Table T1: Experimental and Calculated absolute Solvation free energies in kcal/mol units.

	Experimental	RESP/GAFF	CHelpG/GAFF	AM1/GAFF	RESP/MSI	CHelpG/MSI	AM1/MSI
1,4-dimethylpiperazine	-7.58	-2.50	-2.49	-7.50	-2.87	-2.00	-9.18
Butylamine,	-4.29	-4.34	-3.45	-2.87	-7.39	-6.60	-4.88
1-methylpiperazine	-7.77	-5.13	-4.25	-7.98	-5.96	-5.88	-10.06
1-pentanamine	-4.10	-4.14	-4.05	-3.32	-7.12	-6.15	-4.56
1-Propanamine,	-4.39	-4.55	-4.20	-2.34	-8.24	-7.03	-5.32
azetidine	-5.56	-2.16	-1.89	-3.94	-4.99	-4.80	-6.54
Ethylamine,	-4.50	-3.51	-2.97	-3.04	-6.94	-6.68	-5.68
Methylamine,	-4.56	-3.92	-3.58	-2.59	-6.89	-6.41	-5.35
N,N-diethylethanamine	-4.07	1.77	0.18	-2.24	1.33	0.21	-3.28
N-ethylethanamine	-4.50	-1.56	-1.59	-1.87	-2.51	-2.44	-4.00
N,N-dimethylamine,	-4.56	-1.97	-1.62	-2.37	-3.69	-3.00	-4.46
N-propylpropan-1-amine	-3.66	-1.81	-1.48	-1.41	-3.66	-3.09	-3.27
piperazine	-7.40	-7.09	-6.14	-7.94	-9.83	-9.43	-11.59
Piperidine,	-5.11	-3.88	-2.96	-4.06	-5.48	-4.63	-4.39
Pyrrolidine,	-5.48	-4.08	-3.77	-3.66	-6.12	-4.60	-5.11
Trimethylamine,	-3.42	0.56	0.86	-1.71	1.18	0.68	-3.10
1,2-Ethanediol,	-9.30	-12.89	-12.17	-10.16	-7.85	-6.40	-6.67
1-Butanol,	-4.72	-4.64	-3.38	-3.38	-2.98	-2.78	-1.96
1-Heptanol,	-4.42	-4.98	-3.70	-0.57	-2.84	-2.24	-1.18
1-Hexanol,	-4.36	-4.79	-4.27	-2.88	-3.15	-2.43	-1.48
1-Octanol,	-4.09	-4.53	-4.27	-2.49	-2.59	-2.22	-1.43
1-Pentanol,	-4.47	-4.52	-4.94	-2.71	-3.79	-2.79	-1.87
1-Propanol,	-4.67	-3.92	-3.94	-2.81	-2.61	-2.65	-2.08
2-methylphenol	-5.87	-5.00	-4.12	-5.61	-3.29	-2.03	-3.05
Isopropyl	-4.76	-4.31	-4.32	-2.88	-2.53	-2.08	-1.42
Phenol 3-methyl	-5.49	-5.46	-5.68	-5.13	-3.75	-2.28	-3.09
Phenol 4-methyl	-6.14	-4.06	-5.19	-5.29	-1.51	-1.80	-2.47
Cyclohexanol,	-5.84	-5.82	-5.64	-3.87	-4.10	-3.42	-2.40
Cyclopentanol,	-5.49	-6.35	-6.57	-4.03	-4.48	-3.77	-2.87
Ethanol,	-5.01	-3.79	-3.71	-2.88	-2.59	-2.44	-1.94
Methanol	-5.11	-4.53	-3.88	-2.96	-3.39	-3.02	-2.35
Phenol,	-6.62	-4.50	-4.72	-4.94	-2.34	-2.41	-3.25
Ethanol 1,1-dimethyl,	-4.51	-4.36	-3.97	-3.08	-2.86	-2.67	-1.88
Acetaldehyde,	-3.50	-2.78	-3.31	-3.14	-2.66	-3.08	-3.00
Benzaldehyde,	-4.02	-3.50	-4.26	-4.44	-2.67	-3.07	-3.62
Butanal,	-3.18	-2.83	-3.52	-2.85	-2.49	-2.75	-2.52
Octanal,	-2.29	-2.71	-4.08	-2.25	-2.12	-2.35	-2.02
Pentanal,	-3.44	-3.00	-2.83	-1.94	-2.41	-2.56	-2.22
Propanal,	-3.44	-3.05	-3.27	-3.00	-2.82	-3.22	-2.97
1,3-Butadiene,	0.60	1.51	0.20	1.41	0.70	0.10	-0.75
1-Butene,	1.38	1.89	2.46	2.66	3.24	3.51	3.82
1-Hexene,	1.68	2.23	2.09	2.90	3.25	3.74	4.09
1-Pentene,	1.66	2.33	3.04	2.98	3.47	3.73	4.04
iso-Propene,	1.27	1.96	2.11	2.92	3.04	3.28	3.56
Cyclopentene,	0.56	1.81	1.47	2.19	2.36	2.37	2.20
2-Pentene E	1.34	2.57	2.17	1.99	3.48	3.72	3.68
Ethylene,	1.27	2.03	2.34	2.66	2.89	3.17	3.56
Propene,	1.27	1.95	2.63	2.84	3.00	3.35	3.68
2-Pentene (Z),	1.34	2.41	2.56	2.55	3.23	3.46	3.49
1-Butyne,	-0.16	0.91	1.14	2.06	2.51	2.69	3.65
1-Hexyne,	0.29	0.29	0.90	3.58	2.86	3.18	4.18
1-Pentyne,	0.01	1.24	1.44	1.98	3.12	3.31	4.15
Acetylene,	-0.01	0.60	0.66	2.13	2.22	2.71	3.91
Propyne,	-0.31	0.72	1.58	2.42	2.44	2.76	3.54

Acetamide,	-9.71	-9.15	-8.94	-8.43	-9.46	-7.30	-8.99
N,N-dimethylacetamide	-8.50	-6.53	-7.37	-7.29	-6.58	-7.04	-7.07
N-methylacetamide	-10.00	-7.00	-8.18	-7.07	-7.76	-8.05	-8.68
N-methylformamide	-10.00	-7.37	-7.60	-8.06	-7.12	-7.56	-7.95
Propanamide,	-9.41	-8.10	-7.66	-8.29	-8.25	-6.54	-9.11
1-methyl-1H-pyridin-2-one	-10.00	-8.36	-9.27	-10.23	-7.16	-7.54	-7.67
2,4-dimethylpyridine	-4.86	-2.38	-2.34	-3.55	-1.76	-1.07	-2.18
2,5-dimethylpyridine	-4.72	-2.13	-2.07	-4.42	-1.06	-0.55	-1.66
2,6-dimethylpyridine	-4.60	-2.78	-2.82	-3.93	-1.93	-1.13	-2.79
2-ethylpyrazine	-5.51	-2.43	-3.37	-5.08	-1.10	-0.69	-4.10
2-methylpyrazine	-5.57	-3.12	-2.52	-4.60	-1.45	-0.84	-4.10
2-methylpyridine	-4.63	-2.78	-2.45	-3.80	-1.85	-1.21	-2.39
3-methyl-1H-indole	-5.91	-5.26	-4.31	-6.30	-4.13	-2.79	-5.02
3-methylpyridine	-4.77	-2.68	-2.76	-3.21	-1.93	-1.32	-2.10
4-methyl-1H-imidazole	-10.25	-7.33	-6.60	-6.80	-7.70	-7.04	-7.94
4-methylpyridine	-4.94	-3.25	-2.67	-1.95	-2.01	-1.27	-2.06
aniline	-5.50	-6.74	-6.89	-5.94	-7.39	-6.90	-6.35
propylaminoformamidine	-10.92	-16.16	-14.03	-15.01	-13.68	-13.21	-11.67
Pyridine,	-4.70	-2.82	-2.37	-3.16	-1.36	-0.82	-1.72
Naphthalene,1,3-dimethyl	-2.47	-0.81	-1.23	-2.65	-0.60	0.53	-1.90
Naphthalene,2,7-dimethyl	-2.63	-2.00	-0.41	-3.15	-0.53	0.55	-1.89
Acenaphthylene,	-3.15	-2.41	-1.85	-6.00	-0.82	0.55	-3.39
Anthracene,	-4.23	-3.23	-2.15	-3.93	-1.96	-0.39	-3.71
Benzene,	-0.87	-0.54	0.68	-0.83	0.86	2.08	0.92
Biphenyl,	-2.64	-2.55	-0.90	-2.68	-0.85	1.06	-1.30
Ethylbenzene,	-0.80	0.45	0.93	-0.56	0.72	1.64	0.35
Fluorene,	-3.44	-3.12	-1.73	-4.16	-1.50	-0.11	-2.97
Benzene,1,3-dimethyl	-0.84	0.27	0.83	-0.63	1.08	1.89	0.57
Naphthalene,	-2.29	-2.78	-0.55	-2.92	-0.27	1.04	-1.42
Benzene,1,2-dimethyl	-0.90	-0.43	2.11	-0.65	1.30	2.20	0.79
p-Xylene,	-0.81	-0.09	0.86	-1.01	0.85	1.71	0.46
Phenanthrene,	-3.95	-3.51	-2.35	-5.52	-1.97	-0.28	-3.64
Toluene,	-0.89	-0.26	1.38	0.26	0.80	1.87	0.57
2-methoxyethanamine	-6.55	-7.09	-6.17	-6.52	-10.47	-7.54	-10.34
4-methylmorpholine	-6.34	-2.84	-4.31	-5.25	-2.80	-3.14	-6.38
morpholine	-7.17	-5.30	-4.79	-6.34	-6.74	-6.68	-7.39
1-Buten-3-yne,	0.04	0.79	1.22	0.80	3.03	3.63	3.77
Ethanol,2-methoxy-,	-6.77	-9.12	-10.28	-7.09	-8.54	-5.08	-6.21
2-Propen-1-ol,	-5.08	-4.08	-3.94	-3.30	-2.47	-2.12	-1.99
Benzaldehyde,3-hydroxy-,m096	-9.51	-9.63	-8.66	-8.14	-6.88	-7.10	-6.49
Benzaldehyde,4-hydroxy-,m097	-10.48	-8.76	-10.09	-9.32	-7.49	-8.28	-8.53
Pentane,2,2,4-trimethyl	2.85	2.02	3.61	2.59	2.86	2.81	3.08
Butane,2,2-dimethyl	2.59	2.56	2.40	3.44	3.49	3.43	3.65
Pentane,2,4-dimethyl	2.88	2.51	1.25	3.10	3.16	3.14	3.34
Isobutane,	2.32	2.03	2.23	2.80	3.34	3.34	3.48
Pentane,2-methyl	2.52	2.39	3.67	2.65	2.88	2.84	3.03
Butane,2-methyl	2.38	2.68	2.57	2.60	3.31	3.27	3.42
Propane,2,2-dimethyl	2.50	2.50	3.37	2.35	3.22	3.21	3.42

1,4-dibromobenzene	-2.30	0.27	0.86	-0.03	0.90	0.98	0.72
1-bromobutane	-0.41	1.06	2.45	1.33	1.52	1.50	2.24
1-bromopentane	-0.08	0.86	1.61	2.10	1.57	1.62	2.26
1-bromopropane	-0.56	0.96	0.74	1.44	1.04	1.08	1.75
2-bromopropane	-0.48	0.98	1.37	0.75	1.11	1.22	1.54
bromobenzene	-1.46	-0.28	-0.78	-0.27	0.97	1.28	0.90
bromoethane	-0.70	0.97	1.10	1.77	1.34	1.43	1.83
bromoform	-1.98	0.54	-2.34	1.02	0.89	0.46	1.59
bromomethane	-0.82	0.79	0.76	1.38	0.69	0.75	1.45
dibromomethane	-2.11	-0.06	0.19	1.57	0.23	0.26	1.05
Acetic	-6.70	-8.16	-6.44	-8.31	-13.13	-7.37	-12.52
Butanoic	-6.36	-8.06	-7.60	-6.76	-12.10	-6.00	-11.74
Hexanoic	-6.21	-7.89	-7.51	-6.62	-12.89	-6.34	-11.16
Pentanoic	-6.16	-8.32	-7.21	-6.88	-12.21	-6.51	-11.85
propionic	-6.47	-7.51	-6.82	-7.12	-13.76	-6.80	-11.73
1,1,1,2,2,2-hexachloroethane	-1.40	0.25	1.90	0.80	1.10	2.11	1.76
Ethane,1,1,1-trichloro	-0.25	0.91	0.66	0.72	1.66	1.85	1.67
Tetrachloroethylene,	0.05	1.66	1.16	1.27	2.42	2.32	2.38
1,1,2-trichloroethane	-1.95	-1.46	-1.79	-0.80	-0.60	-0.30	0.10
Propane,1-chloro	-0.27	0.67	-0.02	0.77	1.31	1.47	2.00
Propane,2-chloro	-0.25	0.85	-0.04	0.53	0.96	1.08	1.50
Ethyl chlorida	-0.63	0.50	0.54	0.59	1.09	1.18	1.58
Chloroform,	-1.07	0.54	0.08	1.19	1.38	1.34	1.35
Methyl chloride	-0.56	0.30	0.30	1.36	0.61	0.80	1.25
Methylene chloride	-1.36	0.15	0.62	0.09	0.52	0.53	0.81
Carbon tetrachloride	0.10	-0.50	0.56	1.39	1.82	1.94	1.82
3-chloroprop-1-ene	-0.57	-0.02	0.08	1.08	1.00	1.57	1.98
Ethene,chloro	-0.59	1.23	1.22	1.21	2.05	2.37	2.51
Ethene,1,2-dichloro (E)	-0.76	0.99	1.39	0.98	2.03	2.02	2.23
Trichloroethylene,	-0.39	1.31	1.10	1.22	2.58	2.56	2.47
Ethene,1,2-dichloro (Z)	-1.17	0.90	1.10	0.13	1.25	1.44	1.22
1,2-dichlorobenzene	-1.36	-0.38	-0.67	-0.11	0.76	1.15	0.76
1,4-dichlorobenzene	-1.01	0.11	0.25	-0.50	0.66	0.95	0.76
chlorobenzene	-1.12	-0.17	0.19	-0.04	0.90	1.57	0.85
Cyclohexane,1,2-dimethyl-cis	1.58	1.18	1.55	1.25	2.65	2.63	2.80
Cyclohexane,	1.23	1.40	1.38	1.91	2.34	2.28	2.39
Cyclopentane,	1.20	2.24	1.85	1.90	2.48	2.47	2.51
Cyclopropane,	0.75	2.49	2.74	1.10	1.99	2.13	2.29
Cyclohexane,methyl	1.71	1.20	1.96	2.68	2.44	2.44	2.57
diethyldisulfide	-1.43	0.52	0.63	-0.46	3.16	3.31	2.32
Disulfide,dimethyl	-1.54	0.62	0.37	0.23	3.08	3.53	2.79
Acetic,butyl ester	-2.55	-3.08	-2.82	-2.53	-3.18	-3.23	-3.31
Ethyl acetate	-3.10	-2.83	-3.45	-2.27	-6.24	-6.05	-5.08
Acetic,1-methylethyl	-2.65	-3.78	-4.15	-4.78	-3.92	-3.43	-3.75
Acetic,methyl	-3.32	-4.14	-4.54	-4.02	-3.87	-3.77	-3.56
acetic,pentyl	-2.45	-3.62	-3.84	-3.68	-3.61	-3.24	-2.75
n-Propyl acetate	-2.86	-3.52	-4.29	-3.84	-3.49	-3.39	-3.40
Methyl Benzoate	-4.28	-4.69	-5.19	-4.81	-3.83	-3.28	-4.50
butyric,methyl	-2.55	-3.43	-3.85	-2.21	-3.73	-3.43	-3.40
Ethyl Formate	-2.65	-4.05	-4.34	-2.52	-3.91	-3.67	-3.43
Methyl Formate	-2.78	-6.08	-6.71	-5.39	-5.92	-6.05	-4.84
Hexanoic,methyl	-2.49	-3.50	-3.04	-3.20	-3.45	-3.19	-3.18
Octanoic,methyl	-2.04	-3.37	-2.91	-3.18	-3.59	-3.52	-3.21

pentanoic,methyl	-2.57	-3.31	-3.57	-3.07	-3.42	-3.22	-3.11
Propanoic,ethyl	-2.80	-3.27	-4.05	-2.97	-3.76	-3.43	-3.51
propionic,methyl	-2.93	-3.86	-4.46	-2.45	-3.65	-3.46	-3.64
Ethane,1,2-dimethoxy	-3.86	-4.56	-4.96	-4.26	-4.27	-2.60	-4.51
1,3-Dioxolane,	-4.10	-2.86	-2.80	-2.81	-2.87	-3.59	-3.88
1,4-Dioxane,	-6.69	-3.95	-3.54	-3.93	-4.03	-4.29	-4.02
Methyl propyl ether	-1.59	-0.44	-0.50	-0.79	-0.42	-1.00	-0.71
Propane,2-methoxy-2-methyl	-0.79	-0.21	-0.47	1.21	0.47	-0.36	-0.17
Propane,2-methoxy	-1.31	-0.74	-0.37	-0.72	-0.69	-1.24	-0.33
cis2,5-dimethyltetrahydrofuran	-2.92	-1.45	-1.04	-1.36	-1.73	-1.80	-1.48
Ethoxy ethane	-2.64	0.01	-0.73	-1.43	0.33	-0.77	-0.34
Benzene,methoxy	-3.73	-2.35	-1.73	-1.67	-0.63	-0.23	-1.14
Dimethyl	-2.64	-0.13	-0.73	-0.54	0.00	-0.43	-0.46
Furan,tetrahydro	-3.84	-1.13	-1.72	-0.88	-0.79	-1.79	-1.29
Ethene,tetrafluoro	1.38	2.74	2.42	3.17	2.42	2.53	2.42
Ethane,1,1-difluoro	-0.11	0.66	0.30	0.14	0.38	0.14	0.34
2,2,2-trifluoroethanol	-4.31	-4.53	-4.84	-4.40	-3.11	-3.57	-3.16
Methane,trifluoro	0.81	1.04	1.78	0.53	0.81	0.63	0.03
Methyl fluoride	0.73	0.86	0.49	1.04	0.62	0.38	1.00
Carbon tetrafloride	3.11	2.88	3.24	2.61	1.91	1.87	1.83
1-iodobutane	-0.25	0.22	0.78	0.31	-0.07	-0.36	-0.69
1-iodopentane	-0.12	1.34	2.46	1.35	-0.43	-1.04	-1.04
1-iodopropane	-0.59	0.58	1.54	0.50	-0.54	-0.42	-1.21
2-iodopropane	-0.46	0.83	1.45	0.48	-0.58	-0.79	-1.53
diiodomethane	-2.49	-0.58	1.17	-0.93	-3.29	-2.33	-4.24
iodobenzene	-1.73	-0.63	-9.40	-0.14	-1.19	-9.44	-1.37
iodoethane	-0.72	0.69	0.94	0.23	-1.01	-1.07	-1.98
iodomethane	-0.89	-0.20	1.07	-0.43	-1.19	-0.51	-1.85
1-phenylethanone	-4.58	-4.33	-5.00	-4.58	-3.81	-3.74	-4.39
2-Heptanone,	-3.04	-2.86	-3.79	-3.33	-2.80	-3.12	-2.42
2-hexanone	-3.29	-2.85	-2.45	-2.26	-2.66	-2.93	-2.31
2-Octanone,	-2.88	-2.44	-3.45	-2.73	-3.06	-3.52	-2.80
2-Pentanone,	-3.41	-2.89	-3.66	-2.11	-2.60	-3.24	-2.61
3,3-dimethylbutan-2-one	-2.89	-2.78	-2.59	-2.91	-2.34	-2.76	-2.39
3-Pentanone,	-3.41	-1.92	-2.41	-2.60	-2.36	-2.70	-2.77
4-Heptanone,	-2.93	-2.24	-2.36	-3.31	-1.72	-2.42	-2.43
5-nonanone	-2.67	-2.88	-3.40	-1.93	-2.57	-2.70	-2.14
Acetone,	-3.85	-3.24	-3.88	-3.67	-2.90	-3.37	-2.77
2-Butanone,	-3.64	-2.96	-2.43	-3.16	-2.79	-3.35	-2.91
Cyclopentanone,	-4.68	-4.52	-5.38	-3.84	-4.29	-4.70	-3.30
3-hydroxybenzonitrile	-9.67	-9.41	-8.91	-7.48	-6.80	-5.76	-4.80
Acetonitrile,	-3.89	-2.92	-2.91	-1.72	-2.37	-2.18	-0.82
benzonitrile	-4.10	-3.86	-3.20	-2.76	-2.05	-1.72	-0.74
Butanenitrile,	-3.64	-3.07	-2.46	-1.49	-2.01	-1.76	-0.56
propiononitrile	-3.85	-2.40	-2.86	-1.43	-1.98	-1.89	-0.52
1-methyl-2-nitro-benzene	-3.59	-5.66	-4.68	-4.90	-5.00	-2.93	-3.71
1-nitrobutane	-3.08	-4.45	-3.89	-3.46	-5.30	-4.99	-2.66
1-nitropropane	-3.34	-4.96	-5.03	-3.72	-5.81	-5.26	-3.13
2-nitropropane	-3.14	-4.63	-4.34	-2.23	-5.17	-5.07	-2.92
3-nitrophenol	-9.63	-11.37	-10.26	-8.98	-10.77	-6.82	-7.22
nitrobenzene	-4.12	-4.90	-5.08	-3.18	-2.33	-2.71	-3.53

nitroethane	-3.71	-4.62	-5.62	-4.53	-6.01	-5.99	-3.62
1,1,1,3,3,3-hexafluoropropan-2-ol	-3.77	-5.06	-5.36	-5.90	-3.79	-2.45	-4.50
1,1,1-trifluoropropan-2-ol	-4.16	-5.46	-4.04	-5.11	-3.57	-2.63	-3.78
1,1,2,2-tetrachloroethylene	0.05	1.40	1.90	1.90	2.90	2.80	2.85
1,1,2-trichloro-1,2,2-trifluoro-ethane	1.77	2.04	1.49	2.20	2.03	2.35	1.60
1-bromo-2-chloro-ethane	-1.95	-0.69	0.16	-0.62	0.77	1.26	1.52
1-chloro-2-(2-chloroethylsulfanyl)ethane	-3.92	-5.63	-4.07	-1.73	-3.02	-0.83	-0.42
2,2,2-trifluoroethoxyethylene	-0.12	-0.33	-0.37	-0.87	-0.28	-0.25	-0.63
2-bromo-1,1,1,2-tetrafluoro-ethane	0.52	1.09	0.91	0.73	1.22	1.06	0.14
2-bromo-2-chloro-1,1,1-trifluoro-ethane	-0.13	0.75	0.50	0.49	0.89	0.76	0.92
2-chloro-1,1,1-trifluoro-ethane	0.06	0.71	-0.38	0.14	0.71	0.66	0.60
2-chloro-2-(difluoromethoxy)-1,1,1-trifluoro-ethane	0.11	-0.65	-1.93	-1.34	-1.82	-0.81	-2.15
4-bromophenol	-7.13	-4.77	-4.72	-5.37	-3.12	-2.83	-3.50
bromo-trifluoro-methane	1.79	2.98	2.63	1.89	2.10	2.20	0.94
chloro-difluoro-methane	-0.50	0.88	1.51	0.29	1.33	1.02	0.64
chloro-fluoro-methane	-0.77	0.22	0.15	0.43	0.82	0.17	0.65
1-propylsulfanylpropane	-1.27	-0.60	-0.44	-0.06	0.02	0.93	2.13
Diethyl sulfide	-1.43	0.82	-0.54	0.43	2.03	1.56	1.66
Dimethyl sulfide	-1.54	0.40	0.22	0.93	1.98	2.24	2.14
hydrogen sulfide	-0.70	0.33	0.34	-1.00	0.01	0.37	-2.14
methylsulfanylbenzene	-2.73	-1.55	-0.20	-1.02	0.49	1.38	0.92
1-Propanethiol,	-1.05	-0.26	0.77	-0.82	0.48	1.05	0.90
Benzenethiol	-2.55	-0.76	0.74	-1.69	0.87	1.72	0.16
Ethanethiol,	-1.30	0.27	0.02	0.09	0.49	1.05	0.73
Methanethiol,	-1.24	-0.21	0.12	0.52	-0.11	0.46	0.28
Butane,	2.08	2.47	2.54	3.16	3.18	3.15	3.23
Ethane,	1.83	2.60	2.42	2.58	2.91	2.91	2.92
Heptane,	2.62	3.15	2.47	4.61	3.13	3.08	3.16
Hexane,	2.49	2.78	2.45	1.95	3.27	3.23	3.31
Methane,	2.00	2.60	3.09	2.89	2.45	2.48	2.50
Octane,	2.89	2.78	3.40	3.32	4.00	3.89	4.06
Pentane,	2.33	2.67	1.84	3.04	3.31	3.28	3.36
Propane,	1.96	2.67	3.22	2.05	3.19	3.19	3.24

Figure S1: Figure showing correlation between the electrostatic component of the solvation energy using the PB solvers from CHARMM and Amber ($R^2 > 0.9998$).