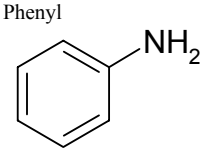
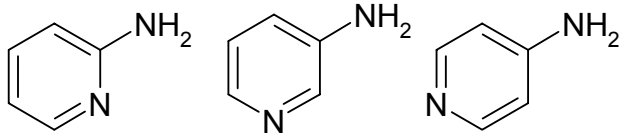
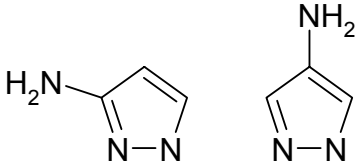
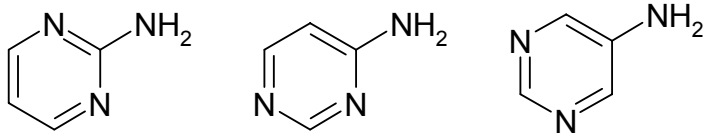
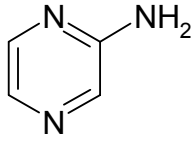
Full citation for Gaussian03:

Gaussian 03, Revision C.02, Frisch, M. J.; Trucks, G. W.; Schlegel, H. B.; Scuseria, G. E.; Robb, M. A.; Cheeseman, J. R.; Montgomery, Jr., J. A.; Vreven, T.; Kudin, K. N.; Burant, J. C.; Millam, J. M.; Iyengar, S. S.; Tomasi, J.; Barone, V.; Mennucci, B.; Cossi, M.; Scalmani, G.; Rega, N.; Petersson, G. A.; Nakatsuji, H.; Hada, M.; Ehara, M.; Toyota, K.; Fukuda, R.; Hasegawa, J.; Ishida, M.; Nakajima, T.; Honda, Y.; Kitao, O.; Nakai, H.; Klene, M.; Li, X.; Knox, J. E.; Hratchian, H. P.; Cross, J. B.; Bakken, V.; Adamo, C.; Jaramillo, J.; Gomperts, R.; Stratmann, R. E.; Yazyev, O.; Austin, A. J.; Cammi, R.; Pomelli, C.; Ochterski, J. W.; Ayala, P. Y.; Morokuma, K.; Voth, G. A.; Salvador, P.; Dannenberg, J. J.; Zakrzewski, V. G.; Dapprich, S.; Daniels, A. D.; Strain, M. C.; Farkas, O.; Malick, D. K.; Rabuck, A. D.; Raghavachari, K.; Foresman, J. B.; Ortiz, J. V.; Cui, Q.; Baboul, A. G.; Clifford, S.; Cioslowski, J.; Stefanov, B. B.; Liu, G.; Liashenko, A.; Piskorz, P.; Komaromi, I.; Martin, R. L.; Fox, D. J.; Keith, T.; Al-Laham, M. A.; Peng, C. Y.; Nanayakkara, A.; Challacombe, M.; Gill, P. M. W.; Johnson, B.; Chen, W.; Wong, M. W.; Gonzalez, C.; and Pople, J. A.; Gaussian, Inc., Wallingford CT, 2004.

Table S1. The representation of amines attached to different positions around different aromatic ring types. The description given is of the ring to which the amine is attached and does not preclude the ring from being fused to other rings (i.e. naphthalene and benzene are both part of the phenyl ring type). The number of compounds in each class that are active is indicated in parentheses. X indicates a position that is not possible and blank boxes indicate substitution types not represented in the dataset.

	Connection point			
Ring type	**2**	**3**	**4**	**5**
Phenyl 	122 (44)			
Pyridine  2 3 4	41 (14)	16 (5)	3 (0)	x
Pyrazole  3 4	x	25 (13)	3 (0)	x
Pyrimidine  2 4 5	5 (2)	x	1 (0)	3 (1)
Pyrazine  2	14 (3)			
Oxazole	2 (1)	x		

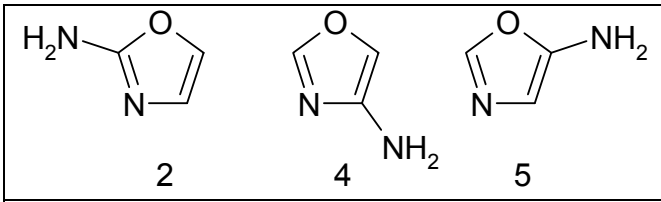
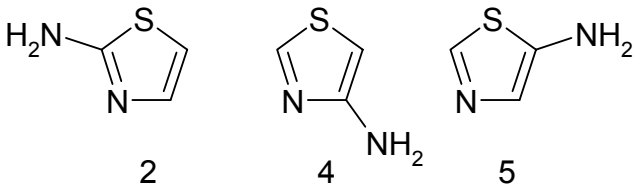
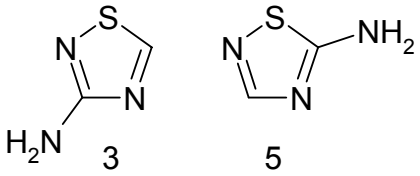
 2 4 5				
Thiazole  2 4 5	48 (22)	x		2 (0)
1,2,4-thiadiazole  3 5	x	1 (0)	x	17 (3)
Others	9 (1)			

Table S2. The mean and standard error in the mean of the distributions of a standard set of QSAR descriptors for active and inactive compounds. The final column is the difference in the means as a product of the sum of the standard errors and indicates whether the two distributions are distinct or not.

QSAR descriptor	Mean for actives	Mean for not actives	SEM for actives	SEM for not actives	Diff
QM descriptors v2: IP	5.38	5.67	0.04	0.03	4.08
Balaban	1.62	1.82	0.03	0.02	4.06
MaxRing2	3.35	1.60	0.30	0.19	3.55
RingCount	1.67	1.32	0.06	0.04	3.46
RigidbondCount	9.39	7.65	0.33	0.19	3.34
GraphDiameter	6.50	5.68	0.16	0.10	3.22
MinEV2	3.84	4.05	0.04	0.03	3.06
QM descriptors v2: SAS_C	90.46	77.05	2.74	1.77	2.97
MM_VDW_EP_N_SUM	-5.75	-5.09	0.13	0.09	2.95
MM_QposVar	0.16	0.18	0.00	0.01	2.91
NEL_HCNOS	83.74	73.72	2.03	1.50	2.84
GraphRadius	3.59	3.25	0.08	0.04	2.83
QM descriptors v2: SumqS	-0.01	0.05	0.00	0.02	2.81
MM_MAXPOS	0.51	0.61	0.02	0.02	2.74
MaxPosChargeGM	0.18	0.22	0.01	0.01	2.73
CMR	4.69	4.18	0.11	0.08	2.71
QM descriptors v2: SAS_H	155.46	136.37	4.03	3.12	2.67
ACDlogP error	0.62	0.50	0.03	0.02	2.64
CarbonCount	8.19	7.08	0.26	0.16	2.64
HalogenCount	0.39	0.80	0.07	0.08	2.63
Chi6p	0.43	0.30	0.03	0.02	2.57
QM descriptors v2: CohesiveE	-49.68	-42.41	1.82	1.01	2.56
MolVol2D	257.34	230.90	6.11	4.21	2.56
AverPosCharge_GM	0.08	0.09	0.00	0.00	2.55

Polarizability	18.16	16.27	0.43	0.31	2.54
Motoc	3.23	2.98	0.06	0.04	2.54
MolFlex	0.99	0.34	0.18	0.08	2.51
AtomCount	20.62	18.53	0.50	0.34	2.49
BondCount	12.43	11.11	0.32	0.21	2.47
Chi3p	2.29	1.99	0.08	0.05	2.46
QM descriptors v2: Molradii	5.11	4.97	0.03	0.03	2.44
QM descriptors v2: SumqH	1.84	1.66	0.04	0.03	2.38
Chi4p	1.43	1.20	0.06	0.04	2.37
MM_SAS_EP_P_AREA	174.10	161.93	2.99	2.16	2.36
Randic	4.35	3.95	0.10	0.07	2.36
QM descriptors v2: DGcdOct	-3.12	-2.06	0.24	0.21	2.35
ChlorineCount	0.06	0.19	0.02	0.03	2.34
Chi5p	0.79	0.62	0.05	0.03	2.34
VOL	141.61	129.95	2.92	2.08	2.33
VOL 2	141.61	129.95	2.92	2.08	2.33
MM_QposMean	0.20	0.22	0.01	0.01	2.31
QM descriptors v2: SAS_Cl	4.35	12.70	1.60	2.03	2.30
SAS_TOT_AREA	345.76	327.89	4.53	3.34	2.27
QM descriptors v2: R2tak	2561.08	2105.80	121.99	79.87	2.26
M1M	46.26	39.05	1.93	1.27	2.25
VDW_AREA	173.28	161.57	3.07	2.25	2.20
ChargeRang_GM	0.49	0.53	0.01	0.01	2.17
MM_QH	1.50	1.38	0.03	0.02	2.17
Wiener	208.20	162.88	12.93	8.02	2.16
IC	2.34	2.26	0.02	0.02	2.15
QM descriptors v2: Polarizability	170.54	155.64	4.05	2.89	2.15
HeavyAtomCount	11.76	10.79	0.27	0.18	2.15
AromCount	7.91	6.99	0.27	0.16	2.14
Kappa2	3.69	3.37	0.09	0.06	2.12
MM_VDW_EP_N_AREA	94.15	87.57	1.87	1.36	2.04
AREA	186.92	174.45	3.54	2.60	2.03
QM descriptors v2: SublEntropy	55.25	54.55	0.19	0.15	2.03
QM descriptors v2: BO_Nsp3	0.68	0.73	0.02	0.01	2.03
MM_VDW_EP_N_VAR	43.40	40.16	0.88	0.73	2.01
QM descriptors v2: SumqF	-0.05	-0.12	0.02	0.02	2.00
QM descriptors v2: SumqCl	0.00	-0.01	0.00	0.00	1.99
SIC	0.33	0.35	0.00	0.00	1.97
HAROM	3.66	3.09	0.18	0.11	1.93
FluorineCount	0.28	0.57	0.07	0.08	1.88
MM_QnegMean	-0.26	-0.29	0.01	0.01	1.85
QM descriptors v2: DGsolvOct	-9.50	-8.30	0.35	0.30	1.85
NPSA	137.46	126.22	3.57	2.60	1.82
NPSA 2	137.46	126.22	3.57	2.60	1.82
DipoleMomGM	2.84	2.59	0.08	0.06	1.82
Chi5c	0.02	0.05	0.01	0.01	1.80
VDW_NONPOL_AREA	123.57	113.77	3.16	2.31	1.79
DipoleMomGH	3.56	2.98	0.21	0.12	1.78

HOMO	-0.71	-0.75	0.01	0.01	1.77
M3M	0.69	1.06	0.10	0.11	1.76
QM descriptors v2: SAS_F	12.15	22.82	2.98	3.12	1.75
MaxRing3	1.38	0.64	0.28	0.14	1.75
MM_VDW_EP_P_AREA	79.14	74.00	1.74	1.23	1.73
MinEV3	4.47	4.61	0.05	0.03	1.68
NitrogenCount	2.31	2.08	0.08	0.06	1.64
LUMO	0.19	0.37	0.06	0.04	1.63
NEL_all	88.68	83.53	1.79	1.38	1.62
M2M	10.61	11.90	0.43	0.37	1.61
Chi3c	0.57	0.67	0.03	0.03	1.60
MaxRing1	6.77	6.27	0.21	0.11	1.58
MM_SAS_EP_N_VAR	13.85	12.86	0.35	0.28	1.58
SAS_NONPOL_AREA	231.71	216.43	5.55	4.18	1.57
QM descriptors v2: DipoleMoment	2.86	3.22	0.13	0.10	1.52
PIAT	8.97	8.31	0.27	0.17	1.50
HuckelPiEnergy	-18.35	-17.02	0.52	0.37	1.49
Chi0	7.61	7.21	0.16	0.12	1.49
MM_FHDSA	0.83	0.90	0.03	0.02	1.47
MM_SAS_EP_N_SUM	-3.41	-3.21	0.08	0.06	1.45
MM_FHADSA	4.10	4.46	0.13	0.12	1.44
Amine2	0.00	0.01	0.00	0.01	1.42
MW	169.43	160.73	3.47	2.74	1.40
Kappa3	4.38	4.10	0.11	0.09	1.38
QM descriptors v2: BO_HC	0.26	0.27	0.00	0.00	1.37
MM_FHASA	3.11	3.36	0.10	0.09	1.34
PAT	3.18	2.91	0.11	0.09	1.34
HBA_Raevsky	2.86	2.62	0.10	0.08	1.32
NonpolarCount	6.74	6.16	0.27	0.18	1.30
Chi2	3.48	3.26	0.10	0.07	1.29
MM_VDW_EP_N_MEAN	-61.50	-58.57	1.25	1.02	1.29
HBA	2.86	2.63	0.10	0.08	1.29
HBAsum	3.40	3.16	0.11	0.08	1.29
Kappa1	8.84	8.41	0.19	0.15	1.28
QM descriptors v2: RawLogP	-0.82	-1.47	0.28	0.24	1.27
MM_MAXNEG	-0.89	-0.90	0.00	0.00	1.25
MM_QMIN	-0.89	-0.90	0.00	0.00	1.25
MM_VDW_EP_P_VAR	38.40	40.02	0.74	0.58	1.23
QM descriptors v2: SumqC	-0.03	0.10	0.06	0.05	1.23
MM_QC	1.53	1.43	0.04	0.03	1.21
SPEC_HB_TOT	0.44	0.46	0.01	0.01	1.16
MM_SAS_EP_N_AREA	171.66	165.96	2.74	2.17	1.16
MM_VDW_EP_P_SUM	4.03	3.82	0.11	0.08	1.15
MM_QN	1.63	1.53	0.05	0.04	1.12
QM descriptors v2: BO_Csp2	0.50	0.46	0.02	0.02	1.12
MaxNegChargeGM	-0.31	-0.31	0.00	0.00	1.11
QM descriptors v2: qHC	0.21	0.20	0.00	0.00	1.10
MM_SAS_EP_P_MEAN	16.59	17.32	0.37	0.30	1.09

Amine1	0.00	0.01	0.00	0.01	1.00
Lipinski	0.01	0.00	0.01	0.00	1.00
Lipinski score	0.01	0.00	0.01	0.00	1.00
QM descriptors v2: qCsp3	0.11	0.14	0.02	0.02	1.00
HBA_Selma	2.69	2.53	0.09	0.07	0.96
MM_SPEC_SAS_EP_P_AREA	0.50	0.49	0.01	0.00	0.96
MM_SPEC_SAS_EP_N_AREA	0.50	0.51	0.01	0.00	0.96
MM_HDSA	0.01	0.01	0.00	0.00	0.96
QM descriptors v2: HBDdispersion	2.36	2.27	0.06	0.04	0.94
MM_PCWT	-8.26	-7.98	0.17	0.13	0.93
MM_HADSA	0.05	0.06	0.00	0.00	0.92
HBsumTotal	6.68	6.37	0.20	0.14	0.91
MM_RNCS	6.44	6.67	0.13	0.12	0.90
NPSA_percentage	73.03	71.63	0.84	0.73	0.89
PSA_percentage	26.97	28.37	0.84	0.73	0.89
NPAT	5.39	4.96	0.29	0.20	0.88
QM descriptors v2: SAS_S	20.80	16.28	3.20	2.08	0.86
MM_HASA	0.04	0.04	0.00	0.00	0.85
MM_QON	1.90	1.81	0.06	0.05	0.85
HBD_Selma	2.28	2.20	0.06	0.03	0.84
ACDlogP	1.08	1.26	0.13	0.08	0.84
AverPosCharge_GH	0.18	0.19	0.01	0.01	0.83
AverNegCharge_GH	-0.19	-0.20	0.01	0.01	0.81
Neutral	0.94	0.90	0.02	0.02	0.81
CHARGED	0.06	0.10	0.02	0.02	0.81
CHARGES	0.06	0.10	0.02	0.02	0.81
MM_VDW_EP_P_MEAN	60.25	61.77	1.02	0.89	0.80
QM descriptors v2: qCsp2	0.63	0.60	0.02	0.01	0.76
Acid	0.05	0.08	0.02	0.02	0.76
NEG_charges	0.05	0.08	0.02	0.02	0.76
QM descriptors v2: BO_Osp3	0.10	0.08	0.01	0.01	0.75
PosIonCenters	1.38	1.31	0.06	0.04	0.74
Amine3	0.02	0.01	0.01	0.01	0.74
MM_SAS_EP_P_SUM	2.76	2.66	0.08	0.06	0.73
MaxEV1	12.90	13.57	0.52	0.40	0.73
AverNegCharge_GM	-0.14	-0.14	0.00	0.00	0.73
SPEC_VDW_HB_D_AREA	0.18	0.19	0.01	0.00	0.71
SPEC_VDW_HB_A_AREA	0.22	0.23	0.01	0.01	0.70
MaxNegChargeGH	-0.54	-0.51	0.02	0.02	0.69
NHCount	2.22	2.16	0.06	0.03	0.69
QM descriptors v2: vdw_HBD	-0.13	-0.13	0.00	0.00	0.69
MaxEV3	8.47	8.40	0.05	0.04	0.68
QM descriptors v2: qNsp2	-0.44	-0.41	0.03	0.02	0.67
VDW_POL_AREA	49.72	47.80	1.64	1.23	0.67
NonpolarCountMW	0.04	0.04	0.00	0.00	0.66
PolarCount	1.83	1.72	0.11	0.07	0.64
SAS_HB_D_AREA	78.14	75.73	2.27	1.60	0.62
SPEC_VDW_POL_AREA	0.29	0.30	0.01	0.01	0.62

SPEC_VDW_NONPOL_AREA	0.71	0.70	0.01	0.01	0.62
MaxEV2	9.41	9.59	0.15	0.14	0.62
HBD	2.33	2.27	0.07	0.04	0.62
HBD 2	2.33	2.27	0.07	0.04	0.62
HBD_Raevsky	2.33	2.27	0.07	0.04	0.62
HBD_nonLipinski	2.33	2.27	0.07	0.04	0.62
VDW_HB_D_AREA	30.15	29.17	0.96	0.64	0.61
QM descriptors v2: qHN	0.39	0.40	0.00	0.00	0.61
QM descriptors v2: BO_Nsp2	0.36	0.33	0.02	0.02	0.59
MinEV1	2.99	3.01	0.03	0.02	0.58
MWPat	27.08	25.90	1.16	0.92	0.57
ACDlogD pH 6.5	0.82	0.97	0.16	0.11	0.56
ACDlogD pH6.5	0.82	0.97	0.16	0.11	0.56
ACDlogD65	0.82	0.97	0.16	0.11	0.56
QM descriptors v2: qOsp3	-0.14	-0.12	0.02	0.02	0.55
SPEC_SAS_NONPOL_AREA	0.67	0.66	0.01	0.01	0.55
SPEC_SAS_POL_AREA	0.33	0.34	0.01	0.01	0.55
QM descriptors v2: Electronegativity	4.25	4.42	0.18	0.14	0.54
QM descriptors v2: SumqN	-1.46	-1.42	0.05	0.03	0.54
RotBond	0.91	0.85	0.06	0.05	0.52
SPEC_SAS_HB_A_AREA	0.22	0.23	0.01	0.01	0.52
NegIonCenters	0.05	0.07	0.02	0.02	0.52
VDW_HB_A_AREA	37.01	35.99	1.11	0.93	0.50
QM descriptors v2: BO_Osp2	0.09	0.08	0.02	0.01	0.50
ACDlogD6.5, with pKa correction library	0.88	1.00	0.15	0.11	0.48
HBAmax	1.42	1.39	0.04	0.03	0.47
ACDlogD (pH 7.4)	0.84	0.97	0.16	0.12	0.47
ACDlogD pH7.4	0.84	0.97	0.16	0.12	0.47
ACDlogD74	0.84	0.97	0.16	0.12	0.47
QM descriptors v2: AromAlif	33.05	33.89	1.05	0.77	0.46
MM_SAS_EP_P_VAR	10.08	10.29	0.28	0.19	0.45
HB_sum	4.94	4.83	0.15	0.10	0.45
PSA 2	49.45	48.23	1.68	1.20	0.42
PSA	49.45	48.24	1.69	1.20	0.42
SulfurCount	0.32	0.29	0.05	0.03	0.42
SPEC_SAS_HB_D_AREA	0.23	0.24	0.01	0.01	0.40
QM descriptors v2: DGsolvH2O	-10.61	-10.30	0.42	0.36	0.40
FractionIonized	0.10	0.12	0.03	0.02	0.40
FractionNeutral	0.90	0.88	0.03	0.02	0.40
ACDlogD7.4, with pKa correction library	0.89	1.00	0.15	0.11	0.40
SAS_POL_AREA	114.04	111.46	3.72	2.89	0.39
GClogP	1.25	1.31	0.09	0.07	0.39
QM descriptors v2: Hardness	1.13	1.25	0.18	0.14	0.38
ChargeRange_GH	0.93	0.91	0.04	0.03	0.38
MWSHDA	41.65	42.59	1.47	1.04	0.37
QM descriptors v2: qOsp2	-0.11	-0.10	0.02	0.01	0.37
SAS_HB_A_AREA	75.95	74.38	2.40	2.02	0.36
QM descriptors v2: qNsp3	-0.89	-0.89	0.01	0.00	0.33

QM descriptors v2: Coul_HBD	-21.41	-21.03	0.69	0.47	0.33
QM descriptors v2: HBAdispersion	-7.01	-6.86	0.24	0.22	0.33
QM descriptors v2: vdw_HBA	-0.50	-0.48	0.03	0.03	0.32
QM descriptors v2: DGcd	-3.60	-3.45	0.26	0.24	0.31
QM descriptors v2: SCF_E	-761.77	-787.91	47.88	37.70	0.31
QM descriptors v2: BO_Csp3	0.67	0.65	0.05	0.04	0.30
MM_SAS_EP_N_MEAN	-19.59	-19.34	0.42	0.40	0.30
HBDsum	-3.28	-3.22	0.13	0.09	0.29
Base	0.02	0.03	0.01	0.01	0.28
POS_charges	0.02	0.03	0.01	0.01	0.28
ClogP 3	1.26	1.30	0.11	0.07	0.27
ClogP	1.26	1.31	0.11	0.07	0.27
SPEC_FLEX_BND	0.07	0.07	0.01	0.00	0.27
HBA_nonLipinski	2.61	2.57	0.10	0.08	0.26
HuckelResEnergy	9.67	9.51	0.36	0.28	0.25
MM_HADCA	0.68	0.69	0.02	0.01	0.25
MM_HDCA	0.14	0.14	0.00	0.00	0.22
OVAL_NEW	0.96	0.96	0.00	0.00	0.22
MM_QnegVar	0.28	0.28	0.00	0.00	0.20
QM descriptors v2: SAS_N	30.98	30.55	1.13	1.03	0.20
HBDmax	-1.55	-1.57	0.05	0.04	0.19
MM_HACA	0.52	0.52	0.01	0.01	0.18
QM descriptors v2: Coul_HBA	92.05	90.79	4.04	3.40	0.17
QM descriptors v2: SumqBr	0.00	0.00	0.00	0.00	0.17
MM_SPEC_VDW_EP_N_AREA	0.54	0.54	0.01	0.00	0.15
MM_SPEC_VDW_EP_P_AREA	0.46	0.46	0.01	0.00	0.15
QM descriptors v2: HBstrength	70.02	69.16	3.60	3.07	0.13
QM descriptors v2: SumqO	-0.27	-0.26	0.03	0.03	0.12
QM descriptors v2: SAS_O	12.99	12.63	1.74	1.48	0.11
BromineCount	0.04	0.04	0.02	0.01	0.11
QM descriptors v2: SAS_Br	2.87	3.14	1.42	1.09	0.10
PolarCountMW	0.01	0.01	0.00	0.00	0.10
QM descriptors v2: EA	3.11	3.16	0.35	0.27	0.08
MM_QO	0.28	0.28	0.04	0.03	0.06
MaxPosChargeGH	0.40	0.40	0.02	0.01	0.06
Chi4c	0.91	0.91	0.05	0.03	0.05
QM descriptors v2: qHO	0.05	0.05	0.01	0.01	0.05
QM descriptors v2: BO_HN	0.26	0.26	0.00	0.00	0.05
NNlogP	1.42	1.41	0.10	0.08	0.03
OxygenCount	0.55	0.55	0.07	0.06	0.02
QM descriptors v2: BO_HO	0.02	0.02	0.01	0.00	0.02
OHCount	0.11	0.11	0.03	0.02	0.01
MWNPat	44.17	44.19	2.30	1.95	0.00
IodineCount	0.00	0.00	0.00	0.00	
PhosphorusCount	0.00	0.00	0.00	0.00	
QUATER	0.00	0.00	0.00	0.00	
SiliconCount	0.00	0.00	0.00	0.00	
Zwitterion	0.00	0.00	0.00	0.00	

Table S3. The mean and standard error in the mean of the distributions of computed QM energy changes for active and inactive compounds. The final column is the difference in the means as a product of the sum of the standard errors and indicates whether the two distributions are distinct or not. dE_GAS is the electronic energy change in the gas phase, dE_THERMAL includes thermal corrections to 298K, dH_GAS includes corrections to enthalpy at 298K and dG_GAS corrections to free energies at 298K. dE_SOLV is the difference in electronic energies after IEFPCM correction and dG_SOLV gas phase free energy changes corrected with solvation free energies according to IEFPCM.

ENERGY_CHANGE	Mean for actives	Mean for not actives	SEM for actives	SEM for not actives	Diff
dE_GAS Equation 4	152.52	164.24	1.35	1.06	4.88
dE_THERMAL Equation 4	148.12	159.69	1.33	1.04	4.88
dH_GAS Equation 4	186.91	197.44	1.20	0.97	4.86
dG_GAS Equation 4	138.05	149.47	1.32	1.04	4.84
dE_GAS Equation 3	-33.69	-21.97	1.40	1.10	4.68
dE_SOLV Equation 4	20.51	29.93	1.16	0.95	4.46
dG_SOLV Equation 4	22.25	31.40	1.13	0.93	4.45
dG_SOLV Equation 3	3.24	12.44	1.16	0.96	4.33
dE_SOLV Equation 2	92.40	94.97	0.37	0.32	3.73
dG_SOLV Equation 2	80.88	83.31	0.35	0.31	3.69
dE_SOLV Equation 5	78.66	79.95	0.24	0.20	2.90
dE_THERMAL Equation 5	68.22	69.53	0.25	0.21	2.87
dG_GAS Equation 5	60.78	62.05	0.24	0.20	2.86
dE_GAS Equation 5	75.71	77.02	0.25	0.21	2.84
dE_GAS Equation 2	91.50	93.38	0.38	0.30	2.78
dG_GAS Equation 2	76.13	77.94	0.37	0.29	2.76
dE_THERMAL Equation 2	83.74	85.57	0.37	0.29	2.76
dH_GAS Equation 2	84.34	86.17	0.37	0.29	2.76
dH_GAS Equation 5	-43.04	-28.93	3.03	2.13	2.73
dG_GAS Equation 6	-10.20	-10.24	0.11	0.06	0.21
dE_GAS Equation 6	-10.22	-10.25	0.11	0.06	0.13
dG_SOLV Equation 6	-6.18	-6.17	0.10	0.05	0.09
dG_SOLV Equation 5	76.40	76.46	0.44	0.32	0.07
dH_GAS Equation 6	-10.94	-10.96	0.11	0.06	0.07
dE_THERMAL Equation 6	-10.94	-10.96	0.11	0.06	0.07
dE_SOLV Equation 6	-10.10	-10.11	0.09	0.05	0.07

Table S4. Correlation between gas phase reaction energies employed in Table 1 expressed as R^2 values.

	2	3	4	5	6
2	X	0.62	0.61	0.48	0.01
3	0.62	X	0.99	0.42	0.02
4	0.61	0.99	X	0.38	0.01
5	0.48	0.42	0.38	X	0.00
6	0.01	0.02	0.01	0.00	X