

Name	SMART
phenol	<chem>[cR1]1[cR1][cR1][cR1][cR1][cR1]1O[H]</chem>
phenoxy	<chem>[cR1]1[cR1][cR1][cR1][cR1][cR1]1[OH0;!R]</chem>
COOH	<chem>C(=O)O[H]</chem>
COOH (aromatic)	<chem>[\$(C(a)(=O)O[H])](=O)O[H]</chem>
COOH (aliphatic)	<chem>[\$(C(C)(=O)O[H])](=O)O[H]</chem>
CH3O (aliphatic)	<chem>[\$([OX2]([CH3])[CX4])]C([H])([H])[H]</chem>
CH3O (aromatic)	<chem>[\$([OX2]([CH3])a)C([H])([H])[H]</chem>
NH2	<chem>[\$([NH2X3][CX4,a])([H])[H]</chem>
nitrile	<chem>[CX4]#[NX3]</chem>
NO2	<chem>[\$([#7X3](~[#8X1])([!#8])(~[#8X1]))(~[#8X1])(~[#8X1])]</chem>
nitrosamine	<chem>[\$([#7X2](-N)=O)=O</chem>
epoxyde	<chem>[#8R1]1~[#6R1]~[#6R1]1</chem>
aziridine	<chem>[#7R1]1~[#6R1]~[#6R1]1</chem>
furan	<chem>[oX2R1]1[cX3R1][cX3R1][cX3R1][cX3R1]1</chem>
pyrrole	<chem>[nX3R1]1[cX3R1][cX3R1][cX3R1][cX3R1]1</chem>
thiophen	<chem>[sX2R1]1[cX3R1][cX3R1][cX3R1][cX3R1]1</chem>
diazole13	<chem>[nX3R1]1[cX3R1][nX2R1][cX3R1][cX3R1]1</chem>
thiazole13	<chem>[sX2R1]1[cX3R1][nX2R1][cX3R1][cX3R1]1</chem>
triazole124	<chem>[nR1]1[cX3R1][nR1][cX3R1][nR1]1</chem>
tetrazole	<chem>[nR1]1[cX3R1][nR1][nR1][nR1]1</chem>
oxazole13	<chem>[oX2R1]1[cX3R1][nX2R1][cX3R1][cX3R1]1</chem>
pyridine	<chem>[nX2R1]1[cX3R1][cX3R1][cX3R1][cX3R1][cX3R1]1</chem>
pyrimidine	<chem>[nX2R1]1[cX3R1][nX2R1][cX3R1][cX3R1][cX3R1]1</chem>
morpholine	<chem>[NR1X3]1[CX4R1][CX4R1][OX2R1][CX4R1][CX4R1]1</chem>
piperazine	<chem>[NR1X3]1[CX4R1][CX4R1][NX3R1][CX4R1][CX4R1]1</chem>
piperidine	<chem>[NR1X3]1[CX4R1][CX4R1][CX4R1][CX4R1][CX4R1]1</chem>
F (aliphatic)	<chem>[\$(F[CX4])]</chem>
F (aromatic)	<chem>[\$(Fa)]</chem>
Cl (aliphatic)	<chem>[\$(Cl[CX4])]</chem>
Cl (aromatic)	<chem>[\$(Cla)]</chem>
Br (aliphatic)	<chem>[\$(Br[CX4])]</chem>
Br (aromatic)	<chem>[\$(Bra)]</chem>
I (aliphatic)	<chem>[\$(I[CX4])]</chem>
I (aromatic)	<chem>[\$(Ia)]</chem>
Hal (aliphatic)	<chem>[\$([F,Cl,Br,I][CX4])]</chem>
Hal (aromatic)	<chem>[\$([F,Cl,Br,I]a)]</chem>
SO2NH	<chem>[\$([SX4]([C,a])(=[OX1])(=[OX1])[NH][#6]))(=[OX1])(=[OX1])[NH][H]</chem>
OH (aromatic)	<chem>[\$([OH1]a)][H]</chem>
hexachlorononbornene	<chem>[CH1]1[CH1]C2(Cl)C(Cl)=C(Cl)C1(Cl)C2(Cl)Cl</chem>
cyano-(3-phenoxyphenyl)methoxy	<chem>[H]c1c([H])c([H])c(Oc2c([H])c([H])c([H])c(c2[H])C([H])(O)C#N)c([H])c1[H]</chem>
bis(4-chlorophenyl)methyl	<chem>[H]c1c([H])c(c([H])c([H])c1Cl)C([H])c1c([H])c([H])c(Cl)c([H])c1[H]</chem>
2-(2,4-dichlorophenoxy)acetyl	<chem>[cH]1[cH]c(O[CH2][CX3]=O)c(Cl)[cH]c1Cl</chem>
dinitrophenoxy	<chem>c1cc(O)c([#7X3](~[#8X1])(~[#8X1]))cc1([#7X3](~[#8X1])(~[#8X1]))</chem>
2-trifluoromethylbenzimidazole	<chem>[H]n1c(nc2ccccc12)C(F)(F)F</chem>
2-fluoroacetyl	<chem>F[CH2][CX3]=O</chem>
phosphoryl	<chem>[PX4H0](=O)([OH0])([OH0])[OH0]</chem>

phosphorothionate	<chem>[\$(([OH0]P(=S)([OH0])[OH0]))P(=S)([OH0])[OH0]</chem>
phosphorodithionate	<chem>[\$([SX2H0]P(=S)([OH0])[OH0]))P(=S)([OH0])[OH0]</chem>
dibenzo-1,4-dioxin	<chem>[F,Cl,Br,I,#1]-c1c(-[F,Cl,Br,I,#1])c(-[F,Cl,Br,I,#1])c2[#8]c3c(-[F,Cl,Br,I,#1])c(-[F,Cl,Br,I,#1])c(-[F,Cl,Br,I,#1])c(-[F,Cl,Br,I,#1])c3[#8]c2c1-[F,Cl,Br,I,#1]</chem>
4-hydroxycoumarin	<chem>[OH1]C1=CC(=O)Oc2[cH][cH][cH]c12</chem>
1,3-indandione	<chem>C1C(=O)c2ccccc2C1=O</chem>
thiourea	<chem>[NX3;!R][CX3;!R](=[SX1])[NX3;!R]</chem>
1-carbox imidoylpiperazine	<chem>[NR1X3]1[CX4R1][CX4R1][NX3R1]([CX3]=[NX2])[CX4R1][CX4R1]1</chem>
phenylpiperazine	<chem>[NR1X3]1[CX4R1][CX4R1][NX3R1](c2ccccc2)[CX4R1][CX4R1]1</chem>
carbamate	<chem>\$(N([!H])C(=O)[OH0])C(=O)[OH0]</chem>
O-(methylamino carbonyl)oxime	<chem>[CX4]NC(=O)ON=C</chem>
4-phenylpiperidine	<chem>[NR1X3]1[CX4R1][CX4R1][CX4R1](c2ccccc2)[CX4R1][CX4R1]1</chem>
4-phenyl aminopiperidine	<chem>[NR1X3]1[CX4R1][CX4R1][CX4R1]([NX3]c2ccccc2)[CX4R1][CX4R1]1</chem>
O,O-diethyl phosphorodithionate	<chem>CCOP(=S)(OCC)SC([*:1])</chem>
O-phenyl phenylphosphonothion ate	<chem>S=P(O([*:1]))(Oc1ccc([*:1])cc1)c1ccccc1</chem>
O-phenyl phosphonothionate	<chem>S=P(O([*:1]))(O([*:1]))Oc1ccc([*:1])cc1</chem>
O,O-diethyl phosphorothionate	<chem>CCOP(=S)(O([*:1]))OCC</chem>
O,O-dimethyl phosphoryl	<chem>COP(=O)(O([*:1]))OC</chem>
2,2-dimethyl-2,3- dihydro-1-benzofuran- 7-yl N-(aminosulfanyl)- N-methylcarbamate	<chem>CN(SN([*:1])([*:1]))C(=O)Oc1cccc2CC(C)(C)Oc12</chem>
phenyl carbamate	<chem>O=C(N([*:1]))Oc1ccccc([*:1])1</chem>
methyl(propoxy sulfanyl) carbamate	<chem>CN(SOCCC([*:1]))C(=O)O([*:1])</chem>
dimethylcarbamate	<chem>CN(C)C(=O)O([*:1])</chem>
2,4-dichloro-benzene- 1,3-dicarbonitrile	<chem>N#Cc1c([*:1])c([*:1])c(Cl)c(C#N)c1Cl</chem>
cyclopentane	<chem>[#6]-1-[#6]-[#6]-[#6]-[#6]-1</chem>
1-benzofuran	<chem>c1cc2ccccc2o1</chem>
Phenothiazine	<chem>*-[#7]-1-c2ccccc2-[#16]-c2ccccc-12</chem>
1H-indole	<chem>c1cc2ccccc2n1</chem>
4,5-dihydro-3H-2,3- benzodiazepine	<chem>[#6]-1-[#6]-c2ccccc2-[#6]=[#7]-[#7]-1</chem>
Pyridazine	<chem>c1ccnnc1</chem>
Anthracyclines	<chem>[H][C@@]1([*:1])C[C@@](O)(Cc2c1c(O)c1c(C(=O)c3cccc(O([*:1]))c3C1=O)c2O)C([*:1])=O</chem>
Aconitine	<chem>[#6]-[#6]-[#7]-1-[#6]C2([#6]-[#8]-[#6])[#6]3-[#6](-[#8]-[#6])-[#6]4-[#6]-1C3([#6]-1-[#6]C3([#8])[#6](-[#8]-[#6])(=O)-[#6]-5=[#6]-[#6]=[#6]-[#6]=[#6]-5)-[#6]-1C4([#8]-[#6](-[#6])=O)[#6](-[#8])-[#6]3-[#8]-[#6])[#6](-[#6]-[#6]2-[#8])-[#8]-[#6]</chem>
2,4,6(1H,3H,5H)- pyrimidinetrione	<chem>*C1(*)[#6](=O)-[#7]-[#6](=O)-[#7]-[#6]1=O</chem>