P	CCL4	-14.23	0.26	-10.87	0.78	-18.15	1.03	-	-	-14.48	0.21	-16.20	0.19
2M2P	CHE	-12.25	0.04	-10.67	0.70	-16.45	0.57	-12.90	0.16	-12.89	0.38	-14.02	0.22
1PL	DAMD	-22.89	-	-	-	-18.23	1.01	-18.16	0.32	-24.30	0.29	-23.65	0.26
1PL	PPN	-20.78	-	-22.72	0.61	-18.16	0.62	-18.77	0.17	-22.31	0.15	-20.98	0.16
1PL	BTN	-20.72	0.03	-21.97	0.61	-17.84	0.62	-18.63	0.16	-21.68	0.20	-21.01	0.20
1PL	PYRI	-23.3	0.06	-	-	-17.71	0.93	-17.07	0.43	-19.70	0.24	-20.17	0.24
1PL	H2O	-20.16	0.08	-20.93	1.47	-12.77	1.40	-18.55	0.17	-19.95	0.15	-12.28	0.16
1PL	C2CL2	-16.75	0.93	-	-	-15.42	0.75	-18.21	0.29	-17.26	0.22	-16.79	0.19
1PL	EAE	-20.31	0.1	-24.21	0.91	-17.36	0.75	-18.20	0.24	-23.30	0.26	-20.86	0.20
1PL	PTL	-22.72	0.0	-30.26	2.11	-18.37	1.30	-18.05	0.47	-23.01	0.70	-19.46	0.34
1PL	MTL	-24.88	0.02	-29.11	1.38	-20.05	0.84	-21.14	0.26	-25.38	0.23	-21.29	0.15
1PL	ETL	-23.97	0.02	-28.87	1.73	-20.40	1.22	-20.67	0.33	-24.40	0.27	-20.43	0.24
1PL	BTL	-21.87	0.0	-26.27	2.30	-18.45	1.71	-19.21	0.39	-24.21	0.44	-19.64	0.51
1PL	2M2P	-21.75	1.05	-27.21	1.41	-20.73	3.57	-19.53	0.53	-24.85	0.84	-19.64	0.49

Table S.1 – Continued on next page

Table S.1 – Continued from previous page

Solute (A)	Solvent (B)	Experimental		GROMOS-54A7		GROMOS-ATB		OPLS-LBCC		AMBER-GAFF2		OpenFF	
		$\Delta_s G_{A:B}^\ominus$	\pm	$\Delta_s G_{A:B}^\ominus$	\pm	$\Delta_s G_{A:B}^\ominus$	\pm	$\Delta_s G_{A:B}^\ominus$	\pm	$\Delta_s G_{A:B}^\ominus$	\pm	$\Delta_s G_{A:B}^\ominus$	\pm
[kJ·mol ⁻¹]													
1PL	1PL	-22.59	0.23	-28.11	1.56	-19.12	1.08	-19.33	0.38	-24.85	0.60	-19.57	0.32
1PL	2PL	-23.22	0.15	-28.35	1.52	-19.49	1.88	-19.48	0.47	-23.63	0.54	-20.03	0.36
1PL	ANLN	-19.69	-	-26.50	3.36	-18.70	1.03	-19.13	0.60	-24.29	0.72	-18.19	0.72
1PL	DEE	-15.93	-	-15.23	0.58	-15.44	0.58	-16.63	0.16	-15.14	0.13	-17.24	0.13
1PL	CHCL3	-18.46	0.07	-16.25	0.77	-16.93	0.93	-21.99	0.18	-19.01	0.21	-17.39	0.20
1PL	DEAN	-18.04	-	-25.32	1.20	-13.74	0.54	-18.46	0.22	-19.95	0.32	-22.30	0.20
1PL	TEAN	-19.07	-	-15.37	0.81	-9.80	0.64	-14.35	0.26	-10.92	0.25	-20.00	0.31
1PL	TOL	-15.55	0.06	-17.19	0.67	-13.73	0.70	-15.21	0.24	-14.93	0.20	-16.20	0.16
1PL	BZN	-16.2	0.01	-19.09	0.77	-15.75	0.80	-15.43	0.18	-17.22	0.21	-16.63	0.18
1PL	HPE	-12.59	0.04	-11.22	0.54	-10.06	0.59	-9.98	0.15	-9.06	0.17	-10.86	0.13
1PL	HXE	-11.9	0.32	-11.48	0.46	-9.81	0.50	-9.78	0.15	-9.70	0.10	-11.62	0.14
1PL	CCL4	-15.13	0.16	-12.24	0.68	-9.88	0.92	-	-	-11.61	0.20	-12.77	0.15
1PL	CHE	-11.48	0.15	-11.98	0.60	-10.19	0.58	-10.20	0.16	-9.13	0.20	-11.65	0.19
2PL	DAMD	-22.64	0.25	-	-	-27.20	1.10	-18.76	0.39	-23.07	0.25	-23.47	0.20
2PL	PPN	-19.64	-	-19.90	0.64	-23.94	0.62	-19.73	0.23	-21.49	0.16	-20.58	0.15
2PL	BTN	-19.5	0.25	-18.92	0.68	-23.66	0.63	-19.16	0.19	-20.64	0.24	-20.46	0.17
2PL	PYRI	-21.45	0.34	-	-	-24.27	1.04	-18.06	0.34	-18.87	0.22	-19.36	0.22
2PL	H2O	-19.86	0.03	-17.33	1.42	-21.93	1.53	-20.11	0.19	-18.08	0.16	-12.75	0.13
2PL	C2CL2	-20.72	-	-	-	-20.47	0.71	-18.30	0.28	-16.32	0.17	-16.53	0.17
2PL	EAE	-17.79	0.25	-20.20	0.87	-23.88	0.81	-18.32	0.22	-22.11	0.22	-20.24	0.22
2PL	PTL	-20.89	0.0	-23.98	2.08	-27.24	1.57	-19.91	0.61	-21.68	0.65	-18.82	0.38
2PL	MTL	-20.66	-	-25.55	1.35	-28.53	0.86	-21.96	0.16	-23.89	0.25	-20.91	0.17
2PL	ETL	-22.03	0.01	-24.11	1.44	-28.05	1.13	-21.62	0.40	-23.20	0.39	-20.46	0.21
2PL	BTL	-21.01	0.0	-25.65	1.82	-26.67	1.93	-20.62	0.42	-22.69	0.60	-19.28	0.37
2PL	2M2P	-21.01	0.0	-24.39	1.45	-26.56	3.69	-21.26	0.54	-22.63	0.75	-19.56	0.40
2PL	1PL	-20.94	0.01	-25.34	1.87	-27.90	1.20	-21.15	0.31	-22.96	0.51	-19.89	0.37
2PL	2PL	-20.67	0.29	-21.69	1.79	-30.52	2.07	-21.07	0.47	-22.95	0.59	-20.40	0.34
2PL	ANLN	-21.81	-	-26.08	3.30	-25.14	0.95	-19.81	0.54	-21.22	0.53	-18.41	0.50
2PL	DEE	-18.21	-	-13.15	0.51	-21.25	0.57	-16.97	0.16	-14.80	0.16	-16.72	0.18
2PL	CHCL3	-17.91	0.02	-13.25	0.73	-20.87	0.90	-22.07	0.28	-17.92	0.15	-17.62	0.20
2PL	DEAN	-16.9	-	-21.36	1.24	-19.37	0.60	-19.24	0.25	-18.72	0.27	-21.37	0.25
2PL	TEAN	-18.1	-	-12.08	0.70	-14.96	0.70	-14.69	0.28	-10.38	0.18	-18.44	0.24
2PL	TOL	-14.73	-	-14.64	0.70	-17.72	0.69	-15.47	0.23	-14.40	0.20	-15.78	0.16
2PL	BZN	-14.55	0.02	-15.88	0.72	-18.71	0.75	-15.54	0.20	-16.44	0.20	-16.46	0.14
2PL	HPE	-10.25	0.66	-9.55	0.54	-12.65	0.53	-9.85	0.12	-8.75	0.13	-10.76	0.14
2PL	HXE	-10.59	0.94	-9.65	0.48	-12.86	0.46	-10.04	0.09	-9.32	0.13	-11.02	0.10
2PL	CCL4	-12.97	0.42	-10.40	0.85	-14.15	0.89	-	-	-11.01	0.15	-12.78	0.15
2PL	CHE	-9.92	0.0	-9.65	0.58	-12.92	0.51	-10.16	0.13	-9.37	0.20	-11.47	0.23
ANLN	DAMD	-30.89	-	-	-	-32.28	1.38	-31.64	0.52	-40.26	0.44	-37.35	0.37
ANLN	PPN	-33.45	0.31	-34.28	0.73	-30.95	0.76	-30.74	0.19	-36.68	0.18	-32.86	0.26
ANLN	BTN	-29.97	-	-32.94	0.81	-30.22	0.77	-30.03	0.24	-35.97	0.30	-32.23	0.25
ANLN	PYRI	-27.23	-	-	-	-25.95	1.14	-29.86	0.31	-34.85	0.29	-32.24	0.28
ANLN	H2O	-23.16	0.15	-31.98	2.00	-21.56	1.66	-21.42	0.14	-27.63	0.18	-22.17	0.29
ANLN	C2CL2	-31.3	0.77	-	-	-25.39	0.95	-29.66	0.39	-31.66	0.21	-28.08	0.25
ANLN	EAE	-32.0	0.33	-37.39	1.22	-30.63	0.96	-30.02	0.32	-37.58	0.30	-33.17	0.41
ANLN	PTL	-27.57	0.63	-33.54	2.32	-25.13	1.58	-27.89	0.54	-30.93	0.80	-27.27	0.55
ANLN	MTL	-31.61	0.02	-39.43	1.85	-26.20	0.94	-29.48	0.26	-32.51	0.31	-30.80	0.21
ANLN	ETL	-30.41	0.03	-36.57	1.90	-24.09	1.14	-28.93	0.26	-31.20	0.36	-29.17	0.26
ANLN	BTL	-28.15	-	-36.41	2.45	-23.62	1.59	-27.94	0.43	-30.58	0.71	-27.98	0.46
ANLN	2M2P	-35.28	-	-32.94	2.14	-26.10	3.09	-28.92	0.50	-29.47	0.81	-26.97	0.66

Table S.1 – Continued on next page

Table S.1 – Continued from previous page

Solute (A)	Solvent (B)	Experimental		GROMOS-54A7		GROMOS-ATB		OPLS-LBCC		AMBER-GAFF2		OpenFF	
		$\Delta_s G_{A:B}^\ominus$	\pm	$\Delta_s G_{A:B}^\ominus$	\pm	$\Delta_s G_{A:B}^\ominus$	\pm	$\Delta_s G_{A:B}^\ominus$	\pm	$\Delta_s G_{A:B}^\ominus$	\pm	$\Delta_s G_{A:B}^\ominus$	\pm
[kJ·mol ⁻¹]													
ANLN	1PL	-28.2	-	-34.13	2.20	-25.70	1.19	-28.66	0.41	-31.49	0.68	-28.23	0.43
ANLN	2PL	-31.46	-	-32.76	1.99	-24.00	2.14	-28.17	0.40	-29.90	0.51	-27.99	0.38
ANLN	ANLN	-31.47	0.26	-45.66	4.01	-25.48	1.07	-28.91	0.63	-39.27	1.11	-30.77	0.73
ANLN	DEE	-31.17	-	-23.86	0.64	-25.76	0.75	-15.93	0.17	-27.73	0.28	-27.14	0.24
ANLN	CHCL3	-30.95	0.58	-26.15	0.94	-26.73	1.22	-31.37	0.28	-32.87	0.28	-28.41	0.32
ANLN	DEAN	-26.66	-	-34.12	1.51	-22.68	0.65	-17.49	0.23	-31.15	0.29	-30.44	0.28
ANLN	TEAN	-23.46	-	-24.07	0.88	-20.42	0.81	-23.52	0.22	-23.84	0.21	-27.83	0.29
ANLN	TOL	-28.07	0.14	-28.63	0.93	-23.17	0.96	-26.12	0.24	-28.58	0.28	-25.79	0.23
ANLN	BZN	-28.81	0.02	-31.00	1.04	-25.03	1.02	-26.72	0.27	-31.42	0.22	-26.88	0.16
ANLN	HPE	-22.52	0.02	-19.00	0.62	-19.58	0.64	-19.88	0.15	-21.44	0.17	-18.57	0.19
ANLN	HXE	-22.75	0.03	-19.27	0.57	-20.02	0.72	-20.09	0.15	-21.52	0.15	-18.85	0.11
ANLN	CCL4	-25.5	0.02	-19.32	0.83	-20.26	1.24	-	-	-23.10	0.23	-20.50	0.18
ANLN	CHE	-23.11	0.01	-19.68	0.73	-19.49	0.70	-20.63	0.18	-21.90	0.29	-19.33	0.24
DEE	DAMD	-13.99	-	-	-	-13.90	1.12	-11.39	0.38	-12.62	0.26	-13.30	0.16
DEE	PPN	-16.67	-	-16.18	0.70	-16.43	0.63	-14.04	0.16	-13.96	0.22	-14.60	0.14
DEE	BTN	-16.27	-	-15.98	0.56	-16.71	0.72	-14.34	0.22	-13.92	0.19	-14.85	0.16
DEE	PYRI	-16.33	-	-	-	-18.11	1.00	-12.38	0.33	-13.94	0.20	-15.27	0.24
DEE	H2O	-7.22	0.33	3.22	1.35	-3.51	1.44	-7.73	0.19	1.32	0.18	-2.14	0.14
DEE	C2CL2	-14.69	0.32	-	-	-17.69	0.76	-14.75	0.39	-15.52	0.21	-17.04	0.17
DEE	EAE	-17.13	-	-14.53	0.85	-16.34	0.82	-14.00	0.31	-13.70	0.19	-14.78	0.21
DEE	PTL	-13.08	0.0	-14.70	0.97	-15.80	1.00	-13.96	0.30	-12.81	0.33	-15.22	0.30
DEE	MTL	-13.64	0.0	-12.21	0.96	-14.99	0.78	-12.44	0.15	-11.65	0.15	-15.43	0.16
DEE	ETL	-16.44	-	-13.37	0.88	-14.78	0.99	-12.94	0.30	-12.17	0.25	-15.11	0.21
DEE	BTL	-12.96	0.0	-13.98	1.01	-15.95	1.30	-13.81	0.30	-12.18	0.34	-14.99	0.36
DEE	2M2P	-14.33	-	-13.96	0.88	-16.03	2.23	-12.77	0.44	-13.15	0.39	-14.69	0.36
DEE	1PL	-15.3	-	-13.72	0.92	-15.98	0.92	-13.30	0.24	-12.41	0.32	-15.27	0.23
DEE	2PL	-14.79	-	-14.10	1.06	-14.71	1.33	-12.59	0.44	-12.84	0.38	-14.92	0.28
DEE	ANLN	-16.55	0.75	-11.28	2.26	-17.69	0.89	-16.63	0.45	-11.92	0.96	-13.51	0.56
DEE	DEE	-14.39	0.0	-16.25	0.52	-17.54	0.60	-14.56	0.15	-14.89	0.11	-15.86	0.14
DEE	CHCL3	-17.92	0.29	-17.33	0.79	-20.92	1.00	-20.07	0.34	-18.10	0.17	-19.22	0.21
DEE	DEAN	-15.07	-	-15.59	0.82	-17.42	0.55	-14.52	0.15	-14.77	0.16	-15.74	0.17
DEE	TEAN	-15.19	-	-15.85	0.66	-16.25	0.70	-13.53	0.16	-13.64	0.26	-15.13	0.18
DEE	TOL	-13.93	0.0	-16.43	0.72	-17.24	0.74	-14.57	0.27	-15.04	0.20	-15.52	0.17
DEE	BZN	-17.76	-	-16.42	0.83	-19.01	0.79	-14.81	0.23	-14.51	0.16	-16.19	0.19
DEE	HPE	-13.7	-	-15.18	0.63	-15.36	0.57	-12.23	0.15	-13.19	0.14	-13.90	0.14
DEE	HXE	-14.61	-	-15.90	0.49	-15.92	0.52	-12.62	0.13	-13.76	0.14	-14.33	0.12
DEE	CCL4	-14.98	0.31	-16.75	0.83	-16.37	0.98	-	-	-15.78	0.20	-16.65	0.26
DEE	CHE	-12.66	0.01	-16.07	0.69	-16.04	0.60	-12.60	0.18	-13.42	0.30	-14.53	0.20
CHCL3	DAMD	-21.47	0.43	-	-	-22.26	1.07	-23.46	0.41	-18.67	0.32	-18.40	0.21
CHCL3	PPN	-19.5	0.02	-17.69	0.71	-21.14	0.65	-24.27	0.19	-18.14	0.17	-18.15	0.17
CHCL3	BTN	-19.79	0.02	-17.64	0.62	-21.13	0.66	-24.93	0.20	-18.42	0.20	-18.09	0.22
CHCL3	PYRI	-19.47	0.13	-	-	-21.17	0.94	-22.24	0.36	-16.91	0.24	-17.20	0.23
CHCL3	H2O	-4.61	0.09	2.14	1.52	-4.68	1.38	-6.29	0.16	0.57	0.15	0.14	0.14
CHCL3	C2CL2	-16.1	1.37	-	-	-20.17	0.68	-19.78	0.34	-15.63	0.18	-16.45	0.16
CHCL3	EAE	-19.37	0.04	-16.86	0.83	-22.54	0.79	-22.80	0.24	-18.74	0.23	-18.26	0.25
CHCL3	PTL	-15.62	-	-15.94	1.04	-19.63	1.12	-25.04	0.39	-15.66	0.47	-16.87	0.32
CHCL3	MTL	-17.69	0.02	-14.54	0.81	-18.12	0.58	-20.61	0.22	-14.27	0.17	-15.91	0.13
CHCL3	ETL	-17.46	0.01	-15.51	0.93	-18.69	0.74	-23.39	0.25	-15.55	0.20	-16.10	0.19
CHCL3	BTL	-16.84	0.0	-15.62	1.01	-20.02	1.06	-24.04	0.38	-15.92	0.41	-16.36	0.30
CHCL3	2M2P	-24.55	-	-15.25	0.98	-19.82	2.26	-25.84	0.41	-15.68	0.57	-16.81	0.42

Table S.1 – Continued on next page

Table S.1 – Continued from previous page

Solute (A)	Solvent (B)	Experimental		GROMOS-54A7		GROMOS-ATB		OPLS-LBCC		AMBER-GAFF2		OpenFF	
		$\Delta_s G_{A:B}^\ominus$	\pm	$\Delta_s G_{A:B}^\ominus$	\pm	$\Delta_s G_{A:B}^\ominus$	\pm	$\Delta_s G_{A:B}^\ominus$	\pm	$\Delta_s G_{A:B}^\ominus$	\pm	$\Delta_s G_{A:B}^\ominus$	\pm
[kJ·mol ⁻¹]													
CHCL3	1PL	-17.59	-	-15.94	1.03	-19.41	0.88	-24.29	0.33	-16.17	0.37	-16.81	0.26
CHCL3	2PL	-19.36	-	-15.12	1.02	-20.40	1.33	-25.12	0.28	-15.72	0.33	-16.39	0.25
CHCL3	ANLN	-16.21	0.01	-15.56	2.62	-20.78	0.94	-21.33	0.43	-12.75	0.70	-14.43	0.66
CHCL3	DEE	-16.1	-	-17.44	0.49	-21.94	0.60	-24.62	0.18	-17.31	0.19	-18.43	0.15
CHCL3	CHCL3	-17.47	0.11	-18.03	0.65	-20.94	1.01	-20.39	0.27	-15.70	0.19	-16.42	0.26
CHCL3	DEAN	-18.56	-	-16.77	0.83	-20.12	0.51	-27.80	0.19	-18.37	0.18	-19.76	0.20
CHCL3	TEAN	-23.58	-	-16.72	0.70	-19.26	0.68	-24.23	0.27	-16.01	0.18	-19.29	0.29
CHCL3	TOL	-16.3	1.52	-17.20	0.69	-21.39	0.71	-22.77	0.24	-17.45	0.21	-17.85	0.22
CHCL3	BZN	-13.25	-	-17.57	0.69	-21.62	0.93	-22.31	0.38	-18.10	0.22	-17.42	0.19
CHCL3	HPE	-15.02	0.12	-16.46	0.56	-17.25	0.59	-16.37	0.15	-14.47	0.14	-14.89	0.17
CHCL3	HXE	-13.59	0.69	-16.13	0.51	-17.44	0.51	-16.38	0.12	-14.91	0.16	-15.39	0.13
CHCL3	CCL4	-16.79	0.0	-17.12	0.88	-19.71	0.87	-	-	-14.52	0.17	-15.15	0.31
CHCL3	CHE	-16.53	1.05	-17.29	0.65	-17.46	0.64	-17.14	0.23	-15.08	0.21	-15.89	0.20
DEAN	DAMD	-12.62	-	-	-	-14.54	1.13	-14.99	0.32	-17.82	0.24	-16.62	0.26
DEAN	PPN	-16.41	0.71	-19.81	0.66	-16.94	0.69	-17.21	0.18	-17.91	0.18	-17.39	0.16
DEAN	BTN	-14.79	-	-19.38	0.73	-17.65	0.68	-16.86	0.17	-17.73	0.19	-17.54	0.23
DEAN	PYRI	-19.3	-	-	-	-17.00	0.89	-16.72	0.28	-17.42	0.24	-18.00	0.29
DEAN	H2O	-17.01	0.01	-9.18	1.72	-3.34	1.75	-15.32	0.19	-6.68	0.20	-12.16	0.14
DEAN	C2CL2	-16.72	0.02	-	-	-16.78	0.80	-17.65	0.35	-18.12	0.24	-19.41	0.24
DEAN	EAE	-15.98	0.29	-19.64	1.01	-18.11	0.72	-17.48	0.20	-18.27	0.26	-17.23	0.28
DEAN	PTL	-19.39	2.79	-18.11	2.64	-15.93	1.00	-17.45	0.44	-15.45	0.73	-21.33	0.39
DEAN	MTL	-21.29	0.02	-20.98	1.53	-14.74	0.71	-18.01	0.25	-16.71	0.24	-23.87	0.20
DEAN	ETL	-16.56	-	-21.34	1.87	-14.87	0.87	-17.38	0.35	-17.06	0.37	-22.57	0.34
DEAN	BTL	-19.43	2.12	-22.41	2.16	-15.20	1.05	-17.61	0.35	-16.13	0.50	-21.83	0.45
DEAN	2M2P	-22.1	-	-17.87	1.57	-18.02	2.04	-16.54	0.38	-15.46	0.50	-19.83	0.55
DEAN	1PL	-17.98	-	-17.73	2.00	-15.66	0.91	-17.66	0.37	-16.57	0.63	-21.86	0.33
DEAN	2PL	-17.3	-	-19.40	1.97	-15.44	1.32	-17.88	0.44	-15.35	0.49	-21.13	0.35
DEAN	ANLN	-24.04	-	-18.91	3.50	-16.77	0.91	-19.03	0.50	-16.94	1.07	-17.52	0.65
DEAN	DEE	-15.07	-	-17.28	0.59	-18.61	0.57	-16.72	0.20	-16.74	0.14	-17.32	0.14
DEAN	CHCL3	-21.84	0.13	-18.31	0.87	-18.51	0.94	-24.51	0.25	-20.66	0.25	-22.44	0.20
DEAN	DEAN	-16.79	-	-19.48	1.10	-17.76	0.66	-17.06	0.20	-16.97	0.24	-17.84	0.20
DEAN	TEAN	-17.3	-	-16.32	0.76	-17.28	0.71	-15.57	0.28	-15.12	0.16	-16.39	0.19
DEAN	TOL	-15.69	0.0	-18.71	0.80	-19.15	0.75	-16.67	0.24	-16.82	0.30	-17.61	0.19
DEAN	BZN	-16.82	0.02	-19.79	0.92	-19.71	0.91	-17.41	0.23	-16.75	0.24	-17.96	0.17
DEAN	HPE	-13.93	0.46	-14.95	0.64	-16.72	0.58	-14.31	0.15	-14.60	0.12	-14.91	0.19
DEAN	HXE	-14.88	0.09	-14.95	0.57	-17.09	0.60	-14.58	0.13	-14.66	0.16	-15.23	0.11
DEAN	CCL4	-17.23	0.02	-15.78	0.83	-18.90	1.07	-	-	-16.78	0.16	-17.55	0.23
DEAN	CHE	-15.12	0.01	-15.09	0.68	-17.46	0.61	-14.58	0.17	-14.58	0.26	-15.34	0.16
TEAN	DAMD	-16.9	-	-	-	-21.55	1.33	-15.40	0.46	-18.21	0.30	-18.84	0.30
TEAN	PPN	-18.44	1.48	-22.18	0.82	-22.30	0.81	-19.35	0.21	-19.69	0.17	-20.03	0.16
TEAN	BTN	-17.41	0.0	-22.51	0.96	-23.69	0.89	-19.52	0.29	-19.81	0.20	-20.44	0.22
TEAN	PYRI	-19.18	-	-	-	-25.44	1.17	-19.05	0.60	-19.51	0.23	-22.13	0.24
TEAN	H2O	-12.86	0.35	1.61	1.90	2.01	1.92	-8.30	0.25	4.56	0.15	-9.23	0.18
TEAN	C2CL2	-19.26	0.85	-	-	-24.70	0.92	-20.02	0.38	-22.42	0.31	-23.91	0.25
TEAN	EAE	-17.6	0.19	-21.42	1.12	-24.43	0.91	-20.26	0.33	-19.94	0.26	-20.78	0.28
TEAN	PTL	-20.78	0.0	-21.25	1.37	-23.59	1.01	-19.80	0.47	-19.73	0.27	-25.30	0.57
TEAN	MTL	-21.91	0.02	-17.03	1.29	-19.82	0.73	-16.75	0.27	-15.53	0.20	-25.75	0.29
TEAN	ETL	-20.37	0.02	-19.15	1.37	-21.15	0.98	-18.28	0.35	-18.46	0.19	-25.50	0.39
TEAN	BTL	-20.33	0.0	-20.11	1.32	-22.22	1.30	-19.72	0.37	-18.57	0.31	-24.79	0.52
TEAN	2M2P	-18.33	0.0	-20.45	1.13	-26.39	2.28	-19.23	0.39	-20.01	0.41	-21.36	0.51

Table S.1 – Continued on next page

Table S.1 – Continued from previous page

Solute (A)	Solvent (B)	Experimental		GROMOS-54A7		GROMOS-ATB		OPLS-LBCC		AMBER-GAFF2		OpenFF	
		$\Delta_s G_{A:B}^\ominus$	\pm	$\Delta_s G_{A:B}^\ominus$	\pm	$\Delta_s G_{A:B}^\ominus$	\pm	$\Delta_s G_{A:B}^\ominus$	\pm	$\Delta_s G_{A:B}^\ominus$	\pm	$\Delta_s G_{A:B}^\ominus$	\pm
[kJ·mol ⁻¹]													
TEAN	1PL	-19.98	0.01	-19.98	1.42	-22.56	0.97	-19.56	0.31	-17.88	0.31	-24.73	0.53
TEAN	2PL	-18.89	0.0	-20.16	1.25	-22.27	1.52	-18.66	0.50	-18.81	0.33	-23.85	0.60
TEAN	ANLN	-29.97	-	-20.80	3.18	-23.81	1.08	-21.25	0.65	-16.89	0.85	-17.58	0.86
TEAN	DEE	-18.61	0.0	-22.64	0.74	-26.12	0.74	-21.27	0.19	-21.89	0.22	-22.18	0.25
TEAN	CHCL3	-24.09	0.0	-24.85	1.05	-27.54	1.15	-27.62	0.30	-24.92	0.29	-27.61	0.28
TEAN	DEAN	-21.35	-	-21.26	0.96	-26.52	0.72	-20.94	0.23	-21.72	0.18	-21.45	0.27
TEAN	TEAN	-19.0	0.42	-22.86	0.92	-26.83	0.92	-21.56	0.23	-22.04	0.29	-21.67	0.29
TEAN	TOL	-19.61	0.08	-23.55	0.97	-27.56	0.82	-21.30	0.31	-22.00	0.27	-22.23	0.28
TEAN	BZN	-19.61	0.31	-23.14	0.92	-27.74	1.03	-21.99	0.41	-21.13	0.23	-22.83	0.25
TEAN	HPE	-18.69	0.03	-22.03	0.68	-26.00	0.66	-20.45	0.20	-21.91	0.21	-20.48	0.18
TEAN	HXE	-18.87	0.08	-22.33	0.69	-26.25	0.70	-20.72	0.20	-22.10	0.18	-20.65	0.12
TEAN	CCL4	-19.68	0.75	-23.83	0.97	-27.14	1.11	-	-	-25.17	0.22	-24.04	0.29
TEAN	CHE	-19.55	0.2	-23.18	0.99	-26.07	0.74	-21.08	0.19	-22.76	0.30	-21.50	0.25
TOL	DAMD	-20.88	0.1	-	-	-20.09	1.23	-19.94	0.46	-20.21	0.27	-17.77	0.21
TOL	PPN	-20.8	0.06	-21.79	0.66	-21.52	0.67	-22.35	0.23	-20.65	0.19	-18.73	0.17
TOL	BTN	-21.31	0.06	-21.79	0.77	-21.82	0.67	-21.78	0.21	-20.63	0.19	-19.02	0.17
TOL	PYRI	-21.43	0.04	-	-	-22.47	1.10	-21.36	0.44	-20.13	0.33	-18.55	0.34
TOL	H2O	-3.45	0.24	-3.14	1.50	-1.94	1.66	-7.15	0.21	-2.98	0.17	-3.40	0.18
TOL	C2CL2	-22.21	0.0	-	-	-22.22	0.76	-22.17	0.30	-22.97	0.23	-20.74	0.21
TOL	EAE	-21.07	0.03	-20.99	0.93	-21.69	0.81	-21.80	0.22	-20.30	0.20	-18.26	0.30
TOL	PTL	-18.53	0.43	-18.90	1.28	-20.73	0.97	-20.39	0.42	-18.73	0.46	-18.08	0.30
TOL	MTL	-18.21	0.0	-17.58	0.99	-18.16	0.71	-18.21	0.26	-16.55	0.28	-18.41	0.17
TOL	ETL	-18.8	0.16	-18.39	1.01	-18.98	0.88	-19.22	0.25	-18.17	0.24	-18.34	0.24
TOL	BTL	-18.91	0.05	-20.04	1.16	-19.75	1.02	-19.70	0.26	-18.18	0.35	-18.10	0.33
TOL	2M2P	-18.44	0.0	-19.17	1.00	-19.80	2.04	-20.33	0.39	-18.66	0.43	-17.34	0.43
TOL	1PL	-18.85	0.07	-19.13	1.07	-19.55	0.91	-20.33	0.31	-18.47	0.43	-17.82	0.27
TOL	2PL	-18.36	0.02	-18.95	1.06	-19.55	1.47	-19.58	0.33	-18.27	0.37	-17.54	0.27
TOL	ANLN	-19.35	0.1	-18.92	2.58	-20.68	1.09	-21.34	0.57	-16.13	0.93	-17.47	0.72
TOL	DEE	-21.18	0.0	-21.59	0.61	-22.63	0.63	-21.83	0.15	-20.71	0.16	-19.42	0.13
TOL	CHCL3	-22.98	0.09	-22.62	0.97	-24.05	1.13	-27.48	0.33	-24.81	0.23	-23.00	0.25
TOL	DEAN	-19.87	-	-21.13	1.00	-22.52	0.68	-21.56	0.23	-21.18	0.28	-19.51	0.19
TOL	TEAN	-20.58	0.15	-20.67	0.70	-22.04	0.76	-21.17	0.20	-19.85	0.22	-18.42	0.18
TOL	TOL	-21.58	0.09	-21.37	0.80	-21.96	0.81	-22.02	0.23	-20.66	0.20	-19.03	0.17
TOL	BZN	-22.25	0.02	-22.03	0.83	-22.76	0.83	-22.75	0.21	-20.91	0.26	-19.60	0.19
TOL	HPE	-19.98	0.08	-20.12	0.59	-21.35	0.60	-19.29	0.20	-19.13	0.10	-17.20	0.20
TOL	HXE	-20.19	0.14	-19.69	0.62	-21.26	0.58	-19.19	0.14	-19.56	0.14	-17.35	0.17
TOL	CCL4	-21.59	0.29	-20.31	1.14	-21.86	1.17	-	-	-21.18	0.22	-18.84	0.24
TOL	CHE	-20.48	0.02	-20.22	0.65	-21.53	0.71	-19.68	0.24	-19.72	0.19	-17.78	0.25
BZN	DAMD	-18.66	0.01	-	-	-17.77	1.20	-16.96	0.41	-17.97	0.23	-15.16	0.27
BZN	PPN	-18.31	0.02	-18.70	0.67	-18.32	0.69	-18.70	0.16	-18.57	0.17	-16.09	0.16
BZN	BTN	-18.68	0.05	-18.65	0.73	-18.40	0.71	-18.82	0.21	-18.18	0.19	-16.02	0.16
BZN	PYRI	-18.88	0.01	-	-	-18.57	1.09	-17.83	0.28	-18.48	0.32	-15.96	0.23
BZN	H2O	-3.67	0.05	-5.40	1.57	-4.03	1.52	-5.97	0.20	-7.07	0.16	-3.36	0.14
BZN	C2CL2	-18.92	0.03	-	-	-18.93	0.74	-18.78	0.26	-20.04	0.22	-17.44	0.22
BZN	EAE	-18.58	0.04	-17.98	0.90	-18.80	0.71	-19.03	0.20	-18.43	0.23	-16.22	0.19
BZN	PTL	-15.81	0.6	-16.57	1.18	-17.67	0.89	-16.96	0.32	-15.17	0.33	-14.14	0.38
BZN	MTL	-15.89	0.04	-16.23	0.91	-15.98	0.59	-15.61	0.17	-15.42	0.17	-15.32	0.15
BZN	ETL	-15.87	0.0	-16.47	1.05	-16.70	0.77	-16.43	0.20	-16.03	0.25	-14.75	0.20
BZN	BTL	-15.83	0.95	-15.81	1.12	-16.19	0.97	-16.84	0.37	-15.19	0.36	-14.51	0.32
BZN	2M2P	-15.53	0.0	-16.43	1.06	-17.95	2.01	-17.64	0.47	-15.54	0.56	-14.73	0.33

Table S.1 – Continued on next page

Table S.1 – Continued from previous page

Solute (A)	Solvent (B)	Experimental		GROMOS-54A7		GROMOS-ATB		OPLS-LBCC		AMBER-GAFF2		OpenFF	
		$\Delta_s G_{A:B}^\ominus$	\pm	$\Delta_s G_{A:B}^\ominus$	\pm	$\Delta_s G_{A:B}^\ominus$	\pm	$\Delta_s G_{A:B}^\ominus$	\pm	$\Delta_s G_{A:B}^\ominus$	\pm	$\Delta_s G_{A:B}^\ominus$	\pm
[kJ·mol ⁻¹]													
BZN	1PL	-15.87	0.0	-15.61	1.07	-16.87	0.81	-17.28	0.26	-15.55	0.24	-14.87	0.22
BZN	2PL	-15.74	0.25	-16.02	1.05	-15.88	1.21	-16.74	0.25	-15.16	0.20	-14.54	0.30
BZN	ANLN	-17.01	0.03	-14.98	3.05	-17.09	1.09	-17.76	0.41	-16.98	0.85	-14.25	0.87
BZN	DEE	-27.69	-	-18.04	0.53	-19.23	0.51	-18.59	0.18	-17.41	0.17	-15.88	0.17
BZN	CHCL3	-19.5	0.24	-18.80	0.94	-20.68	0.99	-22.65	0.30	-22.17	0.20	-18.65	0.22
BZN	DEAN	-18.56	-	-18.60	0.87	-19.24	0.52	-18.01	0.16	-18.03	0.21	-15.91	0.16
BZN	TEAN	-18.84	-	-17.12	0.71	-18.31	0.62	-17.82	0.19	-15.69	0.15	-15.32	0.13
BZN	TOL	-18.55	0.08	-17.59	0.81	-18.52	0.73	-18.71	0.24	-17.71	0.14	-15.79	0.15
BZN	BZN	-19.06	0.01	-18.06	0.91	-19.13	0.88	-18.85	0.18	-18.47	0.22	-16.13	0.17
BZN	HPE	-16.74	0.07	-16.17	0.55	-17.91	0.59	-16.21	0.17	-15.21	0.21	-13.77	0.16
BZN	HXE	-16.63	0.08	-16.61	0.57	-17.55	0.51	-16.51	0.14	-15.67	0.10	-13.96	0.12
BZN	CCL4	-18.76	0.13	-16.50	0.75	-18.26	1.05	-	-	-17.19	0.24	-15.23	0.20
BZN	CHE	-17.42	0.2	-17.32	0.68	-17.63	0.58	-16.84	0.23	-15.48	0.30	-14.06	0.24
HPE	DAMD	-14.5	0.03	-	-	-13.21	1.47	-9.15	0.48	-17.98	0.26	-12.52	0.27
HPE	PPN	-16.17	0.06	-20.09	0.72	-17.57	0.73	-14.37	0.20	-19.15	0.21	-16.45	0.22
HPE	BTN	-17.19	0.05	-20.40	0.82	-18.62	0.73	-15.03	0.23	-20.17	0.15	-16.97	0.24
HPE	PYRI	-16.15	0.01	-	-	-19.00	1.19	-11.32	0.36	-19.60	0.29	-16.83	0.25
HPE	H2O	11.1	0.08	10.43	1.83	9.98	1.85	11.30	0.15	9.52	0.20	11.72	0.20
HPE	C2CL2	-16.9	0.08	-	-	-19.64	0.93	-11.56	0.36	-22.03	0.21	-19.40	0.27
HPE	EAE	-17.23	0.11	-17.75	1.09	-18.62	0.92	-14.64	0.31	-19.59	0.23	-16.12	0.30
HPE	PTL	-16.5	-	-19.42	1.24	-19.71	1.00	-15.00	0.25	-19.65	0.55	-17.74	0.29
HPE	MTL	-14.27	0.0	-15.03	1.01	-15.59	0.85	-7.97	0.23	-15.09	0.20	-15.36	0.15
HPE	ETL	-15.46	0.01	-17.10	1.09	-18.20	0.90	-12.30	0.22	-17.73	0.21	-15.85	0.21
HPE	BTL	-16.44	0.0	-19.78	1.32	-18.44	1.20	-14.34	0.35	-18.78	0.47	-16.91	0.22
HPE	2M2P	-16.56	0.0	-18.73	1.05	-19.69	2.38	-15.06	0.42	-20.48	0.42	-17.93	0.29
HPE	1PL	-15.63	0.01	-19.07	1.29	-18.17	1.05	-14.18	0.16	-18.31	0.30	-16.47	0.24
HPE	2PL	-16.0	0.18	-19.10	1.19	-18.80	1.44	-14.10	0.31	-18.95	0.29	-16.95	0.30
HPE	ANLN	-12.35	0.06	-13.45	2.68	-17.97	1.06	-10.71	0.62	-14.11	0.82	-10.69	0.96
HPE	DEE	-17.98	-	-22.86	0.71	-22.06	0.74	-18.04	0.21	-22.68	0.14	-20.15	0.13
HPE	CHCL3	-19.36	0.0	-23.56	0.87	-21.05	1.03	-17.54	0.27	-25.09	0.21	-22.52	0.24
HPE	DEAN	-16.5	-	-19.78	0.80	-22.11	0.66	-17.72	0.19	-22.04	0.23	-19.25	0.21
HPE	TEAN	-19.58	0.0	-22.00	0.85	-22.44	0.94	-18.52	0.22	-23.02	0.25	-20.00	0.22
HPE	TOL	-19.06	0.01	-22.02	0.85	-22.89	0.93	-17.00	0.19	-22.75	0.22	-20.05	0.23
HPE	BZN	-19.08	0.01	-21.34	0.91	-23.69	1.00	-17.14	0.28	-21.44	0.23	-19.50	0.26
HPE	HPE	-19.54	0.06	-22.03	0.78	-22.05	0.74	-18.68	0.19	-22.65	0.21	-20.46	0.29
HPE	HXE	-19.98	0.0	-21.97	0.77	-22.03	0.77	-18.95	0.24	-23.05	0.25	-20.72	0.13
HPE	CCL4	-19.9	0.02	-22.95	1.06	-22.15	1.28	-	-	-26.10	0.26	-23.05	0.32
HPE	CHE	-20.05	0.02	-22.96	0.84	-22.89	0.81	-18.69	0.25	-22.89	0.27	-20.86	0.36
HXE	DAMD	-11.85	0.07	-	-	-10.58	1.30	-6.89	0.45	-14.89	0.33	-10.13	0.24
HXE	PPN	-13.52	0.01	-16.44	0.69	-14.58	0.72	-11.52	0.15	-15.65	0.12	-13.39	0.15
HXE	BTN	-14.42	0.02	-17.24	0.80	-15.75	0.66	-11.59	0.20	-16.50	0.12	-14.06	0.15
HXE	PYRI	-13.52	0.01	-	-	-15.40	1.08	-8.12	0.36	-16.01	0.18	-13.83	0.20
HXE	H2O	10.4	0.02	9.43	1.56	8.32	1.53	10.59	0.14	9.26	0.16	11.13	0.20
HXE	C2CL2	-14.22	0.08	-	-	-16.40	0.80	-9.00	0.22	-18.24	0.20	-15.79	0.28
HXE	EAE	-14.49	0.01	-14.69	1.05	-15.68	0.85	-12.02	0.25	-16.00	0.15	-13.25	0.16
HXE	PTL	-13.93	0.0	-17.02	1.14	-16.83	0.97	-11.71	0.32	-15.64	0.40	-13.92	0.24
HXE	MTL	-11.69	0.01	-12.89	0.93	-13.03	0.66	-6.36	0.22	-12.64	0.25	-12.19	0.12
HXE	ETL	-12.78	0.01	-14.49	1.08	-14.07	0.82	-9.90	0.29	-15.08	0.23	-13.30	0.18
HXE	BTL	-13.86	0.05	-15.89	1.15	-16.41	1.11	-12.03	0.21	-15.69	0.26	-13.93	0.29
HXE	2M2P	-13.93	0.0	-16.72	0.99	-19.09	2.10	-12.09	0.31	-17.56	0.44	-14.55	0.36

Table S.1 – Continued on next page

Table S.1 – Continued from previous page

Solute (A)	Solvent (B)	Experimental		GROMOS-54A7		GROMOS-ATB		OPLS-LBCC		AMBER-GAFF2		OpenFF	
		$\Delta_s G_{A:B}^\ominus$	\pm	$\Delta_s G_{A:B}^\ominus$	\pm	$\Delta_s G_{A:B}^\ominus$	\pm	$\Delta_s G_{A:B}^\ominus$	\pm	$\Delta_s G_{A:B}^\ominus$	\pm	$\Delta_s G_{A:B}^\ominus$	\pm
[kJ·mol ⁻¹]													
HXE	IPL	-13.02	0.0	-16.30	1.07	-15.54	0.84	-11.70	0.25	-14.86	0.27	-13.92	0.18
HXE	2PL	-13.53	0.2	-16.04	1.02	-16.60	1.37	-11.43	0.20	-15.57	0.31	-14.12	0.25
HXE	ANLN	-10.02	0.14	-10.66	2.59	-14.89	1.00	-8.43	0.51	-10.89	0.66	-8.30	0.53
HXE	DEE	-15.76	-	-19.24	0.63	-18.21	0.64	-15.01	0.14	-18.84	0.11	-17.11	0.19
HXE	CHCL3	-16.42	0.03	-19.94	0.88	-17.78	1.01	-14.73	0.27	-21.06	0.18	-18.83	0.24
HXE	DEAN	-15.41	-	-17.27	0.84	-18.90	0.62	-14.96	0.20	-18.95	0.18	-15.98	0.14
HXE	TEAN	-16.62	0.01	-19.13	0.73	-18.13	0.81	-14.79	0.17	-19.26	0.18	-16.51	0.21
HXE	TOL	-16.1	0.0	-18.42	0.83	-19.08	0.80	-14.09	0.17	-18.99	0.13	-16.34	0.33
HXE	BZN	-15.31	0.37	-18.57	0.98	-19.82	0.89	-14.38	0.17	-17.94	0.25	-16.13	0.21
HXE	HPE	-16.56	0.0	-18.36	0.71	-18.63	0.67	-15.78	0.22	-19.12	0.15	-16.85	0.22
HXE	HXE	-16.88	0.08	-18.40	0.68	-18.82	0.58	-15.89	0.21	-19.17	0.20	-17.25	0.10
HXE	CCL4	-16.98	0.02	-20.44	0.96	-19.06	1.24	-	-	-22.28	0.36	-19.33	0.21
HXE	CHE	-17.01	0.0	-19.11	0.79	-19.16	0.67	-15.78	0.26	-18.87	0.20	-16.98	0.27
CCL4	DAMD	-18.88	0.01	-	-	-18.26	1.05	-	-	-15.79	0.18	-15.01	0.30
CCL4	PPN	-17.17	0.1	-16.99	0.58	-18.22	0.66	-	-	-16.14	0.16	-16.36	0.18
CCL4	BTN	-17.35	0.01	-17.26	0.73	-18.66	0.64	-	-	-16.77	0.19	-16.93	0.16
CCL4	PYRI	-22.38	-	-	-	-20.89	1.04	-	-	-15.38	0.17	-16.61	0.16
CCL4	H2O	0.3	0.02	5.81	1.52	0.67	1.38	-	-	5.78	0.18	4.36	0.10
CCL4	C2CL2	-16.36	1.0	-	-	-18.95	0.78	-	-	-16.38	0.24	-17.64	0.21
CCL4	EAE	-17.69	0.02	-15.72	0.83	-20.59	0.79	-	-	-16.82	0.24	-17.03	0.19
CCL4	PTL	-14.16	-	-16.49	1.24	-19.19	0.83	-	-	-16.69	0.32	-17.98	0.28
CCL4	MTL	-15.18	0.02	-13.47	0.86	-15.71	0.67	-	-	-12.72	0.19	-15.29	0.20
CCL4	ETL	-15.7	0.0	-14.66	0.92	-17.23	0.74	-	-	-15.20	0.13	-16.54	0.18
CCL4	BTL	-16.21	0.0	-15.36	1.05	-18.58	1.26	-	-	-16.32	0.26	-17.57	0.29
CCL4	2M2P	-16.93	1.29	-15.41	0.95	-19.74	1.79	-	-	-17.91	0.38	-17.36	0.26
CCL4	IPL	-15.7	0.0	-15.22	0.98	-18.05	0.71	-	-	-15.10	0.37	-16.92	0.21
CCL4	2PL	-16.44	-	-14.80	0.90	-18.78	1.38	-	-	-15.29	0.30	-16.92	0.24
CCL4	ANLN	-14.72	0.02	-10.42	2.46	-18.67	1.12	-	-	-9.64	0.41	-13.25	0.86
CCL4	DEE	-18.38	0.0	-18.03	0.55	-21.36	0.47	-	-	-18.46	0.16	-19.28	0.16
CCL4	CHCL3	-18.56	0.0	-18.61	0.86	-23.10	0.95	-	-	-17.54	0.22	-18.63	0.15
CCL4	DEAN	-17.98	-	-16.26	0.73	-21.33	0.58	-	-	-18.29	0.13	-18.64	0.18
CCL4	TEAN	-18.04	-	-18.35	0.67	-22.39	0.68	-	-	-18.82	0.22	-19.50	0.16
CCL4	TOL	-18.2	0.07	-17.87	0.87	-22.07	0.85	-	-	-18.33	0.19	-18.62	0.18
CCL4	BZN	-15.93	-	-16.71	0.76	-22.58	0.78	-	-	-17.53	0.22	-18.20	0.18
CCL4	HPE	-17.62	0.49	-18.10	0.65	-20.36	0.57	-	-	-18.72	0.21	-19.16	0.16
CCL4	HXE	-17.59	0.29	-18.38	0.53	-20.47	0.57	-	-	-18.93	0.16	-19.52	0.18
CCL4	CCL4	-18.5	0.0	-18.68	0.92	-23.86	1.12	-	-	-18.25	0.17	-19.14	0.21
CCL4	CHE	-17.93	-	-18.55	0.81	-20.39	0.63	-	-	-19.26	0.25	-20.33	0.24
CHE	DAMD	-13.8	0.21	-	-	-9.20	1.22	-9.75	0.49	-16.70	0.29	-13.72	0.22
CHE	PPN	-14.83	0.01	-18.96	0.67	-13.52	0.66	-13.40	0.16	-17.34	0.20	-15.58	0.18
CHE	BTN	-15.69	0.01	-18.52	0.57	-14.03	0.69	-13.64	0.19	-18.08	0.16	-16.06	0.15
CHE	PYRI	-15.57	0.02	-	-	-14.57	1.06	-11.87	0.31	-18.11	0.31	-16.41	0.23
CHE	H2O	4.77	0.31	5.52	1.34	6.70	1.48	6.27	0.17	4.39	0.14	5.84	0.11
CHE	C2CL2	-15.97	0.03	-	-	-15.39	0.78	-12.16	0.32	-19.69	0.25	-18.29	0.16
CHE	EAE	-15.71	0.03	-17.30	0.89	-14.64	0.82	-13.59	0.25	-18.33	0.27	-16.54	0.18
CHE	PTL	-15.53	0.0	-17.84	1.07	-15.19	0.95	-14.16	0.21	-17.65	0.27	-16.55	0.36
CHE	MTL	-13.86	0.01	-14.29	0.71	-11.67	0.62	-8.65	0.19	-13.88	0.21	-14.67	0.13
CHE	ETL	-14.55	0.02	-15.66	1.05	-13.35	0.78	-11.56	0.30	-16.87	0.16	-15.65	0.18
CHE	BTL	-15.4	0.14	-17.67	1.19	-14.47	1.13	-13.46	0.30	-17.53	0.40	-16.54	0.24
CHE	2M2P	-15.36	0.0	-17.71	1.01	-15.24	2.10	-14.18	0.30	-18.27	0.44	-16.89	0.30

Table S.1 – Continued on next page

Table S.1 – Continued from previous page

Solute (A)	Solvent (B)	Experimental		GROMOS-54A7		GROMOS-ATB		OPLS-LBCC		AMBER-GAFF2		OpenFF	
		$\Delta_s G_{A:B}^\ominus$	\pm	$\Delta_s G_{A:B}^\ominus$	\pm	$\Delta_s G_{A:B}^\ominus$	\pm	$\Delta_s G_{A:B}^\ominus$	\pm	$\Delta_s G_{A:B}^\ominus$	\pm	$\Delta_s G_{A:B}^\ominus$	\pm
[kJ·mol ⁻¹]													
CHE	1PL	-14.8	0.27	-17.22	1.04	-14.29	0.86	-12.96	0.20	-16.63	0.31	-16.48	0.20
CHE	2PL	-14.85	0.2	-17.65	1.18	-13.16	1.24	-13.02	0.28	-17.90	0.28	-16.25	0.25
CHE	ANLN	-12.74	0.07	-15.79	2.85	-13.77	1.01	-11.27	0.34	-13.34	1.10	-12.32	0.51
CHE	DEE	-17.53	0.0	-20.14	0.50	-16.39	0.66	-16.26	0.23	-20.42	0.17	-18.64	0.12
CHE	CHCL3	-18.61	0.01	-21.55	0.77	-15.67	0.98	-16.49	0.18	-22.70	0.23	-20.62	0.19
CHE	DEAN	-16.5	-	-18.41	0.76	-17.36	0.58	-16.43	0.22	-19.61	0.17	-18.07	0.14
CHE	TEAN	-17.47	0.0	-20.03	0.84	-16.84	0.79	-16.44	0.26	-20.83	0.23	-18.68	0.20
CHE	TOL	-17.46	0.01	-20.15	0.75	-17.34	0.88	-15.57	0.23	-20.32	0.23	-18.16	0.20
CHE	BZN	-17.36	0.33	-19.88	0.84	-17.54	0.87	-16.08	0.23	-18.89	0.15	-18.18	0.23
CHE	HPE	-17.53	0.0	-19.99	0.71	-16.76	0.68	-16.37	0.13	-20.51	0.25	-18.57	0.17
CHE	HXE	-17.7	0.0	-20.19	0.61	-16.98	0.67	-16.56	0.14	-20.59	0.15	-18.61	0.12
CHE	CCL4	-18.5	0.08	-20.80	1.17	-16.81	1.14	-	-	-22.84	0.21	-21.54	0.26
CHE	CHE	-18.55	0.01	-21.03	0.77	-16.92	0.68	-17.05	0.31	-21.75	0.20	-20.03	0.26

Table S.2: Numerical values of the electrostatic (ELE) and van der Waals (VDW) contributions to the calculated cross-solvation free energies $\Delta_s G_{A:B}^\ominus$. The results are reported for the the five force fields newly considered in this work (Main Article Tab. 1). The molecules considered and their acronyms are shown in Main Article Fig. 1. This data is displayed graphically in Figs. S.2 and S.3.

Solute (A)	Solvent (B)	GROMOS-54A7		GROMOS-ATB		OPLS-LBCC		AMBER-GAFF2		OpenFF	
		ELE	VDW	ELE	VDW	ELE	VDW	ELE	VDW	ELE	VDW
[kJ·mol ⁻¹]											
DAMD	DAMD	-	-	-17.28	-22.85	-21.35	-12.45	-12.97	-15.64	-16.99	-13.38
DAMD	PPN	-	-	-14.87	-23.62	-18.05	-15.28	-12.58	-16.06	-15.37	-15.29
DAMD	BTN	-	-	-14.40	-22.82	-16.71	-15.87	-11.60	-16.64	-13.98	-15.86
DAMD	PYRI	-	-	-11.71	-27.10	-20.45	-13.76	-13.12	-16.50	-15.50	-16.16
DAMD	H2O	-	-	-34.26	-0.53	-40.00	5.38	-30.26	5.30	-37.62	6.00
DAMD	C2CL2	-	-	-15.34	-22.80	-22.72	-13.61	-12.14	-18.11	-15.47	-17.70
DAMD	EAE	-	-	-11.87	-25.80	-16.34	-16.16	-11.16	-16.49	-14.02	-16.48
DAMD	PTL	-	-	-14.68	-22.27	-15.61	-16.24	-14.33	-16.50	-19.92	-15.84
DAMD	MTL	-	-	-18.54	-20.24	-24.17	-10.40	-18.77	-12.57	-25.92	-14.29
DAMD	ETL	-	-	-16.65	-21.76	-20.22	-13.26	-17.24	-15.37	-23.08	-15.08
DAMD	BTL	-	-	-12.98	-23.12	-16.51	-15.54	-13.67	-16.13	-21.11	-16.55
DAMD	2M2P	-	-	-14.81	-26.97	-15.78	-16.12	-13.88	-17.12	-19.99	-16.33
DAMD	1PL	-	-	-15.79	-22.51	-17.52	-14.99	-15.35	-15.95	-21.66	-16.06
DAMD	2PL	-	-	-14.72	-24.91	-17.04	-15.20	-14.97	-15.87	-21.40	-15.86
DAMD	ANLN	-	-	-20.37	-25.64	-23.76	-12.64	-21.81	-12.30	-24.35	-11.91
DAMD	DEE	-	-	-8.87	-25.57	-10.64	-17.71	-5.97	-18.60	-7.52	-18.15
DAMD	CHCL3	-	-	-18.01	-26.29	-22.94	-18.57	-14.50	-20.42	-16.12	-19.66
DAMD	DEAN	-	-	-6.97	-26.22	-11.83	-18.09	-10.85	-18.49	-10.56	-17.83
DAMD	TEAN	-	-	-1.44	-26.36	-6.38	-19.06	-1.95	-19.27	-6.27	-18.04
DAMD	TOL	-	-	-7.19	-25.65	-12.38	-17.76	-7.15	-19.19	-8.94	-17.72
DAMD	BZN	-	-	-9.56	-26.21	-12.67	-17.59	-10.04	-17.89	-9.88	-17.91
DAMD	HPE	-	-	-0.10	-24.68	-0.66	-18.56	-0.11	-18.63	-0.04	-18.19
DAMD	HXE	-	-	-0.06	-24.63	-0.63	-18.66	-0.09	-19.11	-0.05	-18.29
DAMD	CCL4	-	-	-0.68	-26.43	-	-	-0.42	-21.23	-0.57	-20.84
DAMD	CHE	-	-	-0.00	-24.26	-0.71	-19.66	-0.03	-19.58	-0.05	-18.82
PPN	DAMD	-	-	-12.48	-6.65	-15.08	-3.32	-10.35	-6.45	-12.10	-4.87
PPN	PPN	-6.57	-12.10	-9.42	-9.95	-12.84	-6.82	-9.90	-7.56	-10.64	-7.47
PPN	BTN	-5.71	-12.37	-10.07	-9.15	-11.89	-7.19	-9.13	-7.95	-9.82	-7.56
PPN	PYRI	-	-	-6.45	-12.04	-14.25	-4.76	-10.02	-7.24	-10.50	-7.41
PPN	H2O	-14.88	4.81	-21.58	7.48	-23.89	7.64	-21.71	8.18	-22.70	8.42
PPN	C2CL2	-	-	-11.09	-8.55	-15.88	-5.16	-9.16	-8.94	-10.04	-8.78
PPN	EAE	-6.96	-11.18	-7.09	-11.47	-11.57	-6.99	-8.82	-7.99	-9.79	-7.08
PPN	PTL	-3.37	-10.91	-7.64	-9.91	-10.23	-7.10	-6.65	-7.29	-10.66	-7.73
PPN	MTL	-7.31	-8.38	-10.02	-8.90	-15.92	-3.26	-12.08	-5.81	-14.47	-6.90
PPN	ETL	-5.51	-9.93	-8.13	-9.62	-13.55	-5.45	-10.59	-7.32	-12.85	-7.41
PPN	BTL	-3.89	-10.68	-6.75	-9.27	-11.08	-7.04	-7.73	-7.88	-10.75	-7.65
PPN	2M2P	-4.04	-11.40	-10.84	-7.33	-10.91	-7.21	-8.92	-7.44	-11.05	-7.92
PPN	1PL	-4.82	-11.07	-8.54	-8.83	-12.21	-6.77	-9.36	-7.23	-11.66	-7.47
PPN	2PL	-4.12	-11.35	-7.09	-10.23	-11.68	-6.57	-9.30	-7.38	-11.72	-7.66
PPN	ANLN	-9.67	-9.25	-12.61	-10.88	-16.49	-4.10	-16.54	-3.52	-15.41	-4.61
PPN	DEE	-2.28	-13.19	-5.51	-11.97	-7.81	-9.46	-4.46	-10.01	-5.07	-9.71
PPN	CHCL3	-3.80	-14.31	-10.84	-10.69	-16.61	-8.87	-9.92	-10.51	-9.93	-10.68
PPN	DEAN	-6.28	-11.40	-4.09	-12.70	-8.77	-9.13	-7.70	-9.40	-7.31	-9.24
PPN	TEAN	-1.93	-13.20	-1.04	-11.32	-4.56	-9.52	-1.34	-9.72	-4.17	-9.33
PPN	TOL	-3.96	-12.70	-4.83	-10.92	-9.04	-8.35	-5.58	-9.45	-6.23	-9.33

Table S.2 – Continued on next page

Table S.2 – Continued from previous page

Solute (A)	Solvent (B)	GROMOS-54A7		GROMOS-ATB		OPLS-LBCC		AMBER-GAFF2		OpenFF	
		ELE	VDW	ELE	VDW	ELE	VDW	ELE	VDW	ELE	VDW
[kJ·mol ⁻¹]											
PPN	BZN	-5.21	-11.91	-5.78	-11.74	-9.02	-8.63	-7.77	-8.62	-6.84	-9.16
PPN	HPE	-0.00	-12.77	-0.07	-10.97	-0.39	-9.85	-0.07	-9.45	-0.02	-9.49
PPN	HXE	-0.00	-13.11	-0.04	-10.92	-0.37	-9.88	-0.07	-10.11	-0.01	-9.95
PPN	CCL4	-0.00	-13.84	0.56	-11.71	-	-	-0.24	-11.22	-0.43	-11.08
PPN	CHE	-0.00	-13.50	-0.00	-11.50	-0.38	-10.21	-0.03	-9.62	0.02	-9.70
BTN	DAMD	-	-	-10.95	-7.68	-14.55	-5.27	-9.97	-10.12	-11.48	-7.57
BTN	PPN	-6.14	-14.81	-9.03	-12.02	-12.29	-9.25	-9.61	-10.77	-10.21	-10.13
BTN	BTN	-5.46	-15.03	-9.14	-11.16	-11.40	-9.59	-8.82	-11.37	-9.33	-10.65
BTN	PYRI	-	-	-4.40	-16.22	-13.84	-6.70	-9.74	-10.83	-10.22	-9.95
BTN	H2O	-14.75	5.38	-19.68	8.25	-23.78	8.24	-21.62	8.32	-22.72	8.96
BTN	C2CL2	-	-	-10.78	-11.10	-15.37	-7.33	-8.78	-12.66	-9.84	-12.05
BTN	EAE	-6.53	-14.13	-5.81	-13.91	-11.02	-9.61	-8.55	-11.20	-9.33	-10.36
BTN	PTL	-3.66	-13.81	-6.27	-12.27	-9.73	-9.93	-7.27	-10.93	-10.41	-11.01
BTN	MTL	-6.85	-10.77	-8.51	-10.89	-15.53	-5.11	-12.08	-8.49	-14.39	-9.42
BTN	ETL	-5.20	-12.22	-7.17	-11.76	-12.90	-7.89	-10.79	-10.17	-12.53	-10.02
BTN	BTL	-3.14	-14.40	-5.10	-11.77	-10.73	-9.88	-7.50	-10.27	-10.89	-10.89
BTN	2M2P	-3.93	-14.47	-10.19	-10.21	-10.41	-10.07	-8.93	-11.36	-10.96	-11.38
BTN	1PL	-4.48	-12.66	-7.00	-11.70	-11.77	-9.06	-8.92	-10.15	-11.73	-10.87
BTN	2PL	-4.52	-12.93	-5.33	-11.60	-10.79	-9.11	-8.68	-10.50	-11.48	-10.75
BTN	ANLN	-8.98	-9.44	-10.63	-13.72	-15.83	-6.40	-15.63	-6.46	-14.76	-7.41
BTN	DEE	-2.15	-16.42	-4.43	-14.52	-7.29	-12.18	-4.21	-13.76	-4.94	-13.03
BTN	CHCL3	-3.78	-17.52	-9.66	-13.36	-16.24	-11.90	-9.82	-14.71	-9.74	-14.11
BTN	DEAN	-5.87	-14.17	-3.39	-15.53	-8.02	-12.14	-7.37	-13.03	-6.78	-11.84
BTN	TEAN	-1.77	-15.65	-1.07	-13.48	-4.19	-12.47	-1.26	-13.18	-3.95	-12.60
BTN	TOL	-3.68	-15.64	-4.20	-14.84	-8.43	-10.81	-5.26	-13.25	-6.00	-12.74
BTN	BZN	-4.82	-15.13	-4.57	-15.25	-8.66	-11.37	-7.27	-12.34	-6.60	-12.56
BTN	HPE	-0.00	-15.99	-0.07	-13.44	-0.40	-12.55	-0.05	-13.12	-0.06	-13.00
BTN	HXE	-0.00	-15.63	-0.04	-14.30	-0.39	-12.95	-0.07	-13.61	-0.04	-13.09
BTN	CCL4	-0.00	-16.71	1.46	-16.03	-	-	-0.24	-15.30	-0.38	-14.83
BTN	CHE	-0.00	-16.44	-0.00	-14.14	-0.38	-13.50	-0.03	-13.99	-0.03	-13.48
PYRI	DAMD	-	-	-6.10	-19.24	-15.85	-12.46	-9.70	-12.02	-10.75	-11.98
PYRI	PPN	-	-	-4.45	-20.17	-12.74	-14.40	-8.79	-13.08	-8.95	-13.44
PYRI	BTN	-	-	-3.36	-21.49	-11.83	-15.28	-8.03	-13.38	-8.20	-14.06
PYRI	PYRI	-	-	-3.76	-21.28	-14.70	-12.67	-8.82	-12.42	-8.54	-13.96
PYRI	H2O	-	-	-17.48	-0.66	-22.63	3.61	-17.59	5.67	-18.95	4.90
PYRI	C2CL2	-	-	-3.53	-21.08	-15.72	-12.76	-8.05	-14.09	-7.91	-15.07
PYRI	EAE	-	-	-3.78	-21.20	-11.34	-15.11	-8.14	-13.03	-8.28	-14.35
PYRI	PTL	-	-	-3.91	-18.96	-8.75	-15.44	-5.19	-13.16	-7.93	-14.63
PYRI	MTL	-	-	-4.17	-18.81	-15.44	-9.71	-9.06	-10.25	-11.17	-12.68
PYRI	ETL	-	-	-3.64	-18.97	-12.49	-13.06	-7.42	-12.51	-9.63	-13.49
PYRI	BTL	-	-	-1.67	-20.53	-9.74	-14.52	-5.50	-12.85	-7.75	-14.33
PYRI	2M2P	-	-	-3.70	-19.91	-9.60	-15.87	-5.69	-13.70	-8.23	-14.15
PYRI	1PL	-	-	-3.78	-19.07	-11.11	-14.29	-6.40	-12.71	-8.72	-14.13
PYRI	2PL	-	-	-2.09	-21.77	-10.54	-14.68	-5.56	-12.40	-8.73	-14.48
PYRI	ANLN	-	-	-5.13	-18.84	-15.80	-12.85	-12.72	-9.55	-13.13	-9.96
PYRI	DEE	-	-	-3.98	-20.28	-7.67	-16.85	-3.65	-15.36	-4.25	-16.36
PYRI	CHCL3	-	-	-7.45	-19.91	-15.12	-16.31	-7.69	-16.02	-7.55	-17.19
PYRI	DEAN	-	-	-1.72	-21.29	-8.16	-16.84	-5.77	-14.98	-5.90	-15.87
PYRI	TEAN	-	-	-0.33	-21.18	-4.59	-18.06	-1.19	-15.68	-3.64	-16.06
PYRI	TOL	-	-	-4.47	-19.14	-8.97	-16.53	-4.56	-15.03	-5.11	-15.49

Table S.2 – Continued on next page

Table S.2 – Continued from previous page

Solute (A)	Solvent (B)	GROMOS-54A7		GROMOS-ATB		OPLS-LBCC		AMBER-GAFF2		OpenFF	
		ELE	VDW	ELE	VDW	ELE	VDW	ELE	VDW	ELE	VDW
[kJ·mol ⁻¹]											
PYRI	BZN	-	-	-7.40	-17.64	-9.31	-16.41	-6.91	-14.50	-5.79	-15.54
PYRI	HPE	-	-	-0.02	-20.08	-0.46	-17.78	-0.08	-15.28	0.03	-16.22
PYRI	HXE	-	-	-0.02	-19.64	-0.44	-17.87	-0.08	-15.46	0.00	-16.14
PYRI	CCL4	-	-	-1.48	-19.99	-	-	-0.32	-16.79	-0.32	-17.81
PYRI	CHE	-	-	-0.00	-19.41	-0.55	-18.93	0.00	-15.65	-0.07	-16.83
H2O	DAMD	-	-	-26.19	6.75	-26.49	7.81	-26.54	6.36	-30.10	6.91
H2O	PPN	-16.60	4.31	-19.59	4.26	-22.03	4.84	-21.35	4.40	-21.84	4.44
H2O	BTN	-15.31	4.23	-17.36	3.74	-20.95	4.82	-20.09	4.58	-20.89	4.45
H2O	PYRI	-	-	-19.70	4.45	-20.92	7.61	-18.13	5.59	-20.27	5.84
H2O	H2O	-35.19	8.70	-35.23	8.90	-35.44	9.19	-35.55	9.15	-35.55	9.15
H2O	C2CL2	-	-	-11.65	3.95	-17.86	6.79	-11.42	4.44	-10.80	4.48
H2O	EAE	-20.43	5.61	-18.46	4.77	-20.02	5.35	-22.47	4.93	-21.82	5.59
H2O	PTL	-19.40	2.53	-19.97	3.82	-22.31	4.86	-21.87	5.21	-19.73	4.95
H2O	MTL	-27.06	4.21	-24.88	3.56	-29.34	5.82	-26.15	3.98	-24.52	4.19
H2O	ETL	-22.62	3.88	-22.84	3.70	-27.26	5.26	-23.80	4.34	-22.68	4.55
H2O	BTL	-19.95	1.76	-20.37	2.78	-23.90	4.83	-21.99	4.94	-20.44	4.72
H2O	2M2P	-19.30	1.85	-21.85	4.77	-24.71	4.67	-21.30	4.53	-20.24	4.74
H2O	1PL	-21.19	2.68	-21.07	2.65	-25.45	4.89	-23.91	4.95	-21.58	4.73
H2O	2PL	-20.73	3.31	-22.09	5.40	-24.86	4.93	-22.64	4.71	-21.09	4.74
H2O	ANLN	-27.39	9.81	-20.96	3.23	-24.49	7.97	-24.66	7.77	-21.84	7.39
H2O	DEE	-4.62	2.70	-10.13	2.89	-16.60	3.18	-8.44	3.15	-10.99	3.47
H2O	CHCL3	-4.67	3.86	-10.85	5.53	-14.73	5.45	-9.44	3.70	-8.53	3.98
H2O	DEAN	-18.05	3.97	-7.73	1.98	-22.27	3.83	-15.54	3.86	-19.97	3.92
H2O	TEAN	-5.02	3.55	-2.14	3.93	-14.65	3.96	-2.94	4.20	-15.00	4.01
H2O	TOL	-8.03	4.02	-7.39	3.94	-11.86	5.04	-8.90	4.57	-9.92	4.19
H2O	BZN	-11.41	4.21	-9.32	4.19	-11.87	5.04	-12.75	4.66	-10.73	4.04
H2O	HPE	-0.00	3.06	-0.05	3.05	-0.56	3.13	-0.06	3.94	-0.05	3.51
H2O	HXE	-0.00	2.84	-0.03	2.73	-0.53	2.88	-0.06	3.65	-0.07	3.22
H2O	CCL4	-0.00	3.73	-1.56	5.06	-	-	-0.51	3.86	-0.43	4.24
H2O	CHE	-0.00	3.37	-0.00	2.51	-0.54	3.65	-0.01	4.64	-0.09	4.25
C2CL2	DAMD	-	-	-9.15	-7.95	-18.92	-7.27	-8.47	-10.55	-9.71	-9.33
C2CL2	PPN	-	-	-6.67	-11.70	-15.95	-10.68	-7.35	-11.65	-7.83	-10.91
C2CL2	BTN	-	-	-7.29	-10.96	-14.98	-11.19	-6.76	-12.13	-7.37	-11.50
C2CL2	PYRI	-	-	-2.31	-15.16	-16.81	-8.45	-7.18	-11.05	-7.27	-10.78
C2CL2	H2O	-	-	-10.66	7.20	-19.75	6.68	-9.73	6.91	-9.24	6.84
C2CL2	C2CL2	-	-	-7.28	-10.47	-16.16	-8.27	-5.29	-12.31	-5.39	-12.30
C2CL2	EAE	-	-	-3.97	-13.52	-13.40	-10.89	-6.98	-11.92	-7.05	-10.99
C2CL2	PTL	-	-	-3.14	-11.53	-11.90	-11.30	-3.22	-12.21	-4.04	-11.60
C2CL2	MTL	-	-	-4.57	-10.84	-17.10	-6.51	-5.59	-8.93	-6.22	-10.54
C2CL2	ETL	-	-	-3.34	-11.20	-15.33	-9.08	-4.22	-10.96	-5.49	-11.18
C2CL2	BTL	-	-	-2.40	-12.05	-12.76	-11.25	-3.66	-11.56	-4.25	-11.53
C2CL2	2M2P	-	-	-1.67	-13.46	-13.69	-11.79	-2.35	-12.58	-4.15	-11.76
C2CL2	1PL	-	-	-3.63	-11.65	-14.59	-10.61	-4.43	-10.99	-4.68	-11.71
C2CL2	2PL	-	-	-2.66	-12.15	-13.93	-10.94	-3.64	-11.34	-4.65	-10.77
C2CL2	ANLN	-	-	-5.08	-12.35	-17.30	-6.72	-10.82	-6.84	-9.51	-7.54
C2CL2	DEE	-	-	-2.86	-13.93	-10.23	-13.27	-3.14	-14.09	-4.02	-14.02
C2CL2	CHCL3	-	-	-4.37	-13.66	-13.44	-11.99	-3.54	-14.06	-3.99	-13.73
C2CL2	DEAN	-	-	-1.30	-14.46	-12.06	-13.16	-4.12	-13.22	-5.53	-13.27
C2CL2	TEAN	-	-	-0.67	-13.63	-6.86	-13.85	-1.11	-14.02	-3.89	-13.72
C2CL2	TOL	-	-	-3.17	-13.37	-10.78	-12.18	-4.84	-13.50	-4.95	-12.72

Table S.2 – Continued on next page

Table S.2 – Continued from previous page

Solute (A)	Solvent (B)	GROMOS-54A7		GROMOS-ATB		OPLS-LBCC		AMBER-GAFF2		OpenFF	
		ELE	VDW	ELE	VDW	ELE	VDW	ELE	VDW	ELE	VDW
[kJ·mol ⁻¹]											
C2CL2	BZN	-	-	-3.25	-14.64	-10.56	-12.27	-6.64	-12.59	-5.16	-13.02
C2CL2	HPE	-	-	-0.04	-13.63	-0.37	-14.11	-0.01	-14.16	-0.04	-13.56
C2CL2	HXE	-	-	-0.02	-13.73	-0.36	-14.09	-0.03	-14.45	-0.04	-13.91
C2CL2	CCL4	-	-	0.85	-14.82	-	-	-0.26	-14.42	-0.16	-14.45
C2CL2	CHE	-	-	-0.00	-13.50	-0.27	-14.50	0.00	-14.46	-0.03	-14.58
EAE	DAMD	-	-	-8.26	-14.68	-13.74	-8.17	-9.15	-11.51	-10.92	-12.22
EAE	PPN	-10.03	-19.19	-4.94	-18.12	-11.15	-12.06	-8.53	-12.76	-9.26	-14.30
EAE	BTN	-8.92	-19.41	-6.42	-16.52	-10.22	-12.20	-7.83	-13.20	-8.31	-14.59
EAE	PYRI	-	-	-2.19	-21.68	-12.88	-9.09	-9.26	-12.17	-9.38	-14.89
EAE	H2O	-23.58	5.10	-19.61	7.04	-22.40	8.32	-23.75	8.81	-22.95	6.88
EAE	C2CL2	-	-	-7.82	-16.98	-13.23	-10.11	-8.41	-14.60	-8.59	-16.48
EAE	EAE	-10.61	-18.14	-4.35	-18.89	-10.36	-12.24	-7.96	-12.89	-8.91	-14.63
EAE	PTL	-8.42	-19.45	-4.80	-16.56	-8.70	-12.79	-7.70	-12.95	-9.58	-15.21
EAE	MTL	-12.80	-14.63	-6.48	-15.60	-14.26	-7.35	-12.53	-9.73	-13.76	-13.23
EAE	ETL	-10.55	-15.14	-5.21	-16.66	-11.48	-10.14	-10.95	-11.90	-12.07	-13.91
EAE	BTL	-8.48	-17.53	-3.38	-18.73	-9.11	-12.41	-8.82	-12.50	-10.13	-15.30
EAE	2M2P	-7.81	-17.69	-2.43	-19.62	-9.57	-12.65	-9.91	-13.05	-10.45	-14.65
EAE	1PL	-8.31	-16.69	-5.27	-17.71	-10.56	-11.69	-9.12	-12.21	-11.23	-14.40
EAE	2PL	-10.27	-17.75	-2.80	-18.57	-9.72	-11.81	-9.30	-12.70	-11.26	-14.45
EAE	ANLN	-15.28	-15.28	-8.61	-19.88	-15.73	-8.85	-15.50	-8.14	-15.46	-11.08
EAE	DEE	-3.86	-20.87	-3.59	-19.36	-6.87	-14.58	-3.70	-15.53	-4.57	-17.22
EAE	CHCL3	-6.14	-21.82	-9.26	-18.50	-13.24	-14.92	-9.62	-16.87	-8.76	-19.05
EAE	DEAN	-10.47	-17.99	-2.78	-20.13	-7.56	-14.76	-7.55	-14.92	-6.47	-16.67
EAE	TEAN	-3.19	-20.14	-0.75	-19.03	-4.24	-15.17	-1.25	-15.69	-3.76	-16.95
EAE	TOL	-6.31	-20.21	-3.67	-19.21	-8.61	-14.03	-5.13	-14.99	-6.03	-16.79
EAE	BZN	-7.93	-19.66	-4.64	-18.73	-8.83	-14.16	-7.34	-14.18	-6.60	-16.96
EAE	HPE	-0.00	-20.33	-0.05	-17.78	-0.55	-15.41	-0.04	-15.40	-0.05	-17.47
EAE	HXE	-0.00	-19.81	-0.03	-18.26	-0.53	-15.63	-0.05	-15.58	-0.05	-17.38
EAE	CCL4	-0.00	-21.73	-0.11	-19.86	-	-	-0.41	-17.62	-0.31	-19.65
EAE	CHE	-0.00	-21.04	-0.00	-18.69	-0.55	-16.71	-0.01	-15.98	-0.06	-17.76
PTL	DAMD	-	-	-13.97	-10.11	-16.41	-7.03	-18.72	-12.69	-17.25	-12.60
PTL	PPN	-12.81	-16.25	-10.11	-13.70	-13.24	-11.22	-15.21	-13.66	-12.27	-15.12
PTL	BTN	-11.74	-16.83	-8.90	-14.60	-12.13	-12.08	-14.32	-14.07	-11.82	-15.50
PTL	PYRI	-	-	-7.32	-17.11	-13.82	-8.98	-12.93	-13.79	-11.09	-15.76
PTL	H2O	-28.72	7.13	-22.74	10.27	-27.33	9.08	-28.40	9.51	-19.85	7.87
PTL	C2CL2	-	-	-6.89	-15.24	-13.80	-9.49	-8.47	-15.77	-6.26	-17.28
PTL	EAE	-15.50	-14.75	-8.63	-15.09	-11.89	-11.68	-15.81	-14.18	-11.97	-14.86
PTL	PTL	-17.60	-13.44	-10.92	-14.78	-12.71	-11.41	-14.85	-14.11	-9.99	-15.29
PTL	MTL	-21.83	-12.43	-12.92	-12.55	-18.88	-6.55	-19.33	-10.97	-13.07	-13.90
PTL	ETL	-19.59	-14.86	-11.70	-13.93	-15.69	-9.96	-17.58	-13.06	-11.71	-14.95
PTL	BTL	-18.04	-16.36	-10.90	-15.40	-13.06	-11.85	-16.73	-13.72	-10.42	-15.98
PTL	2M2P	-16.43	-15.56	-13.77	-16.88	-12.89	-12.52	-14.90	-15.21	-10.90	-15.43
PTL	1PL	-18.76	-14.72	-11.18	-14.44	-13.84	-11.62	-17.31	-13.54	-10.94	-15.43
PTL	2PL	-18.37	-15.88	-11.70	-14.62	-14.12	-11.74	-16.61	-13.09	-11.12	-15.55
PTL	ANLN	-22.56	-7.62	-10.21	-15.08	-16.40	-8.23	-19.19	-7.93	-13.00	-10.17
PTL	DEE	-3.52	-19.03	-5.41	-16.80	-7.91	-14.43	-5.63	-17.01	-6.21	-17.97
PTL	CHCL3	-4.02	-19.32	-7.50	-16.50	-13.55	-14.69	-8.05	-18.31	-5.35	-19.55
PTL	DEAN	-15.83	-15.44	-3.18	-18.04	-10.40	-14.54	-11.06	-16.20	-11.88	-17.59
PTL	TEAN	-3.86	-18.55	-0.90	-17.00	-5.58	-15.34	-1.66	-16.90	-9.09	-17.79
PTL	TOL	-5.99	-18.20	-4.38	-16.96	-7.64	-13.98	-6.25	-16.54	-5.65	-17.62

Table S.2 – Continued on next page

Table S.2 – Continued from previous page

Solute (A)	Solvent (B)	GROMOS-54A7		GROMOS-ATB		OPLS-LBCC		AMBER-GAFF2		OpenFF	
		ELE	VDW	ELE	VDW	ELE	VDW	ELE	VDW	ELE	VDW
[kJ·mol ⁻¹]											
PTL	BZN	-8.22	-17.80	-5.07	-17.67	-7.63	-14.22	-9.09	-15.75	-6.05	-17.61
PTL	HPE	-0.00	-18.05	-0.04	-16.80	-0.43	-15.44	-0.04	-16.64	-0.04	-18.05
PTL	HXE	-0.00	-18.56	-0.02	-17.11	-0.41	-15.81	-0.04	-17.20	-0.06	-18.32
PTL	CCL4	-0.00	-19.84	-0.42	-17.23	-	-	-0.35	-19.16	-0.20	-21.08
PTL	CHE	-0.00	-19.73	-0.00	-17.08	-0.42	-16.07	-0.01	-16.29	-0.12	-18.58
MTL	DAMD	-	-	-15.51	0.45	-17.71	2.31	-19.34	1.95	-18.06	-0.50
MTL	PPN	-13.72	-3.71	-11.31	-2.06	-14.39	-0.71	-15.67	0.18	-12.84	-2.54
MTL	BTN	-12.60	-3.93	-10.02	-2.71	-13.46	-0.80	-14.94	0.20	-12.36	-2.60
MTL	PYRI	-	-	-8.74	-3.74	-15.00	1.93	-13.38	1.23	-11.73	-1.83
MTL	H2O	-29.67	7.09	-23.17	8.26	-27.61	7.94	-26.52	9.16	-19.52	6.60
MTL	C2CL2	-	-	-7.45	-2.71	-14.46	1.12	-8.58	-0.37	-6.55	-3.11
MTL	EAE	-16.66	-2.62	-10.24	-2.31	-12.85	-0.55	-16.32	0.23	-12.62	-2.05
MTL	PTL	-19.11	-4.01	-11.57	-2.09	-13.84	-0.91	-15.45	0.60	-9.69	-2.35
MTL	MTL	-22.96	-3.13	-13.79	-2.86	-19.82	1.43	-18.58	0.58	-13.07	-2.29
MTL	ETL	-20.74	-4.16	-12.82	-2.41	-17.75	0.25	-17.14	0.15	-12.04	-2.32
MTL	BTL	-19.29	-5.42	-11.72	-2.26	-14.82	-1.01	-16.24	0.56	-10.68	-2.57
MTL	2M2P	-18.50	-3.68	-13.94	-2.46	-15.03	-0.91	-15.62	0.39	-11.38	-2.31
MTL	1PL	-21.09	-1.97	-12.33	-2.78	-16.06	-0.46	-17.71	0.58	-11.11	-2.59
MTL	2PL	-19.61	-5.17	-12.28	-2.57	-15.67	-0.63	-17.44	0.57	-11.65	-2.34
MTL	ANLN	-22.46	-2.81	-11.38	-2.97	-17.95	1.95	-19.35	2.90	-13.84	0.15
MTL	DEE	-3.98	-5.01	-6.47	-3.12	-9.63	-2.59	-6.17	-1.59	-6.73	-3.99
MTL	CHCL3	-4.42	-4.88	-7.97	-2.14	-13.99	-1.41	-7.53	-1.58	-5.51	-4.24
MTL	DEAN	-17.91	-4.29	-3.83	-4.21	-12.75	-2.24	-12.10	-0.91	-13.10	-3.56
MTL	TEAN	-4.66	-4.61	-1.05	-2.52	-7.36	-2.40	-1.93	-0.78	-10.18	-3.40
MTL	TOL	-6.73	-4.78	-4.99	-2.63	-8.65	-1.25	-6.67	-0.53	-6.08	-3.39
MTL	BZN	-9.41	-4.11	-6.07	-2.84	-8.59	-1.51	-9.72	-0.04	-6.52	-3.58
MTL	HPE	-0.00	-4.55	-0.03	-2.93	-0.42	-2.98	-0.05	-0.89	-0.03	-3.82
MTL	HXE	-0.00	-4.87	-0.02	-3.15	-0.39	-3.19	-0.05	-1.18	-0.04	-4.08
MTL	CCL4	-0.00	-5.06	-0.93	-2.49	-	-	-0.38	-1.64	-0.25	-4.37
MTL	CHE	-0.00	-5.05	-0.00	-3.03	-0.41	-2.81	-0.01	-0.35	-0.06	-3.75
ETL	DAMD	-	-	-15.68	-1.73	-17.36	-0.41	-18.11	-1.89	-17.62	-3.88
ETL	PPN	-13.01	-6.87	-11.27	-5.49	-14.11	-3.56	-14.60	-3.71	-12.53	-5.82
ETL	BTN	-12.00	-6.88	-10.11	-5.86	-13.13	-3.83	-13.88	-3.85	-11.99	-6.05
ETL	PYRI	-	-	-9.07	-7.04	-14.71	-0.83	-12.28	-2.74	-11.44	-5.83
ETL	H2O	-29.19	7.43	-24.59	8.07	-28.64	8.35	-24.72	9.08	-20.06	7.13
ETL	C2CL2	-	-	-7.11	-5.52	-14.52	-1.61	-7.71	-4.54	-6.37	-6.69
ETL	EAE	-15.88	-5.64	-10.61	-5.40	-12.69	-3.55	-15.29	-3.77	-12.17	-5.29
ETL	PTL	-17.64	-7.78	-12.43	-5.99	-13.69	-3.78	-14.26	-3.44	-10.11	-5.86
ETL	MTL	-22.21	-4.54	-14.57	-6.03	-20.27	-0.90	-17.11	-2.57	-13.15	-5.33
ETL	ETL	-20.59	-5.90	-14.19	-5.53	-17.39	-2.63	-15.66	-3.62	-12.17	-5.80
ETL	BTL	-18.51	-4.78	-11.84	-8.01	-14.69	-3.88	-15.09	-3.36	-10.65	-6.17
ETL	2M2P	-16.58	-6.74	-17.69	-6.07	-14.84	-3.92	-14.92	-3.71	-11.01	-5.97
ETL	1PL	-18.71	-7.88	-13.43	-5.25	-15.59	-3.37	-15.93	-2.91	-10.96	-5.69
ETL	2PL	-17.69	-8.02	-13.79	-5.56	-15.58	-3.43	-14.83	-3.33	-11.24	-5.96
ETL	ANLN	-24.28	-1.09	-11.09	-6.00	-17.92	-0.91	-17.68	0.58	-13.83	-3.99
ETL	DEE	-3.68	-8.36	-6.60	-6.67	-9.15	-5.82	-5.51	-5.96	-6.27	-7.78
ETL	CHCL3	-4.16	-8.31	-7.94	-5.24	-14.16	-4.74	-6.87	-6.18	-5.44	-8.09
ETL	DEAN	-16.02	-6.64	-3.88	-7.46	-11.99	-5.35	-10.59	-4.92	-12.14	-6.89
ETL	TEAN	-4.02	-7.63	-1.02	-6.09	-7.07	-5.60	-1.63	-5.20	-9.33	-7.43
ETL	TOL	-6.11	-7.67	-4.81	-6.33	-8.36	-4.75	-6.01	-4.83	-5.70	-7.22

Table S.2 – Continued on next page

Table S.2 – Continued from previous page

Solute (A)	Solvent (B)	GROMOS-54A7		GROMOS-ATB		OPLS-LBCC		AMBER-GAFF2		OpenFF	
		ELE	VDW	ELE	VDW	ELE	VDW	ELE	VDW	ELE	VDW
[kJ·mol ⁻¹]											
ETL	BZN	-8.52	-7.62	-6.12	-6.20	-8.32	-5.00	-8.68	-4.20	-6.15	-6.96
ETL	HPE	-0.00	-7.94	-0.04	-6.08	-0.43	-6.29	-0.04	-5.23	-0.02	-7.54
ETL	HXE	-0.00	-7.99	-0.02	-6.66	-0.41	-6.42	-0.04	-5.68	-0.04	-7.83
ETL	CCL4	-0.00	-8.66	-0.81	-5.86	-	-	-0.33	-6.29	-0.23	-8.78
ETL	CHE	-0.00	-7.92	-0.00	-6.54	-0.42	-6.19	-0.01	-5.06	-0.07	-7.66
BTL	DAMD	-	-	-16.83	-7.94	-16.17	-4.53	-19.13	-8.84	-17.09	-9.87
BTL	PPN	-12.77	-13.29	-12.50	-11.00	-13.06	-8.66	-15.55	-10.47	-12.20	-11.95
BTL	BTN	-11.66	-13.72	-11.46	-11.96	-12.08	-9.01	-14.70	-11.08	-11.78	-12.22
BTL	PYRI	-	-	-9.07	-15.01	-13.77	-6.02	-13.26	-10.38	-11.04	-11.90
BTL	H2O	-28.76	7.02	-27.99	9.41	-27.20	8.92	-29.23	9.09	-19.65	7.40
BTL	C2CL2	-	-	-8.32	-12.11	-13.59	-7.06	-8.59	-11.95	-6.18	-13.75
BTL	EAE	-15.40	-11.83	-10.94	-12.08	-11.70	-9.07	-16.17	-10.79	-11.92	-12.25
BTL	PTL	-17.18	-12.27	-14.64	-11.87	-12.21	-9.27	-17.87	-10.68	-9.88	-12.39
BTL	MTL	-22.04	-9.96	-17.13	-10.61	-18.64	-4.73	-19.93	-8.13	-12.99	-10.87
BTL	ETL	-19.73	-12.03	-16.69	-11.24	-15.82	-7.03	-18.53	-9.38	-11.45	-11.92
BTL	BTL	-17.42	-14.40	-16.75	-11.12	-13.08	-8.92	-17.75	-10.40	-10.21	-12.75
BTL	2M2P	-16.84	-12.15	-18.35	-9.13	-12.90	-9.86	-17.07	-10.97	-10.68	-12.39
BTL	1PL	-18.16	-12.83	-15.44	-12.28	-14.30	-8.57	-17.78	-9.88	-10.76	-12.37
BTL	2PL	-18.43	-12.61	-17.99	-12.13	-13.61	-8.36	-17.16	-10.34	-11.04	-11.81
BTL	ANLN	-21.05	-11.79	-11.43	-12.52	-16.08	-6.08	-20.59	-5.13	-12.49	-7.67
BTL	DEE	-3.52	-15.19	-6.85	-14.12	-8.09	-11.72	-5.84	-13.21	-6.10	-14.83
BTL	CHCL3	-4.04	-16.29	-8.45	-12.59	-13.49	-11.53	-8.15	-14.33	-5.39	-16.37
BTL	DEAN	-15.75	-13.99	-4.05	-15.19	-10.18	-11.61	-11.60	-13.10	-11.79	-14.00
BTL	TEAN	-3.75	-14.86	-1.19	-13.44	-5.57	-12.09	-1.77	-12.89	-9.13	-14.34
BTL	TOL	-5.92	-14.49	-5.11	-14.12	-7.63	-10.95	-6.46	-12.63	-5.50	-14.21
BTL	BZN	-8.28	-14.76	-5.66	-14.63	-7.66	-11.24	-9.27	-11.72	-5.90	-13.85
BTL	HPE	-0.00	-14.53	-0.05	-13.55	-0.42	-12.80	-0.04	-13.10	0.00	-14.72
BTL	HXE	-0.00	-15.00	-0.02	-13.47	-0.40	-12.73	-0.05	-13.34	-0.02	-15.02
BTL	CCL4	-0.00	-15.55	-0.30	-13.76	-	-	-0.37	-15.08	-0.24	-16.89
BTL	CHE	-0.00	-15.55	-0.00	-13.65	-0.41	-12.64	-0.01	-13.00	-0.05	-15.21
2M2P	DAMD	-	-	-15.72	-13.17	-14.82	-4.22	-17.10	-8.45	-16.18	-8.73
2M2P	PPN	-10.17	-9.42	-11.36	-15.06	-12.19	-8.50	-13.82	-10.20	-11.75	-11.24
2M2P	BTN	-9.27	-9.41	-11.36	-14.53	-11.17	-8.74	-12.96	-10.68	-11.27	-11.45
2M2P	PYRI	-	-	-6.87	-19.29	-13.08	-6.01	-11.44	-9.28	-10.66	-10.86
2M2P	H2O	-23.66	10.79	-27.55	5.81	-28.52	8.91	-25.38	8.99	-20.36	7.54
2M2P	C2CL2	-	-	-9.18	-13.61	-13.37	-6.56	-7.52	-11.54	-6.14	-13.29
2M2P	EAE	-12.50	-6.56	-8.99	-17.16	-10.96	-9.04	-14.36	-10.54	-11.50	-11.07
2M2P	PTL	-11.97	-9.78	-14.44	-16.37	-11.70	-9.09	-13.99	-10.35	-9.87	-11.27
2M2P	MTL	-16.67	-5.97	-16.14	-14.03	-18.26	-4.50	-16.85	-7.75	-13.07	-10.49
2M2P	ETL	-13.73	-9.39	-15.29	-15.88	-14.76	-6.89	-15.60	-9.88	-11.73	-10.76
2M2P	BTL	-13.24	-6.01	-16.07	-15.33	-12.28	-8.79	-14.90	-10.25	-10.14	-11.75
2M2P	2M2P	-11.62	-8.75	-20.70	-14.98	-11.84	-9.74	-13.05	-10.26	-9.49	-11.81
2M2P	1PL	-12.79	-7.04	-14.90	-15.10	-12.59	-8.76	-14.93	-9.45	-10.44	-11.26
2M2P	2PL	-12.35	-6.26	-15.21	-17.61	-13.22	-8.08	-14.40	-9.36	-10.31	-11.78
2M2P	ANLN	-16.67	-5.91	-9.76	-17.83	-14.86	-6.66	-16.53	-3.20	-12.50	-8.31
2M2P	DEE	-2.59	-11.05	-6.24	-17.31	-6.42	-11.33	-4.58	-12.91	-4.91	-13.82
2M2P	CHCL3	-3.31	-11.24	-7.96	-16.19	-13.74	-11.24	-6.90	-13.91	-5.44	-15.14
2M2P	DEAN	-10.22	-9.54	-3.55	-18.04	-8.05	-11.34	-8.31	-12.02	-9.35	-13.04
2M2P	TEAN	-2.40	-10.42	-1.33	-16.88	-4.09	-11.33	-1.17	-12.32	-6.19	-13.31
2M2P	TOL	-4.68	-10.63	-4.53	-17.31	-6.87	-10.55	-5.20	-11.78	-5.00	-13.23

Table S.2 – Continued on next page

Table S.2 – Continued from previous page

Solute (A)	Solvent (B)	GROMOS-54A7		GROMOS-ATB		OPLS-LBCC		AMBER-GAFF2		OpenFF	
		ELE	VDW	ELE	VDW	ELE	VDW	ELE	VDW	ELE	VDW
[kJ·mol ⁻¹]											
2M2P	BZN	-6.50	-10.21	-4.53	-17.52	-6.95	-10.85	-7.44	-11.48	-5.41	-13.04
2M2P	HPE	-0.00	-10.23	-0.05	-16.28	-0.40	-12.06	-0.04	-12.21	0.02	-13.53
2M2P	HXE	-0.00	-10.75	-0.03	-16.28	-0.37	-12.10	-0.04	-12.78	-0.01	-13.90
2M2P	CCL4	-0.00	-10.87	1.03	-19.18	-	-	-0.24	-14.24	-0.24	-15.96
2M2P	CHE	-0.00	-10.67	-0.00	-16.45	-0.39	-12.51	-0.01	-12.88	-0.04	-13.98
1PL	DAMD	-	-	-13.62	-4.61	-15.69	-2.47	-18.66	-5.64	-17.05	-6.60
1PL	PPN	-12.78	-9.94	-9.72	-8.44	-12.70	-6.07	-15.21	-7.10	-12.16	-8.82
1PL	BTN	-11.67	-10.30	-9.14	-8.70	-11.76	-6.87	-14.39	-7.29	-11.71	-9.30
1PL	PYRI	-	-	-6.95	-10.76	-13.56	-3.51	-13.06	-6.64	-11.20	-8.97
1PL	H2O	-28.74	7.81	-22.31	9.54	-27.17	8.62	-28.90	8.95	-19.80	7.52
1PL	C2CL2	-	-	-7.25	-8.16	-13.65	-4.56	-8.63	-8.63	-6.19	-10.60
1PL	EAE	-15.50	-8.71	-8.31	-9.05	-11.40	-6.80	-15.83	-7.47	-12.10	-8.76
1PL	PTL	-18.67	-11.59	-10.54	-7.83	-11.63	-6.42	-16.20	-6.81	-10.01	-9.45
1PL	MTL	-21.50	-7.61	-12.42	-7.63	-18.16	-2.98	-19.88	-5.50	-12.81	-8.48
1PL	ETL	-19.84	-9.03	-11.18	-9.21	-15.41	-5.26	-17.78	-6.62	-11.65	-8.78
1PL	BTL	-16.82	-9.45	-11.12	-7.34	-12.37	-6.84	-17.34	-6.87	-10.45	-9.19
1PL	2M2P	-16.09	-11.12	-13.52	-7.20	-12.45	-7.08	-16.41	-8.44	-10.26	-9.38
1PL	1PL	-18.40	-9.71	-11.10	-8.02	-13.35	-5.98	-17.86	-6.99	-10.90	-8.67
1PL	2PL	-17.70	-10.65	-10.89	-8.60	-13.50	-5.98	-17.02	-6.61	-11.13	-8.90
1PL	ANLN	-21.90	-4.59	-9.44	-9.26	-15.79	-3.34	-20.28	-4.01	-12.82	-5.37
1PL	DEE	-3.52	-11.71	-5.24	-10.20	-7.53	-9.10	-5.56	-9.58	-6.04	-11.20
1PL	CHCL3	-4.00	-12.25	-7.43	-9.50	-13.64	-8.35	-8.42	-10.59	-5.30	-12.09
1PL	DEAN	-15.33	-9.98	-2.88	-10.86	-9.81	-8.65	-11.04	-8.91	-11.74	-10.56
1PL	TEAN	-3.78	-11.59	-0.89	-8.91	-5.27	-9.08	-1.65	-9.27	-9.15	-10.85
1PL	TOL	-5.96	-11.23	-4.14	-9.58	-7.43	-7.78	-6.26	-8.67	-5.58	-10.62
1PL	BZN	-8.29	-10.81	-4.87	-10.87	-7.54	-7.89	-9.00	-8.22	-6.01	-10.62
1PL	HPE	-0.00	-11.22	-0.04	-10.03	-0.38	-9.60	-0.04	-9.02	-0.03	-10.83
1PL	HXE	-0.00	-11.48	-0.02	-9.79	-0.36	-9.42	-0.04	-9.66	-0.05	-11.57
1PL	CCL4	-0.00	-12.24	0.02	-9.90	-	-	-0.35	-11.26	-0.21	-12.56
1PL	CHE	-0.00	-11.98	-0.00	-10.19	-0.36	-9.84	-0.01	-9.12	-0.09	-11.56
2PL	DAMD	-	-	-17.21	-9.99	-16.58	-2.18	-17.68	-5.39	-17.02	-6.45
2PL	PPN	-11.64	-8.26	-12.34	-11.60	-13.53	-6.20	-14.37	-7.12	-12.11	-8.47
2PL	BTN	-10.67	-8.25	-11.87	-11.79	-12.58	-6.58	-13.56	-7.08	-11.66	-8.80
2PL	PYRI	-	-	-10.13	-14.15	-14.26	-3.80	-12.25	-6.62	-11.16	-8.20
2PL	H2O	-26.37	9.04	-28.27	6.34	-28.90	8.79	-27.09	9.01	-20.28	7.53
2PL	C2CL2	-	-	-8.43	-12.03	-14.06	-4.24	-8.17	-8.15	-6.31	-10.22
2PL	EAE	-14.28	-5.92	-11.29	-12.59	-12.10	-6.22	-14.94	-7.17	-11.92	-8.32
2PL	PTL	-14.36	-9.62	-14.92	-12.32	-13.22	-6.69	-15.11	-6.57	-9.81	-9.01
2PL	MTL	-19.56	-5.99	-17.81	-10.72	-19.40	-2.56	-18.59	-5.30	-13.11	-7.80
2PL	ETL	-17.70	-6.41	-16.78	-11.27	-16.57	-5.05	-16.84	-6.36	-12.06	-8.40
2PL	BTL	-14.77	-10.88	-16.12	-10.55	-14.11	-6.51	-15.69	-7.00	-10.29	-8.99
2PL	2M2P	-14.05	-10.34	-19.41	-7.15	-14.15	-7.11	-14.13	-8.50	-10.40	-9.16
2PL	1PL	-15.55	-9.78	-16.04	-11.86	-14.96	-6.19	-16.56	-6.40	-10.92	-8.97
2PL	2PL	-14.80	-6.89	-16.59	-13.93	-15.09	-5.98	-16.24	-6.71	-11.33	-9.07
2PL	ANLN	-18.46	-7.62	-12.50	-12.64	-16.75	-3.06	-18.99	-2.23	-12.61	-5.80
2PL	DEE	-3.08	-10.07	-7.92	-13.33	-8.24	-8.73	-5.21	-9.59	-5.81	-10.91
2PL	CHCL3	-3.69	-9.56	-8.62	-12.25	-14.06	-8.01	-7.77	-10.15	-5.47	-12.15
2PL	DEAN	-12.86	-8.50	-4.89	-14.48	-10.64	-8.60	-9.91	-8.81	-10.87	-10.50
2PL	TEAN	-3.06	-9.02	-1.69	-13.28	-5.92	-8.77	-1.37	-9.01	-7.81	-10.63
2PL	TOL	-5.27	-9.37	-5.61	-12.11	-7.80	-7.67	-5.78	-8.62	-5.36	-10.42

Table S.2 – Continued on next page

Table S.2 – Continued from previous page

Solute (A)	Solvent (B)	GROMOS-54A7		GROMOS-ATB		OPLS-LBCC		AMBER-GAFF2		OpenFF	
		ELE	VDW	ELE	VDW	ELE	VDW	ELE	VDW	ELE	VDW
[kJ·mol ⁻¹]											
2PL	BZN	-7.36	-8.52	-6.27	-12.45	-7.74	-7.80	-8.30	-8.14	-5.82	-10.64
2PL	HPE	-0.00	-9.55	-0.04	-12.61	-0.42	-9.43	-0.05	-8.70	-0.01	-10.75
2PL	HXE	-0.00	-9.65	-0.02	-12.83	-0.38	-9.66	-0.05	-9.27	-0.03	-10.99
2PL	CCL4	-0.00	-10.40	-0.30	-13.85	-	-	-0.31	-10.70	-0.23	-12.55
2PL	CHE	-0.00	-9.65	-0.00	-12.92	-0.40	-9.76	-0.01	-9.36	-0.07	-11.40
ANLN	DAMD	-	-	-15.51	-16.77	-18.99	-12.65	-22.43	-17.83	-23.36	-13.99
ANLN	PPN	-17.35	-16.92	-11.39	-19.56	-15.10	-15.64	-18.75	-17.93	-17.24	-15.62
ANLN	BTN	-15.57	-17.37	-9.10	-21.12	-13.66	-16.37	-17.23	-18.74	-16.15	-16.08
ANLN	PYRI	-	-	-4.82	-21.13	-16.29	-13.57	-16.34	-18.51	-16.05	-16.19
ANLN	H2O	-40.73	8.75	-22.86	1.30	-26.09	4.67	-31.26	3.63	-27.57	5.40
ANLN	C2CL2	-	-	-5.15	-20.23	-15.87	-13.79	-12.12	-19.54	-10.64	-17.44
ANLN	EAE	-20.67	-16.72	-9.56	-21.08	-13.62	-16.40	-18.89	-18.69	-16.79	-16.38
ANLN	PTL	-17.47	-16.07	-6.05	-19.07	-10.97	-16.92	-12.06	-18.87	-10.34	-16.93
ANLN	MTL	-25.32	-14.10	-6.65	-19.55	-19.12	-10.36	-18.07	-14.44	-16.56	-14.24
ANLN	ETL	-20.92	-15.64	-5.88	-18.21	-14.91	-14.02	-14.22	-16.98	-13.57	-15.60
ANLN	BTL	-17.02	-19.39	-4.24	-19.38	-11.68	-16.26	-11.99	-18.59	-11.12	-16.86
ANLN	2M2P	-16.14	-16.81	-5.29	-20.81	-11.57	-17.35	-10.42	-19.05	-10.69	-16.28
ANLN	1PL	-19.10	-15.03	-6.39	-19.31	-13.15	-15.51	-14.09	-17.40	-12.20	-16.03
ANLN	2PL	-17.60	-15.16	-5.01	-18.99	-12.30	-15.87	-12.45	-17.45	-11.97	-16.02
ANLN	ANLN	-28.35	-17.31	-5.52	-19.97	-15.96	-12.95	-23.93	-15.34	-18.03	-12.74
ANLN	DEE	-4.93	-18.93	-5.23	-20.53	-6.68	-9.25	-7.02	-20.71	-8.26	-18.88
ANLN	CHCL3	-6.86	-19.29	-7.82	-18.91	-13.86	-17.51	-10.62	-22.25	-8.99	-19.42
ANLN	DEAN	-16.41	-17.71	-1.53	-21.15	-7.07	-10.42	-10.63	-20.52	-12.42	-18.02
ANLN	TEAN	-4.96	-19.11	0.19	-20.61	-3.87	-19.65	-2.31	-21.53	-9.02	-18.81
ANLN	TOL	-10.35	-18.29	-4.02	-19.15	-8.40	-17.72	-7.34	-21.24	-7.80	-17.99
ANLN	BZN	-14.43	-16.57	-7.57	-17.46	-8.80	-17.92	-11.65	-19.77	-9.03	-17.85
ANLN	HPE	-0.00	-19.00	-0.03	-19.55	-0.48	-19.40	-0.12	-21.32	0.08	-18.65
ANLN	HXE	-0.00	-19.27	-0.04	-19.98	-0.47	-19.62	-0.11	-21.41	0.01	-18.86
ANLN	CCL4	-0.00	-19.32	-0.56	-19.71	-	-	-0.54	-22.56	-0.35	-20.15
ANLN	CHE	-0.00	-19.68	-0.00	-19.49	-0.63	-20.00	0.02	-21.92	-0.21	-19.12
DEE	DAMD	-	-	-3.82	-10.07	-7.86	-3.53	-3.52	-9.10	-4.51	-8.79
DEE	PPN	-1.76	-14.42	-2.17	-14.26	-6.08	-7.96	-3.08	-10.88	-3.54	-11.06
DEE	BTN	-1.52	-14.45	-2.81	-13.89	-5.42	-8.92	-2.74	-11.18	-3.24	-11.61
DEE	PYRI	-	-	-2.52	-15.60	-7.44	-4.94	-3.32	-10.62	-3.68	-11.59
DEE	H2O	-4.27	7.49	-10.12	6.61	-18.11	10.38	-8.12	9.44	-10.85	8.71
DEE	C2CL2	-	-	-2.82	-14.87	-8.45	-6.30	-2.87	-12.65	-3.47	-13.57
DEE	EAE	-1.97	-12.56	-2.44	-13.90	-5.61	-8.39	-2.81	-10.89	-3.57	-11.21
DEE	PTL	-0.65	-14.05	-1.92	-13.89	-4.56	-9.40	-1.76	-11.05	-3.26	-11.96
DEE	MTL	-1.93	-10.28	-3.18	-11.81	-8.99	-3.45	-3.31	-8.34	-5.19	-10.24
DEE	ETL	-1.28	-12.09	-2.13	-12.65	-6.55	-6.39	-2.44	-9.73	-4.14	-10.97
DEE	BTL	-0.73	-13.25	-1.11	-14.83	-4.91	-8.90	-1.68	-10.50	-3.04	-11.95
DEE	2M2P	-0.65	-13.31	-0.86	-15.17	-4.19	-8.58	-1.38	-11.77	-2.70	-11.99
DEE	1PL	-0.92	-12.80	-2.06	-13.92	-5.56	-7.74	-2.10	-10.31	-3.70	-11.57
DEE	2PL	-0.74	-13.36	-1.37	-13.35	-4.74	-7.85	-1.83	-11.01	-3.28	-11.64
DEE	ANLN	-2.56	-8.72	-3.71	-13.98	-7.15	-9.48	-5.29	-6.63	-5.57	-7.94
DEE	DEE	-0.51	-15.74	-1.57	-15.97	-3.18	-11.38	-1.34	-13.55	-1.69	-14.17
DEE	CHCL3	-1.03	-16.31	-4.84	-16.08	-8.96	-11.11	-3.08	-15.02	-3.61	-15.61
DEE	DEAN	-1.28	-14.31	-1.22	-16.20	-3.30	-11.22	-1.85	-12.92	-2.18	-13.56
DEE	TEAN	-0.48	-15.37	-0.09	-16.16	-1.82	-11.71	-0.46	-13.18	-1.34	-13.79
DEE	TOL	-1.04	-15.39	-1.48	-15.77	-4.24	-10.33	-1.67	-13.37	-2.16	-13.36

Table S.2 – Continued on next page

Table S.2 – Continued from previous page

Solute (A)	Solvent (B)	GROMOS-54A7		GROMOS-ATB		OPLS-LBCC		AMBER-GAFF2		OpenFF	
		ELE	VDW	ELE	VDW	ELE	VDW	ELE	VDW	ELE	VDW
[kJ·mol ⁻¹]											
DEE	BZN	-1.41	-15.00	-2.52	-16.49	-4.40	-10.41	-2.52	-11.99	-2.43	-13.76
DEE	HPE	-0.00	-15.18	-0.01	-15.35	-0.39	-11.84	-0.01	-13.18	-0.01	-13.89
DEE	HXE	-0.00	-15.90	-0.02	-15.90	-0.36	-12.26	-0.01	-13.75	-0.03	-14.30
DEE	CCL4	-0.00	-16.75	-0.40	-15.97	-	-	-0.18	-15.60	0.01	-16.66
DEE	CHE	-0.00	-16.07	-0.00	-16.04	-0.40	-12.20	0.01	-13.43	-0.07	-14.46
CHCL3	DAMD	-	-	-7.14	-15.12	-12.88	-10.58	-7.30	-11.37	-7.17	-11.23
CHCL3	PPN	-2.25	-15.44	-5.98	-15.16	-12.03	-12.24	-6.07	-12.07	-5.59	-12.56
CHCL3	BTN	-2.10	-15.53	-4.59	-16.54	-11.55	-13.38	-5.81	-12.61	-5.37	-12.72
CHCL3	PYRI	-	-	-4.59	-16.58	-11.31	-10.93	-5.10	-11.81	-4.87	-12.33
CHCL3	H2O	-2.58	4.72	-6.30	1.62	-11.36	5.07	-5.56	6.13	-5.31	5.45
CHCL3	C2CL2	-	-	-2.49	-17.67	-10.23	-9.55	-3.08	-12.55	-3.06	-13.39
CHCL3	EAE	-2.47	-14.40	-5.77	-16.78	-10.13	-12.67	-6.14	-12.60	-5.13	-13.13
CHCL3	PTL	-1.07	-14.88	-3.77	-15.86	-10.83	-14.21	-3.22	-12.44	-3.05	-13.82
CHCL3	MTL	-2.26	-12.28	-4.59	-13.54	-11.98	-8.63	-4.80	-9.47	-4.15	-11.76
CHCL3	ETL	-1.75	-13.75	-4.33	-14.36	-12.17	-11.22	-4.06	-11.49	-3.83	-12.27
CHCL3	BTL	-1.20	-14.42	-3.32	-16.70	-10.99	-13.05	-3.98	-11.94	-3.16	-13.20
CHCL3	2M2P	-0.81	-14.44	-3.08	-16.75	-12.57	-13.27	-2.50	-13.18	-3.33	-13.48
CHCL3	1PL	-1.36	-14.58	-4.30	-15.11	-11.84	-12.45	-4.46	-11.71	-3.60	-13.21
CHCL3	2PL	-1.17	-13.94	-4.25	-16.15	-11.96	-13.16	-3.96	-11.76	-3.49	-12.90
CHCL3	ANLN	-2.92	-12.64	-5.60	-15.18	-11.38	-9.95	-6.53	-6.22	-5.66	-8.77
CHCL3	DEE	-0.86	-16.58	-4.58	-17.36	-9.43	-15.19	-2.82	-14.49	-3.13	-15.30
CHCL3	CHCL3	-0.61	-17.41	-2.70	-18.24	-7.14	-13.25	-1.91	-13.79	-2.00	-14.42
CHCL3	DEAN	-1.83	-14.94	-2.13	-17.99	-12.53	-15.27	-4.20	-14.17	-5.16	-14.60
CHCL3	TEAN	-0.93	-15.79	-0.72	-18.54	-8.46	-15.77	-1.12	-14.89	-4.21	-15.08
CHCL3	TOL	-1.43	-15.77	-3.82	-17.57	-8.34	-14.43	-3.55	-13.90	-3.58	-14.27
CHCL3	BZN	-1.97	-15.60	-5.06	-16.56	-7.88	-14.43	-4.87	-13.23	-3.55	-13.87
CHCL3	HPE	-0.00	-16.46	-0.01	-17.24	-0.23	-16.14	-0.01	-14.46	-0.06	-14.83
CHCL3	HXE	-0.00	-16.13	-0.00	-17.44	-0.23	-16.15	-0.02	-14.89	-0.04	-15.35
CHCL3	CCL4	-0.00	-17.12	-1.39	-18.32	-	-	-0.22	-14.30	-0.09	-15.06
CHCL3	CHE	-0.00	-17.29	-0.00	-17.46	-0.16	-16.98	0.00	-15.08	-0.02	-15.87
DEAN	DAMD	-	-	-2.37	-12.17	-9.04	-5.95	-7.43	-10.39	-6.97	-9.65
DEAN	PPN	-6.90	-12.91	-1.15	-15.79	-6.93	-10.28	-5.97	-11.94	-5.46	-11.93
DEAN	BTN	-6.19	-13.18	-0.73	-16.92	-6.10	-10.76	-5.40	-12.33	-4.94	-12.60
DEAN	PYRI	-	-	-0.83	-16.17	-8.58	-8.14	-5.47	-11.95	-5.66	-12.34
DEAN	H2O	-19.10	9.91	-6.97	3.64	-24.15	8.83	-15.64	8.96	-20.83	8.67
DEAN	C2CL2	-	-	0.24	-17.02	-9.68	-7.97	-4.23	-13.89	-5.21	-14.20
DEAN	EAE	-8.20	-11.44	-1.78	-16.33	-6.55	-10.93	-6.00	-12.27	-5.33	-11.90
DEAN	PTL	-9.21	-8.90	-0.34	-15.59	-6.15	-11.30	-3.37	-12.08	-8.70	-12.63
DEAN	MTL	-11.33	-9.65	-0.91	-13.83	-12.54	-5.47	-7.59	-9.12	-12.53	-11.34
DEAN	ETL	-8.41	-12.93	-0.46	-14.41	-9.11	-8.27	-6.00	-11.06	-10.55	-12.02
DEAN	BTL	-7.33	-15.08	0.26	-15.45	-7.04	-10.57	-3.99	-12.14	-8.90	-12.93
DEAN	2M2P	-5.46	-12.41	1.73	-19.75	-5.12	-11.42	-2.76	-12.70	-6.88	-12.95
DEAN	1PL	-8.10	-9.63	-0.32	-15.34	-7.63	-10.03	-5.31	-11.26	-9.60	-12.26
DEAN	2PL	-7.08	-12.32	-0.12	-15.32	-7.38	-10.50	-3.70	-11.65	-8.50	-12.63
DEAN	ANLN	-8.94	-9.96	-1.18	-15.58	-8.88	-10.15	-7.96	-8.98	-9.21	-8.31
DEAN	DEE	-1.86	-15.42	-1.24	-17.38	-3.53	-13.19	-1.96	-14.78	-2.37	-14.95
DEAN	CHCL3	-2.84	-15.47	-2.00	-16.51	-11.24	-13.27	-4.57	-16.09	-5.71	-16.73
DEAN	DEAN	-5.90	-13.57	-0.36	-17.39	-3.86	-13.20	-2.95	-14.02	-3.34	-14.50
DEAN	TEAN	-1.56	-14.76	0.15	-17.42	-1.88	-13.69	-0.48	-14.64	-1.73	-14.66
DEAN	TOL	-3.57	-15.14	-1.09	-18.06	-4.20	-12.47	-2.58	-14.24	-2.95	-14.66

Table S.2 – Continued on next page

Table S.2 – Continued from previous page

Solute (A)	Solvent (B)	GROMOS-54A7		GROMOS-ATB		OPLS-LBCC		AMBER-GAFF2		OpenFF	
		ELE	VDW	ELE	VDW	ELE	VDW	ELE	VDW	ELE	VDW
[kJ·mol ⁻¹]											
DEAN	BZN	-4.90	-14.89	-2.40	-17.31	-4.39	-13.02	-3.73	-13.02	-3.36	-14.60
DEAN	HPE	-0.00	-14.95	0.00	-16.72	-0.36	-13.95	-0.02	-14.58	-0.02	-14.89
DEAN	HXE	-0.00	-14.95	-0.00	-17.09	-0.34	-14.24	-0.02	-14.64	-0.06	-15.17
DEAN	CCL4	-0.00	-15.78	-1.03	-17.87	-	-	-0.18	-16.60	-0.06	-17.49
DEAN	CHE	-0.00	-15.09	-0.00	-17.46	-0.39	-14.19	0.00	-14.58	-0.14	-15.20
TEAN	DAMD	-	-	0.32	-21.87	-5.55	-9.85	-1.36	-16.85	-4.28	-14.56
TEAN	PPN	-1.82	-20.36	1.73	-24.03	-3.75	-15.60	-1.10	-18.59	-3.27	-16.76
TEAN	BTN	-1.55	-20.96	1.23	-24.93	-3.41	-16.11	-0.97	-18.84	-2.92	-17.52
TEAN	PYRI	-	-	-1.24	-24.20	-5.34	-13.71	-1.32	-18.19	-3.93	-18.20
TEAN	H2O	-7.86	9.47	-2.71	4.72	-16.71	8.41	-3.50	8.06	-18.07	8.84
TEAN	C2CL2	-	-	2.01	-26.71	-5.96	-14.06	-1.06	-21.36	-3.83	-20.08
TEAN	EAE	-1.87	-19.55	-0.53	-23.91	-3.81	-16.45	-1.09	-18.85	-3.31	-17.47
TEAN	PTL	-0.56	-20.69	0.28	-23.87	-3.31	-16.49	-0.41	-19.32	-7.03	-18.27
TEAN	MTL	-2.04	-14.99	0.64	-20.46	-6.85	-9.90	-1.18	-14.35	-9.95	-15.80
TEAN	ETL	-1.21	-17.94	0.48	-21.63	-4.59	-13.69	-0.76	-17.70	-8.41	-17.09
TEAN	BTL	-0.66	-19.45	0.54	-22.76	-3.20	-16.52	-0.50	-18.07	-6.47	-18.32
TEAN	2M2P	-0.50	-19.95	3.05	-29.45	-2.40	-16.83	-0.34	-19.67	-3.40	-17.96
TEAN	1PL	-0.92	-19.06	0.64	-23.20	-3.77	-15.79	-0.78	-17.10	-7.11	-17.62
TEAN	2PL	-0.75	-19.41	0.99	-23.25	-3.24	-15.42	-0.60	-18.21	-6.41	-17.44
TEAN	ANLN	-2.22	-18.58	0.03	-23.85	-6.04	-15.21	-2.18	-14.71	-7.18	-10.40
TEAN	DEE	-0.54	-22.10	-0.32	-25.80	-1.97	-19.30	-0.49	-21.40	-1.61	-20.57
TEAN	CHCL3	-1.10	-23.75	-0.99	-26.55	-7.53	-20.09	-1.20	-23.72	-4.71	-22.90
TEAN	DEAN	-1.10	-20.17	-0.11	-26.40	-1.93	-19.01	-0.50	-21.22	-1.80	-19.65
TEAN	TEAN	-0.44	-22.42	0.32	-27.15	-1.19	-20.37	-0.18	-21.86	-1.18	-20.49
TEAN	TOL	-1.00	-22.55	-0.27	-27.29	-2.66	-18.64	-0.67	-21.33	-2.14	-20.09
TEAN	BZN	-1.40	-21.74	-1.82	-25.92	-2.85	-19.14	-1.04	-20.09	-2.46	-20.37
TEAN	HPE	-0.00	-22.03	0.02	-26.02	-0.35	-20.10	0.00	-21.91	0.04	-20.52
TEAN	HXE	-0.00	-22.33	-0.01	-26.24	-0.33	-20.39	-0.01	-22.09	-0.02	-20.63
TEAN	CCL4	-0.00	-23.83	-1.38	-25.76	-	-	-0.12	-25.05	0.04	-24.08
TEAN	CHE	-0.00	-23.18	-0.00	-26.07	-0.37	-20.71	0.01	-22.77	-0.11	-21.39
TOL	DAMD	-	-	-3.49	-16.61	-9.32	-10.62	-5.01	-15.20	-6.54	-11.23
TOL	PPN	-3.68	-18.11	-2.24	-19.28	-7.23	-15.12	-4.49	-16.16	-5.07	-13.66
TOL	BTN	-3.14	-18.65	-1.53	-20.28	-6.50	-15.28	-3.92	-16.71	-4.59	-14.43
TOL	PYRI	-	-	-4.66	-17.81	-8.94	-12.42	-4.32	-15.81	-4.87	-13.68
TOL	H2O	-8.77	5.63	-7.95	6.01	-13.87	6.72	-9.80	6.82	-11.68	8.28
TOL	C2CL2	-	-	-0.80	-21.42	-9.67	-12.50	-4.51	-18.46	-4.85	-15.89
TOL	EAE	-4.12	-16.86	-2.93	-18.76	-6.60	-15.20	-4.05	-16.25	-4.66	-13.60
TOL	PTL	-1.28	-17.62	-1.04	-19.69	-4.15	-16.24	-1.88	-16.85	-2.73	-15.35
TOL	MTL	-4.05	-13.53	-2.13	-16.03	-9.02	-9.19	-4.35	-12.20	-5.38	-13.03
TOL	ETL	-2.53	-15.86	-1.50	-17.49	-6.52	-12.70	-2.91	-15.26	-4.17	-14.17
TOL	BTL	-1.58	-18.46	-0.56	-19.19	-4.56	-15.14	-2.14	-16.04	-2.84	-15.26
TOL	2M2P	-1.30	-17.88	-0.41	-19.39	-4.26	-16.07	-1.42	-17.24	-2.65	-14.69
TOL	1PL	-1.83	-17.30	-1.15	-18.40	-5.41	-14.92	-2.84	-15.63	-3.48	-14.34
TOL	2PL	-1.57	-17.38	-0.97	-18.58	-4.78	-14.80	-2.15	-16.12	-3.29	-14.25
TOL	ANLN	-7.08	-11.84	-3.49	-17.20	-8.49	-12.85	-5.25	-10.88	-7.19	-10.28
TOL	DEE	-1.02	-20.57	-1.47	-21.16	-3.87	-17.96	-1.67	-19.04	-2.21	-17.21
TOL	CHCL3	-2.02	-20.59	-4.22	-19.83	-9.90	-17.58	-4.33	-20.48	-4.73	-18.27
TOL	DEAN	-2.58	-18.55	-1.02	-21.50	-3.64	-17.92	-2.34	-18.84	-2.82	-16.69
TOL	TEAN	-0.92	-19.75	0.29	-22.34	-2.24	-18.93	-0.59	-19.26	-1.82	-16.60
TOL	TOL	-2.33	-19.04	-1.55	-20.41	-4.77	-17.25	-1.69	-18.97	-2.47	-16.56

Table S.2 – Continued on next page

Table S.2 – Continued from previous page

Solute (A)	Solvent (B)	GROMOS-54A7		GROMOS-ATB		OPLS-LBCC		AMBER-GAFF2		OpenFF	
		ELE	VDW	ELE	VDW	ELE	VDW	ELE	VDW	ELE	VDW
[kJ·mol ⁻¹]											
TOL	BZN	-3.45	-18.58	-4.03	-18.73	-5.12	-17.63	-3.09	-17.82	-3.05	-16.55
TOL	HPE	-0.00	-20.12	-0.01	-21.34	-0.32	-18.97	-0.06	-19.07	0.09	-17.29
TOL	HXE	-0.00	-19.69	-0.02	-21.25	-0.32	-18.87	-0.07	-19.49	0.03	-17.38
TOL	CCL4	-0.00	-20.31	-1.17	-20.69	-	-	-0.17	-21.01	-0.14	-18.70
TOL	CHE	-0.00	-20.22	-0.00	-21.53	-0.44	-19.24	0.02	-19.74	-0.11	-17.67
BZN	DAMD	-	-	-3.87	-13.90	-8.31	-8.65	-6.20	-11.77	-6.34	-8.82
BZN	PPN	-4.39	-14.31	-2.53	-15.80	-6.41	-12.29	-5.63	-12.94	-4.94	-11.15
BZN	BTN	-3.66	-14.98	-1.14	-17.26	-5.84	-12.98	-4.96	-13.22	-4.44	-11.58
BZN	PYRI	-	-	-6.10	-12.46	-7.87	-9.96	-5.79	-12.69	-4.87	-11.09
BZN	H2O	-12.21	6.81	-8.69	4.66	-11.74	5.77	-13.34	6.27	-11.08	7.72
BZN	C2CL2	-	-	0.09	-19.02	-8.30	-10.48	-5.68	-14.36	-4.63	-12.81
BZN	EAE	-4.86	-13.12	-3.86	-14.94	-5.82	-13.21	-5.22	-13.21	-4.72	-11.50
BZN	PTL	-1.50	-15.07	-1.02	-16.65	-3.47	-13.49	-2.55	-12.62	-2.47	-11.67
BZN	MTL	-4.80	-11.43	-2.65	-13.34	-7.91	-7.70	-5.60	-9.82	-5.11	-10.21
BZN	ETL	-3.05	-13.41	-1.85	-14.85	-5.70	-10.73	-3.89	-12.14	-3.92	-10.83
BZN	BTL	-1.75	-14.06	-0.70	-15.49	-4.05	-12.79	-2.70	-12.49	-2.80	-11.71
BZN	2M2P	-1.56	-14.87	0.16	-18.11	-3.91	-13.73	-2.04	-13.50	-2.74	-11.99
BZN	1PL	-2.11	-13.50	-1.40	-15.47	-4.78	-12.50	-3.50	-12.05	-3.27	-11.60
BZN	2PL	-1.81	-14.21	-1.56	-14.32	-4.28	-12.46	-2.79	-12.37	-3.23	-11.31
BZN	ANLN	-8.00	-6.98	-5.09	-12.00	-7.60	-10.16	-8.64	-8.34	-7.44	-6.81
BZN	DEE	-1.21	-16.83	-1.93	-17.29	-3.53	-15.06	-2.05	-15.36	-2.12	-13.76
BZN	CHCL3	-2.57	-16.23	-4.52	-16.16	-8.27	-14.38	-6.05	-16.12	-4.28	-14.37
BZN	DEAN	-3.35	-15.25	-1.32	-17.92	-3.30	-14.71	-3.12	-14.91	-2.77	-13.14
BZN	TEAN	-0.97	-16.15	0.05	-18.35	-2.02	-15.80	-0.68	-15.01	-1.81	-13.51
BZN	TOL	-2.99	-14.60	-2.20	-16.32	-4.31	-14.40	-2.56	-15.15	-2.59	-13.20
BZN	BZN	-4.15	-13.91	-5.60	-13.53	-4.66	-14.19	-4.22	-14.25	-3.26	-12.87
BZN	HPE	-0.00	-16.17	0.00	-17.91	-0.30	-15.91	-0.07	-15.14	0.07	-13.84
BZN	HXE	-0.00	-16.61	-0.01	-17.54	-0.30	-16.21	-0.06	-15.61	0.01	-13.97
BZN	CCL4	-0.00	-16.50	-2.15	-16.11	-	-	-0.25	-16.94	-0.12	-15.11
BZN	CHE	-0.00	-17.32	-0.00	-17.63	-0.39	-16.45	0.02	-15.50	-0.11	-13.95
HPE	DAMD	-	-	-0.02	-13.18	-1.09	-8.06	-0.04	-17.94	-0.10	-12.42
HPE	PPN	-0.00	-20.09	-0.03	-17.54	-0.69	-13.68	-0.02	-19.13	-0.04	-16.41
HPE	BTN	-0.00	-20.40	-0.05	-18.57	-0.63	-14.40	-0.02	-20.15	-0.08	-16.89
HPE	PYRI	-	-	0.03	-19.03	-0.87	-10.45	-0.05	-19.55	0.02	-16.85
HPE	H2O	-0.00	10.43	-0.07	10.05	-0.43	11.73	-0.03	9.55	0.19	11.53
HPE	C2CL2	-	-	-0.11	-19.53	-0.46	-11.10	-0.03	-22.00	-0.02	-19.38
HPE	EAE	-0.00	-17.75	0.05	-18.67	-0.79	-13.85	-0.02	-19.57	-0.09	-16.03
HPE	PTL	-0.00	-19.42	-0.00	-19.71	-0.47	-14.53	0.02	-19.67	-0.01	-17.73
HPE	MTL	-0.00	-15.03	0.01	-15.60	-0.89	-7.08	-0.01	-15.08	0.00	-15.36
HPE	ETL	-0.00	-17.10	0.01	-18.21	-0.69	-11.61	0.00	-17.73	0.01	-15.86
HPE	BTL	-0.00	-19.78	-0.01	-18.43	-0.53	-13.81	0.01	-18.79	0.06	-16.97
HPE	2M2P	-0.00	-18.73	-0.01	-19.68	-0.50	-14.56	0.00	-20.48	0.08	-18.01
HPE	1PL	-0.00	-19.07	-0.00	-18.16	-0.61	-13.57	0.02	-18.33	-0.01	-16.46
HPE	2PL	-0.00	-19.10	0.03	-18.83	-0.53	-13.57	0.01	-18.96	0.03	-16.98
HPE	ANLN	-0.00	-13.45	-0.01	-17.96	-0.83	-9.88	-0.12	-13.99	0.10	-10.79
HPE	DEE	-0.00	-22.86	0.01	-22.07	-0.51	-17.53	-0.01	-22.67	0.00	-20.15
HPE	CHCL3	-0.00	-23.56	-0.01	-21.04	-0.01	-17.53	-0.02	-25.07	-0.07	-22.45
HPE	DEAN	-0.00	-19.78	0.00	-22.12	-0.49	-17.23	-0.01	-22.03	-0.01	-19.24
HPE	TEAN	-0.00	-22.00	-0.00	-22.44	-0.40	-18.12	0.00	-23.02	0.04	-20.04
HPE	TOL	-0.00	-22.02	-0.01	-22.88	-0.53	-16.47	-0.06	-22.69	0.09	-20.14

Table S.2 – Continued on next page

Table S.2 – Continued from previous page

Solute (A)	Solvent (B)	GROMOS-54A7		GROMOS-ATB		OPLS-LBCC		AMBER-GAFF2		OpenFF	
		ELE	VDW	ELE	VDW	ELE	VDW	ELE	VDW	ELE	VDW
[kJ·mol ⁻¹]											
HPE	BZN	-0.00	-21.34	0.02	-23.71	-0.52	-16.62	-0.07	-21.37	0.09	-19.59
HPE	HPE	-0.00	-22.03	0.00	-22.05	-0.19	-18.49	0.00	-22.65	0.11	-20.57
HPE	HXE	-0.00	-21.97	-0.00	-22.03	-0.18	-18.77	0.00	-23.05	0.08	-20.80
HPE	CCL4	-0.00	-22.95	0.06	-22.20	-	-	0.00	-26.10	-0.06	-22.99
HPE	CHE	-0.00	-22.96	-0.00	-22.89	-0.22	-18.47	0.00	-22.89	0.05	-20.91
HXE	DAMD	-	-	-0.02	-10.56	-0.95	-5.94	-0.02	-14.87	-0.13	-10.00
HXE	PPN	-0.00	-16.44	-0.05	-14.53	-0.60	-10.92	-0.02	-15.63	-0.03	-13.36
HXE	BTN	-0.00	-17.24	-0.01	-15.74	-0.54	-11.05	-0.01	-16.49	-0.07	-13.99
HXE	PYRI	-	-	0.03	-15.43	-0.77	-7.35	-0.05	-15.96	-0.02	-13.81
HXE	H2O	-0.00	9.43	-0.04	8.37	-0.35	10.94	-0.04	9.30	0.12	11.01
HXE	C2CL2	-	-	-0.04	-16.36	-0.40	-8.60	-0.02	-18.22	-0.02	-15.77
HXE	EAE	-0.00	-14.69	0.00	-15.68	-0.69	-11.33	-0.01	-15.99	-0.09	-13.16
HXE	PTL	-0.00	-17.02	0.00	-16.83	-0.41	-11.30	0.02	-15.66	-0.05	-13.87
HXE	MTL	-0.00	-12.89	-0.00	-13.03	-0.78	-5.58	-0.01	-12.63	-0.03	-12.16
HXE	ETL	-0.00	-14.49	0.02	-14.09	-0.59	-9.31	0.02	-15.10	-0.03	-13.27
HXE	BTL	-0.00	-15.89	0.02	-16.43	-0.46	-11.57	0.01	-15.70	0.01	-13.94
HXE	2M2P	-0.00	-16.72	-0.01	-19.08	-0.46	-11.63	0.01	-17.57	0.02	-14.57
HXE	1PL	-0.00	-16.30	-0.01	-15.54	-0.52	-11.18	0.03	-14.89	-0.05	-13.87
HXE	2PL	-0.00	-16.04	0.01	-16.61	-0.46	-10.97	0.03	-15.60	-0.02	-14.10
HXE	ANLN	-0.00	-10.66	-0.03	-14.86	-0.76	-7.67	-0.13	-10.76	-0.03	-8.27
HXE	DEE	-0.00	-19.24	-0.01	-18.20	-0.45	-14.56	0.00	-18.84	-0.03	-17.08
HXE	CHCL3	-0.00	-19.94	-0.01	-17.77	0.00	-14.73	-0.01	-21.05	-0.03	-18.80
HXE	DEAN	-0.00	-17.27	-0.01	-18.89	-0.42	-14.54	-0.02	-18.93	-0.07	-15.91
HXE	TEAN	-0.00	-19.13	-0.02	-18.11	-0.34	-14.45	0.00	-19.26	-0.02	-16.49
HXE	TOL	-0.00	-18.42	-0.03	-19.05	-0.48	-13.61	-0.06	-18.93	0.02	-16.36
HXE	BZN	-0.00	-18.57	-0.00	-19.82	-0.47	-13.91	-0.05	-17.89	0.01	-16.14
HXE	HPE	-0.00	-18.36	-0.00	-18.63	-0.16	-15.62	0.00	-19.12	0.07	-16.92
HXE	HXE	-0.00	-18.40	0.00	-18.82	-0.15	-15.74	0.00	-19.17	0.04	-17.29
HXE	CCL4	-0.00	-20.44	0.01	-19.07	-	-	0.00	-22.28	-0.03	-19.30
HXE	CHE	-0.00	-19.11	-0.00	-19.16	-0.18	-15.60	0.00	-18.87	0.01	-16.99
CCL4	DAMD	-	-	0.74	-19.00	-	-	-0.52	-15.27	-0.02	-14.99
CCL4	PPN	-0.00	-16.99	0.90	-19.12	-	-	-0.34	-15.80	-0.15	-16.21
CCL4	BTN	-0.00	-17.26	2.32	-20.97	-	-	-0.30	-16.47	-0.10	-16.83
CCL4	PYRI	-	-	-1.00	-19.89	-	-	-0.38	-15.00	-0.15	-16.46
CCL4	H2O	-0.00	5.81	-0.69	1.36	-	-	-0.26	6.04	-0.56	4.92
CCL4	C2CL2	-	-	3.88	-22.83	-	-	-0.20	-16.18	-0.16	-17.48
CCL4	EAE	-0.00	-15.72	-1.17	-19.41	-	-	-0.42	-16.40	-0.06	-16.97
CCL4	PTL	-0.00	-16.49	0.28	-19.47	-	-	-0.20	-16.49	0.02	-18.00
CCL4	MTL	-0.00	-13.47	0.80	-16.50	-	-	-0.36	-12.36	-0.09	-15.20
CCL4	ETL	-0.00	-14.66	0.52	-17.75	-	-	-0.27	-14.93	-0.01	-16.53
CCL4	BTL	-0.00	-15.36	0.89	-19.47	-	-	-0.23	-16.09	-0.02	-17.55
CCL4	2M2P	-0.00	-15.41	2.49	-22.23	-	-	-0.14	-17.77	0.00	-17.36
CCL4	1PL	-0.00	-15.22	0.78	-18.83	-	-	-0.28	-14.82	0.02	-16.94
CCL4	2PL	-0.00	-14.80	0.12	-18.90	-	-	-0.27	-15.02	0.04	-16.96
CCL4	ANLN	-0.00	-10.42	-0.99	-17.68	-	-	-0.48	-9.16	-0.11	-13.14
CCL4	DEE	-0.00	-18.03	-0.70	-20.66	-	-	-0.17	-18.29	0.02	-19.30
CCL4	CHCL3	-0.00	-18.61	-0.11	-22.99	-	-	-0.15	-17.39	-0.11	-18.52
CCL4	DEAN	-0.00	-16.26	-0.12	-21.21	-	-	-0.15	-18.14	0.01	-18.65
CCL4	TEAN	-0.00	-18.35	0.41	-22.80	-	-	-0.09	-18.73	0.05	-19.55
CCL4	TOL	-0.00	-17.87	-0.68	-21.39	-	-	-0.22	-18.11	-0.08	-18.54

Table S.2 – Continued on next page

Table S.2 – Continued from previous page

Solute (A)	Solvent (B)	GROMOS-54A7		GROMOS-ATB		OPLS-LBCC		AMBER-GAFF2		OpenFF	
		ELE	VDW	ELE	VDW	ELE	VDW	ELE	VDW	ELE	VDW
[kJ·mol ⁻¹]											
CCL4	BZN	-0.00	-16.71	-2.89	-19.69	-	-	-0.33	-17.20	-0.08	-18.12
CCL4	HPE	-0.00	-18.10	0.02	-20.38	-	-	0.00	-18.72	-0.04	-19.12
CCL4	HXE	-0.00	-18.38	0.01	-20.47	-	-	0.00	-18.93	-0.02	-19.50
CCL4	CCL4	-0.00	-18.68	-3.04	-20.82	-	-	-0.07	-18.18	-0.02	-19.12
CCL4	CHE	-0.00	-18.55	-0.00	-20.39	-	-	0.01	-19.27	0.01	-20.34
CHE	DAMD	-	-	-0.00	-9.20	-0.78	-8.97	0.02	-16.72	-0.12	-13.60
CHE	PPN	-0.00	-18.96	-0.00	-13.52	-0.46	-12.94	0.01	-17.35	0.00	-15.58
CHE	BTN	-0.00	-18.52	-0.00	-14.03	-0.42	-13.22	0.00	-18.08	-0.06	-16.00
CHE	PYRI	-	-	-0.00	-14.57	-0.67	-11.20	0.01	-18.12	-0.10	-16.31
CHE	H2O	-0.00	5.52	-0.00	6.70	-0.16	6.43	-0.04	4.43	0.09	5.75
CHE	C2CL2	-	-	-0.00	-15.39	-0.24	-11.92	0.00	-19.69	-0.01	-18.28
CHE	EAE	-0.00	-17.30	-0.00	-14.64	-0.57	-13.02	0.01	-18.34	-0.10	-16.44
CHE	PTL	-0.00	-17.84	-0.00	-15.19	-0.34	-13.82	0.00	-17.65	-0.08	-16.47
CHE	MTL	-0.00	-14.29	-0.00	-11.67	-0.62	-8.03	0.01	-13.89	-0.05	-14.62
CHE	ETL	-0.00	-15.66	-0.00	-13.35	-0.49	-11.07	0.01	-16.88	-0.05	-15.60
CHE	BTL	-0.00	-17.67	-0.00	-14.47	-0.39	-13.07	0.01	-17.54	-0.02	-16.52
CHE	2M2P	-0.00	-17.71	-0.00	-15.24	-0.37	-13.81	0.01	-18.28	-0.04	-16.85
CHE	1PL	-0.00	-17.22	-0.00	-14.29	-0.44	-12.52	0.01	-16.64	-0.08	-16.40
CHE	2PL	-0.00	-17.65	-0.00	-13.16	-0.38	-12.64	0.01	-17.91	-0.06	-16.19
CHE	ANLN	-0.00	-15.79	-0.00	-13.77	-0.74	-10.53	0.03	-13.37	-0.19	-12.13
CHE	DEE	-0.00	-20.14	-0.00	-16.39	-0.38	-15.88	0.01	-20.43	-0.06	-18.58
CHE	CHCL3	-0.00	-21.55	-0.00	-15.67	0.04	-16.53	0.00	-22.70	0.00	-20.62
CHE	DEAN	-0.00	-18.41	-0.00	-17.36	-0.38	-16.05	0.01	-19.62	-0.14	-17.93
CHE	TEAN	-0.00	-20.03	-0.00	-16.84	-0.31	-16.13	0.01	-20.84	-0.09	-18.59
CHE	TOL	-0.00	-20.15	-0.00	-17.34	-0.47	-15.10	0.02	-20.34	-0.10	-18.06
CHE	BZN	-0.00	-19.88	-0.00	-17.54	-0.46	-15.62	0.02	-18.91	-0.12	-18.06
CHE	HPE	-0.00	-19.99	-0.00	-16.76	-0.15	-16.22	0.00	-20.51	0.04	-18.61
CHE	HXE	-0.00	-20.19	-0.00	-16.98	-0.14	-16.42	0.00	-20.59	0.01	-18.62
CHE	CCL4	-0.00	-20.80	-0.00	-16.81	-	-	0.01	-22.85	0.01	-21.55
CHE	CHE	-0.00	-21.03	-0.00	-16.92	-0.16	-16.89	0.00	-21.75	-0.03	-20.00

Table S.3: Numerical values of the difference between experimental and calculated cross-solvation free energies $\Delta_s G_{A:B}^\ominus$. The differences (simulation minus experiment) are calculated based on the data in Tab. S.1. The results are reported for the the five force fields newly considered in this work (Main Article Tab. 1). The molecules considered and their acronyms are shown in Main Article Fig. 1.

Solute (A)	Solvent (B)	GROMOS-54A7	GROMOS-ATB	OPLS-LBCC	AMBER-GAFF2	OpenFF
		[kJ·mol ⁻¹]				
DAMD	DAMD	-	-16.81	-10.48	-5.29	-7.05
DAMD	PPN	-	-12.40	-7.24	-2.55	-4.57
DAMD	BTN	-	-12.74	-8.09	-3.75	-5.35
DAMD	PYRI	-	-15.40	-10.80	-6.21	-8.25
DAMD	H2O	-	-12.91	-12.75	-3.09	-9.75
DAMD	C2CL2	-	-12.05	-10.24	-4.16	-7.08
DAMD	EAE	-	-10.90	-5.73	-0.88	-3.73
DAMD	PTL	-	-13.54	-8.44	-7.42	-12.35
DAMD	MTL	-	-16.56	-12.36	-9.13	-18.00
DAMD	ETL	-	-16.26	-11.33	-10.46	-16.01
DAMD	BTL	-	-15.67	-11.61	-9.36	-17.22
DAMD	2M2P	-	-15.97	-6.09	-5.19	-10.51
DAMD	1PL	-	-15.41	-9.62	-8.41	-14.83
DAMD	2PL	-	-15.76	-8.37	-6.97	-13.39
DAMD	ANLN	-	-18.89	-9.28	-6.99	-9.14
DAMD	DEE	-	-12.86	-6.77	-2.99	-4.09
DAMD	CHCL3	-	-14.07	-11.27	-4.68	-5.54
DAMD	DEAN	-	-11.10	-7.82	-7.24	-6.29
DAMD	TEAN	-	-9.76	-7.40	-3.18	-6.27
DAMD	TOL	-	-12.24	-9.53	-5.73	-6.05
DAMD	BZN	-	-13.16	-7.65	-5.32	-5.18
DAMD	HPE	-	-9.32	-3.75	-3.27	-2.76
DAMD	HXE	-	-7.28	-1.88	-1.79	-0.93
DAMD	CCL4	-	-7.41	-	-1.96	-1.72
DAMD	CHE	-	-6.56	-2.67	-1.91	-1.17
PPN	DAMD	-	-2.64	-1.91	-0.31	-0.48
PPN	PPN	-1.32	-2.02	-2.31	-0.11	-0.76
PPN	BTN	-1.39	-2.52	-2.38	-0.38	-0.68
PPN	PYRI	-	-1.78	-2.30	-0.55	-1.20
PPN	H2O	5.88	1.86	-0.30	2.42	1.67
PPN	C2CL2	-	-1.96	-3.37	-0.43	-1.15
PPN	EAE	-1.81	-2.23	-2.24	-0.49	-0.55
PPN	PTL	-0.82	-4.09	-3.87	-0.48	-4.93
PPN	MTL	0.81	-2.42	-2.68	-1.39	-4.87
PPN	ETL	0.38	-1.94	-3.19	-2.10	-4.45
PPN	BTL	0.10	-1.35	-3.45	-0.94	-3.73
PPN	2M2P	-1.68	-4.42	-4.36	-2.60	-5.21
PPN	1PL	-1.62	-3.10	-4.71	-2.32	-4.86
PPN	2PL	-1.02	-2.87	-3.80	-2.23	-4.93
PPN	ANLN	-1.64	-6.21	-3.31	-2.78	-2.74
PPN	DEE	-1.03	-3.04	-2.83	-0.03	-0.34
PPN	CHCL3	0.41	-3.00	-6.95	-1.90	-2.08
PPN	DEAN	-4.39	-3.48	-4.60	-3.80	-3.25
PPN	TEAN	-2.29	0.48	-1.24	1.78	-0.66
PPN	TOL	-1.71	-0.79	-2.43	-0.07	-0.60
PPN	BZN	-1.25	-1.64	-1.77	-0.51	-0.12

Table S.3 – Continued on next page

Table S.3 – Continued from previous page

Solute (A)	Solvent (B)	GROMOS-54A7	GROMOS-ATB	OPLS-LBCC	AMBER-GAFF2	OpenFF
		[kJ·mol ⁻¹]				
PPN	HPE	-1.87	-0.14	0.66	1.38	1.39
PPN	HXE	-2.17	-0.03	0.69	0.76	0.98
PPN	CCL4	0.15	2.84	-	2.53	2.48
PPN	CHE	-2.41	-0.41	0.50	1.44	1.41
BTN	DAMD	-	0.15	-1.04	-1.31	-0.27
BTN	PPN	-1.50	-1.60	-2.09	-0.93	-0.89
BTN	BTN	-1.45	-1.27	-1.95	-1.15	-0.94
BTN	PYRI	-	-1.16	-1.08	-1.11	-0.71
BTN	H2O	5.69	3.63	-0.48	1.76	1.30
BTN	C2CL2	-	-1.09	-1.92	-0.66	-1.11
BTN	EAE	-2.10	-1.15	-2.07	-1.19	-1.13
BTN	PTL	-1.20	-2.26	-3.39	-1.93	-5.15
BTN	MTL	1.41	-0.37	-1.62	-1.55	-4.79
BTN	ETL	0.62	-0.89	-2.75	-2.92	-4.51
BTN	BTL	-0.26	0.40	-3.34	-0.50	-4.51
BTN	2M2P	-0.61	-2.61	-2.69	-2.50	-4.55
BTN	1PL	0.36	-1.22	-3.34	-1.58	-5.11
BTN	2PL	-0.32	0.20	-2.77	-2.05	-5.10
BTN	ANLN	1.87	-4.06	-1.94	-1.80	-1.88
BTN	DEE	-1.27	-1.65	-2.17	-0.67	-0.67
BTN	CHCL3	1.31	-0.41	-5.53	-1.92	-1.24
BTN	DEAN	-2.67	-1.56	-2.80	-3.04	-1.26
BTN	TEAN	-1.82	1.05	-1.06	1.16	-0.95
BTN	TOL	-1.45	-1.17	-1.37	-0.64	-0.87
BTN	BZN	-1.29	-1.16	-1.37	-0.95	-0.50
BTN	HPE	-1.88	0.60	1.16	0.94	1.05
BTN	HXE	-1.14	0.15	1.15	0.81	1.36
BTN	CCL4	0.43	2.57	-	1.60	1.93
BTN	CHE	-1.98	0.32	0.58	0.44	0.95
PYRI	DAMD	-	-0.65	-3.62	2.97	1.96
PYRI	PPN	-	-1.96	-4.48	0.79	0.27
PYRI	BTN	-	-2.33	-4.59	1.11	0.26
PYRI	PYRI	-	-2.01	-4.34	1.79	0.53
PYRI	H2O	-	1.18	0.30	7.40	5.27
PYRI	C2CL2	-	-1.33	-5.21	1.13	0.29
PYRI	EAE	-	3.23	1.75	7.03	5.57
PYRI	PTL	-	-2.78	-4.09	1.75	-2.46
PYRI	MTL	-	1.35	-0.82	5.02	0.48
PYRI	ETL	-	0.69	-2.24	3.38	0.19
PYRI	BTL	-	0.36	-1.71	4.20	0.47
PYRI	2M2P	-	-1.95	-3.81	2.27	-0.72
PYRI	1PL	-	-0.08	-2.62	3.67	-0.07
PYRI	2PL	-	-1.81	-3.18	4.08	-1.17
PYRI	ANLN	-	15.48	10.80	17.18	16.36
PYRI	DEE	-	6.34	6.08	11.59	9.99
PYRI	CHCL3	-	-0.37	-4.44	3.28	2.25
PYRI	DEAN	-	-3.60	-5.59	-1.34	-2.36
PYRI	TEAN	-	-0.90	-2.04	3.74	0.91
PYRI	TOL	-	-2.19	-4.08	1.83	0.82
PYRI	BZN	-	-2.96	-3.64	0.67	0.75
PYRI	HPE	-	-2.18	-0.32	2.56	1.73

Table S.3 – Continued on next page

Table S.3 – Continued from previous page

Solute (A)	Solvent (B)	GROMOS-54A7	GROMOS-ATB	OPLS-LBCC	AMBER-GAFF2	OpenFF
[kJ·mol ⁻¹]						
PYRI	HXE	-	-3.37	-2.03	0.74	0.14
PYRI	CCL4	-	-0.39	-	3.97	2.95
PYRI	CHE	-	-1.46	-1.53	2.30	1.05
H2O	DAMD	-	5.21	5.98	4.48	1.47
H2O	PPN	2.50	-0.54	-2.40	-2.16	-2.61
H2O	BTN	-0.24	-2.76	-5.28	-4.66	-5.59
H2O	PYRI	-	2.20	4.14	4.91	3.02
H2O	H2O	-0.03	0.12	0.20	0.05	0.05
H2O	C2CL2	-	2.58	-0.79	3.30	3.96
H2O	EAE	1.46	2.58	1.60	-1.27	0.04
H2O	PTL	2.13	2.85	1.56	2.35	4.23
H2O	MTL	0.37	1.89	-0.30	1.05	2.89
H2O	ETL	2.49	2.09	-0.77	1.77	3.10
H2O	BTL	-1.81	-1.21	-2.69	-0.67	0.66
H2O	2M2P	17.36	17.74	14.78	18.05	19.32
H2O	1PL	5.92	6.01	3.87	5.47	7.58
H2O	2PL	1.17	1.89	-1.35	0.65	2.23
H2O	ANLN	-3.48	-3.63	-2.42	-2.79	-0.35
H2O	DEE	2.36	-2.96	-9.14	-1.01	-3.24
H2O	CHCL3	7.80	3.29	-0.67	2.87	4.06
H2O	DEAN	5.22	13.55	0.86	7.62	3.25
H2O	TEAN	10.86	14.11	1.64	13.59	1.34
H2O	TOL	3.06	3.62	0.26	2.75	1.35
H2O	BZN	-0.07	2.00	0.30	-0.96	0.44
H2O	HPE	4.49	4.43	4.00	5.31	4.89
H2O	HXE	8.29	8.15	7.80	9.04	8.60
H2O	CCL4	7.29	7.06	-	6.91	7.37
H2O	CHE	5.03	4.17	4.77	6.29	5.82
C2CL2	DAMD	-	3.98	-5.11	2.06	2.04
C2CL2	PPN	-	1.16	-7.10	0.53	0.79
C2CL2	BTN	-	1.86	-6.05	1.23	1.25
C2CL2	PYRI	-	-0.63	-8.42	-1.39	-1.21
C2CL2	H2O	-	4.07	-5.54	4.71	5.13
C2CL2	C2CL2	-	2.12	-4.56	2.27	2.18
C2CL2	EAE	-	2.34	-4.46	0.93	1.79
C2CL2	PTL	-	1.66	-6.87	0.90	0.69
C2CL2	MTL	-	3.26	-4.94	4.15	1.91
C2CL2	ETL	-	3.10	-6.77	2.46	0.97
C2CL2	BTL	-	2.23	-7.34	1.45	0.89
C2CL2	2M2P	-	-2.63	-12.98	-2.43	-3.41
C2CL2	1PL	-	1.51	-8.41	1.37	0.40
C2CL2	2PL	-	2.89	-7.17	2.72	2.28
C2CL2	ANLN	-	-0.07	-6.66	-0.30	0.31
C2CL2	DEE	-	1.82	-4.89	1.38	0.57
C2CL2	CHCL3	-	0.61	-6.79	1.04	0.92
C2CL2	DEAN	-	3.41	-6.04	1.84	0.38
C2CL2	TEAN	-	-1.17	-7.58	-2.00	-4.48
C2CL2	TOL	-	1.78	-4.63	-0.01	0.66
C2CL2	BZN	-	1.52	-3.42	0.18	1.23
C2CL2	HPE	-	3.30	2.50	2.81	3.38
C2CL2	HXE	-	1.72	1.02	0.99	1.52

Table S.3 – Continued on next page

Table S.3 – Continued from previous page

Solute (A)	Solvent (B)	GROMOS-54A7	GROMOS-ATB	OPLS-LBCC	AMBER-GAFF2	OpenFF
[kJ·mol ⁻¹]						
C2CL2	CCL4	-	5.55	-	4.84	4.91
C2CL2	CHE	-	2.54	1.27	1.58	1.43
EAE	DAMD	-	-5.54	-4.51	-3.26	-5.74
EAE	PPN	-9.47	-3.31	-3.46	-1.54	-3.81
EAE	BTN	-9.52	-4.13	-3.60	-2.21	-4.08
EAE	PYRI	-	-3.55	-1.64	-1.10	-3.94
EAE	H2O	-5.69	0.22	-1.29	-2.15	-3.28
EAE	C2CL2	-	-4.23	-2.77	-2.44	-4.50
EAE	EAE	-9.95	-4.44	-3.80	-2.05	-4.74
EAE	PTL	-11.66	-5.15	-5.28	-4.44	-8.58
EAE	MTL	-9.79	-4.44	-3.97	-4.62	-9.35
EAE	ETL	-8.52	-4.70	-4.45	-5.68	-8.81
EAE	BTL	-9.40	-5.50	-4.91	-4.71	-8.82
EAE	2M2P	-4.95	-1.49	-1.67	-2.41	-4.55
EAE	1PL	-7.76	-5.74	-5.01	-4.09	-8.39
EAE	2PL	-11.29	-4.63	-4.80	-5.27	-8.98
EAE	ANLN	-12.28	-10.20	-6.29	-5.35	-8.25
EAE	DEE	-7.31	-5.54	-4.04	-1.82	-4.38
EAE	CHCL3	-4.73	-4.53	-4.93	-3.26	-4.58
EAE	DEAN	-12.13	-6.58	-5.99	-6.14	-6.81
EAE	TEAN	-2.44	1.11	1.48	3.95	0.18
EAE	TOL	-8.16	-4.51	-4.27	-1.75	-4.45
EAE	BZN	-8.68	-4.47	-4.08	-2.61	-4.65
EAE	HPE	-5.65	-3.15	-1.28	-0.76	-2.84
EAE	HXE	-4.66	-3.14	-1.01	-0.48	-2.28
EAE	CCL4	-3.44	-1.68	-	0.26	-1.67
EAE	CHE	-6.25	-3.90	-2.47	-1.20	-3.03
PTL	DAMD	-	3.79	4.42	-3.55	-1.99
PTL	PPN	-4.00	1.26	0.60	-3.81	-2.33
PTL	BTN	-5.11	-0.04	-0.75	-4.93	-3.86
PTL	PYRI	-	2.40	4.03	0.11	-0.02
PTL	H2O	-2.83	6.29	0.51	-0.13	6.78
PTL	C2CL2	-	1.99	0.83	-0.12	0.58
PTL	EAE	-7.61	-1.07	-0.93	-7.35	-4.19
PTL	PTL	-1.56	3.78	5.36	0.52	4.20
PTL	MTL	-6.13	2.67	2.71	-2.16	1.17
PTL	ETL	-6.13	2.69	2.67	-2.32	1.66
PTL	BTL	-6.08	2.02	3.41	-2.13	1.92
PTL	2M2P	-2.87	-1.53	3.71	-0.99	2.79
PTL	1PL	-5.11	2.75	2.91	-2.48	2.00
PTL	2PL	-5.65	2.29	2.74	-1.10	1.93
PTL	ANLN	-1.86	3.03	3.69	1.20	5.15
PTL	DEE	2.97	3.32	3.18	2.88	1.34
PTL	CHCL3	1.44	0.77	-3.47	-1.59	-0.13
PTL	DEAN	-7.40	2.65	-1.07	-3.39	-5.60
PTL	TEAN	0.77	5.28	2.26	4.62	-3.70
PTL	TOL	-2.50	0.34	0.07	-1.10	-1.58
PTL	BZN	-4.69	-1.40	-0.51	-3.50	-2.32
PTL	HPE	-0.65	0.57	1.53	0.72	-0.69
PTL	HXE	-0.08	1.35	2.26	1.24	0.10
PTL	CCL4	0.28	2.47	-	0.61	-1.16

Table S.3 – Continued on next page

Table S.3 – Continued from previous page

Solute (A)	Solvent (B)	GROMOS-54A7	GROMOS-ATB	OPLS-LBCC	AMBER-GAFF2	OpenFF
[kJ·mol ⁻¹]						
PTL	CHE	-4.20	-1.55	-0.96	-0.77	-3.17
MTL	DAMD	-	5.38	5.03	3.04	1.87
MTL	PPN	-0.14	3.91	2.19	1.80	1.91
MTL	BTN	-0.51	3.30	1.77	1.29	1.07
MTL	PYRI	-	6.25	5.67	6.59	5.18
MTL	H2O	-1.28	6.41	1.64	3.95	8.39
MTL	C2CL2	-	0.79	-2.39	2.00	1.29
MTL	EAE	-4.06	2.67	1.82	-0.87	0.55
MTL	PTL	-5.59	3.87	2.78	2.68	5.49
MTL	MTL	-5.55	3.89	2.15	2.54	5.18
MTL	ETL	-5.50	4.17	1.90	2.41	5.04
MTL	BTL	-6.83	3.90	2.05	2.20	4.63
MTL	2M2P	-2.82	2.96	3.42	4.13	5.67
MTL	1PL	-5.08	2.86	1.45	0.84	4.27
MTL	2PL	-5.65	4.28	2.82	2.25	5.13
MTL	ANLN	-9.12	1.80	0.15	-0.30	2.46
MTL	DEE	5.17	4.57	1.94	6.40	3.44
MTL	CHCL3	4.65	3.84	-1.45	4.84	4.20
MTL	DEAN	-7.70	6.46	-0.49	1.49	-2.16
MTL	TEAN	5.57	11.27	5.08	12.13	1.26
MTL	TOL	-2.22	1.66	-0.61	2.09	-0.18
MTL	BZN	-2.75	1.88	0.68	1.02	0.68
MTL	HPE	1.10	2.69	2.25	4.71	1.80
MTL	HXE	1.41	3.11	2.70	5.05	2.16
MTL	CCL4	4.21	5.85	-	7.25	4.65
MTL	CHE	0.65	2.67	2.48	5.34	1.89
ETL	DAMD	-	4.48	4.12	1.89	0.39
ETL	PPN	-1.43	1.71	0.79	0.15	0.11
ETL	BTN	-0.70	2.21	1.22	0.45	0.14
ETL	PYRI	-	4.97	5.54	6.06	3.81
ETL	H2O	-0.75	4.49	0.72	5.37	8.08
ETL	C2CL2	-	1.37	-2.13	1.75	0.94
ETL	EAE	-4.23	1.28	1.05	-1.77	-0.17
ETL	PTL	-5.95	1.06	2.00	1.77	3.50
ETL	MTL	-4.55	1.60	1.03	2.52	3.72
ETL	ETL	-5.24	1.52	1.23	1.97	3.28
ETL	BTL	-2.79	0.65	1.93	2.05	3.68
ETL	2M2P	-2.19	-2.63	2.37	2.50	4.15
ETL	1PL	-6.37	1.54	1.26	1.38	3.57
ETL	2PL	-5.07	1.30	1.63	2.48	3.44
ETL	ANLN	-7.25	1.04	-0.71	1.02	0.30
ETL	DEE	-0.73	-1.96	-3.66	-0.16	-2.74
ETL	CHCL3	3.99	3.28	-2.44	3.41	2.93
ETL	DEAN	-2.45	8.88	2.87	4.70	1.18
ETL	TEAN	5.62	10.16	4.60	10.44	0.51
ETL	TOL	-0.09	2.56	0.58	2.85	0.77
ETL	BZN	-1.96	1.86	0.86	1.30	1.07
ETL	HPE	1.13	2.95	2.35	3.80	1.51
ETL	HXE	2.81	4.12	3.97	5.08	2.93
ETL	CCL4	3.39	5.38	-	5.43	3.04
ETL	CHE	2.57	3.95	3.88	5.42	2.76

Table S.3 – Continued on next page

Table S.3 – Continued from previous page

Solute (A)	Solvent (B)	GROMOS-54A7	GROMOS-ATB	OPLS-LBCC	AMBER-GAFF2	OpenFF
[kJ·mol ⁻¹]						
BTL	DAMD	-	1.03	5.10	-2.17	-1.16
BTL	PPN	-2.08	0.48	2.26	-2.04	-0.17
BTL	BTN	-1.85	0.12	2.45	-2.24	-0.46
BTL	PYRI	-	1.92	6.22	2.37	3.07
BTL	H2O	-2.06	1.10	1.40	-0.46	7.43
BTL	C2CL2	-	0.17	-0.05	0.06	0.67
BTL	EAE	-4.20	0.01	2.26	-3.93	-1.14
BTL	PTL	-4.04	-1.10	3.93	-3.14	3.14
BTL	MTL	-5.97	-1.72	2.65	-2.04	2.16
BTL	ETL	-5.30	-1.46	3.62	-1.44	3.10
BTL	BTL	-6.38	-2.42	3.45	-2.70	2.49
BTL	2M2P	-2.68	-1.16	3.56	-1.72	3.25
BTL	1PL	-5.47	-2.20	2.64	-2.15	2.38
BTL	2PL	-5.08	-4.16	3.99	-1.54	3.11
BTL	ANLN	-10.31	-1.43	0.37	-3.19	2.37
BTL	DEE	-0.27	-2.53	-1.37	-0.61	-2.49
BTL	CHCL3	1.76	1.05	-2.93	-0.39	0.33
BTL	DEAN	-6.73	3.76	1.22	-1.69	-2.78
BTL	TEAN	2.40	6.39	3.35	6.35	-2.46
BTL	TOL	-2.22	-1.04	-0.39	-0.90	-1.52
BTL	BZN	-4.44	-1.70	-0.30	-2.39	-1.15
BTL	HPE	0.87	1.81	2.18	2.26	0.68
BTL	HXE	0.77	2.27	2.64	2.38	0.73
BTL	CCL4	2.29	3.79	-	2.39	0.71
BTL	CHE	-0.82	1.08	1.68	1.72	-0.53
2M2P	DAMD	-	-7.71	2.14	-4.37	-3.73
2M2P	PPN	1.07	-5.76	-0.03	-3.36	-2.33
2M2P	BTN	1.55	-5.66	0.32	-3.41	-2.49
2M2P	PYRI	-	-4.33	2.73	1.10	0.30
2M2P	H2O	5.84	-3.03	-0.90	2.32	5.89
2M2P	C2CL2	-	-0.18	2.68	3.55	3.18
2M2P	EAE	2.34	-4.74	1.41	-3.49	-1.16
2M2P	PTL	-0.80	-9.86	0.16	-3.39	-0.19
2M2P	MTL	2.07	-5.46	1.95	0.11	1.15
2M2P	ETL	0.33	-7.72	1.80	-2.03	0.96
2M2P	BTL	2.21	-9.94	0.39	-3.69	-0.43
2M2P	2M2P	0.64	-14.67	-0.57	-2.30	-0.29
2M2P	1PL	2.21	-7.95	0.69	-2.34	0.34
2M2P	2PL	3.70	-10.51	1.01	-1.45	0.22
2M2P	ANLN	-2.76	-7.79	-1.71	0.08	-1.00
2M2P	DEE	3.83	-6.08	-0.28	-0.02	-1.26
2M2P	CHCL3	4.18	-5.42	-6.25	-2.08	-1.85
2M2P	DEAN	-0.07	-1.90	0.30	-0.64	-2.70
2M2P	TEAN	6.02	0.63	3.42	5.35	-0.66
2M2P	TOL	0.28	-6.25	-1.83	-1.39	-2.64
2M2P	BZN	-1.25	-6.60	-2.34	-3.46	-2.99
2M2P	HPE	2.47	-3.62	0.24	0.45	-0.81
2M2P	HXE	2.15	-3.41	0.43	0.08	-1.01
2M2P	CCL4	3.36	-3.92	-	-0.25	-1.97
2M2P	CHE	1.58	-4.20	-0.65	-0.64	-1.77
1PL	DAMD	-	4.66	4.73	-1.41	-0.76

Table S.3 – Continued on next page

Table S.3 – Continued from previous page

Solute (A)	Solvent (B)	GROMOS-54A7	GROMOS-ATB	OPLS-LBCC	AMBER-GAFF2	OpenFF
[kJ·mol ⁻¹]						
1PL	PPN	-1.94	2.62	2.01	-1.53	-0.20
1PL	BTN	-1.25	2.88	2.09	-0.96	-0.29
1PL	PYRI	-	5.59	6.23	3.60	3.13
1PL	H2O	-0.77	7.39	1.61	0.21	7.88
1PL	C2CL2	-	1.33	-1.46	-0.51	-0.04
1PL	EAE	-3.90	2.95	2.11	-2.99	-0.55
1PL	PTL	-7.54	4.35	4.67	-0.29	3.26
1PL	MTL	-4.23	4.83	3.74	-0.50	3.59
1PL	ETL	-4.90	3.57	3.30	-0.43	3.54
1PL	BTL	-4.40	3.42	2.66	-2.34	2.23
1PL	2M2P	-5.46	1.02	2.22	-3.10	2.11
1PL	1PL	-5.52	3.47	3.26	-2.26	3.02
1PL	2PL	-5.13	3.73	3.74	-0.41	3.19
1PL	ANLN	-6.81	0.99	0.56	-4.60	1.50
1PL	DEE	0.70	0.49	-0.70	0.79	-1.31
1PL	CHCL3	2.21	1.53	-3.53	-0.55	1.07
1PL	DEAN	-7.28	4.30	-0.42	-1.91	-4.26
1PL	TEAN	3.70	9.27	4.72	8.15	-0.93
1PL	TOL	-1.64	1.82	0.34	0.62	-0.65
1PL	BZN	-2.89	0.45	0.77	-1.02	-0.43
1PL	HPE	1.37	2.53	2.61	3.53	1.73
1PL	HXE	0.42	2.09	2.12	2.20	0.28
1PL	CCL4	2.89	5.25	-	3.52	2.36
1PL	CHE	-0.50	1.29	1.28	2.35	-0.17
2PL	DAMD	-	-4.56	3.88	-0.43	-0.83
2PL	PPN	-0.26	-4.30	-0.09	-1.85	-0.94
2PL	BTN	0.58	-4.16	0.34	-1.14	-0.96
2PL	PYRI	-	-2.82	3.39	2.58	2.09
2PL	H2O	2.53	-2.07	-0.25	1.78	7.11
2PL	C2CL2	-	0.25	2.42	4.40	4.19
2PL	EAE	-2.41	-6.09	-0.53	-4.32	-2.45
2PL	PTL	-3.09	-6.35	0.98	-0.79	2.07
2PL	MTL	-4.89	-7.87	-1.30	-3.23	-0.25
2PL	ETL	-2.08	-6.02	0.41	-1.17	1.57
2PL	BTL	-4.64	-5.66	0.39	-1.68	1.73
2PL	2M2P	-3.38	-5.55	-0.25	-1.62	1.45
2PL	1PL	-4.40	-6.96	-0.21	-2.02	1.05
2PL	2PL	-1.02	-9.85	-0.40	-2.28	0.27
2PL	ANLN	-4.27	-3.33	2.00	0.59	3.40
2PL	DEE	5.06	-3.04	1.24	3.41	1.49
2PL	CHCL3	4.66	-2.96	-4.16	-0.01	0.29
2PL	DEAN	-4.46	-2.47	-2.34	-1.82	-4.47
2PL	TEAN	6.02	3.14	3.41	7.72	-0.34
2PL	TOL	0.09	-2.99	-0.74	0.33	-1.05
2PL	BZN	-1.33	-4.16	-0.99	-1.89	-1.91
2PL	HPE	0.70	-2.40	0.40	1.50	-0.51
2PL	HXE	0.94	-2.27	0.55	1.27	-0.43
2PL	CCL4	2.57	-1.18	-	1.96	0.19
2PL	CHE	0.27	-3.00	-0.24	0.55	-1.55
ANLN	DAMD	-	-1.39	-0.75	-9.37	-6.46
ANLN	PPN	-0.83	2.50	2.71	-3.23	0.59

Table S.3 – Continued on next page

Table S.3 – Continued from previous page

Solute (A)	Solvent (B)	GROMOS-54A7	GROMOS-ATB	OPLS-LBCC	AMBER-GAFF2	OpenFF
[kJ·mol ⁻¹]						
ANLN	BTN	-2.97	-0.25	-0.06	-6.00	-2.26
ANLN	PYRI	-	1.28	-2.63	-7.62	-5.01
ANLN	H2O	-8.82	1.60	1.74	-4.47	0.99
ANLN	C2CL2	-	5.91	1.64	-0.36	3.22
ANLN	EAE	-5.39	1.37	1.98	-5.58	-1.17
ANLN	PTL	-5.97	2.44	-0.32	-3.36	0.30
ANLN	MTL	-7.82	5.41	2.13	-0.90	0.81
ANLN	ETL	-6.16	6.32	1.48	-0.79	1.24
ANLN	BTL	-8.26	4.53	0.21	-2.43	0.17
ANLN	2M2P	2.34	9.18	6.36	5.81	8.31
ANLN	1PL	-5.93	2.50	-0.46	-3.29	-0.03
ANLN	2PL	-1.30	7.46	3.29	1.56	3.47
ANLN	ANLN	-14.19	5.99	2.56	-7.80	0.70
ANLN	DEE	7.31	5.41	15.24	3.44	4.03
ANLN	CHCL3	4.80	4.22	-0.42	-1.92	2.54
ANLN	DEAN	-7.46	3.98	9.17	-4.49	-3.78
ANLN	TEAN	-0.61	3.04	-0.06	-0.38	-4.37
ANLN	TOL	-0.56	4.90	1.95	-0.51	2.28
ANLN	BZN	-2.19	3.78	2.09	-2.61	1.93
ANLN	HPE	3.52	2.94	2.64	1.08	3.95
ANLN	HXE	3.48	2.73	2.66	1.23	3.90
ANLN	CCL4	6.18	5.24	-	2.40	5.00
ANLN	CHE	3.43	3.62	2.48	1.21	3.78
DEE	DAMD	-	0.09	2.60	1.37	0.69
DEE	PPN	0.49	0.24	2.63	2.71	2.07
DEE	BTN	0.29	-0.44	1.93	2.35	1.42
DEE	PYRI	-	-1.78	3.95	2.39	1.06
DEE	H2O	10.44	3.71	-0.51	8.54	5.08
DEE	C2CL2	-	-3.00	-0.06	-0.83	-2.35
DEE	EAE	2.60	0.79	3.13	3.43	2.35
DEE	PTL	-1.62	-2.72	-0.88	0.27	-2.14
DEE	MTL	1.43	-1.35	1.20	1.99	-1.79
DEE	ETL	3.07	1.66	3.50	4.27	1.33
DEE	BTL	-1.02	-2.99	-0.85	0.78	-2.03
DEE	2M2P	0.37	-1.70	1.56	1.18	-0.36
DEE	1PL	1.58	-0.68	2.00	2.89	0.03
DEE	2PL	0.69	0.08	2.20	1.95	-0.13
DEE	ANLN	5.27	-1.14	-0.08	4.63	3.04
DEE	DEE	-1.86	-3.15	-0.17	-0.50	-1.47
DEE	CHCL3	0.59	-3.00	-2.15	-0.18	-1.30
DEE	DEAN	-0.52	-2.35	0.55	0.30	-0.67
DEE	TEAN	-0.66	-1.06	1.66	1.55	0.06
DEE	TOL	-2.50	-3.31	-0.64	-1.11	-1.59
DEE	BZN	1.34	-1.25	2.95	3.25	1.57
DEE	HPE	-1.48	-1.66	1.47	0.51	-0.20
DEE	HXE	-1.29	-1.31	1.99	0.85	0.28
DEE	CCL4	-1.77	-1.39	-	-0.80	-1.67
DEE	CHE	-3.41	-3.38	0.06	-0.76	-1.87
CHCL3	DAMD	-	-0.79	-1.99	2.80	3.07
CHCL3	PPN	1.81	-1.64	-4.77	1.36	1.35
CHCL3	BTN	2.15	-1.34	-5.14	1.37	1.70

Table S.3 – Continued on next page

Table S.3 – Continued from previous page

Solute (A)	Solvent (B)	GROMOS-54A7	GROMOS-ATB	OPLS-LBCC	AMBER-GAFF2	OpenFF
		[kJ·mol ⁻¹]				
CHCL3	PYRI	-	-1.70	-2.77	2.56	2.27
CHCL3	H2O	6.75	-0.07	-1.68	5.18	4.75
CHCL3	C2CL2	-	-4.07	-3.68	0.47	-0.35
CHCL3	EAE	2.51	-3.17	-3.43	0.63	1.11
CHCL3	PTL	-0.32	-4.01	-9.42	-0.04	-1.25
CHCL3	MTL	3.15	-0.43	-2.92	3.42	1.78
CHCL3	ETL	1.95	-1.23	-5.93	1.91	1.36
CHCL3	BTL	1.22	-3.18	-7.20	0.92	0.48
CHCL3	2M2P	9.30	4.73	-1.29	8.87	7.74
CHCL3	1PL	1.65	-1.82	-6.70	1.42	0.78
CHCL3	2PL	4.24	-1.04	-5.76	3.64	2.97
CHCL3	ANLN	0.65	-4.57	-5.12	3.46	1.78
CHCL3	DEE	-1.34	-5.84	-8.52	-1.21	-2.33
CHCL3	CHCL3	-0.56	-3.47	-2.92	1.77	1.05
CHCL3	DEAN	1.79	-1.56	-9.24	0.19	-1.20
CHCL3	TEAN	6.86	4.32	-0.65	7.57	4.29
CHCL3	TOL	-0.90	-5.09	-6.47	-1.15	-1.55
CHCL3	BZN	-4.32	-8.37	-9.06	-4.85	-4.17
CHCL3	HPE	-1.44	-2.23	-1.35	0.55	0.13
CHCL3	HXE	-2.54	-3.85	-2.79	-1.32	-1.80
CHCL3	CCL4	-0.33	-2.92	-	2.27	1.64
CHCL3	CHE	-0.76	-0.93	-0.61	1.45	0.64
DEAN	DAMD	-	-1.92	-2.37	-5.20	-4.00
DEAN	PPN	-3.40	-0.53	-0.80	-1.50	-0.98
DEAN	BTN	-4.59	-2.86	-2.07	-2.94	-2.75
DEAN	PYRI	-	2.30	2.58	1.88	1.30
DEAN	H2O	7.83	13.67	1.69	10.33	4.85
DEAN	C2CL2	-	-0.06	-0.93	-1.40	-2.69
DEAN	EAE	-3.66	-2.13	-1.50	-2.29	-1.25
DEAN	PTL	1.28	3.46	1.94	3.94	-1.94
DEAN	MTL	0.31	6.55	3.28	4.58	-2.58
DEAN	ETL	-4.78	1.69	-0.82	-0.50	-6.01
DEAN	BTL	-2.98	4.23	1.82	3.30	-2.40
DEAN	2M2P	4.23	4.08	5.56	6.64	2.27
DEAN	1PL	0.25	2.32	0.32	1.41	-3.88
DEAN	2PL	-2.10	1.86	-0.58	1.95	-3.83
DEAN	ANLN	5.13	7.27	5.01	7.10	6.52
DEAN	DEE	-2.21	-3.54	-1.65	-1.67	-2.25
DEAN	CHCL3	3.53	3.33	-2.67	1.18	-0.60
DEAN	DEAN	-2.69	-0.97	-0.27	-0.18	-1.05
DEAN	TEAN	0.98	0.02	1.73	2.18	0.91
DEAN	TOL	-3.02	-3.46	-0.98	-1.13	-1.92
DEAN	BZN	-2.97	-2.89	-0.59	0.07	-1.14
DEAN	HPE	-1.02	-2.79	-0.38	-0.67	-0.98
DEAN	HXE	-0.07	-2.21	0.30	0.22	-0.35
DEAN	CCL4	1.45	-1.67	-	0.45	-0.32
DEAN	CHE	0.03	-2.34	0.54	0.54	-0.22
TEAN	DAMD	-	-4.65	1.50	-1.31	-1.94
TEAN	PPN	-3.74	-3.86	-0.91	-1.25	-1.59
TEAN	BTN	-5.10	-6.28	-2.11	-2.40	-3.03
TEAN	PYRI	-	-6.26	0.13	-0.33	-2.95

Table S.3 – Continued on next page

Table S.3 – Continued from previous page

Solute (A)	Solvent (B)	GROMOS-54A7	GROMOS-ATB	OPLS-LBCC	AMBER-GAFF2	OpenFF
[kJ·mol ⁻¹]						
TEAN	H2O	14.47	14.87	4.56	17.42	3.63
TEAN	C2CL2	-	-5.44	-0.76	-3.16	-4.65
TEAN	EAE	-3.82	-6.83	-2.66	-2.34	-3.18
TEAN	PTL	-0.47	-2.81	0.98	1.05	-4.52
TEAN	MTL	4.88	2.09	5.16	6.38	-3.84
TEAN	ETL	1.22	-0.78	2.09	1.91	-5.13
TEAN	BTL	0.22	-1.89	0.61	1.76	-4.46
TEAN	2M2P	-2.12	-8.06	-0.90	-1.68	-3.03
TEAN	1PL	-0.00	-2.58	0.42	2.10	-4.75
TEAN	2PL	-1.27	-3.38	0.23	0.08	-4.96
TEAN	ANLN	9.17	6.16	8.72	13.08	12.39
TEAN	DEE	-4.03	-7.51	-2.66	-3.28	-3.57
TEAN	CHCL3	-0.76	-3.45	-3.53	-0.83	-3.52
TEAN	DEAN	0.09	-5.17	0.41	-0.37	-0.10
TEAN	TEAN	-3.86	-7.83	-2.56	-3.04	-2.67
TEAN	TOL	-3.94	-7.95	-1.69	-2.39	-2.62
TEAN	BZN	-3.53	-8.13	-2.38	-1.52	-3.22
TEAN	HPE	-3.34	-7.31	-1.76	-3.22	-1.79
TEAN	HXE	-3.46	-7.38	-1.85	-3.23	-1.78
TEAN	CCL4	-4.15	-7.46	-	-5.49	-4.36
TEAN	CHE	-3.63	-6.52	-1.53	-3.21	-1.95
TOL	DAMD	-	0.79	0.94	0.67	3.11
TOL	PPN	-0.99	-0.72	-1.55	0.15	2.07
TOL	BTN	-0.48	-0.51	-0.47	0.68	2.29
TOL	PYRI	-	-1.04	0.07	1.30	2.88
TOL	H2O	0.31	1.51	-3.70	0.47	0.05
TOL	C2CL2	-	-0.01	0.04	-0.76	1.47
TOL	EAE	0.08	-0.62	-0.73	0.77	2.81
TOL	PTL	-0.37	-2.20	-1.86	-0.20	0.45
TOL	MTL	0.63	0.05	0.00	1.66	-0.20
TOL	ETL	0.41	-0.18	-0.42	0.63	0.46
TOL	BTL	-1.13	-0.84	-0.79	0.73	0.81
TOL	2M2P	-0.73	-1.36	-1.89	-0.22	1.10
TOL	1PL	-0.28	-0.70	-1.48	0.38	1.03
TOL	2PL	-0.59	-1.19	-1.22	0.09	0.82
TOL	ANLN	0.43	-1.33	-1.99	3.22	1.88
TOL	DEE	-0.41	-1.45	-0.65	0.47	1.76
TOL	CHCL3	0.36	-1.07	-4.50	-1.83	-0.02
TOL	DEAN	-1.26	-2.65	-1.69	-1.31	0.36
TOL	TEAN	-0.09	-1.46	-0.59	0.73	2.16
TOL	TOL	0.21	-0.38	-0.44	0.92	2.55
TOL	BZN	0.22	-0.51	-0.50	1.34	2.65
TOL	HPE	-0.14	-1.37	0.69	0.85	2.78
TOL	HXE	0.50	-1.07	1.00	0.63	2.84
TOL	CCL4	1.28	-0.27	-	0.41	2.75
TOL	CHE	0.26	-1.05	0.80	0.76	2.70
BZN	DAMD	-	0.89	1.70	0.69	3.50
BZN	PPN	-0.39	-0.01	-0.39	-0.26	2.22
BZN	BTN	0.03	0.28	-0.14	0.50	2.66
BZN	PYRI	-	0.31	1.05	0.40	2.92
BZN	H2O	-1.73	-0.36	-2.30	-3.40	0.31

Table S.3 – Continued on next page

Table S.3 – Continued from previous page

Solute (A)	Solvent (B)	GROMOS-54A7	GROMOS-ATB	OPLS-LBCC	AMBER-GAFF2	OpenFF
[kJ·mol ⁻¹]						
BZN	C2CL2	-	-0.01	0.14	-1.12	1.48
BZN	EAE	0.60	-0.22	-0.45	0.15	2.36
BZN	PTL	-0.76	-1.86	-1.15	0.64	1.67
BZN	MTL	-0.34	-0.09	0.28	0.47	0.57
BZN	ETL	-0.60	-0.83	-0.56	-0.16	1.12
BZN	BTL	0.02	-0.36	-1.01	0.64	1.32
BZN	2M2P	-0.90	-2.42	-2.11	-0.01	0.80
BZN	1PL	0.26	-1.00	-1.41	0.32	1.00
BZN	2PL	-0.28	-0.14	-1.00	0.58	1.20
BZN	ANLN	2.03	-0.08	-0.75	0.03	2.76
BZN	DEE	9.65	8.46	9.10	10.28	11.81
BZN	CHCL3	0.70	-1.18	-3.15	-2.67	0.85
BZN	DEAN	-0.04	-0.68	0.55	0.53	2.65
BZN	TEAN	1.72	0.53	1.02	3.15	3.52
BZN	TOL	0.96	0.03	-0.16	0.84	2.76
BZN	BZN	1.00	-0.07	0.21	0.59	2.93
BZN	HPE	0.57	-1.17	0.53	1.53	2.97
BZN	HXE	0.02	-0.92	0.12	0.96	2.67
BZN	CCL4	2.26	0.50	-	1.57	3.53
BZN	CHE	0.10	-0.21	0.58	1.94	3.36
HPE	DAMD	-	1.29	5.35	-3.48	1.98
HPE	PPN	-3.92	-1.40	1.80	-2.98	-0.28
HPE	BTN	-3.21	-1.43	2.16	-2.98	0.22
HPE	PYRI	-	-2.85	4.83	-3.45	-0.68
HPE	H2O	-0.67	-1.12	0.20	-1.58	0.62
HPE	C2CL2	-	-2.74	5.34	-5.13	-2.50
HPE	EAE	-0.52	-1.39	2.59	-2.36	1.11
HPE	PTL	-2.92	-3.21	1.50	-3.15	-1.24
HPE	MTL	-0.76	-1.32	6.30	-0.82	-1.09
HPE	ETL	-1.64	-2.74	3.16	-2.27	-0.39
HPE	BTL	-3.34	-2.00	2.10	-2.34	-0.47
HPE	2M2P	-2.17	-3.13	1.50	-3.92	-1.37
HPE	1PL	-3.44	-2.54	1.45	-2.68	-0.84
HPE	2PL	-3.10	-2.80	1.90	-2.95	-0.95
HPE	ANLN	-1.10	-5.62	1.64	-1.76	1.66
HPE	DEE	-4.88	-4.08	-0.06	-4.70	-2.17
HPE	CHCL3	-4.20	-1.69	1.82	-5.73	-3.16
HPE	DEAN	-3.28	-5.61	-1.22	-5.54	-2.75
HPE	TEAN	-2.42	-2.86	1.06	-3.44	-0.42
HPE	TOL	-2.96	-3.83	2.06	-3.69	-0.99
HPE	BZN	-2.26	-4.61	1.94	-2.36	-0.42
HPE	HPE	-2.49	-2.51	0.86	-3.11	-0.92
HPE	HXE	-1.99	-2.05	1.03	-3.07	-0.74
HPE	CCL4	-3.05	-2.25	-	-6.20	-3.15
HPE	CHE	-2.91	-2.84	1.36	-2.84	-0.81
HXE	DAMD	-	1.27	4.96	-3.04	1.72
HXE	PPN	-2.92	-1.06	2.00	-2.13	0.13
HXE	BTN	-2.82	-1.33	2.83	-2.08	0.36
HXE	PYRI	-	-1.88	5.40	-2.49	-0.31
HXE	H2O	-0.97	-2.08	0.19	-1.14	0.73
HXE	C2CL2	-	-2.18	5.22	-4.02	-1.57

Table S.3 – Continued on next page

Table S.3 – Continued from previous page

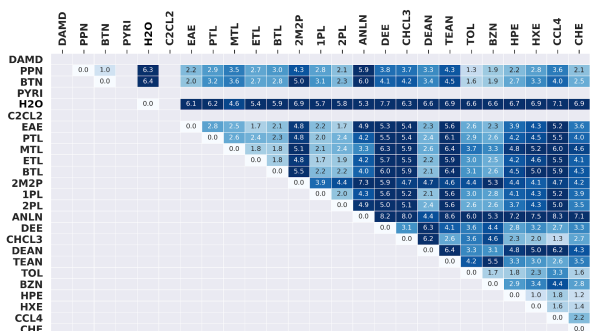
Solute (A)	Solvent (B)	GROMOS-54A7	GROMOS-ATB	OPLS-LBCC	AMBER-GAFF2	OpenFF
[kJ·mol ⁻¹]						
HXE	EAE	-0.20	-1.19	2.47	-1.51	1.24
HXE	PTL	-3.09	-2.90	2.22	-1.71	0.01
HXE	MTL	-1.20	-1.34	5.33	-0.95	-0.50
HXE	ETL	-1.71	-1.29	2.88	-2.30	-0.52
HXE	BTL	-2.03	-2.55	1.83	-1.83	-0.07
HXE	2M2P	-2.79	-5.16	1.84	-3.63	-0.62
HXE	1PL	-3.28	-2.52	1.32	-1.84	-0.90
HXE	2PL	-2.51	-3.07	2.10	-2.04	-0.59
HXE	ANLN	-0.64	-4.87	1.59	-0.87	1.72
HXE	DEE	-3.48	-2.45	0.75	-3.08	-1.35
HXE	CHCL3	-3.52	-1.36	1.69	-4.64	-2.41
HXE	DEAN	-1.86	-3.49	0.45	-3.54	-0.57
HXE	TEAN	-2.51	-1.51	1.83	-2.64	0.11
HXE	TOL	-2.32	-2.98	2.01	-2.89	-0.24
HXE	BZN	-3.26	-4.51	0.93	-2.63	-0.82
HXE	HPE	-1.80	-2.07	0.78	-2.56	-0.29
HXE	HXE	-1.52	-1.94	0.99	-2.29	-0.37
HXE	CCL4	-3.46	-2.08	-	-5.30	-2.35
HXE	CHE	-2.10	-2.15	1.23	-1.86	0.03
CCL4	DAMD	-	0.62	-	3.09	3.87
CCL4	PPN	0.18	-1.05	-	1.03	0.81
CCL4	BTN	0.09	-1.31	-	0.58	0.42
CCL4	PYRI	-	1.49	-	7.00	5.77
CCL4	H2O	5.51	0.37	-	5.48	4.06
CCL4	C2CL2	-	-2.59	-	-0.02	-1.28
CCL4	EAE	1.97	-2.90	-	0.87	0.66
CCL4	PTL	-2.33	-5.03	-	-2.53	-3.82
CCL4	MTL	1.71	-0.53	-	2.46	-0.11
CCL4	ETL	1.04	-1.53	-	0.50	-0.84
CCL4	BTL	0.85	-2.37	-	-0.11	-1.36
CCL4	2M2P	1.52	-2.81	-	-0.98	-0.43
CCL4	1PL	0.48	-2.35	-	0.60	-1.22
CCL4	2PL	1.64	-2.34	-	1.15	-0.48
CCL4	ANLN	4.30	-3.95	-	5.08	1.47
CCL4	DEE	0.35	-2.98	-	-0.08	-0.90
CCL4	CHCL3	-0.05	-4.54	-	1.02	-0.07
CCL4	DEAN	1.72	-3.35	-	-0.31	-0.66
CCL4	TEAN	-0.31	-4.35	-	-0.78	-1.46
CCL4	TOL	0.33	-3.87	-	-0.13	-0.42
CCL4	BZN	-0.78	-6.65	-	-1.60	-2.27
CCL4	HPE	-0.48	-2.74	-	-1.10	-1.54
CCL4	HXE	-0.79	-2.88	-	-1.34	-1.93
CCL4	CCL4	-0.18	-5.36	-	0.25	-0.64
CCL4	CHE	-0.62	-2.46	-	-1.33	-2.40
CHE	DAMD	-	4.60	4.05	-2.90	0.08
CHE	PPN	-4.13	1.31	1.43	-2.51	-0.75
CHE	BTN	-2.83	1.66	2.05	-2.39	-0.37
CHE	PYRI	-	1.00	3.70	-2.54	-0.84
CHE	H2O	0.75	1.93	1.50	-0.38	1.07
CHE	C2CL2	-	0.58	3.81	-3.72	-2.32
CHE	EAE	-1.59	1.07	2.12	-2.62	-0.83

Table S.3 – Continued on next page

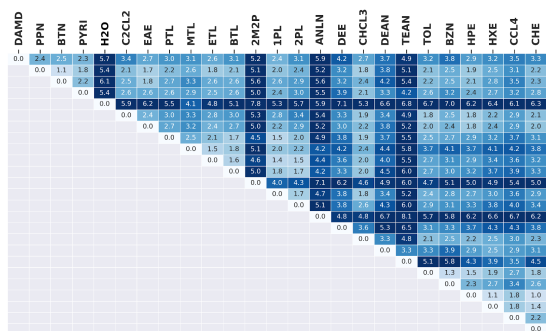
Table S.3 – *Continued from previous page*

Solute (A)	Solvent (B)	GROMOS-54A7	GROMOS-ATB	OPLS-LBCC	AMBER-GAFF2	OpenFF
[kJ·mol ⁻¹]						
CHE	PTL	-2.31	0.34	1.37	-2.12	-1.02
CHE	MTL	-0.43	2.19	5.21	-0.02	-0.81
CHE	ETL	-1.11	1.20	2.99	-2.32	-1.10
CHE	BTL	-2.27	0.93	1.94	-2.13	-1.14
CHE	2M2P	-2.35	0.12	1.18	-2.91	-1.53
CHE	1PL	-2.42	0.51	1.84	-1.83	-1.68
CHE	2PL	-2.80	1.69	1.83	-3.05	-1.40
CHE	ANLN	-3.05	-1.03	1.47	-0.60	0.42
CHE	DEE	-2.61	1.14	1.27	-2.89	-1.11
CHE	CHCL3	-2.94	2.94	2.12	-4.09	-2.01
CHE	DEAN	-1.91	-0.86	0.07	-3.11	-1.57
CHE	TEAN	-2.56	0.63	1.03	-3.36	-1.21
CHE	TOL	-2.69	0.12	1.89	-2.86	-0.70
CHE	BZN	-2.52	-0.18	1.28	-1.53	-0.82
CHE	HPE	-2.46	0.77	1.16	-2.98	-1.04
CHE	HXE	-2.49	0.72	1.14	-2.89	-0.91
CHE	CCL4	-2.30	1.69	-	-4.34	-3.04
CHE	CHE	-2.48	1.63	1.50	-3.20	-1.48

GROMOS-54A7

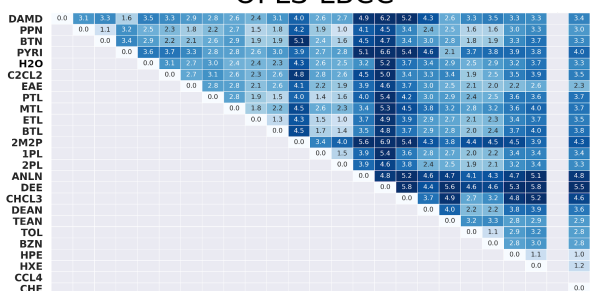


GROMOS-ATB

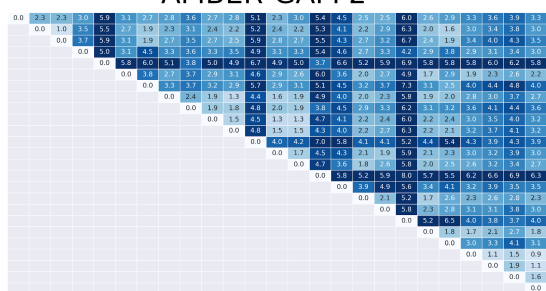


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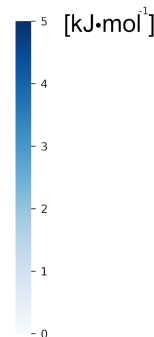
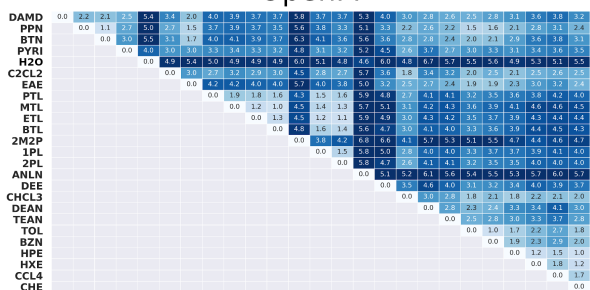
Solvent A



AMBER-GAFF2



OpenFF



Solvent B

Figure S.4: Root-mean-square error relative to experiment for the transfer free energies of all possible solutes C between any pair of solvents A and B, considering the FULL set. For each solvent pair, the RMSE of $\Delta_t G_{C:A \rightarrow B}^{\ominus}$ is obtained by considering the entire series of solutes C. The values are shown for the five force fields newly considered in this work (Main Article Tab. 1). The molecules considered and their acronyms are shown in Main Article Fig. 1. This figure is the analog of Main Article Fig. 6 for the FULL set.

S.2 Force-field comparison for individual compounds

The numerical values pertaining to Main Article Fig. 4 are reported in Tab. S.4. An analog of Main Article Fig. 4 for the FULL set is also displayed in Fig. S.5, with the corresponding numerical values in Tab. S.5.

Table S.4: Numerical values pertaining to Main Article Fig. 4. See the corresponding caption.

	RMSE As Solute [kJ·mol ⁻¹]										RMSE As Solvent [kJ·mol ⁻¹]									
	GROMOS-2016H66	GROMOS-54A7	GROMOS-ATB	CHARMM-CGenFF	OPLS-AA	OPLS-LBCC	AMBER-GAFF	AMBER-GAFF2	OpenFF	GROMOS-2016H66	GROMOS-54A7	GROMOS-ATB	CHARMM-CGenFF	OPLS-AA	OPLS-LBCC	AMBER-GAFF	AMBER-GAFF2	OpenFF		
DAMD	4.7	-	13.6	11.5	5.1	8.7	6.1	5.9	9.7	2.9	-	5.1	3.5	3.8	4.3	3.5	3.5	3.0		
PPN	2.5	2.2	2.7	2.7	1.8	2.8	1.9	1.7	2.9	2.6	3.1	3.6	3.2	1.6	2.5	2.6	2.1	1.9		
BTN	2.1	1.9	1.7	2.8	1.4	2.1	1.4	1.6	2.9	2.7	3.3	3.9	1.9	2.9	3.6	2.7	2.5			
PYR	2.5	-	2.5	2.6	3.3	3.4	3.7	4.2	3.0	2.2	-	4.6	4.1	3.2	4.4	2.7	3.5	3.1		
H2O	4.8	4.3	5.5	5.5	4.4	3.8	4.9	5.0	3.8	2.7	5.6	6.0	6.4	4.6	3.2	5.5	5.4	5.2		
EAE	2.5	8.7	4.8	2.0	3.6	3.9	5.1	3.5	6.0	2.9	4.6	3.7	2.7	3.0	2.3	4.6	3.3	2.4		
PTL	3.3	4.5	2.8	2.3	2.2	2.7	3.8	2.9	3.2	2.6	4.2	2.3	3.7	2.2	3.3	2.8	2.7	4.4		
MTL	2.6	4.7	4.6	2.3	3.4	2.7	2.7	4.2	3.8	2.4	4.2	4.9	5.2	2.9	4.0	4.1	3.3	5.0		
ETL	2.7	3.8	3.9	2.8	3.0	2.6	2.7	3.8	3.0	2.5	3.9	4.7	4.3	2.4	3.4	3.9	3.2	4.8		
BTL	3.0	4.5	2.3	1.9	2.7	3.0	3.7	2.5	2.6	2.6	4.3	4.8	4.5	2.3	3.4	3.5	3.1	4.7		
2M2P	2.9	2.7	7.0	1.6	1.4	1.5	3.8	2.6	2.1	2.5	2.8	6.0	4.3	3.2	3.2	4.4	3.2	4.0		
IPL	2.8	4.2	4.0	1.9	2.8	3.0	3.6	2.7	3.0	4.1	4.8	4.2	4.2	2.3	3.2	3.5	3.1	4.7		
2PL	1.9	3.2	4.9	1.9	1.9	1.6	3.8	2.6	2.3	2.2	4.0	5.4	3.8	2.3	3.1	3.5	2.7	4.4		
ANLN	3.9	6.0	4.3	2.7	5.5	4.4	3.7	4.3	3.5	5.6	6.5	6.2	5.9	4.2	3.7	5.9	4.6	4.6		
DEE	1.2	3.1	2.0	2.0	2.6	2.0	3.1	2.9	1.8	4.3	4.2	5.0	4.3	3.9	5.0	4.0	4.2	4.1		
DEAN	2.7	3.3	4.3	8.4	2.6	2.2	3.9	3.8	3.0	3.3	5.1	5.4	4.2	2.3	3.5	3.7	3.7	3.3		
TEAN	4.2	4.9	6.6	5.7	3.0	2.8	5.9	5.2	4.2	3.0	4.0	5.9	3.0	4.2	3.3	4.9	5.9	2.3		
TOL	0.7	0.6	1.2	0.9	0.7	1.3	3.1	1.1	2.0	2.4	2.8	4.2	2.4	2.4	2.7	2.0	2.2	2.2		
BZN	2.2	2.3	2.0	2.3	2.4	2.2	3.4	2.5	3.4	2.5	3.1	4.3	2.4	2.5	2.4	2.4	2.3	2.2		
HPE	2.6	2.7	3.1	1.3	1.6	2.6	1.1	3.1	1.2	2.2	2.4	3.4	2.1	2.5	1.8	2.0	2.6	2.1		
HXE	2.2	2.3	2.7	1.2	1.4	2.5	1.1	2.3	0.8	2.7	2.8	3.5	2.3	2.8	2.4	2.5	2.9	2.5		
CRE	2.3	2.4	1.5	1.3	1.5	2.2	0.9	2.5	1.1	2.3	2.8	3.2	2.0	2.3	1.9	2.2	2.7	2.3		

	AVEE As Solute [kJ·mol ⁻¹]										AVEE As Solvent [kJ·mol ⁻¹]									
	GROMOS-2016H66	GROMOS-54A7	GROMOS-ATB	CHARMM-CGenFF	OPLS-AA	OPLS-LBCC	AMBER-GAFF	AMBER-GAFF2	OpenFF	GROMOS-2016H66	GROMOS-54A7	GROMOS-ATB	CHARMM-CGenFF	OPLS-AA	OPLS-LBCC	AMBER-GAFF	AMBER-GAFF2	OpenFF		
DAMD	-4.2	-	-13.2	-10.8	-4.5	-8.2	-5.4	-5.3	-8.3	-1.2	-	-0.6	0.3	1.5	1.4	-1.4	-1.5	-0.8		
PPN	-1.9	-1.1	-2	-0.8	0.7	-2.4	-0.6	-0.6	-1.8	-1.5	-1.9	-1.2	-0.9	0.6	-0.3	-1.3	-1.3	-0.6		
BTN	-1.7	-0.5	-0.7	-0.9	0.3	-1.7	-0.3	-0.9	-1.8	-1.6	-2.1	-1.7	-1.5	0.2	-0.7	-1.6	-1.7	-1.1		
PYR	0.9	-	-0.8	0.6	1.5	-2.2	2.6	3.2	1.1	0.1	-	-0.8	0.5	1.5	1.7	0.7	0.4	0.2		
H2O	1	2.6	3	0.4	2.6	0.6	2.5	2.5	1.9	0.8	1.4	2.2	1.2	3.7	-0.3	2.3	2.1	2.9		
EAE	-2	-8.3	-4.2	0.3	-2.4	-3.5	-4.5	-2.7	-5.4	-1	-2.4	-1.2	-0.6	1.5	0.2	-1.6	-1.6	-0.5		
PTL	-2.6	-3.5	1.9	-0.6	1.6	1.9	-2.6	-1.3	0	-1.7	-2.8	-1.8	-0.4	0.9	0	-0.8	-0.8	-0.7		
MTL	-1	-2.5	4.1	1.1	3	2.2	0.2	3.2	3	-0.7	-2	-0.5	0.2	1.9	0.9	-0.9	0	-1.2		
ETL	-0.5	-2	2.6	0.6	2.5	1.8	0.3	2.8	2.1	-1.4	-2.3	-0.9	-0.3	1.2	0.2	-1.2	-0.9	-0.9		
BTL	-1.8	-3.3	0	-0.2	2.1	2.4	-2.5	-0.9	0.9	-1.7	-3.1	-1.5	-0.8	0.8	-0.3	-1	-1	-1.1		
2M2P	2.3	1.7	-6.2	-0.5	0.4	0.4	-2.8	-1.2	-0.8	-0.4	-1.6	-2.7	0.2	1.5	0.4	-1.2	-0.6	0		
IPL	-1.4	-2.9	3.4	0.1	2.4	2.4	-2.1	-0.1	1.2	-1.4	-2.3	-1.4	-0.6	0.9	-0.2	-0.7	-0.9	-0.9		
2PL	0.5	-1	-4.2	0.4	1.1	0.4	-2.4	-0.2	0.3	-1.3	-2.4	-1.6	-0.5	1	0	-0.8	-0.7	-0.9		
ANLN	1.8	-2.9	3.6	0.1	4.6	2.5	0.9	-2.2	0.6	-1.7	-2.7	-2.1	0.7	-1	0	0.5	-0.4	1.1		
DEE	-0.2	0.7	-1.1	1.5	2.2	1.4	2.2	1.9	0.3	-0.9	0.3	-1.5	-0.4	0.9	0.1	0.8	0.7	0.1		
DEAN	0	-0.7	1	6.9	0.8	0.6	1	1.3	-1	-2.3	-3.4	-0.4	1.8	-0.4	-0.8	-1.6	-1.6	-2		
TEAN	-1.6	-0.6	-3.7	3.5	0.1	0.2	2	0.6	-2	0.5	1.2	1.9	2.6	1.7	1.1	3.4	3.2	-0.6		
TOL	0	-0.2	-0.8	0.3	0	-0.7	3	0.7	1.7	-0.8	-1.7	-0.3	0.2	-0.9	-0.3	-0.6	-0.8	-0.8		
BZN	0.9	0.6	0	1.1	1.2	0.2	2.6	0.9	2.6	-1	-2.2	-2.2	0.3	0.7	-0.6	-0.8	-1.1	-0.6		
HPE	-2.4	-2.5	-2.7	0.2	0.6	2	0.3	-3	-0.5	0.2	-0.3	-0.9	0.7	1	0.8	0.8	0.7	0.5		
HXE	-2	-2.2	-2.3	0.3	0.8	2.1	0.8	-2.2	-0.1	0.7	0.1	-0.5	1	1.3	1.2	1.2	0.9	0.8		
CRE	-2.1	-2.2	1	1	1	1.9	0.2	-2.3	-0.9	0	-0.8	-0.9	0.5	0.7	0.6	0.8	0.6	0.3		

Table S.5: Numerical values pertaining to Fig. S.5. See the corresponding caption.

	RMSE As Solute [kJ·mol ⁻¹]										RMSE As Solvent [kJ·mol ⁻¹]									
	GROMOS-2016H66	GROMOS-54A7	GROMOS-ATB	CHARMM-CGenFF	OPLS-AA	OPLS-LBCC	AMBER-GAFF	AMBER-GAFF2	OpenFF	GROMOS-2016H66	GROMOS-54A7	GROMOS-ATB	CHARMM-CGenFF	OPLS-AA	OPLS-LBCC	AMBER-GAFF	AMBER-GAFF2	OpenFF		
DAMD	4.4	-	13.4	11.3	5.0	8.9	5.9	5.7	9.3	3.0	-	4.8	3.8	3.6	4.2	3.3	3.4	3.0		
PPN	2.4	2.1	2.7	2.8	1.9	3.1	2.0	1.7	2.8	2.6	3.0	3.4	3.3	1.6	3.0	2.5	2.0	1.8		
BTN	2.1	1.9	1.7	2.9	1.4	2.3	1.4	1.6	2.7	2.6	3.1	3.7	4.0	1.8	3.2	2.9	2.6	2.4		
PYRI	4.3	-	3.8	3.7	4.1	4.1	4.8	5.3	4.3	2.9	-	4.3	4.1	3.3	4.6	3.0	3.6	3.2		
HEO	6.2	5.9	6.4	5.6	4.7	6.1	5.6	6.0	5.5	3.3	5.6	5.7	6.5	4.6	3.5	5.4	5.4	5.1		
CSCL2	2.5	-	2.6	4.0	2.2	6.3	2.1	2.2	2.3	3.4	-	3.5	3.7	2.1	3.5	1.9	2.5	2.8		
EAE	2.4	8.4	4.7	2.1	3.4	3.9	5.0	3.4	5.8	2.8	2.8	3.8	3.6	2.7	2.9	2.5	3.7	3.1		
PTL	3.2	4.3	2.7	2.2	2.1	2.7	3.6	2.8	3.0	2.5	4.1	4.6	3.7	2.1	4.0	2.7	2.6	4.2		
MTL	2.9	4.7	4.5	2.3	3.5	2.7	2.8	4.3	3.8	2.7	4.1	4.7	5.3	2.9	4.0	3.9	3.3	4.7		
ETL	2.9	3.8	3.9	2.8	3.1	2.6	2.6	3.8	3.0	2.5	3.8	4.5	4.3	2.3	3.8	3.6	3.1	4.6		
BTL	3.0	4.3	2.3	1.9	2.6	2.9	3.6	2.4	2.5	2.5	4.1	4.6	4.4	2.2	3.8	3.2	2.9	4.5		
2M2P	3.4	6.8	6.7	1.9	1.5	2.0	3.7	2.6	2.1	4.6	4.9	6.7	5.2	4.8	5.0	5.8	5.0	5.6		
1PL	2.8	4.1	3.9	1.9	2.8	3.0	3.4	2.7	2.6	2.8	4.0	4.5	4.2	2.2	3.7	3.3	2.9	4.4		
2PL	2.6	3.3	4.7	2.3	2.0	1.8	3.6	2.6	2.3	2.4	3.9	5.1	3.8	2.3	3.5	3.3	2.7	4.2		
ANLN	4.4	5.9	4.4	2.9	5.5	4.3	3.6	4.1	3.5	6.2	6.3	6.6	6.3	4.9	4.4	6.4	5.6	5.3		
DEE	1.2	3.0	2.1	2.0	2.5	2.0	2.9	2.7	1.8	4.1	4.0	4.9	4.3	3.6	5.2	3.8	3.9	3.9		
CHCL3	3.5	3.5	3.5	-	2.8	5.3	3.1	3.2	2.6	3.8	3.4	4.0	-	2.6	4.4	2.2	2.8	2.5		
DEAN	2.6	3.3	4.1	8.2	2.4	2.2	3.7	3.5	2.8	3.2	4.9	5.2	4.2	2.2	4.0	3.5	3.1	3.1		
TEAN	4.2	4.7	6.5	5.6	3.1	2.8	5.6	5.1	4.2	3.1	4.1	5.7	4.1	3.4	3.2	4.9	5.7	2.5		
TOL	0.7	0.6	1.2	0.9	0.7	1.6	3.1	1.1	2.0	2.3	2.6	4.1	2.4	2.2	3.0	1.9	2.1	2.1		
BZN	2.2	2.3	1.9	2.3	2.3	2.2	3.3	2.4	3.3	3.5	3.1	4.6	2.4	2.5	3.0	3.4	2.3	2.3		
HPE	2.8	2.8	3.0	1.6	1.6	2.7	1.2	3.5	1.5	2.1	2.3	3.3	2.1	2.4	1.9	2.1	2.5	2.1		
HXE	2.3	2.5	2.6	1.4	1.5	2.7	1.2	2.7	1.0	2.6	2.7	3.5	2.3	2.7	2.4	2.4	2.8	2.4		
CCL4	2.7	1.8	3.2	-	2.3	-	2.2	2.4	2.1	3.4	3.2	4.1	-	3.2	-	3.1	3.7	3.1		
CHE	2.5	2.4	1.6	1.4	1.5	2.3	1.0	2.7	1.3	2.2	2.7	3.1	1.9	2.2	1.9	2.2	2.6	2.3		

	AVEE As Solute [kJ·mol ⁻¹]										AVEE As Solvent [kJ·mol ⁻¹]									
	GROMOS-2016H66	GROMOS-54A7	GROMOS-ATB	CHARMM-CGenFF	OPLS-AA	OPLS-LBCC	AMBER-GAFF	AMBER-GAFF2	OpenFF	GROMOS-2016H66	GROMOS-54A7	GROMOS-ATB	CHARMM-CGenFF	OPLS-AA	OPLS-LBCC	AMBER-GAFF	AMBER-GAFF2	OpenFF		
DAMD	-3.7	-	-13.0	-10.5	-4.4	-8.4	-5.2	-5.1	-7.9	-0.6	-	-0.3	0.7	1.6	1.0	-1.1	-1.0	-0.3		
PPN	-1.6	-0.9	-1.9	-0.6	0.8	-2.6	-0.5	-0.5	-1.6	-1.1	-1.1	-0.7	0.6	-0.8	-1.1	-1.0	-0.4	-0.4		
BTN	-1.3	-0.4	-0.6	-0.7	0.4	-1.8	-0.2	-0.9	-1.6	-1.2	-1.8	-1.6	-1.2	0.3	-1.1	-1.4	-0.9	-0.5		
PYRI	1.8	-	-0.1	1.2	2.0	-1.9	3.0	3.7	1.8	0.6	-	-0.7	0.6	1.5	1.1	0.9	0.7	0.5		
HEO	2.4	3.7	3.8	1.4	3.5	1.1	3.3	3.3	3.0	1.4	1.8	2.1	1.5	3.9	-0.6	2.6	2.4	3.1		
CSCL2	1.6	-	1.9	2.9	0.0	-5.5	0.1	1.3	1.1	0.1	-	-1.0	1.6	0.5	-0.8	-0.2	-0.4	-0.3		
EAE	-1.7	-7.9	-4.1	0.5	-2.3	-3.5	-4.3	-2.6	-5.2	-0.7	-2.0	-1.2	-0.4	1.4	-0.2	-1.4	-1.3	-0.3		
PTL	-2.1	-3.1	1.8	-0.5	1.6	1.6	-2.5	-1.2	-0.0	-1.6	-2.7	-1.8	-0.3	0.6	-0.7	-0.9	-0.8	-0.8		
MTL	-0.4	-1.9	4.0	1.2	3.1	1.9	0.3	3.4	3.0	-0.1	-1.6	-0.3	0.5	2.0	0.5	-0.6	0.4	-0.9		
ETL	-0.0	-1.5	2.7	0.6	2.5	1.5	0.4	2.9	2.1	-0.9	-1.9	-0.8	-0.1	1.2	-0.3	-1.0	-0.6	-0.8		
BTL	-1.3	-2.8	0.2	-0.1	2.1	2.1	-2.3	-0.7	0.9	-1.3	-2.7	-1.4	-0.7	0.6	-0.9	-0.9	-0.8	-1.0		
2M2P	2.7	1.9	-5.8	-0.2	0.4	0.2	-2.6	-1.0	-0.7	0.7	-0.1	-1.6	0.8	2.1	0.4	-0.0	0.4	0.9		
1PL	-0.9	-2.4	3.3	0.1	2.3	2.0	-1.9	0.0	1.2	-1.0	-2.0	-1.3	-0.5	0.8	-0.9	-0.6	-0.6	-0.8		
2PL	1.1	-0.6	-3.9	0.6	1.2	0.3	-2.1	0.1	0.4	-0.8	-1.9	-1.4	-0.3	1.0	-0.3	-0.3	-0.3	-0.6		
ANLN	2.4	-2.2	3.8	0.3	4.7	2.3	1.1	-1.9	1.0	-0.5	-2.3	-1.5	0.6	-0.1	1.2	0.7	1.7	1.7		
DEE	-0.2	0.5	-1.2	1.4	2.0	1.2	1.9	1.6	0.1	-0.7	0.3	-1.6	-0.3	0.7	-0.4	0.7	0.6	0.0		
CHCL3	1.7	1.4	-2.2	-	0.9	-4.6	1.6	1.7	1.0	2.1	1.2	-1.0	-	1.1	-3.3	-0.6	-0.8	-0.3		
DEAN	0.1	-0.4	0.9	6.8	0.4	0.9	0.9	1.1	-1.0	-1.8	-3.0	-0.4	1.8	-0.4	-1.4	-1.3	-1.3	-1.9		
TEAN	-1.9	-0.8	-3.9	3.3	-0.3	-0.0	1.6	0.2	-2.3	0.5	1.4	1.6	2.4	1.4	0.6	3.2	3.0	0.6		
TOL	0.0	-0.1	-0.8	0.3	0.0	-0.9	2.9	0.5	1.7	-0.7	-1.5	-1.8	0.4	0.2	-1.3	-0.3	-0.6	-0.7		
BZN	1.0	0.7	-0.0	1.0	1.1	0.0	2.5	0.7	2.5	-1.1	-2.3	-2.5	0.4	-1.1	-1.0	-1.3	-0.8	-0.8		
HPE	-2.6	-2.6	-2.6	-0.0	0.4	2.1	0.1	-3.3	-0.8	0.2	-0.2	-0.9	0.8	0.9	0.8	0.9	0.7	0.5		
HXE	-2.2	-2.3	-2.3	0.1	0.6	2.2	0.6	-2.5	-0.3	0.5	-0.1	-0.7	0.9	1.0	1.0	1.0	0.7	0.6		
CCL4	1.3	0.7	-2.6	-	0.4	-	0.6	0.8	-0.2	1.8	0.9	0.4	-	1.1	-	1.3	1.0	0.9		
CHE	-2.3	-2.3	-2.3	0.9	0.8	2.0	0.0	-2.5	-1.0	-0.1	-0.8	-0.9	0.5	0.6	0.6	0.7	0.6	0.2		

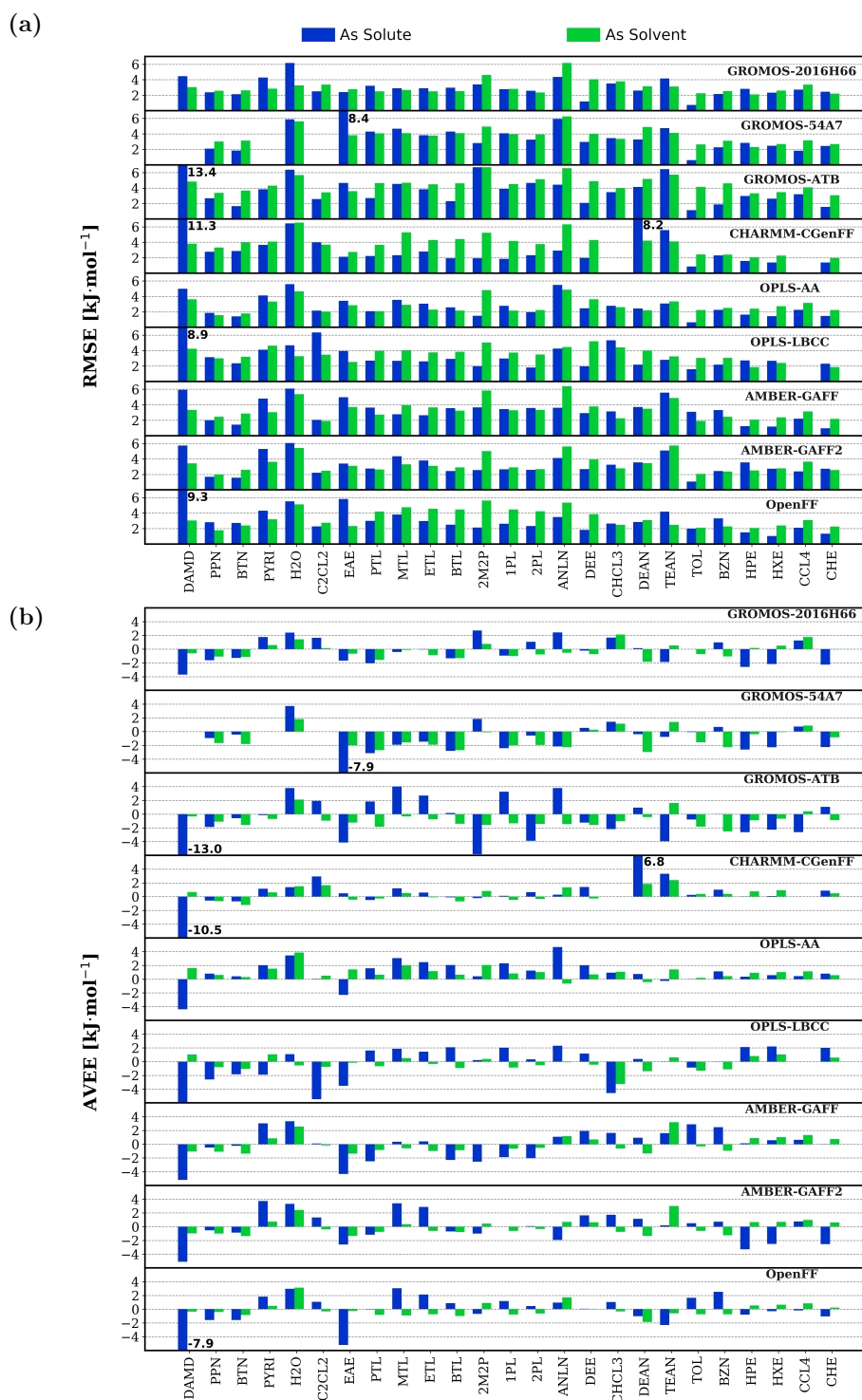


Figure S.5: Deviations between experimental and calculated cross-solvation free energies for the nine force fields, considering the FULL set and individual compounds as solute or solvent. The quantities displayed are (a) the root-mean-square error (RMSE) and (b) the average error (AVEE). Each molecule is considered as solute (blue bars) or as solvent (green bars). The molecules considered and their acronyms are shown in Main Article Fig. 1. They are listed in order of decreasing polarity, as estimated by the molecular dipole moment μ . The numerical values can be found in Tab. S.5. A corresponding comparison considering the COMP set is shown in Main Article Fig. 4, with numerical values in Tab. S.4.

S.3 Single-value and two-solvent models

To provide a baseline in assessing the relative accuracies of the nine force fields, two very simple models have also been considered for estimating the entire set of 625 experimental cross-solvation free energies based on a highly reduced number of experimental parameters. These have been termed the single-value and the two-solvent model. The statistical parameters characterizing the correlation between experimental and calculated cross-solvation free energies for these two models are also reported along the values for the nine force fields in Main Article Tab. 2. The goal of this section is to provide more detailed information concerning these two models and the corresponding results.

The single-value model assumes that all cross-solvation free energies are identical and equal to $-18.4 \text{ kJ}\cdot\text{mol}^{-1}$, which is the average of the 625 entries of the matrix (-18.4 and $-17.8 \text{ kJ}\cdot\text{mol}^{-1}$ for the COMP and CONF sets, respectively)

Clearly, one would expect any decent physics-based model to outperform such a crude model relying on a unique $\Delta_s G_{A:B}^\ominus$ value. The deviations between experimental and calculated cross-solvation free energies for this single-value model are shown in Fig. S.6a.

The two-solvent model relies on the assumption that the solvation free energies measured in two solvents only, one polar and one non-polar, should encompass most of the information contained in the 625 entries of the cross-solvation matrix. The idea here is to test the validity of this assumption, commonly made in force-field refinement³². Given the choice of these two solvents, labelled 1 and 2, the rest of the matrix is fitted against an equation of the form

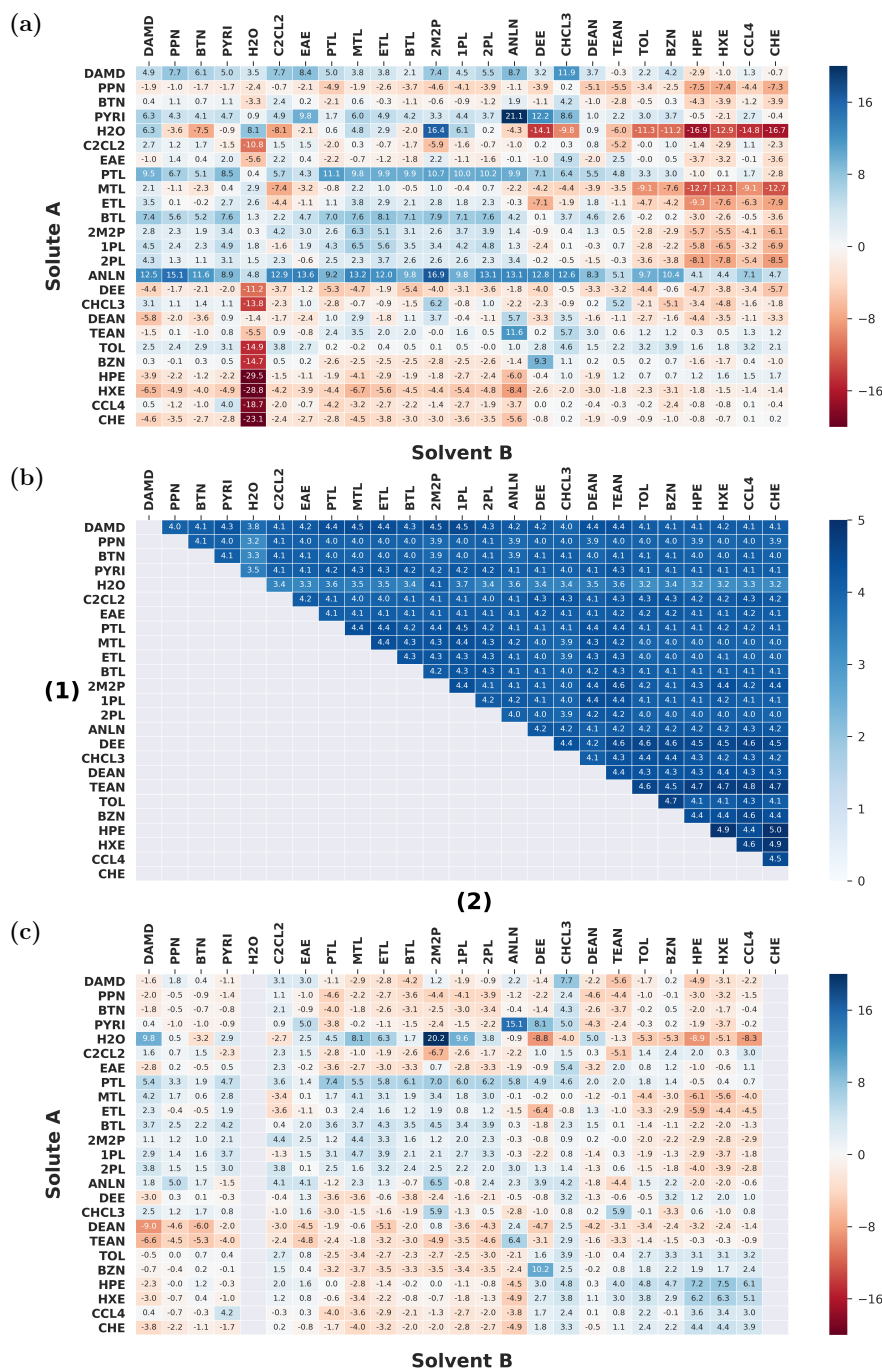
$$\Delta_s G_{A:B}^\ominus = \alpha_0 + \alpha_{A:1} \cdot \Delta_s G_{A:1}^\ominus + \alpha_{A:2} \cdot \Delta_s G_{A:2}^\ominus + \alpha_{B:1} \cdot \Delta_s G_{B:1}^\ominus + \alpha_{B:2} \cdot \Delta_s G_{B:2}^\ominus, \quad (\text{S.1})$$

which involves five empirical coefficients α . The RMSE of this fit is shown in Fig. S.6b considering all possible pairs of solvents 1 and 2. Both the fitting and the RSME calculation are performed considering the FULL set excluding the two columns corresponding to 1 or 2 as solvent. To achieve a good correlation, it is necessary to select water as one of the

two solvents, while the second solvent should preferentially be among the least polar ones. Accordingly, the solvent pair H2O and CHE has been selected as a choice commonly used in force-field refinement³². The corresponding equation reads (with units of $\text{kJ}\cdot\text{mol}^{-1}$)

$$\Delta_s G_{A:B}^{\ominus} = -2.71 + 0.29 \cdot \Delta_s G_{A:H_2O}^{\ominus} + 0.74 \cdot \Delta_s G_{A:CHE}^{\ominus} + 0.12 \cdot \Delta_s G_{B:H_2O}^{\ominus} - 0.01 \cdot \Delta_s G_{B:CHE}^{\ominus}. \quad (\text{S.2})$$

Thus, $\Delta_s G_{A:B}^{\ominus}$ depends mainly on the solvation free energy of A in CHE (0.74), less pronouncedly on the solvation free energy of A in H2O (0.29), and marginally on the solvation free energy of B in H2O (0.12), while it is essentially independent of the solvation free energy of B in CHE (-0.01). The deviations between experimental and calculated cross-solvation free energies for this H2O+CHE two-solvent model are shown in Fig. S.6c.



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