A Reliable and Efficient First Principles-based Method for Predicting pK_a Values. 4. Organic Bases

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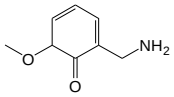
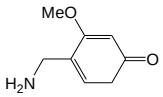
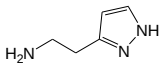
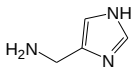
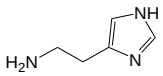
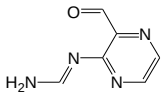
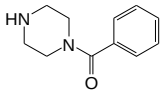
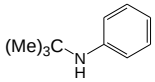
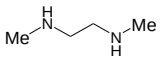
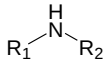
Table S1a Calculated energies and experimental pKas for aliphatic and alicyclic amines --- training set

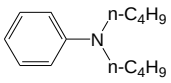
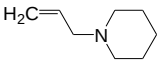
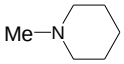
Compounds	Structure	Experimental pKa [ref]	E_B	E_{BH+}	$\Delta E^{\$}$
		Primary amines			
	$R\text{-}NH_2$				
2,2,2-trichloroethanamine	CH_2CCl_3	5.47 [1]	-1514.046508	-1514.494228	280.95
methylamine	Me	10.657, 10.62, 10.67, 10.68, 10.58 [1]; 10.66 [7]	-95.855831	-96.324161	293.88
ethylamine	Et	10.70, 10.67, 10.75, 10.60, 10.79 (20°C) [1]; 10.65 [7]	-135.161487	-135.630015	294.01
2-methylpropan-1-amine	$CH_2CH(Me)_2$	10.15 [1]	-213.765603	-214.233633	293.69
1-acetoxy-2-aminoethane*	$CH_2CH_2OC(=O)Me$	9.10 [1]	-363.044525	-363.505645	289.36
propylamine	$n\text{-}C_3H_7$	10.65 (23°C), 10.75, 10.69, 10.708 (20°C) [1]; 10.57 [3]; 10.54 [7]	-174.464254	-174.932745	293.98
ammonia	H	9.25 [1, 6]	-56.567827	-57.031630	291.04
allylamine*	CH_2CHCH_2	9.49 [1]; 9.69 [3,6]	-173.239623	-173.704013	291.41
1,2-ethanediamine (pKa1)*	$CH_2CH_2NH_2$	9.928 [1]; 9.92 [3]	-190.512192	-190.978654	292.71
1,2-ethanediamine (pKa2)*		6.848 [1]; 6.85 [3]	-190.978654	-191.433703	285.55
cyclohexylamine	C_6H_{11}	10.49 [1]; 10.64 [3]	-291.174354	-291.642348	293.67
1,3-propanediamine*	$(CH_2)_3NH_2$	10.62 (20°C), 10.32 (30°C) [1]; 10.47[3]	-229.815397	-230.283500	293.74
1,3-propanediamine*		8.64 (20°C), 8.33 (30°C) [1]; 8.49 [3]	-230.283500	-230.745040	289.62
phenylmethanamine	$CH_2C_6H_5$	9.34 [6, 7]; 9.15 [11]	-326.875575	-327.342630	293.08
n-butylamine*	$n\text{-}C_4H_7$	10.61, 10.66, 10.72 (20°C), 10.777 (20°C), 10.77 (16°C) [1]; 10.60 [7]	-213.767059	-214.235661	294.05
tert-butylamine	$C(Me)_3$	10.68, 10.40 (20°C), 10.83 (18°C), 10.79 (16°C) [1]; 10.69 [3]	-213.769817	-214.237769	293.64
undecylamine	$n\text{-}C_{11}H_{21}$	10.63 [1, 7]	-488.886986	-489.355702	294.12
2-amino-1-ethanol (ethanolamine)*	$(CH_2)_2OH$	9.4980, 9.500, 9.45, 9.49 (23°C), 9.58 (20°C), 9.6467 (20°C), 9.50 (22°C), 9.60 (20°C) [1]; 9.51 [7]	-210.384552	-210.848663	291.23
2-amino-1-propanol*	$CH(Me)CH_2OH$	9.43 [1]; 9.47 [3]; 9.51 [7]	-249.689599	-250.152026	290.18
3-amino-1-propanol	$(CH_2)_3OH$	9.96 [3, 7]	-249.688893	-250.155184	292.60
2-amino-2-methylpropanol*	$C(Me)_2CH_2OH$	9.71 [1]; 9.65 [3]	-288.991736	-289.453914	290.02
iso-propylamine*	$CH(Me)_2$	10.63, 3.40 (pKb) [1]	-174.466777	-174.934829	293.71
neo-pentylamine*	$CH_2C(Me)_3$	10.15, 10.24, 10.16 (20°C), 10.40 (17°C), 10.55 (16°C) [1]	-253.064566	-253.533205	294.08
n-heptylamine	$n\text{-}C_7H_{13}$	10.66 [1]	-331.675613	-332.144288	294.10
n-octylamine	$n\text{-}C_8H_{15}$	10.65, 10.57, 10.70 (19°C), 11.18 (18.5°C) [1]; 10.65[3, 7]	-370.978486	-371.447178	294.11
n-pentylamine	$n\text{-}C_5H_9$	10.64, 10.57, 10.63, 10.71 (22°C) [1]	-331.675613	-332.144288	294.10
sec-butylamine	$CH(Me)CH_2Me$	10.56 [1, 3, 7]	-213.767541	-214.235810	293.84
2-amino-2-cyanopropane	$C(Me)_2CN$	5.30 [1]	-266.708440	-267.161447	284.27

2-oxy-3-methoxybenzylamine*		10.52 [1]	-516.611064	-517.080179	294.37
4-oxo-2-methoxybenzylamine*		10.42 [1]	-516.618151	-517.086204	293.71
3-(2-aminoethyl)pyrazole*		9.61 [1]	-360.169326	-360.635787	292.71
4-aminomethylimidazole*		9.37 [1]	-320.885483	-321.344852	288.26
4-(2-aminoethyl)imidazole*		9.88 [1]	-360.188685	-360.655338	292.83
2-aminomethyleneamino-3-formylpyrazine*		5.15 (20°C), 5.3 (20°C) [1]	-581.860583	-582.312257	283.43
Secondary amines					
N-benzoylpiperazine*		7.75, 7.73 [1]	-612.274888	-612.737108	290.05
azetidine		11.29 [1,3,7]	-173.221869	-173.692085	295.07
pyrrolidine		11.11 [1]; 11.20 [2]; 11.12 [3, 7]; 11.13 [6]	-212.552025	-213.023635	295.94
piperidine		11.27 [1]; 11.305, 11.469 (20°C), 11.147 (30°C) [2]; 11.31 [3,7]	-251.859775	-252.330482	295.37
piperazine (pKa1)		5.68(20°C), 5.55, 5.56 (23.5°C), 5.63 (20°C), 5.54 (30°C) [1]; 5.333, 5.424 (20°C), 5.246 (30°C), 5.153 (35°C), 5.60 (20°C), 5.57 [2]	-268.354416	-268.809986	285.87
piperazine (pKa2)		9.82 (20°C), 9.81, 9.83 (23.5°C), 9.89 (20°C), 9.68 (30°C) [1]; 9.731, 9.864 (20°C), 9.609 (30°C), 9.485 (35°C), 9.72 (20°C), 9.81 [2]	-267.887137	-268.354416	293.22
α-ethylpyrroline*		7.43 [3]; 7.87 [7]	-289.951471	-290.409164	287.21
N-tert-butylaniline*		7.00, 7.10 (19°C) [2]; 7.10 [3]	-444.779577	-445.233812	285.04
2,5-diazahexane		10.40 [1]; 10.43 [6]	-269.095433	-269.562491	293.08
dimethylamine	 R_1, R_2=Me	10.73, 10.81, 10.77, 10.922 (20°C) [1]; 10.77 [3]; 10.73 [7]	-135.147983	-135.616996	294.31

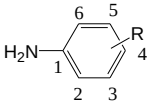
N-methylmethoxyamine	R_1=Me, R_2=OMe	4.75 [1]	-210.318360	-210.766429	281.17
allylmethylamine*	R_1=Me, R_2=CH_2CHCH_2	10.11 [1]	-212.530448	-212.996781	292.63
diethylamine	R_1, R_2=diMe	10.98, 11.04, 10.98, 11.090 (20°C), 11.11 (20°C), 1.16 [1]; 11.380 (15°C), 10.797 (35°C) [2]; 10.80 [3]	-213.758514	-214.228240	294.76
benzylmethylamine	R_1=Me, R_2=$CH_2C_6H_5$	9.58 [1]	-366.167379	-366.635611	293.82
di-n-propylamine	R_1, R_2=di-n-C_3H_7	11.00 [1]	-292.363782	-292.833676	294.86
diisopropylamine*	R_1, R_2=di-$CH(Me)_2$	11.05 [1]; 11.20 [2]	-292.362457	-292.832745	295.11
diethanolamine*	R_1, R_2=di-$(CH)_2OH$	8.96, 8.883, 9.005 (20°C) [1]; 8.88 [3]	-364.204633	-364.665155	288.98
diisopropanolamine*	R_1, R_2=di-CH(Me)OH	8.89 [2]	-442.821586	-443.281098	288.35
N-n-butylethanolamine*	R_1=n-C_4H_9, R_2=$(CH)_2OH$	9.90 [2]	-367.586759	-368.052509	292.26
di-isobutylamine*	R_1, R_2=$CH_2CH(Me)_2$	10.50 [1]	-370.966060	-371.434687	294.07
di-sec-butylamine*	R_1, R_2=CH(Me)CH_2Me	11.01 [1]	-370.963752	-371.433617	294.84
tert-butylcyclohexylamine*	R_1=$C(Me)_3$, R_2=C_6H_{11}	11.23 [1]	-448.367710	-448.838545	295.45
cyanomethylamine*	R_1=Me, R_2=CN	5.34, 5.3 (29°C) [1]; 5.34 [3, 7]	-188.105886	-188.557026	283.09

Tertiary amines

N-chloro-N-methylmethanamine	R_1, R_2=diMe; R_3=Cl	0.46 [1]	-594.743971	-595.182653	275.28
N-chloro-N-ethylmethanamine*	R_1, R_2=diEt; R_3=Cl	1.02 [1]	-673.352506	-673.793302	276.60
dimethyl-n-propylamine	R_1, R_2=diMe; R_3=n-C_3H_7	9.99 [1]	-253.046469	-253.514328	293.59
dimethy-isobutylamine	R_1, R_2=diMe; R_3=CH(Me)CH_2Me	9.91 [1]	-292.343752	-292.811296	293.39
bis(2-cyanoethyl)aminoethane*	R_1, R_2=diMe; R_3=CN	4.55 [1]	-476.852491	-477.301906	282.01
bis(2-chloroethyl)aminoethane*	R_1, R_2=diMe; R_3=Cl	6.55 [1]	-1211.61770	-1212.06929	283.38
trimethylamine	R_1, R_2, R_3=triMe	9.752, 9.81, 9.80, 9.784 (20°C) [1]; 9.801, 9.987 [2]	-174.441553	-174.908410	292.96
triallyamine	R_1, R_2, R_3 = tri-CH_2CHCH_2Me	8.31 [1]	-406.577322	-407.039213	289.84
N-ethyl-N-methylethanamine	R_1=Me; R_2, R_3=diEt	10.46 [1]	-253.045964	-253.514851	294.23
Tripropylamine*	R_1, R_2, R_3=tri-n-C_3H_7	10.65 [1]	-410.254098	-410.724734	295.33
triethylamine	R_1, R_2, R_3=triEt	10.75, 10.67, 10.8, 10.78 (20°C) [1]; 10.82, 10.778, 10.848(20°C), 10.859 (30°C) [2]	-292.345830	-292.815258	294.57
dimethylcyclohexylamine	R_1, R_2=diMe; R_3=C_6H_{11}	10.70 [5]	-369.748588	-370.218153	294.66
dimethylbenzylamine	R_1, R_2=diMe; R_3=C_6H_5	9.00 [1]; 9.02 [3]	-405.459201	-405.924017	291.68
diethylbenzylamine	R_1, R_2=diMe; R_3=Cl	9.50 [1]; 9.48 [3]	-484.061787	-484.528177	292.66
N-methyldiethanolamine*	R_1=Me; R_2, R_3=di-CH_2H_2OH	8.63 [2]	-403.514267	-403.975277	289.29
dimethyl-sec-butylamine	R_1, R_2=diMe; R_3=CH(Me)CH_2Me	10.40 [1]	-292.343773	-292.812787	294.31
dimethyl-tert-butylamine	R_1, R_2=diMe; R_3=$C(Me)_3$	10.52 [1]	-292.339258	-292.809382	295.01
dimethylethylamine	R_1, R_2=diMe; R_3=Et	9.99 [1]	-213.743996	-214.211906	293.62
tri-n-butylamine	R_1, R_2, R_3=tri-C_4H_9	10.89 [1]	-528.162326	-528.633489	295.66

N,N-di-n-butylaniline*		4.74 [2]	-601.981125	-602.430749	282.14
N-allylpiperidine*		9.70 [1]	-368.533784	-369.000644	292.96
1-methylpiperidine		10.08, 10.19 [1]; 10.38 [2]	-291.153830	-291.622544	294.12

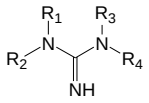
Anilines

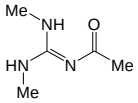
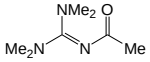
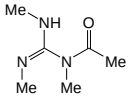
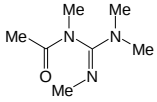


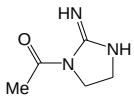
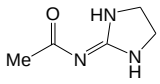
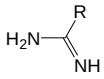
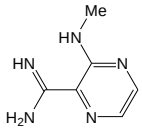
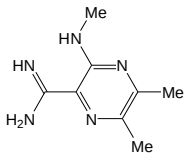
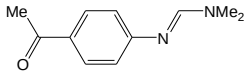
2-cyanoaniline	2-CN	0.95 [1]; 0.77 [2];	-379.842170	-380.275151	271.70
4-nitroaniline	4-NO_2	1.00, 1.02, 0.99, 1.13, 1.04 (20°C) [1]; 1.019, 0.88 [2]; 0.98, 1.11 [6]; 1.01 [3]	-492.129687	-492.559714	269.85
4-methylsulfonylaniline*	4-SO_2Me	1.364, 1.35 [1]; 1.48 [3]	-875.523166	-875.960519	274.44
4-cyanoaniline	4-CN	1.75, 1.739 [1]; 1.71 [2]	-379.845786	-380.281518	273.43
3-methylsulfonylaniline*	3-SO_2Me	2.58, 2.561 [1]; 2.68 [3]	-875.519343	-875.959987	276.51
2-fluoroaniline	2-F	2.96, 3.20 [1]; 3.17 [2]; 3.20 [3]; 2.96 [6]; 3.00 [8]; 3.23 [10]	-386.833495	-387.275523	277.38
3-chloroaniline	3-Cl	3.46, 3.67, 3.52, 3.33, 3.4 [1]; 3.521, 3.52, 3.45 [2]; 3.52 [3]; 3.32 [6]	-747.219989	-747.663359	278.22
4-bromoaniline	4-Br	3.88, 3.86, 3.95[1]; 3.86, 4.289, 3.888 [2]; 3.88 [3]; 3.91 [6]; 3.93 [13]	-2861.834166	-2862.279747	279.61
2-n-butylaniline*	2-n-C_4H_9	4.26 [1]	-444.795954	-445.243802	281.03
3,5-dimethylaniline	3, 5-diMe	4.76 [2,3]; 4.53 [1]	-366.196737	-366.646855	282.45
aniline	H	4.61 [8]; 4.21, 4.53 [9]; 4.80 [10]; 4.58 [12]; 4.67 [13]	-287.584939	-288.032610	280.92
4-tert-butylaniline*	4-$C(Me)_3$	4.95[1]; 3.78[3]	-444.789452	-445.239493	282.41
4-methoxyaniline	4-OMe	5.31, 5.34, 5.40 [1]; 5.357, 5.36 [2]; 5.29 [6]; 5.36 [3]	-402.098039	-402.550503	283.93
2-aminoaniline (pKa2)	2-NH_2	4.246, 4.47 [1]; 4.74, 4.60, 4.85 [2]; 4.47 [6]	-342.940429	-343.385532	279.31
2-aminoaniline (pKa1)	2-NH_2	1.30 (20°C), 0.6 [1]; 0.397, 0.67 [2]	-343.385532	-343.823124	274.59
2,4-dimethylaniline	2, 4-diMe	4.89, 4.84 [1]; 4.85, 4.60 [2]; 4.89 [3]	-366.194556	-366.644820	282.55
2,3-dimethylaniline	2, 3-diMe	4.72, 4.70 [1]; 4.70 [3]	-366.191787	-366.641221	282.02
2,5-dimethylaniline	2, 5-diMe	4.57, 4.53 [1]; 4.53 [3]	-366.195500	-366.644711	281.88
2,6-dimethylaniline	2, 6-diMe	3.95, 3.89, 4.25(22°C) [1]; 3.937, 3.95 [2]; 3.95 [3]	-366.194084	-366.641292	280.63
3,4-dimethylaniline	3, 4-diMe	5.15 [6]; 5.17 [1,3]	-366.194308	-366.645442	283.09
3,5-dichloroaniline	3, 3-diMe	2.05 (22°C), 2.55 (22°C), 2.00, 2.14 (21°C) [1]; 2.42, 2.371, 2.383 [2]; 2.37 [3]	-1206.852965	-1207.292191	275.62
4-methylthioaniline*	4-SMe	4.35 [1]; 4.31 [2]; 4.40 [3]	-725.102839	-725.550482	280.90
2-chloroaniline	2-Cl	2.65, 2.64, 2.63, 2.71, 2.6, 2.57 [1]; 2.661, 2.615, 2.42 [2]; 2.64 [3]; 2.62 [6]	-747.218114	-747.659233	276.81

4-chloroaniline	4-Cl	4.15, 3.98, 4.00, 4.05, 3.93, 3.82 [1]; 3.95, 3.982 [2]; 3.95 [3]; 4.03 [10] 3.81 [6]	-747.219176	-747.664188	279.25
2-bromoaniline	2-Br	2.53, 2.55, 2.45 [1]; 2.527, 2.61 [2]; 2.53 [3]; 2.60 [6]; 2.65 [13]	-2861.833977	-2862.274518	276.44
3-bromoaniline	3-Br	3.58, 3.53, 3.54, 3.55, 3.21 (24°C), 3.60 (20°C), 3.46 (30°C) [1]	-2861.835967	-2862.279248	278.16
3-fluoroaniline	3-F	3.50, 3.59, 3.57, 3.41, 3.39, 3.66 (20°C) [1]; 3.38 [6]; 3.57 [2]	-386.836709	-387.280280	278.35
4-fluoroaniline	4-F	4.65, 4.64, 4.53, 4.73 (20°C) [1]; 4.61 [2]; 4.52 [6]; 4.65 [3]	-386.833802	-387.281152	280.72
3-nitroaniline	3-NO_2	2.466, 2.47, 2.50, 2.46 [1]; 2.39, 2.460, 2.42 [2]; 2.46 [3]; 2.45 [6]	-492.120265	-492.559151	275.41
2-nitroaniline	2-NO_2	-0.26, -0.29, -0.25, -0.36, -0.31 (22°C), -0.30 (22°C) [1]; -0.29, -0.246, -0.26 [2]; -0.28 [3,6]	-492.121466	-492.549754	268.76
3-methoxyaniline*	3-OMe	4.20, 4.23, 4.24(22°C), 4.30 (20°C) [1]; 4.23, 4.20 [2]; 4.20 [3,6]	-402.102028	-402.550120	281.18
2-methoxyaniline*	2-OMe	4.52, 4.56(20°C), 4.61 (20°C) [1]; 4.527, 4.48 [2]; 4.49 [6]; 4.53 [3]	-402.099248	-402.547867	281.51
2,4-dichloro-6-nitroaniline	2, 4-diMe; 6-NO_2	-3.01, -3.28, -3.33 [2]; -3.00 [3]	-1411.378815	-1411.799676	264.09
2,5-dichloro-4-nitroaniline	2, 5-diMe; 4-NO_2	-1.79, -1.74 [2]; -1.74 [3]	-1411.376542	-1411.798297	264.66
2,6-dichloro-4-nitroaniline	2, 6-diMe; 4-NO_2	-3.27, -3.20 [2]; -3.31[3]	-1411.385520	-1411.803920	262.55

guanidines



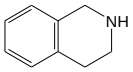
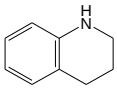
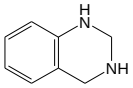
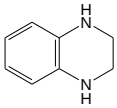
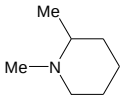
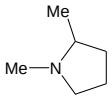
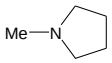
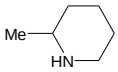
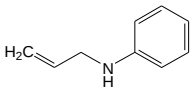
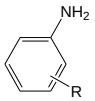
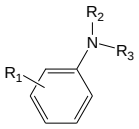
guanidine	R_1, R_2, R_3, R_4=tetraH	13.59 (24.2°C), 13.60[1]	-205.395274	-205.872273	299.32
methylguanidine	R_1=Me; R_2, R_3, R_4=triH	13.40 [1]	-244.686332	-245.163648	299.52
Acetylguanidine*	R_1=COMe; R_2, R_3, R_4=triH	8.26 (20°C) [1]; 8.20 (23°C) [2]; 8.23 [3]	-358.055369	-358.516946	292.67
Aminoguanidane*	R_1=NH_2 ; R_2, R_3, R_4=triH	2.96 (pKb) [1]	-260.710490	-261.188765	300.12
N,N'-dimethylguanidine	R_1, R_3=diMe; R_2, R_4=diH	13.60 [1]	-283.975541	-284.454512	300.56
1,1,3,3,-tetramethylguanidine	R_1, R_2, R_3, R_4=tetraMe	13.60 [1]	-362.547159	-363.028288	301.91
2-acetyl-1,3-dimethylguanidine*		7.50 [2]	-436.636344	-437.100496	291.26
2-acetyl-1,1,3,3-tetramethylguanidine*		7.50 [2]	-515.201341	-515.666308	291.77
(Z)-acetyl-1,2,3-trimethylguanidine*		8.93 [2]	-475.912673	-476.380364	293.48
(Z)-acetyl-1,2,3,3-tetramethylguanidine*		9.10 [2]	-515.199550	-515.668507	294.27

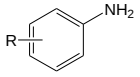
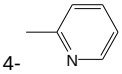
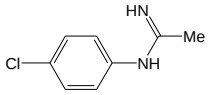
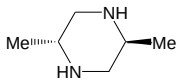
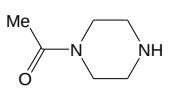
1-(2-iminoimidazolidin-1-yl)-ethanone		9.06 [2]	-435.433147	-435.898057	291.74
N-(imidazolidin-2-ylidene)-Acetamide		7.48 [2]	-435.441732	-435.903717	289.90
		amidines			
					
acetamidine	R=H	12.1, 12.40 [1]; 12.10 [4]	-189.331971	-189.807106	298.15
α-hydroxy-alpha-methylbutyramidine	R=C(OH)(CH_3)CH_2CH_3	11.60 [4]	-382.460961	-382.931918	295.53
hydroxy-isobutyramidine	R=CH(CH_3)CH_2OH	11.35 [4]	-343.155074	-343.628844	297.30
phenylglycolamidine	R=CH(OH)C_6H_5	10.82 [4]	-495.566936	-496.038774	296.08
2-amidino-3-methylaminopyrazine		8.96 (20°C) [1]; 8.98 (20°C) [14]	-507.805224	-508.267085	289.82
2-amidino-5,6-dimethyl-3-methylaminopyrazine		9.43 (20°C) [1]; 9.45 (20°C) [14]	-586.421832	-586.886939	291.86
(E)-N'-(4-acetylphenyl)-N,N-dimethylformamidine		7.02 [15]	-612.276828	-612.735880	288.06

*A conformational search was carried out on these compounds using the GMMX feature of PCModel (see text for more details)

$ kcal/mol

Table S1b Calculated energies and experimental pKas for aliphatic and alicyclic amines --- test set

Compounds	Structure	Experimental pKa [ref]	E_B	E_{BH+}	$\Delta E^{\$}$
1,2,3,4-tetrahydroisoquinoline*		9.41 [1]	-404.276773	-404.742430	292.20
1,2,3,4-tetrahydroquinoline*		5.03 [1]	-404.287289	-404.737360	282.42
1,2,3,4-tetrahydroquinazoline*		7.63 [1]	-420.324601	-420.787916	290.73
2-ethylaziridine		8.31[1,14]; 8.29 [1]	-212.529946	-212.992330	290.15
1,2,3,4-tetrahydroquinoxaline		4.48 [1]	-420.333049	-420.784325	283.18
N,2-dimethylpiperidine		10.26 [14]	-330.454120	-330.923658	294.64
N,2-dimethylpyrrolidine		10.26 [14]	-291.151038	-291.620050	294.31
N-methylazetidine*		10.40 [1,14]	-212.519225	-212.987577	293.90
N-methylpyrrolidine		10.46 [14]	-251.847634	-252.315683	293.71
2-methylpiperidine		10.92 (30°C), 11.02 (23.2°C), 11.08, 10.95, 11.15 (20.1C) [1]; 10.98 [14]	-291.165162	-291.635720	295.28
N-allylaniline*		4.17 [1]	-404.256782	-404.703486	280.31
					
2-acetylaniline	R=2-COMe	2.22, 2.4 [1]	-440.232605	-440.673653	276.76
3-acetylaniline	R=3-COMe	3.56, 3.59, 3.60 [1]	-440.230839	-440.675409	278.97
					
N-t-butyl-N-ethylaniline	R_1=H; R_2=t-butyl; R_3=Et	8.02 [1]	-523.355932	-523.818453	290.24
N-t-butyl-2-methylaniline	R_1=H; R_2=t-butyl; R_3=Me	6.49 [1]	-484.083109	-484.534949	283.53
N-cyclohexylaniline	R_1,R_2=diH; R_3=cyclohexyl	5.60 [1]	-522.191877	-522.641233	281.98

3-cyano-N,N-dimethylaniline	R_1=3-CN; R_2, R_3=diMe	2.969 [1]	-458.418907	-458.862710	278.49
N-n-butylaniline	R_1,R_2=diH; R_3=n-butyl	5.12, 4.95 (30°C) [1]; 5.44 [2]	-444.785934	-445.235158	281.89
N,N-dimethylaniline	R_1=H; R_2, R_3=diMe	5.12, 5.15, 5.150, 5.068, 5.178 (20°C), 5.05 (25.5°C) [1]; 5.07, 4.22 [2]	-366.162979	-366.614752	283.49
N,2-dimethylaniline	R_1, R_2=diMe; R_3=H	4.62 [1]; 4.60, 5.08 [2]	-366.180554	-366.628893	281.34
N-methyl-N-n-propylaniline	R_1=H; R_2=n-propyl; R_3=Me	5.67 [1]	-444.769456	-445.221705	283.79
4-bromo-N-t-butylaniline	R_1=4-Br; R_2=t-butyl; R_3=H	5.93 [1]	-3019.03045	-3019.48124	282.88
2-bromo-N, N-dimethylaniline	R_1=2-Br; R_2, R_3=diMe	4.31 [1]	-2940.40425	-2940.85587	283.40
4-bromo-N, N-dimethylaniline	R_1=4-Br; R_2, R_3=diMe	4.232, 4.282 (20°C) [1]	-2940.41388	-2940.86209	281.26
					
4-bromo-2,6-dinitroaniline	4-Br; 2,6-diNO_2	3.54 [1]	-2940.445404	-2940.889333	278.57
2-bromo-4,6-dinitroaniline	2-Br; 4,6-diNO_2	-6.54, -6.71 (25±3°C) [1]	-3270.895925	-3271.306380	257.56
3-bromo-4-methylaniline	3-Br, 4-Me	3.98 (23°C), 4.04 (18.5°C) [1]	-2901.139548	-2901.585262	279.69
2-n-butylaniline	2-n-Butyl	4.26 [1]	-444.794633	-445.243174	281.46
4-chloro-2-nitroaniline	2-NO_2, 4-Cl	-1.02, -1.03 (25±3°C), -1.11 (20°C), 1.05 (22±2°C), -1.02 (22±2°C), -0.46 (22±2°C), -1.06, -0.91, -1.01(19 2°C) [1]	-951.752515	-952.178144	267.09
3-trifluoromethylaniline	3-CF3	3.49 [1,5]	-624.655447	-625.097278	277.25
4-trifluoromethylaniline	4-CF3	2.45 [1]; 2.57 [6]	-624.658634	-625.097873	275.63
2-p-aminophenylpyridine	4- 	2.47 [14]	-534.659877	-535.104210	278.82
DABCD (triethylenediamine)		8.19 (20°C), 8.8 [1]; 8.28.82 [2]	-345.274136	-345.741766	293.44
N-methylaziridine		7.86 [14]	-173.212502	-173.676067	290.89
N-acetimido-4-chloroaniline*		9.5 (22.5±2.5°C) [1]	-879.982398	-880.446645	291.32
trans-2,5-dimethylpiperazine		5.20 [1]	-346.969965	-347.419542	282.12
trans-2,5-dimethylpiperazine (pKa2)		9.66 [1]	-346.500103	-346.969965	294.85
1-acetylpiperazine		7.94 [1]	-420.563580	-421.026553	290.52

*A conformational search was carried out on these compounds using the GMMX feature of PCModel (see text for more details)

$ kcal/mol

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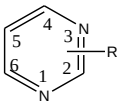
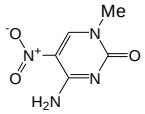
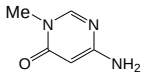
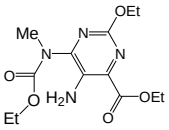
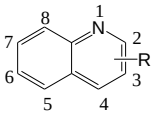
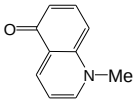
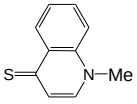
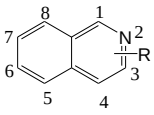
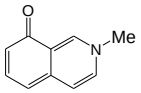
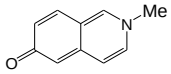
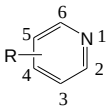
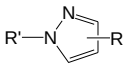
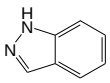
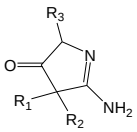
Table S2a Calculated energies and experimental pKas for heteroaromatic bases --- training set

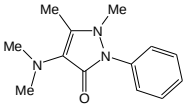
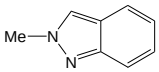
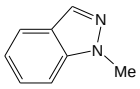
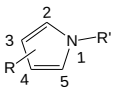
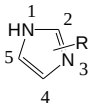
Compounds	Structures	Experimental pKa [ref]	E_B	E_{BH+}	$\Delta E^{\$}$
		pyrimidines			
					
pyrimidine	H	1.23 (20°C) [1]; 1.30 (20°C) [9]	-264.317277	-264.762723	279.52
pyrimidine		-6.30 (20°C) [1]; -7.70, -6.92 [2]	-264.762723	-265.177832	260.49
2-aminopyrimidine	2-NH_2	3.45 (20°C) [1]; 3.54 (20°C) [9]; 3.81 [11]	-319.698047	-320.149201	283.10
4-aminopyrimidine	4-NH_2	5.69 (20°C) [1]; 5.71 (20°C) [9]	-319.698572	-320.156819	287.55
5-aminopyrimidine	5-NH_2	2.51, 2.83 (20°C) [1]; 2.60 [9]	-319.683618	-320.134490	282.93
4-ethylthiopyrimidine*	4-SCH_2CH_3	2.60 (20°C) [2]	-741.144446	-741.595966	283.33
2-ethylthiopyrimidine*	2-SCH_2CH_3	0.70 (20°C) [2]	-741.144722	-741.588331	278.37
2-amino-5-chloropyrimidine	2-NH_2, 5-Cl	1.73 (20°C) [2]	-779.327762	-779.772181	278.88
2-amino-4-chloro-6-dimethylaminopyrimidine*	2-NH_2, 4-Cl, 6-$N(Me)_2$	3.95 (20°C) [2]	-913.294076	-913.744731	282.79
4-amino-6-chloro-2-dimethylaminopyrimidine*	2-$N(Me)_2$, 4-NH_2, 6-Cl	3.75 (20°C) [2]	-913.293893	-913.743676	282.24
2-amino-5-chloro-4-hydroxypyrimidine*	2-NH_2, 4-OH, 5-Cl	2.53 [2]	-854.575014	-855.023304	281.31
2-amino-5-chloro-4-hydroxypyrimidine*		7.97 [2]	-854.112862	-854.575014	290.01
2-amino-6-chloro-4-hydroxypyrimidine	2-NH_2, 4-OH, 6-Cl	0.50 [2]	-854.584413	-855.025154	276.57
2-amino-5-(4-chlorophenyl)pyrimidine	2-NH_2, 5-p-C_6H_5CL	3.14 (20°C) [2]	-1010.356518	-1010.805501	281.74
2-amino-5-cyanopyrimidine*	2-NH_2, 5-CN	-1.48 (20°C) [2]	-411.951939	-412.390465	275.18
4-amino-5-cyanopyrimidine	4-NH_2, 5-CN	2.49 (20°C) [1]	-411.948904	-412.395299	280.12
4-amino-6-methoxypyrimidine	4-NH_2, 6-OMe	4.00 (20°C), 4.16[1]; 4.02 [20°C] [9]	-434.226561	-434.680483	284.84
2-amino-4-methylpyrimidine	2-NH_2, 4-Me	4.11(20°C) [1]; 4.15 (20°C) [9]	-359.009237	-359.462886	284.67
4-amino-6-methylpyrimidine	2-NH_2, 6-Me	6.16 [1]	-359.009583	-359.469546	288.63
4-amino-2-methylaminopyrimidine	2-NHMe, 4-NH_2	7.53 (20°C) [1]; 7.55 (23°C) [9]	-414.368421	-414.831313	290.47
4-amino-6-methylaminopyrimidine	4-NH_2, 6-NHMe	6.30 (20°C) [1]; 6.32 (20°C) [9]	-414.365618	-414.824940	288.23
2-chloro-4-methylaminopyrimidine*	2-Cl, 4-NHMe	2.80 (20°C) [1]; 2.83 (20°C) [9]	-818.628596	-819.076360	280.98
4-amino-5-aminomethyl-2-methyl-pyrimidine	2-Me, 4-NH_2, 5-CH_2NH_2	4.00 [1]	-453.659089	-454.113985	285.45
4-amino-6-chloropyrimidine*	4-NH_2, 6-Cl	2.10 (20°C) [1, 13]	-779.335275	-779.780389	279.31
4-amino-6-chloro-2-methylpyrimidine*	2-Me, 4-NH_2, 6-Cl	3.79 (20°C) [1]	-818.646611	-819.094830	281.26
2-amino-4,6-dimethylpyrimidine	2-NH_2; 4,6-diMe	4.95, 5.0, 4.82(20°C) [1]; 4.85 (20°C) [9]	-398.320184	-398.775883	285.96
4-amino-6-hydroxypyrimidine*	4-NH_2, 6-OH	1.36 [1]	-394.946365	-395.393151	280.36
4-amino-2-mercaptopyrimidine*	4-NH_2, 2-SH	3.29 (20°C) [1]	-717.919303	-718.371997	284.07
4-amino-1,2-dihydro-1-methyl-5-nitro -2-oxo-pyrimidine		1.35 [1]	-638.783449	-639.225940	277.67
4-amino-1,6-dihydro-1-methyl-6-oxo-pyrimidine		0.98 (20°C) [1]	-434.251745	-434.696923	279.35

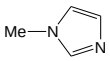
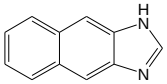
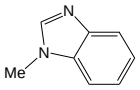
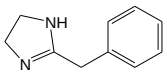
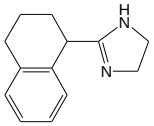
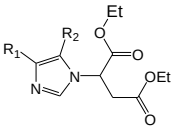
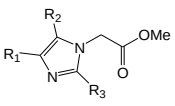
5-amino-2-ethoxy-4-ethoxycarbonyl-6-ethoxy-carbonylmethylaminopyrimidine		4.58 [1]	-1141.826922	-1142.281386	285.18
	quinolines				
					
quinoline	H	4.81, 4.89, 4.95, 4.93, 4.96 (20°C) [1] 4.97 [10]; 5.05 [11]; 4.87, 4.94 (20°C) [9]	-401.894291	-402.350499	286.28
2-aminoquinoline	2-NH_2	7.30 (20°C), 7.04(35°C) [1]; 7.34 (20°C) [9]	-457.269793	-457.730935	289.37
3-aminoquinoline	3-NH_2	4.91(20°C), 4.94 (20°C), 4.73 (35°C) [1]; 4.95 (20°C) [9]	-457.258967	-457.716251	286.95
4-aminoquinoline	4-NH_2	9.13 (20°C); 9.17 [1]; 5.46 (20°C) [9]	-457.263235	-457.730847	293.43
5-aminoquinoline*	5-NH_2	5.42 (20°C), 5.27 (35°C) [1]; 5.63 (20°C) [9]	-457.256114	-457.716511	288.90
6-aminoquinoline	6-NH_2	5.59 (20°C), 5.45 (35°C) [1]; 5.63 (20°C) [9]	-457.259678	-457.720274	289.03
7-aminoquinoline	7-NH_2	6.61 (20°C) [1]; 6.65 (20°C) [9]	-457.260852	-457.724898	291.19
8-aminoquinoline	8-NH_2	3.95 (20°C) [1]; 3.99 (20°C) [9]	-457.259318	-457.710920	283.38
4-amino-7-chloroquinoline	4-NH_2, 7-Cl	8.23 (30°C) [1]; 8.22 (23°C) [9]	-916.897046	-917.361798	291.64
5-amino-8-hydroxyquinoline*	5-NH_2, 8-OH	5.67 (20°C) [1]	-532.488826	-532.944468	285.92
4-amino-6-methoxyquinoline*	4-NH_2, 6-OMe	8.93 (30°C) [1]	-571.779022	-572.247488	293.97
8-amino-6-methoxyquinoline*	8-NH_2, 6-OMe	3.38 (30°C) [1]	-571.776114	-572.228716	284.01
4-amino-2-methylquinoline	2-Me, 4-NH_2	9.42 (20°C) [1]	-496.572131	-497.041864	294.76
4-amino-2,6,8-trimethylquinoline	2, 6, 8-triMe; 4-NH_2	10.40 (20°C) [1]	-575.181713	-575.653497	296.05
2-bromoquinoline	2-Br	1.50 [1]	-2976.147385	-2976.589957	277.72
5-bromoquinoline	5-Br	3.62 [1]	-2976.140535	-2976.592714	283.75
3-hydroxyquinoline*	3-OH	4.18 (20°C), 4.28 (20°C) [1]; 44.30 (20°C) [9]	-477.128372	-477.581866	284.57
5-hydroxyquinoline*	5-OH	5.18 (20°C) [1]; 5.20 (20°C) [9]	-477.127957	-477.584895	286.73
6-hydroxyquinoline*	6-OH	5.15 (20°C) [1]]; 5.17 (20°C) [9]	-477.129404	-477.586329	286.73
7-hydroxyquinoline*	7-OH	5.46 (20°C) [1]; 5.48 (20°C) [9]	-477.130547	-477.588690	287.49
8-hydroxyquinoline*	8-OH	5.11 (20°C), 5.017 (20°C), 4.910, 4.88 (20±3°C), 5.13 (20°C) [1]; 5.13(20°°C) [9]	-477.131286	-477.583220	283.59
8-hydroxy-2-methylquinoline*	2-Me, 8-OH	5.61 [1]; 5.55 [3]	-516.440717	-516.895273	285.24
8-hydroxy-4-methylquinoline*	4-Me, 8-OH	5.56 [1, 3]	-516.438145	-516.891992	284.79
6-bromo-4-chloroquinoline	4-Cl, 6-Br	2.83 [1]	-3435.773511	-3436.223412	282.32
3-chloroquinoline	3-Cl	2.63 [1]	-861.526165	-861.974912	281.59
1,5-dihydro-1-methyl-5-oxo-quinoline		6.09 (20°C) [1]	-516.418609	-516.875938	286.98

1,4-dihydro-1-methyl-4-thioquinoline		0.56 (20°C) [1]	-839.415444	-839.857811	277.59
		isoquinolines			
					
isoquinoline	H	5.38 (20°C), 5.42 (20°C), 5.36 [1] 5.59 [10]; 5.59 [11]; 5.40 (20°C) [9]	-401.892756	-402.350382	287.16
3-aminoisoquinoline	3-NH_2	5.03 (20°C), 4.85 (35°C) [1]; 5.05 (20°C) [9]	-457.263796	-457.720074	286.32
4-aminoisoquinoline	4-NH_2	6.26 (20°C) [1]; 6.28 (20°C) [9]	-457.255006	-457.716871	289.82
5-aminoisoquinoline*	5-NH_2	5.57 (20°C) [1]; 5.59 (20°C) [9]	-457.255161	-457.714600	288.30
6-aminoisoquinoline	6-NH_2	7.16 (20°C) [1]; 7.17 (20°C) [9]	-457.260744	-457.726088	292.01
7-aminoisoquinoline	7-NH_2	6.19 (20°C) [1]; 6.20 (20°C) [9]	-457.258371	-457.720554	290.02
8-aminoisoquinoline	8-NH_2	6.04 (20°C) [1]; 6.06 (20°C) [9]	-457.255485	-457.716718	289.43
1-methoxyisoquinoline	1-OMe	3.01 (20°C)[1]; 3.05 [9]	-516.420380	-516.870462	282.43
4-nitroisoquinoline	4-NO_2	1.35 [1]; 1.35 [9]	-606.413736	-606.858741	279.25
5-nitroisoquinoline	5-NO_2	3.49 (20°C) [1]; 3.53 [9]	-606.415662	-606.866199	282.72
3-methylisoquinoline	3-Me	5.64 [1]	-441.202167	-441.661057	287.96
1-methylthioisoquinoline	1-SMe	3.89 (20°C) [1]	-839.412178	-839.864936	284.11
1-mercaptoisoquinoline	1-SH	10.86 (20°C) [1]; 10.82 (20°C) [9]	-799.558268	-800.029722	295.84
4-hydroxyisoquinoline*	4-OH	4.78 (20°C), 4.70 [1]; 4.80 (20°C) [9]	-477.125793	-477.582668	286.69
5-hydroxyisoquinoline*	5-OH	5.38 (20°C) [1]; 5.40 (20°C) [9]	-477.126500	-477.584156	287.18
6-hydroxyisoquinoline*	6-OH	5.83 (20°C) [1]; 5.85 (20°C) [9]	-477.129243	-477.589630	288.90
7-hydroxyisoquinoline*	7-OH	5.68 (20°C) [1]; 5.70 (20°C) [9]	-477.127897	-477.586640	287.87
8-hydroxyisoquinoline*	8-OH	5.64 (20°C) [1]; 5.66 (20°C) [9]	-477.126589	-477.585284	287.84
2,8-dihydro-2-methyl-8-oxo-isoquinoline		5.99 (20°C) [1]	-516.425377	-516.882919	287.11
2,6-dihydro-2-methyl-6-oxo-isoquinoline		5.78 (20°C) [1]	-516.422034	-516.878716	286.57
		pyrazines			
					
pyrazine	H	1.10, 0.65 (27±2°C), 0.6, 0.51 (20°C) [1]; 0.65 (27°C) [9]	-264.310142	-264.754033	278.55
2-hydroxypyrazine*	2-OH	8.25 (20°C) [1]	-339.555783	-339.999866	278.67
2-aminopyrazine	2-NH_2	2.93, 3.07 (20°C) [1]; 3.14 (20°C) [9]	-319.685704	-320.135895	282.50
2-amino-3-carboxypyrazine	2-NH_2, 3-COOH	3.70 [1]	-507.816652	-508.265373	281.58
2-amino-3-carboxy-5,6-dimethylpyrazine	2-NH_2; 3-COOH; 5, 6-diMe	4.48 [1]	-586.433111	-586.886874	284.74
2-carbamylpyrazine	2-$CONH_2$	-0.5 [1]	-433.029581	-433.471246	277.15
2-carbamyl-3-methylaminopyrazine*	2-$CONH_2$, 3-NHMe	2.09 (20°C) [1]	-527.704465	-528.151137	280.29

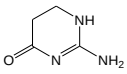
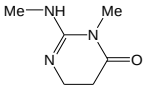
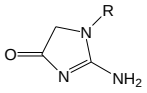
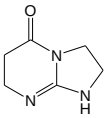
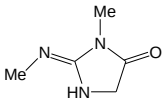
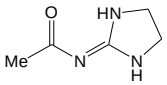
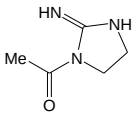
2,5-dimethylpyrazine	2, 5-diMe	2.1, 1.97, 1.9, 1.85 (27±2°C) [1]	-342.931662	-343.380068	281.38
2,6-dimethylpyrazine	2, 6-diMe	2.5, 1.90 (27±2°C) [1]	-342.931871	-343.380662	281.62
2-dimethylaminopyrazine	2-$N(Me)_2$	3.24 [1]	-398.264388	-398.715997	283.39
2-methyoxypyrazine*	2-OMe	0.75 (20C) [1]	-378.838006	-379.283558	279.59
2-methylpyrazine	2-Me	1.50, 1.47, 1.4, 1.45 (27±2°C) [1]	-303.621111	-304.067466	280.09
2-methylaminopyrazine*	2-NHMe	3.39 [1]	-358.977070	-359.428246	283.12
2-methylthiopyrazine*	2-SMe	0.55, 0.48 (20°C) [1]	-701.831955	-702.276707	279.09
tetramethylpyrazine	2, 3, 5, 6-tetraMe	2.8, 3.6 (25±0.5°C), 3.7, 3.55 (27±2°C) [1]	-421.547661	-421.999051	283.25
1,2-dihydro-1-methyl-2-oxo-pyrazine*		-0.04 (20°C) [1]	-378.861187	-379.305460	278.79
1,2-dihydro-1-methyl-2-thio-pyrazine*		-0.18, -0.45 (20°C) [1]	-701.834825	-702.276493	277.15
		pyridines			
					
2-chloropyridine	2-Cl	0.49, 0.72 [1]; 0.72 [9]	-707.906015	-708.348256	277.51
3-hydroxypyridine*	3-OH	5.10 [1]; 4.80 [3]	-323.505080	-323.958799	284.71
2-bromopyridine	2-Br	0.71, 0.90 [1]; 0.90 [9]	-2822.521307	-2822.964096	277.85
3-nitropyridine	3-NO_2	0.77 [1]; 1.18 [2]; 0.81[9]	-452.796701	-453.239362	277.77
3-cyanopyridine	3-CN	1.36, 1.39 [1]; 1.35 [2]; 1.45 (24°C) [9]	-340.519250	-340.963746	278.93
3-bromopyridine	3-Br	2.84, 2.91 (20°C) [1]; 2.85 [2]; 2.84 [9]	-2822.517234	-2822.966318	281.80
3-fluoropyridine	3-F	2.97 [1, 9]	-347.516796	-347.966355	282.10
3-formylpyridine*	3-CHO	3.76, 3.84 [1]; 3.73, 3.70, 3.75 [2]; 3.80 (20°C) [9]	-361.600685	-362.049426	281.59
3-methoxypyridine*	3-OMe	4.91 [1]; 4.78 [2]; 4.88 (20°C) [9]	-362.785866	-363.241869	286.15
2-vinylpyridine*	2-CH_2-CH=CH_2	4.98, 4.92 [1]	-364.957518	-365.414388	286.69
Pyridine	H	5.25 [2]; 5.215, 5.23, 5.22 [2]; 5.17 [9]; 5.31 [10]; 5.42 [15]	-248.269028	-248.725510	286.45
3-ethylpyridine	3-Et	5.56 [1]; 5.70 [9]	-326.876563	-327.334739	287.51
2-isopropylpyridine*	2-$CH(Me)_2$	5.83 [1, 9]	-366.180862	-366.639476	287.78
2-methylpyridine	2-Me	5.97 [1]; 5.957, 6.06 [2]; 5.943, 5.97 [9]	-287.578561	-288.037303	287.87
4-methoxypyridine	4-OMe	6.47 [1]; 6.62 (20°C) [9]	-362.790281	-363.251064	289.15
2,4-dimethylpyridine	2, 4-diMe	6.77, 6.99 [1]; 6.85 (20°C), 6.64 (30°C) [2]; 6.75 [11]	-326.886912	-327.348072	289.38
2,4,6-trimethylpyridine	2, 4, 6-triMe	7.59, 7.43 [1]; 7.25[2]; 7.59 [15]	-366.196007	-366.659372	290.77
2-aminopyridine	2-NH_2	6.71 [1]; 6.86 (20°C) [2, 13]; 6.71 [14]; 6.70 [15]	-303.642149	-304.102237	288.71
3-aminopyridine*	3-NH_2	6.03 [1]; 6.04 [2]; 5.98 (20°C) [9]	-303.633709	-304.094571	289.20
4-aminopyridine	4-NH_2	9.18 [1]; 9.12 [2]; 9.17 (20°C) [9]; 9.22 [14]; 9.18 [15]	-303.640134	-304.107737	293.43
3-methylpyridine	3-Me	5.52, 5.63, 5.68, 5.66 [1]; 5.703, 5.67 [2]; 5.68 [3]; 5.68, 5.657 [9]	-287.576519	-288.034433	287.35

4-methylpyridine	4-Me	6.03, 6.08, 5.98, 6.02, 6.00 [1]; 6.03, 5.992 [2]; 6.00 [3]; 6.02, 6.025 [9]	-287.577558	-288.036569	288.03
2-methoxypyridine	2-OMe	3.06, 3.25 (20°C), 3.40 (20°C) [1]; 3.28 [2]; 3.06 [3]	-362.796268	-363.244514	281.28
4-ethylpyridine	4-Et	5.87, 6.02 [1]; 6.03 [2]; 5.87 [3]; 6.02[9]	-326.878007	-327.337436	288.30
2-ethylpyridine*	2-Et	5.89, 5.97 [1]; 5.89 [3]; 5.97 [9]	-326.878924	-327.339071	288.75
4-bromopyridine	4-Br	3.78 [1]; 3.75[2]; 3.71[3]	-2822.518031	-2822.970262	283.78
2-nitropyridine	2-NO_2	-2.06 [3]	-452.800482	-453.233931	271.99
4-nitropyridine	4-NO_2	1.39 [2]; 1.23 [3]	-452.795456	-453.239977	278.94
2-fluoropyridine	2-F	-0.44 [1,3,9]	-347.527778	-347.966490	275.30
3-cloropyridine	3-Cl	2.84 [1, 3, 9]; 2.81[2]	-707.901017	-708.350232	281.89
4-cloropyridine	4-Cl	3.84 (20°C) [1]; 3.83 [2,3]	-707.902281	-708.354629	283.85
2-cyanopyridine	2-CN	-0.26 [1,3,9]	-340.517929	-340.957112	275.59
4-cyanopyridine	3-CN	1.9 [1,3, 13]; 1.86 [2]	-340.517354	-340.964010	280.28
2,5-dimethylpyridine	2, 5-diMe	6.40, 6.47 (20°C) [1]; 6.55 (20°C) [2]; 6.43 [3]; 6.53 [11]	-326.885734	-327.345945	288.79
2,6-dimethylpyridine	2, 6-diMe	6.75, 6.64, 6.72, 6.60 [1]; 6.64 [2]; 6.71 [3]	-326.887883	-327.348934	289.31
3,4-dimethylpyridine	3, 4-diMe	6.46, 6.52 (20°C) [1]; 6.48 [2]; 6.47 [3]; 6.64 [11]	-326.883586	-327.343897	288.85
3,5-dimethylpyridine	3, 5-diMe	6.15, 6.14 (20°C), 6.25 (20°C) [1]; 6.14 [2]; 6.09 [3]	-326.883583	-327.342845	288.19
2-isopropylpyridine	2-$CH(Me)_2$	5.72 (25±1°C), 5.88 (20°C), 5.68 (35°C) [1]; 5.72 [3, 9]	-366.180863	-366.639464	287.78
4-isopropylpyridine	4-$CH(Me)_2$	6.02 (25±1°C) [1]; 6.04 [2]; 6.02 [3,9]	-366.180703	-366.639662	288.00
2-tert-butylpyridine	2-$C(Me)_3$	5.76 [1,3,9]; 5.90 [2]	-405.477976	-405.936480	287.72
3-tert-butylpyridine	3-$C(Me)_3$	5.82 [1, 3, 9]	-405.475992	-405.934279	287.58
4-tert-butylpyridine	4-$C(Me)_3$	5.99 [1, 3, 9]	-405.477485	-405.936550	288.07
		pyrazoles			
					
Pyrazole	R=H; R'=H	2.48 [1]; 2.52 (20°C), 2.52, 2.61 [2]	-226.206341	-226.652707	280.10
1,3-dimethylpyrazole	R=3-Me; R'=Me	3.11 [1]; 2.82 (20°C) [2]	-304.812804	-305.263194	282.62
3,5-dimethylpyrazole	R=3, 5-Me; R'=H	4.38 [1,9]; 4.12 (20°C) [2]	-304.824770	-305.277368	284.01
3-methylpyrazole	R=3-Me; R'=H	3.56 [1, 3]; 3.32 (20°C) [2]	-265.515263	-265.965107	282.28
3-(2-aminoethyl)pyrazole	R=3-$CH_2CH_2NH_2$, R'=H	2.02 (20°C) [1]	-360.169326	-360.617840	281.45
N-methylpyrazole	R=H; R'=Me	2.09 [2]; 2.10 [6]; 2.04 [9]	-265.503586	-265.950920	280.71
benzpyrazole		1.30 [6]	-379.829397	-380.272146	277.83
					
3-amino-4,5-dihydro-4-	R_1=$CHMe_2$; R_2, R_3=diH	2.80 [1]	-474.715580	-475.161229	279.65

isopropyl-5-oxo-pyrazole					
3-amino-4,5-dihydro-4,4-dimethyl-5-oxo-pyrazole	R_1, R_2=diMe; R_3=H	2.10 [1]	-435.415196	-435.858799	278.37
3-amino-4,5-dihydro-5-oxo-pyrazole	R_1, R_2, R_3=triH	2.90 [1]	-356.817351	-357.261996	279.02
3-amino-4,5-dihydro-5-oxo-1-phenyl-pyrazole	R_1, R_2=diMe; R_3=C_6H_5	1.20 [1]	-587.830145	-588.270836	276.54
2,3-dihydro-4-dimethylamino-1,5-dimethyl-3-oxo-2-phenylpyrazole		5.04 [1]	-744.988117	-745.443617	285.83
N-methylbenz-[3,4]-pyrazole		2.00 [6]	-419.123273	-419.570984	280.94
N-methylbenzpyrazole		0.40 [6]	-419.126234	-419.569171	277.95
	pyrroles (c2 protonation)				
					
Pyrrole	R=H, R'=H	-3.80 [1]; -4.40 [2]	-210.164016	-210.598018	272.34
1-methylpyrrole	R=H, R'=-Me	-2.90 [1]; -3.40 [2]	-249.458217	-249.895965	274.69
2-methylpyrrole	R=2-Me, R'=H	-0.21 [1]	-249.472273	-249.914019	277.20
3-methylpyrrole	R=3-Me, R'=H	-1.00 [1]	-249.469142	-249.907269	274.93
2,5-dimethylpyrrole	R=2, 5-Me; R'=H	-0.71 [1]; -0.80 [3]	-288.780319	-289.219078	275.33
2,4-dimethylpyrrole	R=2, 4-Me; R'=H	2.55, 1.98 [1]; 2.12 [2]; 2.0 [9]	-288.777182	-289.227906	282.83
3,4-dimethylpyrrole	R=3, 4-Me; R'=H	0.66 [1]	-288.775702	-289.220167	278.91
1,2,5-trimethylpyrrole	R=2, 5-Me; R'=H	-0.24 [1]; -0.20 [3]	-328.071226	-328.513956	277.82
2,5-dimethyl-1-phenylpyrrole	R=2, 5-Me; R'=C_6H_5	-2.30 [2]	-519.787593	-520.227050	275.76
2,3,5-trimethylpyrrole	R=2, 3, 5-Me; R'=H	2.00 [1]; 3.50 [9]	-328.084618	-328.528480	278.53
3-ethyl-2,4-dimethylpyrrole	R=2, 5-Me, 3-Et; R'=H	3.54 [1]	-367.383577	-367.836214	284.03
2,3,4,5-tetramethylpyrrole	R=2, 3, 4, 5-Me; R'=H	3.77 [1]; 3.80 [9]	-367.388379	-367.840784	283.89
2,3,4-trimethylpyrrole	R=2, 3, 4-Me; R'=H	3.94 [1]; 3.90 [9]	-328.082189	-328.533706	283.33
	imidazoles				
					
Imidazole	H	7.10, 6.853, 7.09, 7.12, 7.65, 7.11 (23°C), 7.50 (23°C), 7.12 (27°C) [1]; 6.9929, 7.1028 (20°C), 6.8867 (30°C) [2]; 7.22 [1]; 7.13[7]; 6.95[9]	-226.226010	-226.685417	288.28
4-(2-acetoxyethyl)imidazole	4-$CH_2CH_2OC(=O)Me$	6.97 (26°C) [1]; 6.97 [2]	-532.717645	-533.179914	290.08
N-acetylimidazole	1-COMe	3.60 [1]	-378.867189	-379.318056	282.92
5-(2-aminoethyl)imidazole	5-$CH_2CH_2NH_2$	6.13, 5.94, 5.91, 5.88, 5.97 (20°C), 6.05 (20°C) [1]; 6.04 [2]	-360.188685	-360.649772	289.34
4(5)-phenylimidazole	5-C_6H_5	5.997, 6.10 [1]; 6.00 [9]	-457.253306	-457.711205	287.34
4-(2-pyridyl)imidazole	4- 	5.42 [1]; 5.492 [2]	-473.302456	-473.761804	288.25
2,4,5-trimethylimidazole	2, 4, 5-Me	8.92 [1]	-344.152296	-344.619773	293.35

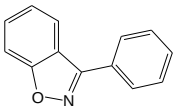
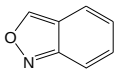
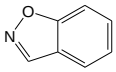
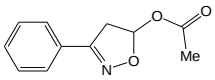
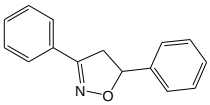
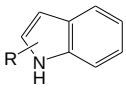
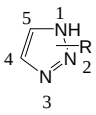
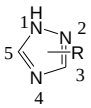
4-carbamoylimidazole	4-$CONH_2$	3.70 [1]	-394.958008	-395.407567	282.10
4-chloro-1-methylimidazole	1-Me, 4-Cl	3.10 [1, 2]	-725.153913	-725.602261	281.34
2,4-dimethylimidazole	2, 4-diMe	8.36 [1, 9]	-304.845777	-305.310872	291.85
2,4-diphenylimidazole	2,4-diC_6H_5	5.64 [1]	-688.282019	-688.738200	286.26
2-ethylimidazole	2-Et	8.00 [1]	-304.837186	-305.301420	291.31
2-methylimidazole	2-Me	7.851 [1]; 7.86 [2]	-265.536619	-265.999477	290.45
2-phenylimidazole	2-C_6H_5	6.48, 6.402 [1]; 6.39 [9]	-457.254340	-457.712012	287.19
4(5)-nitroimidazole*	4-NO_2	-0.05 [1,9]; -0.16 [2]	-430.762627	-431.197824	273.09
4(5)-hydroxymethylimidazole	4-CH_2OH	6.385 [1]	-340.753505	-341.213513	288.66
1-methyl-4-phenylimidazole	1-Me, 4-C_6H_5	5.78 [1]	-496.549708	-497.007525	287.28
4-(3-methoxycarbonylpropyl)imidazole	$(CH_2)_3COOMe$	7.30 [1]	-572.018067	-572.479360	289.47
2-chloroimidazole	2-Cl	3.55 [8]	-685.854796	-686.303282	281.43
2-aminoimidazole	2-NH_2	8.76 [2]	-281.589065	-282.054787	292.25
N-methylimidazole		5.24 [2]; 5.57 [9]	-265.521204	-265.981626	288.92
benzimidazole		5.59 [7]; 5.53 [9]	-379.855940	-380.311716	286.00
naphthimidazole		5.24 [7]	-533.476376	-533.931292	285.46
N-methylbenzimidazole		7.30 [6], 7.33 [9]	-419.151558	-419.608153	286.52
Tolazoline		10.30 [16]	-497.736944	-498.209222	296.36
tetrahydrozoline		10.51 [16]	-614.443471	-614.917200	297.27
					
diethyl 2-(1H-imidazol-1-yl)-succinate	R_1, R_2=H	6.02 [5]	-839.173683	-839.631253	287.13
diethyl 2-(2-methyl-1H-imidazol-1-yl)succinate	R_1=H, R_2=Me	6.70 [5]	-878.485141	-878.947910	290.39
diethyl 2-(4,5-dimethyl-1H-imidazol-1-yl)succinate	R_1, R_2=Me	6.82 [5]	-917.796893	-918.258999	289.98
					
methyl 2-(1H-imidazol-1-yl)acetate*	R_1, R_2, R_3=H	6.35 [5]	-493.394668	-493.850560	286.08
methyl 2-(2-methyl-1H-imidazol-1-yl)acetate	R_1, R_2=H, R_3=Me	7.09 [5]	-532.703243	-533.164322	289.33
methyl 2-(4,5-dimethyl-1H-imidazol-1-yl)acetate	R_1, R_2=Me, R_3=H	7.42 [5]	-572.009639	-572.471669	289.93

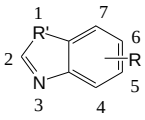
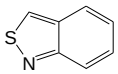
guanidines

2-amino-5,6-dihydropyrimidin-4-one		7.05 [2]	-396.153650	-396.614461	289.16
5,6-dihydro-3-methyl-2-(methyl-amino)-pyrimidin-4(3H)-one		9.48 [2,4]	-474.726860	-475.195244	293.92
					
2-amino-1H-imidazol-4(5H)-one	R=H	4.80 [2]	-356.854821	-357.309896	285.56
2-amino-1-methyl-1H-imidazol-4(5H)-one	R=Me	4.83 [2]	-396.148084	-396.603977	286.08
2,3,6,7-tetrahydroimidazo [1,2-a]pyrimidin-5(1H)-one		8.25 [2, 4]	-473.538357	-474.003683	292.00
3-methyl-2-(methylimino)-imidazolidin-4-one		7.96 [4]	-396.142013	-396.605334	290.74
N-(imidazolidin-2-ylidene)-Acetamide		7.48 [2,4]	-435.441732	-435.903717	289.90
1-(2-iminoimidazolidin-1-yl)ethanone		9.06 [2, 4]	-435.436928	-435.904141	293.18

isoxazoles

					
isoxazole	R=H	1.30 [1,9]; -2.03 [2]	-246.040532	-246.469767	269.35
3-phenylisoxazole	3-C_6H_5	-3.18 [2]	-477.067497	-477.498120	270.22
5-phenylisoxazole	5-C_6H_5	-3.22 [2]	-477.071304	-477.503348	271.11
4-bromo-5-phenylisoxazole	3-C_6H_5, 4-Br	-5.58 [2]	-3051.309281	-3051.735120	267.22
3-bromo-5-phenylisoxazole	3-C_6H_5, 3-Br	-6.68 [2]	-3051.315552	-3051.739915	266.29
3,4-dichloro-5-phenylisoxazole	3, 4-diCl, 5-C_6H_5	-7.66 [2]	-1396.318805	-1396.737155	262.52
3,4,5-trimethylisoxazole	3, 4-diMe; 5-Me	-1.00 [1]; -0.76 [2]; 0.47 [9]	-363.970474	-364.410542	276.15
4-benzyl-3,5-dimethylisoxazole	3, 5-diMe; 4-CH_2-C_6H_5	-1.60 [2]	-594.989281	-595.426041	274.07
3-methyl-4-chloro-5-phenylisoxazole	3-Me, 4-Cl, 5-C_6H_5	-4.35 [2]	-516.381933	-516.817956	273.61
3,5-diphenylisoxazole	3, 5-diC_6H_5	-3.24 [2]	-708.098054	-708.530853	271.59
4-bromo-3,5-diphenylisoxazole	3, 5-diC_6H_5; 4-Br	-5.14 [2]	-3282.332166	-3282.759857	268.38
4-bromo-3,5-dimethylisoxazole	3, 5-diMe; 4-Br	-2.32 [2]	-2898.907136	-2899.338192	270.49
(3,5-dimethylisoxazole-4-yl)-methyl acetate	3, 5-diMe; 4-$CH_2OC(=O)Me$	-1.82 [2]	-591.851622	-592.284810	271.83
4-methyl-3,5-diphenylisoxazole	3, 5-diC_6H_5; 4-Me	-3.18 [2]	-747.400861	-747.835639	272.83
3-methyl-5-phenylisoxazole	3-Me, 5-C_6H_5	-2.45 [2]	-516.381932	-516.817925	273.59
3,5-dimethylisoxazole	3-Me, 5-Me	-2.00 [1,9]; -1.26 [2]	-324.665194	-325.102509	274.42

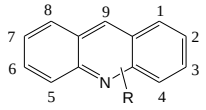
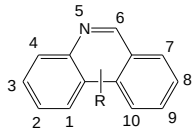
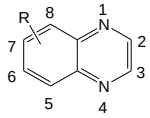
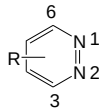
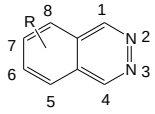
4-chloro-3-methyl-5-phenylisoxazole	3-Me, 4-Cl, 5-C_6H_5	-4.35 [2]	-976.003981	-976.434050	269.87
4-chloro-3,5-diphenylisoxazole	3, 5-diC_6H_5; 4-Cl	-5.2 [2]	-1167.717889	-1168.145453	268.30
4-chloro-3,5-dimethylisoxazole	3, 5-diMe; 4-Cl	-2.48 [2]	-784.290803	-784.721765	270.43
3-phenyl-4,5-benzisoxazole		-4.31 [2]	-630.693897	-631.123770	269.75
benz-[3,4]-isoxazole		-2.20 [6]	-399.652664	-400.086262	272.09
benz-[4,5]-isoxazole		-4.70 [6]	-399.668112	-400.096423	268.77
5-acetoxy-4,5-dihydro-3-phenyl-isoxazole (5-acetoxy-3-phenyl-2-isoxazoline*)*		-3.67 [2]	-706.151299	-706.580067	269.06
4,5-dihydro-3,5-diphenylisoxazole (3,5-diphenyl-2-isoxazoline)		-3.28 [2]	-709.279291	-709.714502	273.10
	indoles (C3 protonation)				
					
indoles	H	-2.48 [1]; -2.47, -3.62, -3.50, -2.46 [2]	-363.793714	-364.227026	271.91
1-methylindole	1-Me	-1.80 [1]; -2.30, -2.32 [2]	-403.088003	-403.525514	274.54
2-methylindole	2-Me	-0.10 [1, 9]; -0.28 [2]	-403.103687	-403.544850	276.83
3-methylindole	3-Me	-3.35 [1]; -4.55 [2]; -3.30 [9]	-403.100318	-403.529281	269.18
3-tert-butylindole	1, 3, 3-Et	-3.43, - 2.2 [2]	-521.006847	-521.436968	269.91
1,3-diethylindole	1, 2-diMe	0.34 [1]; 0.30 [2]	-520.999986	-521.433851	272.25
1,2-dimethylindole	1, 3-diMe	-3.37 [2]	-442.395678	-442.839942	278.78
1,3-dimethylindole	2, 3-diMe	-1.10 [1,9]; -1.49, -1.44, -1.34 [2]	-442.394440	-442.827763	271.91
2,3-dimethylindole		-3.58, -3.70 [2]	-442.408503	-442.846191	274.65
1,2-dimethyl-5-nitroindole	1, 2-diMe; 5-NO_2	-2.94 [2]	-607.643630	-608.072983	269.42
5-nitroindole	5-NO_2	-7.40, -4.49 (20°C), -4.61 (20°C) [2]	-568.332622	-568.753889	264.35
2-methyl-3-n-propylindole	2-Me, 3-n-C_3H_7	-1.40 [2]	-521.013181	-521.448586	273.22
	Others				
1,2,3-triazoles					
1,2,3-triazole	R=H	1.17 (20°C) [1,9]	-242.242370	-242.686881	278.94
1-methyl-1,2,3-triazole	R=1-Me	1.25 (20°C) [1,9]	-281.540730	-281.986843	279.94
1,2,4-triazoles					
1,2,4-triazole*	H	2.27(20°C), 2.45 [2]; 2.30 [1, 9]	-242.267653	-242.713040	279.48
1-methyl-1,2,4-triazole*	1-Me	10.80(pKb) [2]	-281.566197	-282.013251	280.53
3,5-diethyl-1,2,4-triazole	3,5-diEt	3.75 [1,9]	-399.494391	-399.947170	284.12

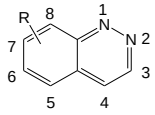
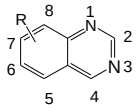
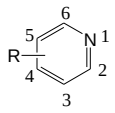
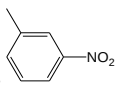
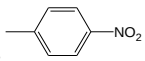
3,5-dimethyl-1,2,4-triazole	3, 5-diMe	3.79 [1,9]	-320.892592	-321.343164	282.74
benzothiazoles					
benzoxazole*	R=H, R'=O	-2.20 [6]	-399.707205	-400.146202	275.48
benzothiazole	R=H, R'=S	1.20 [6]	-722.707010	-723.149829	277.87
2-amino-benzothiazole	R=2-NH_2, R'=S	4.48 (20°C), 4.3 [1]	-778.080155	-778.529798	282.16
2-amino-5-methoxybenzothiazole*	R=2-NH_2, 5-OMe, R'=S	4.29 [1]	-892.595656	-893.046030	282.61
2-amino-7-methybenzothiazole*	R=2-NH_2, 7-Me, R'=S	4.25 [1]	-817.386926	-817.837395	282.67
isothiazole		-0.50 [6]	-569.068691	-569.507239	275.19
benz-[3,4]-isothiazole		-0.10 [6]	-722.685633	-723.126501	276.65
oxazole		0.80 (33°C) [2,3]	-246.074902	-246.516639	277.19

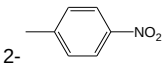
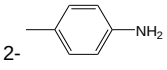
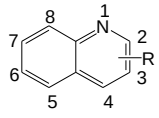
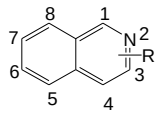
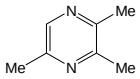
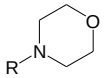
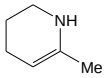
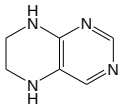
*A conformational search was carried out on these compounds using the GMMX feature of PCModel (see text for more details)

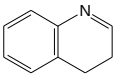
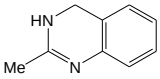
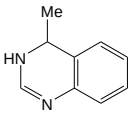
$ kcal/mol

Table S2b Calculated energies and experimental pKas for heteroaromatic bases --- test set

Compounds	Structure	Experimental pKa [ref]	E_B	E_{BH+}	$\Delta E^{\$}$
acridines					
acridine	H	5.58 (20°C), 5.15 (30°C), 5.45 (15°C) [1]; 5.60 [9]	-555.514056	-555.972287	287.54
9-methoxycarbonylacridine	9-COOMe	3.41 (20°C) [1]; 3.45 (20°C) [9]	-783.376423	-783.830971	285.23
1-aminoacridine	1-NH_2	6.00 (20°C) [1]; 6.04 (20°C) [9]	-610.876494	-611.339543	290.57
2-aminoacridine	2-NH_2	5.48 (20°C) [1]; 5.88 (20°C) [9]	-610.879956	-611.340892	289.24
phenanthridines					
phenanthridine	H	4.61 (20°C), 4.48 (20°C) [1]; 4.47 (22°C) [2]; 4.52 (20°C) [9]	-555.519271	-555.975020	285.99
6-aminophenanthridine*	6-NH_2	7.27 (20°C) [1]; 6.88 (20°C) [9]	-610.891799	-611.352833	289.31
6-methoxyphenanthridine	6-OMe	2.38 (20°C) [1,9]	-670.047722	-670.496498	281.61
quinoxalines					
quinoxaline	H	0.56 (20°C) [1,9]; 0.70 (20°C) [1]	-417.937431	-418.382056	279.01
2-methoxy-3-methylquinoxaline	2-OMe, 3-Me	1.38 (20±5°C) [1]; 1.38 [9]	-571.775935	-572.223334	280.75
2-methylthioquinoxaline	2-SMe	0.95 (20°C) [1]; 0.26 [9]	-855.460577	-855.904334	278.46
2-methoxyquinoxaline	2-OMe	0.28 (20±5°C) [1]; 0.28 [9]	-532.467222	-532.910841	278.38
2,3-dimethoxyquinoxaline	2,3-diOMe	-1.15 [9]	-646.995321	-647.433741	275.11
pyridazines					
pyridazine	H	2.24 (20°C), 2.96 (20.5°C) [1]; 2.33 (20°C) [9]	-264.284737	-264.7353216	282.75
3,6-dimethylpyridazine	3,6-diMe	3.99 (20°C) [1]	-342.904949	-343.360377	285.79
4-methylthiopyridazine	4-SMe	3.24 (20°C) [1]; 3.26 (20°C) [9]	-701.806016	-702.261345	285.73
3-methylthiopyridazine	3-SMe	2.26 (20°C) [1,9]	-701.805586	-702.257060	283.31
4-methoxypyridazine	4-OMe	3.66 (20°C) [1]; 3.70 (20°C) [9]	-378.805534	-379.261072	285.86
3-methoxypyridazine	3-OMe	2.48 (20°C) [1]; 2.52 (20°C) [9]	-378.811401	-379.263471	283.68
phthalazines					
phthalazine	H	3.48 (20°C) [1]; 3.47 (20°C) [1,9]	-417.911444	-418.366347	285.46
1-methylthiophthalazine	1-SMe	3.44 (20°C) [1]; 3.48 (20°C) [9]	-855.430831	-855.886322	285.83
1-aminophthalazine	1-NH_2	6.57 (20°C) [1]; 6.60 (20°C) [9]	-473.285167	-473.746475	289.48

Cinnolines					
cinnoline	H	2.27 (20°C), 2.37 (20°C) [1]; 2.42 (20°C) [9]	-417.909019	-418.361584	283.99
3-aminocinnoline	3-NH_2	3.69 (20°C), 3.61 (20°C) [1]; 3.70 (20°C) [1,9]	-473.280709	-473.734796	284.94
4-methylthiocinnoline*	4-SMe	3.09 (20°C) [1]; 3.21 (20°C) [9]	-855.428014	-855.883087	285.56
4-methoxycinnoline	4-OMe	3.15 (20°C) [1]; 3.13 (20°C) [9]	-532.429318	-532.885350	286.16
quinazolines					
2-aminoquinazoline	2-NH_2	4.75 (20°C), 4.81 (20°C)[1]; 4.82 (20°C) [9]	-473.323763	-473.778164	285.14
4-aminoquinazoline	4-NH_2	5.70 (20°C), 5.84 (20°C) [1]; 5.73 (20°C) [9]	-473.324077	-473.783253	288.14
2-methylquinazoline	2-Me	4.50 (20°C) [1]; 4.52 (20°C) [9]	-457.254224	-457.705022	282.88
4-methylquinazoline	4-Me	2.44 (20°C), 2.35 (20°C) [1]; 2.52 (20°C) [9]	-457.253143	-457.703018	282.30
5-methylquinazoline	5-Me	3.61 (20°C) [1]; 3.63 (20°C) [9]	-457.248684	-457.696875	281.24
6-methylquinazoline	6-Me	3.39 (20°C) [1]; 3.41 (20°C) [9]	-457.250248	-457.698549	281.31
7-methylquinazoline	7-Me	3.15 (20°C) [1]; 3.17 (20°C) [9]	-457.251610	-457.700504	281.69
8-methylquinazoline	8-Me	3.18 (20°C) [1]; 3.20 (20°C) [9]	-457.249340	-457.696720	280.74
pyrimidines					
2-chloro-4-methylaminopyrimidine	2-Cl, 4-NHMe	2.80 (20°C) [1]; 2.83 (20°C) [9]	-818.628458	-819.076589	281.21
4-chloro-2-methylaminopyrimidine	4-Cl, 2-Me	2.59 (20°C) [1]; 2.63 (20°C) [9]	-818.627850	-819.075679	281.02
4-dimethylamino-2-methoxypyrimidine	2-Me, 4-$N(Me)_2$	6.13 (20°C) [1]; 6.17(20°C), 6.17 [2]	-512.8091688	-513.269569	288.91
4-dimethylamino-6-methoxypyrimidine	6-Me, 4-$N(Me)_2$	4.27 (20°C) [1]; 4.29 (20°C) [9]	-512.806084	-513.259853	284.74
4-chloro-6-dimethylaminopyrimidine	4-Cl, 6-$N(Me)_2$	2.42 (20°C) [1]	-857.9151033	-858.362724	280.89
2-bromopyrimidine	2-Br	-1.63 (20°C) [2]	-2838.567957	-2839.002471	272.66
4-methylpyrimidine	4-Me	1.91 (20°C), 1.90 [1]; 1.98 (20°C) [9]	-303.629269	-304.0778783	281.51
4,6-dimethylpyrimidine	2,6-diMe	2.70 [1]	-342.940953	-343.391847	282.94
Pyridines					
4-phenylpyridine	4-C_6H_5	5.55 (20°C) [1,9]	-479.294116	-479.751833	287.22
3-acetylpyridine	3-COMe	3.18 [1,9]; 3.26, 3.20 (35°C) [2]	-400.912203	-401.363000	282.88
4-acetylpyridine	4-COMe	3.59 [1]; 3.51, 3.43 (35°C) [2]	-400.910846	-401.362328	283.31
4-vinylprridine	4-CH_2-CH=CH_2	5.62 [1,9]	-364.956720	-365.414587	287.32
4-m-nitrophenylpyridine	4- 	4.90 (20°C) [1,9]	-683.825794	-684.280998	285.65
4-p-nitrophenylpyridine	4- 	4.87 (20°C) [1,9]	-683.826644	-684.281208	285.24

2-p-nitrophenylpyridine		3.63 (20°C) [1,9]	-683.827193	-684.278519	283.21
2-p-aminophenylpyridine		5.70 (20°C) [1,9]	-534.659877	-535.121464	289.65
quinolines					
6-methoxyquinoline	6-OMe	5.03 (20°C) [1]	-516.410898	-516.868231	286.98
7-methoxyquinoline*	7-OMe	5.03 [17]	-516.413515	-516.872441	287.98
2-methylquinoline	2-Me	5.71 (22±2°C), 5.83 (20°C), 5.65, 5.42, 5.69 [1]	-441.203821	-441.662664	287.93
3-methylquinoline	3-Me	5.17 (20°C), 5.14, 4.54 [1]; 5.14 [9]	-441.201800	-441.658582	286.64
4-methylquinoline	4-Me	5.67, 5.20, 5.59 [1]; 5.20 [9]	-441.200793	-441.659172	287.64
6-methylquinoline	6-Me	5.22, 4.92, 5.15 [1]	-441.200633	-441.657950	286.97
6-chloroquinoline	6-Cl	3.99, 4.10, 3.27 [1]	-861.527353	-861.980752	284.51
7-chloroquinoline	7-Cl	3.85 [1]	-861.527567	-861.980992	284.53
8-chloroquinoline	8-Cl	3.12 [1]	-861.524607	-861.976200	283.38
isoquinolines					
4-bromoisoquinoline	4-Br	3.31 [1, 9]	-2976.138756	-2976.590008	283.17
6-nitroisoquinoline	6-NO_2	3.43 (20°C) [1]; 3.47 (20°C) [9]	-606.422453	-606.873473	283.02
7-nitroisoquinoline	7-NO_2	3.57(20°C) [1]; 3.61 (20°C) [9]	-606.423850	-606.874612	282.86
8-nitroisoquinoline	8-NO_2	3.55 (20°C) [1]; 3.59 (20°C) [9]	-606.413532	-606.865145	283.39
3-methylthioisoquinoline	3-SMe	3.37(20°C) [1]; 3.41 (20°C) [9]	-839.412199	-839.864824	284.03
trimethylpyrazine		-3.5 (27°C) [1]	-382.688597	-383.114259	267.11
trimethylpyrazine		2.8 (27°C) [1]	-382.240006	-382.688597	281.50
dihydropyrrols					
2-ethyl-Δ^2-dihydropyrrol*	R=Et	7.91 [15]	-289.965127	-290.430952	292.31
2-cyclohexyl-Δ^2-dihydropyrrol*	R=cyclohexyl	7.95 [15]	-445.974316	-446.440089	292.28
morphines					
morpholine	R=H	8.33, 8.39, 8.30(20°C), 8.5 [1]; 8.492, 8.608 (20°C), 8.380 (30°C) [2]; 8.50 [13]	-287.767805	-288.232083	291.34
N-ethylmorpholine	R=Et	7.67 [1]; 7.70 [9]	-366.364865	-366.828181	290.74
N-methylmorpholine	R=Me	7.38 [1]; 7.41 [9]	-327.062474	-327.524742	290.08
2-methyl-Δ^2-tetrahydropyridine*		9.55 [9]	-289.963916	-290.433737	294.82
5,6,7,8-tetrahydropteridine		6.63 (20°C) [9]	-452.448107	-452.911363	290.70

3,4-dihydroquinoline		9.19 (20°C) [9]	-419.139716	-419.606066	292.64
2-methyl-3,4-dihydroquinazoline		10.16 (20°C) [9]	-458.449590	-458.919257	294.72
4-methyl-3,4-dihydroquinazoline		9.19 (20°C) [9]	-458.445276	-458.910976	292.23

*A conformational search was carried out on these compounds using the GMMX feature of PCModel (see text for more details)

$ kcal/mol

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