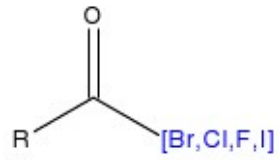
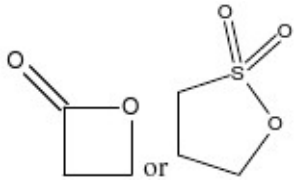
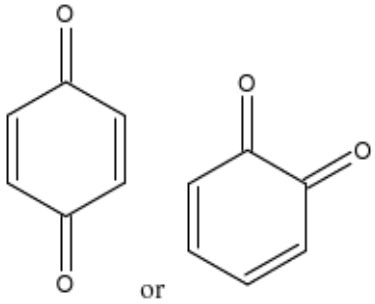
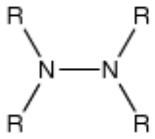
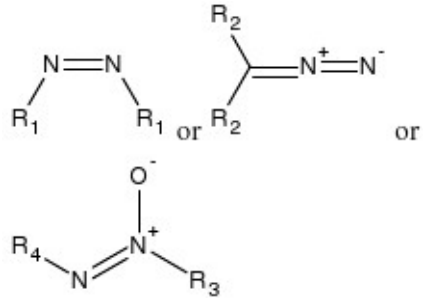
1st SAs RULESET	
Structural Alert	**SMARTS or details**
SA_1: Acyl halides  R = any atom/group, except OH, SH	`[!$([OH1,SH1])]C(=O)[Br,Cl,F,I]`

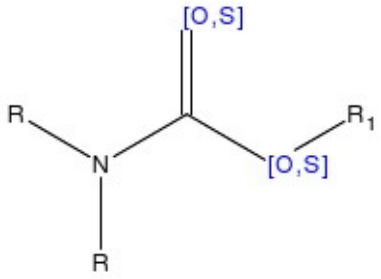
SA_6: Propiolactones or propiosultones
 
 	
	`[O,S]=C1[O,S]CC1`
	OR
	`O=S1(=O)(CCCO1)`

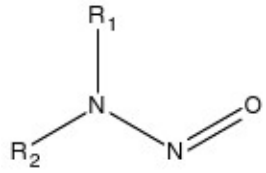
SA_12: Quinones
 
 	
R = any atom/group
	`O=[#6]1[#6]=,:[#6][#6](=O)[#6]=,:[#6]1`
	OR
	`O=[#6]1[#6]=,:[#6][#6]=,:[#6][#6]1(=O)`

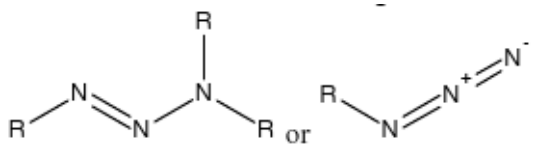
SA_13: Hydrazine
 
 	
	`[N+0]!@;-[N+0](=[!O;!N])`
	OR
	`[N+0]([#1,*])!@;-[N+0]([#1,*])`

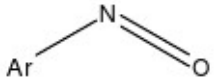
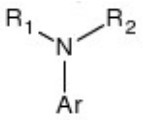
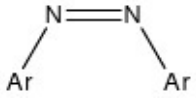
1st SAs RULESET	
Structural Alert	**SMARTS or details**

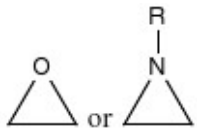
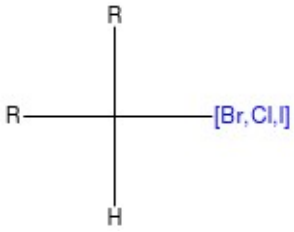
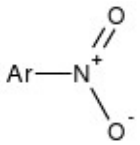
SA_14: Aliphatic azo and azoxy
 
R1= Aliphatic carbon or hydrogen
R2, R3 = Any atom/group
R4 = Aliphatic carbon
	`[C,#1]N=[NX2][C,#1]`
	OR
	`[$(C=[N+]=[N-]);!$(C=[N+]=[N-]=N);!$(C=[N+]=[N-]N)]`
	OR
	`C=[$(N=N);!$(N=N=N);!$(N=NN)]`
	OR
	`CN=NO`

SA_16: alkyl carbamate and thiocarbamate  R = Aliphatic carbon or hydrogen R1 = Aliphatic carbon	`[NX3]([CX4,#1])([CX4,#1])C(=[O,S])[O,S][CX4]`
SA_18: Polycyclic Aromatic Hydrocarbons	Three or more fused rings, not heteroaromatic

1st SAs RULESET	
Structural Alert	**SMARTS or details**
SA_21: alkyl and aryl N-nitroso groups  R1= Aliphatic or aromatic carbon, R2= Any atom/group	`[C,c]N[NX2;v3]=O`

SA_22: azide and triazene groups
 
R= Any atom/group
	`[N]=[N]-[N]`
	OR
	`[N]=[N]=[N]`

SA_25: aromatic nitroso group  Ar = Any aromatic/heteroaromatic ring	
SA_28bis: Aromatic mono- and dialkylamine  Ar = Any aromatic/heteroaromatic ring R1 = Hydrogen, methyl, ethyl R2 = Methyl, ethyl	• Chemicals with ortho-disubstitution, or with an ortho carboxylic acid substituent are excluded. • Chemicals with a sulfonic acid group (- SO3H) on the same ring of the amino group are excluded .
SA_29: Aromatic diazo  Ar = Any aromatic/heteroaromatic ring	• Chemicals with a sulfonic acid group (-SO3H) on both rings linked to the diazo group are excluded.

2nd SAs RULESET	
Structural Alert	**SMARTS or details**
SA_7:Epoxides and aziridines  R = any atom/group	`C1[O,N]C1`
SA_8: Aliphatic halogens  R = any atom/group	
SA_19: Heterocyclic Polycyclic Aromatic Hydrocarbons	Three or more fused rings, heteroaromatic
SA_27: Nitro-aromatic  Ar = Any aromatic/heteroaromatic ring	• Chemicals with ortho-disubstitution, or with an ortho carboxylic acid substituent are excluded. • Chemicals with a sulfonic acid group (-SO3H) on the same ring of the nitro group are excluded .