Supporting Information

The pK_{BHX} Database: Towards a Better Understanding of Hydrogen-Bond Basicity for Medicinal Chemists

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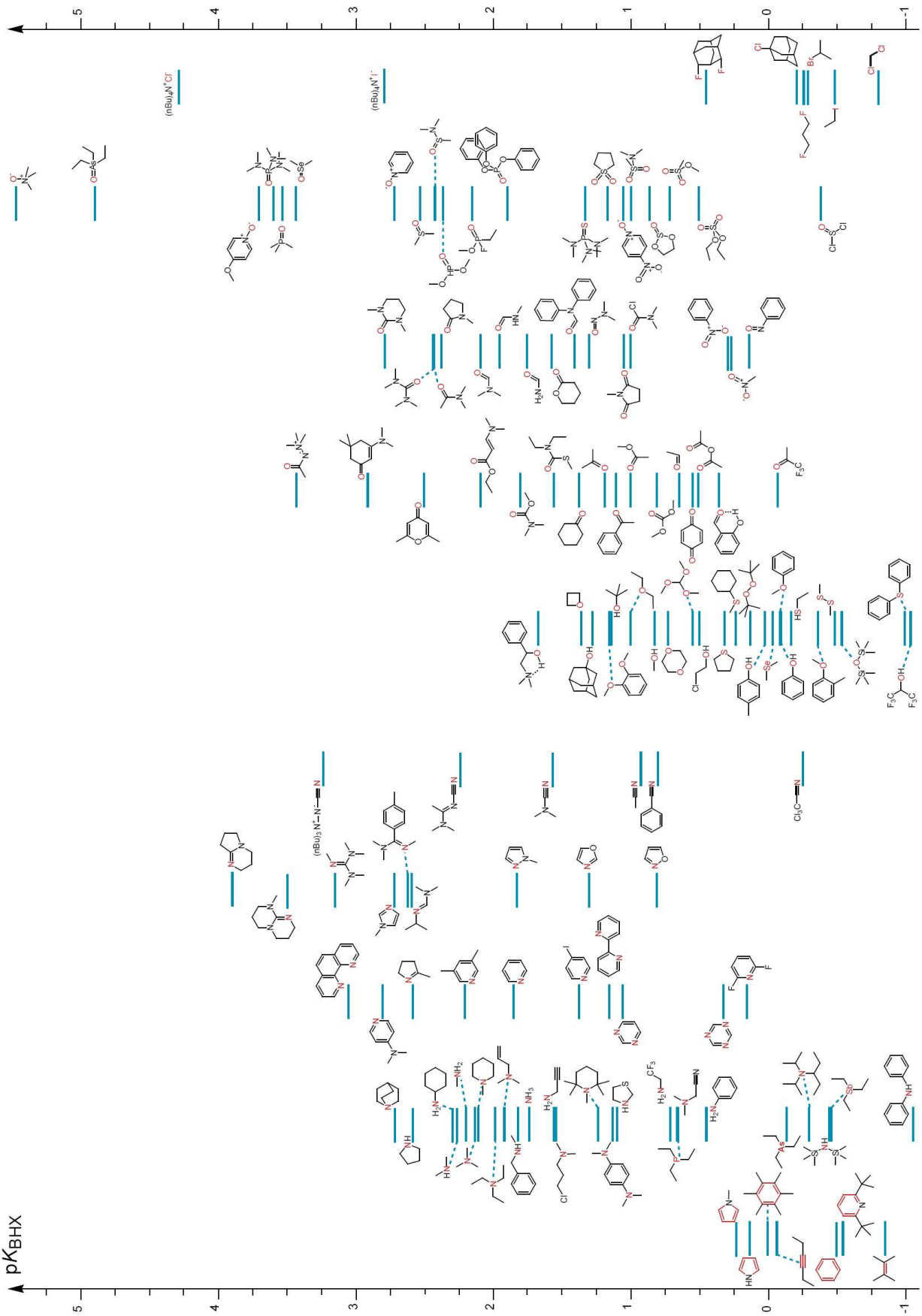
Contents of Supporting Information

I. Graphical representation of the pK_{BHX} scale depicting functional groups contained in the database.



II. The pK_{BHX} and pK_{BH}^{+} values used for the comparison of the HB and proton basicity scales.

Base	pK_{BH+}	pK_{BHX}
Acetonitrile	-10.1	0.91
Benzonitrile	-10.4	0.80
Chloroacetonitrile	-12.8	0.39
1-Acetyl-1H-imidazole	3.6	1.86
1-Methyl-1H-imidazole	7.12	2.72
1,3-Oxazole	0.8	1.30
Isoxazole	1.3	0.81
1,3-Thiazole	2.518	1.37
1-Methyl-1H-pyrazole	2.06	1.84
1,1-Diphenylmethanimine	7.18	1.80
2-Methyl-N-(phenylmethylene)propan-2-amine	6.7	1.29
N,N-Dimethyl-N'-phenylimidoformamide	8.15	1.90
N,N-Dimethyl-N'-(4-nitrophenyl)imidoformamide	6.02	1.20
N'-(4-Cyanophenyl)-N,N-dimethylimidoformamide	6.44	1.32
N'-(4-Acetylphenyl)-N,N-dimethylimidoformamide	7.02	1.52
N'-(4-Bromophenyl)-N,N-dimethylimidoformamide	7.40	1.65
N,N-Dimethyl-N'-(4-methylphenyl)imidoformamide	8.45	2.07
N'-(2-Bromophenyl)-N,N-dimethylimidoformamide	6.71	1.37
N,N-Dimethyl-N'-(2-methylphenyl)imidoformamide	8.27	1.63
N'-(3,5-Dichlorobenzyl)-N,N-dimethylimidoformamide	9.86	2.00
N'-(3-Chlorobenzyl)-N,N-dimethylimidoformamide	10.15	2.10
N'-(4-Chlorobenzyl)-N,N-dimethylimidoformamide	10.32	2.12
N'-Benzyl-N,N-dimethylimidoformamide	10.65	2.35
N,N-Dimethyl-N'-(4-methylbenzyl)imidoformamide	10.91	2.36
N'-Isobutyl-N,N-dimethylimidoformamide	11.30	2.52
N,N-Dimethyl-N'-propylimidoformamide	11.46	2.59
1,1,3,3-Tetramethylguanidine	13.6	3.21
1,1,2,3,3-Pentamethylguanidine	13.8	3.16
Aniline	4.61	0.46
3-Chloroaniline	3.52	0.13

Base	pK_{BH+}	pK_{BHX}
p-Toluidine	5.08	0.56
3-Fluoroaniline	3.59	0.20
2,6-Dimethylaniline	3.95	0.47
N-Methylaniline	4.85	0.26
N,4-Dimethylaniline	5.36	0.43
4-Chloro-N-methylaniline	3.9	0.05
N,N-Dimethylaniline	5.070	0.39
N,N-Dimethyl-3-toluidine	5.34	0.41
4-Bromo-N,N-dimethylaniline	4.23	0.17
1-Phenylpyrrolidine	4.3	0.16
1,2,3,4-Tetrahydroquinoline	5.03	0.70
N,N,4-Trimethylaniline	5.63	0.69
N,N-Diethylaniline	6.61	0.05
Proton sponge	12.1	-0.55
Diphenylamine	0.79	-1.05
N,N,N',N'-Tetramethylbenzene-1,4-diamine	6.05	1.13
2-N,N-Dimethylaminopyridine	6.99	1.61
2-Aminopyridine	6.71	2.12
2-Methoxypyridine	3.06	0.99
2-Tert-butylpyridine	5.76	1.42
2-Isopropylpyridine	5.83	1.76
2-Ethylpyridine	5.89	1.94
2-Methylpyridine	5.96	2.03
2-Phenylpyridine	4.77	1.43
2-Vinylpyridine	4.92	1.65
2-Fluoropyridine	-0.44	0.95
2-Chloropyridine	0.72	1.05
2-Bromopyridine	0.90	1.03
2-Cyanopyridine	-0.26	0.48
2,6-Dimethylpyridine	6.72	2.14
2,4,6-Trimethylpyridine	7.43	2.29

Base	pK_{BH+}	pK_{BHX}
Pyridine	5.20	1.86
3-Methylpyridine	5.66	2.00
3-Ethylpyridine	5.73	2.01
3-Fluoropyridine	3.00	1.35
3-Chloropyridine	2.80	1.31
3-Bromopyridine	2.84	1.31
3-Iodopyridine	3.28	1.37
3,5-Dichloropyridine	0.66	0.85
3-Aminopyridine	6.03	2.20
3-Benzoylpyridine	3.18	1.42
3-Cyanopyridine	1.34	0.82
Methylnicotinate	3.08	1.44
3,5-Dimethylpyridine	6.34	2.21
3,4-Dimethylpyridine	6.47	2.24
4-Methylpyridine	6.03	2.07
4-Ethylpyridine	6.02	2.07
4-Tert-butylpyridine	5.99	2.11
4-Chloropyridine	3.83	1.54
4-Methoxypyridine	6.58	2.13
4-Aminopyridine	9.12	2.56
4-N,N-Dimethylaminopyridine	9.58	2.80
4-Phenylpyridine	5.35	1.96
4-Cyanopyridine	1.86	0.92
4-Acetylpyridine	3.51	1.41
4-Vinylpyridine	5.62	1.95
Quinoline	4.85	1.89
Acridine	5.24	1.95
Isoquinoline	5.40	1.94
Phenantridine	4.47	1.87
Phenazine	0.90	1.22
7,8-Benzoquinoline	3.95	1.16

Base	pK_{BH+}	pK_{BHX}
Pyridazine	2.00	1.65
Pyrimidine	0.93	1.07
Pyrazine	0.37	0.92
Phtalazine	3.17	1.97
2-Aminopyrimidine	3.54	1.85
Ammonia	9.2445	1.74
Methylamine	10.6532	2.20
Ethylamine	10.6784	2.17
n-Propylamine	10.5685	2.20
Isopropylamine	10.67	2.20
n-Butylamine	10.6385	2.19
Tert-butylamine	10.6837	2.23
c-Propylamine	9.10	1.72
c-Hexylamine	10.58	2.29
Allylamine	9.52	1.93
Adamantanamine	10.58	2.30
n-Octylamine	10.61	2.27
n-Hexadecylamine	10.61	2.26
2-Phenylethanamine	9.83	2.16
Benzylamine	9.34	1.84
Propargylamine	8.15	1.56
3-Aminopropionitrile	7.80	1.33
2,2,2-Trifluoroethylamine	5.61	0.71
1,4-Diaminobutane	10.35	2.21
1,6-Diaminohexane	10.63	2.21
Ethylenediamine	9.626	2.25
1,3-Diaminopropane	10.17	2.31
2-Methoxyethylamine	9.44	2.26
3-Methoxypropylamine	9.92	2.22
Dimethylamine	10.7788	2.26
Diethylamine	11.0151	2.25

Base	pK_{BH+}	pK_{BHX}
N-Methylcyclohexylamine	11.04	2.24
Azetidine	11.29	2.59
Pyrrolidine	11.3060	2.59
Piperidine	11.1236	2.38
Azepane	11.1000	2.24
Morpholine	8.4918	1.78
Diallylamine	9.24	1.70
Piperazine	9.432	2.11
N-methylbutylamine	10.90	2.24
N,N'-dimethylethylenediamine	9.94	2.29
Thiazolidine	6.22	1.10
1,2,3,4-Tetrahydroisoquinoline	9.41	2.04
N-Methylphenetylamine	10.08	2.14
N-Methylallylamine	10.11	2.00
N-Methylbenzylamine	9.56	1.82
3-Methylaminopropionitrile	8.10	1.37
2-Phenylpyrrolidine	9.60	1.93
Dibutylamine	11.25	2.11
Diisopropylamine	11.20	2.00
2,2,6,6-Tetramethylpiperidine	11.0725	1.88
Dibenzylamine	8.52	1.34
Trimethylamine	9.7977	2.13
Triethylamine	10.7174	1.98
N,N-Dimethylcyclohexylamine	10.72	2.15
N-Methylpyrrolidine	10.46	2.19
N-Methylpiperidine	10.08	2.11
Quinuclidine	11.1516	2.71
N-Methylmorpholine	7.41	1.56
Triallylamine	8.28	1.34
Hexamethylenetetramine	7.4696	1.33
N,N-Dimethylethylamine	10.16	2.17

Base	pK_{BH+}	pK_{BHX}
N,N-Dimethylisopropylamine	10.47	2.11
N,N,N',N'-Tetramethylethylenediamine	8.85	2.02
N-Butylpyrrolidine	10.36	2.04
N-Methyl-2-phenylpyrrolidine	8.8	1.38
N,N-Dimethylallylamine	8.64	1.92
N,N-Dimethylpropargylamine	7.45	1.60
N,N-Dimethylbenzylamine	8.91	1.59
Tripropylamine	10.66	1.47
Tributylamine	9.93	1.55
Diazabicyclooctane	8.52	2.33
1,2,2,6,6-Pentamethylpiperidine	11.19	1.23
Tripropargylamine	3.09	0.83
Dimethylaminoacetonitrile	4.2	0.67
Acetone	-3.06	1.18
Butan-2-one	-3.06	1.22
3-Methylbutan-2-one	-3.29	1.2
3,3-Dimethylbutan-2-one	-3.37	1.17
2,2,4,4-Tetramethylpentan-3-one	-6.8	0.96
2,6-Dimethylheptan-4-one	-4.3	1.07
3,5-Dimethylheptan-4-one	-3.86	1.07
Nonan-5-one	-3.89	1.21
3-Chloro-5,5-dimethylcyclohexenone	-3.36	1.21
3-Methyl-5,5-dimethylcyclohexenone	-2.5	1.74
3-Dimethylamino-5,5-dimethylcyclohexenone	3.14	2.92
Acetophenone	-3.46	1.11
4-Methylacetophenone	-3.78	1.24
4-Ethylacetophenone	-3.71	1.25
4-Isopropylacetophenone	-3.69	1.21
4-Tert-butylacetophenone	-3.97	1.25
4-Methoxyacetophenone	-3.02	1.33
4-Trifluoromethylacetophenone	-4.13	0.78

Base	pK_{BH+}	pK_{BHX}
4-Fluoroacetophenone	-3.53	1.00
4-Nitroacetophenone	-5.02	0.57
Benzophenone	-4.71	1.07
Acetamide	-0.66	2.06
Formamide	-1.47	1.75
N-Methylformamide	-1.1	1.96
N-Methylacetamide	-0.56	2.30
N-Methylpropanamide	-0.7	2.24
N,N-Dimethylacetamide	-0.21	2.44
1-Methyl-2-pyrrolidone	-0.71	2.38
N,N-Dimethylformamide	-1.13	2.10
N,N-Dimethylpropanamide	-0.56	2.36
N,N,2-Trimethylpropanamide	-1.61	2.26
N,N,2,2-Tetramethylpropanamide	-2.03	2.10
1,1,3,3-Tetramethylurea	-0.14	2.44
N,N-Dimethylthioacetamide	-2.25	1.22
Hexamethylphosphoramide	-0.97	3.60
Dimethyl sulfoxide	-1.54	2.54
Methyl 4-nitrophenyl sulfoxide	-3.11	1.58
Diphenyl sulfoxide	-2.54	2.04
Methyl phenyl sulfoxide	-2.27	2.24
Tetramethylene sulfone	-0.65	1.17
Dimethyl sulfone	-3.5	1.10
Methyl acetate	-3.9	1.00
Methyl benzoate	-7.05	0.89
Ethyl benzoate	-6.16	0.94
Ethyl acetate	-3.45	1.07
Diethyl ether	-2.39	1.01
Methanol	-2.05	0.82
Ethanol	-1.94	1.02
Propan-1-ol	-2.12	1.00

Base	pK_{BH+}	pK_{BHX}
2-Chloroethanol	-2.45	0.50
2-Bromethanol	-2.41	0.54
Propan-2-ol	-2.02	1.06
Pyridine 1-oxide	0.79	2.72
4-Methylpyridine 1-oxide	1.29	3.12
4-Chloropyridine 1-oxide	0.33	2.44
3,5-Dichloropyridine 1-oxide	-0.94	1.56
4-Methoxypyridine 1-oxide	2.05	3.70
3-Methylpyridine 1-oxide	0.93	2.92
4-Phenylpyridine 1-oxide	0.83	2.85
4-Nitropyridine 1-oxide	-1.51	1.05
1H-Pyrrole	-3.8	0.15
1-Methyl-1H-pyrrole	-2.9	0.23
Hexamethylbenzene	-14.65	0.02
Dimethyl sulfide	-6.95	0.12
t-Butyl methyl sulfide	-6.68	0.25

III. Table listing a representative sample of the data contained in the pK_{BHX} database.

Hydrogen-bond acceptor	pK_{BHX}	Hydrogen-bond acceptor	pK_{BHX}
Arenes		**Tertiary amines**	
Pyrene	-0.56	Tripropargylamine	0.83 (N)
Phenanthrene	-0.53	N,N-Diisopropylethylamine	1.05
Benzene	-0.49	1,2,2,6,6-Pentamethylpiperidine	1.23
Naphtalene	-0.48	Hexamethylenetetramine	1.33
Biphenyl	-0.47	N-Ethyl-N-methylbenzylamine	1.47
Methylbenzene, toluene	-0.36	Tri-n-butylamine	1.55
1,3-Dimethylbenzene, m-xylene	-0.28	N-Methylmorpholine	1.56 (N)
Hexamethylbenzene	0.02	1,3,5-Trimethylhexahydrotriazine	1.58
Thiophene	-0.50	N,N-Dimethylbenzylamine	1.59
Alkenes		N-Methyl-1,2,3,4-tetrahydroisoquinoline	1.80
Cyclohexene	-0.82	N,N'-Dimethylpiperazine	1.88
1-Heptene	-0.67	Triethylamine	1.98
Alkynes		N-Methyl-1,2,3,6-tetrahydropyridine	2.02
1-Hexyne	-0.22	N,N,N',N'-Tetramethylethylenediamine	2.02
2-Hexyne	-0.09	N-Methylpiperidine	2.11
Primary amines		Trimethylamine	2.13
2,2,2-Trifluoroethylamine	0.71	N,N-Dimethylcyclohexylamine	2.15
Ammonia	1.74	N,N-Dimethylethylamine	2.17
Benzylamine	1.88	N-Methylpyrrolidine	2.19
Allylamine	1.94	Diazabicyclooctane (DABCO)	2.33
Phenethylamine	2.16	Tropane	2.39
Ethylamine	2.17	Quinuclidine	2.71
Methylamine	2.20	**Six-membered N-heteroaromatics**	
n-Butylamine	2.21	2,6-Difluoropyridine	0.14
Isopropylamine	2.22	1,3,5-Triazine	0.32
Ethylenediamine	2.25	3,5-Dichloropyridine	0.85
tert-Butylamine	2.26	Pyrazine	0.92
Secondary amines		2-Fluoropyridine	0.95
Thiazolidine	1.10 (N)	Pyrimidine	1.07

Hydrogen-bond acceptor	pK_{BHX}	Hydrogen-bond acceptor	pK_{BHX}
Dibenzylamine	1.34	2,2'-Bipyridine	1.15
Morpholine	1.78 (N)	7,8-Benzoquinoline	1.16
N-Methylbenzylamine	1.82	Phenazine	1.22
2,2,6,6-Tetramethylpiperidine	1.88	3-Chloropyridine	1.31
2-Phenylpyrrolidine	1.93	2-tert-Butylpyridine	1.42
1,2,3,4-Tetrahydroisoquinoline	2.04	Methyl nicotinate	1.45 (N)
Piperazine	2.11	4-Chloropyridine	1.54
1,2,3,6-Tetrahydropyridine	2.16	5-N,N-Dimethylaminopyrimidine	1.58
N-Methyl-tert-butylamine	2.21	2-N,N-Dimethylaminopyridine	1.61
N-Methylcyclohexylamine	2.24	Pyridazine	1.65
Dimethylamine	2.26	Pyridine	1.86
2-Methylaziridine	2.28	Phenanthridine	1.87
Piperidine	2.38	2-n-Butylpyridine	1.88
Pyrrolidine	2.59	Quinoline	1.89
Azetidine	2.59	Isoquinoline	1.94
Acridine	1.95	Propionitrile	0.93
Phtalazine	1.97	Trimethylacetonitrile	1.00
3-Methylpyridine, 3-picoline	2.00	2-Methoxybenzonitrile	1.06
2-Methylpyridine, 2-picoline	2.03	4-Dimethylaminobenzonitrile	1.23
4-Ethylpyridine	2.07	Cyanamide	1.40
2-Methylaminopyridine	2.11	Dimethylcyanamide	1.56
2-Aminopyridine	2.12	1-Piperidinecarbonitrile	1.58
4-Methoxypyridine	2.13	Diethylcyanamide	1.63
2,6-Dimethylpyridine ; 2,6-lutidine	2.14	1-Pyrrolidinecarbonitrile	1.66
3,4-Dimethylpyridine ; 3,4-lutidine	2.24	Trans-3-dimethylaminoacrylonitrile	1.70
9-N,N-Dimethylaminoacridine	2.31	N_1,N_1-Dimethyl-N_2-cyanoacetamidine	2.24
4-N,N-Dimethylaminoquinoline	2.43	**Water, alcohols, and phenols**	
4-Aminopyridine	2.56	2,2,2-Trifluoroethanol	-0.28
4-Piperidinopyridine	2.68	Phenol	-0.07
4-N,N-Dimethylaminopyridine	2.80	3-Methylphenol	0.01
4-Pyrrolidinopyridine	2.93	Propargyl alcohol	0.38

Hydrogen-bond acceptor	pK_{BHX}
Five-membered N-heteroaromatics	
Pyrrole	0.15
1-Methylpyrrole	0.23
Isoxazole	0.81
2-Phenylbenzoxazole	1.18
Oxazole	1.30
Benzothiazole	1.35
Thiazole	1.37
1-Methylpyrazole	1.84
4-Butyl-1,2,4-triazole	2.29
Imidazole	2.42
1-Methylimidazole	2.72
Guanidines	
Pentaisopropylguanidine	1.06
Tetramethylguanidine	3.21
Imines	
N-Benzylideneaniline	0.87
N-Benzilidene-tert-butylamine	1.29
N-Benzylidenemethylamine	1.49
2-Phenyl-1-pyrroline	1.98
Nitriles	
Pentafluorobenzonitrile	0.01
Chloroacetonitrile	0.39
2-Chlorobenzonitrile	0.67
Acrylonitrile	0.70
4-Fluorobenzonitrile	0.72
Methyl thiocyanate	0.73
Benzonitrile	0.80
Allyl cyanide	0.87
Acetonitrile	0.91
Aldehydes	
2-Chloroethanol	0.50
Water	0.65
Allyl alcohol	0.79
Methanol	0.82
Benzyl alcohol	0.86
Phenethyl alcohol	0.97
Ethanol	1.02
n-Octanol	1.04
Cyclohexanol	1.14
Ethers	
Furan	-0.40
1,3,5-Trioxane	0.02
3,4-Dihydro-2H-pyran	0.41
1,3-Dioxolane	0.45
2,3-Dihydrofuran	0.53
Dimethoxymethane	0.58
1,4-Dioxane	0.73
Di-tert-butyl ether	0.75
Propylene oxide	0.97
Diethyl ether	1.01
Cyclohexene oxide	1.13
Tetrahydrofuran	1.28
2-Methyltetrahydrofuran	1.34
Oxetane, trimethylene oxide	1.36
Cineole, eucalyptol	1.38
2,3-Diadamant-2-yl oxirane	1.44
Peroxides	
tert-Butyl peroxide	0.13
Ascaridole	0.92
Tropolone	1.31

Hydrogen-bond acceptor	pK_{BHX}	Hydrogen-bond acceptor	pK_{BHX}
Salicylaldehyde	0.36	Xanthone	1.36
Acetaldehyde	0.65	1,4-Androstadiene-3,17-dione	1.36 (O17)
Benzaldehyde	0.78		1.84 (O3)
4-Methoxybenzaldehyde	1.10	Acetylferrocene	1.65
trans-Cinnamaldehyde	1.13	10-Methyl-9(10H)-acridone	1.92
4-Dimethylaminobenzaldehyde	1.53	Flavone	1.99
Aliphatic ketones		2,6-Dimethyl-γ-pyrone	2.50
Biacetyl	0.23	**Esters, lactones, and carbonates.**	
2,2,4,4-Tetramethylpentan-3-one	0.96	Methyl trichloroacetate	0.11
2,4-Dimethylpentan-3-one	1.08	Diethyl oxalate	0.65
Hexan-3-one	1.13	Methyl formate	0.65
Pentan-2-one	1.17	Ethyl fluoroacetate	0.74
4-Methylpentan-2-one	1.17	Diethyl terephtalate	0.76
Hexan-2-one	1.18	Ethyl 4-bromobenzoate	0.78
Propan-2-one, acetone	1.18	Dimethyl carbonate	0.82
Cyclohexyl methyl ketone	1.24	Triacetin	0.84
Cycloalkanones		β-Propiolactone	0.86
Cyclobutanone	1.00	β-Butyrolactone	0.97
Cyclopentadecanone	1.22	Methyl acetate	1.00
Camphor	1.31	Ethyl 1-adamantanecarboxylate	1.06
5-α-Androstane-17-one	1.36	Ethyl acetate	1.07
Cyclohexanone	1.39	Ethyl isovalerate	1.11
Cyclooctanone	1.45	Ethyl 4-methoxybenzoate	1.13
Ring-substituted acetophenones		(E)-Ethyl cinnamate	1.14
2-Hydroxyacetophenone	0.56	Coumarin	1.30
3-Fluoroacetophenone	0.83	γ-Valerolactone	1.43
1,3-Diacetylbenzene	0.86	δ-Valerolactone	1.57
2-Chloroacetophenone	0.90	ε-Caprolactone	1.63
4-Chloroacetophenone	0.93	Ethyl 3-dimethylaminoacrylate	2.09
3-Methylacetophenone	1.10	**Amides, lactams, carbamates, ureas**	

Hydrogen-bond acceptor	pK_{BHX}
Acetophenone	1.11
2-Methoxyacetophenone	1.34
4-Dimethylaminoacetophenone	1.76
Ring-substituted benzophenones	
2-Hydroxybenzophenone	0.49
Benzophenone	1.07
4,4'-Dimethoxybenzophenone	1.49
4,4'-Bis(diethylamino)benzophenone	2.33
Miscellaneous conjugated ketones	
1,4-Benzoquinone	0.51
Acetylacetone (ketoenol tautomer)	0.90
Butyrophenone	1.04
9-Fluorenone	1.09
Anthrone	1.16
Thioxanthen-9-one	1.18
N-Methylacetanilide	2.19
N-Formylpyrrolidine	2.31
1-Methyl-2-pyrrolidone	2.38
N,N -Dimethylacetamide	2.44
1,1,3,3-Tetramethylurea	2.44
4-(Dimethylamino)antipyrine	2.45
1-Methyl-2-pyridone	2.50
N-Methylcaprolactam	2.53
1-Methyl-2-piperidone	2.60
1-Acetylpyrrolidine	2.61
Antipyrine	2.79
Nitro compounds	
Nitromethane	0.27
1,2-Dimethyl-4-nitrobenzene	0.46
Dimethylnitramine	0.82
N,N-Dimethyl-4-nitroaniline	0.83

Hydrogen-bond acceptor	pK_{BHX}
Dimethylcarbamoyl chloride	1.00
N,N -Dimethylsalicylamide	1.27
Acetanilide	1.69
Phenyl dimethylcarbamate	1.70
N,N -Dimethyl-2-chloroacetamide	1.74
Formamide	1.75
Benzamide	1.81
Ethyl dimethylcarbamate	1.83
N-Formylmorpholine	1.93
N,N -Diphenylacetamide	1.94
N-Methylformamide	1.96
N,N-Diethylnicotinamide	1.98 (O)
	1.63 (N)
Acetamide	2.06
N-Acetylmorpholine	2.16
Thiocarbonyl compounds	
Thiocamphor	0.34
1,4,5-Trimethylthiazoline-2-thione	1.13
N-methylthioacetamide	1.14
1,3-Dimethylbenzimidazole-2-thione	1.19
N,N-Dimethylthioacetamide	1.22
Benzoxazole-2-thione	1.24
N,N'-Dimethyl-N,N'-ethylenethiourea	1.32
1,3-Oxazolidine-2-thione	1.38
1-Methylbenzimidazole-2-thione	1.53
ε-Thiocaprolactam	1.60
N-Methyl-N,N'-propylenethiourea	2.00
Methimazole	2.11
Single-bonded sulfur bases	
Diphenyl sulfide	-0.93 (S)
Thioanisole	-0.32 (S)

Hydrogen-bond acceptor	pK_{BHX}
Nitroso compounds	
Nitrosobenzene	0.15
N-Nitrosodiphenylamine	0.64
1-Nitrosopyrrolidine	1.49
Sulfonyl compounds	
Diethyl sulfate	0.80
N,N-Dimethylmethanesulfonamide	1.30
Dimethyl sulfone	1.40
N,N,N',N'-Tetraethylsulfamide	1.47
Sulfinyl compounds	
Thionyl chloride	-0.38
Dimethyl sulfite	0.94
Bis(4-chlorophenyl) sulfoxide	1.68
N,N-Dimethybenzenesulfinamide	2.15
Dimethyl sulfoxide	2.54
Amine oxides	
Pyridine N-oxide	2.72
Trimethylamine N-oxide	5.46
Phosphoroso compounds	
Phosphoryl chloride	0.56
Triethyl phosphate	2.68
Trimethylphosphine oxide	3.53
Hexamethylphosphoric triamide (HMPA)	3.60
Triethylphosphine oxide	3.66
Arsine oxides	
Triethylarsine oxide	4.89
Isothiocyanates	
Phenyl isothiocyanate	-0.55 (S)
1,4-Dithiane	-0.14
2-Propanethiol	-0.10
1,3-Dithiane	-0.06
Methyl sulfide	0.12
n-Butyl sulfide	0.23
Tetrahydrothiophene	0.32
tert-Butyl sulfide	0.40
Halogenoalkanes	
trans-1,2-Dichlorocyclohexane	-0.50
1,4-Dibromobutane	-0.47
Iodoethane	-0.47
1,4-Diiodobutane	-0.46
Bromoethane	-0.40
1,5-Dichloropentane	-0.39
2-Iodo-2-methylpropane	-0.33
2-Chloropropane	-0.30
2-Bromo-2-methylpropane	-0.22
1-Fluoropentane	-0.06
Fluorocyclohexane	0.09
Imides	
N-Ethylmaleimide	0.68
N-Methylsuccinimide	1.06
Ion pairs	
Tetrabutylammonium iodide	2.80
Tetrabutylammonium acetate	5.60