MATERIAL SUPLEMENTAR

Solvent selection for chemical reactions: automated computational screening of solvents using the SMD model

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Table 1S. Gas phase contribution to the reaction[a]

process	$\Delta E^{\ddagger}$ [b]	$\Delta G_g^{\ddagger}$ [c]
2-bromoacetophenone + Pyridine → TS	18.70	29.29

a – Units in kcal mol^{-1}, 25 °C, 1 mol L^{-1} standard state. b – Energy obtained at M08-HX/def2-TZVPP level. c – gas phase free energy.

Table 2S. Solvent contribution to the reaction[a]

	Pyridine	2-bromoacetophenone	TS		
	ΔG_{solv} [b]	ΔG_{solv} [b]	ΔG_{solv} [b]	$\Delta\Delta G_{solv}$ [c]	$\Delta G_{sol}^{\ddagger}$ [d]
sulfolane	-2.66	-5.73	-13.40	-5.01	24.28
formamide	-1.85	-2.67	-9.38	-4.86	24.43
dimethyl sulfoxide	-3.73	-7.28	-15.69	-4.68	24.61
1,2-ethanediol	-2.07	-3.49	-10.21	-4.65	24.64
N-methylformamide	-3.79	-6.55	-14.85	-4.51	24.78
N,N-dimethylformamide	-4.57	-8.4	-17.42	-4.45	24.84
N,N-dimethylacetamide	-4.61	-8.54	-17.59	-4.44	24.85
nitromethane	-4.95	-8.1	-17.44	-4.39	24.90
formic acid	-3.02	-3.35	-10.76	-4.39	24.90
nitrobenzene	-5.64	-9.48	-19.47	-4.35	24.94
o-nitrotoluene	-5.42	-9.14	-18.9	-4.34	24.95
benzonitrile	-5.54	-9.4	-19.21	-4.27	25.02
nitroethane	-5.28	-8.75	-18.3	-4.27	25.02
acetonitrile	-5.34	-8.66	-18.24	-4.24	25.05
acetophenone	-5.05	-8.97	-18.25	-4.23	25.06
cyclohexanone	-4.67	-8.4	-17.28	-4.21	25.08
1-nitropropane	-5.49	-9.1	-18.78	-4.19	25.10
2-nitropropane	-5.51	-9.15	-18.85	-4.19	25.10
2-methoxyethanol	-3.53	-6.72	-14.43	-4.18	25.11
propanonitrile	-5.54	-9.15	-18.87	-4.18	25.11
butanonitrile	-5.57	-9.29	-19.01	-4.15	25.14
benzaldehyde	-5.5	-9.53	-19.18	-4.15	25.14
cyclopentanol	-4.02	-7.07	-15.23	-4.14	25.15
cyclopentanone	-4.75	-8.48	-17.35	-4.12	25.17
diiodomethane	-2.9	-5.84	-12.82	-4.08	25.21
acetone	-5.33	-9.06	-18.46	-4.07	25.22
methanol	-4.51	-7.33	-15.9	-4.06	25.23
butanone	-5.37	-9.27	-18.69	-4.05	25.24
pyridine	-5.06	-9.09	-18.2	-4.05	25.24
2,2,2-trifluoroethanol	-4.15	-5.65	-13.85	-4.05	25.24

3-pentanone	-5.32	-9.22	-18.58	-4.04	25.25
propanal	-5.54	-9.41	-18.98	-4.03	25.26
4-methylpyridine	-4.97	-9	-17.98	-4.01	25.28
phenylmethanol	-4.09	-7.34	-15.44	-4.01	25.28
Etanol	-4.67	-7.75	-16.43	-4.01	25.28
2-hexanone	-5.2	-9.1	-18.3	-4.00	25.29
3-methylpyridine	-4.98	-9.02	-18	-4.00	25.29
2-propen-1-ol	-4.46	-7.51	-15.96	-3.99	25.30
2-pentanone	-5.36	-9.32	-18.66	-3.98	25.31
1-propanol	-4.57	-7.65	-16.2	-3.98	25.31
1-butanol	-4.43	-7.46	-15.85	-3.96	25.33
2-propanol	-4.65	-7.91	-16.52	-3.96	25.33
Butanal	-5.32	-9.17	-18.43	-3.94	25.35
2-butanol	-4.51	-7.74	-16.18	-3.93	25.36
4-heptanone	-5.17	-9.1	-18.19	-3.92	25.37
2-methyl-1-propanol	-4.57	-7.67	-16.16	-3.92	25.37
2-heptanone	-5.07	-8.96	-17.95	-3.92	25.37
m-cresol	-3.97	-5.94	-13.83	-3.92	25.37
1-pentanol	-4.37	-7.38	-15.67	-3.92	25.37
4-methyl-2-pentanone	-5.28	-9.23	-18.42	-3.91	25.38
dimethyl disulfide	-5.19	-9	-18.09	-3.90	25.39
2-methylpyridine	-4.88	-8.97	-17.75	-3.90	25.39
2,4-dimethylpyridine	-4.72	-8.83	-17.44	-3.89	25.40
5-nonanone	-5.02	-8.93	-17.83	-3.88	25.41
1-hexanol	-4.25	-7.22	-15.34	-3.87	25.42
1-heptanol	-4.14	-7.07	-15.06	-3.85	25.44
o-dichlorobenzene	-5.89	-9.71	-19.42	-3.82	25.47
pentanal	-5.09	-8.91	-17.82	-3.82	25.47
2-octanone	-4.96	-8.86	-17.63	-3.81	25.48
2-methyl-2-propanol	-4.5	-7.82	-16.13	-3.81	25.48
1,2-dichloroethane	-5.4	-8.74	-17.92	-3.78	25.51
1-octanol	-4.04	-6.93	-14.74	-3.77	25.52
tributyl phosphate	-4	-8.63	-16.38	-3.75	25.54
aniline	-3.96	-7.11	-14.79	-3.72	25.57
methyl benzoate	-4.46	-8.29	-16.47	-3.72	25.57
methyl formate	-5.06	-8.72	-17.5	-3.72	25.57
1-nonanol	-3.89	-6.71	-14.32	-3.72	25.57
2,6-dimethylpyridine	-4.58	-8.71	-16.98	-3.69	25.60
tetrahydrofuran	-4.68	-8.46	-16.82	-3.68	25.61
ethyl formate	-5.14	-8.88	-17.69	-3.67	25.62

benzyl chloride	-4.91	-8.82	-17.38	-3.65	25.64
2-bromopropane	-5.92	-9.74	-19.31	-3.65	25.64
1-decanol	-3.74	-6.5	-13.89	-3.65	25.64
dibromomethane	-5.09	-8.49	-17.23	-3.65	25.64
bromoethane	-5.94	-9.75	-19.32	-3.63	25.66
iodoethane	-5.55	-9.4	-18.58	-3.63	25.66
cis-dichloroethylene	-5.72	-9.16	-18.5	-3.62	25.67
o-cresol	-3.6	-5.54	-12.74	-3.60	25.69
1-bromopropane	-5.72	-9.47	-18.78	-3.59	25.70
iodomethane	-5.42	-9.26	-18.27	-3.59	25.70
1-iodopropane	-5.42	-9.23	-18.23	-3.58	25.71
methyl acetate	-4.73	-8.45	-16.75	-3.57	25.72
1,1,2-trichloroethane	-5.03	-8.3	-16.9	-3.57	25.72
1-bromo-2-methylpropane	-5.75	-9.53	-18.84	-3.56	25.73
sec-butyl chloride	-5.89	-9.65	-19.1	-3.56	25.73
dichloromethane	-5.87	-9.36	-18.79	-3.56	25.73
N-methylaniline	-4.22	-7.7	-15.47	-3.55	25.74
1-chloropropane	-5.94	-9.69	-19.17	-3.54	25.75
acetic acid	-2.93	-4.05	-10.48	-3.50	25.79
1-iodobutane	-5.32	-9.12	-17.92	-3.48	25.81
Ethanethiol	-5.4	-9.25	-18.12	-3.47	25.82
methyl propanoate	-4.67	-8.44	-16.58	-3.47	25.82
1-bromopentane	-5.36	-9.04	-17.86	-3.46	25.83
1-chloropentane	-5.52	-9.19	-18.16	-3.45	25.84
ethyl acetate	-4.71	-8.5	-16.65	-3.44	25.85
1,2-dibromoethane	-4.31	-7.56	-15.29	-3.42	25.87
1-iodopentane	-5.18	-8.93	-17.53	-3.42	25.87
1,1,1-trichloroethane	-5.95	-9.83	-19.2	-3.42	25.87
methyl butanoate	-4.58	-8.37	-16.35	-3.40	25.89
1-chlorohexane	-5.35	-8.98	-17.72	-3.39	25.90
diethyl sulfide	-5.01	-8.89	-17.29	-3.39	25.90
propyl acetate	-4.62	-8.43	-16.43	-3.38	25.91
chlorobenzene	-5.56	-9.44	-18.36	-3.36	25.93
bromobenzene	-5.4	-9.31	-18.06	-3.35	25.94
butyl acetate	-4.45	-8.24	-16	-3.31	25.98
1-bromooctane	-4.99	-8.6	-16.89	-3.30	25.99
pentyl acetate	-4.38	-8.18	-15.82	-3.26	26.03
propylamine	-3.93	-7.36	-14.55	-3.26	26.03
iodobenzene	-5.03	-8.98	-17.27	-3.26	26.03
bromoform	-4.28	-7.39	-14.91	-3.24	26.05

butylamine	-3.75	-7.15	-14.12	-3.22	26.07
fluorobenzene	-5.73	-9.7	-18.64	-3.21	26.08
o-chlorotoluene	-5.21	-9.02	-17.43	-3.20	26.09
anisole	-4.48	-8.31	-15.98	-3.19	26.10
thiophenol	-4.58	-8.13	-15.9	-3.19	26.10
ethylphenyl ether	-4.5	-8.38	-16.04	-3.16	26.13
pentylamine	-3.66	-7.12	-13.91	-3.13	26.16
chloroform	-5.33	-8.68	-17.02	-3.01	26.28
1-iodohexadecane	-4.25	-7.78	-15.02	-2.99	26.30
diethyl ether	-4.77	-8.7	-16.44	-2.97	26.32
1-fluorooctane	-4.87	-8.46	-16.26	-2.93	26.36
diethylamine	-3.64	-7.4	-13.94	-2.90	26.39
propanoic acid	-2.25	-3.14	-8.28	-2.89	26.40
water	-3.33	-3.32	-9.47	-2.82	26.47
diphenyl ether	-5.38	-9.73	-17.92	-2.81	26.48
trichloroethene	-4.78	-8.21	-15.75	-2.76	26.53
dibutyl ether	-3.72	-7.46	-13.9	-2.72	26.57
diisopropyl ether	-4.42	-8.35	-15.48	-2.71	26.58
butanoic acid	-2.05	-2.88	-7.63	-2.70	26.59
Dipropylamine	-3.18	-6.85	-12.68	-2.65	26.64
tetralin	-4.07	-7.86	-14.54	-2.61	26.68
pentanoic acid	-1.84	-2.59	-6.99	-2.56	26.73
hexanoic acid	-1.74	-2.44	-6.7	-2.52	26.77
carbon disulfide	-4.33	-8.26	-15.09	-2.50	26.79
thiophene	-4.41	-8.32	-15.22	-2.49	26.80
1,4-dioxane	-2.27	-5.87	-10.54	-2.40	26.89
o-xylene	-4.22	-8.07	-14.66	-2.37	26.92
Triethylamine	-2.95	-7.07	-12.35	-2.33	26.96
1-hexyne	-4.14	-7.3	-13.75	-2.31	26.98
Ethylbenzene	-4.19	-8.04	-14.52	-2.29	27.00
n-butylbenzene	-4	-7.76	-14.03	-2.27	27.02
1,2,4-trimethylbenzene	-3.99	-7.83	-14.08	-2.26	27.03
xylene (mixture)	-4.15	-8.01	-14.41	-2.25	27.04
isopropylbenzene	-4.12	-7.96	-14.31	-2.23	27.06
cis-decalin	-3.73	-7.13	-13.09	-2.23	27.06
sec-butylbenzene	-4.02	-7.81	-14.06	-2.23	27.06
tert-butylbenzene	-4.05	-7.87	-14.15	-2.23	27.06
m-xylene	-4.13	-7.99	-14.33	-2.21	27.08
decalin (cis/trans mixture)	-3.77	-7.2	-13.17	-2.20	27.09
toluene	-4.32	-8.24	-14.76	-2.20	27.09

trans-decalin	-3.82	-7.27	-13.25	-2.16	27.13
mesitylene	-4	-7.88	-14.04	-2.16	27.13
tetrachloroethene	-4.26	-7.98	-14.39	-2.15	27.14
p-isopropyltoluene	-3.96	-7.82	-13.92	-2.14	27.15
p-xylene	-4.09	-7.96	-14.19	-2.14	27.15
benzene	-4.37	-8.38	-14.84	-2.09	27.20
trans-dichloroethylene	-3.86	-7.11	-12.98	-2.01	27.28
n-hexadecane	-3.74	-7.17	-12.91	-2.00	27.29
carbon tetrachloride	-4.63	-8.49	-15.1	-1.98	27.31
cis-1,2-dimethylcyclohexane	-3.89	-7.4	-13.27	-1.98	27.31
n-pentadecane	-3.76	-7.19	-12.93	-1.98	27.31
cyclohexane	-3.86	-7.35	-13.15	-1.94	27.35
n-dodecane	-3.82	-7.28	-13.03	-1.93	27.36
methylcyclohexane	-3.95	-7.49	-13.36	-1.92	27.37
n-undecane	-3.9	-7.45	-13.24	-1.89	27.40
n-decane	-3.87	-7.36	-13.11	-1.88	27.41
1-hexene	-4.14	-7.81	-13.82	-1.87	27.42
n-nonane	-3.9	-7.41	-13.15	-1.84	27.45
cyclopentane	-3.94	-7.47	-13.24	-1.83	27.46
E-2-pentene	-4.21	-7.92	-13.95	-1.82	27.47
n-octane	-3.94	-7.47	-13.21	-1.80	27.49
perfluorobenzene	-4.3	-7.94	-14.04	-1.80	27.49
1-pentene	-4.19	-7.91	-13.85	-1.75	27.54
n-heptane	-3.99	-7.54	-13.27	-1.74	27.55
2,2,4-trimethylpentane	-4.11	-7.74	-13.59	-1.74	27.55
2,4-dimethylpentane	-4.09	-7.7	-13.47	-1.68	27.61
n-hexane	-4.04	-7.62	-13.33	-1.67	27.62
2-methylpentane	-4.11	-7.72	-13.49	-1.66	27.63
n-pentane	-4.1	-7.72	-13.41	-1.59	27.70

a – Units in kcal mol^{-1}, 25 ^{o}C, 1 mol L^{-1} standard state. b – Solvation free energy calculated at the SMD/X3LYP/6-31G(d) level of theory. c – variation in the solvation free energy. d – Solution phase activation free energy.