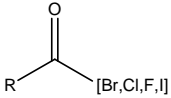
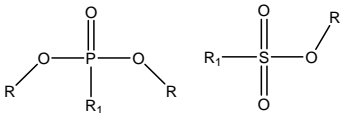
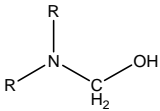
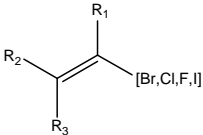
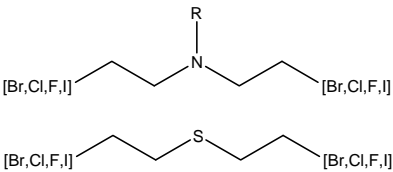
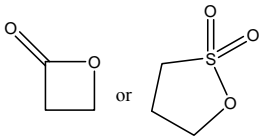
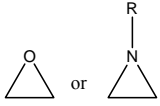
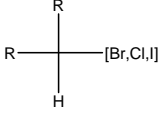
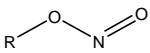
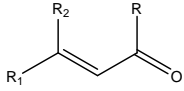
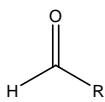
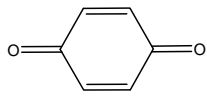
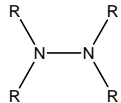
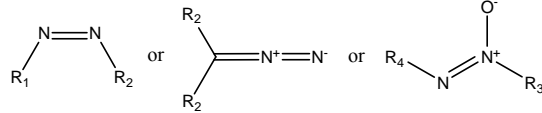
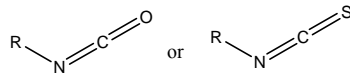
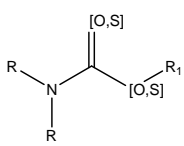
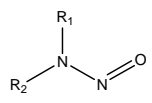
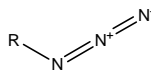
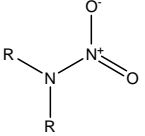
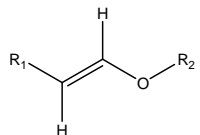
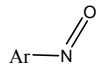
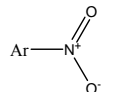
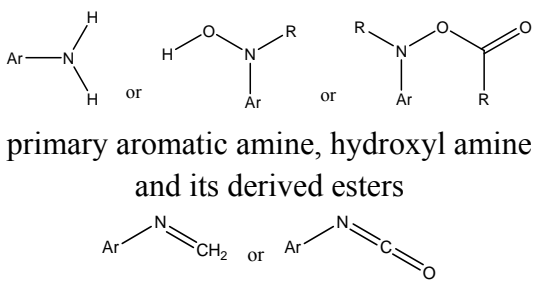
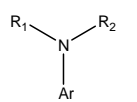
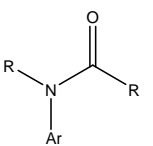
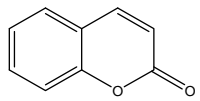


Table S3: SAs (Benigni) and examples matching SAs in our dataset

SAs	Examples
 <p>acyl halides</p>	<p>dimethylcarbamylyl chloride (CID000006598) benzoyl chloride (CID000007412)</p>
 <p>alkyl (C<5) or benzyl ester of sulphonic or phosphonic acid</p>	<p>trichlorfon (CID000005853) ethyl p-toluenesulfonate (CID000006638)</p>
 <p>N-methylol derivatives</p>	<p>N-methylolacrylamide (CID000013543)</p>
 <p>monohaloalkene</p>	<p>vinyl fluoride (CID000006339) 1-chloro-2-methylpropene (CID000010555)</p>
 <p>S or N mustard</p>	<p>2,2',2''-trichlorotriethylamine (CID000005561) sulfur mustard (CID000010461)</p>
 <p>propiolactones or propiosultones</p>	<p>propiolactone (CID000002365) 1,3-propane sultone (CID000014264)</p>
 <p>epoxides and aziridines</p>	<p>3,4-epoxy-1-butene (CID000013586) aziridine (CID000009033)</p>
 <p>aliphatic halogens</p>	<p>2-bromobutane (CID000006554) 2-iodobutane (CID000010559)</p>
 <p>alkyl nitrite</p>	<p>isobutyl nitrite (CID000010958)</p>

 <p>α,β unsaturated carbonyls</p>	<p>acrylamide (CID000006579) 2-butenal (CID000447466)</p>
 <p>simple aldehyde</p>	<p>acetaldehyde (CID000000177) bromoacetaldehyde (CID000105131)</p>
 <p>quinones</p>	<p>phenylbenzoquinone (CID000009688) chloranil (CID000008371)</p>
 <p>hydrazine</p>	<p>1,1-dibutylhydrazine (CID000023902) hydrazine (CID000009321)</p>
 <p>aliphatic azo and azoxy</p>	<p>diazomethane (CID000009550) methylazoxymethanol acetate (CID005964719)</p>
 <p>isocyanate and isothiocyanate groups</p>	<p>toluene 2,4-diisocyanate (CID000011443) benzyl isothiocyanate (CID000002346)</p>
 <p>alkyl carbamate and thiocarbamate</p>	<p>ethyl butylcarbamate (CID000011577) pebulate (CID000014215)</p>
<p>polycyclic aromatic hydrocarbons</p>	<p>dibenzo(a,i)pyrene (CID000009106) dibenzo(a,h)pyrene (CID000009108)</p>
<p>heterocyclic polycyclic aromatic hydrocarbons</p>	<p>benzo(f)quinoline (CID000006796) benzo(b)naphtho(2,1-d)thiophene (CID000009198)</p>
 <p>alkyl and aryl <i>N</i>-nitroso groups</p>	<p>2-methylnitrosopiperidine (CID000023677) <i>N</i>-nitroso-<i>N</i>-butyl-<i>N</i>-propylamine (CID000032965)</p>
 <p>triazene groups</p>	<p>zidovudine (CID000035370)</p>

 <p>aliphatic <i>N</i>-nitro group</p>	<p>dimethylnitramine (CID000020120) <i>N</i>-nitrodiethylamine (CID000023505)</p>
 <p>α,β unsaturated aliphatic alkoxy group</p>	<p>sterigmatocystin (CID005284457) aflatoxin G1 (CID000014421)</p>
 <p>aromatic nitroso group</p>	<p>2-nitrosofluorene (CID000017271) 3,2'-dimethyl-4-nitrosobiphenyl (CID000051168)</p>
 <p>nitro-aromatic</p>	<p>4,4'-dinitrobiphenyl (CID000015216) 4-nitrophenyl (CID000119211)</p>
 <p>primary aromatic amine, hydroxyl amine and its derived esters or amine generating group</p>	<p>4-aminophenyl (CID0000181201) <i>N</i>-hydroxy-4-aminobiphenyl (CID000081261) <i>N</i>-acetoxy-4-acetylamino-biphenyl (CID000091584) toluene 2,4-diisocyanate (CID000011443) DADI (CID000007069)</p>
 <p>aromatic mono- and dialkylamine</p>	<p><i>N,N,N',N'</i>-tetramethyl-4,4'-methylenedianiline (CID000007567) 4-dimethylaminostilbene (CID000640024)</p>
 <p>aromatic <i>N</i>-alkyl amine</p>	<p><i>N,N'</i>-diacetylbenzidine (CID000011942) 4-acetylamino-biphenyl (CID000019998)</p>
 <p>coumarins and Furocoumarins</p>	<p>6-methylcoumarin (CID000007092) coumarin (CID000000323)</p>