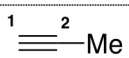
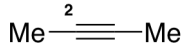
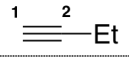
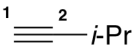
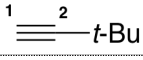
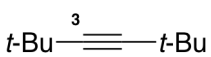
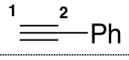
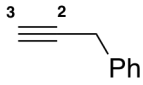
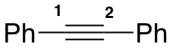
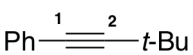
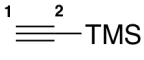
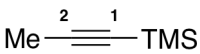
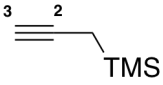
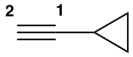
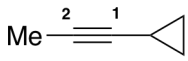
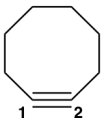
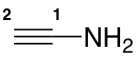
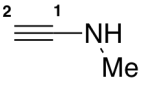
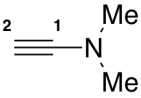
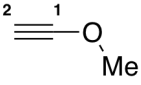
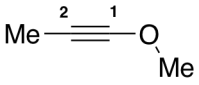
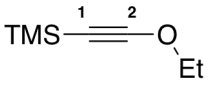
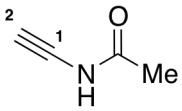
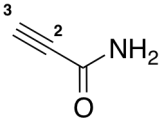
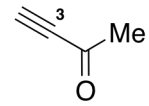
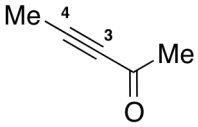
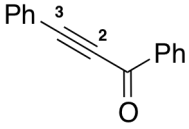
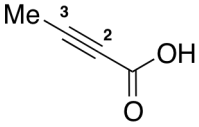
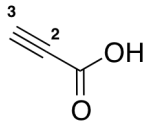
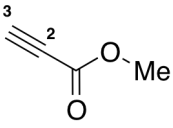
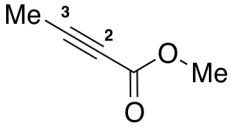
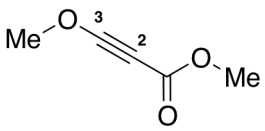
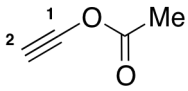
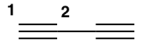
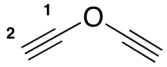
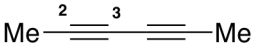
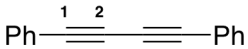
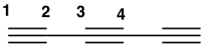
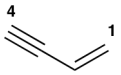
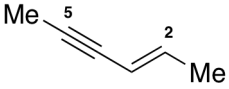
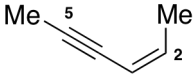
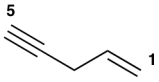
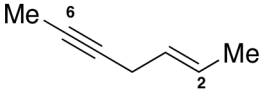
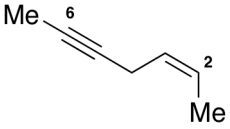
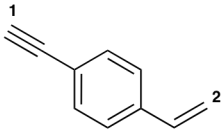
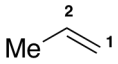
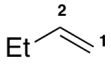
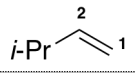
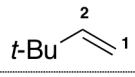
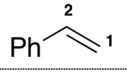
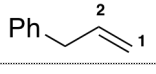
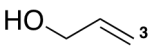
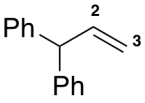
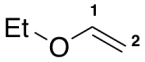
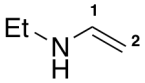
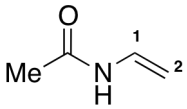
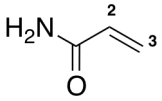
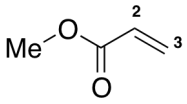
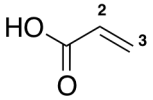
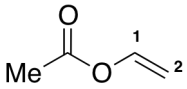
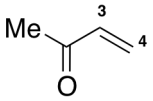
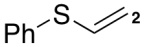
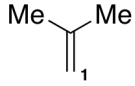
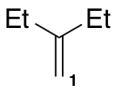
ALKENES, ALKYNES AND AROMATICS BASED ACCEPTORS

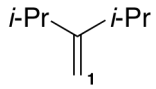
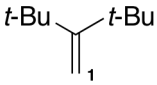
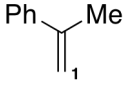
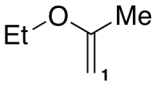
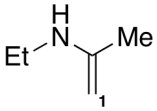
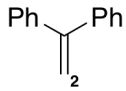
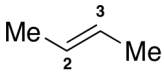
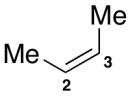
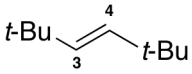
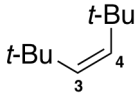
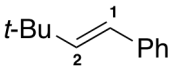
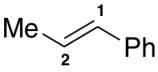
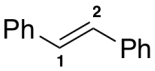
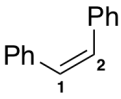
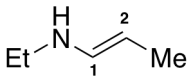
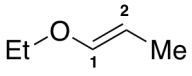
Label	Name	Structure	Binding Site	Cl^+ affinity kcal/mol	X-Cl distance (Å)
A1	ethyne		C1-C2	114.5	1.902
A2	prop-1-yne		C1	136.9	1.722
A3	but-2-yne		C2	143.3	1.768
A4	but-1-yne		C1	142.0	1.724
A5	3-methylbut-1-yne		C1	181.9	1.681
A6	3,3-dimethylbut-1-yne		C1	192.0	1.689
A7	2,2,5,5-tetramethylhex-3-yne		C3	156.6	1.781
A8	ethynylbenzene		C1	168.1	1.727
A9	prop-2-yn-1-ylbenzene		C3	195.0	1.703
A10	1,2-diphenylethyne		C1	169.3	1.674
A11	(3,3-dimethylbut-1-yn-1-yl)benzene		C2	172.6	1.755
A12	ethynyltrimethylsilane		C1	187.0	1.833
A13	trimethyl(prop-1-yn-1-yl)silane		C2	148.6	1.789
A14	trimethyl(prop-2-yn-1-yl)silane		C3	171.9	1.727
A15	ethynylcyclopropane		C2	164.9	1.721
A16	prop-1-yn-1-ylcyclopropane		C2	168.0	1.743
A17	cyclooctyne		C1-C2	164.0	1.749
A18	ethynamine		C2	177.1	1.709
A19	*N*-methylethynamine		C2	187.4	1.713
A20	*N,N*-dimethylethynamine		C2	195.0	1.718
AO42	methoxyethyne		C2 O	162.8 NA	1.717 NA

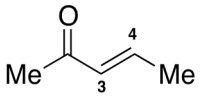
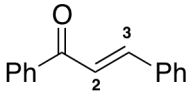
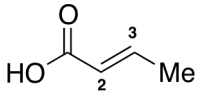
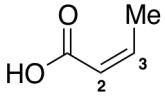
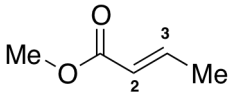
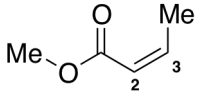
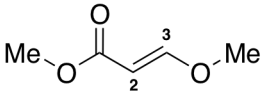
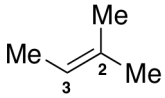
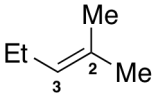
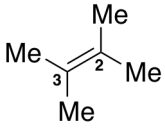
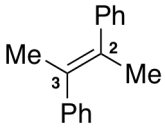
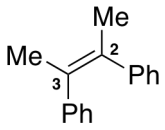
Label	Name	Structure	Binding Site	Cl^+ affinity kcal/mol	X-Cl distance (Å)
A21	1-methoxyprop-1-yne		C2	202.9	1.738
AO43	(ethoxyethynyl)trimethylsilane		C1 O	175.9 NA	1.732 NA
A22	*N*-ethynylacetamide		C2	172.3	1.712
A23	propiolamide		C2-C3	146.4	1.699
A24	but-3-yn-2-one		C3-C4	138.7	1.692
A25	pent-3-yn-2-one		C3-C4	140.2	1.696
A26	1,3-diphenylprop-2-yn-1-one		C2	167.8	1.730
A27	but-2-ynoic acid		C2-C3	133.3	1.720
A28	propiolic acid		C2-C3	125.6	1.697
A29	methyl propiolate		C2-C3	135.1	1.695
A30	methyl but-2-ynoate		C2	154.8	1.687
A31	methyl 3-methoxypropiolate		C2	162.4	1.711

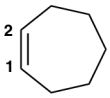
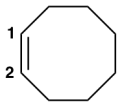
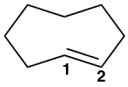
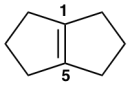
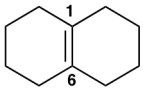
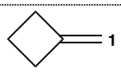
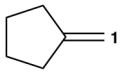
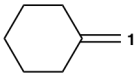
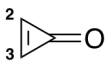
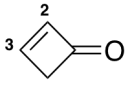
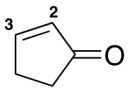
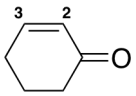
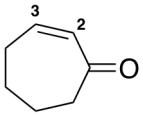
Label	Name	Structure	Binding Site	Cl^+ affinity kcal/mol	X-Cl distance (Å)
A32	ethynyl acetate		C2	170.8	1.731
A33	buta-1,3-diyne		C1	140.7	1.705
AO41	(ethynyloxy)ethyne		C2 O	144.2 NA	1.715 NA
A34	hexa-2,4-diyne		C2	160.1	1.733
A35	1,4-diphenylbuta-1,3-diyne		C1	177.4	1.751
A36	hexa-1,3,5-triyne		C3 C1	134.8 156.5	1.733 1.707
A37	but-1-en-3-yne		C4 C1	151.6 142.1	1.721 1.828
A38	(*E*)-hex-2-en-4-yne		C5 C2	168.6 160.0	1.745 1.848
A39	(*Z*)-hex-2-en-4-yne		C5 C2	166.2 159.3	1.747 1.855
A40	pent-1-en-4-yne		C5 C1	168.5 147.9	1.683 1.811
A41	(*E*)-hept-2-en-5-yne		C6 C2	203.6 162.1	1.711 1.829
A42	(*Z*)-hept-2-en-5-yne		C6 C2	169.4 162.4	1.745 1.830
A43	1-ethynyl-4-vinylbenzene		C1 C2	177.1 171.2	1.733 1.815
A44	ethene		C1-C2	136.2	1.892
A45	prop-1-ene		C1-C2	146.0	1.862
A46	but-1-ene		C1-C2	148.4	1.855

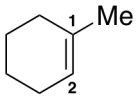
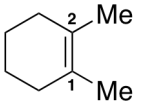
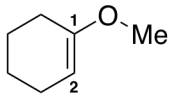
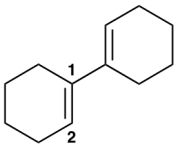
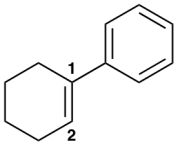
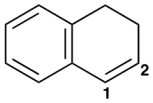
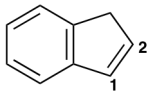
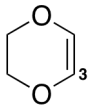
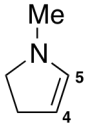
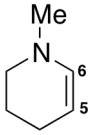
Label	Name	Structure	Binding Site	Cl^+ affinity kcal/mol	X-Cl distance (Å)
A47	3-methylbut-1-ene		C1-C2	150.9	1.848
A48	3,3-dimethylbut-1-ene		C1	153.6	1.836
A49	styrene		C1	167.4	1.815
A50	3-phenylpropene		C1	165.0	1.804
AO11*	prop-2-en-1-ol		O C3	109.8 147.4	1.746 1.799
A51	prop-2-ene-1,1-diyldibenzene		C3	181.1	1.808
AO37	ethoxyethene		C2 O	165.5 NA	1.808 NA
A52	*N*-ethylethenamine		C2	193.0	1.801
A53	*N*-vinylacetamide		C2	169.7	1.804
A54	acrylamide		C2-C3	135.4	1.882
A55	methyl acrylate		C2-C3	133.1	1.882
A56	acrylic acid		C2-C3	128.0	1.884
A57	vinyl acetate		C2	158.9	1.806
A58	but-3-en-2-one		C3-C4	133.4	1.882
AS20	phenyl(vinyl)sulfane		S C2	159.4 171.5	2.089 1.811
A59	2-methylprop-1-ene		C1	155.8	1.831
A60	3-methylenepentane		C1	161.6	1.824

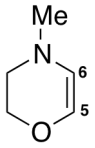
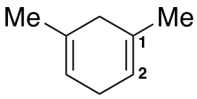
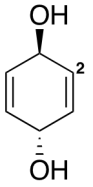
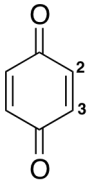
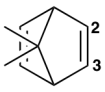
*Addition of Cl^+ to the olefin leads to the epoxide during geometry optimization.

Label	Name	Structure	Binding Site	Cl^+ affinity kcal/mol	X-Cl distance (Å)
A61	2,4-dimethyl-3-methylenepentane		C1	202.9	1.818
A62	2,2,4,4-tetramethyl-3-methylenepentane		C1	165.7	1.819
A63	α-methylstyrene		C1	173.7	1.813
AO39	2-ethoxyprop-1-ene		C1 O	176.9 NA	1.808 NA
A64	*N*-ethylprop-1-en-2-amine		C1	200.9	1.802
A65	ethene-1,1-diyldibenzene		C2	182.2	1.814
A66	*trans*-but-2-ene		C2-C3	153.7	1.955
A67	*cis*-but-2-ene		C2-C3	154.1	1.957
A68	*trans*-2,2,5,5-tetramethylhex-3-ene		C3-C4	163.2	1.972
A69	*cis*-2,2,5,5-tetramethylhex-3-ene		C3-C4	162.9	1.957
A70	(*E*)-(3,3-dimethylbut-1-en-1-yl)benzene		C2 C1	171.7 172.9	1.846 1.848
A71	β-methylstyrene		C2	170.1	1.838
A72	*trans*-stilbene		C1	169.7	1.815
A73	*cis*-stilbene		C1	168.1	1.846
A74	(*E*)-*N*-ethylprop-1-en-1-amine		C2	196.1	1.821
AO38	(*E*)-1-ethoxyprop-1-ene		C2 O	171.3 NA	1.835 NA

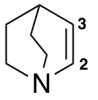
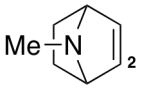
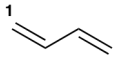
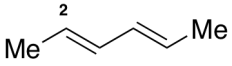
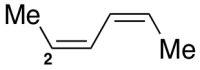
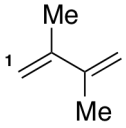
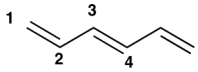
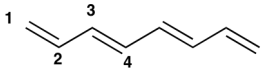
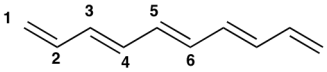
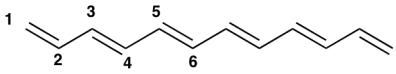
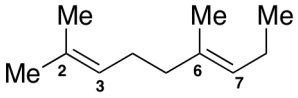
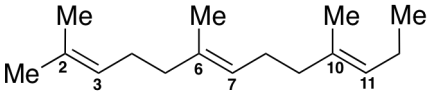
Label	Name	Structure	Binding Site	Cl^+ affinity kcal/mol	X-Cl distance (Å)
A75	(*E*)-pent-3-en-2-one		C3-C4	141.1	1.883
A76	*(E)*-1,3-diphenyl-2-propene-1-one (chalcone)		C2	168.9	1.781
A77	(*E*)-but-2-enoic acid		C2-C3	136.5	1.874
A78	(*Z*)-but-2-enoic acid		C2-C3	136.9	1.871
A79	(*E*)-methyl but-2-enoate		C2-C3	140.4	1.881
A80	(*Z*)-methyl but-2-enoate		C2-C3	141.1	1.876
AO40	(*E*)-methyl 3-methoxyacrylate		C2 O	160.6 NA	1.787 NA
A81	2-methylbut-2-ene		C3	161.0	1.887
A82	2-methylpent-2-ene		C3	166.3	1.870
A83	2,3-dimethylbut-2-ene		C2-C3	166.3	2.001
A84	(*E*)-2,3-diphenyl-2-butene		C2	170.2	1.874
A85	(*Z*)-2,3-diphenyl-2-butene		C2	174.7	1.867
A86	cyclopropene		C1-C2	141.1	1.899
A87	cyclobutene		C1-C2	147.9	1.935
A88	cyclopentene		C1-C2	155.5	1.958

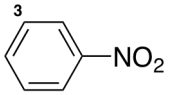
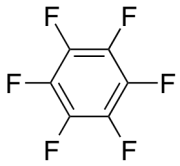
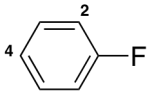
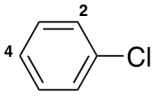
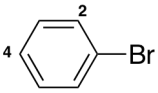
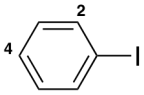
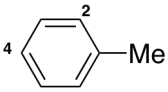
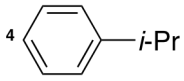
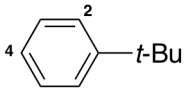
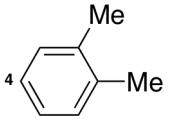
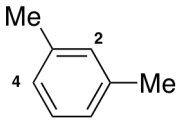
Label	Name	Structure	Binding Site	Cl^+ affinity kcal/mol	X-Cl distance (Å)
A89	cyclohexene		C1-C2	154.8	1.962
A90	cycloheptene		C1-C2	156.9	1.962
A91	*cis*-cyclooctene		C1-C2	159.2	1.827
A92	*trans*-cyclooctene		C1-C2	170.3	1.970
A93	bicyclo[2.2.0]hex-1(4)-ene		C1-C4	162.2	1.950
A94	1,2,3,4,5,6-hexahydropentalene		C1-C5	169.1	2.005
A95	1,2,3,4,5,6,7,8-octahydronaphthalene		C1-C6	165.2	2.029
A96	methylenecyclopropane		C1	147.9	1.871
A97	methylenecyclobutane		C1	155.9	1.830
A98	methylenecyclopentane		C1	161.5	1.819
A99	methylenecyclohexane		C1	162.1	1.822
A100	cycloprop-2-enone		C2-C3	101.1	1.875
A101	cyclobut-2-enone		C2-C3	127.2	1.896
A102	cyclopent-2-enone		C2-C3	131.9	1.893
A103	cyclohex-2-enone		C2-C3	137.7	1.891
A104	cyclohept-2-enone		C2-C3	140.1	1.906

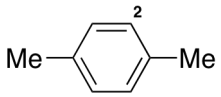
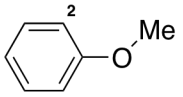
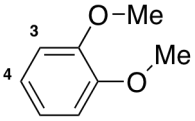
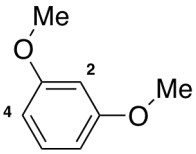
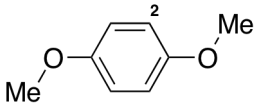
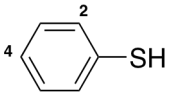
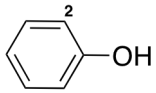
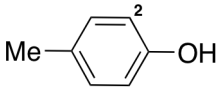
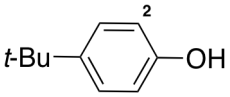
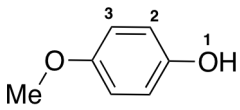
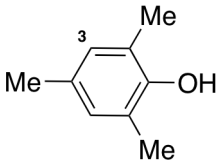
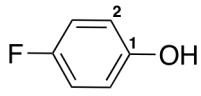
Label	Name	Structure	Binding Site	Cl^+ affinity kcal/mol	X-Cl distance (Å)
A105	1-methylcyclohex-1-ene		C2	162.2	1.867
A106	1,2-dimethylcyclohex-1-ene		C1-C2	166.1	1.974
A107	1-methoxycyclohex-1-ene		C2	180.2	1.830
A108	[1,1'-bi(cyclohexane)]-1,1'-diene		C2	181.4	1.835
A109	2,3,4,5-tetrahydro-1,1'-biphenyl		C2	177.5	1.830
A110	1,2-dihydronaphthalene		C2	173.7	1.842
A111	1*H*-indene		C2	170.4	1.813
A112	2,3-dihydrofuran		C3	169.9	1.822
A113	3,4-dihydro-2*H*-pyran		C3	169.2	1.810
A114	2,3-dihydro-1,4-dioxine		C3	164.6	1.878
A115	1-methyl-2,3-dihydro-1*H*-pyrrole		C4	201.7	1.819
A116	1-methyl-1,2,3,4-tetrahydropyridine		C5	200.0	1.812

Label	Name	Structure	Binding Site	Cl^+ affinity kcal/mol	X-Cl distance (Å)
ANO44	4-methyl-3,4-dihydro-2*H*-1,4-oxazine		C5 O N	196.1 NA NA	1.851 NA NA
A117	cyclobuta-1,3-diene		C1	193.4	1.754
A118	cyclopenta-1,3-diene		C1	162.4	1.804
A119	cyclohexa-1,4-diene		C1-C2	153.6	1.960
A120	1,5-dimethylcyclohexa-1,4-diene		C2	162.2	1.887
A121*	*trans*-cyclohexa-2,5-diene-1,4-diol		C2	165.4	1.799
A122	*para*-benzoquinone		C2-C3	118.4	1.918
A123	bicyclo[2.2.1]hept-2-ene		C2-C3	161.0	1.960
A124	bicyclo[2.2.2]oct-2-ene		C2-C3	158.2	1.953
A125	7,7-dimethylbicyclo[2.2.1]hept-2-ene		C2-C3	155.7	1.969
A126**	bicyclo[2.2.2]octa-2,5-diene		C2	174.1	1.792
A127	bicyclo[2.2.1]hepta-2,5-diene		C2	175.1	1.783
A128	7,7-dimethylbicyclo[2.2.1]hepta-2,5-diene		C2	180.7	1.795

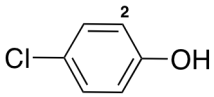
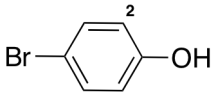
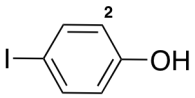
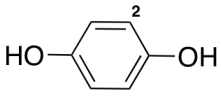
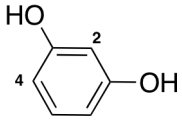
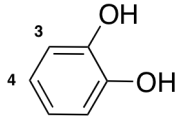
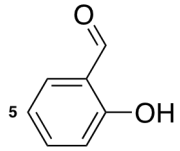
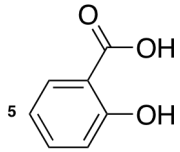
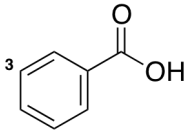
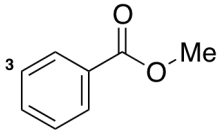
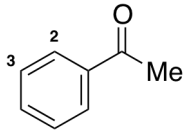
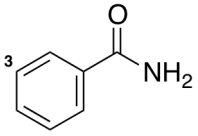
*Addition of Cl^+ to the olefin leads to the epoxide during geometry optimization. **Addition of Cl^+ to the olefin results in anchimeric assistance of the other olefin leading to a C-C bond formation.

Label	Name	Structure	Binding Site	Cl^+ affinity kcal/mol	X-Cl distance (Å)
AN66	1-azabicyclo[2.2.2]oct-2-ene		C2-C3 N	152.6 168.2	1.924 1.780
AN64	7-methyl-7-azabicyclo[2.2.1]hept-2-ene		N (N-Cl *syn* to C=C) N (N-Cl *anti* to C=C) C2	169.0 170.8 188.4	1.796 1.794 1.781
A129	buta-1,3-diene		C1	149.8	1.822
A130	(2*E*,4*E*)-hexadiene		C2	165.1	1.839
A131	(2*Z*,4*Z*)-hexadiene		C2	167.2	1.850
A132	2,3-dimethylbuta-1,3-diene		C1	163.8	1.818
A133	(*E*)-hexa-1,3,5-triene		C1 C3-C4	171.8 152.8	1.815 1.981
A134	(3*E*,5*E*)-octa-1,3,5,7-tetraene		C1 C3	184.7 168.0	1.814 1.854
A135	(3*E*,5*E*,7*E*)-deca-1,3,5,7,9-pentaene		C1 C3 C5	194.1 178.8 169.9	1.817 1.847 1.820
A136	(3*E*,5*E*,7*E*,9*E*)-dodeca-1,3,5,7,9,11-hexaene		C1 C3 C5	200.7 186.8 179.3	1.819 1.848 1.843
A137	(*E*)-2,6-dimethylnona-2,6-diene		C3 C7	164.5 170.3	1.918 1.850
A138	(6*E*,10*E*)-2,6,10-trimethyltrideca-2,6,10-triene		C3 C7 C11	167.7 171.5 172.3	1.929 1.853 1.837

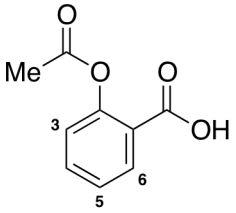
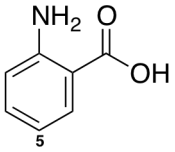
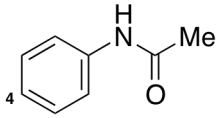
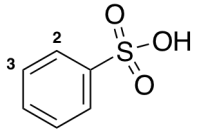
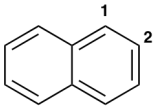
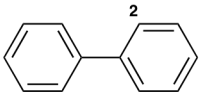
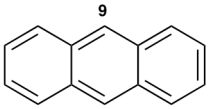
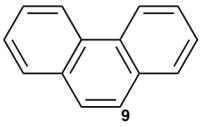
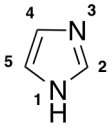
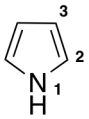
Label	Name	Structure	Binding Site	Cl^+ affinity kcal/mol	X-Cl distance (Å)
A139	cyclohexa-1,3-dien-5-yne		C5	170.8	1.698
A140	benzene		C	139.0	1.805
AO141	nitrobenzene		O C3	118.2 121.8	1.709 1.804
A142	hexafluorobenzene		C	121.4	1.797
A143	fluorobenzene		C2 C4	137.9 141.0	1.807 1.814
A144	chlorobenzene		C2 C4	136.6 139.5	1.815 1.816
A145	bromobenzene		C2 C4	137.1 140.1	1.815 1.820
A146	iodobenzene		C2 C4	139.3 142.2	1.822 1.821
A147	toluene		C2 C4	147.2 148.4	1.803 1.812
A148	cumene		C4	150.7	1.816
A149	*tert*-butylbenzene		C2 C4	146.6 151.5	1.842 1.817
A150	*o*-xylene		C4	151.2	1.817
A151	*m*-xylene		C2 C4	153.0 155.5	1.831 1.813

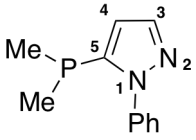
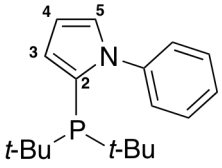
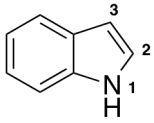
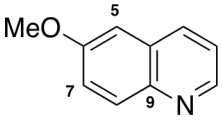
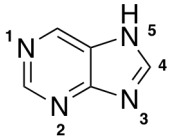
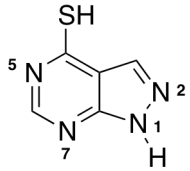
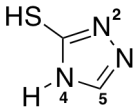
Label	Name	Structure	Binding Site	Cl^+ affinity kcal/mol	X-Cl distance (Å)
A152	*p*-xylene		C2	150.7	1.805
AO153	anisole		C2 O	155.6 112.1	1.826 2.026
A154	1,2-dimethoxybenzene		C3 C4	161.3 166.7	1.821 1.830
A155	1,3-dimethoxybenzene		C2 C4	171.3 174.3	1.819 1.821
A156	1,4-dimethoxybenzene		C2	158.4	1.825
AS3	benzenethiol		C2 C4 S	149.2 152.9 146.8	1.804 1.824 2.089
AO12	phenol		C2 O	152.3 106.3	1.814 2.138
AO13	*p*-cresol		C2 O	157.9 113.9	1.806 2.205
AO14	4-(*tert*-butyl)phenol		C2 O	159.1 116.5	1.818 2.247
AO15	4-methoxyphenol		C2 C3 O1	156.0 158.4 124.8	1.807 1.877 2.326
AO16	2,4,6-trimethylphenol		C3 O	159.3 124.6	1.816 2.321
AO17*	4-fluorophenol		C1 C2 O	137.4 146.1 NA	1.886 1.821 NA

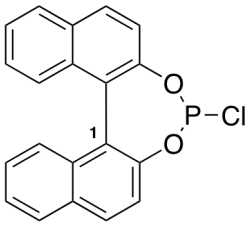
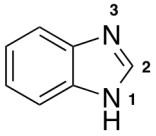
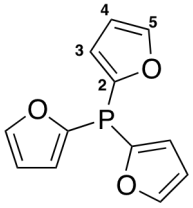
*Attempts for the geometry optimization of the structure in which Cl^+ was attached to OH resulted in the migration of the halogen to C1.

Label	Name	Structure	Binding Site	Cl^+ affinity kcal/mol	X-Cl distance (Å)
AO18	4-chlorophenol		C2 O	145.3 106.4	1.816 2.211
AO19	4-bromophenol		C2 O	145.7 107.2	1.816 2.222
AO20	4-iodophenol		C2 O	147.2 110.1	1.816 2.240
AO21	hydroquinone		C2 O	153.9 120.5	1.807 2.216
AO22	resorcinol		C2 C4 O	162.4 165.9 108.4	1.816 1.816 2.178
AO23*	pyrocatechol		C3 C4 O	152.9 154.1 NA	1.808 1.823 NA
AO157	2-hydroxybenzaldehyde		C5 O	149.5 125.3	1.822 1.727
AO158	2-hydroxybenzoic acid		C5 O	153.7 124.7	1.823 1.731
A159	benzoic acid		C3	133.7	1.804
A160	methyl benzoate		C3	137.2	1.807
A161	acetophenone		C2 C3	134.8 134.7	1.830 1.803
AN162	benzamide		C3 N	137.2 133.0	1.808 1.763

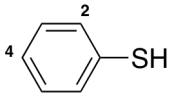
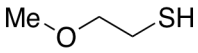
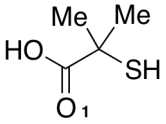
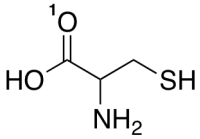
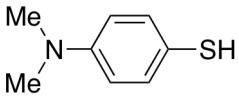
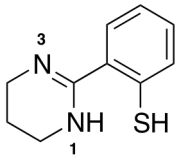
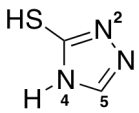
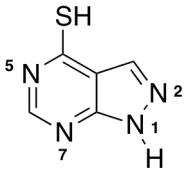
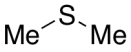
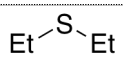
*Attempts for the geometry optimization of the structure in which Cl^+ was attached to OH resulted in the migration of the halogen to C3.

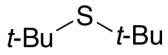
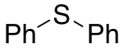
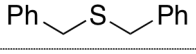
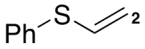
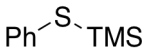
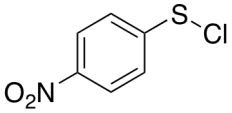
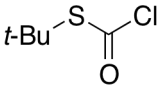
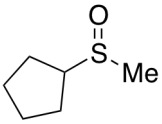
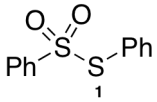
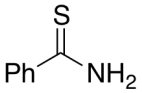
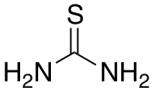
Label	Name	Structure	Binding Site	Cl^+ affinity kcal/mol	X-Cl distance (Å)
A163	2-acetoxybenzoic acid		C3 C5 C6	135.8 137.0 116.8	1.818 1.819 1.836
AN164	2-aminobenzoic acid		C5 N	168.6 150.0	1.827 1.810
A165	*N*-phenylacetamide		C4	162.2	1.824
A166	benzenesulfonic acid		C2 C3	123.8 126.1	1.814 1.803
A167	naphthalene		C1 C2	156.5 152.8	1.834 1.827
A168	1,1'-biphenyl		C2	154.9	1.833
A169	anthracene		C9	175.7	1.848
A170	phenanthrene		C9	161.4	1.854
AN104	1*H*-imidazole		N1 N3 C2 C4	107.7 159.5 151.8 149.9	1.791 1.704 1.770 1.792
AN105	1*H*-pyrrole		N1 C2 C3	122.2 169.8 162.0	1.796 1.785 1.801

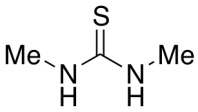
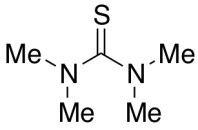
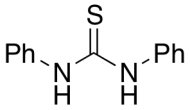
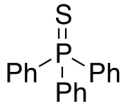
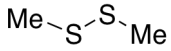
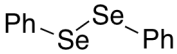
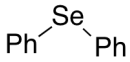
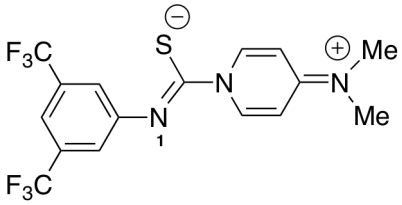
Label	Name	Structure	Binding Site	Cl^+ affinity kcal/mol	X-Cl distance (Å)
ANP27	5-(dimethylphosphino)-1-phenyl-1*H*-pyrazole		P	205.9	2.036
			N2	160.4	1.696
			N1	NA	Cl transfer to C3
			C5	160.1	1.780
			C4	171.2	1.805
			C3	159.3	1.798
ANP28	2-(di-*tert*-butylphosphino)-1-phenyl-1*H*-pyrrole		P	217.9	2.038
			N	131.8	1.830
			C2	173.8	1.798
			C3	177.6	1.817
AN106	1*H*-indole		N1	135.1	1.829
			C2	170.1	1.801
			C3	173.8	1.812
AN107	6-methoxyquinoline		N	167.0	1.734
			C5	165.9	1.838
			C7	153.2	1.829
			C9	142.1	1.892
AN108	7*H*-purine		N1	154.2	1.728
			N2	156.6	1.723
			N3	151.7	1.702
			N5	106.2	1.803
			C4	128.2	1.775
ANS10	1*H*-pyrazolo[3,4-*d*]pyrimidine-4-thiol		S	132.3	2.059
			N5	147.8	1.730
			N7	148.2	1.723
			N1	115.5	1.772
			N2	140.3	1.694
ANS9	4*H*-1,2,4-triazole-3-thiol		S	128.7	2.086
			N4	96.5	1.782
			C5	145.3	1.769
			N2	153.0	1.695

Label	Name	Structure	Binding Site	Cl^+ affinity kcal/mol	X-Cl distance (Å)
AOP25	4-chlorodinaphtho[2,1-*d*:1',2'-*f*][1,3,2]dioxaphosphepine		P	181.0	1.984
			O	NA	Cl transfer to C1
			C1	152.0	1.886
AN109	1*H*-benzimidazole		N1	122.4	1.811
			C2	153.7	1.782
			N3	163.0	1.703
AP29	tri(furan-2-yl)phosphine		P	205.5	2.046
			C2	180.6	1.706
			C3	165.2	1.807
			C4	154.6	1.827
			C5	178.2	1.778

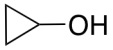
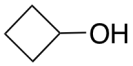
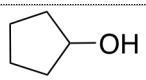
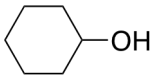
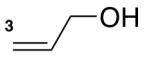
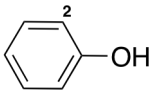
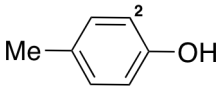
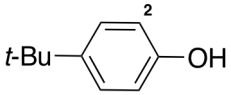
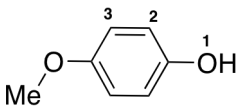
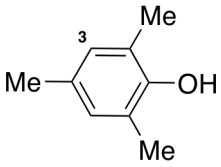
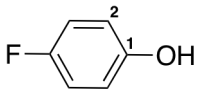
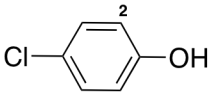
SULFUR BASED ACCEPTORS

Label	Name	Structure	Binding Site	Cl^+ affinity kcal/mol	X-Cl distance (Å)
S1	ethanethiol	Et—SH	S	141.1	2.034
S2	2-methylpropane-2-thiol	*i*-Pr—SH	S	149.4	2.037
AS3	benzenethiol		S C2 C4	146.8 149.2 152.9	2.089 1.804 1.824
OS4	2-methoxyethanethiol		S O	149.1 107.0	2.044 1.757
OS5	2-mercapto-2-methylpropanoic acid		S O1	142.9 119.4	2.071 1.751
NOS6	2-amino-3-mercaptopropanoic acid		S O1 N	175.6 107.5 139.7	2.070 1.747 1.777
NS7	4-(dimethyl amino)benzenethiol		S N	167.6 157.3	2.213 1.976
NS8	2-(1,4,5,6-tetrahydropyrimidin-2-yl)benzenethiol		S N1 N3	180.5 156.4 181.4	2.103 1.793 1.725
ANS9	4*H*-1,2,4-triazole-3-thiol		S N4 C5 N2	128.7 96.5 145.3 153.0	2.086 1.782 1.769 1.695
ANS10	1*H*-pyrazolo[3,4-*d*]pyrimidine-4-thiol		S N5 N7 N1 N2	132.3 147.8 148.2 115.5 140.3	2.059 1.730 1.723 1.772 1.694
S11	dimethylsulfane		S	153.3	2.037
S12	diethylsulfane		S	161.3	2.042

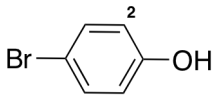
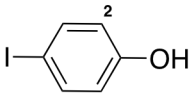
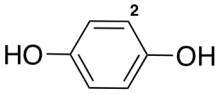
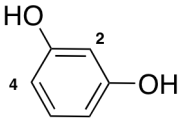
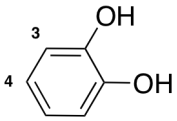
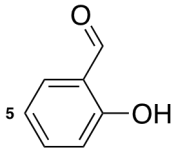
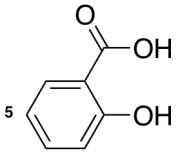
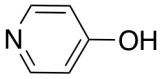
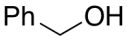
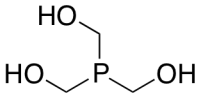
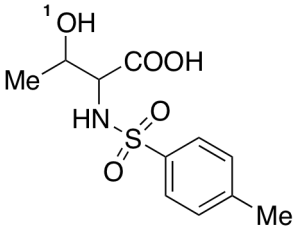
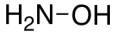
Label	Name	Structure	Binding Site	Cl^+ affinity kcal/mol	X-Cl distance (Å)
S13	thiirane		S	147.3	2.031
S14	thietane		S	155.2	2.027
S15	tetrahydrothiophene		S	159.1	2.045
S16	tetrahydro-2*H*-thiopyran		S	161.5	2.041
S17	di-*tert*-butylsulfane		S	170.7	2.048
S18	diphenylsulfane		S	163.5	2.094
S19	dibenzylsulfane		S	168.1	2.050
AS20	phenyl(vinyl)sulfane		S C2	159.4 171.5	2.089 1.811
S21	trimethyl(phenylthio)silane		S	165.8	2.087
S22	4-nitrophenyl hypochlorothioite		S	142.7	2.047
OS23	*S*-*tert*-butyl carbonochloridothioate		S O	136.6 105.9	2.024 1.742
OS24	(methylsulfinyl)cyclopentane		O	144.6	1.747
OS25	*S*-phenyl benzenesulfonothioate		S1 O	156.2 126.6	2.058 1.744
NS26	benzothioamide		S N	175.8 129.3	2.056 1.796
NS27	thiourea		S N	169.6 NA	2.045 NA

Label	Name	Structure	Binding Site	Cl^+ affinity kcal/mol	X-Cl distance (Å)
NS28	1,3-dimethylthiourea		S N	173.2 NA	2.056 NA
NS29	1,1,3,3-tetramethylthiourea		S N	181.9 NA	2.059 NA
NS30	1,3-diphenylthiourea		S N	180.2 NA	2.058 NA
S31	triphenylphosphine sulfide		S	184.2	2.075
S32	carbon disulfide	S=C=S	S	109.1	2.052
S33	1,2-dimethyldisulfane		S	150.1	2.078
S34	1,2-diphenyldiselane		Se	173.2	2.222
S35	diphenylselane		Se	173.1	2.210
NS36	(Z)-N-(3,5-bis(trifluoromethyl)phenyl)-4-(dimethyliminio)pyridine-1(4H)-carbimidothioate		S N1	189.3 172.5	2.079 1.777

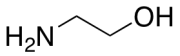
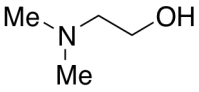
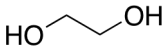
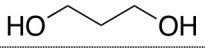
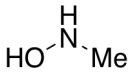
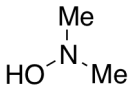
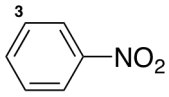
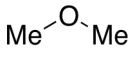
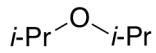
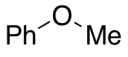
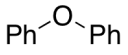
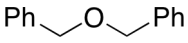
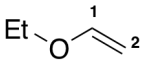
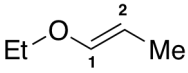
OXYGEN BASED ACCEPTORS

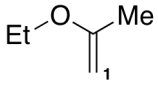
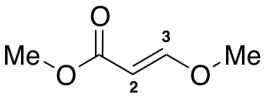
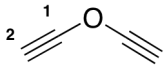
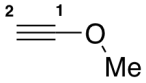
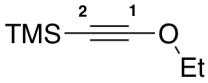
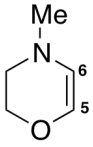
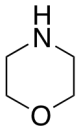
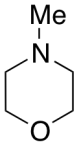
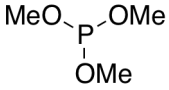
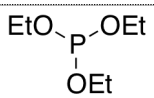
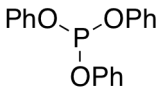
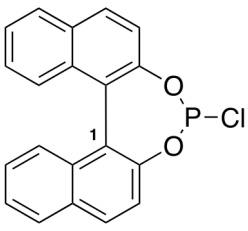
Label	Name	Structure	Binding Site	Cl^+ affinity kcal/mol	X-Cl distance (Å)
O1	water	H_2O	O	81.0	1.774
O2	methanol	Me−OH	O	98.3	1.762
O3	ethanol	Et−OH	O	104.9	1.757
O4	propan-2-ol	*i*-Pr−OH	O	110.5	1.751
O5	butan-1-ol	*n*-Bu−OH	O	106.1	1.753
O6	2-methylpropan-2-ol	*t*-Bu−OH	O	117.4	1.731
O7	cyclopropanol		O	104.9	1.805
O8	cyclobutanol		O	109.9	1.766
O9	cyclopentanol		O	113.5	1.750
O10	cyclohexanol		O	114.3	1.747
AO11*	prop-2-en-1-ol		O C3	109.8 147.4	1.746 1.799
AO12	phenol		O C2	106.3 152.3	2.138 1.814
AO13	*p*-cresol		O C2	113.9 157.9	2.205 1.806
AO14	4-(*tert*-butyl)phenol		O C2	116.5 159.1	2.247 1.818
AO15	4-methoxyphenol		O1 C2 C3	124.8 156.0 158.4	2.326 1.807 1.877
AO16	2,4,6-trimethylphenol		O C3	124.6 159.3	2.321 1.816
AO17**	4-fluorophenol		C1 C2 O	137.4 146.1 NA	1.886 1.821 NA
AO18	4-chlorophenol		O C2	106.4 145.3	2.211 1.816

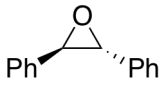
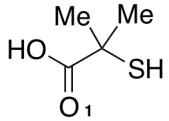
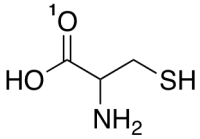
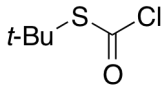
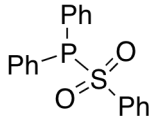
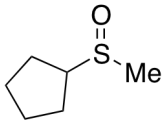
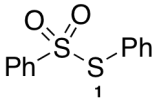
*Addition of Cl^+ to the olefin leads to the epoxide during geometry optimization. **Attempts for the geometry optimization of the structure in which Cl^+ was attached to OH resulted in the migration of the halogen to C2.

Label	Name	Structure	Binding Site	Cl^+ affinity kcal/mol	X-Cl distance (Å)
AO19	4-bromophenol		O C2	107.2 145.7	2.222 1.816
AO20	4-iodophenol		C2 O	147.2 110.1	1.816 2.240
AO21	hydroquinone		O C2	120.5 153.9	2.216 1.807
AO22	resorcinol		O C2 C4	108.4 162.4 165.9	2.178 1.816 1.816
AO23*	pyrocatechol		O C3 C4	NA 152.9 154.1	NA 1.808 1.823
AO157	2-hydroxybenzaldehyde		O C5	125.3 149.5	1.727 1.822
AO158	2-hydroxybenzoic acid		O C5	124.7 153.7	1.731 1.823
NO24	pyridin-4-ol		O N	90.3 161.7	1.917 1.725
O25	phenylmethanol		O	118.4	1.786
OP16	phosphinetriyltrimethanol		O P	123.6 191.3	1.757 2.017
NO26	3-hydroxy-2-(4-methylphenylsulfonamido) butanoic acid		O1 N	137.0 138.5	1.779 1.749
NO27	hydroxylamine		O N	95.0 131.2	1.883 1.784

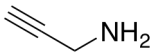
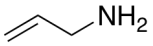
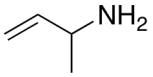
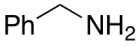
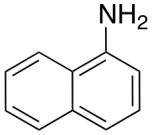
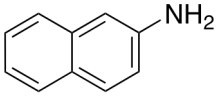
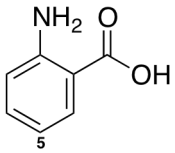
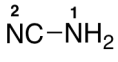
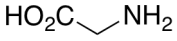
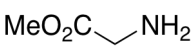
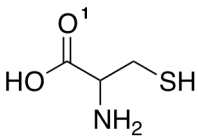
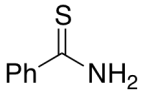
*Attempts for the geometry optimization of the structure in which Cl^+ was attached to OH resulted in the migration of the halogen to C3.

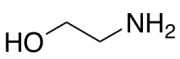
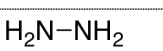
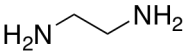
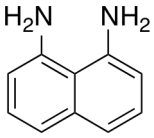
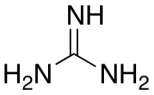
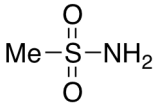
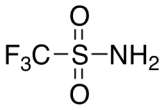
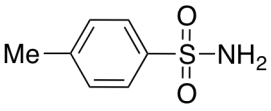
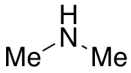
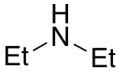
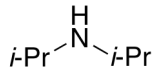
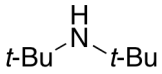
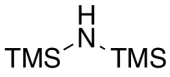
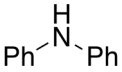
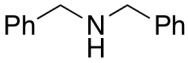
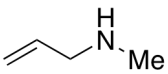
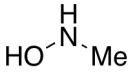
Label	Name	Structure	Binding Site	Cl^+ affinity kcal/mol	X-Cl distance (Å)
NO28	2-aminoethanol		O N	148.2 153.5	1.725 1.763
NO55	2-(dimethylamino)ethanol		O N	158.0 161.8	1.725 1.807
O29	ethane-1,2-diol		O	117.4	1.745
O30	propane-1,3-diol		O	129.9	1.743
NO31	*N*-methylhydroxylamine		O N	106.7 142.9	2.006 1.798
NO32	*N*,*N*-dimethylhydroxylamine		N O	150.5 117.4	1.798 1.798
AO141	nitrobenzene		O C3	118.2 121.8	1.709 1.804
O33	methoxymethane		O	107.9	1.760
O34	2-isopropoxypropane		O	123.8	1.743
AO153	anisole		O C1	112.1 155.6	2.026 1.826
O35	oxydibenzene		O	115.0	2.240
O36	(oxybis(methylene))dibenzene		O	129.2	1.762
AO37	ethoxyethene		O C2	NA 165.5	NA 1.808
AO38	(*E*)-1-ethoxyprop-1-ene		O C2	NA 171.3	NA 1.835

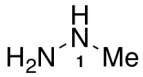
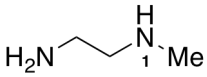
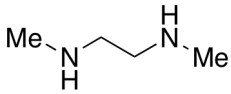
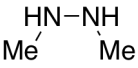
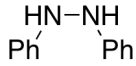
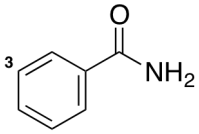
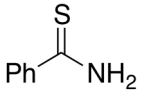
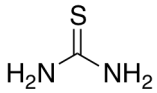
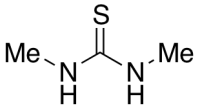
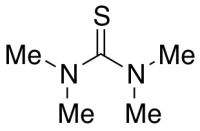
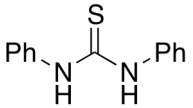
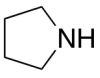
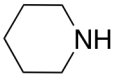
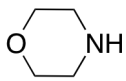
Label	Name	Structure	Binding Site	Cl^+ affinity kcal/mol	X-Cl distance (Å)
AO39	2-ethoxyprop-1-ene		O C1	NA 176.9	NA 1.806
AO40	(*E*)-methyl 3-methoxyacrylate		O C2	NA 160.6	NA 1.787
AO41	(ethynyloxy)ethyne		C2 O	144.2 NA	1.715 NA
AO42	methoxyethyne		C2 O	162.8 NA	1.717 NA
AO43	(ethoxyethynyl)trimethylsilane		C2 O	175.9 NA	1.732 NA
ANO44	4-methyl-3,4-dihydro-2*H*-1,4-oxazine		C5 N O	196.1 NA NA	1.851 NA NA
NO45	morpholine		O (eq) N (ax) N (eq)	117.8 156.0 157.5	1.883 1.791 1.790
NO46	4-methylmorpholine		O N (ax) N (eq)	118.5 159.7 158.5	1.804 1.804 1.811
OP17	trimethyl phosphite		O P	130.9 202.1	1.740 2.006
OP18	triethyl phosphite		O P	135.7 209.1	1.742 2.013
OP19	triphenyl phosphite		O P	128.1 198.4	1.846 2.000
AOP25	4-chlorodinaphtho[2,1-*d*:1',2'-*f*][1,3,2]dioxaphosphepine		O P C1	NA 181.0 152.0	Cl transfer to C1 1.985, 1.84 1.886

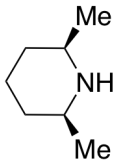
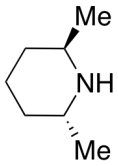
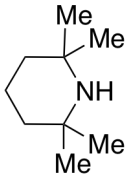
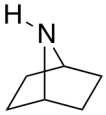
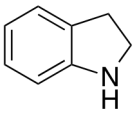
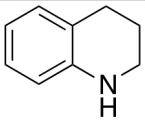
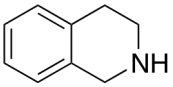
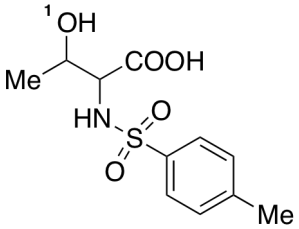
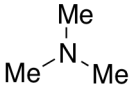
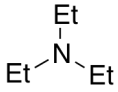
Label	Name	Structure	Binding Site	Cl^+ affinity kcal/mol	X-Cl distance (Å)
O47	oxirane		O	104.4	1.752
O48	*cis*-2,3-dimethyloxirane		O (*syn*) O (*anti*)	117.6 119.8	1.738 1.746
O49	*trans*-2,3-dimethyloxirane		O	118.6	1.742
O50	*trans*-2,3-di-*tert*-butyloxirane		O	122.5	1.742
O51	*trans*-2,3-diphenyloxirane		O	141.4	1.743
O52	*trans*-2,3-dibenzyloxirane		O	124.5	1.754
OS5	2-mercapto-2-methyl propanoic acid		O1 S	119.4 142.9	1.751 2.071
NOS6	2-amino-3-mercapto propanoic acid		O1 S N	107.5 175.6 139.7	1.747 2.070 1.777
OS23	*S*-*tert*-butyl carbonochloridothioate		O S	105.9 136.6	1.742 2.024
OP24	diphenyl(phenylsulfonyl)phosphine		O P	141.7 198.8	1.739 2.030
OS24	(methylsulfinyl)cyclopentane		O	144.6	1.747
OS25	*S*-phenyl benzenesulfonothioate		O S1	126.6 156.2	1.744 2.058

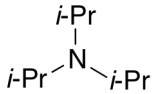
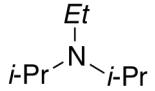
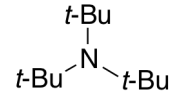
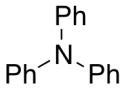
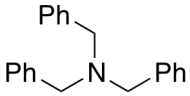
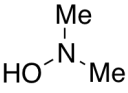
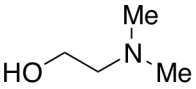
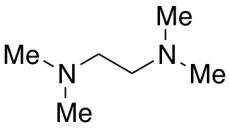
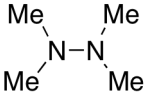
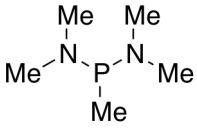
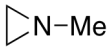
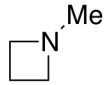
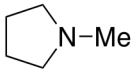
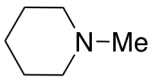
NIROGEN BASED ACCEPTORS

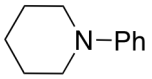
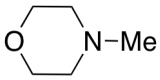
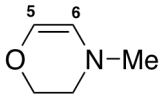
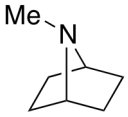
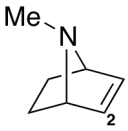
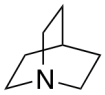
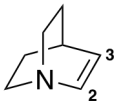
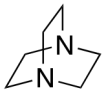
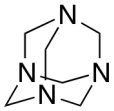
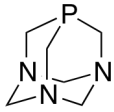
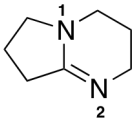
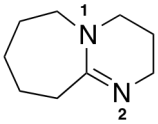
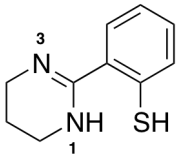
Label	Name	Structure	Binding Site	Cl^+ affinity kcal/mol	X-Cl distance (Å)
N1	ammonia	NH_3	N	132.5	1.764
N2	methanamine	$Me-NH_2$	N	146.7	1.773
N3	ethanamine	$Et-NH_2$	N	151.0	1.772
N4	propan-2-amine	i-$Pr-NH_2$	N	154.3	1.772
N5	2-methylpropan-2-amine	t-$Bu-NH_2$	N	156.9	1.774
N6	prop-2-yn-1-amine		N	146.1	1.773
N7	prop-2-en-1-amine		N	152.8	1.778
N8	but-3-en-2-amine		N	153.4	1.780
N9	cyclohexanamine	$Cy-NH_2$	N (eq)	157.8	1.777
N10	aniline	$Ph-NH_2$	N	146.8	1.865
N11	phenylmethanamine		N	157.8	1.788
N12	naphthalen-1-amine		N	153.5	2.072
N13	naphthalen-2-amine		N	152.2	2.004
AN164	2-aminobenzoic acid		N C5	150.0 168.6	1.810 1.827
N14	cyanamide		N1 N2	93.7 125.4	1.858 1.637
N15	2-aminoacetic acid		N	146.7	1.764
N16	methyl 2-aminoacetate		N	146.0	1.778
NOS6	2-amino-3-mercaptopropanoic acid		N O1 S	139.7 107.5 175.6	1.777 1.747 2.070
NS26	benzothioamide		N S	129.3 175.8	1.796 2.056
NO27	hydroxylamine	$HO-NH_2$	N O	131.2 95.0	1.784 1.883

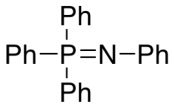
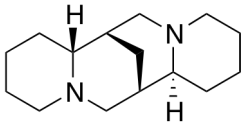
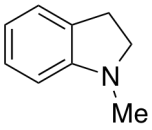
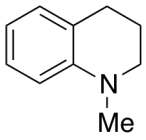
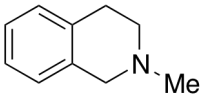
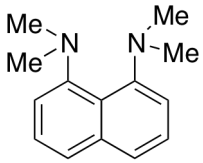
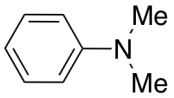
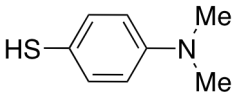
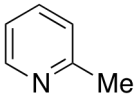
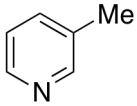
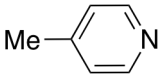
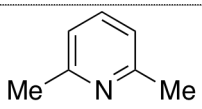
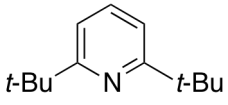
Label	Name	Structure	Binding Site	Cl^+ affinity kcal/mol	X-Cl distance (Å)
NO28	2-aminoethanol		N O	153.5 148.2	1.763 1.725
N17	hydrazine		N	147.7	1.858
N18	ethane-1,2-diamine		N	164.2	1.758
N19	naphthalene-1,8-diamine		N	168.4	1.835
N20	guanidine		N	173.9	1.709
N21	methanesulfonamide		N	124.9	1.747
N22	trifluoromethanesulfonamide		N	113.8	1.744
N23	4-methyl benzenesulfonamide		N	142.8	1.744
N24	dimethylamine		N	155.6	1.786
N25	diethylamine		N	161.7	1.786
N26	diisopropylamine		N	164.7	1.793
N27	di-*tert*-butylamine		N	164.7	1.797
N28	bis(trimethylsilyl)amine		N	162.6	1.798
N29	diphenylamine		N	151.3	1.901
N30	dibenzylamine		N	167.4	1.785
N31	*N*-methylprop-2-en-1-amine		N	153.7	1.780
NO31	*N*-methylhydroxylamine		N O	142.9 106.7	1.798 2.006

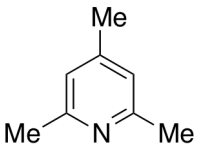
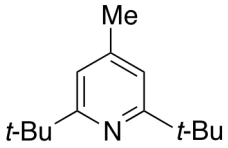
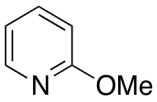
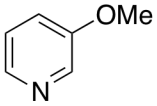
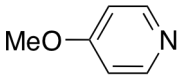
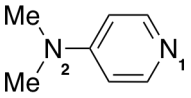
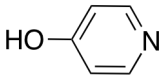
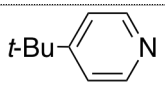
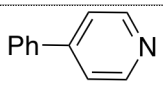
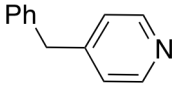
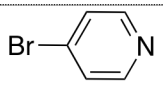
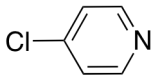
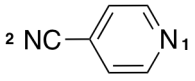
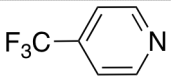
Label	Name	Structure	Binding Site	Cl^+ affinity kcal/mol	X-Cl distance (Å)
N32	methylhydrazine		N1	159.0	1.870
N33	N^1-methylethane-1,2-diamine		N1	171.1	1.781
N34	N^1,N^2-dimethylethane-1,2-diamine		N	170.9	1.782
N35	1,2-dimethylhydrazine		N	163.1	1.939
N36	1,2-diphenylhydrazine		N	161.7	2.196
AN162	benzamide		C3 N	137.2 133.0	1.808 1.763
NS26	benzothioamide		S N	175.8 129.3	2.056 1.796
NS27	thiourea		S N	169.6 NA	2.045 NA
NS28	1,3-dimethylthiourea		N S	NA 173.2	NA 2.056
NS29	1,1,3,3-tetramethylthiourea		S N	181.9 NA	2.059 NA
NS30	1,3-diphenylthiourea		S N	180.2 NA	2.058 NA
N37	aziridine		N	150.5	1.740
N38	azetidine		N	161.8	1.761
N39	pyrrolidine		N	162.3	1.770
N40	piperidine		N (ax) N (eq)	162.7 164.3	1.789 1.785
NO45	morpholine		N (ax) N (eq) O (eq)	156.0 157.5 117.8	1.791 1.790 1.883

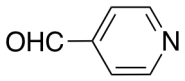
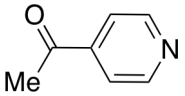
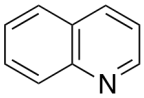
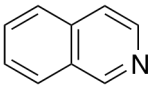
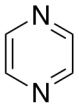
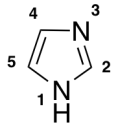
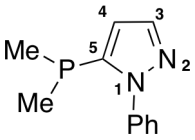
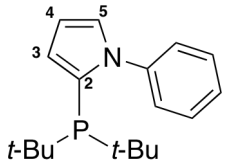
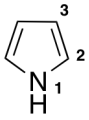
Label	Name	Structure	Binding Site	Cl^+ affinity kcal/mol	X-Cl distance (Å)
N41	*cis*-2,6-dimethylpiperidine		N (ax)	165.5	1.789
			N (eq)	166.2	1.794
N42	*trans*-2,6-dimethylpiperidine		N (ax)	167.5	1.791
			N (eq)	167.5	1.791
N43	2,2,6,6-tetramethylpiperidine		N (ax)	163.5	1.797
			N (eq)	168.9	1.798
N44	7-azabicyclo[2.2.1]heptane		N	166.9	1.766
N45	indoline		N	158.8	1.869
N46	1,2,3,4-tetrahydroquinoline		N	155.4	1.832
N47	1,2,3,4-tetrahydroisoquinoline		N (ax)	162.1	1.788
			N (eq)	163.9	1.786
NO26	3-hydroxy-2-(4-methylphenylsulfonamido)butanoic acid		N	138.5	1.749
			O1	137.0	1.779
N48	trimethylamine		N	160.1	1.799
N49	triethylamine		N	167.7	1.805

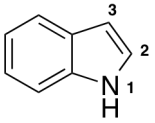
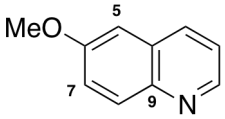
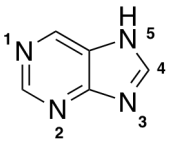
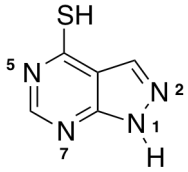
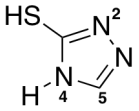
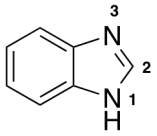
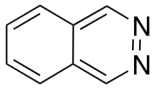
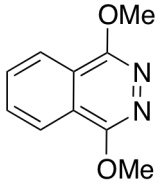
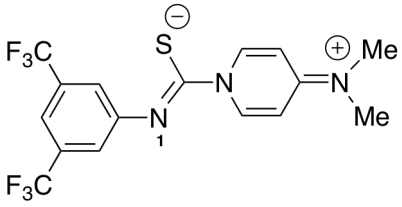
Label	Name	Structure	Binding Site	Cl^+ affinity kcal/mol	X-Cl distance (Å)
N50	triisopropylamine		N	160.4	1.834
N51	*N*-ethyl-*N*-isopropylpropan-2-amine		N	166.3	1.820
N52	tri-*tert*-butylamine		N	169.2	1.800
N53	triphenylamine		N	202.9	2.409
N54	tribenzylamine		N	170.1	1.794
NO32	*N*,*N*-dimethylhydroxylamine		N O	150.5 117.4	1.798 1.798
NO55	2-(dimethylamino)ethanol		N O	161.8 158.0	1.807 1.725
N56	N^1,N^1,N^2,N^2-tetramethylethane-1,2-diamine		N	164.4	1.802
N57	1,1,2,2-tetramethylhydrazine		N	168.9	2.068
NP20	*N*,*N*,*N*',*N*',1-pentamethylphosphinediamine		N P	177.8 219.9	1.792 2.045
N58	1-methylaziridine		N	157.4	1.758
N59	1-methylazetidine		N	164.3	1.785
N60	1-methylpyrrolidine		N	165.4	1.799
N61	1-methylpiperidine		N (ax) N (eq)	165.9 165.1	1.803 1.804

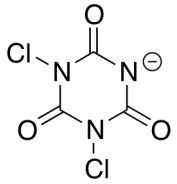
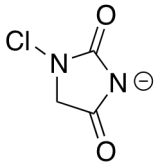
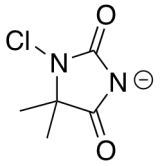
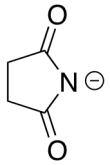
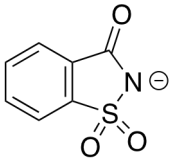
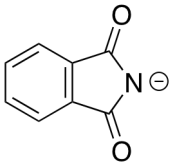
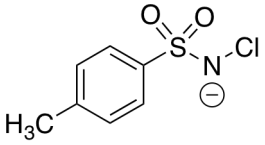
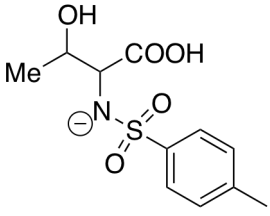
Label	Name	Structure	Binding Site	Cl^+ affinity kcal/mol	X-Cl distance (Å)
N62	1-phenylpiperidine		N	161.8	1.838
NO46	4-methylmorpholine		N (ax) N (eq) O (eq)	159.7 158.5 118.5	1.804 1.811 1.804
ANO44	4-methyl-3,4-dihydro-2*H*-1,4-oxazine		N O C5	NA NA 196.1	NA NA 1.851
N63	7-methyl-7-azabicyclo[2.2.1]heptane		N	169.0	1.793
AN64	7-methyl-7-azabicyclo[2.2.1]hept-2-ene		N (Cl syn to C=C) N (Cl anti to C=C) C2	169.0 170.8 188.4	1.796 1.794 1.781
N65	quinuclidine		N	171.3	1.791
AN66	1-azabicyclo[2.2.2]oct-2-ene		C2-C3 N	152.6 168.2	1.924 1.780
N67	1,4-diazabicyclo[2.2.2]octane		N (1^{st}-Cl) N (2^{nd}-Cl)	167.5 55.3	1.796 1.783
N68	1,3,5,7-Tetraazatricyclo[3.3.1.$1^{3,7}$]decane (HMTA)		N	169.6	1.773
NP22	1,3,5-triaza-7-phosphaadamantane		N P	170.0 200.5	1.800 2.021
N69	1,5-diazabicyclo [4.3.0] non-5-ene (DBN)		N1 N2	148.6 184.9	1.806 1.723
N70	1,8-diazabicyclo [5.4.0] undec-7-ene (DBU)		N1 N2	148.9 184.2	1.816 1.730
NS8	2-(1,4,5,6-tetrahydropyrimidin-2-yl)benzenethiol		S N1 N3	180.5 156.4 181.4	2.103 1.793 1.725

Label	Name	Structure	Binding Site	Cl^+ affinity kcal/mol	X-Cl distance (Å)
NP23	*N*-(triphenyl phosphoranylidene)aniline		N	189.3	1.773
N71	Sparteine		N	171.8	1.817
N72	1-methylindoline		N	162.1	1.876
N73	1-methyl-1,2,3,4-tetrahydroquinoline		N (pseudo-ax) N (pseudo-eq)	161.0 159.7	1.866 1.837
N74	2-methyl-1,2,3,4-tetrahydroisoquinoline		N	165.5	1.803
N75	N^1,N^1,N^8,N^8-tetramethylnaphthalene-1,8-diamine		N	154.4	1.844
N76	*N*,*N*-dimethylaniline		N	156.8	1.843
NS7	4-(dimethylamino)benzenethiol		N S	157.3 167.6	1.976 2.213
N77	pyridine		N	157.3	1.728
N78	2-methylpyridine		N	161.3	1.732
N79	3-methylpyridine		N	160.8	1.730
N80	4-methylpyridine		N	161.8	1.727
N81	2,6-dimethylpyridine		N	164.4	1.736
N82	2,6-di-*tert*-butylpyridine		N N (SM8-acetone)	150.5 126.1	1.743 1.749

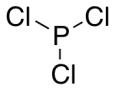
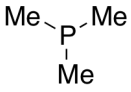
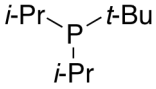
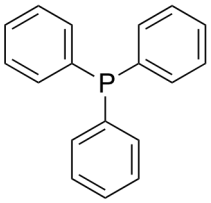
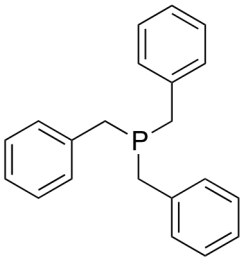
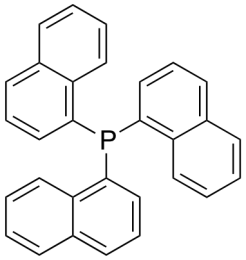
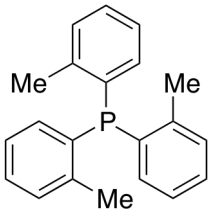
Label	Name	Structure	Binding Site	Cl^+ affinity kcal/mol	X-Cl distance (Å)
N83	2,4,6-trimethylpyridine		N N (SM8-acetone)	168.2 148.2	1.735 1.743
N84	2,6-di-*tert*-butyl-4-methylpyridine		N N (SM8-acetone)	153.1 127.2	1.742 1.742
N85	2-methoxypyridine		N	161.9	1.725
N86	3-methoxypyridine		N	160.9	1.731
N87	4-methoxypyridine		N	165.2	1.725
N88	*N*,*N*-dimethylpyridin-4-amine		N1 N1 (SM8-acetone) N2	176.0 154.3 145.7	1.724 1.732 1.823
NO24	4-hydroxypyridine		N O	161.7 90.3	1.725 1.917
N89	4-(*tert*-butyl)pyridine		N N (SM8-acetone)	164.6 146.3	1.727 1.737
N90	4-phenylpyridine		N N (SM8-acetone)	165.7 145.7	1.725 1.735
N91	4-benzylpyridine		N	164.7	1.728
N92	4-bromopyridine		N N (SM8-acetone)	153.4 138.8	1.726 1.735
N93	4-chloropyridine		N	152.9	1.726
N94	4-cyanopyridine		N1 N1 (SM8-acetone) N2	145.2 138.0 120.5	1.725 1.737 1.614
N95	4-(trifluoromethyl)pyridine		N N (SM8-acetone)	149.3 137.2	1.726 1.736

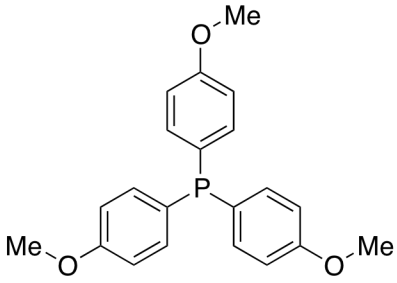
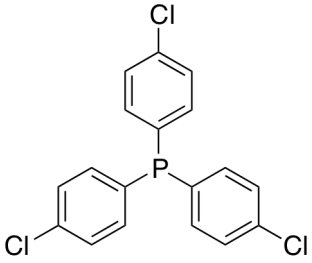
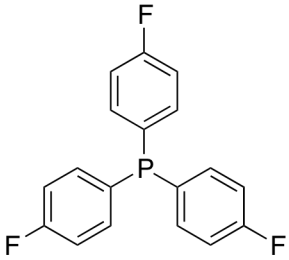
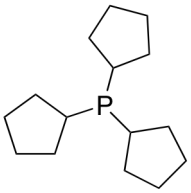
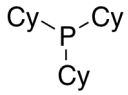
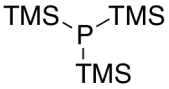
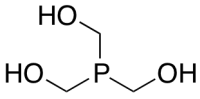
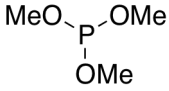
Label	Name	Structure	Binding Site	Cl^+ affinity kcal/mol	X-Cl distance (Å)
N96	pyridine-4-carbaldehye		N N (SM8-acetone)	150.8 140.8	1.726 1.737
N97	4-pyridyl methyl ketone		N	154.6	1.726
N98	quinoline		N	163.3	1.733
N99	isoquinoline		N	164.7	1.728
N100	pyridazine		N	154.4	1.728
N101	pyrimidine		N	146.7	1.729
N102	pyrazine		N	144.2	1.727
N103	1,3,5-triazine		N	135.0	1.725
AN104	1*H*-imidazole		N1 N3 C2 C4	107.7 159.5 151.8 149.9	1.791 1.704 1.770 1.792
ANP27	5-(dimethylphosphino)-1-phenyl-1*H*-pyrazole		P N2 N1 C5 C4 C3	205.9 160.4 NA 160.1 171.2 159.3	2.036 1.696 Cl transfers to C3 1.780 1.805 1.798
ANP28	2-(di-*tert*-butylphosphino)-1-phenyl-1*H*-pyrrole		P N C2 C3 C4 C5	217.9 131.8 173.8 177.6 177.3 185.6	2.038 1.830 1.798 1.817 1.811 1.793
AN105	1*H*-pyrrole		N1 C2 C3	122.2 169.8 162.0	1.796 1.785 1.801

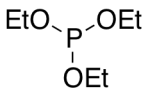
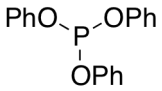
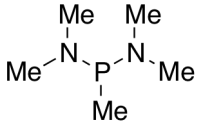
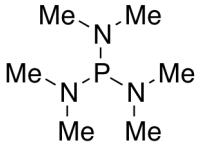
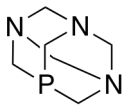
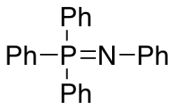
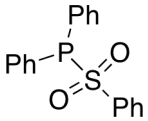
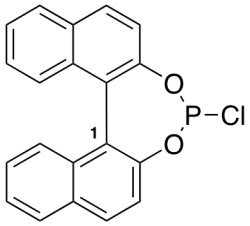
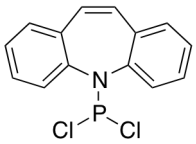
Label	Name	Structure	Binding Site	Cl^+ affinity kcal/mol	X-Cl distance (Å)
AN106	1*H*-indole		N1	135.1	1.829
			C2	170.1	1.801
			C3	173.8	1.812
AN107	6-methoxyquinoline		N	167.0	1.734
			C5	165.9	1.838
			C7	153.2	1.829
			C9	142.1	1.892
AN108	7*H*-purine		N1	154.2	1.728
			N2	156.6	1.723
			N3	151.7	1.702
			N5	106.2	1.803
			C4	128.2	1.775
ANS10	1*H*-pyrazolo[3,4-*d*]pyrimidine-4-thiol		S	132.3	2.059
			N5	147.8	1.730
			N7	148.2	1.723
			N1	115.5	1.772
			N2	140.3	1.694
ANS9	4*H*-1,2,4-triazole-3-thiol		S	128.7	2.086
			N4	96.5	1.782
			C5	145.3	1.769
			N2	153.0	1.695
AN109	1*H*-benzimidazole		N1	122.4	1.811
			C2	153.7	1.782
			N3	163.0	1.703
N110	phthalazine		N	164.9	1.726
N111	1,4-dimethoxyphthalazine		N	162.7	1.731
NS36	Z)-N-(3,5-bis(trifluoromethyl)phenyl)-4-(dimethyliminio)pyridine-1(4H)-carbimidothioate		S	189.3	2.079
			N1	172.5	1.777

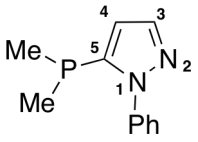
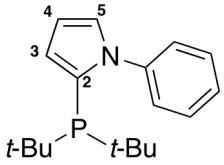
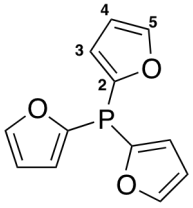
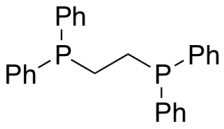
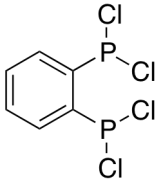
Label	Name	Structure	Binding Site	Cl^+ affinity kcal/mol	X-Cl distance (Å)
N112	3,5-dichloro-2,4,6-trioxo-1,3,5-triazinan-1-ide		N N (SM8-acetone)	252.1 148.1	1.715 1.715
N113	3-chloro-2,5-dioxoimidazolidin-1-ide		N	273.6	1.703
N114	3-chloro-4,4-dimethyl-2,5-dioxoimidazolidin-1-ide		N N (SM8-acetone)	275.7 168.3	1.705 1.708
N115	2,5-dioxopyrrolidin-1-ide		N N (SM8-acetone)	290.1 181.1	1.707 1.716
N116	3-oxo-3*H*-benzo[*d*]isothiazol-2-ide 1,1-dioxide		N	265.0	1.712
N117	1,3-dioxoisoindolin-2-ide		N N (SM8-acetone)	286.7 177.7	1.702 1.705
N118	chloro(tosyl)amide		N	273.3	1.778
N119	(1-carboxy-2-hydroxypropyl)(tosyl)amide		N	268.2	1.768

PHOSPHORUS BASED ACCEPTORS

Label	Name	Structure	Binding Site	Cl^+ affinity kcal/mol	X-Cl distance (Å)
P1	phosphine		P	156.0	1.978
P2	phenylphosphine		P	184.6	2.012
P3	trichlorophosphine		P	142.6	1.980
P4	trimethylphosphine		P	205.9	2.015
P5	*tert*-butyl diisopropylphosphine		P	220.5	2.039
P6	triphenylphosphine		P	215.0	2.049
P7	tribenzylphosphine		P	215.0	2.022
P8	tri(naphthalen-1-yl)phosphine		P	221.3	2.057
P9	tri-*o*-tolylphosphine		P	214.5	2.055

Label	Name	Structure	Binding Site	Cl^+ affinity kcal/mol	X-Cl distance (Å)
P10	tris(4-methoxyphenyl)phosphine		P	227.8	2.066
P11	tris(4-chlorophenyl)phosphine		P	207.7	2.049
P12	tris(4-fluorophenyl)phosphine		P	211.3	2.051
P13	tricyclopentylphosphine		P	222.2	2.037
P14	tricyclohexylphosphine		P	223.5	2.046
P15	1,1,1,3,3,3-hexamethyl-2-(trimethylsilyl)disilaphosphane		P	216.7	2.091
OP16	phosphinetriyltrimethanol		P O	191.3 123.6	2.017 1.757
OP17	trimethyl phosphite		P O	202.1 130.9	2.006 1.740

Label	Name	Structure	Binding Site	Cl^+ affinity kcal/mol	X-Cl distance (Å)
OP18	triethyl phosphite		P	209.1	2.013
			O	135.7	1.742
OP19	triphenyl phosphite		P	198.4	2.000
			O	128.1	1.846
NP20	*N*,*N*,*N*',*N*',1-pentamethylphosphinediamine		P	219.9	2.045
			N	177.8	1.792
NP21	*N*,*N*,*N*',*N*',*N*'',*N*''-hexamethylphosphinetriamine		P	221.4	2.075
			N	180.2	1.792
NP22	1,3,5-triaza-7-phosphaadamantane		P	200.5	2.021
			N	170.0	1.800
NP23	*N*-(triphenyl phosphoranylidene)aniline		N	189.3	1.773
OP24	diphenyl(phenylsulfonyl)phosphine		P	198.7	2.030
			O	141.7	1.739
AOP25	4-chlorodinaphtho[2,1-*d*:1',2'-*f*][1,3,2]dioxaphosphepine		P	181.0	1.984
			O	NA	Cl transfers to C1
			C1	152.0	1.886
NP26	5-(dichlorophosphino)-5*H*-dibenzo[*b*,*f*]azepine		P	175.3	2.001
			N	NA	Cl transfers to P

Label	Name	Structure	Binding Site	Cl^+ affinity kcal/mol	X-Cl distance (Å)
ANP27	5-(dimethylphosphino)-1-phenyl-1*H*-pyrazole		P	205.9	2.036
			N2	160.4	1.696
			N1	NA	*Cl transfers to C3*
			C5	160.1	1.780
			C4	171.2	1.805
			C3	159.3	1.798
ANP28	2-(di-*tert*-butylphosphino)-1-phenyl-1*H*-pyrrole		P	217.9	2.038
			N	131.8	1.830
			C2	173.8	1.798
			C3	177.6	1.817
			C4	177.3	1.811
			C5	185.6	1.793
AP29	tri(furan-2-yl)phosphine		P	205.5	2.046
			C3	165.2	1.807
			C4	154.6	1.827
			C5	178.2	1.778
P30	1,2-bis(diphenyl phosphino)ethane		P	217.6	2.041
P31	1,2-bis(dichloro phosphino)benzene		P	162.2	1.988