

Table 1

Molecular weight, SMILES structure and carcinogenicity of air pollutants.

Name	Molecular weight (g/mol)	SMILES structure	carcinogenicity (admetlab3.0)	hematotoxicity (admetlab3.0)	Carcinogenicity (ProTox3)
benzene	78.11	<chem>C1=CC=CC=C1</chem>	0.969	0.901	0.92
SO ₂	64.069	<chem>O=S=O</chem>	0.786	0.39	0.6
NO	30.006	<chem>[N]=O</chem>	0.635	0.441	0.59
CO	28.01	<chem>[C-]#[O+]</chem>	1	0	0.51
NO ₂	46.006	<chem>N(=O)[O-]</chem>	0.897	0.672	0.6
Toluene	92.14	<chem>CC1=CC=CC=C1</chem>	0.957	0.837	0.88
Formaldehyde	30.026	<chem>C=O</chem>	0.654	0.396	0.78
Naphthalene	128.169	<chem>C1=CC=C2C=CC=CC2=C1</chem>	0.676	0.315	0.88
O ₃	47.998	<chem>[O-][O+]=O</chem>	0.981	0.802	0.56

This table summarizes the molecular weights, SMILES structures, carcinogenicity and hematotoxicity evaluations of nine air pollutants (benzene, SO₂, NO, CO, NO₂, toluene, formaldehyde, naphthalene and O₃). The carcinogenicity and hematotoxicity were evaluated using the ADMETLAB 3.0 and ProTox-3 databases.