

List of functional groups recognized by checkmol

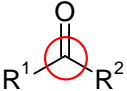
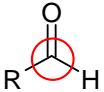
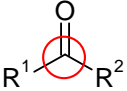
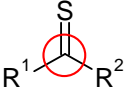
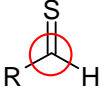
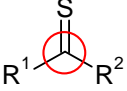
Current program version: v0.5

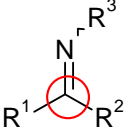
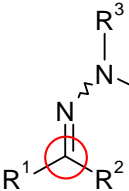
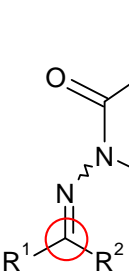
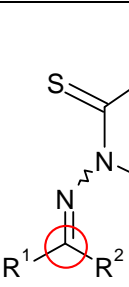
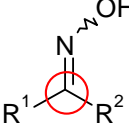
Norbert Haider, University of Vienna, 2005–2013

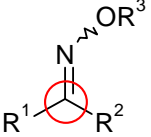
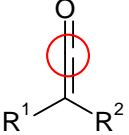
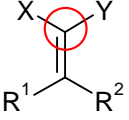
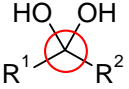
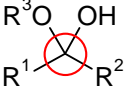
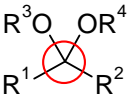
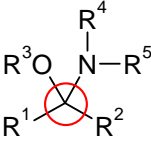
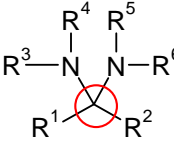
<http://merian.pch.univie.ac.at/~nhaider/cheminf/cmmm.html>

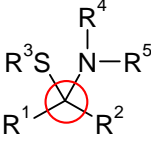
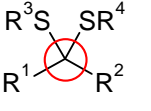
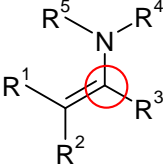
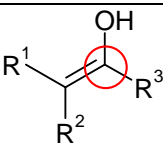
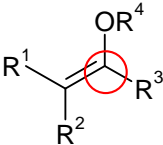


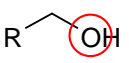
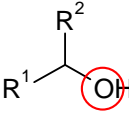
For background information and for appropriate citation, please refer to this article: [Haider, N., Functionality Pattern Matching as an Efficient Complementary Structure/Reaction Search Tool: an Open-Source Approach. *Molecules*, 15, 5079-5092 \(2010\).](#)

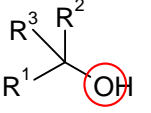
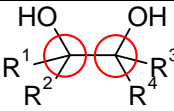
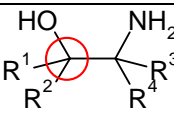
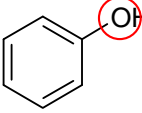
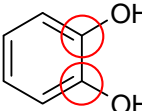
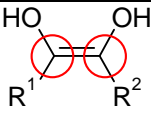
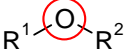
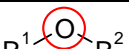



The table below lists the functional group ID number, the English name (as obtained with the –e option), the 8-letter code (as obtained with the –c option [deprecated]) and the structures of the groups recognized by checkmol. The red circles in the structure drawing indicate the “key atoms” which are assigned to each functionality (as listed with the –p option). Wherever possible, a single “key atom” is used to identify and localize a functional group, but in some cases (e.g., for disulfides, peroxides, etc.) a pair of connected atoms serves as a key.

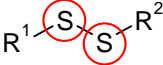
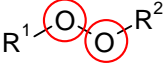
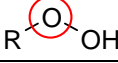
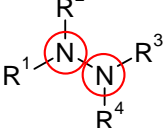
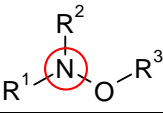
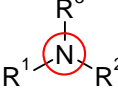



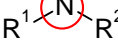
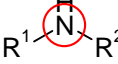
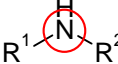
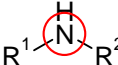
No.	functional group name	code	general structure	remarks
001	cation	000000T2	any positive charge	
002	anion	000000T1	any negative charge	
003	carbonyl compound	C2O10000	 $R^1 = \text{H, alkyl, aryl}$ $R^2 = \text{H, alkyl, aryl}$	ketone or aldehyde
004	aldehyde	C2O1H000	 $R = \text{H, alkyl, aryl}$	
005	ketone	C2O1C000	 $R^1 = \text{alkyl, aryl}$ $R^2 = \text{alkyl, aryl}$	
006	thiocarbonyl compound	C2S10000	 $R^1 = \text{H, alkyl, aryl}$ $R^2 = \text{H, alkyl, aryl}$	thioketone or thioaldehyde
007	thioaldehyde	C2S1H000	 $R = \text{H, alkyl, aryl}$	
008	thioketone	C2S1C000	 $R^1 = \text{alkyl, aryl}$ $R^2 = \text{alkyl, aryl}$	

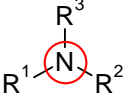
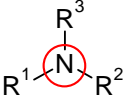
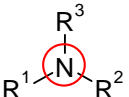
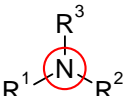
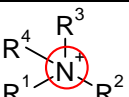
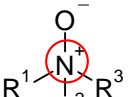
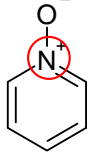







009	imine	C2N1000	 <p> $R^1 = \text{H, alkyl, aryl}$ $R^2 = \text{H, alkyl, aryl}$ $R^3 = \text{H, alkyl, aryl}$ </p>	
010	hydrazone	C2N1N000	 <p> $R^1 = \text{H, alkyl, aryl}$ $R^2 = \text{H, alkyl, aryl}$ $R^3 = \text{H, alkyl, aryl}$ $R^4 = \text{H, alkyl, aryl}$ </p>	
011	semicarbazone	C2NNC4ON	 <p> $R^1 = \text{H, alkyl, aryl}$ $R^2 = \text{H, alkyl, aryl}$ $R^3 = \text{H, alkyl, aryl}$ $R^4 = \text{H, alkyl, aryl,}$ $R^5 = \text{H, alkyl, aryl}$ </p>	
012	thiosemicarbazone	C2NNC4SN	 <p> $R^1 = \text{H, alkyl, aryl}$ $R^2 = \text{H, alkyl, aryl}$ $R^3 = \text{H, alkyl, aryl}$ $R^4 = \text{H, alkyl, aryl,}$ $R^5 = \text{H, alkyl, aryl}$ </p>	
013	oxime	C2N1OH00	 <p> $R^1 = \text{H, alkyl, aryl}$ $R^2 = \text{H, alkyl, aryl}$ </p>	

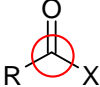
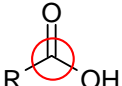
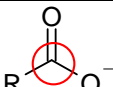
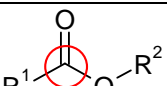
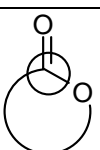
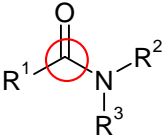
014	oxime ether	C2N1OC00	 <p>R¹ = H, alkyl, aryl R² = H, alkyl, aryl R³ = alkyl, aryl</p>	
015	ketene	C3OC0000	 <p>R¹ = H, alkyl, aryl R² = H, alkyl, aryl</p>	
016	ketene acetal derivative	C3OCC000	 <p>R¹ = H, alkyl, aryl R² = H, alkyl, aryl X = any hetero atom Y = any hetero atom</p>	
017	carbonyl hydrate	C2O2H200	 <p>R¹ = H, alkyl, aryl R² = H, alkyl, aryl</p>	
018	hemiacetal	C2O2HC00	 <p>R¹ = H, alkyl, aryl R² = H, alkyl, aryl R³ = alkyl, aryl</p>	
019	acetal	C2O2CC00	 <p>R¹ = H, alkyl, aryl R² = H, alkyl, aryl R³ = alkyl, aryl R⁴ = alkyl, aryl</p>	
020	hemiaminal	C2NOHC10	 <p>R¹ = H, alkyl, aryl R² = H, alkyl, aryl R³ = H, alkyl, aryl R⁴ = H, alkyl, aryl R⁵ = H, alkyl, aryl</p>	in a true hemiaminal, R ³ would be H
021	aminal	C2N2CC10	 <p>R¹ = H, alkyl, aryl R² = H, alkyl, aryl R³ = H, alkyl, aryl R⁴ = H, alkyl, aryl R⁵ = H, alkyl, aryl R⁶ = H, alkyl, aryl</p>	

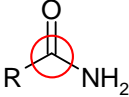
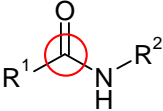
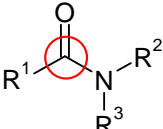
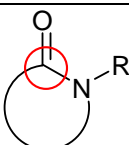
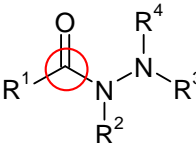
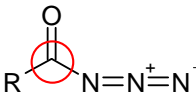
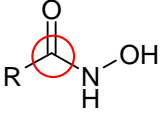
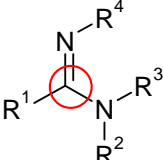
022	thiohemiaminal	C2NSHC10	 <p> $R^1 = \text{H, alkyl, aryl}$ $R^2 = \text{H, alkyl, aryl}$ $R^3 = \text{H, alkyl, aryl}$ $R^4 = \text{H, alkyl, aryl}$ $R^5 = \text{H, alkyl, aryl}$ </p>	
023	thioacetal	C2S2CC00	 <p> $R^1 = \text{H, alkyl, aryl}$ $R^2 = \text{H, alkyl, aryl}$ $R^3 = \text{alkyl, aryl}$ $R^4 = \text{alkyl, aryl}$ </p>	
024	enamine	C2CNH000	 <p> $R^1 = \text{H, acyl, alkyl, aryl}$ $R^2 = \text{H, acyl, alkyl, aryl}$ $R^3 = \text{H, acyl, alkyl, aryl}$ $R^4 = \text{H, acyl, alkyl, aryl}$ $R^5 = \text{H, acyl, alkyl, aryl}$ </p>	$R^4, R^5 = \text{acyl}$ should be types as enamide
025	enol	C2COH000	 <p> $R^1 = \text{H, acyl, alkyl, aryl}$ $R^2 = \text{H, acyl, alkyl, aryl}$ $R^3 = \text{H, acyl, alkyl, aryl}$ </p>	
026	enoether	C2COC000	 <p> $R^1 = \text{H, acyl, alkyl, aryl}$ $R^2 = \text{H, acyl, alkyl, aryl}$ $R^3 = \text{H, acyl, alkyl, aryl}$ $R^4 = \text{alkyl, aryl}$ </p>	
027	hydroxy compound	O1H00000	 <p>$R = \text{alkyl, aryl}$</p>	alcohol or phenol
028	alcohol	O1H0C000	 <p>$R = \text{alkyl}$</p>	
029	prim. alcohol	O1H1C000	 <p>$R = \text{alkyl, aryl}$</p>	
030	sec. alcohol	O1H2C000	 <p> $R^1 = \text{alkyl, aryl}$ $R^2 = \text{alkyl, aryl}$ </p>	

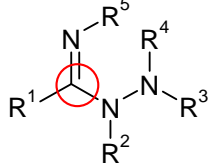

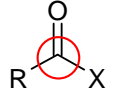
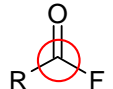
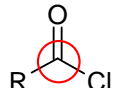
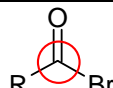
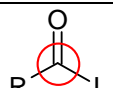
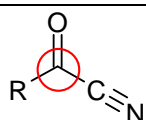
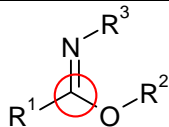
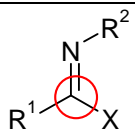
031	tert. alcohol	O1H3C000	 <p> $R^1 = \text{alkyl, aryl}$ $R^2 = \text{alkyl, aryl}$ $R^3 = \text{alkyl, aryl}$ </p>	
032	1,2-diol	O1H0CO1H	 <p> $R^1 = \text{H, alkyl, aryl}$ $R^2 = \text{H, alkyl, aryl}$ $R^3 = \text{H, alkyl, aryl}$ $R^4 = \text{H, alkyl, aryl}$ </p>	
033	1,2-aminoalcohol	O1H0CN1C	 <p> $R^1 = \text{H, alkyl, aryl}$ $R^2 = \text{H, alkyl, aryl}$ $R^3 = \text{H, alkyl, aryl}$ $R^4 = \text{H, alkyl, aryl}$ </p>	
034	phenol	O1H1A000		any aromatic or heteroaromatic ring with an OH substituent
035	1,2-diphenol	O1H2A000		any aromatic or heteroaromatic ring with two adjacent OH substituents (except tautomeric lactams)
036	enediol	C2COH200	 <p> $R^1 = \text{H, alkyl, aryl}$ $R^2 = \text{H, alkyl, aryl}$ </p>	
037	ether	O1C00000	 <p> $R^1 = \text{alkyl, aryl}$ $R^2 = \text{alkyl, aryl}$ </p>	
038	dialkylether	O1C0CC00	 <p> $R^1 = \text{alkyl}$ $R^2 = \text{alkyl}$ </p>	
039	alkylarylether	O1C0CA00	 <p> $R^1 = \text{alkyl}$ $R^2 = \text{aryl}$ </p>	
040	diarylether	O1C0AA00	 <p> $R^1 = \text{aryl}$ $R^2 = \text{aryl}$ </p>	
041	thioether	S1C00000	 <p> $R^1 = \text{alkyl, aryl}$ $R^2 = \text{alkyl, aryl}$ </p>	

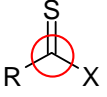
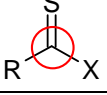
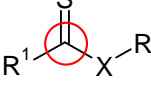
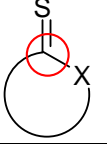
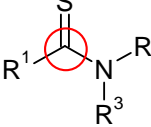
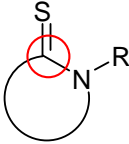
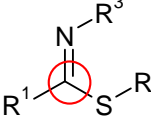
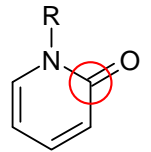
042	disulfide	S1S1C000		R ¹ = alkyl, aryl R ² = alkyl, aryl	
043	peroxide	O1O1C000		R ¹ = alkyl, aryl R ² = alkyl, aryl	
044	hydroperoxide	O1O1H000		R = alkyl, aryl	
045	hydrazine derivative	N1N10000		R ¹ = H, acyl, alkyl, aryl R ² = H, acyl, alkyl, aryl R ³ = H, acyl, alkyl, aryl R ⁴ = H, acyl, alkyl, aryl	
046	hydroxylamine	N1O1H000		R ¹ = H, alkyl, aryl R ² = H, alkyl, aryl R ³ = H, alkyl, aryl	
047	amine	N1C00000		R ¹ = alkyl, aryl R ² = H, alkyl, aryl R ³ = H, alkyl, aryl	
048	prim. amine	N1C10000		R = alkyl, aryl	
049	prim. aliphatic amine	N1C1C000		R = alkyl	
050	prim. aromatic amine	N1C1A000		R = aryl	
051	sec. amine	N1C20000		R ¹ = alkyl, aryl R ² = alkyl, aryl	
052	sec. aliphatic amine	N1C2CC00		R ¹ = alkyl R ² = alkyl	
053	sec. mixed amine (aryl alkyl)	N1C2AC00		R ¹ = alkyl R ² = aryl	
054	sec. aromatic amine	N1C2AA00		R ¹ = aryl R ² = aryl	

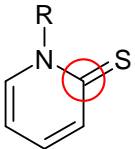
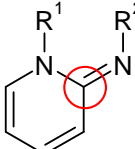
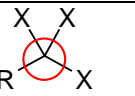
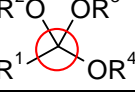
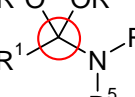
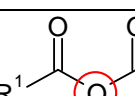
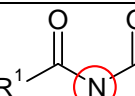
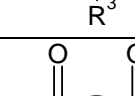
055	tert. amine	N1C30000		$R^1 = \text{alkyl, aryl}$ $R^2 = \text{alkyl, aryl}$ $R^3 = \text{alkyl, aryl}$		
056	tert. aliphatic amine	N1C3CC00		$R^1 = \text{alkyl}$ $R^2 = \text{alkyl}$ $R^3 = \text{alkyl}$		
057	tert. mixed amine	N1C3AC00		$R^1 = \text{alkyl}$ $R^2 = \text{aryl}$ $R^3 = \text{alkyl, aryl}$		
058	tert. aromatic amine	N1C3AA00		$R^1 = \text{aryl}$ $R^2 = \text{aryl}$ $R^3 = \text{aryl}$		
059	quaternary ammonium salt	N1C400T2		$R^1 = \text{alkyl, aryl}$ $R^2 = \text{alkyl, aryl}$ $R^3 = \text{alkyl, aryl}$ $R^4 = \text{alkyl, aryl}$		
060	N-oxide	N0O10000		$R^1 = \text{alkyl, aryl}$ $R^2 = \text{alkyl, aryl}$ $R^3 = \text{alkyl, aryl}$		the N-O bond may be formulated as a double bond
061	halogen deriv.	XX000000		$X = \text{F, Cl, Br, I}$ $R = \text{alkyl, alkenyl, aryl}$		
062	alkyl halide	XX00C000		$X = \text{F, Cl, Br, I}$ $R = \text{alkyl}$		
063	alkyl fluoride	XF00C000		$R = \text{alkyl}$		
064	alkyl chloride	XC00C000		$R = \text{alkyl}$		
065	alkyl bromide	XB00C000		$R = \text{alkyl}$		
066	alkyl iodide	XI00C000		$R = \text{alkyl}$		
067	aryl halide	XX00A000		$X = \text{F, Cl, Br, I}$ $R = \text{aryl}$		

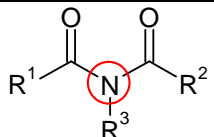
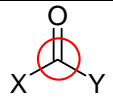
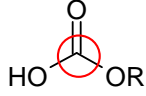
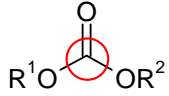
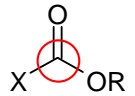
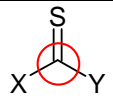
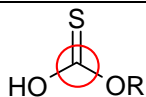
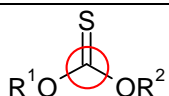
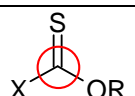
068	aryl fluoride	XF00A000	$R-\text{F}$ R = aryl	
069	aryl chloride	XC00A000	$R-\text{Cl}$ R = aryl	
070	aryl bromide	XB00A000	$R-\text{Br}$ R = aryl	
071	aryl iodide	XI00A000	$R-\text{I}$ R = aryl	
072	organometallic compound	000000MX	$R-\text{M}$ M = any metal R = alkyl, aryl	
073	organolithium compound	000000ML	$R-\text{Li}$ R = alkyl, aryl	
074	organomagnesium compound	000000MM	$R-\text{Mg}$ R = alkyl, aryl	
075	carboxylic acid deriv.	C3O20000	 R = H, alkyl, aryl X = any hetero atom	
076	carboxylic acid	C3O2H000	 R = H, alkyl, aryl	
077	carboxylic acid salt	C3O200T1	 R = H, alkyl, aryl	
078	carboxylic acid ester	C3O2C000	 R ¹ = H, alkyl, aryl R ² = alkyl, aryl	
079	lactone	C3O2CZ00		a cyclic ester (any ring size)
080	carboxylic acid amide	C3ONC000	 R ¹ = H, alkyl, aryl R ² = H, alkyl, aryl R ³ = H, alkyl, aryl	

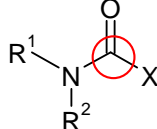
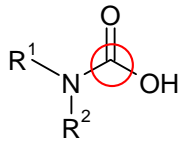
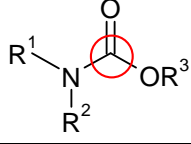
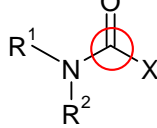
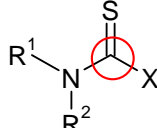
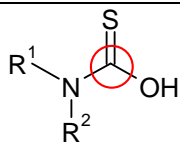
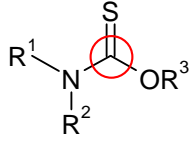
081	carboxylic acid prim. amide	C3ONC100	 $R = \text{H, alkyl, aryl}$	
082	carboxylic acid sec. amide	C3ONC200	 $R^1 = \text{H, alkyl, aryl}$ $R^2 = \text{alkyl, aryl}$	
083	carboxylic acid tert. amide	C3ONC300	 $R^1 = \text{H, alkyl, aryl}$ $R^2 = \text{alkyl, aryl}$ $R^3 = \text{alkyl, aryl}$	
084	lactam	C3ONCZ00	 $R = \text{H, alkyl, aryl}$	a cyclic amide (any ring size)
085	carboxylic acid hydrazide	C3ONN100	 $R^1 = \text{H, alkyl, aryl}$ $R^2 = \text{H, alkyl, aryl}$ $R^3 = \text{H, alkyl, aryl}$ $R^4 = \text{H, alkyl, aryl}$	
086	carboxylic acid azide	C3ONN200	 $R = \text{H, alkyl, aryl}$	
087	hydroxamic acid	C3ONOH00	 $R = \text{H, alkyl, aryl}$	
088	carboxylic acid amidine	C3N2H000	 $R^1 = \text{H, alkyl, aryl}$ $R^2 = \text{H, alkyl, aryl}$ $R^3 = \text{H, alkyl, aryl}$ $R^4 = \text{H, alkyl, aryl}$	

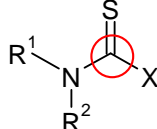
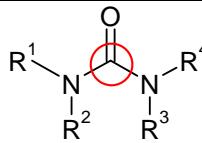
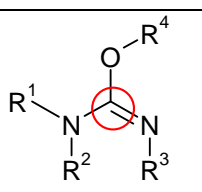
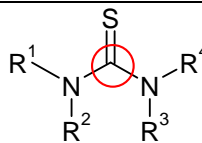
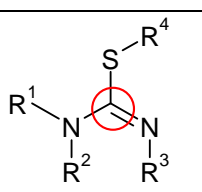
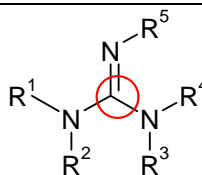
089	carboxylic acid amidrazone	C3NNN100	 <p> $R^1 = \text{H, alkyl, aryl}$ $R^2 = \text{H, alkyl, aryl}$ $R^3 = \text{H, alkyl, aryl}$ $R^4 = \text{H, alkyl, aryl}$ $R^5 = \text{H, alkyl, aryl}$ </p>	
090	nitrile	C3N00000	 <p>$R = \text{H, alkyl, aryl}$</p>	
091	acyl halide	C3OXX000	 <p> $R = \text{H, alkyl, aryl}$ $X = \text{F, Cl, Br, I}$ </p>	
092	acyl fluoride	C3OXF000	 <p>$R = \text{H, alkyl, aryl}$</p>	
093	acyl chloride	C3OXC000	 <p>$R = \text{H, alkyl, aryl}$</p>	
094	acyl bromide	C3OXB000	 <p>$R = \text{H, alkyl, aryl}$</p>	
095	acyl iodide	C3OXI000	 <p>$R = \text{H, alkyl, aryl}$</p>	
096	acyl cyanide	C2OC3N00	 <p>$R = \text{H, alkyl, aryl}$</p>	
097	imido ester	C3NOC000	 <p> $R^1 = \text{H, alkyl, aryl}$ $R^2 = \text{alkyl, aryl}$ $R^3 = \text{H, alkyl, aryl}$ </p>	
098	imidoyl halide	C3NXX000	 <p> $R^1 = \text{H, alkyl, aryl}$ $R^2 = \text{H, alkyl, aryl}$ $X = \text{F, Cl, Br, I}$ </p>	

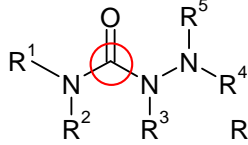
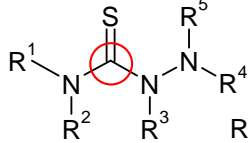
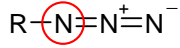
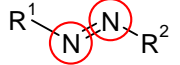

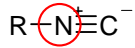
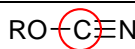
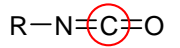
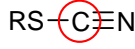
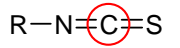
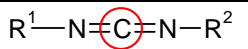
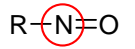
099	thiocarboxylic acid deriv.	C3SO0000	 <p>R = H, alkyl, aryl X = any hetero atom</p>	
100	thiocarboxylic acid	C3SOH000	 <p>R = H, alkyl, aryl X = OH, SH</p>	
101	thiocarboxylic acid ester	C3SOC000	 <p>R¹ = H, alkyl, aryl R² = alkyl, aryl X = O, S</p>	
102	thiolactone	C3SOCZ00	 <p>X = O, S</p>	a cyclic thioester (any ring size)
103	thiocarboxylic acid amide	C3SNH000	 <p>R¹ = H, alkyl, aryl R² = H, alkyl, aryl R³ = H, alkyl, aryl</p>	
104	thiolactam	C3SNCZ00	 <p>R = H, alkyl, aryl</p>	
105	imidothioester	C3NSC000	 <p>R¹ = H, alkyl, aryl R² = alkyl, aryl R³ = H, alkyl, aryl</p>	
106	oxohetarene	C3ONAZ00	 <p>R = H, alkyl, aryl</p>	any (hetero)aromatic compound with a C=O structure

107	thioxohetarene	C3SNAZ00	 <p>R = H, alkyl, aryl</p>	any (hetero)aromatic compound with a C=S structure
108	iminohetarene	C3NNAZ00	 <p>R¹ = H, alkyl, aryl R² = H, alkyl, aryl</p>	
109	orthocarboxylic acid deriv.	C3O30000	 <p>R = H, alkyl, aryl X = OH, alkoxy, aryloxy, (substituted) amino, etc.</p>	
110	carboxylic acid orthoester	C3O3C000	 <p>R¹ = H, alkyl, aryl R², R³, R⁴ = alkyl, aryl</p>	
111	carboxylic acid amide acetal	C3O3NC00	 <p>R¹ = H, alkyl, aryl R², R³ = alkyl, aryl R⁴, R⁵ = H, alkyl, aryl</p>	
112	carboxylic acid anhydride	C3O2C3O2	 <p>R¹, R² = H, alkyl, aryl</p>	
113	carboxylic acid imide	C3ONC000	 <p>R¹, R² = H, alkyl, aryl R³ = H, alkyl, aryl, ...</p>	
114	carboxylic acid unsubst. imide	C3ONCH10	 <p>R¹, R² = H, alkyl, aryl</p>	

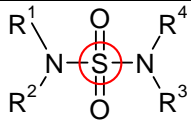
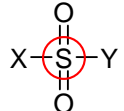
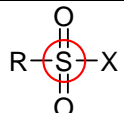
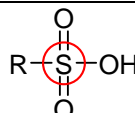
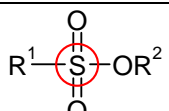
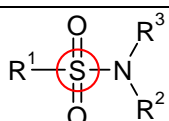
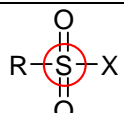
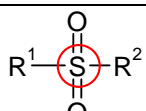
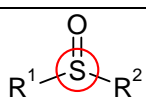
115	carboxylic acid subst. imide	C3ONCC10	 <p>R¹, R² = H, alkyl, aryl R³ = anything but H</p>	
116	CO ₂ deriv. (general)	C4000000	any carbon with 4 valences to hetero atoms (a double bond counts as 2 valences, a triple bond as 3 valences)	
117	carbonic acid deriv.	C4O30000	 <p>X, Y = any hetero atom</p>	output only if none of the more specific types apply
118	carbonic acid monoester	C4O3C100	 <p>R = alkyl, aryl</p>	
119	carbonic acid diester	C4O3C200	 <p>R¹, R² = alkyl, aryl</p>	
120	carbonic acid ester halide	C4O3CX00	 <p>R = alkyl, aryl X = F, Cl, Br, I</p>	
121	thiocarbonic acid deriv.	C4SO0000	 <p>X, Y = any hetero atom</p>	
122	thiocarbonic acid monoester	C4SOC100	 <p>R = alkyl, aryl</p>	S may be in any other position (replacing O)
123	thiocarbonic acid diester	C4SOC200	 <p>R¹, R² = alkyl, aryl</p>	S may be in any other position (replacing O)
124	thiocarbonic acid ester halide	C4SOX_00	 <p>R = alkyl, aryl X = F, Cl, Br, I</p>	

125	carbamic acid deriv	C4O2N000		$R^1, R^2 = \text{H, alkyl, aryl}$ $X = \text{OH, alkoxy, aryloxy, halogen}$	
126	carbamic acid	C4O2NH00		$R^1, R^2 = \text{H, alkyl, aryl}$	
127	carbamic acid ester (urethane)	C4O2NC00		$R^1, R^2 = \text{H, alkyl, aryl}$ $R^3 = \text{alkyl, aryl}$	
128	carbamic acid halide	C4O2NX00		$R^1, R^2 = \text{H, alkyl, aryl}$ $X = \text{F, Cl, Br, I}$	
129	thiocarbamic acid deriv.	C4SN0000		$R^1, R^2 = \text{H, alkyl, aryl}$ $X = \text{OH, alkoxy, aryloxy, halogen}$	
130	thiocarbamic acid	C4SNOH00		$R^1, R^2 = \text{H, alkyl, aryl}$	also possible: SH instead of OH
131	thiocarbamic acid ester	C4SNOC00		$R^1, R^2 = \text{H, alkyl, aryl}$ $R^3 = \text{alkyl, aryl}$	

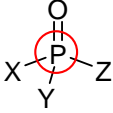
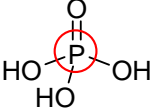
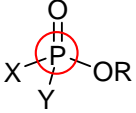
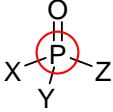
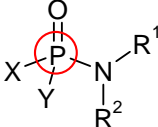
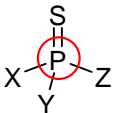
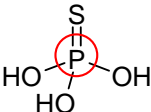
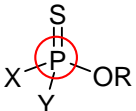
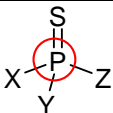
132	thiocarbamic acid halide	C4SNXX00	 <p>R¹, R² = H, alkyl, aryl X = F, Cl, Br, I</p>	
133	urea	C4O1N200	 <p>R¹, R², R³, R⁴ = H, alkyl, aryl</p>	
134	isourea	C4N2O100	 <p>R¹, R², R³, R⁴ = H, alkyl, aryl</p>	
135	thiourea	C4S1N200	 <p>R¹, R², R³, R⁴ = H, alkyl, aryl</p>	
136	isothiurea	C4N2S100	 <p>R¹, R², R³, R⁴ = H, alkyl, aryl</p>	
137	guanidine	C4N30000	 <p>R¹, R², R³, R⁴, R⁵ = H, alkyl, aryl</p>	

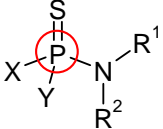
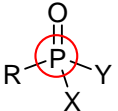
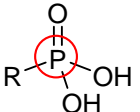
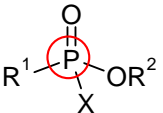
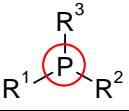
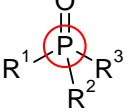
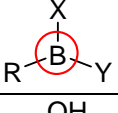
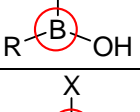
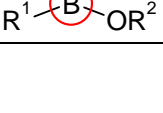
138	semicarbazide	C4ON2N00	 $R^1-N(R^2)-C(=O)-N(R^3)-N(R^4)-R^5$ <p>$R^1, R^2, R^3, R^4, R^5 = H, \text{ alkyl, aryl}$</p>	
139	thiosemicarbazide	C4SN2N00	 $R^1-N(R^2)-C(=S)-N(R^3)-N(R^4)-R^5$ <p>$R^1, R^2, R^3, R^4, R^5 = H, \text{ alkyl, aryl}$</p>	
140	azide	N4N20000	 $R-N=N^+=N^-$ <p>$R = \text{ alkyl, aryl}$</p>	
141	azo compound	N2N10000	 $R^1-N^+=N-R^2$ <p>$R^1, R^2 = \text{ alkyl, aryl}$</p>	
142	diazonium salt	N3N100T2	 $R-N^+=N^+$ <p>$R = \text{ alkyl, aryl}$</p>	
143	isonitrile	N3C10000	 $R-N=C^-$ <p>$R = \text{ alkyl, aryl}$</p>	
144	cyanate	C4NO1000	 $RO-C\equiv N$ <p>$R = \text{ alkyl, aryl}$</p>	
145	isocyanate	C4NO2000	 $R-N=C=O$ <p>$R = \text{ alkyl, aryl}$</p>	
146	thiocyanate	C4NS1000	 $RS-C\equiv N$ <p>$R = \text{ alkyl, aryl}$</p>	
147	isothiocyanate	C4NS2000	 $R-N=C=S$ <p>$R = \text{ alkyl, aryl}$</p>	
148	carbodiimide	C4N20000	 $R^1-N=C=N-R^2$ <p>$R^1, R^2 = H, \text{ alkyl, aryl}$</p>	
149	nitroso compound	N2O10000	 $R-N=O$ <p>$R = \text{ alkyl, aryl}$</p>	

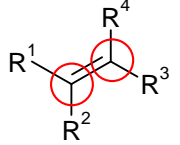
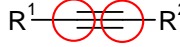
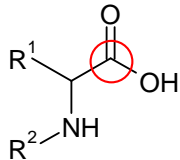
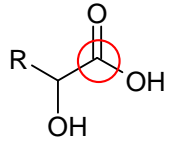
150	nitro compound	N4O20000	$\text{R}-\overset{\text{O}}{\underset{\text{O}}{\text{N}}}$	R = alkyl, aryl	
151	nitrite	N3O20000	$\text{RO}-\overset{\text{O}}{\text{N}}$	R = alkyl, aryl	
152	nitrate	N4O30000	$\text{RO}-\overset{\text{O}}{\underset{\text{O}}{\text{N}}}$	R = alkyl, aryl	
153	sulfuric acid deriv.	S6O00000	$\text{X}-\overset{\text{O}}{\underset{\text{O}}{\text{S}}}-\text{Y}$	X, Y = any hetero atom	for query purposes only
154	sulfuric acid	S6O4H000	$\text{HO}-\overset{\text{O}}{\underset{\text{O}}{\text{S}}}-\text{OH}$		
155	sulfuric acid monoester	S6O4HC00	$\text{RO}-\overset{\text{O}}{\underset{\text{O}}{\text{S}}}-\text{OH}$	R = alkyl, aryl	
156	sulfuric acid diester	S6O4CC00	$\text{R}^1\text{O}-\overset{\text{O}}{\underset{\text{O}}{\text{S}}}-\text{OR}^2$	R ¹ , R ² = alkyl, aryl	
157	sulfuric acid amide ester	S6O3NC00	$\text{R}^1\text{O}-\overset{\text{O}}{\underset{\text{O}}{\text{S}}}-\text{N}\begin{matrix} \text{R}^3 \\ \text{R}^2 \end{matrix}$	R ¹ = alkyl, aryl R ² , R ³ = H, alkyl, aryl	
158	sulfuric acid amide	S6O3N100	$\text{HO}-\overset{\text{O}}{\underset{\text{O}}{\text{S}}}-\text{N}\begin{matrix} \text{R}^2 \\ \text{R}^1 \end{matrix}$	R ¹ , R ² = H, alkyl, aryl	

159	sulfuric acid diamide	S6O2N200	 $\begin{array}{c} R^1 \quad O \quad R^4 \\ \diagdown \quad \quad / \\ N \quad S \quad N \\ / \quad \backslash \quad \backslash \\ R^2 \quad O \quad R^3 \end{array}$ <p>R¹, R², R³, R⁴ = H, alkyl, aryl</p>	
160	sulfuryl halide	S6O3XX00	 $\begin{array}{c} O \\ \\ X-S-Y \\ \\ O \end{array}$ <p>X = F, Cl, Br, I Y = any hetero atom</p>	
161	sulfonic acid deriv.	S5O00000	 $\begin{array}{c} O \\ \\ R-S-X \\ \\ O \end{array}$ <p>R = alkyl, aryl X = any hetero atom</p>	for query purposes only
162	sulfonic acid	S5O3H000	 $\begin{array}{c} O \\ \\ R-S-OH \\ \\ O \end{array}$ <p>R = alkyl, aryl</p>	
163	sulfonic acid ester	S5O3C000	 $\begin{array}{c} O \\ \\ R^1-S-OR^2 \\ \\ O \end{array}$ <p>R¹, R² = alkyl, aryl</p>	
164	sulfonamide	S5O2N000	 $\begin{array}{c} O \\ \\ R^1-S-N \\ \quad \diagup \quad \diagdown \\ O \quad R^2 \quad R^3 \end{array}$ <p>R¹ = alkyl, aryl R², R³ = H, alkyl, aryl</p>	
165	sulfonyl halide	S5O2XX00	 $\begin{array}{c} O \\ \\ R-S-X \\ \\ O \end{array}$ <p>R = alkyl, aryl X = F, Cl, Br, I</p>	
166	sulfone	S4O20000	 $\begin{array}{c} O \\ \\ R^1-S-R^2 \\ \\ O \end{array}$ <p>R¹, R² = alkyl, aryl</p>	
167	sulfoxide	S2O10000	 $\begin{array}{c} O \\ \\ R^1-S-R^2 \end{array}$ <p>R¹, R² = alkyl, aryl</p>	

168	sulfinic acid deriv.	S3O00000	$\begin{array}{c} \text{O} \\ \parallel \\ \text{R}-\text{S}-\text{X} \end{array}$ R = alkyl, aryl X = any hetero atom	for query purposes only
169	sulfinic acid	S3O2H000	$\begin{array}{c} \text{O} \\ \parallel \\ \text{R}-\text{S}-\text{OH} \end{array}$ R = alkyl, aryl	
170	sulfinic acid ester	S3O2C000	$\begin{array}{c} \text{O} \\ \parallel \\ \text{R}^1-\text{S}-\text{OR}^2 \end{array}$ R ¹ , R ² = alkyl, aryl	
171	sulfinic acid halide	S3O1XX00	$\begin{array}{c} \text{O} \\ \parallel \\ \text{R}-\text{S}-\text{X} \end{array}$ R = alkyl, aryl X = F, Cl, Br, I	
172	sulfinic acid amide	S3O1N000	$\begin{array}{c} \text{O} \\ \parallel \\ \text{R}^1-\text{S}-\text{N} \begin{array}{l} \nearrow \text{R}^3 \\ \downarrow \text{R}^2 \end{array} \end{array}$ R ¹ = alkyl, aryl R ² , R ³ = H, alkyl, aryl	
173	sulfenic acid deriv.	S1O00000	$\text{R}-\text{S}-\text{X}$ R = alkyl, aryl X = any hetero atom	for query purposes only
174	sulfenic acid	S1O1H000	$\text{R}-\text{S}-\text{OH}$ R = alkyl, aryl	
175	sulfenic acid ester	S1O1C000	$\text{R}^1-\text{S}-\text{OR}^2$ R ¹ , R ² = alkyl, aryl	
176	sulfenic acid halide	S1O0XX00	$\text{R}-\text{S}-\text{X}$ R = alkyl, aryl X = F, Cl, Br, I	
177	sulfenic acid amide	S1O0N100	$\text{R}^1-\text{S}-\text{N} \begin{array}{l} \nearrow \text{R}^3 \\ \downarrow \text{R}^2 \end{array}$ R ¹ = alkyl, aryl R ² , R ³ = H, alkyl, aryl	
178	thiol	S1H10000	$\text{R}-\text{SH}$ R = alkyl, aryl	
179	alkylthiol	S1H1C000	$\text{R}-\text{SH}$ R = alkyl	
180	arylthiol	S1H1A000	$\text{R}-\text{SH}$ R = aryl	

181	phosphoric acid deriv.	P5O0H000		X, Y, Z = O, N, Hal residue	for query purposes only
182	phosphoric acid	P5O4H200			
183	phosphoric acid ester	P5O4HC00		R = alkyl, aryl X, Y = any O, N, Hal residue	
184	phosphoric acid halide	P5O3HX00		X = F, Cl, Br, I Y, Z = any O, N, Hal residue	
185	phosphoric acid amide	P5O3HN00		R ¹ , R ² = H, alkyl, aryl X, Y = any O, N, Hal residue	
186	thiophosphoric acid deriv.	P5O0S000		X, Y, Z = any O, N, Hal residue	for query purposes only
187	thiophosphoric acid	P5O3SH00			
188	thiophosphoric acid ester	P5O3SC00		R = alkyl, aryl X, Y = any O, N, Hal residue	
189	thiophosphoric acid halide	P5O2SX00		X = F, Cl, Br, I Y, Z = any O, N, Hal residue	

190	thiophosphoric acid amide	P5O2SN00	 <p>R¹, R² = H, alkyl, aryl X, Y = any O, N, Hal residue</p>	
191	phosphonic acid deriv.	P4O30000	 <p>R = alkyl, aryl X, Y = any O, N, Hal residue</p>	
192	phosphonic acid	P4O3H000	 <p>R = alkyl, aryl</p>	
193	phosphonic acid ester	P4O3C000	 <p>R¹, R² = alkyl, aryl X = any O, N, Hal residue</p>	
194	phosphine	P3000000	 <p>R¹, R², R³ = alkyl, aryl</p>	
195	phosphin oxide	P2O00000	 <p>R¹, R², R³ = alkyl, aryl</p>	
196	boronic acid deriv.	B2O20000	 <p>R = alkyl, aryl X, Y = any O, N, Hal residue</p>	
197	boronic acid	B2O2H000	 <p>R = alkyl, aryl</p>	
198	boronic acid ester	B2O2C000	 <p>R¹, R² = alkyl, aryl X = any O, N, Hal residue</p>	

199	alkene	000C2C00	 $R^1, R^2, R^3, R^4 = \text{H, alkyl, aryl}$	
200	alkyne	000C3C00	 $R^1, R^2 = \text{H, alkyl, aryl}$	
201	aromatic compound	0000A000	any aromatic carbocyclic or heterocyclic structure, including cyclopentadienyl anion, tropylium cation, fulvene, tropone, pyridone-type lactams, etc.	criteria: conjugated system, Hückel's rule must apply ($4n + 2$ pi electrons); planar geometry is not checked
202	heterocyclic compound	0000CZ00	any cyclic structure with at least one non-carbon atom incorporated	starting with v0.3b, metal atoms are not accepted as ring members, unless option -M is used
203	alpha-aminoacid	C3O2HN1C	 $R^1, R^2 = \text{H, alkyl, aryl}$	
204	alpha-hydroxyacid	C3O2HO1H	 $R = \text{H, alkyl, aryl}$	