

SUPPLEMENTARY DATA: TABLE S1

acetal

11_diethoxyethane
dimethoxymethane

acid

3_methylbutanoic_acid
acetic_acid
butanoic_acid
hexanoic_acid
pentanoic_acid
propanoic_acid

alcohol

111_trifluoropropan_2_ol
12_ethanediol
222_trifluoroethanol
2_butoxyethanol
2_ethoxyethanol
2_methoxyethanol
2_methylbutan_1_ol
2_methylbutan_2_ol
2_methylpentan_2_ol
2_methylpentan_3_ol
2_methylpropan_1_ol
2_methylpropan_2_ol
2_phenylethanol
2_propoxyethanol
3_methylbutan_1_ol
3_phenylpropanol
4_methylpentan_2_ol
benzyl_alcohol
butan_1_ol
butan_2_ol
cycloheptanol
cyclohexanol
cyclopentanol
decan_1_ol
ethanol
heptan_1_ol
hexan_1_ol
hexan_3_ol
methanol
nonan_1_ol
octan_1_ol
pentan_1_ol
pentan_2_ol
pentan_3_ol
prop_2_en_1_ol
propan_1_ol
propan_2_ol
triacetyl_glycerol

aldehyde

3_formylpyridine

3_hydroxybenzaldehyde
4_formylpyridine
4_hydroxybenzaldehyde
4_methylbenzaldehyde
acetaldehyde
benzaldehyde
butyraldehyde
e_but_2_enal
e_hex_2_enal
e_oct_2_enal
formaldehyde
heptanal
hexanal
isobutyraldehyde
nonanal
octanal
pentanal
propionaldehyde

alkane

224_trimethylpentane
225_trimethylhexane
22_dimethylbutane
22_dimethylpentane
22_dimethylpropane
234_trimethylpentane
23_dimethylbutane
23_dimethylpentane
24_dimethylpentane
2_methylbutane
2_methylhexane
2_methylpentane
2_methylpropane
33_dimethylpentane
3_methylheptane
3_methylhexane
3_methylpentane
ethane
methane
n_butane
n_decane
n_heptane
n_hexane
n_nonane
n_octane
n_pentane
propane

alkene

1_methylcyclohexene
23_dimethylbuta_13_diene
2_methylbut_2_ene
2_methylbuta_13_diene
2_methylpent_1_ene

2_methylpropene
3_chloroprop_1_ene
3_methylbut_1_ene
alpha_methylstyrene
but_1_ene
buta_13_diene
chloroethylene
cyclohepta_135_triene
cyclohexene
cyclopentene
e_12_dichloroethene
e_but_2_enal
e_hept_2_ene
e_hex_2_enal
e_oct_2_enal
ethene
hept_1_ene
hex_1_ene
hexa_15_diene
non_1_ene
oct_1_ene
pent_1_ene
penta_14_diene
prop_2_en_1_ol
propene
styrene
z_12_dichloroethene
z_pent_2_ene
trichloroethene
tetrachloroethene

alkyne

but_1_yne
hept_1_yne
hex_1_yne
oct_1_yne
pent_1_yne
propyne

amine

14_dimethyl_piperazine
1_naphthylamine
26_dimethylaniline
2_chloroaniline
2_methoxyaniline
2_methoxyethanamine
2_naphthylamine
2_nitroaniline
3_chloroaniline
3_methoxyaniline
3_nitroaniline
4_chloroaniline
4_methoxyaniline
4_nitroaniline

aniline
azetidine
cyclohexylamine
diethylamine
diisopropylamine
dimethylamine
di_n_butylamine
di_n_propylamine
ethylamine
methylamine
morpholine
n_butylamine
n_heptylamine
n_hexylamine
n_methylaniline
n_methylmorpholine
n_methyl_n_222_trifluoroethyl_aniline
n_methylpiperazine
n_methylpiperidine
nn_dimethylaniline
n_octylamine
n_pentylamine
n_propylamine
o_toluidine
piperazine
piperidine
p_toluidine
pyrrolidine
triethylamine
trimethylamine

aromatic

1234_tetrachlorobenzene
1235_tetrachlorobenzene
123_trichlorobenzene
123_trimethylbenzene
1245_tetrachlorobenzene
124_trichlorobenzene
124_trimethylbenzene
12_dichlorobenzene
135_trichlorobenzene
135_trimethylbenzene
13_dichlorobenzene
13_dimethylnaphthalene
14_dichlorobenzene
14_dimethylnaphthalene
1_ethylnaphthalene
1_methyl_imidazole
1_methylnaphthalene
1_methyl_pyrrole
1_naphthol
1_naphthylamine
23_dimethylnaphthalene
23_dimethylphenol
23_dimethylpyridine

24_dimethylphenol
24_dimethylpyridine
25_dimethylphenol
25_dimethylpyridine
26_dimethylaniline
26_dimethylnaphthalene
26_dimethylphenol
26_dimethylpyridine
2_chloroaniline
2_chlorophenol
2_chloropyridine
2_chlorotoluene
2_ethylpyrazine
2_ethylpyridine
2_ethyltoluene
2_fluorophenol
2_iodophenol
2_isobutylpyrazine
2_methoxyaniline
2_methoxyphenol
2_methylpyrazine
2_methylpyridine
2_methylthiophene
2_naphthol
2_naphthylamine
2_nitroaniline
2_nitrophenol
2_nitrotoluene
2_phenylethanol
34_dimethylphenol
34_dimethylpyridine
35_dimethylphenol
35_dimethylpyridine
3_acetylpyridine
3_chloroaniline
3_chlorophenol
3_chloropyridine
3_cyanophenol
3_cyanopyridine
3_ethylphenol
3_ethylpyridine
3_formylpyridine
3_hydroxybenzaldehyde
3_methoxyaniline
3_methoxyphenol
3_methyl_1h_indole
3_methylpyridine
3_nitroaniline
3_nitrophenol
3_nitrotoluene
3_phenylpropanol
4_acetylpyridine
4_bromophenol
4_bromotoluene
4_chloro_3_methylphenol
4_chloroaniline

4_chlorophenol
4_cyanophenol
4_cyanopyridine
4_ethylphenol
4_ethylpyridine
4_ethyltoluene
4_fluorophenol
4_formylpyridine
4_hydroxybenzaldehyde
4_isopropyltoluene
4_methoxyacetophenone
4_methoxyaniline
4_methyl_1h_imidazole
4_methylacetophenone
4_methylbenzaldehyde
4_methylpyridine
4_nitroaniline
4_nitrophenol
4_n_propylphenol
4_tert_butylphenol
acenaphthene
acetophenone
alpha_methylstyrene
aniline
anisole
anthracene
benzaldehyde
benzamide
benzene
benzonitrile
benzotrifluoride
benzyl_alcohol
benzyl_bromide
benzyl_chloride
biphenyl
bromobenzene
chlorobenzene
diethoxymethoxybenzene
ethylbenzene
ethyl_benzoate
ethyl_phenyl_ether
fluorene
fluorobenzene
imidazole
indane
iodobenzene
isobutylbenzene
isopropylbenzene
m_bis_trifluoromethyl_benzene
m_cresol
methyl_benzoate
methyl_p_methoxybenzoate
methyl_p_nitrobenzoate
m_xylene
naphthalene

n_butylbenzene
n_hexylbenzene
nitrobenzene
n_methylaniline
n_methyl_n_222_trifluoroet
hyl__aniline
nn_dimethylaniline
nn_dimethylbenzamide
nn_dimethyl_p_methoxybenz
amide
nn_dimethyl_p_methylbenza
mide
nn_dimethyl_p_nitrobenzami
de
n_pentylbenzene
n_propylbenzene
o_cresol
o_toluidine
o_xylene
p_cresol
p_dibromobenzene
phenanthrene
phenol
phenyl_formate
phenyl_methyl_sulfide
phenyl_trifluoroethyl_ether
p_toluidine
p_xylene
pyrene
pyridine
pyrrole
quinoline
sec_butylbenzene
styrene
tert_butylbenzene
thiophene
thiophenol
toluene
trimethoxymethylbenzene

bromo

12_dibromoethane
1_bromo_2_chloroethane
1_bromo_2_methylpropane
1_bromobutane
1_bromoheptane
1_bromohexane
1_bromooctane
1_bromopentane
1_bromopropane
2_bromo_2_methylpropane
2_bromopropane
4_bromophenol
4_bromotoluene
benzyl_bromide
bromobenzene

bromoethane
bromomethane
dibromomethane
halothane
p_dibromobenzene
teflurane

ca_amide

benzamide
ethanamide
n_acetylpyrrolidine
n_butylacetamide
n_methylacetamide
nn_dimethylbenzamide
nn_dimethylformamide
nn_dimethyl_p_methoxybenz
amide
nn_dimethyl_p_methylbenza
mide
nn_dimethyl_p_nitrobenzami
de

ca_ester

11_diacetoxyethane
12_diacetoxyethane
diethyl_malonate
diethyl_succinate
dimethyl_sulfate
ethyl_acetate
ethyl_benzoate
ethyl_butanoate
ethyl_formate
ethyl_hexanoate
ethyl_pentanoate
ethyl_propanoate
isoamyl_acetate
isoamyl_formate
isobutyl_acetate
isobutyl_formate
isobutyl_isobutanoate
isopropyl_acetate
isopropyl_formate
methyl_acetate
methyl_benzoate
methyl_butanoate
methyl_chloroacetate
methyl_cyanoacetate
methyl_cyclohexanecarboxyl
ate
methyl_cyclopropanecarboxyl
ate
methyl_formate
methyl_hexanoate
methyl_methanesulfonate
methyl_octanoate
methyl_pentanoate

methyl_p_methoxybenzoate
methyl_p_nitrobenzoate
methyl_propanoate
methyl_trifluoroacetate
methyl_trimethylacetate
n_butyl_acetate
n_hexyl_acetate
n_pentyl_acetate
n_pentyl_propanoate
n_propyl_acetate
n_propyl_butyrate
n_propyl_formate
n_propyl_propanoate
phenyl_formate
triethyl_phosphate
trimethyl_phosphate

ca_ortho

111_trifluoro_222_trimethoxy
ethane
111_trimethoxyethane
2_chloro_111_trimethoxyetha
ne
2_methoxy_111_trimethoxyet
hane
333_trimethoxypropionitrile
diethoxymethoxybenzene
isoflurane
methoxyflurane
trimethoxy_methane
trimethoxymethylbenzene

carbonitrile

333_trimethoxypropionitrile
3_cyanophenol
3_cyanopyridine
4_cyanophenol
4_cyanopyridine
acetonitrile
benzonitrile
butanenitrile
methyl_cyanoacetate
pentanenitrile
propanenitrile

chloro_alkyl

1112_tetrachloroethane
1122_tetrachloroethane
112_trichloroethane
11_dichloroethane
12_dichloroethane
12_dichloropropane
13_dichloropropane
14_dichlorobutane
1_bromo_2_chloroethane
1_chloro_222_trifluoroethane

1_chlorobutane
1_chloroheptane
1_chlorohexane
1_chloropentane
1_chloropropane
2_chloro_111_trimethoxyethane
2_chloro_2_methylpropane
2_chlorobutane
2_chloropropane
3_chloroprop_1_ene
benzyl_chloride
bis_2_chloroethyl__ether
chloroethane
chlorofluoromethane
chloromethane
dichloromethane
halothane
isoflurane
methoxyflurane
methyl_chloroacetate
pentachloroethane

chloro_aryl

1234_tetrachlorobenzene
1235_tetrachlorobenzene
123_trichlorobenzene
1245_tetrachlorobenzene
124_trichlorobenzene
12_dichlorobenzene
135_trichlorobenzene
13_dichlorobenzene
14_dichlorobenzene
2_chloroaniline
2_chlorophenol
2_chloropyridine
2_chlorotoluene
3_chloroaniline
3_chlorophenol
3_chloropyridine
4_chloro_3_methylphenol
4_chloroaniline
4_chlorophenol
chlorobenzene

cyclohydrocarbon

cis_12_dimethylcyclohexane
cyclohexane
cyclopentane
cyclopropane
methylcyclohexane
methylcyclopentane
n_pentylcyclopentane
n_propylcyclopentane
trans_14_dimethylcyclohexane

ether_alkyl

12_diethoxyethane
12_dimethoxyethane
14_dioxane
25_dimethyltetrahydrofuran
2_butoxyethanol
2_ethoxyethanol
2_methoxy_111_trimethoxyethane
2_methoxyethanamine
2_methoxyethanol
2_methyltetrahydrofuran
2_propoxyethanol
bis_2_chloroethyl__ether
diethyl_ether
diisopropyl_ether
dimethyl_ether
di_n_butyl_ether
di_n_propyl_ether
methyl_ethyl_ether
methyl_isopropyl_ether
methyl_propyl_ether
methyl_t_butyl_ether
morpholine
n_methylmorpholine
tetrahydrofuran
tetrahydropyran

ether_aryl

2_methoxyaniline
2_methoxyphenol
3_methoxyaniline
3_methoxyphenol
4_methoxyacetophenone
4_methoxyaniline
anisole
ethyl_phenyl_ether
methyl_p_methoxybenzoate
nn_dimethyl_p_methoxybenzamide

fluoro

11_difluoroethane
2_fluorophenol
4_fluorophenol
chlorofluoromethane
fluorobenzene
fluoromethane
phenyl_trifluoroethyl_ether
teflurane
112_trichloro_122_trifluoroethane
chlorodifluoromethane

halogen

111_trichloroethane

111_trifluoro_222_trimethoxyethane
111_trifluoropropan_2_ol
112_trichloro_122_trifluoroethane
11_dichloroethene
222_trifluoroethanol
benzotrifluoride
bromotrifluoromethane
chlorodifluoromethane
chloroethylene
e_12_dichloroethene
hexafluoropropene
m_bis_trifluoromethyl__benzene
methyl_trifluoroacetate
n_methyl_n_222_trifluoroethyl__aniline
tetrachloroethene
tetrachloromethane
tetrafluoromethane
tribromomethane
trichloroethene
trichloromethane
z_12_dichloroethene

heterocyclic

14_dimethyl_piperazine
14_dioxane
1_methyl_imidazole
1_methyl_pyrrole
23_dimethylpyridine
24_dimethylpyridine
25_dimethylpyridine
25_dimethyltetrahydrofuran
26_dimethylpyridine
2_chloropyridine
2_ethylpyrazine
2_ethylpyridine
2_isobutylpyrazine
2_methylpyrazine
2_methylpyridine
2_methyltetrahydrofuran
2_methylthiophene
34_dimethylpyridine
35_dimethylpyridine
3_acetylpyridine
3_chloropyridine
3_cyanopyridine
3_ethylpyridine
3_formylpyridine
3_methyl_1h_indole
3_methylpyridine
4_acetylpyridine
4_cyanopyridine
4_ethylpyridine

4_formylpyridine
4_methyl_1h_imidazole
4_methylpyridine
azetidine
imidazole
morpholine
n_acetylpyrrolidine
n_methylmorpholine
n_methylpiperazine
n_methylpiperidine
piperazine
piperidine
pyridine
pyrrole
pyrrolidine
quinoline
tetrahydrofuran
tetrahydropyran
thiophene

hypervalents

dimethyl_sulfate
dimethyl_sulfone
methyl_methanesulfonate
methanesulfonyl_chloride

iodo

1_iodobutane
1_iodoheptane
1_iodohexane
1_iodopentane
1_iodopropane
2_iodophenol
2_iodopropane
diiodomethane
iodobenzene
iodoethane
iodomethane

ketone

24_dimethylpentan_3_one
33_dimethylbutan_2_one
3_acetylpyridine
3_methylbutan_2_one
4_acetylpyridine
4_methoxyacetophenone
4_methylacetophenone
4_methylpentan_2_one
acetophenone
cyclohexanone
cyclopentanone
decan_2_one
heptan_2_one
heptan_4_one
hexan_2_one
methyl_cyclohexyl_ketone

methyl_cyclopropyl_ketone
nonan_2_one
nonan_5_one
octan_2_one
pentan_2_one
pentan_3_one
propanone
triacetyl_glycerol
undecan_2_one

nitro

1_nitrobutane
1_nitropentane
1_nitropropane
2_nitroaniline
2_nitrophenol
2_nitropropane
2_nitrotoluene
3_nitroaniline
3_nitrophenol
3_nitrotoluene
4_nitroaniline
4_nitrophenol
methyl_p_nitrobenzoate
nitrobenzene
nitroethane
nitromethane
nn_dimethyl_p_nitrobenzami
de

nitrogen

ammonia
hydrazine

orthoester

111_trifluoro_222_trimethoxy
ethane
111_trimethoxyethane
2_chloro_111_trimethoxyetha
ne
2_methoxy_111_trimethoxyet
hane
333_trimethoxypropionitrile
diethoxymethoxybenzene
trimethoxy_methane
trimethoxymethylbenzene

other

ammonia
hydrazine
11_diethoxyethane
diethyl_disulfide
dimethoxymethane
dimethyl_disulfide
dimethyl_sulfoxide
hydrogen_sulfide

phenol

1_naphthol
23_dimethylphenol
24_dimethylphenol
25_dimethylphenol
26_dimethylphenol
2_chlorophenol
2_fluorophenol
2_iodophenol
2_methoxyphenol
2_naphthol
2_nitrophenol
34_dimethylphenol
35_dimethylphenol
3_chlorophenol
3_cyanophenol
3_ethylphenol
3_hydroxybenzaldehyde
3_methoxyphenol
3_nitrophenol
4_bromophenol
4_chloro_3_methylphenol
4_chlorophenol
4_cyanophenol
4_ethylphenol
4_fluorophenol
4_hydroxybenzaldehyde
4_nitrophenol
4_n_propylphenol
4_tert_butylphenol
m_cresol
o_cresol
p_cresol
phenol

sulfur

diethyl_disulfide
dimethyl_disulfide
dimethyl_sulfoxide
hydrogen_sulfide

thioether

diethyl_sulfide
di_isopropyl_sulfide
dimethyl_sulfide
di_n_propyl_sulfide
methyl_ethyl_sulfide
phenyl_methyl_sulfide

thiol

ethanethiol
methanethiol
n_butanethiol
n_propanethiol
thiophenol

