Supporting information

Approach for Predicting the Standard Free Energy Solvation of H^+ and Acidity Constant in Nonaqueous Organic Solvents

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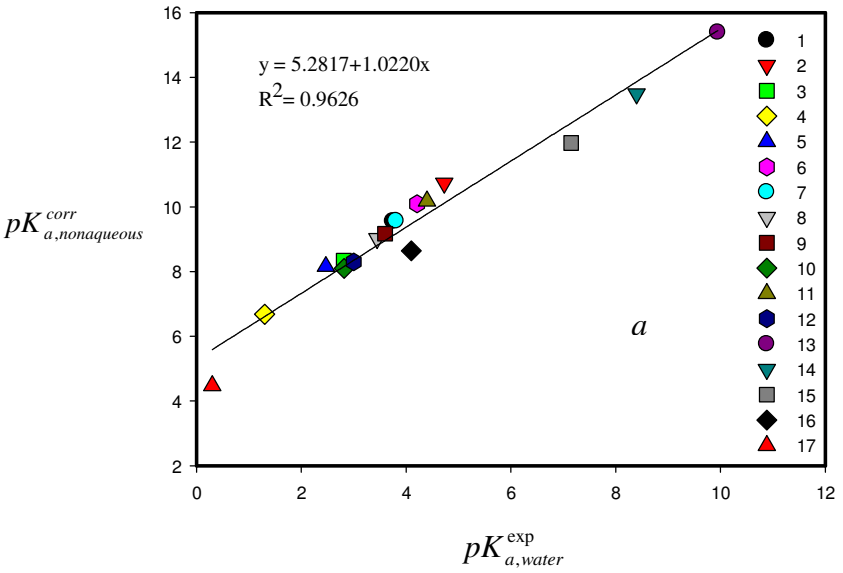
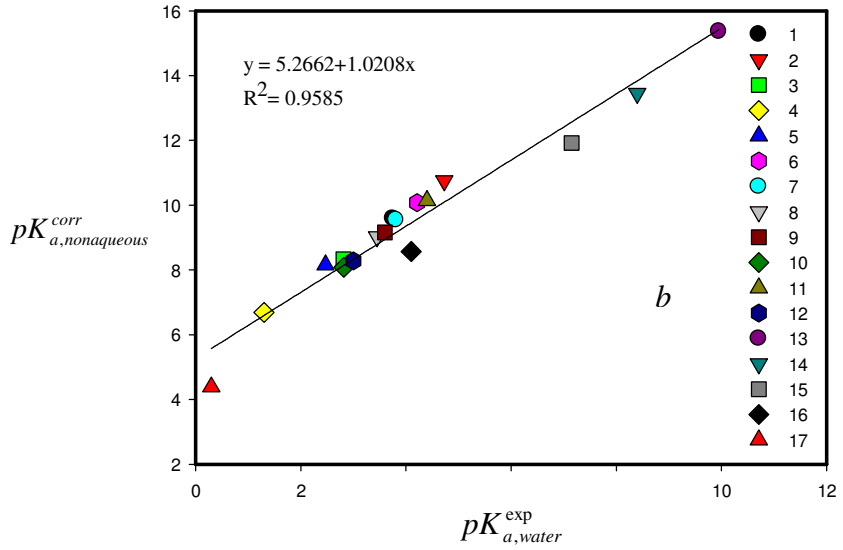
Figure S1. The variation of $pK^{corr}_{a,nonaqueous}$ versus $pK^{exp}_{a,water}$ for the compounds reported in Table 4 in methanol solvent. The numbering of symbols in the figure is the same as the numbering of compounds in Table 4. (*a*) B3LYP (*b*) M062X and (*c*) MP2.





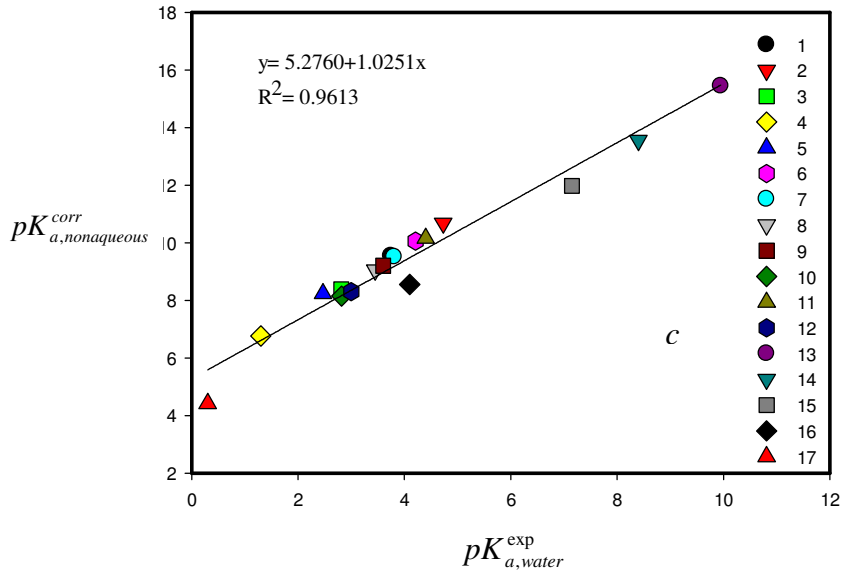
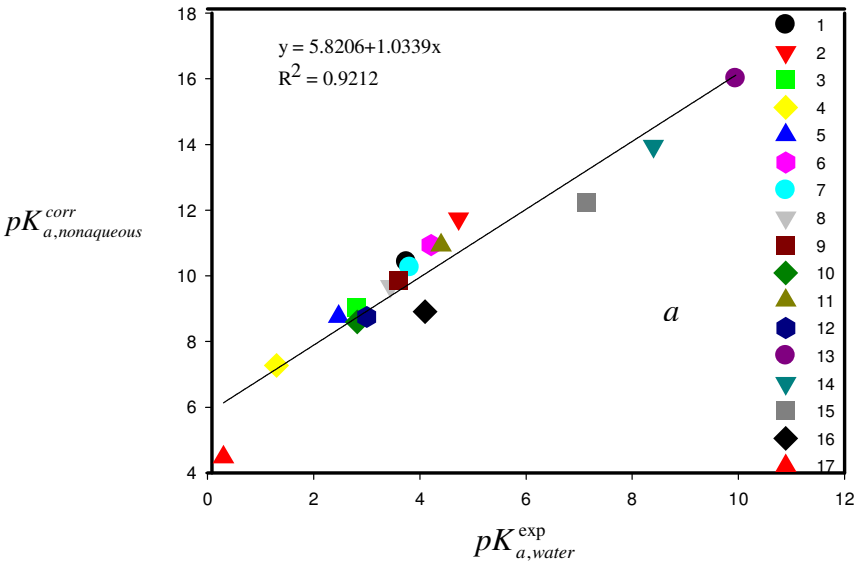
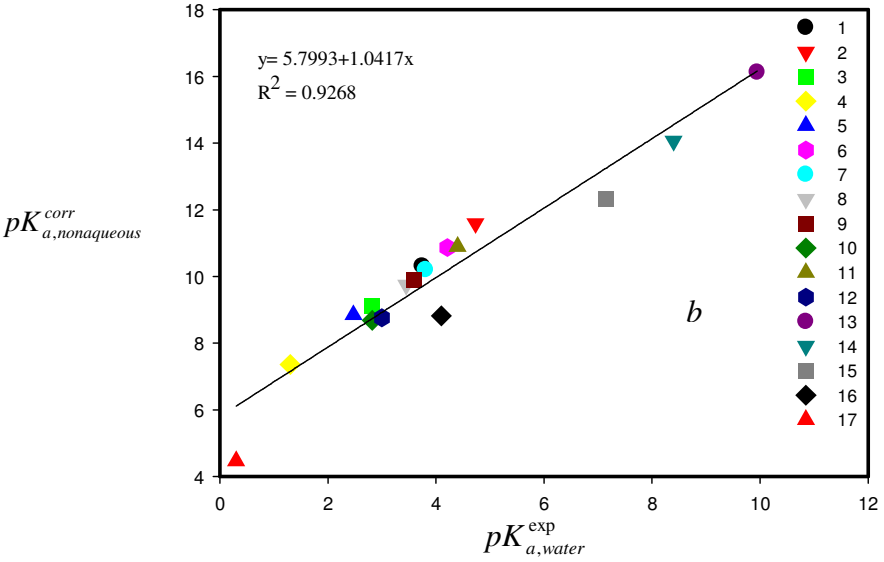


Figure S2. The variation of $pK_{a,nonaqueous}^{corr}$ versus $pK_{a,water}^{exp}$ for the compounds reported in Table 4 in 2-propanol solvent. The numbering of symbols in the figure is the same as the numbering of compounds in Table 4. (*a*) B3LYP (*b*) M062X and (*c*) MP2.





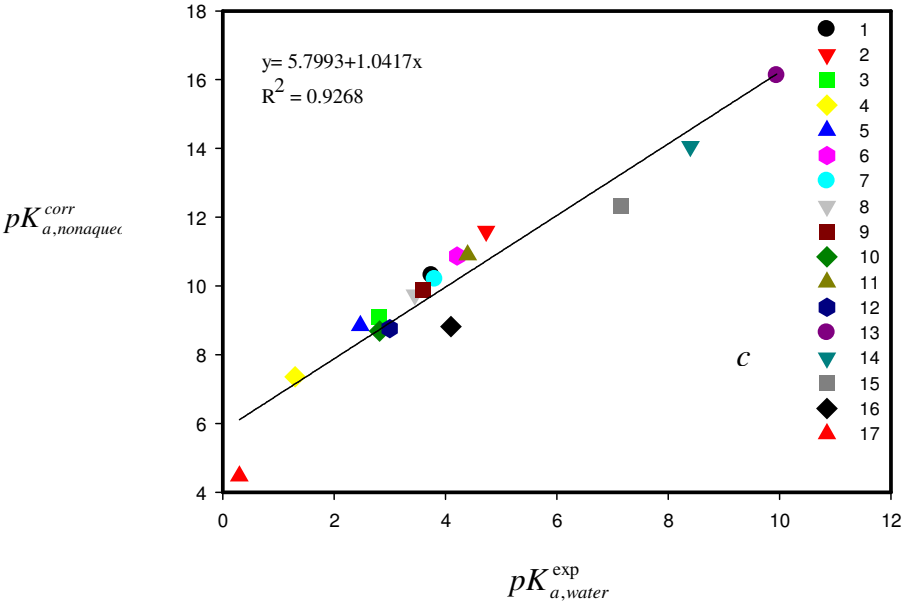
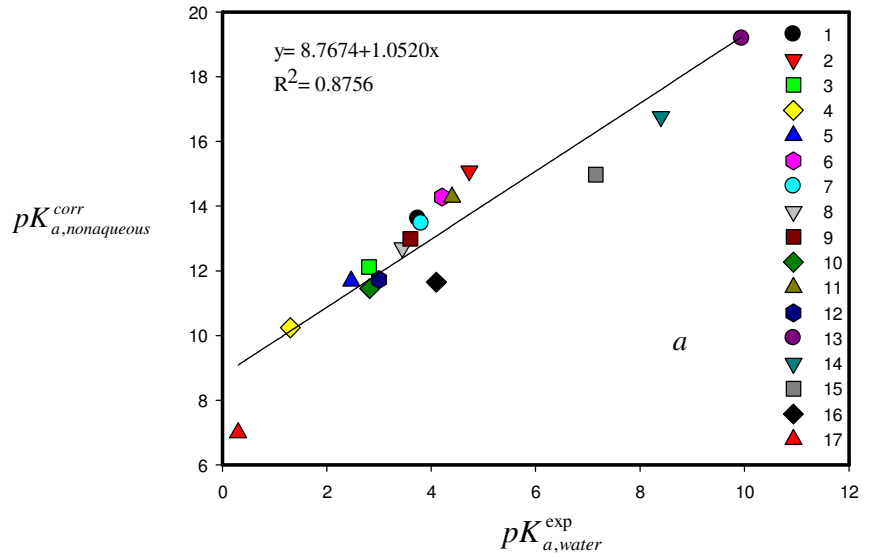
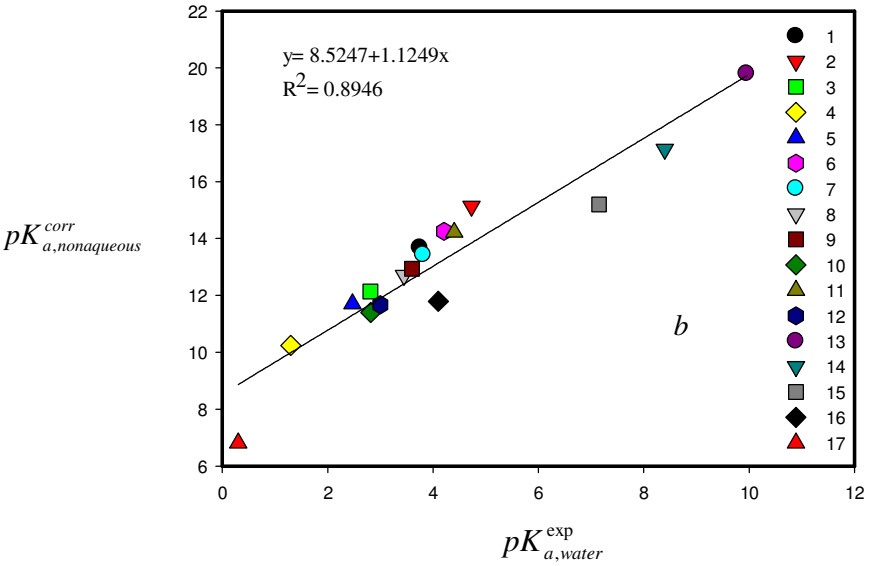


Figure S3. The variation of $pK_{a,nonaqueous}^{corr}$ versus $pK_{a,water}^{exp}$ for the compounds reported in Table 4 in 2-methyl-2-propanol solvent. The numbering of symbols in the figure is the same as the numbering of compounds in Table 4. (*a*) B3LYP (*b*) M062X and (*c*) MP2.





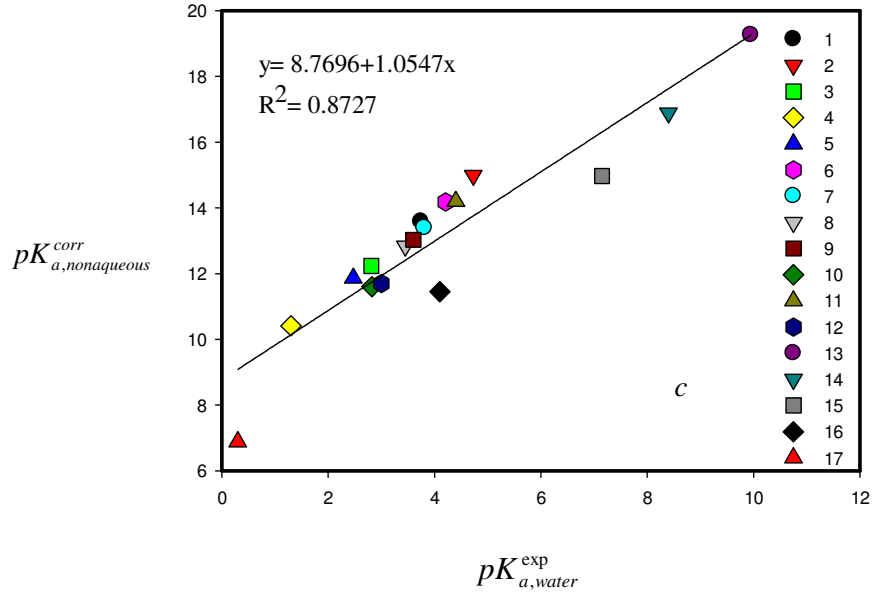


Figure S4. The variation of $pK_{a,nonaqueous}^{corr}$ versus $pK_{a,water}^{exp}$ for the compounds reported in Table 4 in ACN solvent. The numbering of symbols in the figure is the same as the numbering of compounds in Table 4. (*a*) B3LYP (*b*) M062X and (*c*) MP2.

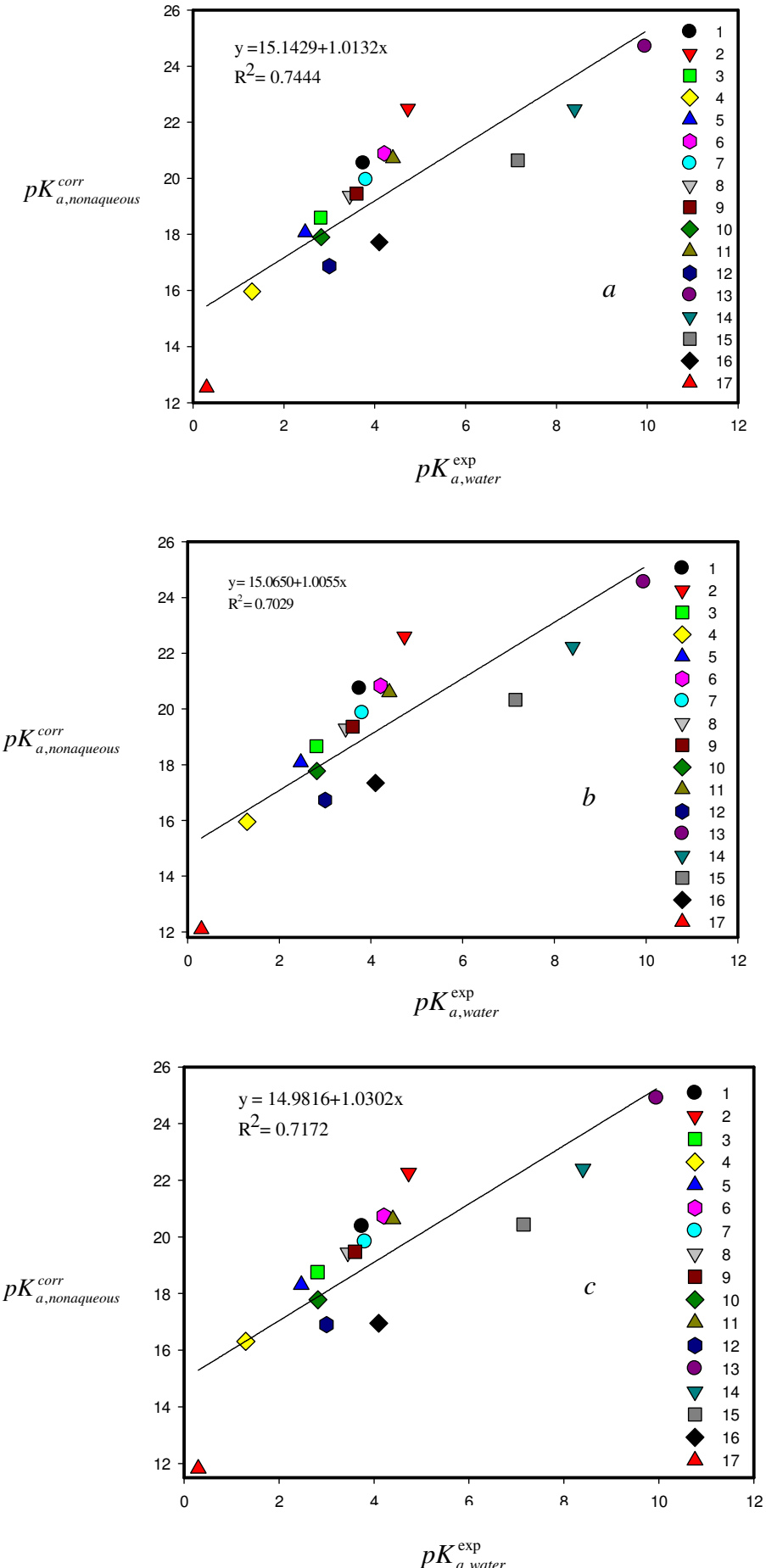
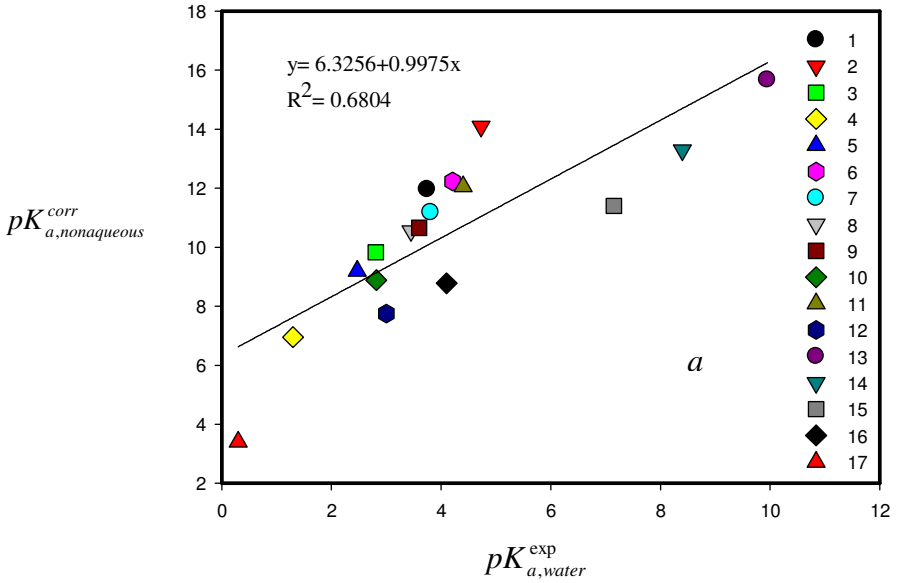
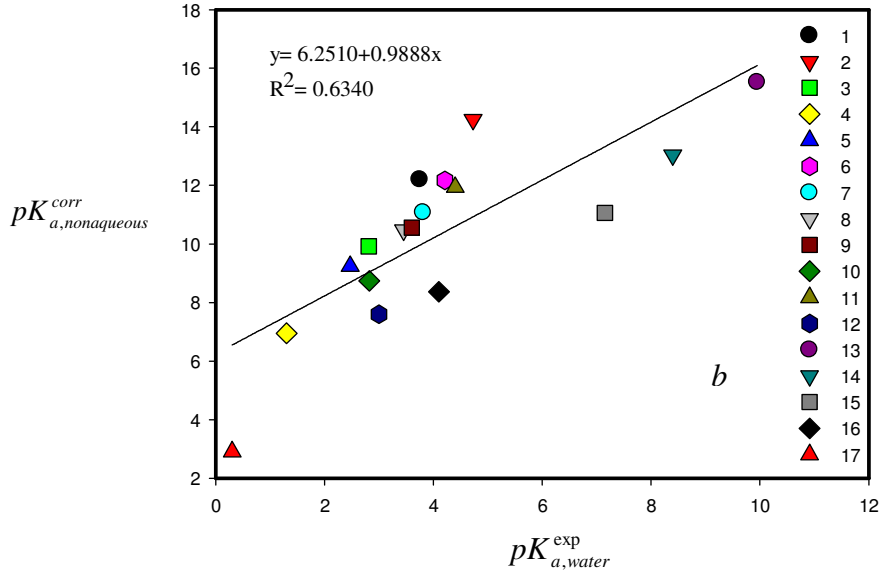


Figure S5. The variation of $pK_{a,nonaqueous}^{corr}$ versus $pK_{a,water}^{exp}$ for the compounds reported in Table 4 in DMF solvent. The numbering of symbols in the figure is the same as the numbering of compounds in Table 4. (*a*) B3LYP (*b*) M062X and (*c*) MP2.





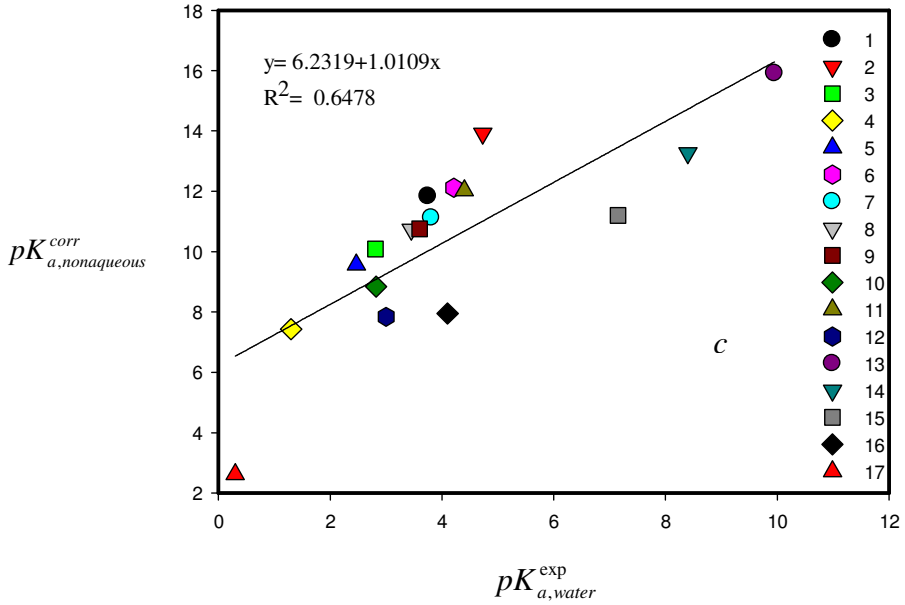
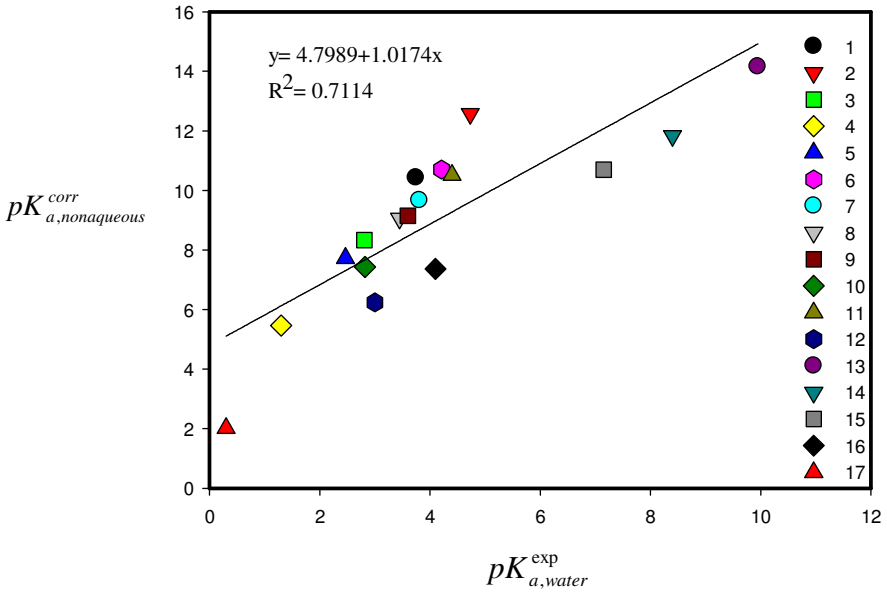
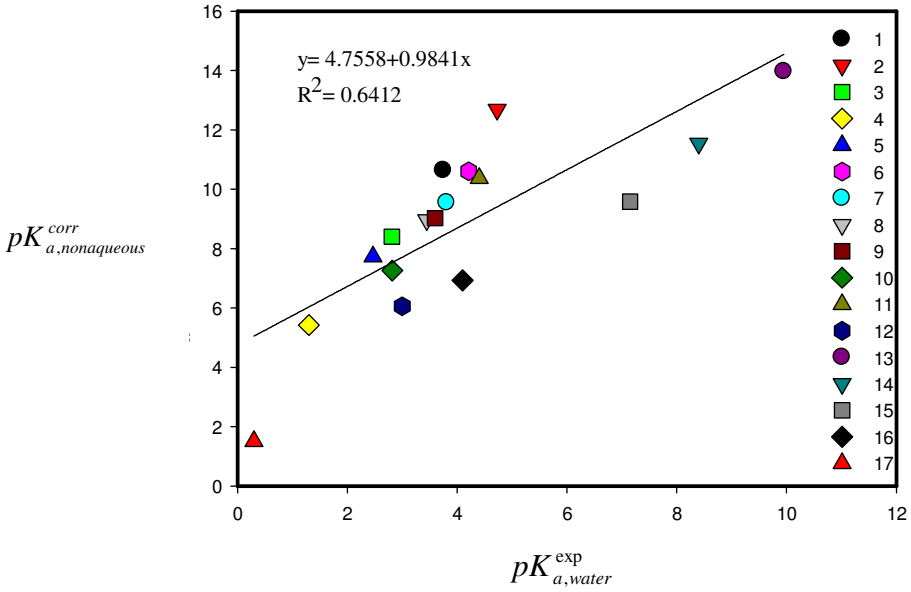


Figure S6. The variation of $pK_{a,nonaqueous}^{corr}$ versus $pK_{a,water}^{exp}$ for the compounds reported in Table 4 in DMSO solvent. The numbering of symbols in the figure is the same as the numbering of compounds in Table 4. (*a*) B3LYP (*b*) M062X and (*c*) MP2.





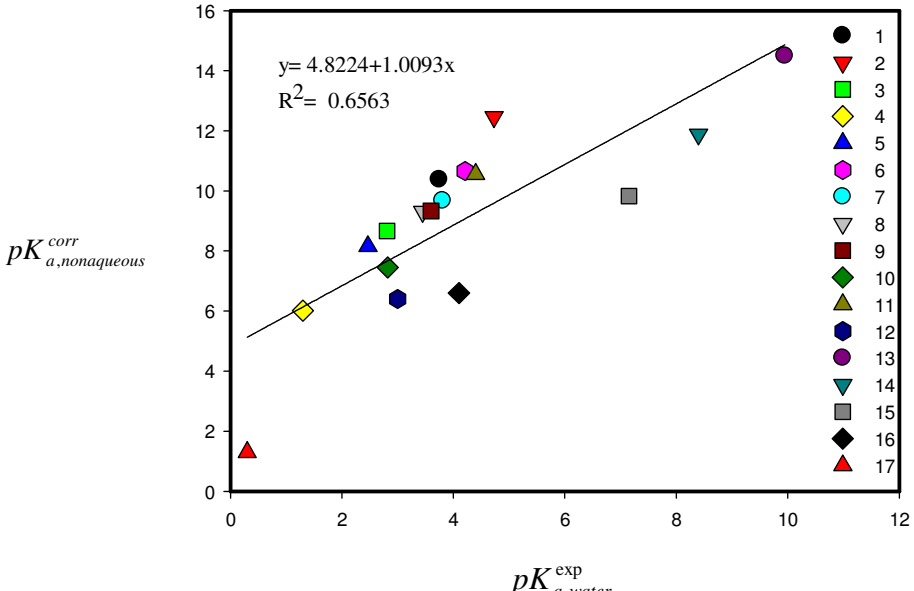


Table S1. The values of ΔG_g , $\Delta G_{sol}^{A^-}$, ΔG_{sol}^{AH} of selected compounds calculated at different levels of theory, the value of $\Delta G_{sol}^{H^+}$ obtained from eq. 3 using the $pK_a^{\exp}$ of compounds in ethanol (column 6) and; the calculated values of $\Delta G_{sol}^{H^+}$ in ethanol (last column), corrected using the computational error in water solvent reported in the last column of Table 1. The values of $\Delta G_{sol}^{A^-}$ and ΔG_{sol}^{AH} have been calculated in ethanol solvent.

compound	ΔG_g (kcal.mol^{-1})	$\Delta G_{sol}^{A^-}$	ΔG_{sol}^{AH}	$pK_a^{\exp}$	$(\Delta G_{sol}^{H^+})^e$	$(\Delta G_{sol}^{H^+})^f$
acetic acid	338.11[a]	-68.50	-7.41	10.3	-264.95	-262.41
	339.88[b]	-69.86	-7.62		-265.48	-262.64
	340.80[c]	-64.10	-4.91		-269.45	-261.75
	344.50[d]	-65.90	-5.35		-271.78	-262.15
chloroacetic acid	324.26	-63.19	-10.50	8.3	-262.14	-261.88
	325.96	-64.47	-10.68		-262.74	-262.07
	328.66	-59.29	-7.27		-267.20	-261.36
	333.14	-61.16	-7.70		-270.25	-261.74
dichloroacetic acid	315.72	-59.54	-10.11	7.3	-258.26	-260.99
	317.26	-60.59	-10.27		-258.88	-261.20
	320.83	-56.55	-7.59		-263.80	-260.51
	325.30	-58.42	-7.89		-266.70	-260.88
benzoic acid	330.97	-64.94	-9.03	10.1	-263.18	-261.83
	330.84	-66.47	-9.50		-261.99	-262.01
	332.61	-59.88	-6.39		-267.23	-261.18
formic acid *	340.67*	-64.29	-4.01	10.1	-268.51	-261.45
3-boromobenzoic acid	325.18	-61.71	-10.14	9.4	-262.68	-262.06
	325.18	-62.97	-10.47		-261.75	-262.23
	327.27	-57.45	-7.53		-266.42	-261.39
Cyanoacetic acid*	326.74*	-58.28	-8.67	9.4	-266.21	-261.47

[a]B3LYP/6-311++G(d,p); [b]M062X/6-311++G(d,p); [c]MP2/6-311++G(d,p); [d] CCSD/6-311++G(d,p)

[e] Calculated using eq. (3).

[f] The corrected calculated value of $\Delta G_{sol}^{H^+}$ obtained using the computational error in water reported in the last column of Table 1.

Table S2. The values of ΔG_g , $\Delta G_{sol}^{A^-}$, ΔG_{sol}^{AH} of selected compounds calculated at different levels of theory, the value of $\Delta G_{sol}^{H^+}$ obtained from eq. 3 using the $pK_a^{\exp}$ of compounds in 2-propanol (column 6) and; the calculated values of $\Delta G_{sol}^{H^+}$ in 2-propanol (last column), corrected using the computational error in water solvent reported in the last column of Table 1. The values of $\Delta G_{sol}^{A^-}$ and ΔG_{sol}^{AH} have been calculated in 2-propanol solvent.

compound	ΔG_g (kcal.mol^{-1})	$\Delta G_{sol}^{A^-}$	ΔG_{sol}^{AH}	$pK_a^{\exp}$	$(\Delta G_{sol}^{H^+})^e$	$(\Delta G_{sol}^{H^+})^f$
acetic acid	338.11[a]	-66.76	-7.47	11.3	-265.39	-262.85
	339.88[b]	-67.96	-7.66		-266.06	-263.22
	340.80[c]	-62.95	-5.21		-269.54	-261.84
	344.49[d]	-64.51	-5.58		-272.04	-262.41
chloroacetic acid	324.26	-61.76	-10.52	9.2	-262.37	-262.11
	325.96	-62.90	-10.68		-263.08	-262.42
	328.65	-58.37	-7.52		-267.14	-261.31
	333.14	-60.01	-7.89		-270.36	-261.86
dichloroacetic acid	315.72	-58.36	-10.21	7.8	-258.82	-261.59
	317.26	-59.30	-10.36		-259.57	-261.90
	320.83	-55.82	-7.88		-264.14	-260.85
	325.30	-57.45	-8.13		-267.23	-261.45
4-nitrobenzoic acid	318.08	-54.93	-10.40	9.6	-262.35	-262.45
	318.43	-55.99	-10.58		-261.82	-262.74
	321.91	-51.09	-5.66		-265.28	-261.63
	-	-	-		-	-
3-boromobenzoic acid	325.18	-60.28	-10.19	10.1	-263.21	-262.58
	325.18	-61.43	-10.50		-262.37	-262.84
	327.27	-56.60	-7.82		-266.61	-261.57
	-	-	-		-	-

[a]B3LYP/6-311++G(d,p); [b]M062X/6-311++G(d,p); [c]MP2/6-311++G(d,p); [d] CCSD/6-311++G(d,p)
[e] Calculated using eq. (3).
[f] The corrected calculated value of $\Delta G_{sol}^{H^+}$ obtained using the computational error in water reported in the last column of Table 1.

Table S3. The values of ΔG_g , $\Delta G_{sol}^{A^-}$, ΔG_{sol}^{AH} of selected compounds calculated at different levels of theory, the value of $\Delta G_{sol}^{H^+}$ obtained from eq. 3 using the $pK_a^{\exp}$ of compounds in 2-methyl-2-propanol (column 6) and; the calculated values of $\Delta G_{sol}^{H^+}$ in 2-methyl-2-propanol (last column), corrected using the computational error in water solvent reported in the last column of Table 1. The values of $\Delta G_{sol}^{A^-}$ and ΔG_{sol}^{AH} have been calculated in 2-methyl-2-propanol solvent.

compound	ΔG_g (kcal.mol^{-1})	$\Delta G_{sol}^{A^-}$	ΔG_{sol}^{AH}	$pK_a^{\exp}$	$(\Delta G_{sol}^{H^+})^e$	$(\Delta G_{sol}^{H^+})^f$
acetic acid	338.11[a]	-64.11	-7.21	14.2	-263.83	-261.29
	339.88[b]	-65.21	-7.37		-264.57	-261.73
	340.80[c]	-60.68	-5.13		-267.77	-260.08
	344.49[d]	-62.08	-5.45		-270.38	-260.76
chloroacetic acid	324.26	-59.42	-10.13	12.2	-260.22	-259.97
	325.96	-60.46	-10.28		-261.03	-260.37
	328.65	-56.37	-7.35		-264.88	-259.05
	333.14	-57.84	-7.68		-268.23	-259.73
dichloroacetic acid	315.72	-56.24	-9.90	10.2	-257.36	-260.12
	317.26	-57.10	-10.04		-258.18	-260.50
	320.83	-53.97	-7.74		-262.58	-259.28
	325.30	-55.45	-7.97		-265.80	-259.97
benzoic acid	330.97	-60.75	-8.78	15.1	-260.30	-258.95
	330.84	-62.07	-9.20		-259.27	-259.29
	332.61	-56.70	-6.59		-263.80	-257.74
	-	-	-		-	-
3-boromobenzoic acid	325.18	-57.94	-9.93	13.5	-260.65	-260.03
	325.18	-59.01	-10.23		-259.88	-260.36
	327.27	-54.61	-7.75		-263.89	-258.86
	-	-	-		-	-

[a]B3LYP/6-311++G(d,p); [b]M062X/6-311++G(d,p); [c]MP2/6-311++G(d,p); [d] CCSD/6-311++G(d,p)

[e] Calculated using eq. (3).

[f] The corrected calculated value of $\Delta G_{sol}^{H^+}$ obtained using the computational error in water reported in the last column of Table 1.

Table S4. The values of ΔG_g , $\Delta G_{sol}^{A^-}$, ΔG_{sol}^{AH} of selected compounds calculated at different levels of theory, the value of $\Delta G_{sol}^{H^+}$ obtained from eq. 3 using the $pK_a^{\exp}$ of compounds in DMSO (column 6) and; the calculated values of $\Delta G_{sol}^{H^+}$ in DMSO (last column), corrected using the computational error in water solvent reported in the last column of Table 1. The values of $\Delta G_{sol}^{A^-}$ and ΔG_{sol}^{AH} have been calculated in DMSO solvent.

compound	ΔG_g (kcal.mol^{-1})	$\Delta G_{sol}^{A^-}$	ΔG_{sol}^{AH}	$pK_a^{\exp}$	$(\Delta G_{sol}^{H^+})^e$	$(\Delta G_{sol}^{H^+})^f$
acetic acid	338.11[a]	-59.20	-6.39	12.3	-270.51	-267.97
	339.88[b]	-59.73	-6.48		-271.75	-268.91
	340.80[c]	-57.91	-5.15		-273.16	-265.46
	344.49[d]	-58.40	-5.29		-276.50	-266.87
formic acid	333.76	-58.78	-5.43	10.3	-268.25	-267.77
	335.29	-59.21	-5.56		-269.49	-268.85
	336.36	-57.97	-4.12		-270.36	-265.36
	340.67	-58.34	-4.33		-274.50	-266.82
3,4-dichlorobenzoic acid	322.36	-51.76	-8.08	9.2	-268.02	-267.53
	322.16	-52.32	-8.27		-267.46	-268.13
	325.53	-50.78	-6.60		-270.69	-265.41
	-	-	-		-	-
benzoic acid	330.97	-56.85	-7.53	11	-268.54	-267.19
	330.84	-57.86	-7.95		-267.82	-267.84
	332.61	-54.81	-6.15		-270.84	-264.78
	-	-	-		-	-
3-boromobenzoic acid	325.18	-54.05	-8.37	9.7	-268.16	-267.54
	325.18	-54.81	-8.66		-267.69	-268.17
	327.27	-52.67	-6.98		-270.24	-265.21
	-	-	-		-	-

[a]B3LYP/6311++G(d,p); [b]M062X/6-311++G(d,p); [c]MP2/6-311++G(d,p); [d] CCSD/6-311++G(d,p)

[e] Calculated using eq. (3).

[f] The corrected calculated value of $\Delta G_{sol}^{H^+}$ obtained using the computational error in water reported in the last column of Table 1.

Table S5. The values of ΔG_g, $\Delta G_{sol}^{A^-}$, ΔG_{sol}^{AH} of selected compounds calculated at different levels of theory, the value of $\Delta G_{sol}^{H^+}$ obtained from eq. 3 using the $pK_a^{\exp}$ of compounds in ACN (column 6) and; the calculated values of $\Delta G_{sol}^{H^+}$ in ACN (last column), corrected using the computational error in water solvent reported in the last column of Table 1. The values of $\Delta G_{sol}^{A^-}$ and ΔG_{sol}^{AH} have been calculated in ACN solvent.

compound	ΔG_g (kcal.mol^{-1})	$\Delta G_{sol}^{A^-}$	ΔG_{sol}^{AH}	$pK_a^{\exp}$	$(\Delta G_{sol}^{H^+})^e$	$(\Delta G_{sol}^{H^+})^f$
acetic acid	338.11[a]	-60.20	-6.42	22.3	-255.90	-253.36
	339.88[b]	-60.82	-6.52		-257.06	-254.22
	340.80[c]	-58.59	-5.02		-258.71	-251.01
	344.49[d]	-59.21	-5.18		-261.94	-252.31
chloroacetic acid	324.26	-56.76	-9.34	18.8	-253.09	-252.84
	325.96	-57.38	-9.45		-254.28	-253.62
	328.65	-55.14	-7.08		-256.84	-251.01
	333.14	-55.87	-7.27		-260.79	-252.29
dichloroacetic acid	315.72	-54.38	-8.88	15.8	-250.56	-253.33
	317.26	-54.92	-9.01		-251.69	-254.02
	320.83	-53.31	-7.19		-255.05	-251.76
	325.30	-54.09	-7.31		-258.86	-253.04
benzoic acid	330.97	-58.64	-8.72	20.7	-254.71	-253.36
	330.84	-59.68	-9.15		-253.97	-253.99
	332.61	-56.30	-7.20		-257.17	-251.11
	-	-	-		-	-
3-boromobenzoic acid	325.18	-55.76	-9.62	20.3	-253.25	-252.62
	325.18	-56.56	-9.91		-252.74	-253.21
	327.27	-54.10	-8.07		-255.45	-250.41
	-	-	-		-	-

[a]B3LYP/6-311++G(d,p); [b]M062X/6-311++G(d,p); [c]MP2/6-311++G(d,p); [d] CCSD/6-311++G(d,p)

[e] Calculated using eq. (3).

[f] The corrected calculated value of $\Delta G_{sol}^{H^+}$ obtained using the computational error in water reported in the last column of Table 1.

Table S6. The values of ΔG_g , $\Delta G_{sol}^{A^-}$, ΔG_{sol}^{AH} of selected compounds calculated at different levels of theory, the value of $\Delta G_{sol}^{H^+}$ obtained from eq. 3 using the $pK_a^{\exp}$ of compounds in DMF (column 6) and; the calculated values of $\Delta G_{sol}^{H^+}$ in DMF (last column), corrected using the computational error in water solvent reported in the last column of Table 1. The values of $\Delta G_{sol}^{A^-}$ and ΔG_{sol}^{AH} have been calculated in DMF solvent.

compound	ΔG_g (kcal.mol^{-1})	$\Delta G_{sol}^{A^-}$	ΔG_{sol}^{AH}	$pK_a^{\exp}$	$(\Delta G_{sol}^{H^+})^e$	$(\Delta G_{sol}^{H^+})^f$
acetic acid	338.11[a]	-59.12	-6.66	13.3	-269.49	-266.95
	339.88[b]	-59.64	-6.76		-270.75	-267.91
	340.80[c]	-57.83	-5.44		-272.16	-264.46
	344.49[d]	-58.32	-5.57		-275.49	-265.86
chloroacetic acid	324.26	-56.17	-9.56	10.1	-265.77	-265.51
	325.96	-56.70	-9.66		-267.04	-266.37
	328.65	-54.80	-7.48		-269.44	-263.61
	333.14	-55.39	-7.66		-281.057	-265.02
3,4-dichlorobenzoic acid	322.36	-52.38	-9.03	11	-265.90	-265.41
	322.16	-52.94	-9.22		-265.33	-266.01
	325.53	-51.41	-7.57		-268.58	-263.30
	-	-	-		-	-
benzoic acid	330.97	-57.33	-8.37	12.3	-267.13	-265.78
	330.84	-58.33	-8.79		-266.42	-266.44
	332.61	-55.30	-7.01		-269.43	-263.38
	-	-	-		-	-
3-boromobenzoic acid	325.18	-54.64	-9.31	11.3	-266.33	-265.71
	325.18	-55.39	-9.59		-265.86	-266.34
	327.27	-53.27	-7.93		-268.41	-263.38
	-	-	-		-	-

[a]B3LYP/6-311++G(d,p); [b]M062X/6-311++G(d,p); [c]MP2/6-311++G(d,p); [d] CCSD/6-311++G(d,p)

[e] Calculated using eq. (3).

[f] The corrected calculated value of $\Delta G_{sol}^{H^+}$ obtained using the computational error in water reported in the last column of Table 1.

Table S7. The values of pK_a of selected compounds in ethanol solvent, calculated at the different levels of theory using the values of $\Delta G_{sol}^{H^+}$ reported in Table 3 (columns 3, 4 and 5) along with the corresponding $pK_{a,nonaqueous}^{corr}$ values obtained from eq. (5) (columns 6, 7 and 8).

No	compound	[a] pK_a (B3LYP)	[a] pK_a (M062X)	[a] pK_a (MP2)	[b] pK_a (B3LYP)	[b] pK_a (M062X)	[b] pK_a (MP2)	[c] $pK_{a,nonaqueous}^{exp}$
1	Formic	9.70	9.88	13.20	9.55	9.59	9.54	9.15
2	Acetic	12.52	12.83	16.32	10.73	10.75	10.68	10.30
3	Choloro acetic	8.53	8.82	12.67	8.34	8.33	8.39	8.30
4	Di choloro acetic	4.65	4.99	9.18	6.68	6.69	6.76	7.30
5	Cyano acetic	8.89	7.12	10.92	8.16	8.16	8.24	7.49
6	Benzoic	11.08	10.07	14.50	10.10	10.08	10.06	10.10
7	3-bromo benzoic	10.01	9.20	13.20	9.56	9.54	9.51	9.40
8	4-nitro benzoic	8.94	8.34	11.73	9.02	9.02	9.05	8.9
9	3,4-di choloro benzoic	9.53	8.66	13.07	9.17	9.16	9.20	-
10	3,5-di nitro benzoic	7.24	6.82	8.98	8.10	8.08	8.15	-
11	3,4-dimethylbenzoic	12.78	11.65	15.30	10.18	10.14	10.16	-
12	Salicylic	6.78	5.49	9.36	8.30	8.28	8.30	8.68
13	Phenol	19.16	18.66	23.32	15.39	15.36	15.44	-
14	3-nitro phenol	15.88	15.65	18.26	13.49	13.45	13.55	-
15	4-nitro phenol	11.76	12.23	16.00	11.97	11.92	11.98	-
16	2,4-di nitro phenol	8.69	7.54	12.40	8.64	8.57	8.55	-
17	2,4,6-tri nitro phenol	2.22	1.44	5.93	4.48	4.39	4.42	4.1

[a] The calculated pK_a values obtained using the values of $\Delta G_{sol}^{H^+}$ reported in Table 3.

[b] The calculated pK_a values (named as $pK_{a,nonaqueous}^{corr}$ in the text) corrected with the corresponding values of Δ reported in Table 4.

[c] The experimental pK_a values of the compounds in ethanol solvent.

Table S8. The values of pK_a of selected compounds in 2-propanol solvent, calculated at the different levels of theory using the values of $\Delta G_{sol}^{H^+}$ reported in Table 3 (columns 3, 4 and 5) along with the corresponding $pK_{a,nonaqueous}^{corr}$ values obtained from eq. (5) (columns 6, 7 and 8).

number	compound	[a] pK_a (B3LYP)	[a] pK_a (M062X)	[a] pK_a (MP2)	[b] pK_a (B3LYP)	[b] pK_a (M062X)	[b] pK_a (MP2)	[c] $pK_{a,nonaqueous}^{exp}$
1	Formic	10.51	10.70	13.97	10.36	10.42	10.31	-
2	Acetic	13.49	13.82	17.24	11.69	11.74	11.59	11.3
3	Choloro acetic	9.24	9.54	13.38	9.05	9.05	9.10	9.2
4	Di choloro acetic	5.24	5.56	9.78	7.26	7.27	7.36	7.8
5	Cyano acetic	9.49	7.72	11.52	8.76	8.76	8.85	-
6	Benzoic	11.95	10.92	15.31	10.96	10.94	10.87	1175
7	3-bromo benzoic	10.75	9.91	13.89	10.30	10.26	10.20	10.1
8	4-nitro benzoic	9.62	9.01	12.42	9.70	9.69	9.74	9.6
9	3,4-di choloro benzoic	10.25	9.36	13.76	9.89	9.86	9.89	9.8
10	3,5-di nitro benzoic	7.77	7.35	9.51	8.64	8.60	8.69	8.3
11	3,4-dimethylbenzoic	13.57	12.43	16.04	10.97	10.93	10.90	11.7
12	Salicylic	7.28	5.96	9.82	8.80	8.75	8.76	-
13	Phenol	19.83	19.31	24.00	16.06	16.01	16.12	-
14	3-nitro phenol	16.40	16.15	18.77	14.01	13.95	14.06	13.92
15	4-nitro phenol	12.14	12.56	16.34	12.35	12.24	12.32	12.45
16	2,4-di nitro phenol	9.07	7.88	12.67	9.02	8.91	8.82	-
17	2,4,6-tri nitro phenol	2.36	1.54	5.98	4.63	4.48	4.47	3.7

[a] The calculated pK_a values obtained using the values of $\Delta G_{sol}^{H^+}$ reported in Table 3.

[b] The calculated pK_a values (named as $pK_{a,nonaqueous}^{corr}$ in the text) corrected with the corresponding values of Δ reported in Table 4.

[c] The experimental pK_a values of the compounds in 2-propanol solvent.

Table S9. The values of pK_a of selected compounds in 2-methyl-2-propanol solvent, calculated at the different levels of theory using the values of $\Delta G_{sol}^{H^+}$ reported in Table 3 (columns 3, 4 and 5) along with the corresponding $pK_{a,nonaqueous}^{corr}$ values obtained from eq. (5) (columns 6, 7 and 8).

No	compound	[a] pK_a (B3LYP)	[a] pK_a (M062X)	[a] pK_a (MP2)	[b] pK_a (B3LYP)	[b] pK_a (M062X)	[b] pK_a (MP2)	[c] $pK_{a,nonaqueous}^{exp}$
1	Formic	13.76	13.96	17.24	13.61	13.68	13.58	-
2	Acetic	16.89	17.22	20.63	15.09	15.14	14.99	14.2
3	Choloro acetic	12.31	12.63	16.51	12.12	12.14	12.23	12.2
4	Di choloro acetic	8.21	8.54	12.82	10.24	10.24	10.41	10.2
5	Cyano acetic	12.43	10.66	14.54	11.69	11.70	11.86	10.6
6	Benzoic	15.27	14.24	18.62	14.28	14.25	14.18	15.1
7	3-bromo benzoic	13.92	13.08	17.09	13.47	13.43	13.39	13.5
8	4-nitro benzoic	12.64	12.02	15.52	12.71	12.70	12.84	12
9	3,4-di choloro benzoic	13.35	12.44	16.90	12.99	12.94	13.03	13
10	3,5-di nitro benzoic	10.59	10.14	12.42	11.45	11.40	11.60	10.6
11	3,4-dimethylbenzoic	16.88	15.72	19.34	14.28	14.22	14.20	15.4
12	Salicylic	10.21	8.88	12.76	11.73	11.67	11.70	-
13	Phenol	22.96	23.10	27.14	19.18	19.80	19.26	-
14	3-nitro phenol	19.16	19.34	21.60	16.77	17.14	16.89	16.99
15	4-nitro phenol	14.76	15.51	19.00	14.97	15.20	14.97	14.6
16	2,4-di nitro phenol	11.70	10.76	15.31	11.65	11.79	11.45	-
17	2,4,6-tri nitro phenol	4.73	3.86	8.39	7.00	6.81	6.88	4.8

[a] The calculated pK_a values obtained using the values of $\Delta G_{sol}^{H^+}$ reported in Table 3.

[b] The calculated pK_a values (named as $pK_{a,nonaqueous}^{corr}$ in the text) corrected with the corresponding values of Δ reported in Table 4.

[c] The experimental pK_a values of the compounds in 2–methyl-2-propanol solvent.

Table S10. The values of pK_a of selected compounds in DMSO solvent, calculated at the different levels of theory using the values of $\Delta G_{sol}^{H^+}$ reported in Table 3 (columns 3, 4 and 5) along with the corresponding $pK_{a,nonaqueous}^{corr}$ values obtained from eq. (5) (columns 6, 7 and 8).

Acid	[a] pK_a (B3LYP)	[a] pK_a (M062X)	[a] pK_a (MP2)	[b] pK_a (B3LYP)	[b] pK_a (M062X)	[b] pK_a (MP2)	[c] $pK_{a,nonaqueous}^{exp}$
Formic	10.57	10.93	14.05	10.42	10.64	10.38	10.3
Acetic	14.37	14.77	18.10	12.57	12.69	12.46	12.3
Choloro acetic	8.52	8.89	12.94	8.33	8.40	8.67	-
Di choloro acetic	3.43	3.72	8.42	5.46	5.42	6.01	-
Cyano acetic	8.46	6.69	10.84	7.73	7.73	8.16	-
Benzoic	11.69	10.59	15.10	10.70	10.61	10.66	11
3-bromo benzoic	10.11	9.20	13.37	9.66	9.55	9.67	9.7
4-nitro benzoic	8.98	8.28	11.99	9.06	8.96	9.31	9
3,4-di choloro benzoic	9.51	8.52	13.20	9.15	9.03	9.33	9.2
3,5-di nitro benzoic	6.56	6.00	8.27	7.43	7.26	7.45	7.4
3,4-dimethylbenzoic	13.12	11.87	15.70	10.52	10.37	10.56	11.4
Salicylic	4.72	3.27	7.46	6.24	6.06	6.40	6.9
Phenol	17.93	17.27	22.37	14.15	13.97	14.49	18
3-nitro phenol	14.22	13.74	16.59	11.83	11.54	11.88	-
4-nitro phenol	10.48	9.89	13.85	10.69	9.58	9.83	9.9
2,4-di nitro phenol	7.42	5.90	10.46	7.37	6.93	6.60	6.36
2,4,6-tri nitro phenol	-0.24	-1.44	2.81	2.02	1.51	1.30	-1.9

[a] The calculated pK_a values obtained using the values of $\Delta G_{sol}^{H^+}$ reported in Table 3.

[b] The calculated pK_a values (named as $pK_{a,nonaqueous}^{corr}$ in the text) corrected with the corresponding values of Δ reported in Table 4.

[c] The experimental pK_a values of the compounds in DMSO solvent.

Table S11. The values of pK_a of selected compounds in ACN solvent, calculated at the different levels of theory using the values of $\Delta G_{sol}^{H^+}$ reported in Table 3 (columns 3, 4 and 5) along with the corresponding $pK_{a,nonaqueous}^{corr}$ values obtained from eq. (5) (columns 6, 7 and 8).

Acid	[a] pK_a (B3LYP)	[a] pK_a (M062X)	[a] pK_a (MP2)	[b] pK_a (B3LYP)	[b] pK_a (M062X)	[b] pK_a (MP2)	[c] $pK_{a,nonaqueous}^{exp}$
Formic	20.69	21.02	24.03	20.54	20.73	20.37	-
Acetic	24.29	24.68	27.91	22.49	22.60	22.26	22.3
Choloro acetic	18.79	19.15	23.04	18.60	18.66	18.76	18.8
Di choloro acetic	13.94	14.25	18.73	15.96	15.95	16.31	15.8
Cyano acetic	18.81	17.04	20.98	18.07	18.08	18.31	18.0
Benzoic	21.88	20.82	25.18	20.89	20.83	20.74	20.7
3-bromo benzoic	20.40	19.51	23.52	19.95	19.86	19.83	20.3
4-nitro benzoic	19.31	18.62	22.12	19.38	19.30	19.45	18.7
3,4-di choloro benzoic	19.81	18.86	23.35	19.45	19.36	19.48	19
3,5-di nitro benzoic	17.03	16.51	18.60	17.90	17.77	17.78	16.9
3,4-dimethylbenzoic	23.32	22.10	25.77	20.71	20.60	20.63	21.2
Salicylic	15.35	13.94	17.97	16.87	16.73	16.90	16.7
Phenol	28.47	27.85	32.77	24.70	24.55	24.90	26.7
3-nitro phenol	24.86	24.43	27.13	22.47	22.23	22.41	23.9
4-nitro phenol	20.43	20.64	24.46	20.64	20.33	20.44	20.8
2,4-di nitro phenol	14.63	16.31	20.81	14.58	17.34	16.95	16.66
2,4,6-tri nitro phenol	10.27	9.14	13.33	12.54	12.09	11.82	11

[a] The calculated pK_a values obtained using the values of $\Delta G_{sol}^{H^+}$ reported in Table 3.

[b] The calculated pK_a values (named as $pK_{a,nonaqueous}^{corr}$ in the text) corrected with the corresponding values of Δ reported in Table 4.

[c] The experimental pK_a values of the compounds in ACN solvent.

Table S12. The values of pK_a of selected compounds in DMF solvent, calculated at the different levels of theory using the values of $\Delta G_{sol}^{H^+}$ reported in Table 3 (columns 3, 4 and 5) along with the corresponding $pK_{a,nonaqueous}^{corr}$ values obtained from eq. (5) (columns 6, 7 and 8).

Acid	[a] pK_a (B3LYP)	[a] pK_a (M062X)	[a] pK_a (MP2)	[c] pK_a (B3LYP)	[c] pK_a (M062X)	[c] pK_a (MP2)	[c] $pK_{a,nonaqueous}^{exp}$
Formic	12.11	12.49	15.51	11.96	12.20	11.84	-
Acetic	15.89	16.34	19.56	14.09	14.25	13.91	13.3
Choloro acetic	10.02	10.41	14.37	9.83	9.92	10.09	10.1
Di choloro acetic	4.92	5.25	9.84	6.95	6.95	7.43	7.2
Cyano acetic	9.94	8.20	12.24	9.20	9.24	9.57	-
Benzoic	13.22	12.16	16.56	12.23	12.17	12.12	12.3
3-bromo benzoic	11.63	10.73	14.81	11.18	11.07	11.12	11.3
4-nitro benzoic	10.47	9.79	13.40	10.55	10.47	10.73	10.6
3,4-di choloro benzoic	11.02	10.06	14.63	10.66	10.56	10.76	11
3,5-di nitro benzoic	8.01	7.49	9.66	8.88	8.74	8.84	8.9
3,4-dimethylbenzoic	14.66	13.44	17.17	12.06	11.94	12.03	13
Salicylic	6.23	4.82	8.90	7.75	7.60	7.84	-
Phenol	19.44	18.82	23.79	15.67	15.52	15.91	<15
3-nitro phenol	15.68	15.23	17.98	13.29	13.03	13.27	13.8
4-nitro phenol	11.19	11.37	15.22	11.40	11.06	11.20	10.9
2,4-di nitro phenol	8.83	7.34	11.80	8.78	8.37	7.95	6.3
2,4,6-tri nitro phenol	1.13	-0.04	4.13	3.40	2.91	2.62	1.2

[a] The calculated pK_a values obtained using the values of $\Delta G_{sol}^{H^+}$ reported in Table 3.

[b] The calculated pK_a values (named as $pK_{a,nonaqueous}^{corr}$ in the text) corrected with the corresponding values of Δ reported in Table 4.

[c] The experimental pK_a values of the compounds in DMF solvent.

Table S13. The pK_a values of the selected phenol derivatives in methanol solvent estimated from the correlation equations of different levels of theory.

Compound	$pK_{a,water}^{exp}$	pK_a^{exp}	$pK_{a,B3LYP}$	$pK_{a,M062X}$	$pK_{a,MP2}$
1-Naphthol	9.4		14.89	14.86	14.91
2-Chlorophenol	8.51		13.98	13.95	14.00
2-Fluorophenol	8.73		14.20	14.18	14.23
2-Nitrophenol	7.23		12.67	12.65	12.69
2-Methylphenol	10.31		15.82	15.79	15.84
2-Methoxyphenol	9.9		15.40	15.37	15.42
2-tert-Butylphenol	11.34		16.87	16.84	16.90
3-Bromophenol	9.01		14.49	14.46	14.51
2-trifuoromethylphenol	8.42		13.89	13.86	13.91
3-trifluoromethylphenol	9.06		14.50	14.47	14.52
4-trifuoromethylphenol	8.68		14.15	14.13	14.17
3,5-Ditrifuoromethylphenol	8.26		13.72	13.70	13.74
3-Chlorophenol	9.02		14.54	14.51	14.56
3-Methylphenol	10.1		15.60	15.58	15.63
4-Bromophenol	9.36		14.85	14.82	14.87
4-cyanophenol	7.95		14.87	14.84	14.89
4-Chlorophenol	9.38		13.41	13.38	13.43
4-Methylphenol	10.28		15.79	15.76	15.81
4-Hydroxybenzaldehyde	7.51		12.96	12.93	12.97
4-tert-Butylphenol	10.31		15.82	15.79	15.84
4-[(E)-2-(4-Nitrophenyl)-1-ethenyl]phenol	9.39		14.88	14.85	14.90
2,3-Dimethylphenol	10.54		16.05	16.03	16.08
3-chloro-4-nitrophenol	6.49		13.09	13.07	13.11
2,4-Dinitrophenol	4.1		11.91	11.89	11.93
2-Chloro-4-bromophenol	7.64		9.47	9.45	9.48

2,4-Dimethylphenol	10.6	16.11	16.09	16.14
2-Chloro-4-phenylphenol	8.07	13.53	13.50	13.55
2,4-Di-tert-butylphenol	11.57	17.11	17.08	17.14
2,5-Dinitrophenol	5.22	10.62	10.59	10.63
2,5-Dimethylphenol	10.41	15.92	15.89	15.95
2,6-Dinitrophenol	3.74	9.10	9.08	9.11
3,4-Dinitrophenol	5.42	16.10	16.08	16.13
2,6-Dimethylphenol	10.59	10.82	10.80	10.83
3,4-Dichloroohenol	8.58	15.87	15.84	15.90
3,4-Dimethylphenol	10.36	14.05	14.02	14.07
3,5-Dichlorophenol	8.18	13.64	13.62	13.66
3,5-Dinitrophenol	6.66	12.09	12.06	12.10
3,5-Dimethylphenol	10.2	15.71	15.68	15.73
3,5-Di-tert-butylphenol	10.29	15.80	15.77	15.82
2,4,6-Tribromophenol	6.1	11.52	11.49	11.53
2,6-Dinitro-4-chlorophenol	2.97	8.74	8.72	8.74
3,4,5-Trichlorophenol	7.9	8.32	8.30	8.32
2,6-Dibromo-4-nitrophenol	3.38	13.36	13.33	13.37
2,4,6-trimethylphenol	10.86	16.38	16.35	16.41
2,6-Di-tert-butyl-4-nitrophenol	6.65	12.08	12.05	12.09
3,3-Di-tert-butyl-4-hydroxybenzaldehyde	8.05	13.51	13.48	13.53
Bromophenol blue	4.17	9.54	9.52	9.55
Bromocresol green	4.93	10.32	10.30	10.33
Bromocresol purple	6.39	11.81	11.79	11.83
Bromothymol blue	7.35	12.79	12.77	12.81
thymol blue	7.1	12.54	12.51	12.55
phenol red	7.9	13.36	13.33	13.37
phenolphthalein	9.5	14.99	14.96	15.01

Table S14. The pK_a values of the selected carboxylic acids (aliphatic and aromatic derivatives) in ethanol solvent estimated from the correlation equation.

compound	$pK_{a,water}^{exp}$	pK_a^{exp}	$pK_{a,B3LYP}$	$pK_{a,M062X}$	$pK_{a,MP2}$
2-Bromoacetic acid	2.9		8.25	8.23	8.25
2-Fluoroacetic acid	2.82		8.16	8.14	8.17
2-Lodoacetic acid	3.13		8.48	8.46	8.48
2-Hydroxyacetic acid	3.85		9.22	9.20	9.22
2-Sulfanylacetic acid	3.73		9.09	9.07	9.10
2-Phenylacetic acid	4.31		9.69	9.67	9.69
Propanoic acid	4.88		10.27	10.25	10.28
3-Bromopropanoic acid	4.04		9.41	9.39	9.42
3-Chloropropanoic acid	4.09		9.46	9.44	9.47
3-Iodopropanoic acid	4.05		9.42	9.40	9.43
3-Hydroxypropanoic acid	4.51		9.89	9.87	9.90
2-Bromopropanoic acid	3		8.35	8.33	8.35
2-Chloropropanoic acid	2.9		8.25	8.23	8.25
2,3-Dibromopropanoic acid	2.36		7.69	7.68	7.70
2,3-Dichloropropanoic acid	2.85		8.19	8.18	8.20
Malonic acid (pK1)	2.83		8.17	8.16	8.18
Malonic acid (pK2)	5.66		11.07	11.04	11.08
Methylmalonic(pK1)	2.94		8.29	8.27	8.29
methylmalonic(pK2)	5.76		11.17	11.15	11.18
Ethylmalonic(pK1)	3.35		8.71	8.69	8.71
Ethylmalonic(pK2)	5.83		11.24	11.22	11.25
Acrylic acid	4.25		9.63	9.60	9.63
(E)-4-Oxo-4-[4-vinyloxy)anilino]-2-butenoic acid	3.66		9.02	9.00	9.03
(E)-4-[4-Ethoxyanilino]-4-	3.63		8.99	8.97	9.00

oxo-2-butenoic acid				
Fumaric acid (pK2)	4.6	9.98	9.96	9.99
Atropic acid	4.44	9.82	9.80	9.83
2-(3-Chlorophenyl)acrylic acid	4.29	9.67	9.65	9.67
2-(3-Nitrophenyl)acrylic acid	4.12	9.49	9.47	9.50
2-(4-Nitrophenyl)acrylic acid	4.05	9.42	9.40	9.43
1-Cyclopropanecarboxilic acid	4.83	10.22	10.20	10.23
Butanoic acid	4.82	10.21	10.19	10.22
3-Bromobutanoic acid	4.01	9.38	9.36	9.39
3-Chlorobutanoic acid	4.17	9.54	9.52	9.55
2-Chlorobutanoic acid	2.92	8.27	8.25	8.27
Succinic acid (pK1)	4.2	9.57	9.55	9.58
Succinic acid (pK2)	5.61	11.02	10.99	11.03
Methylsuccinic(pK1)	4.49	9.87	9.85	9.88
Tartaric acid (pK1)	3.01	8.36	8.34	8.36
d-(sec-Butyl)tartrate	3.38	8.74	8.72	8.74
meso-(sec-Butyl)tartrate	3.68	9.04	9.02	9.05
4-Oxo-4-[4-(vinylox)anilino]butanoic acid	4.64	10.02	10.00	10.03
4-(4-Ethoxyanilino]-4-oxobutanoic acid	4.55	9.93	9.91	9.94
1-Cyclobutanecarboxylic acid	4.79	10.18	10.16	10.19
1-Cyclobutanecarboxylic acid	4.99	10.38	10.36	10.39
1-Cyclohexanecarboxylic	4.9	10.29	10.27	10.30

acid				
cis-2-Hydroxy-1-cyclohexanecarboxylic acid	4.8	10.19	10.17	10.20
trans-2-Hydroxy-1-cyclohexanecarboxylic acid	4.82	10.21	10.19	10.22
cis-3-Hydroxy-1-cyclophexanecarboxylic acid	4.6	9.98	9.96	9.99
trans-3-Hydroxy-1-cyclohexanecarboxcylic acid	4.82	10.21	10.19	10.22
cis-4-Hydroxy-1-cyclohexanecarboxylic acid	4.84	10.23	10.21	10.24
trans-4-Hydroxy-1-cyclohexanecarboxylic acid	4.69	10.07	10.05	10.08
Heptanedioic acid	4.46	9.84	9.82	9.85
Octanedioic acid	4.5	9.88	9.86	9.89
Bicyclo[2,2,2]octane-1-carboxylic acid	5.08	10.47	10.45	10.48
4-Bromobicyclo[2,2,2]octane-1-carboxylic acid	4.62	10.00	9.98	10.01
4-Cyanobicyclo[2,2,2]octane-1-carboxylic acid	4.55	9.93	9.91	9.94
Bicyclo[2,2,2]octane-1,4-dicarboxylic acid (pK1)	4.47	9.85	9.83	9.86
Bicyclo[2,2,2]octane-1,4-dicarboxylic acid (pK2)	5.46	10.86	10.84	10.87
4-(1,1,1-Trimethylammonio)bicyclo	4.08	9.45	9.43	9.46

[2,2,2]octane-1-oDecanedioic acid				
Decanedioic acid	4.5	9.88	9.86	9.89
2-Fluorobenzoic acid	3.57	8.93	8.91	8.94
2-Bromobenzoic acid	2.85	8.19	8.18	8.20
2-Chlorobenzoic acid	2.92	8.27	8.25	8.27
2-lodobenzoic acid	2.85	8.19	8.18	8.20
2-Methylbenzoic acid	3.91	9.28	9.26	9.28
2-Nitrobenzoic acid	2.19	7.52	7.50	7.52
2-Methoxybenzoic acid	4.09	9.46	9.44	9.47
2-[4-(Vinyloxy)anilino]benzoic acid	3.8	9.17	9.15	9.17
2-[Methyl-4-(vinyloxy)anilino]benzoic acid	4.34	9.72	9.70	9.72
3-Fluorobenzoic acid	3.88	9.25	9.23	9.25
3-Chlorobenzoic acid	3.8	9.17	9.15	9.17
3-lodobenzoic acid	3.82	9.19	9.17	9.19
3-Hydroxybenzoic acid	4.01	9.38	9.36	9.39
3-Acetamidobenzoic acid	4.06	9.43	9.41	9.44
3-Nitrobenzoic acid	3.47	8.83	8.81	8.83
3-Methoxynbenzoic acid	4.12	9.49	9.47	9.50
3-Phenoxybenzoic acid	3.95	9.32	9.30	9.33
3-Mercaptgobenzoic acid	3.96	9.33	9.31	9.34
3-Sulfamylbenzoic acid	3.68	9.04	9.02	9.05
3-(Methylsulfonyl)benzoic acid	3.53	8.89	8.87	8.89
3-Methylbenzoic acid	4.28	9.66	9.64	9.66
3-(Trifluoromethyl)benzoic acid	3.75	9.11	9.09	9.12

3-Cyanobenzoic acid	3.6	8.96	8.94	8.97
3-Acetylbenzoic acid	3.83	9.20	9.18	9.20
4-Fluorobenzoic acid	4.15	9.52	9.50	9.53
4-Bromobenzoic acid	3.99	9.36	9.34	9.37
4-Chlorobenzoic acid	4	9.37	9.35	9.38
4-lodobenzoic acid	3.98	9.35	9.33	9.36
4-Aminobenzoic acid	4.82	10.21	10.19	10.22
4-Acetamidobenzoic acid	4.3	9.68	9.66	9.68
4-(Dimethylamino)benzoic acid	5.03	10.42	10.40	10.43
4-Hydroxybenzoic acid	4.55	9.93	9.91	9.94
4-Methoxybenzoic acid	4.25	9.63	9.60	9.63
4-(Methylmercapto)benzoic acid	4.2	9.57	9.55	9.58
4-Sulfamylbenzoic acid	3.63	8.99	8.97	9.00
4-(Methylsulfonyl)benzoic acid	3.48	8.84	8.82	8.84
4-Methylbenzoic acid	4.38	9.76	9.74	9.77
4-Cyanobenzoic acid	3.53	8.89	8.87	8.89
4-Acetylbenzoic acid	3.7	9.06	9.04	9.07
4-tert-Butylbenzoic acid	4.36	9.74	9.72	9.75
2,4-Dichlorobenzoic acid	2.76	8.10	8.08	8.11
2,4-Dinitrobenzoic acid	1.43	6.74	6.73	6.74
2,4-Dimethylbenzoic acid	4.22	9.59	9.57	9.60
2,6-Dichlorobenzoic acid	1.82	7.14	7.12	7.14
2,6-Dinitrobenzoic acid	1.14	6.45	6.43	6.44
3,4-Dimethoxybenzoic acid	4.44	9.82	9.80	9.83
3,4-Dinitrobenzoic acid	2.82	8.16	8.14	8.17
3-Methyl-4-chlorobenzoic acid	4.07	9.44	9.42	9.45
3-Methyl-4-nitrobenzoic	3.65	9.01	8.99	9.02

acid				
4-Chloro-3-nitrobenzoic acid	3.34	8.70	8.68	8.70
3,5-Dichlorobenzoic acid	3.56	8.92	8.90	8.93
3,5-Dinitrobenzoic acid	2.82	8.16	8.14	8.17
2,4,6-Trimethylbenzoic acid	3.45	8.81	8.79	8.81

Table S15. The pK_a values of the selected phenol derivatives in methanol solvent estimated from the correlation equation.

Compound	$pK_{a,water}^{exp}$	pK_a^{exp}	$pK_{a,B3LYP}$	$pK_{a,M062X}$	$pK_{a,MP2}$
1-Naphthol	9.4	13.91	14.27	14.26	14.27
2-Chlorophenol	8.51	12.97	13.38	13.37	13.38
2-Fluorophenol	8.73	12.94	13.60	13.59	13.60
2-Nitrophenol	7.23	11.53	12.10	12.09	12.10
2-Methylphenol	10.31	14.86	15.18	15.17	15.18
2-Methoxyphenol	9.9	14.48	14.77	14.76	14.77
2-tert-Butylphenol	11.34	16.5	16.22	16.20	16.21
3-Bromophenol	9.01	13.3	13.88	13.87	13.88
2-trifuoromethylphenol	8.42		13.29	13.28	13.29
3-trifluoromethylphenol	9.06		13.93	13.92	13.93
4-trifuoromethylphenol	8.68		13.55	13.54	13.55
3,5-Ditrifuoromethylphenol	8.26		13.13	13.12	13.13
3-Chlorophenol	9.02	13.1	13.89	13.88	13.89
3-Methylphenol	10.1	14.43	14.97	14.96	14.97
4-Bromophenol	9.36	13.63	14.23	14.22	14.23
4-cyanophenol	7.95		12.82	12.81	12.82
4-Chlorophenol	9.38	13.59	14.25	14.24	14.25
4-Methylphenol	10.28	14.54	15.15	15.14	15.15
4-Hydroxybenzaldehyde	7.51	12.01	12.38	12.37	12.38
4-tert-Butylphenol	10.31	14.52	15.18	15.17	15.18
4-[(E)-2-(4-Nitrophenyl)-1-ethenyl]phenol	9.39	13.11	14.26	14.25	14.26
2,3-Dimethylphenol	10.54	15.08	15.42	15.40	15.41
3-chloro-4-nitrophenol	6.49		11.36	11.34	11.36
2,4-Dinitrophenol	4.1		8.96	8.95	8.97
2-Chloro-4-bromophenol	7.64	12.14	12.51	12.50	12.51

2,4-Dimethylphenol	10.6	15.04	15.48	15.46	15.47
2-Chloro-4-phenylphenol	8.07	12.7	12.94	12.93	12.94
2,4-Di-tert-butylphenol	11.57	16.77	16.45	16.43	16.44
2,5-Dinitrophenol	5.22	8.94	10.09	10.07	10.09
2,5-Dimethylphenol	10.41	14.91	15.28	15.27	15.28
2,6-Dinitrophenol	3.74	7.64	8.60	8.59	8.61
3,4-Dinitrophenol	5.42		10.29	10.27	10.29
2,6-Dimethylphenol	10.59	15.26	15.47	15.45	15.46
3,4-Dichloroohenol	8.58		13.45	13.44	13.45
3,4-Dimethylphenol	10.36	14.63	15.23	15.22	15.23
3,5-Dichlorophenol	8.18	12.11	13.05	13.04	13.05
3,5-Dinitrophenol	6.66	10.29	11.53	11.51	11.53
3,5-Dimethylphenol	10.2	14.57	15.07	15.06	15.07
3,5-Di-tert-butylphenol	10.29	14.89	15.16	15.15	15.16
2,4,6-Tribromophenol	6.1	10.1	10.97	10.95	10.97
2,6-Dinitro-4-chlorophenol	2.97		7.83	7.82	7.84
3,4,5-Trichlorophenol	7.9		12.77	12.76	12.77
2,6-Dibromo-4-nitrophenol	3.38	7.31	8.24	8.23	8.25
2,4,6-trimethylphenol	10.86	15.53	15.74	15.72	15.73
2,6-Di-tert-butyl-4-nitrophenol	6.65	11.07	11.52	11.50	11.52
3,3-Di-tert-butyl-4-hydroxybenzaldehyde	8.05	12.4	12.92	12.91	12.92
Bromophenol blue	4.17	8.9	9.03	9.02	9.04
Bromocresol green	4.93	9.8	9.80	9.78	9.80
Bromocresol purple	6.39	11.3	11.26	11.24	11.26
Bromothymol blue	7.35	12.4	12.22	12.21	12.22
thymol blue	7.1		11.97	11.96	11.97
phenol red	7.9		12.77	12.76	12.77
phenolphthalein	9.5		14.37	14.36	14.37

Table S16. The pK_a values of the selected carboxylic acids (aliphatic and aromatic derivatives) in Methanol solvent estimated from the correlation equation.

compound	$pK_{a,water}^{exp}$	pK_a^{exp}	$pK_{a,B3LYP}$	$pK_{a,M062X}$	$pK_{a,MP2}$
2-Bromoacetic acid	2.9	8.06	7.76	7.75	7.77
2-Fluoroacetic acid	2.82	7.99	7.68	7.67	7.69
2-Lodoacetic acid	3.13	8.38	7.99	7.98	8.00
2-Hydroxyacetic acid	3.85	8.68	8.71	8.70	8.72
2-Sulfanylacetic acid	3.73	8.52	8.59	8.58	8.60
2-Phenylacetic acid	4.31	9.43	9.17	9.16	9.18
Propanoic acid	4.88	9.71	9.75	9.73	9.75
3-Bromopropanoic acid	4.04	9	8.90	8.89	8.91
3-Chloropropanoic acid	4.09	9.18	8.95	8.94	8.96
3-Iodopropanoic acid	4.05	8.89	8.91	8.90	8.92
3-Hydroxypropanoic acid	4.51	9.42	9.37	9.36	9.38
2-Bromopropanoic acid	3	8.22	7.86	7.85	7.87
2-Chloropropanoic acid	2.9	8.06	7.76	7.75	7.77
2,3-Dibromopropanoic acid	2.36	7.38	7.22	7.21	7.23
2,3-Dichloropropanoic acid	2.85	7.5	7.71	7.70	7.72
Malonic acid (pK1)	2.83	7.66	7.69	7.68	7.70
Malonic acid (pK2)	5.66	10.64	10.53	10.51	10.53
Methylmalonic(pK1)	2.94		7.80	7.79	7.81
methylmalonic(pK2)	5.76		10.63	10.61	10.63
Ethylmalonic(pK1)	3.35		8.21	8.20	8.22
Ethylmalonic(pK2)	5.83		10.70	10.68	10.70
Acrylic acid	4.25	9.27	9.11	9.10	9.12
(E)-4-Oxo-4-[4-vinyloxy)anilino]-2-butenoic acid	3.66	8.15	8.52	8.51	8.53
(E)-4-[4-Ethoxyanilino]-4-	3.63	8.18	8.49	8.48	8.50

oxo-2-butenoic acid					
Fumaric acid (pK2)	4.6	9.78	9.47	9.45	9.47
Atropic acid	4.44	9.31	9.30	9.29	9.31
2-(3-Chlorophenyl)acrylic acid	4.29	9.06	9.15	9.14	9.16
2-(3-Nitrophenyl)acrylic acid	4.12	9.89	8.98	8.97	8.99
2-(4-Nitrophenyl)acrylic acid	4.05	8.83	8.91	8.90	8.92
1-Cyclopropanecarboxilic acid	4.83	9.83	9.70	9.68	9.70
Butanoic acid	4.82	9.69	9.69	9.67	9.69
3-Bromobutanoic acid	4.01	9.12	8.87	8.86	8.88
3-Chlorobutanoic acid	4.17	9.18	9.03	9.02	9.04
2-Chlorobutanoic acid	2.92	8.11	7.78	7.77	7.79
Succinic acid (pK1)	4.2	9.14	9.06	9.05	9.07
Succinic acid (pK2)	5.61	11.3	10.48	10.46	10.48
Methylsuccinic(pK1)	4.49		9.35	9.34	9.36
Tartaric acid (pK1)	3.01	8.12	7.87	7.86	7.88
d-(sec-Butyl)tartrate	3.38	8.45	8.24	8.23	8.25
meso-(sec-Butyl)tartrate	3.68	8.7	8.54	8.53	8.55
4-Oxo-4-[4-(vinylox)anilino]butanoic acid	4.64	9.51	9.51	9.49	9.51
4-(4-Ethoxyanilino]-4-oxobutanoic acid	4.55	9.55	9.41	9.40	9.42
1-Cyclobutanecarboxylic acid	4.79	9.89	9.66	9.64	9.66
1-Cyclobutanecarboxylic acid	4.99	10.15	9.86	9.84	9.86
1-Cyclohexanecarboxylic	4.9	9.98	9.77	9.75	9.77

acid					
cis-2-Hydroxy-1-cyclohexanecarboxylic acid	4.8	9.35	9.67	9.65	9.67
trans-2-Hydroxy-1-cyclohexanecarboxylic acid	4.82	9.63	9.69	9.67	9.69
cis-3-Hydroxy-1-cyclophexanecarboxylic acid	4.6	9.77	9.47	9.45	9.47
trans-3-Hydroxy-1-cyclohexanecarboxcylic acid	4.82	10.09	9.69	9.67	9.69
cis-4-Hydroxy-1-cyclohexanecarboxylic acid	4.84	10.12	9.71	9.69	9.71
trans-4-Hydroxy-1-cyclohexanecarboxylic acid	4.69	9.82	9.56	9.54	9.56
Heptanedioic acid	4.46	9.11	9.32	9.31	9.33
Octanedioic acid	4.5	9.22	9.36	9.35	9.37
Bicyclo[2,2,2]octane-1-carboxylic acid	5.08	10.23	9.95	9.93	9.95
4-Bromobicyclo[2,2,2]octane-1-carboxylic acid	4.62	9.75	9.49	9.47	9.49
4-Cyanobicyclo[2,2,2]octane-1-carboxylic acid	4.55	9.62	9.41	9.40	9.42
Bicyclo[2,2,2]octane-1,4-dicarboxylic acid (pK1)	4.47	9.57	9.33	9.32	9.34
Bicyclo[2,2,2]octane-1,4-dicarboxylic acid (pK2)	5.46	10.57	10.33	10.31	10.33
4-(1,1,1-Trimethylammonio)bicyclo	4.08	9.38	8.94	8.93	8.95

[2,2,2]octane-1-oDecanedioic acid					
Decanedioic acid	4.5	9.25	9.36	9.35	9.37
2-Fluorobenzoic acid	3.57	8.41	8.43	8.42	8.44
2-Bromobenzoic acid	2.85	8.19	7.71	7.70	7.72
2-Chlorobenzoic acid	2.92	8.31	7.78	7.77	7.79
2-lodobenzoic acid	2.85	8.24	7.71	7.70	7.72
2-Methylbenzoic acid	3.91	9.24	8.77	8.76	8.78
2-Nitrobenzoic acid	2.19	7.64	7.05	7.04	7.06
2-Methoxybenzoic acid	4.09	9.26	8.95	8.94	8.96
2-[4-(Vinyloxy)anilino]benzoic acid	3.8	8.99	8.66	8.65	8.67
2-[Methyl-4-(vinyloxy)anilino]benzoic acid	4.34	9.45	9.20	9.19	9.21
3-Fluorobenzoic acid	3.88	8.87	8.74	8.73	8.75
3-Chlorobenzoic acid	3.8	8.83	8.66	8.65	8.67
3-lodobenzoic acid	3.82	8.89	8.68	8.67	8.69
3-Hydroxybenzoic acid	4.01	9.58	8.87	8.86	8.88
3-Acetamidobenzoic acid	4.06	9.25	8.92	8.91	8.93
3-Nitrobenzoic acid	3.47	8.32	8.33	8.32	8.34
3-Methoxynbenzoic acid	4.12	9.3	8.98	8.97	8.99
3-Phenoxybenzoic acid	3.95	9	8.81	8.80	8.82
3-Mercaptgobenzoic acid	3.96	8.9	8.82	8.81	8.83
3-Sulfamylbenzoic acid	3.68	8.65	8.54	8.53	8.55
3-(Methylsulfonyl)benzoic acid	3.53	8.43	8.39	8.38	8.40
3-Methylbenzoic acid	4.28	9.39	9.14	9.13	9.15
3-(Trifluoromethyl)benzoic acid	3.75	8.69	8.61	8.60	8.62

3-Cyanobenzoic acid	3.6	8.53	8.46	8.45	8.47
3-Acetylbenzoic acid	3.83	8.87	8.69	8.68	8.70
4-Fluorobenzoic acid	4.15	9.23	9.01	9.00	9.02
4-Bromobenzoic acid	3.99	8.93	8.85	8.84	8.86
4-Chlorobenzoic acid	4	9.09	8.86	8.85	8.87
4-lodobenzoic acid	3.98	9.04	8.84	8.83	8.85
4-Aminobenzoic acid	4.82	10.25	9.69	9.67	9.69
4-Acetamidobenzoic acid	4.3	9.57	9.16	9.15	9.17
4-(Dimethylamino)benzoic acid	5.03	10.4	9.90	9.88	9.90
4-Hydroxybenzoic acid	4.55	9.99	9.41	9.40	9.42
4-Methoxybenzoic acid	4.25	9.79	9.11	9.10	9.12
4-(Methylmercapto)benzoic acid	4.2	9.43	9.06	9.05	9.07
4-Sulfamylbenzoic acid	3.63	8.55	8.49	8.48	8.50
4-(Methylsulfonyl)benzoic acid	3.48	8.36	8.34	8.33	8.35
4-Methylbenzoic acid	4.38	9.51	9.24	9.23	9.25
4-Cyanobenzoic acid	3.53	8.42	8.39	8.38	8.40
4-Acetylbenzoic acid	3.7	8.72	8.56	8.55	8.57
4-tert-Butylbenzoic acid	4.36	9.61	9.22	9.21	9.23
2,4-Dichlorobenzoic acid	2.76	7.8	7.62	7.61	7.63
2,4-Dinitrobenzoic acid	1.43	6.45	6.29	6.28	6.30
2,4-Dimethylbenzoic acid	4.22	9.7	9.08	9.07	9.09
2,6-Dichlorobenzoic acid	1.82	7.05	6.68	6.67	6.69
2,6-Dinitrobenzoic acid	1.14	6.3	6.00	5.99	6.01
3,4-Dimethoxybenzoic acid	4.44	9.54	9.30	9.29	9.31
3,4-Dinitrobenzoic acid	2.82	7.44	7.68	7.67	7.69
3-Methyl-4-chlorobenzoic acid	4.07	9.12	8.93	8.92	8.94
3-Methyl-4-nitrobenzoic	3.65	8.54	8.51	8.50	8.52

acid					
4-Chloro-3-nitrobenzoic acid	3.34	8.1	8.20	8.19	8.21
3,5-Dichlorobenzoic acid	3.56	8.26	8.42	8.41	8.43
3,5-Dinitrobenzoic acid	2.82	7.38	7.68	7.67	7.69
2,4,6-Trimethylbenzoic acid	3.45	8.6	8.31	8.30	8.32

Table S17. The pK_a values of the selected phenol derivatives in 2-propanol solvent estimated from the correlation equation.

Compound	$pK_{a,water}^{exp}$	pK_a^{exp}	$pK_{a,B3LYP}$	$pK_{a,M062X}$	$pK_{a,MP2}$
1-Naphthol	9.4		15.58	15.54	15.59
2-Chlorophenol	8.51		14.66	14.62	14.66
2-Fluorophenol	8.73		14.89	14.85	14.89
2-Nitrophenol	7.23		13.34	13.30	13.33
2-Methylphenol	10.31		16.53	16.48	16.54
2-Methoxyphenol	9.9		16.10	16.06	16.11
2-tert-Butylphenol	11.34		17.59	17.55	17.61
3-Bromophenol	9.01	14.83	15.18	15.14	15.19
2-trifuoromethylphenol	8.42		14.57	14.53	14.57
3-trifluoromethylphenol	9.06		15.19	15.15	15.20
4-trifuoromethylphenol	8.68		14.84	14.79	14.84
3,5-Ditrifuoromethylphenol	8.26		14.40	14.36	14.40
3-Chlorophenol	9.02	13.7	15.23	15.19	15.24
3-Methylphenol	10.1		16.31	16.26	16.32
4-Bromophenol	9.36	15.36	15.54	15.50	15.55
4-cyanophenol	7.95	15.31	15.56	15.52	15.57
4-Chlorophenol	9.38		14.08	14.04	14.08
4-Methylphenol	10.28		16.50	16.45	16.51
4-Hydroxybenzaldehyde	7.51		13.63	13.59	13.62
4-tert-Butylphenol	10.31		16.53	16.48	16.54
4-[(E)-2-(4-Nitrophenyl)-1-ethenyl]phenol	9.39		15.57	15.53	15.58
2,3-Dimethylphenol	10.54		16.76	16.72	16.78
3-chloro-4-nitrophenol	6.49		13.76	13.72	13.76
2,4-Dinitrophenol	4.1		12.57	12.53	12.56
2-Chloro-4-bromophenol	7.64		10.09	10.06	10.07
2,4-Dimethylphenol	10.6		16.83	16.78	16.84

2-Chloro-4-phenylphenol	8.07		14.21	14.16	14.21
2,4-Di-tert-butylphenol	11.57		17.83	17.78	17.85
2,5-Dinitrophenol	5.22		11.25	11.22	11.24
2,5-Dimethylphenol	10.41		16.63	16.58	16.64
2,6-Dinitrophenol	3.74		9.72	9.69	9.70
3,4-Dinitrophenol	5.42		16.82	16.77	16.83
2,6-Dimethylphenol	10.59		11.46	11.42	11.45
3,4-Dichloroohenol	8.58		16.58	16.53	16.59
3,4-Dimethylphenol	10.36		14.73	14.69	14.74
3,5-Dichlorophenol	8.18	14.05	14.32	14.28	14.32
3,5-Dinitrophenol	6.66	10.84	12.75	12.71	12.74
3,5-Dimethylphenol	10.2		16.41	16.37	16.42
3,5-Di-tert-butylphenol	10.29		16.51	16.46	16.52
2,4,6-Tribromophenol	6.1		12.17	12.13	12.15
2,6-Dinitro-4-chlorophenol	2.97		9.35	9.32	9.32
3,4,5-Trichlorophenol	7.9		8.92	8.89	8.89
2,6-Dibromo-4-nitrophenol	3.38		14.03	13.99	14.03
2,4,6-trimethylphenol	10.86		17.10	17.05	17.11
2,6-Di-tert-butyl-4-nitrophenol	6.65		12.74	12.70	12.73
3,3-Di-tert-butyl-4-hydroxybenzaldehyde	8.05		14.19	14.14	14.18
Bromophenol blue	4.17		10.17	10.13	10.14
Bromocresol green	4.93		10.95	10.92	10.93
Bromocresol purple	6.39		12.47	12.43	12.46
Bromothymol blue	7.35		13.46	13.42	13.46
thymol blue	7.1		13.20	13.16	13.20
phenol red	7.9		14.03	13.99	14.03
phenolphthalein	9.5		15.69	15.64	15.70

Table S18. The pK_a values of the selected carboxylic acids (aliphatic and aromatic derivatives) in 2-propanol solvent estimated from the correlation equation.

compound	$pK_{a,water}^{exp}$	pK_a^{exp}	$pK_{a,B3LYP}$	$pK_{a,M062X}$	$pK_{a,MP2}$
2-Bromoacetic acid	2.9		8.85	8.82	8.82
2-Fluoroacetic acid	2.82		7.68	7.67	7.69
2-Lodoacetic acid	3.13		7.99	7.98	8.00
2-Hydroxyacetic acid	3.85		8.71	8.70	8.72
2-Sulfanylacetic acid	3.73		8.59	8.58	8.60
2-Phenylacetic acid	4.31		9.17	9.16	9.18
Propanoic acid	4.88		9.75	9.73	9.75
3-Bromopropanoic acid	4.04		8.90	8.89	8.91
3-Chloropropanoic acid	4.09		8.95	8.94	8.96
3-Iodopropanoic acid	4.05		8.91	8.90	8.92
3-Hydroxypropanoic acid	4.51		9.37	9.36	9.38
2-Bromopropanoic acid	3		7.86	7.85	7.87
2-Chloropropanoic acid	2.9		7.76	7.75	7.77
2,3-Dibromopropanoic acid	2.36		7.22	7.21	7.23
2,3-Dichloropropanoic acid	2.85		7.71	7.70	7.72
Malonic acid (pK1)	2.83		7.69	7.68	7.70
Malonic acid (pK2)	5.66		10.53	10.51	10.53
Methylmalonic(pK1)	2.94	9.81	7.80	7.79	7.81
methylmalonic(pK2)	5.76		10.63	10.61	10.63
Ethylmalonic(pK1)	3.35	9.96	8.21	8.20	8.22
Ethylmalonic(pK2)	5.83		10.70	10.68	10.70
Acrylic acid	4.25		9.11	9.10	9.12
(E)-4-Oxo-4-[4-vinyloxy)anilino]-2-butenoic acid	3.66		8.52	8.51	8.53
(E)-4-[4-Ethoxyanilino]-4-	3.63		8.49	8.48	8.50

oxo-2-butenoic acid					
Fumaric acid (pK2)	4.6		9.47	9.45	9.47
Atropic acid	4.44		9.30	9.29	9.31
2-(3-Chlorophenyl)acrylic acid	4.29		9.15	9.14	9.16
2-(3-Nitrophenyl)acrylic acid	4.12		8.98	8.97	8.99
2-(4-Nitrophenyl)acrylic acid	4.05		8.91	8.90	8.92
1-Cyclopropanecarboxilic acid	4.83		9.70	9.68	9.70
Butanoic acid	4.82		9.69	9.67	9.69
3-Bromobutanoic acid	4.01		8.87	8.86	8.88
3-Chlorobutanoic acid	4.17		9.03	9.02	9.04
2-Chlorobutanoic acid	2.92		7.78	7.77	7.79
Succinic acid (pK1)	4.2		9.06	9.05	9.07
Succinic acid (pK2)	5.61		10.48	10.46	10.48
Methylsuccinic(pK1)	4.49	10.96	9.35	9.34	9.36
Tartaric acid (pK1)	3.01		7.87	7.86	7.88
d-(sec-Butyl)tartrate	3.38		8.24	8.23	8.25
meso-(sec-Butyl)tartrate	3.68		8.54	8.53	8.55
4-Oxo-4-[4-(vinylox)anilino]butanoic acid	4.64		9.51	9.49	9.51
4-(4-Ethoxyanilino]-4-oxobutanoic acid	4.55		9.41	9.40	9.42
1-Cyclobutanecarboxylic acid	4.79		9.66	9.64	9.66
1-Cyclobutanecarboxylic acid	4.99		9.86	9.84	9.86
1-Cyclohexanecarboxylic	4.9		9.77	9.75	9.77

acid				
cis-2-Hydroxy-1-cyclohexanecarboxylic acid	4.8	9.67	9.65	9.67
trans-2-Hydroxy-1-cyclohexanecarboxylic acid	4.82	9.69	9.67	9.69
cis-3-Hydroxy-1-cyclophexanecarboxylic acid	4.6	9.47	9.45	9.47
trans-3-Hydroxy-1-cyclohexanecarboxcylic acid	4.82	9.69	9.67	9.69
cis-4-Hydroxy-1-cyclohexanecarboxylic acid	4.84	9.71	9.69	9.71
trans-4-Hydroxy-1-cyclohexanecarboxylic acid	4.69	9.56	9.54	9.56
Heptanedioic acid	4.46	9.32	9.31	9.33
Octanedioic acid	4.5	9.36	9.35	9.37
Bicyclo[2,2,2]octane-1-carboxylic acid	5.08	9.95	9.93	9.95
4-Bromobicyclo[2,2,2]octane-1-carboxylic acid	4.62	9.49	9.47	9.49
4-Cyanobicyclo[2,2,2]octane-1-carboxylic acid	4.55	9.41	9.40	9.42
Bicyclo[2,2,2]octane-1,4-dicarboxylic acid (pK1)	4.47	9.33	9.32	9.34
Bicyclo[2,2,2]octane-1,4-dicarboxylic acid (pK2)	5.46	10.33	10.31	10.33
4-(1,1,1-Trimethylammonio)bicyclo	4.08	8.94	8.93	8.95

[2,2,2]octane-1-oDecanedioic acid				
Decanedioic acid	4.5	9.36	9.35	9.37
2-Fluorobenzoic acid	3.57	8.43	8.42	8.44
2-Bromobenzoic acid	2.85	7.71	7.70	7.72
2-Chlorobenzoic acid	2.92	7.78	7.77	7.79
2-lodobenzoic acid	2.85	7.71	7.70	7.72
2-Methylbenzoic acid	3.91	8.77	8.76	8.78
2-Nitrobenzoic acid	2.19	7.05	7.04	7.06
2-Methoxybenzoic acid	4.09	8.95	8.94	8.96
2-[4-(Vinyloxy)anilino]benzoic acid	3.8	8.66	8.65	8.67
2-[Methyl-4-(vinyloxy)anilino]benzoic acid	4.34	9.20	9.19	9.21
3-Fluorobenzoic acid	3.88	8.74	8.73	8.75
3-Chlorobenzoic acid	3.8	8.66	8.65	8.67
3-lodobenzoic acid	3.82	8.68	8.67	8.69
3-Hydroxybenzoic acid	4.01	8.87	8.86	8.88
3-Acetamidobenzoic acid	4.06	8.92	8.91	8.93
3-Nitrobenzoic acid	3.47	8.33	8.32	8.34
3-Methoxynbenzoic acid	4.12	8.98	8.97	8.99
3-Phenoxybenzoic acid	3.95	8.81	8.80	8.82
3-Mercaptgobenzoic acid	3.96	8.82	8.81	8.83
3-Sulfamylbenzoic acid	3.68	8.54	8.53	8.55
3-(Methylsulfonyl)benzoic acid	3.53	8.39	8.38	8.40
3-Methylbenzoic acid	4.28	9.14	9.13	9.15
3-(Trifluoromethyl)benzoic acid	3.75	8.61	8.60	8.62

3-Cyanobenzoic acid	3.6	8.46	8.45	8.47
3-Acetylbenzoic acid	3.83	8.69	8.68	8.70
4-Fluorobenzoic acid	4.15	9.01	9.00	9.02
4-Bromobenzoic acid	3.99	8.85	8.84	8.86
4-Chlorobenzoic acid	4	8.86	8.85	8.87
4-lodobenzoic acid	3.98	8.84	8.83	8.85
4-Aminobenzoic acid	4.82	9.69	9.67	9.69
4-Acetamidobenzoic acid	4.3	9.16	9.15	9.17
4-(Dimethylamino)benzoic acid	5.03	9.90	9.88	9.90
4-Hydroxybenzoic acid	4.55	9.41	9.40	9.42
4-Methoxybenzoic acid	4.25	9.11	9.10	9.12
4-(Methylmercapto)benzoic acid	4.2	9.06	9.05	9.07
4-Sulfamylbenzoic acid	3.63	8.49	8.48	8.50
4-(Methylsulfonyl)benzoic acid	3.48	8.34	8.33	8.35
4-Methylbenzoic acid	4.38	9.24	9.23	9.25
4-Cyanobenzoic acid	3.53	8.39	8.38	8.40
4-Acetylbenzoic acid	3.7	8.56	8.55	8.57
4-tert-Butylbenzoic acid	4.36	9.22	9.21	9.23
2,4-Dichlorobenzoic acid	2.76	7.62	7.61	7.63
2,4-Dinitrobenzoic acid	1.43	6.29	6.28	6.30
2,4-Dimethylbenzoic acid	4.22	9.08	9.07	9.09
2,6-Dichlorobenzoic acid	1.82	6.68	6.67	6.69
2,6-Dinitrobenzoic acid	1.14	6.00	5.99	6.01
3,4-Dimethoxybenzoic acid	4.44	9.30	9.29	9.31
3,4-Dinitrobenzoic acid	2.82	7.68	7.67	7.69
3-Methyl-4-chlorobenzoic acid	4.07	8.93	8.92	8.94
3-Methyl-4-nitrobenzoic	3.65	8.51	8.50	8.52

acid					
4-Chloro-3-nitrobenzoic acid	3.34	9.34	8.20	8.19	8.21
3,5-Dichlorobenzoic acid	3.56		8.42	8.41	8.43
3,5-Dinitrobenzoic acid	2.82	8.31	7.68	7.67	7.69
2,4,6-Trimethylbenzoic acid	3.45		8.31	8.30	8.32

Table S19. The pK_a values of the selected phenol derivatives in 2-methyl-2-propanol solvent estimated from the correlation equation.

Compound	$pK_{a,water}^{exp}$	pK_a^{exp}	$pK_{a,B3LYP}$	$pK_{a,M062X}$	$pK_{a,MP2}$
1-Naphthol	9.4		18.66	19.10	18.68
2-Chlorophenol	8.51	18.54	17.72	18.10	17.75
2-Fluorophenol	8.73		17.95	18.35	17.98
2-Nitrophenol	7.23	15.88	16.37	16.66	16.40
2-Methylphenol	10.31		19.61	20.12	19.64
2-Methoxyphenol	9.9		19.18	19.66	19.21
2-tert-Butylphenol	11.34		20.70	21.28	20.73
3-Bromophenol	9.01	18.52	18.25	18.66	18.27
2-trifuoromethylphenol	8.42		17.63	18.00	17.65
3-trifluoromethylphenol	9.06		18.26	18.67	18.28
4-trifuoromethylphenol	8.68		17.90	18.29	17.92
3,5-Ditrifuoromethylphenol	8.26		17.46	17.82	17.48
3-Chlorophenol	9.02		18.30	18.72	18.33
3-Methylphenol	10.1		19.39	19.89	19.42
4-Bromophenol	9.36	18.88	18.61	19.05	18.64
4-cyanophenol	7.95	18.96	18.64	19.08	18.66
4-Chlorophenol	9.38		17.13	17.47	17.15
4-Methylphenol	10.28		19.58	20.09	19.61
4-Hydroxybenzaldehyde	7.51		16.67	16.97	16.69
4-tert-Butylphenol	10.31		19.61	20.12	19.64
4-[(E)-2-(4-Nitrophenyl)-1-ethenyl]phenol	9.39		18.65	19.09	18.67
2,3-Dimethylphenol	10.54		19.86	20.38	19.89
3-chloro-4-nitrophenol	6.49		16.80	17.12	16.83
2,4-Dinitrophenol	4.1		15.59	15.83	15.61
2-Chloro-4-bromophenol	7.64		13.08	13.14	13.09

2,4-Dimethylphenol	10.6		19.92	20.45	19.95
2-Chloro-4-phenylphenol	8.07		17.26	17.60	17.28
2,4-Di-tert-butylphenol	11.57		20.94	21.54	20.97
2,5-Dinitrophenol	5.22		14.26	14.40	14.28
2,5-Dimethylphenol	10.41		19.72	20.23	19.75
2,6-Dinitrophenol	3.74		12.70	12.73	12.71
3,4-Dinitrophenol	5.42		19.91	20.44	19.94
2,6-Dimethylphenol	10.59		14.47	14.62	14.49
3,4-Dichloroohenol	8.58		19.67	20.18	19.70
3,4-Dimethylphenol	10.36		17.79	18.18	17.82
3,5-Dichlorophenol	8.18	17.04	17.37	17.73	17.40
3,5-Dinitrophenol	6.66	13.4	15.77	16.02	15.79
3,5-Dimethylphenol	10.2		19.50	20.00	19.53
3,5-Di-tert-butylphenol	10.29		19.59	20.10	19.62
2,4,6-Tribromophenol	6.1		15.18	15.39	15.20
2,6-Dinitro-4-chlorophenol	2.97		12.32	12.33	12.33
3,4,5-Trichlorophenol	7.9		11.89	11.87	11.90
2,6-Dibromo-4-nitrophenol	3.38		17.08	17.41	17.10
2,4,6-trimethylphenol	10.86		20.19	20.74	20.22
2,6-Di-tert-butyl-4-nitrophenol	6.65		15.76	16.01	15.78
3,3-Di-tert-butyl-4-hydroxybenzaldehyde	8.05		17.24	17.58	17.26
Bromophenol blue	4.17		13.15	13.22	13.17
Bromocresol green	4.93		13.95	14.07	13.97
Bromocresol purple	6.39		15.49	15.71	15.51
Bromothymol blue	7.35		16.50	16.79	16.52
thymol blue	7.1		16.24	16.51	16.26
phenol red	7.9		17.08	17.41	17.10
phenolphthalein	9.5		18.76	19.21	18.79

Table S20. The pK_a values of the selected carboxylic acids (aliphatic and aromatic derivatives) in 2-methyl-2-propanol solvent estimated from the correlation equation.

compound	$pK_{a,water}^{exp}$	pK_a^{exp}	$pK_{a,B3LYP}$	$pK_{a,M062X}$	$pK_{a,MP2}$
2-Bromoacetic acid	2.9		11.82	11.79	11.83
2-Fluoroacetic acid	2.82		11.73	11.70	11.74
2-Lodoacetic acid	3.13		12.06	12.05	12.07
2-Hydroxyacetic acid	3.85		12.82	12.86	12.83
2-Sulfanylacetic acid	3.73		12.69	12.72	12.70
2-Phenylacetic acid	4.31		13.30	13.37	13.32
Propanoic acid	4.88		13.90	14.01	13.92
3-Bromopropanoic acid	4.04		13.02	13.07	13.03
3-Chloropropanoic acid	4.09		13.07	13.13	13.08
3-Iodopropanoic acid	4.05		13.03	13.08	13.04
3-Hydroxypropanoic acid	4.51		13.51	13.60	13.53
2-Bromopropanoic acid	3		11.92	11.90	11.93
2-Chloropropanoic acid	2.9		11.82	11.79	11.83
2,3-Dibromopropanoic acid	2.36	11.71	11.25	11.18	11.26
2,3-Dichloropropanoic acid	2.85		11.77	11.73	11.78
Malonic acid (pK1)	2.83		11.74	11.71	11.75
Malonic acid (pK2)	5.66		14.72	14.89	14.74
Methylmalonic(pK1)	2.94	12.77	11.86	11.83	11.87
methylmalonic(pK2)	5.76		14.83	15.00	14.84
Ethylmalonic(pK1)	3.35	12.52	12.29	12.29	12.30
Ethylmalonic(pK2)	5.83		14.90	15.08	14.92
Acrylic acid	4.25		13.24	13.31	13.25
(E)-4-Oxo-4-[4-vinyloxy)anilino]-2-butenoic acid	3.66		12.62	12.64	12.63

(E)-4-[4-Ethoxyanilino]-4-oxo-2-butenoic acid	3.63		12.59	12.61	12.60
Fumaric acid (pK2)	4.6		13.61	13.70	13.62
Atropic acid	4.44		13.44	13.52	13.45
2-(3-Chlorophenyl)acrylic acid	4.29		13.28	13.35	13.29
2-(3-Nitrophenyl)acrylic acid	4.12		13.10	13.16	13.11
2-(4-Nitrophenyl)acrylic acid	4.05		13.03	13.08	13.04
1-Cyclopropanecarboxilic acid	4.83		13.85	13.96	13.86
Butanoic acid	4.82		13.84	13.95	13.85
3-Bromobutanoic acid	4.01		12.99	13.04	13.00
3-Chlorobutanoic acid	4.17		13.15	13.22	13.17
2-Chlorobutanoic acid	2.92		11.84	11.81	11.85
Succinic acid (pK1)	4.2		13.19	13.25	13.20
Succinic acid (pK2)	5.61		14.67	14.84	14.69
Methylsuccinic(pK1)	4.49	14.22	13.49	13.58	13.51
Tartaric acid (pK1)	3.01		11.93	11.91	11.94
d-(sec-Butyl)tartrate	3.38		12.32	12.33	12.33
meso-(sec-Butyl)tartrate	3.68		12.64	12.66	12.65
4-Oxo-4-[4-(vinylox)anilino]butanoic acid	4.64		13.65	13.74	13.66
4-(4-Ethoxyanilino]-4-oxobutanoic acid	4.55		13.55	13.64	13.57
1-Cyclobutanecarboxylic acid	4.79		13.81	13.91	13.82
1-Cyclobutanecarboxylic acid	4.99		14.02	14.14	14.03

1-Cyclohexanecarboxylic acid	4.9	13.92	14.04	13.94
cis-2-Hydroxy-1-cyclohexanecarboxylic acid	4.8	13.82	13.92	13.83
trans-2-Hydroxy-1-cyclohexanecarboxylic acid	4.82	13.84	13.95	13.85
cis-3-Hydroxy-1-cyclophexanecarboxylic acid	4.6	13.61	13.70	13.62
trans-3-Hydroxy-1-cyclohexanecarboxcylic acid	4.82	13.84	13.95	13.85
cis-4-Hydroxy-1-cyclohexanecarboxylic acid	4.84	13.86	13.97	13.87
trans-4-Hydroxy-1-cyclohexanecarboxylic acid	4.69	13.70	13.80	13.72
Heptanedioic acid	4.46	13.46	13.54	13.47
Octanedioic acid	4.5	13.50	13.59	13.52
Bicyclo[2,2,2]octane-1-carboxylic acid	5.08	14.11	14.24	14.13
4-Bromobicyclo[2,2,2]octane-1-carboxylic acid	4.62	13.63	13.72	13.64
4-Cyanobicyclo[2,2,2]octane-1-carboxylic acid	4.55	13.55	13.64	13.57
Bicyclo[2,2,2]octane-1,4-dicarboxylic acid (pK1)	4.47	13.47	13.55	13.48
Bicyclo[2,2,2]octane-1,4-dicarboxylic acid (pK2)	5.46	14.51	14.67	14.53
4-(1,1,1-	4.08	13.06	13.11	13.07

Trimethylammonio)bicyclo [2,2,2]octane-1-oDecanedioic acid				
Decanedioic acid	4.5	13.50	13.59	13.52
2-Fluorobenzoic acid	3.57	12.52	12.54	12.53
2-Bromobenzoic acid	2.85	11.77	11.73	11.78
2-Chlorobenzoic acid	2.92	11.84	11.81	11.85
2-lodobenzoic acid	2.85	11.77	11.73	11.78
2-Methylbenzoic acid	3.91	12.88	12.92	12.89
2-Nitrobenzoic acid	2.19	11.07	10.99	11.08
2-Methoxybenzoic acid	4.09	13.07	13.13	13.08
2-[4-(Vinyloxy)anilino]benzoic acid	3.8	12.77	12.80	12.78
2-[Methyl-4-(vinyloxy)anilino]benzoic acid	4.34	13.33	13.41	13.35
3-Fluorobenzoic acid	3.88	12.85	12.89	12.86
3-Chlorobenzoic acid	3.8	12.77	12.80	12.78
3-lodobenzoic acid	3.82	12.79	12.82	12.80
3-Hydroxybenzoic acid	4.01	12.99	13.04	13.00
3-Acetamidobenzoic acid	4.06	13.04	13.09	13.05
3-Nitrobenzoic acid	3.47	12.42	12.43	12.43
3-Methoxynbenzoic acid	4.12	13.10	13.16	13.11
3-Phenoxybenzoic acid	3.95	12.92	12.97	12.94
3-Mercaptgobenzoic acid	3.96	12.93	12.98	12.95
3-Sulfamylbenzoic acid	3.68	12.64	12.66	12.65
3-(Methylsulfonyl)benzoic acid	3.53	12.48	12.50	12.49
3-Methylbenzoic acid	4.28	13.27	13.34	13.28
3-(Trifluoromethyl)benzoic	3.75	12.71	12.74	12.72

acid				
3-Cyanobenzoic acid	3.6	12.55	12.57	12.57
3-Acetylbenzoic acid	3.83	12.80	12.83	12.81
4-Fluorobenzoic acid	4.15	13.13	13.19	13.15
4-Bromobenzoic acid	3.99	12.96	13.01	12.98
4-Chlorobenzoic acid	4	12.98	13.02	12.99
4-lodobenzoic acid	3.98	12.95	13.00	12.97
4-Aminobenzoic acid	4.82	13.84	13.95	13.85
4-Acetamidobenzoic acid	4.3	13.29	13.36	13.30
4-(Dimethylamino)benzoic acid	5.03	14.06	14.18	14.07
4-Hydroxybenzoic acid	4.55	13.55	13.64	13.57
4-Methoxybenzoic acid	4.25	13.24	13.31	13.25
4-(Methylmercapto)benzoic acid	4.2	13.19	13.25	13.20
4-Sulfamylbenzoic acid	3.63	12.59	12.61	12.60
4-(Methylsulfonyl)benzoic acid	3.48	12.43	12.44	12.44
4-Methylbenzoic acid	4.38	13.38	13.45	13.39
4-Cyanobenzoic acid	3.53	12.48	12.50	12.49
4-Acetylbenzoic acid	3.7	12.66	12.69	12.67
4-tert-Butylbenzoic acid	4.36	13.35	13.43	13.37
2,4-Dichlorobenzoic acid	2.76	11.67	11.63	11.68
2,4-Dinitrobenzoic acid	1.43	10.27	10.13	10.28
2,4-Dimethylbenzoic acid	4.22	13.21	13.27	13.22
2,6-Dichlorobenzoic acid	1.82	10.68	10.57	10.69
2,6-Dinitrobenzoic acid	1.14	9.97	9.81	9.97
3,4-Dimethoxybenzoic acid	4.44	13.44	13.52	13.45
3,4-Dinitrobenzoic acid	2.82	11.73	11.70	11.74
3-Methyl-4-chlorobenzoic acid	4.07	13.05	13.10	13.06

3-Methyl-4-nitrobenzoic acid	3.65		12.61	12.63	12.62
4-Chloro-3-nitrobenzoic acid	3.34	11.77	12.28	12.28	12.29
3,5-Dichlorobenzoic acid	3.56		12.51	12.53	12.52
3,5-Dinitrobenzoic acid	2.82	10.6	11.73	11.70	11.74
2,4,6-Trimethylbenzoic acid	3.45		12.40	12.41	12.41

Table S21. The pK_a values of the selected phenol derivatives in ACN solvent estimated from the correlation equation.

Compound	$pK_{a,water}^{exp}$	pK_a^{exp}	$pK_{a,B3LYP}$	$pK_{a,M062X}$	$pK_{a,MP2}$
1-Naphthol	9.4		24.67	24.52	24.67
2-Chlorophenol	8.51		23.77	23.62	23.75
2-Fluorophenol	8.73		23.99	23.84	23.98
2-Nitrophenol	7.23	22.1	22.47	22.33	22.43
2-Methylphenol	10.31		25.59	25.43	25.60
2-Methoxyphenol	9.9		25.17	25.02	25.18
2-tert-Butylphenol	11.34		26.63	26.47	26.66
3-Bromophenol	9.01		24.27	24.12	24.26
2-trifuoromethylphenol	8.42		23.67	23.53	23.66
3-trifluoromethylphenol	9.06	25	24.28	24.13	24.27
4-trifuoromethylphenol	8.68		23.94	23.79	23.92
3,5-Ditrifuoromethylphenol	8.26		23.51	23.37	23.49
3-Chlorophenol	9.02	24.9	24.32	24.17	24.32
3-Methylphenol	10.1		25.38	25.22	25.39
4-Bromophenol	9.36	25.6	24.63	24.48	24.62
4-cyanophenol	7.95		24.65	24.50	24.64
4-Chlorophenol	9.38	22.7	23.20	23.06	23.17
4-Methylphenol	10.28		25.56	25.40	25.57
4-Hydroxybenzaldehyde	7.51		22.75	22.62	22.72
4-tert-Butylphenol	10.31		25.59	25.43	25.60
4-[(E)-2-(4-Nitrophenyl)-1-ethenyl]phenol	9.39		24.66	24.51	24.66
2,3-Dimethylphenol	10.54		25.82	25.66	25.84
3-chloro-4-nitrophenol	6.49		22.88	22.75	22.85
2,4-Dinitrophenol	4.1	19.9	21.72	21.59	21.67
2-Chloro-4-bromophenol	7.64	16	19.30	19.19	19.21

2,4-Dimethylphenol	10.6		25.88	25.72	25.90
2-Chloro-4-phenylphenol	8.07		23.32	23.18	23.30
2,4-Di-tert-butylphenol	11.57		26.87	26.70	26.90
2,5-Dinitrophenol	5.22		20.43	20.31	20.36
2,5-Dimethylphenol	10.41		25.69	25.53	25.71
2,6-Dinitrophenol	3.74	16.45	18.93	18.83	18.83
3,4-Dinitrophenol	5.42		25.87	25.71	25.89
2,6-Dimethylphenol	10.59	17.9	20.63	20.51	20.57
3,4-Dichloroohenol	8.58		25.64	25.48	25.65
3,4-Dimethylphenol	10.36	24	23.84	23.69	23.82
3,5-Dichlorophenol	8.18	23.3	23.43	23.29	23.41
3,5-Dinitrophenol	6.66	20.5	21.89	21.76	21.84
3,5-Dimethylphenol	10.2		25.48	25.32	25.49
3,5-Di-tert-butylphenol	10.29		25.57	25.41	25.58
2,4,6-Tribromophenol	6.1		21.32	21.20	21.27
2,6-Dinitro-4-chlorophenol	2.97		18.57	18.46	18.46
3,4,5-Trichlorophenol	7.9	15	18.15	18.05	18.04
2,6-Dibromo-4-nitrophenol	3.38	22.5	23.15	23.01	23.12
2,4,6-trimethylphenol	10.86		26.15	25.98	26.17
2,6-Di-tert-butyl-4-nitrophenol	6.65	19	21.88	21.75	21.83
3,3-Di-tert-butyl-4-hydroxybenzaldehyde	8.05		23.30	23.16	23.27
Bromophenol blue	4.17		19.37	19.26	19.28
Bromocresol green	4.93		20.14	20.02	20.06
Bromocresol purple	6.39		21.62	21.49	21.56
Bromothymol blue	7.35		22.59	22.46	22.55
thymol blue	7.1		22.34	22.20	22.30
phenol red	7.9		23.15	23.01	23.12
phenolphthalein	9.5		24.77	24.62	24.77

Table S22. The pK_a values of the selected carboxylic acids (aliphatic and aromatic derivatives) in ACN solvent estimated from the correlation equation.

compound	$pK_{a,water}^{exp}$	pK_a^{exp}	$pK_{a,B3LYP}$	$pK_{a,M062X}$	$pK_{a,MP2}$
2-Bromoacetic acid	2.9		18.08	17.98	17.97
2-Fluoroacetic acid	2.82		18.00	17.90	17.89
2-Lodoacetic acid	3.13		18.31	18.21	18.21
2-Hydroxyacetic acid	3.85		19.04	18.94	18.95
2-Sulfanylacetic acid	3.73		18.92	18.82	18.82
2-Phenylacetic acid	4.31		19.51	19.40	19.42
Propanoic acid	4.88		20.09	19.97	20.01
3-Bromopropanoic acid	4.04		19.24	19.13	19.14
3-Chloropropanoic acid	4.09		19.29	19.18	19.20
3-Iodopropanoic acid	4.05		19.25	19.14	19.15
3-Hydroxypropanoic acid	4.51		19.71	19.60	19.63
2-Bromopropanoic acid	3		18.18	18.08	18.07
2-Chloropropanoic acid	2.9		18.08	17.98	17.97
2,3-Dibromopropanoic acid	2.36	17.1	17.53	17.44	17.41
2,3-Dichloropropanoic acid	2.85		18.03	17.93	17.92
Malonic acid (pK1)	2.83		18.01	17.91	17.90
Malonic acid (pK2)	5.66		20.88	20.76	20.81
Methylmalonic(pK1)	2.94		18.12	18.02	18.01
methylmalonic(pK2)	5.76		20.98	20.86	20.92
Ethylmalonic(pK1)	3.35		18.54	18.43	18.43
Ethylmalonic(pK2)	5.83		21.05	20.93	20.99
Acrylic acid	4.25		19.45	19.34	19.36
(E)-4-Oxo-4-[4-vinyloxy)anilino]-2-butenoic acid	3.66		18.85	18.75	18.75

(E)-4-[4-Ethoxyanilino]-4-oxo-2-butenoic acid	3.63	18.82	18.71	18.72
Fumaric acid (pK2)	4.6	19.80	19.69	19.72
Atropic acid	4.44	19.64	19.53	19.56
2-(3-Chlorophenyl)acrylic acid	4.29	19.49	19.38	19.40
2-(3-Nitrophenyl)acrylic acid	4.12	19.32	19.21	19.23
2-(4-Nitrophenyl)acrylic acid	4.05	19.25	19.14	19.15
1-Cyclopropanecarboxilic acid	4.83	20.04	19.92	19.96
Butanoic acid	4.82	20.03	19.91	19.95
3-Bromobutanoic acid	4.01	19.21	19.10	19.11
3-Chlorobutanoic acid	4.17	19.37	19.26	19.28
2-Chlorobutanoic acid	2.92	18.10	18.00	17.99
Succinic acid (pK1)	4.2	19.40	19.29	19.31
Succinic acid (pK2)	5.61	20.83	20.71	20.76
Methylsuccinic(pK1)	4.49	19.69	19.58	19.61
Tartaric acid (pK1)	3.01	18.19	18.09	18.08
d-(sec-Butyl)tartrate	3.38	18.57	18.46	18.46
meso-(sec-Butyl)tartrate	3.68	18.87	18.77	18.77
4-Oxo-4-[4-(vinylox)anilino]butanoic acid	4.64	19.84	19.73	19.76
4-(4-Ethoxyanilino]-4-oxobutanoic acid	4.55	19.75	19.64	19.67
1-Cyclobutanecarboxylic acid	4.79	20.00	19.88	19.92
1-Cyclobutanecarboxylic acid	4.99	20.20	20.08	20.12

1-Cyclohexanecarboxylic acid	4.9	20.11	19.99	20.03
cis-2-Hydroxy-1-cyclohexanecarboxylic acid	4.8	20.01	19.89	19.93
trans-2-Hydroxy-1-cyclohexanecarboxylic acid	4.82	20.03	19.91	19.95
cis-3-Hydroxy-1-cyclophexanecarboxylic acid	4.6	19.80	19.69	19.72
trans-3-Hydroxy-1-cyclohexanecarboxcylic acid	4.82	20.03	19.91	19.95
cis-4-Hydroxy-1-cyclohexanecarboxylic acid	4.84	20.05	19.93	19.97
trans-4-Hydroxy-1-cyclohexanecarboxylic acid	4.69	19.89	19.78	19.81
Heptanedioic acid	4.46	19.66	19.55	19.58
Octanedioic acid	4.5	19.70	19.59	19.62
Bicyclo[2,2,2]octane-1-carboxylic acid	5.08	20.29	20.17	20.22
4-Bromobicyclo[2,2,2]octane-1-carboxylic acid	4.62	19.82	19.71	19.74
4-Cyanobicyclo[2,2,2]octane-1-carboxylic acid	4.55	19.75	19.64	19.67
Bicyclo[2,2,2]octane-1,4-dicarboxylic acid (pK1)	4.47	19.67	19.56	19.59
Bicyclo[2,2,2]octane-1,4-dicarboxylic acid (pK2)	5.46	20.67	20.56	20.61
4-(1,1,1-	4.08	19.28	19.17	19.18

Trimethylammonio)bicyclo [2,2,2]octane-1-oDecanedioic acid				
Decanedioic acid	4.5	19.70	19.59	19.62
2-Fluorobenzoic acid	3.57	18.76	18.65	18.66
2-Bromobenzoic acid	2.85	18.03	17.93	17.92
2-Chlorobenzoic acid	2.92	18.10	18.00	17.99
2-lodobenzoic acid	2.85	18.03	17.93	17.92
2-Methylbenzoic acid	3.91	19.10	19.00	19.01
2-Nitrobenzoic acid	2.19	17.36	17.27	17.24
2-Methoxybenzoic acid	4.09	19.29	19.18	19.20
2-[4-(Vinyloxy)anilino]benzoic acid	3.8	18.99	18.89	18.90
2-[Methyl-4-(vinyloxy)anilino]benzoic acid	4.34	19.54	19.43	19.45
3-Fluorobenzoic acid	3.88	19.07	18.97	18.98
3-Chlorobenzoic acid	3.8	18.99	18.89	18.90
3-lodobenzoic acid	3.82	19.01	18.91	18.92
3-Hydroxybenzoic acid	4.01	19.21	19.10	19.11
3-Acetamidobenzoic acid	4.06	19.26	19.15	19.16
3-Nitrobenzoic acid	3.47	18.66	18.55	18.56
3-Methoxynbenzoic acid	4.12	19.32	19.21	19.23
3-Phenoxybenzoic acid	3.95	19.15	19.04	19.05
3-Mercaptgobenzoic acid	3.96	19.16	19.05	19.06
3-Sulfamylbenzoic acid	3.68	18.87	18.77	18.77
3-(Methylsulfonyl)benzoic acid	3.53	18.72	18.61	18.62
3-Methylbenzoic acid	4.28	19.48	19.37	19.39
3-(Trifluoromethyl)benzoic	3.75	18.94	18.84	18.84

acid				
3-Cyanobenzoic acid	3.6	18.79	18.68	18.69
3-Acetylbenzoic acid	3.83	19.02	18.92	18.93
4-Fluorobenzoic acid	4.15	19.35	19.24	19.26
4-Bromobenzoic acid	3.99	19.19	19.08	19.09
4-Chlorobenzoic acid	4	19.20	19.09	19.10
4-Iodobenzoic acid	3.98	19.18	19.07	19.08
4-Aminobenzoic acid	4.82	20.03	19.91	19.95
4-Acetamidobenzoic acid	4.3	19.50	19.39	19.41
4-(Dimethylamino)benzoic acid	5.03	20.24	20.12	20.16
4-Hydroxybenzoic acid	4.55	19.75	19.64	19.67
4-Methoxybenzoic acid	4.25	19.45	19.34	19.36
4-(Methylmercapto)benzoic acid	4.2	19.40	19.29	19.31
4-Sulfamylbenzoic acid	3.63	18.82	18.71	18.72
4-(Methylsulfonyl)benzoic acid	3.48	18.67	18.56	18.57
4-Methylbenzoic acid	4.38	19.58	19.47	19.49
4-Cyanobenzoic acid	3.53	18.72	18.61	18.62
4-Acetylbenzoic acid	3.7	18.89	18.79	18.79
4-tert-Butylbenzoic acid	4.36	19.56	19.45	19.47
2,4-Dichlorobenzoic acid	2.76	17.94	17.84	17.82
2,4-Dinitrobenzoic acid	1.43	16.59	16.50	16.45
2,4-Dimethylbenzoic acid	4.22	19.42	19.31	19.33
2,6-Dichlorobenzoic acid	1.82	16.99	16.90	16.86
2,6-Dinitrobenzoic acid	1.14	16.30	16.21	16.16
3,4-Dimethoxybenzoic acid	4.44	19.64	19.53	19.56
3,4-Dinitrobenzoic acid	2.82	18.00	17.90	17.89
3-Methyl-4-chlorobenzoic acid	4.07	19.27	19.16	19.17

3-Methyl-4-nitrobenzoic acid	3.65		18.84	18.74	18.74
4-Chloro-3-nitrobenzoic acid	3.34	18.5	18.53	18.42	18.42
3,5-Dichlorobenzoic acid	3.56		18.75	18.64	18.65
3,5-Dinitrobenzoic acid	2.82		18.00	17.90	17.89
2,4,6-Trimethylbenzoic acid	3.45		18.64	18.53	18.54

Table S23. The pK_a values of the selected phenol derivatives in DMF solvent estimated from the correlation equation.

Compound	$pK_{a,water}^{exp}$	pK_a^{exp}	$pK_{a,B3LYP}$	$pK_{a,M062X}$	$pK_{a,MP2}$
1-Naphthol	9.4		15.70	15.55	15.73
2-Chlorophenol	8.51		14.81	14.67	14.83
2-Fluorophenol	8.73		15.03	14.88	15.06
2-Nitrophenol	7.23	12.2	13.54	13.40	13.54
2-Methylphenol	10.31		16.61	16.45	16.65
2-Methoxyphenol	9.9		16.20	16.04	16.24
2-tert-Butylphenol	11.34		17.64	17.46	17.70
3-Bromophenol	9.01		15.31	15.16	15.34
2-trifuoromethylphenol	8.42	16.2	15.32	15.17	15.35
3-trifluoromethylphenol	9.06	15.7	14.72	14.58	14.74
4-trifuoromethylphenol	8.68		15.36	15.21	15.39
3,5-Ditrifuoromethylphenol	8.26		14.98	14.83	15.01
3-Chlorophenol	9.02		14.56	14.42	14.58
3-Methylphenol	10.1		16.40	16.24	16.44
4-Bromophenol	9.36		15.66	15.51	15.69
4-cyanophenol	7.95	16.7	15.68	15.53	15.71
4-Chlorophenol	9.38		14.26	14.11	14.27
4-Methylphenol	10.28		16.58	16.42	16.62
4-Hydroxybenzaldehyde	7.51		13.82	13.68	13.82
4-tert-Butylphenol	10.31		16.61	16.45	16.65
4-[(E)-2-(4-Nitrophenyl)-1-ethenyl]phenol	9.39		15.69	15.54	15.72
2,3-Dimethylphenol	10.54		16.84	16.67	16.89
3-chloro-4-nitrophenol	6.49		13.95	13.81	13.96
2,4-Dinitrophenol	4.1		12.80	12.67	12.79

2-Chloro-4-bromophenol	7.64	6.3	10.42	10.31	10.38
2,4-Dimethylphenol	10.6		16.90	16.73	16.95
2-Chloro-4-phenylphenol	8.07		14.38	14.23	14.39
2,4-Di-tert-butylphenol	11.57		17.87	17.69	17.93
2,5-Dinitrophenol	5.22	8.7	11.53	11.41	11.51
2,5-Dimethylphenol	10.41		16.71	16.54	16.76
2,6-Dinitrophenol	3.74	6.18	10.06	9.95	10.01
3,4-Dinitrophenol	5.42		16.89	16.72	16.94
2,6-Dimethylphenol	10.59		11.73	11.61	11.71
3,4-Dichloroohenol	8.58		16.66	16.49	16.70
3,4-Dimethylphenol	10.36		14.88	14.73	14.91
3,5-Dichlorophenol	8.18		14.49	14.34	14.50
3,5-Dinitrophenol	6.66		12.97	12.84	12.96
3,5-Dimethylphenol	10.2		16.50	16.34	16.54
3,5-Di-tert-butylphenol	10.29		16.59	16.43	16.63
2,4,6-Tribromophenol	6.1		12.41	12.28	12.40
2,6-Dinitro-4-chlorophenol	2.97	4.7	9.70	9.59	9.65
3,4,5-Trichlorophenol	7.9		9.29	9.19	9.23
2,6-Dibromo-4-nitrophenol	3.38		14.21	14.06	14.22
2,4,6-trimethylphenol	10.86		17.16	16.99	17.21
2,6-Di-tert-butyl-4-nitrophenol	6.65		12.96	12.83	12.95
3,3-Di-tert-butyl-4-hydroxybenzaldehyde	8.05		14.36	14.21	14.37
Bromophenol blue	4.17		10.49	10.37	10.45
Bromocresol green	4.93		11.24	11.13	11.22
Bromocresol purple	6.39		12.70	12.57	12.69
Bromothymol blue	7.35		13.66	13.52	13.66
thymol blue	7.1		13.41	13.27	13.41

phenol red	7.9	14.21	14.06	14.22
phenolphthalein	9.5	15.80	15.64	15.84

Table S24. The pK_a values of the selected carboxylic acids (aliphatic and aromatic derivatives) in DMF solvent estimated from the correlation equation.

compound	$pK_{a,water}^{exp}$	pK_a^{exp}	$pK_{a,B3LYP}$	$pK_{a,M062X}$	$pK_{a,MP2}$
2-Bromoacetic acid	2.9		9.22	9.12	9.16
2-Fluoroacetic acid	2.82		9.14	9.04	9.08
2-Lodoacetic acid	3.13		9.45	9.35	9.40
2-Hydroxyacetic acid	3.85		10.17	10.06	10.12
2-Sulfanylacetic acid	3.73		10.05	9.94	10.00
2-Phenylacetic acid	4.31		10.62	10.51	10.59
Propanoic acid	4.88		11.19	11.08	11.17
3-Bromopropanoic acid	4.04		10.36	10.25	10.32
3-Chloropropanoic acid	4.09		10.41	10.30	10.37
3-Iodopropanoic acid	4.05		10.37	10.26	10.33
3-Hydroxypropanoic acid	4.51		10.82	10.71	10.79
2-Bromopropanoic acid	3		9.32	9.22	9.26
2-Chloropropanoic acid	2.9		9.22	9.12	9.16
2,3-Dibromopropanoic acid	2.36		8.68	8.58	8.62
2,3-Dichloropropanoic acid	2.85		9.17	9.07	9.11
Malonic acid (pK1)	2.83		9.15	9.05	9.09
Malonic acid (pK2)	5.66		11.97	11.85	11.95
Methylmalonic(pK1)	2.94		9.26	9.16	9.20
methylmalonic(pK2)	5.76		12.07	11.95	12.05
Ethylmalonic(pK1)	3.35		9.67	9.56	9.62
Ethylmalonic(pK2)	5.83		12.14	12.02	12.13
Acrylic acid	4.25		10.56	10.45	10.53
(E)-4-Oxo-4-[4-vinyloxy)anilino]-2-	3.66		9.98	9.87	9.93

butenoic acid				
(E)-4-[4-Ethoxyanilino]-4-oxo-2-butenoic acid	3.63	9.95	9.84	9.90
Fumaric acid (pK2)	4.6	10.91	10.80	10.88
Atropic acid	4.44	10.75	10.64	10.72
2-(3-Chlorophenyl)acrylic acid	4.29	10.60	10.49	10.57
2-(3-Nitrophenyl)acrylic acid	4.12	10.44	10.32	10.40
2-(4-Nitrophenyl)acrylic acid	4.05	10.37	10.26	10.33
1-Cyclopropanecarboxilic acid	4.83	11.14	11.03	11.11
Butanoic acid	4.82	11.13	11.02	11.10
3-Bromobutanoic acid	4.01	10.33	10.22	10.29
3-Chlorobutanoic acid	4.17	10.49	10.37	10.45
2-Chlorobutanoic acid	2.92	9.24	9.14	9.18
Succinic acid (pK1)	4.2	10.52	10.40	10.48
Succinic acid (pK2)	5.61	11.92	11.80	11.90
Methylsuccinic(pK1)	4.49	10.80	10.69	10.77
Tartaric acid (pK1)	3.01	9.33	9.23	9.27
d-(sec-Butyl)tartrate	3.38	9.70	9.59	9.65
meso-(sec-Butyl)tartrate	3.68	10.00	9.89	9.95
4-Oxo-4-[4-(vinylox)anilino]butanoic acid	4.64	10.95	10.84	10.92
4-(4-Ethoxyanilino]-4-oxobutanoic acid	4.55	10.86	10.75	10.83
1-Cyclobutanecarboxylic acid	4.79	11.10	10.99	11.07
1-Cyclobutanecarboxylic	4.99	11.30	11.19	11.28

acid				
1-Cyclohexanecarboxylic acid	4.9	11.21	11.10	11.19
cis-2-Hydroxy-1-cyclohexanecarboxylic acid	4.8	11.11	11.00	11.08
trans-2-Hydroxy-1-cyclohexanecarboxylic acid	4.82	11.13	11.02	11.10
cis-3-Hydroxy-1-cyclophexanecarboxylic acid	4.6	10.91	10.80	10.88
trans-3-Hydroxy-1-cyclohexanecarboxcylic acid	4.82	11.13	11.02	11.10
cis-4-Hydroxy-1-cyclohexanecarboxylic acid	4.84	11.15	11.04	11.12
trans-4-Hydroxy-1-cyclohexanecarboxylic acid	4.69	11.00	10.89	10.97
Heptanedioic acid	4.46	10.77	10.66	10.74
Octanedioic acid	4.5	10.81	10.70	10.78
Bicyclo[2,2,2]octane-1-carboxylic acid	5.08	11.39	11.27	11.37
4-Bromobicyclo[2,2,2]octane-1-carboxylic acid	4.62	10.93	10.82	10.90
4-Cyanobicyclo[2,2,2]octane-1-carboxylic acid	4.55	10.86	10.75	10.83
Bicyclo[2,2,2]octane-1,4-dicarboxylic acid (pK1)	4.47	10.78	10.67	10.75
Bicyclo[2,2,2]octane-1,4-dicarboxylic acid (pK2)	5.46	11.77	11.65	11.75

4-(1,1,1-Trimethylammonio)bicyclo [2,2,2]octane-1-	4.08			
oDecanedioic acid		10.40	10.29	10.36
Decanedioic acid	4.5	10.81	10.70	10.78
2-Fluorobenzoic acid	3.57	9.89	9.78	9.84
2-Bromobenzoic acid	2.85	9.17	9.07	9.11
2-Chlorobenzoic acid	2.92	9.24	9.14	9.18
2-lodobenzoic acid	2.85	9.17	9.07	9.11
2-Methylbenzoic acid	3.91	10.23	10.12	10.18
2-Nitrobenzoic acid	2.19	8.51	8.42	8.45
2-Methoxybenzoic acid	4.09	10.41	10.30	10.37
2-[4-(Vinyloxy)anilino]benzoic	3.8			
acid		10.12	10.01	10.07
2-[Methyl-4-(vinyloxy)anilino]benzoic	4.34			
acid		10.65	10.54	10.62
3-Fluorobenzoic acid	3.88	10.20	10.09	10.15
3-Chlorobenzoic acid	3.8	10.12	10.01	10.07
3-lodobenzoic acid	3.82	10.14	10.03	10.09
3-Hydroxybenzoic acid	4.01	10.33	10.22	10.29
3-Acetamidobenzoic acid	4.06	10.38	10.27	10.34
3-Nitrobenzoic acid	3.47	9.79	9.68	9.74
3-Methoxynbenzoic acid	4.12	10.44	10.32	10.40
3-Phenoxybenzoic acid	3.95	10.27	10.16	10.22
3-Mercaptgobenzoic acid	3.96	10.28	10.17	10.24
3-Sulfamylbenzoic acid	3.68	10.00	9.89	9.95
3-(Methylsulfonyl)benzoic	3.53			
acid		9.85	9.74	9.80
3-Methylbenzoic acid	4.28	10.59	10.48	10.56

3-(Trifluoromethyl)benzoic acid	3.75	10.07	9.96	10.02
3-Cyanobenzoic acid	3.6	9.92	9.81	9.87
3-Acetylbenzoic acid	3.83	10.15	10.04	10.10
4-Fluorobenzoic acid	4.15	10.47	10.35	10.43
4-Bromobenzoic acid	3.99	10.31	10.20	10.27
4-Chlorobenzoic acid	4	10.32	10.21	10.28
4-lodobenzoic acid	3.98	10.30	10.19	10.26
4-Aminobenzoic acid	4.82	11.13	11.02	11.10
4-Acetamidobenzoic acid	4.3	10.61	10.50	10.58
4-(Dimethylamino)benzoic acid	5.03	11.34	11.22	11.32
4-Hydroxybenzoic acid	4.55	10.86	10.75	10.83
4-Methoxybenzoic acid	4.25	10.56	10.45	10.53
4-(Methylmercapto)benzoic acid	4.2	10.52	10.40	10.48
4-Sulfamylbenzoic acid	3.63	9.95	9.84	9.90
4-(Methylsulfonyl)benzoic acid	3.48	9.80	9.69	9.75
4-Methylbenzoic acid	4.38	10.69	10.58	10.66
4-Cyanobenzoic acid	3.53	9.85	9.74	9.80
4-Acetylbenzoic acid	3.7	10.02	9.91	9.97
4-tert-Butylbenzoic acid	4.36	10.67	10.56	10.64
2,4-Dichlorobenzoic acid	2.76	9.08	8.98	9.02
2,4-Dinitrobenzoic acid	1.43	7.75	7.66	7.68
2,4-Dimethylbenzoic acid	4.22	10.54	10.42	10.50
2,6-Dichlorobenzoic acid	1.82	8.14	8.05	8.07
2,6-Dinitrobenzoic acid	1.14	7.46	7.38	7.38
3,4-Dimethoxybenzoic acid	4.44	10.75	10.64	10.72
3,4-Dinitrobenzoic acid	2.82	9.14	9.04	9.08
3-Methyl-4-chlorobenzoic	4.07	10.39	10.28	10.35

acid				
3-Methyl-4-nitrobenzoic acid	3.65	9.97	9.86	9.92
4-Chloro-3-nitrobenzoic acid	3.34	9.66	9.55	9.61
3,5-Dichlorobenzoic acid	3.56	9.88	9.77	9.83
3,5-Dinitrobenzoic acid	2.82	9.14	9.04	9.08
2,4,6-Trimethylbenzoic acid	3.45	9.77	9.66	9.72

Table S25. The pK_a values of the selected phenol derivatives in DMSO solvent estimated from the correlation equation.

Compound	$pK_{a,water}^{exp}$	pK_{ar}^{exp}	$pK_{a,B3LYP}$	$pK_{a,M062X}$	$pK_{a,MP2}$
1-Naphthol	9.4		14.36	14.01	14.31
2-Chlorophenol	8.51		13.46	13.13	13.41
2-Fluorophenol	8.73		13.68	13.35	13.63
2-Nitrophenol	7.23	11	12.15	11.87	12.12
2-Methylphenol	10.31		15.29	14.90	15.23
2-Methoxyphenol	9.9		14.87	14.50	14.81
2-tert-Butylphenol	11.34		16.34	15.92	16.27
3-Bromophenol	9.01		13.97	13.62	13.92
2-trifuoromethylphenol	8.42		13.98	13.63	13.93
3-trifluoromethylphenol	9.06	14.4	13.37	13.04	13.32
4-trifuoromethylphenol	8.68	14.3	14.02	13.67	13.97
3,5-Ditrifuoromethylphenol	8.26	14.6	13.63	13.30	13.58
3-Chlorophenol	9.02	13.2	13.20	12.88	13.16
3-Methylphenol	10.1		15.07	14.70	15.02
4-Bromophenol	9.36	15.7	14.32	13.97	14.27
4-cyanophenol	7.95		14.34	13.99	14.29
4-Chlorophenol	9.38	13.1	12.89	12.58	12.85
4-Methylphenol	10.28		15.26	14.87	15.20
4-Hydroxybenzaldehyde	7.51		12.44	12.15	12.40
4-tert-Butylphenol	10.31		15.29	14.90	15.23
4-[(E)-2-(4-Nitrophenyl)-1-ethenyl]phenol	9.39		14.35	14.00	14.30
2,3-Dimethylphenol	10.54		15.52	15.13	15.46
3-chloro-4-nitrophenol	6.49		12.57	12.27	12.53
2,4-Dinitrophenol	4.1	9.8	11.40	11.14	11.37

2-Chloro-4-bromophenol	7.64	5.4	8.97	8.79	8.96
2,4-Dimethylphenol	10.6		15.58	15.19	15.52
2-Chloro-4-phenylphenol	8.07		13.01	12.70	12.97
2,4-Di-tert-butylphenol	11.57		16.57	16.14	16.50
2,5-Dinitrophenol	5.22		10.11	9.89	10.09
2,5-Dimethylphenol	10.41		15.39	15.00	15.33
2,6-Dinitrophenol	3.74	4.9	8.60	8.44	8.60
3,4-Dinitrophenol	5.42		15.57	15.18	15.51
2,6-Dimethylphenol	10.59	7.9	10.31	10.09	10.29
3,4-Dichloroohenol	8.58		15.34	14.95	15.28
3,4-Dimethylphenol	10.36	14.2	13.53	13.20	13.48
3,5-Dichlorophenol	8.18	13	13.12	12.81	13.08
3,5-Dinitrophenol	6.66	10.6	11.57	11.31	11.54
3,5-Dimethylphenol	10.2		15.18	14.79	15.12
3,5-Di-tert-butylphenol	10.29		15.27	14.88	15.21
2,4,6-Tribromophenol	6.1		11.01	10.76	10.98
2,6-Dinitro-4-chlorophenol	2.97		8.24	8.08	8.23
3,4,5-Trichlorophenol	7.9	3.6	7.82	7.68	7.82
2,6-Dibromo-4-nitrophenol	3.38	12.5	12.84	12.53	12.80
2,4,6-trimethylphenol	10.86		15.85	15.44	15.78
2,6-Di-tert-butyl-4-nitrophenol	6.65	7.6	11.56	11.30	11.53
3,3-Di-tert-butyl-4-hydroxybenzaldehyde	8.05		12.99	12.68	12.95
Bromophenol blue	4.17		9.04	8.86	9.03
Bromocresol green	4.93	7.3	9.81	9.61	9.80
Bromocresol purple	6.39		11.30	11.04	11.27
Bromothymol blue	7.35	11.3	12.28	11.99	12.24
thymol blue	7.1	11.3	12.02	11.74	11.99
phenol red	7.9	13.7	12.84	12.53	12.80
phenolphthalein	9.5	16.3	14.46	14.10	14.41

Table S26. The pK_a values of the selected carboxylic acids (aliphatic and aromatic derivatives) in DMSO solvent estimated from the correlation equation.

compound	$pK_{a,water}^{exp}$	pK_a^{exp}	$pK_{a,B3LYP}$	$pK_{a,M062X}$	$pK_{a,MP2}$
2-Bromoacetic acid	2.9		7.75	7.61	7.75
2-Fluoroacetic acid	2.82		7.67	7.53	7.67
2-Lodoacetic acid	3.13		7.98	7.84	7.98
2-Hydroxyacetic acid	3.85		8.72	8.54	8.71
2-Sulfanylacetic acid	3.73		8.59	8.43	8.59
2-Phenylacetic acid	4.31		9.18	9.00	9.17
Propanoic acid	4.88		9.76	9.56	9.75
3-Bromopropanoic acid	4.04		8.91	8.73	8.90
3-Chloropropanoic acid	4.09		8.96	8.78	8.95
3-Iodopropanoic acid	4.05		8.92	8.74	8.91
3-Hydroxypropanoic acid	4.51		9.39	9.19	9.37
2-Bromopropanoic acid	3		7.85	7.71	7.85
2-Chloropropanoic acid	2.9		7.75	7.61	7.75
2,3-Dibromopropanoic acid	2.36		7.20	7.08	7.20
2,3-Dichloropropanoic acid	2.85		7.70	7.56	7.70
Malonic acid (pK1)	2.83		7.68	7.54	7.68
Malonic acid (pK2)	5.66		10.56	10.33	10.54
Methylmalonic(pK1)	2.94		7.79	7.65	7.79
methylmalonic(pK2)	5.76		10.66	10.42	10.64
Ethylmalonic(pK1)	3.35		8.21	8.05	8.20
Ethylmalonic(pK2)	5.83		10.73	10.49	10.71
Acrylic acid	4.25		9.12	8.94	9.11
(E)-4-Oxo-4-[4-vinyloxy)anilino]-2-butenoic acid	3.66		8.52	8.36	8.52
(E)-4-[4-Ethoxyanilino]-4-	3.63		8.49	8.33	8.49

oxo-2-butenoic acid				
Fumaric acid (pK2)	4.6	9.48	9.28	9.47
Atropic acid	4.44	9.32	9.13	9.30
2-(3-Chlorophenyl)acrylic acid	4.29	9.16	8.98	9.15
2-(3-Nitrophenyl)acrylic acid	4.12	8.99	8.81	8.98
2-(4-Nitrophenyl)acrylic acid	4.05	8.92	8.74	8.91
1-Cyclopropanecarboxilic acid	4.83	9.71	9.51	9.70
Butanoic acid	4.82	9.70	9.50	9.69
3-Bromobutanoic acid	4.01	8.88	8.70	8.87
3-Chlorobutanoic acid	4.17	9.04	8.86	9.03
2-Chlorobutanoic acid	2.92	7.77	7.63	7.77
Succinic acid (pK1)	4.2	9.07	8.89	9.06
Succinic acid (pK2)	5.61	10.51	10.28	10.48
Methylsuccinic(pK1)	4.49	9.37	9.17	9.35
Tartaric acid (pK1)	3.01	7.86	7.72	7.86
d-(sec-Butyl)tartrate	3.38	8.24	8.08	8.23
meso-(sec-Butyl)tartrate	3.68	8.54	8.38	8.54
4-Oxo-4-[4-(vinylox)anilino]butanoic acid	4.64	9.52	9.32	9.51
4-(4-Ethoxyanilino]-4-oxobutanoic acid	4.55	9.43	9.23	9.41
1-Cyclobutanecarboxylic acid	4.79	9.67	9.47	9.66
1-Cyclobutanecarboxylic acid	4.99	9.88	9.67	9.86
1-Cyclohexanecarboxylic	4.9	9.78	9.58	9.77

acid				
cis-2-Hydroxy-1-cyclohexanecarboxylic acid	4.8	9.68	9.48	9.67
trans-2-Hydroxy-1-cyclohexanecarboxylic acid	4.82	9.70	9.50	9.69
cis-3-Hydroxy-1-cyclophexanecarboxylic acid	4.6	9.48	9.28	9.47
trans-3-Hydroxy-1-cyclohexanecarboxcylic acid	4.82	9.70	9.50	9.69
cis-4-Hydroxy-1-cyclohexanecarboxylic acid	4.84	9.72	9.52	9.71
trans-4-Hydroxy-1-cyclohexanecarboxylic acid	4.69	9.57	9.37	9.56
Heptanedioic acid	4.46	9.34	9.14	9.32
Octanedioic acid	4.5	9.38	9.18	9.36
Bicyclo[2,2,2]octane-1-carboxylic acid	5.08	9.97	9.76	9.95
4-Bromobicyclo[2,2,2]octane-1-carboxylic acid	4.62	9.50	9.30	9.49
4-Cyanobicyclo[2,2,2]octane-1-carboxylic acid	4.55	9.43	9.23	9.41
Bicyclo[2,2,2]octane-1,4-dicarboxylic acid (pK1)	4.47	9.35	9.15	9.33
Bicyclo[2,2,2]octane-1,4-dicarboxylic acid (pK2)	5.46	10.35	10.13	10.33
4-(1,1,1-Trimethylammonio)bicyclo	4.08	8.95	8.77	8.94

[2,2,2]octane-1-oDecanedioic acid				
Decanedioic acid	4.5	9.38	9.18	9.36
2-Fluorobenzoic acid	3.57	8.43	8.27	8.43
2-Bromobenzoic acid	2.85	7.70	7.56	7.70
2-Chlorobenzoic acid	2.92	7.77	7.63	7.77
2-lodobenzoic acid	2.85	7.70	7.56	7.70
2-Methylbenzoic acid	3.91	8.78	8.60	8.77
2-Nitrobenzoic acid	2.19	7.03	6.91	7.03
2-Methoxybenzoic acid	4.09	8.96	8.78	8.95
2-[4-(Vinyloxy)anilino]benzoic acid	3.8	8.67	8.50	8.66
2-[Methyl-4-(vinyloxy)anilino]benzoic acid	4.34	9.21	9.03	9.20
3-Fluorobenzoic acid	3.88	8.75	8.57	8.74
3-Chlorobenzoic acid	3.8	8.67	8.50	8.66
3-lodobenzoic acid	3.82	8.69	8.52	8.68
3-Hydroxybenzoic acid	4.01	8.88	8.70	8.87
3-Acetamidobenzoic acid	4.06	8.93	8.75	8.92
3-Nitrobenzoic acid	3.47	8.33	8.17	8.32
3-Methoxynbenzoic acid	4.12	8.99	8.81	8.98
3-Phenoxybenzoic acid	3.95	8.82	8.64	8.81
3-Mercaptgobenzoic acid	3.96	8.83	8.65	8.82
3-Sulfamylbenzoic acid	3.68	8.54	8.38	8.54
3-(Methylsulfonyl)benzoic acid	3.53	8.39	8.23	8.39
3-Methylbenzoic acid	4.28	9.15	8.97	9.14
3-(Trifluoromethyl)benzoic acid	3.75	8.61	8.45	8.61

3-Cyanobenzoic acid	3.6	8.46	8.30	8.46
3-Acetylbenzoic acid	3.83	8.70	8.52	8.69
4-Fluorobenzoic acid	4.15	9.02	8.84	9.01
4-Bromobenzoic acid	3.99	8.86	8.68	8.85
4-Chlorobenzoic acid	4	8.87	8.69	8.86
4-lodobenzoic acid	3.98	8.85	8.67	8.84
4-Aminobenzoic acid	4.82	9.70	9.50	9.69
4-Acetamidobenzoic acid	4.3	9.17	8.99	9.16
4-(Dimethylamino)benzoic acid	5.03	9.92	9.71	9.90
4-Hydroxybenzoic acid	4.55	9.43	9.23	9.41
4-Methoxybenzoic acid	4.25	9.12	8.94	9.11
4-(Methylmercapto)benzoic acid	4.2	9.07	8.89	9.06
4-Sulfamylbenzoic acid	3.63	8.49	8.33	8.49
4-(Methylsulfonyl)benzoic acid	3.48	8.34	8.18	8.33
4-Methylbenzoic acid	4.38	9.26	9.07	9.24
4-Cyanobenzoic acid	3.53	8.39	8.23	8.39
4-Acetylbenzoic acid	3.7	8.56	8.40	8.56
4-tert-Butylbenzoic acid	4.36	9.23	9.05	9.22
2,4-Dichlorobenzoic acid	2.76	7.61	7.47	7.61
2,4-Dinitrobenzoic acid	1.43	6.25	6.16	6.27
2,4-Dimethylbenzoic acid	4.22	9.09	8.91	9.08
2,6-Dichlorobenzoic acid	1.82	6.65	6.55	6.66
2,6-Dinitrobenzoic acid	1.14	5.96	5.88	5.97
3,4-Dimethoxybenzoic acid	4.44	9.32	9.13	9.30
3,4-Dinitrobenzoic acid	2.82	7.67	7.53	7.67
3-Methyl-4-chlorobenzoic acid	4.07	8.94	8.76	8.93
3-Methyl-4-nitrobenzoic	3.65	8.51	8.35	8.51

acid				
4-Chloro-3-nitrobenzoic acid	3.34	8.20	8.04	8.19
3,5-Dichlorobenzoic acid	3.56	8.42	8.26	8.42
3,5-Dinitrobenzoic acid	2.82	7.67	7.53	7.67
2,4,6-Trimethylbenzoic acid	3.45	8.31	8.15	8.30

Table S27. The pK_a values of the selected pharmaceutical ingredients and some anti-inflammatory agents in methanol solvent estimated from the correlation equation.

compound	$pK_{a,water}^{exp}$	pK_a^{exp}	$pK_{a,B3LYP}$	$pK_{a,M062X}$	$pK_{a,MP2}$
Diclofenac	4.21	-	9.07	9.06	9.08
Ketoprofen	4.36	-	9.22	9.21	9.23
Flurbiprofen	4.35	-	9.21	9.20	9.22
Naproxen	4.57	-	9.43	9.42	9.44
Ibuprofen	4.52	-	9.38	9.37	9.39
Carprofen	4.63	-	9.50	9.48	9.50
Butibufen	4.64	-	9.51	9.49	9.51
Fenbufen	4.56	-	9.42	9.41	9.43
Ciprofloxacin	6.68	-	11.55	11.53	11.55
Danofloxacin	6.32	-	11.19	11.17	11.19
Difloxacin	6.49	-	11.36	11.34	11.36
Enoxacin	6.43	-	11.30	11.28	11.30
Fleroxacin	6.42	-	11.29	11.27	11.29
Flumequine	6.65	-	11.52	11.50	11.52
Lomefloxacin	6.56	-	11.43	11.41	11.43
Marbofloxacin	5.51	-	10.38	10.36	10.38
Nalidixic acid	6.5	-	11.37	11.35	11.37
Norfloxacine	6.36	-	11.23	11.21	11.23
Pefloxacin	6.68	-	11.55	11.53	11.55
Pipemidic acid	6.16	-	11.03	11.01	11.03
Ofloxacin	6.67	-	11.54	11.52	11.54
Amoxillin	3.39	-	8.25	8.24	8.26
Ampicillin	3.39	-	8.25	8.24	8.26
penicillin G (benzylpenicillin)	3.42	-	8.28	8.27	8.29

Table S28. The pK_a values of the selected pharmaceutical ingredients and some anti-inflammatory agents in ethanol solvent estimated from the correlation equation.

compound	$pK_{a,water}^{exp}$	pK_a^{exp}	$pK_{a,B3LYP}$	$pK_{a,M062X}$	$pK_{a,MP2}$
Diclofenac	4.21	-	9.58	9.56	9.59
Ketoprofen	4.36	-	9.74	9.72	9.75
Flurbiprofen	4.35	-	9.73	9.71	9.74
Naproxen	4.57	-	9.95	9.93	9.96
Ibuprofen	4.52	-	9.90	9.88	9.91
Carprofen	4.63	-	10.01	9.99	10.02
Butibufen	4.64	-	10.02	10.00	10.03
Fenbufen	4.56	-	9.94	9.92	9.95
Ciprofloxacin	6.68	-	12.11	12.09	12.12
Danofloxacin	6.32	-	11.74	11.72	11.75
Difloxacin	6.49	-	11.91	11.89	11.93
Enoxacin	6.43	-	11.85	11.83	11.87
Fleroxacin	6.42	-	11.84	11.82	11.86
Flumequine	6.65	-	12.08	12.05	12.09
Lomefloxacin	6.56	-	11.99	11.96	12.00
Marbofloxacin	5.51	-	10.91	10.89	10.92
Nalidixic acid	6.5	-	11.92	11.90	11.94
Norfloxacine	6.36	-	11.78	11.76	11.80
Pefloxacin	6.68	-	12.11	12.09	12.12
Pipemidic acid	6.16	-	11.58	11.55	11.59
Ofloxacin	6.67	-	12.10	12.07	12.11
Amoxillin	3.39	-	8.75	8.73	8.75
Ampicillin	3.39	-	8.75	8.73	8.75
penicillin G (benzylpenicillin)	3.42	-	8.78	8.76	8.78

Table S29. The pK_a values of the selected pharmaceutical ingredients and some anti-inflammatory agents in 2-propanol solvent estimated from the correlation equation.

compound	$pK_{a,water}^{exp}$	pK_a^{exp}	$pK_{a,B3LYP}$	$pK_{a,M062X}$	$pK_{a,MP2}$
Diclofenac	4.21	11.03	10.21	10.17	10.18
Ketoprofen	4.36	11.45	10.36	10.33	10.34
Flurbiprofen	4.35	11.43	10.35	10.32	10.33
Naproxen	4.57	11.87	10.58	10.55	10.56
Ibuprofen	4.52	11.77	10.53	10.49	10.51
Carprofen	4.63	11.99	10.64	10.61	10.62
Butibufen	4.64	12.03	10.65	10.62	10.63
Fenbufen	4.56	11.85	10.57	10.54	10.55
Ciprofloxacin	6.68	-	12.77	12.73	12.76
Danofloxacin	6.32	-	12.39	12.35	12.38
Difloxacin	6.49	-	12.57	12.53	12.56
Enoxacin	6.43	-	12.51	12.47	12.50
Fleroxacin	6.42	-	12.50	12.46	12.49
Flumequine	6.65	-	12.74	12.70	12.73
Lomefloxacin	6.56	-	12.64	12.60	12.63
Marbofloxacin	5.51	-	11.55	11.52	11.54
Nalidixic acid	6.5	-	12.58	12.54	12.57
Norfloxacine	6.36	-	12.43	12.40	12.42
Pefloxacin	6.68	-	12.77	12.73	12.76
Pipemidic acid	6.16	-	12.23	12.19	12.22
Ofloxacin	6.67	-	12.76	12.72	12.75
Amoxillin	3.39	-	9.36	9.33	9.33
Ampicillin	3.39	-	9.36	9.33	9.33
penicillin G (benzylpenicillin)	3.42	-	9.39	9.36	9.36

Table S30. The pK_a values of the selected pharmaceutical ingredients and some anti-inflammatory agents in ACN solvent estimated from the correlation equation.

compound	$pK_{a,water}^{exp}$	pK_a^{exp}	$pK_{a,B3LYP}$	$pK_{a,M062X}$	$pK_{a,MP2}$
Diclofenac	4.21	-	19.41	19.30	19.32
Ketoprofen	4.36	-	19.56	19.45	19.47
Flurbiprofen	4.35	-	19.55	19.44	19.46
Naproxen	4.57	-	19.77	19.66	19.69
Ibuprofen	4.52	-	19.72	19.61	19.64
Carprofen	4.63	-	19.83	19.72	19.75
Butibufen	4.64	-	19.84	19.73	19.76
Fenbufen	4.56	-	19.76	19.65	19.68
Ciprofloxacin	6.68	-	21.91	21.78	21.86
Danofloxacin	6.32	-	21.55	21.42	21.49
Difloxacin	6.49	-	21.72	21.59	21.67
Enoxacin	6.43	-	21.66	21.53	21.61
Fleroxacin	6.42	-	21.65	21.52	21.60
Flumequine	6.65	-	21.88	21.75	21.83
Lomefloxacin	6.56	-	21.79	21.66	21.74
Marbofloxacin	5.51	-	20.73	20.61	20.66
Nalidixic acid	6.5	-	21.73	21.60	21.68
Norfloxacine	6.36	-	21.59	21.46	21.53
Pefloxacin	6.68	-	21.91	21.78	21.86
Pipemidic acid	6.16	-	21.38	21.26	21.33
Ofloxacin	6.67	-	21.90	21.77	21.85
Amoxillin	3.39	-	18.58	18.47	18.47
Ampicillin	3.39	-	18.58	18.47	18.47
penicillin G (benzylpenicillin)	3.42	-	18.61	18.50	18.50

Table S31. The pK_a values of the selected pharmaceutical ingredients and some anti-inflammatory agents in DMF solvent estimated from the correlation equation.

compound	$pK_{a,water}^{exp}$	pK_a^{exp}	$pK_{a,B3LYP}$	$pK_{a,M062X}$	$pK_{a,MP2}$
Diclofenac	4.21	-	10.53	10.41	10.49
Ketoprofen	4.36	-	10.67	10.56	10.64
Flurbiprofen	4.35	-	10.66	10.55	10.63
Naproxen	4.57	-	10.88	10.77	10.85
Ibuprofen	4.52	-	10.83	10.72	10.80
Carprofen	4.63	-	10.94	10.83	10.91
Butibufen	4.64	-	10.95	10.84	10.92
Fenbufen	4.56	-	10.87	10.76	10.84
Ciprofloxacin	6.68	-	12.99	12.86	12.98
Danofloxacin	6.32	-	12.63	12.50	12.62
Difloxacin	6.49	-	12.80	12.67	12.79
Enoxacin	6.43	-	12.74	12.61	12.73
Fleroxacin	6.42	-	12.73	12.60	12.72
Flumequine	6.65	-	12.96	12.83	12.95
Lomefloxacin	6.56	-	12.87	12.74	12.86
Marbofloxacin	5.51	-	11.82	11.70	11.80
Nalidixic acid	6.5	-	12.81	12.68	12.80
Norfloxacine	6.36	-	12.67	12.54	12.66
Pefloxacin	6.68	-	12.99	12.86	12.98
Pipemidic acid	6.16	-	12.47	12.34	12.46
Ofloxacin	6.67	-	12.98	12.85	12.97
Amoxillin	3.39	-	9.71	9.60	9.66
Ampicillin	3.39	-	9.71	9.60	9.66
penicillin G (benzylpenicillin)	3.42	-	9.74	9.63	9.69

Table S32. The pK_a values of the selected pharmaceutical ingredients and some anti-inflammatory agents in DMSO solvent estimated from the correlation equation.

compound	$pK_{a,water}^{exp}$	pK_a^{exp}	$pK_{a,B3LYP}$	$pK_{a,M062X}$	$pK_{a,MP2}$
Diclofenac	4.21	-	9.08	8.90	9.07
Ketoprofen	4.36	-	9.23	9.05	9.22
Flurbiprofen	4.35	-	9.22	9.04	9.21
Naproxen	4.57	-	9.45	9.25	9.43
Ibuprofen	4.52	-	9.40	9.20	9.38
Carprofen	4.63	-	9.51	9.31	9.50
Butibufen	4.64	-	9.52	9.32	9.51
Fenbufen	4.56	-	9.44	9.24	9.42
Ciprofloxacin	6.68	-	11.60	11.33	11.56
Danofloxacin	6.32	-	11.23	10.98	11.20
Difloxacin	6.49	-	11.40	11.14	11.37
Enoxacin	6.43	-	11.34	11.08	11.31
Fleroxacin	6.42	-	11.33	11.07	11.30
Flumequine	6.65	-	11.56	11.30	11.53
Lomefloxacin	6.56	-	11.47	11.21	11.44
Marbofloxacin	5.51	-	10.40	10.18	10.38
Nalidixic acid	6.5	-	11.41	11.15	11.38
Norfloxacine	6.36	-	11.27	11.01	11.24
Pefloxacin	6.68	-	11.60	11.33	11.56
Pipemidic acid	6.16	-	11.07	10.82	11.04
Ofloxacin	6.67	-	11.58	11.32	11.55
Amoxillin	3.39	-	8.25	8.09	8.24
Ampicillin	3.39	-	8.25	8.09	8.24
penicillin G (benzylpenicillin)	3.42	-	8.28	8.12	8.27