

[a;!\$(a[a[A;!#1;]H])(a[A;!#1;]H));!\$(aa[CX3](=O)[OX2H1]);!\$(aa[SX4](=[OX1])(=[OX1])([OX2H1]));!\$(aaa[SX4](=[OX1])(=[OX1])([OX 2H1]));!\$(aaaa[SX4](=[OX1])(=[OX1])([OX2H1]));!\$(aaaaa[SX4](=[OX1])(=[OX1])([OX2H1]));!\$(aaaaaa[SX4](=[OX1])(=[OX1])([OX2H 1])))([!\$([N+](([O-])=O))])	SA27_gen. Nitro aromatic,SA27 Nitro aromatic: Nitro aromatic. However: Aromatic nitro groups with ortho-disubstitution or with a carboxylic acid substituent in ortho position should be excluded. Please note that a molecule like this CC1=CC=CC(=C1[N+](=O)[O-])[N+](=O)[O-] should be included in the alert: one of the two nitro groups is ortho disubstituted, but the other one is ortho-monosubstituted. Also the following molecule CC2=CC=CC(CCC1=CC=CC(=C1)[N+](=O)[O-])=C2[N+](=O)[O-] Should fire the alert (one nitro group is ortho disubstituted, but the other is not). If a sulfonic acid group (-SO3H) is present on the ring that contains also the nitro group, the substance should be excluded
[a;!\$(a[a[A;!#1;])(a[A;!#1;]));!\$(aa[CX3](=O)[OX2H1]);!\$(aa[SX4](=[OX1])(=[OX1])([O]));!\$(aaa[SX4](=[OX1])(=[OX1])([O]));!\$(aaaa[X4](=[OX1])(=[OX1])([O]));!\$(aaaaa[SX4](=[OX1])(=[OX1])([O]));!\$(aaaaaa[SX4](=[OX1])(=[OX1])([O]))!@[!\$([N+O;H2;D1]),!\$([N+O;H1 ;D2][OH;D1]),!\$([N+O;H0;D3][OH;D1])C,!\$([N+O;H1;D2]OC=O),!\$([N+O;H0;D3](C)OC=O)]	SA28_gen. Primary aromatic amine, hydroxyl amine and its derived esters (with restrictions). SA28 Primary aromatic amine, hydroxyl amine and its derived esters (with restrictions): Primary aromatic amine, hydroxyl amine and its derived esters (with restrictions). However: Aromatic amino groups with ortho disubstitutions or with a carboxylic acid substituent in ortho position are excluded. If a sulfonic acid group (-SO3H) is present on the ring that contains also the amino group, the substance should be excluded from the alert. The following structures should also be included: O=C=NC1=CC=CC=C1 and C([H])([H])=NC1=CC=CC=C1. The possibility that the Nitrogen atom of hydroxyl amine is part of a cycle, should be excluded
aN=C=O	
aN=[CH2]	
aN=[CH2]	SA28_gen. Primary aromatic amine, hydroxyl amine and its derived esters (with restrictions). SA28 Primary aromatic amine, hydroxyl amine and its derived esters (with restrictions): Primary aromatic amine, hydroxyl amine and its derived esters (with restrictions). However: Aromatic amino groups with ortho disubstitutions or with a carboxylic acid substituent in ortho position are excluded. If a sulfonic acid group (-SO3H) is present on the ring that contains also the amino group, the substance should be excluded from the alert. The following structures should also be included: O=C=NC1=CC=CC=C1 and C([H])([H])=NC1=CC=CC=C1. The possibility that the Nitrogen atom of hydroxyl amine is part of a cycle, should be excluded
[a;!\$(a[a[A;!#1;])(a[A;!#1;]));!\$(aa[CX3](=O)[OX2H1]);!\$(aa[SX4](=[OX1])(=[OX1])([O]));!\$(aaa[SX4](=[OX1])(=[OX1])([O]));!\$(aaaa[X4](=[OX1])(=[OX1])([O]));!\$(aaaaa[SX4](=[OX1])(=[OX1])([O]));!\$(aaaaaa[SX4](=[OX1])(=[OX1])([O]))!@[!\$([NX3;v3]([#1,CH3])([CH 3])),!\$([NX3;v3]([#1,CH3])([CH2][CH3])),!\$([NX3;v3]([CH2][CH3])([CH2][CH3]))]	SA28bis_gen. Mono- or di- methyl or ethyl aromatic amines, are included. SA28bis Aromatic mono- and dialkylamine: Mono- or di- methyl or ethyl aromatic amines, are included. However:Aromatic amino groups with ortho-disubstitution or with a carboxylic acid substituent in ortho position should be excluded. If a sulfonic acid group (-SO3H) is present on the ring that contains also the amino group, the substance should be excluded from the alert
[a;!\$(a[a[A;!#1;])(a[A;!#1;]));!\$(aa[CX3](=O)[OX2H1]);!\$(aa[SX4](=[OX1])(=[OX1])([O]));!\$(aaa[SX4](=[OX1])(=[OX1])([O]));!\$(aaaa[X4](=[OX1])(=[OX1])([O]));!\$(aaaaa[SX4](=[OX1])(=[OX1])([O]));!\$(aaaaaa[SX4](=[OX1])(=[OX1])([O]))!@[!\$([NX3;v3]([#1,CH3])C(=O)([#1,CH3]))]	'SA28ter_gen. Aromatic N-acyl amine
a[N]=[N]a [!\$([N](a)=[N]a);!\$([N](a:aS(=[OD1])(=[OD1])[OD1])=[N]a:aS(=[OD 1])(=[OD1])[OD1]);!\$([N](a:aS(=[OD1])(=[OD1])[OD1])=[N]a:a:aS(=[OD1])(=[OD1])[OD1]);!\$([N](a:aS(=[OD1])(=[OD1])[OD1])=[N]a: a:a:aS(=[OD1])(=[OD1])[OD1]);!\$([N](a:aS(=[OD1])(=[OD1])[OD1] =[N]a:a:a:aS(=[OD1])(=[OD1])[OD1]);!\$([N](a:aS(=[OD1])(=[OD1] [OD1])=[N]a:a:a:a:aS(=[OD1])(=[OD1])[OD1]);!\$([N](a:aS(=[OD 1])(=[OD1])[OD1])=[N]a:a:a:a:a:aS(=[OD1])(=[OD1])[OD1]);!\$([N)a:a:aS(=[OD1])(=[OD1])[OD1])=[N]a:aS(=[OD1])(=[OD1])[OD1]);! [!\$([N](a:a:aS(=[OD1])(=[OD1])[OD1])=[N]a:a:aS(=[OD1])(=[OD1])[OD1]);!\$([N](a:a:aS(=[OD1])(=[OD1])[OD1])=[N]a:a:a:aS(=[OD1])(=[OD1])[OD1]);!\$([N](a:a:aS(=[OD1])(=[OD1])[OD1])=[N]a:a:a:a: S(=[OD1])(=[OD1])[OD1]);!\$([N](a:a:aS(=[OD1])(=[OD1])[OD1])=[N]a:a:a:a:aS(=[OD1])(=[OD1])[OD1]);!\$([N](a:a:aS(=[OD1])(=[O D1])[OD1])=[N]a:a:a:a:a:a:aS(=[OD1])(=[OD1])[OD1]);!\$([N](a:a: aS(=[OD1])(=[OD1])[OD1])=[N]a:aS(=[OD1])(=[OD1])[OD1]);!\$([N (a:a:aS(=[OD1])(=[OD1])[OD1])=[N]a:a:aS(=[OD1])(=[OD1])[OD1]);!\$([N](a:a:aS(=[OD1])(=[OD1])[OD1])=[N]a:a:a:aS(=[OD1])(= OD1])[OD1]);!\$([N](a:a:a:aS(=[OD1])(=[OD1])[OD1])=[N]a:a:a:a: S(=[OD1])(=[OD1])[OD1]);!\$([N](a:a:a:aS(=[OD1])(=[OD1])[OD1])= [N]a:a:a:a:aS(=[OD1])(=[OD1])[OD1]);!\$([N](a:a:a:aS(=[OD1])(=[OD1])[OD1])=[N]a:a:a:a:a:aS(=[OD1])(=[OD1])[OD1]);!\$([N](a:a: a:aS(=[OD1])(=[OD1])[OD1])=[N]a:aS(=[OD1])(=[OD1])[OD1]);!\$([N](a:a:a:aS(=[OD1])(=[OD1])[OD1])=[N]a:a:aS(=[OD1])(=[OD1])][OD1]);!\$([N](a:a:a:aS(=[OD1])(=[OD1])[OD1])=[N]a:a:a:aS(=[O D1])(=[OD1])[OD1]);!\$([N](a:a:a:aS(=[OD1])(=[OD1])[OD1])=[N] a:a:a:aS(=[OD1])(=[OD1])[OD1]);!\$([N](a:a:a:aS(=[OD1])(=[OD 1])[OD1])=[N]a:a:a:a:aS(=[OD1])(=[OD1])[OD1]);!\$([N](a:a:a:a	SA29_gen. Aromatic diazo
O=c1ccc2ccccc2(o1) O=C1C=Cc2ccccc2O1 C12CCCCN1CC=C2 c1ccccc1C[C;IR]=C C[C@]12CCC3c4c(CCC3C1CC[C@H]2O)cc(O)cc4 [!a,#1;!\$(C1(=O)C=CC(=O)C=C1)][#6]([!a,#1;!\$(C1(=O)C=CC(=O)C =C1))];;=#6][#6](=O)!O;!\$([#6]1;=#6)[#6](=O)[#6];=#6][#6](= O)1]]	SA30_gen. Coumarins and Furocoumarins
	SA37_gen. Genotoxic mechanism. Pyrrolizidine Alkaloids
	SA38_gen. Genotoxic mechanism. Alkenylbenzenes: Alkenylbenzenes
	SA39_gen_and_nogen. Mixed genotoxic and non genotoxic mechanism. Steroidal estrogens: Steroidal estrogens
[!\$([#6]);!\$([#6]1C(=O)[#6];=#6]C(=O)[#6];=1;!\$([#6]C!;- [C;R]!;-[C;R]!;-[C;R]!;-[C;R]!;-[C;R]!;-[C;R]!;-[C;R]!;-[C;R]! [C;R])!;;=[!\$([#6]);!\$(C=C[a])][!\$([#6]);!\$([#6]- O)];!\$(C1(=O)[#6];=#6]C(=O)[#6];=#6]1))=(O) [#7X3][#6](=[SX1])[!\$([O,S][CX4])!\$([OH,SH])!\$([O,-S-])]	SA10_gen. ?,? unsaturated carbonyls
	SA17_nogen. Thiocarbonyl (Nongenotoxic carcinogens)

<div>[c;!\$(c[N+](=O)[O]);!\$(c[N]([#1,C])([#1,C]));!\$(cN([OX2H])([#1,C])) ;!\$(cN([#1,C])OC=O);!\$(c[NX3v3]([#1,CH3])([#1,CH3]));!\$(c[NX3v 3]([#1,CH3])([CH2][CH3]));!\$(c[NX3v3]([CH2][CH3])([CH2][CH3])); !\$(cNC(=O)[#1,CH3]);!\$(cN=[N]a);!\$(c!@[cR1r6]1cccc1);!\$(c!@* !@c1cccc1);!\$([R2])]1[c;!\$(c[N+](=O)[O]);!\$(c[N]([#1,C])([#1,C])); !\$(cN([OX2H])([#1,C]));!\$(cN([#1,C])OC=O);!\$(c[NX3v3]([#1,CH3]) ([#1,CH3]));!\$(c[NX3v3]([#1,CH3])([CH2][CH3]));!\$(c[NX3v3]([CH 2][CH3])([CH2][CH3]));!\$(cNC(=O)[#1,CH3]);!\$(cN=[N]a);!\$(c!@[c R1r6]1cccc1);!\$(c!@*!@c1cccc1);!\$([R2])]1[c;!\$(c[N+](=O)[O]);! \$(c[N]([#1,C])([#1,C]));!\$(cN([OX2H])([#1,C]));!\$(cN([#1,C])OC=O);!\$(c[NX3v3]([#1,CH3])([#1,CH3]));!\$(c[NX3v3]([#1,CH3])([CH2][C H3]));!\$(c[NX3v3]([CH2][CH3])([CH2][CH3]));!\$(cNC(=O)[#1,CH3]) ;!\$(cN=[N]a);!\$(c!@[cR1r6]1cccc1);!\$(c!@*!@c1cccc1);!\$([R2])]1[c;!\$(c[N+](=O)[O]);!\$(c[N]([#1,C])([#1,C]));!\$(cN([OX2H])([#1,C]));!\$(cN([#1,C])OC=O);!\$(c[NX3v3]([#1,CH3])([#1,CH3]));!\$(c[NX3v 3]([#1,CH3])([CH2][CH3]));!\$(c[NX3v3]([CH2][CH3])([CH2][CH3])); !\$(cNC(=O)[#1,CH3]);!\$(cN=[N]a);!\$(c!@[cR1r6]1cccc1);!\$(c!@* !@c1cccc1);!\$([R2])]1[c;!\$(c[N+](=O)[O]);!\$(c[N]([#1,C])([#1,C]));! \$(cN([OX2H])([#1,C]));!\$(cN([#1,C])OC=O);!\$(c[NX3v3]([#1,CH3])([#1,CH3]));!\$(c[NX3v3]([#1,CH3])([CH2][CH3]));!\$(c[NX3v3]([CH2][CH3])([CH2][CH3]);!\$(cNC(=O)[#1,CH3]);!\$(cN=[N]a);!\$(c!@[cR 1r6]1cccc1);!\$(c!@*!@c1cccc1);!\$([R2])]1[c!([Cl,Br,F,I];!\$([Cl,Br,I, F]cc([Cl,Br,I,F]);!\$([Cl,Br,I,F]ccc([Cl,Br,I,F]);!\$([Cl,Br,I,F]c1c([OX2H])c ([OX2H])c([OX2H])cc1);!\$([Cl,Br,I,F]c1c([OX2H])c([OX2H])cc([OX2 H])c1);!\$([Cl,Br,I,F]c1c([OX2H])c([OX2H])ccc1([OX2H]));!\$([Cl,Br,I, F]c1c([OX2H])cc([OX2H])c([OX2H])c1);!\$([Cl,Br,I,F]c1c([OX2H])cc([OX2H])cc1([OX2H]));!\$([Cl,Br,I,F]c1cc([OX2H])c([OX2H])c([OX2H] [Cl,Br,F,I])c1ccc2cccc2(c1)</div>	SA31a_nogen. Halogenated benzene (Nongenotoxic carcinogens)
<div>[Cl,Br,F,I]c1ccc(cc1)!@c2ccc(cc2)[Cl,Br,F,I] c1cc(ccc1[!R]c2ccc(cc2)[Cl,Br,F,I])[Cl,Br,F,I]</div>	SA31b_nogen. Halogenated PAH (naphthalenes, biphenyls, diphenyls) (Nongenotoxic carcinogens)
<div>c1ccc2Oc3cc(ccc3(Oc2(c1)))[Cl,Br,F,I] c1(OC(C)(C)C(=O)O)ccc([#6,#17])cc1</div>	SA31c_nogen. Halogenated dibenzodioxins (Nongenotoxic carcinogens)
<div>c1(OCC(=O)[O;H0])cc(Cl)c(Cl)cc1 c1(OCC(=O)[O;H0])c(Cl)cc(Cl)cc1</div>	SA40_nogen. Nongenotoxic mechanism. Substituted phenoxyacid: Substituted phenoxyacid
<div>[C;!R&\$ (C([C;!R])([C;!R])[C;!R][C;!R])&!\$(CCCCCCCCCCC)[C;!R& \$(C[OX2;!R]),\$(C(=O)[OX2;!R])] O=C(O)c1cccc1C(=O)O O=C(O)[CX4;!R][CX4;!R][CX4;!R][CX4;!R]C(=O)O</div>	SA41_nogen. Nongenotoxic mechanism. Substituted n-alkylcarboxylic acids: Substituted n-alkylcarboxylic acids
	SA42_nogen. Nongenotoxic mechanism. Phthalate diesters and monoesters: Phthalate diesters and monoesters
<div>CC(F)(F)C(F)(F)C(F)(F)C(F)(F)C(F)(F)F [Cl,F][C;!\$(Cc)]=C([Cl,F])[Cl,F]</div>	SA43_nogen. Nongenotoxic mechanism. SA43 Perfluorooctanoic acid (PFOA): Perfluorooctanoic acid (PFOA)
<div>Cl[C;!\$(Cc)]=C(Cl)Cl [Cl,F]C#C[Cl,F]</div>	SA44_nogen. Nongenotoxic mechanism. SA44 Trichloro (or fluoro) ethylene and Tetrachloro (or fluoro) ethylene: Trichloro (or fluoro) ethylene and Tetrachloro (or fluoro) ethylene
<div>OCc1c[nH]c2cccc12 Clc1c(Cl)c(Cl)c(Cl)c(Cl)c1O Oc2cccc2c1cccc1 Oc1c(c2cccc2)cccc1</div>	SA45_nogen. Ngenotoxic mechanisms. Indole-3-carbinol: Indole-3-carbinol
	SA46_nogen. Nongenotoxic mechanism. Pentachlorophenol: Pentachlorophenol
	SA47_nogen. Nongenotoxic mechanisms. O-phenylphenol: O-phenylphenol
<div>Oc1cc(O)c2C(=O)C(O)=C(Oc2c1)c3ccc(O)c(O)c3 n1c[nH]cc1</div>	SA48_nogen. Nongenotoxic mechanisms. SA48 Quercetin-type flavonoids: Quercetin-type flavonoids
<div>n2c1cccc1nc2</div>	SA49_nogen. Nongenotoxic mechanism. Imidazole and benzimidazole: Imidazole and benzimidazole
<div>[#6]1[#6](=O)[#7][#6](=O)[#6]1 [CX4H3]c1cccc([CX4H3])n1 [As,Cu,Cr,Hg,Co] c1cc(N)ccc1S(=O)(=O)N</div>	SA50_nogen. Nongenotoxic mechanism. Dicarboximide: Dicarboximide
	SA51_nogen. Nongenotoxic mechanism. Dimethylpyridine: Dimethylpyridine
	SA52_nogen. Nongenotoxic mechanism. Metals, oxidative stress: Metals, oxidative stress
<div>c1cc(S)ccc1S(=O)(=O)N c1cccc1S(=O)(=O)[N;-1] c1cc(C)ccc1S(=O)(=O)O</div>	SA53_nogen. Nongenotoxic mechanism. SA53 Benzensulfonic ethers: Benzensulfonic ethers
<div>[C;!\$(C(C)(C))]1Oc2cccc2O1 c1cc(O)ccc1OC(C)C(=O)[O;!\$(OCCCC)] [C;H1,!\$(CCOP)&!\$(CCP)&!\$(CF)&!\$(CN)&!\$(C[CH3])](Cl)(Cl)(Cl)</div>	SA54_nogen. Nongenotoxic mechanism. 1,3-Benzodioxoles: 1,3-Benzodioxoles
	SA55_nogen. Nongenotoxic mechanisms. Phenoxy herbicides: Phenoxy herbicides
	SA56_nogen. Nongenotoxic mechanism
<div>[N+O;!R;!\$(N=*);!\$(N#*)][C+O;!R;!\$(C=*);!\$(C#*)][C+O;!R;!\$(C=*) ;!\$(C#*)][N+O;!R;!\$(N=*);!\$(N#*)]Cc1c2aaaac2aaa1</div>	
<div>[N+O;!R;!\$(N=*);!\$(N#*)][C+O;!R;!\$(C=*);!\$(C#*)][C+O;!R;!\$(C=*) [N+O;!R;!\$(N=*);!\$(N#*)][C+O;!R;!\$(C=*);!\$(C#*)][C+O;!R;!\$(C=*) ;!\$(C#*)][N+O;!R;!\$(N=*);!\$(N#*)]Cc1c2[A][A]=[A][A]c2aaa1</div>	
<div>[N+O;!R;!\$(N=*);!\$(N#*)][C+O;!R;!\$(C=*);!\$(C#*)][C+O;!R;!\$(C=*) ;!\$(C#*)][N+O;!R;!\$(N=*);!\$(N#*)]Cc1c2[A][A]=[A]c2aaa1</div>	SA57 DNA Intercalating Agents with a basic side chain: DNA intercalating agents are defined as those compounds that are able to insert partially or completely between adjacent DNA base pairs
<div>[N+O;!R;!\$(N=*);!\$(N#*)][C+O;!R;!\$(C=*);!\$(C#*)][C+O;!R;!\$(C=*) ;!\$(C#*)][N+O;!R;!\$(N=*);!\$(N#*)]Cc1c2Cc3aaaac3c2aaa1</div>	
<div>[N+O;!R;!\$(N=*);!\$(N#*)][C+O;!R;!\$(C=*);!\$(C#*)][C+O;!R;!\$(C=*) ;!\$(C#*)][N+O;!R;!\$(N=*);!\$(N#*)]Cc1c2c3aaaac3Cc2aaa1</div>	

