



QSAR-WB Descriptors Manual

Software and models development

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1 Introduction

QSAR-WB Descriptors (Quantitative Structure-Activity Relationship WorkBench Descriptors) is a software for the calculation of 1D and 2D molecular descriptors and fingerprints. QSAR-WB Descriptors is designed to run on multiple operating systems ¹ and can be run either as a Graphical User Interface (GUI) application or as a command line application.

2 Getting started

2.1 Software requirements

QSAR-WB Descriptors requires Java[®] SE 21 runtime environment or a more recent version.

2.2 Installing QSAR-WB Descriptors

Unzip the downloaded file in a folder of choice.

2.3 Running QSAR-WB Descriptors

To run QSAR-WB Descriptors as a GUI application, double click on the [QSAR-WB-Descriptors.jar](#) icon. Alternatively, you can run QSAR-WB Descriptors as a GUI application by opening a terminal pointing to the QSAR-WB Descriptors main folder ², and by typing

```
java -jar QSAR-WB-Descriptors
```

To run QSAR-WB Descriptors as a command line application see section 4.

¹The ones supporting Java[®] SE runtime environments.

²The folder where [QSAR-WB-Descriptors.jar](#) is located

3 Calculating descriptors and fingerprints

Figure 1 shows the main window of QSAR-WB Descriptors when run as a GUI application.

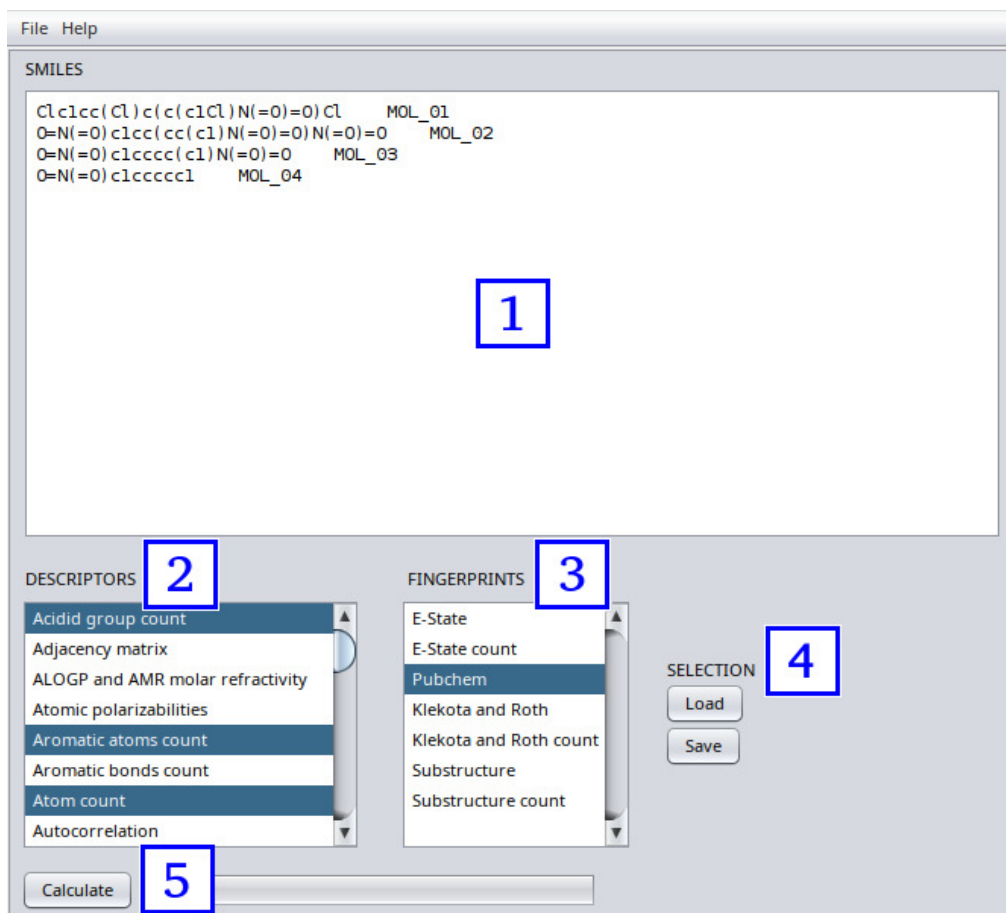


Figure 1: QSAR-WB Descriptors main window.

To calculate descriptors and/or fingerprints you first need to type the chemical SMILES, in the `.smi` format ³, in the **SMILES edit area** (Figure 1, box 1). SMILES can be typed directly in the edit area and, in addition, a drop-down menu is available by right clicking on the edit area, allowing to copy/paste SMILES or to import SMILES from a `.smi` file.

Concerning SMILES themselves, dative bonds must be converted to covalent ones like, for example, [N+](=[O-])=O (dative bond) as N(=O)=O (covalent bond). Chiral and isotopic markings should be also removed. Aromaticity is automatically detected by QSAR-WB Descriptors using the CDK Daylight aromaticity model.

Descriptors and fingerprints can be selected respectively by clicking on the **DESCRIPTORS** list (Figure 1, box 2) and the **FINGERPRINTS** list (Figure 1, box 3). In addition, by right-clicking on the lists, a drop-down menu will allow to either select or unselect all descriptors/fingerprints. If needed, selections can be loaded as saved as `.ini` config files (Figure 1, box 4).

By pressing the **Calculate** button (Figure 1, box 5) a dialog will appear asking for the name of the calculated descriptors/fingerprints `.csv` output file, then descriptors/fingerprints will be calculated and saved in this file.

³SMILES strings are followed by one or more spaces/tabulations followed by the chemicals name.

4 Running QSAR-WB Descriptors as a command line application

Section 2.3 explains how to run QSAR-WB Descriptors as a GUI application from terminal. By adding one or more options after [QSAR-WB-Descriptors.jar](#), will run as a command line application. To get help about the command line options type

```
java -jar QSAR-WB-Descriptors --help
```

the following output will be generated

```
Usage -i [SMILES FILE] -o [OUTPUT FILE] ...
```

```
Example: 'java -jar QSAR-MD-Calculator.java -i smiles.smi -o output.csv'
```

File options:

```
-i <file>      SMILES file (.smi format)
```

```
-o <file>      Output file (.csv format)
```

```
-c <file>      Use selected descriptors configuration file (optional)
```

```
-g <file>      Generate default descriptors configuration .ini file (skips descriptors calculation)
```

4.1 Choosing descriptors and fingerprints

QSAR-WB Descriptors selects descriptors and/or fingerprints to be calculated from a [.ini](#) configuration file. The [-g](#) option creates a default configuration file, which name must be specified, like in the following example

```
java -jar QSAR-WB-Descriptors.jar -g config.ini
```

A configuration file is a text structured as

```
[descriptors]
```

```
Acidid group count=yes
```

```
Adjacency matrix=no
```

```
ALOGP and AMR molar refractivity=no
```

```
...
```

```
[fingerprints]
```

```
E-State fingerprint=no
```

```
E-State count fingerprint=no
```

```
Pubchem fingerprint=yes
```

```
...
```

By opening the configuration file with a text editor, descriptors and fingerprints can be selected or not by typing [yes](#) or [no](#) after [=](#). Anything else in the configuration file must be left untouched.

4.2 Calculating descriptors and fingerprints

To calculate descriptors, a [.smi](#) input file and a [.csv](#) output file must be specified. Optionally a configuration [.ini](#) file can also be specified ⁴. Here it follows example using a configuration file

```
java -jar QSAR-WB-Descriptors.jar -i example.smi -o example.csv -c config.ini
```

⁴If a configuration file is not specified the list of available descriptors is automatically selected.

5 Descriptors

5.1 Acidic groups count

Name	Description
nAromBond	Number of acidic groups

5.2 Adjacency distance matrix

Name	Description
SpMax_A	Leading eigenvalue
SpDiam_A	Spectral diameter
SpAD_A	Spectral absolute deviation
SpMAD_A	Spectral mean absolute deviation
EE_A	Estrada-like index
VE1_A	Coefficient sum of the last eigenvector
VE2_A	Average coefficient sum of the last eigenvector
VE3_A	Logarithmic coefficient sum of the last eigenvector
VR1_A	Randic-like eigenvector-based index
VR2_A	Normalized Randic-like eigenvector-based index
VR3_A	Logarithmic Randic-like eigenvector-based index

5.3 ALogP

Name	Description
ALogP	Ghose-Crippen LogKow
ALogp2	Squared Ghose-Crippen LogKow
AMR	Ghose-Crippen molar refractivity

5.4 Atomic polarizabilities

Name	Description
apol	Sum of the atomic polarizabilities (including implicit hydrogens)

5.5 Aromatic atoms count

Name	Description
naAromAtom	Number of aromatic atoms

5.6 Aromatic bonds count

Name	Description
nAromBond	Number of aromatic bonds

5.7 Atom count

Name	Description
nHeavyAtom	Number of heavy atoms
nAtom	Number of all atoms
nH	Number of hydrogen atoms
nB	Number of boron atoms
nC	Number of carbon atoms
nN	Number of nitrogen atoms
nO	Number of oxygen atoms
nS	Number of sulphur atoms
nP	Number of phosphorus atoms
nF	Number of fluorine atoms
nCl	Number of chlorine atoms
nBr	Number of bromine atoms
nI	Number of iodine atoms
nX	Number of halogen atoms

5.8 Autocorrelation

5.8.1 Broto-Moreau autocorrelation

Name	Description
ATS0d	Broto-Moreau autocorrelation of lag 0 weighted by sigma electrons
ATS1d	Broto-Moreau autocorrelation of lag 1 weighted by sigma electrons
ATS2d	Broto-Moreau autocorrelation of lag 2 weighted by sigma electrons
ATS3d	Broto-Moreau autocorrelation of lag 3 weighted by sigma electrons
ATS4d	Broto-Moreau autocorrelation of lag 4 weighted by sigma electrons
ATS5d	Broto-Moreau autocorrelation of lag 5 weighted by sigma electrons
ATS6d	Broto-Moreau autocorrelation of lag 6 weighted by sigma electrons
ATS7d	Broto-Moreau autocorrelation of lag 7 weighted by sigma electrons
ATS8d	Broto-Moreau autocorrelation of lag 8 weighted by sigma electrons

Name	Description
ATS0e	Broto-Moreau autocorrelation of lag 0 weighted by Sanderson atomic electronegativity
ATS1e	Broto-Moreau autocorrelation of lag 1 weighted by Sanderson atomic electronegativity
ATS2e	Broto-Moreau autocorrelation of lag 2 weighted by Sanderson atomic electronegativity
ATS3e	Broto-Moreau autocorrelation of lag 3 weighted by Sanderson atomic electronegativity
ATS4e	Broto-Moreau autocorrelation of lag 4 weighted by Sanderson atomic electronegativity
ATS5e	Broto-Moreau autocorrelation of lag 5 weighted by Sanderson atomic electronegativity
ATS6e	Broto-Moreau autocorrelation of lag 6 weighted by Sanderson atomic electronegativity
ATS7e	Broto-Moreau autocorrelation of lag 7 weighted by Sanderson atomic electronegativity
ATS8e	Broto-Moreau autocorrelation of lag 8 weighted by Sanderson atomic electronegativity

Name	Description
ATS0i	Broto-Moreau autocorrelation of lag 0 weighted by atomic first ionization potential
ATS1i	Broto-Moreau autocorrelation of lag 1 weighted by atomic first ionization potential
ATS2i	Broto-Moreau autocorrelation of lag 2 weighted by atomic first ionization potential
ATS3i	Broto-Moreau autocorrelation of lag 3 weighted by atomic first ionization potential
ATS4i	Broto-Moreau autocorrelation of lag 4 weighted by atomic first ionization potential
ATS5i	Broto-Moreau autocorrelation of lag 5 weighted by atomic first ionization potential
ATS6i	Broto-Moreau autocorrelation of lag 6 weighted by atomic first ionization potential
ATS7i	Broto-Moreau autocorrelation of lag 7 weighted by atomic first ionization potential
ATS8i	Broto-Moreau autocorrelation of lag 8 weighted by atomic first ionization potential

Name	Description
ATS0m	Broto-Moreau autocorrelation of lag 0 weighted by atomic mass
ATS1m	Broto-Moreau autocorrelation of lag 1 weighted by atomic mass
ATS2m	Broto-Moreau autocorrelation of lag 2 weighted by atomic mass
ATS3m	Broto-Moreau autocorrelation of lag 3 weighted by atomic mass
ATS4m	Broto-Moreau autocorrelation of lag 4 weighted by atomic mass
ATS5m	Broto-Moreau autocorrelation of lag 5 weighted by atomic mass
ATS6m	Broto-Moreau autocorrelation of lag 6 weighted by atomic mass
ATS7m	Broto-Moreau autocorrelation of lag 7 weighted by atomic mass
ATS8m	Broto-Moreau autocorrelation of lag 8 weighted by atomic mass

Name	Description
ATS0p	Broto-Moreau autocorrelation of lag 0 weighted by atomic polarizability
ATS1p	Broto-Moreau autocorrelation of lag 1 weighted by atomic polarizability
ATS2p	Broto-Moreau autocorrelation of lag 2 weighted by atomic polarizability
ATS3p	Broto-Moreau autocorrelation of lag 3 weighted by atomic polarizability
ATS4p	Broto-Moreau autocorrelation of lag 4 weighted by atomic polarizability
ATS5p	Broto-Moreau autocorrelation of lag 5 weighted by atomic polarizability
ATS6p	Broto-Moreau autocorrelation of lag 6 weighted by atomic polarizability
ATS7p	Broto-Moreau autocorrelation of lag 7 weighted by atomic polarizability
ATS8p	Broto-Moreau autocorrelation of lag 8 weighted by atomic polarizability

Name	Description
ATS0s	Broto-Moreau autocorrelation of lag 0 weighted by atomic intrinsic state
ATS1s	Broto-Moreau autocorrelation of lag 1 weighted by atomic intrinsic state
ATS2s	Broto-Moreau autocorrelation of lag 2 weighted by atomic intrinsic state
ATS3s	Broto-Moreau autocorrelation of lag 3 weighted by atomic intrinsic state
ATS4s	Broto-Moreau autocorrelation of lag 4 weighted by atomic intrinsic state
ATS5s	Broto-Moreau autocorrelation of lag 5 weighted by atomic intrinsic state
ATS6s	Broto-Moreau autocorrelation of lag 6 weighted by atomic intrinsic state
ATS7s	Broto-Moreau autocorrelation of lag 7 weighted by atomic intrinsic state
ATS8s	Broto-Moreau autocorrelation of lag 8 weighted by atomic intrinsic state

Name	Description
ATS0v	Broto-Moreau autocorrelation of lag 0 weighted by van der Waals atomic volume
ATS1v	Broto-Moreau autocorrelation of lag 1 weighted by van der Waals atomic volume
ATS2v	Broto-Moreau autocorrelation of lag 2 weighted by van der Waals atomic volume
ATS3v	Broto-Moreau autocorrelation of lag 3 weighted by van der Waals atomic volume
ATS4v	Broto-Moreau autocorrelation of lag 4 weighted by van der Waals atomic volume
ATS5v	Broto-Moreau autocorrelation of lag 5 weighted by van der Waals atomic volume

Name	Description
ATS6v	Broto-Moreau autocorrelation of lag 6 weighted by van der Waals atomic volume
ATS7v	Broto-Moreau autocorrelation of lag 7 weighted by van der Waals atomic volume
ATS8v	Broto-Moreau autocorrelation of lag 8 weighted by van der Waals atomic volume

Name	Description
ATS0Z	Broto-Moreau autocorrelation of lag 0 weighted by atomic number
ATS1Z	Broto-Moreau autocorrelation of lag 1 weighted by atomic number
ATS2Z	Broto-Moreau autocorrelation of lag 2 weighted by atomic number
ATS3Z	Broto-Moreau autocorrelation of lag 3 weighted by atomic number
ATS4Z	Broto-Moreau autocorrelation of lag 4 weighted by atomic number
ATS5Z	Broto-Moreau autocorrelation of lag 5 weighted by atomic number
ATS6Z	Broto-Moreau autocorrelation of lag 6 weighted by atomic number
ATS7Z	Broto-Moreau autocorrelation of lag 7 weighted by atomic number
ATS8Z	Broto-Moreau autocorrelation of lag 8 weighted by atomic number

Name	Description
ATS0dv	Broto-Moreau autocorrelation of lag 0 weighted by atomic valence
ATS1dv	Broto-Moreau autocorrelation of lag 1 weighted by atomic valence
ATS2dv	Broto-Moreau autocorrelation of lag 2 weighted by atomic valence
ATS3dv	Broto-Moreau autocorrelation of lag 3 weighted by atomic valence
ATS4dv	Broto-Moreau autocorrelation of lag 4 weighted by atomic valence
ATS5dv	Broto-Moreau autocorrelation of lag 5 weighted by atomic valence
ATS6dv	Broto-Moreau autocorrelation of lag 6 weighted by atomic valence
ATS7dv	Broto-Moreau autocorrelation of lag 7 weighted by atomic valence
ATS8dv	Broto-Moreau autocorrelation of lag 8 weighted by atomic valence

Name	Description
ATS0pe	Broto-Moreau autocorrelation of lag 0 weighted by Pauling electronegativity
ATS1pe	Broto-Moreau autocorrelation of lag 1 weighted by Pauling electronegativity
ATS2pe	Broto-Moreau autocorrelation of lag 2 weighted by Pauling electronegativity
ATS3pe	Broto-Moreau autocorrelation of lag 3 weighted by Pauling electronegativity
ATS4pe	Broto-Moreau autocorrelation of lag 4 weighted by Pauling electronegativity
ATS5pe	Broto-Moreau autocorrelation of lag 5 weighted by Pauling electronegativity
ATS6pe	Broto-Moreau autocorrelation of lag 6 weighted by Pauling electronegativity
ATS7pe	Broto-Moreau autocorrelation of lag 7 weighted by Pauling electronegativity
ATS8pe	Broto-Moreau autocorrelation of lag 8 weighted by Pauling electronegativity

Name	Description
ATS0are	Broto-Moreau autocorrelation of lag 0 weighted by Allred-Rocow electronegativity
ATS1are	Broto-Moreau autocorrelation of lag 1 weighted by Allred-Rocow electronegativity
ATS2are	Broto-Moreau autocorrelation of lag 2 weighted by Allred-Rocow electronegativity
ATS3are	Broto-Moreau autocorrelation of lag 3 weighted by Allred-Rocow electronegativity
ATS4are	Broto-Moreau autocorrelation of lag 4 weighted by Allred-Rocow electronegativity
ATS5are	Broto-Moreau autocorrelation of lag 5 weighted by Allred-Rocow electronegativity
ATS6are	Broto-Moreau autocorrelation of lag 6 weighted by Allred-Rocow electronegativity
ATS7are	Broto-Moreau autocorrelation of lag 7 weighted by Allred-Rocow electronegativity
ATS8are	Broto-Moreau autocorrelation of lag 8 weighted by Allred-Rocow electronegativity

5.8.2 Averaged Broto-Moreau autocorrelation

Name	Description
AATS0d	Averaged Broto-Moreau autocorrelation of lag 0 weighted by sigma electrons
AATS1d	Averaged Broto-Moreau autocorrelation of lag 1 weighted by sigma electrons
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AATS3d	Averaged Broto-Moreau autocorrelation of lag 3 weighted by sigma electrons
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AATS8Z	Averaged Broto-Moreau autocorrelation of lag 8 weighted by atomic number

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AATS5dv	Averaged Broto-Moreau autocorrelation of lag 5 weighted by atomic valence
AATS6dv	Averaged Broto-Moreau autocorrelation of lag 6 weighted by atomic valence
AATS7dv	Averaged Broto-Moreau autocorrelation of lag 7 weighted by atomic valence
AATS8dv	Averaged Broto-Moreau autocorrelation of lag 8 weighted by atomic valence

Name	Description
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AATS3pe	Averaged Broto-Moreau autocorrelation of lag 3 weighted by Pauling electronegativity
AATS4pe	Averaged Broto-Moreau autocorrelation of lag 4 weighted by Pauling electronegativity
AATS5pe	Averaged Broto-Moreau autocorrelation of lag 5 weighted by Pauling electronegativity
AATS6pe	Averaged Broto-Moreau autocorrelation of lag 6 weighted by Pauling electronegativity
AATS7pe	Averaged Broto-Moreau autocorrelation of lag 7 weighted by Pauling electronegativity
AATS8pe	Averaged Broto-Moreau autocorrelation of lag 8 weighted by Pauling electronegativity

Name	Description
AATS0are	Averaged Broto-Moreau autocorrelation of lag 0 weighted by Allred-Rocow electronegativity
AATS1are	Averaged Broto-Moreau autocorrelation of lag 1 weighted by Allred-Rocow electronegativity
AATS2are	Averaged Broto-Moreau autocorrelation of lag 2 weighted by Allred-Rocow electronegativity
AATS3are	Averaged Broto-Moreau autocorrelation of lag 3 weighted by Allred-Rocow electronegativity
AATS4are	Averaged Broto-Moreau autocorrelation of lag 4 weighted by Allred-Rocow electronegativity
AATS5are	Averaged Broto-Moreau autocorrelation of lag 5 weighted by Allred-Rocow electronegativity
AATS6are	Averaged Broto-Moreau autocorrelation of lag 6 weighted by Allred-Rocow electronegativity
AATS7are	Averaged Broto-Moreau autocorrelation of lag 7 weighted by Allred-Rocow electronegativity
AATS8are	Averaged Broto-Moreau autocorrelation of lag 8 weighted by Allred-Rocow electronegativity

5.8.3 Centered Broto-Moreau autocorrelation

Name	Description
ATSC0c	Centered Broto-Moreau autocorrelation of lag 0 weighted by atomic charge
ATSC1c	Centered Broto-Moreau autocorrelation of lag 1 weighted by atomic charge
ATSC2c	Centered Broto-Moreau autocorrelation of lag 2 weighted by atomic charge
ATSC3c	Centered Broto-Moreau autocorrelation of lag 3 weighted by atomic charge
ATSC4c	Centered Broto-Moreau autocorrelation of lag 4 weighted by atomic charge
ATSC5c	Centered Broto-Moreau autocorrelation of lag 5 weighted by atomic charge
ATSC6c	Centered Broto-Moreau autocorrelation of lag 6 weighted by atomic charge
ATSC7c	Centered Broto-Moreau autocorrelation of lag 7 weighted by atomic charge
ATSC8c	Centered Broto-Moreau autocorrelation of lag 8 weighted by atomic charge

Name	Description
ATSC0d	Centered Broto-Moreau autocorrelation of lag 0 weighted by sigma electrons
ATSC1d	Centered Broto-Moreau autocorrelation of lag 1 weighted by sigma electrons
ATSC2d	Centered Broto-Moreau autocorrelation of lag 2 weighted by sigma electrons
ATSC3d	Centered Broto-Moreau autocorrelation of lag 3 weighted by sigma electrons
ATSC4d	Centered Broto-Moreau autocorrelation of lag 4 weighted by sigma electrons
ATSC5d	Centered Broto-Moreau autocorrelation of lag 5 weighted by sigma electrons
ATSC6d	Centered Broto-Moreau autocorrelation of lag 6 weighted by sigma electrons
ATSC7d	Centered Broto-Moreau autocorrelation of lag 7 weighted by sigma electrons
ATSC8d	Centered Broto-Moreau autocorrelation of lag 8 weighted by sigma electrons

Name	Description
ATSC0e	Centered Broto-Moreau autocorrelation of lag 0 weighted by Sanderson atomic electronegativity
ATSC1e	Centered Broto-Moreau autocorrelation of lag 1 weighted by Sanderson atomic electronegativity
ATSC2e	Centered Broto-Moreau autocorrelation of lag 2 weighted by Sanderson atomic electronegativity
ATSC3e	Centered Broto-Moreau autocorrelation of lag 3 weighted by Sanderson atomic electronegativity

Name	Description
ATSC4e	Centered Broto-Moreau autocorrelation of lag 4 weighted by Sanderson atomic electronegativity
ATSC5e	Centered Broto-Moreau autocorrelation of lag 5 weighted by Sanderson atomic electronegativity
ATSC6e	Centered Broto-Moreau autocorrelation of lag 6 weighted by Sanderson atomic electronegativity
ATSC7e	Centered Broto-Moreau autocorrelation of lag 7 weighted by Sanderson atomic electronegativity
ATSC8e	Centered Broto-Moreau autocorrelation of lag 8 weighted by Sanderson atomic electronegativity

Name	Description
ATSC0i	Centered Broto-Moreau autocorrelation of lag 0 weighted by atomic first ionization potential
ATSC1i	Centered Broto-Moreau autocorrelation of lag 1 weighted by atomic first ionization potential
ATSC2i	Centered Broto-Moreau autocorrelation of lag 2 weighted by atomic first ionization potential
ATSC3i	Centered Broto-Moreau autocorrelation of lag 3 weighted by atomic first ionization potential
ATSC4i	Centered Broto-Moreau autocorrelation of lag 4 weighted by atomic first ionization potential
ATSC5i	Centered Broto-Moreau autocorrelation of lag 5 weighted by atomic first ionization potential
ATSC6i	Centered Broto-Moreau autocorrelation of lag 6 weighted by atomic first ionization potential
ATSC7i	Centered Broto-Moreau autocorrelation of lag 7 weighted by atomic first ionization potential
ATSC8i	Centered Broto-Moreau autocorrelation of lag 8 weighted by atomic first ionization potential

Name	Description
ATSC0m	Centered Broto-Moreau autocorrelation of lag 0 weighted by atomic mass
ATSC1m	Centered Broto-Moreau autocorrelation of lag 1 weighted by atomic mass
ATSC2m	Centered Broto-Moreau autocorrelation of lag 2 weighted by atomic mass
ATSC3m	Centered Broto-Moreau autocorrelation of lag 3 weighted by atomic mass
ATSC4m	Centered Broto-Moreau autocorrelation of lag 4 weighted by atomic mass
ATSC5m	Centered Broto-Moreau autocorrelation of lag 5 weighted by atomic mass
ATSC6m	Centered Broto-Moreau autocorrelation of lag 6 weighted by atomic mass
ATSC7m	Centered Broto-Moreau autocorrelation of lag 7 weighted by atomic mass
ATSC8m	Centered Broto-Moreau autocorrelation of lag 8 weighted by atomic mass

Name	Description
ATSC0p	Centered Broto-Moreau autocorrelation of lag 0 weighted by atomic polarizability
ATSC1p	Centered Broto-Moreau autocorrelation of lag 1 weighted by atomic polarizability
ATSC2p	Centered Broto-Moreau autocorrelation of lag 2 weighted by atomic polarizability
ATSC3p	Centered Broto-Moreau autocorrelation of lag 3 weighted by atomic polarizability
ATSC4p	Centered Broto-Moreau autocorrelation of lag 4 weighted by atomic polarizability
ATSC5p	Centered Broto-Moreau autocorrelation of lag 5 weighted by atomic polarizability
ATSC6p	Centered Broto-Moreau autocorrelation of lag 6 weighted by atomic polarizability
ATSC7p	Centered Broto-Moreau autocorrelation of lag 7 weighted by atomic polarizability
ATSC8p	Centered Broto-Moreau autocorrelation of lag 8 weighted by atomic polarizability

Name	Description
ATSC0s	Centered Broto-Moreau autocorrelation of lag 0 weighted by atomic intrinsic state
ATSC1s	Centered Broto-Moreau autocorrelation of lag 1 weighted by atomic intrinsic state
ATSC2s	Centered Broto-Moreau autocorrelation of lag 2 weighted by atomic intrinsic state
ATSC3s	Centered Broto-Moreau autocorrelation of lag 3 weighted by atomic intrinsic state
ATSC4s	Centered Broto-Moreau autocorrelation of lag 4 weighted by atomic intrinsic state
ATSC5s	Centered Broto-Moreau autocorrelation of lag 5 weighted by atomic intrinsic state
ATSC6s	Centered Broto-Moreau autocorrelation of lag 6 weighted by atomic intrinsic state
ATSC7s	Centered Broto-Moreau autocorrelation of lag 7 weighted by atomic intrinsic state
ATSC8s	Centered Broto-Moreau autocorrelation of lag 8 weighted by atomic intrinsic state

Name	Description
ATSC0v	Centered Broto-Moreau autocorrelation of lag 0 weighted by van der Waals atomic volume
ATSC1v	Centered Broto-Moreau autocorrelation of lag 1 weighted by van der Waals atomic volume
ATSC2v	Centered Broto-Moreau autocorrelation of lag 2 weighted by van der Waals atomic volume
ATSC3v	Centered Broto-Moreau autocorrelation of lag 3 weighted by van der Waals atomic volume
ATSC4v	Centered Broto-Moreau autocorrelation of lag 4 weighted by van der Waals atomic volume
ATSC5v	Centered Broto-Moreau autocorrelation of lag 5 weighted by van der Waals atomic volume
ATSC6v	Centered Broto-Moreau autocorrelation of lag 6 weighted by van der Waals atomic volume
ATSC7v	Centered Broto-Moreau autocorrelation of lag 7 weighted by van der Waals atomic volume
ATSC8v	Centered Broto-Moreau autocorrelation of lag 8 weighted by van der Waals atomic volume

Name	Description
ATSC0Z	Centered Broto-Moreau autocorrelation of lag 0 weighted by atomic number
ATSC1Z	Centered Broto-Moreau autocorrelation of lag 1 weighted by atomic number
ATSC2Z	Centered Broto-Moreau autocorrelation of lag 2 weighted by atomic number
ATSC3Z	Centered Broto-Moreau autocorrelation of lag 3 weighted by atomic number
ATSC4Z	Centered Broto-Moreau autocorrelation of lag 4 weighted by atomic number
ATSC5Z	Centered Broto-Moreau autocorrelation of lag 5 weighted by atomic number
ATSC6Z	Centered Broto-Moreau autocorrelation of lag 6 weighted by atomic number
ATSC7Z	Centered Broto-Moreau autocorrelation of lag 7 weighted by atomic number
ATSC8Z	Centered Broto-Moreau autocorrelation of lag 8 weighted by atomic number

Name	Description
ATSC0dv	Centered Broto-Moreau autocorrelation of lag 0 weighted by atomic valence
ATSC1dv	Centered Broto-Moreau autocorrelation of lag 1 weighted by atomic valence
ATSC2dv	Centered Broto-Moreau autocorrelation of lag 2 weighted by atomic valence
ATSC3dv	Centered Broto-Moreau autocorrelation of lag 3 weighted by atomic valence
ATSC4dv	Centered Broto-Moreau autocorrelation of lag 4 weighted by atomic valence
ATSC5dv	Centered Broto-Moreau autocorrelation of lag 5 weighted by atomic valence
ATSC6dv	Centered Broto-Moreau autocorrelation of lag 6 weighted by atomic valence
ATSC7dv	Centered Broto-Moreau autocorrelation of lag 7 weighted by atomic valence
ATSC8dv	Centered Broto-Moreau autocorrelation of lag 8 weighted by atomic valence

Name	Description
ATSC0pe	Centered Broto-Moreau autocorrelation of lag 0 weighted by Pauling electronegativity
ATSC1pe	Centered Broto-Moreau autocorrelation of lag 1 weighted by Pauling electronegativity
ATSC2pe	Centered Broto-Moreau autocorrelation of lag 2 weighted by Pauling electronegativity
ATSC3pe	Centered Broto-Moreau autocorrelation of lag 3 weighted by Pauling electronegativity
ATSC4pe	Centered Broto-Moreau autocorrelation of lag 4 weighted by Pauling electronegativity
ATSC5pe	Centered Broto-Moreau autocorrelation of lag 5 weighted by Pauling electronegativity
ATSC6pe	Centered Broto-Moreau autocorrelation of lag 6 weighted by Pauling electronegativity
ATSC7pe	Centered Broto-Moreau autocorrelation of lag 7 weighted by Pauling electronegativity
ATSC8pe	Centered Broto-Moreau autocorrelation of lag 8 weighted by Pauling electronegativity

Name	Description
ATSC0are	Centered Broto-Moreau autocorrelation of lag 0 weighted by Allred-Rocow electronegativity
ATSC1are	Centered Broto-Moreau autocorrelation of lag 1 weighted by Allred-Rocow electronegativity
ATSC2are	Centered Broto-Moreau autocorrelation of lag 2 weighted by Allred-Rocow electronegativity
ATSC3are	Centered Broto-Moreau autocorrelation of lag 3 weighted by Allred-Rocow electronegativity

Name	Description
ATSC4are	Centered Broto-Moreau autocorrelation of lag 4 weighted by Allred-Rocow electronegativity
ATSC5are	Centered Broto-Moreau autocorrelation of lag 5 weighted by Allred-Rocow electronegativity
ATSC6are	Centered Broto-Moreau autocorrelation of lag 6 weighted by Allred-Rocow electronegativity
ATSC7are	Centered Broto-Moreau autocorrelation of lag 7 weighted by Allred-Rocow electronegativity
ATSC8are	Centered Broto-Moreau autocorrelation of lag 8 weighted by Allred-Rocow electronegativity

5.8.4 Average centered Broto-Moreau autocorrelation

Name	Description
AATSC0c	Average centered Broto-Moreau autocorrelation of lag 0 weighted by atomic charge
AATSC1c	Average centered Broto-Moreau autocorrelation of lag 1 weighted by atomic charge
AATSC2c	Average centered Broto-Moreau autocorrelation of lag 2 weighted by atomic charge
AATSC3c	Average centered Broto-Moreau autocorrelation of lag 3 weighted by atomic charge
AATSC4c	Average centered Broto-Moreau autocorrelation of lag 4 weighted by atomic charge
AATSC5c	Average centered Broto-Moreau autocorrelation of lag 5 weighted by atomic charge
AATSC6c	Average centered Broto-Moreau autocorrelation of lag 6 weighted by atomic charge
AATSC7c	Average centered Broto-Moreau autocorrelation of lag 7 weighted by atomic charge
AATSC8c	Average centered Broto-Moreau autocorrelation of lag 8 weighted by atomic charge

Name	Description
AATSC0d	Average centered Broto-Moreau autocorrelation of lag 0 weighted by sigma electrons
AATSC1d	Average centered Broto-Moreau autocorrelation of lag 1 weighted by sigma electrons
AATSC2d	Average centered Broto-Moreau autocorrelation of lag 2 weighted by sigma electrons
AATSC3d	Average centered Broto-Moreau autocorrelation of lag 3 weighted by sigma electrons
AATSC4d	Average centered Broto-Moreau autocorrelation of lag 4 weighted by sigma electrons
AATSC5d	Average centered Broto-Moreau autocorrelation of lag 5 weighted by sigma electrons
AATSC6d	Average centered Broto-Moreau autocorrelation of lag 6 weighted by sigma electrons
AATSC7d	Average centered Broto-Moreau autocorrelation of lag 7 weighted by sigma electrons
AATSC8d	Average centered Broto-Moreau autocorrelation of lag 8 weighted by sigma electrons

Name	Description
AATSC0e	Average centered Broto-Moreau autocorrelation of lag 0 weighted by Sanderson atomic electronegativity
AATSC1e	Average centered Broto-Moreau autocorrelation of lag 1 weighted by Sanderson atomic electronegativity
AATSC2e	Average centered Broto-Moreau autocorrelation of lag 2 weighted by Sanderson atomic electronegativity
AATSC3e	Average centered Broto-Moreau autocorrelation of lag 3 weighted by Sanderson atomic electronegativity
AATSC4e	Average centered Broto-Moreau autocorrelation of lag 4 weighted by Sanderson atomic electronegativity
AATSC5e	Average centered Broto-Moreau autocorrelation of lag 5 weighted by Sanderson atomic electronegativity
AATSC6e	Average centered Broto-Moreau autocorrelation of lag 6 weighted by Sanderson atomic electronegativity
AATSC7e	Average centered Broto-Moreau autocorrelation of lag 7 weighted by Sanderson atomic electronegativity
AATSC8e	Average centered Broto-Moreau autocorrelation of lag 8 weighted by Sanderson atomic electronegativity

Name	Description
AATSC0i	Average centered Broto-Moreau autocorrelation of lag 0 weighted by atomic first ionization potential
AATSC1i	Average centered Broto-Moreau autocorrelation of lag 1 weighted by atomic first ionization potential
AATSC2i	Average centered Broto-Moreau autocorrelation of lag 2 weighted by atomic first ionization potential
AATSC3i	Average centered Broto-Moreau autocorrelation of lag 3 weighted by atomic first ionization potential
AATSC4i	Average centered Broto-Moreau autocorrelation of lag 4 weighted by atomic first ionization potential
AATSC5i	Average centered Broto-Moreau autocorrelation of lag 5 weighted by atomic first ionization potential
AATSC6i	Average centered Broto-Moreau autocorrelation of lag 6 weighted by atomic first ionization potential
AATSC7i	Average centered Broto-Moreau autocorrelation of lag 7 weighted by atomic first ionization potential
AATSC8i	Average centered Broto-Moreau autocorrelation of lag 8 weighted by atomic first ionization potential

Name	Description
AATSC0m	Average centered Broto-Moreau autocorrelation of lag 0 weighted by atomic mass
AATSC1m	Average centered Broto-Moreau autocorrelation of lag 1 weighted by atomic mass
AATSC2m	Average centered Broto-Moreau autocorrelation of lag 2 weighted by atomic mass
AATSC3m	Average centered Broto-Moreau autocorrelation of lag 3 weighted by atomic mass
AATSC4m	Average centered Broto-Moreau autocorrelation of lag 4 weighted by atomic mass
AATSC5m	Average centered Broto-Moreau autocorrelation of lag 5 weighted by atomic mass
AATSC6m	Average centered Broto-Moreau autocorrelation of lag 6 weighted by atomic mass
AATSC7m	Average centered Broto-Moreau autocorrelation of lag 7 weighted by atomic mass
AATSC8m	Average centered Broto-Moreau autocorrelation of lag 8 weighted by atomic mass

Name	Description
AATSC0p	Average centered Broto-Moreau autocorrelation of lag 0 weighted by atomic polarizability
AATSC1p	Average centered Broto-Moreau autocorrelation of lag 1 weighted by atomic polarizability
AATSC2p	Average centered Broto-Moreau autocorrelation of lag 2 weighted by atomic polarizability
AATSC3p	Average centered Broto-Moreau autocorrelation of lag 3 weighted by atomic polarizability
AATSC4p	Average centered Broto-Moreau autocorrelation of lag 4 weighted by atomic polarizability
AATSC5p	Average centered Broto-Moreau autocorrelation of lag 5 weighted by atomic polarizability
AATSC6p	Average centered Broto-Moreau autocorrelation of lag 6 weighted by atomic polarizability
AATSC7p	Average centered Broto-Moreau autocorrelation of lag 7 weighted by atomic polarizability
AATSC8p	Average centered Broto-Moreau autocorrelation of lag 8 weighted by atomic polarizability

Name	Description
AATSC0s	Average centered Broto-Moreau autocorrelation of lag 0 weighted by atomic intrinsic state
AATSC1s	Average centered Broto-Moreau autocorrelation of lag 1 weighted by atomic intrinsic state
AATSC2s	Average centered Broto-Moreau autocorrelation of lag 2 weighted by atomic intrinsic state
AATSC3s	Average centered Broto-Moreau autocorrelation of lag 3 weighted by atomic intrinsic state
AATSC4s	Average centered Broto-Moreau autocorrelation of lag 4 weighted by atomic intrinsic state
AATSC5s	Average centered Broto-Moreau autocorrelation of lag 5 weighted by atomic intrinsic state
AATSC6s	Average centered Broto-Moreau autocorrelation of lag 6 weighted by atomic intrinsic state
AATSC7s	Average centered Broto-Moreau autocorrelation of lag 7 weighted by atomic intrinsic state
AATSC8s	Average centered Broto-Moreau autocorrelation of lag 8 weighted by atomic intrinsic state

Name	Description
AATSC0v	Average centered Broto-Moreau autocorrelation of lag 0 weighted by van der Waals atomic volume
AATSC1v	Average centered Broto-Moreau autocorrelation of lag 1 weighted by van der Waals atomic volume
AATSC2v	Average centered Broto-Moreau autocorrelation of lag 2 weighted by van der Waals atomic volume
AATSC3v	Average centered Broto-Moreau autocorrelation of lag 3 weighted by van der Waals atomic volume
AATSC4v	Average centered Broto-Moreau autocorrelation of lag 4 weighted by van der Waals atomic volume
AATSC5v	Average centered Broto-Moreau autocorrelation of lag 5 weighted by van der Waals atomic volume

Name	Description
AATSC6v	Average centered Broto-Moreau autocorrelation of lag 6 weighted by van der Waals atomic volume
AATSC7v	Average centered Broto-Moreau autocorrelation of lag 7 weighted by van der Waals atomic volume
AATSC8v	Average centered Broto-Moreau autocorrelation of lag 8 weighted by van der Waals atomic volume

Name	Description
AATSC0Z	Average centered Broto-Moreau autocorrelation of lag 0 weighted by atomic number
AATSC1Z	Average centered Broto-Moreau autocorrelation of lag 1 weighted by atomic number
AATSC2Z	Average centered Broto-Moreau autocorrelation of lag 2 weighted by atomic number
AATSC3Z	Average centered Broto-Moreau autocorrelation of lag 3 weighted by atomic number
AATSC4Z	Average centered Broto-Moreau autocorrelation of lag 4 weighted by atomic number
AATSC5Z	Average centered Broto-Moreau autocorrelation of lag 5 weighted by atomic number
AATSC6Z	Average centered Broto-Moreau autocorrelation of lag 6 weighted by atomic number
AATSC7Z	Average centered Broto-Moreau autocorrelation of lag 7 weighted by atomic number
AATSC8Z	Average centered Broto-Moreau autocorrelation of lag 8 weighted by atomic number

Name	Description
AATSC0dv	Average centered Broto-Moreau autocorrelation of lag 0 weighted by atomic valence
AATSC1dv	Average centered Broto-Moreau autocorrelation of lag 1 weighted by atomic valence
AATSC2dv	Average centered Broto-Moreau autocorrelation of lag 2 weighted by atomic valence
AATSC3dv	Average centered Broto-Moreau autocorrelation of lag 3 weighted by atomic valence
AATSC4dv	Average centered Broto-Moreau autocorrelation of lag 4 weighted by atomic valence
AATSC5dv	Average centered Broto-Moreau autocorrelation of lag 5 weighted by atomic valence
AATSC6dv	Average centered Broto-Moreau autocorrelation of lag 6 weighted by atomic valence
AATSC7dv	Average centered Broto-Moreau autocorrelation of lag 7 weighted by atomic valence
AATSC8dv	Average centered Broto-Moreau autocorrelation of lag 8 weighted by atomic valence

Name	Description
AATSC0pe	Average centered Broto-Moreau autocorrelation of lag 0 weighted by Pauling electronegativity
AATSC1pe	Average centered Broto-Moreau autocorrelation of lag 1 weighted by Pauling electronegativity
AATSC2pe	Average centered Broto-Moreau autocorrelation of lag 2 weighted by Pauling electronegativity
AATSC3pe	Average centered Broto-Moreau autocorrelation of lag 3 weighted by Pauling electronegativity
AATSC4pe	Average centered Broto-Moreau autocorrelation of lag 4 weighted by Pauling electronegativity
AATSC5pe	Average centered Broto-Moreau autocorrelation of lag 5 weighted by Pauling electronegativity
AATSC6pe	Average centered Broto-Moreau autocorrelation of lag 6 weighted by Pauling electronegativity
AATSC7pe	Average centered Broto-Moreau autocorrelation of lag 7 weighted by Pauling electronegativity
AATSC8pe	Average centered Broto-Moreau autocorrelation of lag 8 weighted by Pauling electronegativity

Name	Description
AATSC0are	Average centered Broto-Moreau autocorrelation of lag 0 weighted by Allred-Rocow electronegativity
AATSC1are	Average centered Broto-Moreau autocorrelation of lag 1 weighted by Allred-Rocow electronegativity
AATSC2are	Average centered Broto-Moreau autocorrelation of lag 2 weighted by Allred-Rocow electronegativity
AATSC3are	Average centered Broto-Moreau autocorrelation of lag 3 weighted by Allred-Rocow electronegativity
AATSC4are	Average centered Broto-Moreau autocorrelation of lag 4 weighted by Allred-Rocow electronegativity
AATSC5are	Average centered Broto-Moreau autocorrelation of lag 5 weighted by Allred-Rocow electronegativity

Name	Description
AATSC6are	Average centered Broto-Moreau autocorrelation of lag 6 weighted by Allred-Rocow electronegativity
AATSC7are	Average centered Broto-Moreau autocorrelation of lag 7 weighted by Allred-Rocow electronegativity
AATSC8are	Average centered Broto-Moreau autocorrelation of lag 8 weighted by Allred-Rocow electronegativity

5.8.5 Moran autocorrelation

Name	Description
MATS1c	Moran autocorrelation of lag 1 weighted by atomic charge
MATS2c	Moran autocorrelation of lag 2 weighted by atomic charge
MATS3c	Moran autocorrelation of lag 3 weighted by atomic charge
MATS4c	Moran autocorrelation of lag 4 weighted by atomic charge
MATS5c	Moran autocorrelation of lag 5 weighted by atomic charge
MATS6c	Moran autocorrelation of lag 6 weighted by atomic charge
MATS7c	Moran autocorrelation of lag 7 weighted by atomic charge
MATS8c	Moran autocorrelation of lag 8 weighted by atomic charge

Name	Description
MATS1d	Moran autocorrelation of lag 1 weighted by sigma electrons
MATS2d	Moran autocorrelation of lag 2 weighted by sigma electrons
MATS3d	Moran autocorrelation of lag 3 weighted by sigma electrons
MATS4d	Moran autocorrelation of lag 4 weighted by sigma electrons
MATS5d	Moran autocorrelation of lag 5 weighted by sigma electrons
MATS6d	Moran autocorrelation of lag 6 weighted by sigma electrons
MATS7d	Moran autocorrelation of lag 7 weighted by sigma electrons
MATS8d	Moran autocorrelation of lag 8 weighted by sigma electrons

Name	Description
MATS1e	Moran autocorrelation of lag 1 weighted by Sanderson atomic electronegativity
MATS2e	Moran autocorrelation of lag 2 weighted by Sanderson atomic electronegativity
MATS3e	Moran autocorrelation of lag 3 weighted by Sanderson atomic electronegativity
MATS4e	Moran autocorrelation of lag 4 weighted by Sanderson atomic electronegativity
MATS5e	Moran autocorrelation of lag 5 weighted by Sanderson atomic electronegativity
MATS6e	Moran autocorrelation of lag 6 weighted by Sanderson atomic electronegativity
MATS7e	Moran autocorrelation of lag 7 weighted by Sanderson atomic electronegativity
MATS8e	Moran autocorrelation of lag 8 weighted by Sanderson atomic electronegativity

Name	Description
MATS1i	Moran autocorrelation of lag 1 weighted by atomic first ionization potential
MATS2i	Moran autocorrelation of lag 2 weighted by atomic first ionization potential
MATS3i	Moran autocorrelation of lag 3 weighted by atomic first ionization potential
MATS4i	Moran autocorrelation of lag 4 weighted by atomic first ionization potential
MATS5i	Moran autocorrelation of lag 5 weighted by atomic first ionization potential
MATS6i	Moran autocorrelation of lag 6 weighted by atomic first ionization potential
MATS7i	Moran autocorrelation of lag 7 weighted by atomic first ionization potential
MATS8i	Moran autocorrelation of lag 8 weighted by atomic first ionization potential

Name	Description
MATS1m	Moran autocorrelation of lag 1 weighted by atomic mass
MATS2m	Moran autocorrelation of lag 2 weighted by atomic mass
MATS3m	Moran autocorrelation of lag 3 weighted by atomic mass
MATS4m	Moran autocorrelation of lag 4 weighted by atomic mass
MATS5m	Moran autocorrelation of lag 5 weighted by atomic mass
MATS6m	Moran autocorrelation of lag 6 weighted by atomic mass
MATS7m	Moran autocorrelation of lag 7 weighted by atomic mass
MATS8m	Moran autocorrelation of lag 8 weighted by atomic mass

Name	Description
MATS1p	Moran autocorrelation of lag 1 weighted by atomic polarizability
MATS2p	Moran autocorrelation of lag 2 weighted by atomic polarizability
MATS3p	Moran autocorrelation of lag 3 weighted by atomic polarizability
MATS4p	Moran autocorrelation of lag 4 weighted by atomic polarizability
MATS5p	Moran autocorrelation of lag 5 weighted by atomic polarizability
MATS6p	Moran autocorrelation of lag 6 weighted by atomic polarizability
MATS7p	Moran autocorrelation of lag 7 weighted by atomic polarizability
MATS8p	Moran autocorrelation of lag 8 weighted by atomic polarizability

Name	Description
MATS1s	Moran autocorrelation of lag 1 weighted by atomic intrinsic state
MATS2s	Moran autocorrelation of lag 2 weighted by atomic intrinsic state
MATS3s	Moran autocorrelation of lag 3 weighted by atomic intrinsic state
MATS4s	Moran autocorrelation of lag 4 weighted by atomic intrinsic state
MATS5s	Moran autocorrelation of lag 5 weighted by atomic intrinsic state
MATS6s	Moran autocorrelation of lag 6 weighted by atomic intrinsic state
MATS7s	Moran autocorrelation of lag 7 weighted by atomic intrinsic state
MATS8s	Moran autocorrelation of lag 8 weighted by atomic intrinsic state

Name	Description
MATS1v	Moran autocorrelation of lag 1 weighted by van der Waals atomic volume
MATS2v	Moran autocorrelation of lag 2 weighted by van der Waals atomic volume
MATS3v	Moran autocorrelation of lag 3 weighted by van der Waals atomic volume
MATS4v	Moran autocorrelation of lag 4 weighted by van der Waals atomic volume
MATS5v	Moran autocorrelation of lag 5 weighted by van der Waals atomic volume
MATS6v	Moran autocorrelation of lag 6 weighted by van der Waals atomic volume
MATS7v	Moran autocorrelation of lag 7 weighted by van der Waals atomic volume
MATS8v	Moran autocorrelation of lag 8 weighted by van der Waals atomic volume

Name	Description
MATS1Z	Moran autocorrelation of lag 1 weighted by atomic number
MATS2Z	Moran autocorrelation of lag 2 weighted by atomic number
MATS3Z	Moran autocorrelation of lag 3 weighted by atomic number
MATS4Z	Moran autocorrelation of lag 4 weighted by atomic number
MATS5Z	Moran autocorrelation of lag 5 weighted by atomic number
MATS6Z	Moran autocorrelation of lag 6 weighted by atomic number
MATS7Z	Moran autocorrelation of lag 7 weighted by atomic number
MATS8Z	Moran autocorrelation of lag 8 weighted by atomic number

Name	Description
MATS1dv	Moran autocorrelation of lag 1 weighted by atomic valence
MATS2dv	Moran autocorrelation of lag 2 weighted by atomic valence
MATS3dv	Moran autocorrelation of lag 3 weighted by atomic valence
MATS4dv	Moran autocorrelation of lag 4 weighted by atomic valence
MATS5dv	Moran autocorrelation of lag 5 weighted by atomic valence
MATS6dv	Moran autocorrelation of lag 6 weighted by atomic valence
MATS7dv	Moran autocorrelation of lag 7 weighted by atomic valence
MATS8dv	Moran autocorrelation of lag 8 weighted by atomic valence

Name	Description
MATS1pe	Moran autocorrelation of lag 1 weighted by Pauling electronegativity
MATS2pe	Moran autocorrelation of lag 2 weighted by Pauling electronegativity
MATS3pe	Moran autocorrelation of lag 3 weighted by Pauling electronegativity
MATS4pe	Moran autocorrelation of lag 4 weighted by Pauling electronegativity
MATS5pe	Moran autocorrelation of lag 5 weighted by Pauling electronegativity
MATS6pe	Moran autocorrelation of lag 6 weighted by Pauling electronegativity
MATS7pe	Moran autocorrelation of lag 7 weighted by Pauling electronegativity
MATS8pe	Moran autocorrelation of lag 8 weighted by Pauling electronegativity

Name	Description
MATS1are	Moran autocorrelation of lag 1 weighted by Allred-Rocow electronegativity
MATS2are	Moran autocorrelation of lag 2 weighted by Allred-Rocow electronegativity
MATS3are	Moran autocorrelation of lag 3 weighted by Allred-Rocow electronegativity
MATS4are	Moran autocorrelation of lag 4 weighted by Allred-Rocow electronegativity
MATS5are	Moran autocorrelation of lag 5 weighted by Allred-Rocow electronegativity
MATS6are	Moran autocorrelation of lag 6 weighted by Allred-Rocow electronegativity
MATS7are	Moran autocorrelation of lag 7 weighted by Allred-Rocow electronegativity
MATS8are	Moran autocorrelation of lag 8 weighted by Allred-Rocow electronegativity

5.8.6 Geary autocorrelation

Name	Description
GATS1c	Geary autocorrelation of lag 1 weighted by atomic charge
GATS2c	Geary autocorrelation of lag 2 weighted by atomic charge
GATS3c	Geary autocorrelation of lag 3 weighted by atomic charge
GATS4c	Geary autocorrelation of lag 4 weighted by atomic charge
GATS5c	Geary autocorrelation of lag 5 weighted by atomic charge
GATS6c	Geary autocorrelation of lag 6 weighted by atomic charge
GATS7c	Geary autocorrelation of lag 7 weighted by atomic charge
GATS8c	Geary autocorrelation of lag 8 weighted by atomic charge

Name	Description
GATS1d	Geary autocorrelation of lag 1 weighted by sigma electrons
GATS2d	Geary autocorrelation of lag 2 weighted by sigma electrons
GATS3d	Geary autocorrelation of lag 3 weighted by sigma electrons
GATS4d	Geary autocorrelation of lag 4 weighted by sigma electrons
GATS5d	Geary autocorrelation of lag 5 weighted by sigma electrons
GATS6d	Geary autocorrelation of lag 6 weighted by sigma electrons
GATS7d	Geary autocorrelation of lag 7 weighted by sigma electrons
GATS8d	Geary autocorrelation of lag 8 weighted by sigma electrons

Name	Description
GATS1e	Geary autocorrelation of lag 1 weighted by Sanderson atomic electronegativity
GATS2e	Geary autocorrelation of lag 2 weighted by Sanderson atomic electronegativity
GATS3e	Geary autocorrelation of lag 3 weighted by Sanderson atomic electronegativity
GATS4e	Geary autocorrelation of lag 4 weighted by Sanderson atomic electronegativity
GATS5e	Geary autocorrelation of lag 5 weighted by Sanderson atomic electronegativity
GATS6e	Geary autocorrelation of lag 6 weighted by Sanderson atomic electronegativity
GATS7e	Geary autocorrelation of lag 7 weighted by Sanderson atomic electronegativity
GATS8e	Geary autocorrelation of lag 8 weighted by Sanderson atomic electronegativity

Name	Description
GATS1i	Geary autocorrelation of lag 1 weighted by atomic first ionization potential
GATS2i	Geary autocorrelation of lag 2 weighted by atomic first ionization potential
GATS3i	Geary autocorrelation of lag 3 weighted by atomic first ionization potential
GATS4i	Geary autocorrelation of lag 4 weighted by atomic first ionization potential
GATS5i	Geary autocorrelation of lag 5 weighted by atomic first ionization potential
GATS6i	Geary autocorrelation of lag 6 weighted by atomic first ionization potential
GATS7i	Geary autocorrelation of lag 7 weighted by atomic first ionization potential
GATS8i	Geary autocorrelation of lag 8 weighted by atomic first ionization potential

Name	Description
GATS1m	Geary autocorrelation of lag 1 weighted by atomic mass
GATS2m	Geary autocorrelation of lag 2 weighted by atomic mass
GATS3m	Geary autocorrelation of lag 3 weighted by atomic mass
GATS4m	Geary autocorrelation of lag 4 weighted by atomic mass
GATS5m	Geary autocorrelation of lag 5 weighted by atomic mass
GATS6m	Geary autocorrelation of lag 6 weighted by atomic mass
GATS7m	Geary autocorrelation of lag 7 weighted by atomic mass
GATS8m	Geary autocorrelation of lag 8 weighted by atomic mass

Name	Description
GATS1p	Geary autocorrelation of lag 1 weighted by atomic polarizability
GATS2p	Geary autocorrelation of lag 2 weighted by atomic polarizability
GATS3p	Geary autocorrelation of lag 3 weighted by atomic polarizability
GATS4p	Geary autocorrelation of lag 4 weighted by atomic polarizability
GATS5p	Geary autocorrelation of lag 5 weighted by atomic polarizability
GATS6p	Geary autocorrelation of lag 6 weighted by atomic polarizability
GATS7p	Geary autocorrelation of lag 7 weighted by atomic polarizability
GATS8p	Geary autocorrelation of lag 8 weighted by atomic polarizability

Name	Description
GATS1s	Geary autocorrelation of lag 1 weighted by atomic intrinsic state
GATS2s	Geary autocorrelation of lag 2 weighted by atomic intrinsic state
GATS3s	Geary autocorrelation of lag 3 weighted by atomic intrinsic state
GATS4s	Geary autocorrelation of lag 4 weighted by atomic intrinsic state
GATS5s	Geary autocorrelation of lag 5 weighted by atomic intrinsic state
GATS6s	Geary autocorrelation of lag 6 weighted by atomic intrinsic state
GATS7s	Geary autocorrelation of lag 7 weighted by atomic intrinsic state
GATS8s	Geary autocorrelation of lag 8 weighted by atomic intrinsic state

Name	Description
GATS1v	Geary autocorrelation of lag 1 weighted by van der Waals atomic volume
GATS2v	Geary autocorrelation of lag 2 weighted by van der Waals atomic volume
GATS3v	Geary autocorrelation of lag 3 weighted by van der Waals atomic volume
GATS4v	Geary autocorrelation of lag 4 weighted by van der Waals atomic volume
GATS5v	Geary autocorrelation of lag 5 weighted by van der Waals atomic volume
GATS6v	Geary autocorrelation of lag 6 weighted by van der Waals atomic volume
GATS7v	Geary autocorrelation of lag 7 weighted by van der Waals atomic volume
GATS8v	Geary autocorrelation of lag 8 weighted by van der Waals atomic volume

Name	Description
GATS1Z	Geary autocorrelation of lag 1 weighted by atomic number
GATS2Z	Geary autocorrelation of lag 2 weighted by atomic number
GATS3Z	Geary autocorrelation of lag 3 weighted by atomic number
GATS4Z	Geary autocorrelation of lag 4 weighted by atomic number
GATS5Z	Geary autocorrelation of lag 5 weighted by atomic number
GATS6Z	Geary autocorrelation of lag 6 weighted by atomic number
GATS7Z	Geary autocorrelation of lag 7 weighted by atomic number
GATS8Z	Geary autocorrelation of lag 8 weighted by atomic number

Name	Description
GATS1dv	Geary autocorrelation of lag 1 weighted by atomic valence
GATS2dv	Geary autocorrelation of lag 2 weighted by atomic valence
GATS3dv	Geary autocorrelation of lag 3 weighted by atomic valence
GATS4dv	Geary autocorrelation of lag 4 weighted by atomic valence
GATS5dv	Geary autocorrelation of lag 5 weighted by atomic valence
GATS6dv	Geary autocorrelation of lag 6 weighted by atomic valence
GATS7dv	Geary autocorrelation of lag 7 weighted by atomic valence
GATS8dv	Geary autocorrelation of lag 8 weighted by atomic valence

Name	Description
GATS1pe	Geary autocorrelation of lag 1 weighted by Pauling electronegativity
GATS2pe	Geary autocorrelation of lag 2 weighted by Pauling electronegativity
GATS3pe	Geary autocorrelation of lag 3 weighted by Pauling electronegativity
GATS4pe	Geary autocorrelation of lag 4 weighted by Pauling electronegativity
GATS5pe	Geary autocorrelation of lag 5 weighted by Pauling electronegativity
GATS6pe	Geary autocorrelation of lag 6 weighted by Pauling electronegativity
GATS7pe	Geary autocorrelation of lag 7 weighted by Pauling electronegativity
GATS8pe	Geary autocorrelation of lag 8 weighted by Pauling electronegativity

Name	Description
GATS1are	Geary autocorrelation of lag 1 weighted by Allred-Rocow electronegativity
GATS2are	Geary autocorrelation of lag 2 weighted by Allred-Rocow electronegativity
GATS3are	Geary autocorrelation of lag 3 weighted by Allred-Rocow electronegativity
GATS4are	Geary autocorrelation of lag 4 weighted by Allred-Rocow electronegativity
GATS5are	Geary autocorrelation of lag 5 weighted by Allred-Rocow electronegativity
GATS6are	Geary autocorrelation of lag 6 weighted by Allred-Rocow electronegativity
GATS7are	Geary autocorrelation of lag 7 weighted by Allred-Rocow electronegativity
GATS8are	Geary autocorrelation of lag 8 weighted by Allred-Rocow electronegativity

5.9 Barysz matrix

Name	Description
SpAbs_DzZ	Graph energy weighted by atomic number
SpMax_DzZ	Leading eigenvalue weighted by atomic number
SpDiam_DzZ	Spectral diameter weighted by atomic number
SpAD_DzZ	Spectral absolute deviation weighted by atomic number
SpMAD_DzZ	Spectral mean absolute deviation weighted by atomic number
EE_DzZ	Estrada-like index weighted by atomic number
SM1_DzZ	Order 1 spectral moment weighted by atomic number
VE1_DzZ	Coefficient sum of the last eigenvector weighted by atomic number
VE2_DzZ	Average coefficient sum of the last eigenvector weighted by atomic number
VE3_DzZ	Logarithmic coefficient sum of the last eigenvector weighted by atomic number
VR1_DzZ	Randic-like eigenvector-based index weighted by atomic number
VR2_DzZ	Normalized Randic-like eigenvector-based index weighted by atomic number
VR3_DzZ	Logarithmic Randic-like eigenvector-based index weighted by atomic number

Name	Description
SpAbs_Dzm	Graph energy weighted by atomic mass
SpMax_Dzm	Leading eigenvalue weighted by atomic mass
SpDiam_Dzm	Spectral diameter weighted by atomic mass
SpAD_Dzm	Spectral absolute deviation weighted by atomic mass
SpMAD_Dzm	Spectral mean absolute deviation weighted by atomic mass
EE_Dzm	Estrada-like index weighted by atomic mass
SM1_Dzm	Order 1 spectral moment weighted by atomic mass
VE1_Dzm	Coefficient sum of the last eigenvector weighted by atomic mass
VE2_Dzm	Average coefficient sum of the last eigenvector weighted by atomic mass
VE3_Dzm	Logarithmic coefficient sum of the last eigenvector weighted by atomic mass
VR1_Dzm	Randic-like eigenvector-based index weighted by atomic mass
VR2_Dzm	Normalized Randic-like eigenvector-based index weighted by atomic mass
VR3_Dzm	Logarithmic Randic-like eigenvector-based index weighted by atomic mass

Name	Description
SpAbs_Dze	Graph energy weighted by Sanderson atomic electronegativity
SpMax_Dze	Leading eigenvalue weighted by Sanderson atomic electronegativity
SpDiam_Dze	Spectral diameter weighted by Sanderson atomic electronegativity
SpAD_Dze	Spectral absolute deviation weighted by Sanderson atomic electronegativity
SpMAD_Dze	Spectral mean absolute deviation weighted by Sanderson atomic electronegativity
EE_Dze	Estrada-like index weighted by Sanderson atomic electronegativity
SM1_Dze	Order 1 spectral moment weighted by Sanderson atomic electronegativity
VE1_Dze	Coefficient sum of the last eigenvector weighted by Sanderson atomic electronegativity
VE2_Dze	Average coefficient sum of the last eigenvector weighted by Sanderson atomic electronegativity
VE3_Dze	Logarithmic coefficient sum of the last eigenvector weighted by Sanderson atomic electronegativity
VR1_Dze	Randic-like eigenvector-based index weighted by Sanderson atomic electronegativity
VR2_Dze	Normalized Randic-like eigenvector-based index weighted by Sanderson atomic electronegativity
VR3_Dze	Logarithmic Randic-like eigenvector-based index weighted by Sanderson atomic electronegativity

Name	Description
SpAbs_Dzp	Graph energy weighted by atomic polarizability
SpMax_Dzp	Leading eigenvalue weighted by atomic polarizability

Name	Description
SpDiam_Dzp	Spectral diameter weighted by atomic polarizability
SpAD_Dzp	Spectral absolute deviation weighted by atomic polarizability
SpMAD_Dzp	Spectral mean absolute deviation weighted by atomic polarizability
EE_Dzp	Estrada-like index weighted by atomic polarizability
SM1_Dzp	Order 1 spectral moment weighted by atomic polarizability
VE1_Dzp	Coefficient sum of the last eigenvector weighted by atomic polarizability
VE2_Dzp	Average coefficient sum of the last eigenvector weighted by atomic polarizability
VE3_Dzp	Logarithmic coefficient sum of the last eigenvector weighted by atomic polarizability
VR1_Dzp	Randic-like eigenvector-based index weighted by atomic polarizability
VR2_Dzp	Normalized Randic-like eigenvector-based index weighted by atomic polarizability
VR3_Dzp	Logarithmic Randic-like eigenvector-based index weighted by atomic polarizability

Name	Description
SpAbs_Dzi	Graph energy weighted by atomic first ionization potential
SpMax_Dzi	Leading eigenvalue weighted by atomic first ionization potential
SpDiam_Dzi	Spectral diameter weighted by atomic first ionization potential
SpAD_Dzi	Spectral absolute deviation weighted by atomic first ionization potential
SpMAD_Dzi	Spectral mean absolute deviation weighted by atomic first ionization potential
EE_Dzi	Estrada-like index weighted by atomic first ionization potential
SM1_Dzi	Order 1 spectral moment weighted by atomic first ionization potential
VE1_Dzi	Coefficient sum of the last eigenvector weighted by atomic first ionization potential
VE2_Dzi	Average coefficient sum of the last eigenvector weighted by atomic first ionization potential
VE3_Dzi	Logarithmic coefficient sum of the last eigenvector weighted by atomic first ionization potential
VR1_Dzi	Randic-like eigenvector-based index weighted by atomic first ionization potential
VR2_Dzi	Normalized Randic-like eigenvector-based index weighted by atomic first ionization potential
VR3_Dzi	Logarithmic Randic-like eigenvector-based index weighted by atomic first ionization potential

Name	Description
SpAbs_Dzs	Graph energy weighted by atomic intrinsic state (hydrogens included)
SpMax_Dzs	Leading eigenvalue weighted by atomic intrinsic state (hydrogens included)
SpDiam_Dzs	Spectral diameter weighted by atomic intrinsic state (hydrogens included)
SpAD_Dzs	Spectral absolute deviation weighted by atomic intrinsic state (hydrogens included)
SpMAD_Dzs	Spectral mean absolute deviation weighted by atomic intrinsic state (hydrogens included)
EE_Dzs	Estrada-like index weighted by atomic intrinsic state (hydrogens included)
SM1_Dzs	Order 1 spectral moment weighted by atomic intrinsic state (hydrogens included)
VE1_Dzs	Coefficient sum of the last eigenvector weighted by atomic intrinsic state (hydrogens included)
VE2_Dzs	Average coefficient sum of the last eigenvector weighted by atomic intrinsic state (hydrogens included)
VE3_Dzs	Logarithmic coefficient sum of the last eigenvector weighted by atomic intrinsic state (hydrogens included)
VR1_Dzs	Randic-like eigenvector-based index weighted by atomic intrinsic state (hydrogens included)
VR2_Dzs	Normalized Randic-like eigenvector-based index weighted by atomic intrinsic state (hydrogens included)
VR3_Dzs	Logarithmic Randic-like eigenvector-based index weighted by atomic intrinsic state (hydrogens included)

Name	Description
SpAbs_Dzpe	Graph energy weighted by Pauling electronegativity
SpMax_Dzpe	Leading eigenvalue weighted by Pauling electronegativity
SpDiam_Dzpe	Spectral diameter weighted by Pauling electronegativity
SpAD_Dzpe	Spectral absolute deviation weighted by Pauling electronegativity

Name	Description
SpMAD_Dzpe	Spectral mean absolute deviation weighted by Pauling electronegativity
EE_Dzpe	Estrada-like index weighted by Pauling electronegativity
SM1_Dzpe	Order 1 spectral moment weighted by Pauling electronegativity
VE1_Dzpe	Coefficient sum of the last eigenvector weighted by Pauling electronegativity
VE2_Dzpe	Average coefficient sum of the last eigenvector weighted by Pauling electronegativity
VE3_Dzpe	Logarithmic coefficient sum of the last eigenvector weighted by Pauling electronegativity
VR1_Dzpe	Randic-like eigenvector-based index weighted by Pauling electronegativity
VR2_Dzpe	Normalized Randic-like eigenvector-based index weighted by Pauling electronegativity
VR3_Dzpe	Logarithmic Randic-like eigenvector-based index weighted by Pauling electronegativity

Name	Description
SpAbs_Dzare	Graph energy weighted by Allred-Rocow electronegativity
SpMax_Dzare	Leading eigenvalue weighted by Allred-Rocow electronegativity
SpDiam_Dzare	Spectral diameter weighted by Allred-Rocow electronegativity
SpAD_Dzare	Spectral absolute deviation weighted by Allred-Rocow electronegativity
SpMAD_Dzare	Spectral mean absolute deviation weighted by Allred-Rocow electronegativity
EE_Dzare	Estrada-like index weighted by Allred-Rocow electronegativity
SM1_Dzare	Order 1 spectral moment weighted by Allred-Rocow electronegativity
VE1_Dzare	Coefficient sum of the last eigenvector weighted by Allred-Rocow electronegativity
VE2_Dzare	Average coefficient sum of the last eigenvector weighted by Allred-Rocow electronegativity
VE3_Dzare	Logarithmic coefficient sum of the last eigenvector weighted by Allred-Rocow electronegativity
VR1_Dzare	Randic-like eigenvector-based index weighted by Allred-Rocow electronegativity
VR2_Dzare	Normalized Randic-like eigenvector-based index weighted by Allred-Rocow electronegativity
VR3_Dzare	Logarithmic Randic-like eigenvector-based index weighted by Allred-Rocow electronegativity

Name	Description
SpAbs_Dzv	Graph energy weighted by van der Waals atomic volume
SpMax_Dzv	Leading eigenvalue weighted by van der Waals atomic volume
SpDiam_Dzv	Spectral diameter weighted by van der Waals atomic volume
SpAD_Dzv	Spectral absolute deviation weighted by van der Waals atomic volume
SpMAD_Dzv	Spectral mean absolute deviation weighted by van der Waals atomic volume
EE_Dzv	Estrada-like index weighted by van der Waals atomic volume
SM1_Dzv	Order 1 spectral moment weighted by van der Waals atomic volume
VE1_Dzv	Coefficient sum of the last eigenvector weighted by van der Waals atomic volume
VE2_Dzv	Average coefficient sum of the last eigenvector weighted by van der Waals atomic volume
VE3_Dzv	Logarithmic coefficient sum of the last eigenvector weighted by van der Waals atomic volume
VR1_Dzv	Randic-like eigenvector-based index weighted by van der Waals atomic volume
VR2_Dzv	Normalized Randic-like eigenvector-based index weighted by van der Waals atomic volume
VR3_Dzv	Logarithmic Randic-like eigenvector-based index weighted by van der Waals atomic volume

5.10 Basic groups count

Name	Description
nBase	Number of basic groups

5.11 BCUT

Name	Description
BCUTw-1l	First lowest eigenvalue of Burden matrix weighted by atomic weight

Name	Description
BCUTw-1h	First highest eigenvalue of Burden matrix weighted by atomic weight
BCUTc-1l	First lowest eigenvalue of Burden matrix weighted by partial charge (Gasteiger Marsilli)
BCUTc-1h	First highest eigenvalue of Burden matrix weighted by partial charge (Gasteiger Marsilli)
BCUTp-1l	First lowest eigenvalue of Burden matrix weighted by atomic polarizability
BCUTp-1h	First highest eigenvalue of Burden matrix weighted by atomic polarizability

5.12 Bond count

Name	Description
nBonds	Bonds count (no hydrogens)
nBonds2	Bonds count
nBondsS	Single bonds count
nBondsS2	Single bonds count (no aromatic bonds)
nBondsS3	Single bonds count (no hydrogens and aromatic bonds)
nBondsD	Double bonds count
nBondsD2	Double bonds count (no aromatic bonds)
nBondsT	Triple bonds count
nBondsQ	Quadruple bonds count
nBondsM	Bonds of order bigger than 1 count

5.13 Bonded atoms polarizabilities

Name	Description
bpol	Sum of the absolute value of the difference between atomic polarizabilities of all bonded atoms in the molecule (including implicit hydrogens)

5.14 Burden modified eigenvalues

Name	Description
SpMin1_Bhe	1st lowest absolute eigenvalue of Burden modified matrix weighted by Sanderson atomic electronegativity
SpMin2_Bhe	2nd lowest absolute eigenvalue of Burden modified matrix weighted by Sanderson atomic electronegativity
SpMin3_Bhe	3rd lowest absolute eigenvalue of Burden modified matrix weighted by Sanderson atomic electronegativity
SpMin4_Bhe	4th lowest absolute eigenvalue of Burden modified matrix weighted by Sanderson atomic electronegativity
SpMin5_Bhe	5th lowest absolute eigenvalue of Burden modified matrix weighted by Sanderson atomic electronegativity
SpMin6_Bhe	6th lowest absolute eigenvalue of Burden modified matrix weighted by Sanderson atomic electronegativity
SpMin7_Bhe	7th lowest absolute eigenvalue of Burden modified matrix weighted by Sanderson atomic electronegativity
SpMin8_Bhe	8th lowest absolute eigenvalue of Burden modified matrix weighted by Sanderson atomic electronegativity

Name	Description
SpMax1_Bhe	1st highest absolute eigenvalue of Burden modified matrix weighted by Sanderson atomic electronegativity
SpMax2_Bhe	2nd highest absolute eigenvalue of Burden modified matrix weighted by Sanderson atomic electronegativity
SpMax3_Bhe	3rd highest absolute eigenvalue of Burden modified matrix weighted by Sanderson atomic electronegativity
SpMax4_Bhe	4th highest absolute eigenvalue of Burden modified matrix weighted by Sanderson atomic electronegativity
SpMax5_Bhe	5th highest absolute eigenvalue of Burden modified matrix weighted by Sanderson atomic electronegativity
SpMax6_Bhe	6th highest absolute eigenvalue of Burden modified matrix weighted by Sanderson atomic electronegativity
SpMax7_Bhe	7th highest absolute eigenvalue of Burden modified matrix weighted by Sanderson atomic electronegativity
SpMax8_Bhe	8th highest absolute eigenvalue of Burden modified matrix weighted by Sanderson atomic electronegativity

Name	Description
SpMin1_Bhi	1st lowest absolute eigenvalue of Burden modified matrix weighted by atomic first ionization potential
SpMin2_Bhi	2nd lowest absolute eigenvalue of Burden modified matrix weighted by atomic first ionization potential
SpMin3_Bhi	3rd lowest absolute eigenvalue of Burden modified matrix weighted by atomic first ionization potential
SpMin4_Bhi	4th lowest absolute eigenvalue of Burden modified matrix weighted by atomic first ionization potential
SpMin5_Bhi	5th lowest absolute eigenvalue of Burden modified matrix weighted by atomic first ionization potential
SpMin6_Bhi	6th lowest absolute eigenvalue of Burden modified matrix weighted by atomic first ionization potential
SpMin7_Bhi	7th lowest absolute eigenvalue of Burden modified matrix weighted by atomic first ionization potential
SpMin8_Bhi	8th lowest absolute eigenvalue of Burden modified matrix weighted by atomic first ionization potential

Name	Description
SpMax1_Bhi	1st highest absolute eigenvalue of Burden modified matrix weighted by atomic first ionization potential
SpMax2_Bhi	2nd highest absolute eigenvalue of Burden modified matrix weighted by atomic first ionization potential
SpMax3_Bhi	3rd highest absolute eigenvalue of Burden modified matrix weighted by atomic first ionization potential
SpMax4_Bhi	4th highest absolute eigenvalue of Burden modified matrix weighted by atomic first ionization potential
SpMax5_Bhi	5th highest absolute eigenvalue of Burden modified matrix weighted by atomic first ionization potential
SpMax6_Bhi	6th highest absolute eigenvalue of Burden modified matrix weighted by atomic first ionization potential
SpMax7_Bhi	7th highest absolute eigenvalue of Burden modified matrix weighted by atomic first ionization potential
SpMax8_Bhi	8th highest absolute eigenvalue of Burden modified matrix weighted by atomic first ionization potential

Name	Description
SpMin1_Bhm	1st lowest absolute eigenvalue of Burden modified matrix weighted by atomic mass
SpMin2_Bhm	2nd lowest absolute eigenvalue of Burden modified matrix weighted by atomic mass
SpMin3_Bhm	3rd lowest absolute eigenvalue of Burden modified matrix weighted by atomic mass
SpMin4_Bhm	4th lowest absolute eigenvalue of Burden modified matrix weighted by atomic mass
SpMin5_Bhm	5th lowest absolute eigenvalue of Burden modified matrix weighted by atomic mass
SpMin6_Bhm	6th lowest absolute eigenvalue of Burden modified matrix weighted by atomic mass
SpMin7_Bhm	7th lowest absolute eigenvalue of Burden modified matrix weighted by atomic mass
SpMin8_Bhm	8th lowest absolute eigenvalue of Burden modified matrix weighted by atomic mass

Name	Description
SpMax1_Bhm	1st highest absolute eigenvalue of Burden modified matrix weighted by atomic mass
SpMax2_Bhm	2nd highest absolute eigenvalue of Burden modified matrix weighted by atomic mass
SpMax3_Bhm	3rd highest absolute eigenvalue of Burden modified matrix weighted by atomic mass
SpMax4_Bhm	4th highest absolute eigenvalue of Burden modified matrix weighted by atomic mass
SpMax5_Bhm	5th highest absolute eigenvalue of Burden modified matrix weighted by atomic mass
SpMax6_Bhm	6th highest absolute eigenvalue of Burden modified matrix weighted by atomic mass
SpMax7_Bhm	7th highest absolute eigenvalue of Burden modified matrix weighted by atomic mass
SpMax8_Bhm	8th highest absolute eigenvalue of Burden modified matrix weighted by atomic mass

Name	Description
SpMin1_Bhp	1st lowest absolute eigenvalue of Burden modified matrix weighted by atomic polarizability
SpMin2_Bhp	2nd lowest absolute eigenvalue of Burden modified matrix weighted by atomic polarizability
SpMin3_Bhp	3rd lowest absolute eigenvalue of Burden modified matrix weighted by atomic polarizability
SpMin4_Bhp	4th lowest absolute eigenvalue of Burden modified matrix weighted by atomic polarizability
SpMin5_Bhp	5th lowest absolute eigenvalue of Burden modified matrix weighted by atomic polarizability
SpMin6_Bhp	6th lowest absolute eigenvalue of Burden modified matrix weighted by atomic polarizability
SpMin7_Bhp	7th lowest absolute eigenvalue of Burden modified matrix weighted by atomic polarizability
SpMin8_Bhp	8th lowest absolute eigenvalue of Burden modified matrix weighted by atomic polarizability

Name	Description
SpMax1_Bhp	1st highest absolute eigenvalue of Burden modified matrix weighted by atomic polarizability
SpMax2_Bhp	2nd highest absolute eigenvalue of Burden modified matrix weighted by atomic polarizability
SpMax3_Bhp	3rd highest absolute eigenvalue of Burden modified matrix weighted by atomic polarizability
SpMax4_Bhp	4th highest absolute eigenvalue of Burden modified matrix weighted by atomic polarizability
SpMax5_Bhp	5th highest absolute eigenvalue of Burden modified matrix weighted by atomic polarizability
SpMax6_Bhp	6th highest absolute eigenvalue of Burden modified matrix weighted by atomic polarizability
SpMax7_Bhp	7th highest absolute eigenvalue of Burden modified matrix weighted by atomic polarizability
SpMax8_Bhp	8th highest absolute eigenvalue of Burden modified matrix weighted by atomic polarizability

Name	Description
SpMin1_Bhs	1st lowest absolute eigenvalue of Burden modified matrix weighted by atomic intrinsic state
SpMin2_Bhs	2nd lowest absolute eigenvalue of Burden modified matrix weighted by atomic intrinsic state
SpMin3_Bhs	3rd lowest absolute eigenvalue of Burden modified matrix weighted by atomic intrinsic state
SpMin4_Bhs	4th lowest absolute eigenvalue of Burden modified matrix weighted by atomic intrinsic state
SpMin5_Bhs	5th lowest absolute eigenvalue of Burden modified matrix weighted by atomic intrinsic state
SpMin6_Bhs	6th lowest absolute eigenvalue of Burden modified matrix weighted by atomic intrinsic state
SpMin7_Bhs	7th lowest absolute eigenvalue of Burden modified matrix weighted by atomic intrinsic state
SpMin8_Bhs	8th lowest absolute eigenvalue of Burden modified matrix weighted by atomic intrinsic state

Name	Description
SpMax1_Bhs	1st highest absolute eigenvalue of Burden modified matrix weighted by atomic intrinsic state
SpMax2_Bhs	2nd highest absolute eigenvalue of Burden modified matrix weighted by atomic intrinsic state
SpMax3_Bhs	3rd highest absolute eigenvalue of Burden modified matrix weighted by atomic intrinsic state
SpMax4_Bhs	4th highest absolute eigenvalue of Burden modified matrix weighted by atomic intrinsic state
SpMax5_Bhs	5th highest absolute eigenvalue of Burden modified matrix weighted by atomic intrinsic state
SpMax6_Bhs	6th highest absolute eigenvalue of Burden modified matrix weighted by atomic intrinsic state
SpMax7_Bhs	7th highest absolute eigenvalue of Burden modified matrix weighted by atomic intrinsic state
SpMax8_Bhs	8th highest absolute eigenvalue of Burden modified matrix weighted by atomic intrinsic state

Name	Description
SpMin1_Bhv	1st lowest absolute eigenvalue of Burden modified matrix weighted by van der Waals atomic volume
SpMin2_Bhv	2nd lowest absolute eigenvalue of Burden modified matrix weighted by van der Waals atomic volume
SpMin3_Bhv	3rd lowest absolute eigenvalue of Burden modified matrix weighted by van der Waals atomic volume
SpMin4_Bhv	4th lowest absolute eigenvalue of Burden modified matrix weighted by van der Waals atomic volume
SpMin5_Bhv	5th lowest absolute eigenvalue of Burden modified matrix weighted by van der Waals atomic volume
SpMin6_Bhv	6th lowest absolute eigenvalue of Burden modified matrix weighted by van der Waals atomic volume
SpMin7_Bhv	7th lowest absolute eigenvalue of Burden modified matrix weighted by van der Waals atomic volume
SpMin8_Bhv	8th lowest absolute eigenvalue of Burden modified matrix weighted by van der Waals atomic volume

Name	Description
SpMax1_Bhv	1st highest absolute eigenvalue of Burden modified matrix weighted by van der Waals atomic volume
SpMax2_Bhv	2nd highest absolute eigenvalue of Burden modified matrix weighted by van der Waals atomic volume
SpMax3_Bhv	3rd highest absolute eigenvalue of Burden modified matrix weighted by van der Waals atomic volume
SpMax4_Bhv	4th highest absolute eigenvalue of Burden modified matrix weighted by van der Waals atomic volume
SpMax5_Bhv	5th highest absolute eigenvalue of Burden modified matrix weighted by van der Waals atomic volume
SpMax6_Bhv	6th highest absolute eigenvalue of Burden modified matrix weighted by van der Waals atomic volume
SpMax7_Bhv	7th highest absolute eigenvalue of Burden modified matrix weighted by van der Waals atomic volume
SpMax8_Bhv	8th highest absolute eigenvalue of Burden modified matrix weighted by van der Waals atomic volume

5.15 Carbon types

Name	Description
C1SP1	Triply bonded carbon bound to one other carbon
C2SP1	Triply bonded carbon bound to two other carbons
C1SP2	Doubly bonded carbon bound to one other carbon
C2SP2	Doubly bonded carbon bound to two other carbons
C3SP2	Doubly bonded carbon bound to three other carbons
C1SP3	Singly bonded carbon bound to one other carbon
C2SP3	Singly bonded carbon bound to two other carbons
C3SP3	Singly bonded carbon bound to three other carbons
C4SP3	Singly bonded carbon bound to four other carbons

5.16 Chi chain

Name	Description
SCH-3	Simple chain of order 3
SCH-4	Simple chain of order 4
SCH-5	Simple chain of order 5
SCH-6	Simple chain of order 6
SCH-7	Simple chain of order 7
VCH-3	Valence chain order 3
VCH-4	Valence chain order 4
VCH-5	Valence chain order 5
VCH-6	Valence chain order 6
VCH-7	Valence chain order 7

5.17 Chi cluster

Name	Description
SC-3	Simple cluster of order 3
SC-4	Simple cluster of order 4
SC-5	Simple cluster of order 5
SC-6	Simple cluster of order 6
VC-3	Valence cluster order 3
VC-4	Valence cluster order 4
VC-5	Valence cluster order 5
VC-6	Valence cluster order 6

5.18 Chi path

Name	Description
SP-0	Simple path of order 0
SP-1	Simple path of order 1
SP-2	Simple path of order 2
SP-3	Simple path of order 3
SP-4	Simple path of order 4
SP-5	Simple path of order 5
SP-6	Simple path of order 6
SP-7	Simple path of order 7
ASP-0	Average simple path of order 0
ASP-1	Average simple path of order 1

Name	Description
ASP-2	Average simple path of order 2
ASP-3	Average simple path of order 3
ASP-4	Average simple path of order 4
ASP-5	Average simple path of order 5
ASP-6	Average simple path of order 6
ASP-7	Average simple path of order 7
VP-0	Valence path order 0
VP-1	Valence path order 1
VP-2	Valence path order 2
VP-3	Valence path order 3
VP-4	Valence path order 4
VP-5	Valence path order 5
VP-6	Valence path order 6
VP-7	Valence path order 7
AVP-0	Average valence path order 0
AVP-1	Average valence path order 1
AVP-2	Average valence path order 2
AVP-3	Average valence path order 3
AVP-4	Average valence path order 4
AVP-5	Average valence path order 5
AVP-6	Average valence path order 6
AVP-7	Average valence path order 7

5.19 Chi path cluster

Name	Description
SPC-4	Simple path cluster of order 4
SPC-5	Simple path cluster of order 5
SPC-6	Simple path cluster of order 6
VPC-4	Valence path cluster order 4
VPC-5	Valence path cluster order 5
VPC-6	Valence path cluster order 6

5.20 Constitutional

Name	Description
MZ	Mean of atomic number
Mi	Mean of atomic first ionization potential
Mp	Mean of atomic polarizability
Mpe	Mean of Pauling atomic electronegativity
Mv	Mean of van der Waals volume
Mse	Mean of Sanderson atomic electronegativity
Mare	Mean of Allred-Rochow atomic electronegativity
Si	Sum of atomic first ionization potential
Sp	Sum of atomic polarizability
Spe	Sum of Pauling atomic electronegativity
Sv	Sum of van der Waals volume
Sse	Sum of Sanderson atomic electronegativity
Sare	Sum of Allred-Rochow atomic electronegativity

5.21 Crippen LogP

Name	Description
CrippenLogP	Crippen LogP
CrippenMR	Crippen molar refractivity

5.22 Detour matrix

Name	Description
SpMax_Dz	Leading eigenvalue
SpDiam_Dz	Spectral diameter
SpAD_Dz	Spectral absolute deviation
SpMAD_Dz	Spectral mean absolute deviation
EE_Dz	Estrada-like index
VE1_Dz	Coefficient sum of the last eigenvector
VE2_Dz	Average coefficient sum of the last eigenvector
VE3_Dz	Logarithmic coefficient sum of the last eigenvector
VR1_Dz	Randic-like eigenvector-based index
VR2_Dz	Normalized Randic-like eigenvector-based index
VR3_Dz	Logarithmic Randic-like eigenvector-based index

5.23 Eccentric connectivity index

Name	Description
ECCEN	Eccentric connectivity index

5.24 Electrotological state index

Name	Description
nsLi	Count of (-Li) atom type E-State
nssBe	Count of (-Be-) atom type E-State
nssssBem	Count of (>Be<-2) atom type E-State
nssBH	Count of (-BH-) atom type E-State
nsssb	Count of (-B<) atom type E-State
nssssBm	Count of (>B<-) atom type E-State
nsCH3	Count of (-CH3) atom type E-State
ndCH2	Count of (=CH2) atom type E-State
nssCH2	Count of (-CH2-) atom type E-State
ntCH	Count of (#CH) atom type E-State
ndsCH	Count of (=CH-) atom type E-State
naaCH	Count of (:CH:) atom type E-State
nssCH	Count of (>CH-) atom type E-State
nddC	Count of (=C=) atom type E-State
ntsC	Count of (#C-) atom type E-State
ndssC	Count of (=C<) atom type E-State
naasC	Count of (:C:-) atom type E-State
naaaC	Count of (::C:) atom type E-State
nssssC	Count of (>C<) atom type E-State
nsNH3p	Count of (-NH3+) atom type E-State

Name	Description
nsNH2	Count of (-NH2) atom type E-State
nssNH2p	Count of (-NH2+) atom type E-State
ndNH	Count of (=NH) atom type E-State
nssNH	Count of (-NH-) atom type E-State
naaNH	Count of (:NH:) atom type E-State
ntN	Count of (#N) atom type E-State
nsssNHp	Count of (>NH+) atom type E-State
ndsN	Count of (=N-) atom type E-State
naaN	Count of (:N:) atom type E-State
nsssN	Count of (>N-) atom type E-State
nddsN	Count of (-N<<) atom type E-State
naasN	Count of (:N-) atom type E-State
nssssNp	Count of (>N<+) atom type E-State
nsOH	Count of (-OH) atom type E-State
ndO	Count of (=O) atom type E-State
nssO	Count of (-O-) atom type E-State
naaO	Count of (:O:) atom type E-State
nsF	Count of (-F) atom type E-State
nsSiH3	Count of (-SiH3) atom type E-State
nssSiH2	Count of (-SiH2-) atom type E-State
nsssSiH	Count of (>SiH-) atom type E-State
nssssSi	Count of (>Si<) atom type E-State
nsPH2	Count of (-PH2) atom type E-State
nssPH	Count of (-PH-) atom type E-State
nsssP	Count of (>P-) atom type E-State
ndsssP	Count of (->P=) atom type E-State
nsssssP	Count of (->P<) atom type E-State
nsSH	Count of (-SH) atom type E-State
ndS	Count of (=S) atom type E-State
nssS	Count of (-S-) atom type E-State
naaS	Count of (aSa) atom type E-State
ndssS	Count of (>S=) atom type E-State
nddsS	Count of (>S==) atom type E-State
nsCl	Count of (-Cl) atom type E-State
nsGeH3	Count of (-GeH3) atom type E-State
nssGeH2	Count of (-GeH2-) atom type E-State
nsssGeH	Count of (>GeH-) atom type E-State
nssssGe	Count of (>Ge<) atom type E-State
nsAsH2	Count of (-AsH2) atom type E-State
nssAsH	Count of (-AsH-) atom type E-State
nsssAs	Count of (>As-) atom type E-State
ndsssAs	Count of (->As=) atom type E-State
nsssssAs	Count of (->As<) atom type E-State
nsSeH	Count of (-SeH) atom type E-State
ndSe	Count of (=Se) atom type E-State
nssSe	Count of (-Se-) atom type E-State
naaSe	Count of (aSea) atom type E-State
ndssSe	Count of (>Se=) atom type E-State
nddsSe	Count of (-=Se=-) atom type E-State
nsBr	Count of (-Br) atom type E-State
nsSnH3	Count of (-SnH3) atom type E-State
nssSnH2	Count of (-SnH2-) atom type E-State
nsssSnH	Count of (>SnH-) atom type E-State
nssssSn	Count of (>Sn<) atom type E-State

Name	Description
nsI	Count of (-I) atom type E-State
nsPbH3	Count of (-PbH3) atom type E-State
nssPbH2	Count of (-PbH2-) atom type E-State
nsssPbH	Count of (>PbH-) atom type E-State
nssssPb	Count of (>Pb<) atom type E-State
nsBH2	Count of (-BH2) atom type E-State
naOm	Count of (:O-0.5) atom type E-State
nsOm	Count of (-O-) atom type E-State
nddsP	Count of (-=P=) atom type E-State
nssssssS	Count of (>S<<) atom type E-State
nSm	Count of (-S-) atom type E-State
nddsAs	Count of (-=As=) atom type E-State
nssssssSe	Count of (>Se<<) atom type E-State

Name	Description
nHBd	Count of (strong) hydrogen bond donors E-State
nwHBd	Count of weak hydrogen bond donors E-State
nHBa	Count of (strong) hydrogen bond acceptors E-State
nwHBa	Count of weak hydrogen bond acceptors E-State
nHBint2	Count of potential internal hydrogen bonds of path length 2 E-State
nHBint3	Count of potential internal hydrogen bonds of path length 3 E-State
nHBint4	Count of potential internal hydrogen bonds of path length 4 E-State
nHBint5	Count of potential internal hydrogen bonds of path length 5 E-State
nHBint6	Count of potential internal hydrogen bonds of path length 6 E-State
nHBint7	Count of potential internal hydrogen bonds of path length 7 E-State
nHBint8	Count of potential internal hydrogen bonds of path length 8 E-State
nHBint9	Count of potential internal hydrogen bonds of path length 9 E-State
nHBint10	Count of potential internal hydrogen bonds of path length 10 E-State
nHCHnX	Count of (CHnX) atom type H E-State
nHCsats	Count of (H on C sp3 bonded to saturated C) atom type E-State
nHCsatu	Count of (H on C sp3 bonded to unsaturated C) atom type E-State
nHAvin	Count of (H on C vinyl bonded to C aromatic) atom type E-State
nHother	Count of (H on aaCH, dCH2 or dsCH) atom type E-State
nHmisc	Count of atom types (H bonded to B, Si, P, Ge, As, Se, Sn or Pb) atom type E-State
nHsOH	Count (-OH) atom type H E-State
nHdNH	Count of (=NH) atom type H E-State
nHsSH	Count of (-SH) atom type H E-State
nHsNH2	Count of (-NH2) atom type H E-State
nHssNH	Count of (-NH-) atom type H E-State
nHaaNH	Count of (:NH:) atom type H E-State
nHsNpH3	Count of (-NH3+) atom type H E-State
nHssNpH2	Count of (-NH2+) atom type H E-State
nHssNpH	Count of (>NH+) atom type H E-State
nHtCH	Count of (#CH) atom type H E-State
nHdCH2	Count of (=CH2) atom type H E-State
nHdsCH	Count of (=CH-) atom type H E-State
nHaaCH	Count of (:CH:) atom type H E-State

Name	Description
SsLi	Sum of (-Li) atom type E-State
SssBe	Sum of (-Be-) atom type E-State
SssssBem	Sum of (>Be<-2) atom type E-State

Name	Description
SssBH	Sum of (-BH-) atom type E-State
SsssB	Sum of (-B<) atom type E-State
SssssBm	Sum of (>B<-) atom type E-State
SsCH3	Sum of (-CH3) atom type E-State
SdCH2	Sum of (=CH2) atom type E-State
SssCH2	Sum of (-CH2-) atom type E-State
StCH	Sum of (#CH) atom type E-State
SdsCH	Sum of (=CH-) atom type E-State
SaaCH	Sum of (:CH:) atom type E-State
SsssCH	Sum of (>CH-) atom type E-State
SddC	Sum of (=C=) atom type E-State
StsC	Sum of (#C-) atom type E-State
SdssC	Sum of (=C<) atom type E-State
SaasC	Sum of (:C:-) atom type E-State
SaaaC	Sum of (::C:) atom type E-State
SssssC	Sum of (>C<) atom type E-State
SsNH3p	Sum of (-NH3+) atom type E-State
SsNH2	Sum of (-NH2) atom type E-State
SssNH2p	Sum of (-NH2-+) atom type E-State
SdNH	Sum of (=NH) atom type E-State
SssNH	Sum of (-NH-) atom type E-State
SaaNH	Sum of (:NH:) atom type E-State
StN	Sum of (#N) atom type E-State
SsssNHp	Sum of (>NH-+) atom type E-State
SdsN	Sum of (=N-) atom type E-State
SaaN	Sum of (:N:) atom type E-State
SsssN	Sum of (>N-) atom type E-State
SddsN	Sum of (-N<<) atom type E-State
SaasN	Sum of (:N:-) atom type E-State
SssssNp	Sum of (>N<+) atom type E-State
SsOH	Sum of (-OH) atom type E-State
SdO	Sum of (=O) atom type E-State
SssO	Sum of (-O-) atom type E-State
SaaO	Sum of (:O:) atom type E-State
SsF	Sum of (-F) atom type E-State
SsSiH3	Sum of (-SiH3) atom type E-State
SssSiH2	Sum of (-SiH2-) atom type E-State
SsssSiH	Sum of (>SiH-) atom type E-State
SssssSi	Sum of (>Si<) atom type E-State
SsPH2	Sum of (-PH2) atom type E-State
SssPH	Sum of (-PH-) atom type E-State
SsssP	Sum of (>P-) atom type E-State
SdssP	Sum of (->P=) atom type E-State
SssssP	Sum of (->P<) atom type E-State
SsSH	Sum of (-SH) atom type E-State
SdS	Sum of (=S) atom type E-State
SssS	Sum of (-S-) atom type E-State
SaaS	Sum of (aSa) atom type E-State
SdssS	Sum of (>S=) atom type E-State
SddssS	Sum of (>S==) atom type E-State
SsCl	Sum of (-Cl) atom type E-State
SsGeH3	Sum of (-GeH3) atom type E-State
SssGeH2	Sum of (-GeH2-) atom type E-State
SsssGeH	Sum of (>GeH-) atom type E-State

Name	Description
SssssGe	Sum of (>Ge<) atom type E-State
SsAsH2	Sum of (-AsH2) atom type E-State
SssAsH	Sum of (-AsH-) atom type E-State
SsssAs	Sum of (>As-) atom type E-State
SdsssAs	Sum of (->As=) atom type E-State
SsssssAs	Sum of (->As<) atom type E-State
SsSeH	Sum of (-SeH) atom type E-State
SdSe	Sum of (=Se) atom type E-State
SssSe	Sum of (-Se-) atom type E-State
SaaSe	Sum of (aSea) atom type E-State
SdssSe	Sum of (>Se=) atom type E-State
SddssSe	Sum of (-=Se=-) atom type E-State
SsBr	Sum of (-Br) atom type E-State
SsSnH3	Sum of (-SnH3) atom type E-State
SssSnH2	Sum of (-SnH2-) atom type E-State
SsssSnH	Sum of (>SnH-) atom type E-State
SssssSn	Sum of (>Sn<) atom type E-State
SsI	Sum of (-I) atom type E-State
SsPbH3	Sum of (-PbH3) atom type E-State
SssPbH2	Sum of (-PbH2-) atom type E-State
SsssPbH	Sum of (>PbH-) atom type E-State
SssssPb	Sum of (>Pb<) atom type E-State
SsBH2	Sum of (-BH2) atom type E-State
SaOm	Sum of (:O-0.5) atom type E-State
SsOm	Sum of (-O-) atom type E-State
SddsP	Sum of (-=P=) atom type E-State
SssssssS	Sum of (>S<<) atom type E-State
SSm	Sum of (-S-) atom type E-State
SddsAs	Sum of (-=As=) atom type E-State
SssssssSe	Sum of (>Se<<) atom type E-State

Name	Description
SHBd	Sum of (strong) hydrogen bond donors E-State
SwHBd	Sum of weak hydrogen bond donors E-State
SHBa	Sum of (strong) hydrogen bond acceptors E-State
SwHBa	Sum of weak hydrogen bond acceptors E-State
SHBint2	Sum of potential internal hydrogen bonds of path length 2 E-State
SHBint3	Sum of potential internal hydrogen bonds of path length 3 E-State
SHBint4	Sum of potential internal hydrogen bonds of path length 4 E-State
SHBint5	Sum of potential internal hydrogen bonds of path length 5 E-State
SHBint6	Sum of potential internal hydrogen bonds of path length 6 E-State
SHBint7	Sum of potential internal hydrogen bonds of path length 7 E-State
SHBint8	Sum of potential internal hydrogen bonds of path length 8 E-State
SHBint9	Sum of potential internal hydrogen bonds of path length 9 E-State
SHBint10	Sum of potential internal hydrogen bonds of path length 10 E-State
SHCHnX	Sum of (CHnX) atom type H E-State
SHCsats	Sum of (H on C sp3 bonded to saturated C) atom type E-State
SHCsatu	Sum of (H on C sp3 bonded to unsaturated C) atom type E-State
SHAvin	Sum of (H on C vinyl bonded to C aromatic) atom type E-State
SHoher	Sum of (H on aaCH, dCH2 or dsCH) atom type E-State
SHmisc	Sum of atom types (H bonded to B, Si, P, Ge, As, Se, Sn or Pb) atom type E-State
SHsOH	Sum of (-OH) atom type H E-State
SHdNH	Sum of (=NH) atom type H E-State

Name	Description
SHsSH	Sum of (-SH) atom type H E-State
SHsNH2	Sum of (-NH2) atom type H E-State
SHssNH	Sum of (-NH-) atom type H E-State
SHaaNH	Sum of (:NH:) atom type H E-State
SHsNpH3	Sum of (-NH3+) atom type H E-State
SHssNpH2	Sum of (-NH2-+) atom type H E-State
SHssNpH	Sum of (>NH-+) atom type H E-State
SHtCH	Sum of (#CH) atom type H E-State
SHdCH2	Sum of (=CH2) atom type H E-State
SHdsCH	Sum of (=CH-) atom type H E-State
SHaaCH	Sum of (:CH:) atom type H E-State

Name	Description
minsLi	Minimum value of (-Li) atom type E-State
minssBe	Minimum value of (-Be-) atom type E-State
minssssBem	Minimum value of (>Be<-2) atom type E-State
minssBH	Minimum value of (-BH-) atom type E-State
minsssB	Minimum value of (-B<) atom type E-State
minssssBm	Minimum value of (>B<-) atom type E-State
minsCH3	Minimum value of (-CH3) atom type E-State
mindCH2	Minimum value of (=CH2) atom type E-State
minssCH2	Minimum value of (-CH2-) atom type E-State
mintCH	Minimum value of (#CH) atom type E-State
mindsCH	Minimum value of (=CH-) atom type E-State
minaaCH	Minimum value of (:CH:) atom type E-State
minsssCH	Minimum value of (>CH-) atom type E-State
minddC	Minimum value of (=C=) atom type E-State
mitsC	Minimum value of (#C-) atom type E-State
mindssC	Minimum value of (=C<) atom type E-State
minaasC	Minimum value of (:C:-) atom type E-State
minaaaC	Minimum value of (::C:) atom type E-State
minssssC	Minimum value of (>C<) atom type E-State
minsNH3p	Minimum value of (-NH3+) atom type E-State
minsNH2	Minimum value of (-NH2) atom type E-State
minssNH2p	Minimum value of (-NH2-+) atom type E-State
mindNH	Minimum value of (=NH) atom type E-State
minssNH	Minimum value of (-NH-) atom type E-State
minaaNH	Minimum value of (:NH:) atom type E-State
mintN	Minimum value of (#N) atom type E-State
minssNHp	Minimum value of (>NH-+) atom type E-State
mindsN	Minimum value of (=N-) atom type E-State
minaaN	Minimum value of (:N:) atom type E-State
minsssN	Minimum value of (>N-) atom type E-State
minddsN	Minimum value of (-N<<) atom type E-State
minaasN	Minimum value of (:N:-) atom type E-State
minssssNp	Minimum value of (>N<+) atom type E-State
minsOH	Minimum value of (-OH) atom type E-State
mindO	Minimum value of (=O) atom type E-State
minssO	Minimum value of (-O-) atom type E-State
minaaO	Minimum value of (:O:) atom type E-State
minsF	Minimum value of (-F) atom type E-State
minsSiH3	Minimum value of (-SiH3) atom type E-State
minssSiH2	Minimum value of (-SiH2-) atom type E-State

Name	Description
minsssSiH	Minimum value of (>SiH-) atom type E-State
minsssSi	Minimum value of (>Si<) atom type E-State
minsPH2	Minimum value of (-PH2) atom type E-State
minssPH	Minimum value of (-PH-) atom type E-State
minsssP	Minimum value of (>P-) atom type E-State
mindsssP	Minimum value of (->P=) atom type E-State
minsssssP	Minimum value of (->P<) atom type E-State
minsSH	Minimum value of (-SH) atom type E-State
mindS	Minimum value of (=S) atom type E-State
minssS	Minimum value of (-S-) atom type E-State
minaaS	Minimum value of (aSa) atom type E-State
mindssS	Minimum value of (>S=) atom type E-State
minddssS	Minimum value of (>S==) atom type E-State
minsCl	Minimum value of (-Cl) atom type E-State
minsGeH3	Minimum value of (-GeH3) atom type E-State
minssGeH2	Minimum value of (-GeH2-) atom type E-State
minsssGeH	Minimum value of (>GeH-) atom type E-State
minsssssGe	Minimum value of (>Ge<) atom type E-State
minsAsH2	Minimum value of (-AsH2) atom type E-State
minssAsH	Minimum value of (-AsH-) atom type E-State
minsssAs	Minimum value of (>As-) atom type E-State
mindsssAs	Minimum value of (->As=) atom type E-State
minsssssAs	Minimum value of (->As<) atom type E-State
minsSeH	Minimum value of (-SeH) atom type E-State
mindSe	Minimum value of (=Se) atom type E-State
minssSe	Minimum value of (-Se-) atom type E-State
minaaSe	Minimum value of (aSea) atom type E-State
mindssSe	Minimum value of (>Se=) atom type E-State
minddssSe	Minimum value of (-=Se=) atom type E-State
minsBr	Minimum value of (-Br) atom type E-State
minsSnH3	Minimum value of (-SnH3) atom type E-State
minssSnH2	Minimum value of (-SnH2-) atom type E-State
minsssSnH	Minimum value of (>SnH-) atom type E-State
minsssssSn	Minimum value of (>Sn<) atom type E-State
minsl	Minimum value of (-I) atom type E-State
minsPbH3	Minimum value of (-PbH3) atom type E-State
minssPbH2	Minimum value of (-PbH2-) atom type E-State
minsssPbH	Minimum value of (>PbH-) atom type E-State
minsssssPb	Minimum value of (>Pb<) atom type E-State
minsBH2	Minimum value of (-BH2) atom type E-State
minaOm	Minimum value of (:O-0.5) atom type E-State
minsOm	Minimum value of (-O-) atom type E-State
minddsP	Minimum value of (-=P=) atom type E-State
minssssssS	Minimum value of (>S<<) atom type E-State
minSm	Minimum value of (-S-) atom type E-State
minddsAs	Minimum value of (-=As=) atom type E-State
minssssssSe	Minimum value of (>Se<<) atom type E-State

Name	Description
minHBd	Minimum value of (strong) hydrogen bond donors E-State
minwHBd	Minimum value of weak hydrogen bond donors E-State
minHBa	Minimum value of (strong) hydrogen bond acceptors E-State
minwHBa	Minimum value of weak hydrogen bond acceptors E-State

Name	Description
minHBint2	Minimum value of potential internal hydrogen bonds of path length 2 E-State
minHBint3	Minimum value of potential internal hydrogen bonds of path length 3 E-State
minHBint4	Minimum value of potential internal hydrogen bonds of path length 4 E-State
minHBint5	Minimum value of potential internal hydrogen bonds of path length 5 E-State
minHBint6	Minimum value of potential internal hydrogen bonds of path length 6 E-State
minHBint7	Minimum value of potential internal hydrogen bonds of path length 7 E-State
minHBint8	Minimum value of potential internal hydrogen bonds of path length 8 E-State
minHBint9	Minimum value of potential internal hydrogen bonds of path length 9 E-State
minHBint10	Minimum value of potential internal hydrogen bonds of path length 10 E-State
minHCHnX	Minimum value of (CHnX) atom type H E-State
minHCsats	Minimum value of (H on C sp ³ bonded to saturated C) atom type E-State
minHCsatu	Minimum value of (H on C sp ³ bonded to unsaturated C) atom type E-State
minHAvin	Minimum value of (H on C vinyl bonded to C aromatic) atom type E-State
minHother	Minimum value of (H on aaCH, dCH ₂ or dsCH) atom type E-State
minHmisc	Minimum value of atom types (H bonded to B, Si, P, Ge, As, Se, Sn or Pb) atom type E-State
minHsOH	Minimum value (-OH) atom type H E-State
minHdNH	Minimum value of (=NH) atom type H E-State
minHsSH	Minimum value of (-SH) atom type H E-State
minHsNH ₂	Minimum value of (-NH ₂) atom type H E-State
minHssNH	Minimum value of (-NH-) atom type H E-State
minHaaNH	Minimum value of (:NH:) atom type H E-State
minHsNpH ₃	Minimum value of (-NH ₃ +) atom type H E-State
minHssNpH ₂	Minimum value of (-NH ₂ -) atom type H E-State
minHsssNpH	Minimum value of (>NH-) atom type H E-State
minHtCH	Minimum value of (#CH) atom type H E-State
minHdCH ₂	Minimum value of (=CH ₂) atom type H E-State
minHdsCH	Minimum value of (=CH-) atom type H E-State
minHaaCH	Minimum value of (:CH:) atom type H E-State

Name	Description
maxsLi	Maximum value of (-Li) atom type E-State
maxssBe	Maximum value of (-Be-) atom type E-State
maxssssBem	Maximum value of (>Be<-2) atom type E-State
maxssBH	Maximum value of (-BH-) atom type E-State
maxsssB	Maximum value of (-B<) atom type E-State
maxssssBm	Maximum value of (>B<-) atom type E-State
maxsCH ₃	Maximum value of (-CH ₃) atom type E-State
maxdCH ₂	Maximum value of (=CH ₂) atom type E-State
maxssCH ₂	Maximum value of (-CH ₂ -) atom type E-State
maxtCH	Maximum value of (#CH) atom type E-State
maxdsCH	Maximum value of (=CH-) atom type E-State
maxaaCH	Maximum value of (:CH:) atom type E-State
maxsssCH	Maximum value of (>CH-) atom type E-State
maxddC	Maximum value of (=C=) atom type E-State
maxtsC	Maximum value of (#C-) atom type E-State
maxdssC	Maximum value of (=C<) atom type E-State
maxaasC	Maximum value of (:C:-) atom type E-State
maxaaaC	Maximum value of (::C:) atom type E-State
maxssssC	Maximum value of (>C<) atom type E-State
maxsNH ₃ p	Maximum value of (-NH ₃ +) atom type E-State
maxsNH ₂	Maximum value of (-NH ₂) atom type E-State
maxssNH ₂ p	Maximum value of (-NH ₂ -) atom type E-State
maxdNH	Maximum value of (=NH) atom type E-State

Name	Description
maxssNH	Maximum value of (-NH-) atom type E-State
maxaaNH	Maximum value of (:NH:) atom type E-State
maxtN	Maximum value of (#N) atom type E-State
maxsssNHp	Maximum value of (>NH+) atom type E-State
maxdsN	Maximum value of (=N-) atom type E-State
maxaaN	Maximum value of (:N:) atom type E-State
maxssN	Maximum value of (>N-) atom type E-State
maxddsN	Maximum value of (-N<<) atom type E-State
maxaasN	Maximum value of (:N:-) atom type E-State
maxssssNp	Maximum value of (>N<+) atom type E-State
maxsOH	Maximum value of (-OH) atom type E-State
maxdO	Maximum value of (=O) atom type E-State
maxssO	Maximum value of (-O-) atom type E-State
maxaaO	Maximum value of (:O:) atom type E-State
maxsF	Maximum value of (-F) atom type E-State
maxsSiH3	Maximum value of (-SiH3) atom type E-State
maxssSiH2	Maximum value of (-SiH2-) atom type E-State
maxsssSiH	Maximum value of (>SiH-) atom type E-State
maxssssSi	Maximum value of (>Si<) atom type E-State
maxsPH2	Maximum value of (-PH2) atom type E-State
maxssPH	Maximum value of (-PH-) atom type E-State
maxsssP	Maximum value of (>P-) atom type E-State
maxdsssP	Maximum value of (->P=) atom type E-State
maxsssssP	Maximum value of (->P<) atom type E-State
maxsSH	Maximum value of (-SH) atom type E-State
maxdS	Maximum value of (=S) atom type E-State
maxssS	Maximum value of (-S-) atom type E-State
maxaaS	Maximum value of (aSa) atom type E-State
maxdssS	Maximum value of (>S=) atom type E-State
maxddssS	Maximum value of (>S==) atom type E-State
maxsCl	Maximum value of (-Cl) atom type E-State
maxsGeH3	Maximum value of (-GeH3) atom type E-State
maxssGeH2	Maximum value of (-GeH2-) atom type E-State
maxsssGeH	Maximum value of (>GeH-) atom type E-State
maxssssGe	Maximum value of (>Ge<) atom type E-State
maxsAsH2	Maximum value of (-AsH2) atom type E-State
maxssAsH	Maximum value of (-AsH-) atom type E-State
maxsssAs	Maximum value of (>As-) atom type E-State
maxdsssAs	Maximum value of (->As=) atom type E-State
maxsssssAs	Maximum value of (->As<) atom type E-State
maxsSeH	Maximum value of (-SeH) atom type E-State
maxdSe	Maximum value of (=Se) atom type E-State
maxssSe	Maximum value of (-Se-) atom type E-State
maxaaSe	Maximum value of (aSea) atom type E-State
maxdssSe	Maximum value of (>Se=) atom type E-State
maxddssSe	Maximum value of (-=Se=-) atom type E-State
maxsBr	Maximum value of (-Br) atom type E-State
maxsSnH3	Maximum value of (-SnH3) atom type E-State
maxssSnH2	Maximum value of (-SnH2-) atom type E-State
maxsssSnH	Maximum value of (>SnH-) atom type E-State
maxssssSn	Maximum value of (>Sn<) atom type E-State
maxsl	Maximum value of (-I) atom type E-State
maxsPbH3	Maximum value of (-PbH3) atom type E-State
maxssPbH2	Maximum value of (-PbH2-) atom type E-State

Name	Description
maxsssPbH	Maximum value of (>PbH-) atom type E-State
maxsssPb	Maximum value of (>Pb<) atom type E-State
maxsBH2	Maximum value of (-BH2) atom type E-State
maxaOm	Maximum value of (:O-0.5) atom type E-State
maxsOm	Maximum value of (-O-) atom type E-State
maxddsP	Maximum value of (-=P=) atom type E-State
maxsssssS	Maximum value of (>S<<) atom type E-State
maxSm	Maximum value of (-S-) atom type E-State
maxddsAs	Maximum value of (-=As=) atom type E-State
maxsssssSe	Maximum value of (>Se<<) atom type E-State

Name	Description
maxHBd	Maximum value of (strong) hydrogen bond donors E-State
maxwHBd	Maximum value of weak hydrogen bond donors E-State
maxHBa	Maximum value of (strong) hydrogen bond acceptors E-State
maxwHBa	Maximum value of weak hydrogen bond acceptors E-State
maxHBint2	Maximum value of potential internal hydrogen bonds of path length 2 E-State
maxHBint3	Maximum value of potential internal hydrogen bonds of path length 3 E-State
maxHBint4	Maximum value of potential internal hydrogen bonds of path length 4 E-State
maxHBint5	Maximum value of potential internal hydrogen bonds of path length 5 E-State
maxHBint6	Maximum value of potential internal hydrogen bonds of path length 6 E-State
maxHBint7	Maximum value of potential internal hydrogen bonds of path length 7 E-State
maxHBint8	Maximum value of potential internal hydrogen bonds of path length 8 E-State
maxHBint9	Maximum value of potential internal hydrogen bonds of path length 9 E-State
maxHBint10	Maximum value of potential internal hydrogen bonds of path length 10 E-State
maxHCHnX	Maximum value of (CHnX) atom type H E-State
maxHCsats	Maximum value of (H on C sp3 bonded to saturated C) atom type E-State
maxHCsatu	Maximum value of (H on C sp3 bonded to unsaturated C) atom type E-State
maxHAvin	Maximum value of (H on C vinyl bonded to C aromatic) atom type E-State
maxHother	Maximum value of (H on aaCH, dCH2 or dsCH) atom type E-State
maxHmisc	Maximum value of atom types (H bonded to B, Si, P, Ge, As, Se, Sn or Pb) atom type E-State
maxHsOH	Maximum value (-OH) atom type H E-State
maxHdNH	Maximum value of (=NH) atom type H E-State
maxHsSH	Maximum value of (-SH) atom type H E-State
maxHsNH2	Maximum value of (-NH2) atom type H E-State
maxHssNH	Maximum value of (-NH-) atom type H E-State
maxHaaNH	Maximum value of (:NH:) atom type H E-State
maxHsNpH3	Maximum value of (-NH3+) atom type H E-State
maxHssNpH2	Maximum value of (-NH2-+) atom type H E-State
maxHsssNpH	Maximum value of (>NH-+) atom type H E-State
maxHtCH	Maximum value of (#CH) atom type H E-State
maxHdCH2	Maximum value of (=CH2) atom type H E-State
maxHdsCH	Maximum value of (=CH-) atom type H E-State
maxHaaCH	Maximum value of (:CH:) atom type H E-State

Name	Description
gmin	Minimum E-State
hmin	Minimum hydrogen E-State
gmax	Maximum E-State
hmax	Maximum hydrogen E-State
sumI	Sum of the intrinsic state values I
meanI	Mean of the intrinsic state values I

Name	Description
MAXDN	Maximum negative intrinsic state difference (molecular connectivity delta value calculated according to the Molconn definition)
MAXDP	Maximum positive intrinsic state difference (molecular connectivity delta value calculated according to the Molconn definition)
DELS	Sum of all atoms intrinsic state differences (molecular connectivity delta value calculated according to the Molconn definition)
MAXDN2	Maximum negative intrinsic state difference (molecular connectivity delta value calculated according to the Kier and Hall definition)
MAXDP2	Maximum positive intrinsic state difference (molecular connectivity delta value calculated according to the Kier and Hall definition)
DELS2	Sum of all atoms intrinsic state differences (molecular connectivity delta value calculated according to the Kier and Hall definition)

5.25 Extended topochemical index

Name	Description
ETA_Alpha	Sum of alpha values of molecule non-hydrogen vertices
ETA_AlphaP	Sum of alpha values of molecule non-hydrogen vertices relative to molecular size
ETA_dAlpha_A	A measure of count of non-hydrogen heteroatoms
ETA_dAlpha_B	A measure of count of hydrogen bond acceptor atoms and/or polar surface area
ETA_Epsilon_1	A measure of electronegative atom count
ETA_Epsilon_2	A measure of electronegative atom count
ETA_Epsilon_3	A measure of electronegative atom count
ETA_Epsilon_4	A measure of electronegative atom count
ETA_Epsilon_5	A measure of electronegative atom count
ETA_dEpsilon_A	A measure of contribution of unsaturation and electronegative atom count
ETA_dEpsilon_B	A measure of contribution of unsaturation
ETA_dEpsilon_C	A measure of contribution of electronegativity
ETA_dEpsilon_D	A measure of contribution of hydrogen bond donor atoms
ETA_Psi_1	A measure of hydrogen bonding propensity of the molecules and/or polar surface area
ETA_dPsi_A	A measure of hydrogen bonding propensity of the molecules
ETA_dPsi_B	A measure of hydrogen bonding propensity of the molecules
ETA_Shape_P	Shape index P
ETA_Shape_Y	Shape index Y
ETA_Shape_X	Shape index X
ETA_Beta	A measure of electronic features of the molecule
ETA_BetaP	A measure of electronic features of the molecule relative to molecular size
ETA_Beta_s	A measure of electronegative atom count of the molecule
ETA_BetaP_s	A measure of electronegative atom count of the molecule relative to molecular size
ETA_Beta_ns	A measure of electron-richness of the molecule
ETA_BetaP_ns	A measure of electron-richness of the molecule relative to molecular size
ETA_dBeta	A measure of relative unsaturation content
ETA_dBetaP	A measure of relative unsaturation content relative to molecular size
ETA_Beta_ns_d	A measure of lone electrons entering into resonance
ETA_BetaP_ns_d	A measure of lone electrons entering into resonance relative to molecular size
ETA_Eta	Composite index Eta
ETA_EtaP	Composite index Eta relative to molecular size
ETA_Eta_R	Composite index Eta for reference alkane
ETA_Eta_F	Functionality index EtaF
ETA_EtaP_F	Functionality index EtaF relative to molecular size
ETA_Eta_L	Local index Eta_local
ETA_EtaP_L	Local index Eta_local relative to molecular size
ETA_Eta_R_L	Local index Eta_local for reference alkane

Name	Description
ETA_Eta_F_L	Local functionality contribution EtaF_local
ETA_EtaP_F_L	Local functionality contribution EtaF_local relative to molecular size
ETA_Eta_B	Branching index EtaB
ETA_EtaP_B	Branching index EtaB relative to molecular size
ETA_Eta_B_RC	Branching index EtaB with ring correction
ETA_EtaP_B_RC	Branching index EtaB, with ring correction, relative to molecular size

5.26 FMF

Name	Description
FMF	Molecular complexity

5.27 CSP3

Name	Description
Fsp3	Molecular complexity

5.28 Polar surface area

Name	Description
tpsaEfficiency	Polar surface area expressed as a ratio to molecular size

5.29 Hydrogen bond acceptors count

Name	Description
nHBAcc	Number of hydrogen bond acceptors
nHBAcc2	Number of hydrogen bond acceptors (any oxygen; any nitrogen where the formal charge of the nitrogen is non-positive (i.e. formal charge smaller or equal to 0) except a non-aromatic nitrogen that is adjacent to an oxygen and aromatic ring, or an aromatic nitrogen with a hydrogen atom in a ring, or an aromatic nitrogen with 3 neighbouring atoms in a ring, or a nitrogen with total bond order (≥ 4); any fluorine)
nHBAcc3	Number of hydrogen bond acceptors (any oxygen; any nitrogen where the formal charge of the nitrogen is non-positive (i.e. formal charge smaller or equal to 0) except a non-aromatic nitrogen that is adjacent to an oxygen and aromatic ring, or an aromatic nitrogen with a hydrogen atom in a ring, or an aromatic nitrogen with 3 neighbouring atoms in a ring, or a nitrogen with total bond order (≥ 4), or a nitrogen
nHBAcc_Lipinski	Number of hydrogen bond acceptors (using Lipinski's definition: any nitrogen; any oxygen)

5.30 Hydrogen bond donors count

Name	Description
nHBDon	Number of hydrogen bond donors
nHBDon_Lipinski	Number of hydrogen bond donors (using Lipinski's definition: Any OH or NH. Each available hydrogen atom is counted as one hydrogen bond donor)

5.31 Hybridization ratio

Name	Description
IC0	0-ordered neighborhood symmetry information content index
IC1	1-ordered neighborhood symmetry information content index
IC2	2-ordered neighborhood symmetry information content index
IC3	3-ordered neighborhood symmetry information content index
IC4	4-ordered neighborhood symmetry information content index
IC5	5-ordered neighborhood symmetry information content index

5.32 Information content

Name	Description
TIC0	0-ordered neighborhood symmetry total information content index
TIC1	1-ordered neighborhood symmetry total information content index
TIC2	2-ordered neighborhood symmetry total information content index
TIC3	3-ordered neighborhood symmetry total information content index
TIC4	4-ordered neighborhood symmetry total information content index
TIC5	5-ordered neighborhood symmetry total information content index

Name	Description
SIC0	0-ordered neighborhood symmetry structural information content index
SIC1	1-ordered neighborhood symmetry structural information content index
SIC2	2-ordered neighborhood symmetry structural information content index
SIC3	3-ordered neighborhood symmetry structural information content index
SIC4	4-ordered neighborhood symmetry structural information content index
SIC5	5-ordered neighborhood symmetry structural information content index

Name	Description
CIC0	0-ordered neighborhood symmetry complementary information content index
CIC1	1-ordered neighborhood symmetry complementary information content index
CIC2	2-ordered neighborhood symmetry complementary information content index
CIC3	3-ordered neighborhood symmetry complementary information content index
CIC4	4-ordered neighborhood symmetry complementary information content index
CIC5	5-ordered neighborhood symmetry complementary information content index

Name	Description
BIC0	0-ordered neighborhood symmetry bond information content index
BIC1	1-ordered neighborhood symmetry bond information content index
BIC2	2-ordered neighborhood symmetry bond information content index
BIC3	3-ordered neighborhood symmetry bond information content index
BIC4	4-ordered neighborhood symmetry bond information content index
BIC5	5-ordered neighborhood symmetry bond information content index

Name	Description
MIC0	0-ordered neighborhood symmetry modified information content index
MIC1	1-ordered neighborhood symmetry modified information content index
MIC2	2-ordered neighborhood symmetry modified information content index
MIC3	3-ordered neighborhood symmetry modified information content index

Name	Description
MIC4	4-ordered neighborhood symmetry modified information content index
MIC5	5-ordered neighborhood symmetry modified information content index

Name	Description
ZMIC0	0-ordered neighborhood symmetry Z-modified information content index
ZMIC1	1-ordered neighborhood symmetry Z-modified information content index
ZMIC2	2-ordered neighborhood symmetry Z-modified information content index
ZMIC3	3-ordered neighborhood symmetry Z-modified information content index
ZMIC4	4-ordered neighborhood symmetry Z-modified information content index
ZMIC5	5-ordered neighborhood symmetry Z-modified information content index

5.33 JPLogP

Name	Description
JPLogP	Plante-Werner JPLogP

5.34 Kappa shape index

Name	Description
Kier1	First kappa shape index
Kier2	Second kappa shape index
Kier3	Third kappa shape index

5.35 Largest chain

Name	Description
nAtomLC	Largest chain atoms count

5.36 Largest Pi system

Name	Description
nAtomP	Largest Pi system atoms count

5.37 Largest aliphatic chain

Name	Description
nAtomLAC	Largest aliphatic chain atoms count

5.38 Mannhold LogP

Name	Description
MLogP	Mannhold LogP

5.39 Molecular linear free energy relation

Name	Description
MLFER_A	Overall or summation solute hydrogen bond acidity
MLFER_E	Excess molar refraction
MLFER_S	Combined dipolarity/polarizability
MLFER_BH	Overall or summation solute hydrogen bond basicity
MLFER_BO	Overall or summation solute hydrogen bond basicity
MLFER_L	Solute gas-hexadecane partition coefficient

5.40 Molecular distance edge

Name	Description
MDEC-11	Molecular distance edge between all primary carbons
MDEC-12	Molecular distance edge between all primary and secondary carbons
MDEC-13	Molecular distance edge between all primary and tertiary carbons
MDEC-14	Molecular distance edge between all primary and quaternary carbons
MDEC-22	Molecular distance edge between all secondary carbons
MDEC-23	Molecular distance edge between all secondary and tertiary carbons
MDEC-24	Molecular distance edge between all secondary and quaternary carbons
MDEC-33	Molecular distance edge between all tertiary carbons
MDEC-34	Molecular distance edge between all tertiary and quaternary carbons
MDEC-44	Molecular distance edge between all quaternary carbons

Name	Description
MDEO-11	Molecular distance edge between all primary oxygens
MDEO-12	Molecular distance edge between all primary and secondary oxygens
MDEO-22	Molecular distance edge between all secondary oxygens

Name	Description
MDEN-11	Molecular distance edge between all primary nitrogens
MDEN-12	Molecular distance edge between all primary and secondary nitrogens
MDEN-13	Molecular distance edge between all primary and tertiary nitrogens
MDEN-22	Molecular distance edge between all secondary nitrogens
MDEN-23	Molecular distance edge between all secondary and tertiary nitrogens
MDEN-33	Molecular distance edge between all tertiary nitrogens

5.41 Path count

Name	Description
MPC1	Order 1 path count
MPC2	Order 2 path count
MPC3	Order 3 path count
MPC4	Order 4 path count
MPC5	Order 5 path count
MPC6	Order 6 path count
MPC7	Order 7 path count
MPC8	Order 8 path count
MPC9	Order 9 path count

Name	Description
MPC10	Order 0 path count

Name	Description
piPC1	Order 1 pi-path count $\log(1 + x)$ scale
piPC2	Order 2 pi-path count $\log(1 + x)$ scale
piPC3	Order 3 pi-path count $\log(1 + x)$ scale
piPC4	Order 4 pi-path count $\log(1 + x)$ scale
piPC5	Order 5 pi-path count $\log(1 + x)$ scale
piPC6	Order 6 pi-path count $\log(1 + x)$ scale
piPC7	Order 7 pi-path count $\log(1 + x)$ scale
piPC8	Order 8 pi-path count $\log(1 + x)$ scale
piPC9	Order 9 pi-path count $\log(1 + x)$ scale
piPC10	Order 10 pi-path count $\log(1 + x)$ scale

Name	Description
TPC	Total path count (orders from 1 to 10)
TpiPC	Total pi-path count (orders from 1 to 10) $\log(1 + x)$ scale
R_TpiPCTPC	Total bond count (orders from 1 to 10) divided by total path count (orders from 1 to 10)

5.42 Petitjean number

Name	Description
PetitjeanNumber	Petitjean number

5.43 Ring count

Name	Description
nRing	rings count
n3Ring	3-membered rings count
n4Ring	4-membered rings count
n5Ring	5-membered rings count
n6Ring	6-membered rings count
n7Ring	7-membered rings count
n8Ring	8-membered rings count
n9Ring	9-membered rings count
n10Ring	10-membered rings count
n11Ring	11-membered rings count
n12Ring	12-membered rings count
n12GRing	Greater than 12-membered rings count

Name	Description
nFRing	Fused rings count
nF4Ring	4-membered fused rings count
nF5Ring	5-membered fused rings count
nF6Ring	6-membered fused rings count
nF7Ring	7-membered fused rings count
nF8Ring	8-membered fused rings count
nF9Ring	9-membered fused rings count

Name	Description
nF10Ring	10-membered fused rings count
nF11Ring	11-membered fused rings count
nF12Ring	12-membered fused rings count
nF12GRing	Greater than 12-membered fused rings count

Name	Description
nTRing	Rings count (including counts from fused rings)
nT4Ring	4-membered rings count (including counts from fused rings)
nT5Ring	5-membered rings count (including counts from fused rings)
nT6Ring	6-membered rings count (including counts from fused rings)
nT7Ring	7-membered rings count (including counts from fused rings)
nT8Ring	8-membered rings count (including counts from fused rings)
nT9Ring	9-membered rings count (including counts from fused rings)
nT10Ring	10-membered rings count (including counts from fused rings)
nT11Ring	11-membered rings count (including counts from fused rings)
nT12Ring	12-membered rings count (including counts from fused rings)
nT12GRing	Greater than 12-membered rings count (including counts from fused rings)

Name	Description
nHeteroRing	Rings containing heteroatoms (N, O, P, S, or halogens) count
n3HeteroRing	3-membered rings containing heteroatoms (N, O, P, S, or halogens) count
n4HeteroRing	4-membered rings containing heteroatoms (N, O, P, S, or halogens) count
n5HeteroRing	5-membered rings containing heteroatoms (N, O, P, S, or halogens) count
n6HeteroRing	6-membered rings containing heteroatoms (N, O, P, S, or halogens) count
n7HeteroRing	7-membered rings containing heteroatoms (N, O, P, S, or halogens) count
n8HeteroRing	8-membered rings containing heteroatoms (N, O, P, S, or halogens) count
n9HeteroRing	9-membered rings containing heteroatoms (N, O, P, S, or halogens) count
n10HeteroRing	10-membered rings containing heteroatoms (N, O, P, S, or halogens) count
n11HeteroRing	11-membered rings containing heteroatoms (N, O, P, S, or halogens) count
n12HeteroRing	12-membered rings containing heteroatoms (N, O, P, S, or halogens) count
n12GHeteroRing	Greater than 12-membered rings containing heteroatoms (N, O, P, S, or halogens) count

Name	Description
nFHeteroRing	Fused rings containing heteroatoms (N, O, P, S, or halogens) count
nF4HeteroRing	4-membered fused rings containing heteroatoms (N, O, P, S, or halogens) count
nF5HeteroRing	5-membered fused rings containing heteroatoms (N, O, P, S, or halogens) count
nF6HeteroRing	6-membered fused rings containing heteroatoms (N, O, P, S, or halogens) count
nF7HeteroRing	7-membered fused rings containing heteroatoms (N, O, P, S, or halogens) count
nF8HeteroRing	8-membered fused rings containing heteroatoms (N, O, P, S, or halogens) count
nF9HeteroRing	9-membered fused rings containing heteroatoms (N, O, P, S, or halogens) count
nF10HeteroRing	10-membered fused rings containing heteroatoms (N, O, P, S, or halogens) count
nF11HeteroRing	11-membered fused rings containing heteroatoms (N, O, P, S, or halogens) count
nF12HeteroRing	12-membered fused rings containing heteroatoms (N, O, P, S, or halogens) count
nF12GHeteroRing	Greater than 12-membered fused rings containing heteroatoms (N, O, P, S, or halogens) count

Name	Description
nTHeteroRing	Rings containing heteroatoms (N, O, P, S, or halogens) count (including counts from fused rings)
nT4HeteroRing	4-membered rings containing heteroatoms (N, O, P, S, or halogens) count (including counts from fused rings)

Name	Description
nT5HeteroRing	5-membered rings containing heteroatoms (N, O, P, S, or halogens) count (including counts from fused rings)
nT6HeteroRing	6-membered rings containing heteroatoms (N, O, P, S, or halogens) count (including counts from fused rings)
nT7HeteroRing	7-membered rings containing heteroatoms (N, O, P, S, or halogens) count (including counts from fused rings)
nT8HeteroRing	8-membered rings containing heteroatoms (N, O, P, S, or halogens) count (including counts from fused rings)
nT9HeteroRing	9-membered rings containing heteroatoms (N, O, P, S, or halogens) count (including counts from fused rings)
nT10HeteroRing	10-membered rings containing heteroatoms (N, O, P, S, or halogens) count (including counts from fused rings)
nT11HeteroRing	11-membered rings containing heteroatoms (N, O, P, S, or halogens) count (including counts from fused rings)
nT12HeteroRing	12-membered rings containing heteroatoms (N, O, P, S, or halogens) count (including counts from fused rings)
nT12GHeteroRing	Number of Greater than 12-membered rings containing heteroatoms (N, O, P, S, or halogens) count (including counts from fused rings)

5.44 Rotatable bonds count

Name	Description
nRotB	Rotatable bonds count, excluding terminal bonds.
nRotBt	Rotatable bonds count, including terminal bonds.
RotBFrac	Rotatable bonds fraction, excluding terminal bonds.
RotBtFrac	Rotatable bonds fraction, including terminal bonds.

5.45 Rule of five

Name	Description
LipinskiFailures	Lipinski's Rule of 5 failures count

5.46 Spiro atom count

Name	Description
nSpiroAtoms	Spiro atom count

5.47 Topological

Name	Description
topoRadius	Topological radius (minimum atom eccentricity)
topoDiameter	Topological diameter (maximum atom eccentricity)
topoShape	Petitjean topological shape index

5.48 Topological charge

Name	Description
GGI1	Order 1 topological charge index
GGI2	Order 2 topological charge index
GGI3	Order 3 topological charge index
GGI4	Order 4 topological charge index
GGI5	Order 5 topological charge index
GGI6	Order 6 topological charge index
GGI7	Order 7 topological charge index
GGI8	Order 8 topological charge index
GGI9	Order 9 topological charge index
GGI10	Order 10 topological charge index

Name	Description
JGI1	Order 1 mean topological charge index
JGI2	Order 2 mean topological charge index
JGI3	Order 3 mean topological charge index
JGI4	Order 4 mean topological charge index
JGI5	Order 5 mean topological charge index
JGI6	Order 6 mean topological charge index
JGI7	Order 7 mean topological charge index
JGI8	Order 8 mean topological charge index
JGI9	Order 9 mean topological charge index
JGI10	Order 10 mean topological charge index

Name	Description
JGT	Global topological charge index

5.49 Topological distance matrix

Name	Description
SpMax_D	Leading eigenvalue
SpDiam_D	Spectral diameter
SpAD_D	Spectral absolute deviation
SpMAD_D	Spectral mean absolute deviation
EE_D	Estrada-like index
VE1_D	Coefficient sum of the last eigenvector
VE2_D	Average coefficient sum of the last eigenvector
VE3_D	Logarithmic coefficient sum of the last eigenvector
VR1_D	Randic-like eigenvector-based index
VR2_D	Normalized Randic-like eigenvector-based index
VR3_D	Logarithmic Randic-like eigenvector-based index

5.50 Topological polar surface area

Name	Description
TopoPSA	topological polar surface area based on fragment contributions (TPSA)

5.51 Van der Waals volume

Name	Description
VABC	Van der Waals volume

5.52 Vertex adjacency matrix

Name	Description
vAdjMat	Vertex adjacency information (magnitude)

5.53 Walk count

Name	Description
MWC2	Order 2 walk count $\log(1 + x)$ scale
MWC3	Order 3 walk count $\log(1 + x)$ scale
MWC4	Order 4 walk count $\log(1 + x)$ scale
MWC5	Order 5 walk count $\log(1 + x)$ scale
MWC6	Order 6 walk count $\log(1 + x)$ scale
MWC7	Order 7 walk count $\log(1 + x)$ scale
MWC8	Order 8 walk count $\log(1 + x)$ scale
MWC9	Order 9 walk count $\log(1 + x)$ scale
MWC10	Order 10 walk count $\log(1 + x)$ scale

Name	Description
SRW2	Order 2 self-returning walk count $\log(1 + x)$ scale
SRW3	Order 3 self-returning walk count $\log(1 + x)$ scale
SRW4	Order 4 self-returning walk count $\log(1 + x)$ scale
SRW5	Order 5 self-returning walk count $\log(1 + x)$ scale
SRW6	Order 6 self-returning walk count $\log(1 + x)$ scale
SRW7	Order 7 self-returning walk count $\log(1 + x)$ scale
SRW8	Order 8 self-returning walk count $\log(1 + x)$ scale
SRW9	Order 9 self-returning walk count $\log(1 + x)$ scale
SRW10	Order 10 self-returning walk count $\log(1 + x)$ scale

Name	Description
TWC	Total walk count (orders from 2 to 10)
TSRW	Total self-return walk count (up to order 10) $\log(1 + x)$ scale

5.54 Weight

Name	Description
MW	Molecular weight
AMW	Average molecular weight calculated as molecular weight / atoms count

5.55 Weighted path

Name	Description
WTPT1	Molecular ID
WTPT2	Molecular ID / atoms count

Name	Description
WTPT3	Sum of path lengths starting from heteroatoms
WTPT4	Sum of path lengths starting from oxygens
WTPT5	Sum of path lengths starting from nitrogens

5.56 Wiener number

Name	Description
WPATH	Wiener path number
WPOL	Wiener polarity number

5.57 XLogP

Name	Description
XLogP	XLogP

5.58 Zagreb index

Name	Description
Zagreb	Sum of the squares of atom degree over all heavy atoms

6 Fingerprints

6.1 EState - Kier and Hall fragment count

Name	Count name	Atom group	Pattern
EstateFP1	khs.sLi	sLi	[LiD1]-*
EstateFP2	khs.ssBe	ssBe	[BeD2](-*)-*
EstateFP3	khs.ssssBe	ssssBe	[BeD4](-*)(-*)(-*)-*
EstateFP4	khs.ssBH	ssBH	[BD2H](-*)-*
EstateFP5	khs.sssB	sssB	[BD3](-*)(-*)-*
EstateFP6	khs.ssssB	ssssB	[BD4](-*)(-*)(-*)-*
EstateFP7	khs.sCH3	sCH3	[CD1H3]-*
EstateFP8	khs.dCH2	dCH2	[CD1H2]=*
EstateFP9	khs.ssCH2	ssCH2	[CD2H2](-*)-*
EstateFP10	khs.tCH	tCH	[CD1H]#*
EstateFP11	khs.dsCH	dsCH	[CD2H](=*)-*
EstateFP12	khs.aaCH	aaCH	[C,c;D2H](:*):*
EstateFP13	khs.sssCH	sssCH	[CD3H](-*)(-*)-*
EstateFP14	khs.ddC	ddC	[CD2H0](=*)=*
EstateFP15	khs.tsC	tsC	[CD2H0](#*)-*
EstateFP16	khs.dssC	dssC	[CD3H0](=*)(-*)-*
EstateFP17	khs.aasC	aasC	[C,c;D3H0](:*)(:*)-*
EstateFP18	khs.aaaC	aaaC	[C,c;D3H0](:*)(:*)(:*)-*
EstateFP19	khs.ssssC	ssssC	[CD4H0](-*)(-*)(-*)-*
EstateFP20	khs.sNH3	sNH3	[ND1H3]-*
EstateFP21	khs.sNH2	sNH2	[ND1H2]-*
EstateFP22	khs.ssNH2	ssNH2	[ND2H2](-*)-*
EstateFP23	khs.dNH	dNH	[ND1H]=*
EstateFP24	khs.ssNH	ssNH	[ND2H](-*)-*
EstateFP25	khs.aaNH	aaNH	[N,nD2H](:*):*
EstateFP26	khs.tN	tN	[ND1H0]#*
EstateFP27	khs.sssNH	sssNH	[ND3H](-*)(-*)-*
EstateFP28	khs.dsN	dsN	[ND2H0](=*)-*
EstateFP29	khs.aaN	aaN	[N,nD2H0](:*):*
EstateFP30	khs.sssN	sssN	[ND3H0](-*)(-*)-*
EstateFP31	khs.ddsN	ddsN	[ND3H0]([OD1H0])([OD1H0])-,*
EstateFP32	khs.aasN	aasN	[N,nD3H0](:*)(:*)-,*
EstateFP33	khs.ssssN	ssssN	[ND4H0](-*)(-*)(-*)-*
EstateFP34	khs.sOH	sOH	[OD1H]-*
EstateFP35	khs.dO	dO	[OD1H0]=*
EstateFP36	khs.ssO	ssO	[OD2H0](-*)-*
EstateFP37	khs.aaO	aaO	[O,oD2H0](:*):*
EstateFP38	khs.sF	sF	[FD1]-*
EstateFP39	khs.sSiH3	sSiH3	[SiD1H3]-*
EstateFP40	khs.ssSiH2	ssSiH2	[SiD2H2](-*)-*
EstateFP41	khs.sssSiH	sssSiH	[SiD3H1](-*)(-*)-*
EstateFP42	khs.ssssSi	ssssSi	[SiD4H0](-*)(-*)(-*)-*
EstateFP43	khs.sPH2	sPH2	[PD1H2]-*
EstateFP44	khs.ssPH	ssPH	[PD2H1](-*)-*
EstateFP45	khs.sssP	sssP	[PD3H0](-*)(-*)-*
EstateFP46	khs.dsssP	dsssP	[PD4H0](=*)(-*)(-*)-*
EstateFP47	khs.sssssP	sssssP	[PD5H0](-*)(-*)(-*)(-*)-*
EstateFP48	khs.sSH	sSH	[SD1H1]-*

Name	Count name	Atom group	Pattern
EstateFP49	khs.dS	dS	[SD1H0]=*
EstateFP50	khs.ssS	ssS	[SD2H0](-*)-*
EstateFP51	khs.aaS	aaS	[S,sD2H0](.*):
EstateFP52	khs.dssS	dssS	[SD3H0](=*)(-*)-*
EstateFP53	khs.ddssS	ddssS	[SD4H0]([OD1H0])([OD1H0])(-*)-*
EstateFP54	khs.sCl	sCl	[CID1]-*
EstateFP55	khs.sGeH3	sGeH3	[GeD1H3](-*)
EstateFP56	khs.ssGeH2	ssGeH2	[GeD2H2](-*)-*
EstateFP57	khs.sssGeH	sssGeH	[GeD3H1](-*)(-*)-*
EstateFP58	khs.ssssGe	ssssGe	[GeD4H0](-*)(-*)(-*)-*
EstateFP59	khs.sAsH2	sAsH2	[AsD1H2]-*
EstateFP60	khs.ssAsH	ssAsH	[AsD2H1](-*)-*
EstateFP61	khs.sssAs	sssAs	[AsD3H0](-*)(-*)-*
EstateFP62	khs.sssdAs	sssdAs	[AsD4H0](=*)(-*)(-*)-*
EstateFP63	khs.sssssAs	sssssAs	[AsD5H0](-*)(-*)(-*)(-*)-*
EstateFP64	khs.sSeH	sSeH	[SeD1H1]-*
EstateFP65	khs.dSe	dSe	[SeD1H0]=*
EstateFP66	khs.ssSe	ssSe	[SeD2H0](-*)-*
EstateFP67	khs.aaSe	aaSe	[SeD2H0](.*):
EstateFP68	khs.dssSe	dssSe	[SeD3H0](=*)(-*)-*
EstateFP69	khs.ddssSe	ddssSe	[SeD4H0](=*)(=*)(-*)-*
EstateFP70	khs.sBr	sBr	[BrD1]-*
EstateFP71	khs.sSnH3	sSnH3	[SnD1H3]-*
EstateFP72	khs.ssSnH2	ssSnH2	[SnD2H2](-*)-*
EstateFP73	khs.sssSnH	sssSnH	[SnD3H1](-*)(-*)-*
EstateFP74	khs.ssssSn	ssssSn	[SnD4H0](-*)(-*)(-*)-*
EstateFP75	khs.sl	sl	[ID1]-*
EstateFP76	khs.sPbH3	sPbH3	[PbD1H3]-*
EstateFP77	khs.ssPbH2	ssPbH2	[PbD2H2](-*)-*
EstateFP78	khs.sssPbH	sssPbH	[PbD3H1](-*)(-*)-*
EstateFP79	khs.ssssPb	ssssPb	[PbD4H0](-*)(-*)(-*)-*

6.2 PubChem

The following tables are adapted from PubChem Substructure Fingerprint V1.3 (see <http://pubchem.ncbi.nlm.nih.gov>)

6.2.1 Section 1

Hierarchic Element Counts - These bits test for the presence or count of individual chemical atoms represented by their atomic symbol.

Name	Substructure	Name	Substructure
PubchemFP0	>= 4 H	PubchemFP58	>= 1 Fe
PubchemFP1	>= 8 H	PubchemFP59	>= 1 Co
PubchemFP2	>= 16 H	PubchemFP60	>= 1 Ni
PubchemFP3	>= 32 H	PubchemFP61	>= 1 Cu
PubchemFP4	>= 1 Li	PubchemFP62	>= 1 Zn
PubchemFP5	>= 2 Li	PubchemFP63	>= 1 Ga
PubchemFP6	>= 1 B	PubchemFP64	>= 1 Ge
PubchemFP7	>= 2 B	PubchemFP65	>= 1 As
PubchemFP8	>= 4 B	PubchemFP66	>= 1 Se
PubchemFP9	>= 2 C	PubchemFP67	>= 1 Kr
PubchemFP10	>= 4 C	PubchemFP68	>= 1 Rb

Name	Substructure	Name	Substructure
PubchemFP11	>= 8 C	PubchemFP69	>= 1 Sr
PubchemFP12	>= 16 C	PubchemFP70	>= 1 Y
PubchemFP13	>= 32 C	PubchemFP71	>= 1 Zr
PubchemFP14	>= 1 N	PubchemFP72	>= 1 Nb
PubchemFP15	>= 2 N	PubchemFP73	>= 1 Mo
PubchemFP16	>= 4 N	PubchemFP74	>= 1 Ru
PubchemFP17	>= 8 N	PubchemFP75	>= 1 Rh
PubchemFP18	>= 1 O	PubchemFP76	>= 1 Pd
PubchemFP19	>= 2 O	PubchemFP77	>= 1 Ag
PubchemFP20	>= 4 O	PubchemFP78	>= 1 Cd
PubchemFP21	>= 8 O	PubchemFP79	>= 1 In
PubchemFP22	>= 16 O	PubchemFP80	>= 1 Sn
PubchemFP23	>= 1 F	PubchemFP81	>= 1 Sb
PubchemFP24	>= 2 F	PubchemFP82	>= 1 Te
PubchemFP25	>= 4 F	PubchemFP83	>= 1 Xe
PubchemFP26	>= 1 Na	PubchemFP84	>= 1 Cs
PubchemFP27	>= 2 Na	PubchemFP85	>= 1 Ba
PubchemFP28	>= 1 Si	PubchemFP86	>= 1 Lu
PubchemFP29	>= 2 Si	PubchemFP87	>= 1 Hf
PubchemFP30	>= 1 P	PubchemFP88	>= 1 Ta
PubchemFP31	>= 2 P	PubchemFP89	>= 1 W
PubchemFP32	>= 4 P	PubchemFP90	>= 1 Re
PubchemFP33	>= 1 S	PubchemFP91	>= 1 Os
PubchemFP34	>= 2 S	PubchemFP92	>= 1 Ir
PubchemFP35	>= 4 S	PubchemFP93	>= 1 Pt
PubchemFP36	>= 8 S	PubchemFP94	>= 1 Au
PubchemFP37	>= 1 Cl	PubchemFP95	>= 1 Hg
PubchemFP38	>= 2 Cl	PubchemFP96	>= 1 Tl
PubchemFP39	>= 4 Cl	PubchemFP97	>= 1 Pb
PubchemFP40	>= 8 Cl	PubchemFP98	>= 1 Bi
PubchemFP41	>= 1 K	PubchemFP99	>= 1 La
PubchemFP42	>= 2 K	PubchemFP100	>= 1 Ce
PubchemFP43	>= 1 Br	PubchemFP101	>= 1 Pr
PubchemFP44	>= 2 Br	PubchemFP102	>= 1 Nd
PubchemFP45	>= 4 Br	PubchemFP103	>= 1 Pm
PubchemFP46	>= 1 I	PubchemFP104	>= 1 Sm
PubchemFP47	>= 2 I	PubchemFP105	>= 1 Eu
PubchemFP48	>= 4 I	PubchemFP106	>= 1 Gd
PubchemFP49	>= 1 Be	PubchemFP107	>= 1 Tb
PubchemFP50	>= 1 Mg	PubchemFP108	>= 1 Dy
PubchemFP51	>= 1 Al	PubchemFP109	>= 1 Ho
PubchemFP52	>= 1 Ca	PubchemFP110	>= 1 Er
PubchemFP53	>= 1 Sc	PubchemFP111	>= 1 Tm
PubchemFP54	>= 1 Ti	PubchemFP112	>= 1 Yb
PubchemFP55	>= 1 V	PubchemFP113	>= 1 Tc
PubchemFP56	>= 1 Cr	PubchemFP114	>= 1 U
PubchemFP57	>= 1 Mn		

6.2.2 Section 2

Rings in a canonic Extended Smallest Set of Smallest Rings (ESSSR) ring set - These bits test for the presence or count of the described chemical ring system. An ESSSR ring is any ring which does not share three consecutive atoms with any other ring in the chemical structure. For example, naphthalene has three ESSSR rings (two phenyl fragments and the 10-membered envelope), while biphenyl will yield a count of only two ESSSR rings.

Name	Substructure	Name	Substructure
PubchemFP115	>= 1 any ring size 3	PubchemFP189	>= 2 unsaturated non-aromatic carbon-only ring size 6
PubchemFP116	>= 1 saturated or aromatic carbon-only ring size 3	PubchemFP190	>= 2 unsaturated non-aromatic nitrogen-containing ring size 6
PubchemFP117	>= 1 saturated or aromatic nitrogen-containing ring size 3	PubchemFP191	>= 2 unsaturated non-aromatic heteroatom-containing ring size 6
PubchemFP118	>= 1 saturated or aromatic heteroatom-containing ring size 3	PubchemFP192	>= 3 any ring size 6
PubchemFP119	>= 1 unsaturated non-aromatic carbon-only ring size 3	PubchemFP193	>= 3 saturated or aromatic carbon-only ring size 6
PubchemFP120	>= 1 unsaturated non-aromatic nitrogen-containing ring size 3	PubchemFP194	>= 3 saturated or aromatic nitrogen-containing ring size 6
PubchemFP121	>= 1 unsaturated non-aromatic heteroatom-containing ring size 3	PubchemFP195	>= 3 saturated or aromatic heteroatom-containing ring size 6
PubchemFP122	>= 2 any ring size 3	PubchemFP196	>= 3 unsaturated non-aromatic carbon-only ring size 6
PubchemFP123	>= 2 saturated or aromatic carbon-only ring size 3	PubchemFP197	>= 3 unsaturated non-aromatic nitrogen-containing ring size 6
PubchemFP124	>= 2 saturated or aromatic nitrogen-containing ring size 3	PubchemFP198	>= 3 unsaturated non-aromatic heteroatom-containing ring size 6
PubchemFP125	>= 2 saturated or aromatic heteroatom-containing ring size 3	PubchemFP199	>= 4 any ring size 6
PubchemFP126	>= 2 unsaturated non-aromatic carbon-only ring size 3	PubchemFP200	>= 4 saturated or aromatic carbon-only ring size 6
PubchemFP127	>= 2 unsaturated non-aromatic nitrogen-containing ring size 3	PubchemFP201	>= 4 saturated or aromatic nitrogen-containing ring size 6
PubchemFP128	>= 2 unsaturated non-aromatic heteroatom-containing ring size 3	PubchemFP202	>= 4 saturated or aromatic heteroatom-containing ring size 6
PubchemFP129	>= 1 any ring size 4	PubchemFP203	>= 4 unsaturated non-aromatic carbon-only ring size 6
PubchemFP130	>= 1 saturated or aromatic carbon-only ring size 4	PubchemFP204	>= 4 unsaturated non-aromatic nitrogen-containing ring size 6
PubchemFP131	>= 1 saturated or aromatic nitrogen-containing ring size 4	PubchemFP205	>= 4 unsaturated non-aromatic heteroatom-containing ring size 6
PubchemFP132	>= 1 saturated or aromatic heteroatom-containing ring size 4	PubchemFP206	>= 5 any ring size 6
PubchemFP133	>= 1 unsaturated non-aromatic carbon-only ring size 4	PubchemFP207	>= 5 saturated or aromatic carbon-only ring size 6
PubchemFP134	>= 1 unsaturated non-aromatic nitrogen-containing ring size 4	PubchemFP208	>= 5 saturated or aromatic nitrogen-containing ring size 6
PubchemFP135	>= 1 unsaturated non-aromatic heteroatom-containing ring size 4	PubchemFP209	>= 5 saturated or aromatic heteroatom-containing ring size 6
PubchemFP136	>= 2 any ring size 4	PubchemFP210	>= 5 unsaturated non-aromatic carbon-only ring size 6
PubchemFP137	>= 2 saturated or aromatic carbon-only ring size 4	PubchemFP211	>= 5 unsaturated non-aromatic nitrogen-containing ring size 6
PubchemFP138	>= 2 saturated or aromatic nitrogen-containing ring size 4	PubchemFP212	>= 5 unsaturated non-aromatic heteroatom-containing ring size 6
PubchemFP139	>= 2 saturated or aromatic heteroatom-containing ring size 4	PubchemFP213	>= 1 any ring size 7
PubchemFP140	>= 2 unsaturated non-aromatic carbon-only ring size 4	PubchemFP214	>= 1 saturated or aromatic carbon-only ring size 7
PubchemFP141	>= 2 unsaturated non-aromatic nitrogen-containing ring size 4	PubchemFP215	>= 1 saturated or aromatic nitrogen-containing ring size 7

Name	Substructure	Name	Substructure
PubchemFP142	>= 2 unsaturated non-aromatic heteroatom-containing ring size 4	PubchemFP216	>= 1 saturated or aromatic heteroatom-containing ring size 7
PubchemFP143	>= 1 any ring size 5	PubchemFP217	>= 1 unsaturated non-aromatic carbon-only ring size 7
PubchemFP144	>= 1 saturated or aromatic carbon-only ring size 5	PubchemFP218	>= 1 unsaturated non-aromatic nitrogen-containing ring size 7
PubchemFP145	>= 1 saturated or aromatic nitrogen-containing ring size 5	PubchemFP219	>= 1 unsaturated non-aromatic heteroatom-containing ring size 7
PubchemFP146	>= 1 saturated or aromatic heteroatom-containing ring size 5	PubchemFP220	>= 2 any ring size 7
PubchemFP147	>= 1 unsaturated non-aromatic carbon-only ring size 5	PubchemFP221	>= 2 saturated or aromatic carbon-only ring size 7
PubchemFP148	>= 1 unsaturated non-aromatic nitrogen-containing ring size 5	PubchemFP222	>= 2 saturated or aromatic nitrogen-containing ring size 7
PubchemFP149	>= 1 unsaturated non-aromatic heteroatom-containing ring size 5	PubchemFP223	>= 2 saturated or aromatic heteroatom-containing ring size 7
PubchemFP150	>= 2 any ring size 5	PubchemFP224	>= 2 unsaturated non-aromatic carbon-only ring size 7
PubchemFP151	>= 2 saturated or aromatic carbon-only ring size 5	PubchemFP225	>= 2 unsaturated non-aromatic nitrogen-containing ring size 7
PubchemFP152	>= 2 saturated or aromatic nitrogen-containing ring size 5	PubchemFP226	>= 2 unsaturated non-aromatic heteroatom-containing ring size 7
PubchemFP153	>= 2 saturated or aromatic heteroatom-containing ring size 5	PubchemFP227	>= 1 any ring size 8
PubchemFP154	>= 2 unsaturated non-aromatic carbon-only ring size 5	PubchemFP228	>= 1 saturated or aromatic carbon-only ring size 8
PubchemFP155	>= 2 unsaturated non-aromatic nitrogen-containing ring size 5	PubchemFP229	>= 1 saturated or aromatic nitrogen-containing ring size 8
PubchemFP156	>= 2 unsaturated non-aromatic heteroatom-containing ring size 5	PubchemFP230	>= 1 saturated or aromatic heteroatom-containing ring size 8
PubchemFP157	>= 3 any ring size 5	PubchemFP231	>= 1 unsaturated non-aromatic carbon-only ring size 8
PubchemFP158	>= 3 saturated or aromatic carbon-only ring size 5	PubchemFP232	>= 1 unsaturated non-aromatic nitrogen-containing ring size 8
PubchemFP159	>= 3 saturated or aromatic nitrogen-containing ring size 5	PubchemFP233	>= 1 unsaturated non-aromatic heteroatom-containing ring size 8
PubchemFP160	>= 3 saturated or aromatic heteroatom-containing ring size 5	PubchemFP234	>= 2 any ring size 8
PubchemFP161	>= 3 unsaturated non-aromatic carbon-only ring size 5	PubchemFP235	>= 2 saturated or aromatic carbon-only ring size 8
PubchemFP162	>= 3 unsaturated non-aromatic nitrogen-containing ring size 5	PubchemFP236	>= 2 saturated or aromatic nitrogen-containing ring size 8
PubchemFP163	>= 3 unsaturated non-aromatic heteroatom-containing ring size 5	PubchemFP237	>= 2 saturated or aromatic heteroatom-containing ring size 8
PubchemFP164	>= 4 any ring size 5	PubchemFP238	>= 2 unsaturated non-aromatic carbon-only ring size 8
PubchemFP165	>= 4 saturated or aromatic carbon-only ring size 5	PubchemFP239	>= 2 unsaturated non-aromatic nitrogen-containing ring size 8
PubchemFP166	>= 4 saturated or aromatic nitrogen-containing ring size 5	PubchemFP240	>= 2 unsaturated non-aromatic heteroatom-containing ring size 8
PubchemFP167	>= 4 saturated or aromatic heteroatom-containing ring size 5	PubchemFP241	>= 1 any ring size 9
PubchemFP168	>= 4 unsaturated non-aromatic carbon-only ring size 5	PubchemFP242	>= 1 saturated or aromatic carbon-only ring size 9

Name	Substructure	Name	Substructure
PubchemFP169	>= 4 unsaturated non-aromatic nitrogen-containing ring size 5	PubchemFP243	>= 1 saturated or aromatic nitrogen-containing ring size 9
PubchemFP170	>= 4 unsaturated non-aromatic heteroatom-containing ring size 5	PubchemFP244	>= 1 saturated or aromatic heteroatom-containing ring size 9
PubchemFP171	>= 5 any ring size 5	PubchemFP245	>= 1 unsaturated non-aromatic carbon-only ring size 9
PubchemFP172	>= 5 saturated or aromatic carbon-only ring size 5	PubchemFP246	>= 1 unsaturated non-aromatic nitrogen-containing ring size 9
PubchemFP173	>= 5 saturated or aromatic nitrogen-containing ring size 5	PubchemFP247	>= 1 unsaturated non-aromatic heteroatom-containing ring size 9
PubchemFP174	>= 5 saturated or aromatic heteroatom-containing ring size 5	PubchemFP248	>= 1 any ring size 10
PubchemFP175	>= 5 unsaturated non-aromatic carbon-only ring size 5	PubchemFP249	>= 1 saturated or aromatic carbon-only ring size 10
PubchemFP176	>= 5 unsaturated non-aromatic nitrogen-containing ring size 5	PubchemFP250	>= 1 saturated or aromatic nitrogen-containing ring size 10
PubchemFP177	>= 5 unsaturated non-aromatic heteroatom-containing ring size 5	PubchemFP251	>= 1 saturated or aromatic heteroatom-containing ring size 10
PubchemFP178	>= 1 any ring size 6	PubchemFP252	>= 1 unsaturated non-aromatic carbon-only ring size 10
PubchemFP179	>= 1 saturated or aromatic carbon-only ring size 6	PubchemFP253	>= 1 unsaturated non-aromatic nitrogen-containing ring size 10
PubchemFP180	>= 1 saturated or aromatic nitrogen-containing ring size 6	PubchemFP254	>= 1 unsaturated non-aromatic heteroatom-containing ring size 10
PubchemFP181	>= 1 saturated or aromatic heteroatom-containing ring size 6	PubchemFP255	>= 1 aromatic ring
PubchemFP182	>= 1 unsaturated non-aromatic carbon-only ring size 6	PubchemFP256	>= 1 hetero-aromatic ring
PubchemFP183	>= 1 unsaturated non-aromatic nitrogen-containing ring size 6	PubchemFP257	>= 2 aromatic rings
PubchemFP184	>= 1 unsaturated non-aromatic heteroatom-containing ring size 6	PubchemFP258	>= 2 hetero-aromatic rings
PubchemFP185	>= 2 any ring size 6	PubchemFP259	>= 3 aromatic rings
PubchemFP186	>= 2 saturated or aromatic carbon-only ring size 6	PubchemFP260	>= 3 hetero-aromatic rings
PubchemFP187	>= 2 saturated or aromatic nitrogen-containing ring size 6	PubchemFP261	>= 4 aromatic rings
PubchemFP188	>= 2 saturated or aromatic heteroatom-containing ring size 6	PubchemFP262	>= 4 hetero-aromatic rings

6.2.3 Section 3

Simple atom pairs - These bits test for the presence of patterns of bonded atom pairs, regardless of bond order or count.

Name	Substructure	Name	Substructure
PubchemFP263	Li-H	PubchemFP295	C-As
PubchemFP264	Li-Li	PubchemFP296	C-Se
PubchemFP265	Li-B	PubchemFP297	C-Br
PubchemFP266	Li-C	PubchemFP298	C-I
PubchemFP267	Li-O	PubchemFP299	N-H
PubchemFP268	Li-F	PubchemFP300	N-N
PubchemFP269	Li-P	PubchemFP301	N-O
PubchemFP270	Li-S	PubchemFP302	N-F

Name	Substructure	Name	Substructure
PubchemFP271	Li-Cl	PubchemFP303	N-Si
PubchemFP272	B-H	PubchemFP304	N-P
PubchemFP273	B-B	PubchemFP305	N-S
PubchemFP274	B-C	PubchemFP306	N-Cl
PubchemFP275	B-N	PubchemFP307	N-Br
PubchemFP276	B-O	PubchemFP308	O-H
PubchemFP277	B-F	PubchemFP309	O-O
PubchemFP278	B-Si	PubchemFP310	O-Mg
PubchemFP279	B-P	PubchemFP311	O-Na
PubchemFP280	B-S	PubchemFP312	O-Al
PubchemFP281	B-Cl	PubchemFP313	O-Si
PubchemFP282	B-Br	PubchemFP314	O-P
PubchemFP283	C-H	PubchemFP315	O-K
PubchemFP284	C-C	PubchemFP316	F-P
PubchemFP285	C-N	PubchemFP317	F-S
PubchemFP286	C-O	PubchemFP318	Al-H
PubchemFP287	C-F	PubchemFP319	Al-Cl
PubchemFP288	C-Na	PubchemFP320	Si-H
PubchemFP289	C-Mg	PubchemFP321	Si-Si
PubchemFP290	C-Al	PubchemFP322	Si-Cl
PubchemFP291	C-Si	PubchemFP323	P-H
PubchemFP292	C-P	PubchemFP324	P-P
PubchemFP293	C-S	PubchemFP325	As-H
PubchemFP294	C-Cl	PubchemFP326	As-As

6.2.4 Section 4

Simple atom nearest neighbors - These bits test for the presence of atom nearest neighbor patterns, regardless of bond order (denoted by "~") or count, but where bond aromaticity (denoted by ":") is significant.

Name	Substructure	Name	Substructure
PubchemFP327	C(~Br)(~C)	PubchemFP372	C(~H)(:C)(:N)
PubchemFP328	C(~Br)(~C)(~C)	PubchemFP373	C(~H)(:N)
PubchemFP329	C(~Br)(~H)	PubchemFP374	C(~H)(~H)(~H)
PubchemFP330	C(~Br)(:C)	PubchemFP375	C(~N)(~N)
PubchemFP331	C(~Br)(:N)	PubchemFP376	C(~N)(:C)
PubchemFP332	C(~C)(~C)	PubchemFP377	C(~N)(:C)(:C)
PubchemFP333	C(~C)(~C)(~C)	PubchemFP378	C(~N)(:C)(:N)
PubchemFP334	C(~C)(~C)(~C)(~C)	PubchemFP379	C(~N)(:N)
PubchemFP335	C(~C)(~C)(~C)(~H)	PubchemFP380	C(~O)(~O)
PubchemFP336	C(~C)(~C)(~C)(~N)	PubchemFP381	C(~O)(:C)
PubchemFP337	C(~C)(~C)(~C)(~O)	PubchemFP382	C(~O)(:C)(:C)
PubchemFP338	C(~C)(~C)(~H)(~N)	PubchemFP383	C(~S)(:C)
PubchemFP339	C(~C)(~C)(~H)(~O)	PubchemFP384	C(:C)(:C)
PubchemFP340	C(~C)(~C)(~N)	PubchemFP385	C(:C)(:C)(:C)
PubchemFP341	C(~C)(~C)(~O)	PubchemFP386	C(:C)(:C)(:N)
PubchemFP342	C(~C)(~Cl)	PubchemFP387	C(:C)(:N)
PubchemFP343	C(~C)(~Cl)(~H)	PubchemFP388	C(:C)(:N)(:N)
PubchemFP344	C(~C)(~H)	PubchemFP389	C(:N)(:N)
PubchemFP345	C(~C)(~H)(~N)	PubchemFP390	N(~C)(~C)
PubchemFP346	C(~C)(~H)(~O)	PubchemFP391	N(~C)(~C)(~C)
PubchemFP347	C(~C)(~H)(~O)(~O)	PubchemFP392	N(~C)(~C)(~H)
PubchemFP348	C(~C)(~H)(~P)	PubchemFP393	N(~C)(~H)
PubchemFP349	C(~C)(~H)(~S)	PubchemFP394	N(~C)(~H)(~N)

Name	Substructure	Name	Substructure
PubchemFP350	C(~C)(~I)	PubchemFP395	N(~C)(~O)
PubchemFP351	C(~C)(~N)	PubchemFP396	N(~C)(:C)
PubchemFP352	C(~C)(~O)	PubchemFP397	N(~C)(:C)(:C)
PubchemFP353	C(~C)(~S)	PubchemFP398	N(~H)(~N)
PubchemFP354	C(~C)(~Si)	PubchemFP399	N(~H)(:C)
PubchemFP355	C(~C)(:C)	PubchemFP400	N(~H)(:C)(:C)
PubchemFP356	C(~C)(:C)(:C)	PubchemFP401	N(~O)(~O)
PubchemFP357	C(~C)(:C)(:N)	PubchemFP402	N(~O)(:O)
PubchemFP358	C(~C)(:N)	PubchemFP403	N(:C)(:C)
PubchemFP359	C(~C)(:N)(:N)	PubchemFP404	N(:C)(:C)(:C)
PubchemFP360	C(~Cl)(~Cl)	PubchemFP405	O(~C)(~C)
PubchemFP361	C(~Cl)(~H)	PubchemFP406	O(~C)(~H)
PubchemFP362	C(~Cl)(:C)	PubchemFP407	O(~C)(~P)
PubchemFP363	C(~F)(~F)	PubchemFP408	O(~H)(~S)
PubchemFP364	C(~F)(:C)	PubchemFP409	O(:C)(:C)
PubchemFP365	C(~H)(~N)	PubchemFP410	P(~C)(~C)
PubchemFP366	C(~H)(~O)	PubchemFP411	P(~O)(~O)
PubchemFP367	C(~H)(~O)(~O)	PubchemFP412	S(~C)(~C)
PubchemFP368	C(~H)(~S)	PubchemFP413	S(~C)(~H)
PubchemFP369	C(~H)(~Si)	PubchemFP414	S(~C)(~O)
PubchemFP370	C(~H)(:C)	PubchemFP415	Si(~C)(~C)
PubchemFP371	C(~H)(:C)(:C)		

6.2.5 Section 5

Detailed atom neighborhoods - These bits test for the presence of detailed atom neighborhood patterns, regardless of count, but where bond orders are specific, bond aromaticity matches both single and double bonds, and where "-", "=", and "#" matches a single bond, double bond, and triple bond order, respectively.

Name	Substructure	Name	Substructure
PubchemFP416	C=C	PubchemFP438	C(-C)(-N)(=N)
PubchemFP417	C#C	PubchemFP439	C(-C)(-N)(=O)
PubchemFP418	C=N	PubchemFP440	C(-C)(-O)(=O)
PubchemFP419	C#N	PubchemFP441	C(-C)(=C)
PubchemFP420	C=O	PubchemFP442	C(-C)(=N)
PubchemFP421	C=S	PubchemFP443	C(-C)(=O)
PubchemFP422	N=N	PubchemFP444	C(-Cl)(=O)
PubchemFP423	N=O	PubchemFP445	C(-H)(-N)(=C)
PubchemFP424	N=P	PubchemFP446	C(-H)(=C)
PubchemFP425	P=O	PubchemFP447	C(-H)(=N)
PubchemFP426	P=P	PubchemFP448	C(-H)(=O)
PubchemFP427	C(#C)(-C)	PubchemFP449	C(-N)(=C)
PubchemFP428	C(#C)(-H)	PubchemFP450	C(-N)(=N)
PubchemFP429	C(#N)(-C)	PubchemFP451	C(-N)(=O)
PubchemFP430	C(-C)(-C)(=C)	PubchemFP452	C(-O)(=O)
PubchemFP431	C(-C)(-C)(=N)	PubchemFP453	N(-C)(=C)
PubchemFP432	C(-C)(-C)(=O)	PubchemFP454	N(-C)(=O)
PubchemFP433	C(-C)(-Cl)(=O)	PubchemFP455	N(-O)(=O)
PubchemFP434	C(-C)(-H)(=C)	PubchemFP456	P(-O)(=O)
PubchemFP435	C(-C)(-H)(=N)	PubchemFP457	S(-C)(=O)
PubchemFP436	C(-C)(-H)(=O)	PubchemFP458	S(-O)(=O)
PubchemFP437	C(-C)(-N)(=C)	PubchemFP459	S(=O)(=O)

6.2.6 Section 6

Simple SMARTS patterns - These bits test for the presence of simple SMARTS patterns, regardless of count, but where bond orders are specific and bond aromaticity matches both single and double bonds.

Name	Substructure	Name	Substructure
PubchemFP460	C-C-C#C	PubchemFP587	N-C:C-O-[#1]
PubchemFP461	O-C-C=N	PubchemFP588	O=C-C-C=O
PubchemFP462	O-C-C=O	PubchemFP589	C-C:C-O-C
PubchemFP463	N:C-S-[#1]	PubchemFP590	C-C:C-O-[#1]
PubchemFP464	N-C-C=C	PubchemFP591	Cl-C-C-C-C
PubchemFP465	O=S-C-C	PubchemFP592	N-C-C-C-C
PubchemFP466	N#C-C=C	PubchemFP593	N-C-C-C-N
PubchemFP467	C=N-N-C	PubchemFP594	C-O-C-C=C
PubchemFP468	O=S-C-N	PubchemFP595	C:C-C-C-C
PubchemFP469	S-S-C:C	PubchemFP596	N=C-N-C-C
PubchemFP470	C:C-C=C	PubchemFP597	O=C-C-C:C
PubchemFP471	S:C:C:C	PubchemFP598	Cl-C:C:C-C
PubchemFP472	C:N:C-C	PubchemFP599	[#1]-C-C=C-[#1]
PubchemFP473	S-C:N:C	PubchemFP600	N-C:C:C-C
PubchemFP474	S:C:C:N	PubchemFP601	N-C:C:C-N
PubchemFP475	S-C=N-C	PubchemFP602	O=C-C-N-C
PubchemFP476	C-O-C=C	PubchemFP603	C-C:C:C-C
PubchemFP477	N-N-C:C	PubchemFP604	C-O-C-C:C
PubchemFP478	S-C=N-[#1]	PubchemFP605	O=C-C-O-C
PubchemFP479	S-C-S-C	PubchemFP606	O-C:C-C-C
PubchemFP480	C:S:C-C	PubchemFP607	N-C-C-C:C
PubchemFP481	O-S-C:C	PubchemFP608	C-C-C-C:C
PubchemFP482	C:N-C:C	PubchemFP609	Cl-C-C-N-C
PubchemFP483	N-S-C:C	PubchemFP610	C-O-C-O-C
PubchemFP484	N-C:N:C	PubchemFP611	N-C-C-N-C
PubchemFP485	N:C:C:N	PubchemFP612	N-C-O-C-C
PubchemFP486	N-C:N:N	PubchemFP613	C-N-C-C-C
PubchemFP487	N-C=N-C	PubchemFP614	C-C-O-C-C
PubchemFP488	N-C=N-[#1]	PubchemFP615	N-C-C-O-C
PubchemFP489	N-C-S-C	PubchemFP616	C:C:N:N:C
PubchemFP490	C-C-C=C	PubchemFP617	C-C-C-O-[#1]
PubchemFP491	C-N:C-[#1]	PubchemFP618	C:C-C-C:C
PubchemFP492	N-C:O:C	PubchemFP619	O-C-C=C-C
PubchemFP493	O=C-C:C	PubchemFP620	C:C-O-C-C
PubchemFP494	O=C-C:N	PubchemFP621	N-C:C:C:N
PubchemFP495	C-N-C:C	PubchemFP622	O=C-O-C:C
PubchemFP496	N:N-C-[#1]	PubchemFP623	O=C-C:C-C
PubchemFP497	O-C:C:N	PubchemFP624	O=C-C:C-N
PubchemFP498	O-C=C-C	PubchemFP625	O=C-C:C-O
PubchemFP499	N-C:C:N	PubchemFP626	C-O-C:C-C
PubchemFP500	C-S-C:C	PubchemFP627	O=[As]-C:C:C
PubchemFP501	Cl-C:C-C	PubchemFP628	C-N-C-C:C
PubchemFP502	N-C=C-[#1]	PubchemFP629	S-C:C:C-N
PubchemFP503	Cl-C:C-[#1]	PubchemFP630	O-C:C-O-C
PubchemFP504	N:C:N-C	PubchemFP631	O-C:C-O-[#1]
PubchemFP505	Cl-C:C-O	PubchemFP632	C-C-O-C:C
PubchemFP506	C-C:N:C	PubchemFP633	N-C-C:C-C
PubchemFP507	C-C-S-C	PubchemFP634	C-C-C:C-C
PubchemFP508	S=C-N-C	PubchemFP635	N-N-C-N-[#1]
PubchemFP509	Br-C:C-C	PubchemFP636	C-N-C-N-C

Name	Substructure	Name	Substructure
PubchemFP510	[#1]-N-N-[#1]	PubchemFP637	O-C-C-C-C
PubchemFP511	S=C-N-[#1]	PubchemFP638	O-C-C-C-N
PubchemFP512	C-[As]-O-[#1]	PubchemFP639	O-C-C-C-O
PubchemFP513	S:C-C-[#1]	PubchemFP640	C=C-C-C-C
PubchemFP514	O-N-C-C	PubchemFP641	O-C-C-C=C
PubchemFP515	N-N-C-C	PubchemFP642	O-C-C-C=O
PubchemFP516	[#1]-C=C-[#1]	PubchemFP643	[#1]-C-C-N-[#1]
PubchemFP517	N-N-C-N	PubchemFP644	C-C=N-N-C
PubchemFP518	O=C-N-N	PubchemFP645	O=C-N-C-C
PubchemFP519	N=C-N-C	PubchemFP646	O=C-N-C-[#1]
PubchemFP520	C=C-C:C	PubchemFP647	O=C-N-C-N
PubchemFP521	C:N-C-[#1]	PubchemFP648	O=N-C:C-N
PubchemFP522	C-N-N-[#1]	PubchemFP649	O=N-C:C-O
PubchemFP523	N:C:C-C	PubchemFP650	O=C-N-C=O
PubchemFP524	C-C=C-C	PubchemFP651	O-C:C:C-C
PubchemFP525	[As]-C:C-[#1]	PubchemFP652	O-C:C:C-N
PubchemFP526	Cl-C:C-Cl	PubchemFP653	O-C:C:C-O
PubchemFP527	C:C:N-[#1]	PubchemFP654	N-C-N-C-C
PubchemFP528	[#1]-N-C-[#1]	PubchemFP655	O-C-C-C:C
PubchemFP529	Cl-C-C-Cl	PubchemFP656	C-C-N-C-C
PubchemFP530	N:C-C:C	PubchemFP657	C-N-C:C-C
PubchemFP531	S-C:C-C	PubchemFP658	C-C-S-C-C
PubchemFP532	S-C:C-[#1]	PubchemFP659	O-C-C-N-C
PubchemFP533	S-C:C-N	PubchemFP660	C-C=C-C-C
PubchemFP534	S-C:C-O	PubchemFP661	O-C-O-C-C
PubchemFP535	O=C-C-C	PubchemFP662	O-C-C-O-C
PubchemFP536	O=C-C-N	PubchemFP663	O-C-C-O-[#1]
PubchemFP537	O=C-C-O	PubchemFP664	C-C=C-C=C
PubchemFP538	N=C-C-C	PubchemFP665	N-C:C-C-C
PubchemFP539	N=C-C-[#1]	PubchemFP666	C=C-C-O-C
PubchemFP540	C-N-C-[#1]	PubchemFP667	C=C-C-O-[#1]
PubchemFP541	O-C:C-C	PubchemFP668	C-C:C-C-C
PubchemFP542	O-C:C-[#1]	PubchemFP669	Cl-C:C-C=O
PubchemFP543	O-C:C-N	PubchemFP670	Br-C:C:C-C
PubchemFP544	O-C:C-O	PubchemFP671	O=C-C=C-C
PubchemFP545	N-C:C-C	PubchemFP672	O=C-C=C-[#1]
PubchemFP546	N-C:C-[#1]	PubchemFP673	O=C-C=C-N
PubchemFP547	N-C:C-N	PubchemFP674	N-C-N-C:C
PubchemFP548	O-C-C:C	PubchemFP675	Br-C-C-C:C
PubchemFP549	N-C-C:C	PubchemFP676	N#C-C-C-C
PubchemFP550	Cl-C-C-C	PubchemFP677	C-C=C-C:C
PubchemFP551	Cl-C-C-O	PubchemFP678	C-C-C=C-C
PubchemFP552	C:C-C:C	PubchemFP679	C-C-C-C-C-C
PubchemFP553	O=C-C=C	PubchemFP680	O-C-C-C-C-C
PubchemFP554	Br-C-C-C	PubchemFP681	O-C-C-C-C-O
PubchemFP555	N=C-C=C	PubchemFP682	O-C-C-C-C-N
PubchemFP556	C=C-C-C	PubchemFP683	N-C-C-C-C-C
PubchemFP557	N:C-O-[#1]	PubchemFP684	O=C-C-C-C-C
PubchemFP558	O=N-C:C	PubchemFP685	O=C-C-C-C-N
PubchemFP559	O-C-N-[#1]	PubchemFP686	O=C-C-C-C-O
PubchemFP560	N-C-N-C	PubchemFP687	O=C-C-C-C=O
PubchemFP561	Cl-C-C=O	PubchemFP688	C-C-C-C-C-C
PubchemFP562	Br-C-C=O	PubchemFP689	O-C-C-C-C-C
PubchemFP563	O-C-O-C	PubchemFP690	O-C-C-C-C-C-O

Name	Substructure	Name	Substructure
PubchemFP564	C=C-C=C	PubchemFP691	O-C-C-C-C-C-N
PubchemFP565	C:C-O-C	PubchemFP692	O=C-C-C-C-C-C
PubchemFP566	O-C-C-N	PubchemFP693	O=C-C-C-C-C-O
PubchemFP567	O-C-C-O	PubchemFP694	O=C-C-C-C-C=O
PubchemFP568	N#C-C-C	PubchemFP695	O=C-C-C-C-C-N
PubchemFP569	N-C-C-N	PubchemFP696	C-C-C-C-C-C-C
PubchemFP570	C:C-C-C	PubchemFP697	C-C-C-C-C-C(C)-C
PubchemFP571	[#1]-C-O-[#1]	PubchemFP698	O-C-C-C-C-C-C-C
PubchemFP572	N:C:N:C	PubchemFP699	O-C-C-C-C-C(C)-C
PubchemFP573	O-C-C=C	PubchemFP700	O-C-C-C-C-C-O-C
PubchemFP574	O-C-C:C-C	PubchemFP701	O-C-C-C-C-C(O)-C
PubchemFP575	O-C-C:C-O	PubchemFP702	O-C-C-C-C-C-N-C
PubchemFP576	N=C-C:C-[#1]	PubchemFP703	O-C-C-C-C-C(N)-C
PubchemFP577	C:C-N-C:C	PubchemFP704	O=C-C-C-C-C-C-C
PubchemFP578	C-C:C-C:C	PubchemFP705	O=C-C-C-C-C(O)-C
PubchemFP579	O=C-C-C-C	PubchemFP706	O=C-C-C-C-C(=O)-C
PubchemFP580	O=C-C-C-N	PubchemFP707	O=C-C-C-C-C(N)-C
PubchemFP581	O=C-C-C-O	PubchemFP708	C-C(C)-C-C
PubchemFP582	C-C-C-C-C	PubchemFP709	C-C(C)-C-C-C
PubchemFP583	Cl-C:C-O-C	PubchemFP710	C-C-C(C)-C-C
PubchemFP584	C:C-C=C-C	PubchemFP711	C-C(C)(C)-C-C
PubchemFP585	C-C:C-N-C	PubchemFP712	C-C(C)-C(C)-C
PubchemFP586	C-S-C-C-C		

6.2.7 Section 7

Complex SMARTS patterns - These bits test for the presence of complex SMARTS patterns, regardless of count, but where bond orders and bond aromaticity are specific.

Name	Substructure	Name	Substructure
PubchemFP713	Cc1ccc(C)cc1	PubchemFP797	CC1CC(C)CCC1
PubchemFP714	Cc1ccc(O)cc1	PubchemFP798	CC1CC(O)CCC1
PubchemFP715	Cc1ccc(S)cc1	PubchemFP799	CC1CC(S)CCC1
PubchemFP716	Cc1ccc(N)cc1	PubchemFP800	CC1CC(N)CCC1
PubchemFP717	Cc1ccc(Cl)cc1	PubchemFP801	CC1CC(Cl)CCC1
PubchemFP718	Cc1ccc(Br)cc1	PubchemFP802	CC1CC(Br)CCC1
PubchemFP719	Oc1ccc(O)cc1	PubchemFP803	OC1CC(O)CCC1
PubchemFP720	Oc1ccc(S)cc1	PubchemFP804	OC1CC(S)CCC1
PubchemFP721	Oc1ccc(N)cc1	PubchemFP805	OC1CC(N)CCC1
PubchemFP722	Oc1ccc(Cl)cc1	PubchemFP806	OC1CC(Cl)CCC1
PubchemFP723	Oc1ccc(Br)cc1	PubchemFP807	OC1CC(Br)CCC1
PubchemFP724	Sc1ccc(S)cc1	PubchemFP808	SC1CC(S)CCC1
PubchemFP725	Sc1ccc(N)cc1	PubchemFP809	SC1CC(N)CCC1
PubchemFP726	Sc1ccc(Cl)cc1	PubchemFP810	SC1CC(Cl)CCC1
PubchemFP727	Sc1ccc(Br)cc1	PubchemFP811	SC1CC(Br)CCC1
PubchemFP728	Nc1ccc(N)cc1	PubchemFP812	NC1CC(N)CCC1
PubchemFP729	Nc1ccc(Cl)cc1	PubchemFP813	NC1CC(Cl)CCC1
PubchemFP730	Nc1ccc(Br)cc1	PubchemFP814	NC1CC(Br)CCC1
PubchemFP731	Clc1ccc(Cl)cc1	PubchemFP815	ClC1CC(Cl)CCC1
PubchemFP732	Clc1ccc(Br)cc1	PubchemFP816	ClC1CC(Br)CCC1
PubchemFP733	BrC1ccc(Br)cc1	PubchemFP817	BrC1CC(Br)CCC1
PubchemFP734	Cc1cc(C)ccc1	PubchemFP818	CC1C(C)CCCC1
PubchemFP735	Cc1cc(O)ccc1	PubchemFP819	CC1C(O)CCCC1
PubchemFP736	Cc1cc(S)ccc1	PubchemFP820	CC1C(S)CCCC1

Name	Substructure	Name	Substructure
PubchemFP737	Cc1cc(N)ccc1	PubchemFP821	CC1C(N)CCCC1
PubchemFP738	Cc1cc(Cl)ccc1	PubchemFP822	CC1C(Cl)CCCC1
PubchemFP739	Cc1cc(Br)ccc1	PubchemFP823	CC1C(Br)CCCC1
PubchemFP740	Oc1cc(O)ccc1	PubchemFP824	OC1C(O)CCCC1
PubchemFP741	Oc1cc(S)ccc1	PubchemFP825	OC1C(S)CCCC1
PubchemFP742	Oc1cc(N)ccc1	PubchemFP826	OC1C(N)CCCC1
PubchemFP743	Oc1cc(Cl)ccc1	PubchemFP827	OC1C(Cl)CCCC1
PubchemFP744	Oc1cc(Br)ccc1	PubchemFP828	OC1C(Br)CCCC1
PubchemFP745	Sc1cc(S)ccc1	PubchemFP829	SC1C(S)CCCC1
PubchemFP746	Sc1cc(N)ccc1	PubchemFP830	SC1C(N)CCCC1
PubchemFP747	Sc1cc(Cl)ccc1	PubchemFP831	SC1C(Cl)CCCC1
PubchemFP748	Sc1cc(Br)ccc1	PubchemFP832	SC1C(Br)CCCC1
PubchemFP749	Nc1cc(N)ccc1	PubchemFP833	NC1C(N)CCCC1
PubchemFP750	Nc1cc(Cl)ccc1	PubchemFP834	NC1C(Cl)CCCC1
PubchemFP751	Nc1cc(Br)ccc1	PubchemFP835	NC1C(Br)CCCC1
PubchemFP752	Clc1cc(Cl)ccc1	PubchemFP836	ClC1C(Cl)CCCC1
PubchemFP753	Clc1cc(Br)ccc1	PubchemFP837	ClC1C(Br)CCCC1
PubchemFP754	BrC1cc(Br)ccc1	PubchemFP838	BrC1C(Br)CCCC1
PubchemFP755	Cc1c(C)cccc1	PubchemFP839	CC1CC(C)CC1
PubchemFP756	Cc1c(O)cccc1	PubchemFP840	CC1CC(O)CC1
PubchemFP757	Cc1c(S)cccc1	PubchemFP841	CC1CC(S)CC1
PubchemFP758	Cc1c(N)cccc1	PubchemFP842	CC1CC(N)CC1
PubchemFP759	Cc1c(Cl)cccc1	PubchemFP843	CC1CC(Cl)CC1
PubchemFP760	Cc1c(Br)cccc1	PubchemFP844	CC1CC(Br)CC1
PubchemFP761	Oc1c(O)cccc1	PubchemFP845	OC1CC(O)CC1
PubchemFP762	Oc1c(S)cccc1	PubchemFP846	OC1CC(S)CC1
PubchemFP763	Oc1c(N)cccc1	PubchemFP847	OC1CC(N)CC1
PubchemFP764	Oc1c(Cl)cccc1	PubchemFP848	OC1CC(Cl)CC1
PubchemFP765	Oc1c(Br)cccc1	PubchemFP849	OC1CC(Br)CC1
PubchemFP766	Sc1c(S)cccc1	PubchemFP850	SC1CC(S)CC1
PubchemFP767	Sc1c(N)cccc1	PubchemFP851	SC1CC(N)CC1
PubchemFP768	Sc1c(Cl)cccc1	PubchemFP852	SC1CC(Cl)CC1
PubchemFP769	Sc1c(Br)cccc1	PubchemFP853	SC1CC(Br)CC1
PubchemFP770	Nc1c(N)cccc1	PubchemFP854	NC1CC(N)CC1
PubchemFP771	Nc1c(Cl)cccc1	PubchemFP855	NC1CC(Cl)CC1
PubchemFP772	Nc1c(Br)cccc1	PubchemFP856	NC1CC(Br)CC1
PubchemFP773	Clc1c(Cl)cccc1	PubchemFP857	ClC1CC(Cl)CC1
PubchemFP774	Clc1c(Br)cccc1	PubchemFP858	ClC1CC(Br)CC1
PubchemFP775	BrC1c(Br)cccc1	PubchemFP859	BrC1CC(Br)CC1
PubchemFP776	CC1CCC(C)CC1	PubchemFP860	CC1C(C)CCC1
PubchemFP777	CC1CCC(O)CC1	PubchemFP861	CC1C(O)CCC1
PubchemFP778	CC1CCC(S)CC1	PubchemFP862	CC1C(S)CCC1
PubchemFP779	CC1CCC(N)CC1	PubchemFP863	CC1C(N)CCC1
PubchemFP780	CC1CCC(Cl)CC1	PubchemFP864	CC1C(Cl)CCC1
PubchemFP781	CC1CCC(Br)CC1	PubchemFP865	CC1C(Br)CCC1
PubchemFP782	OC1CCC(O)CC1	PubchemFP866	OC1C(O)CCC1
PubchemFP783	OC1CCC(S)CC1	PubchemFP867	OC1C(S)CCC1
PubchemFP784	OC1CCC(N)CC1	PubchemFP868	OC1C(N)CCC1
PubchemFP785	OC1CCC(Cl)CC1	PubchemFP869	OC1C(Cl)CCC1
PubchemFP786	OC1CCC(Br)CC1	PubchemFP870	OC1C(Br)CCC1
PubchemFP787	SC1CCC(S)CC1	PubchemFP871	SC1C(S)CCC1
PubchemFP788	SC1CCC(N)CC1	PubchemFP872	SC1C(N)CCC1
PubchemFP789	SC1CCC(Cl)CC1	PubchemFP873	SC1C(Cl)CCC1
PubchemFP790	SC1CCC(Br)CC1	PubchemFP874	SC1C(Br)CCC1

Name	Substructure	Name	Substructure
PubchemFP791	NC1CCC(N)CC1	PubchemFP875	NC1C(N)CCC1
PubchemFP792	NC1CCC(Cl)CC1	PubchemFP876	NC1C(Cl)CC1
PubchemFP793	NC1CCC(Br)CC1	PubchemFP877	NC1C(Br)CCC1
PubchemFP794	ClC1CCC(Cl)CC1	PubchemFP878	ClC1C(Cl)CCC1
PubchemFP795	ClC1CCC(Br)CC1	PubchemFP879	ClC1C(Br)CCC1
PubchemFP796	BrC1CCC(Br)CC1	PubchemFP880	BrC1C(Br)CCC1

6.3 Klekota and Roth

The following table is adapted from PaDEL-Descriptor v2.21 documentation.

Name	Count name	Pattern
KRFP1	KRFPC1	[!#1][CH](!!#1)!!#1
KRFP2	KRFPC2	[!#1][CH](!!#1)[CH](!!#1)!!#1
KRFP3	KRFPC3	[!#1][CH](!!#1)[CH](!!#1)C([CH3])([CH3])[CH3]
KRFP4	KRFPC4	[!#1][CH](!!#1)[CH](C(=O)O[CH3])C(=O)O[CH3]
KRFP5	KRFPC5	[!#1][CH](!!#1)[CH]1[CH2][CH](!!#1)!!#1)[CH]([CH]1C(=O)!!#1)C(=O)[OH]
KRFP6	KRFPC6	[!#1][CH](!!#1)[CH2][CH](!!#1)[CH2][CH](!!#1)!!#1)C(=O)!!#1)C(=O)!!#1
KRFP7	KRFPC7	[!#1][CH](!!#1)[CH2][CH2][CH3]
KRFP8	KRFPC8	[!#1][CH](!!#1)[CH2][CH2]C(!!#1)(!!#1)[CH3]
KRFP9	KRFPC9	[!#1][CH](!!#1)[CH2]C(=N[NH]C(=S)[NH2])[CH2][CH3]
KRFP10	KRFPC10	[!#1][CH](!!#1)[CH2]C(=O)!!#1
KRFP11	KRFPC11	[!#1][CH](!!#1)[CH2]C(=O)[CH2][CH3]
KRFP12	KRFPC12	[!#1][CH](!!#1)[CH2]C(=O)[CH3]
KRFP13	KRFPC13	[!#1][CH](!!#1)[CH2]N(!!#1)[CH2][CH](!!#1)!!#1
KRFP14	KRFPC14	[!#1][CH](!!#1)[CH3]
KRFP15	KRFPC15	[!#1][CH](!!#1)[N+](=O)[O-]
KRFP16	KRFPC16	[!#1][CH](!!#1)[NH]C(=O)!!#1
KRFP17	KRFPC17	[!#1][CH](!!#1)[OH]
KRFP18	KRFPC18	[!#1][CH](!!#1)C(!!#1)(!!#1)!!#1
KRFP19	KRFPC19	[!#1][CH](!!#1)C(!!#1)([CH3])[CH3]
KRFP20	KRFPC20	[!#1][CH](!!#1)C(=O)!!#1
KRFP21	KRFPC21	[!#1][CH](!!#1)C(=O)[CH](!!#1)!!#1
KRFP22	KRFPC22	[!#1][CH](!!#1)C(=O)[CH2]C([CH3])([CH3])[CH2]C(!!#1)(!!#1)!!#1
KRFP23	KRFPC23	[!#1][CH](!!#1)C(=O)[CH3]
KRFP24	KRFPC24	[!#1][CH](!!#1)C(=O)[NH][NH]C(=O)[CH2][CH2][CH2][CH2][CH2][CH2][CH3]
KRFP25	KRFPC25	[!#1][CH](!!#1)C(=O)[OH]
KRFP26	KRFPC26	[!#1][CH](!!#1)C(=O)c1[cH][cH][cH][cH]1
KRFP27	KRFPC27	[!#1][CH](!!#1)C(=O)c1[cH][cH]c(!!#1)[cH][cH]1
KRFP28	KRFPC28	[!#1][CH](!!#1)C(=O)c1[cH][cH]c(Cl)[cH][cH]1
KRFP29	KRFPC29	[!#1][CH](!!#1)C(=O)c1c([CH3])[cH]c([CH3])[nH]c1=O
KRFP30	KRFPC30	[!#1][CH](!!#1)C(=O)c1c([CH3])[nH]c2[cH][cH][cH][cH]c12
KRFP31	KRFPC31	[!#1][CH](!!#1)C(=O)c1c([OH])[cH]c([CH3])oc1=O
KRFP32	KRFPC32	[!#1][CH](!!#1)C(=O)O[CH2][CH2]N([CH2][CH3])[CH2][CH3]
KRFP33	KRFPC33	[!#1][CH](!!#1)c1[cH][cH][cH][cH]1
KRFP34	KRFPC34	[!#1][CH](!!#1)c1[cH][cH][cH][cH]c1!!#1
KRFP35	KRFPC35	[!#1][CH](!!#1)c1[cH][cH][cH][cH]c1[N+](=O)[O-]
KRFP36	KRFPC36	[!#1][CH](!!#1)c1[cH][cH][cH][cH]c1[OH]
KRFP37	KRFPC37	[!#1][CH](!!#1)c1[cH][cH][cH][cH]c1Cl
KRFP38	KRFPC38	[!#1][CH](!!#1)c1[cH][cH][cH][cH]c1F
KRFP39	KRFPC39	[!#1][CH](!!#1)c1[cH][cH][cH][cH]c1N(!!#1)c2[cH][cH][cH][cH]c2[CH](!!#1)!!#1

Name	Count name	Pattern
KRFP40	KRFPC40	[!#1][CH]([!#1])c1[cH][cH][cH]c([cH]1)[N+](=O)[O-]
KRFP41	KRFPC41	[!#1][CH]([!#1])c1[cH][cH][cH]c(Br)[cH]1
KRFP42	KRFPC42	[!#1][CH]([!#1])c1[cH][cH][cH]n[cH]1
KRFP43	KRFPC43	[!#1][CH]([!#1])c1[cH][cH][cH]o1
KRFP44	KRFPC44	[!#1][CH]([!#1])c1[cH][cH][cH]s1
KRFP45	KRFPC45	[!#1][CH]([!#1])c1[cH][cH]c([!#1])[cH][cH]1
KRFP46	KRFPC46	[!#1][CH]([!#1])c1[cH][cH]c([!#1])o1
KRFP47	KRFPC47	[!#1][CH]([!#1])c1[cH][cH]c([cH][cH]1)[CH]([!#1])[!#1]
KRFP48	KRFPC48	[!#1][CH]([!#1])c1[cH][cH]c([cH][cH]1)[N+](=O)[O-]
KRFP49	KRFPC49	[!#1][CH]([!#1])c1[cH][cH]c([cH][cH]1)N([!#1])[CH3]
KRFP50	KRFPC50	[!#1][CH]([!#1])c1[cH][cH]c([CH3])[cH]c1[CH3]
KRFP51	KRFPC51	[!#1][CH]([!#1])c1[cH][cH]c([CH3])o1
KRFP52	KRFPC52	[!#1][CH]([!#1])c1[cH][cH]c([OH])[cH][cH]1
KRFP53	KRFPC53	[!#1][CH]([!#1])c1[cH][cH]c(Br)[cH][cH]1
KRFP54	KRFPC54	[!#1][CH]([!#1])c1[cH][cH]c(Cl)[cH][cH]1
KRFP55	KRFPC55	[!#1][CH]([!#1])c1[cH][cH]c(Cl)[cH]c1Cl
KRFP56	KRFPC56	[!#1][CH]([!#1])c1[cH][cH]c(F)[cH][cH]1
KRFP57	KRFPC57	[!#1][CH]([!#1])c1[cH][cH]c2O[CH2]Oc2[cH]1
KRFP58	KRFPC58	[!#1][CH]([!#1])c1[cH][cH]n[cH][cH]1
KRFP59	KRFPC59	[!#1][CH]([!#1])c1[cH][nH]c2[cH][cH][cH][cH]c12
KRFP60	KRFPC60	[!#1][CH]([!#1])c1[cH]c([!#1])nn1[!#1]
KRFP61	KRFPC61	[!#1][CH]([!#1])c1[cH]c([cH][cH]c1[OH])[N+](=O)[O-]
KRFP62	KRFPC62	[!#1][CH]([!#1])c1[cH]c(Br)[cH]c(Br)c1[OH]
KRFP63	KRFPC63	[!#1][CH]([!#1])C1=C([OH])[CH2]C([CH3])([CH3])[CH2]C1=O
KRFP64	KRFPC64	[!#1][CH]([!#1])c1c([OH])[cH][cH]c2[cH][cH][cH][cH]c12
KRFP65	KRFPC65	[!#1][CH]([!#1])c1c2[cH][cH][cH][cH]c2[cH]c3[cH][cH][cH][cH]c13
KRFP66	KRFPC66	[!#1][CH]([!#1])c1sc2[cH][cH][cH][cH]c2[n+][CH2][CH2][CH2]S(=O)(=O)[OH]
KRFP67	KRFPC67	[!#1][CH]([!#1])N([!#1])[CH3]
KRFP68	KRFPC68	[!#1][CH]([!#1])N([!#1])c1[cH][cH][cH][cH][cH]1
KRFP69	KRFPC69	[!#1][CH]([!#1])N([CH3])[CH3]
KRFP70	KRFPC70	[!#1][CH]([!#1])N1[CH2][CH2]O[CH2][CH2]1
KRFP71	KRFPC71	[!#1][CH]([!#1])O[CH2][CH2]N([CH3])[CH3]
KRFP72	KRFPC72	[!#1][CH]([!#1])OC(=O)[!#1]
KRFP73	KRFPC73	[!#1][CH]([!#1])S(=O)(=O)[!#1]
KRFP74	KRFPC74	[!#1][CH]([CH]([CH3])[CH3])C(=O)[OH]
KRFP75	KRFPC75	[!#1][CH]([CH]=[CH]c1[cH][cH]c(Cl)[cH]c1Cl)C([CH3])([CH3])[CH3]
KRFP76	KRFPC76	[!#1][CH]([CH2][CH2]C(=O)[OH])C(=O)[OH]
KRFP77	KRFPC77	[!#1][CH]([CH2][CH2]S[CH3])C(=O)[OH]
KRFP78	KRFPC78	[!#1][CH]([CH2][N+](=O)[O-])SC(=O)[CH3]
KRFP79	KRFPC79	[!#1][CH]([CH2]C(=N[NH]C(=O)[!#1])[!#1])C(=O)[OH]
KRFP80	KRFPC80	[!#1][CH]([CH2]C(=O)[!#1])C(=O)N([!#1])c1[cH][cH][cH][cH][cH]1
KRFP81	KRFPC81	[!#1][CH]([CH2]C(=O)[!#1])C(=O)N([!#1])c1[cH][cH][cH]c([CH3])[cH]1
KRFP82	KRFPC82	[!#1][CH]([CH2]C(=O)[!#1])C(=O)N([!#1])c1[cH][cH][cH]c(Br)[cH]1
KRFP83	KRFPC83	[!#1][CH]([CH2]C(=O)[!#1])C(=O)N([!#1])c1[cH][cH][cH]c(Cl)[cH]1
KRFP84	KRFPC84	[!#1][CH]([CH2]C(=O)[!#1])C(=O)N([!#1])c1[cH][cH]c([cH][cH]1)[N+](=O)[O-]
KRFP85	KRFPC85	[!#1][CH]([CH2]C(=O)[!#1])C(=O)N([!#1])c1[cH][cH]c([cH][cH]1)C(=O)[OH]
KRFP86	KRFPC86	[!#1][CH]([CH2]C(=O)[!#1])C(=O)N([!#1])c1[cH][cH]c(Br)[cH][cH]1
KRFP87	KRFPC87	[!#1][CH]([CH2]C(=O)[!#1])C(=O)N([!#1])c1[cH][cH]c(Cl)[cH][cH]1
KRFP88	KRFPC88	[!#1][CH]([CH2]C(=O)[NH2])C(=O)[OH]
KRFP89	KRFPC89	[!#1][CH]([CH2]C(=O)[OH])[NH]C(=O)C(F)(F)F
KRFP90	KRFPC90	[!#1][CH]([CH2]C(=O)[OH])C(=O)[OH]
KRFP91	KRFPC91	[!#1][CH]([CH3])[CH2][CH3]
KRFP92	KRFPC92	[!#1][CH]([CH3])[CH3]

Name	Count name	Pattern
KRFP93	KRFPC93	[!#1][CH]([CH3])[NH]C(=O)[!#1]
KRFP94	KRFPC94	[!#1][CH]([CH3])[NH]C(=O)[NH][CH2]C(=O)O[CH2][CH3]
KRFP95	KRFPC95	[!#1][CH]([CH3])[NH]C(=S)[!#1]
KRFP96	KRFPC96	[!#1][CH]([CH3])[NH]C(=S)[NH]C([!#1])([!#1])[!#1]
KRFP97	KRFPC97	[!#1][CH]([CH3])[NH]S(=O)(=O)[!#1]
KRFP98	KRFPC98	[!#1][CH]([CH3])C(=O)[!#1]
KRFP99	KRFPC99	[!#1][CH]([CH3])C(=O)[OH]
KRFP100	KRFPC100	[!#1][CH]([CH3])C(=O)O[CH2]C(=O)[!#1]
KRFP101	KRFPC101	[!#1][CH]([CH3])c1[cH][cH][cH][cH][cH]1
KRFP102	KRFPC102	[!#1][CH]([CH3])N([!#1])C(=O)[!#1]
KRFP103	KRFPC103	[!#1][CH]([NH]C(=O)[!#1])[NH]C(=O)[!#1]
KRFP104	KRFPC104	[!#1][CH]([NH]C(=O)[!#1])C(=O)[OH]
KRFP105	KRFPC105	[!#1][CH]([NH]C(=O)[!#1])C(Br)(Br)Br
KRFP106	KRFPC106	[!#1][CH]([NH]C(=O)[!#1])C(Cl)(Cl)Cl
KRFP107	KRFPC107	[!#1][CH]([NH]C(=O)[CH2][CH2][CH2][CH2][CH3])C(Cl)(Cl)Cl
KRFP108	KRFPC108	[!#1][CH]([NH]S(=O)(=O)[!#1])C(Cl)(Cl)Cl
KRFP109	KRFPC109	[!#1][CH]([NH2])[CH2][CH3]
KRFP110	KRFPC110	[!#1][CH]([NH2])[CH2]C(=O)[OH]
KRFP111	KRFPC111	[!#1][CH]([NH2])C(=O)[OH]
KRFP112	KRFPC112	[!#1][CH]([OH])[CH]([NH2])[CH2][OH]
KRFP113	KRFPC113	[!#1][CH]([OH])[CH2][NH]C(=O)[!#1]
KRFP114	KRFPC114	[!#1][CH]([OH])[CH2][NH2]
KRFP115	KRFPC115	[!#1][CH]([OH])[CH2][OH]
KRFP116	KRFPC116	[!#1][CH]([OH])C(=N[NH]C(=O)[!#1])[!#1]
KRFP117	KRFPC117	[!#1][CH]([OH])C(Cl)(Cl)Cl
KRFP118	KRFPC118	[!#1][CH]([OH])C(F)(F)F
KRFP119	KRFPC119	[!#1][CH]([OH])c1[cH][cH][cH][cH][cH]1
KRFP120	KRFPC120	[!#1][CH](C(=O)[CH3])C(=O)[CH3]
KRFP121	KRFPC121	[!#1][CH](C(=O)O[CH2][CH3])C(=O)O[CH2][CH3]
KRFP122	KRFPC122	[!#1][CH](C(=O)O[CH3])C(=O)O[CH3]
KRFP123	KRFPC123	[!#1][CH](F)C(F)(F)F
KRFP124	KRFPC124	[!#1][CH](F)OC(F)(F)F
KRFP125	KRFPC125	[!#1][CH](OC(=O)[CH3])OC(=O)[CH3]
KRFP126	KRFPC126	[!#1][CH]=[CH][!#1]
KRFP127	KRFPC127	[!#1][CH]=[CH][CH]([!#1])C([CH3])([CH3])[CH3]
KRFP128	KRFPC128	[!#1][CH]=[CH][CH]=C1SC(=S)N([!#1])C1=O
KRFP129	KRFPC129	[!#1][CH]=[CH][CH]=N[!#1]
KRFP130	KRFPC130	[!#1][CH]=[CH][CH]=N[NH]C(=O)[!#1]
KRFP131	KRFPC131	[!#1][CH]=[CH]C(=N[NH]C(=O)[!#1])[!#1]
KRFP132	KRFPC132	[!#1][CH]=[CH]C(=N[NH]C(=O)[!#1])[CH3]
KRFP133	KRFPC133	[!#1][CH]=[CH]C(=O)[!#1]
KRFP134	KRFPC134	[!#1][CH]=[CH]C(=O)[NH][NH]C(=O)[!#1]
KRFP135	KRFPC135	[!#1][CH]=[CH]C(=O)[NH]C(=S)[!#1]
KRFP136	KRFPC136	[!#1][CH]=[CH]C(=O)[OH]
KRFP137	KRFPC137	[!#1][CH]=[CH]N([!#1])[CH3]
KRFP138	KRFPC138	[!#1][CH]=[CH2]
KRFP139	KRFPC139	[!#1][CH]=C([NH]C(=O)[!#1])C(=O)[!#1]
KRFP140	KRFPC140	[!#1][CH]=C([NH]C(=O)[!#1])C(=O)[NH][CH2][CH2][CH2]N([CH3])[CH3]
KRFP141	KRFPC141	[!#1][CH]=C(C#N)C#N
KRFP142	KRFPC142	[!#1][CH]=C(C#N)C(=O)[NH2]
KRFP143	KRFPC143	[!#1][CH]=C(C#N)C(=O)O[CH2][CH3]
KRFP144	KRFPC144	[!#1][CH]=C(Cl)Cl
KRFP145	KRFPC145	[!#1][CH]=C1[CH2]N([!#1])[CH2]C(=[CH][!#1])C1=O
KRFP146	KRFPC146	[!#1][CH]=c1[nH]c(=O)c(=[CH][!#1])[nH]c1=O

Name	Count name	Pattern
KRFP147	KRFPC147	[!#1][CH]=C1C(=NN(C1=O)c2[cH][cH]c(!#1)[cH][cH]2)[!#1]
KRFP148	KRFPC148	[!#1][CH]=C1C(=O)[NH]C(=O)[NH]C1=O
KRFP149	KRFPC149	[!#1][CH]=C1C(=O)[NH]C(=O)N(!#1)C1=O
KRFP150	KRFPC150	[!#1][CH]=C1C(=O)[NH]C(=O)N(C1=O)c2[cH][cH][cH]c3[cH][cH][cH][cH]c23
KRFP151	KRFPC151	[!#1][CH]=C1C(=O)c2[cH][cH][cH][cH]c2C1=O
KRFP152	KRFPC152	[!#1][CH]=C1C(=O)N(N=C1c2[cH][cH][cH][cH][cH]2)c3[cH][cH]c(!#1)[cH][cH]3
KRFP153	KRFPC153	[!#1][CH]=C1C(=O)OC(!#1)([CH3])OC1=O
KRFP154	KRFPC154	[!#1][CH]=C1N=C(OC1=O)c2[cH][cH][cH][cH]2
KRFP155	KRFPC155	[!#1][CH]=C1OC(=O)c2c1[cH]c(!#1)[nH]c2=O
KRFP156	KRFPC156	[!#1][CH]=C1SC(=N(!#1))[NH]C1=O
KRFP157	KRFPC157	[!#1][CH]=C1SC(=O)N(!#1)C1=O
KRFP158	KRFPC158	[!#1][CH]=C1SC(=S)[NH]C1=O
KRFP159	KRFPC159	[!#1][CH]=C1SC(=S)N(!#1)C1=O
KRFP160	KRFPC160	[!#1][CH]=C1SC(=S)N(C1=O)c2[cH][cH]c(!#1)[cH][cH]2
KRFP161	KRFPC161	[!#1][CH]=N(!#1)
KRFP162	KRFPC162	[!#1][CH]=N[CH](!#1)[CH3]
KRFP163	KRFPC163	[!#1][CH]=N[CH2][CH2][CH2][CH2][CH2]N=[CH](!#1)
KRFP164	KRFPC164	[!#1][CH]=N[CH2][CH2][NH]C(=O)[!#1]
KRFP165	KRFPC165	[!#1][CH]=N[CH2][CH2]N=[CH](!#1)
KRFP166	KRFPC166	[!#1][CH]=N[NH]C(=[NH])[NH][N+](=O)[O-]
KRFP167	KRFPC167	[!#1][CH]=N[NH]C(=[NH])[NH2]
KRFP168	KRFPC168	[!#1][CH]=N[NH]C(=O)[!#1]
KRFP169	KRFPC169	[!#1][CH]=N[NH]C(=O)[CH](!#1)[CH3]
KRFP170	KRFPC170	[!#1][CH]=N[NH]C(=O)[CH](!#1)[NH]C(=O)[!#1]
KRFP171	KRFPC171	[!#1][CH]=N[NH]C(=O)[CH](!#1)[OH]
KRFP172	KRFPC172	[!#1][CH]=N[NH]C(=O)[CH2][CH2][CH]([CH3])[OH]
KRFP173	KRFPC173	[!#1][CH]=N[NH]C(=O)[CH2][CH2][CH2][CH2][CH2][CH2][CH3]
KRFP174	KRFPC174	[!#1][CH]=N[NH]C(=O)[CH2][CH2][CH2][CH2][CH3]
KRFP175	KRFPC175	[!#1][CH]=N[NH]C(=O)[CH2][NH]C(=O)[!#1]
KRFP176	KRFPC176	[!#1][CH]=N[NH]C(=O)[CH2][OH]
KRFP177	KRFPC177	[!#1][CH]=N[NH]C(=O)[CH2]C(=O)[NH]N=[CH](!#1)
KRFP178	KRFPC178	[!#1][CH]=N[NH]C(=O)[NH2]
KRFP179	KRFPC179	[!#1][CH]=N[NH]C(=O)C(=O)[NH]N=[CH](!#1)
KRFP180	KRFPC180	[!#1][CH]=N[NH]C(=O)O[CH2][CH3]
KRFP181	KRFPC181	[!#1][CH]=N[NH]C(=S)[NH2]
KRFP182	KRFPC182	[!#1][CH]=N[NH]C(=S)S[CH3]
KRFP183	KRFPC183	[!#1][CH]=N[NH]S(=O)(=O)[!#1]
KRFP184	KRFPC184	[!#1][CH]=N[OH]
KRFP185	KRFPC185	[!#1][CH]=NC(=N[NH]C(=O)[!#1])[!#1]
KRFP186	KRFPC186	[!#1][CH]=NN(!#1)[CH3]
KRFP187	KRFPC187	[!#1][CH]=NN=[CH](!#1)
KRFP188	KRFPC188	[!#1][CH]=NOC(=O)[!#1]
KRFP189	KRFPC189	[!#1][CH]=O
KRFP190	KRFPC190	[!#1][CH]1[CH](!#1)[CH]2[CH2][CH]1[CH]=[CH]2
KRFP191	KRFPC191	[!#1][CH]1[CH](!#1)[CH]2c3[cH][cH][cH][cH]c3[CH]1c4[cH][cH][cH][cH] c24
KRFP192	KRFPC192	[!#1][CH]1[CH]([CH]2[CH2][CH]1[CH]=[CH]2)C(=O)[OH]
KRFP193	KRFPC193	[!#1][CH]1[CH]([CH]2c3[cH][cH][cH][cH]c3[CH]1c4[cH][cH][cH][cH]c24)C(=O)[OH]
KRFP194	KRFPC194	[!#1][CH]1[CH]([OH])O[CH]([CH2][OH])[CH]([OH])[CH]1[OH]
KRFP195	KRFPC195	[!#1][CH]1[CH]2[CH2][CH]3[CH2][CH]([CH2]2)[CH2][CH]1[CH2]3
KRFP196	KRFPC196	[!#1][CH]1[CH]2[CH2][CH2][CH2][CH2][CH]12
KRFP197	KRFPC197	[!#1][CH]1[CH]2S[CH2]C1(!#1)[CH2][CH2][CH]2[!#1]
KRFP198	KRFPC198	[!#1][CH]1[CH2][CH]([CH3])[CH2][CH2][CH]1[CH]([CH3])[CH3]

Name	Count name	Pattern
KRFP199	KRFPC199	[!#1][CH]1[CH2][CH]=[CH][CH2][CH]1[!#1]
KRFP200	KRFPC200	[!#1][CH]1[CH2][CH]=[CH][CH2][CH]1C(=O)[OH]
KRFP201	KRFPC201	[!#1][CH]1[CH2][CH]1[!#1]
KRFP202	KRFPC202	[!#1][CH]1[CH2][CH]1c2[cH][cH][cH][cH]2
KRFP203	KRFPC203	[!#1][CH]1[CH2][CH]2[CH2][CH2][CH]([CH2]1)N2[!#1]
KRFP204	KRFPC204	[!#1][CH]1[CH2][CH]2[CH2][CH2][CH]([CH2]1)N2[CH3]
KRFP205	KRFPC205	[!#1][CH]1[CH2][CH]2[CH2][CH2][CH]1[CH2]2
KRFP206	KRFPC206	[!#1][CH]1[CH2][CH]2[CH2][CH2]N1[CH2][CH]2[CH]=[CH2]
KRFP207	KRFPC207	[!#1][CH]1[CH2][CH2][CH]([!#1])[CH]([!#1])[CH2]1
KRFP208	KRFPC208	[!#1][CH]1[CH2][CH2][CH]([!#1])[CH2][CH2]1
KRFP209	KRFPC209	[!#1][CH]1[CH2][CH2][CH]([CH2][CH2]1)C([CH3])([CH3])[CH3]
KRFP210	KRFPC210	[!#1][CH]1[CH2][CH2][CH]2[CH2][CH2][CH2][NH][CH]2[CH2]1
KRFP211	KRFPC211	[!#1][CH]1[CH2][CH2][CH2][CH]([!#1)N1[!#1]
KRFP212	KRFPC212	[!#1][CH]1[CH2][CH2][CH2][CH2][CH]1[!#1]
KRFP213	KRFPC213	[!#1][CH]1[CH2][CH2][CH2][CH2][CH2][CH2][CH2]1
KRFP214	KRFPC214	[!#1][CH]1[CH2][CH2][CH2][CH2][CH2]1
KRFP215	KRFPC215	[!#1][CH]1[CH2][CH2][CH2][CH2][NH]C1=O
KRFP216	KRFPC216	[!#1][CH]1[CH2][CH2][CH2][CH2]1
KRFP217	KRFPC217	[!#1][CH]1[CH2][CH2][CH2][CH2]C1=O
KRFP218	KRFPC218	[!#1][CH]1[CH2][CH2][CH2][CH2]N1[!#1]
KRFP219	KRFPC219	[!#1][CH]1[CH2][CH2][CH2]C1=N[NH]C(=S)[NH2]
KRFP220	KRFPC220	[!#1][CH]1[CH2][CH2][CH2]c2c1[nH]c3[cH][cH]c([!#1])[cH]c23
KRFP221	KRFPC221	[!#1][CH]1[CH2][CH2][CH2]c2c1[nH]c3[cH][cH]c([cH]c23)c4[cH][cH][cH][cH]cH]4
KRFP222	KRFPC222	[!#1][CH]1[CH2][CH2][CH2]c2c1[nH]c3[cH][cH]c([CH3])[cH]c23
KRFP223	KRFPC223	[!#1][CH]1[CH2][CH2][CH2]N([!#1])[CH2]1
KRFP224	KRFPC224	[!#1][CH]1[CH2][CH2][CH2]N1[!#1]
KRFP225	KRFPC225	[!#1][CH]1[CH2][CH2][CH2]O1
KRFP226	KRFPC226	[!#1][CH]1[CH2][CH2][NH][CH2][CH2]1
KRFP227	KRFPC227	[!#1][CH]1[CH2][CH2][NH]C(=O)[NH]1
KRFP228	KRFPC228	[!#1][CH]1[CH2][CH2]1
KRFP229	KRFPC229	[!#1][CH]1[CH2][CH2]C([!#1])(C(=O)[OH])C1([!#1])[CH3]
KRFP230	KRFPC230	[!#1][CH]1[CH2][CH2]C([CH3])(C(=O)[OH])C1([CH3])[CH3]
KRFP231	KRFPC231	[!#1][CH]1[CH2][CH2]c2c([!#1])c([!#1])sc2C1=O
KRFP232	KRFPC232	[!#1][CH]1[CH2][CH2]N([!#1])[CH2][CH2]1
KRFP233	KRFPC233	[!#1][CH]1[CH2][CH2]OC1=O
KRFP234	KRFPC234	[!#1][CH]1[CH2][CH2]S(=O)(=O)[CH2]1
KRFP235	KRFPC235	[!#1][CH]1[CH2][NH]c2[cH][cH][cH][cH]c12
KRFP236	KRFPC236	[!#1][CH]1[CH2]C([!#1])([CH]([!#1])[CH2]N1[!#1])c2[cH][cH][cH][cH] [cH]2
KRFP237	KRFPC237	[!#1][CH]1[CH2]C([!#1])([CH3])[NH]C([!#1])([CH3])[CH2]1
KRFP238	KRFPC238	[!#1][CH]1[CH2]C([CH3])([CH3])[NH]C([CH3])([CH3])[CH2]1
KRFP239	KRFPC239	[!#1][CH]1[CH2]C(=O)N(C1=O)c2[cH][cH][cH][cH][cH]2
KRFP240	KRFPC240	[!#1][CH]1[CH2]C(=O)N(C1=O)c2[cH][cH][cH]c([!#1])[cH]2
KRFP241	KRFPC241	[!#1][CH]1[CH2]C(=O)N(C1=O)c2[cH][cH][cH]c(Cl)[cH]2
KRFP242	KRFPC242	[!#1][CH]1[CH2]C(=O)N(C1=O)c2[cH][cH][cH]c3[cH][cH][cH][cH]c23
KRFP243	KRFPC243	[!#1][CH]1[CH2]C(=O)N(C1=O)c2[cH][cH]c([!#1])[cH][cH]2
KRFP244	KRFPC244	[!#1][CH]1[CH2]C(=O)N(C1=O)c2[cH][cH]c(Br)[cH][cH]2
KRFP245	KRFPC245	[!#1][CH]1[CH2]C(=O)N(C1=O)c2[cH][cH]c(Cl)[cH][cH]2
KRFP246	KRFPC246	[!#1][CH]1[CH2]C(=O)N(C1=O)c2[cH][cH]c(O[CH3])[cH][cH]2
KRFP247	KRFPC247	[!#1][CH]1[CH2]C(=O)N(N([CH3])[CH3])C1=O
KRFP248	KRFPC248	[!#1][CH]1[CH2]C(=O)O[CH]1c2[cH][cH][cH][cH][cH]2
KRFP249	KRFPC249	[!#1][CH]1[CH2]C1([!#1])[CH3]
KRFP250	KRFPC250	[!#1][CH]1[CH2]C1([CH3])[CH3]
KRFP251	KRFPC251	[!#1][CH]1[CH2]C1(c2[cH][cH][cH][cH][cH]2)c3[cH][cH][cH][cH][cH]3

Name	Count name	Pattern
KRFP252	KRFPC252	[!#1][CH]1[CH2]C1(c2[cH][cH]c([!#1])[cH][cH]2)c3[cH][cH]c([!#1])[cH][cH]3
KRFP253	KRFPC253	[!#1][CH]1[CH2]C1(c2[cH][cH]c([CH3])[cH][cH]2)c3[cH][cH]c([CH3])[cH][cH]3
KRFP254	KRFPC254	[!#1][CH]1[CH2]C2([!#1])[CH2]C([!#1])([CH2][CH]([!#1])C2=O)C1=O
KRFP255	KRFPC255	[!#1][CH]1[CH2]c2[cH][cH][cH]c3[cH][cH][cH]c1c23
KRFP256	KRFPC256	[!#1][CH]1[CH2]C21[CH2][CH2][CH2]2
KRFP257	KRFPC257	[!#1][CH]1[CH2]c2c([nH]c3[cH][cH][cH][cH]c23)[CH]([!#1])[NH]1
KRFP258	KRFPC258	[!#1][CH]1[CH2]c2c([nH]c3[cH][cH][cH][cH]c23)[CH]([NH]1)c4[cH][cH]c([!#1])[cH][cH]4
KRFP259	KRFPC259	[!#1][CH]1[CH2]N2[CH2][CH2][CH]1[CH2][CH]2[!#1]
KRFP260	KRFPC260	[!#1][CH]1[CH2]O[CH]([!#1])O1
KRFP261	KRFPC261	[!#1][CH]1[CH2]O1
KRFP262	KRFPC262	[!#1][CH]1[CH2]OC([!#1])([CH3])O1
KRFP263	KRFPC263	[!#1][CH]1[CH2]OC2([CH2][CH2][CH2][CH2]2)O1
KRFP264	KRFPC264	[!#1][CH]1[CH2]Oc2[cH][cH][cH][cH]c2O1
KRFP265	KRFPC265	[!#1][CH]1[CH2]S(=O)(=O)[CH]=[CH]1
KRFP266	KRFPC266	[!#1][CH]1[CH2]S(=O)(=O)[CH2][CH]1[!#1]
KRFP267	KRFPC267	[!#1][CH]1[CH2]S(=O)(=O)[CH2][CH]1[OH]
KRFP268	KRFPC268	[!#1][CH]1[CH2]S[CH]([NH]1)c2[cH][cH]c([!#1])[cH][cH]2
KRFP269	KRFPC269	[!#1][CH]1[CH2]S[CH](N1[!#1])c2[cH][cH]c([!#1])[cH][cH]2
KRFP270	KRFPC270	[!#1][CH]1[CH2]S[CH2][CH]1[!#1]
KRFP271	KRFPC271	[!#1][CH]1[NH][CH2][CH2]n2[cH][cH][cH]c12
KRFP272	KRFPC272	[!#1][CH]1[NH]c2[cH][cH][cH][cH]c2[NH]C1=O
KRFP273	KRFPC273	[!#1][CH]1C(=NN(C1=O)c2[cH][cH][cH][cH]2)[!#1]
KRFP274	KRFPC274	[!#1][CH]1C(=NN(C1=O)c2c([!#1])c([!#1])c([!#1])c([!#1])c2[!#1])[!#1]
KRFP275	KRFPC275	[!#1][CH]1C(=NN(C1=O)c2c(F)c(F)c(F)c(F)c2F)[CH3]
KRFP276	KRFPC276	[!#1][CH]1C(=O)[CH2]C([!#1])([CH3])[CH2]C1=O
KRFP277	KRFPC277	[!#1][CH]1C(=O)[CH2]C([CH3])([CH3])[CH2]C1=O
KRFP278	KRFPC278	[!#1][CH]1C(=O)[NH]C(=O)[NH]C1=O
KRFP279	KRFPC279	[!#1][CH]1C(=O)c2[cH][cH][cH][cH]c2C1=O
KRFP280	KRFPC280	[!#1][CH]1c2[cH][cH][cH][cH]c2-c3[cH][cH][cH][cH]c13
KRFP281	KRFPC281	[!#1][CH]1c2[cH][cH][cH][cH]c2Oc3[cH][cH][cH][cH]c13
KRFP282	KRFPC282	[!#1][CH]1N([!#1])[CH2][CH2]c2[cH][cH][cH][cH]c12
KRFP283	KRFPC283	[!#1][CH]1N(C(=O)N([!#1])C1([!#1])[CH3])c2[cH][cH][cH]c3[cH][cH][cH]c23
KRFP284	KRFPC284	[!#1][CH]1N(C(=O)N([!#1])C1([!#1])[CH3])c2[cH][cH]c([!#1])c([!#1])[cH]2
KRFP285	KRFPC285	[!#1][CH]1N(C(=O)N([!#1])C1([CH3])[CH3])c2[cH][cH][cH]c3[cH][cH][cH]c23
KRFP286	KRFPC286	[!#1][CH]1N2[CH2][CH2][CH]([CH2][CH2]2)C1=O
KRFP287	KRFPC287	[!#1][CH]1O[CH]([!#1])[CH]([!#1])[CH]([!#1])[CH]1[!#1]
KRFP288	KRFPC288	[!#1][CH]1O[CH]([CH]([!#1])[CH]1[!#1])n2[cH][cH]c(=O)[nH]c2=O
KRFP289	KRFPC289	[!#1][CH]1O[CH]([CH]([!#1])[CH]1[!#1])n2[cH]nc3c([!#1])n[cH]nc23
KRFP290	KRFPC290	[!#1][CH]1O[CH]([CH2][OH])[CH]([OH])[CH]([OH])[CH]1[OH]
KRFP291	KRFPC291	[!#1][CH]1O[CH]([CH2][OH])[CH]([OH])[CH]1[OH]
KRFP292	KRFPC292	[!#1][CH]1O[CH]([CH3])[CH]([OH])[CH]([OH])[CH]1[OH]
KRFP293	KRFPC293	[!#1][CH]1O[CH2][CH2]O[CH]1[!#1]
KRFP294	KRFPC294	[!#1][CH]1OC([!#1])([CH3])O[CH]1[!#1]
KRFP295	KRFPC295	[!#1][CH]1S(=O)(=O)[CH2][CH]([CH2]S1(=O)=O)c2[cH][cH][cH][cH]c2
KRFP296	KRFPC296	[!#1][CH]1S(c2[cH][cH][cH][cH]c2[NH]C1=O)
KRFP297	KRFPC297	[!#1][CH2][!#1]
KRFP298	KRFPC298	[!#1][CH2][CH]([!#1])[!#1]
KRFP299	KRFPC299	[!#1][CH2][CH]([!#1])[CH3]
KRFP300	KRFPC300	[!#1][CH2][CH]([!#1])[OH]
KRFP301	KRFPC301	[!#1][CH2][CH]([!#1])C#[CH]
KRFP302	KRFPC302	[!#1][CH2][CH]([!#1])C(=O)[!#1]

Name	Count name	Pattern
KRFP303	KRFPC303	[!#1][CH2][CH]([!#1])C(=O)[NH][!#1]
KRFP304	KRFPC304	[!#1][CH2][CH]([!#1])C(=O)[OH]
KRFP305	KRFPC305	[!#1][CH2][CH]([!#1])C(=O)O[CH2][CH3]
KRFP306	KRFPC306	[!#1][CH2][CH]([CH2][CH3])[NH]C(=O)[!#1]
KRFP307	KRFPC307	[!#1][CH2][CH]([CH3])[CH3]
KRFP308	KRFPC308	[!#1][CH2][CH]([CH3])[NH][CH2]C(=O)[NH][!#1]
KRFP309	KRFPC309	[!#1][CH2][CH]([CH3])[NH]C(=O)[!#1]
KRFP310	KRFPC310	[!#1][CH2][CH]([CH3])[NH2]
KRFP311	KRFPC311	[!#1][CH2][CH]([CH3])[OH]
KRFP312	KRFPC312	[!#1][CH2][CH]([CH3])O[!#1]
KRFP313	KRFPC313	[!#1][CH2][CH]([CH3])S[CH2][CH3]
KRFP314	KRFPC314	[!#1][CH2][CH]([NH]C(=O)[!#1])C(=O)[NH][!#1]
KRFP315	KRFPC315	[!#1][CH2][CH]([NH]C(=O)[!#1])C(=O)[OH]
KRFP316	KRFPC316	[!#1][CH2][CH]([NH]C(=O)[!#1])C(=O)O[CH2][CH3]
KRFP317	KRFPC317	[!#1][CH2][CH]([NH]C(=O)[!#1])C(=O)O[CH3]
KRFP318	KRFPC318	[!#1][CH2][CH]([NH]C(=O)[CH2]O[!#1])C(=O)[OH]
KRFP319	KRFPC319	[!#1][CH2][CH]([NH]C(=O)[CH2]O[!#1])C(=O)O[CH3]
KRFP320	KRFPC320	[!#1][CH2][CH]([NH]C(=O)[CH3])C(=O)[OH]
KRFP321	KRFPC321	[!#1][CH2][CH]([NH]C(=O)[CH3])C(=O)O[CH2][CH3]
KRFP322	KRFPC322	[!#1][CH2][CH]([NH]C(=O)OC([CH3])([CH3])[CH3])C(=O)O[!#1]
KRFP323	KRFPC323	[!#1][CH2][CH]([NH]S(=O)(=O)[!#1])C(=O)[OH]
KRFP324	KRFPC324	[!#1][CH2][CH]([NH]S(=O)(=O)[!#1])C(=O)O[CH3]
KRFP325	KRFPC325	[!#1][CH2][CH]([NH2])C(=O)[OH]
KRFP326	KRFPC326	[!#1][CH2][CH]([OH])[CH2][!#1]
KRFP327	KRFPC327	[!#1][CH2][CH]([OH])[CH2][NH][!#1]
KRFP328	KRFPC328	[!#1][CH2][CH]([OH])[CH2][OH]
KRFP329	KRFPC329	[!#1][CH2][CH]([OH])[CH2]Br
KRFP330	KRFPC330	[!#1][CH2][CH]([OH])[CH2]Cl
KRFP331	KRFPC331	[!#1][CH2][CH]([OH])[CH2]N([!#1])[!#1]
KRFP332	KRFPC332	[!#1][CH2][CH]([OH])[CH2]N([!#1])[CH3]
KRFP333	KRFPC333	[!#1][CH2][CH]([OH])[CH2]N([CH2][CH2][OH])[CH2][CH2][OH]
KRFP334	KRFPC334	[!#1][CH2][CH]([OH])[CH2]N([CH2][CH3])[CH2][CH3]
KRFP335	KRFPC335	[!#1][CH2][CH]([OH])[CH2]N([CH3])[CH3]
KRFP336	KRFPC336	[!#1][CH2][CH]([OH])[CH2]O[!#1]
KRFP337	KRFPC337	[!#1][CH2][CH](O[CH3])O[CH3]
KRFP338	KRFPC338	[!#1][CH2][CH]=[CH][!#1]
KRFP339	KRFPC339	[!#1][CH2][CH]=[CH2]
KRFP340	KRFPC340	[!#1][CH2][CH]1[CH2]OC2([CH2][CH2][CH2][CH2][CH2]2)O1
KRFP341	KRFPC341	[!#1][CH2][CH2][!#1]
KRFP342	KRFPC342	[!#1][CH2][CH2][CH]([CH3])[CH3]
KRFP343	KRFPC343	[!#1][CH2][CH2][CH]=C([CH3])[CH3]
KRFP344	KRFPC344	[!#1][CH2][CH2][CH2][!#1]
KRFP345	KRFPC345	[!#1][CH2][CH2][CH2][CH]([CH2]O[!#1])O[!#1]
KRFP346	KRFPC346	[!#1][CH2][CH2][CH2][CH2][!#1]
KRFP347	KRFPC347	[!#1][CH2][CH2][CH2][CH2][CH2][!#1]
KRFP348	KRFPC348	[!#1][CH2][CH2][CH2][CH2][CH2][CH2][!#1]
KRFP349	KRFPC349	[!#1][CH2][CH2][CH2][CH2][CH2][CH2][CH3]
KRFP350	KRFPC350	[!#1][CH2][CH2][CH2][CH2][CH2][CH3]
KRFP351	KRFPC351	[!#1][CH2][CH2][CH2][CH2][CH2]C(=O)[NH][!#1]
KRFP352	KRFPC352	[!#1][CH2][CH2][CH2][CH2][CH2]C(=O)[OH]
KRFP353	KRFPC353	[!#1][CH2][CH2][CH2][CH2][CH2]C(=O)N([!#1])[CH2][!#1]
KRFP354	KRFPC354	[!#1][CH2][CH2][CH2][CH2][CH3]
KRFP355	KRFPC355	[!#1][CH2][CH2][CH2][CH2][NH]C(=O)[!#1]
KRFP356	KRFPC356	[!#1][CH2][CH2][CH2][CH2][NH]C(=S)[NH][CH3]

Name	Count name	Pattern
KRFP357	KRFPC357	[!#1][CH2][CH2][CH2][CH2][OH]
KRFP358	KRFPC358	[!#1][CH2][CH2][CH2][CH2]C(=O)[OH]
KRFP359	KRFPC359	[!#1][CH2][CH2][CH2][CH2]C(=O)O[CH3]
KRFP360	KRFPC360	[!#1][CH2][CH2][CH2][CH2]N(!#1)C(=O)[!#1]
KRFP361	KRFPC361	[!#1][CH2][CH2][CH2][CH2]S[!#1]
KRFP362	KRFPC362	[!#1][CH2][CH2][CH2][CH3]
KRFP363	KRFPC363	[!#1][CH2][CH2][CH2][NH][!#1]
KRFP364	KRFPC364	[!#1][CH2][CH2][CH2][NH]C(=O)[!#1]
KRFP365	KRFPC365	[!#1][CH2][CH2][CH2][NH]S(=O)(=O)[!#1]
KRFP366	KRFPC366	[!#1][CH2][CH2][CH2][NH2]
KRFP367	KRFPC367	[!#1][CH2][CH2][CH2][OH]
KRFP368	KRFPC368	[!#1][CH2][CH2][CH2]C(=O)[!#1]
KRFP369	KRFPC369	[!#1][CH2][CH2][CH2]C(=O)[NH][!#1]
KRFP370	KRFPC370	[!#1][CH2][CH2][CH2]C(=O)[OH]
KRFP371	KRFPC371	[!#1][CH2][CH2][CH2]C(=O)O[CH3]
KRFP372	KRFPC372	[!#1][CH2][CH2][CH2]Cl
KRFP373	KRFPC373	[!#1][CH2][CH2][CH2]N([CH2][CH3])[CH2][CH3]
KRFP374	KRFPC374	[!#1][CH2][CH2][CH2]N([CH3])[CH3]
KRFP375	KRFPC375	[!#1][CH2][CH2][CH2]O[!#1]
KRFP376	KRFPC376	[!#1][CH2][CH2][CH2]OC(=O)[!#1]
KRFP377	KRFPC377	[!#1][CH2][CH2][CH2]OC(=O)C(!#1)(!#1)[OH]
KRFP378	KRFPC378	[!#1][CH2][CH2][CH2]OC(=O)C([CH3])([CH3])[CH3]
KRFP379	KRFPC379	[!#1][CH2][CH2][CH2]S(=O)(=O)[OH]
KRFP380	KRFPC380	[!#1][CH2][CH2][CH2]S(=O)(=O)O[Na]
KRFP381	KRFPC381	[!#1][CH2][CH2][CH2]S[!#1]
KRFP382	KRFPC382	[!#1][CH2][CH2][CH3]
KRFP383	KRFPC383	[!#1][CH2][CH2][NH][!#1]
KRFP384	KRFPC384	[!#1][CH2][CH2][NH][CH2]C(=O)[NH][!#1]
KRFP385	KRFPC385	[!#1][CH2][CH2][NH]C(!#1)(!#1)[!#1]
KRFP386	KRFPC386	[!#1][CH2][CH2][NH]C(=C1C(=O)O[CH](C1=O)c2[cH][cH][cH][cH][cH]2)[CH3]
KRFP387	KRFPC387	[!#1][CH2][CH2][NH]C(=O)[!#1]
KRFP388	KRFPC388	[!#1][CH2][CH2][NH]C(=O)[CH](!#1)[CH3]
KRFP389	KRFPC389	[!#1][CH2][CH2][NH]C(=O)[CH]=[CH][!#1]
KRFP390	KRFPC390	[!#1][CH2][CH2][NH]C(=O)[CH2][!#1]
KRFP391	KRFPC391	[!#1][CH2][CH2][NH]C(=O)[CH2][CH2][!#1]
KRFP392	KRFPC392	[!#1][CH2][CH2][NH]C(=O)[CH2]O[!#1]
KRFP393	KRFPC393	[!#1][CH2][CH2][NH]C(=O)[CH3]
KRFP394	KRFPC394	[!#1][CH2][CH2][NH]C(=O)[NH][!#1]
KRFP395	KRFPC395	[!#1][CH2][CH2][NH]C(=O)O[CH2][CH2]Cl
KRFP396	KRFPC396	[!#1][CH2][CH2][NH]S(=O)(=O)[!#1]
KRFP397	KRFPC397	[!#1][CH2][CH2][NH2]
KRFP398	KRFPC398	[!#1][CH2][CH2][OH]
KRFP399	KRFPC399	[!#1][CH2][CH2]C#N
KRFP400	KRFPC400	[!#1][CH2][CH2]C(=N[OH])[!#1]
KRFP401	KRFPC401	[!#1][CH2][CH2]C(=O)[!#1]
KRFP402	KRFPC402	[!#1][CH2][CH2]C(=O)[CH3]
KRFP403	KRFPC403	[!#1][CH2][CH2]C(=O)[NH][!#1]
KRFP404	KRFPC404	[!#1][CH2][CH2]C(=O)[NH][NH]C(=O)[!#1]
KRFP405	KRFPC405	[!#1][CH2][CH2]C(=O)[NH][NH]S(=O)(=O)[!#1]
KRFP406	KRFPC406	[!#1][CH2][CH2]C(=O)[NH][NH2]
KRFP407	KRFPC407	[!#1][CH2][CH2]C(=O)[NH]N=[CH][!#1]
KRFP408	KRFPC408	[!#1][CH2][CH2]C(=O)[NH2]
KRFP409	KRFPC409	[!#1][CH2][CH2]C(=O)[OH]
KRFP410	KRFPC410	[!#1][CH2][CH2]C(=O)O[!#1]

Name	Count name	Pattern
KRFP411	KRFPC411	[!#1][CH2][CH2]C(=O)O[CH2][CH3]
KRFP412	KRFPC412	[!#1][CH2][CH2]C(=O)O[CH3]
KRFP413	KRFPC413	[!#1][CH2][CH2]c1[cH][cH][cH][cH][cH]1
KRFP414	KRFPC414	[!#1][CH2][CH2]c1[cH][cH]c(O[!#1])c(O[!#1])[cH]1
KRFP415	KRFPC415	[!#1][CH2][CH2]c1c(nc2[cH][cH][cH][cH]c2c1[NH][!#1])N([!#1])[CH2]c3[cH][cH][cH][cH][cH]3
KRFP416	KRFPC416	[!#1][CH2][CH2]c1c(nc2[cH][cH][cH][cH]c2c1[NH][!#1])N([!#1])[CH3]
KRFP417	KRFPC417	[!#1][CH2][CH2]N([!#1])[CH]1[CH2][CH2][CH2]c2c1n([!#1])c3[cH][cH]c([CH3])[cH]c23
KRFP418	KRFPC418	[!#1][CH2][CH2]N([!#1])[CH2][CH2][NH][!#1]
KRFP419	KRFPC419	[!#1][CH2][CH2]N([!#1])[CH2][CH2]N([!#1])[CH2][CH]([!#1])[!#1]
KRFP420	KRFPC420	[!#1][CH2][CH2]N([!#1])[CH2][CH2]N([!#1])[CH2][CH]([OH])[CH2]O[!#1]
KRFP421	KRFPC421	[!#1][CH2][CH2]N([!#1])[CH2][CH2]N([!#1])[CH2]C(=O)[!#1]
KRFP422	KRFPC422	[!#1][CH2][CH2]N([!#1])[CH2][CH2]N([!#1])[CH2]c1[cH][cH][cH][cH][cH]1
KRFP423	KRFPC423	[!#1][CH2][CH2]N([!#1])[CH2][CH2]N([!#1])[CH2]c1[cH][cH]c2O[CH2]Oc2[cH]1
KRFP424	KRFPC424	[!#1][CH2][CH2]N([!#1])[CH2][CH2]N([!#1])[CH3]
KRFP425	KRFPC425	[!#1][CH2][CH2]N([!#1])[CH2][CH2]N([!#1])c1[cH][cH][cH][cH][cH]1
KRFP426	KRFPC426	[!#1][CH2][CH2]N([!#1])[CH2][CH2]N([!#1])c1[cH][cH][cH][cH]c1O[!#1]
KRFP427	KRFPC427	[!#1][CH2][CH2]N([!#1])[CH2][CH2]N([!#1])c1[cH][cH][cH][cH]n1
KRFP428	KRFPC428	[!#1][CH2][CH2]N([!#1])[CH2][CH2]N([!#1])c1[cH][cH]c([!#1])[cH][cH]1
KRFP429	KRFPC429	[!#1][CH2][CH2]N([!#1])[CH2][CH2]N([!#1])c1[cH][cH]c([cH][cH]1)[N+](=O)[O-]
KRFP430	KRFPC430	[!#1][CH2][CH2]N([!#1])[CH2][CH2]N([!#1])c1[cH][cH]c(Cl)[cH][cH]1
KRFP431	KRFPC431	[!#1][CH2][CH2]N([!#1])[CH2][CH2]N([!#1])c1[cH][cH]c(F)[cH][cH]1
KRFP432	KRFPC432	[!#1][CH2][CH2]N([!#1])[CH2][CH2]N([!#1])c1n[cH][cH][cH]n1
KRFP433	KRFPC433	[!#1][CH2][CH2]N([!#1])[CH2][CH2]O[!#1]
KRFP434	KRFPC434	[!#1][CH2][CH2]N([!#1])[CH2][CH3]
KRFP435	KRFPC435	[!#1][CH2][CH2]N([!#1])[CH3]
KRFP436	KRFPC436	[!#1][CH2][CH2]N([!#1])[NH2]
KRFP437	KRFPC437	[!#1][CH2][CH2]N([!#1])c1[cH][cH][cH][cH][cH]1
KRFP438	KRFPC438	[!#1][CH2][CH2]N([CH2][!#1])[CH2][!#1]
KRFP439	KRFPC439	[!#1][CH2][CH2]N([CH2][CH2]O[!#1])C(=O)[!#1]
KRFP440	KRFPC440	[!#1][CH2][CH2]N([CH2][CH3])[CH2][CH3]
KRFP441	KRFPC441	[!#1][CH2][CH2]N([CH3])[CH2]C(=O)[NH][!#1]
KRFP442	KRFPC442	[!#1][CH2][CH2]N([CH3])[CH3]
KRFP443	KRFPC443	[!#1][CH2][CH2]N=[CH][!#1]
KRFP444	KRFPC444	[!#1][CH2][CH2]O[!#1]
KRFP445	KRFPC445	[!#1][CH2][CH2]O[CH2][CH]([OH])[CH2][!#1]
KRFP446	KRFPC446	[!#1][CH2][CH2]O[CH2][CH]([OH])[CH2][NH2]
KRFP447	KRFPC447	[!#1][CH2][CH2]OC(=O)[!#1]
KRFP448	KRFPC448	[!#1][CH2][CH2]OC(=O)[CH2][CH2]C(=O)[NH][!#1]
KRFP449	KRFPC449	[!#1][CH2][CH2]OC(=O)[CH3]
KRFP450	KRFPC450	[!#1][CH2][CH2]OC(=O)[NH][CH]([!#1])C(Cl)(Cl)Cl
KRFP451	KRFPC451	[!#1][CH2][CH2]OC(=O)[NH][CH]([NH][!#1])C(Cl)(Cl)Cl
KRFP452	KRFPC452	[!#1][CH2][CH2]P(=O)([!#1])[CH2][CH3]
KRFP453	KRFPC453	[!#1][CH2][CH2]S(=O)(=O)[!#1]
KRFP454	KRFPC454	[!#1][CH2][CH2]S(=O)(=O)[CH2][CH2][!#1]
KRFP455	KRFPC455	[!#1][CH2][CH2]S(=O)(=O)[CH2][CH2]C(=O)[NH2]
KRFP456	KRFPC456	[!#1][CH2][CH2]S(=O)(=O)O[!#1]
KRFP457	KRFPC457	[!#1][CH2][CH2]S(=O)[!#1]
KRFP458	KRFPC458	[!#1][CH2][CH2]S[!#1]
KRFP459	KRFPC459	[!#1][CH2][CH2]S[CH2][!#1]
KRFP460	KRFPC460	[!#1][CH2][CH2]S[CH2][CH2][!#1]

Name	Count name	Pattern
KRFP461	KRFPC461	[!#1][CH2][CH2]S[CH2][CH2]S[CH2][CH2][!#1]
KRFP462	KRFPC462	[!#1][CH2][CH2]S[CH2]C(=O)[OH]
KRFP463	KRFPC463	[!#1][CH2][CH2]SC(=[NH])[NH2]
KRFP464	KRFPC464	[!#1][CH2][CH2]SC(=O)[CH3]
KRFP465	KRFPC465	[!#1][CH2][CH2]SC(=S)[!#1]
KRFP466	KRFPC466	[!#1][CH2][CH3]
KRFP467	KRFPC467	[!#1][CH2][NH][!#1]
KRFP468	KRFPC468	[!#1][CH2][NH][CH]([CH2][!#1])C(=O)[OH]
KRFP469	KRFPC469	[!#1][CH2][NH][CH]([CH3])[CH2][CH3]
KRFP470	KRFPC470	[!#1][CH2][NH][CH]([CH3])[CH3]
KRFP471	KRFPC471	[!#1][CH2][NH][CH]([NH]C(=O)[!#1])C(Br)(Br)Br
KRFP472	KRFPC472	[!#1][CH2][NH][CH]([NH]C(=O)[!#1])C(Cl)(Cl)Cl
KRFP473	KRFPC473	[!#1][CH2][NH][CH]=C1C(=O)[CH2][NH]C1=O
KRFP474	KRFPC474	[!#1][CH2][NH][CH]=C1C(=O)[NH]C(=O)[NH]C1=O
KRFP475	KRFPC475	[!#1][CH2][NH][CH]=C1C(=O)[NH]C(=O)N([!#1])C1=O
KRFP476	KRFPC476	[!#1][CH2][NH][CH2][!#1]
KRFP477	KRFPC477	[!#1][CH2][NH]C([CH3])([CH3])[CH3]
KRFP478	KRFPC478	[!#1][CH2][NH]C(=[NH])[NH]C(=[NH])[NH2]
KRFP479	KRFPC479	[!#1][CH2][NH]C(=N[OH])[!#1]
KRFP480	KRFPC480	[!#1][CH2][NH]C(=O)[!#1]
KRFP481	KRFPC481	[!#1][CH2][NH]C(=O)[CH]([!#1])[CH2][!#1]
KRFP482	KRFPC482	[!#1][CH2][NH]C(=O)[CH]=[CH]C(=O)[OH]
KRFP483	KRFPC483	[!#1][CH2][NH]C(=O)[CH2][!#1]
KRFP484	KRFPC484	[!#1][CH2][NH]C(=O)[CH2][CH2]C(=O)[OH]
KRFP485	KRFPC485	[!#1][CH2][NH]C(=O)[CH2]Cl
KRFP486	KRFPC486	[!#1][CH2][NH]C(=O)[CH2]O[!#1]
KRFP487	KRFPC487	[!#1][CH2][NH]C(=O)[CH3]
KRFP488	KRFPC488	[!#1][CH2][NH]C(=O)[NH][!#1]
KRFP489	KRFPC489	[!#1][CH2][NH]C(=O)C(=[CH][!#1])[NH]C(=O)[!#1]
KRFP490	KRFPC490	[!#1][CH2][NH]C(=S)[NH][!#1]
KRFP491	KRFPC491	[!#1][CH2][NH]C(=S)[NH]C(=O)[!#1]
KRFP492	KRFPC492	[!#1][CH2][NH]S(=O)(=O)[!#1]
KRFP493	KRFPC493	[!#1][CH2][NH2]
KRFP494	KRFPC494	[!#1][CH2][OH]
KRFP495	KRFPC495	[!#1][CH2]Br
KRFP496	KRFPC496	[!#1][CH2]C#C[!#1]
KRFP497	KRFPC497	[!#1][CH2]C([CH3])([CH3])[CH3]
KRFP498	KRFPC498	[!#1][CH2]C(=[CH2])[CH3]
KRFP499	KRFPC499	[!#1][CH2]C(=N[NH][!#1])[CH3]
KRFP500	KRFPC500	[!#1][CH2]C(=N[NH]C(=O)[!#1])[CH3]
KRFP501	KRFPC501	[!#1][CH2]C(=N[NH]C(=O)[!#1])C(=O)[OH]
KRFP502	KRFPC502	[!#1][CH2]C(=N[NH]C(=O)[CH2]O[!#1])[CH3]
KRFP503	KRFPC503	[!#1][CH2]C(=N[OH])[!#1]
KRFP504	KRFPC504	[!#1][CH2]C(=O)[!#1]
KRFP505	KRFPC505	[!#1][CH2]C(=O)[CH3]
KRFP506	KRFPC506	[!#1][CH2]C(=O)[NH][!#1]
KRFP507	KRFPC507	[!#1][CH2]C(=O)[NH][CH]([!#1])[CH3]
KRFP508	KRFPC508	[!#1][CH2]C(=O)[NH][CH]([!#1])C(=O)[NH][!#1]
KRFP509	KRFPC509	[!#1][CH2]C(=O)[NH][CH]([!#1])C(Cl)(Cl)Cl
KRFP510	KRFPC510	[!#1][CH2]C(=O)[NH][CH]([NH][!#1])C(Cl)(Cl)Cl
KRFP511	KRFPC511	[!#1][CH2]C(=O)[NH][CH]([NH]C(=S)[NH][!#1])C(Cl)(Cl)Cl
KRFP512	KRFPC512	[!#1][CH2]C(=O)[NH][CH](S[!#1])C(Cl)(Cl)Cl
KRFP513	KRFPC513	[!#1][CH2]C(=O)[NH][CH2][CH2][OH]
KRFP514	KRFPC514	[!#1][CH2]C(=O)[NH][CH2][CH2]S(=O)(=O)[OH]

Name	Count name	Pattern
KRFP515	KRFPC515	[!#1][CH2]C(=O)[NH][NH][!#1]
KRFP516	KRFPC516	[!#1][CH2]C(=O)[NH][NH]C(=O)[!#1]
KRFP517	KRFPC517	[!#1][CH2]C(=O)[NH][NH2]
KRFP518	KRFPC518	[!#1][CH2]C(=O)[NH][OH]
KRFP519	KRFPC519	[!#1][CH2]C(=O)[NH]N([!#1])[CH3]
KRFP520	KRFPC520	[!#1][CH2]C(=O)[NH]N=[CH][!#1]
KRFP521	KRFPC521	[!#1][CH2]C(=O)[NH]N=[CH][CH]([!#1])[!#1]
KRFP522	KRFPC522	[!#1][CH2]C(=O)[NH]N=[CH]c1[cH][cH][cH][cH]1
KRFP523	KRFPC523	[!#1][CH2]C(=O)[NH]N=[CH]c1[cH][cH][cH][cH]c1[N+](=O)[O-]
KRFP524	KRFPC524	[!#1][CH2]C(=O)[NH]N=[CH]c1[cH][cH][cH][cH]c1[OH]
KRFP525	KRFPC525	[!#1][CH2]C(=O)[NH]N=[CH]c1[cH][cH][cH][cH]c1Br
KRFP526	KRFPC526	[!#1][CH2]C(=O)[NH]N=[CH]c1[cH][cH][cH][cH]c1Cl
KRFP527	KRFPC527	[!#1][CH2]C(=O)[NH]N=[CH]c1[cH][cH][cH]c([cH]1)[N+](=O)[O-]
KRFP528	KRFPC528	[!#1][CH2]C(=O)[NH]N=[CH]c1[cH][cH][cH]c(l)[cH]1
KRFP529	KRFPC529	[!#1][CH2]C(=O)[NH]N=[CH]c1[cH][cH][cH]o1
KRFP530	KRFPC530	[!#1][CH2]C(=O)[NH]N=[CH]c1[cH][cH][cH]s1
KRFP531	KRFPC531	[!#1][CH2]C(=O)[NH]N=[CH]c1[cH][cH]c([cH][cH]1)[N+](=O)[O-]
KRFP532	KRFPC532	[!#1][CH2]C(=O)[NH]N=[CH]c1[cH][cH]c([OH])[cH]c1[OH]
KRFP533	KRFPC533	[!#1][CH2]C(=O)[NH]N=[CH]c1[cH][cH]c(Br)[cH][cH]1
KRFP534	KRFPC534	[!#1][CH2]C(=O)[NH]N=[CH]c1[cH][cH]c(Cl)[cH][cH]1
KRFP535	KRFPC535	[!#1][CH2]C(=O)[NH]N=[CH]c1[cH][cH]c2O[CH2]Oc2[cH]1
KRFP536	KRFPC536	[!#1][CH2]C(=O)[NH]N=[CH]c1[cH][nH]c2[cH][cH][cH]c12
KRFP537	KRFPC537	[!#1][CH2]C(=O)[NH]N=[CH]c1[cH]c([cH][cH]c1[OH])[N+](=O)[O-]
KRFP538	KRFPC538	[!#1][CH2]C(=O)[NH]N=[CH]c1[cH]c(N=Nc2[cH][cH][cH][cH]2)[cH][cH]c1[OH]
KRFP539	KRFPC539	[!#1][CH2]C(=O)[NH]N=[CH]c1[cH]c2[cH][cH][cH][cH]c2nc1Cl
KRFP540	KRFPC540	[!#1][CH2]C(=O)[NH]N=[CH]c1[cH]c2O[CH2]Oc2[cH]c1[N+](=O)[O-]
KRFP541	KRFPC541	[!#1][CH2]C(=O)[NH]N=[CH]c1c([OH])[cH][cH]c2[cH][cH][cH]c12
KRFP542	KRFPC542	[!#1][CH2]C(=O)[NH]N=[CH]c1c(Cl)[cH][cH][cH]c1Cl
KRFP543	KRFPC543	[!#1][CH2]C(=O)[NH]N=C([!#1])[CH3]
KRFP544	KRFPC544	[!#1][CH2]C(=O)[NH]N=C([CH3])c1[cH][cH]c(Br)[cH][cH]1
KRFP545	KRFPC545	[!#1][CH2]C(=O)[NH]N=C1[CH2][CH2][CH2]c2c1non2=O
KRFP546	KRFPC546	[!#1][CH2]C(=O)[NH]S(=O)(=O)[!#1]
KRFP547	KRFPC547	[!#1][CH2]C(=O)[NH2]
KRFP548	KRFPC548	[!#1][CH2]C(=O)[OH]
KRFP549	KRFPC549	[!#1][CH2]C(=O)C([CH3])([CH3])[CH3]
KRFP550	KRFPC550	[!#1][CH2]C(=O)c1[cH][cH][cH][cH]1
KRFP551	KRFPC551	[!#1][CH2]C(=O)c1[cH][cH]c([!#1])[cH][cH]1
KRFP552	KRFPC552	[!#1][CH2]C(=O)c1[cH][cH]c([CH3])[cH][cH]1
KRFP553	KRFPC553	[!#1][CH2]C(=O)c1[cH][cH]c(Cl)c(Cl)[cH]1
KRFP554	KRFPC554	[!#1][CH2]C(=O)N([!#1])[CH3]
KRFP555	KRFPC555	[!#1][CH2]C(=O)N([CH3])[CH]([!#1])C(=O)[NH][!#1]
KRFP556	KRFPC556	[!#1][CH2]C(=O)N=[CH][NH][NH][!#1]
KRFP557	KRFPC557	[!#1][CH2]C(=O)O[!#1]
KRFP558	KRFPC558	[!#1][CH2]C(=O)O[CH2][CH2][CH2][CH3]
KRFP559	KRFPC559	[!#1][CH2]C(=O)O[CH2][CH2][NH]C(=O)[!#1]
KRFP560	KRFPC560	[!#1][CH2]C(=O)O[CH2][CH3]
KRFP561	KRFPC561	[!#1][CH2]C(=O)O[CH2]C(=O)[!#1]
KRFP562	KRFPC562	[!#1][CH2]C(=O)O[CH3]
KRFP563	KRFPC563	[!#1][CH2]C(=O)O[Na]
KRFP564	KRFPC564	[!#1][CH2]C(=S)[!#1]
KRFP565	KRFPC565	[!#1][CH2]C1([CH2][CH]2[CH2][CH]3[CH2][CH]([CH2]2)[CH2]1)[CH2]3
KRFP566	KRFPC566	[!#1][CH2]c1[cH][cH][cH][cH]1
KRFP567	KRFPC567	[!#1][CH2]c1[cH][cH][cH][cH]c1Br

Name	Count name	Pattern
KRFP568	KRFPC568	[!#1][CH2]c1[cH][cH][cH][cH]c1C(F)(F)F
KRFP569	KRFPC569	[!#1][CH2]c1[cH][cH][cH][cH]c1Cl
KRFP570	KRFPC570	[!#1][CH2]c1[cH][cH][cH][cH]c1F
KRFP571	KRFPC571	[!#1][CH2]c1[cH][cH][cH]c([CH3])[cH]1
KRFP572	KRFPC572	[!#1][CH2]c1[cH][cH][cH]c([OH])[cH]1
KRFP573	KRFPC573	[!#1][CH2]c1[cH][cH][cH]c(Br)[cH]1
KRFP574	KRFPC574	[!#1][CH2]c1[cH][cH][cH]c(Cl)[cH]1
KRFP575	KRFPC575	[!#1][CH2]c1[cH][cH][cH]c(Cl)c1Cl
KRFP576	KRFPC576	[!#1][CH2]c1[cH][cH][cH]c(F)[cH]1
KRFP577	KRFPC577	[!#1][CH2]c1[cH][cH][cH]c(O[!#1])[cH]1
KRFP578	KRFPC578	[!#1][CH2]c1[cH][cH][cH]c2[cH][cH][cH][cH]c12
KRFP579	KRFPC579	[!#1][CH2]c1[cH][cH][cH]n[cH]1
KRFP580	KRFPC580	[!#1][CH2]c1[cH][cH][cH]o1
KRFP581	KRFPC581	[!#1][CH2]c1[cH][cH][cH]s1
KRFP582	KRFPC582	[!#1][CH2]c1[cH][cH]c([!#1])[cH][cH]1
KRFP583	KRFPC583	[!#1][CH2]c1[cH][cH]c([cH][cH]1)[N+](=O)[O-]
KRFP584	KRFPC584	[!#1][CH2]c1[cH][cH]c([cH][cH]1)C(F)(F)F
KRFP585	KRFPC585	[!#1][CH2]c1[cH][cH]c([CH3])[cH][cH]1
KRFP586	KRFPC586	[!#1][CH2]c1[cH][cH]c(Br)[cH][cH]1
KRFP587	KRFPC587	[!#1][CH2]c1[cH][cH]c(Br)s1
KRFP588	KRFPC588	[!#1][CH2]c1[cH][cH]c(Cl)[cH][cH]1
KRFP589	KRFPC589	[!#1][CH2]c1[cH][cH]c(Cl)[cH]c1Cl
KRFP590	KRFPC590	[!#1][CH2]c1[cH][cH]c(F)[cH][cH]1
KRFP591	KRFPC591	[!#1][CH2]c1[cH][cH]c(F)[cH]c1F
KRFP592	KRFPC592	[!#1][CH2]c1[cH][cH]c(O[!#1])[cH][cH]1
KRFP593	KRFPC593	[!#1][CH2]c1[cH][cH]c(O[!#1])c(O[!#1])[cH]1
KRFP594	KRFPC594	[!#1][CH2]c1[cH][cH]c(S[CH3])[cH][cH]1
KRFP595	KRFPC595	[!#1][CH2]c1[cH][cH]c2[cH][cH][cH][cH]c2[cH]1
KRFP596	KRFPC596	[!#1][CH2]c1[cH][cH]c2O[CH2]Oc2[cH]1
KRFP597	KRFPC597	[!#1][CH2]c1[cH][cH]o[cH]1
KRFP598	KRFPC598	[!#1][CH2]c1[cH][cH]s[cH]1
KRFP599	KRFPC599	[!#1][CH2]c1[cH][nH]c2[cH][cH][cH][cH]c12
KRFP600	KRFPC600	[!#1][CH2]c1[cH]c([CH2][!#1])c([OH])c([!#1])n1
KRFP601	KRFPC601	[!#1][CH2]c1c([!#1])[cH][cH]c2[cH][cH][cH][cH]c12
KRFP602	KRFPC602	[!#1][CH2]c1c([NH][!#1])sc2[CH2][CH2][CH2][CH2]c12
KRFP603	KRFPC603	[!#1][CH2]c1nc2[cH][cH][cH][cH]c2[nH]1
KRFP604	KRFPC604	[!#1][CH2]Cl
KRFP605	KRFPC605	[!#1][CH2]N([!#1])[CH2][!#1]
KRFP606	KRFPC606	[!#1][CH2]N([!#1])[CH2][CH2][OH]
KRFP607	KRFPC607	[!#1][CH2]N([!#1])[CH2][CH3]
KRFP608	KRFPC608	[!#1][CH2]N([!#1])[CH3]
KRFP609	KRFPC609	[!#1][CH2]N([!#1])[NH]C(=O)[CH2][!#1]
KRFP610	KRFPC610	[!#1][CH2]N([!#1])C(=O)[!#1]
KRFP611	KRFPC611	[!#1][CH2]N([!#1])C(=O)[CH2][CH2]C(=O)[!#1]
KRFP612	KRFPC612	[!#1][CH2]N([!#1])C(=O)[CH2]O[!#1]
KRFP613	KRFPC613	[!#1][CH2]N([!#1])C(=O)[CH3]
KRFP614	KRFPC614	[!#1][CH2]N([!#1])C(=O)c1[cH][cH][cH][cH]c1C(=O)[!#1]
KRFP615	KRFPC615	[!#1][CH2]N([!#1])C(=O)c1[cH]c([cH][cH]c1C(=O)[!#1])[N+](=O)[O-]
KRFP616	KRFPC616	[!#1][CH2]N([!#1])C(=O)c1[cH]c(Br)[cH][cH]c1C(=O)[!#1]
KRFP617	KRFPC617	[!#1][CH2]N([!#1])c1[cH][cH][cH][cH]c1C(=O)C(=O)[!#1]
KRFP618	KRFPC618	[!#1][CH2]N([!#1])N=[CH][!#1]
KRFP619	KRFPC619	[!#1][CH2]N([!#1])S(=O)(=O)[NH]C(=O)[NH][!#1]
KRFP620	KRFPC620	[!#1][CH2]N([CH2][!#1])[CH2][!#1]
KRFP621	KRFPC621	[!#1][CH2]N([CH2][!#1])C(=O)[!#1]

Name	Count name	Pattern
KRFP622	KRFPC622	[!#1][CH2]N([CH2][!#1])C(=O)[NH][!#1]
KRFP623	KRFPC623	[!#1][CH2]N([CH2][!#1])S(=O)(=O)[!#1]
KRFP624	KRFPC624	[!#1][CH2]N([CH2][CH]([OH])[CH2]O[!#1])C([CH3])([CH3])[CH3]
KRFP625	KRFPC625	[!#1][CH2]N([CH2][CH]=[CH2])[CH2][CH]=[CH2]
KRFP626	KRFPC626	[!#1][CH2]N([CH2][CH2][OH])[CH2][CH2][OH]
KRFP627	KRFPC627	[!#1][CH2]N([CH2][CH3])[CH2][CH3]
KRFP628	KRFPC628	[!#1][CH2]N([CH2]C(=O)[OH])[CH2]C(=O)[OH]
KRFP629	KRFPC629	[!#1][CH2]N([CH3])[CH3]
KRFP630	KRFPC630	[!#1][CH2]N([CH3])C(=O)[!#1]
KRFP631	KRFPC631	[!#1][CH2]N([CH3])S(=O)(=O)[!#1]
KRFP632	KRFPC632	[!#1][CH2]N([OH])[CH2][!#1]
KRFP633	KRFPC633	[!#1][CH2]N(C([CH3])([CH3])[CH3])S(=O)(=O)[!#1]
KRFP634	KRFPC634	[!#1][CH2]N(C(=O)[!#1])C([CH3])([CH3])[CH3]
KRFP635	KRFPC635	[!#1][CH2]N(C(=O)[CH2][CH2]C(=O)[OH])C([CH3])([CH3])[CH3]
KRFP636	KRFPC636	[!#1][CH2]N=[CH][!#1]
KRFP637	KRFPC637	[!#1][CH2]N=c1[cH][cH]n([!#1])[cH][cH]1
KRFP638	KRFPC638	[!#1][CH2]N1[CH2][CH2][CH]([!#1])[CH2][CH2]1
KRFP639	KRFPC639	[!#1][CH2]N1[CH2][CH2][CH2][CH2][CH2]1
KRFP640	KRFPC640	[!#1][CH2]N1[CH2][CH2]N([CH2][CH2]1)c2[cH][cH][cH][cH]2
KRFP641	KRFPC641	[!#1][CH2]N1[CH2][CH2]N([CH2][CH2]1)c2[cH][cH][cH][cH]n2
KRFP642	KRFPC642	[!#1][CH2]N1[CH2][CH2]N([CH2][CH2]1)c2[cH][cH]c(Cl)[cH][cH]2
KRFP643	KRFPC643	[!#1][CH2]N1[CH2][CH2]N([CH2][CH2]1)c2[cH][cH]c(F)[cH][cH]2
KRFP644	KRFPC644	[!#1][CH2]N1[CH2][CH2]O[CH2][CH2]1
KRFP645	KRFPC645	[!#1][CH2]N1C(=O)c2[cH][cH][cH][cH]c2C1=O
KRFP646	KRFPC646	[!#1][CH2]n1nnc2[cH][cH][cH][cH]c12
KRFP647	KRFPC647	[!#1][CH2]O[!#1]
KRFP648	KRFPC648	[!#1][CH2]O[CH2][!#1]
KRFP649	KRFPC649	[!#1][CH2]O[CH2][CH]([OH])[CH2][!#1]
KRFP650	KRFPC650	[!#1][CH2]O[CH2][CH]([OH])[CH2][NH][CH]([CH3])[CH3]
KRFP651	KRFPC651	[!#1][CH2]O[CH2][CH3]
KRFP652	KRFPC652	[!#1][CH2]O[CH3]
KRFP653	KRFPC653	[!#1][CH2]OC([!#1])([!#1])[!#1]
KRFP654	KRFPC654	[!#1][CH2]OC(=O)[!#1]
KRFP655	KRFPC655	[!#1][CH2]OC(=O)[CH]([CH]([!#1])S[CH2][!#1])[N+](=O)[O-]
KRFP656	KRFPC656	[!#1][CH2]OC(=O)[CH2][CH2]C(=O)[OH]
KRFP657	KRFPC657	[!#1][CH2]OC(=O)[CH2][CH3]
KRFP658	KRFPC658	[!#1][CH2]OC(=O)[CH3]
KRFP659	KRFPC659	[!#1][CH2]OC(=O)[NH][!#1]
KRFP660	KRFPC660	[!#1][CH2]OC(=O)[NH][CH]([NH]C(=S)[NH][!#1])C(Cl)(Cl)Cl
KRFP661	KRFPC661	[!#1][CH2]OP(=S)(O[CH2][CH3])O[CH2][CH3]
KRFP662	KRFPC662	[!#1][CH2]OS(=O)(=O)[!#1]
KRFP663	KRFPC663	[!#1][CH2]S(=O)(=O)[!#1]
KRFP664	KRFPC664	[!#1][CH2]S(=O)(=O)[NH][!#1]
KRFP665	KRFPC665	[!#1][CH2]S[!#1]
KRFP666	KRFPC666	[!#1][CH2]S[CH2]C(=O)[NH]N=[CH][!#1]
KRFP667	KRFPC667	[!#1][CH2]S[CH2]S[CH2][!#1]
KRFP668	KRFPC668	[!#1][CH2]SC(=[NH])[NH2]
KRFP669	KRFPC669	[!#1][CH3]
KRFP670	KRFPC670	[!#1][N]([CH3])([CH3])[CH3]
KRFP671	KRFPC671	[!#1][N+](CH3)(CH3)[CH3]
KRFP672	KRFPC672	[!#1][N+](=O)[O-]
KRFP673	KRFPC673	[!#1][n+]1[cH][cH][cH][cH][cH]1
KRFP674	KRFPC674	[!#1][n+]1[cH][cH]c2[cH][cH][cH][cH]c2[cH]1
KRFP675	KRFPC675	[!#1][n+]1c([CH3])sc2[cH][cH]c(O[CH3])[cH]c12

Name	Count name	Pattern
KRFP676	KRFPC676	[!#1][NH](=O)[OH]
KRFP677	KRFPC677	[!#1][NH][!#1]
KRFP678	KRFPC678	[!#1][NH][CH]([!#1])[!#1]
KRFP679	KRFPC679	[!#1][NH][CH]([!#1])[CH]([CH3])[CH3]
KRFP680	KRFPC680	[!#1][NH][CH]([!#1])[CH2][CH]([!#1])[CH3]
KRFP681	KRFPC681	[!#1][NH][CH]([!#1])[CH2][CH2][CH3]
KRFP682	KRFPC682	[!#1][NH][CH]([!#1])[CH2]C(=O)[!#1]
KRFP683	KRFPC683	[!#1][NH][CH]([!#1])[CH3]
KRFP684	KRFPC684	[!#1][NH][CH]([!#1])C(Br)(Br)Br
KRFP685	KRFPC685	[!#1][NH][CH]([!#1])C(Cl)(Cl)Cl
KRFP686	KRFPC686	[!#1][NH][CH]([!#1])P(=O)(O[CH]([CH3])[CH3])O[CH]([CH3])[CH3]
KRFP687	KRFPC687	[!#1][NH][CH]([!#1])P(=O)(O[CH2][CH3])O[CH2][CH3]
KRFP688	KRFPC688	[!#1][NH][CH]([!#1])P(=O)(O[CH3])O[CH3]
KRFP689	KRFPC689	[!#1][NH][CH]([CH]([CH3])[CH3])C(=O)[OH]
KRFP690	KRFPC690	[!#1][NH][CH]([CH2][CH]([CH3])[CH3])C(=O)[!#1]
KRFP691	KRFPC691	[!#1][NH][CH]([CH2][CH]([CH3])[CH3])C(=O)[OH]
KRFP692	KRFPC692	[!#1][NH][CH]([CH2][CH2][OH])C(=O)[NH][!#1]
KRFP693	KRFPC693	[!#1][NH][CH]([CH2][CH2]S[CH3])C(=O)[OH]
KRFP694	KRFPC694	[!#1][NH][CH]([CH2][CH3])C(=O)[OH]
KRFP695	KRFPC695	[!#1][NH][CH]([CH2]C([!#1])([CH3])[CH3])[CH2]C([CH3])([CH3])[NH][!#1]
KRFP696	KRFPC696	[!#1][NH][CH]([CH2]C(=O)[OH])c1[cH][cH][cH][cH]1
KRFP697	KRFPC697	[!#1][NH][CH]([CH2]c1[cH][cH][cH][cH]1)C(=O)[!#1]
KRFP698	KRFPC698	[!#1][NH][CH]([CH2]c1[cH][cH][cH][cH]1)C(=O)[OH]
KRFP699	KRFPC699	[!#1][NH][CH]([CH2]c1[cH][cH]c([OH])[cH][cH]1)C(=O)[!#1]
KRFP700	KRFPC700	[!#1][NH][CH]([CH2]c1[cH][nH]c2[cH][cH][cH][cH]c12)C(=O)[!#1]
KRFP701	KRFPC701	[!#1][NH][CH]([CH2]c1[cH][nH]c2[cH][cH][cH][cH]c12)C(=O)[OH]
KRFP702	KRFPC702	[!#1][NH][CH]([CH3])[CH2][CH2][CH2]N([CH2][CH3])[CH2][CH3]
KRFP703	KRFPC703	[!#1][NH][CH]([CH3])[CH2][CH3]
KRFP704	KRFPC704	[!#1][NH][CH]([CH3])[CH2]c1[cH][cH][cH][cH]1
KRFP705	KRFPC705	[!#1][NH][CH]([CH3])[CH2]c1[cH][nH]c2[cH][cH][cH][cH]c12
KRFP706	KRFPC706	[!#1][NH][CH]([CH3])[CH3]
KRFP707	KRFPC707	[!#1][NH][CH]([CH3])C(=O)[!#1]
KRFP708	KRFPC708	[!#1][NH][CH]([CH3])c1[cH][cH][cH][cH]1
KRFP709	KRFPC709	[!#1][NH][CH]([NH]C(=O)[!#1])C(=O)[!#1]
KRFP710	KRFPC710	[!#1][NH][CH]([NH]C(=O)[!#1])C(Br)(Br)Br
KRFP711	KRFPC711	[!#1][NH][CH]([NH]C(=O)[!#1])C(Cl)(Cl)Cl
KRFP712	KRFPC712	[!#1][NH][CH]([NH]C(=O)[CH]([CH3])[CH3])C(Cl)(Cl)Cl
KRFP713	KRFPC713	[!#1][NH][CH]([NH]C(=O)[CH2][CH2][CH2][CH2][CH2][CH3])C(Cl)(Cl)Cl
KRFP714	KRFPC714	[!#1][NH][CH]([NH]C(=O)[CH2][CH2][CH3])C(Cl)(Cl)Cl
KRFP715	KRFPC715	[!#1][NH][CH]([NH]C(=O)[CH2][CH3])C(Cl)(Cl)Cl
KRFP716	KRFPC716	[!#1][NH][CH]([NH]C(=O)[CH2]F)C(Cl)(Cl)Cl
KRFP717	KRFPC717	[!#1][NH][CH]([NH]C(=O)[NH][!#1])C(Cl)(Cl)Cl
KRFP718	KRFPC718	[!#1][NH][CH]([NH]C(=O)[NH][CH]([NH][!#1])C(Cl)(Cl)Cl)C(Cl)(Cl)Cl
KRFP719	KRFPC719	[!#1][NH][CH]([NH]C(=S)[NH]c1[cH][cH][cH][cH]1)C(Cl)(Cl)Cl
KRFP720	KRFPC720	[!#1][NH][CH]([NH]C(=S)[NH]c1[cH][cH][cH][cH]c1[CH3])C(Cl)(Cl)Cl
KRFP721	KRFPC721	[!#1][NH][CH]([NH]C(=S)[NH]c1[cH][cH][cH][cH]c1[N+](=O)[O-])C(Cl)(Cl)Cl
KRFP722	KRFPC722	[!#1][NH][CH]([NH]C(=S)[NH]c1[cH][cH][cH][cH]c1[OH])C(Cl)(Cl)Cl
KRFP723	KRFPC723	[!#1][NH][CH]([NH]C(=S)[NH]c1[cH][cH][cH][cH]c1C(=O)[!#1])C(Cl)(Cl)Cl
KRFP724	KRFPC724	[!#1][NH][CH]([NH]C(=S)[NH]c1[cH][cH][cH][cH]c1C(=O)[OH])C(Cl)(Cl)Cl
KRFP725	KRFPC725	[!#1][NH][CH]([NH]C(=S)[NH]c1[cH][cH][cH][cH]c1O[!#1])C(Cl)(Cl)Cl
KRFP726	KRFPC726	[!#1][NH][CH]([NH]C(=S)[NH]c1[cH][cH][cH]c([cH]1)[N+](=O)[O-])C(Cl)(Cl)Cl
KRFP727	KRFPC727	[!#1][NH][CH]([NH]C(=S)[NH]c1[cH][cH][cH]c([cH]1)C(=O)[OH])C(Cl)(Cl)Cl
KRFP728	KRFPC728	[!#1][NH][CH]([NH]C(=S)[NH]c1[cH][cH][cH]c([CH3])[cH]1)C(Cl)(Cl)Cl

Name	Count name	Pattern
KRFP729	KRFPC729	[!#1][NH][CH]([NH]C(=S)[NH]c1[cH][cH][cH]c([OH])[cH]1)C(Cl)(Cl)Cl
KRFP730	KRFPC730	[!#1][NH][CH]([NH]C(=S)[NH]c1[cH][cH][cH]c2[cH][cH][cH][cH]c12)C(Cl)(Cl)Cl
KRFP731	KRFPC731	[!#1][NH][CH]([NH]C(=S)[NH]c1[cH][cH][cH]c2[cH][cH][cH]nc12)C(Cl)(Cl)Cl
KRFP732	KRFPC732	[!#1][NH][CH]([NH]C(=S)[NH]c1[cH][cH]c([cH][cH]1)[N+](=O)[O-])C(Cl)(Cl)Cl
KRFP733	KRFPC733	[!#1][NH][CH]([NH]C(=S)[NH]c1[cH][cH]c([cH][cH]1)C(=O)[OH])C(Cl)(Cl)Cl
KRFP734	KRFPC734	[!#1][NH][CH]([NH]C(=S)[NH]c1[cH][cH]c([cH][cH]1)S(=O)(=O)[!#1])C(Cl)(Cl)Cl
KRFP735	KRFPC735	[!#1][NH][CH]([NH]C(=S)[NH]c1[cH][cH]c([CH3])[cH][cH]1)C(Cl)(Cl)Cl
KRFP736	KRFPC736	[!#1][NH][CH]([NH]C(=S)[NH]c1[cH][cH]c([NH][!#1])[cH][cH]1)C(Cl)(Cl)Cl
KRFP737	KRFPC737	[!#1][NH][CH]([NH]C(=S)[NH]c1[cH][cH]c(N=Nc2[cH][cH][cH][cH]2)[cH]1)C(Cl)(Cl)Cl
KRFP738	KRFPC738	[!#1][NH][CH]([NH]C(=S)[NH]c1[cH][cH]c(N=Nc2[cH][cH][cH][cH]c2[CH3])[cH]c1[CH3])C(Cl)(Cl)Cl
KRFP739	KRFPC739	[!#1][NH][CH]([NH]C(=S)[NH]c1[cH][cH]c(O[!#1])[cH][cH]1)C(Cl)(Cl)Cl
KRFP740	KRFPC740	[!#1][NH][CH]([NH]C(=S)[NH]c1[cH][cH]c(O[!#1])[cH]c1[N+](=O)[O-])C(Cl)(Cl)Cl
KRFP741	KRFPC741	[!#1][NH][CH]([NH]C(=S)[NH]c1[cH]c([cH][cH]c1Cl)C(F)(F)F)C(Cl)(Cl)Cl
KRFP742	KRFPC742	[!#1][NH][CH]([NH]C(=S)[NH]c1[cH]c([cH][cH]c1O[!#1])[N+](=O)[O-])C(Cl)(Cl)Cl
KRFP743	KRFPC743	[!#1][NH][CH]([NH]C(=S)[NH]c1[cH]c(Cl)[cH][cH]c1Cl)C(Cl)(Cl)Cl
KRFP744	KRFPC744	[!#1][NH][CH]([NH]C(=S)[NH]c1sc2[CH2][CH2][CH2][CH2]c2c1C(=O)[!#1])C(Cl)(Cl)Cl
KRFP745	KRFPC745	[!#1][NH][CH](c1[cH][cH][cH][cH][cH]1)C([!#1])([!#1])C(=O)[!#1]
KRFP746	KRFPC746	[!#1][NH][CH](c1[cH][cH][cH][cH][cH]1)c2c([OH])[cH][cH]c3[cH][cH][cH]c23
KRFP747	KRFPC747	[!#1][NH][CH](c1[cH][cH][cH][cH][cH]c1[!#1])c2[cH][cH][cH][cH]c2O[!#1]
KRFP748	KRFPC748	[!#1][NH][CH]=[CH][!#1]
KRFP749	KRFPC749	[!#1][NH][CH]=C1C(=O)[CH2][NH]C1=O
KRFP750	KRFPC750	[!#1][NH][CH]=C1C(=O)[CH2]C([!#1])([CH3])[CH]([!#1])C1=O
KRFP751	KRFPC751	[!#1][NH][CH]=C1C(=O)[CH2]C([!#1])([CH3])[CH2]C1=O
KRFP752	KRFPC752	[!#1][NH][CH]1[CH2][CH2][CH2][CH2][CH2]1
KRFP753	KRFPC753	[!#1][NH][CH]1[CH2][CH2][CH2][CH2]1
KRFP754	KRFPC754	[!#1][NH][CH]1[CH2][CH2]1
KRFP755	KRFPC755	[!#1][NH][CH]1[CH2][CH2]S(=O)(=O)[CH2]1
KRFP756	KRFPC756	[!#1][NH][CH]1O[CH]([CH2][OH])[CH]([OH])[CH]([OH])[CH]1[OH]
KRFP757	KRFPC757	[!#1][NH][CH]1O[CH2][CH]([OH])[CH]([OH])[CH]1[OH]
KRFP758	KRFPC758	[!#1][NH][CH2][CH]([!#1])[!#1]
KRFP759	KRFPC759	[!#1][NH][CH2][CH]([CH3])[CH3]
KRFP760	KRFPC760	[!#1][NH][CH2][CH]([OH])[CH]([OH])[CH]([OH])[CH2][OH]
KRFP761	KRFPC761	[!#1][NH][CH2][CH]([OH])[CH2]O[!#1]
KRFP762	KRFPC762	[!#1][NH][CH2][CH]=[CH2]
KRFP763	KRFPC763	[!#1][NH][CH2][CH2][CH2][CH2][CH2][CH2][NH][!#1]
KRFP764	KRFPC764	[!#1][NH][CH2][CH2][CH2][CH2][CH2][CH2][OH]
KRFP765	KRFPC765	[!#1][NH][CH2][CH2][CH2][CH2][CH2]C(=O)[OH]
KRFP766	KRFPC766	[!#1][NH][CH2][CH2][CH2][CH2][CH3]
KRFP767	KRFPC767	[!#1][NH][CH2][CH2][CH2][CH2][OH]
KRFP768	KRFPC768	[!#1][NH][CH2][CH2][CH2][CH3]
KRFP769	KRFPC769	[!#1][NH][CH2][CH2][CH2][NH2]
KRFP770	KRFPC770	[!#1][NH][CH2][CH2][CH2][OH]
KRFP771	KRFPC771	[!#1][NH][CH2][CH2][CH2]C(=O)[OH]
KRFP772	KRFPC772	[!#1][NH][CH2][CH2][CH2]O[CH3]
KRFP773	KRFPC773	[!#1][NH][CH2][CH2][CH3]
KRFP774	KRFPC774	[!#1][NH][CH2][CH2][NH][!#1]

Name	Count name	Pattern
KRFP775	KRFPC775	[!#1][NH][CH2][CH2][NH2]
KRFP776	KRFPC776	[!#1][NH][CH2][CH2][OH]
KRFP777	KRFPC777	[!#1][NH][CH2][CH2]C#N
KRFP778	KRFPC778	[!#1][NH][CH2][CH2]C(=O)[!#1]
KRFP779	KRFPC779	[!#1][NH][CH2][CH2]C(=O)[OH]
KRFP780	KRFPC780	[!#1][NH][CH2][CH2]c1[cH][cH][cH][cH]1
KRFP781	KRFPC781	[!#1][NH][CH2][CH2]c1[cH][cH]c(O[!#1])[cH][cH]1
KRFP782	KRFPC782	[!#1][NH][CH2][CH2]c1[cH][cH]c(O[!#1])c(O[!#1])[cH]1
KRFP783	KRFPC783	[!#1][NH][CH2][CH2]c1[cH][nH]c2[cH][cH][cH][cH]c12
KRFP784	KRFPC784	[!#1][NH][CH2][CH2]c1[cH][nH]c2[cH][cH]c(O[!#1])[cH]c12
KRFP785	KRFPC785	[!#1][NH][CH2][CH2]N([CH2][CH3])[CH2][CH3]
KRFP786	KRFPC786	[!#1][NH][CH2][CH2]O[!#1]
KRFP787	KRFPC787	[!#1][NH][CH2][CH2]S(=O)(=O)[OH]
KRFP788	KRFPC788	[!#1][NH][CH2][CH3]
KRFP789	KRFPC789	[!#1][NH][CH2][NH][!#1]
KRFP790	KRFPC790	[!#1][NH][CH2]C(=O)[!#1]
KRFP791	KRFPC791	[!#1][NH][CH2]C(=O)[NH][!#1]
KRFP792	KRFPC792	[!#1][NH][CH2]C(=O)[NH]N=[CH][!#1]
KRFP793	KRFPC793	[!#1][NH][CH2]C(=O)[NH]N=[CH]c1[cH][cH]c([OH])[cH][cH]1
KRFP794	KRFPC794	[!#1][NH][CH2]C(=O)[NH]N=[CH]c1[cH][cH]c2O[CH2]Oc2[cH]1
KRFP795	KRFPC795	[!#1][NH][CH2]C(=O)[NH]N=[CH]c1[cH]c(N=Nc2[cH][cH][cH][cH]2)[cH]c1[OH]
KRFP796	KRFPC796	[!#1][NH][CH2]C(=O)[NH]N=[CH]c1[cH]c2[cH][cH][cH][cH]c2nc1Cl
KRFP797	KRFPC797	[!#1][NH][CH2]C(=O)[OH]
KRFP798	KRFPC798	[!#1][NH][CH2]C(=O)C([!#1])([!#1])C(=O)[!#1]
KRFP799	KRFPC799	[!#1][NH][CH2]C(=O)O[CH2][CH2][CH2][CH3]
KRFP800	KRFPC800	[!#1][NH][CH2]C(=O)O[CH2][CH3]
KRFP801	KRFPC801	[!#1][NH][CH2]C(=O)O[CH3]
KRFP802	KRFPC802	[!#1][NH][CH2]c1[cH][cH][cH][cH]1
KRFP803	KRFPC803	[!#1][NH][CH2]c1[cH][cH][cH]n[cH]1
KRFP804	KRFPC804	[!#1][NH][CH2]c1[cH][cH][cH]o1
KRFP805	KRFPC805	[!#1][NH][CH2]c1[cH][cH][cH]s1
KRFP806	KRFPC806	[!#1][NH][CH2]c1[cH][cH]c(Cl)[cH][cH]1
KRFP807	KRFPC807	[!#1][NH][CH2]c1[cH]c(Br)[cH]c(Br)c1O[!#1]
KRFP808	KRFPC808	[!#1][NH][CH2]c1[cH]c(Br)[cH]c(C(=O)[OH])c1O[!#1]
KRFP809	KRFPC809	[!#1][NH][CH2]c1c(O[!#1])[cH][cH]c2[cH][cH][cH][cH]c12
KRFP810	KRFPC810	[!#1][NH][CH3]
KRFP811	KRFPC811	[!#1][NH][NH][!#1]
KRFP812	KRFPC812	[!#1][NH][NH][CH]=O
KRFP813	KRFPC813	[!#1][NH][NH]C(=O)[!#1]
KRFP814	KRFPC814	[!#1][NH][NH]C(=O)[CH2][CH2][CH3]
KRFP815	KRFPC815	[!#1][NH][NH]C(=O)[CH3]
KRFP816	KRFPC816	[!#1][NH][NH]C(=O)[NH][!#1]
KRFP817	KRFPC817	[!#1][NH][NH]C(=S)[NH][!#1]
KRFP818	KRFPC818	[!#1][NH][NH]C(=S)[NH2]
KRFP819	KRFPC819	[!#1][NH][NH]S(=O)(=O)[!#1]
KRFP820	KRFPC820	[!#1][NH][NH2]
KRFP821	KRFPC821	[!#1][NH]C([!#1])([!#1])[!#1]
KRFP822	KRFPC822	[!#1][NH]C([!#1])([!#1])[CH3]
KRFP823	KRFPC823	[!#1][NH]C([!#1])([!#1])C(=O)[!#1]
KRFP824	KRFPC824	[!#1][NH]C([!#1])([!#1])C(=O)c1[cH][cH][cH][cH]c1C(=O)[CH]([!#1])[!#1]
KRFP825	KRFPC825	[!#1][NH]C([!#1])([CH3])[CH2][CH3]
KRFP826	KRFPC826	[!#1][NH]C([!#1])([CH3])[CH3]
KRFP827	KRFPC827	[!#1][NH]C([CH3])([CH3])[CH2][CH]([!#1])[CH2]C([!#1])([CH3])[CH3]

Name	Count name	Pattern
KRFP828	KRFPC828	[!#1][NH]C([CH3])([CH3])[CH2][OH]
KRFP829	KRFPC829	[!#1][NH]C([CH3])([CH3])[CH3]
KRFP830	KRFPC830	[!#1][NH]C(=[NH])[NH]C(=[NH])[NH][!#1]
KRFP831	KRFPC831	[!#1][NH]C(=[NH])[NH]C(=[NH])N([CH3])[CH3]
KRFP832	KRFPC832	[!#1][NH]C(=[NH])[NH]C(=O)[NH2]
KRFP833	KRFPC833	[!#1][NH]C(=[NH])[NH2]
KRFP834	KRFPC834	[!#1][NH]C(=C(S(=O)(=O)[CH2][CH3])S(=O)(=O)[CH2][CH3])[NH][!#1]
KRFP835	KRFPC835	[!#1][NH]C(=C1C(=O)[CH2]SC1=O)[CH3]
KRFP836	KRFPC836	[!#1][NH]C(=C1C(=O)[NH]C(=O)N([!#1])C1=O)[CH3]
KRFP837	KRFPC837	[!#1][NH]C(=N[!#1])[NH][!#1]
KRFP838	KRFPC838	[!#1][NH]C(=N[!#1])SC([!#1])([!#1])C(=O)[!#1]
KRFP839	KRFPC839	[!#1][NH]C(=O)[!#1]
KRFP840	KRFPC840	[!#1][NH]C(=O)[CH]([!#1])[!#1]
KRFP841	KRFPC841	[!#1][NH]C(=O)[CH]([!#1])[CH]([CH3])[CH3]
KRFP842	KRFPC842	[!#1][NH]C(=O)[CH]([!#1])[CH3]
KRFP843	KRFPC843	[!#1][NH]C(=O)[CH]([!#1])C(=O)[NH][!#1]
KRFP844	KRFPC844	[!#1][NH]C(=O)[CH]([!#1])C(=O)O[CH2][CH3]
KRFP845	KRFPC845	[!#1][NH]C(=O)[CH]([CH](C(=O)[OH])C(=O)O[!#1])C(=O)O[!#1]
KRFP846	KRFPC846	[!#1][NH]C(=O)[CH]([CH2][CH2][CH3])[CH2][CH2][CH3]
KRFP847	KRFPC847	[!#1][NH]C(=O)[CH]([CH3])[CH2][SH](=O)=O
KRFP848	KRFPC848	[!#1][NH]C(=O)[CH]([CH3])[NH]C(=O)[!#1]
KRFP849	KRFPC849	[!#1][NH]C(=O)[CH]([CH3])Br
KRFP850	KRFPC850	[!#1][NH]C(=O)[CH](C(=O)[!#1])S(=O)(=O)[!#1]
KRFP851	KRFPC851	[!#1][NH]C(=O)[CH](OC(=O)[!#1])[CH](OC(=O)[!#1])C(=O)[OH]
KRFP852	KRFPC852	[!#1][NH]C(=O)[CH]=[CH][!#1]
KRFP853	KRFPC853	[!#1][NH]C(=O)[CH]=[CH][CH3]
KRFP854	KRFPC854	[!#1][NH]C(=O)[CH]=[CH]C(=O)[OH]
KRFP855	KRFPC855	[!#1][NH]C(=O)[CH]=[CH]C(=O)O[CH2]C(F)(F)[CH](F)F
KRFP856	KRFPC856	[!#1][NH]C(=O)[CH]=[CH]c1[cH][cH][cH][cH][cH]1
KRFP857	KRFPC857	[!#1][NH]C(=O)[CH]=[CH]c1[cH][cH][cH]c([cH]1)[N+](=O)[O-]
KRFP858	KRFPC858	[!#1][NH]C(=O)[CH2][CH]([!#1])[NH]C(=O)C(F)(F)F
KRFP859	KRFPC859	[!#1][NH]C(=O)[CH2][CH2][CH2][CH2][CH2][CH2]C(=O)[NH][!#1]
KRFP860	KRFPC860	[!#1][NH]C(=O)[CH2][CH2][CH2][CH3]
KRFP861	KRFPC861	[!#1][NH]C(=O)[CH2][CH2][CH2]C(=O)[NH][!#1]
KRFP862	KRFPC862	[!#1][NH]C(=O)[CH2][CH2][CH2]C(=O)[OH]
KRFP863	KRFPC863	[!#1][NH]C(=O)[CH2][CH2][CH2]C(=O)O[!#1]
KRFP864	KRFPC864	[!#1][NH]C(=O)[CH2][CH2][CH2]C(=O)O[CH2]C#[CH]
KRFP865	KRFPC865	[!#1][NH]C(=O)[CH2][CH2][CH2]O[!#1]
KRFP866	KRFPC866	[!#1][NH]C(=O)[CH2][CH2][CH3]
KRFP867	KRFPC867	[!#1][NH]C(=O)[CH2][CH2]C([CH3])([CH3])C(=O)[NH][!#1]
KRFP868	KRFPC868	[!#1][NH]C(=O)[CH2][CH2]C(=O)[OH]
KRFP869	KRFPC869	[!#1][NH]C(=O)[CH2][CH2]C(=O)O[!#1]
KRFP870	KRFPC870	[!#1][NH]C(=O)[CH2][CH2]C(=O)O[CH2][CH]=[CH2]
KRFP871	KRFPC871	[!#1][NH]C(=O)[CH2][CH2]C(=O)O[CH2]C(=C(Cl)Cl)Cl
KRFP872	KRFPC872	[!#1][NH]C(=O)[CH2][CH2]C(=O)O[CH3]
KRFP873	KRFPC873	[!#1][NH]C(=O)[CH2][CH2]Cl
KRFP874	KRFPC874	[!#1][NH]C(=O)[CH2][CH3]
KRFP875	KRFPC875	[!#1][NH]C(=O)[CH2][NH][CH]([CH3])[CH3]
KRFP876	KRFPC876	[!#1][NH]C(=O)[CH2][NH]C([CH3])([CH3])[CH3]
KRFP877	KRFPC877	[!#1][NH]C(=O)[CH2][SH]
KRFP878	KRFPC878	[!#1][NH]C(=O)[CH2]C(=N[NH]C(=O)[!#1])[CH3]
KRFP879	KRFPC879	[!#1][NH]C(=O)[CH2]C(=O)[!#1]
KRFP880	KRFPC880	[!#1][NH]C(=O)[CH2]C(=O)[CH3]
KRFP881	KRFPC881	[!#1][NH]C(=O)[CH2]C(=O)[NH][!#1]

Name	Count name	Pattern
KRFP882	KRFPC882	[!#1][NH]C(=O)[CH2]Cl
KRFP883	KRFPC883	[!#1][NH]C(=O)[CH2]N([CH2][CH2][CH2][CH3])[CH2][CH2][CH2][CH3]
KRFP884	KRFPC884	[!#1][NH]C(=O)[CH2]N([CH2][CH3])[CH2][CH3]
KRFP885	KRFPC885	[!#1][NH]C(=O)[CH2]N([CH3])[CH3]
KRFP886	KRFPC886	[!#1][NH]C(=O)[CH2]O[!#1]
KRFP887	KRFPC887	[!#1][NH]C(=O)[CH2]S[!#1]
KRFP888	KRFPC888	[!#1][NH]C(=O)[CH2]S[CH2][CH2][NH2]
KRFP889	KRFPC889	[!#1][NH]C(=O)[CH2]SC(=O)[!#1]
KRFP890	KRFPC890	[!#1][NH]C(=O)[CH3]
KRFP891	KRFPC891	[!#1][NH]C(=O)[NH][!#1]
KRFP892	KRFPC892	[!#1][NH]C(=O)[NH][CH]([!#1])[CH3]
KRFP893	KRFPC893	[!#1][NH]C(=O)[NH][CH]([CH2]C(=O)[!#1])C(Cl)(Cl)Cl
KRFP894	KRFPC894	[!#1][NH]C(=O)[NH][CH2][CH2][CH2][OH]
KRFP895	KRFPC895	[!#1][NH]C(=O)[NH][CH2][CH2][OH]
KRFP896	KRFPC896	[!#1][NH]C(=O)[NH][CH3]
KRFP897	KRFPC897	[!#1][NH]C(=O)[NH][NH]C(=O)[!#1]
KRFP898	KRFPC898	[!#1][NH]C(=O)[NH][NH]C(=O)[CH2]O[!#1]
KRFP899	KRFPC899	[!#1][NH]C(=O)[NH][NH]C(=O)O[CH3]
KRFP900	KRFPC900	[!#1][NH]C(=O)[NH]C(=O)[!#1]
KRFP901	KRFPC901	[!#1][NH]C(=O)[NH]C(=O)[CH2]O[!#1]
KRFP902	KRFPC902	[!#1][NH]C(=O)[NH]C(=O)[NH2]
KRFP903	KRFPC903	[!#1][NH]C(=O)[NH]C(=O)C(Cl)(Cl)Cl
KRFP904	KRFPC904	[!#1][NH]C(=O)[NH]N=[CH][!#1]
KRFP905	KRFPC905	[!#1][NH]C(=O)[NH]N=C([!#1])[CH3]
KRFP906	KRFPC906	[!#1][NH]C(=O)[NH]S(=O)(=O)[!#1]
KRFP907	KRFPC907	[!#1][NH]C(=O)[NH]S(=O)(=O)[NH][!#1]
KRFP908	KRFPC908	[!#1][NH]C(=O)[NH2]
KRFP909	KRFPC909	[!#1][NH]C(=O)C([!#1])([!#1])[NH][!#1]
KRFP910	KRFPC910	[!#1][NH]C(=O)C([!#1])([!#1])[OH]
KRFP911	KRFPC911	[!#1][NH]C(=O)C([!#1])(F)F
KRFP912	KRFPC912	[!#1][NH]C(=O)C([CH3])([CH3])[CH3]
KRFP913	KRFPC913	[!#1][NH]C(=O)C(=[CH][!#1])[NH]C(=O)[CH3]
KRFP914	KRFPC914	[!#1][NH]C(=O)C(=[CH]c1[cH][cH][cH][cH]1)[NH]C(=O)[CH3]
KRFP915	KRFPC915	[!#1][NH]C(=O)C(=[CH2])[CH3]
KRFP916	KRFPC916	[!#1][NH]C(=O)C(=O)[NH]N=C1C(=O)[NH]c2[cH][cH][cH][cH]c12
KRFP917	KRFPC917	[!#1][NH]C(=O)C(Cl)(Cl)Cl
KRFP918	KRFPC918	[!#1][NH]C(=O)C(F)(F)C(F)(F)F
KRFP919	KRFPC919	[!#1][NH]C(=O)C(F)(F)F
KRFP920	KRFPC920	[!#1][NH]C(=O)C(F)(F)OC(F)(F)C(F)(F)OC(F)(F)F
KRFP921	KRFPC921	[!#1][NH]C(=O)C(F)(OC(F)(F)C(F)(F)C(F)(F)F)C(F)(F)F
KRFP922	KRFPC922	[!#1][NH]C(=O)N([!#1])[OH]
KRFP923	KRFPC923	[!#1][NH]C(=O)N([CH]([CH3])[CH3])[CH]([CH3])[CH3]
KRFP924	KRFPC924	[!#1][NH]C(=O)O[!#1]
KRFP925	KRFPC925	[!#1][NH]C(=O)O[CH]([CH3])[CH3]
KRFP926	KRFPC926	[!#1][NH]C(=O)O[CH2][CH2][CH2][NH]C(=O)[!#1]
KRFP927	KRFPC927	[!#1][NH]C(=O)O[CH2][CH2][NH]C(=O)[!#1]
KRFP928	KRFPC928	[!#1][NH]C(=O)O[CH2][CH2][NH]C(=O)O[CH3]
KRFP929	KRFPC929	[!#1][NH]C(=O)O[CH2][CH2][NH]S(=O)(=O)[!#1]
KRFP930	KRFPC930	[!#1][NH]C(=O)O[CH2][CH2]O[CH3]
KRFP931	KRFPC931	[!#1][NH]C(=O)O[CH2][CH3]
KRFP932	KRFPC932	[!#1][NH]C(=O)O[CH3]
KRFP933	KRFPC933	[!#1][NH]C(=O)ON=[CH][!#1]
KRFP934	KRFPC934	[!#1][NH]C(=O)ON=C([CH3])[CH3]
KRFP935	KRFPC935	[!#1][NH]C(=O)S[CH2]C(=O)[!#1]

Name	Count name	Pattern
KRFP936	KRFPC936	[!#1][NH]C(=S)[!#1]
KRFP937	KRFPC937	[!#1][NH]C(=S)[NH][!#1]
KRFP938	KRFPC938	[!#1][NH]C(=S)[NH][CH]([NH]C(=O)[!#1])C(Cl)(Cl)Cl
KRFP939	KRFPC939	[!#1][NH]C(=S)[NH][CH]([NH]C(=O)[CH]([!#1])[!#1])C(Cl)(Cl)Cl
KRFP940	KRFPC940	[!#1][NH]C(=S)[NH][CH]([NH]C(=O)[CH]([CH3])[CH3])C(Cl)(Cl)Cl
KRFP941	KRFPC941	[!#1][NH]C(=S)[NH][CH]([NH]C(=O)[CH]=[CH][!#1])C(Cl)(Cl)Cl
KRFP942	KRFPC942	[!#1][NH]C(=S)[NH][CH]([NH]C(=O)[CH]=[CH]c1[cH][cH][cH][cH][cH]1)C(Cl)(Cl)Cl
KRFP943	KRFPC943	[!#1][NH]C(=S)[NH][CH]([NH]C(=O)[CH2][CH]([CH3])[CH3])C(Cl)(Cl)Cl
KRFP944	KRFPC944	[!#1][NH]C(=S)[NH][CH]([NH]C(=O)[CH2][CH2][CH2][CH2][CH2][CH3])C(Cl)(Cl)Cl
KRFP945	KRFPC945	[!#1][NH]C(=S)[NH][CH]([NH]C(=O)[CH2][CH2][CH2][CH2][CH3])C(Cl)(Cl)Cl
KRFP946	KRFPC946	[!#1][NH]C(=S)[NH][CH]([NH]C(=O)[CH2][CH2][CH3])C(Cl)(Cl)Cl
KRFP947	KRFPC947	[!#1][NH]C(=S)[NH][CH]([NH]C(=O)[CH2][CH3])C(Cl)(Cl)Cl
KRFP948	KRFPC948	[!#1][NH]C(=S)[NH][CH]([NH]C(=O)[CH2]F)C(Cl)(Cl)Cl
KRFP949	KRFPC949	[!#1][NH]C(=S)[NH][CH]([NH]C(=O)[CH3])C(Cl)(Cl)Cl
KRFP950	KRFPC950	[!#1][NH]C(=S)[NH][CH]([NH]C(=O)C([CH3])([CH3])[CH3])C(Cl)(Cl)Cl
KRFP951	KRFPC951	[!#1][NH]C(=S)[NH][CH](N=C([!#1])O[CH3])C(Cl)(Cl)Cl
KRFP952	KRFPC952	[!#1][NH]C(=S)[NH]C(=C(C(F)(F)F)C(F)(F)F)C(F)(F)C(F)(F)C(F)(F)F
KRFP953	KRFPC953	[!#1][NH]C(=S)[NH]C(=N[CH2]S(=O)(=O)[!#1])[!#1]
KRFP954	KRFPC954	[!#1][NH]C(=S)[NH]C(=O)[!#1]
KRFP955	KRFPC955	[!#1][NH]C(=S)[NH]C(=O)[CH]=[CH][!#1]
KRFP956	KRFPC956	[!#1][NH]C(=S)[NH]C(=O)[CH]=[CH]c1[cH][cH][cH][cH][cH]1
KRFP957	KRFPC957	[!#1][NH]C(=S)[NH]C(=O)[CH]=[CH]c1[cH][cH][cH]o1
KRFP958	KRFPC958	[!#1][NH]C(=S)[NH]C(=O)[CH]=[CH]c1[cH][cH]c(F)[cH][cH]1
KRFP959	KRFPC959	[!#1][NH]C(=S)[NH]C(=O)[CH]=[CH]c1[cH][cH]c(O[CH3])c(O[CH3])[cH]1
KRFP960	KRFPC960	[!#1][NH]C(=S)[NH]c1[cH][cH]c([cH][cH]1)S(=O)(=O)[!#1]
KRFP961	KRFPC961	[!#1][NH]C(=S)[NH]N=[CH][!#1]
KRFP962	KRFPC962	[!#1][NH]C(=S)[NH]N=C([!#1])[CH3]
KRFP963	KRFPC963	[!#1][NH]C(=S)[NH2]
KRFP964	KRFPC964	[!#1][NH]C(=S)O[CH2][CH2][CH3]
KRFP965	KRFPC965	[!#1][NH]C(=S)SC([!#1])([!#1])C(=O)[!#1]
KRFP966	KRFPC966	[!#1][NH]C1([CH2][CH]2[CH2][CH]3[CH2][CH]([CH2]2)[CH2]1)[CH2]3
KRFP967	KRFPC967	[!#1][NH]C1([CH2][CH2][CH2][CH2][CH2]1)C(=O)[!#1]
KRFP968	KRFPC968	[!#1][NH]C1([CH2][CH2][CH2][CH2][CH2]1)c2nnnn2[!#1]
KRFP969	KRFPC969	[!#1][NH]C1([CH2][CH2][CH2][CH2]1)C(=O)[!#1]
KRFP970	KRFPC970	[!#1][NH]C1([CH3])C(=O)c2[cH][cH][cH][cH]c2C1=O
KRFP971	KRFPC971	[!#1][NH]C1(C(=O)c2[cH][cH][cH][cH]c2C1=O)c3[cH][cH][cH][cH][cH]3
KRFP972	KRFPC972	[!#1][NH]c1[cH][cH][cH][cH][cH]1
KRFP973	KRFPC973	[!#1][NH]c1[cH][cH][cH][cH]c1[!#1]
KRFP974	KRFPC974	[!#1][NH]c1[cH][cH][cH][cH]c1[CH2][CH3]
KRFP975	KRFPC975	[!#1][NH]c1[cH][cH][cH][cH]c1[CH3]
KRFP976	KRFPC976	[!#1][NH]c1[cH][cH][cH][cH]c1[N+](=O)[O-]
KRFP977	KRFPC977	[!#1][NH]c1[cH][cH][cH][cH]c1[NH][!#1]
KRFP978	KRFPC978	[!#1][NH]c1[cH][cH][cH][cH]c1[OH]
KRFP979	KRFPC979	[!#1][NH]c1[cH][cH][cH][cH]c1Br
KRFP980	KRFPC980	[!#1][NH]c1[cH][cH][cH][cH]c1C([!#1])([!#1])C(=O)[!#1]
KRFP981	KRFPC981	[!#1][NH]c1[cH][cH][cH][cH]c1C([OH])([CH2]C(=N[NH]C(=O)[CH2]O[!#1])[CH3])C(=O)[!#1]
KRFP982	KRFPC982	[!#1][NH]c1[cH][cH][cH][cH]c1C(=N[!#1])C(=O)[!#1]
KRFP983	KRFPC983	[!#1][NH]c1[cH][cH][cH][cH]c1C(=O)[!#1]
KRFP984	KRFPC984	[!#1][NH]c1[cH][cH][cH][cH]c1C(=O)[OH]
KRFP985	KRFPC985	[!#1][NH]c1[cH][cH][cH][cH]c1C(F)(F)F
KRFP986	KRFPC986	[!#1][NH]c1[cH][cH][cH][cH]c1Cl

Name	Count name	Pattern
KRFP987	KRFPC987	[!#1][NH]c1[cH][cH][cH][cH]c1F
KRFP988	KRFPC988	[!#1][NH]c1[cH][cH][cH][cH]c1I
KRFP989	KRFPC989	[!#1][NH]c1[cH][cH][cH][cH]c1O[!#1]
KRFP990	KRFPC990	[!#1][NH]c1[cH][cH][cH][cH]c1S[CH]([CH2]C(=O)[!#1])C(=O)[!#1]
KRFP991	KRFPC991	[!#1][NH]c1[cH][cH][cH][cH]c1n
KRFP992	KRFPC992	[!#1][NH]c1[cH][cH][cH]c([!#1])[cH]1
KRFP993	KRFPC993	[!#1][NH]c1[cH][cH][cH]c([cH]1)[CH]([!#1])[!#1]
KRFP994	KRFPC994	[!#1][NH]c1[cH][cH][cH]c([cH]1)[N+](=O)[O-]
KRFP995	KRFPC995	[!#1][NH]c1[cH][cH][cH]c([cH]1)C(=O)[!#1]
KRFP996	KRFPC996	[!#1][NH]c1[cH][cH][cH]c([cH]1)C(=O)[CH3]
KRFP997	KRFPC997	[!#1][NH]c1[cH][cH][cH]c([cH]1)C(=O)[OH]
KRFP998	KRFPC998	[!#1][NH]c1[cH][cH][cH]c([cH]1)C(F)(F)F
KRFP999	KRFPC999	[!#1][NH]c1[cH][cH][cH]c([CH3])[cH]1
KRFP1000	KRFPC1000	[!#1][NH]c1[cH][cH][cH]c([CH3])c1[CH3]
KRFP1001	KRFPC1001	[!#1][NH]c1[cH][cH][cH]c([NH][!#1])[cH]1
KRFP1002	KRFPC1002	[!#1][NH]c1[cH][cH][cH]c([OH])[cH]1
KRFP1003	KRFPC1003	[!#1][NH]c1[cH][cH][cH]c(Br)[cH]1
KRFP1004	KRFPC1004	[!#1][NH]c1[cH][cH][cH]c(Cl)[cH]1
KRFP1005	KRFPC1005	[!#1][NH]c1[cH][cH][cH]c(Cl)c1[CH3]
KRFP1006	KRFPC1006	[!#1][NH]c1[cH][cH][cH]c(Cl)c1Cl
KRFP1007	KRFPC1007	[!#1][NH]c1[cH][cH][cH]c(F)[cH]1
KRFP1008	KRFPC1008	[!#1][NH]c1[cH][cH][cH]c(O[!#1])[cH]1
KRFP1009	KRFPC1009	[!#1][NH]c1[cH][cH][cH]c2[cH][cH][cH]c12
KRFP1010	KRFPC1010	[!#1][NH]c1[cH][cH][cH]c2[cH][cH][cH]nc12
KRFP1011	KRFPC1011	[!#1][NH]c1[cH][cH][cH]c2c([NH][!#1])[cH][cH][cH]c12
KRFP1012	KRFPC1012	[!#1][NH]c1[cH][cH][cH]c2C(=O)c3[cH][cH][cH]c3C(=O)c12
KRFP1013	KRFPC1013	[!#1][NH]c1[cH][cH][cH]c([!#1])[cH][cH]1
KRFP1014	KRFPC1014	[!#1][NH]c1[cH][cH][cH]c([!#1])[cH]c1[CH3]
KRFP1015	KRFPC1015	[!#1][NH]c1[cH][cH][cH]c([!#1])[cH]c1[N+](=O)[O-]
KRFP1016	KRFPC1016	[!#1][NH]c1[cH][cH][cH]c([!#1])c([cH]1)S(=O)(=O)c2[cH]c([NH][!#1])[cH] [cH]c2[!#1]
KRFP1017	KRFPC1017	[!#1][NH]c1[cH][cH][cH]c([CH]([!#1])[!#1])c([cH]1)S(=O)(=O)[OH]
KRFP1018	KRFPC1018	[!#1][NH]c1[cH][cH][cH]c([cH][cH]1)[CH]([!#1])[!#1]
KRFP1019	KRFPC1019	[!#1][NH]c1[cH][cH][cH]c([cH][cH]1)[CH]([CH3])[CH3]
KRFP1020	KRFPC1020	[!#1][NH]c1[cH][cH][cH]c([cH][cH]1)[N+](=O)[O-]
KRFP1021	KRFPC1021	[!#1][NH]c1[cH][cH][cH]c([cH][cH]1)C(=O)[!#1]
KRFP1022	KRFPC1022	[!#1][NH]c1[cH][cH][cH]c([cH][cH]1)C(=O)[CH3]
KRFP1023	KRFPC1023	[!#1][NH]c1[cH][cH][cH]c([cH][cH]1)C(=O)[OH]
KRFP1024	KRFPC1024	[!#1][NH]c1[cH][cH][cH]c([cH][cH]1)S(=O)(=O)[!#1]
KRFP1025	KRFPC1025	[!#1][NH]c1[cH][cH][cH]c([cH]c1[N+](=O)[O-])[N+](=O)[O-]
KRFP1026	KRFPC1026	[!#1][NH]c1[cH][cH][cH]c([cH]c1[N+](=O)[O-])C(=O)[OH]
KRFP1027	KRFPC1027	[!#1][NH]c1[cH][cH][cH]c([cH]c1C(=N[NH])C(=O)[CH2]O[!#1])C(=O)[!#1])[N+] (=O)[O-]
KRFP1028	KRFPC1028	[!#1][NH]c1[cH][cH][cH]c([CH2][CH2]c2[cH][cH][cH]c2[!#1])c([NH][!#1])[cH]1
KRFP1029	KRFPC1029	[!#1][NH]c1[cH][cH][cH]c([CH2]c2[cH][cH]c([NH][!#1])[cH][cH]2)[cH][cH]1
KRFP1030	KRFPC1030	[!#1][NH]c1[cH][cH][cH]c([CH3])[cH][cH]1
KRFP1031	KRFPC1031	[!#1][NH]c1[cH][cH][cH]c([CH3])[cH]c1[CH3]
KRFP1032	KRFPC1032	[!#1][NH]c1[cH][cH][cH]c([CH3])[cH]c1[N+](=O)[O-]
KRFP1033	KRFPC1033	[!#1][NH]c1[cH][cH][cH]c([CH3])c([cH]1)[N+](=O)[O-]
KRFP1034	KRFPC1034	[!#1][NH]c1[cH][cH][cH]c([CH3])c([CH3])[cH]1
KRFP1035	KRFPC1035	[!#1][NH]c1[cH][cH][cH]c([CH3])c([NH][!#1])[cH]1
KRFP1036	KRFPC1036	[!#1][NH]c1[cH][cH][cH]c([N+](=O)[O-])c2nonc12
KRFP1037	KRFPC1037	[!#1][NH]c1[cH][cH][cH]c([NH][!#1])[cH][cH]1
KRFP1038	KRFPC1038	[!#1][NH]c1[cH][cH][cH]c([OH])[cH][cH]1

Name	Count name	Pattern
KRFP1039	KRFPC1039	[!#1][NH]c1[cH][cH]c(Br)[cH][cH]1
KRFP1040	KRFPC1040	[!#1][NH]c1[cH][cH]c(Br)[cH]c1C(=O)[!#1]
KRFP1041	KRFPC1041	[!#1][NH]c1[cH][cH]c(Br)[cH]n1
KRFP1042	KRFPC1042	[!#1][NH]c1[cH][cH]c(Cl)[cH][cH]1
KRFP1043	KRFPC1043	[!#1][NH]c1[cH][cH]c(Cl)[cH]c1[N+](=O)[O-]
KRFP1044	KRFPC1044	[!#1][NH]c1[cH][cH]c(Cl)[cH]c1C(=O)[!#1]
KRFP1045	KRFPC1045	[!#1][NH]c1[cH][cH]c(Cl)[cH]c1Cl
KRFP1046	KRFPC1046	[!#1][NH]c1[cH][cH]c(Cl)[cH]n1
KRFP1047	KRFPC1047	[!#1][NH]c1[cH][cH]c(Cl)c([cH]1)[N+](=O)[O-]
KRFP1048	KRFPC1048	[!#1][NH]c1[cH][cH]c(Cl)c(Cl)[cH]1
KRFP1049	KRFPC1049	[!#1][NH]c1[cH][cH]c(F)[cH][cH]1
KRFP1050	KRFPC1050	[!#1][NH]c1[cH][cH]c(F)c(Cl)[cH]1
KRFP1051	KRFPC1051	[!#1][NH]c1[cH][cH]c(I)[cH][cH]1
KRFP1052	KRFPC1052	[!#1][NH]c1[cH][cH]c(N(!#1)[CH2][CH3])c2c([cH][cH][cH]c12)C(=O) [!#1]
KRFP1053	KRFPC1053	[!#1][NH]c1[cH][cH]c(N=Nc2[cH][cH][cH][cH]2)[cH][cH]1
KRFP1054	KRFPC1054	[!#1][NH]c1[cH][cH]c(N=Nc2[cH][cH][cH][cH]c2[CH3])[cH]c1[CH3]
KRFP1055	KRFPC1055	[!#1][NH]c1[cH][cH]c(O(!#1))[cH][cH]1
KRFP1056	KRFPC1056	[!#1][NH]c1[cH][cH]c(O(!#1))[cH]c1[N+](=O)[O-]
KRFP1057	KRFPC1057	[!#1][NH]c1[cH][cH]c(O[CH3])nn1
KRFP1058	KRFPC1058	[!#1][NH]c1[cH][cH]c2[cH][cH][cH][cH]c2[cH]1
KRFP1059	KRFPC1059	[!#1][NH]c1[cH][cH]c2[cH][cH][cH]c([OH])c2n1
KRFP1060	KRFPC1060	[!#1][NH]c1[cH][cH]c2[CH2][CH2]c3[cH][cH][cH][cH]c3N(!#1)c2[cH]1
KRFP1061	KRFPC1061	[!#1][NH]c1[cH][cH]c2c([cH]1)oc3[cH][cH][cH][cH]c32
KRFP1062	KRFPC1062	[!#1][NH]c1[cH][cH]c2nc(!#1)[nH]c2[cH]1
KRFP1063	KRFPC1063	[!#1][NH]c1[cH][cH]c2nonc2c1[N+](=O)[O-]
KRFP1064	KRFPC1064	[!#1][NH]c1[cH][cH]c2O[CH2]Oc2[cH]1
KRFP1065	KRFPC1065	[!#1][NH]c1[cH][cH]c2oc(!#1)nc2[cH]1
KRFP1066	KRFPC1066	[!#1][NH]c1[cH][cH]n[cH][cH]1
KRFP1067	KRFPC1067	[!#1][NH]c1[cH][cH]nc2[cH]c3[cH][cH][cH][cH]c3[cH]c12
KRFP1068	KRFPC1068	[!#1][NH]c1[cH]c(!#1)nc2[cH][cH][cH][cH]c12
KRFP1069	KRFPC1069	[!#1][NH]c1[cH]c([cH][cH]c1[CH3])[N+](=O)[O-]
KRFP1070	KRFPC1070	[!#1][NH]c1[cH]c([cH][cH]c1C(=O)[OH])[N+](=O)[O-]
KRFP1071	KRFPC1071	[!#1][NH]c1[cH]c([cH][cH]c1Cl)C(F)(F)F
KRFP1072	KRFPC1072	[!#1][NH]c1[cH]c([cH]c([cH]1)[N+](=O)[O-])C(=O)[OH]
KRFP1073	KRFPC1073	[!#1][NH]c1[cH]c([cH]c([cH]1)C(=O)[OH])C(=O)[OH]
KRFP1074	KRFPC1074	[!#1][NH]c1[cH]c([CH3])[cH][cH]c1[CH3]
KRFP1075	KRFPC1075	[!#1][NH]c1[cH]c([CH3])[cH][cH]n1
KRFP1076	KRFPC1076	[!#1][NH]c1[cH]c([CH3])[cH]c([CH3])[cH]1
KRFP1077	KRFPC1077	[!#1][NH]c1[cH]c([CH3])nc2[cH][cH][cH][cH]c12
KRFP1078	KRFPC1078	[!#1][NH]c1[cH]c(Cl)[cH][cH]c1Cl
KRFP1079	KRFPC1079	[!#1][NH]c1[cH]c(Cl)[cH][cH]c1O(!#1)
KRFP1080	KRFPC1080	[!#1][NH]c1[cH]c(O(!#1))c(O(!#1))[cH]c1C(=O)[!#1]
KRFP1081	KRFPC1081	[!#1][NH]c1[cH]c(O[CH3])nc(O[CH3])n1
KRFP1082	KRFPC1082	[!#1][NH]c1[cH]nc2[cH][cH][cH][cH]c2[cH]1
KRFP1083	KRFPC1083	[!#1][NH]c1[nH]nc([CH3])c1[N+](=O)[O-]
KRFP1084	KRFPC1084	[!#1][NH]C1=[CH]C(=O)c2[cH][cH][cH][cH]c2C1=O
KRFP1085	KRFPC1085	[!#1][NH]c1c([cH][cH]c2nonc12)[N+](=O)[O-]
KRFP1086	KRFPC1086	[!#1][NH]c1c([cH]c([cH]c1[N+](=O)[O-])[N+](=O)[O-])C(=O)[OH]
KRFP1087	KRFPC1087	[!#1][NH]c1c([cH]c([cH]c1[N+](=O)[O-])C(=O)[OH])[N+](=O)[O-]
KRFP1088	KRFPC1088	[!#1][NH]c1c([cH]c([N+](=O)[O-])c2[cH][cH][cH][cH]c12)[N+](=O)[O-]
KRFP1089	KRFPC1089	[!#1][NH]c1c([CH3])[cH][cH][cH]c1[CH3]
KRFP1090	KRFPC1090	[!#1][NH]c1c([CH3])[cH]c([CH3])[cH]c1[CH3]
KRFP1091	KRFPC1091	[!#1][NH]c1c([CH3])c([CH2][CH3])nc2[cH][cH][cH][cH]c12
KRFP1092	KRFPC1092	[!#1][NH]c1c([CH3])n(!#1)n(!#1)c1=O

Name	Count name	Pattern
KRFP1093	KRFPC1093	[!#1][NH]c1c([N+](=O)[O-])c(=O)oc2[cH][cH][cH][cH]c12
KRFP1094	KRFPC1094	[!#1][NH]c1c2[cH][cH][cH][cH]c2nc3[cH][cH][cH][cH]c13
KRFP1095	KRFPC1095	[!#1][NH]c1c2[CH2][CH2][CH2]c2nc3[cH][cH][cH][cH]c13
KRFP1096	KRFPC1096	[!#1][NH]c1c2[CH2][CH2][CH2]c2nc3[CH2][CH2][CH2][CH2]c13
KRFP1097	KRFPC1097	[!#1][NH]c1n[cH][cH][cH]n1
KRFP1098	KRFPC1098	[!#1][NH]c1n[cH][cH]nc1O[CH3]
KRFP1099	KRFPC1099	[!#1][NH]c1n[cH][cH]s1
KRFP1100	KRFPC1100	[!#1][NH]c1n[cH][nH]n1
KRFP1101	KRFPC1101	[!#1][NH]c1n[cH]nc2n(!#1)[cH]nc12
KRFP1102	KRFPC1102	[!#1][NH]c1n[cH]nc2sc3[CH2][CH2][CH2][CH2]c3c12
KRFP1103	KRFPC1103	[!#1][NH]c1n[nH]c(=O)[nH]c1=O
KRFP1104	KRFPC1104	[!#1][NH]c1nc(!#1)[cH]s1
KRFP1105	KRFPC1105	[!#1][NH]c1nc(!#1)nc(!#1)n1
KRFP1106	KRFPC1106	[!#1][NH]c1nc(!#1)nc(Cl)n1
KRFP1107	KRFPC1107	[!#1][NH]c1nc(!#1)nc(n1)N2[CH2][CH2]O[CH2][CH2]2
KRFP1108	KRFPC1108	[!#1][NH]c1nc(!#1)nc(O[CH](C(F)(F)F)C(F)(F)F)n1
KRFP1109	KRFPC1109	[!#1][NH]c1nc([cH]s1)c2[cH][cH][cH][cH][cH]2
KRFP1110	KRFPC1110	[!#1][NH]c1nc([cH]s1)c2[cH][cH]c(!#1)[cH][cH]2
KRFP1111	KRFPC1111	[!#1][NH]c1nc([CH3])[cH]c([CH3])n1
KRFP1112	KRFPC1112	[!#1][NH]c1nc(Cl)nc(Cl)n1
KRFP1113	KRFPC1113	[!#1][NH]c1nc(O[CH](C(F)(F)F)C(F)(F)F)nc(O[CH](C(F)(F)F)C(F)(F)F)n1
KRFP1114	KRFPC1114	[!#1][NH]c1nc2[cH][cH][cH][cH]c2n1(!#1)
KRFP1115	KRFPC1115	[!#1][NH]c1nc2[cH][cH][cH][cH]c2nc1(!#1)
KRFP1116	KRFPC1116	[!#1][NH]c1nc2[cH][cH][cH][cH]c2nc1[NH](!#1)
KRFP1117	KRFPC1117	[!#1][NH]c1nc2[cH][cH][cH][cH]c2s1
KRFP1118	KRFPC1118	[!#1][NH]c1nc2[CH2][CH2][CH2][CH2]c2s1
KRFP1119	KRFPC1119	[!#1][NH]c1nc2nonc2nc1(!#1)
KRFP1120	KRFPC1120	[!#1][NH]c1nnc([CH2][CH3])s1
KRFP1121	KRFPC1121	[!#1][NH]c1nnc([CH3])s1
KRFP1122	KRFPC1122	[!#1][NH]c1sc([CH3])c([CH3])c1C(=O)(!#1)
KRFP1123	KRFPC1123	[!#1][NH]c1sc2[CH2][CH2][CH2][CH2]c2c1C(=O)(!#1)
KRFP1124	KRFPC1124	[!#1][NH]N(!#1)(!#1)
KRFP1125	KRFPC1125	[!#1][NH]N=[CH](!#1)
KRFP1126	KRFPC1126	[!#1][NH]N=C(!#1)(!#1)
KRFP1127	KRFPC1127	[!#1][NH]N=C(!#1)[CH3]
KRFP1128	KRFPC1128	[!#1][NH]N=C(!#1)N=N(!#1)
KRFP1129	KRFPC1129	[!#1][NH]N=C1C(=N[NH]C1=O)(!#1)
KRFP1130	KRFPC1130	[!#1][NH]N=C1C(=NN(C1=O)c2[cH][cH][cH][cH]2)(!#1)
KRFP1131	KRFPC1131	[!#1][NH]N=C1C(=NN(C1=O)c2nc([cH]s2)c3[cH][cH][cH][cH]3)(!#1)
KRFP1132	KRFPC1132	[!#1][NH]N=C1C(=O)[NH]C(=O)[NH]C1=O
KRFP1133	KRFPC1133	[!#1][NH]N=C1C(=O)[NH]C(=S)[NH]C1=O
KRFP1134	KRFPC1134	[!#1][NH]N=N(!#1)
KRFP1135	KRFPC1135	[!#1][NH]n1[cH]nn[cH]1
KRFP1136	KRFPC1136	[!#1][NH]P(=O)(O[CH]([CH3])[CH3])O[CH]([CH3])[CH3]
KRFP1137	KRFPC1137	[!#1][NH]P(=O)(O[CH2][CH]([CH3])[CH3])O[CH2][CH]([CH3])[CH3]
KRFP1138	KRFPC1138	[!#1][NH]P(=O)(O[CH2][CH3])O[CH2][CH3]
KRFP1139	KRFPC1139	[!#1][NH]S(=O)(=O)(!#1)
KRFP1140	KRFPC1140	[!#1][NH]S(=O)(=O)[CH2][CH]=[CH2]
KRFP1141	KRFPC1141	[!#1][NH]S(=O)(=O)[CH3]
KRFP1142	KRFPC1142	[!#1][NH]S(=O)(=O)[NH]C([CH3])([CH3])[CH3]
KRFP1143	KRFPC1143	[!#1][NH]S(=O)(=O)[NH]C(=O)N(!#1)[CH3]
KRFP1144	KRFPC1144	[!#1][NH]S(=O)(!#1)
KRFP1145	KRFPC1145	[!#1][NH]S(!#1)
KRFP1146	KRFPC1146	[!#1][NH2]

Name	Count name	Pattern
KRFP1147	KRFPC1147	[!#1][O-]
KRFP1148	KRFPC1148	[!#1][OH]
KRFP1149	KRFPC1149	[!#1][SH]
KRFP1150	KRFPC1150	[!#1]Br
KRFP1151	KRFPC1151	[!#1]C#C[!#1]
KRFP1152	KRFPC1152	[!#1]C#CC([CH3])([CH3])[OH]
KRFP1153	KRFPC1153	[!#1]C#N
KRFP1154	KRFPC1154	[!#1]C([!#1])([!#1])[!#1]
KRFP1155	KRFPC1155	[!#1]C([!#1])([!#1])[CH2][CH3]
KRFP1156	KRFPC1156	[!#1]C([!#1])([!#1])[CH3]
KRFP1157	KRFPC1157	[!#1]C([!#1])([!#1])[OH]
KRFP1158	KRFPC1158	[!#1]C([!#1])([!#1])c1[cH][cH][cH][cH]1
KRFP1159	KRFPC1159	[!#1]C([!#1])([CH3])[CH2][CH3]
KRFP1160	KRFPC1160	[!#1]C([!#1])([CH3])[CH3]
KRFP1161	KRFPC1161	[!#1]C([!#1])([CH3])[OH]
KRFP1162	KRFPC1162	[!#1]C([!#1])([OH])c1[cH][cH][cH][cH]1
KRFP1163	KRFPC1163	[!#1]C([!#1])(C#N)C#N
KRFP1164	KRFPC1164	[!#1]C([!#1])(Cl)C([!#1])([!#1])[N+](=O)[O-]
KRFP1165	KRFPC1165	[!#1]C([!#1])(Cl)Cl
KRFP1166	KRFPC1166	[!#1]C([CH3])([CH3])[CH2][CH]([CH3])[OH]
KRFP1167	KRFPC1167	[!#1]C([CH3])([CH3])[CH2][CH]([CH3])OC(=O)C([CH3])([CH3])[CH3]
KRFP1168	KRFPC1168	[!#1]C([CH3])([CH3])[CH2][CH]=C([CH3])[CH2][CH2][CH]=C([CH3])[CH3]
KRFP1169	KRFPC1169	[!#1]C([CH3])([CH3])[CH2][CH3]
KRFP1170	KRFPC1170	[!#1]C([CH3])([CH3])[CH2][OH]
KRFP1171	KRFPC1171	[!#1]C([CH3])([CH3])[CH2]C([CH3])([CH3])[CH3]
KRFP1172	KRFPC1172	[!#1]C([CH3])([CH3])[CH2]N([CH3])[CH3]
KRFP1173	KRFPC1173	[!#1]C([CH3])([CH3])[CH3]
KRFP1174	KRFPC1174	[!#1]C([OH])([CH2][CH]=[CH2])[CH2][CH]=[CH2]
KRFP1175	KRFPC1175	[!#1]C([OH])(C(=O)O[CH2][CH3])C(F)(F)F
KRFP1176	KRFPC1176	[!#1]C([OH])(C(=O)O[CH3])C(F)(F)F
KRFP1177	KRFPC1177	[!#1]C([OH])(C(F)(F)F)C(F)(F)F
KRFP1178	KRFPC1178	[!#1]C(=[CH]C(=O)[CH3])[CH3]
KRFP1179	KRFPC1179	[!#1]C(=[CH]C(=O)O[CH2][CH3])[CH3]
KRFP1180	KRFPC1180	[!#1]C(=N[NH]C(=O)[!#1])[!#1]
KRFP1181	KRFPC1181	[!#1]C(=N[NH]C(=O)[!#1])[CH3]
KRFP1182	KRFPC1182	[!#1]C(=N[NH]C(=O)[NH2])[CH3]
KRFP1183	KRFPC1183	[!#1]C(=N[NH]S(=O)(=O)[!#1])[CH3]
KRFP1184	KRFPC1184	[!#1]C(=N[OH])[!#1]
KRFP1185	KRFPC1185	[!#1]C(=N[OH])[CH2][CH]([CH3])[CH3]
KRFP1186	KRFPC1186	[!#1]C(=N[OH])[CH2][CH3]
KRFP1187	KRFPC1187	[!#1]C(=N[OH])[CH3]
KRFP1188	KRFPC1188	[!#1]C(=N[OH])N([CH2][CH3])[CH2][CH3]
KRFP1189	KRFPC1189	[!#1]C(=NN=C([!#1])[CH3])[CH3]
KRFP1190	KRFPC1190	[!#1]C(=NO[CH2][CH3])[CH2][CH2][CH3]
KRFP1191	KRFPC1191	[!#1]C(=NO[CH2]ON=C([!#1])[CH3])[CH3]
KRFP1192	KRFPC1192	[!#1]C(=NOC(=O)[!#1])[CH3]
KRFP1193	KRFPC1193	[!#1]C(=O)[!#1]
KRFP1194	KRFPC1194	[!#1]C(=O)[CH]([CH]1[CH2][CH2][CH2][CH2][CH2]1)C(=O)[!#1]
KRFP1195	KRFPC1195	[!#1]C(=O)[CH]([CH3])[CH3]
KRFP1196	KRFPC1196	[!#1]C(=O)[CH]([CH3])c1[cH][cH]c([CH2][CH]([CH3])[CH3])[cH][cH]1
KRFP1197	KRFPC1197	[!#1]C(=O)[CH]([CH3])N([CH3])[CH3]
KRFP1198	KRFPC1198	[!#1]C(=O)[CH](c1[cH][cH][cH][cH]1)c2[cH][cH][cH][cH][cH]2
KRFP1199	KRFPC1199	[!#1]C(=O)[CH](F)F

Name	Count name	Pattern
KRFP1200	KRFPC1200	[!#1]C(=O)[CH]1[CH]([CH]2c3[cH][cH][cH]c3[CH]1c4[cH][cH][cH][cH]c24)C(=O)[OH]
KRFP1201	KRFPC1201	[!#1]C(=O)[CH]1[CH]2[CH2][CH2][CH2][CH2][CH]12
KRFP1202	KRFPC1202	[!#1]C(=O)[CH]1[CH2][CH]1c2[cH][cH][cH][cH][cH]2
KRFP1203	KRFPC1203	[!#1]C(=O)[CH]1[CH2][CH2][CH2][CH2][CH2]1
KRFP1204	KRFPC1204	[!#1]C(=O)[CH]1[CH2][CH2]1
KRFP1205	KRFPC1205	[!#1]C(=O)[CH]1[CH2][CH2]C([CH3])(C(=O)[OH])C1([CH3])[CH3]
KRFP1206	KRFPC1206	[!#1]C(=O)[CH]1[CH2]C1([CH3])[CH3]
KRFP1207	KRFPC1207	[!#1]C(=O)[CH]1[CH2]C1(c2[cH][cH][cH][cH]c2)c3[cH][cH][cH][cH]c3
KRFP1208	KRFPC1208	[!#1]C(=O)[CH]1[CH2]C1(c2[cH][cH]c([CH3])[cH][cH]2)c3[cH][cH]c([CH3])[cH][cH]3
KRFP1209	KRFPC1209	[!#1]C(=O)[CH]1[CH2]C21[CH2][CH2][CH2]2
KRFP1210	KRFPC1210	[!#1]C(=O)[CH]1C(=O)C(!#1)(!#1)C(=O)[CH2]C1([CH3])[CH3]
KRFP1211	KRFPC1211	[!#1]C(=O)[CH2][CH]([CH3])[CH2]C(=O)[!#1]
KRFP1212	KRFPC1212	[!#1]C(=O)[CH2][CH]([CH3])[CH3]
KRFP1213	KRFPC1213	[!#1]C(=O)[CH2][CH]([NH2])C(Cl)(Cl)Cl
KRFP1214	KRFPC1214	[!#1]C(=O)[CH2][CH2][CH2][CH2][CH2][CH2][CH2][CH2]C(=O)[!#1]
KRFP1215	KRFPC1215	[!#1]C(=O)[CH2][CH2][CH2][CH2][CH2][CH2][CH3]
KRFP1216	KRFPC1216	[!#1]C(=O)[CH2][CH2][CH2][CH2][CH2][CH2]C(=O)[!#1]
KRFP1217	KRFPC1217	[!#1]C(=O)[CH2][CH2][CH2][CH2][CH2][CH3]
KRFP1218	KRFPC1218	[!#1]C(=O)[CH2][CH2][CH2][CH2][CH3]
KRFP1219	KRFPC1219	[!#1]C(=O)[CH2][CH2][CH2][CH2]C(=O)[!#1]
KRFP1220	KRFPC1220	[!#1]C(=O)[CH2][CH2][CH2][CH2]C(=O)[OH]
KRFP1221	KRFPC1221	[!#1]C(=O)[CH2][CH2][CH2][CH3]
KRFP1222	KRFPC1222	[!#1]C(=O)[CH2][CH2][CH2]C(=O)[!#1]
KRFP1223	KRFPC1223	[!#1]C(=O)[CH2][CH2][CH2]C(=O)[OH]
KRFP1224	KRFPC1224	[!#1]C(=O)[CH2][CH2][CH2]c1[cH][cH][cH][cH][cH]1
KRFP1225	KRFPC1225	[!#1]C(=O)[CH2][CH2][CH3]
KRFP1226	KRFPC1226	[!#1]C(=O)[CH2][CH2]Br
KRFP1227	KRFPC1227	[!#1]C(=O)[CH2][CH2]C([CH3])([CH3])C(=O)[!#1]
KRFP1228	KRFPC1228	[!#1]C(=O)[CH2][CH2]C(=O)[!#1]
KRFP1229	KRFPC1229	[!#1]C(=O)[CH2][CH2]C(=O)[OH]
KRFP1230	KRFPC1230	[!#1]C(=O)[CH2][CH2]C(=O)O[CH2]C(=O)[!#1]
KRFP1231	KRFPC1231	[!#1]C(=O)[CH2][CH2]C(=O)O[CH3]
KRFP1232	KRFPC1232	[!#1]C(=O)[CH2][CH2]c1[cH][cH][cH][cH][cH]1
KRFP1233	KRFPC1233	[!#1]C(=O)[CH2][CH2]c1[cH][cH]c([CH3])o1
KRFP1234	KRFPC1234	[!#1]C(=O)[CH2][CH2]N([CH2][CH3])[CH2][CH3]
KRFP1235	KRFPC1235	[!#1]C(=O)[CH2][CH2]N([CH3])[CH3]
KRFP1236	KRFPC1236	[!#1]C(=O)[CH2][CH3]
KRFP1237	KRFPC1237	[!#1]C(=O)[CH2][NH][CH2][CH2][OH]
KRFP1238	KRFPC1238	[!#1]C(=O)[CH2][NH][CH2][CH3]
KRFP1239	KRFPC1239	[!#1]C(=O)[CH2][NH]C([CH3])([CH3])[CH3]
KRFP1240	KRFPC1240	[!#1]C(=O)[CH2][NH]C(=O)[!#1]
KRFP1241	KRFPC1241	[!#1]C(=O)[CH2][NH2]
KRFP1242	KRFPC1242	[!#1]C(=O)[CH2]C(!#1)([OH])C(F)(F)[CH](F)F
KRFP1243	KRFPC1243	[!#1]C(=O)[CH2]C(!#1)([OH])C(F)(F)F
KRFP1244	KRFPC1244	[!#1]C(=O)[CH2]C(=N[NH]c1[cH][cH][cH][cH][cH]1)[CH3]
KRFP1245	KRFPC1245	[!#1]C(=O)[CH2]C(=O)[!#1]
KRFP1246	KRFPC1246	[!#1]C(=O)[CH2]C(=O)[CH3]
KRFP1247	KRFPC1247	[!#1]C(=O)[CH2]C(=O)O[CH2][CH3]
KRFP1248	KRFPC1248	[!#1]C(=O)[CH2]C1([CH2][CH]2[CH2][CH]3[CH2][CH]([CH2]2)[CH2]1)[CH2]3
KRFP1249	KRFPC1249	[!#1]C(=O)[CH2]C1(C(=O)c2[cH][cH][cH][cH]c2C1=O)c3[cH][cH][cH][cH]c3
KRFP1250	KRFPC1250	[!#1]C(=O)[CH2]c1[cH][cH][cH][cH][cH]1

Name	Count name	Pattern
KRFP1251	KRFPC1251	[!#1]C(=O)[CH2]c1[cH][cH][cH]c2[cH][cH][cH]c12
KRFP1252	KRFPC1252	[!#1]C(=O)[CH2]Cl
KRFP1253	KRFPC1253	[!#1]C(=O)[CH2]F
KRFP1254	KRFPC1254	[!#1]C(=O)[CH2]N([CH2][CH3])[CH2][CH3]
KRFP1255	KRFPC1255	[!#1]C(=O)[CH2]N([CH3])[CH3]
KRFP1256	KRFPC1256	[!#1]C(=O)[CH2]OC(=O)[!#1]
KRFP1257	KRFPC1257	[!#1]C(=O)[CH2]OC(=O)[CH2][CH2][CH2][CH3]
KRFP1258	KRFPC1258	[!#1]C(=O)[CH2]OC(=O)[CH2][CH2]C(=O)C(=O)O[CH2]C(=O)[!#1]
KRFP1259	KRFPC1259	[!#1]C(=O)[CH2]OC(=O)[CH2][CH2]S(=O)(=O)[!#1]
KRFP1260	KRFPC1260	[!#1]C(=O)[CH2]OC(=O)C(=O)O[CH2]C(=O)[!#1]
KRFP1261	KRFPC1261	[!#1]C(=O)[CH2]SC(=S)[!#1]
KRFP1262	KRFPC1262	[!#1]C(=O)[CH2]SS(=O)(=O)[OH]
KRFP1263	KRFPC1263	[!#1]C(=O)[CH3]
KRFP1264	KRFPC1264	[!#1]C(=O)[NH][CH]([CH]([CH3])[CH3])C(=O)[OH]
KRFP1265	KRFPC1265	[!#1]C(=O)[NH][CH]([CH2][CH]([CH3])[CH3])C(=O)[OH]
KRFP1266	KRFPC1266	[!#1]C(=O)[NH][CH]([CH2][CH]([CH3])[CH3])C(=O)O[CH3]
KRFP1267	KRFPC1267	[!#1]C(=O)[NH][CH]([CH2][CH2][CH2][NH]C(=[NH])[NH2])C(=O)[NH2]
KRFP1268	KRFPC1268	[!#1]C(=O)[NH][CH]([CH2][OH])[CH]([CH3])[CH3]
KRFP1269	KRFPC1269	[!#1]C(=O)[NH][CH]([CH2]C(=O)O[CH3])C(=O)O[CH3]
KRFP1270	KRFPC1270	[!#1]C(=O)[NH][CH]([CH3])[CH2][CH2][CH2][CH2][CH3]
KRFP1271	KRFPC1271	[!#1]C(=O)[NH][CH]([CH3])[CH2][CH3]
KRFP1272	KRFPC1272	[!#1]C(=O)[NH][CH]([CH3])[CH3]
KRFP1273	KRFPC1273	[!#1]C(=O)[NH][CH]([CH3])C(=O)[OH]
KRFP1274	KRFPC1274	[!#1]C(=O)[NH][CH]([NH]C([CH3])([CH3])[CH3])C(Cl)(Cl)Cl
KRFP1275	KRFPC1275	[!#1]C(=O)[NH][CH](N([CH2][CH3])[CH2][CH3])C(Cl)(Cl)Cl
KRFP1276	KRFPC1276	[!#1]C(=O)[NH][CH2][CH]([CH3])[CH3]
KRFP1277	KRFPC1277	[!#1]C(=O)[NH][CH2][CH]=[CH2]
KRFP1278	KRFPC1278	[!#1]C(=O)[NH][CH2][CH2][CH2][CH2][CH2][CH2][NH]C(=O)[!#1]
KRFP1279	KRFPC1279	[!#1]C(=O)[NH][CH2][CH2][CH2][CH2][CH2][CH3]
KRFP1280	KRFPC1280	[!#1]C(=O)[NH][CH2][CH2][CH2][CH2][CH2]C(=O)[OH]
KRFP1281	KRFPC1281	[!#1]C(=O)[NH][CH2][CH2][CH2][CH2][CH3]
KRFP1282	KRFPC1282	[!#1]C(=O)[NH][CH2][CH2][CH2][CH2][NH]C(=O)[!#1]
KRFP1283	KRFPC1283	[!#1]C(=O)[NH][CH2][CH2][CH2][CH3]
KRFP1284	KRFPC1284	[!#1]C(=O)[NH][CH2][CH2][CH2][OH]
KRFP1285	KRFPC1285	[!#1]C(=O)[NH][CH2][CH2][CH2]C(=O)[OH]
KRFP1286	KRFPC1286	[!#1]C(=O)[NH][CH2][CH2][CH2]N([CH3])[CH3]
KRFP1287	KRFPC1287	[!#1]C(=O)[NH][CH2][CH2][CH3]
KRFP1288	KRFPC1288	[!#1]C(=O)[NH][CH2][CH2][NH]C(=O)[!#1]
KRFP1289	KRFPC1289	[!#1]C(=O)[NH][CH2][CH2][OH]
KRFP1290	KRFPC1290	[!#1]C(=O)[NH][CH2][CH2]C(=O)[OH]
KRFP1291	KRFPC1291	[!#1]C(=O)[NH][CH2][CH2]N([CH2][CH3])[CH2][CH3]
KRFP1292	KRFPC1292	[!#1]C(=O)[NH][CH2][CH2]OC(=O)[!#1]
KRFP1293	KRFPC1293	[!#1]C(=O)[NH][CH2][CH2]OC(=O)[CH3]
KRFP1294	KRFPC1294	[!#1]C(=O)[NH][CH2][CH3]
KRFP1295	KRFPC1295	[!#1]C(=O)[NH][CH2]C(=O)[OH]
KRFP1296	KRFPC1296	[!#1]C(=O)[NH][CH2]C(=O)O[CH2][CH3]
KRFP1297	KRFPC1297	[!#1]C(=O)[NH][CH2]C(=O)O[CH3]
KRFP1298	KRFPC1298	[!#1]C(=O)[NH][CH2]OC(=O)[!#1]
KRFP1299	KRFPC1299	[!#1]C(=O)[NH][CH3]
KRFP1300	KRFPC1300	[!#1]C(=O)[NH][NH]C(=O)[!#1]
KRFP1301	KRFPC1301	[!#1]C(=O)[NH][NH]C(=O)[CH]=[CH]C(=O)[OH]
KRFP1302	KRFPC1302	[!#1]C(=O)[NH][NH]C(=O)[CH2][CH2][CH2][CH2][CH2][CH3]
KRFP1303	KRFPC1303	[!#1]C(=O)[NH][NH]C(=O)[CH2][CH2]C(=O)[OH]
KRFP1304	KRFPC1304	[!#1]C(=O)[NH][NH]C(=O)[CH3]

Name	Count name	Pattern
KRFP1305	KRFPC1305	[!#1]C(=O)[NH][NH]C(=O)C(F)(F)F
KRFP1306	KRFPC1306	[!#1]C(=O)[NH][NH]C(=S)[NH]C(=O)[!#1]
KRFP1307	KRFPC1307	[!#1]C(=O)[NH][NH]C(=S)[NH2]
KRFP1308	KRFPC1308	[!#1]C(=O)[NH][NH]S(=O)(=O)[!#1]
KRFP1309	KRFPC1309	[!#1]C(=O)[NH][NH2]
KRFP1310	KRFPC1310	[!#1]C(=O)[NH][OH]
KRFP1311	KRFPC1311	[!#1]C(=O)[NH]C([!#1])([!#1])[CH3]
KRFP1312	KRFPC1312	[!#1]C(=O)[NH]C([CH2][OH])([CH2][OH])[CH2][OH]
KRFP1313	KRFPC1313	[!#1]C(=O)[NH]C([CH3])([CH3])[CH3]
KRFP1314	KRFPC1314	[!#1]C(=O)[NH]C(=S)[!#1]
KRFP1315	KRFPC1315	[!#1]C(=O)[NH]c1[cH][cH][cH][cH][cH]1
KRFP1316	KRFPC1316	[!#1]C(=O)[NH]c1[cH][cH][cH]c(Cl)[cH]1
KRFP1317	KRFPC1317	[!#1]C(=O)[NH]c1[cH][cH][cH]c2[cH][cH][cH]c12
KRFP1318	KRFPC1318	[!#1]C(=O)[NH]c1[cH][cH]c([cH][cH]1)S(=O)(=O)[!#1]
KRFP1319	KRFPC1319	[!#1]C(=O)[NH]c1[cH][cH]c(Cl)[cH][cH]1
KRFP1320	KRFPC1320	[!#1]C(=O)[NH]c1[cH][cH]c(Cl)c(Cl)[cH]1
KRFP1321	KRFPC1321	[!#1]C(=O)[NH]c1nc([CH3])[cH]c([CH3])n1
KRFP1322	KRFPC1322	[!#1]C(=O)[NH]c1nc([CH3])nc(O[CH3])n1
KRFP1323	KRFPC1323	[!#1]C(=O)[NH]N=[CH][CH]=[CH]c1[cH][cH][cH][cH][cH]1
KRFP1324	KRFPC1324	[!#1]C(=O)[NH]N=[CH][CH]=N[NH]C(=O)[!#1]
KRFP1325	KRFPC1325	[!#1]C(=O)[NH]N=[CH][CH2][CH2][CH3]
KRFP1326	KRFPC1326	[!#1]C(=O)[NH]N=[CH]c1[cH][cH][cH][cH][cH]1
KRFP1327	KRFPC1327	[!#1]C(=O)[NH]N=[CH]c1[cH][cH][cH][cH]c1[N+](=O)[O-]
KRFP1328	KRFPC1328	[!#1]C(=O)[NH]N=[CH]c1[cH][cH][cH][cH]c1[OH]
KRFP1329	KRFPC1329	[!#1]C(=O)[NH]N=[CH]c1[cH][cH][cH][cH]c1Cl
KRFP1330	KRFPC1330	[!#1]C(=O)[NH]N=[CH]c1[cH][cH][cH][cH]c1F
KRFP1331	KRFPC1331	[!#1]C(=O)[NH]N=[CH]c1[cH][cH][cH][cH]c1O[CH3]
KRFP1332	KRFPC1332	[!#1]C(=O)[NH]N=[CH]c1[cH][cH][cH][cH][nH]1
KRFP1333	KRFPC1333	[!#1]C(=O)[NH]N=[CH]c1[cH][cH][cH]c([cH]1)[N+](=O)[O-]
KRFP1334	KRFPC1334	[!#1]C(=O)[NH]N=[CH]c1[cH][cH][cH]c([CH2][CH]=[CH2])c1[OH]
KRFP1335	KRFPC1335	[!#1]C(=O)[NH]N=[CH]c1[cH][cH][cH]n[cH]1
KRFP1336	KRFPC1336	[!#1]C(=O)[NH]N=[CH]c1[cH][cH][cH]o1
KRFP1337	KRFPC1337	[!#1]C(=O)[NH]N=[CH]c1[cH][cH][cH]s1
KRFP1338	KRFPC1338	[!#1]C(=O)[NH]N=[CH]c1[cH][cH]c([!#1])[cH][cH]1
KRFP1339	KRFPC1339	[!#1]C(=O)[NH]N=[CH]c1[cH][cH]c([!#1])[cH]c1[OH]
KRFP1340	KRFPC1340	[!#1]C(=O)[NH]N=[CH]c1[cH][cH]c([cH][cH]1)[N+](=O)[O-]
KRFP1341	KRFPC1341	[!#1]C(=O)[NH]N=[CH]c1[cH][cH]c([cH][cH]1)c2[cH][cH][cH][cH]2
KRFP1342	KRFPC1342	[!#1]C(=O)[NH]N=[CH]c1[cH][cH]c([cH][cH]1)N([CH3])[CH3]
KRFP1343	KRFPC1343	[!#1]C(=O)[NH]N=[CH]c1[cH][cH]c([CH3])o1
KRFP1344	KRFPC1344	[!#1]C(=O)[NH]N=[CH]c1[cH][cH]c([OH])[cH][cH]1
KRFP1345	KRFPC1345	[!#1]C(=O)[NH]N=[CH]c1[cH][cH]c([OH])c(O[CH3])[cH]1
KRFP1346	KRFPC1346	[!#1]C(=O)[NH]N=[CH]c1[cH][cH]c(Br)[cH][cH]1
KRFP1347	KRFPC1347	[!#1]C(=O)[NH]N=[CH]c1[cH][cH]c(Cl)[cH][cH]1
KRFP1348	KRFPC1348	[!#1]C(=O)[NH]N=[CH]c1[cH][cH]c(Cl)[cH]c1Cl
KRFP1349	KRFPC1349	[!#1]C(=O)[NH]N=[CH]c1[cH][cH]c(F)[cH][cH]1
KRFP1350	KRFPC1350	[!#1]C(=O)[NH]N=[CH]c1[cH][cH]c(O[CH3])[cH][cH]1
KRFP1351	KRFPC1351	[!#1]C(=O)[NH]N=[CH]c1[cH][cH]c(O[CH3])[cH]c1O[CH3]
KRFP1352	KRFPC1352	[!#1]C(=O)[NH]N=[CH]c1[cH][cH]c(O[CH3])c(O[CH3])[cH]1
KRFP1353	KRFPC1353	[!#1]C(=O)[NH]N=[CH]c1[cH][cH]c(o1)[N+](=O)[O-]
KRFP1354	KRFPC1354	[!#1]C(=O)[NH]N=[CH]c1[cH][cH]c(s1)[N+](=O)[O-]
KRFP1355	KRFPC1355	[!#1]C(=O)[NH]N=[CH]c1[cH][cH]c2n([CH2][CH3])c3[cH][cH][cH][cH]c3c2[cH]1
KRFP1356	KRFPC1356	[!#1]C(=O)[NH]N=[CH]c1[cH][cH]c2O[CH2]O2[cH]1
KRFP1357	KRFPC1357	[!#1]C(=O)[NH]N=[CH]c1[cH][cH]n[cH][cH]1

Name	Count name	Pattern
KRFP1358	KRFPC1358	[!#1]C(=O)[NH]N=[CH]c1[cH][nH]c2[cH][cH][cH][cH]c12
KRFP1359	KRFPC1359	[!#1]C(=O)[NH]N=[CH]c1[cH]c([cH][cH]c1[OH])[N+](=O)[O-]
KRFP1360	KRFPC1360	[!#1]C(=O)[NH]N=[CH]c1[cH]c([CH3])[cH][cH]c1[OH]
KRFP1361	KRFPC1361	[!#1]C(=O)[NH]N=[CH]c1[cH]c(Cl)[cH][cH]c1[OH]
KRFP1362	KRFPC1362	[!#1]C(=O)[NH]N=[CH]c1[cH]c(Cl)[cH]c(Cl)c1O[CH3]
KRFP1363	KRFPC1363	[!#1]C(=O)[NH]N=[CH]c1[cH]c2O[CH2]Oc2[cH]c1[N+](=O)[O-]
KRFP1364	KRFPC1364	[!#1]C(=O)[NH]N=[CH]c1[cH]c2O[CH2]Oc2[cH]c1Br
KRFP1365	KRFPC1365	[!#1]C(=O)[NH]N=[CH]c1c([OH])[cH][cH]c2[cH][cH][cH][cH]c12
KRFP1366	KRFPC1366	[!#1]C(=O)[NH]N=[CH]c1nc2[cH][cH][cH][cH]c2[nH]1
KRFP1367	KRFPC1367	[!#1]C(=O)[NH]N=C(!#1)[CH2][CH2][CH2][CH2][CH3]
KRFP1368	KRFPC1368	[!#1]C(=O)[NH]N=C(!#1)[CH2][CH2][CH2][CH3]
KRFP1369	KRFPC1369	[!#1]C(=O)[NH]N=C(!#1)[CH2][CH2][CH3]
KRFP1370	KRFPC1370	[!#1]C(=O)[NH]N=C(!#1)[CH2][CH3]
KRFP1371	KRFPC1371	[!#1]C(=O)[NH]N=C([CH3])[CH]=[CH]c1[cH][cH][cH][cH][cH]1
KRFP1372	KRFPC1372	[!#1]C(=O)[NH]N=C([CH3])[CH]1[CH2][CH2]1
KRFP1373	KRFPC1373	[!#1]C(=O)[NH]N=C([CH3])[CH2][CH]([CH3])[CH3]
KRFP1374	KRFPC1374	[!#1]C(=O)[NH]N=C([CH3])[CH2][CH2][CH]=[CH2]
KRFP1375	KRFPC1375	[!#1]C(=O)[NH]N=C([CH3])[CH2][CH2][CH2][CH3]
KRFP1376	KRFPC1376	[!#1]C(=O)[NH]N=C([CH3])[CH2][NH]C(=O)[CH3]
KRFP1377	KRFPC1377	[!#1]C(=O)[NH]N=C([CH3])[CH2]C(=O)[CH3]
KRFP1378	KRFPC1378	[!#1]C(=O)[NH]N=C([CH3])[CH3]
KRFP1379	KRFPC1379	[!#1]C(=O)[NH]N=C([CH3])C(=N[OH])[CH3]
KRFP1380	KRFPC1380	[!#1]C(=O)[NH]N=C([CH3])c1[cH][cH][cH][cH][cH]1
KRFP1381	KRFPC1381	[!#1]C(=O)[NH]N=C([CH3])c1[cH][cH][cH][cH]c1[OH]
KRFP1382	KRFPC1382	[!#1]C(=O)[NH]N=C([CH3])c1[cH][cH][cH]c([cH]1)[N+](=O)[O-]
KRFP1383	KRFPC1383	[!#1]C(=O)[NH]N=C([CH3])c1[cH][cH][cH]c([NH2])[cH]1
KRFP1384	KRFPC1384	[!#1]C(=O)[NH]N=C([CH3])c1[cH][cH][cH]o1
KRFP1385	KRFPC1385	[!#1]C(=O)[NH]N=C([CH3])c1[cH][cH]c(!#1)[cH][cH]1
KRFP1386	KRFPC1386	[!#1]C(=O)[NH]N=C([CH3])c1[cH][cH]c([cH][cH]1)[N+](=O)[O-]
KRFP1387	KRFPC1387	[!#1]C(=O)[NH]N=C([CH3])c1[cH][cH]c([cH][cH]1)c2[cH][cH][cH][cH]c2
KRFP1388	KRFPC1388	[!#1]C(=O)[NH]N=C([CH3])c1[cH][cH]c([NH2])[cH][cH]1
KRFP1389	KRFPC1389	[!#1]C(=O)[NH]N=C([CH3])c1[cH][cH]c([OH])[cH][cH]1
KRFP1390	KRFPC1390	[!#1]C(=O)[NH]N=C([CH3])c1[cH][cH]c(Br)[cH][cH]1
KRFP1391	KRFPC1391	[!#1]C(=O)[NH]N=C([CH3])c1[cH][cH]c(Cl)[cH][cH]1
KRFP1392	KRFPC1392	[!#1]C(=O)[NH]N=C([CH3])c1[cH][cH]c(Cl)s1
KRFP1393	KRFPC1393	[!#1]C(=O)[NH]N=C([CH3])c1[cH][cH]c(F)[cH][cH]1
KRFP1394	KRFPC1394	[!#1]C(=O)[NH]N=C([CH3])c1[cH][cH]c(O[CH3])[cH][cH]1
KRFP1395	KRFPC1395	[!#1]C(=O)[NH]N=C([CH3])c1[cH][cH]c(O[CH3])[cH]c1O[CH3]
KRFP1396	KRFPC1396	[!#1]C(=O)[NH]N=C([CH3])c1[cH]c([OH])[cH][cH]c1[OH]
KRFP1397	KRFPC1397	[!#1]C(=O)[NH]N=C1[CH2][CH2][CH2][CH2][CH2]1
KRFP1398	KRFPC1398	[!#1]C(=O)[NH]N=C1[CH2][CH2][CH2][CH2]1
KRFP1399	KRFPC1399	[!#1]C(=O)[NH]N=C1[CH2]C(=O)[CH2]C([CH3])([CH3])[CH2]1
KRFP1400	KRFPC1400	[!#1]C(=O)[NH]N=C1C(=O)[NH]c2[cH][cH][cH][cH]c12
KRFP1401	KRFPC1401	[!#1]C(=O)[NH]N=C1C(=O)[NH]c2[cH][cH]c(!#1)[cH]c12
KRFP1402	KRFPC1402	[!#1]C(=O)[NH]N=c1c(=O)c2[cH][cH][cH][cH]c2c1=O
KRFP1403	KRFPC1403	[!#1]C(=O)[NH]N=C1c2nn(!#1)nc2C(=N[NH]C(=O)[!#1])c3nn(!#1)nc13
KRFP1404	KRFPC1404	[!#1]C(=O)[NH]S(=O)(=O)[!#1]
KRFP1405	KRFPC1405	[!#1]C(=O)[NH2]
KRFP1406	KRFPC1406	[!#1]C(=O)[OH]
KRFP1407	KRFPC1407	[!#1]C(=O)C(!#1)(!#1)[CH3]
KRFP1408	KRFPC1408	[!#1]C(=O)C(!#1)(!#1)[OH]
KRFP1409	KRFPC1409	[!#1]C(=O)C(!#1)(!#1)C#N
KRFP1410	KRFPC1410	[!#1]C(=O)C(!#1)(!#1)C(=O)[!#1]
KRFP1411	KRFPC1411	[!#1]C(=O)C([CH2][CH3])([CH2][CH3])C(=O)[!#1]

Name	Count name	Pattern
KRFP1412	KRFPC1412	[!#1]C(=O)C([CH3])([CH3])[CH3]
KRFP1413	KRFPC1413	[!#1]C(=O)C([OH])(c1[cH][cH][cH][cH][cH]1)c2[cH][cH][cH][cH][cH]2
KRFP1414	KRFPC1414	[!#1]C(=O)C([OH])(c1[cH][cH]c(Br)[cH][cH]1)c2[cH][cH]c(Br)[cH][cH]2
KRFP1415	KRFPC1415	[!#1]C(=O)C(=N[NH]c1[cH][cH]c([cH][cH]1)[N+](=O)[O-])C(=O)[!#1]
KRFP1416	KRFPC1416	[!#1]C(=O)C(=N[NH]c1[cH][cH]c([cH][cH]1)S(=O)(=O)[OH])C(=O)[!#1]
KRFP1417	KRFPC1417	[!#1]C(=O)C(=N[OH])C(=O)O[CH2][CH3]
KRFP1418	KRFPC1418	[!#1]C(=O)C(=O)[!#1]
KRFP1419	KRFPC1419	[!#1]C(=O)C(Cl)(Cl)Cl
KRFP1420	KRFPC1420	[!#1]C(=O)C(F)(F)C(F)(F)F
KRFP1421	KRFPC1421	[!#1]C(=O)C(F)(F)F
KRFP1422	KRFPC1422	[!#1]C(=O)C(F)(F)OC(F)(F)C(F)(F)OC(F)(F)F
KRFP1423	KRFPC1423	[!#1]C(=O)C(F)(OC(F)(F)C(F)(F)C(F)(F)F)C(F)(F)F
KRFP1424	KRFPC1424	[!#1]C(=O)C1([CH2][CH]2[CH2][CH]3[CH2][CH]([CH2]2)[CH2]1)[CH2]3
KRFP1425	KRFPC1425	[!#1]C(=O)C1([CH2][CH]2[CH2][CH]3[CH2]1)[CH2][CH]([CH2]2)[CH2][CH2]3
KRFP1426	KRFPC1426	[!#1]C(=O)c1[cH][cH][cH][cH][cH]1
KRFP1427	KRFPC1427	[!#1]C(=O)c1[cH][cH][cH][cH]c1[!#1]
KRFP1428	KRFPC1428	[!#1]C(=O)c1[cH][cH][cH][cH]c1[CH3]
KRFP1429	KRFPC1429	[!#1]C(=O)c1[cH][cH][cH][cH]c1[N+](=O)[O-]
KRFP1430	KRFPC1430	[!#1]C(=O)c1[cH][cH][cH][cH]c1[OH]
KRFP1431	KRFPC1431	[!#1]C(=O)c1[cH][cH][cH][cH]c1Br
KRFP1432	KRFPC1432	[!#1]C(=O)c1[cH][cH][cH][cH]c1C(=O)[!#1]
KRFP1433	KRFPC1433	[!#1]C(=O)c1[cH][cH][cH][cH]c1C(=O)[OH]
KRFP1434	KRFPC1434	[!#1]C(=O)c1[cH][cH][cH][cH]c1Cl
KRFP1435	KRFPC1435	[!#1]C(=O)c1[cH][cH][cH][cH]c1F
KRFP1436	KRFPC1436	[!#1]C(=O)c1[cH][cH][cH][cH]c1I
KRFP1437	KRFPC1437	[!#1]C(=O)c1[cH][cH][cH][cH]n1
KRFP1438	KRFPC1438	[!#1]C(=O)c1[cH][cH][cH]c([!#1])[cH]1
KRFP1439	KRFPC1439	[!#1]C(=O)c1[cH][cH][cH]c([cH]1)[N+](=O)[O-]
KRFP1440	KRFPC1440	[!#1]C(=O)c1[cH][cH][cH]c([cH]1)C(=O)[!#1]
KRFP1441	KRFPC1441	[!#1]C(=O)c1[cH][cH][cH]c([cH]1)S(=O)(=O)[!#1]
KRFP1442	KRFPC1442	[!#1]C(=O)c1[cH][cH][cH]c([CH3])[cH]1
KRFP1443	KRFPC1443	[!#1]C(=O)c1[cH][cH][cH]c(Br)[cH]1
KRFP1444	KRFPC1444	[!#1]C(=O)c1[cH][cH][cH]c(Cl)[cH]1
KRFP1445	KRFPC1445	[!#1]C(=O)c1[cH][cH][cH]c(F)[cH]1
KRFP1446	KRFPC1446	[!#1]C(=O)c1[cH][cH][cH]c(I)[cH]1
KRFP1447	KRFPC1447	[!#1]C(=O)c1[cH][cH][cH]c2[cH][cH][cH][cH]c12
KRFP1448	KRFPC1448	[!#1]C(=O)c1[cH][cH][cH]n[cH]1
KRFP1449	KRFPC1449	[!#1]C(=O)c1[cH][cH][cH]o1
KRFP1450	KRFPC1450	[!#1]C(=O)c1[cH][cH][cH]s1
KRFP1451	KRFPC1451	[!#1]C(=O)c1[cH][cH][n+](([O-])[cH][cH]1
KRFP1452	KRFPC1452	[!#1]C(=O)c1[cH][cH]c([!#1])[cH][cH]1
KRFP1453	KRFPC1453	[!#1]C(=O)c1[cH][cH]c([!#1])c([cH]1)[N+](=O)[O-]
KRFP1454	KRFPC1454	[!#1]C(=O)c1[cH][cH]c([cH][cH]1)[N+](=O)[O-]
KRFP1455	KRFPC1455	[!#1]C(=O)c1[cH][cH]c([cH][cH]1)C([CH3])([CH3])[CH3]
KRFP1456	KRFPC1456	[!#1]C(=O)c1[cH][cH]c([cH][cH]1)C(=O)[!#1]
KRFP1457	KRFPC1457	[!#1]C(=O)c1[cH][cH]c([cH][cH]1)c2[cH][cH][cH][cH]2
KRFP1458	KRFPC1458	[!#1]C(=O)c1[cH][cH]c([cH][cH]1)S(=O)(=O)[!#1]
KRFP1459	KRFPC1459	[!#1]C(=O)c1[cH][cH]c([cH]c1[N+](=O)[O-])[N+](=O)[O-]
KRFP1460	KRFPC1460	[!#1]C(=O)c1[cH][cH]c([cH]c1C(=O)[OH])[N+](=O)[O-]
KRFP1461	KRFPC1461	[!#1]C(=O)c1[cH][cH]c([CH3])[cH][cH]1
KRFP1462	KRFPC1462	[!#1]C(=O)c1[cH][cH]c([CH3])c([cH]1)S(=O)(=O)[!#1]
KRFP1463	KRFPC1463	[!#1]C(=O)c1[cH][cH]c([OH])[cH][cH]1
KRFP1464	KRFPC1464	[!#1]C(=O)c1[cH][cH]c(Br)[cH][cH]1
KRFP1465	KRFPC1465	[!#1]C(=O)c1[cH][cH]c(Br)c([cH]1)[N+](=O)[O-]

Name	Count name	Pattern
KRFP1466	KRFPC1466	[!#1]C(=O)c1[cH][cH]c(Br)o1
KRFP1467	KRFPC1467	[!#1]C(=O)c1[cH][cH]c(Cl)[cH][cH]1
KRFP1468	KRFPC1468	[!#1]C(=O)c1[cH][cH]c(Cl)[cH]c1Cl
KRFP1469	KRFPC1469	[!#1]C(=O)c1[cH][cH]c(Cl)c([cH]1)[N+](=O)[O-]
KRFP1470	KRFPC1470	[!#1]C(=O)c1[cH][cH]c(Cl)c(Cl)[cH]1
KRFP1471	KRFPC1471	[!#1]C(=O)c1[cH][cH]c(F)[cH][cH]1
KRFP1472	KRFPC1472	[!#1]C(=O)c1[cH][cH]c(F)c(F)[cH]1
KRFP1473	KRFPC1473	[!#1]C(=O)c1[cH][cH]c(o1)[N+](=O)[O-]
KRFP1474	KRFPC1474	[!#1]C(=O)c1[cH][cH]c2[cH][cH][cH][cH]c2[cH]1
KRFP1475	KRFPC1475	[!#1]C(=O)c1[cH][cH]c2n(!#1)c([CH3])c([CH3])c2[cH]1
KRFP1476	KRFPC1476	[!#1]C(=O)c1[cH][cH]n[cH][cH]1
KRFP1477	KRFPC1477	[!#1]C(=O)c1[cH]c([cH][cH]c1Cl)[N+](=O)[O-]
KRFP1478	KRFPC1478	[!#1]C(=O)c1[cH]c([cH]c([cH]1)[N+](=O)[O-])[N+](=O)[O-]
KRFP1479	KRFPC1479	[!#1]C(=O)c1[cH]c([cH]c([cH]1)C([CH3])([CH3])[CH3])C([CH3])([CH3])[CH3]
KRFP1480	KRFPC1480	[!#1]C(=O)c1[cH]c([N+](=O)[O-])c([CH3])c([cH]1)[N+](=O)[O-]
KRFP1481	KRFPC1481	[!#1]C(=O)c1[cH]c(Cl)[cH][cH]c1[OH]
KRFP1482	KRFPC1482	[!#1]C(=O)c1[cH]c(Cl)[cH]c(Cl)[cH]1
KRFP1483	KRFPC1483	[!#1]C(=O)c1[cH]c2[cH][cH][cH][cH]c2oc1=O
KRFP1484	KRFPC1484	[!#1]C(=O)c1[cH]n(!#1)nc1(!#1)
KRFP1485	KRFPC1485	[!#1]C(=O)c1c(!#1)[cH]nn1(!#1)
KRFP1486	KRFPC1486	[!#1]C(=O)c1c(!#1)n(!#1)c2nc3[cH][cH][cH][cH]c3nc12
KRFP1487	KRFPC1487	[!#1]C(=O)c1c([cH][cH][cH]c1[N+](=O)[O-])C(=O)[OH]
KRFP1488	KRFPC1488	[!#1]C(=O)c1c([cH]nn1(!#1))[N+](=O)[O-]
KRFP1489	KRFPC1489	[!#1]C(=O)c1c([OH])c2[cH][cH][cH][cH]c2oc1=O
KRFP1490	KRFPC1490	[!#1]C(=O)c1c(F)[cH][cH][cH]c1F
KRFP1491	KRFPC1491	[!#1]C(=O)c1c(n[cH]n1(!#1))[N+](=O)[O-]
KRFP1492	KRFPC1492	[!#1]C(=O)c1n[cH][cH]nc1C(=O)[OH]
KRFP1493	KRFPC1493	[!#1]C(=O)c1nn(!#1)[cH]c1Br
KRFP1494	KRFPC1494	[!#1]C(=O)c1sc(!#1)nc1(!#1)
KRFP1495	KRFPC1495	[!#1]C(=O)c1sc2[cH][cH][cH][cH]c2c1Cl
KRFP1496	KRFPC1496	[!#1]C(=O)N([CH])([CH3])[CH3][CH]([CH3])[CH3]
KRFP1497	KRFPC1497	[!#1]C(=O)N([CH2][CH2][CH2][CH2][CH3])[CH2][CH2][CH2][CH2][CH3]
KRFP1498	KRFPC1498	[!#1]C(=O)N([CH2][CH2]C(=O)[OH])[CH2]C(=O)[OH]
KRFP1499	KRFPC1499	[!#1]C(=O)N([CH2][CH3])[CH2][CH3]
KRFP1500	KRFPC1500	[!#1]C(=O)N([CH3])[CH3]
KRFP1501	KRFPC1501	[!#1]C(=O)n1[cH]nc2[cH][cH][cH][cH]c12
KRFP1502	KRFPC1502	[!#1]C(=O)N1[CH2][CH2][CH2][CH2][CH2][CH2]1
KRFP1503	KRFPC1503	[!#1]C(=O)N1[CH2][CH2][CH2][CH2][CH2]1
KRFP1504	KRFPC1504	[!#1]C(=O)N1[CH2][CH2][CH2][CH2]1
KRFP1505	KRFPC1505	[!#1]C(=O)N1[CH2][CH2]c2[cH][cH][cH][cH]c12
KRFP1506	KRFPC1506	[!#1]C(=O)N1[CH2][CH2]O[CH2][CH2]1
KRFP1507	KRFPC1507	[!#1]C(=O)n1nnc2[cH][cH][cH][cH]c12
KRFP1508	KRFPC1508	[!#1]C(=O)O[CH]([CH3])[CH3]
KRFP1509	KRFPC1509	[!#1]C(=O)O[CH]([CH3])C(=C(Cl)Cl)Cl
KRFP1510	KRFPC1510	[!#1]C(=O)O[CH2][CH]([CH3])[CH3]
KRFP1511	KRFPC1511	[!#1]C(=O)O[CH2][CH2][CH2][CH2][CH2][CH3]
KRFP1512	KRFPC1512	[!#1]C(=O)O[CH2][CH2][CH2][CH2][CH3]
KRFP1513	KRFPC1513	[!#1]C(=O)O[CH2][CH2][CH2][CH3]
KRFP1514	KRFPC1514	[!#1]C(=O)O[CH2][CH2][CH2]N([CH3])[CH3]
KRFP1515	KRFPC1515	[!#1]C(=O)O[CH2][CH2][CH3]
KRFP1516	KRFPC1516	[!#1]C(=O)O[CH2][CH2][NH2]
KRFP1517	KRFPC1517	[!#1]C(=O)O[CH2][CH2][OH]
KRFP1518	KRFPC1518	[!#1]C(=O)O[CH2][CH2]N([CH2][CH3])[CH2][CH3]
KRFP1519	KRFPC1519	[!#1]C(=O)O[CH2][CH2]N([CH3])[CH3]

Name	Count name	Pattern
KRFP1520	KRFPC1520	[!#1]C(=O)O[CH2][CH3]
KRFP1521	KRFPC1521	[!#1]C(=O)O[CH2]C#[CH]
KRFP1522	KRFPC1522	[!#1]C(=O)O[CH2]C(=C(Cl)Cl)Cl
KRFP1523	KRFPC1523	[!#1]C(=O)O[CH2]C(F)(F)C(F)(F)F
KRFP1524	KRFPC1524	[!#1]C(=O)O[CH3]
KRFP1525	KRFPC1525	[!#1]C(=O)OC([CH3])([CH3])[CH3]
KRFP1526	KRFPC1526	[!#1]C(=O)ON=[CH]c1[cH][cH]c(Br)[cH][cH]1
KRFP1527	KRFPC1527	[!#1]C(=O)ON=C([CH3])C([CH3])([CH3])[CH3]
KRFP1528	KRFPC1528	[!#1]C(=O)ON=C([CH3])c1[cH][cH][cH][cH][cH]1
KRFP1529	KRFPC1529	[!#1]C(=S)[NH][CH2]C(=[CH2])[CH3]
KRFP1530	KRFPC1530	[!#1]C(=S)[NH2]
KRFP1531	KRFPC1531	[!#1]C(=S)S[CH2][CH2]C(=O)[OH]
KRFP1532	KRFPC1532	[!#1]C(Cl)(Cl)Cl
KRFP1533	KRFPC1533	[!#1]C(F)(F)[CH](F)F
KRFP1534	KRFPC1534	[!#1]C(F)(F)C(F)(F)[CH](F)F
KRFP1535	KRFPC1535	[!#1]C(F)(F)C(F)(F)F
KRFP1536	KRFPC1536	[!#1]C(F)(F)F
KRFP1537	KRFPC1537	[!#1]C1([!#1])[CH]2[CH2][CH2]C([CH3])(C1=O)C2([CH3])[CH3]
KRFP1538	KRFPC1538	[!#1]C1([!#1])[CH2][CH2][CH2][CH2][CH2]1
KRFP1539	KRFPC1539	[!#1]C1([!#1])[CH2][CH2][CH2][CH2]1
KRFP1540	KRFPC1540	[!#1]C1([!#1])C(=NN(C1=O)c2[cH][cH]c([cH][cH]2)[N+](=O)[O-])[CH3]
KRFP1541	KRFPC1541	[!#1]C1([!#1])C(=O)[CH2]C([CH3])([CH3])[CH2]C1=O
KRFP1542	KRFPC1542	[!#1]C1([!#1])C(=O)c2[cH][cH][cH][cH]c2C1=O
KRFP1543	KRFPC1543	[!#1]C1([!#1])C(=O)N(N=C1c2[cH][cH][cH][cH][cH]2)c3[cH][cH]c([cH][cH]3)[N+](=O)[O-]
KRFP1544	KRFPC1544	[!#1]C1([!#1])C(=O)OC([CH3])([CH3])OC1=O
KRFP1545	KRFPC1545	[!#1]C1([!#1])S(c2[cH][cH][cH][cH]c2C1=O)
KRFP1546	KRFPC1546	[!#1]C1([CH2][CH]2[CH2][CH]3[CH2][CH]([CH2]2)[CH2]1)[CH2]3
KRFP1547	KRFPC1547	[!#1]C1([CH2][CH]2[CH2][CH]3[CH2][CH]2[CH2]1)[CH2]3
KRFP1548	KRFPC1548	[!#1]C1([CH2][CH]2[CH2][CH]3[CH2]1)[CH2][CH]([CH2]2)[CH2][CH2]3
KRFP1549	KRFPC1549	[!#1]C1([CH2][CH]2[CH2][CH]3[CH2]1)[CH2]C([!#1])([CH2]2)[CH2]3
KRFP1550	KRFPC1550	[!#1]C1([CH2][CH]2[CH2][CH]3[CH2]1)[CH2]C([OH])([CH2]2)[CH2]3
KRFP1551	KRFPC1551	[!#1]C1([CH2][CH3])C(=[NH])[NH]C(=O)[NH]C1=O
KRFP1552	KRFPC1552	[!#1]C1([CH2]N2[CH2]N3[CH2]1)C(=O)C([!#1])([CH2]2)[CH2]3
KRFP1553	KRFPC1553	[!#1]C1([CH3])O[CH2][CH2]O1
KRFP1554	KRFPC1554	[!#1]C1([OH])[CH2][CH2][CH2][CH2][CH2]1
KRFP1555	KRFPC1555	[!#1]C1([OH])[CH2][CH2][CH2][CH2]1
KRFP1556	KRFPC1556	[!#1]C1([OH])C(=O)[NH]c2[cH][cH][cH][cH]c21
KRFP1557	KRFPC1557	[!#1]C1([OH])N(C(=O)[NH]c2[cH][cH][cH][cH]c21)c3[cH][cH][cH][cH][cH]3
KRFP1558	KRFPC1558	[!#1]C1(C(=O)c2[cH][cH][cH][cH]c2C1=O)c3[cH][cH][cH][cH][cH]3
KRFP1559	KRFPC1559	[!#1]C1(C(=O)N(c2[cH][cH][cH][cH]c21)c3[cH][cH][cH][cH][cH]3)C(F)(F)F
KRFP1560	KRFPC1560	[!#1]C1(F)OC([!#1])(F)C([!#1])(F)C1([!#1])F
KRFP1561	KRFPC1561	[!#1]C1(F)OC(F)(F)C(F)(F)C1(F)F
KRFP1562	KRFPC1562	[!#1]C1(O[CH]2[CH]=[CH]1)[CH]3[CH]2C(=O)N(C3=O)c4[cH][cH][cH][cH]4
KRFP1563	KRFPC1563	[!#1]C1(Oc2[cH][cH][cH][cH]c2O1)C(Cl)(Cl)Cl
KRFP1564	KRFPC1564	[!#1]c1[cH][cH][cH][cH][cH]1
KRFP1565	KRFPC1565	[!#1]c1[cH][cH][cH][cH][n+][!#1]
KRFP1566	KRFPC1566	[!#1]c1[cH][cH][cH][cH]c1[!#1]
KRFP1567	KRFPC1567	[!#1]c1[cH][cH][cH][cH]c1[CH2][CH3]
KRFP1568	KRFPC1568	[!#1]c1[cH][cH][cH][cH]c1[CH3]
KRFP1569	KRFPC1569	[!#1]c1[cH][cH][cH][cH]c1[N+](=O)[O-]
KRFP1570	KRFPC1570	[!#1]c1[cH][cH][cH][cH]c1[NH2]
KRFP1571	KRFPC1571	[!#1]c1[cH][cH][cH][cH]c1[OH]

Name	Count name	Pattern
KRFP1572	KRFPC1572	[!#1]c1[cH][cH][cH][cH]c1Br
KRFP1573	KRFPC1573	[!#1]c1[cH][cH][cH][cH]c1C#N
KRFP1574	KRFPC1574	[!#1]c1[cH][cH][cH][cH]c1C(=O)[CH3]
KRFP1575	KRFPC1575	[!#1]c1[cH][cH][cH][cH]c1C(=O)[OH]
KRFP1576	KRFPC1576	[!#1]c1[cH][cH][cH][cH]c1C(=O)c2[cH]c(!#1)nnc2[!#1]
KRFP1577	KRFPC1577	[!#1]c1[cH][cH][cH][cH]c1C(F)(F)F
KRFP1578	KRFPC1578	[!#1]c1[cH][cH][cH][cH]c1c2[cH][cH][cH][cH]2
KRFP1579	KRFPC1579	[!#1]c1[cH][cH][cH][cH]c1c2[cH][cH][cH][cH]c2[!#1]
KRFP1580	KRFPC1580	[!#1]c1[cH][cH][cH][cH]c1c2n[nH]c(=S)[nH]c2=O
KRFP1581	KRFPC1581	[!#1]c1[cH][cH][cH][cH]c1c2nc3[cH][cH][cH][cH]c3c(=O)[nH]2
KRFP1582	KRFPC1582	[!#1]c1[cH][cH][cH][cH]c1c2nc3[cH][cH][cH][cH]c3s2
KRFP1583	KRFPC1583	[!#1]c1[cH][cH][cH][cH]c1Cl
KRFP1584	KRFPC1584	[!#1]c1[cH][cH][cH][cH]c1F
KRFP1585	KRFPC1585	[!#1]c1[cH][cH][cH][cH]c1I
KRFP1586	KRFPC1586	[!#1]c1[cH][cH][cH][cH]c1N2C(=O)[CH]=[CH]C2=O
KRFP1587	KRFPC1587	[!#1]c1[cH][cH][cH][cH]c1N2C(=O)[CH]3[CH]([CH]([CH]=[CH][CH]3c4[cH] [cH][cH][cH][cH]4)c5[cH][cH][cH][cH]5)C2=O
KRFP1588	KRFPC1588	[!#1]c1[cH][cH][cH][cH]c1O[CH3]
KRFP1589	KRFPC1589	[!#1]c1[cH][cH][cH][cH]n1
KRFP1590	KRFPC1590	[!#1]c1[cH][cH][cH][nH]1
KRFP1591	KRFPC1591	[!#1]c1[cH][cH][cH]c(!#1)[cH]1
KRFP1592	KRFPC1592	[!#1]c1[cH][cH][cH]c(!#1)c1[!#1]
KRFP1593	KRFPC1593	[!#1]c1[cH][cH][cH]c(!#1)c1n2nnnc2C3(!#1)[CH2][CH2][CH2][CH2] [CH2]3
KRFP1594	KRFPC1594	[!#1]c1[cH][cH][cH]c(!#1)n1
KRFP1595	KRFPC1595	[!#1]c1[cH][cH][cH]c([CH]=[CH]C(=O)[OH])[cH]1
KRFP1596	KRFPC1596	[!#1]c1[cH][cH][cH]c([cH]1)[CH]2[CH2]C(=N[CH2][CH2]S2)c3c(!#1)[cH] c(!#1)oc3=O
KRFP1597	KRFPC1597	[!#1]c1[cH][cH][cH]c([cH]1)[N+](=O)[O-]
KRFP1598	KRFPC1598	[!#1]c1[cH][cH][cH]c([cH]1)C(=O)[CH3]
KRFP1599	KRFPC1599	[!#1]c1[cH][cH][cH]c([cH]1)C(=O)[OH]
KRFP1600	KRFPC1600	[!#1]c1[cH][cH][cH]c([cH]1)C(F)(F)F
KRFP1601	KRFPC1601	[!#1]c1[cH][cH][cH]c([cH]1)c2[cH]nc3[cH][cH][cH][cH]c3n2
KRFP1602	KRFPC1602	[!#1]c1[cH][cH][cH]c([cH]1)c2nc3[cH][cH][cH][cH]c3o2
KRFP1603	KRFPC1603	[!#1]c1[cH][cH][cH]c([cH]1)c2nc3[cH]c(!#1)[cH][cH]c3o2
KRFP1604	KRFPC1604	[!#1]c1[cH][cH][cH]c([cH]1)N2[CH2][CH2][CH2]C2=O
KRFP1605	KRFPC1605	[!#1]c1[cH][cH][cH]c([cH]1)N2C(=O)c3[cH][cH][cH][cH]c3C2=O
KRFP1606	KRFPC1606	[!#1]c1[cH][cH][cH]c([cH]1)S(=O)(=O)[!#1]
KRFP1607	KRFPC1607	[!#1]c1[cH][cH][cH]c([CH2][CH3])[cH]1
KRFP1608	KRFPC1608	[!#1]c1[cH][cH][cH]c([CH2][OH])[cH]1
KRFP1609	KRFPC1609	[!#1]c1[cH][cH][cH]c([CH3])[cH]1
KRFP1610	KRFPC1610	[!#1]c1[cH][cH][cH]c([CH3])c1[CH3]
KRFP1611	KRFPC1611	[!#1]c1[cH][cH][cH]c([CH3])n1
KRFP1612	KRFPC1612	[!#1]c1[cH][cH][cH]c([N+](=O)[O-])c1[!#1]
KRFP1613	KRFPC1613	[!#1]c1[cH][cH][cH]c([NH2])[cH]1
KRFP1614	KRFPC1614	[!#1]c1[cH][cH][cH]c([OH])[cH]1
KRFP1615	KRFPC1615	[!#1]c1[cH][cH][cH]c(Br)[cH]1
KRFP1616	KRFPC1616	[!#1]c1[cH][cH][cH]c(Cl)[cH]1
KRFP1617	KRFPC1617	[!#1]c1[cH][cH][cH]c(Cl)c1[CH3]
KRFP1618	KRFPC1618	[!#1]c1[cH][cH][cH]c(Cl)c1Cl
KRFP1619	KRFPC1619	[!#1]c1[cH][cH][cH]c(F)[cH]1
KRFP1620	KRFPC1620	[!#1]c1[cH][cH][cH]c(I)[cH]1
KRFP1621	KRFPC1621	[!#1]c1[cH][cH][cH]c(O[CH3])[cH]1
KRFP1622	KRFPC1622	[!#1]c1[cH][cH][cH]c2[cH][cH][cH][cH]c12
KRFP1623	KRFPC1623	[!#1]c1[cH][cH][cH]c2[cH][cH][cH]c(!#1)c12

Name	Count name	Pattern
KRFP1624	KRFPC1624	[!#1]c1[cH][cH][cH]c2[cH][cH][cH]nc12
KRFP1625	KRFPC1625	[!#1]c1[cH][cH][cH]c2[CH2][CH2][CH2][CH2]c12
KRFP1626	KRFPC1626	[!#1]c1[cH][cH][cH]c2c(!#1)[cH][cH][cH]c12
KRFP1627	KRFPC1627	[!#1]c1[cH][cH][cH]c2c(=O)[nH][nH]c(=O)c12
KRFP1628	KRFPC1628	[!#1]c1[cH][cH][cH]c2C(=O)c3[cH][cH][cH][cH]c3C(=O)c12
KRFP1629	KRFPC1629	[!#1]c1[cH][cH][cH]c2C(=O)c3[cH][cH][cH]c(!#1)c3C(=O)c12
KRFP1630	KRFPC1630	[!#1]c1[cH][cH][cH]c2c3[CH2][CH2][CH2][CH2]c3oc12
KRFP1631	KRFPC1631	[!#1]c1[cH][cH][cH]c2n[cH][cH][cH]c12
KRFP1632	KRFPC1632	[!#1]c1[cH][cH][cH]c2nsnc12
KRFP1633	KRFPC1633	[!#1]c1[cH][cH][cH]n[cH]1
KRFP1634	KRFPC1634	[!#1]c1[cH][cH][cH]nc1[!#1]
KRFP1635	KRFPC1635	[!#1]c1[cH][cH][cH]nc1c2[cH]c(!#1)c(!#1)c(!#1)[cH]2
KRFP1636	KRFPC1636	[!#1]c1[cH][cH][cH]nc1c2n[cH][cH][cH]c2[!#1]
KRFP1637	KRFPC1637	[!#1]c1[cH][cH][cH]o1
KRFP1638	KRFPC1638	[!#1]c1[cH][cH][cH]s1
KRFP1639	KRFPC1639	[!#1]c1[cH][cH][n+](!#1)[cH][cH]1
KRFP1640	KRFPC1640	[!#1]c1[cH][cH][n+](!#1)c2[cH][cH][cH][cH]c12
KRFP1641	KRFPC1641	[!#1]c1[cH][cH][n+](O-)[cH][cH]1
KRFP1642	KRFPC1642	[!#1]c1[cH][cH]c(!#1)[cH][cH]1
KRFP1643	KRFPC1643	[!#1]c1[cH][cH]c(!#1)[cH]c1S(=O)(=O)c2[cH]c(!#1)[cH][cH]c2 [!#1]
KRFP1644	KRFPC1644	[!#1]c1[cH][cH]c(!#1)[n+](!#1)[cH]1
KRFP1645	KRFPC1645	[!#1]c1[cH][cH]c(!#1)c(!#1)[cH]1
KRFP1646	KRFPC1646	[!#1]c1[cH][cH]c(!#1)c(!#1)c1[!#1]
KRFP1647	KRFPC1647	[!#1]c1[cH][cH]c(!#1)c(!#1)n1
KRFP1648	KRFPC1648	[!#1]c1[cH][cH]c(!#1)c([cH]1)[N+](=O)[O-]
KRFP1649	KRFPC1649	[!#1]c1[cH][cH]c(!#1)c([cH]1)C(=O)[OH]
KRFP1650	KRFPC1650	[!#1]c1[cH][cH]c(!#1)c([cH]1)c2[cH][cH][cH][cH]c2
KRFP1651	KRFPC1651	[!#1]c1[cH][cH]c(!#1)c([cH]1)c2nc3[cH][cH][cH][cH]c3s2
KRFP1652	KRFPC1652	[!#1]c1[cH][cH]c(!#1)c([CH3])[cH]1
KRFP1653	KRFPC1653	[!#1]c1[cH][cH]c(!#1)c([OH])[cH]1
KRFP1654	KRFPC1654	[!#1]c1[cH][cH]c(!#1)c(Cl)[cH]1
KRFP1655	KRFPC1655	[!#1]c1[cH][cH]c(!#1)c2[cH][cH][cH][cH]c12
KRFP1656	KRFPC1656	[!#1]c1[cH][cH]c(!#1)c2c(!#1)[cH][cH][cH]c12
KRFP1657	KRFPC1657	[!#1]c1[cH][cH]c(!#1)c2n[cH][cH][cH]c12
KRFP1658	KRFPC1658	[!#1]c1[cH][cH]c(!#1)c2nonc12
KRFP1659	KRFPC1659	[!#1]c1[cH][cH]c(!#1)n[cH]1
KRFP1660	KRFPC1660	[!#1]c1[cH][cH]c(!#1)n1c2[cH][cH]c(!#1)[cH][cH]2
KRFP1661	KRFPC1661	[!#1]c1[cH][cH]c(!#1)nn1
KRFP1662	KRFPC1662	[!#1]c1[cH][cH]c(!#1)o1
KRFP1663	KRFPC1663	[!#1]c1[cH][cH]c(!#1)s1
KRFP1664	KRFPC1664	[!#1]c1[cH][cH]c([cH][cH]1)[CH]([CH3])[CH3]
KRFP1665	KRFPC1665	[!#1]c1[cH][cH]c([cH][cH]1)[CH]2[CH]3[CH2][CH]4[CH2][CH]([CH2]3)[CH2] [CH]2[CH2]4
KRFP1666	KRFPC1666	[!#1]c1[cH][cH]c([cH][cH]1)[CH]2[CH2][CH2][CH2][CH2][CH2]2
KRFP1667	KRFPC1667	[!#1]c1[cH][cH]c([cH][cH]1)[CH]2[NH]c3[cH][cH]c4n[cH][cH][cH] c4c3C5=C2C(=O)[CH2][CH2][CH2]5
KRFP1668	KRFPC1668	[!#1]c1[cH][cH]c([cH][cH]1)[CH]2N([CH2][CH2]N2c3[cH][cH][cH][cH] [cH]3)c4[cH][cH][cH][cH]4
KRFP1669	KRFPC1669	[!#1]c1[cH][cH]c([cH][cH]1)[CH]2N=NC(=[CH][CH]2c3[cH][cH][cH][cH] [cH]3)[CH]4C(=O)c5[cH][cH][cH][cH]c5C4=O
KRFP1670	KRFPC1670	[!#1]c1[cH][cH]c([cH][cH]1)[N+](=O)[O-]
KRFP1671	KRFPC1671	[!#1]c1[cH][cH]c([cH][cH]1)[NH](=O)[OH]
KRFP1672	KRFPC1672	[!#1]c1[cH][cH]c([cH][cH]1)C(!#1)([CH3])[CH3]
KRFP1673	KRFPC1673	[!#1]c1[cH][cH]c([cH][cH]1)C([CH3])([CH3])[CH3]

Name	Count name	Pattern
KRFP1674	KRFPC1674	[!#1]c1[cH][cH]c([cH][cH]1)C(=N[NH]c2[cH][cH]c([cH]c2[N+](=O)[O-])[N+](=O)[O-])[CH3]
KRFP1675	KRFPC1675	[!#1]c1[cH][cH]c([cH][cH]1)C(=N[OH])[CH3]
KRFP1676	KRFPC1676	[!#1]c1[cH][cH]c([cH][cH]1)C(=O)[CH3]
KRFP1677	KRFPC1677	[!#1]c1[cH][cH]c([cH][cH]1)C(=O)[OH]
KRFP1678	KRFPC1678	[!#1]c1[cH][cH]c([cH][cH]1)C(=O)C(=O)c2[cH][cH][cH][cH]c2
KRFP1679	KRFPC1679	[!#1]c1[cH][cH]c([cH][cH]1)C2(!#1)C(=O)c3[cH][cH][cH][cH]c3C2=O
KRFP1680	KRFPC1680	[!#1]c1[cH][cH]c([cH][cH]1)C2([CH2][CH]3[CH2][CH]4[CH2][CH]([CH2]3)[CH2]2)[CH2]4
KRFP1681	KRFPC1681	[!#1]c1[cH][cH]c([cH][cH]1)C2([NH]C(=O)c3[cH][cH][cH][cH]c32)c4[cH][cH]c(!#1)[cH][cH]4
KRFP1682	KRFPC1682	[!#1]c1[cH][cH]c([cH][cH]1)C2(c3[cH][cH][cH][cH]c3-c4[cH][cH][cH][cH]c42)c5[cH][cH]c(!#1)[cH][cH]5
KRFP1683	KRFPC1683	[!#1]c1[cH][cH]c([cH][cH]1)C2(OC(=O)c3[cH][cH][cH][cH]c32)c4[cH][cH]c(!#1)[cH][cH]4
KRFP1684	KRFPC1684	[!#1]c1[cH][cH]c([cH][cH]1)c2[cH][cH][cH][cH]c2
KRFP1685	KRFPC1685	[!#1]c1[cH][cH]c([cH][cH]1)c2[cH][cH][cH]c(n2)c3[cH][cH]c(!#1)[cH][cH]3
KRFP1686	KRFPC1686	[!#1]c1[cH][cH]c([cH][cH]1)c2[cH][cH]c(!#1)[cH][cH]2
KRFP1687	KRFPC1687	[!#1]c1[cH][cH]c([cH][cH]1)c2[cH][cH]c([cH][cH]2)S(=O)(=O)!#1
KRFP1688	KRFPC1688	[!#1]c1[cH][cH]c([cH][cH]1)c2[cH]c(nc(n2)c3[cH][cH][cH][cH]c3)c4[cH][cH]c(!#1)[cH][cH]4
KRFP1689	KRFPC1689	[!#1]c1[cH][cH]c([cH][cH]1)c2[cH]nc(n[cH]2)c3[cH][cH]c(!#1)[cH][cH]3
KRFP1690	KRFPC1690	[!#1]c1[cH][cH]c([cH][cH]1)c2[cH]nc3[cH][cH][cH][cH]c3n2
KRFP1691	KRFPC1691	[!#1]c1[cH][cH]c([cH][cH]1)c2n[cH][cH][cH]c2!#1
KRFP1692	KRFPC1692	[!#1]c1[cH][cH]c([cH][cH]1)c2nc(!#1)[cH][cH]c2!#1
KRFP1693	KRFPC1693	[!#1]c1[cH][cH]c([cH][cH]1)c2nc(!#1)[cH]c(!#1)c2!#1
KRFP1694	KRFPC1694	[!#1]c1[cH][cH]c([cH][cH]1)c2nc(c3[cH][cH]c(!#1)[cH][cH]3)c4[cH][cH][cH]c4n2
KRFP1695	KRFPC1695	[!#1]c1[cH][cH]c([cH][cH]1)c2nc3[cH][cH][cH][cH]c3[nH]2
KRFP1696	KRFPC1696	[!#1]c1[cH][cH]c([cH][cH]1)c2nc3[cH][cH][cH][cH]c3nc2c4[cH][cH][cH][cH]c4
KRFP1697	KRFPC1697	[!#1]c1[cH][cH]c([cH][cH]1)c2nc3[cH][cH][cH][cH]c3nc2c4[cH][cH]c(!#1)[cH][cH]4
KRFP1698	KRFPC1698	[!#1]c1[cH][cH]c([cH][cH]1)c2nc3[cH][cH][cH][cH]c3o2
KRFP1699	KRFPC1699	[!#1]c1[cH][cH]c([cH][cH]1)c2nc3[cH][cH][cH][cH]c3s2
KRFP1700	KRFPC1700	[!#1]c1[cH][cH]c([cH][cH]1)c2nc3[cH][cH]c(!#1)[cH]c3[nH]2
KRFP1701	KRFPC1701	[!#1]c1[cH][cH]c([cH][cH]1)c2nc3[cH][cH]c(!#1)[cH]c3o2
KRFP1702	KRFPC1702	[!#1]c1[cH][cH]c([cH][cH]1)c2nc3[cH][cH]c(!#1)[cH]c3s2
KRFP1703	KRFPC1703	[!#1]c1[cH][cH]c([cH][cH]1)c2nc3[cH][cH]c([cH]c3[nH]2)c4nc5[cH][cH]c(!#1)[cH]c5[nH]4
KRFP1704	KRFPC1704	[!#1]c1[cH][cH]c([cH][cH]1)c2nc3[cH]c(!#1)[cH][cH]c3[nH]2
KRFP1705	KRFPC1705	[!#1]c1[cH][cH]c([cH][cH]1)c2nc3[cH]c(!#1)[cH][cH]c3o2
KRFP1706	KRFPC1706	[!#1]c1[cH][cH]c([cH][cH]1)c2sc(c(c2c3[cH][cH][cH][cH]c3)c4[cH][cH][cH][cH]c4)c5[cH][cH]c(!#1)[cH][cH]5
KRFP1707	KRFPC1707	[!#1]c1[cH][cH]c([cH][cH]1)N([CH3])[CH3]
KRFP1708	KRFPC1708	[!#1]c1[cH][cH]c([cH][cH]1)N2[CH2][CH2][CH2]C2=O
KRFP1709	KRFPC1709	[!#1]c1[cH][cH]c([cH][cH]1)N2[CH2][CH2]C(=N2)c3[cH][cH]c(!#1)[cH][cH]3
KRFP1710	KRFPC1710	[!#1]c1[cH][cH]c([cH][cH]1)N2[CH2][CH2]O[CH2][CH2]2
KRFP1711	KRFPC1711	[!#1]c1[cH][cH]c([cH][cH]1)n2c([CH3])[cH][cH]c2[CH3]
KRFP1712	KRFPC1712	[!#1]c1[cH][cH]c([cH][cH]1)N2C(=O)[CH]=[CH]C2=O
KRFP1713	KRFPC1713	[!#1]c1[cH][cH]c([cH][cH]1)N2C(=O)[CH]3[CH]4[CH2][CH]([CH]=[CH]4)[CH]3C2=O
KRFP1714	KRFPC1714	[!#1]c1[cH][cH]c([cH][cH]1)N2C(=O)[CH2][CH](N3[CH2][CH2][CH2][CH2][CH2]3)C2=O

Name	Count name	Pattern
KRFP1715	KRFPC1715	[!#1]c1[cH][cH]c([cH][cH]1)N2C(=O)[CH2][CH](N3[CH2][CH2][CH2][CH2]3)C2=O
KRFP1716	KRFPC1716	[!#1]c1[cH][cH]c([cH][cH]1)N2C(=O)[CH2][CH](N3[CH2][CH2]N([CH2][CH2]3)[CH]4[CH2]C(=O)N(C4=O)c5[cH][cH]c(!#1)[cH][cH]5)C2=O
KRFP1717	KRFPC1717	[!#1]c1[cH][cH]c([cH][cH]1)N2C(=O)[CH2][CH](N3[CH2][CH2]N([CH2][CH2]3)c4n[cH][cH][cH]n4)C2=O
KRFP1718	KRFPC1718	[!#1]c1[cH][cH]c([cH][cH]1)N2C(=O)[CH2][CH](N3[CH2][CH2]O[CH2][CH2]3)C2=O
KRFP1719	KRFPC1719	[!#1]c1[cH][cH]c([cH][cH]1)N2C(=O)c3[cH][cH][cH][cH]c3C2=O
KRFP1720	KRFPC1720	[!#1]c1[cH][cH]c([cH][cH]1)N2C(=O)c3[cH][cH][cH]c(!#1)c3C2=O
KRFP1721	KRFPC1721	[!#1]c1[cH][cH]c([cH][cH]1)N2C(=O)c3[cH][cH]c(!#1)[cH]c3C2=O
KRFP1722	KRFPC1722	[!#1]c1[cH][cH]c([cH][cH]1)N2C(=O)c3[cH][cH]c([cH]c3C2=O)C(=O)[OH]
KRFP1723	KRFPC1723	[!#1]c1[cH][cH]c([cH][cH]1)n2c(=O)c3[cH]c4c(=O)n(c5[cH][cH]c(!#1)[cH][cH]5)c(=O)c4[cH]c3c2=O
KRFP1724	KRFPC1724	[!#1]c1[cH][cH]c([cH][cH]1)S(=O)(=O)[!#1]
KRFP1725	KRFPC1725	[!#1]c1[cH][cH]c([cH][cH]1)S(=O)(=O)[NH2]
KRFP1726	KRFPC1726	[!#1]c1[cH][cH]c([cH][cH]1)S(=O)(=O)[OH]
KRFP1727	KRFPC1727	[!#1]c1[cH][cH]c([cH][cH]1)S(=O)(=O)c2[cH][cH]c(!#1)[cH][cH]2
KRFP1728	KRFPC1728	[!#1]c1[cH][cH]c([cH][cH]1)S(=O)(=O)c2[cH][cH][cH][cH]c2[cH][cH]1
KRFP1729	KRFPC1729	[!#1]c1[cH][cH]c([cH][cH]1)S(=O)(=O)c2[cH][cH]c(!#1)[cH]c2S(=O)(=O)[OH]c([cH]1)S(=O)(=O)[OH]
KRFP1730	KRFPC1730	[!#1]c1[cH][cH]c([cH][cH]1)S(=O)(=O)[OH]
KRFP1731	KRFPC1731	[!#1]c1[cH][cH]c([cH][cH]1)S(=O)(=O)[OH]
KRFP1732	KRFPC1732	[!#1]c1[cH][cH]c([cH][cH]1)S(=O)(=O)[OH]
KRFP1733	KRFPC1733	[!#1]c1[cH][cH]c([cH][cH]1)S(=O)(=O)[OH]
KRFP1734	KRFPC1734	[!#1]c1[cH][cH]c([cH][cH]1)S(=O)(=O)[OH]
KRFP1735	KRFPC1735	[!#1]c1[cH][cH]c([cH][cH]1)S(=O)(=O)[OH]
KRFP1736	KRFPC1736	[!#1]c1[cH][cH]c([cH][cH]1)S(=O)(=O)[OH]
KRFP1737	KRFPC1737	[!#1]c1[cH][cH]c([cH][cH]1)S(=O)(=O)[OH]
KRFP1738	KRFPC1738	[!#1]c1[cH][cH]c([cH][cH]1)S(=O)(=O)[OH]
KRFP1739	KRFPC1739	[!#1]c1[cH][cH]c([cH][cH]1)S(=O)(=O)[OH]
KRFP1740	KRFPC1740	[!#1]c1[cH][cH]c([cH][cH]1)S(=O)(=O)[OH]
KRFP1741	KRFPC1741	[!#1]c1[cH][cH]c([cH][cH]1)S(=O)(=O)[OH]
KRFP1742	KRFPC1742	[!#1]c1[cH][cH]c([cH][cH]1)S(=O)(=O)[OH]
KRFP1743	KRFPC1743	[!#1]c1[cH][cH]c([cH][cH]1)S(=O)(=O)[OH]
KRFP1744	KRFPC1744	[!#1]c1[cH][cH]c([cH][cH]1)S(=O)(=O)[OH]
KRFP1745	KRFPC1745	[!#1]c1[cH][cH]c([cH][cH]1)S(=O)(=O)[OH]
KRFP1746	KRFPC1746	[!#1]c1[cH][cH]c([cH][cH]1)S(=O)(=O)[OH]
KRFP1747	KRFPC1747	[!#1]c1[cH][cH]c([cH][cH]1)S(=O)(=O)[OH]
KRFP1748	KRFPC1748	[!#1]c1[cH][cH]c([cH][cH]1)S(=O)(=O)[OH]
KRFP1749	KRFPC1749	[!#1]c1[cH][cH]c([cH][cH]1)S(=O)(=O)[OH]
KRFP1750	KRFPC1750	[!#1]c1[cH][cH]c([cH][cH]1)S(=O)(=O)[OH]
KRFP1751	KRFPC1751	[!#1]c1[cH][cH]c([cH][cH]1)S(=O)(=O)[OH]
KRFP1752	KRFPC1752	[!#1]c1[cH][cH]c([cH][cH]1)S(=O)(=O)[OH]
KRFP1753	KRFPC1753	[!#1]c1[cH][cH]c([cH][cH]1)S(=O)(=O)[OH]
KRFP1754	KRFPC1754	[!#1]c1[cH][cH]c([cH][cH]1)S(=O)(=O)[OH]
KRFP1755	KRFPC1755	[!#1]c1[cH][cH]c([cH][cH]1)S(=O)(=O)[OH]
KRFP1756	KRFPC1756	[!#1]c1[cH][cH]c([cH][cH]1)S(=O)(=O)[OH]
KRFP1757	KRFPC1757	[!#1]c1[cH][cH]c([cH][cH]1)S(=O)(=O)[OH]
KRFP1758	KRFPC1758	[!#1]c1[cH][cH]c([cH][cH]1)S(=O)(=O)[OH]
KRFP1759	KRFPC1759	[!#1]c1[cH][cH]c([cH][cH]1)S(=O)(=O)[OH]
KRFP1760	KRFPC1760	[!#1]c1[cH][cH]c([cH][cH]1)S(=O)(=O)[OH]
KRFP1761	KRFPC1761	[!#1]c1[cH][cH]c([cH][cH]1)S(=O)(=O)[OH]

Name	Count name	Pattern
KRFP1762	KRFPC1762	[!#1]c1[cH][cH]c([CH3])c(l)[cH]1
KRFP1763	KRFPC1763	[!#1]c1[cH][cH]c([CH3])n[cH]1
KRFP1764	KRFPC1764	[!#1]c1[cH][cH]c([CH3])o1
KRFP1765	KRFPC1765	[!#1]c1[cH][cH]c([N+](=O)[O-])c([CH3])[cH]1
KRFP1766	KRFPC1766	[!#1]c1[cH][cH]c([N+](=O)[O-])c2nonc12
KRFP1767	KRFPC1767	[!#1]c1[cH][cH]c([NH2])[cH][cH]1
KRFP1768	KRFPC1768	[!#1]c1[cH][cH]c([NH2])c([cH]1)[N+](=O)[O-]
KRFP1769	KRFPC1769	[!#1]c1[cH][cH]c([OH])[cH][cH]1
KRFP1770	KRFPC1770	[!#1]c1[cH][cH]c([OH])[cH]c1[OH]
KRFP1771	KRFPC1771	[!#1]c1[cH][cH]c([OH])c(!#1))[cH]1
KRFP1772	KRFPC1772	[!#1]c1[cH][cH]c([OH])c([cH]1)C(=O)[OH]
KRFP1773	KRFPC1773	[!#1]c1[cH][cH]c([OH])c([OH])[cH]1
KRFP1774	KRFPC1774	[!#1]c1[cH][cH]c(=S)[nH]n1
KRFP1775	KRFPC1775	[!#1]c1[cH][cH]c(Br)[cH][cH]1
KRFP1776	KRFPC1776	[!#1]c1[cH][cH]c(Br)[cH]c1[!#1]
KRFP1777	KRFPC1777	[!#1]c1[cH][cH]c(Br)[cH]c1Br
KRFP1778	KRFPC1778	[!#1]c1[cH][cH]c(Br)[cH]n1
KRFP1779	KRFPC1779	[!#1]c1[cH][cH]c(Br)c(!#1))[cH]1
KRFP1780	KRFPC1780	[!#1]c1[cH][cH]c(Br)c([cH]1)[N+](=O)[O-]
KRFP1781	KRFPC1781	[!#1]c1[cH][cH]c(Br)c(Cl)[cH]1
KRFP1782	KRFPC1782	[!#1]c1[cH][cH]c(Br)c2[cH][cH][cH]c12
KRFP1783	KRFPC1783	[!#1]c1[cH][cH]c(Br)o1
KRFP1784	KRFPC1784	[!#1]c1[cH][cH]c(C(=O)[OH])c(!#1))[cH]1
KRFP1785	KRFPC1785	[!#1]c1[cH][cH]c(C(=O)[OH])c([cH]1)C(=O)[OH]
KRFP1786	KRFPC1786	[!#1]c1[cH][cH]c(Cl)[cH][cH]1
KRFP1787	KRFPC1787	[!#1]c1[cH][cH]c(Cl)[cH]c1[!#1]
KRFP1788	KRFPC1788	[!#1]c1[cH][cH]c(Cl)[cH]c1[CH3]
KRFP1789	KRFPC1789	[!#1]c1[cH][cH]c(Cl)[cH]c1[N+](=O)[O-]
KRFP1790	KRFPC1790	[!#1]c1[cH][cH]c(Cl)[cH]c1Br
KRFP1791	KRFPC1791	[!#1]c1[cH][cH]c(Cl)[cH]c1Cl
KRFP1792	KRFPC1792	[!#1]c1[cH][cH]c(Cl)[cH]n1
KRFP1793	KRFPC1793	[!#1]c1[cH][cH]c(Cl)c(!#1))[cH]1
KRFP1794	KRFPC1794	[!#1]c1[cH][cH]c(Cl)c([cH]1)[N+](=O)[O-]
KRFP1795	KRFPC1795	[!#1]c1[cH][cH]c(Cl)c([CH3])[cH]1
KRFP1796	KRFPC1796	[!#1]c1[cH][cH]c(Cl)c(Cl)[cH]1
KRFP1797	KRFPC1797	[!#1]c1[cH][cH]c(Cl)c2[cH][cH][cH]c12
KRFP1798	KRFPC1798	[!#1]c1[cH][cH]c(F)[cH][cH]1
KRFP1799	KRFPC1799	[!#1]c1[cH][cH]c(F)[cH]c1F
KRFP1800	KRFPC1800	[!#1]c1[cH][cH]c(F)c(Cl)[cH]1
KRFP1801	KRFPC1801	[!#1]c1[cH][cH]c(F)c(F)[cH]1
KRFP1802	KRFPC1802	[!#1]c1[cH][cH]c(l)[cH][cH]1
KRFP1803	KRFPC1803	[!#1]c1[cH][cH]c(N=[CH]c2[cH][cH][cH][cH]c2[OH])[cH][cH]1
KRFP1804	KRFPC1804	[!#1]c1[cH][cH]c(N=[CH]c2[cH][cH]c([cH][cH]2)[N+](=O)[O-])[cH][cH]1
KRFP1805	KRFPC1805	[!#1]c1[cH][cH]c(N=[CH]c2[cH]c([cH][cH]c2[OH])[N+](=O)[O-])[cH][cH]1
KRFP1806	KRFPC1806	[!#1]c1[cH][cH]c(N=[CH]c2c([OH])[cH][cH]c3[cH][cH][cH]c23)[cH] [cH]1
KRFP1807	KRFPC1807	[!#1]c1[cH][cH]c(N=[N+]=[N-])[cH][cH]1
KRFP1808	KRFPC1808	[!#1]c1[cH][cH]c(N=Nc2[cH][cH][cH][cH]2)[cH][cH]1
KRFP1809	KRFPC1809	[!#1]c1[cH][cH]c(N=Nc2[cH][cH][cH][cH]c2[CH3])[cH]c1[CH3]
KRFP1810	KRFPC1810	[!#1]c1[cH][cH]c(N2[CH2][CH2][CH2]C2=O)c(!#1))[cH]1
KRFP1811	KRFPC1811	[!#1]c1[cH][cH]c(O[CH3])[cH][cH]1
KRFP1812	KRFPC1812	[!#1]c1[cH][cH]c(O[CH3])[cH]c1[N+](=O)[O-]
KRFP1813	KRFPC1813	[!#1]c1[cH][cH]c(O[CH3])[cH]c1Br
KRFP1814	KRFPC1814	[!#1]c1[cH][cH]c(O[CH3])[cH]c1O[CH3]
KRFP1815	KRFPC1815	[!#1]c1[cH][cH]c(O[CH3])c(Cl)[cH]1

Name	Count name	Pattern
KRFP1816	KRFPC1816	[!#1]c1[cH][cH]c(O[CH3])c(O[CH3])[cH]1
KRFP1817	KRFPC1817	[!#1]c1[cH][cH]c(O[CH3])nn1
KRFP1818	KRFPC1818	[!#1]c1[cH][cH]c(o1)[CH]2[CH2][CH]2[CH]3[CH2][CH2]3
KRFP1819	KRFPC1819	[!#1]c1[cH][cH]c(o1)c2[cH][cH][cH]c(!#1)[cH]2
KRFP1820	KRFPC1820	[!#1]c1[cH][cH]c(o1)c2[cH][cH]c(!#1)[cH][cH]2
KRFP1821	KRFPC1821	[!#1]c1[cH][cH]c(S[CH2][CH2]c2[cH][cH]n[cH][cH]2)[cH][cH]1
KRFP1822	KRFPC1822	[!#1]c1[cH][cH]c(S[CH3])[cH][cH]1
KRFP1823	KRFPC1823	[!#1]c1[cH][cH]c(s1)C(=O)[OH]
KRFP1824	KRFPC1824	[!#1]c1[cH][cH]c2[cH][cH][cH][cH]c2[cH]1
KRFP1825	KRFPC1825	[!#1]c1[cH][cH]c2[cH][cH][cH][cH]c2[n+]1[!#1]
KRFP1826	KRFPC1826	[!#1]c1[cH][cH]c2[cH][cH][cH][cH]c2c1[!#1]
KRFP1827	KRFPC1827	[!#1]c1[cH][cH]c2[cH][cH][cH][cH]c2c1Br
KRFP1828	KRFPC1828	[!#1]c1[cH][cH]c2[cH][cH][cH][cH]c2n1
KRFP1829	KRFPC1829	[!#1]c1[cH][cH]c2[cH][cH][cH]c(!#1)c2n1
KRFP1830	KRFPC1830	[!#1]c1[cH][cH]c2[cH][cH][cH]c([OH])c2n1
KRFP1831	KRFPC1831	[!#1]c1[cH][cH]c2[cH][cH]c(!#1)[cH]c2[cH]1
KRFP1832	KRFPC1832	[!#1]c1[cH][cH]c2[CH]3c4[cH][cH][cH][cH]c4[CH](c5[cH][cH][cH][cH]c35) c2[cH]1
KRFP1833	KRFPC1833	[!#1]c1[cH][cH]c2[CH]3c4[cH][cH][cH][cH]c4[CH](c5[cH][cH]c(!#1)) [cH]c35)c2[cH]1
KRFP1834	KRFPC1834	[!#1]c1[cH][cH]c2[cH]c(!#1)[cH][cH]c2[cH]1
KRFP1835	KRFPC1835	[!#1]c1[cH][cH]c2[cH]c(!#1)c(=O)oc2[cH]1
KRFP1836	KRFPC1836	[!#1]c1[cH][cH]c2[cH]c([OH])[cH][cH]c2[cH]1
KRFP1837	KRFPC1837	[!#1]c1[cH][cH]c2[CH2][CH2]c3[cH][cH][cH][cH]c3[NH]c2[cH]1
KRFP1838	KRFPC1838	[!#1]c1[cH][cH]c2[CH2][CH2]c3[cH][cH][cH]c1c32
KRFP1839	KRFPC1839	[!#1]c1[cH][cH]c2[CH2]OC(=O)c2[cH]1
KRFP1840	KRFPC1840	[!#1]c1[cH][cH]c2[n+](!#1)[cH][cH][cH]c2[cH]1
KRFP1841	KRFPC1841	[!#1]c1[cH][cH]c2[n+](!#1)c(!#1)[cH][cH]c2[cH]1
KRFP1842	KRFPC1842	[!#1]c1[cH][cH]c2[nH]c(=O)[nH]c2[cH]1
KRFP1843	KRFPC1843	[!#1]c1[cH][cH]c2[NH]C(=O)C(=O)c2[cH]1
KRFP1844	KRFPC1844	[!#1]c1[cH][cH]c2[nH]c(=O)oc2[cH]1
KRFP1845	KRFPC1845	[!#1]c1[cH][cH]c2[nH]c3C(=O)[CH2][CH2][CH2]c3c2[cH]1
KRFP1846	KRFPC1846	[!#1]c1[cH][cH]c2[nH]c3C(=O)[NH][CH2][CH2]c3c2[cH]1
KRFP1847	KRFPC1847	[!#1]c1[cH][cH]c2c(!#1)[cH]c(=O)oc2[cH]1
KRFP1848	KRFPC1848	[!#1]c1[cH][cH]c2c(!#1)[n+](!#1)[cH][cH]n12
KRFP1849	KRFPC1849	[!#1]c1[cH][cH]c2c(!#1)c(!#1)[cH][cH]c2[cH]1
KRFP1850	KRFPC1850	[!#1]c1[cH][cH]c2c(!#1)nc(!#1)nc2[cH]1
KRFP1851	KRFPC1851	[!#1]c1[cH][cH]c2c([cH]1)-c3[cH]c(!#1)[cH][cH]c3S2(=O)=O
KRFP1852	KRFPC1852	[!#1]c1[cH][cH]c2c([cH]1)nc3c4[cH][cH]c(!#1)c5[cH][cH][cH]c(c(=O) n23)c54
KRFP1853	KRFPC1853	[!#1]c1[cH][cH]c2c([cH]1)oc3[cH][cH][cH][cH]c32
KRFP1854	KRFPC1854	[!#1]c1[cH][cH]c-2c([CH2]c3[cH][cH][cH][cH]c32)[cH]1
KRFP1855	KRFPC1855	[!#1]c1[cH][cH]c-2c([CH2]c3[cH]c(!#1)[cH][cH]c32)[cH]1
KRFP1856	KRFPC1856	[!#1]c1[cH][cH]c2c([CH3])[cH]c(=O)oc2[cH]1
KRFP1857	KRFPC1857	[!#1]c1[cH][cH]c2c(=O)c(!#1)[cH]oc2[cH]1
KRFP1858	KRFPC1858	[!#1]c1[cH][cH]c2c(=O)c(!#1)c(!#1)oc2[cH]1
KRFP1859	KRFPC1859	[!#1]c1[cH][cH]c2c(=O)c(!#1)c([CH3])oc2[cH]1
KRFP1860	KRFPC1860	[!#1]c1[cH][cH]c2c(=O)c([cH]oc2[cH]1)c3[cH][cH]c4O[CH2][CH2]Oc4[cH]3
KRFP1861	KRFPC1861	[!#1]c1[cH][cH]c2C(=O)c3[cH][cH][cH][cH]c3C(=O)c2[cH]1
KRFP1862	KRFPC1862	[!#1]c1[cH][cH]c2C(=O)c3[cH][cH][cH][cH]c3-c2[cH]1
KRFP1863	KRFPC1863	[!#1]c1[cH][cH]c2C(=O)N(C(=O)c2[cH]1)c3[cH][cH][cH][cH]c3[!#1]
KRFP1864	KRFPC1864	[!#1]c1[cH][cH]c2C(=O)N(C(=O)c2[cH]1)c3[cH][cH][cH]c(!#1)[cH]3
KRFP1865	KRFPC1865	[!#1]c1[cH][cH]c2C(=O)N(C(=O)c2[cH]1)c3[cH][cH][cH]c(n3)N4C(=O)c5[cH] [cH]c(!#1)[cH]c5C4=O
KRFP1866	KRFPC1866	[!#1]c1[cH][cH]c2C(=O)N(C(=O)c2[cH]1)c3[cH][cH][cH]c4[cH][cH][cH][cH] c34

Name	Count name	Pattern
KRFP1867	KRFPC1867	[!#1]c1[cH][cH]c2C(=O)OC(=O)c2[cH]1
KRFP1868	KRFPC1868	[!#1]c1[cH][cH]c2-c3[cH][cH]c(!#1)[cH]c3S(=O)(=O)c2[cH]1
KRFP1869	KRFPC1869	[!#1]c1[cH][cH]c2n(!#1)c([CH3])c([CH3])c2[cH]1
KRFP1870	KRFPC1870	[!#1]c1[cH][cH]c2n(!#1)c(=O)oc2[cH]1
KRFP1871	KRFPC1871	[!#1]c1[cH][cH]c2n(!#1)c3[cH][cH][cH][cH]c3c2[cH]1
KRFP1872	KRFPC1872	[!#1]c1[cH][cH]c2n(!#1)c3[cH][cH]c(!#1)[cH]c3c2[cH]1
KRFP1873	KRFPC1873	[!#1]c1[cH][cH]c2N([CH2][CH3])C(=O)c3[cH][cH][cH]c1c23
KRFP1874	KRFPC1874	[!#1]c1[cH][cH]c2n[cH][cH][cH]c2[cH]1
KRFP1875	KRFPC1875	[!#1]c1[cH][cH]c2n[cH][nH]c2[cH]1
KRFP1876	KRFPC1876	[!#1]c1[cH][cH]c2n[cH]nc3-c4[cH][cH][cH][cH]c4C(=O)c1c32
KRFP1877	KRFPC1877	[!#1]c1[cH][cH]c2N=C(c3[cH][cH][cH][cH]c3)c4[cH]c(!#1)[cH][cH]c4N=C(c5[cH][cH][cH][cH]c5)c2[cH]1
KRFP1878	KRFPC1878	[!#1]c1[cH][cH]c2n3[CH2][CH2][CH2]c3nc2[cH]1
KRFP1879	KRFPC1879	[!#1]c1[cH][cH]c2n3[CH2][CH2][NH][CH]4[CH2][CH2][CH2]c(c43)c2[cH]1
KRFP1880	KRFPC1880	[!#1]c1[cH][cH]c2nc([CH3])[nH]c2[cH]1
KRFP1881	KRFPC1881	[!#1]c1[cH][cH]c2nc(nc(c3[cH][cH][cH][cH]c3)c2[cH]1)c4[cH][cH]c([cH][cH]4)c5nc(c6[cH][cH][cH][cH]c6)c7[cH]c(!#1)[cH][cH]c7n5
KRFP1882	KRFPC1882	[!#1]c1[cH][cH]c2nc(oc(=O)c2[cH]1)c3[cH][cH][cH][cH]c3
KRFP1883	KRFPC1883	[!#1]c1[cH][cH]c2nc3[cH][cH][cH][cH]c3[n+](!#1)c2[cH]1
KRFP1884	KRFPC1884	[!#1]c1[cH][cH]c2nc3[CH2][CH2][CH2][CH2]c3n2[cH]1
KRFP1885	KRFPC1885	[!#1]c1[cH][cH]c2nc3c([cH]c2[cH]1)n(!#1)c4[cH][cH][cH][cH]c43
KRFP1886	KRFPC1886	[!#1]c1[cH][cH]c2nc3c(=O)[nH]c(=O)nc3[nH]c2[cH]1
KRFP1887	KRFPC1887	[!#1]c1[cH][cH]c2nc3c(=O)n(!#1)c(=O)[nH]c3nc2[cH]1
KRFP1888	KRFPC1888	[!#1]c1[cH][cH]c2nn(nc2[cH]1)c3[cH][cH][cH][cH]c3
KRFP1889	KRFPC1889	[!#1]c1[cH][cH]c2nn[nH]c2[cH]1
KRFP1890	KRFPC1890	[!#1]c1[cH][cH]c2nonc2c1!#1
KRFP1891	KRFPC1891	[!#1]c1[cH][cH]c2nsnc2c1[N+](=O)[O-]
KRFP1892	KRFPC1892	[!#1]c1[cH][cH]c2o[cH]nc2[cH]1
KRFP1893	KRFPC1893	[!#1]c1[cH][cH]c2O[CH2][CH2]O[CH2][CH2]O[CH2][CH2]O[CH2][CH2]O[CH2][CH2]Oc2[cH]1
KRFP1894	KRFPC1894	[!#1]c1[cH][cH]c2O[CH2][CH2]Oc2[cH]1
KRFP1895	KRFPC1895	[!#1]c1[cH][cH]c2O[CH2]Oc2[cH]1
KRFP1896	KRFPC1896	[!#1]c1[cH][cH]c2oc(nc2[cH]1)c3[cH][cH][cH][cH]c3
KRFP1897	KRFPC1897	[!#1]c1[cH][cH]c2oc(nc2[cH]1)c3[cH][cH][cH][cH]c3!#1
KRFP1898	KRFPC1898	[!#1]c1[cH][cH]c2oc(nc2[cH]1)c3[cH][cH][cH]n[cH]3
KRFP1899	KRFPC1899	[!#1]c1[cH][cH]c2oc(nc2[cH]1)c3[cH][cH]c(!#1)c(!#1)[cH]3
KRFP1900	KRFPC1900	[!#1]c1[cH][cH]c2oc(nc2[cH]1)c3[cH][cH]c([CH2][CH3])[cH][cH]3
KRFP1901	KRFPC1901	[!#1]c1[cH][cH]c2oc(nc2[cH]1)c3[cH][cH]c(c4nc5[cH]c(!#1)[cH][cH]c5o4)c6[cH][cH][cH][cH]c36
KRFP1902	KRFPC1902	[!#1]c1[cH][cH]c2oc3[cH][cH]c(!#1)[cH]c3c2[cH]1
KRFP1903	KRFPC1903	[!#1]c1[cH][cH]c2S(=O)c3[cH][cH][cH][cH]c3[NH]c2[cH]1
KRFP1904	KRFPC1904	[!#1]c1[cH][cH]c2sc([CH3])nc2[cH]1
KRFP1905	KRFPC1905	[!#1]c1[cH][cH]n(!#1)n1
KRFP1906	KRFPC1906	[!#1]c1[cH][cH]n(n1)c2[cH][cH][cH][cH]c2
KRFP1907	KRFPC1907	[!#1]c1[cH][cH]n[cH][cH]1
KRFP1908	KRFPC1908	[!#1]c1[cH][cH]n[nH]1
KRFP1909	KRFPC1909	[!#1]c1[cH][cH]nc(!#1)[cH]1
KRFP1910	KRFPC1910	[!#1]c1[cH][cH]nc(!#1)n1
KRFP1911	KRFPC1911	[!#1]c1[cH][cH]nc2[cH][cH][cH][cH]c12
KRFP1912	KRFPC1912	[!#1]c1[cH][cH]nc2[cH]c3[cH][cH][cH][cH]c3[cH]c12
KRFP1913	KRFPC1913	[!#1]c1[cH][cH]nn1!#1
KRFP1914	KRFPC1914	[!#1]c1[cH][cH]nn1[CH3]
KRFP1915	KRFPC1915	[!#1]c1[cH][cH]o[cH]1
KRFP1916	KRFPC1916	[!#1]c1[cH][cH]s[cH]1

Name	Count name	Pattern
KRFP1917	KRFPC1917	[!#1]c1[cH][cH]sc1[!#1]
KRFP1918	KRFPC1918	[!#1]c1[cH][cH]sc1c2[cH][cH][cH][cH]2
KRFP1919	KRFPC1919	[!#1]c1[cH][nH]c(=O)[nH]c1=O
KRFP1920	KRFPC1920	[!#1]c1[cH][nH]c2[cH][cH][cH]c12
KRFP1921	KRFPC1921	[!#1]c1[cH][nH]c2[cH][cH][cH]nc12
KRFP1922	KRFPC1922	[!#1]c1[cH][nH]c2[cH][cH]c([!#1])[cH]c12
KRFP1923	KRFPC1923	[!#1]c1[cH][nH]c2[cH][cH]c(O[CH3])[cH]c12
KRFP1924	KRFPC1924	[!#1]c1[cH][nH]c2c([!#1])[cH][cH][cH]c12
KRFP1925	KRFPC1925	[!#1]c1[cH][nH]nc1c2[cH][cH][cH][cH]2
KRFP1926	KRFPC1926	[!#1]c1[cH]c([!#1])[cH]c([!#1])[cH]1
KRFP1927	KRFPC1927	[!#1]c1[cH]c([!#1])[cH]c([CH3]1)N2C(=O)c3[cH][cH][cH][cH]c3C2=O
KRFP1928	KRFPC1928	[!#1]c1[cH]c([!#1])[cH]c([CH3])[cH]1
KRFP1929	KRFPC1929	[!#1]c1[cH]c([!#1])[nH]c(=O)n1
KRFP1930	KRFPC1930	[!#1]c1[cH]c([!#1])[nH]n1
KRFP1931	KRFPC1931	[!#1]c1[cH]c([!#1])c([!#1])[cH]c1[!#1]
KRFP1932	KRFPC1932	[!#1]c1[cH]c([!#1])c([!#1])c([!#1])[cH]1
KRFP1933	KRFPC1933	[!#1]c1[cH]c([!#1])c([!#1])c([!#1])c1[!#1]
KRFP1934	KRFPC1934	[!#1]c1[cH]c([!#1])c([!#1])c([!#1])n1
KRFP1935	KRFPC1935	[!#1]c1[cH]c([!#1])c([!#1])c(=O)[nH]1
KRFP1936	KRFPC1936	[!#1]c1[cH]c([!#1])c([!#1])c(=O)o1
KRFP1937	KRFPC1937	[!#1]c1[cH]c([!#1])c([!#1])s1
KRFP1938	KRFPC1938	[!#1]c1[cH]c([!#1])c([OH])c(n1)C([CH3])([CH3])[CH3]
KRFP1939	KRFPC1939	[!#1]c1[cH]c([!#1])c2[cH][cH][cH][cH]c2c1[!#1]
KRFP1940	KRFPC1940	[!#1]c1[cH]c([!#1])c2[cH][cH][cH][cH]c2n1
KRFP1941	KRFPC1941	[!#1]c1[cH]c([!#1])c2[cH][cH][cH]nc2c1[!#1]
KRFP1942	KRFPC1942	[!#1]c1[cH]c([!#1])c2n([!#1])n[cH][n+]2n1
KRFP1943	KRFPC1943	[!#1]c1[cH]c([!#1])n([!#1])c(=O)c1[!#1]
KRFP1944	KRFPC1944	[!#1]c1[cH]c([!#1])n([!#1])c(=O)n1
KRFP1945	KRFPC1945	[!#1]c1[cH]c([!#1])n([!#1])n1
KRFP1946	KRFPC1946	[!#1]c1[cH]c([!#1])n(n1)c2[cH][cH][cH][cH]2
KRFP1947	KRFPC1947	[!#1]c1[cH]c([!#1])nc([!#1])n1
KRFP1948	KRFPC1948	[!#1]c1[cH]c([!#1])on1
KRFP1949	KRFPC1949	[!#1]c1[cH]c([cH][cH]c1[CH3])[CH]([CH3])[CH3]
KRFP1950	KRFPC1950	[!#1]c1[cH]c([cH][cH]c1[CH3])[N+](=O)[O-]
KRFP1951	KRFPC1951	[!#1]c1[cH]c([cH][cH]c1[OH])[N+](=O)[O-]
KRFP1952	KRFPC1952	[!#1]c1[cH]c([cH][cH]c1[OH])S(=O)(=O)c2[cH][cH]c([OH])c([!#1])[cH]2
KRFP1953	KRFPC1953	[!#1]c1[cH]c([cH][cH]c1C(=O)[OH])[N+](=O)[O-]
KRFP1954	KRFPC1954	[!#1]c1[cH]c([cH][cH]c1C(=O)[OH])C(=O)[OH]
KRFP1955	KRFPC1955	[!#1]c1[cH]c([cH][cH]c1Cl)[N+](=O)[O-]
KRFP1956	KRFPC1956	[!#1]c1[cH]c([cH][cH]c1Cl)C(F)(F)F
KRFP1957	KRFPC1957	[!#1]c1[cH]c([cH][cH]c1O[CH3])[N+](=O)[O-]
KRFP1958	KRFPC1958	[!#1]c1[cH]c([cH]c([cH]1)[N+](=O)[O-])[N+](=O)[O-]
KRFP1959	KRFPC1959	[!#1]c1[cH]c([cH]c([cH]1)C([CH3])([CH3])[CH3])C([CH3])([CH3])[CH3]
KRFP1960	KRFPC1960	[!#1]c1[cH]c([cH]c([cH]1)C(=O)[OH])C(=O)[OH]
KRFP1961	KRFPC1961	[!#1]c1[cH]c([cH]c(c1[OH])C([CH3])([CH3])[CH3])C([CH3])([CH3])[CH3]
KRFP1962	KRFPC1962	[!#1]c1[cH]c([CH3])[cH][cH]c1[CH]([CH3])[CH3]
KRFP1963	KRFPC1963	[!#1]c1[cH]c([CH3])[cH][cH]c1[CH3]
KRFP1964	KRFPC1964	[!#1]c1[cH]c([CH3])[cH][cH]n1
KRFP1965	KRFPC1965	[!#1]c1[cH]c([CH3])[cH]c([CH3])[cH]1
KRFP1966	KRFPC1966	[!#1]c1[cH]c([CH3])c(Br)[cH]c1[CH]([CH3])[CH3]
KRFP1967	KRFPC1967	[!#1]c1[cH]c([CH3])c(Cl)c([CH3])[cH]1
KRFP1968	KRFPC1968	[!#1]c1[cH]c([CH3])n[nH]1
KRFP1969	KRFPC1969	[!#1]c1[cH]c([CH3])nc([!#1])c1[OH]
KRFP1970	KRFPC1970	[!#1]c1[cH]c([CH3])nc2[cH][cH][cH][cH]c12

Name	Count name	Pattern
KRFP1971	KRFPC1971	[!#1]c1[cH]c([N+](=O)[O-])c([CH3])c([cH]1)[N+](=O)[O-]
KRFP1972	KRFPC1972	[!#1]c1[cH]c([N+](=O)[O-])c(Cl)[cH]c1Cl
KRFP1973	KRFPC1973	[!#1]c1[cH]c([nH]n1)c2[cH][cH][cH][cH]c2
KRFP1974	KRFPC1974	[!#1]c1[cH]c([OH])[cH][cH]c1[OH]
KRFP1975	KRFPC1975	[!#1]c1[cH]c([OH])[cH]c([OH])[cH]1
KRFP1976	KRFPC1976	[!#1]c1[cH]c(=O)[nH]c([!#1])n1
KRFP1977	KRFPC1977	[!#1]c1[cH]c(=O)oc2[cH][cH][cH][cH]c12
KRFP1978	KRFPC1978	[!#1]c1[cH]c(=O)oc2[cH][cH]c([cH]c12)[N+](=O)[O-]
KRFP1979	KRFPC1979	[!#1]c1[cH]c(Br)[cH]c(Br)c1[!#1]
KRFP1980	KRFPC1980	[!#1]c1[cH]c(Br)[cH]c(Br)c1[OH]
KRFP1981	KRFPC1981	[!#1]c1[cH]c(Br)[cH]c(C(=O)[OH])c1[!#1]
KRFP1982	KRFPC1982	[!#1]c1[cH]c(Br)c([OH])c(Br)[cH]1
KRFP1983	KRFPC1983	[!#1]c1[cH]c(c([OH])c([cH]1)C([CH3])([CH3])[CH3])C([CH3])([CH3])[CH3]
KRFP1984	KRFPC1984	[!#1]c1[cH]c(C(=O)[OH])c([!#1])[cH]c1C(=O)[OH]
KRFP1985	KRFPC1985	[!#1]c1[cH]c(Cl)[cH][cH]c1[OH]
KRFP1986	KRFPC1986	[!#1]c1[cH]c(Cl)[cH][cH]c1Cl
KRFP1987	KRFPC1987	[!#1]c1[cH]c(Cl)[cH]c(Cl)[cH]1
KRFP1988	KRFPC1988	[!#1]c1[cH]c(Cl)[cH]c(Cl)c1O[CH3]
KRFP1989	KRFPC1989	[!#1]c1[cH]c(Cl)c([!#1])c(Cl)[cH]1
KRFP1990	KRFPC1990	[!#1]c1[cH]c(Cl)c(Cl)[cH]c1Cl
KRFP1991	KRFPC1991	[!#1]c1[cH]c(n[nH]1)c2[cH][cH][cH][cH]c2
KRFP1992	KRFPC1992	[!#1]c1[cH]c(n[nH]1)c2[cH][cH]c([!#1])[cH][cH]c2
KRFP1993	KRFPC1993	[!#1]c1[cH]c(nc2[cH][cH][cH][cH]c12)c3[cH][cH][cH][cH]c3
KRFP1994	KRFPC1994	[!#1]c1[cH]c(nc2[cH][cH][cH][cH]c12)N([CH3])[CH3]
KRFP1995	KRFPC1995	[!#1]c1[cH]c(nn1c2[cH][cH][cH][cH]c2)c3[cH][cH][cH][cH]c3
KRFP1996	KRFPC1996	[!#1]c1[cH]c(nn1c2[cH][cH][cH][cH]c2)c3[cH][cH]c([!#1])[cH][cH]c3
KRFP1997	KRFPC1997	[!#1]c1[cH]c(O[CH3])[cH][cH]c1O[CH3]
KRFP1998	KRFPC1998	[!#1]c1[cH]c(O[CH3])[cH]c(O[CH3])[cH]1
KRFP1999	KRFPC1999	[!#1]c1[cH]c(O[CH3])c(O[CH3])[cH]c1[!#1]
KRFP2000	KRFPC2000	[!#1]c1[cH]c(O[CH3])c(O[CH3])c(O[CH3])[cH]1
KRFP2001	KRFPC2001	[!#1]c1[cH]c(O[CH3])nc(O[CH3])n1
KRFP2002	KRFPC2002	[!#1]c1[cH]c2[cH][cH][cH][cH]c2[cH]c1[!#1]
KRFP2003	KRFPC2003	[!#1]c1[cH]c2[cH][cH][cH][cH]c2[cH]c1[OH]
KRFP2004	KRFPC2004	[!#1]c1[cH]c2[cH][cH][cH][cH]c2[cH]c1O[CH3]
KRFP2005	KRFPC2005	[!#1]c1[cH]c2[cH][cH][cH][cH]c2[nH]1
KRFP2006	KRFPC2006	[!#1]c1[cH]c2[cH][cH][cH][cH]c2nc1[!#1]
KRFP2007	KRFPC2007	[!#1]c1[cH]c2[cH][cH][cH][cH]c2o1
KRFP2008	KRFPC2008	[!#1]c1[cH]c2[cH][cH][cH][cH]c2oc1=O
KRFP2009	KRFPC2009	[!#1]c1[cH]c2C(=N[OH])[CH2][CH2][CH2][CH2]c2s1
KRFP2010	KRFPC2010	[!#1]c1[cH]c2nc3[cH][cH][cH][cH]c3nc2[cH]c1[!#1]
KRFP2011	KRFPC2011	[!#1]c1[cH]c2O[CH2][CH2]Oc2[cH]c1[!#1]
KRFP2012	KRFPC2012	[!#1]c1[cH]c2O[CH2]Oc2[cH]c1[!#1]
KRFP2013	KRFPC2013	[!#1]c1[cH]n([!#1])c2[cH][cH][cH][cH]c12
KRFP2014	KRFPC2014	[!#1]c1[cH]n([!#1])c2[cH][cH]c([!#1])[cH]c12
KRFP2015	KRFPC2015	[!#1]c1[cH]n([!#1])nc1[!#1]
KRFP2016	KRFPC2016	[!#1]c1[cH]n(C(=O)[CH3])c2[cH][cH][cH][cH]c12
KRFP2017	KRFPC2017	[!#1]c1[cH]n(nc1c2[cH][cH][cH][cH]c2)c3[cH][cH][cH][cH]c3
KRFP2018	KRFPC2018	[!#1]c1[cH]n[cH]c([!#1])[cH]1
KRFP2019	KRFPC2019	[!#1]c1[cH]n[cH]c(Br)[cH]1
KRFP2020	KRFPC2020	[!#1]c1[cH]n[nH]c1[!#1]
KRFP2021	KRFPC2021	[!#1]c1[cH]n2[cH][cH][cH][cH]c2n1
KRFP2022	KRFPC2022	[!#1]c1[cH]n2[CH2][CH2][CH2]c2n1
KRFP2023	KRFPC2023	[!#1]c1[cH]n2c(n1)n([!#1])c3[cH][cH][cH][cH]c32
KRFP2024	KRFPC2024	[!#1]c1[cH]nc([!#1])c([!#1])[cH]1

Name	Count name	Pattern
KRFP2025	KRFPC2025	[!#1]c1[cH]nc(!#1)n[cH]1
KRFP2026	KRFPC2026	[!#1]c1[cH]nc(!#1)n1[!#1]
KRFP2027	KRFPC2027	[!#1]c1[cH]nc(!#1)o1
KRFP2028	KRFPC2028	[!#1]c1[cH]nc2[cH][cH][cH][cH]c2[cH]1
KRFP2029	KRFPC2029	[!#1]c1[cH]nc2[cH][cH][cH][cH]c2n1
KRFP2030	KRFPC2030	[!#1]c1[cH]nn(!#1)c1[!#1]
KRFP2031	KRFPC2031	[!#1]c1[cH]nn([cH]1)c2[cH][cH][cH][cH]c2
KRFP2032	KRFPC2032	[!#1]c1[cH]oc2[cH][cH]c(!#1)c(!#1)c12
KRFP2033	KRFPC2033	[!#1]c1[cH]oc2c1[cH]c(!#1)c3[cH][cH][cH][cH]c23
KRFP2034	KRFPC2034	[!#1]c1[cH]sc(!#1)n1
KRFP2035	KRFPC2035	[!#1]c1[cH]sc([NH2])n1
KRFP2036	KRFPC2036	[!#1]c1[n+](!#1)[cH][cH]c2[cH][cH][cH][cH]c12
KRFP2037	KRFPC2037	[!#1]c1[nH]c(!#1)c(!#1)c1[!#1]
KRFP2038	KRFPC2038	[!#1]c1[nH]c2[cH][cH][cH][cH]c2c1[!#1]
KRFP2039	KRFPC2039	[!#1]c1[nH]c2[cH][cH]c(!#1)[cH]c2c1[!#1]
KRFP2040	KRFPC2040	[!#1]c1[nH]n[cH]c1l
KRFP2041	KRFPC2041	[!#1]c1[nH]nc([CH3])c1[N+](=O)[O-]
KRFP2042	KRFPC2042	[!#1]c1[nH]nc([CH3])c1Br
KRFP2043	KRFPC2043	[!#1]C1=[CH][CH2][CH2][CH2][CH2]1
KRFP2044	KRFPC2044	[!#1]C1=[CH][NH][CH]2[CH]=[CH][CH]=[CH][CH]21
KRFP2045	KRFPC2045	[!#1]C1=[CH]C(=O)[CH]=[CH]C1=O
KRFP2046	KRFPC2046	[!#1]C1=[CH]C(=O)[CH2]C(!#1)([CH3])[CH2]1
KRFP2047	KRFPC2047	[!#1]C1=[CH]C(=O)[CH2]C([CH3])([CH3])[CH2]1
KRFP2048	KRFPC2048	[!#1]C1=[CH]C(=O)c2[cH][cH][cH][cH]c2C1=O
KRFP2049	KRFPC2049	[!#1]C1=[CH]C(=O)OC21[CH2][CH2][CH2][CH2][CH2]2
KRFP2050	KRFPC2050	[!#1]C1=[CH]O[CH2][CH2]O1
KRFP2051	KRFPC2051	[!#1]C1=C(!#1)[CH]([NH]C(=O)[NH]1)c2[cH][cH][cH][cH]c2
KRFP2052	KRFPC2052	[!#1]C1=C(!#1)[CH]([NH]C(=O)[NH]1)c2[cH][cH][cH]c(!#1)[cH]2
KRFP2053	KRFPC2053	[!#1]C1=C(!#1)[CH](C2=C([CH2]C(!#1)([CH3])[CH2]C2=O)[NH]1)c3 [cH][cH][cH]c(!#1)[cH]3
KRFP2054	KRFPC2054	[!#1]C1=C(!#1)C(=O)[CH2]C(!#1)([CH3])[CH2]1
KRFP2055	KRFPC2055	[!#1]C1=C(!#1)C(=O)c2[cH][cH][cH][cH]c2C1=O
KRFP2056	KRFPC2056	[!#1]C1=C([OH])[CH2]C([CH3])([CH3])[CH2]C1=O
KRFP2057	KRFPC2057	[!#1]C1=C([OH])C(=O)c2[cH][cH][cH][cH]c2C1=O
KRFP2058	KRFPC2058	[!#1]C1=C(C(=O)c2[cH][cH][cH][cH]c12)c3[cH][cH][cH][cH]c3
KRFP2059	KRFPC2059	[!#1]C1=C2[NH]c3[cH][cH][cH][cH]c3N2[CH2][CH2]C1=O
KRFP2060	KRFPC2060	[!#1]C1=N[CH2][CH2][NH]1
KRFP2061	KRFPC2061	[!#1]C1=N[CH2][CH2]c2[cH][cH][cH][cH]c12
KRFP2062	KRFPC2062	[!#1]C1=N[CH2][CH2]n2[cH][cH][cH]c12
KRFP2063	KRFPC2063	[!#1]C1=N[NH]C([CH2]1)(c2[cH][cH][cH][cH]c2)c3[cH][cH][cH][cH]c3
KRFP2064	KRFPC2064	[!#1]C1=Nc2[cH][cH][cH][cH]c2[CH2][CH2][CH2]1
KRFP2065	KRFPC2065	[!#1]C12[CH2][CH2][CH2][CH]2[CH]3[CH2][CH2][CH]1[CH2]3
KRFP2066	KRFPC2066	[!#1]c1c(!#1)c(!#1)c(!#1)c(!#1)c1[!#1]
KRFP2067	KRFPC2067	[!#1]c1c(!#1)c(=O)n(c2[cH][cH][cH][cH]c2n1[!#1])
KRFP2068	KRFPC2068	[!#1]c1c(!#1)c2[cH][cH][cH][cH]c2n1[!#1]
KRFP2069	KRFPC2069	[!#1]c1c(!#1)c2[cH][cH][cH][cH]c2oc1=O
KRFP2070	KRFPC2070	[!#1]c1c(!#1)c2[cH][cH][cH][cH]c2sc1=O
KRFP2071	KRFPC2071	[!#1]c1c(!#1)c2[cH]c(!#1)[cH][cH]c2n1[!#1]
KRFP2072	KRFPC2072	[!#1]c1c(!#1)c2[cH]c(!#1)[cH][cH]c2n1c3[cH][cH][cH][cH]c3
KRFP2073	KRFPC2073	[!#1]c1c(!#1)c2[cH]c(!#1)c(!#1)[cH]c2n1[!#1]
KRFP2074	KRFPC2074	[!#1]c1c([cH][cH][cH]c1[N+](=O)[O-])C(=O)[OH]
KRFP2075	KRFPC2075	[!#1]c1c([cH][cH]c2nonc12)[N+](=O)[O-]
KRFP2076	KRFPC2076	[!#1]c1c([cH]c([cH]c1[CH]([CH3])[CH3])[CH]([CH3])[CH3])[CH]([CH3])[CH3]
KRFP2077	KRFPC2077	[!#1]c1c([cH]c([cH]c1[N+](=O)[O-])C(=O)[OH])[N+](=O)[O-]

Name	Count name	Pattern
KRFP2078	KRFPC2078	[!#1]c1c([cH]c([cH]c1[N+](=O)[O-])C(F)(F)F)[N+](=O)[O-]
KRFP2079	KRFPC2079	[!#1]c1c([cH]c([CH3])[cH]c1[N+](=O)[O-])[N+](=O)[O-]
KRFP2080	KRFPC2080	[!#1]c1c([cH]c([N+](=O)[O-])c2[cH][cH]nc12)[N+](=O)[O-]
KRFP2081	KRFPC2081	[!#1]c1c([cH]nn1[CH3])[N+](=O)[O-]
KRFP2082	KRFPC2082	[!#1]c1c([CH3])[cH][cH][cH]c1[CH3]
KRFP2083	KRFPC2083	[!#1]c1c([CH3])[cH][cH]c([CH3])c1[CH3]
KRFP2084	KRFPC2084	[!#1]c1c([CH3])[cH]c([CH3])[cH]c1[CH3]
KRFP2085	KRFPC2085	[!#1]c1c([CH3])[cH]c([CH3])c([CH]=N[OH])c1[CH3]
KRFP2086	KRFPC2086	[!#1]c1c([CH3])[cH]c(Br)[cH]c1[CH3]
KRFP2087	KRFPC2087	[!#1]c1c([CH3])[nH]c2[cH][cH][cH][cH]c12
KRFP2088	KRFPC2088	[!#1]c1c([CH3])c([CH2][CH3])nc2[cH][cH][cH][cH]c12
KRFP2089	KRFPC2089	[!#1]c1c([CH3])n(!#1)n(!#1)c1=O
KRFP2090	KRFPC2090	[!#1]c1c([CH3])n([CH3])n(c2[cH][cH][cH][cH]2)c1=O
KRFP2091	KRFPC2091	[!#1]c1c([CH3])nn(!#1)c1[CH3]
KRFP2092	KRFPC2092	[!#1]c1c([N+](=O)[O-])c(!#1)c([N+](=O)[O-])c(!#1)c1[N+](=O)[O-]
KRFP2093	KRFPC2093	[!#1]c1c([nH]c2[cH][cH]c(!#1)[cH]c12)C(=O)[OH]
KRFP2094	KRFPC2094	[!#1]c1c([OH])[cH][cH]c2[cH][cH][cH][cH]c12
KRFP2095	KRFPC2095	[!#1]c1c([OH])[cH]c([OH])[cH]c1[OH]
KRFP2096	KRFPC2096	[!#1]c1c([OH])c2[cH][cH][cH][cH]c2oc1=O
KRFP2097	KRFPC2097	[!#1]c1c([OH])c2[cH][cH][cH][cH]c2sc1=O
KRFP2098	KRFPC2098	[!#1]c1c(Br)[cH]c(Br)[cH]c1Br
KRFP2099	KRFPC2099	[!#1]c1c(Br)[cH]c(Br)c2[cH][cH][cH]nc12
KRFP2100	KRFPC2100	[!#1]c1c(c2[cH][cH][cH][cH][cH]2)c3[cH]c(!#1)[cH][cH]c3n1(!#1)
KRFP2101	KRFPC2101	[!#1]c1c(Cl)[cH][cH][cH]c1Cl
KRFP2102	KRFPC2102	[!#1]c1c(Cl)[cH]c(Cl)[cH]c1Cl
KRFP2103	KRFPC2103	[!#1]c1c(F)[cH][cH][cH]c1F
KRFP2104	KRFPC2104	[!#1]c1c(F)c(F)c(!#1)c(F)c1F
KRFP2105	KRFPC2105	[!#1]c1c(F)c(F)c(F)c(F)c1F
KRFP2106	KRFPC2106	[!#1]c1c(n[cH]n1[CH3])[N+](=O)[O-]
KRFP2107	KRFPC2107	[!#1]c1c(nc([CH3])n1(!#1))[N+](=O)[O-]
KRFP2108	KRFPC2108	[!#1]c1c2[CH]([OH])[CH2]C([CH3])([CH3])[CH2]c2nc3[cH][cH][cH][cH]c13
KRFP2109	KRFPC2109	[!#1]c1c2[cH][cH][cH][cH]c2[cH]c3[cH][cH][cH][cH]c13
KRFP2110	KRFPC2110	[!#1]c1c2[cH][cH][cH][cH]c2c(!#1)c3[cH][cH][cH][cH]c13
KRFP2111	KRFPC2111	[!#1]c1c2[cH][cH][cH][cH]c2n3c([CH3])nc4[cH][cH][cH][cH]c4c13
KRFP2112	KRFPC2112	[!#1]c1c2[cH][cH][cH][cH]c2nc3[cH][cH][cH][cH]c13
KRFP2113	KRFPC2113	[!#1]c1c2[CH2][CH2][CH2][CH2]c2nc3[cH][cH][cH][cH]c13
KRFP2114	KRFPC2114	[!#1]c1c2[CH2][CH2][CH2]c2nc3[cH][cH][cH][cH]c13
KRFP2115	KRFPC2115	[!#1]c1c2[CH2][CH2][CH2]c2nc3[CH2][CH2][CH2][CH2]c13
KRFP2116	KRFPC2116	[!#1]c1c2[CH2][CH2][CH2]c2nc3[CH2][CH2][CH2]c31
KRFP2117	KRFPC2117	[!#1]c1c2[CH2][CH2]N([CH3])c2nc3[cH][cH][cH][cH]c13
KRFP2118	KRFPC2118	[!#1]c1c2C(=O)[CH2]C(!#1)([CH3])[CH2]c2nc3[cH][cH][cH][cH]c13
KRFP2119	KRFPC2119	[!#1]c1c2C(=O)[CH2]C([CH3])([CH3])[CH2]c2nc3[cH][cH][cH][cH]c13
KRFP2120	KRFPC2120	[!#1]c1n(!#1)c2[cH][cH][cH][cH]c2[n+]1(!#1)
KRFP2121	KRFPC2121	[!#1]c1n(!#1)c2[cH][cH]c(!#1)[cH]c2[n+]1(!#1)
KRFP2122	KRFPC2122	[!#1]c1n([CH3])c2[cH][cH][cH][cH]c2[n+]1[CH3]
KRFP2123	KRFPC2123	[!#1]c1n[cH][cH][cH]c1[CH3]
KRFP2124	KRFPC2124	[!#1]c1n[cH][cH][cH]c1[OH]
KRFP2125	KRFPC2125	[!#1]c1n[cH][cH][cH]n1
KRFP2126	KRFPC2126	[!#1]c1n[cH][cH]c(n1)c2[cH][cH][cH][cH]c12
KRFP2127	KRFPC2127	[!#1]c1n[cH][cH]n1(!#1)
KRFP2128	KRFPC2128	[!#1]c1n[cH][cH]nc1(!#1)
KRFP2129	KRFPC2129	[!#1]c1n[cH][cH]nc1C(=O)[OH]
KRFP2130	KRFPC2130	[!#1]c1n[cH][cH]nc1O[CH3]
KRFP2131	KRFPC2131	[!#1]c1n[cH][cH]s1

Name	Count name	Pattern
KRFP2132	KRFPC2132	[!#1]c1n[cH][nH]c1[!#1]
KRFP2133	KRFPC2133	[!#1]c1n[cH][nH]n1
KRFP2134	KRFPC2134	[!#1]c1n[cH]c(s1)c2[cH][cH][cH][cH]2
KRFP2135	KRFPC2135	[!#1]c1n[cH]n([!#1])c1[!#1]
KRFP2136	KRFPC2136	[!#1]c1n[cH]n[nH]1
KRFP2137	KRFPC2137	[!#1]c1n[cH]nc([!#1])c1[!#1]
KRFP2138	KRFPC2138	[!#1]c1n[cH]nc2[nH][cH]nc12
KRFP2139	KRFPC2139	[!#1]c1n[cH]nc2n[cH][nH]c12
KRFP2140	KRFPC2140	[!#1]c1n[cH]nc2sc([CH3])c([CH3])c12
KRFP2141	KRFPC2141	[!#1]c1n[cH]nc2sc3[CH2][CH2][CH2][CH2]c3c12
KRFP2142	KRFPC2142	[!#1]c1n[nH]c([!#1])c1[!#1]
KRFP2143	KRFPC2143	[!#1]c1n[nH]c([!#1])n1
KRFP2144	KRFPC2144	[!#1]c1n[nH]c([NH2])n1
KRFP2145	KRFPC2145	[!#1]c1n[nH]c(=O)[nH]c1=O
KRFP2146	KRFPC2146	[!#1]c1n[nH]c(=O)c2[cH][cH][cH][cH]c12
KRFP2147	KRFPC2147	[!#1]c1n[nH]c(=S)[nH]c1=O
KRFP2148	KRFPC2148	[!#1]c1n[nH]c2[CH2][CH2][CH2][CH2]c12
KRFP2149	KRFPC2149	[!#1]c1nc([!#1])c([!#1])[nH]1
KRFP2150	KRFPC2150	[!#1]c1nc([!#1])c([!#1])c([!#1])n1
KRFP2151	KRFPC2151	[!#1]c1nc([!#1])c([!#1])s1
KRFP2152	KRFPC2152	[!#1]c1nc([!#1])c2[cH][cH][cH][cH]c2n1
KRFP2153	KRFPC2153	[!#1]c1nc([!#1])c2c3[CH2][CH2][CH2][CH2]c3sc2n1
KRFP2154	KRFPC2154	[!#1]c1nc([!#1])n([!#1])n1
KRFP2155	KRFPC2155	[!#1]c1nc([!#1])nc([!#1])n1
KRFP2156	KRFPC2156	[!#1]c1nc([!#1])nc([NH][CH3])n1
KRFP2157	KRFPC2157	[!#1]c1nc([!#1])nc([NH]N=[CH]c2[cH][cH][cH]c([N+](=O)[O-])c2[OH])n1
KRFP2158	KRFPC2158	[!#1]c1nc([!#1])nc(Cl)n1
KRFP2159	KRFPC2159	[!#1]c1nc([!#1])nc(n1)N2[CH2][CH2][CH2][CH2][CH2]2
KRFP2160	KRFPC2160	[!#1]c1nc([!#1])nc(n1)N2[CH2][CH2][NH][CH2][CH2]2
KRFP2161	KRFPC2161	[!#1]c1nc([!#1])nc(n1)N2[CH2][CH2]O[CH2][CH2]2
KRFP2162	KRFPC2162	[!#1]c1nc([!#1])nc(O[CH](C(F)(F)F)C(F)(F)F)n1
KRFP2163	KRFPC2163	[!#1]c1nc([!#1])nc(O[CH3])n1
KRFP2164	KRFPC2164	[!#1]c1nc([cH]c(n1)c2[cH][cH][cH][cH]c2)c3[cH][cH][cH][cH]3
KRFP2165	KRFPC2165	[!#1]c1nc([cH]s1)C2([CH2][CH]3[CH2][CH]4[CH2][CH]([CH2]3)[CH2]2) [CH2]4
KRFP2166	KRFPC2166	[!#1]c1nc([cH]s1)c2[cH][cH][cH][cH]c2
KRFP2167	KRFPC2167	[!#1]c1nc([cH]s1)c2[cH][cH]c([!#1])[cH]c2
KRFP2168	KRFPC2168	[!#1]c1nc([cH]s1)c2[cH][cH]c([!#1])c([!#1])c2
KRFP2169	KRFPC2169	[!#1]c1nc([CH3])[cH][cH]c1[OH]
KRFP2170	KRFPC2170	[!#1]c1nc([CH3])[cH]c([CH3])n1
KRFP2171	KRFPC2171	[!#1]c1nc([CH3])[cH]s1
KRFP2172	KRFPC2172	[!#1]c1nc([CH3])nc(O[CH3])n1
KRFP2173	KRFPC2173	[!#1]c1nc([CH3])nc2sc3[CH2][CH2][CH2][CH2]c3c12
KRFP2174	KRFPC2174	[!#1]c1nc([NH2])nc(Cl)n1
KRFP2175	KRFPC2175	[!#1]c1nc([OH])[cH]c(=O)[nH]1
KRFP2176	KRFPC2176	[!#1]c1nc(=O)c([!#1])c([!#1])[nH]1
KRFP2177	KRFPC2177	[!#1]c1nc(c([!#1])s1)c2[cH][cH][cH][cH]c2
KRFP2178	KRFPC2178	[!#1]c1nc(c([!#1])s1)c2[cH][cH]c([!#1])[cH]c2
KRFP2179	KRFPC2179	[!#1]c1nc(Cl)nc(Cl)n1
KRFP2180	KRFPC2180	[!#1]c1nc(l)[cH][cH]c1[OH]
KRFP2181	KRFPC2181	[!#1]c1nc(nc(n1)N2[CH2][CH2]O[CH2][CH2]2)N3[CH2][CH2][CH2][CH2][CH2]3
KRFP2182	KRFPC2182	[!#1]c1nc(nc(n1)N2[CH2][CH2]O[CH2][CH2]2)N3[CH2][CH2]O[CH2][CH2]3
KRFP2183	KRFPC2183	[!#1]c1nc(O[CH3])nc(O[CH3])n1
KRFP2184	KRFPC2184	[!#1]c1nc2[cH][cH][cH][cH]c2[nH]1
KRFP2185	KRFPC2185	[!#1]c1nc2[cH][cH][cH][cH]c2[nH]c1=O

Name	Count name	Pattern
KRFP2186	KRFPC2186	[!#1]c1nc2[cH][cH][cH][cH]c2c(!#1)c1(!#1)
KRFP2187	KRFPC2187	[!#1]c1nc2[cH][cH][cH][cH]c2c(=O)[nH]1
KRFP2188	KRFPC2188	[!#1]c1nc2[cH][cH][cH][cH]c2c(=O)n1c3[cH][cH][cH][cH][cH]3
KRFP2189	KRFPC2189	[!#1]c1nc2[cH][cH][cH][cH]c2c(=O)o1
KRFP2190	KRFPC2190	[!#1]c1nc2[cH][cH][cH][cH]c2c3[cH][cH][cH][cH]c13
KRFP2191	KRFPC2191	[!#1]c1nc2[cH][cH][cH][cH]c2n1(!#1)
KRFP2192	KRFPC2192	[!#1]c1nc2[cH][cH][cH][cH]c2nc1(!#1)
KRFP2193	KRFPC2193	[!#1]c1nc2[cH][cH][cH][cH]c2o1
KRFP2194	KRFPC2194	[!#1]c1nc2[cH][cH][cH][cH]c2s1
KRFP2195	KRFPC2195	[!#1]c1nc2[cH][cH][cH][cH]n2c1(!#1)
KRFP2196	KRFPC2196	[!#1]c1nc2[cH][cH]c(!#1)[cH]c2[nH]1
KRFP2197	KRFPC2197	[!#1]c1nc2[cH][cH]c(!#1)[cH]c2o1
KRFP2198	KRFPC2198	[!#1]c1nc2[cH][cH]c(!#1)[cH]c2s1
KRFP2199	KRFPC2199	[!#1]c1nc2[cH][cH]c([CH3])[cH]c2s1
KRFP2200	KRFPC2200	[!#1]c1nc2[cH]c(!#1)[cH][cH]c2[nH]1
KRFP2201	KRFPC2201	[!#1]c1nc2[cH]c(!#1)[cH][cH]c2o1
KRFP2202	KRFPC2202	[!#1]c1nc2[cH]c(!#1)[cH][cH]c2s1
KRFP2203	KRFPC2203	[!#1]c1nc2[cH]c(Cl)[cH][cH]c2o1
KRFP2204	KRFPC2204	[!#1]c1nc2n(!#1)c(=O)[nH]c(=O)c2n1(!#1)
KRFP2205	KRFPC2205	[!#1]c1nc2n(!#1)c(=O)n(!#1)c(=O)c2n1(!#1)
KRFP2206	KRFPC2206	[!#1]c1nc2nc(!#1)[cH]c(!#1)n2n1
KRFP2207	KRFPC2207	[!#1]c1nc2nc([cH]c(c3[cH][cH][cH][cH][cH]3)n2n1)c4[cH][cH][cH][cH][cH]4
KRFP2208	KRFPC2208	[!#1]c1nc2nc([CH3])[cH]c([CH3])n2n1
KRFP2209	KRFPC2209	[!#1]c1nc2nonc2nc1(!#1)
KRFP2210	KRFPC2210	[!#1]c1nc2sc3[CH2][CH2][CH2][CH2]c3c2c(=O)n1(!#1)
KRFP2211	KRFPC2211	[!#1]c1nc2sc3[CH2][CH2][CH2][CH2]c3c2s1
KRFP2212	KRFPC2212	[!#1]c1nn(!#1)c(!#1)c1(!#1)
KRFP2213	KRFPC2213	[!#1]c1nn([CH3])[cH]c1Br
KRFP2214	KRFPC2214	[!#1]c1nn(c(!#1)c1(!#1))c2[cH][cH][cH][cH][cH]2
KRFP2215	KRFPC2215	[!#1]c1nn(c(!#1)c1(!#1))c2[cH][cH]c(!#1)[cH][cH]2
KRFP2216	KRFPC2216	[!#1]c1nn[cH][nH]1
KRFP2217	KRFPC2217	[!#1]c1nn[cH]n1c2[cH][cH][cH][cH][cH]2
KRFP2218	KRFPC2218	[!#1]c1nnc(!#1)n1(!#1)
KRFP2219	KRFPC2219	[!#1]c1nnc(!#1)n1c2[cH][cH][cH][cH][cH]2
KRFP2220	KRFPC2220	[!#1]c1nnc(!#1)o1
KRFP2221	KRFPC2221	[!#1]c1nnc(!#1)s1
KRFP2222	KRFPC2222	[!#1]c1nnc([CH2][CH3])s1
KRFP2223	KRFPC2223	[!#1]c1nnc([CH3])s1
KRFP2224	KRFPC2224	[!#1]c1nnc([NH2])s1
KRFP2225	KRFPC2225	[!#1]c1nnc2c(!#1)nc3nonc3n12
KRFP2226	KRFPC2226	[!#1]c1nnc2c3[cH][cH][cH][cH]c3[nH]c2n1
KRFP2227	KRFPC2227	[!#1]c1nnn[nH]1
KRFP2228	KRFPC2228	[!#1]c1nnnn1(!#1)
KRFP2229	KRFPC2229	[!#1]c1nnnn1c2[cH][cH][cH][cH][cH]2
KRFP2230	KRFPC2230	[!#1]c1nnnn1c2c(!#1)[cH][cH][cH]c2(!#1)
KRFP2231	KRFPC2231	[!#1]c1nnnn1c2c([CH3])[cH][cH][cH]c2[CH3]
KRFP2232	KRFPC2232	[!#1]c1no[n+](!#1)c1(!#1)
KRFP2233	KRFPC2233	[!#1]c1nonc1(!#1)
KRFP2234	KRFPC2234	[!#1]c1oc2[cH][cH][cH][cH]c2[n+](!#1)
KRFP2235	KRFPC2235	[!#1]c1oc2[cH][cH]c(!#1)[cH]c2c1(!#1)
KRFP2236	KRFPC2236	[!#1]c1oc2[cH][cH]c(!#1)c(!#1)c2c1(!#1)
KRFP2237	KRFPC2237	[!#1]c1oc2[cH]c(!#1)c(!#1)[cH]c2c1(!#1)
KRFP2238	KRFPC2238	[!#1]c1oc2c(!#1)c(!#1)c(!#1)[cH]c2c1(!#1)
KRFP2239	KRFPC2239	[!#1]c1s[cH][n+](!#1)c1(!#1)

Name	Count name	Pattern
KRFP2240	KRFPC2240	[!#1]c1s[cH][n+](!!#1)c1[CH3]
KRFP2241	KRFPC2241	[!#1]c1s[cH]c(c1!!#1)c2[cH][cH][cH][cH]2
KRFP2242	KRFPC2242	[!#1]c1sc(!!#1)c(!!#1)c1!!#1
KRFP2243	KRFPC2243	[!#1]c1sc(!!#1)c(c1!!#1)c2[cH][cH][cH][cH]2
KRFP2244	KRFPC2244	[!#1]c1sc([CH3])c([CH3])c1!!#1
KRFP2245	KRFPC2245	[!#1]c1sc2[cH][cH][cH][cH]c2[n+]1!!#1
KRFP2246	KRFPC2246	[!#1]c1sc2[cH][cH][cH][cH]c2c1!!#1
KRFP2247	KRFPC2247	[!#1]c1sc2[cH][cH][cH][cH]c2c1Cl
KRFP2248	KRFPC2248	[!#1]c1sc2[cH][cH]c(!!#1)[cH]c2[n+]1!!#1
KRFP2249	KRFPC2249	[!#1]c1sc2[cH][cH]c3[cH][cH][cH][cH]c3c2[n+]1!!#1
KRFP2250	KRFPC2250	[!#1]c1sc2[cH]c(!!#1)[cH][cH]c2c1!!#1
KRFP2251	KRFPC2251	[!#1]c1sc2[cH]c(F)[cH][cH]c2c1Cl
KRFP2252	KRFPC2252	[!#1]c1sc2[CH2][CH2][CH2][CH2]c2c1!!#1
KRFP2253	KRFPC2253	[!#1]c1sc2[CH2][CH2][CH2][CH2]c2c1C(=O)[NH2]
KRFP2254	KRFPC2254	[!#1]c1sc2c(!!#1)[cH][cH][cH]c2c1!!#1
KRFP2255	KRFPC2255	[!#1]c1sc2c(!!#1)c(!!#1)[cH][cH]c2c1!!#1
KRFP2256	KRFPC2256	[!#1]c1sc2C(=N[OH])[CH2][CH2][CH2]c2c1!!#1
KRFP2257	KRFPC2257	[!#1]c1sc2C(=O)[CH2][CH2][CH2]c2c1!!#1
KRFP2258	KRFPC2258	[!#1]c1sc2n[cH]nc(!!#1)c2c1!!#1
KRFP2259	KRFPC2259	[!#1]Cl
KRFP2260	KRFPC2260	[!#1]F
KRFP2261	KRFPC2261	[!#1]I
KRFP2262	KRFPC2262	[!#1]N(!!#1)!!#1
KRFP2263	KRFPC2263	[!#1]N(!!#1)[CH2]c1[cH][cH][cH][cH]1
KRFP2264	KRFPC2264	[!#1]N(!!#1)[CH3]
KRFP2265	KRFPC2265	[!#1]N(!!#1)C(=O)!!#1
KRFP2266	KRFPC2266	[!#1]N(!!#1)C(=O)O[CH2][CH3]
KRFP2267	KRFPC2267	[!#1]N(!!#1)c1[cH][cH][cH][cH]1
KRFP2268	KRFPC2268	[!#1]N(!!#1)c1[cH][cH][cH]c2[cH][cH][cH]c12
KRFP2269	KRFPC2269	[!#1]N([CH]([CH]([CH3])[CH3])C(=O)!!#1)C(=O)c1[cH][cH][cH][cH]c1C(=O)!!#1
KRFP2270	KRFPC2270	[!#1]N([CH]([CH]([CH3])[CH3])C(=O)[OH])C(=S)SC(!!#1)(!!#1)C(=O)!!#1
KRFP2271	KRFPC2271	[!#1]N([CH]([CH2]c1[cH][cH][cH][cH]1)C(=O)!!#1)C(=O)c2[cH][cH][cH][cH]c2C(=O)!!#1
KRFP2272	KRFPC2272	[!#1]N([CH]([CH2]c1[cH][cH]c([cH][cH]1)[N+](=O)[O-])C(=O)!!#1)C(=O)c2[cH][cH][cH][cH]c2C(=O)!!#1
KRFP2273	KRFPC2273	[!#1]N([CH]([CH3])[CH3])[CH]([CH3])[CH3]
KRFP2274	KRFPC2274	[!#1]N([CH]1[CH2][CH2][CH2][CH2][CH2]1)[CH]2[CH2][CH2][CH2][CH2][CH2]2
KRFP2275	KRFPC2275	[!#1]N([CH2][CH2][CH2][CH2]C(=O)!!#1)C(=O)c1[cH][cH][cH][cH]c1C(=O)!!#1
KRFP2276	KRFPC2276	[!#1]N([CH2][CH2][CH2][CH3])[CH2][CH2][CH2][CH3]
KRFP2277	KRFPC2277	[!#1]N([CH2][CH2][CH2][CH3])C(=O)!!#1
KRFP2278	KRFPC2278	[!#1]N([CH2][CH2][CH2]C(=O)!!#1)[CH2]C(=O)!!#1
KRFP2279	KRFPC2279	[!#1]N([CH2][CH2][CH2]C(=O)!!#1)C(=O)c1[cH][cH][cH][cH]c1C(=O)!!#1
KRFP2280	KRFPC2280	[!#1]N([CH2][CH2][CH2]C(=O)!!#1)C(=S)SC(!!#1)(!!#1)C(=O)!!#1
KRFP2281	KRFPC2281	[!#1]N([CH2][CH2][CH2]C(=O)!!#1)c1[cH][cH]c([cH][cH]1)S(=O)(=O)!!#1
KRFP2282	KRFPC2282	[!#1]N([CH2][CH2][CH2]S(=O)(=O)[OH])c1[cH][cH][cH][cH]c1SC(!!#1)(!!#1)!!#1
KRFP2283	KRFPC2283	[!#1]N([CH2][CH2][OH])[CH2][CH2][OH]
KRFP2284	KRFPC2284	[!#1]N([CH2][CH2]C(=O)!!#1)C(=O)c1[cH][cH][cH][cH]c1C(=O)!!#1
KRFP2285	KRFPC2285	[!#1]N([CH2][CH2]C(=O)!!#1)C(=S)SC(!!#1)(!!#1)C(=O)!!#1
KRFP2286	KRFPC2286	[!#1]N([CH2][CH2]C(=O)[OH])C(=S)SC(!!#1)(!!#1)C(=O)!!#1
KRFP2287	KRFPC2287	[!#1]N([CH2][CH3])[CH2][CH2][OH]

Name	Count name	Pattern
KRFP2288	KRFPC2288	[!#1]N([CH2][CH3])[CH2][CH3]
KRFP2289	KRFPC2289	[!#1]N([CH2][CH3])C(=O)[!#1]
KRFP2290	KRFPC2290	[!#1]N([CH2][CH3])c1[cH][cH][cH][cH]1
KRFP2291	KRFPC2291	[!#1]N([CH2]C([CH3])([CH3])[CH2][CH]=C([CH3])[CH3])C(=O)[CH3]
KRFP2292	KRFPC2292	[!#1]N([CH2]C(=O)[!#1])C(=O)c1[cH][cH][cH][cH]c1C(=O)[!#1]
KRFP2293	KRFPC2293	[!#1]N([CH2]C(=O)[!#1])C(=O)c1[cH][cH][cH]c2[cH][cH][cH]c(C(=O)[!#1])c12
KRFP2294	KRFPC2294	[!#1]N([CH2]C(=O)[!#1])C(=O)SC([!#1])([!#1])C(=O)[!#1]
KRFP2295	KRFPC2295	[!#1]N([CH2]C(=O)[!#1])C(=S)SC([!#1])([!#1])C(=O)[!#1]
KRFP2296	KRFPC2296	[!#1]N([CH2]C(=O)[OH])[CH2]C(=O)[OH]
KRFP2297	KRFPC2297	[!#1]N([CH2]C(=O)[OH])C(=S)SC([!#1])([!#1])C(=O)[!#1]
KRFP2298	KRFPC2298	[!#1]N([CH2]c1[cH][cH][cH][cH]1)[CH2]c2[cH][cH][cH][cH]2
KRFP2299	KRFPC2299	[!#1]N([CH2]c1[cH][cH][cH][cH]1)C([CH3])([CH3])[CH3]
KRFP2300	KRFPC2300	[!#1]N([CH2]c1[cH][cH][cH][cH]1)C(=S)SC([!#1])([!#1])C(=O)[!#1]
KRFP2301	KRFPC2301	[!#1]N([CH2]c1[cH][cH]c(Cl)[cH]c1Cl)c2[cH][cH][cH]c(Cl)[cH]2
KRFP2302	KRFPC2302	[!#1]N([CH2]c1[cH][cH]c(F)[cH][cH]1)c2[cH][cH]c(I)[cH][cH]2
KRFP2303	KRFPC2303	[!#1]N([CH3])[CH2][CH2][OH]
KRFP2304	KRFPC2304	[!#1]N([CH3])[CH2]C(=O)[OH]
KRFP2305	KRFPC2305	[!#1]N([CH3])[CH2]c1[cH][cH][cH][cH]1
KRFP2306	KRFPC2306	[!#1]N([CH3])[CH3]
KRFP2307	KRFPC2307	[!#1]N([CH3])C(=[NH])[NH]C(=[NH])[NH2]
KRFP2308	KRFPC2308	[!#1]N([CH3])C(=O)[!#1]
KRFP2309	KRFPC2309	[!#1]N([CH3])C(=O)[CH3]
KRFP2310	KRFPC2310	[!#1]N([CH3])c1[cH][cH][cH][cH]1
KRFP2311	KRFPC2311	[!#1]N([CH3])c1[cH][cH][cH][cH]c1C([!#1])([!#1])C(=O)[!#1]
KRFP2312	KRFPC2312	[!#1]N([CH3])c1[cH][cH]c([!#1])[cH][cH]1
KRFP2313	KRFPC2313	[!#1]N([CH3])c1[cH]c([!#1])c2[cH][cH][cH][cH]c2n1
KRFP2314	KRFPC2314	[!#1]N([CH3])S(=O)(=O)[!#1]
KRFP2315	KRFPC2315	[!#1]N(C(=O)[!#1])S(=O)(=O)[!#1]
KRFP2316	KRFPC2316	[!#1]N(C(=O)[CH]([CH2]C(=O)[!#1])S[CH2]C(=O)[!#1])c1[cH][cH][cH]c(Cl)[cH]1
KRFP2317	KRFPC2317	[!#1]N(C(=O)[CH2][CH2][CH3])S(=O)(=O)[!#1]
KRFP2318	KRFPC2318	[!#1]N(C(=O)[CH3])C(=O)[CH3]
KRFP2319	KRFPC2319	[!#1]N(C(=O)c1[cH]c([cH][cH]c1C(=O)[!#1])C(=O)[!#1])c2[cH][cH]c([cH][cH]2)C(=O)[!#1]
KRFP2320	KRFPC2320	[!#1]N(C(=O)c1[cH]c([cH][cH]c1C(=O)[!#1])C(=O)[OH])c2[cH][cH]c([!#1])[cH][cH]2
KRFP2321	KRFPC2321	[!#1]N(C(=S)SC([!#1])([!#1])C(=O)[!#1])c1[cH][cH]c([cH][cH]1)C(=O)[OH]
KRFP2322	KRFPC2322	[!#1]N(c1[cH][cH][cH][cH]1)c2[cH][cH][cH][cH]2
KRFP2323	KRFPC2323	[!#1]N=[CH][CH]([!#1])[!#1]
KRFP2324	KRFPC2324	[!#1]N=[CH][CH]=N[!#1]
KRFP2325	KRFPC2325	[!#1]N=[CH]c1[cH][cH][cH][cH]1
KRFP2326	KRFPC2326	[!#1]N=[CH]c1[cH][cH][cH][cH]c1[N+](=O)[O-]
KRFP2327	KRFPC2327	[!#1]N=[CH]c1[cH][cH][cH][cH]c1[OH]
KRFP2328	KRFPC2328	[!#1]N=[CH]c1[cH][cH][cH][cH]c1F
KRFP2329	KRFPC2329	[!#1]N=[CH]c1[cH][cH][cH][nH]1
KRFP2330	KRFPC2330	[!#1]N=[CH]c1[cH][cH][cH]c([cH]1)[N+](=O)[O-]
KRFP2331	KRFPC2331	[!#1]N=[CH]c1[cH][cH][cH]c([OH])[cH]1
KRFP2332	KRFPC2332	[!#1]N=[CH]c1[cH][cH][cH]c(Cl)[cH]1
KRFP2333	KRFPC2333	[!#1]N=[CH]c1[cH][cH][cH]c2[cH][cH][cH][cH]c12
KRFP2334	KRFPC2334	[!#1]N=[CH]c1[cH][cH][cH]n[cH]1
KRFP2335	KRFPC2335	[!#1]N=[CH]c1[cH][cH][cH]o1
KRFP2336	KRFPC2336	[!#1]N=[CH]c1[cH][cH]c([!#1])[cH][cH]1
KRFP2337	KRFPC2337	[!#1]N=[CH]c1[cH][cH]c([!#1])o1

Name	Count name	Pattern
KRFP2338	KRFPC2338	[!#1]N=[CH]c1[cH][cH]c([cH][cH]1)[N+](=O)[O-]
KRFP2339	KRFPC2339	[!#1]N=[CH]c1[cH][cH]c([cH][cH]1)N(!#1)[CH2][CH3]
KRFP2340	KRFPC2340	[!#1]N=[CH]c1[cH][cH]c([cH][cH]1)N(!#1)[CH3]
KRFP2341	KRFPC2341	[!#1]N=[CH]c1[cH][cH]c([CH]=N(!#1))[cH][cH]1
KRFP2342	KRFPC2342	[!#1]N=[CH]c1[cH][cH]c([CH3])o1
KRFP2343	KRFPC2343	[!#1]N=[CH]c1[cH][cH]c([OH])[cH][cH]1
KRFP2344	KRFPC2344	[!#1]N=[CH]c1[cH][cH]c([OH])[cH]c1[OH]
KRFP2345	KRFPC2345	[!#1]N=[CH]c1[cH][cH]c([OH])c([OH])[cH]1
KRFP2346	KRFPC2346	[!#1]N=[CH]c1[cH][cH]c(Br)[cH][cH]1
KRFP2347	KRFPC2347	[!#1]N=[CH]c1[cH][cH]c(Br)s1
KRFP2348	KRFPC2348	[!#1]N=[CH]c1[cH][cH]c(C#Cc2[cH][cH][cH][cH]2)[cH][cH]1
KRFP2349	KRFPC2349	[!#1]N=[CH]c1[cH][cH]c(Cl)[cH][cH]1
KRFP2350	KRFPC2350	[!#1]N=[CH]c1[cH][cH]c(Cl)[cH]c1Cl
KRFP2351	KRFPC2351	[!#1]N=[CH]c1[cH][cH]c(s1)[N+](=O)[O-]
KRFP2352	KRFPC2352	[!#1]N=[CH]c1[cH][cH]c2n(!#1)c3[cH][cH][cH][cH]c3c2[cH]1
KRFP2353	KRFPC2353	[!#1]N=[CH]c1[cH][cH]c2O[CH2]Oc2[cH]1
KRFP2354	KRFPC2354	[!#1]N=[CH]c1[cH][nH]c2[cH][cH][cH][cH]c12
KRFP2355	KRFPC2355	[!#1]N=[CH]c1[cH]c([cH][cH]c1[OH])[N+](=O)[O-]
KRFP2356	KRFPC2356	[!#1]N=[CH]c1[cH]c(Br)[cH][cH]c1[OH]
KRFP2357	KRFPC2357	[!#1]N=[CH]c1[cH]c(Br)[cH]c(c1[OH])C([CH3])([CH3])[CH3]
KRFP2358	KRFPC2358	[!#1]N=[CH]c1[cH]c(c([OH])c([cH]1)C([CH3])([CH3])[CH3])C([CH3])([CH3])[CH3]
KRFP2359	KRFPC2359	[!#1]N=[CH]c1[cH]c(Cl)[cH]c(Cl)c1[OH]
KRFP2360	KRFPC2360	[!#1]N=[CH]c1[cH]c2O[CH2]Oc2[cH]c1[N+](=O)[O-]
KRFP2361	KRFPC2361	[!#1]N=[CH]c1c([CH3])[nH]n(!#1)c1=O
KRFP2362	KRFPC2362	[!#1]N=[CH]c1c([OH])[cH][cH]c2[cH][cH][cH][cH]c12
KRFP2363	KRFPC2363	[!#1]N=[CH]c1c2[cH][cH][cH][cH]c2[cH]c3[cH][cH][cH][cH]c13
KRFP2364	KRFPC2364	[!#1]N=[CH]c1s[cH][cH]c1[CH3]
KRFP2365	KRFPC2365	[!#1]N=[CH]N([CH3])[CH3]
KRFP2366	KRFPC2366	[!#1]N=[N+](!#1)[O-]
KRFP2367	KRFPC2367	[!#1]N=[N+]=[N-]
KRFP2368	KRFPC2368	[!#1]N=C([CH](!#1)!#1)[CH](!#1)!#1
KRFP2369	KRFPC2369	[!#1]N=C([CH3])N([CH3])[CH3]
KRFP2370	KRFPC2370	[!#1]N=C(O[CH3])c1[cH][cH]c([CH3])[cH][cH]1
KRFP2371	KRFPC2371	[!#1]N=C(OC(=O)C(!#1)(!#1)!#1)c1[cH][cH][cH][cH]1
KRFP2372	KRFPC2372	[!#1]N=C1[CH](C(=O)c2[cH][cH][cH][cH]c12)c3[cH][cH][cH][cH]c3
KRFP2373	KRFPC2373	[!#1]N=c1[cH][cH]n(!#1)[cH][cH]1
KRFP2374	KRFPC2374	[!#1]N=C1[CH2][CH2][CH2]c2[cH][cH][cH][cH]c2[NH]1
KRFP2375	KRFPC2375	[!#1]N=C1[NH]C(=[NH])c2[cH][cH][cH][cH]c12
KRFP2376	KRFPC2376	[!#1]N=C1C(=O)[NH]c2[cH][cH][cH][cH]c12
KRFP2377	KRFPC2377	[!#1]N=c1s[cH]c(!#1)n1!#1
KRFP2378	KRFPC2378	[!#1]N=c1s[cH]c(c2[cH][cH]c(!#1)[cH][cH]2)n1!#1
KRFP2379	KRFPC2379	[!#1]N=N!#1
KRFP2380	KRFPC2380	[!#1]N=O
KRFP2381	KRFPC2381	[!#1]N1[CH]([CH3])[CH2][CH2][CH2][CH]1[CH3]
KRFP2382	KRFPC2382	[!#1]N1[CH](S[CH2]C1=O)c2[cH][cH][cH][cH]c2
KRFP2383	KRFPC2383	[!#1]n1[cH][cH][cH][cH]c1=[NH]
KRFP2384	KRFPC2384	[!#1]n1[cH][cH][cH]c([CH3])c1=[NH]
KRFP2385	KRFPC2385	[!#1]n1[cH][cH][cH]c1[CH]=O
KRFP2386	KRFPC2386	[!#1]n1[cH][cH][cH]n1
KRFP2387	KRFPC2387	[!#1]n1[cH][cH][cH]nc1=[NH]
KRFP2388	KRFPC2388	[!#1]n1[cH][cH]c([CH3])n1
KRFP2389	KRFPC2389	[!#1]n1[cH][cH]c(=[NH])[cH][cH]1
KRFP2390	KRFPC2390	[!#1]n1[cH][cH]c(=N[CH2]c2[cH][cH][cH][cH]2)[cH][cH]1

Name	Count name	Pattern
KRFP2391	KRFPC2391	[!#1]n1[cH][cH]c(=O)[nH]c1=O
KRFP2392	KRFPC2392	[!#1]n1[cH][cH]c2[cH][cH][cH]c12
KRFP2393	KRFPC2393	[!#1]n1[cH][cH]n[cH]1
KRFP2394	KRFPC2394	[!#1]n1[cH][cH]nc1[CH3]
KRFP2395	KRFPC2395	[!#1]n1[cH][cH]nc1[N+](=O)[O-]
KRFP2396	KRFPC2396	[!#1]n1[cH][cH]sc1=[NH]
KRFP2397	KRFPC2397	[!#1]n1[cH]c(Br)[cH][cH]c1=[NH]
KRFP2398	KRFPC2398	[!#1]n1[cH]n[cH]n1
KRFP2399	KRFPC2399	[!#1]n1[cH]n[n+](!#1)[cH]1
KRFP2400	KRFPC2400	[!#1]n1[cH]nc([cH]1)[N+](=O)[O-]
KRFP2401	KRFPC2401	[!#1]n1[cH]nc(=O)[cH]n1
KRFP2402	KRFPC2402	[!#1]n1[cH]nc2[cH][cH][cH]c12
KRFP2403	KRFPC2403	[!#1]n1[cH]nn[cH]1
KRFP2404	KRFPC2404	[!#1]N1[CH2][CH]([CH2]C1=O)c2[cH][cH][cH][cH]2
KRFP2405	KRFPC2405	[!#1]N1[CH2][CH]([CH3])C([OH])([CH2][CH]1[CH3])c2[cH][cH][cH][cH] [cH]2
KRFP2406	KRFPC2406	[!#1]N1[CH2][CH2][CH]([CH2]1)c2[cH][cH][cH][cH]2
KRFP2407	KRFPC2407	[!#1]N1[CH2][CH2][CH]([CH2]c2[cH][cH][cH][cH]2)[CH2][CH2]1
KRFP2408	KRFPC2408	[!#1]N1[CH2][CH2][CH]([CH3])[CH2][CH2]1
KRFP2409	KRFPC2409	[!#1]N1[CH2][CH2][CH]=[CH][CH2]1
KRFP2410	KRFPC2410	[!#1]N1[CH2][CH2][CH2][CH]1C(=O)[OH]
KRFP2411	KRFPC2411	[!#1]N1[CH2][CH2][CH2][CH2][CH]1[CH2][CH3]
KRFP2412	KRFPC2412	[!#1]N1[CH2][CH2][CH2][CH2][CH2][CH2]1
KRFP2413	KRFPC2413	[!#1]N1[CH2][CH2][CH2][CH2][CH2]1
KRFP2414	KRFPC2414	[!#1]N1[CH2][CH2][CH2][CH2]1
KRFP2415	KRFPC2415	[!#1]N1[CH2][CH2][CH2]C1=O
KRFP2416	KRFPC2416	[!#1]N1[CH2][CH2][CH2]c2[cH][cH][cH][cH]c12
KRFP2417	KRFPC2417	[!#1]N1[CH2][CH2][CH2]c2c(!#1)c3[cH][cH][cH][cH]c3nc12
KRFP2418	KRFPC2418	[!#1]N1[CH2][CH2][CH2]N(!#1)[CH2][CH2]1
KRFP2419	KRFPC2419	[!#1]N1[CH2][CH2][NH][CH2][CH2]1
KRFP2420	KRFPC2420	[!#1]N1[CH2][CH2]C(=[CH][CH2]1)!#1
KRFP2421	KRFPC2421	[!#1]N1[CH2][CH2]C(=O)[CH2][CH2]1
KRFP2422	KRFPC2422	[!#1]N1[CH2][CH2]C2([CH2][CH2]1)O[CH2][CH2]O2
KRFP2423	KRFPC2423	[!#1]N1[CH2][CH2]c2[cH][cH][cH][cH]c12
KRFP2424	KRFPC2424	[!#1]N1[CH2][CH2]c2c([CH2]1)c3[cH][cH][cH][cH]c3n2!#1
KRFP2425	KRFPC2425	[!#1]N1[CH2][CH2]c2c1nc3[cH][cH][cH][cH]c3c2!#1
KRFP2426	KRFPC2426	[!#1]N1[CH2][CH2]c2c1nc3[cH][cH]c(!#1)[cH]c3c2!#1
KRFP2427	KRFPC2427	[!#1]N1[CH2][CH2]N(!#1)[CH]1c2[cH][cH]c(!#1)[cH][cH]2
KRFP2428	KRFPC2428	[!#1]N1[CH2][CH2]N(!#1)[CH2][CH2]1
KRFP2429	KRFPC2429	[!#1]N1[CH2][CH2]N([CH2][CH]=[CH]c2[cH][cH][cH][cH]2)[CH2][CH2]1
KRFP2430	KRFPC2430	[!#1]N1[CH2][CH2]N([CH2][CH2]1)[CH]2[CH2]C(=O)N(C2=O)c3[cH][cH][cH][cH]3
KRFP2431	KRFPC2431	[!#1]N1[CH2][CH2]N([CH2][CH2]1)[CH]2[CH2]C(=O)N(C2=O)c3[cH][cH][cH]c(!#1)[cH]3
KRFP2432	KRFPC2432	[!#1]N1[CH2][CH2]N([CH2][CH2]1)[CH]2[CH2]C(=O)N(C2=O)c3[cH][cH]c(!#1)[cH][cH]3
KRFP2433	KRFPC2433	[!#1]N1[CH2][CH2]N([CH2][CH2]1)C(=O)!#1
KRFP2434	KRFPC2434	[!#1]N1[CH2][CH2]N([CH2][CH2]1)c2[cH][cH][cH][cH]2
KRFP2435	KRFPC2435	[!#1]N1[CH2][CH2]N([CH2][CH2]1)c2[cH][cH][cH][cH]c2!#1
KRFP2436	KRFPC2436	[!#1]N1[CH2][CH2]N([CH2][CH2]1)c2[cH][cH][cH][cH]c2O[CH3]
KRFP2437	KRFPC2437	[!#1]N1[CH2][CH2]N([CH2][CH2]1)c2[cH][cH][cH][cH]n2
KRFP2438	KRFPC2438	[!#1]N1[CH2][CH2]N([CH2][CH2]1)c2[cH][cH]c(!#1)[cH][cH]2
KRFP2439	KRFPC2439	[!#1]N1[CH2][CH2]N([CH2][CH2]1)c2[cH][cH]c([cH][cH]2)[N+](=O)[O-]
KRFP2440	KRFPC2440	[!#1]N1[CH2][CH2]N([CH2][CH2]1)c2[cH][cH]c(Cl)[cH][cH]2
KRFP2441	KRFPC2441	[!#1]N1[CH2][CH2]N([CH2][CH2]1)c2[cH][cH]c(F)[cH][cH]2

Name	Count name	Pattern
KRFP2442	KRFPC2442	[!#1]N1[CH2][CH2]N([CH2][CH2]1)c2[cH][cH]c3[cH][cH][cH]c3n2
KRFP2443	KRFPC2443	[!#1]N1[CH2][CH2]N([CH2][CH2]1)S(=O)(=O)[!#1]
KRFP2444	KRFPC2444	[!#1]N1[CH2][CH2]N([CH3])[CH2][CH2]1
KRFP2445	KRFPC2445	[!#1]N1[CH2][CH2]N2[CH2][CH2][CH2][CH2]2[CH2]1
KRFP2446	KRFPC2446	[!#1]N1[CH2][CH2]n2c3[CH]1[CH2][CH2][CH2]c3c4[cH]c(!#1)[cH][cH]c24
KRFP2447	KRFPC2447	[!#1]N1[CH2][CH2]n2c3[CH]1[CH2][CH2][CH2]c3c4[cH]c([CH3])[cH][cH]c24
KRFP2448	KRFPC2448	[!#1]N1[CH2][CH2]O[CH2][CH2]1
KRFP2449	KRFPC2449	[!#1]N1[CH2][CH2]O[CH2][CH2]O[CH2][CH2][NH][CH2][CH2]O[CH2][CH2]O[CH2][CH2]1
KRFP2450	KRFPC2450	[!#1]N1[CH2][CH2]O[CH2][CH2]O[CH2][CH2]N(!#1)[CH2][CH2]O[CH2][CH2]O[CH2][CH2]1
KRFP2451	KRFPC2451	[!#1]N1[CH2][CH2]O[CH2][CH2]O[CH2][CH2]O[CH2][CH2]O[CH2][CH2]1
KRFP2452	KRFPC2452	[!#1]N1[CH2][CH2]O[CH2][CH2]O[CH2][CH2]O[CH2][CH2]O[CH2][CH2]O[CH2][CH2]1
KRFP2453	KRFPC2453	[!#1]N1[CH2][CH2]SC1=[NH]
KRFP2454	KRFPC2454	[!#1]N1[CH2]C(!#1)(!#1)C(=O)C(!#1)(!#1)[CH2]1
KRFP2455	KRFPC2455	[!#1]N1[CH2]C(=O)[NH]c2[cH][cH][cH][cH]c12
KRFP2456	KRFPC2456	[!#1]N1[CH2]C(=O)N(!#1)C(=O)[CH2]1
KRFP2457	KRFPC2457	[!#1]N1[CH2]c2[cH][cH][cH][cH]c2[CH2]1
KRFP2458	KRFPC2458	[!#1]N1[CH2]c2[cH][cH][cH][cH]c2C1=O
KRFP2459	KRFPC2459	[!#1]n1c([CH3])[cH][cH]c1[CH3]
KRFP2460	KRFPC2460	[!#1]n1c([CH3])[cH]c([CH3])nc1=O
KRFP2461	KRFPC2461	[!#1]n1c([CH3])n[cH]c1[N+](=O)[O-]
KRFP2462	KRFPC2462	[!#1]n1c([CH3])nc2[cH][cH][cH][cH]c12
KRFP2463	KRFPC2463	[!#1]n1c(=[NH])n(!#1)c2[cH][cH][cH][cH]c12
KRFP2464	KRFPC2464	[!#1]n1c(=[NH])sc2[cH][cH][cH][cH]c12
KRFP2465	KRFPC2465	[!#1]N1C(=O)[CH]=[CH]C1=O
KRFP2466	KRFPC2466	[!#1]N1C(=O)[CH]2[CH]([CH]3[CH]=[CH][CH]2[CH]4[CH]3C(=O)N(!#1)C4=O)C1=O
KRFP2467	KRFPC2467	[!#1]N1C(=O)[CH]2[CH]([CH]3[CH]=[CH][CH]2[CH]4[CH2][CH]43)C1=O
KRFP2468	KRFPC2468	[!#1]N1C(=O)[CH]2[CH]([CH]3c4[cH][cH][cH][cH]c4[CH]2c5[cH][cH][cH]c35)C1=O
KRFP2469	KRFPC2469	[!#1]N1C(=O)[CH]2[CH]3[CH2][CH]([CH]=[CH]3)[CH]2C1=O
KRFP2470	KRFPC2470	[!#1]N1C(=O)[CH]2[CH]3OC(!#1)([CH]=[CH]3)[CH]2C1=O
KRFP2471	KRFPC2471	[!#1]N1C(=O)[CH2][CH2]C1=O
KRFP2472	KRFPC2472	[!#1]N1C(=O)[CH2][NH][CH2]C1=O
KRFP2473	KRFPC2473	[!#1]N1C(=O)[CH2]SC1=S
KRFP2474	KRFPC2474	[!#1]N1C(=O)[NH]C2([CH2][CH2][CH2][CH2]2)C1=O
KRFP2475	KRFPC2475	[!#1]N1C(=O)[NH]C2([CH2][CH2][CH2][CH2]2)C1=O
KRFP2476	KRFPC2476	[!#1]N1C(=O)C(!#1)([OH])c2[cH][cH][cH][cH]c12
KRFP2477	KRFPC2477	[!#1]N1C(=O)C(=[CH]c2[cH][cH][cH][cH]c2)SC1=S
KRFP2478	KRFPC2478	[!#1]N1C(=O)C(=[CH]c2[cH][cH]c(Cl)[cH][cH]2)SC1=S
KRFP2479	KRFPC2479	[!#1]N1C(=O)C(=[CH]c2[cH][cH]c(F)[cH][cH]2)SC1=S
KRFP2480	KRFPC2480	[!#1]N1C(=O)C(=[CH]c2[cH][cH]c(O[CH3])[cH][cH]2)SC1=S
KRFP2481	KRFPC2481	[!#1]N1C(=O)C(=C2C(=O)[NH]c3[cH][cH][cH][cH]c23)SC1=S
KRFP2482	KRFPC2482	[!#1]N1C(=O)C(=C2SC(=S)N(!#1)C2=O)SC1=S
KRFP2483	KRFPC2483	[!#1]N1C(=O)C(=C2S(c3[cH][cH][cH][cH]c3N2(!#1))SC1=S)
KRFP2484	KRFPC2484	[!#1]N1C(=O)C(=O)c2[cH][cH][cH][cH]c12
KRFP2485	KRFPC2485	[!#1]N1C(=O)C(=O)c2[cH]c(!#1)[cH][cH]c12
KRFP2486	KRFPC2486	[!#1]N1C(=O)c2[cH][cH][cH][cH]c2C1=O
KRFP2487	KRFPC2487	[!#1]N1C(=O)c2[cH][cH][cH]c3[cH][cH][cH]c(C1=O)c23
KRFP2488	KRFPC2488	[!#1]N1C(=O)c2[cH][cH][cH]c3c(!#1)[cH][cH]c(C1=O)c23
KRFP2489	KRFPC2489	[!#1]N1C(=O)c2[cH][cH][cH]c3c(!#1)[cH][cH]c1c23

Name	Count name	Pattern
KRFP2490	KRFPC2490	[!#1]N1C(=O)c2[cH][cH][cH]c3c([cH][cH]c(C1=O)c23)N4[CH2][CH2]O[CH2][CH2]4
KRFP2491	KRFPC2491	[!#1]N1C(=O)c2[cH][cH]c(!#1)[cH]c2C1=O
KRFP2492	KRFPC2492	[!#1]N1C(=O)c2[cH][cH]c([cH]c2C1=O)[N+](=O)[O-]
KRFP2493	KRFPC2493	[!#1]N1C(=O)c2[cH][cH]c([cH]c2C1=O)C(=O)[OH]
KRFP2494	KRFPC2494	[!#1]N1C(=O)c2[cH][cH]c([cH]c2C1=O)c3[cH][cH]c4C(=O)N(!#1)C(=O)c4[cH]3
KRFP2495	KRFPC2495	[!#1]N1C(=O)c2[cH][cH]c(Br)[cH]c2C1=O
KRFP2496	KRFPC2496	[!#1]n1c(=O)c2[cH]c3c(=O)n(!#1)c(=O)c3[cH]c2c1=O
KRFP2497	KRFPC2497	[!#1]N1C(=O)N(!#1)C(=O)C(!#1)(!#1)C1=O
KRFP2498	KRFPC2498	[!#1]n1c(=O)n(!#1)c(=O)n(!#1)c1=O
KRFP2499	KRFPC2499	[!#1]n1c(=O)oc2[cH][cH][cH][cH]c12
KRFP2500	KRFPC2500	[!#1]n1c(=O)oc2[cH]c(Br)[cH][cH]c12
KRFP2501	KRFPC2501	[!#1]n1c(=O)oc2[cH]c(Cl)[cH][cH]c12
KRFP2502	KRFPC2502	[!#1]n1c(=S)n(!#1)c2[cH][cH][cH][cH]c12
KRFP2503	KRFPC2503	[!#1]n1c(=S)oc2[cH][cH][cH][cH]c12
KRFP2504	KRFPC2504	[!#1]n1c(=S)sc2[cH][cH][cH][cH]c12
KRFP2505	KRFPC2505	[!#1]N1c2[cH][cH][cH][cH]c2[CH]=[CH]c3[cH][cH][cH][cH]c13
KRFP2506	KRFPC2506	[!#1]N1c2[cH][cH][cH][cH]c2[CH]=[CH]c3[cH][cH]c(!#1)[cH]c13
KRFP2507	KRFPC2507	[!#1]N1c2[cH][cH][cH][cH]c2[CH2][CH2]c3[cH][cH][cH][cH]c13
KRFP2508	KRFPC2508	[!#1]N1c2[cH][cH][cH][cH]c2[CH2][CH2]c3[cH][cH]c(!#1)[cH]c13
KRFP2509	KRFPC2509	[!#1]N1c2[cH][cH][cH][cH]c2[CH2][CH2]c3[cH][cH]c([NH]C(=O)!#1)[cH] c13
KRFP2510	KRFPC2510	[!#1]N1c2[cH][cH][cH][cH]c2C([CH3])([CH3])C1(!#1)!#1
KRFP2511	KRFPC2511	[!#1]n1c2[cH][cH][cH][cH]c2c(=O)c3[cH][cH][cH][cH]c13
KRFP2512	KRFPC2512	[!#1]n1c2[cH][cH][cH][cH]c2c3[cH][cH][cH][cH]c13
KRFP2513	KRFPC2513	[!#1]n1c2[cH][cH][cH][cH]c2c3nc4[cH][cH]c([cH]c4[cH]c13)[N+](=O)[O-]
KRFP2514	KRFPC2514	[!#1]N1c2[cH][cH][cH][cH]c2Oc3nnc(Cl)[cH]c13
KRFP2515	KRFPC2515	[!#1]N1c2[cH][cH][cH][cH]c2SC1(!#1)!#1
KRFP2516	KRFPC2516	[!#1]N1c2[cH][cH][cH][cH]c2S(c3[cH][cH][cH][cH]c13)
KRFP2517	KRFPC2517	[!#1]N1c2[cH][cH][cH][cH]c2S(c3[cH][cH]c(!#1)[cH]c13)
KRFP2518	KRFPC2518	[!#1]N1c2[cH][cH][cH][cH]c2S(c3[cH][cH]c([cH]c13)C(F)(F)F)
KRFP2519	KRFPC2519	[!#1]N1c2[cH][cH][cH][cH]c2S(c3[cH][cH]c([NH]C(=O)!#1)[cH]c13)
KRFP2520	KRFPC2520	[!#1]n1c2[cH][cH]c(Br)[cH]c2c3[cH]c(Br)[cH][cH]c13
KRFP2521	KRFPC2521	[!#1]n1c2[cH][cH]c(Cl)[cH]c2c3[cH]c(Cl)[cH][cH]c13
KRFP2522	KRFPC2522	[!#1]n1c2[CH2][CH2][CH2][CH2]c2sc1=[NH]
KRFP2523	KRFPC2523	[!#1]n1c2[CH2][CH2][CH2]c2c(=[NH])c3[cH][cH][cH][cH]c13
KRFP2524	KRFPC2524	[!#1]n1c2[CH2][CH2][CH2]c2c3[cH][cH][cH][cH]c13
KRFP2525	KRFPC2525	[!#1]n1c-2c([CH2][CH2]c3c2[cH]nn3c4[cH][cH][cH][cH][cH]4)c5[cH][cH][cH][cH]c15
KRFP2526	KRFPC2526	[!#1]n1c2C(=O)[CH2][CH2][CH2]c2c3[cH]c([CH3])[cH][cH]c13
KRFP2527	KRFPC2527	[!#1]n1c2c(n(!#1))c3[cH][cH][cH][cH]c23)c4[cH][cH][cH][cH]c14
KRFP2528	KRFPC2528	[!#1]n1n[cH][n+]2nc([CH3])[cH]c([OH])c12
KRFP2529	KRFPC2529	[!#1]N1N=C([CH2][CH](C1=O)c2[cH][nH]c3[cH][cH][cH][cH]c23)c4[cH][cH][cH][cH]c4
KRFP2530	KRFPC2530	[!#1]N1N=C([CH2][CH](C1=O)c2[cH]n(!#1))c3[cH][cH][cH][cH]c23)c4[cH][cH][cH][cH]c4
KRFP2531	KRFPC2531	[!#1]N1N=C2[CH]([CH2][CH2]c3[cH][cH]c(!#1)[cH]c23)[CH]1c4[cH][cH]c(!#1)[cH][cH]c4
KRFP2532	KRFPC2532	[!#1]N1N=C2[CH]([CH2][CH2]c3[cH]c(!#1)[cH][cH]c23)[CH]1c4[cH][cH]c(!#1)[cH][cH]c4
KRFP2533	KRFPC2533	[!#1]n1nc([CH3])[cH]c1[CH3]
KRFP2534	KRFPC2534	[!#1]n1nc([CH3])c(Br)c1[CH3]
KRFP2535	KRFPC2535	[!#1]n1nc(c2[cH][cH][cH][cH]2)c3[cH][cH][cH]c3c1c4[cH][cH][cH][cH]c4
KRFP2536	KRFPC2536	[!#1]n1nc(nc1c2[cH][cH][cH][cH]2)c3[cH][cH][cH][cH]c3

Name	Count name	Pattern
KRFP2537	KRFPC2537	[!#1]n1nc2[cH][cH][cH][cH]c2n1
KRFP2538	KRFPC2538	[!#1]n1nc2C(=N[NH][CH3])c3nn(!#1)nc3C(=N[NH][CH3])c2n1
KRFP2539	KRFPC2539	[!#1]n1nc2C(=N[OH])c3nn(!#1)nc3C(=N[OH])c2n1
KRFP2540	KRFPC2540	[!#1]n1nc2C(=NN=C([CH3])[CH3])c3nn(!#1)nc3C(=NN=C([CH3])[CH3])c2n1
KRFP2541	KRFPC2541	[!#1]n1nc2C(=NOC(=O)[CH3])c3nn(!#1)nc3C(=NOC(=O)[CH3])c2n1
KRFP2542	KRFPC2542	[!#1]n1nnc2[cH][cH][cH][cH]c12
KRFP2543	KRFPC2543	[!#1]n1nnc2c(=O)oc3[cH][cH][cH][cH]c3c12
KRFP2544	KRFPC2544	[!#1]n1nnnc1C2(!#1)[CH2][CH2][CH2][CH2][CH2]2
KRFP2545	KRFPC2545	[!#1]n1nnnc1C2(!#1)[CH2][CH2][CH2][CH2]2
KRFP2546	KRFPC2546	[!#1]n1nnnc1c2[cH][cH][cH][cH]c2
KRFP2547	KRFPC2547	[!#1]O[!#1]
KRFP2548	KRFPC2548	[!#1]O[CH](!#1)[!#1]
KRFP2549	KRFPC2549	[!#1]O[CH]([CH](!#1)[CH2][CH]1[CH2][CH2]N(!#1)[CH2][CH]1[CH](!#1)[!#1])c2[cH][cH]nc3[cH][cH][cH][cH]c23
KRFP2550	KRFPC2550	[!#1]O[CH]([CH3])[CH3]
KRFP2551	KRFPC2551	[!#1]O[CH]([CH3])C(!#1)(!#1)Cl
KRFP2552	KRFPC2552	[!#1]O[CH]([CH3])C(=O)[NH][NH2]
KRFP2553	KRFPC2553	[!#1]O[CH]([CH3])C(=O)[NH]N=[CH][!#1]
KRFP2554	KRFPC2554	[!#1]O[CH]([CH3])C(=O)[NH]N=[CH]c1[cH][cH][cH][cH][cH]1
KRFP2555	KRFPC2555	[!#1]O[CH]([CH3])C(=O)[NH]N=[CH]c1[cH][cH][cH]c([cH]1)[N+](=O)[O-]
KRFP2556	KRFPC2556	[!#1]O[CH]([CH3])C(=O)[NH]N=[CH]c1[cH]c([cH][cH]c1[OH])[N+](=O)[O-]
KRFP2557	KRFPC2557	[!#1]O[CH]([CH3])C(=O)[OH]
KRFP2558	KRFPC2558	[!#1]O[CH]([NH]C(=O)[!#1])C(Br)(Br)Br
KRFP2559	KRFPC2559	[!#1]O[CH]([NH]C(=O)[!#1])C(Cl)(Cl)Cl
KRFP2560	KRFPC2560	[!#1]O[CH](C(F)(F)F)C(F)(F)F
KRFP2561	KRFPC2561	[!#1]O[CH](F)F
KRFP2562	KRFPC2562	[!#1]O[CH]1[CH2][CH]([CH3])[CH2][CH2][CH]1[CH]([CH3])[CH3]
KRFP2563	KRFPC2563	[!#1]O[CH]1[CH2][CH2][CH]([CH2][CH2]1)C([CH3])([CH3])[CH3]
KRFP2564	KRFPC2564	[!#1]O[CH2][CH]([!#1])[!#1]
KRFP2565	KRFPC2565	[!#1]O[CH2][CH]([CH3])[CH3]
KRFP2566	KRFPC2566	[!#1]O[CH2][CH]([OH])[CH2][NH][CH]([CH3])[CH3]
KRFP2567	KRFPC2567	[!#1]O[CH2][CH]([OH])[CH2][NH]C([CH3])([CH3])[CH2]C([CH3])([CH3])[CH3]
KRFP2568	KRFPC2568	[!#1]O[CH2][CH]([OH])[CH2][NH]C([CH3])([CH3])[CH3]
KRFP2569	KRFPC2569	[!#1]O[CH2][CH]([OH])[CH2][NH]S(=O)(=O)[OH]
KRFP2570	KRFPC2570	[!#1]O[CH2][CH]([OH])[CH2]N(!#1)[CH2][CH3]
KRFP2571	KRFPC2571	[!#1]O[CH2][CH]([OH])[CH2]N(!#1)[CH3]
KRFP2572	KRFPC2572	[!#1]O[CH2][CH]([OH])[CH2]N([CH2][CH3])[CH2][CH3]
KRFP2573	KRFPC2573	[!#1]O[CH2][CH]([OH])[CH2]N([CH2][CH3])S(=O)(=O)[OH]
KRFP2574	KRFPC2574	[!#1]O[CH2][CH]([OH])[CH2]N([CH3])[CH2][CH]([OH])[CH2][NH]S(=O)(=O)[OH]
KRFP2575	KRFPC2575	[!#1]O[CH2][CH]([OH])[CH2]N([CH3])S(=O)(=O)[OH]
KRFP2576	KRFPC2576	[!#1]O[CH2][CH]=[CH2]
KRFP2577	KRFPC2577	[!#1]O[CH2][CH]1O[CH](!#1)[CH](O[!#1])[CH]1O[!#1]
KRFP2578	KRFPC2578	[!#1]O[CH2][CH2][CH]([CH3])[CH3]
KRFP2579	KRFPC2579	[!#1]O[CH2][CH2][CH2][CH2][CH2][CH2][CH3]
KRFP2580	KRFPC2580	[!#1]O[CH2][CH2][CH2][CH2][CH2][CH3]
KRFP2581	KRFPC2581	[!#1]O[CH2][CH2][CH2][CH2][CH3]
KRFP2582	KRFPC2582	[!#1]O[CH2][CH2][CH2][CH3]
KRFP2583	KRFPC2583	[!#1]O[CH2][CH2][CH2]C(=O)[!#1]
KRFP2584	KRFPC2584	[!#1]O[CH2][CH2][CH3]
KRFP2585	KRFPC2585	[!#1]O[CH2][CH2][NH]C(=O)[!#1]
KRFP2586	KRFPC2586	[!#1]O[CH2][CH2][NH2]
KRFP2587	KRFPC2587	[!#1]O[CH2][CH2][OH]
KRFP2588	KRFPC2588	[!#1]O[CH2][CH2]c1[cH][cH][cH][cH]1

Name	Count name	Pattern
KRFP2589	KRFPC2589	[!#1]O[CH2][CH2]Cl
KRFP2590	KRFPC2590	[!#1]O[CH2][CH2]F
KRFP2591	KRFPC2591	[!#1]O[CH2][CH2]N([CH2][CH3])[CH2][CH3]
KRFP2592	KRFPC2592	[!#1]O[CH2][CH2]O[!#1]
KRFP2593	KRFPC2593	[!#1]O[CH2][CH2]OC(=O)[!#1]
KRFP2594	KRFPC2594	[!#1]O[CH2][CH2]S(=O)(=O)[!#1]
KRFP2595	KRFPC2595	[!#1]O[CH2][CH3]
KRFP2596	KRFPC2596	[!#1]O[CH2]C#[CH]
KRFP2597	KRFPC2597	[!#1]O[CH2]C([!#1])([!#1])Cl
KRFP2598	KRFPC2598	[!#1]O[CH2]C(=O)[!#1]
KRFP2599	KRFPC2599	[!#1]O[CH2]C(=O)[CH3]
KRFP2600	KRFPC2600	[!#1]O[CH2]C(=O)[NH][CH]([!#1])[CH3]
KRFP2601	KRFPC2601	[!#1]O[CH2]C(=O)[NH][CH]([CH2][CH2]S[CH3])C(=O)O[CH3]
KRFP2602	KRFPC2602	[!#1]O[CH2]C(=O)[NH][CH2][CH2]N([CH3])[CH3]
KRFP2603	KRFPC2603	[!#1]O[CH2]C(=O)[NH][NH]C(=O)[!#1]
KRFP2604	KRFPC2604	[!#1]O[CH2]C(=O)[NH][NH]C(=O)[CH2][CH2][CH2][CH3]
KRFP2605	KRFPC2605	[!#1]O[CH2]C(=O)[NH][NH2]
KRFP2606	KRFPC2606	[!#1]O[CH2]C(=O)[NH]C(=O)O[!#1]
KRFP2607	KRFPC2607	[!#1]O[CH2]C(=O)[NH]N=[CH][!#1]
KRFP2608	KRFPC2608	[!#1]O[CH2]C(=O)[NH]N=[CH][CH]([!#1])[!#1]
KRFP2609	KRFPC2609	[!#1]O[CH2]C(=O)[NH]N=[CH][CH]=[CH][!#1]
KRFP2610	KRFPC2610	[!#1]O[CH2]C(=O)[NH]N=[CH][CH]=[CH]c1[cH][cH][cH]c([cH]1)[N+](=O)[O-]
KRFP2611	KRFPC2611	[!#1]O[CH2]C(=O)[NH]N=[CH]c1[cH][cH][cH][cH]c1[!#1]
KRFP2612	KRFPC2612	[!#1]O[CH2]C(=O)[NH]N=[CH]c1[cH][cH][cH][cH]c1[N+](=O)[O-]
KRFP2613	KRFPC2613	[!#1]O[CH2]C(=O)[NH]N=[CH]c1[cH][cH][cH][cH]c1[OH]
KRFP2614	KRFPC2614	[!#1]O[CH2]C(=O)[NH]N=[CH]c1[cH][cH][cH][cH]c1Cl
KRFP2615	KRFPC2615	[!#1]O[CH2]C(=O)[NH]N=[CH]c1[cH][cH][cH][cH]c1O[CH3]
KRFP2616	KRFPC2616	[!#1]O[CH2]C(=O)[NH]N=[CH]c1[cH][cH][cH]c([!#1])[cH]1
KRFP2617	KRFPC2617	[!#1]O[CH2]C(=O)[NH]N=[CH]c1[cH][cH][cH]c([cH]1)[N+](=O)[O-]
KRFP2618	KRFPC2618	[!#1]O[CH2]C(=O)[NH]N=[CH]c1[cH][cH]c([!#1])[cH][cH]1
KRFP2619	KRFPC2619	[!#1]O[CH2]C(=O)[NH]N=[CH]c1[cH][cH]c([!#1])[cH]c1[OH]
KRFP2620	KRFPC2620	[!#1]O[CH2]C(=O)[NH]N=[CH]c1[cH][cH]c([cH][cH]1)[N+](=O)[O-]
KRFP2621	KRFPC2621	[!#1]O[CH2]C(=O)[NH]N=[CH]c1[cH][cH]c([CH3])o1
KRFP2622	KRFPC2622	[!#1]O[CH2]C(=O)[NH]N=[CH]c1[cH][cH]c([OH])[cH][cH]1
KRFP2623	KRFPC2623	[!#1]O[CH2]C(=O)[NH]N=[CH]c1[cH][cH]c([OH])c([cH]1)[N+](=O)[O-]
KRFP2624	KRFPC2624	[!#1]O[CH2]C(=O)[NH]N=[CH]c1[cH][cH]c(Cl)[cH][cH]1
KRFP2625	KRFPC2625	[!#1]O[CH2]C(=O)[NH]N=[CH]c1[cH][cH]c(Cl)c([cH]1)[N+](=O)[O-]
KRFP2626	KRFPC2626	[!#1]O[CH2]C(=O)[NH]N=[CH]c1[cH][cH]c(O[CH3])c([cH]1)[N+](=O)[O-]
KRFP2627	KRFPC2627	[!#1]O[CH2]C(=O)[NH]N=[CH]c1[cH][cH]c(s1)[N+](=O)[O-]
KRFP2628	KRFPC2628	[!#1]O[CH2]C(=O)[NH]N=[CH]c1[cH]c([cH][cH]c1[OH])[N+](=O)[O-]
KRFP2629	KRFPC2629	[!#1]O[CH2]C(=O)[NH]N=[CH]c1[cH]c(l)[cH]c([!#1])c1[OH]
KRFP2630	KRFPC2630	[!#1]O[CH2]C(=O)[NH]N=[CH]c1[cH]c(N=Nc2[cH][cH][cH][cH][cH]2)[cH][cH]c1[OH]
KRFP2631	KRFPC2631	[!#1]O[CH2]C(=O)[NH]N=[CH]c1[cH]c2[cH][cH][cH][cH]c2nc1Cl
KRFP2632	KRFPC2632	[!#1]O[CH2]C(=O)[NH]N=[CH]c1[cH]c2O[CH2]Oc2[cH]c1[N+](=O)[O-]
KRFP2633	KRFPC2633	[!#1]O[CH2]C(=O)[NH]N=[CH]c1c([OH])[cH][cH]c2[cH][cH][cH][cH]c12
KRFP2634	KRFPC2634	[!#1]O[CH2]C(=O)[NH]N=[CH]c1c(Cl)[cH][cH][cH]c1Cl
KRFP2635	KRFPC2635	[!#1]O[CH2]C(=O)[NH]N=[CH]c1c(O[CH3])[cH][cH]c2[cH][cH][cH][cH]c12
KRFP2636	KRFPC2636	[!#1]O[CH2]C(=O)[NH]N=C([!#1])[CH3]
KRFP2637	KRFPC2637	[!#1]O[CH2]C(=O)[NH]N=C([CH3])[CH]([!#1])[!#1]
KRFP2638	KRFPC2638	[!#1]O[CH2]C(=O)[NH]N=C([CH3])[CH]=[CH][!#1]
KRFP2639	KRFPC2639	[!#1]O[CH2]C(=O)[NH]N=C([CH3])[CH]=[CH]c1[cH][cH][cH]o1
KRFP2640	KRFPC2640	[!#1]O[CH2]C(=O)[NH]N=C([CH3])c1[cH][cH][cH]c([cH]1)[N+](=O)[O-]

Name	Count name	Pattern
KRFP2641	KRFPC2641	[!#1]O[CH2]C(=O)[NH]N=C([CH3])c1[cH][cH][cH]s1
KRFP2642	KRFPC2642	[!#1]O[CH2]C(=O)[NH]N=C([CH3])c1[cH][cH]c(Br)s1
KRFP2643	KRFPC2643	[!#1]O[CH2]C(=O)[NH]N=C(C(=O)[!#1])c1[cH]c(Br)[cH][cH]c1N([!#1])[CH3]
KRFP2644	KRFPC2644	[!#1]O[CH2]C(=O)[NH]N=C1[CH2][CH2][CH2][CH2][CH2]1
KRFP2645	KRFPC2645	[!#1]O[CH2]C(=O)[NH]N=C1C(=O)[NH]c2[cH][cH][cH][cH]c12
KRFP2646	KRFPC2646	[!#1]O[CH2]C(=O)[NH]N=C1C(=O)[NH]c2[cH][cH]c([!#1])[cH]c12
KRFP2647	KRFPC2647	[!#1]O[CH2]C(=O)[NH]N=C1C(=O)[NH]c2[cH][cH]c([cH]c12)[N+](=O)[O-]
KRFP2648	KRFPC2648	[!#1]O[CH2]C(=O)[NH]N=C1C(=O)N([!#1])c2[cH][cH]c([!#1])[cH]c12
KRFP2649	KRFPC2649	[!#1]O[CH2]C(=O)[NH]N=C1C(=O)N([CH3])c2[cH][cH]c(Br)[cH]c12
KRFP2650	KRFPC2650	[!#1]O[CH2]C(=O)[NH2]
KRFP2651	KRFPC2651	[!#1]O[CH2]C(=O)[OH]
KRFP2652	KRFPC2652	[!#1]O[CH2]C(=O)c1[cH][cH][cH][cH][cH]1
KRFP2653	KRFPC2653	[!#1]O[CH2]C(=O)c1[cH][cH]c([cH][cH]1)[N+](=O)[O-]
KRFP2654	KRFPC2654	[!#1]O[CH2]C(=O)c1[cH][cH]c(Br)[cH][cH]1
KRFP2655	KRFPC2655	[!#1]O[CH2]C(=O)c1[cH][cH]c(Cl)[cH][cH]1
KRFP2656	KRFPC2656	[!#1]O[CH2]C(=O)c1[cH][cH]c(O[!#1])[cH][cH]1
KRFP2657	KRFPC2657	[!#1]O[CH2]C(=O)N([!#1])[CH2][CH3]
KRFP2658	KRFPC2658	[!#1]O[CH2]C(=O)N([!#1])[CH3]
KRFP2659	KRFPC2659	[!#1]O[CH2]C(=O)N([CH2][CH3])[CH2][CH3]
KRFP2660	KRFPC2660	[!#1]O[CH2]C(=O)O[!#1]
KRFP2661	KRFPC2661	[!#1]O[CH2]C(=O)O[CH2]C(=O)[!#1]
KRFP2662	KRFPC2662	[!#1]O[CH2]C(=O)O[CH3]
KRFP2663	KRFPC2663	[!#1]O[CH2]C(=O)ON=[CH]c1[cH][cH]c(Br)[cH][cH]1
KRFP2664	KRFPC2664	[!#1]O[CH2]C(=O)ON=C([CH3])C([CH3])([CH3])[CH3]
KRFP2665	KRFPC2665	[!#1]O[CH2]C(F)(F)F
KRFP2666	KRFPC2666	[!#1]O[CH2]c1[cH][cH][cH][cH][cH]1
KRFP2667	KRFPC2667	[!#1]O[CH3]
KRFP2668	KRFPC2668	[!#1]OC([!#1])([!#1])C(=O)[!#1]
KRFP2669	KRFPC2669	[!#1]OC([!#1])([!#1])c1[cH][cH][cH][cH]c1C(=O)[!#1]
KRFP2670	KRFPC2670	[!#1]OC([!#1])([!#1])c1[cH][cH][cH][cH]c1C(=O)C([!#1])([!#1])c2[cH][cH][cH][cH][cH]2
KRFP2671	KRFPC2671	[!#1]OC([!#1])([!#1])c1[cH]c([CH3])[nH]c(=O)c1C(=O)[!#1]
KRFP2672	KRFPC2672	[!#1]OC([CH3])([CH3])[CH3]
KRFP2673	KRFPC2673	[!#1]OC(=O)[!#1]
KRFP2674	KRFPC2674	[!#1]OC(=O)[CH]([CH3])[NH]C(=O)OC([CH3])([CH3])[CH3]
KRFP2675	KRFPC2675	[!#1]OC(=O)[CH]=[CH][!#1]
KRFP2676	KRFPC2676	[!#1]OC(=O)[CH]=[CH]c1[cH][cH][cH][cH][cH]1
KRFP2677	KRFPC2677	[!#1]OC(=O)[CH2][CH2][CH2]C(=O)O[!#1]
KRFP2678	KRFPC2678	[!#1]OC(=O)[CH2][CH2][CH3]
KRFP2679	KRFPC2679	[!#1]OC(=O)[CH2][CH2]C(=O)O[CH3]
KRFP2680	KRFPC2680	[!#1]OC(=O)[CH2][CH3]
KRFP2681	KRFPC2681	[!#1]OC(=O)[CH2]C(=O)[CH3]
KRFP2682	KRFPC2682	[!#1]OC(=O)[CH3]
KRFP2683	KRFPC2683	[!#1]OC(=O)[NH][CH3]
KRFP2684	KRFPC2684	[!#1]OC(=O)[NH]C(=O)[CH2][CH2]Br
KRFP2685	KRFPC2685	[!#1]OC(=O)[NH2]
KRFP2686	KRFPC2686	[!#1]OC(=O)C(=[CH2])[CH3]
KRFP2687	KRFPC2687	[!#1]OC(=O)C(F)(F)F
KRFP2688	KRFPC2688	[!#1]OC(=O)C(F)(OC(F)(F)C(F)(F)C(F)(F)F)C(F)(F)F
KRFP2689	KRFPC2689	[!#1]OC(=O)O[CH3]
KRFP2690	KRFPC2690	[!#1]OC(C(=O)[!#1])(c1[cH][cH][cH][cH][cH]1)c2[cH][cH][cH][cH][cH]2
KRFP2691	KRFPC2691	[!#1]OC(F)(F)[CH](F)Cl
KRFP2692	KRFPC2692	[!#1]OC(F)(F)[CH](F)F
KRFP2693	KRFPC2693	[!#1]OC1([CH2][CH2][CH2][CH2][CH2]1)C([!#1])([!#1])[!#1]

Name	Count name	Pattern
KRFP2694	KRFPC2694	[!#1]Oc1[cH][cH][cH][cH]1
KRFP2695	KRFPC2695	[!#1]Oc1[cH][cH][cH][cH]c1[!#1]
KRFP2696	KRFPC2696	[!#1]Oc1[cH][cH][cH][cH]c1[N+](=O)[O-]
KRFP2697	KRFPC2697	[!#1]Oc1[cH][cH][cH][cH]c1[NH]C(=O)[!#1]
KRFP2698	KRFPC2698	[!#1]Oc1[cH][cH][cH][cH]c1[OH]
KRFP2699	KRFPC2699	[!#1]Oc1[cH][cH][cH][cH]c1C(=O)[!#1]
KRFP2700	KRFPC2700	[!#1]Oc1[cH][cH][cH][cH]c1F
KRFP2701	KRFPC2701	[!#1]Oc1[cH][cH][cH][cH]c1N([!#1])C(=O)[CH]([!#1])[CH2]C(=O)[!#1]
KRFP2702	KRFPC2702	[!#1]Oc1[cH][cH][cH][cH]c1O[!#1]
KRFP2703	KRFPC2703	[!#1]Oc1[cH][cH][cH]c([!#1])[cH]1
KRFP2704	KRFPC2704	[!#1]Oc1[cH][cH][cH]c([CH]=N[!#1])c1[OH]
KRFP2705	KRFPC2705	[!#1]Oc1[cH][cH][cH]c([cH]1)[N+](=O)[O-]
KRFP2706	KRFPC2706	[!#1]Oc1[cH][cH][cH]c([cH]1)C(=O)[!#1]
KRFP2707	KRFPC2707	[!#1]Oc1[cH][cH][cH]c([CH3])[cH]1
KRFP2708	KRFPC2708	[!#1]Oc1[cH][cH][cH]c2[cH][cH][cH]c12
KRFP2709	KRFPC2709	[!#1]Oc1[cH][cH][cH]c2[cH][cH][cH]nc12
KRFP2710	KRFPC2710	[!#1]Oc1[cH][cH][cH]nc1[!#1]
KRFP2711	KRFPC2711	[!#1]Oc1[cH][cH]c([!#1])[cH][cH]1
KRFP2712	KRFPC2712	[!#1]Oc1[cH][cH]c([!#1])[cH]c1[!#1]
KRFP2713	KRFPC2713	[!#1]Oc1[cH][cH]c([!#1])[cH]c1Br
KRFP2714	KRFPC2714	[!#1]Oc1[cH][cH]c([!#1])[cH]c1O[!#1]
KRFP2715	KRFPC2715	[!#1]Oc1[cH][cH]c([!#1])c([cH]1)[N+](=O)[O-]
KRFP2716	KRFPC2716	[!#1]Oc1[cH][cH]c([cH][cH]1)[CH]([!#1])[!#1]
KRFP2717	KRFPC2717	[!#1]Oc1[cH][cH]c([cH][cH]1)[N+](=O)[O-]
KRFP2718	KRFPC2718	[!#1]Oc1[cH][cH]c([cH][cH]1)C([CH3])([CH3])[CH3]
KRFP2719	KRFPC2719	[!#1]Oc1[cH][cH]c([cH][cH]1)C([CH3])([CH3])c2[cH][cH]c([!#1])[cH] [cH]2
KRFP2720	KRFPC2720	[!#1]Oc1[cH][cH]c([cH][cH]1)C([CH3])([CH3])c2[cH][cH]c(O[!#1])[cH] [cH]2
KRFP2721	KRFPC2721	[!#1]Oc1[cH][cH]c([cH][cH]1)C(=O)[!#1]
KRFP2722	KRFPC2722	[!#1]Oc1[cH][cH]c([cH][cH]1)C(=O)[OH]
KRFP2723	KRFPC2723	[!#1]Oc1[cH][cH]c([cH][cH]1)C(c2[cH][cH][cH][cH]c2[!#1])(c3[cH][cH] [cH][cH]c3[!#1])c4[cH][cH]c(O[!#1])[cH][cH]4
KRFP2724	KRFPC2724	[!#1]Oc1[cH][cH]c([cH][cH]1)C(O[!#1])(c2[cH][cH][cH][cH][cH]2)c3[cH] [cH]c([!#1])[cH][cH]3
KRFP2725	KRFPC2725	[!#1]Oc1[cH][cH]c([cH][cH]1)N([!#1])[CH2]c2[cH][cH]c(Br)[cH][cH]2
KRFP2726	KRFPC2726	[!#1]Oc1[cH][cH]c([cH][cH]1)N([!#1])[CH2]c2[cH][cH]c(F)[cH][cH]2
KRFP2727	KRFPC2727	[!#1]Oc1[cH][cH]c([cH][cH]1)N([!#1])C(=O)[CH]([!#1])[CH2]C(=O) [!#1]
KRFP2728	KRFPC2728	[!#1]Oc1[cH][cH]c([cH][cH]1)N([!#1])C(=O)[CH]([CH2]C(=O)[!#1]) S[CH2]C(=O)[!#1]
KRFP2729	KRFPC2729	[!#1]Oc1[cH][cH]c([cH][cH]1)S(=O)(=O)[!#1]
KRFP2730	KRFPC2730	[!#1]Oc1[cH][cH]c([cH][cH]1)S(=O)(=O)c2[cH][cH]c([!#1])[cH][cH]2
KRFP2731	KRFPC2731	[!#1]Oc1[cH][cH]c([CH]=N[!#1])[cH][cH]1
KRFP2732	KRFPC2732	[!#1]Oc1[cH][cH]c([CH]=N[!#1])[cH]c1[OH]
KRFP2733	KRFPC2733	[!#1]Oc1[cH][cH]c([CH]=N[!#1])[cH]c1O[!#1]
KRFP2734	KRFPC2734	[!#1]Oc1[cH][cH]c([CH]=N[!#1])c(O[!#1])[cH]1
KRFP2735	KRFPC2735	[!#1]Oc1[cH][cH]c([CH]=O)[cH][cH]1
KRFP2736	KRFPC2736	[!#1]Oc1[cH][cH]c([cH]c1O[!#1])[CH]([!#1])[!#1]
KRFP2737	KRFPC2737	[!#1]Oc1[cH][cH]c([cH]c1O[!#1])C(=O)[!#1]
KRFP2738	KRFPC2738	[!#1]Oc1[cH][cH]c([CH2][CH2]N([!#1])[CH3])[cH]c1O[!#1]
KRFP2739	KRFPC2739	[!#1]Oc1[cH][cH]c([CH2]C(=O)[!#1])[cH][cH]1
KRFP2740	KRFPC2740	[!#1]Oc1[cH][cH]c([CH2]C(=O)[!#1])[cH]c1O[!#1]
KRFP2741	KRFPC2741	[!#1]Oc1[cH][cH]c([CH3])[cH][cH]1
KRFP2742	KRFPC2742	[!#1]Oc1[cH][cH]c([CH3])[cH]c1[CH3]
KRFP2743	KRFPC2743	[!#1]Oc1[cH][cH]c([CH3])[cH]c1[N+](=O)[O-]
KRFP2744	KRFPC2744	[!#1]Oc1[cH][cH]c([CH3])c([CH3])[cH]1

Name	Count name	Pattern
KRFP2745	KRFPC2745	[!#1]Oc1[cH][cH]c([NH]C(=O)[!#1])[cH]c1Cl
KRFP2746	KRFPC2746	[!#1]Oc1[cH][cH]c([NH2])[cH][cH]1
KRFP2747	KRFPC2747	[!#1]Oc1[cH][cH]c([OH])[cH][cH]1
KRFP2748	KRFPC2748	[!#1]Oc1[cH][cH]c(Br)[cH][cH]1
KRFP2749	KRFPC2749	[!#1]Oc1[cH][cH]c(C(=O)[OH])c([cH]1)C(=O)[OH]
KRFP2750	KRFPC2750	[!#1]Oc1[cH][cH]c(Cl)[cH][cH]1
KRFP2751	KRFPC2751	[!#1]Oc1[cH][cH]c(Cl)[cH]c1Cl
KRFP2752	KRFPC2752	[!#1]Oc1[cH][cH]c(O[!#1])[cH][cH]1
KRFP2753	KRFPC2753	[!#1]Oc1[cH][cH]c2[cH][cH][cH][cH]c2[cH]1
KRFP2754	KRFPC2754	[!#1]Oc1[cH][cH]c2[cH][cH][cH][cH]c2c1[CH2]c3c(O[!#1])[cH][cH]c4[cH][cH][cH]c34
KRFP2755	KRFPC2755	[!#1]Oc1[cH][cH]c2[cH][cH][cH][cH]c2c1Br
KRFP2756	KRFPC2756	[!#1]Oc1[cH][cH]c2c([CH3])[cH]c(=O)oc2[cH]1
KRFP2757	KRFPC2757	[!#1]Oc1[cH][cH]c2c(=O)c([!#1])[cH]oc2[cH]1
KRFP2758	KRFPC2758	[!#1]Oc1[cH][cH]c2c(=O)c([!#1])c([CH3])oc2[cH]1
KRFP2759	KRFPC2759	[!#1]Oc1[cH][cH]c2C(=O)OC(=O)c2[cH]1
KRFP2760	KRFPC2760	[!#1]Oc1[cH]c([cH][cH]c1[!#1])[CH]([!#1])[!#1]
KRFP2761	KRFPC2761	[!#1]Oc1[cH]c([cH][cH]c1[OH])[CH]([!#1])[!#1]
KRFP2762	KRFPC2762	[!#1]Oc1[cH]c([CH]=N[!#1])[cH][cH]c1[OH]
KRFP2763	KRFPC2763	[!#1]Oc1[cH]c([cH]c(O[!#1])c1O[!#1])C(=O)[!#1]
KRFP2764	KRFPC2764	[!#1]Oc1[cH]c([CH3])[cH]c(O[!#1])[cH]1
KRFP2765	KRFPC2765	[!#1]Oc1[cH]c(Br)[cH]c([CH]=N[!#1])c1[OH]
KRFP2766	KRFPC2766	[!#1]Oc1c([!#1])[cH][cH][cH]c1[CH]([!#1])[!#1]
KRFP2767	KRFPC2767	[!#1]Oc1c([CH3])[cH]c(Br)[cH]c1[CH3]
KRFP2768	KRFPC2768	[!#1]Oc1c(Br)[cH]c(Br)c2[cH][cH][cH]nc12
KRFP2769	KRFPC2769	[!#1]Oc1c(Cl)[cH]c(Cl)[cH]c1C(=O)[!#1]
KRFP2770	KRFPC2770	[!#1]Oc1c(F)c(F)c([!#1])c(F)c1F
KRFP2771	KRFPC2771	[!#1]OP(=O)([OH])O[!#1]
KRFP2772	KRFPC2772	[!#1]OP(=O)(O[!#1])O[!#1]
KRFP2773	KRFPC2773	[!#1]OS(=O)(=O)[!#1]
KRFP2774	KRFPC2774	[!#1]OS(=O)(=O)[CH2][CH2]S(=O)(=O)[!#1]
KRFP2775	KRFPC2775	[!#1]OS(=O)(=O)[CH2][CH2]S[!#1]
KRFP2776	KRFPC2776	[!#1]OS(=O)(=O)[CH3]
KRFP2777	KRFPC2777	[!#1]OS(=O)(=O)[OH]
KRFP2778	KRFPC2778	[!#1]P(=O)([OH])O[CH2][CH3]
KRFP2779	KRFPC2779	[!#1]P(=O)(O[CH3])O[CH3]
KRFP2780	KRFPC2780	[!#1]P1(=O)O[CH2][CH2][CH2]O1
KRFP2781	KRFPC2781	[!#1]S(=O)(=O)[!#1]
KRFP2782	KRFPC2782	[!#1]S(=O)(=O)[CH]1[CH2][CH2]S(=O)(=O)[CH2]1
KRFP2783	KRFPC2783	[!#1]S(=O)(=O)[CH2][CH2][CH2][CH2][CH2][CH3]
KRFP2784	KRFPC2784	[!#1]S(=O)(=O)[CH2][CH2][OH]
KRFP2785	KRFPC2785	[!#1]S(=O)(=O)[CH2][CH2]C(=O)[CH3]
KRFP2786	KRFPC2786	[!#1]S(=O)(=O)[CH2][CH2]C(=O)[OH]
KRFP2787	KRFPC2787	[!#1]S(=O)(=O)[CH2][CH2]C(=O)O[CH2][CH3]
KRFP2788	KRFPC2788	[!#1]S(=O)(=O)[CH2][CH2]C(=O)O[CH3]
KRFP2789	KRFPC2789	[!#1]S(=O)(=O)[CH2][CH3]
KRFP2790	KRFPC2790	[!#1]S(=O)(=O)[CH2]Br
KRFP2791	KRFPC2791	[!#1]S(=O)(=O)[CH2]C(=N[NH]C(=S)[NH2])[CH3]
KRFP2792	KRFPC2792	[!#1]S(=O)(=O)[CH2]C(=O)[CH3]
KRFP2793	KRFPC2793	[!#1]S(=O)(=O)[CH2]C(=O)[NH2]
KRFP2794	KRFPC2794	[!#1]S(=O)(=O)[CH2]C(=O)[OH]
KRFP2795	KRFPC2795	[!#1]S(=O)(=O)[CH2]OC(=O)[CH3]
KRFP2796	KRFPC2796	[!#1]S(=O)(=O)[CH3]
KRFP2797	KRFPC2797	[!#1]S(=O)(=O)[NH][CH]([CH]([CH3])[CH3])C(=O)[OH]

Name	Count name	Pattern
KRFP2798	KRFPC2798	[!#1]S(=O)(=O)[NH][CH]([CH2][CH2][CH3])C(=O)[OH]
KRFP2799	KRFPC2799	[!#1]S(=O)(=O)[NH][CH]([CH3])[CH3]
KRFP2800	KRFPC2800	[!#1]S(=O)(=O)[NH][CH2][CH2][CH2][CH2][CH3]
KRFP2801	KRFPC2801	[!#1]S(=O)(=O)[NH][CH2][CH2][CH2][CH2]C(=O)[OH]
KRFP2802	KRFPC2802	[!#1]S(=O)(=O)[NH][CH2][CH2][CH2][CH3]
KRFP2803	KRFPC2803	[!#1]S(=O)(=O)[NH][CH2][CH2][CH2][OH]
KRFP2804	KRFPC2804	[!#1]S(=O)(=O)[NH][CH2][CH2][CH2]C(=O)[OH]
KRFP2805	KRFPC2805	[!#1]S(=O)(=O)[NH][CH2][CH2][OH]
KRFP2806	KRFPC2806	[!#1]S(=O)(=O)[NH][CH2][CH2]C(=O)[OH]
KRFP2807	KRFPC2807	[!#1]S(=O)(=O)[NH][CH2][CH2]OC(=O)[NH][CH2][CH2][CH2][CH3]
KRFP2808	KRFPC2808	[!#1]S(=O)(=O)[NH][CH2]C(=O)[OH]
KRFP2809	KRFPC2809	[!#1]S(=O)(=O)[NH][CH2]C(=O)O[CH2][CH3]
KRFP2810	KRFPC2810	[!#1]S(=O)(=O)[NH][CH3]
KRFP2811	KRFPC2811	[!#1]S(=O)(=O)[NH]C([CH3])([CH3])[CH3]
KRFP2812	KRFPC2812	[!#1]S(=O)(=O)[NH]C(=O)[CH3]
KRFP2813	KRFPC2813	[!#1]S(=O)(=O)[NH]C(=O)[NH2]
KRFP2814	KRFPC2814	[!#1]S(=O)(=O)[NH]C(=O)O[CH2][CH2]N([CH2][CH3])[CH2][CH3]
KRFP2815	KRFPC2815	[!#1]S(=O)(=O)[NH2]
KRFP2816	KRFPC2816	[!#1]S(=O)(=O)[OH]
KRFP2817	KRFPC2817	[!#1]S(=O)(=O)C([CH3])([CH3])[CH2]C(=O)[CH3]
KRFP2818	KRFPC2818	[!#1]S(=O)(=O)C([CH3])([CH3])[CH3]
KRFP2819	KRFPC2819	[!#1]S(=O)(=O)C(F)(F)F
KRFP2820	KRFPC2820	[!#1]S(=O)(=O)c1[cH][cH][cH][cH]1
KRFP2821	KRFPC2821	[!#1]S(=O)(=O)c1[cH][cH][cH][cH]c1[N+](=O)[O-]
KRFP2822	KRFPC2822	[!#1]S(=O)(=O)c1[cH][cH][cH][cH]c1Cl
KRFP2823	KRFPC2823	[!#1]S(=O)(=O)c1[cH][cH][cH]c([cH]1)[N+](=O)[O-]
KRFP2824	KRFPC2824	[!#1]S(=O)(=O)c1[cH][cH][cH]c([cH]1)C(F)(F)F
KRFP2825	KRFPC2825	[!#1]S(=O)(=O)c1[cH][cH][cH]c([cH]1)S(=O)(=O)c2[cH][cH]c(Cl)[cH][cH]2
KRFP2826	KRFPC2826	[!#1]S(=O)(=O)c1[cH][cH][cH]c([cH]1)S(=O)(=O)c2[cH][cH]c(Cl)c(Cl)[cH]2
KRFP2827	KRFPC2827	[!#1]S(=O)(=O)c1[cH][cH][cH]c2[cH][cH][cH]nc12
KRFP2828	KRFPC2828	[!#1]S(=O)(=O)c1[cH][cH][cH]c2nsnc12
KRFP2829	KRFPC2829	[!#1]S(=O)(=O)c1[cH][cH]c([cH][cH]1)[CH]2[CH2][CH2][CH2][CH2][CH2]2
KRFP2830	KRFPC2830	[!#1]S(=O)(=O)c1[cH][cH]c([cH][cH]1)[N+](=O)[O-]
KRFP2831	KRFPC2831	[!#1]S(=O)(=O)c1[cH][cH]c([cH][cH]1)C([CH3])([CH3])[CH3]
KRFP2832	KRFPC2832	[!#1]S(=O)(=O)c1[cH][cH]c([cH][cH]1)C(=O)[OH]
KRFP2833	KRFPC2833	[!#1]S(=O)(=O)c1[cH][cH]c([CH3])[cH][cH]1
KRFP2834	KRFPC2834	[!#1]S(=O)(=O)c1[cH][cH]c([CH3])c([cH]1)[N+](=O)[O-]
KRFP2835	KRFPC2835	[!#1]S(=O)(=O)c1[cH][cH]c(Br)[cH][cH]1
KRFP2836	KRFPC2836	[!#1]S(=O)(=O)c1[cH][cH]c(Cl)[cH][cH]1
KRFP2837	KRFPC2837	[!#1]S(=O)(=O)c1[cH][cH]c(Cl)c([cH]1)[N+](=O)[O-]
KRFP2838	KRFPC2838	[!#1]S(=O)(=O)c1[cH][cH]c(Cl)c(Cl)[cH]1
KRFP2839	KRFPC2839	[!#1]S(=O)(=O)c1[cH][cH]c(S(c2[cH][cH]c([cH][cH]2)S(=O)(=O)[!#1]))[cH][cH]1
KRFP2840	KRFPC2840	[!#1]S(=O)(=O)c1[cH][cH]c2[cH][cH][cH][cH]c2[cH]1
KRFP2841	KRFPC2841	[!#1]S(=O)(=O)c1c([cH]c([cH]c1[CH]([CH3])[CH3])[CH]([CH3])[CH3])[CH]([CH3])[CH3]
KRFP2842	KRFPC2842	[!#1]S(=O)(=O)c1c([CH3])[cH]c([CH3])[cH]c1[CH3]
KRFP2843	KRFPC2843	[!#1]S(=O)(=O)N([CH2][CH]([CH3])[CH3])[CH2][CH]([CH3])[CH3]
KRFP2844	KRFPC2844	[!#1]S(=O)(=O)N([CH2][CH2][CH2][CH3])[CH2][CH2]C(=O)[NH2]
KRFP2845	KRFPC2845	[!#1]S(=O)(=O)N([CH2][CH2][CH3])[CH2][CH2][CH3]
KRFP2846	KRFPC2846	[!#1]S(=O)(=O)N([CH2][CH2][OH])[CH2][CH2][OH]
KRFP2847	KRFPC2847	[!#1]S(=O)(=O)N([CH2][CH3])[CH2][CH3]
KRFP2848	KRFPC2848	[!#1]S(=O)(=O)N([CH3])[CH3]
KRFP2849	KRFPC2849	[!#1]S(=O)(=O)N1[CH2][CH2][CH2][CH2][CH2]1

Name	Count name	Pattern
KRFP2850	KRFPC2850	[!#1]S(=O)(=O)N1[CH2][CH2]O[CH2][CH2]1
KRFP2851	KRFPC2851	[!#1]S(=O)(=O)O[CH2][CH2]S(=O)(=O)[CH2][CH3]
KRFP2852	KRFPC2852	[!#1]S(=O)(=O)O[CH3]
KRFP2853	KRFPC2853	[!#1]S(=O)(=O)O[K]
KRFP2854	KRFPC2854	[!#1]S(=O)(=O)O[Na]
KRFP2855	KRFPC2855	[!#1]S[!#1]
KRFP2856	KRFPC2856	[!#1]S[CH]([!#1])[!#1]
KRFP2857	KRFPC2857	[!#1]S[CH]([!#1])[CH2]C(=O)[!#1]
KRFP2858	KRFPC2858	[!#1]S[CH]([!#1])C(=O)[OH]
KRFP2859	KRFPC2859	[!#1]S[CH]([NH]C(=O)[!#1])C(=O)[!#1]
KRFP2860	KRFPC2860	[!#1]S[CH]([NH]C(=O)[!#1])C(Cl)(Cl)Cl
KRFP2861	KRFPC2861	[!#1]S[CH2][CH2][CH2]S(=O)(=O)[OH]
KRFP2862	KRFPC2862	[!#1]S[CH2][CH2][NH2]
KRFP2863	KRFPC2863	[!#1]S[CH2][CH2][OH]
KRFP2864	KRFPC2864	[!#1]S[CH2][CH2]C(F)(F)F
KRFP2865	KRFPC2865	[!#1]S[CH2][CH2]S(=O)(=O)[!#1]
KRFP2866	KRFPC2866	[!#1]S[CH2][CH2]S[!#1]
KRFP2867	KRFPC2867	[!#1]S[CH2][CH2]SC(=[NH])[NH2]
KRFP2868	KRFPC2868	[!#1]S[CH2][CH3]
KRFP2869	KRFPC2869	[!#1]S[CH2][NH]C(=O)[!#1]
KRFP2870	KRFPC2870	[!#1]S[CH2]C(=O)[!#1]
KRFP2871	KRFPC2871	[!#1]S[CH2]C(=O)[CH3]
KRFP2872	KRFPC2872	[!#1]S[CH2]C(=O)[NH]N=[CH][!#1]
KRFP2873	KRFPC2873	[!#1]S[CH2]C(=O)[NH2]
KRFP2874	KRFPC2874	[!#1]S[CH2]C(=O)[OH]
KRFP2875	KRFPC2875	[!#1]S[CH2]C(=O)O[CH2][CH3]
KRFP2876	KRFPC2876	[!#1]S[CH3]
KRFP2877	KRFPC2877	[!#1]SC([CH3])([CH3])[CH3]
KRFP2878	KRFPC2878	[!#1]SC(=[NH])[NH]N=[CH][!#1]
KRFP2879	KRFPC2879	[!#1]SC(=[NH])[NH2]
KRFP2880	KRFPC2880	[!#1]SC(=C(Cl)Cl)[NH]C(=O)[!#1]
KRFP2881	KRFPC2881	[!#1]SC(=N[CH2][CH3])[NH][CH2][CH3]
KRFP2882	KRFPC2882	[!#1]SC(=O)[!#1]
KRFP2883	KRFPC2883	[!#1]SC(F)(F)C(F)(F)C(F)(F)F
KRFP2884	KRFPC2884	[!#1]SC(F)(F)F
KRFP2885	KRFPC2885	[!#1]S(c1[cH][cH][cH][cH]1)
KRFP2886	KRFPC2886	[!#1]S(c1[cH][cH]c([!#1])[cH][cH]1)
KRFP2887	KRFPC2887	[!#1]S(c1nc2[cH][cH][cH][cH]c2s1)
KRFP2888	KRFPC2888	[Na]OS(=O)=O
KRFP2889	KRFPC2889	[O-][N+](=O)c1cc([N+](=O)[O-])c2ccccc2c1
KRFP2890	KRFPC2890	[O-][N+](=O)c1cc(C=O)cc(c1)[N+](=O)[O-]
KRFP2891	KRFPC2891	[O-][N+](=O)c1cc(C=O)ccc1Br
KRFP2892	KRFPC2892	[O-][N+](=O)c1cc(C=O)ccc1Cl
KRFP2893	KRFPC2893	[O-][N+](=O)c1cc(cc(c1)C(F)(F)F)[N+](=O)[O-]
KRFP2894	KRFPC2894	[O-][N+](=O)c1cc(ccc1Cl)S(=O)=O
KRFP2895	KRFPC2895	[O-][N+](=O)c1cc(NC=O)ccc1Cl
KRFP2896	KRFPC2896	[O-][N+](=O)c1cc2ccccc2oc1=O
KRFP2897	KRFPC2897	[O-][N+](=O)c1cc2OCOc2cc1C=N
KRFP2898	KRFPC2898	[O-][N+](=O)c1cc2OCOc2cc1C=NNC=O
KRFP2899	KRFPC2899	[O-][N+](=O)c1ccc(C=N)cc1
KRFP2900	KRFPC2900	[O-][N+](=O)c1ccc(C=N)s1
KRFP2901	KRFPC2901	[O-][N+](=O)c1ccc(C=NNC=O)cc1
KRFP2902	KRFPC2902	[O-][N+](=O)c1ccc(C=NNC=O)o1
KRFP2903	KRFPC2903	[O-][N+](=O)c1ccc(C=O)c(C=O)c1

Name	Count name	Pattern
KRFP2904	KRFPC2904	[O-][N+](=O)c1ccc(C=O)c(c1)[N+](=O)[O-]
KRFP2905	KRFPC2905	[O-][N+](=O)c1ccc(C=O)cc1
KRFP2906	KRFPC2906	[O-][N+](=O)c1ccc(cc1)C(=O)CCC(Cl)(Cl)Cl
KRFP2907	KRFPC2907	[O-][N+](=O)c1ccc(cc1)C(=O)NN=Cc2ccccc2
KRFP2908	KRFPC2908	[O-][N+](=O)c1ccc(cc1)N2CCNCC2
KRFP2909	KRFPC2909	[O-][N+](=O)c1ccc(cc1)N2N=C(CC2=O)c3ccccc3
KRFP2910	KRFPC2910	[O-][N+](=O)c1ccc(cc1)S(=O)=O
KRFP2911	KRFPC2911	[O-][N+](=O)c1ccc(CCC=O)cc1
KRFP2912	KRFPC2912	[O-][N+](=O)c1ccc(Cl)c(C=O)c1
KRFP2913	KRFPC2913	[O-][N+](=O)c1ccc(Cl)cc1
KRFP2914	KRFPC2914	[O-][N+](=O)c1ccc(NC(=S)NCC(Cl)(Cl)Cl)cc1
KRFP2915	KRFPC2915	[O-][N+](=O)c1ccc(NC=O)cc1
KRFP2916	KRFPC2916	[O-][N+](=O)c1ccc(NN=C(C=O)C=O)cc1
KRFP2917	KRFPC2917	[O-][N+](=O)c1ccc2C(=O)NC(=O)c2c1
KRFP2918	KRFPC2918	[O-][N+](=O)c1ccc2nc3c(cc2c1)[nH]c4ccccc43
KRFP2919	KRFPC2919	[O-][N+](=O)c1ccc2nonc2c1
KRFP2920	KRFPC2920	[O-][N+](=O)c1cccc(Br)c1
KRFP2921	KRFPC2921	[O-][N+](=O)c1cccc(C=N)c1
KRFP2922	KRFPC2922	[O-][N+](=O)c1cccc(C=NNC=O)c1
KRFP2923	KRFPC2923	[O-][N+](=O)c1cccc(C=O)c1
KRFP2924	KRFPC2924	[O-][N+](=O)c1cccc(C=O)c1C=O
KRFP2925	KRFPC2925	[O-][N+](=O)c1cccc(c1)[N+](=O)[O-]
KRFP2926	KRFPC2926	[O-][N+](=O)c1cccc(c1)C(F)(F)F
KRFP2927	KRFPC2927	[O-][N+](=O)c1cccc(c1)S(=O)=O
KRFP2928	KRFPC2928	[O-][N+](=O)c1cccc(Cl)c1
KRFP2929	KRFPC2929	[O-][N+](=O)c1cccc(NC(=S)NCC(Cl)(Cl)Cl)c1
KRFP2930	KRFPC2930	[O-][N+](=O)c1cccc(NC=O)c1
KRFP2931	KRFPC2931	[O-][N+](=O)c1cccc(NS(=O)=O)c1
KRFP2932	KRFPC2932	[O-][N+](=O)c1cccc2nonc12
KRFP2933	KRFPC2933	[O-][N+](=O)c1cccc2nsnc12
KRFP2934	KRFPC2934	[O-][N+](=O)c1cccc1
KRFP2935	KRFPC2935	[O-][N+](=O)c1cccc1C=N
KRFP2936	KRFPC2936	[O-][N+](=O)c1cccc1C=NNC=O
KRFP2937	KRFPC2937	[O-][N+](=O)c1cccc1C=O
KRFP2938	KRFPC2938	[O-][N+](=O)c1cccc1Cl
KRFP2939	KRFPC2939	[O-][N+](=O)c1cccc1NC(=S)NCC(Cl)(Cl)Cl
KRFP2940	KRFPC2940	[O-][N+](=O)c1cccc1NC=O
KRFP2941	KRFPC2941	[O-][N+](=O)c1cccc1S(=O)=O
KRFP2942	KRFPC2942	[O-][N+](=O)c1cn[nH]c1C=O
KRFP2943	KRFPC2943	[O-][N+](=O)c1nc[nH]c1C=O
KRFP2944	KRFPC2944	[O-][N+](=O)CCCl
KRFP2945	KRFPC2945	[O-][N+](=O)NC(=N)NN=C
KRFP2946	KRFPC2946	[O-][n+](=O)1ccc(C=O)cc1
KRFP2947	KRFPC2947	[O-][NH]=N
KRFP2948	KRFPC2948	[O-][NH]=O
KRFP2949	KRFPC2949	[OH]
KRFP2950	KRFPC2950	Br
KRFP2951	KRFPC2951	Brc1c[nH]nc1C=O
KRFP2952	KRFPC2952	Brc1cc(Br)c2ccncc2c1
KRFP2953	KRFPC2953	Brc1cc(Br)cc(Br)c1
KRFP2954	KRFPC2954	Brc1cc2OCOc2cc1C=NNC=O
KRFP2955	KRFPC2955	Brc1ccc(C=N)cc1
KRFP2956	KRFPC2956	Brc1ccc(C=N)s1
KRFP2957	KRFPC2957	Brc1ccc(C=NNC=O)cc1

Name	Count name	Pattern
KRFP2958	KRFPC2958	<chem>Brc1ccc(C=NOC=O)cc1</chem>
KRFP2959	KRFPC2959	<chem>Brc1ccc(C=O)c(C=O)c1</chem>
KRFP2960	KRFPC2960	<chem>Brc1ccc(C=O)cc1</chem>
KRFP2961	KRFPC2961	<chem>Brc1ccc(C=O)o1</chem>
KRFP2962	KRFPC2962	<chem>Brc1ccc(cc1)N2C(=O)CCC2=O</chem>
KRFP2963	KRFPC2963	<chem>Brc1ccc(cc1)S(=O)=O</chem>
KRFP2964	KRFPC2964	<chem>Brc1ccc(NC=O)cc1</chem>
KRFP2965	KRFPC2965	<chem>Brc1ccc(NS(=O)=O)cc1</chem>
KRFP2966	KRFPC2966	<chem>Brc1cccc(Br)c1</chem>
KRFP2967	KRFPC2967	<chem>Brc1cccc(C=O)c1</chem>
KRFP2968	KRFPC2968	<chem>Brc1cccc2ccccc12</chem>
KRFP2969	KRFPC2969	<chem>Brc1ccccc1</chem>
KRFP2970	KRFPC2970	<chem>Brc1ccccc1C=O</chem>
KRFP2971	KRFPC2971	<chem>Brc1ccccc1NC=O</chem>
KRFP2972	KRFPC2972	<chem>Brc1cccnc1</chem>
KRFP2973	KRFPC2973	<chem>Brc1cccocl</chem>
KRFP2974	KRFPC2974	<chem>BrCCC=O</chem>
KRFP2975	KRFPC2975	<chem>C</chem>
KRFP2976	KRFPC2976	<chem>C#C</chem>
KRFP2977	KRFPC2977	<chem>C#N</chem>
KRFP2978	KRFPC2978	<chem>C(#Cc1ccccc1)c2ccccc2</chem>
KRFP2979	KRFPC2979	<chem>C(c1ccccc1)c2ccccc2</chem>
KRFP2980	KRFPC2980	<chem>C(c1nn[nH]1)c2ccccc2</chem>
KRFP2981	KRFPC2981	<chem>C(Cc1ccccc1)c2ccccc2</chem>
KRFP2982	KRFPC2982	<chem>C(Cc1ccncc1)S(c2ccccc2)</chem>
KRFP2983	KRFPC2983	<chem>C(NCc1ccccc1)c2ccccc2</chem>
KRFP2984	KRFPC2984	<chem>C[N+](=O)[O-]</chem>
KRFP2985	KRFPC2985	<chem>C[NH](C)C</chem>
KRFP2986	KRFPC2986	<chem>C=C</chem>
KRFP2987	KRFPC2987	<chem>C=C(C#N)C#N</chem>
KRFP2988	KRFPC2988	<chem>C=C(NC=O)C=O</chem>
KRFP2989	KRFPC2989	<chem>C=c1[nH]c(=O)c(=C)[nH]c1=O</chem>
KRFP2990	KRFPC2990	<chem>C=C1C(=O)c2ccccc2C1=O</chem>
KRFP2991	KRFPC2991	<chem>C=C1C(=O)N(N=C1c2ccccc2)c3ccccc3</chem>
KRFP2992	KRFPC2992	<chem>C=C1C(=O)NC(=O)N(C1=O)c2cccc3ccccc23</chem>
KRFP2993	KRFPC2993	<chem>C=C1C(=O)NC(=O)NC1=O</chem>
KRFP2994	KRFPC2994	<chem>C=C1C(=O)OCOC1=O</chem>
KRFP2995	KRFPC2995	<chem>C=C1C=NN(C1=O)c2ccccc2</chem>
KRFP2996	KRFPC2996	<chem>C=C1CNCC(=C)C1=O</chem>
KRFP2997	KRFPC2997	<chem>C=C1N=C(OC1=O)c2ccccc2</chem>
KRFP2998	KRFPC2998	<chem>C=C1Nc2ccccc2C=C1</chem>
KRFP2999	KRFPC2999	<chem>C=C1OC(=O)c2c1cc[nH]c2=O</chem>
KRFP3000	KRFPC3000	<chem>C=C1SC(=N)NC1=O</chem>
KRFP3001	KRFPC3001	<chem>C=C1SC(=O)NC1=O</chem>
KRFP3002	KRFPC3002	<chem>C=C1SC(=S)N(C1=O)c2ccccc2</chem>
KRFP3003	KRFPC3003	<chem>C=C1SC(=S)NC1=O</chem>
KRFP3004	KRFPC3004	<chem>C=CC(=O)NC=S</chem>
KRFP3005	KRFPC3005	<chem>C=CC(=O)NNC=O</chem>
KRFP3006	KRFPC3006	<chem>C=CC=C1SC(=S)N(C1=O)c2ccccc2</chem>
KRFP3007	KRFPC3007	<chem>C=CC=C1SC(=S)NC1=O</chem>
KRFP3008	KRFPC3008	<chem>C=CC=N</chem>
KRFP3009	KRFPC3009	<chem>C=CC=NNC=O</chem>
KRFP3010	KRFPC3010	<chem>C=CC=O</chem>
KRFP3011	KRFPC3011	<chem>C=CC1CN2CCC1CC2</chem>

Name	Count name	Pattern
KRFP3012	KRFPC3012	C=CCNC=O
KRFP3013	KRFPC3013	C=N
KRFP3014	KRFPC3014	C=NC=NNC=O
KRFP3015	KRFPC3015	C=NCCCCCN=C
KRFP3016	KRFPC3016	C=NCCN=C
KRFP3017	KRFPC3017	C=NCCNC=O
KRFP3018	KRFPC3018	C=NN=C
KRFP3019	KRFPC3019	C=NNC(=O)C(=O)NN=C
KRFP3020	KRFPC3020	C=NNC(=O)CC(=O)NN=C
KRFP3021	KRFPC3021	C=NNC(=O)CNC=O
KRFP3022	KRFPC3022	C=NNC=O
KRFP3023	KRFPC3023	C=NNS(=O)=O
KRFP3024	KRFPC3024	C=NOC=O
KRFP3025	KRFPC3025	C=O
KRFP3026	KRFPC3026	c1[nH]c2cccc2[nH+]1
KRFP3027	KRFPC3027	c1[nH]c2cccc2c1c3cccc3
KRFP3028	KRFPC3028	c1[nH+]c2c(ccc3cccc23)s1
KRFP3029	KRFPC3029	c1[nH+]c2cccc2o1
KRFP3030	KRFPC3030	c1[nH+]c2cccc2s1
KRFP3031	KRFPC3031	C1C(N(N=C1c2cccc2)c3cccc3)c4cccc4
KRFP3032	KRFPC3032	c1c(nc2cccn12)c3cccc3
KRFP3033	KRFPC3033	C1C(NN=C1c2cccc2)c3cccc3
KRFP3034	KRFPC3034	c1c[nH]cn1
KRFP3035	KRFPC3035	c1c[nH+]on1
KRFP3036	KRFPC3036	C1C=NN(C1c2cccc2)c3cccc3
KRFP3037	KRFPC3037	C1C=NNC1(c2cccc2)c3cccc3
KRFP3038	KRFPC3038	C1C2CC3CC1CC(C2)(C3)c4cccc4
KRFP3039	KRFPC3039	C1C2CC3CC1CC(C2)(C3)c4cscn4
KRFP3040	KRFPC3040	C1C2CC3CC1CC(C2)C3
KRFP3041	KRFPC3041	C1C2CC3CC1CC(C2)CC3
KRFP3042	KRFPC3042	C1C2CCCC12
KRFP3043	KRFPC3043	C1c2cccc2-c3cccc13
KRFP3044	KRFPC3044	c1c2cccc2n3cnc4cccc4c13
KRFP3045	KRFPC3045	C1c2cccc2Oc3cccc13
KRFP3046	KRFPC3046	c1cc([nH]n1)c2cccc2
KRFP3047	KRFPC3047	C1CC(=NN1)c2cccc2
KRFP3048	KRFPC3048	C1CC(=NN1c2cccc2)c3cccc3
KRFP3049	KRFPC3049	C1CC(CCN1)c2cccc2
KRFP3050	KRFPC3050	C1CC(CN1)c2cccc2
KRFP3051	KRFPC3051	c1cc(cs1)c2cccc2
KRFP3052	KRFPC3052	c1cc(n[nH]1)c2cccc2
KRFP3053	KRFPC3053	c1cc[n+]2cccn2c1
KRFP3054	KRFPC3054	c1cc[nH]c1
KRFP3055	KRFPC3055	c1cc[nH+]cc1
KRFP3056	KRFPC3056	C1CC=CC=C1
KRFP3057	KRFPC3057	C1CC=CCN1
KRFP3058	KRFPC3058	C1CC1
KRFP3059	KRFPC3059	C1CC1(c2cccc2)c3cccc3
KRFP3060	KRFPC3060	C1CC12CCC2
KRFP3061	KRFPC3061	C1CC1C2CC2c3ccco3
KRFP3062	KRFPC3062	C1CC1c2cccc2
KRFP3063	KRFPC3063	C1Cc2[nH]cnc2C(N1)c3cccc3
KRFP3064	KRFPC3064	C1Cc2c([nH]c3cccc23)C(N1)c4cccc4
KRFP3065	KRFPC3065	C1Cc2c([nH]c3cccc23)-c4cnn(c14)c5cccc5

Name	Count name	Pattern
KRFP3066	KRFPC3066	C1Cc2c(CN1)[nH]c3cccc23
KRFP3067	KRFPC3067	c1cc2c(n[nH]c(c3cccc3)c2c1)c4cccc4
KRFP3068	KRFPC3068	c1cc2c[nH+]ccn2c1
KRFP3069	KRFPC3069	C1CC2c3cccc3C1c4cccc24
KRFP3070	KRFPC3070	C1CC2CC1C=C2
KRFP3071	KRFPC3071	C1Cc2cc3CCCCc3nc2C1
KRFP3072	KRFPC3072	C1Cc2cc3cccc3nc2N1
KRFP3073	KRFPC3073	C1Cc2cc3cccc3nc2N1c4cccc4
KRFP3074	KRFPC3074	C1CC2CCC1C2
KRFP3075	KRFPC3075	c1cc2ccc3cccc3c2o1
KRFP3076	KRFPC3076	C1CC2CCCC1N2
KRFP3077	KRFPC3077	C1Cc2cccc3cccc1c23
KRFP3078	KRFPC3078	c1cc2cccc2[nH]1
KRFP3079	KRFPC3079	C1Cc2cccc2C(N1)c3cccc3
KRFP3080	KRFPC3080	C1Cc2cccc2C3=NNC(C13)c4cccc4
KRFP3081	KRFPC3081	C1Cc2cccc2CN1
KRFP3082	KRFPC3082	C1Cc2cccc2N1
KRFP3083	KRFPC3083	c1cc2cccc2n1c3cccc3
KRFP3084	KRFPC3084	C1Cc2cccc2Nc3cccc13
KRFP3085	KRFPC3085	c1cc2cccc2o1
KRFP3086	KRFPC3086	c1cc2cccc2s1
KRFP3087	KRFPC3087	c1cc2ccnc2s1
KRFP3088	KRFPC3088	C1CC2CNCCN2C1
KRFP3089	KRFPC3089	c1cc2cncnc2s1
KRFP3090	KRFPC3090	C1CC2Nc3cccc3C2CN1
KRFP3091	KRFPC3091	c1cc2nc3cccc3nc2n1c4cccc4
KRFP3092	KRFPC3092	C1Cc2ncn2C1
KRFP3093	KRFPC3093	C1CC2NCCn3c2c(C1)c4cccc34
KRFP3094	KRFPC3094	C1Cc2sc3ncncc3c2C1
KRFP3095	KRFPC3095	C1CCC(C1)c2nnn[nH]2
KRFP3096	KRFPC3096	c1ccc(cc1)C(c2cccc2)c3cccc3
KRFP3097	KRFPC3097	c1ccc(cc1)C2(c3cccc3-c4cccc42)c5cccc5
KRFP3098	KRFPC3098	c1ccc(cc1)c2cc(nc(n2)c3cccc3)c4cccc4
KRFP3099	KRFPC3099	c1ccc(cc1)c2cc(ncn2)c3cccc3
KRFP3100	KRFPC3100	C1CCC(CC1)c2ccc3[nH]c4CCCCc4c3c2
KRFP3101	KRFPC3101	c1ccc(cc1)c2ccc3c(ccc4cccc43)n2
KRFP3102	KRFPC3102	c1ccc(cc1)c2ccc3cccc3n2
KRFP3103	KRFPC3103	c1ccc(cc1)c2cccc(n2)c3cccc3
KRFP3104	KRFPC3104	C1CCC(CC1)c2cccc2
KRFP3105	KRFPC3105	c1ccc(cc1)c2cccn2
KRFP3106	KRFPC3106	c1ccc(cc1)c2ccnc(n2)c3cccc3
KRFP3107	KRFPC3107	c1ccc(cc1)c2ccnnc2
KRFP3108	KRFPC3108	c1ccc(cc1)c2cnc3cccc3n2
KRFP3109	KRFPC3109	c1ccc(cc1)c2n[nH]c(n2)c3cccc3
KRFP3110	KRFPC3110	c1ccc(cc1)c2nc(c3cccc3)c4cccc4n2
KRFP3111	KRFPC3111	c1ccc(cc1)c2nc3cccc3[nH]2
KRFP3112	KRFPC3112	c1ccc(cc1)c2nc3cccc3nc2c4cccc4
KRFP3113	KRFPC3113	c1ccc(cc1)c2nc3cccc3o2
KRFP3114	KRFPC3114	c1ccc(cc1)c2nc3cccc3s2
KRFP3115	KRFPC3115	c1ccc(cc1)c2nccn2
KRFP3116	KRFPC3116	c1ccc(cc1)c2ncnnc2
KRFP3117	KRFPC3117	C1CCC(CC1)c2nnn[nH]2
KRFP3118	KRFPC3118	C1CCC(CC1)c2nnnn2c3cccc3
KRFP3119	KRFPC3119	c1ccc(cc1)n2nc3cccc3n2

Name	Count name	Pattern
KRFP3120	KRFPC3120	C1CCC=CC1
KRFP3121	KRFPC3121	C1CCC1
KRFP3122	KRFPC3122	c1ccc2[nH]nnc2c1
KRFP3123	KRFPC3123	c1ccc2[nH+]c3cccc3nc2c1
KRFP3124	KRFPC3124	c1ccc2[nH+]cccc2c1
KRFP3125	KRFPC3125	c1ccc2c(c1)[nH]c3cc4cccc4nc32
KRFP3126	KRFPC3126	C1CCc2c(C1)[nH]c3ccc(cc23)c4cccc4
KRFP3127	KRFPC3127	C1CCc2c(C1)[nH]c3cccc23
KRFP3128	KRFPC3128	c1ccc2c(c1)[nH]c3cccc32
KRFP3129	KRFPC3129	c1ccc2c(c1)[nH]c3ncnnc23
KRFP3130	KRFPC3130	C1CCc2c(C1)nc3ccccn23
KRFP3131	KRFPC3131	c1ccc2c(c1)oc3cccc32
KRFP3132	KRFPC3132	C1CCc2c(C1)sc3ncncc23
KRFP3133	KRFPC3133	C1CCC2C(NCCC2C1)c3cccc3
KRFP3134	KRFPC3134	c1ccc2c[nH+]ccc2c1
KRFP3135	KRFPC3135	c1ccc2c3[nH]c4cccc4c3[nH]c2c1
KRFP3136	KRFPC3136	c1ccc2C3c4cccc4C(c2c1)c5cccc35
KRFP3137	KRFPC3137	c1ccc2cc3cccc3cc2c1
KRFP3138	KRFPC3138	c1ccc2cc3ncccc3cc2c1
KRFP3139	KRFPC3139	c1ccc2cccc2c1
KRFP3140	KRFPC3140	c1ccc2n[nH]nc2c1
KRFP3141	KRFPC3141	c1ccc2nc3cccc3cc2c1
KRFP3142	KRFPC3142	c1ccc2nc3cccc3nc2c1
KRFP3143	KRFPC3143	c1ccc2ncccc2c1
KRFP3144	KRFPC3144	c1ccc2ncnc2c1
KRFP3145	KRFPC3145	c1ccc2ncncc2c1
KRFP3146	KRFPC3146	c1ccc2nonc2c1
KRFP3147	KRFPC3147	c1ccc2nsnc2c1
KRFP3148	KRFPC3148	C1CCc2sccc2C1
KRFP3149	KRFPC3149	C1CCCC1
KRFP3150	KRFPC3150	C1CCCCC1
KRFP3151	KRFPC3151	C1CCCCC1
KRFP3152	KRFPC3152	C1CCCCCCC1
KRFP3153	KRFPC3153	C1CCCNCC1
KRFP3154	KRFPC3154	c1ccn(c1)c2cccc2
KRFP3155	KRFPC3155	C1CCN(CC1)c2ncncn2
KRFP3156	KRFPC3156	C1CCNC1
KRFP3157	KRFPC3157	C1CCNCC1
KRFP3158	KRFPC3158	c1ccnnc1
KRFP3159	KRFPC3159	c1ccoc1
KRFP3160	KRFPC3160	C1CCOCC1
KRFP3161	KRFPC3161	c1ccsc1
KRFP3162	KRFPC3162	C1CN(C(N1c2cccc2)c3cccc3)c4cccc4
KRFP3163	KRFPC3163	C1CN(CCN1)c2cccc2
KRFP3164	KRFPC3164	C1CN(CCN1)c2ccccn2
KRFP3165	KRFPC3165	C1CN(CCO1)c2cccc2
KRFP3166	KRFPC3166	C1CN(CCO1)c2ncnc(n2)N3CCOCC3
KRFP3167	KRFPC3167	C1CN(CCO1)c2ncncn2
KRFP3168	KRFPC3168	c1cn(nc1c2cccc2)c3cccc3
KRFP3169	KRFPC3169	c1cn[nH]c1
KRFP3170	KRFPC3170	c1cn2c(n1)[nH]c3cccc32
KRFP3171	KRFPC3171	C1CN2CCC1CC2
KRFP3172	KRFPC3172	C1Cn2cccc2C=[NH+]1
KRFP3173	KRFPC3173	C1Cn2cccc2C=N1

Name	Count name	Pattern
KRFP3174	KRFPC3174	C1Cn2cccc2CN1
KRFP3175	KRFPC3175	c1cn2cccc2n1
KRFP3176	KRFPC3176	C1CNC(N1)c2cccc2
KRFP3177	KRFPC3177	C1CNc2cccc2C1
KRFP3178	KRFPC3178	c1cnc2nonc2n1
KRFP3179	KRFPC3179	C1CNCCN1
KRFP3180	KRFPC3180	c1cncnc1
KRFP3181	KRFPC3181	c1cnn(c1)c2cccc2
KRFP3182	KRFPC3182	c1cnoc1
KRFP3183	KRFPC3183	c1cnon1
KRFP3184	KRFPC3184	c1coc(c1)c2cccc2
KRFP3185	KRFPC3185	C1COC(C1)n2cnc3cncnc23
KRFP3186	KRFPC3186	C1COC(N1)c2cccc2
KRFP3187	KRFPC3187	C1COC=CO1
KRFP3188	KRFPC3188	C1COC2(CCCC2)O1
KRFP3189	KRFPC3189	C1COC2C(C1)COc3cccc23
KRFP3190	KRFPC3190	C1COc2cccc2O1
KRFP3191	KRFPC3191	C1COCCN1
KRFP3192	KRFPC3192	C1COCCO1
KRFP3193	KRFPC3193	C1COCCOCCNCCOCCOCCN1
KRFP3194	KRFPC3194	C1COCCOCCOCCOCCOCCN1
KRFP3195	KRFPC3195	c1cocn1
KRFP3196	KRFPC3196	C1COCO1
KRFP3197	KRFPC3197	c1csc(c1)c2cccc2
KRFP3198	KRFPC3198	C1CSC(N1)c2cccc2
KRFP3199	KRFPC3199	c1csc[nH+]1
KRFP3200	KRFPC3200	c1cscn1
KRFP3201	KRFPC3201	c1n[nH]c2cccn[n+]12
KRFP3202	KRFPC3202	c1n[nH+]c[nH]1
KRFP3203	KRFPC3203	c1nc(cs1)c2cccc2
KRFP3204	KRFPC3204	c1nc(oc1c2cccc2)c3cccc3
KRFP3205	KRFPC3205	c1nc[nH]n1
KRFP3206	KRFPC3206	c1nc2cccc2[nH]1
KRFP3207	KRFPC3207	c1nc2cccc2o1
KRFP3208	KRFPC3208	c1nc2cccc2s1
KRFP3209	KRFPC3209	c1nc2cnccc2[nH]1
KRFP3210	KRFPC3210	c1nc2cncnc2[nH]1
KRFP3211	KRFPC3211	c1nc2nc(cc(c3cccc3)n2n1)c4cccc4
KRFP3212	KRFPC3212	c1nc2ncccn2n1
KRFP3213	KRFPC3213	c1nc2ncncc2[nH]1
KRFP3214	KRFPC3214	c1ncc(s1)c2cccc2
KRFP3215	KRFPC3215	c1ncncn1
KRFP3216	KRFPC3216	c1nnc[nH]1
KRFP3217	KRFPC3217	c1nncn1c2cccc2
KRFP3218	KRFPC3218	c1nnco1
KRFP3219	KRFPC3219	c1nncs1
KRFP3220	KRFPC3220	c1nnn[nH]1
KRFP3221	KRFPC3221	c1nnnn1c2cccc2
KRFP3222	KRFPC3222	C1Oc2cccc2O1
KRFP3223	KRFPC3223	CBr
KRFP3224	KRFPC3224	CC
KRFP3225	KRFPC3225	CC#C
KRFP3226	KRFPC3226	CC#CC(O)(c1cccc1)c2cccc2
KRFP3227	KRFPC3227	CC#CCCO

Name	Count name	Pattern
KRFP3228	KRFPC3228	<chem>CC(=C)C(=O)N</chem>
KRFP3229	KRFPC3229	<chem>CC(=N)C</chem>
KRFP3230	KRFPC3230	<chem>CC(=N)CC=O</chem>
KRFP3231	KRFPC3231	<chem>CC(=NN)C</chem>
KRFP3232	KRFPC3232	<chem>CC(=NNC(=O)c1cccc1)c2cccc2</chem>
KRFP3233	KRFPC3233	<chem>CC(=NNC(=O)c1cccc1O)c2cccc2</chem>
KRFP3234	KRFPC3234	<chem>CC(=NNC(=O)CO)C</chem>
KRFP3235	KRFPC3235	<chem>CC(=NNC(=O)CO)C=C</chem>
KRFP3236	KRFPC3236	<chem>CC(=NNC(=O)CO)C=Cc1ccco1</chem>
KRFP3237	KRFPC3237	<chem>CC(=NNC(=O)CO)c1ccc(Br)s1</chem>
KRFP3238	KRFPC3238	<chem>CC(=NNC(=O)CO)c1cccs1</chem>
KRFP3239	KRFPC3239	<chem>CC(=NNC=O)C</chem>
KRFP3240	KRFPC3240	<chem>CC(=NNC=O)C(=O)O</chem>
KRFP3241	KRFPC3241	<chem>CC(=NNC=O)C=C</chem>
KRFP3242	KRFPC3242	<chem>CC(=NNC=O)C=Cc1cccc1</chem>
KRFP3243	KRFPC3243	<chem>CC(=NNC=O)c1cc(O)ccc1O</chem>
KRFP3244	KRFPC3244	<chem>CC(=NNC=O)C1CC1</chem>
KRFP3245	KRFPC3245	<chem>CC(=NNC=O)c1cc2ccc(O)cc2oc1=O</chem>
KRFP3246	KRFPC3246	<chem>CC(=NNC=O)c1ccc(Br)cc1</chem>
KRFP3247	KRFPC3247	<chem>CC(=NNC=O)c1ccc(cc1)[N+](=O)[O-]</chem>
KRFP3248	KRFPC3248	<chem>CC(=NNC=O)c1ccc(cc1)c2cccc2</chem>
KRFP3249	KRFPC3249	<chem>CC(=NNC=O)c1ccc(Cl)s1</chem>
KRFP3250	KRFPC3250	<chem>CC(=NNC=O)c1ccc(F)cc1</chem>
KRFP3251	KRFPC3251	<chem>CC(=NNC=O)c1ccc(N)cc1</chem>
KRFP3252	KRFPC3252	<chem>CC(=NNC=O)c1ccc(O)cc1</chem>
KRFP3253	KRFPC3253	<chem>CC(=NNC=O)c1cccc(c1)[N+](=O)[O-]</chem>
KRFP3254	KRFPC3254	<chem>CC(=NNC=O)c1cccc(N)c1</chem>
KRFP3255	KRFPC3255	<chem>CC(=NNC=O)c1cccc1</chem>
KRFP3256	KRFPC3256	<chem>CC(=NNC=O)c1cccc1O</chem>
KRFP3257	KRFPC3257	<chem>CC(=NNC=O)c1ccco1</chem>
KRFP3258	KRFPC3258	<chem>CC(=NNC=O)c1cccs1</chem>
KRFP3259	KRFPC3259	<chem>CC(=NNC=O)CC(=O)N</chem>
KRFP3260	KRFPC3260	<chem>CC(=NNC=O)CCC=C</chem>
KRFP3261	KRFPC3261	<chem>CC(=NNc1ccc(cc1[N+](=O)[O-])[N+](=O)[O-])c2cccc2</chem>
KRFP3262	KRFPC3262	<chem>CC(=NNc1cccc1)c2cccc2</chem>
KRFP3263	KRFPC3263	<chem>CC(=NNc1cccc1)CC=O</chem>
KRFP3264	KRFPC3264	<chem>CC(=NO)c1cccc1</chem>
KRFP3265	KRFPC3265	<chem>CC(=NOC(=O)N)C</chem>
KRFP3266	KRFPC3266	<chem>CC(=NOC=O)C(C)(C)C</chem>
KRFP3267	KRFPC3267	<chem>CC(=NOC=O)c1cccc1</chem>
KRFP3268	KRFPC3268	<chem>CC(=O)C</chem>
KRFP3269	KRFPC3269	<chem>CC(=O)C1(C(C=O)C(C=O)C2c3cccc31)c4cccc24</chem>
KRFP3270	KRFPC3270	<chem>CC(=O)C1(CC2CC3CC(C2)C1)C3</chem>
KRFP3271	KRFPC3271	<chem>CC(=O)c1c(C)[nH]c2ccc(O)cc12</chem>
KRFP3272	KRFPC3272	<chem>CC(=O)c1c(C)[nH]c2cccc12</chem>
KRFP3273	KRFPC3273	<chem>CC(=O)c1c(C)cc(C)[nH]c1=O</chem>
KRFP3274	KRFPC3274	<chem>CC(=O)c1c(O)cc(C)oc1=O</chem>
KRFP3275	KRFPC3275	<chem>CC(=O)c1ccc(Br)cc1</chem>
KRFP3276	KRFPC3276	<chem>CC(=O)c1ccc(C)cc1</chem>
KRFP3277	KRFPC3277	<chem>CC(=O)c1ccc(cc1)c2cccc2</chem>
KRFP3278	KRFPC3278	<chem>CC(=O)c1ccc(Cl)c(Cl)c1</chem>
KRFP3279	KRFPC3279	<chem>CC(=O)c1ccc(Cl)cc1</chem>
KRFP3280	KRFPC3280	<chem>CC(=O)c1ccc(N)cc1</chem>
KRFP3281	KRFPC3281	<chem>CC(=O)c1ccc(O)cc1</chem>

Name	Count name	Pattern
KRFP3282	KRFPC3282	<chem>CC(=O)c1cccc(c1)[N+](=O)[O-]</chem>
KRFP3283	KRFPC3283	<chem>CC(=O)c1cccc1</chem>
KRFP3284	KRFPC3284	<chem>CC(=O)c1cccc1C(=O)C</chem>
KRFP3285	KRFPC3285	<chem>CC(=O)c1cccc1O</chem>
KRFP3286	KRFPC3286	<chem>CC(=O)c1ccncc1</chem>
KRFP3287	KRFPC3287	<chem>CC(=O)CC(=NNC=O)C</chem>
KRFP3288	KRFPC3288	<chem>CC(=O)CC(=O)C</chem>
KRFP3289	KRFPC3289	<chem>CC(=O)CC(=O)N</chem>
KRFP3290	KRFPC3290	<chem>CC(=O)CC(C)(C)S(=O)=O</chem>
KRFP3291	KRFPC3291	<chem>CC(=O)CC=O</chem>
KRFP3292	KRFPC3292	<chem>CC(=O)CCS(=O)=O</chem>
KRFP3293	KRFPC3293	<chem>CC(=O)CO</chem>
KRFP3294	KRFPC3294	<chem>CC(=O)CS(=O)=O</chem>
KRFP3295	KRFPC3295	<chem>CC(=O)N</chem>
KRFP3296	KRFPC3296	<chem>CC(=O)n1ccc2ccccc12</chem>
KRFP3297	KRFPC3297	<chem>CC(=O)N1CCOCC1</chem>
KRFP3298	KRFPC3298	<chem>CC(=O)NC(=C)C(=O)N</chem>
KRFP3299	KRFPC3299	<chem>CC(=O)NC(=Cc1cccc1)C(=O)N</chem>
KRFP3300	KRFPC3300	<chem>CC(=O)NC(N)C(Cl)(Cl)Cl</chem>
KRFP3301	KRFPC3301	<chem>CC(=O)NC(NC(=S)N)C(Cl)(Cl)Cl</chem>
KRFP3302	KRFPC3302	<chem>CC(=O)NCC(=O)N</chem>
KRFP3303	KRFPC3303	<chem>CC(=O)NN</chem>
KRFP3304	KRFPC3304	<chem>CC(=O)NN=C</chem>
KRFP3305	KRFPC3305	<chem>CC(=O)NN=C(C)c1cccc1</chem>
KRFP3306	KRFPC3306	<chem>CC(=O)NN=C(C=O)c1cccc(Br)c1</chem>
KRFP3307	KRFPC3307	<chem>CC(=O)NN=C(C=O)c1cccc(c1)[N+](=O)[O-]</chem>
KRFP3308	KRFPC3308	<chem>CC(=O)NN=C1CCc2c1non2=O</chem>
KRFP3309	KRFPC3309	<chem>CC(=O)NN=Cc1c(Cl)cccc1Cl</chem>
KRFP3310	KRFPC3310	<chem>CC(=O)NN=Cc1c(O)ccc2ccccc12</chem>
KRFP3311	KRFPC3311	<chem>CC(=O)NN=Cc1c[nH]c2ccccc12</chem>
KRFP3312	KRFPC3312	<chem>CC(=O)NN=Cc1cc(ccc1O)[N+](=O)[O-]</chem>
KRFP3313	KRFPC3313	<chem>CC(=O)NN=Cc1cc(N=Nc2ccccc2)ccc1O</chem>
KRFP3314	KRFPC3314	<chem>CC(=O)NN=Cc1cc2ccccc2nc1Cl</chem>
KRFP3315	KRFPC3315	<chem>CC(=O)NN=Cc1cc2OCOc2cc1[N+](=O)[O-]</chem>
KRFP3316	KRFPC3316	<chem>CC(=O)NN=Cc1ccc(Br)cc1</chem>
KRFP3317	KRFPC3317	<chem>CC(=O)NN=Cc1ccc(cc1)[N+](=O)[O-]</chem>
KRFP3318	KRFPC3318	<chem>CC(=O)NN=Cc1ccc(Cl)cc1</chem>
KRFP3319	KRFPC3319	<chem>CC(=O)NN=Cc1ccc2OCOc2c1</chem>
KRFP3320	KRFPC3320	<chem>CC(=O)NN=Cc1cccc(c1)[N+](=O)[O-]</chem>
KRFP3321	KRFPC3321	<chem>CC(=O)NN=Cc1cccc1</chem>
KRFP3322	KRFPC3322	<chem>CC(=O)NN=Cc1cccc1O</chem>
KRFP3323	KRFPC3323	<chem>CC(=O)NN=Cc1ccco1</chem>
KRFP3324	KRFPC3324	<chem>CC(=O)NN=Cc1cccs1</chem>
KRFP3325	KRFPC3325	<chem>CC(=O)NNC=O</chem>
KRFP3326	KRFPC3326	<chem>CC(=O)NO</chem>
KRFP3327	KRFPC3327	<chem>CC(=O)NS(=O)=O</chem>
KRFP3328	KRFPC3328	<chem>CC(=O)O</chem>
KRFP3329	KRFPC3329	<chem>CC(=O)O[Na]</chem>
KRFP3330	KRFPC3330	<chem>CC(=O)OC(=N)c1cccc1</chem>
KRFP3331	KRFPC3331	<chem>CC(=O)OCC=O</chem>
KRFP3332	KRFPC3332	<chem>CC(=O)OCCNC=O</chem>
KRFP3333	KRFPC3333	<chem>CC(Br)(Br)Br</chem>
KRFP3334	KRFPC3334	<chem>CC(Br)C(=O)N</chem>
KRFP3335	KRFPC3335	<chem>CC(C(C=O)C(C=O)C(C)c1cccc1)c2ccccc2</chem>

Name	Count name	Pattern
KRFP3336	KRFPC3336	CC(C)(C)C
KRFP3337	KRFPC3337	CC(C)(C)C(=O)N
KRFP3338	KRFPC3338	CC(C)(C)C(=O)NC(NC(=S)N)C(Cl)(Cl)Cl
KRFP3339	KRFPC3339	CC(C)(C)C=O
KRFP3340	KRFPC3340	CC(C)(C)c1cc(Br)cc(C=N)c1O
KRFP3341	KRFPC3341	CC(C)(C)c1cc(C=N)cc(c1O)C(C)(C)C
KRFP3342	KRFPC3342	CC(C)(C)c1cc(C=O)cc(c1)C(C)(C)C
KRFP3343	KRFPC3343	CC(C)(C)c1ccc(C=O)cc1
KRFP3344	KRFPC3344	CC(C)(C)c1ccc(cc1)S(=O)=O
KRFP3345	KRFPC3345	CC(C)(C)c1ccc(O)c(c1)C(C)(C)C
KRFP3346	KRFPC3346	CC(C)(C)c1ccc(O)cc1
KRFP3347	KRFPC3347	CC(C)(C)c1cccc(c1)C(C)(C)C
KRFP3348	KRFPC3348	CC(C)(C)c1cccc(c1O)C(C)(C)C
KRFP3349	KRFPC3349	CC(C)(C)c1cccc1
KRFP3350	KRFPC3350	CC(C)(C)c1ncccc1O
KRFP3351	KRFPC3351	CC(C)(C)CC=C
KRFP3352	KRFPC3352	CC(C)(C)CC=Cc1ccc(Cl)cc1Cl
KRFP3353	KRFPC3353	CC(C)(C)N
KRFP3354	KRFPC3354	CC(C)(C)NC(NC=O)C(Cl)(Cl)Cl
KRFP3355	KRFPC3355	CC(C)(C)NC=O
KRFP3356	KRFPC3356	CC(C)(C)NCC(=O)N
KRFP3357	KRFPC3357	CC(C)(C)NCC(O)CO
KRFP3358	KRFPC3358	CC(C)(C)NS(=O)(=O)N
KRFP3359	KRFPC3359	CC(C)(C)NS(=O)=O
KRFP3360	KRFPC3360	CC(C)(C)O
KRFP3361	KRFPC3361	CC(C)(C)OC=O
KRFP3362	KRFPC3362	CC(C)(C)S
KRFP3363	KRFPC3363	CC(C)(C)S(=O)=O
KRFP3364	KRFPC3364	CC(C)(c1ccc(O)cc1)c2ccc(O)cc2
KRFP3365	KRFPC3365	CC(C)(CCC(=O)N)C(=O)N
KRFP3366	KRFPC3366	CC(C)(CCC=O)C=O
KRFP3367	KRFPC3367	CC(C)(N)CO
KRFP3368	KRFPC3368	CC(C)(O)C#C
KRFP3369	KRFPC3369	CC(C)C
KRFP3370	KRFPC3370	CC(C)C(=O)NC(NC(=S)N)C(Cl)(Cl)Cl
KRFP3371	KRFPC3371	CC(C)C(N)C(=O)O
KRFP3372	KRFPC3372	CC(C)C(NC(=S)SCC=O)C(=O)O
KRFP3373	KRFPC3373	CC(C)C(NC=O)C(=O)O
KRFP3374	KRFPC3374	CC(C)C(NS(=O)=O)C(=O)O
KRFP3375	KRFPC3375	CC(C)C=O
KRFP3376	KRFPC3376	CC(C)c1cc(C(C)C)c(S(=O)=O)c(c1)C(C)C
KRFP3377	KRFPC3377	CC(C)c1cc(cc(c1)C(C)C)C(C)C
KRFP3378	KRFPC3378	CC(C)c1ccc(C)c(O)c1
KRFP3379	KRFPC3379	CC(C)c1ccc(C)cc1
KRFP3380	KRFPC3380	CC(C)C1CCC(C)CC1O
KRFP3381	KRFPC3381	CC(C)c1ccc(O)cc1
KRFP3382	KRFPC3382	CC(C)c1cccc1
KRFP3383	KRFPC3383	CC(C)c1nn[nH]1
KRFP3384	KRFPC3384	CC(C)CC(=NNC=O)C
KRFP3385	KRFPC3385	CC(C)CC(=O)N
KRFP3386	KRFPC3386	CC(C)CC(=O)NC(NC(=S)N)C(Cl)(Cl)Cl
KRFP3387	KRFPC3387	CC(C)CC(=O)O
KRFP3388	KRFPC3388	CC(C)CC(C)(C)C
KRFP3389	KRFPC3389	CC(C)CC(C)O

Name	Count name	Pattern
KRFP3390	KRFPC3390	<chem>CC(C)CC=O</chem>
KRFP3391	KRFPC3391	<chem>CC(C)Cc1ccc(cc1)C(C)C=O</chem>
KRFP3392	KRFPC3392	<chem>CC(C)CCC(=O)O</chem>
KRFP3393	KRFPC3393	<chem>CC(C)CCC=O</chem>
KRFP3394	KRFPC3394	<chem>CC(C)CCCC(C)C</chem>
KRFP3395	KRFPC3395	<chem>CC(C)CCO</chem>
KRFP3396	KRFPC3396	<chem>CC(C)CN</chem>
KRFP3397	KRFPC3397	<chem>CC(C)CN(CC(C)C)S(=O)=O</chem>
KRFP3398	KRFPC3398	<chem>CC(C)CNC=O</chem>
KRFP3399	KRFPC3399	<chem>CC(C)CO</chem>
KRFP3400	KRFPC3400	<chem>CC(C)COC=O</chem>
KRFP3401	KRFPC3401	<chem>CC(C)COP(=O)(N)OCC(C)C</chem>
KRFP3402	KRFPC3402	<chem>CC(C)N</chem>
KRFP3403	KRFPC3403	<chem>CC(C)N(C=O)C(C)C</chem>
KRFP3404	KRFPC3404	<chem>CC(C)NC=O</chem>
KRFP3405	KRFPC3405	<chem>CC(C)NCC(=O)N</chem>
KRFP3406	KRFPC3406	<chem>CC(C)NCC(O)CO</chem>
KRFP3407	KRFPC3407	<chem>CC(C)NS(=O)=O</chem>
KRFP3408	KRFPC3408	<chem>CC(C)O</chem>
KRFP3409	KRFPC3409	<chem>CC(C)OC(=O)N</chem>
KRFP3410	KRFPC3410	<chem>CC(C)OC=O</chem>
KRFP3411	KRFPC3411	<chem>CC(C)OP(=O)(N)OC(C)C</chem>
KRFP3412	KRFPC3412	<chem>CC(CC=O)c1ccccc1</chem>
KRFP3413	KRFPC3413	<chem>CC(Cl)(Cl)Cl</chem>
KRFP3414	KRFPC3414	<chem>CC(N)C(=O)O</chem>
KRFP3415	KRFPC3415	<chem>CC(N)c1ccccc1</chem>
KRFP3416	KRFPC3416	<chem>CC(NC(=O)CO)C(=O)O</chem>
KRFP3417	KRFPC3417	<chem>CC(NC(=O)OC(C)(C)C)C(=O)O</chem>
KRFP3418	KRFPC3418	<chem>CC(NC=O)C(=O)N</chem>
KRFP3419	KRFPC3419	<chem>CC(NC=O)C(=O)O</chem>
KRFP3420	KRFPC3420	<chem>CC(NS(=O)=O)C(=O)O</chem>
KRFP3421	KRFPC3421	<chem>CC(O)C(=O)NN</chem>
KRFP3422	KRFPC3422	<chem>CC(O)C(=O)NN=C</chem>
KRFP3423	KRFPC3423	<chem>CC(O)C(=O)NN=Cc1cc(ccc1O)[N+](=O)[O-]</chem>
KRFP3424	KRFPC3424	<chem>CC(O)C(=O)NN=Cc1ccccc1</chem>
KRFP3425	KRFPC3425	<chem>CC(O)C(=O)O</chem>
KRFP3426	KRFPC3426	<chem>CC(O)C(O)C(O)C(C)O</chem>
KRFP3427	KRFPC3427	<chem>CC(O)C(O)C(O)C(O)CO</chem>
KRFP3428	KRFPC3428	<chem>CC(O)C(O)C(O)CO</chem>
KRFP3429	KRFPC3429	<chem>CC(O)c1ccc(cc1)[N+](=O)[O-]</chem>
KRFP3430	KRFPC3430	<chem>CC(O)c1ccccc1</chem>
KRFP3431	KRFPC3431	<chem>CC(O)CBr</chem>
KRFP3432	KRFPC3432	<chem>CC(O)CCC(=O)NN=C</chem>
KRFP3433	KRFPC3433	<chem>CC(O)CCl</chem>
KRFP3434	KRFPC3434	<chem>CC(O)CN</chem>
KRFP3435	KRFPC3435	<chem>CC(O)CN(C)C</chem>
KRFP3436	KRFPC3436	<chem>CC(O)CO</chem>
KRFP3437	KRFPC3437	<chem>CC(OC=O)C(=C(Cl)Cl)Cl</chem>
KRFP3438	KRFPC3438	<chem>CC[n+](c(C)oc2ccccc12</chem>
KRFP3439	KRFPC3439	<chem>CC[n+](c2ccccc2nc3ccccc13</chem>
KRFP3440	KRFPC3440	<chem>CC=C</chem>
KRFP3441	KRFPC3441	<chem>CC=CC(=O)C</chem>
KRFP3442	KRFPC3442	<chem>CC=CC(=O)N</chem>
KRFP3443	KRFPC3443	<chem>CC=N</chem>

Name	Count name	Pattern
KRFP3444	KRFPC3444	CC=NN
KRFP3445	KRFPC3445	CC=NN=CC
KRFP3446	KRFPC3446	CC=NNC(=O)C
KRFP3447	KRFPC3447	CC=NNC(=O)CO
KRFP3448	KRFPC3448	CC=NNC(=O)N
KRFP3449	KRFPC3449	CC=NNC(=S)N
KRFP3450	KRFPC3450	CC=NNC=O
KRFP3451	KRFPC3451	CC=NNS(=O)=O
KRFP3452	KRFPC3452	CC=NO
KRFP3453	KRFPC3453	CC=NOC=O
KRFP3454	KRFPC3454	CC=NOCON=CC
KRFP3455	KRFPC3455	CC=O
KRFP3456	KRFPC3456	CC1(C)C(CCC1(C)C(=O)O)C(=O)N
KRFP3457	KRFPC3457	CC1(C)C(CCC1(C)C(=O)O)C=O
KRFP3458	KRFPC3458	CC1(C)C2CCC1(C)C(=O)C2
KRFP3459	KRFPC3459	CC1(C)CC(=CC(=O)C1)O
KRFP3460	KRFPC3460	CC1(C)CC(=O)c2cc3cccc3nc2C1
KRFP3461	KRFPC3461	CC1(C)CC(=O)c2cncnc2C1
KRFP3462	KRFPC3462	CC1(C)CC(=O)CC(=NNC=O)C1
KRFP3463	KRFPC3463	CC1(C)CC(=O)CC(=O)C1
KRFP3464	KRFPC3464	CC1(C)CC(=O)CC(=O)C1C=O
KRFP3465	KRFPC3465	CC1(C)CC(O)c2cc3cccc3nc2C1
KRFP3466	KRFPC3466	CC1(C)CC=CC(=O)C1
KRFP3467	KRFPC3467	CC1(C)CC1
KRFP3468	KRFPC3468	CC1(C)CC1C=O
KRFP3469	KRFPC3469	CC1(C)CCCC(C)(C)N1
KRFP3470	KRFPC3470	CC1(C)CCCC1(C)C(=O)O
KRFP3471	KRFPC3471	CC1(C)CN(C(=O)N1)c2cccc3cccc23
KRFP3472	KRFPC3472	CC1(C)OC(=O)CC(=O)O1
KRFP3473	KRFPC3473	CC1(CC2CC3CC(C2)C1)C3
KRFP3474	KRFPC3474	CC1(O)CCCCC1
KRFP3475	KRFPC3475	Cc1[nH][nH]c(=O)c1C=N
KRFP3476	KRFPC3476	Cc1[nH]c2ccc(C=O)cc2c1C
KRFP3477	KRFPC3477	Cc1[nH]c2ccc(O)cc2c1C=O
KRFP3478	KRFPC3478	Cc1[nH]c2ccccc2c1C
KRFP3479	KRFPC3479	CC1=CC(NC(=O)N1)c2ccccc2
KRFP3480	KRFPC3480	CC1=NN(C(=O)C1)c2c(F)c(F)c(F)c2F
KRFP3481	KRFPC3481	CC1=NN(C(=O)C1)c2ccc(cc2)[N+](=O)[O-]
KRFP3482	KRFPC3482	CC1C(=O)c2ccccc2C1=O
KRFP3483	KRFPC3483	CC1C(=O)CC(C)(C)CC1=O
KRFP3484	KRFPC3484	CC1C(C=O)C(C=O)C(C)C(C=O)C1C=O
KRFP3485	KRFPC3485	Cc1c(C=O)oc2c(O)cccc12
KRFP3486	KRFPC3486	Cc1c(cc(C=O)cc1[N+](=O)[O-])[N+](=O)[O-]
KRFP3487	KRFPC3487	Cc1c(cc(cc1[N+](=O)[O-])C(=O)N)[N+](=O)[O-]
KRFP3488	KRFPC3488	Cc1c(cccc1[N+](=O)[O-])[N+](=O)[O-]
KRFP3489	KRFPC3489	Cc1c(O)ccc2ccccc12
KRFP3490	KRFPC3490	Cc1c[nH]c2ccccc12
KRFP3491	KRFPC3491	Cc1cc(=O)[nH][nH]1
KRFP3492	KRFPC3492	Cc1cc(=O)c2ccc(O)cc2o1
KRFP3493	KRFPC3493	Cc1cc(=O)c2ccccc2o1
KRFP3494	KRFPC3494	Cc1cc(=O)n(c2ccccc2)n1C
KRFP3495	KRFPC3495	Cc1cc(=O)oc2cc(O)ccc12
KRFP3496	KRFPC3496	Cc1cc(=O)oc2ccccc12
KRFP3497	KRFPC3497	Cc1cc(Br)cc(Br)c1O

Name	Count name	Pattern
KRFP3498	KRFPC3498	<chem>Cc1cc(Br)cc(C(=O)O)c1O</chem>
KRFP3499	KRFPC3499	<chem>Cc1cc(Br)cc(C)c1O</chem>
KRFP3500	KRFPC3500	<chem>Cc1cc(C)[nH]c(=O)n1</chem>
KRFP3501	KRFPC3501	<chem>Cc1cc(C)[nH]n1</chem>
KRFP3502	KRFPC3502	<chem>Cc1cc(C)c(C)c(C)c1C</chem>
KRFP3503	KRFPC3503	<chem>Cc1cc(C)c(C=NO)c(C)c1</chem>
KRFP3504	KRFPC3504	<chem>CC1CC(C)C(C=O)C1C=O</chem>
KRFP3505	KRFPC3505	<chem>CC1CC(C)C(C1C=O)C(=O)O</chem>
KRFP3506	KRFPC3506	<chem>Cc1cc(C)c(O)c(n1)C(C)(C)C</chem>
KRFP3507	KRFPC3507	<chem>Cc1cc(C)c(O)cn1</chem>
KRFP3508	KRFPC3508	<chem>Cc1cc(C)c(S(=O)=O)c(C)c1</chem>
KRFP3509	KRFPC3509	<chem>Cc1cc(C)cc(Br)c1</chem>
KRFP3510	KRFPC3510	<chem>Cc1cc(C)cc(C)c1</chem>
KRFP3511	KRFPC3511	<chem>Cc1cc(C)n2ncnc2n1</chem>
KRFP3512	KRFPC3512	<chem>Cc1cc(C)nc(N)n1</chem>
KRFP3513	KRFPC3513	<chem>Cc1cc(C)nc(NC=O)n1</chem>
KRFP3514	KRFPC3514	<chem>Cc1cc(C)nc(NS(=O)=O)n1</chem>
KRFP3515	KRFPC3515	<chem>Cc1cc(C)ncn1</chem>
KRFP3516	KRFPC3516	<chem>Cc1cc(cc(c1)[N+](=O)[O-])[N+](=O)[O-]</chem>
KRFP3517	KRFPC3517	<chem>Cc1cc(ccc1O)[N+](=O)[O-]</chem>
KRFP3518	KRFPC3518	<chem>Cc1cc(CO)c(C=O)c(=O)[nH]1</chem>
KRFP3519	KRFPC3519	<chem>Cc1cc(O)c2[nH]nc[n+]₂n1</chem>
KRFP3520	KRFPC3520	<chem>Cc1cc(O)cc(O)c1</chem>
KRFP3521	KRFPC3521	<chem>Cc1cc[nH]n1</chem>
KRFP3522	KRFPC3522	<chem>Cc1cc2cc(ccc2[nH]1)[N+](=O)[O-]</chem>
KRFP3523	KRFPC3523	<chem>Cc1cc2ccccc2[nH]1</chem>
KRFP3524	KRFPC3524	<chem>Cc1cc2ccccc2n1C</chem>
KRFP3525	KRFPC3525	<chem>Cc1ccc(Br)cc1</chem>
KRFP3526	KRFPC3526	<chem>Cc1ccc(Br)s1</chem>
KRFP3527	KRFPC3527	<chem>Cc1ccc(C)[nH]1</chem>
KRFP3528	KRFPC3528	<chem>Cc1ccc(C)c(C)c1</chem>
KRFP3529	KRFPC3529	<chem>Cc1ccc(C)cc1</chem>
KRFP3530	KRFPC3530	<chem>Cc1ccc(C)n1c2ccccc2</chem>
KRFP3531	KRFPC3531	<chem>Cc1ccc(C)o1</chem>
KRFP3532	KRFPC3532	<chem>Cc1ccc(C=N)o1</chem>
KRFP3533	KRFPC3533	<chem>Cc1ccc(C=NNC=O)o1</chem>
KRFP3534	KRFPC3534	<chem>Cc1ccc(C=O)cc1</chem>
KRFP3535	KRFPC3535	<chem>Cc1ccc(C=O)cc1S(=O)=O</chem>
KRFP3536	KRFPC3536	<chem>Cc1ccc(cc1)[N+](=O)[O-]</chem>
KRFP3537	KRFPC3537	<chem>Cc1ccc(cc1)C(=O)O</chem>
KRFP3538	KRFPC3538	<chem>Cc1ccc(cc1)C(F)(F)F</chem>
KRFP3539	KRFPC3539	<chem>Cc1ccc(cc1)C2(CC2C=O)c3ccc(C)cc3</chem>
KRFP3540	KRFPC3540	<chem>Cc1ccc(cc1)c2ccccc2</chem>
KRFP3541	KRFPC3541	<chem>Cc1ccc(cc1)S(=O)(=O)C</chem>
KRFP3542	KRFPC3542	<chem>Cc1ccc(cc1)S(=O)(=O)N</chem>
KRFP3543	KRFPC3543	<chem>Cc1ccc(cc1)S(=O)=O</chem>
KRFP3544	KRFPC3544	<chem>Cc1ccc(cc1[N+](=O)[O-])S(=O)=O</chem>
KRFP3545	KRFPC3545	<chem>Cc1ccc(CCC=O)o1</chem>
KRFP3546	KRFPC3546	<chem>Cc1ccc(Cl)cc1</chem>
KRFP3547	KRFPC3547	<chem>Cc1ccc(Cl)cc1Cl</chem>
KRFP3548	KRFPC3548	<chem>Cc1ccc(F)cc1</chem>
KRFP3549	KRFPC3549	<chem>Cc1ccc(F)cc1F</chem>
KRFP3550	KRFPC3550	<chem>Cc1ccc(N)cc1</chem>
KRFP3551	KRFPC3551	<chem>Cc1ccc(NC(=S)NCC(Cl)(Cl)Cl)cc1</chem>

Name	Count name	Pattern
KRFP3552	KRFPC3552	<chem>Cc1ccc(NC(=S)SCC=O)cc1</chem>
KRFP3553	KRFPC3553	<chem>Cc1ccc(NC=O)cc1</chem>
KRFP3554	KRFPC3554	<chem>Cc1ccc(O)c(C)c1</chem>
KRFP3555	KRFPC3555	<chem>Cc1ccc(O)c(C)n1</chem>
KRFP3556	KRFPC3556	<chem>Cc1ccc(O)c(C=NNC=O)c1</chem>
KRFP3557	KRFPC3557	<chem>Cc1ccc(O)c(c1)[N+](=O)[O-]</chem>
KRFP3558	KRFPC3558	<chem>Cc1ccc(O)c(CCc2ccccc2)n1</chem>
KRFP3559	KRFPC3559	<chem>Cc1ccc(O)c(O)c1</chem>
KRFP3560	KRFPC3560	<chem>Cc1ccc(O)cc1</chem>
KRFP3561	KRFPC3561	<chem>Cc1ccc(O)cc1C</chem>
KRFP3562	KRFPC3562	<chem>Cc1ccc(O)cn1</chem>
KRFP3563	KRFPC3563	<chem>Cc1ccc(o1)[N+](=O)[O-]</chem>
KRFP3564	KRFPC3564	<chem>Cc1ccc[nH]1</chem>
KRFP3565	KRFPC3565	<chem>Cc1ccc[nH]c1=N</chem>
KRFP3566	KRFPC3566	<chem>Cc1ccc2[nH]c3C(=O)CCc3c2c1</chem>
KRFP3567	KRFPC3567	<chem>Cc1ccc2[nH]c3CCCCc3c2c1</chem>
KRFP3568	KRFPC3568	<chem>Cc1ccc2ccccc2c1</chem>
KRFP3569	KRFPC3569	<chem>Cc1ccc2ccccc2n1</chem>
KRFP3570	KRFPC3570	<chem>Cc1ccc2n3CCNC4CCc(c43)c2c1</chem>
KRFP3571	KRFPC3571	<chem>Cc1ccc2ncsc2c1</chem>
KRFP3572	KRFPC3572	<chem>Cc1ccc2OCOc2c1</chem>
KRFP3573	KRFPC3573	<chem>Cc1cccc(Br)c1</chem>
KRFP3574	KRFPC3574	<chem>Cc1cccc(C)c1</chem>
KRFP3575	KRFPC3575	<chem>Cc1cccc(C)c1Cl</chem>
KRFP3576	KRFPC3576	<chem>Cc1cccc(C)c1n2cnnn2</chem>
KRFP3577	KRFPC3577	<chem>Cc1cccc(C)c1NC=O</chem>
KRFP3578	KRFPC3578	<chem>Cc1cccc(C)n1</chem>
KRFP3579	KRFPC3579	<chem>Cc1cccc(C=O)c1</chem>
KRFP3580	KRFPC3580	<chem>Cc1cccc(c1)[N+](=O)[O-]</chem>
KRFP3581	KRFPC3581	<chem>Cc1cccc(c1)C(=O)N</chem>
KRFP3582	KRFPC3582	<chem>Cc1cccc(c1)C(=O)O</chem>
KRFP3583	KRFPC3583	<chem>Cc1cccc(c1)C(C)(C)C</chem>
KRFP3584	KRFPC3584	<chem>Cc1cccc(c1)c2cccc(C)c2</chem>
KRFP3585	KRFPC3585	<chem>Cc1cccc(Cl)c1</chem>
KRFP3586	KRFPC3586	<chem>Cc1cccc(F)c1</chem>
KRFP3587	KRFPC3587	<chem>Cc1cccc(N)c1</chem>
KRFP3588	KRFPC3588	<chem>Cc1cccc(N=Nc2ccccc2C)c1</chem>
KRFP3589	KRFPC3589	<chem>Cc1cccc(NC(=S)NCC(Cl)(Cl)Cl)c1</chem>
KRFP3590	KRFPC3590	<chem>Cc1cccc(NC=O)c1</chem>
KRFP3591	KRFPC3591	<chem>Cc1cccc(O)c1</chem>
KRFP3592	KRFPC3592	<chem>Cc1cccc2ccccc12</chem>
KRFP3593	KRFPC3593	<chem>CC1CCCCC1</chem>
KRFP3594	KRFPC3594	<chem>Cc1cccc1[N+](=O)[O-]</chem>
KRFP3595	KRFPC3595	<chem>Cc1cccc1Br</chem>
KRFP3596	KRFPC3596	<chem>Cc1cccc1C</chem>
KRFP3597	KRFPC3597	<chem>Cc1cccc1C(F)(F)F</chem>
KRFP3598	KRFPC3598	<chem>Cc1cccc1C=O</chem>
KRFP3599	KRFPC3599	<chem>Cc1cccc1Cl</chem>
KRFP3600	KRFPC3600	<chem>Cc1cccc1F</chem>
KRFP3601	KRFPC3601	<chem>Cc1cccc1I</chem>
KRFP3602	KRFPC3602	<chem>Cc1cccc1N</chem>
KRFP3603	KRFPC3603	<chem>Cc1cccc1N=Nc2ccc(NC(=S)NCC(Cl)(Cl)Cl)c(C)c2</chem>
KRFP3604	KRFPC3604	<chem>Cc1cccc1NC(=S)NCC(Cl)(Cl)Cl</chem>
KRFP3605	KRFPC3605	<chem>Cc1cccc1NS(=O)=O</chem>

Name	Count name	Pattern
KRFP3606	KRFPC3606	Cc1ccccc1O
KRFP3607	KRFPC3607	Cc1ccccc1S(=O)(=O)O
KRFP3608	KRFPC3608	Cc1cccn1
KRFP3609	KRFPC3609	Cc1ccnc1
KRFP3610	KRFPC3610	Cc1ccco1
KRFP3611	KRFPC3611	Cc1cccs1
KRFP3612	KRFPC3612	Cc1ccn[nH]1
KRFP3613	KRFPC3613	Cc1ccnc(C)c1
KRFP3614	KRFPC3614	Cc1ccnc(N)c1
KRFP3615	KRFPC3615	Cc1ccnc2ccc3ccccc3c12
KRFP3616	KRFPC3616	Cc1ccncc1
KRFP3617	KRFPC3617	Cc1ccnnc1
KRFP3618	KRFPC3618	Cc1ccoc1
KRFP3619	KRFPC3619	Cc1ccsc1
KRFP3620	KRFPC3620	Cc1ccsc1C
KRFP3621	KRFPC3621	Cc1ccsc1C=N
KRFP3622	KRFPC3622	CC1COC2(CCCCC2)O1
KRFP3623	KRFPC3623	Cc1csc[nH+]1
KRFP3624	KRFPC3624	Cc1csc2CCCCc12
KRFP3625	KRFPC3625	Cc1cscn1
KRFP3626	KRFPC3626	Cc1n[nH]cc1[N+](=O)[O-]
KRFP3627	KRFPC3627	Cc1nc2ccccc2[nH]1
KRFP3628	KRFPC3628	Cc1nc2ccccc2c(=O)[nH]1
KRFP3629	KRFPC3629	Cc1nc2ccccc2c3cc4ccccc4n13
KRFP3630	KRFPC3630	Cc1nc2ccccc2s1
KRFP3631	KRFPC3631	Cc1ncc([nH]1)[N+](=O)[O-]
KRFP3632	KRFPC3632	Cc1ncc[nH]1
KRFP3633	KRFPC3633	Cc1ncc2c3CCCCc3sc2n1
KRFP3634	KRFPC3634	Cc1nncc1
KRFP3635	KRFPC3635	CC1OCC(O)C(O)C1O
KRFP3636	KRFPC3636	CC1OCCO1
KRFP3637	KRFPC3637	Cc1sc2ccccc2[n+]1CCCS(=O)(=O)O
KRFP3638	KRFPC3638	Cc1sc2ncncc2c1C
KRFP3639	KRFPC3639	Cc1sc(C=O)c1C
KRFP3640	KRFPC3640	CCC
KRFP3641	KRFPC3641	CCC#N
KRFP3642	KRFPC3642	CCC(=NNC(=S)N)CC
KRFP3643	KRFPC3643	CCC(=O)C
KRFP3644	KRFPC3644	CCC(=O)C1(CC2CC3CC(C2)C1)C3
KRFP3645	KRFPC3645	CCC(=O)c1ccccc1
KRFP3646	KRFPC3646	CCC(=O)CC
KRFP3647	KRFPC3647	CCC(=O)N
KRFP3648	KRFPC3648	CCC(=O)NC
KRFP3649	KRFPC3649	CCC(=O)NC(C)C
KRFP3650	KRFPC3650	CCC(=O)NC(NC(=S)N)C(Cl)(Cl)Cl
KRFP3651	KRFPC3651	CCC(=O)NN
KRFP3652	KRFPC3652	CCC(=O)NN=C
KRFP3653	KRFPC3653	CCC(=O)NNC=O
KRFP3654	KRFPC3654	CCC(=O)O
KRFP3655	KRFPC3655	CCC(=O)OC
KRFP3656	KRFPC3656	CCC(=O)OCC=O
KRFP3657	KRFPC3657	CCC(C)(C)C
KRFP3658	KRFPC3658	CCC(C)(C)CC(=O)C
KRFP3659	KRFPC3659	CCC(C)C

Name	Count name	Pattern
KRFP3660	KRFPC3660	CCC(C)CC
KRFP3661	KRFPC3661	CCC(C)N
KRFP3662	KRFPC3662	CCC(C)NC=O
KRFP3663	KRFPC3663	CCC(C=O)C(CC)C=O
KRFP3664	KRFPC3664	CCC(CC)(C=O)C=O
KRFP3665	KRFPC3665	CCC(CC)Cc1cccc1
KRFP3666	KRFPC3666	CCC(CCC(O)c1ccnc2cccc12)C(C)C
KRFP3667	KRFPC3667	CCC(N)C(=O)O
KRFP3668	KRFPC3668	CCC=C(C)C
KRFP3669	KRFPC3669	CCC=NNC=O
KRFP3670	KRFPC3670	CCC=NO
KRFP3671	KRFPC3671	CCC=O
KRFP3672	KRFPC3672	CCC1(CC2CC3CC(C2)C1)C3
KRFP3673	KRFPC3673	CCC1C(C=O)C(C=O)C(C)(CC=O)C(C=O)C1C=O
KRFP3674	KRFPC3674	CCc1c[nH]c2ccc(O)cc12
KRFP3675	KRFPC3675	CCc1c[nH]c2cccc12
KRFP3676	KRFPC3676	CCC1CC1
KRFP3677	KRFPC3677	CCc1cc2c(=O)ccoc2cc1O
KRFP3678	KRFPC3678	CCc1ccc(C)nc1
KRFP3679	KRFPC3679	CCc1ccc(cc1)c2nc3cccc3o2
KRFP3680	KRFPC3680	CCc1ccc(O)c(O)c1
KRFP3681	KRFPC3681	CCc1ccc(O)cc1
KRFP3682	KRFPC3682	CCc1cccc1
KRFP3683	KRFPC3683	CCC1CCCCN1
KRFP3684	KRFPC3684	CCc1cnc2ccc(Br)cc2c1
KRFP3685	KRFPC3685	CCc1cnc2cccc2c1
KRFP3686	KRFPC3686	CCc1nc(C)ccc1O
KRFP3687	KRFPC3687	CCc1nc2cccc2[nH]1
KRFP3688	KRFPC3688	CCc1nc2cccc2cc1C
KRFP3689	KRFPC3689	CCc1ncccc1O
KRFP3690	KRFPC3690	CCc1nnc(N)s1
KRFP3691	KRFPC3691	CCc1nncs1
KRFP3692	KRFPC3692	CCCC
KRFP3693	KRFPC3693	CCCC(=O)N
KRFP3694	KRFPC3694	CCCC(=O)NC(N)C(Cl)(Cl)Cl
KRFP3695	KRFPC3695	CCCC(=O)NC(NC(=S)N)C(Cl)(Cl)Cl
KRFP3696	KRFPC3696	CCCC(=O)NS(=O)=O
KRFP3697	KRFPC3697	CCCC(=O)O
KRFP3698	KRFPC3698	CCCC(CCC)C(=O)N
KRFP3699	KRFPC3699	CCCC(O)CO
KRFP3700	KRFPC3700	CCCC=NNC=O
KRFP3701	KRFPC3701	CCCC=O
KRFP3702	KRFPC3702	CCc1c[nH]c2cccc12
KRFP3703	KRFPC3703	CCc1ccc(O)cc1
KRFP3704	KRFPC3704	CCc1cccc1
KRFP3705	KRFPC3705	CCc1nc2cccc2cc1CC
KRFP3706	KRFPC3706	CCCCC
KRFP3707	KRFPC3707	CCCCC(=O)N
KRFP3708	KRFPC3708	CCCCC(=O)O
KRFP3709	KRFPC3709	CCCCC=O
KRFP3710	KRFPC3710	CCCCc1cccc1
KRFP3711	KRFPC3711	CCCCc1nc2cccc2cc1CCC
KRFP3712	KRFPC3712	CCCCC
KRFP3713	KRFPC3713	CCCCC(=O)N

Name	Count name	Pattern
KRFP3714	KRFPC3714	CCCCC(=O)NC(NC(=S)N)C(Cl)(Cl)Cl
KRFP3715	KRFPC3715	CCCCC(=O)NN=C
KRFP3716	KRFPC3716	CCCCC(=O)O
KRFP3717	KRFPC3717	CCCCC(C)NC=O
KRFP3718	KRFPC3718	CCCCC=O
KRFP3719	KRFPC3719	CCCCC
KRFP3720	KRFPC3720	CCCCC(=O)NC(NC(=S)N)C(Cl)(Cl)Cl
KRFP3721	KRFPC3721	CCCCC=O
KRFP3722	KRFPC3722	CCCCC
KRFP3723	KRFPC3723	CCCCC(=O)NN=C
KRFP3724	KRFPC3724	CCCCC(=O)NNC=O
KRFP3725	KRFPC3725	CCCCC=O
KRFP3726	KRFPC3726	CCCCCNC=O
KRFP3727	KRFPC3727	CCCCCO
KRFP3728	KRFPC3728	CCCCCOC=O
KRFP3729	KRFPC3729	CCCCCN
KRFP3730	KRFPC3730	CCCCCO
KRFP3731	KRFPC3731	CCCCCOC=O
KRFP3732	KRFPC3732	CCCCI
KRFP3733	KRFPC3733	CCCCN
KRFP3734	KRFPC3734	CCCCN(CCC)CC(=O)N
KRFP3735	KRFPC3735	CCCCNC=O
KRFP3736	KRFPC3736	CCCCNS(=O)=O
KRFP3737	KRFPC3737	CCCCO
KRFP3738	KRFPC3738	CCCCOC=O
KRFP3739	KRFPC3739	CCCCS
KRFP3740	KRFPC3740	CCCN
KRFP3741	KRFPC3741	CCCN(C)C
KRFP3742	KRFPC3742	CCCN=O
KRFP3743	KRFPC3743	CCCN(=O)=O
KRFP3744	KRFPC3744	CCCO
KRFP3745	KRFPC3745	CCCO(=O)CO
KRFP3746	KRFPC3746	CCCO=O
KRFP3747	KRFPC3747	CCCS(=O)(=O)O
KRFP3748	KRFPC3748	CCCS(=O)(=O)O[Na]
KRFP3749	KRFPC3749	CCI
KRFP3750	KRFPC3750	CCN
KRFP3751	KRFPC3751	CCN(C)C
KRFP3752	KRFPC3752	CCN(C)CC
KRFP3753	KRFPC3753	CCN(C)CC(=O)N
KRFP3754	KRFPC3754	CCN(CC(O)CO)S(=O)(=O)O
KRFP3755	KRFPC3755	CCN(CC)C(=S)N
KRFP3756	KRFPC3756	CCN(CC)C=O
KRFP3757	KRFPC3757	CCN(CC)CC
KRFP3758	KRFPC3758	CCN(CC)CC(=O)N
KRFP3759	KRFPC3759	CCN(CC)CC(C)O
KRFP3760	KRFPC3760	CCN(CC)CC=O
KRFP3761	KRFPC3761	CCN(CC)CCC=O
KRFP3762	KRFPC3762	CCN(CC)CCCC(C)N
KRFP3763	KRFPC3763	CCN(CC)CCN
KRFP3764	KRFPC3764	CCN(CC)CCNC=O
KRFP3765	KRFPC3765	CCN(CC)CCOC=O
KRFP3766	KRFPC3766	CCN(CC)S(=O)=O
KRFP3767	KRFPC3767	CCN(CCO)C=O

Name	Count name	Pattern
KRFP3768	KRFPC3768	CCN=C
KRFP3769	KRFPC3769	CCN1C(=O)c2cccc3cccc1c23
KRFP3770	KRFPC3770	CCN1C(=O)c2cccc2C1=O
KRFP3771	KRFPC3771	CCn1c2cccc2c3cc(C=NNC=O)ccc13
KRFP3772	KRFPC3772	CCN1CCOCC1
KRFP3773	KRFPC3773	CCNC
KRFP3774	KRFPC3774	CCNC(=NCC)S
KRFP3775	KRFPC3775	CCNC(=O)C
KRFP3776	KRFPC3776	CCNC(=O)C=C
KRFP3777	KRFPC3777	CCNC(=O)CC
KRFP3778	KRFPC3778	CCNC(=O)CO
KRFP3779	KRFPC3779	CCNC(=O)N
KRFP3780	KRFPC3780	CCNC(=S)NC(CC=O)c1cccc1
KRFP3781	KRFPC3781	CCNC=O
KRFP3782	KRFPC3782	CCNCC
KRFP3783	KRFPC3783	CCNCC(=O)N
KRFP3784	KRFPC3784	CCNCC(O)CO
KRFP3785	KRFPC3785	CCNCC=O
KRFP3786	KRFPC3786	CCNCCO
KRFP3787	KRFPC3787	CCNS(=O)=O
KRFP3788	KRFPC3788	CCO
KRFP3789	KRFPC3789	CCOC
KRFP3790	KRFPC3790	CCOC(=O)C
KRFP3791	KRFPC3791	CCOC(=O)C(=C)C#N
KRFP3792	KRFPC3792	CCOC(=O)C(C)NC(=O)C
KRFP3793	KRFPC3793	CCOC(=O)C(C)NC=O
KRFP3794	KRFPC3794	CCOC(=O)C=CC
KRFP3795	KRFPC3795	CCOC(=O)CC
KRFP3796	KRFPC3796	CCOC(=O)CC(=O)N
KRFP3797	KRFPC3797	CCOC(=O)CC(=O)OCC
KRFP3798	KRFPC3798	CCOC(=O)CC=O
KRFP3799	KRFPC3799	CCOC(=O)CCC(=O)N
KRFP3800	KRFPC3800	CCOC(=O)CN
KRFP3801	KRFPC3801	CCOC(=O)CNC=O
KRFP3802	KRFPC3802	CCOC(=O)CS
KRFP3803	KRFPC3803	CCOC(=O)N
KRFP3804	KRFPC3804	CCOC(=O)NC(N)C(Cl)(Cl)Cl
KRFP3805	KRFPC3805	CCOC(=O)NN=C
KRFP3806	KRFPC3806	CCOC=O
KRFP3807	KRFPC3807	CCOP(=O)(CN)OCC
KRFP3808	KRFPC3808	CCOP(=O)(N)OCC
KRFP3809	KRFPC3809	CCS
KRFP3810	KRFPC3810	CCS(=O)(=O)C(=C(N)N)S(=O)(=O)CC
KRFP3811	KRFPC3811	CCS(=O)(=O)CCC(=O)N
KRFP3812	KRFPC3812	CCS(=O)(=O)CCC=O
KRFP3813	KRFPC3813	CCS(=O)(=O)O
KRFP3814	KRFPC3814	CCS(=O)=O
KRFP3815	KRFPC3815	CCS=O
KRFP3816	KRFPC3816	CCSC
KRFP3817	KRFPC3817	CCSC(=N)N
KRFP3818	KRFPC3818	CCSC(C)C
KRFP3819	KRFPC3819	CCSC=S
KRFP3820	KRFPC3820	CCSCC
KRFP3821	KRFPC3821	Cl

Name	Count name	Pattern
KRFP3822	KRFPC3822	<chem>ClC(=C(Cl)COC=O)Cl</chem>
KRFP3823	KRFPC3823	<chem>ClC(=C)Cl</chem>
KRFP3824	KRFPC3824	<chem>ClC(Cl)(Cl)C=O</chem>
KRFP3825	KRFPC3825	<chem>ClC(Cl)(Cl)CNC(=S)Nc1ccc(cc1)S(=O)=O</chem>
KRFP3826	KRFPC3826	<chem>ClC(Cl)(Cl)CNC(=S)Nc1ccc(N=Nc2ccccc2)cc1</chem>
KRFP3827	KRFPC3827	<chem>ClC(Cl)(Cl)CNC(=S)Nc1cccc2ccccc12</chem>
KRFP3828	KRFPC3828	<chem>ClC(Cl)(Cl)CNC(=S)Nc1cccc2cccn12</chem>
KRFP3829	KRFPC3829	<chem>ClC(Cl)(Cl)CNC(=S)Nc1ccccc1</chem>
KRFP3830	KRFPC3830	<chem>ClC(Cl)(Cl)CNC(=S)Nc1ccccc1C=O</chem>
KRFP3831	KRFPC3831	<chem>ClC(Cl)(Cl)CNC(=S)Nc1sc2CCCCc2c1C=O</chem>
KRFP3832	KRFPC3832	<chem>ClC(Cl)(Cl)CNC=O</chem>
KRFP3833	KRFPC3833	<chem>ClC(Cl)(Cl)CNS(=O)=O</chem>
KRFP3834	KRFPC3834	<chem>ClC(Cl)Cl</chem>
KRFP3835	KRFPC3835	<chem>Clc1c(C=O)sc2ccccc12</chem>
KRFP3836	KRFPC3836	<chem>Clc1cc(Cl)cc(C=O)c1</chem>
KRFP3837	KRFPC3837	<chem>Clc1cc(Cl)cc(Cl)c1</chem>
KRFP3838	KRFPC3838	<chem>Clc1ccc(C=C2SC(=S)NC2=O)cc1</chem>
KRFP3839	KRFPC3839	<chem>Clc1ccc(C=N)c(Cl)c1</chem>
KRFP3840	KRFPC3840	<chem>Clc1ccc(C=N)cc1</chem>
KRFP3841	KRFPC3841	<chem>Clc1ccc(C=NNC=O)c(Cl)c1</chem>
KRFP3842	KRFPC3842	<chem>Clc1ccc(C=NNC=O)cc1</chem>
KRFP3843	KRFPC3843	<chem>Clc1ccc(C=O)c(Cl)c1</chem>
KRFP3844	KRFPC3844	<chem>Clc1ccc(C=O)cc1</chem>
KRFP3845	KRFPC3845	<chem>Clc1ccc(C=O)cc1Cl</chem>
KRFP3846	KRFPC3846	<chem>Clc1ccc(cc1)N2C(=O)CCC2=O</chem>
KRFP3847	KRFPC3847	<chem>Clc1ccc(cc1)N2CCNCC2</chem>
KRFP3848	KRFPC3848	<chem>Clc1ccc(cc1)S(=O)(=O)c2ccc(c2)S(=O)=O</chem>
KRFP3849	KRFPC3849	<chem>Clc1ccc(cc1)S(=O)=O</chem>
KRFP3850	KRFPC3850	<chem>Clc1ccc(cc1Cl)S(=O)(=O)c2ccc(c2)S(=O)=O</chem>
KRFP3851	KRFPC3851	<chem>Clc1ccc(cc1Cl)S(=O)=O</chem>
KRFP3852	KRFPC3852	<chem>Clc1ccc(Cl)c(Cl)c1</chem>
KRFP3853	KRFPC3853	<chem>Clc1ccc(Cl)c(NC(=S)NCC(Cl)(Cl)Cl)c1</chem>
KRFP3854	KRFPC3854	<chem>Clc1ccc(Cl)c(NC=O)c1</chem>
KRFP3855	KRFPC3855	<chem>Clc1ccc(Cl)cc1</chem>
KRFP3856	KRFPC3856	<chem>Clc1ccc(NC=O)c(Cl)c1</chem>
KRFP3857	KRFPC3857	<chem>Clc1ccc(NC=O)cc1</chem>
KRFP3858	KRFPC3858	<chem>Clc1ccc(NC=O)cc1Cl</chem>
KRFP3859	KRFPC3859	<chem>Clc1ccc(NS(=O)=O)cc1</chem>
KRFP3860	KRFPC3860	<chem>Clc1ccc2[nH]c3ccc(Cl)cc3c2c1</chem>
KRFP3861	KRFPC3861	<chem>Clc1ccc2ocnc2c1</chem>
KRFP3862	KRFPC3862	<chem>Clc1cccc(Br)c1</chem>
KRFP3863	KRFPC3863	<chem>Clc1cccc(C=N)c1</chem>
KRFP3864	KRFPC3864	<chem>Clc1cccc(C=O)c1</chem>
KRFP3865	KRFPC3865	<chem>Clc1cccc(c1)N2C(=O)CCC2=O</chem>
KRFP3866	KRFPC3866	<chem>Clc1cccc(Cl)c1</chem>
KRFP3867	KRFPC3867	<chem>Clc1cccc(NC=O)c1</chem>
KRFP3868	KRFPC3868	<chem>Clc1cccc2ccccc12</chem>
KRFP3869	KRFPC3869	<chem>Clc1ccccc1</chem>
KRFP3870	KRFPC3870	<chem>Clc1ccccc1Br</chem>
KRFP3871	KRFPC3871	<chem>Clc1ccccc1C=NNC=O</chem>
KRFP3872	KRFPC3872	<chem>Clc1ccccc1C=O</chem>
KRFP3873	KRFPC3873	<chem>Clc1ccccc1Cl</chem>
KRFP3874	KRFPC3874	<chem>Clc1ccccc1NC=O</chem>
KRFP3875	KRFPC3875	<chem>Clc1ccccc1S(=O)=O</chem>

Name	Count name	Pattern
KRFP3876	KRFPC3876	Clc1cccnc1
KRFP3877	KRFPC3877	Clc1csc2ccccc12
KRFP3878	KRFPC3878	Clc1ncnc(Cl)n1
KRFP3879	KRFPC3879	Clc1ncncn1
KRFP3880	KRFPC3880	CICC=O
KRFP3881	KRFPC3881	CICCI
KRFP3882	KRFPC3882	CN
KRFP3883	KRFPC3883	CN(C(=O)CCC(=O)O)C(C)(C)C
KRFP3884	KRFPC3884	CN(C)C
KRFP3885	KRFPC3885	CN(C)C(=N)C
KRFP3886	KRFPC3886	CN(C)C(=N)NC(=N)N
KRFP3887	KRFPC3887	CN(C)C(=O)N
KRFP3888	KRFPC3888	CN(C)C=N
KRFP3889	KRFPC3889	CN(C)C=O
KRFP3890	KRFPC3890	CN(C)c1ccc(C=NNC=O)cc1
KRFP3891	KRFPC3891	CN(C)c1ccc2ccccc2n1
KRFP3892	KRFPC3892	CN(C)c1ccccc1
KRFP3893	KRFPC3893	CN(C)CC(=O)N
KRFP3894	KRFPC3894	CN(C)CC=O
KRFP3895	KRFPC3895	CN(C)CCC=O
KRFP3896	KRFPC3896	CN(C)CCCNC(=O)C(=C)NC=O
KRFP3897	KRFPC3897	CN(C)CCCNC=O
KRFP3898	KRFPC3898	CN(C)CCOC=O
KRFP3899	KRFPC3899	CN(C)CCOC=O
KRFP3900	KRFPC3900	CN(C)N1C(=O)CCC1=O
KRFP3901	KRFPC3901	CN(C)S(=O)=O
KRFP3902	KRFPC3902	CN(C=O)C(C)(C)C
KRFP3903	KRFPC3903	CN(C=O)c1ccc(l)cc1
KRFP3904	KRFPC3904	CN(CC(O)CO)S(=O)(=O)O
KRFP3905	KRFPC3905	CN(CCO)CCO
KRFP3906	KRFPC3906	CN(S(=O)=O)C(C)(C)C
KRFP3907	KRFPC3907	CN=C
KRFP3908	KRFPC3908	CN=c1cc[nH]cc1
KRFP3909	KRFPC3909	CN1C(=O)C(=NNC(=O)CO)c2cc(Br)ccc12
KRFP3910	KRFPC3910	CN1C(=O)c2ccccc2C1=O
KRFP3911	KRFPC3911	CN1C2CCC1CCC2
KRFP3912	KRFPC3912	Cn1cc(Br)c(n1)C(=O)N
KRFP3913	KRFPC3913	CN1CCc2cc3ccccc3nc12
KRFP3914	KRFPC3914	CN1CCCC1
KRFP3915	KRFPC3915	CN1CCCCC1
KRFP3916	KRFPC3916	Cn1cccn1
KRFP3917	KRFPC3917	CN1CCN(CC1)c2ccc(Cl)cc2
KRFP3918	KRFPC3918	CN1CCN(CC1)c2ccc(F)cc2
KRFP3919	KRFPC3919	CN1CCN(CC1)c2ccccc2
KRFP3920	KRFPC3920	CN1CCN(CC1)c2ccccn2
KRFP3921	KRFPC3921	CN1CCNCC1
KRFP3922	KRFPC3922	CN1CCOCC1
KRFP3923	KRFPC3923	Cn1cnc(c1)[N+](=O)[O-]
KRFP3924	KRFPC3924	Cn1ncc([N+](=O)[O-])c1C(=O)N
KRFP3925	KRFPC3925	Cn1nnc2ccccc12
KRFP3926	KRFPC3926	CNC
KRFP3927	KRFPC3927	CNC(=N)NC(=N)N
KRFP3928	KRFPC3928	CNC(=O)C
KRFP3929	KRFPC3929	CNC(=O)C(=C)NC=O

Name	Count name	Pattern
KRFP3930	KRFPC3930	CNC(=O)CCC(=O)O
KRFP3931	KRFPC3931	CNC(=O)CCl
KRFP3932	KRFPC3932	CNC(=O)CO
KRFP3933	KRFPC3933	CNC(=O)N
KRFP3934	KRFPC3934	CNC(=O)O
KRFP3935	KRFPC3935	CNC(=S)NC
KRFP3936	KRFPC3936	CNC(C)(C)C
KRFP3937	KRFPC3937	CNC(C)C
KRFP3938	KRFPC3938	CNC(C)C(=O)O
KRFP3939	KRFPC3939	CNC(NC=O)C(Cl)(Cl)Cl
KRFP3940	KRFPC3940	CNC=C
KRFP3941	KRFPC3941	CNC=C1C(=O)NC(=O)NC1=O
KRFP3942	KRFPC3942	CNC=O
KRFP3943	KRFPC3943	CNc1ccccc1
KRFP3944	KRFPC3944	CNc1ncncn1
KRFP3945	KRFPC3945	CNCC(=O)N
KRFP3946	KRFPC3946	CNCC(C)O
KRFP3947	KRFPC3947	CNCC(O)CO
KRFP3948	KRFPC3948	CNCCO
KRFP3949	KRFPC3949	CNN
KRFP3950	KRFPC3950	CNN=C
KRFP3951	KRFPC3951	CNN=C1c2n[nH]nc2C(=NNC)c3n[nH]nc13
KRFP3952	KRFPC3952	CNn1cnnc1
KRFP3953	KRFPC3953	CNNC(=O)C
KRFP3954	KRFPC3954	CNS(=O)(=O)NC(=O)N
KRFP3955	KRFPC3955	CNS(=O)=O
KRFP3956	KRFPC3956	CO
KRFP3957	KRFPC3957	COC
KRFP3958	KRFPC3958	COC(=N)c1ccc(C)cc1
KRFP3959	KRFPC3959	COC(=O)C
KRFP3960	KRFPC3960	COC(=O)C(C)NC(=O)CO
KRFP3961	KRFPC3961	COC(=O)C(C)NC=O
KRFP3962	KRFPC3962	COC(=O)C(O)C(F)(F)F
KRFP3963	KRFPC3963	COC(=O)CCC(=O)N
KRFP3964	KRFPC3964	COC(=O)CCC(=O)O
KRFP3965	KRFPC3965	COC(=O)CCS(=O)=O
KRFP3966	KRFPC3966	COC(=O)CN
KRFP3967	KRFPC3967	COC(=O)CO
KRFP3968	KRFPC3968	COC(=O)N
KRFP3969	KRFPC3969	COC(=O)O
KRFP3970	KRFPC3970	COC=NC(NC(=S)N)C(Cl)(Cl)Cl
KRFP3971	KRFPC3971	COC=O
KRFP3972	KRFPC3972	COc1c(Cl)cc(Cl)cc1C=NNC=O
KRFP3973	KRFPC3973	COc1cc(C=NNC=O)ccc1O
KRFP3974	KRFPC3974	COc1cc(cc(OC)c1OC)C(=O)N
KRFP3975	KRFPC3975	COc1cc(N)nc(OC)n1
KRFP3976	KRFPC3976	COc1ccc(C(=NNC=O)C)c(OC)c1
KRFP3977	KRFPC3977	COc1ccc(C=C2SC(=S)NC2=O)cc1
KRFP3978	KRFPC3978	COc1ccc(C=CC(=O)NC(=S)N)cc1OC
KRFP3979	KRFPC3979	COc1ccc(C=NNC(=O)CO)cc1[N+](=O)[O-]
KRFP3980	KRFPC3980	COc1ccc(C=NNC=O)c(OC)c1
KRFP3981	KRFPC3981	COc1ccc(C=NNC=O)cc1
KRFP3982	KRFPC3982	COc1ccc(C=NNC=O)cc1OC
KRFP3983	KRFPC3983	COc1ccc(cc1)[N+](=O)[O-]

Name	Count name	Pattern
KRFP3984	KRFPC3984	<chem>COc1ccc(cc1)C(=NNC=O)C</chem>
KRFP3985	KRFPC3985	<chem>COc1ccc(cc1)C(=O)N</chem>
KRFP3986	KRFPC3986	<chem>COc1ccc(cc1)N2C(=O)CCC2=O</chem>
KRFP3987	KRFPC3987	<chem>COc1ccc(Cl)cc1Cl</chem>
KRFP3988	KRFPC3988	<chem>COc1ccc(N)nn1</chem>
KRFP3989	KRFPC3989	<chem>COc1ccc(OC)cc1</chem>
KRFP3990	KRFPC3990	<chem>COc1ccc2[nH]ccc2c1</chem>
KRFP3991	KRFPC3991	<chem>COc1ccc2ccccc2c1</chem>
KRFP3992	KRFPC3992	<chem>COc1ccc2ccccc2c1C=NNC(=O)CO</chem>
KRFP3993	KRFPC3993	<chem>COc1ccc2sc(C)[nH+]c2c1</chem>
KRFP3994	KRFPC3994	<chem>COc1cccc(Br)c1</chem>
KRFP3995	KRFPC3995	<chem>COc1cccc(C=NNC(=O)CO)c1</chem>
KRFP3996	KRFPC3996	<chem>COc1cccc(c1)[N+](=O)[O-]</chem>
KRFP3997	KRFPC3997	<chem>COc1cccc(c1)C(=O)O</chem>
KRFP3998	KRFPC3998	<chem>COc1cccc(OC)c1</chem>
KRFP3999	KRFPC3999	<chem>COc1cccc(OC)c1OC</chem>
KRFP4000	KRFPC4000	<chem>COc1cccc1</chem>
KRFP4001	KRFPC4001	<chem>COc1cccc1C=NNC(=O)CO</chem>
KRFP4002	KRFPC4002	<chem>COc1cccc1C=NNC=O</chem>
KRFP4003	KRFPC4003	<chem>COc1cccc1Cl</chem>
KRFP4004	KRFPC4004	<chem>COc1cccc1N2CCNCC2</chem>
KRFP4005	KRFPC4005	<chem>COc1cccc1O</chem>
KRFP4006	KRFPC4006	<chem>COc1cccc1OC</chem>
KRFP4007	KRFPC4007	<chem>COc1cccn1</chem>
KRFP4008	KRFPC4008	<chem>COc1ccnc(OC)n1</chem>
KRFP4009	KRFPC4009	<chem>COc1cnccn1</chem>
KRFP4010	KRFPC4010	<chem>COc1nc(C)nc(NC=O)n1</chem>
KRFP4011	KRFPC4011	<chem>COc1nccnc1N</chem>
KRFP4012	KRFPC4012	<chem>COc1ncnc(C)n1</chem>
KRFP4013	KRFPC4013	<chem>COc1ncnc(OC)n1</chem>
KRFP4014	KRFPC4014	<chem>COc1nccn1</chem>
KRFP4015	KRFPC4015	<chem>COCC(C)O</chem>
KRFP4016	KRFPC4016	<chem>COCC(O)CNC(C)C</chem>
KRFP4017	KRFPC4017	<chem>COP(=O)(CN)OC</chem>
KRFP4018	KRFPC4018	<chem>COS(=O)=O</chem>
KRFP4019	KRFPC4019	<chem>CS</chem>
KRFP4020	KRFPC4020	<chem>CS(=O)(=O)c1cccc1</chem>
KRFP4021	KRFPC4021	<chem>CS(=O)(=O)N</chem>
KRFP4022	KRFPC4022	<chem>CS(=O)(=O)O</chem>
KRFP4023	KRFPC4023	<chem>CS(=O)=O</chem>
KRFP4024	KRFPC4024	<chem>CSC(=N)N</chem>
KRFP4025	KRFPC4025	<chem>CSC(=S)NN=C</chem>
KRFP4026	KRFPC4026	<chem>CS(c1ccc(C)cc1)</chem>
KRFP4027	KRFPC4027	<chem>CS(c1ccc(O)cc1)</chem>
KRFP4028	KRFPC4028	<chem>CS(c1ccccc1)</chem>
KRFP4029	KRFPC4029	<chem>CS(c1nc2ccccc2[nH]1)</chem>
KRFP4030	KRFPC4030	<chem>CSCC(=O)NN=C</chem>
KRFP4031	KRFPC4031	<chem>CSCCCC(=O)O</chem>
KRFP4032	KRFPC4032	<chem>F</chem>
KRFP4033	KRFPC4033	<chem>FC(F)(C=O)C1(F)OC(F)(F)C(F)(F)C1(F)F</chem>
KRFP4034	KRFPC4034	<chem>FC(F)(F)C(F)(F)C(F)(F)OC(F)(C=O)C(F)(F)F</chem>
KRFP4035	KRFPC4035	<chem>FC(F)(F)C(F)(F)C(F)(F)S</chem>
KRFP4036	KRFPC4036	<chem>FC(F)(F)C(F)(F)C=O</chem>
KRFP4037	KRFPC4037	<chem>FC(F)(F)C(OC1ncnc(OC(C(F)(F)F)C(F)(F)F)n1)C(F)(F)F</chem>

Name	Count name	Pattern
KRFP4038	KRFPC4038	<chem>FC(F)(F)C(Oc1ncncn1)C(F)(F)F</chem>
KRFP4039	KRFPC4039	<chem>FC(F)(F)C=O</chem>
KRFP4040	KRFPC4040	<chem>FC(F)(F)c1ccc(Cl)c(NC(=S)NCC(Cl)(Cl)Cl)c1</chem>
KRFP4041	KRFPC4041	<chem>FC(F)(F)c1ccc(Cl)cc1</chem>
KRFP4042	KRFPC4042	<chem>FC(F)(F)c1ccc(S(c2ccccc2))cc1</chem>
KRFP4043	KRFPC4043	<chem>FC(F)(F)c1ccc2S(c3ccccc3Nc2c1)</chem>
KRFP4044	KRFPC4044	<chem>FC(F)(F)c1cccc(c1)S(=O)=O</chem>
KRFP4045	KRFPC4045	<chem>FC(F)(F)c1cccc(NC=O)c1</chem>
KRFP4046	KRFPC4046	<chem>FC(F)(F)c1cccc1</chem>
KRFP4047	KRFPC4047	<chem>FC(F)(F)CCS</chem>
KRFP4048	KRFPC4048	<chem>FC(F)(F)COc1ncncn1</chem>
KRFP4049	KRFPC4049	<chem>FC(F)(F)OC(F)(F)C(F)(F)OC(F)(F)C=O</chem>
KRFP4050	KRFPC4050	<chem>FC(F)(F)S</chem>
KRFP4051	KRFPC4051	<chem>FC(F)(F)S(=O)=O</chem>
KRFP4052	KRFPC4052	<chem>FC(F)C(F)F</chem>
KRFP4053	KRFPC4053	<chem>FC(F)F</chem>
KRFP4054	KRFPC4054	<chem>Fc1cc(F)c(F)c(F)c1F</chem>
KRFP4055	KRFPC4055	<chem>Fc1cc(F)c(F)cc1F</chem>
KRFP4056	KRFPC4056	<chem>Fc1ccc(C=C2SC(=S)NC2=O)cc1</chem>
KRFP4057	KRFPC4057	<chem>Fc1ccc(C=NNC=O)cc1</chem>
KRFP4058	KRFPC4058	<chem>Fc1ccc(C=O)c(C=O)c1</chem>
KRFP4059	KRFPC4059	<chem>Fc1ccc(C=O)cc1</chem>
KRFP4060	KRFPC4060	<chem>Fc1ccc(C=O)cc1F</chem>
KRFP4061	KRFPC4061	<chem>Fc1ccc(cc1)N2CCNCC2</chem>
KRFP4062	KRFPC4062	<chem>Fc1ccc(NC=O)cc1</chem>
KRFP4063	KRFPC4063	<chem>Fc1ccc2c(Cl)csc2c1</chem>
KRFP4064	KRFPC4064	<chem>Fc1cccc(C=O)c1</chem>
KRFP4065	KRFPC4065	<chem>Fc1cccc(F)c1</chem>
KRFP4066	KRFPC4066	<chem>Fc1cccc(F)c1C=O</chem>
KRFP4067	KRFPC4067	<chem>Fc1cccc1</chem>
KRFP4068	KRFPC4068	<chem>Fc1cccc1C=N</chem>
KRFP4069	KRFPC4069	<chem>Fc1cccc1C=NNC=O</chem>
KRFP4070	KRFPC4070	<chem>Fc1cccc1C=O</chem>
KRFP4071	KRFPC4071	<chem>Fc1cccc1Cl</chem>
KRFP4072	KRFPC4072	<chem>FC1OC(F)(F)C(F)(F)C1(F)F</chem>
KRFP4073	KRFPC4073	<chem>FCC=O</chem>
KRFP4074	KRFPC4074	<chem>I</chem>
KRFP4075	KRFPC4075	<chem>lc1ccc(NC=O)cc1</chem>
KRFP4076	KRFPC4076	<chem>lc1cccc(C=O)c1</chem>
KRFP4077	KRFPC4077	<chem>lc1cccc1</chem>
KRFP4078	KRFPC4078	<chem>lc1cccc1C=O</chem>
KRFP4079	KRFPC4079	<chem>lc1cn[nH]c1</chem>
KRFP4080	KRFPC4080	<chem>N</chem>
KRFP4081	KRFPC4081	<chem>N#Cc1cccc1</chem>
KRFP4082	KRFPC4082	<chem>N#CCC#N</chem>
KRFP4083	KRFPC4083	<chem>N(=Nc1cccc1)c2cccc2</chem>
KRFP4084	KRFPC4084	<chem>N(=Nc1cccc1)c2nc3cccc3s2</chem>
KRFP4085	KRFPC4085	<chem>N(N=Cc1ccc1)c2ncncn2</chem>
KRFP4086	KRFPC4086	<chem>N=[N+]=[N-]</chem>
KRFP4087	KRFPC4087	<chem>N=C(C=O)c1cccc1</chem>
KRFP4088	KRFPC4088	<chem>N=C(c1cccc1)c2cccc2</chem>
KRFP4089	KRFPC4089	<chem>N=C(Nc1cccc1)SCC=O</chem>
KRFP4090	KRFPC4090	<chem>N=c1[nH]c(cs1)c2cccc2</chem>
KRFP4091	KRFPC4091	<chem>N=c1[nH]c2cccc2[nH]1</chem>

Name	Count name	Pattern
KRFP4092	KRFPC4092	<chem>N=c1[nH]c2CCCCc2s1</chem>
KRFP4093	KRFPC4093	<chem>N=c1[nH]ccs1</chem>
KRFP4094	KRFPC4094	<chem>N=C1C(=O)Nc2ccccc12</chem>
KRFP4095	KRFPC4095	<chem>N=c1c2CCCCc2[nH]c3ccccc13</chem>
KRFP4096	KRFPC4096	<chem>N=C1CC(=O)c2ccccc12</chem>
KRFP4097	KRFPC4097	<chem>N=C1CC(=O)NC(=O)N1</chem>
KRFP4098	KRFPC4098	<chem>N=c1cc[nH]c2ccccc12</chem>
KRFP4099	KRFPC4099	<chem>N=c1cc[nH]cc1</chem>
KRFP4100	KRFPC4100	<chem>N=c1cccc[nH]1</chem>
KRFP4101	KRFPC4101	<chem>N=C1CCCc2ccccc2N1</chem>
KRFP4102	KRFPC4102	<chem>N=C1NC(=O)CS1</chem>
KRFP4103	KRFPC4103	<chem>N=c1nccc[nH]1</chem>
KRFP4104	KRFPC4104	<chem>N=c1ncccn1CC=O</chem>
KRFP4105	KRFPC4105	<chem>N=Cc1c[nH]c2ccccc12</chem>
KRFP4106	KRFPC4106	<chem>N=Cc1c2ccccc2cc3ccccc13</chem>
KRFP4107	KRFPC4107	<chem>N=Cc1ccc(C#Cc2ccccc2)cc1</chem>
KRFP4108	KRFPC4108	<chem>N=Cc1ccc(C=N)cc1</chem>
KRFP4109	KRFPC4109	<chem>N=Cc1ccc[nH]1</chem>
KRFP4110	KRFPC4110	<chem>N=Cc1ccc2[nH]c3ccccc3c2c1</chem>
KRFP4111	KRFPC4111	<chem>N=Cc1ccc2OCOc2c1</chem>
KRFP4112	KRFPC4112	<chem>N=Cc1cccc2ccccc12</chem>
KRFP4113	KRFPC4113	<chem>N=Cc1ccccc1</chem>
KRFP4114	KRFPC4114	<chem>N=Cc1cccnc1</chem>
KRFP4115	KRFPC4115	<chem>N=Cc1cccoc1</chem>
KRFP4116	KRFPC4116	<chem>N=N</chem>
KRFP4117	KRFPC4117	<chem>N=O</chem>
KRFP4118	KRFPC4118	<chem>N1C(Nc2ccccc12)c3ccccc3</chem>
KRFP4119	KRFPC4119	<chem>N1C=CC2C=CC=CC12</chem>
KRFP4120	KRFPC4120	<chem>N1c2ccccc2C=Cc3ccccc13</chem>
KRFP4121	KRFPC4121	<chem>N1c2ccccc2S(c3ccccc13)</chem>
KRFP4122	KRFPC4122	<chem>NC(=N)N</chem>
KRFP4123	KRFPC4123	<chem>NC(=N)NC(=N)N</chem>
KRFP4124	KRFPC4124	<chem>NC(=N)NC(=O)N</chem>
KRFP4125	KRFPC4125	<chem>NC(=N)NCCCC(NC=O)C(=O)N</chem>
KRFP4126	KRFPC4126	<chem>NC(=N)NN=C</chem>
KRFP4127	KRFPC4127	<chem>NC(=N)S</chem>
KRFP4128	KRFPC4128	<chem>NC(=N)SCC=O</chem>
KRFP4129	KRFPC4129	<chem>NC(=Nc1ccccc1)S</chem>
KRFP4130	KRFPC4130	<chem>NC(=O)C(=C)C#N</chem>
KRFP4131	KRFPC4131	<chem>NC(=O)C(=O)NN=C1C(=O)Nc2ccccc12</chem>
KRFP4132	KRFPC4132	<chem>NC(=O)C(C(C(=O)O)C(=O)O)C(=O)O</chem>
KRFP4133	KRFPC4133	<chem>NC(=O)C(C=O)S(=O)=O</chem>
KRFP4134	KRFPC4134	<chem>NC(=O)C(Cl)(Cl)Cl</chem>
KRFP4135	KRFPC4135	<chem>NC(=O)C(F)(F)C(F)(F)F</chem>
KRFP4136	KRFPC4136	<chem>NC(=O)C(F)(F)F</chem>
KRFP4137	KRFPC4137	<chem>NC(=O)C(F)(F)OC(F)(F)C(F)(F)OC(F)(F)F</chem>
KRFP4138	KRFPC4138	<chem>NC(=O)C(F)(OC(F)(F)C(F)(F)C(F)(F)F)C(F)(F)F</chem>
KRFP4139	KRFPC4139	<chem>NC(=O)C=C</chem>
KRFP4140	KRFPC4140	<chem>NC(=O)C=CC(=O)O</chem>
KRFP4141	KRFPC4141	<chem>NC(=O)C=Cc1cccc(c1)[N+](=O)[O-]</chem>
KRFP4142	KRFPC4142	<chem>NC(=O)C=Cc1ccccc1</chem>
KRFP4143	KRFPC4143	<chem>NC(=O)C1(CC2CC3CC(C2)C1)C3</chem>
KRFP4144	KRFPC4144	<chem>NC(=O)C1C(C2CC1C=C2)C(=O)O</chem>
KRFP4145	KRFPC4145	<chem>NC(=O)c1c(cccc1[N+](=O)[O-])C(=O)O</chem>

Name	Count name	Pattern
KRFP4146	KRFPC4146	<chem>NC(=O)C1C2CCCCC12</chem>
KRFP4147	KRFPC4147	<chem>NC(=O)c1cc(cc(c1)[N+](=O)[O-])[N+](=O)[O-]</chem>
KRFP4148	KRFPC4148	<chem>NC(=O)c1cc(ccc1Cl)[N+](=O)[O-]</chem>
KRFP4149	KRFPC4149	<chem>NC(=O)C1CC1(c2ccccc2)c3ccccc3</chem>
KRFP4150	KRFPC4150	<chem>NC(=O)C1CC1c2ccccc2</chem>
KRFP4151	KRFPC4151	<chem>NC(=O)C1CC21CCC2</chem>
KRFP4152	KRFPC4152	<chem>NC(=O)c1cc2ccccc2oc1=O</chem>
KRFP4153	KRFPC4153	<chem>NC(=O)c1ccc(Br)cc1</chem>
KRFP4154	KRFPC4154	<chem>NC(=O)c1ccc(Br)o1</chem>
KRFP4155	KRFPC4155	<chem>NC(=O)c1ccc(cc1)[N+](=O)[O-]</chem>
KRFP4156	KRFPC4156	<chem>NC(=O)c1ccc(cc1)c2ccccc2</chem>
KRFP4157	KRFPC4157	<chem>NC(=O)c1ccc(cc1)N2C(=O)c3ccccc3C2=O</chem>
KRFP4158	KRFPC4158	<chem>NC(=O)c1ccc(cc1C(=O)O)[N+](=O)[O-]</chem>
KRFP4159	KRFPC4159	<chem>NC(=O)c1ccc(Cl)cc1</chem>
KRFP4160	KRFPC4160	<chem>NC(=O)c1ccc(Cl)cc1Cl</chem>
KRFP4161	KRFPC4161	<chem>NC(=O)c1ccc(F)c(F)c1</chem>
KRFP4162	KRFPC4162	<chem>NC(=O)c1ccc(F)cc1</chem>
KRFP4163	KRFPC4163	<chem>NC(=O)c1ccc(N)cc1</chem>
KRFP4164	KRFPC4164	<chem>NC(=O)C1CCC=CC1</chem>
KRFP4165	KRFPC4165	<chem>NC(=O)c1ccc2C(=O)N(C(=O)c2c1)c3ccccc3</chem>
KRFP4166	KRFPC4166	<chem>NC(=O)c1cccc(Br)c1</chem>
KRFP4167	KRFPC4167	<chem>NC(=O)c1cccc(c1)[N+](=O)[O-]</chem>
KRFP4168	KRFPC4168	<chem>NC(=O)c1cccc2ccccc12</chem>
KRFP4169	KRFPC4169	<chem>NC(=O)C1CCCCC1</chem>
KRFP4170	KRFPC4170	<chem>NC(=O)c1cccc1[N+](=O)[O-]</chem>
KRFP4171	KRFPC4171	<chem>NC(=O)c1cccc1Br</chem>
KRFP4172	KRFPC4172	<chem>NC(=O)c1cccc1C(=O)O</chem>
KRFP4173	KRFPC4173	<chem>NC(=O)c1cccc1Cl</chem>
KRFP4174	KRFPC4174	<chem>NC(=O)c1cccc1F</chem>
KRFP4175	KRFPC4175	<chem>NC(=O)c1cccnc1</chem>
KRFP4176	KRFPC4176	<chem>NC(=O)c1ccco1</chem>
KRFP4177	KRFPC4177	<chem>NC(=O)c1cccs1</chem>
KRFP4178	KRFPC4178	<chem>NC(=O)c1ccncc1</chem>
KRFP4179	KRFPC4179	<chem>NC(=O)c1csc2CCCCc12</chem>
KRFP4180	KRFPC4180	<chem>NC(=O)c1nccnc1C(=O)O</chem>
KRFP4181	KRFPC4181	<chem>NC(=O)CC(=O)N</chem>
KRFP4182	KRFPC4182	<chem>NC(=O)CC=O</chem>
KRFP4183	KRFPC4183	<chem>NC(=O)CCC(=O)O</chem>
KRFP4184	KRFPC4184	<chem>NC(=O)CCC(=O)OCC(=C(Cl)Cl)Cl</chem>
KRFP4185	KRFPC4185	<chem>NC(=O)CCCC(=O)O</chem>
KRFP4186	KRFPC4186	<chem>NC(=O)CCCC(=O)OCC#C</chem>
KRFP4187	KRFPC4187	<chem>NC(=O)CCCCCCC(=O)N</chem>
KRFP4188	KRFPC4188	<chem>NC(=O)CCCO</chem>
KRFP4189	KRFPC4189	<chem>NC(=O)CCl</chem>
KRFP4190	KRFPC4190	<chem>NC(=O)CCNC(=O)C(F)(F)F</chem>
KRFP4191	KRFPC4191	<chem>NC(=O)CO</chem>
KRFP4192	KRFPC4192	<chem>NC(=O)CS</chem>
KRFP4193	KRFPC4193	<chem>NC(=O)N</chem>
KRFP4194	KRFPC4194	<chem>NC(=O)NC(=O)C(Cl)(Cl)Cl</chem>
KRFP4195	KRFPC4195	<chem>NC(=O)NC(=O)N</chem>
KRFP4196	KRFPC4196	<chem>NC(=O)NC(CC=O)C(Cl)(Cl)Cl</chem>
KRFP4197	KRFPC4197	<chem>NC(=O)NC=O</chem>
KRFP4198	KRFPC4198	<chem>NC(=O)NN=C</chem>
KRFP4199	KRFPC4199	<chem>NC(=O)NN=C1C(=O)Nc2ccccc12</chem>

Name	Count name	Pattern
KRFP4200	KRFPC4200	<chem>NC(=O)NN=Cc1cccc1</chem>
KRFP4201	KRFPC4201	<chem>NC(=O)NNC=O</chem>
KRFP4202	KRFPC4202	<chem>NC(=O)NO</chem>
KRFP4203	KRFPC4203	<chem>NC(=O)NS(=O)(=O)N</chem>
KRFP4204	KRFPC4204	<chem>NC(=O)NS(=O)=O</chem>
KRFP4205	KRFPC4205	<chem>NC(=O)O</chem>
KRFP4206	KRFPC4206	<chem>NC(=O)OCCNS(=O)=O</chem>
KRFP4207	KRFPC4207	<chem>NC(=O)ON=C</chem>
KRFP4208	KRFPC4208	<chem>NC(=O)SCC=O</chem>
KRFP4209	KRFPC4209	<chem>NC(=S)N</chem>
KRFP4210	KRFPC4210	<chem>NC(=S)NC(=O)C=C</chem>
KRFP4211	KRFPC4211	<chem>NC(=S)NC(=O)C=Cc1ccc(F)cc1</chem>
KRFP4212	KRFPC4212	<chem>NC(=S)NC(=O)C=Cc1cccc1</chem>
KRFP4213	KRFPC4213	<chem>NC(=S)NC(=O)C=Cc1ccco1</chem>
KRFP4214	KRFPC4214	<chem>NC(=S)NC(NC(=O)C=C)C(Cl)(Cl)Cl</chem>
KRFP4215	KRFPC4215	<chem>NC(=S)NC(NC(=O)C=Cc1cccc1)C(Cl)(Cl)Cl</chem>
KRFP4216	KRFPC4216	<chem>NC(=S)NC(NC(=O)CF)C(Cl)(Cl)Cl</chem>
KRFP4217	KRFPC4217	<chem>NC(=S)NC(NC=O)C(Cl)(Cl)Cl</chem>
KRFP4218	KRFPC4218	<chem>NC(=S)NC=O</chem>
KRFP4219	KRFPC4219	<chem>NC(=S)Nc1ccc(cc1)S(=O)=O</chem>
KRFP4220	KRFPC4220	<chem>NC(=S)NCC=O</chem>
KRFP4221	KRFPC4221	<chem>NC(=S)NN=C</chem>
KRFP4222	KRFPC4222	<chem>NC(=S)NN=C1C(=O)Nc2cccc12</chem>
KRFP4223	KRFPC4223	<chem>NC(=S)NNC=O</chem>
KRFP4224	KRFPC4224	<chem>NC(=S)SCC=O</chem>
KRFP4225	KRFPC4225	<chem>NC(CO)CO</chem>
KRFP4226	KRFPC4226	<chem>NC(NC(=O)CF)C(Cl)(Cl)Cl</chem>
KRFP4227	KRFPC4227	<chem>NC(NC(=O)N)C(Cl)(Cl)Cl</chem>
KRFP4228	KRFPC4228	<chem>NC(NC=O)C(Br)(Br)Br</chem>
KRFP4229	KRFPC4229	<chem>NC(NC=O)C(Cl)(Cl)Cl</chem>
KRFP4230	KRFPC4230	<chem>NC(NC=O)C=O</chem>
KRFP4231	KRFPC4231	<chem>NC=C</chem>
KRFP4232	KRFPC4232	<chem>NC=C1C(=O)CCCC1=O</chem>
KRFP4233	KRFPC4233	<chem>NC=C1C(=O)CNC1=O</chem>
KRFP4234	KRFPC4234	<chem>NC=C1C(=O)N(C(=O)c2cccc12)c3cccc3</chem>
KRFP4235	KRFPC4235	<chem>NC=C1C(=O)NC(=O)NC1=O</chem>
KRFP4236	KRFPC4236	<chem>NC=C1SC(=S)NC1=O</chem>
KRFP4237	KRFPC4237	<chem>NC=O</chem>
KRFP4238	KRFPC4238	<chem>NC=S</chem>
KRFP4239	KRFPC4239	<chem>NC1=CC(=O)c2cccc2C1=O</chem>
KRFP4240	KRFPC4240	<chem>Nc1ccc([N+](=O)[O-])c2nonc12</chem>
KRFP4241	KRFPC4241	<chem>Nc1ccc(Br)cc1</chem>
KRFP4242	KRFPC4242	<chem>Nc1ccc(Br)cc1C=O</chem>
KRFP4243	KRFPC4243	<chem>Nc1ccc(C=O)cc1</chem>
KRFP4244	KRFPC4244	<chem>Nc1ccc(cc1)[N+](=O)[O-]</chem>
KRFP4245	KRFPC4245	<chem>Nc1ccc(cc1)C(=O)O</chem>
KRFP4246	KRFPC4246	<chem>Nc1ccc(cc1)S(=O)(=O)N</chem>
KRFP4247	KRFPC4247	<chem>Nc1ccc(cc1)S(=O)=O</chem>
KRFP4248	KRFPC4248	<chem>Nc1ccc(cc1[N+](=O)[O-])[N+](=O)[O-]</chem>
KRFP4249	KRFPC4249	<chem>Nc1ccc(Cl)c(Cl)c1</chem>
KRFP4250	KRFPC4250	<chem>Nc1ccc(Cl)cc1</chem>
KRFP4251	KRFPC4251	<chem>Nc1ccc(Cl)cc1C=O</chem>
KRFP4252	KRFPC4252	<chem>Nc1ccc(F)cc1</chem>
KRFP4253	KRFPC4253	<chem>Nc1ccc(I)cc1</chem>

Name	Count name	Pattern
KRFP4254	KRFPC4254	<chem>Nc1ccc(O)cc1</chem>
KRFP4255	KRFPC4255	<chem>Nc1ccc2ccccc2c1</chem>
KRFP4256	KRFPC4256	<chem>Nc1cccc(c1)[N+](=O)[O-]</chem>
KRFP4257	KRFPC4257	<chem>Nc1cccc(c1)C(=O)O</chem>
KRFP4258	KRFPC4258	<chem>Nc1cccc(c1)C(F)(F)F</chem>
KRFP4259	KRFPC4259	<chem>Nc1cccc(Cl)c1</chem>
KRFP4260	KRFPC4260	<chem>Nc1cccc(O)c1</chem>
KRFP4261	KRFPC4261	<chem>NC1CCCC1</chem>
KRFP4262	KRFPC4262	<chem>Nc1cccc2ccccc12</chem>
KRFP4263	KRFPC4263	<chem>Nc1cccc2ccnc12</chem>
KRFP4264	KRFPC4264	<chem>NC1CCCCC1</chem>
KRFP4265	KRFPC4265	<chem>Nc1cccc1[N+](=O)[O-]</chem>
KRFP4266	KRFPC4266	<chem>Nc1cccc1C(=O)O</chem>
KRFP4267	KRFPC4267	<chem>Nc1cccc1Cl</chem>
KRFP4268	KRFPC4268	<chem>Nc1cccc1O</chem>
KRFP4269	KRFPC4269	<chem>Nc1ccccn1</chem>
KRFP4270	KRFPC4270	<chem>Nc1cnc2ccccc2n1</chem>
KRFP4271	KRFPC4271	<chem>Nc1cnon1</chem>
KRFP4272	KRFPC4272	<chem>Nc1nc(Cl)nc(Cl)n1</chem>
KRFP4273	KRFPC4273	<chem>Nc1nc(cs1)c2ccccc2</chem>
KRFP4274	KRFPC4274	<chem>Nc1ncccn1</chem>
KRFP4275	KRFPC4275	<chem>Nc1nccs1</chem>
KRFP4276	KRFPC4276	<chem>Nc1ncn[nH]1</chem>
KRFP4277	KRFPC4277	<chem>Nc1ncnc(Cl)n1</chem>
KRFP4278	KRFPC4278	<chem>Nc1ncnc(n1)N2CCOCC2</chem>
KRFP4279	KRFPC4279	<chem>Nc1ncncn1</chem>
KRFP4280	KRFPC4280	<chem>Nc1nncs1</chem>
KRFP4281	KRFPC4281	<chem>NCC(=O)N</chem>
KRFP4282	KRFPC4282	<chem>NCC(=O)NN=C</chem>
KRFP4283	KRFPC4283	<chem>NCC(=O)O</chem>
KRFP4284	KRFPC4284	<chem>NCC(O)CO</chem>
KRFP4285	KRFPC4285	<chem>NCC=C</chem>
KRFP4286	KRFPC4286	<chem>NCC=O</chem>
KRFP4287	KRFPC4287	<chem>NCc1ccccc1</chem>
KRFP4288	KRFPC4288	<chem>NCc1ccc(O)c1</chem>
KRFP4289	KRFPC4289	<chem>NCc1ccncc1</chem>
KRFP4290	KRFPC4290	<chem>NCCC(=O)O</chem>
KRFP4291	KRFPC4291	<chem>NCCC=O</chem>
KRFP4292	KRFPC4292	<chem>NCCCC(=O)O</chem>
KRFP4293	KRFPC4293	<chem>NCCCCO</chem>
KRFP4294	KRFPC4294	<chem>NCCN</chem>
KRFP4295	KRFPC4295	<chem>NCCO</chem>
KRFP4296	KRFPC4296	<chem>NCCS</chem>
KRFP4297	KRFPC4297	<chem>NCN1C(=O)c2ccccc2C1=O</chem>
KRFP4298	KRFPC4298	<chem>NCN1C(=O)CCC1=O</chem>
KRFP4299	KRFPC4299	<chem>NCn1cnc2ccccc12</chem>
KRFP4300	KRFPC4300	<chem>NCn1nnc2ccccc12</chem>
KRFP4301	KRFPC4301	<chem>NN</chem>
KRFP4302	KRFPC4302	<chem>NN=C</chem>
KRFP4303	KRFPC4303	<chem>NN=C1C(=O)NC(=O)NC1=O</chem>
KRFP4304	KRFPC4304	<chem>NN=C1C(=O)NC(=S)NC1=O</chem>
KRFP4305	KRFPC4305	<chem>NN=C1C(=O)Nc2ccccc12</chem>
KRFP4306	KRFPC4306	<chem>NN=C1C(C(=NN)c2ccccc12)c3ccccc3</chem>
KRFP4307	KRFPC4307	<chem>NN=C1C=NN(C1=O)c2ccccc2</chem>

Name	Count name	Pattern
KRFP4308	KRFPC4308	<chem>NN=C1C=NN(C1=O)c2nc(cs2)c3ccccc3</chem>
KRFP4309	KRFPC4309	<chem>NN=C1C=NNC1=O</chem>
KRFP4310	KRFPC4310	<chem>NN=CN=N</chem>
KRFP4311	KRFPC4311	<chem>NN=N</chem>
KRFP4312	KRFPC4312	<chem>Nn1cnnc1</chem>
KRFP4313	KRFPC4313	<chem>NNC(=O)c1ccccc1</chem>
KRFP4314	KRFPC4314	<chem>NNC(=O)CO</chem>
KRFP4315	KRFPC4315	<chem>NNC(=O)N</chem>
KRFP4316	KRFPC4316	<chem>NNC(=S)N</chem>
KRFP4317	KRFPC4317	<chem>NNC=O</chem>
KRFP4318	KRFPC4318	<chem>NNc1ccccc1</chem>
KRFP4319	KRFPC4319	<chem>NNS(=O)=O</chem>
KRFP4320	KRFPC4320	<chem>NS</chem>
KRFP4321	KRFPC4321	<chem>NS(=O)(=O)c1ccc(Br)cc1</chem>
KRFP4322	KRFPC4322	<chem>NS(=O)(=O)c1ccc(cc1)[N+](=O)[O-]</chem>
KRFP4323	KRFPC4323	<chem>NS(=O)(=O)c1ccc(cc1)c2ccccc2</chem>
KRFP4324	KRFPC4324	<chem>NS(=O)(=O)c1ccc(Cl)cc1</chem>
KRFP4325	KRFPC4325	<chem>NS(=O)(=O)c1cccc2nsnc12</chem>
KRFP4326	KRFPC4326	<chem>NS(=O)(=O)c1ccccc1</chem>
KRFP4327	KRFPC4327	<chem>NS(=O)(=O)c1ccccc1[N+](=O)[O-]</chem>
KRFP4328	KRFPC4328	<chem>NS(=O)=O</chem>
KRFP4329	KRFPC4329	<chem>NS=O</chem>
KRFP4330	KRFPC4330	<chem>NS(c1ccccc1[N+](=O)[O-])</chem>
KRFP4331	KRFPC4331	<chem>O</chem>
KRFP4332	KRFPC4332	<chem>O[NH2]=O</chem>
KRFP4333	KRFPC4333	<chem>O=[SH2]=O</chem>
KRFP4334	KRFPC4334	<chem>O=C(C(=O)c1ccccc1)c2ccccc2</chem>
KRFP4335	KRFPC4335	<chem>O=C(C=Cc1ccccc1)c2ccccc2</chem>
KRFP4336	KRFPC4336	<chem>O=C(c1ccccc1)c2ccccc2</chem>
KRFP4337	KRFPC4337	<chem>O=C(c1ccccc1)c2cnccc2</chem>
KRFP4338	KRFPC4338	<chem>O=C(NN=Cc1ccccc1)c2ccccc2</chem>
KRFP4339	KRFPC4339	<chem>O=C(NNC(=O)c1ccccc1)c2ccccc2</chem>
KRFP4340	KRFPC4340	<chem>O=c1[nH][nH]c(=O)c2ccccc12</chem>
KRFP4341	KRFPC4341	<chem>O=c1[nH]c(=O)[nH]c(=O)[nH]1</chem>
KRFP4342	KRFPC4342	<chem>O=c1[nH]c(=O)c2[nH]cnc2[nH]1</chem>
KRFP4343	KRFPC4343	<chem>O=c1[nH]c(=O)c2cc3c(=O)[nH]c(=O)c3cc12</chem>
KRFP4344	KRFPC4344	<chem>O=c1[nH]c(=O)c2nc3ccccc3nc2[nH]1</chem>
KRFP4345	KRFPC4345	<chem>O=c1[nH]c(nc2ccccc12)c3ccccc3</chem>
KRFP4346	KRFPC4346	<chem>O=c1[nH]c2ccccc2[nH]1</chem>
KRFP4347	KRFPC4347	<chem>O=c1[nH]c2ccccc2o1</chem>
KRFP4348	KRFPC4348	<chem>O=c1[nH]cnc2ccccc12</chem>
KRFP4349	KRFPC4349	<chem>O=c1[nH]cnc2n(cnc12)C3CCCO3</chem>
KRFP4350	KRFPC4350	<chem>O=c1[nH]cnc2sc3CCCCc3c12</chem>
KRFP4351	KRFPC4351	<chem>O=c1[nH]ncc2ccccc12</chem>
KRFP4352	KRFPC4352	<chem>O=C1C(=Cc2ccccc12)c3ccccc3</chem>
KRFP4353	KRFPC4353	<chem>O=C1C(C(=O)c2ccccc12)C3=CC(C(N=N3)c4ccccc4)c5ccccc5</chem>
KRFP4354	KRFPC4354	<chem>O=C1C(C(=O)c2ccccc12)c3ccccc3</chem>
KRFP4355	KRFPC4355	<chem>O=c1c(coc2ccccc12)c3ccc4OCCOc4c3</chem>
KRFP4356	KRFPC4356	<chem>O=c1c(coc2ccccc12)c3ccccc3</chem>
KRFP4357	KRFPC4357	<chem>O=c1c(coc2ccccc12)c3nc4ccccc4[nH]3</chem>
KRFP4358	KRFPC4358	<chem>O=C1C=C(C(=O)c2ccccc12)c3ccccc3</chem>
KRFP4359	KRFPC4359	<chem>O=C1C=CC(=O)C=C1</chem>
KRFP4360	KRFPC4360	<chem>O=C1C=CC(=O)c2ccccc12</chem>
KRFP4361	KRFPC4361	<chem>O=C1C=CC(=O)N1c2ccccc2</chem>

Name	Count name	Pattern
KRFP4362	KRFPC4362	<chem>O=C1C2C(C(C=CC2c3cccc3)c4cccc4)C(=O)N1c5cccc5</chem>
KRFP4363	KRFPC4363	<chem>O=C1C2C(C3C=CC2C4C3C(=O)N(C4=O)c5cccc5)C(=O)N1c6cccc6</chem>
KRFP4364	KRFPC4364	<chem>O=C1C2C(C3c4cccc4C2c5cccc35)C(=O)N1c6cccc6</chem>
KRFP4365	KRFPC4365	<chem>O=C1C2C3CC(C=C3)C2C(=O)N1c4cccc4</chem>
KRFP4366	KRFPC4366	<chem>O=C1C2C3OC(C=C3)C2C(=O)N1c4cccc4</chem>
KRFP4367	KRFPC4367	<chem>O=c1c2cccc3cccc(c4nc5cccc5n14)c32</chem>
KRFP4368	KRFPC4368	<chem>O=C1c2cccc2C(=O)c3cccc13</chem>
KRFP4369	KRFPC4369	<chem>O=C1c2cccc2C(c3cccc3)(c4cccc4)c5cccc15</chem>
KRFP4370	KRFPC4370	<chem>O=C1c2cccc2-c3cccc13</chem>
KRFP4371	KRFPC4371	<chem>O=C1c2cccc2-c3ncnc4cccc1c34</chem>
KRFP4372	KRFPC4372	<chem>O=C1C2CN3CC1CN(C2)C3</chem>
KRFP4373	KRFPC4373	<chem>O=C1CC(=O)c2cccc12</chem>
KRFP4374	KRFPC4374	<chem>O=C1CC(=O)NC(=O)N1</chem>
KRFP4375	KRFPC4375	<chem>O=C1CC(CN1)c2cccc2</chem>
KRFP4376	KRFPC4376	<chem>O=C1CC(N2CCCC2)C(=O)N1c3cccc3</chem>
KRFP4377	KRFPC4377	<chem>O=C1CC(N2CCCC2)C(=O)N1c3cccc3</chem>
KRFP4378	KRFPC4378	<chem>O=C1CC(N2CCN(CC2)C3CC(=O)N(C3=O)c4cccc4)C(=O)N1c5cccc5</chem>
KRFP4379	KRFPC4379	<chem>O=C1CC(N2CCN(CC2)c3cccc3)C(=O)N1c4cccc4</chem>
KRFP4380	KRFPC4380	<chem>O=C1CC(N2CCN(CC2)c3ncccn3)C(=O)N1c4cccc4</chem>
KRFP4381	KRFPC4381	<chem>O=C1CC(N2CCNCC2)C(=O)N1c3cccc3</chem>
KRFP4382	KRFPC4382	<chem>O=C1CC(N2CCOCC2)C(=O)N1c3cccc3</chem>
KRFP4383	KRFPC4383	<chem>O=c1cc[nH]c(=O)[nH]1</chem>
KRFP4384	KRFPC4384	<chem>O=c1cc[nH]cn1</chem>
KRFP4385	KRFPC4385	<chem>O=c1cc[nH]n1c2cccc2</chem>
KRFP4386	KRFPC4386	<chem>O=C1CC=NN1c2cccc2</chem>
KRFP4387	KRFPC4387	<chem>O=C1Cc2cccc2N1</chem>
KRFP4388	KRFPC4388	<chem>O=C1CCC(=O)N1</chem>
KRFP4389	KRFPC4389	<chem>O=C1CCC(=O)N1c2cccc3cccc23</chem>
KRFP4390	KRFPC4390	<chem>O=C1CCC(=O)N1c2cccc2</chem>
KRFP4391	KRFPC4391	<chem>O=C1CCC(O1)c2cccc2</chem>
KRFP4392	KRFPC4392	<chem>O=c1ccc2c(c3cccc3)c4cccc4oc2c1</chem>
KRFP4393	KRFPC4393	<chem>O=c1ccc2cccc2[nH]1</chem>
KRFP4394	KRFPC4394	<chem>O=c1ccc2cccc2o1</chem>
KRFP4395	KRFPC4395	<chem>O=c1ccc2cccc2s1</chem>
KRFP4396	KRFPC4396	<chem>O=C1CCCC(=O)C1</chem>
KRFP4397	KRFPC4397	<chem>O=c1cccc[nH]1</chem>
KRFP4398	KRFPC4398	<chem>O=C1CCCC=C1</chem>
KRFP4399	KRFPC4399	<chem>O=C1CCCC1</chem>
KRFP4400	KRFPC4400	<chem>O=C1CCCc2[nH]ncc12</chem>
KRFP4401	KRFPC4401	<chem>O=C1CCCC2=C1C(C=CN2)c3cccc3</chem>
KRFP4402	KRFPC4402	<chem>O=C1CCCC2=C1C(C=CO2)c3cccc3</chem>
KRFP4403	KRFPC4403	<chem>O=C1CCCC2=C1C(Nc3ccc4cccc4c23)c5cccc5</chem>
KRFP4404	KRFPC4404	<chem>O=C1CCCC2=C1C(Nc3ccc4ncccc4c23)c5cccc5</chem>
KRFP4405	KRFPC4405	<chem>O=C1CCCc2c1[nH]c3cccc23</chem>
KRFP4406	KRFPC4406	<chem>O=C1CCCc2ccsc12</chem>
KRFP4407	KRFPC4407	<chem>O=C1CCCc2nc3cccc3cc12</chem>
KRFP4408	KRFPC4408	<chem>O=C1CCCCC1</chem>
KRFP4409	KRFPC4409	<chem>O=C1CCCCCN1</chem>
KRFP4410	KRFPC4410	<chem>O=c1cccc1</chem>
KRFP4411	KRFPC4411	<chem>O=C1CCCN1</chem>
KRFP4412	KRFPC4412	<chem>O=C1CCCN1c2cccc2</chem>
KRFP4413	KRFPC4413	<chem>O=C1CCCCO1</chem>
KRFP4414	KRFPC4414	<chem>O=c1ccn(C2CCCO2)c(=O)[nH]1</chem>
KRFP4415	KRFPC4415	<chem>O=C1CCN2C(=C1)Nc3cccc23</chem>

Name	Count name	Pattern
KRFP4416	KRFPC4416	<chem>O=c1ccnc[nH]1</chem>
KRFP4417	KRFPC4417	<chem>O=c1ccnc2cccn12</chem>
KRFP4418	KRFPC4418	<chem>O=c1ccoc2ccccc12</chem>
KRFP4419	KRFPC4419	<chem>O=c1cn[nH]c(=O)[nH]1</chem>
KRFP4420	KRFPC4420	<chem>O=c1cn[nH]c(=S)[nH]1</chem>
KRFP4421	KRFPC4421	<chem>O=c1cnc2ccccc2[nH]1</chem>
KRFP4422	KRFPC4422	<chem>O=C1CNc2ccccc2N1</chem>
KRFP4423	KRFPC4423	<chem>O=C1CNCC(=O)N1</chem>
KRFP4424	KRFPC4424	<chem>O=C1CSC(=S)N1</chem>
KRFP4425	KRFPC4425	<chem>O=C1CSC(N1)c2ccccc2</chem>
KRFP4426	KRFPC4426	<chem>O=C1CS(c2ccccc12)</chem>
KRFP4427	KRFPC4427	<chem>O=C1CS(c2ccccc2N1)</chem>
KRFP4428	KRFPC4428	<chem>O=C1N(C(=O)c2cccc3cccc1c23)c4ccccc4</chem>
KRFP4429	KRFPC4429	<chem>O=C1N(C(=O)c2ccccc12)c3ccccc3</chem>
KRFP4430	KRFPC4430	<chem>O=c1n(c2ccccc2)c(=O)c3cc4c(=O)n(c5ccccc5)c(=O)c4cc13</chem>
KRFP4431	KRFPC4431	<chem>O=c1n(cnc2ccccc12)c3ccccc3</chem>
KRFP4432	KRFPC4432	<chem>O=C1NC(=O)C=C1</chem>
KRFP4433	KRFPC4433	<chem>O=C1NC(=O)C2(CCCCC2)N1</chem>
KRFP4434	KRFPC4434	<chem>O=C1NC(=O)C2C1C3C=CC2C4C3C(=O)NC4=O</chem>
KRFP4435	KRFPC4435	<chem>O=C1NC(=O)C2C1C3c4ccccc4C2c5ccccc35</chem>
KRFP4436	KRFPC4436	<chem>O=C1NC(=O)C2C3CC(C=C3)C21</chem>
KRFP4437	KRFPC4437	<chem>O=C1NC(=O)C2C3OC(C=C3)C21</chem>
KRFP4438	KRFPC4438	<chem>O=C1NC(=O)c2ccc(N3CCOCC3)c4ccccc1c24</chem>
KRFP4439	KRFPC4439	<chem>O=C1NC(=O)c2cccc3cccc1c23</chem>
KRFP4440	KRFPC4440	<chem>O=C1NC(=O)c2ccccc12</chem>
KRFP4441	KRFPC4441	<chem>O=C1NC(=S)SC1=C2C(=O)Nc3ccccc23</chem>
KRFP4442	KRFPC4442	<chem>O=C1NC(=S)SC1=C2Nc3ccccc3S2</chem>
KRFP4443	KRFPC4443	<chem>O=C1NC(=S)SC1=C2SC(=S)NC2=O</chem>
KRFP4444	KRFPC4444	<chem>O=C1NC(=S)SC1=Cc2ccccc2</chem>
KRFP4445	KRFPC4445	<chem>O=C1NC(c2ccccc12)(c3ccccc3)c4ccccc4</chem>
KRFP4446	KRFPC4446	<chem>O=c1nc[nH]c2ccccc12</chem>
KRFP4447	KRFPC4447	<chem>O=C1NC=CC(N1)c2ccccc2</chem>
KRFP4448	KRFPC4448	<chem>O=C1Nc2ccccc3cccc1c23</chem>
KRFP4449	KRFPC4449	<chem>O=C1Nc2ccccc2C1=C3SC(=S)N(C3=O)c4ccccc4</chem>
KRFP4450	KRFPC4450	<chem>O=C1Nc2ccccc2C1=O</chem>
KRFP4451	KRFPC4451	<chem>O=C1NC2NC(=O)NC2N1</chem>
KRFP4452	KRFPC4452	<chem>O=C1NCCc2ccccc12</chem>
KRFP4453	KRFPC4453	<chem>O=c1nccc[nH]1</chem>
KRFP4454	KRFPC4454	<chem>O=C1NCCc2c1[nH]c3ccccc23</chem>
KRFP4455	KRFPC4455	<chem>O=c1ncccn1c2ccccc2</chem>
KRFP4456	KRFPC4456	<chem>O=C1NCCN1c2cccc3ccccc23</chem>
KRFP4457	KRFPC4457	<chem>O=C1NCCN1c2ccccc2</chem>
KRFP4458	KRFPC4458	<chem>O=C1NN=C(CC1c2c[nH]c3ccccc23)c4ccccc4</chem>
KRFP4459	KRFPC4459	<chem>O=C1OC(=O)c2ccccc12</chem>
KRFP4460	KRFPC4460	<chem>O=C1OC(c2ccccc12)(c3ccccc3)c4ccccc4</chem>
KRFP4461	KRFPC4461	<chem>O=c1oc(nc2ccccc12)c3ccccc3</chem>
KRFP4462	KRFPC4462	<chem>O=C1OC2(CCCCC2)C=C1</chem>
KRFP4463	KRFPC4463	<chem>O=c1oc2ccccc2c3[nH]nnc13</chem>
KRFP4464	KRFPC4464	<chem>O=C1OCc2ccccc12</chem>
KRFP4465	KRFPC4465	<chem>O=c1occcc1C2=Nc3ccccc3SC(C2)c4ccccc4</chem>
KRFP4466	KRFPC4466	<chem>O=c1occcc1C2=NCCSC(C2)c3ccccc3</chem>
KRFP4467	KRFPC4467	<chem>O=c1ocnc2ccccc12</chem>
KRFP4468	KRFPC4468	<chem>O=CC(=O)c1ccccc1</chem>
KRFP4469	KRFPC4469	<chem>O=CC(C=O)C1CCCCC1</chem>

Name	Count name	Pattern
KRFP4470	KRFPC4470	<chem>O=CC(c1cccc1)c2cccc2</chem>
KRFP4471	KRFPC4471	<chem>O=CC(Cc1cccc1)C=O</chem>
KRFP4472	KRFPC4472	<chem>O=CC=O</chem>
KRFP4473	KRFPC4473	<chem>O=CC1(CC2CC3C1)CC(C2)CC3</chem>
KRFP4474	KRFPC4474	<chem>O=CC1(CC2CC3CC(C2)C1)C3</chem>
KRFP4475	KRFPC4475	<chem>O=CC1C(C=O)C2c3cccc3C1c4cccc24</chem>
KRFP4476	KRFPC4476	<chem>O=CC1C(C=O)N2C(C(C=O)C(C=O)N2C1c3cccc3)c4cccc4</chem>
KRFP4477	KRFPC4477	<chem>O=Cc1c[nH]c2nc3cccc3nc12</chem>
KRFP4478	KRFPC4478	<chem>O=CC1C2CCCCC12</chem>
KRFP4479	KRFPC4479	<chem>O=CC1CC1</chem>
KRFP4480	KRFPC4480	<chem>O=CC1CC1(c2cccc2)c3cccc3</chem>
KRFP4481	KRFPC4481	<chem>O=CC1CC1c2cccc2</chem>
KRFP4482	KRFPC4482	<chem>O=CC1CC21CCC2</chem>
KRFP4483	KRFPC4483	<chem>O=Cc1cc2cccc2oc1=O</chem>
KRFP4484	KRFPC4484	<chem>O=Cc1ccc(C=O)c(C=O)c1</chem>
KRFP4485	KRFPC4485	<chem>O=Cc1ccc(C=O)cc1</chem>
KRFP4486	KRFPC4486	<chem>O=Cc1ccc(cc1)c2cccc2</chem>
KRFP4487	KRFPC4487	<chem>O=Cc1ccc(cc1)S(=O)=O</chem>
KRFP4488	KRFPC4488	<chem>O=Cc1ccc(cc1C=O)C(=O)c2ccc(C=O)c(C=O)c2</chem>
KRFP4489	KRFPC4489	<chem>O=Cc1ccc2cccc2c1</chem>
KRFP4490	KRFPC4490	<chem>O=Cc1cccc(C=O)c1</chem>
KRFP4491	KRFPC4491	<chem>O=Cc1cccc(c1)S(=O)=O</chem>
KRFP4492	KRFPC4492	<chem>O=CC1CCCC1</chem>
KRFP4493	KRFPC4493	<chem>O=Cc1cccc2cccc(C=O)c12</chem>
KRFP4494	KRFPC4494	<chem>O=Cc1cccc2cccc12</chem>
KRFP4495	KRFPC4495	<chem>O=CC1CCCCC1</chem>
KRFP4496	KRFPC4496	<chem>O=Cc1cccc1C=O</chem>
KRFP4497	KRFPC4497	<chem>O=Cc1cccc1S(=O)=O</chem>
KRFP4498	KRFPC4498	<chem>O=Cc1ccccn1</chem>
KRFP4499	KRFPC4499	<chem>O=Cc1cccnc1</chem>
KRFP4500	KRFPC4500	<chem>O=Cc1cccoc1</chem>
KRFP4501	KRFPC4501	<chem>O=Cc1cccs1</chem>
KRFP4502	KRFPC4502	<chem>O=Cc1ccn[nH]1</chem>
KRFP4503	KRFPC4503	<chem>O=Cc1ccncc1</chem>
KRFP4504	KRFPC4504	<chem>O=Cc1ccsc1</chem>
KRFP4505	KRFPC4505	<chem>O=Cc1cn[nH]c1</chem>
KRFP4506	KRFPC4506	<chem>O=Cc1cnsc1</chem>
KRFP4507	KRFPC4507	<chem>O=Cc1csc2C(=O)CCCc12</chem>
KRFP4508	KRFPC4508	<chem>O=Cc1csc2CCCCc12</chem>
KRFP4509	KRFPC4509	<chem>O=CCC#N</chem>
KRFP4510	KRFPC4510	<chem>O=CCC(NC=O)c1cccc1</chem>
KRFP4511	KRFPC4511	<chem>O=CCC(S(c1cccc1))C=O</chem>
KRFP4512	KRFPC4512	<chem>O=CCC=O</chem>
KRFP4513	KRFPC4513	<chem>O=CCC1(C(=O)c2cccc2C1=O)c3cccc3</chem>
KRFP4514	KRFPC4514	<chem>O=CCC1(CC2CC3CC(C2)C1)C3</chem>
KRFP4515	KRFPC4515	<chem>O=CCc1cccc2cccc12</chem>
KRFP4516	KRFPC4516	<chem>O=CCc1cccc1</chem>
KRFP4517	KRFPC4517	<chem>O=CCc1cccc1C=O</chem>
KRFP4518	KRFPC4518	<chem>O=CCCC(=O)OCC=O</chem>
KRFP4519	KRFPC4519	<chem>O=CCCC=O</chem>
KRFP4520	KRFPC4520	<chem>O=CCc1c[nH]c2cccc12</chem>
KRFP4521	KRFPC4521	<chem>O=CCc1cccc1</chem>
KRFP4522	KRFPC4522	<chem>O=CCCCC=O</chem>
KRFP4523	KRFPC4523	<chem>O=CCCCc1cccc1</chem>

Name	Count name	Pattern
KRFP4524	KRFPC4524	O=CCCCC=O
KRFP4525	KRFPC4525	O=CCCCCCC=O
KRFP4526	KRFPC4526	O=CCCCNC(=S)SCC=O
KRFP4527	KRFPC4527	O=CCCNC(=S)SCC=O
KRFP4528	KRFPC4528	O=CCn1ccc(=NCc2cccc2)cc1
KRFP4529	KRFPC4529	O=CCNC(=O)SCC=O
KRFP4530	KRFPC4530	O=CCNC(=S)SCC=O
KRFP4531	KRFPC4531	O=CCNC=O
KRFP4532	KRFPC4532	O=CCOC(=O)CCS(=O)=O
KRFP4533	KRFPC4533	O=CCOC=O
KRFP4534	KRFPC4534	O=CCSC(=S)Nc1cccc1
KRFP4535	KRFPC4535	O=CCSC(=S)NCc1cccc1
KRFP4536	KRFPC4536	O=CCSC(CC=O)C=O
KRFP4537	KRFPC4537	O=CN1CCc2cccc12
KRFP4538	KRFPC4538	O=CN1CCCC1
KRFP4539	KRFPC4539	O=CN1CCCCC1
KRFP4540	KRFPC4540	O=CN1CCCCC1
KRFP4541	KRFPC4541	O=CN1CCNCC1
KRFP4542	KRFPC4542	O=CN1CCOCC1
KRFP4543	KRFPC4543	O=Cn1cnc2cccc12
KRFP4544	KRFPC4544	O=Cn1nnc2cccc12
KRFP4545	KRFPC4545	O=CNC=S
KRFP4546	KRFPC4546	O=CNc1cc2CCCCc2s1
KRFP4547	KRFPC4547	O=CNc1ccc(cc1)S(=O)=O
KRFP4548	KRFPC4548	O=CNc1ccc(CCc2cccc2)cc1
KRFP4549	KRFPC4549	O=CNc1ccc(S(c2cccc2))cc1
KRFP4550	KRFPC4550	O=CNc1ccc2cccc2c1
KRFP4551	KRFPC4551	O=CNc1cccc2cccc12
KRFP4552	KRFPC4552	O=CNC1CCCCC1
KRFP4553	KRFPC4553	O=CNc1cccc1c2nc3cccc3s2
KRFP4554	KRFPC4554	O=CNc1nc2cccc2s1
KRFP4555	KRFPC4555	O=CNCCCCCNC=O
KRFP4556	KRFPC4556	O=CNCCCCNC=O
KRFP4557	KRFPC4557	O=CNCCNC=O
KRFP4558	KRFPC4558	O=CNCCOC=O
KRFP4559	KRFPC4559	O=CNCNC=O
KRFP4560	KRFPC4560	O=CNCO=O
KRFP4561	KRFPC4561	O=CN=C1C(=O)Nc2cccc12
KRFP4562	KRFPC4562	O=CN=C1CCCC1
KRFP4563	KRFPC4563	O=CN=C1CCCCC1
KRFP4564	KRFPC4564	O=CN=CC=Cc1cccc1
KRFP4565	KRFPC4565	O=CN=CC=NNC=O
KRFP4566	KRFPC4566	O=CN=Cc1c[nH]c2cccc12
KRFP4567	KRFPC4567	O=CN=Cc1ccc(cc1)c2cccc2
KRFP4568	KRFPC4568	O=CN=Cc1ccc[nH]1
KRFP4569	KRFPC4569	O=CN=Cc1ccc2OCOc2c1
KRFP4570	KRFPC4570	O=CN=Cc1cccc2cccc12
KRFP4571	KRFPC4571	O=CN=Cc1cccc1
KRFP4572	KRFPC4572	O=CN=Cc1ccnc1
KRFP4573	KRFPC4573	O=CN=Cc1ccco1
KRFP4574	KRFPC4574	O=CN=Cc1cccs1
KRFP4575	KRFPC4575	O=CN=Cc1ccncc1
KRFP4576	KRFPC4576	O=CN=Cc1nc2cccc2[nH]1
KRFP4577	KRFPC4577	O=CNn1cnnc1

Name	Count name	Pattern
KRFP4578	KRFPC4578	<chem>O=CNNC(=S)NC=O</chem>
KRFP4579	KRFPC4579	<chem>O=CNNC=O</chem>
KRFP4580	KRFPC4580	<chem>O=CNNS(=O)=O</chem>
KRFP4581	KRFPC4581	<chem>O=CNS(=O)=O</chem>
KRFP4582	KRFPC4582	<chem>O=COc1ccc2ccccc2c1</chem>
KRFP4583	KRFPC4583	<chem>O=COc1ccccc1</chem>
KRFP4584	KRFPC4584	<chem>O=COCC#C</chem>
KRFP4585	KRFPC4585	<chem>O=P1OCCCO1</chem>
KRFP4586	KRFPC4586	<chem>O=S(=O)(c1ccccc1)c2ccccc2</chem>
KRFP4587	KRFPC4587	<chem>O=S(=O)c1ccc(cc1)C2CCCCC2</chem>
KRFP4588	KRFPC4588	<chem>O=S(=O)c1ccc(S(c2ccc(cc2)S(=O)=O))cc1</chem>
KRFP4589	KRFPC4589	<chem>O=S(=O)c1ccc2ccccc2c1</chem>
KRFP4590	KRFPC4590	<chem>O=S(=O)c1ccc2nsnc12</chem>
KRFP4591	KRFPC4591	<chem>O=S(=O)c1ccccc1</chem>
KRFP4592	KRFPC4592	<chem>O=S(=O)C1CCS(=O)(=O)C1</chem>
KRFP4593	KRFPC4593	<chem>O=S(=O)N1CCCCC1</chem>
KRFP4594	KRFPC4594	<chem>O=S(=O)N1CCNCC1</chem>
KRFP4595	KRFPC4595	<chem>O=S(=O)N1CCOCC1</chem>
KRFP4596	KRFPC4596	<chem>O=S(=O)n1cnc2ccccc12</chem>
KRFP4597	KRFPC4597	<chem>O=S(=O)Nc1cccc2cccn12</chem>
KRFP4598	KRFPC4598	<chem>O=S(=O)NC1CCCCC1</chem>
KRFP4599	KRFPC4599	<chem>O=S(=O)Nc1cccn1</chem>
KRFP4600	KRFPC4600	<chem>O=S(=O)Nc1cnc2ccccc2n1</chem>
KRFP4601	KRFPC4601	<chem>O=S(=O)Nc1nccs1</chem>
KRFP4602	KRFPC4602	<chem>O=S(=O)Oc1ccccc1</chem>
KRFP4603	KRFPC4603	<chem>O=S1(=O)c2ccccc2-c3ccccc31</chem>
KRFP4604	KRFPC4604	<chem>O=S1(=O)CC(CS(=O)(=O)C1)c2ccccc2</chem>
KRFP4605	KRFPC4605	<chem>O=S1(=O)CCC=C1</chem>
KRFP4606	KRFPC4606	<chem>O=S1(=O)CCCC1</chem>
KRFP4607	KRFPC4607	<chem>O1C=CC(c2cn[nH]c12)c3ccccc3</chem>
KRFP4608	KRFPC4608	<chem>OC(=O)C(F)(F)F</chem>
KRFP4609	KRFPC4609	<chem>OC(=O)C(F)(OC(F)(F)C(F)(F)C(F)(F)F)C(F)(F)F</chem>
KRFP4610	KRFPC4610	<chem>OC(=O)C=C</chem>
KRFP4611	KRFPC4611	<chem>OC(=O)C=CC(=O)NNC=O</chem>
KRFP4612	KRFPC4612	<chem>OC(=O)C=Cc1ccccc1</chem>
KRFP4613	KRFPC4613	<chem>OC(=O)C1(CC2CC3CC(C2)C1)C3</chem>
KRFP4614	KRFPC4614	<chem>OC(=O)C1C(C=O)C2c3ccccc3C1c4ccccc24</chem>
KRFP4615	KRFPC4615	<chem>OC(=O)C1C2CCCCC12</chem>
KRFP4616	KRFPC4616	<chem>OC(=O)c1cc(cc(c1)[N+](=O)[O-])[N+](=O)[O-]</chem>
KRFP4617	KRFPC4617	<chem>OC(=O)c1cc(ccc1C=O)[N+](=O)[O-]</chem>
KRFP4618	KRFPC4618	<chem>OC(=O)C1CC1c2ccccc2</chem>
KRFP4619	KRFPC4619	<chem>OC(=O)C1CC2c3ccccc3C1c4ccccc24</chem>
KRFP4620	KRFPC4620	<chem>OC(=O)C1CC2CC1C=C2</chem>
KRFP4621	KRFPC4621	<chem>OC(=O)c1cc2ccccc2[nH]1</chem>
KRFP4622	KRFPC4622	<chem>OC(=O)c1ccc(C=O)c(C=O)c1</chem>
KRFP4623	KRFPC4623	<chem>OC(=O)c1ccc(C=O)cc1</chem>
KRFP4624	KRFPC4624	<chem>OC(=O)c1ccc(cc1)[N+](=O)[O-]</chem>
KRFP4625	KRFPC4625	<chem>OC(=O)c1ccc(cc1)C(=O)O</chem>
KRFP4626	KRFPC4626	<chem>OC(=O)c1ccc(cc1)c2ccccc2</chem>
KRFP4627	KRFPC4627	<chem>OC(=O)c1ccc(cc1)S(=O)=O</chem>
KRFP4628	KRFPC4628	<chem>OC(=O)c1ccc(Cl)cc1</chem>
KRFP4629	KRFPC4629	<chem>OC(=O)c1ccc(Cl)cc1Cl</chem>
KRFP4630	KRFPC4630	<chem>OC(=O)c1ccc(NC(=S)NCC(Cl)(Cl)Cl)cc1</chem>
KRFP4631	KRFPC4631	<chem>OC(=O)c1ccc(NC(=S)SCC=O)cc1</chem>

Name	Count name	Pattern
KRFP4632	KRFPC4632	<chem>OC(=O)c1ccc(NC=O)cc1</chem>
KRFP4633	KRFPC4633	<chem>OC(=O)c1ccc(O)cc1</chem>
KRFP4634	KRFPC4634	<chem>OC(=O)c1ccc(O)cc1C(=O)O</chem>
KRFP4635	KRFPC4635	<chem>OC(=O)C1CCC=CC1</chem>
KRFP4636	KRFPC4636	<chem>OC(=O)c1ccc2C(=O)N(C(=O)c2c1)c3ccccc3</chem>
KRFP4637	KRFPC4637	<chem>OC(=O)c1cccc([N+](=O)[O-])c1C=O</chem>
KRFP4638	KRFPC4638	<chem>OC(=O)c1cccc(Br)c1</chem>
KRFP4639	KRFPC4639	<chem>OC(=O)c1cccc(c1)[N+](=O)[O-]</chem>
KRFP4640	KRFPC4640	<chem>OC(=O)c1cccc(c1)C(=O)O</chem>
KRFP4641	KRFPC4641	<chem>OC(=O)c1cccc(NC(=S)NCC(Cl)(Cl)Cl)c1</chem>
KRFP4642	KRFPC4642	<chem>OC(=O)c1cccc(NC=O)c1</chem>
KRFP4643	KRFPC4643	<chem>OC(=O)c1cccc(NS(=O)=O)c1</chem>
KRFP4644	KRFPC4644	<chem>OC(=O)c1cccc2ccccc12</chem>
KRFP4645	KRFPC4645	<chem>OC(=O)c1ccccc1</chem>
KRFP4646	KRFPC4646	<chem>OC(=O)c1ccccc1C(=O)O</chem>
KRFP4647	KRFPC4647	<chem>OC(=O)c1ccccc1C=O</chem>
KRFP4648	KRFPC4648	<chem>OC(=O)c1ccccc1NC(=S)NCC(Cl)(Cl)Cl</chem>
KRFP4649	KRFPC4649	<chem>OC(=O)c1ccccc1NC=O</chem>
KRFP4650	KRFPC4650	<chem>OC(=O)c1ccccc1O</chem>
KRFP4651	KRFPC4651	<chem>OC(=O)C1CCCN1</chem>
KRFP4652	KRFPC4652	<chem>OC(=O)c1ccco1</chem>
KRFP4653	KRFPC4653	<chem>OC(=O)c1cccs1</chem>
KRFP4654	KRFPC4654	<chem>OC(=O)c1cnccn1</chem>
KRFP4655	KRFPC4655	<chem>OC(=O)c1csc2CCCCc12</chem>
KRFP4656	KRFPC4656	<chem>OC(=O)c1nccnc1C=O</chem>
KRFP4657	KRFPC4657	<chem>OC(=O)CC(=O)O</chem>
KRFP4658	KRFPC4658	<chem>OC(=O)CC1(CC2CC3CC(C2)C1)C3</chem>
KRFP4659	KRFPC4659	<chem>OC(=O)Cc1ccccc1</chem>
KRFP4660	KRFPC4660	<chem>OC(=O)CCC(=O)NNC=O</chem>
KRFP4661	KRFPC4661	<chem>OC(=O)CCC(=O)O</chem>
KRFP4662	KRFPC4662	<chem>OC(=O)CCC=NNC=O</chem>
KRFP4663	KRFPC4663	<chem>OC(=O)CCC=O</chem>
KRFP4664	KRFPC4664	<chem>OC(=O)CCc1c[nH]c2ccccc12</chem>
KRFP4665	KRFPC4665	<chem>OC(=O)CCc1ccccc1</chem>
KRFP4666	KRFPC4666	<chem>OC(=O)CCCC(=O)O</chem>
KRFP4667	KRFPC4667	<chem>OC(=O)CCCC=O</chem>
KRFP4668	KRFPC4668	<chem>OC(=O)CCCCC=O</chem>
KRFP4669	KRFPC4669	<chem>OC(=O)CCCCCNC=O</chem>
KRFP4670	KRFPC4670	<chem>OC(=O)CCCCCNS(=O)=O</chem>
KRFP4671	KRFPC4671	<chem>OC(=O)CCCNC=O</chem>
KRFP4672	KRFPC4672	<chem>OC(=O)CCCNS(=O)=O</chem>
KRFP4673	KRFPC4673	<chem>OC(=O)CCNC(=S)SCC=O</chem>
KRFP4674	KRFPC4674	<chem>OC(=O)CCNC=O</chem>
KRFP4675	KRFPC4675	<chem>OC(=O)CCNS(=O)=O</chem>
KRFP4676	KRFPC4676	<chem>OC(=O)CCS(=O)=O</chem>
KRFP4677	KRFPC4677	<chem>OC(=O)CNC(=S)SCC=O</chem>
KRFP4678	KRFPC4678	<chem>OC(=O)CNC=O</chem>
KRFP4679	KRFPC4679	<chem>OC(=O)CNCC(=O)O</chem>
KRFP4680	KRFPC4680	<chem>OC(=O)CNS(=O)=O</chem>
KRFP4681	KRFPC4681	<chem>OC(=O)CS</chem>
KRFP4682	KRFPC4682	<chem>OC(=O)CS(=O)=O</chem>
KRFP4683	KRFPC4683	<chem>OC(=O)CSC(CC=O)C=O</chem>
KRFP4684	KRFPC4684	<chem>OC(=O)NC(=O)CCBr</chem>
KRFP4685	KRFPC4685	<chem>OC(C(F)(F)F)C(F)(F)F</chem>

Name	Count name	Pattern
KRFP4686	KRFPC4686	<chem>OC(C=O)(c1ccc(Br)cc1)c2ccc(Br)cc2</chem>
KRFP4687	KRFPC4687	<chem>OC(C=O)(c1ccccc1)C(F)(F)F</chem>
KRFP4688	KRFPC4688	<chem>OC(C=O)(c1ccccc1)c2ccccc2</chem>
KRFP4689	KRFPC4689	<chem>OC(CC=C)CC=C</chem>
KRFP4690	KRFPC4690	<chem>OC(F)(F)C(F)Cl</chem>
KRFP4691	KRFPC4691	<chem>OC(F)(F)C(F)F</chem>
KRFP4692	KRFPC4692	<chem>OC(F)F</chem>
KRFP4693	KRFPC4693	<chem>OC(NC=O)C(Br)(Br)Br</chem>
KRFP4694	KRFPC4694	<chem>OC(NC=O)C(Cl)(Cl)Cl</chem>
KRFP4695	KRFPC4695	<chem>OC=O</chem>
KRFP4696	KRFPC4696	<chem>OC1(CC2CC3CC(C2)C1)C3</chem>
KRFP4697	KRFPC4697	<chem>OC1C(=O)Nc2ccccc12</chem>
KRFP4698	KRFPC4698	<chem>Oc1c(Br)cccc1Br</chem>
KRFP4699	KRFPC4699	<chem>Oc1c(C=O)c(=O)oc2ccccc12</chem>
KRFP4700	KRFPC4700	<chem>Oc1c(CC=C)cccc1C=NNC=O</chem>
KRFP4701	KRFPC4701	<chem>Oc1c(Cl)cc(Cl)cc1C=N</chem>
KRFP4702	KRFPC4702	<chem>Oc1c(F)c(F)c(O)c(F)c1F</chem>
KRFP4703	KRFPC4703	<chem>Oc1c(F)c(F)cc(F)c1F</chem>
KRFP4704	KRFPC4704	<chem>Oc1cc(=O)[nH]cn1</chem>
KRFP4705	KRFPC4705	<chem>Oc1cc(=O)oc2ccccc12</chem>
KRFP4706	KRFPC4706	<chem>Oc1cc(=O)sc2ccccc12</chem>
KRFP4707	KRFPC4707	<chem>Oc1cc(cc2ccccc12)S(=O)(=O)O</chem>
KRFP4708	KRFPC4708	<chem>Oc1cc(O)cc(O)c1</chem>
KRFP4709	KRFPC4709	<chem>Oc1ccc(Br)cc1</chem>
KRFP4710	KRFPC4710	<chem>Oc1ccc(Br)cc1Br</chem>
KRFP4711	KRFPC4711	<chem>Oc1ccc(Br)cc1C=N</chem>
KRFP4712	KRFPC4712	<chem>Oc1ccc(C=N)c(O)c1</chem>
KRFP4713	KRFPC4713	<chem>Oc1ccc(C=N)cc1</chem>
KRFP4714	KRFPC4714	<chem>Oc1ccc(C=N)cc1O</chem>
KRFP4715	KRFPC4715	<chem>Oc1ccc(C=NNC=O)c(O)c1</chem>
KRFP4716	KRFPC4716	<chem>Oc1ccc(C=NNC=O)cc1</chem>
KRFP4717	KRFPC4717	<chem>Oc1ccc(C=O)cc1</chem>
KRFP4718	KRFPC4718	<chem>Oc1ccc(C=O)cc1O</chem>
KRFP4719	KRFPC4719	<chem>Oc1ccc(cc1)[N+](=O)[O-]</chem>
KRFP4720	KRFPC4720	<chem>Oc1ccc(cc1)C(=O)c2ccccc2</chem>
KRFP4721	KRFPC4721	<chem>Oc1ccc(cc1)C(=O)NN=Cc2ccccc2</chem>
KRFP4722	KRFPC4722	<chem>Oc1ccc(cc1)C(c2ccccc2)(c3ccccc3)c4ccc(O)cc4</chem>
KRFP4723	KRFPC4723	<chem>Oc1ccc(cc1)C(O)(c2ccccc2)c3ccccc3</chem>
KRFP4724	KRFPC4724	<chem>Oc1ccc(cc1)S(=O)(=O)c2ccc(O)cc2</chem>
KRFP4725	KRFPC4725	<chem>Oc1ccc(cc1)S(=O)=O</chem>
KRFP4726	KRFPC4726	<chem>Oc1ccc(cc1C=N)[N+](=O)[O-]</chem>
KRFP4727	KRFPC4727	<chem>Oc1ccc(cc1C=NNC=O)[N+](=O)[O-]</chem>
KRFP4728	KRFPC4728	<chem>Oc1ccc(CCC=O)cc1</chem>
KRFP4729	KRFPC4729	<chem>Oc1ccc(Cl)cc1</chem>
KRFP4730	KRFPC4730	<chem>Oc1ccc(Cl)cc1C=N</chem>
KRFP4731	KRFPC4731	<chem>Oc1ccc(Cl)cc1C=NNC=O</chem>
KRFP4732	KRFPC4732	<chem>Oc1ccc(Cl)cc1C=O</chem>
KRFP4733	KRFPC4733	<chem>Oc1ccc(Cl)cc1Cl</chem>
KRFP4734	KRFPC4734	<chem>Oc1ccc(F)cc1</chem>
KRFP4735	KRFPC4735	<chem>Oc1ccc(NC=O)cc1</chem>
KRFP4736	KRFPC4736	<chem>Oc1ccc(O)cc1</chem>
KRFP4737	KRFPC4737	<chem>Oc1ccc2[nH]c3CCCCc3c2c1</chem>
KRFP4738	KRFPC4738	<chem>Oc1ccc2c(=O)ccoc2c1</chem>
KRFP4739	KRFPC4739	<chem>Oc1ccc2C(=O)OC(=O)c2c1</chem>

Name	Count name	Pattern
KRFP4740	KRFPC4740	<chem>Oc1ccc2ccccc2c1</chem>
KRFP4741	KRFPC4741	<chem>Oc1ccc2ccccc2c1C=N</chem>
KRFP4742	KRFPC4742	<chem>Oc1ccc2ccccc2c1C=Nc3ccccc3</chem>
KRFP4743	KRFPC4743	<chem>Oc1ccc2ccccc2c1C=NNC=O</chem>
KRFP4744	KRFPC4744	<chem>Oc1ccc2ccccc2c1Cc3c(O)ccc4ccccc34</chem>
KRFP4745	KRFPC4745	<chem>Oc1ccc2ccccc2c1Cc3ccccc3</chem>
KRFP4746	KRFPC4746	<chem>Oc1cccc(C=N)c1</chem>
KRFP4747	KRFPC4747	<chem>Oc1cccc(C=O)c1</chem>
KRFP4748	KRFPC4748	<chem>Oc1cccc(c1)[N+](=O)[O-]</chem>
KRFP4749	KRFPC4749	<chem>Oc1cccc(CC=O)c1</chem>
KRFP4750	KRFPC4750	<chem>Oc1cccc(NC(=S)NCC(Cl)(Cl)Cl)c1</chem>
KRFP4751	KRFPC4751	<chem>Oc1cccc(NC=O)c1</chem>
KRFP4752	KRFPC4752	<chem>Oc1cccc(O)c1</chem>
KRFP4753	KRFPC4753	<chem>Oc1cccc(O)c1O</chem>
KRFP4754	KRFPC4754	<chem>OC1CCCC1</chem>
KRFP4755	KRFPC4755	<chem>Oc1cccc2ccccc12</chem>
KRFP4756	KRFPC4756	<chem>Oc1cccc2ccncc12</chem>
KRFP4757	KRFPC4757	<chem>OC1CCCCC1</chem>
KRFP4758	KRFPC4758	<chem>Oc1cccc1[N+](=O)[O-]</chem>
KRFP4759	KRFPC4759	<chem>Oc1cccc1Br</chem>
KRFP4760	KRFPC4760	<chem>Oc1cccc1C=N</chem>
KRFP4761	KRFPC4761	<chem>Oc1cccc1C=Nc2ccccc2</chem>
KRFP4762	KRFPC4762	<chem>Oc1cccc1C=NNC=O</chem>
KRFP4763	KRFPC4763	<chem>Oc1cccc1C=O</chem>
KRFP4764	KRFPC4764	<chem>Oc1cccc1Cc2ccccc2</chem>
KRFP4765	KRFPC4765	<chem>Oc1cccc1Cl</chem>
KRFP4766	KRFPC4766	<chem>Oc1cccc1F</chem>
KRFP4767	KRFPC4767	<chem>Oc1cccc1I</chem>
KRFP4768	KRFPC4768	<chem>Oc1cccc1NC(=S)NCC(Cl)(Cl)Cl</chem>
KRFP4769	KRFPC4769	<chem>Oc1cccc1NC=O</chem>
KRFP4770	KRFPC4770	<chem>Oc1cccc1O</chem>
KRFP4771	KRFPC4771	<chem>Oc1cccc1S(=O)(=O)O</chem>
KRFP4772	KRFPC4772	<chem>Oc1cccncc1</chem>
KRFP4773	KRFPC4773	<chem>OC1CCS(=O)(=O)C1</chem>
KRFP4774	KRFPC4774	<chem>OCC#C</chem>
KRFP4775	KRFPC4775	<chem>OCC(=O)c1ccc(Br)cc1</chem>
KRFP4776	KRFPC4776	<chem>OCC(=O)c1ccc(cc1)[N+](=O)[O-]</chem>
KRFP4777	KRFPC4777	<chem>OCC(=O)c1ccc(Cl)cc1</chem>
KRFP4778	KRFPC4778	<chem>OCC(=O)c1ccccc1</chem>
KRFP4779	KRFPC4779	<chem>OCC(=O)NC(=O)O</chem>
KRFP4780	KRFPC4780	<chem>OCC(=O)NN=C</chem>
KRFP4781	KRFPC4781	<chem>OCC(=O)NN=C1C(=O)Nc2ccc(cc12)[N+](=O)[O-]</chem>
KRFP4782	KRFPC4782	<chem>OCC(=O)NN=C1C(=O)Nc2ccccc12</chem>
KRFP4783	KRFPC4783	<chem>OCC(=O)NN=CC=C</chem>
KRFP4784	KRFPC4784	<chem>OCC(=O)NN=CC=Cc1cccc(c1)[N+](=O)[O-]</chem>
KRFP4785	KRFPC4785	<chem>OCC(=O)NN=Cc1c(Cl)ccc1Cl</chem>
KRFP4786	KRFPC4786	<chem>OCC(=O)NN=Cc1c(O)ccc2ccccc12</chem>
KRFP4787	KRFPC4787	<chem>OCC(=O)NN=Cc1cc(ccc1O)[N+](=O)[O-]</chem>
KRFP4788	KRFPC4788	<chem>OCC(=O)NN=Cc1cc(I)ccc1O</chem>
KRFP4789	KRFPC4789	<chem>OCC(=O)NN=Cc1cc(N=Nc2ccccc2)ccc1O</chem>
KRFP4790	KRFPC4790	<chem>OCC(=O)NN=Cc1cc2ccccc2nc1Cl</chem>
KRFP4791	KRFPC4791	<chem>OCC(=O)NN=Cc1cc2OCOc2cc1[N+](=O)[O-]</chem>
KRFP4792	KRFPC4792	<chem>OCC(=O)NN=Cc1ccc(O)c(c1)[N+](=O)[O-]</chem>
KRFP4793	KRFPC4793	<chem>OCC(=O)NN=Cc1ccc(O)cc1</chem>

Name	Count name	Pattern
KRFP4794	KRFPC4794	<chem>OCC(=O)NN=Cc1ccc(s1)[N+](=O)[O-]</chem>
KRFP4795	KRFPC4795	<chem>OCC(=O)NN=Cc1cccc(c1)[N+](=O)[O-]</chem>
KRFP4796	KRFPC4796	<chem>OCC(=O)NN=Cc1cccc(O)c1</chem>
KRFP4797	KRFPC4797	<chem>OCC(=O)NN=Cc1cccc2ccccc12</chem>
KRFP4798	KRFPC4798	<chem>OCC(=O)NN=Cc1ccccc1</chem>
KRFP4799	KRFPC4799	<chem>OCC(=O)NN=Cc1ccccc1[N+](=O)[O-]</chem>
KRFP4800	KRFPC4800	<chem>OCC(=O)NN=Cc1ccccc1Cl</chem>
KRFP4801	KRFPC4801	<chem>OCC(=O)NN=Cc1ccccc1O</chem>
KRFP4802	KRFPC4802	<chem>OCC(=O)NNC=O</chem>
KRFP4803	KRFPC4803	<chem>OCC(=O)O</chem>
KRFP4804	KRFPC4804	<chem>OCC(=O)OCC=O</chem>
KRFP4805	KRFPC4805	<chem>OCC(c1ccccc1)c2ccccc2</chem>
KRFP4806	KRFPC4806	<chem>OCC(Cl)(Cl)Cl</chem>
KRFP4807	KRFPC4807	<chem>OCC(CO)(CO)NC=O</chem>
KRFP4808	KRFPC4808	<chem>OCC(F)(F)F</chem>
KRFP4809	KRFPC4809	<chem>OCC(O)CNS(=O)(=O)O</chem>
KRFP4810	KRFPC4810	<chem>OCC=C</chem>
KRFP4811	KRFPC4811	<chem>OCC=O</chem>
KRFP4812	KRFPC4812	<chem>OCc1cccc(Br)c1</chem>
KRFP4813	KRFPC4813	<chem>OCc1ccccc1</chem>
KRFP4814	KRFPC4814	<chem>OCc1ccccc1C(=O)Cc2ccccc2</chem>
KRFP4815	KRFPC4815	<chem>OCc1ccccc1C=O</chem>
KRFP4816	KRFPC4816	<chem>OCc1nc2ccccc2[nH]1</chem>
KRFP4817	KRFPC4817	<chem>OCC1OCC(O)C(O)C1O</chem>
KRFP4818	KRFPC4818	<chem>OCC1OCC(O)C1O</chem>
KRFP4819	KRFPC4819	<chem>OCCC(O)c1ccc(cc1)[N+](=O)[O-]</chem>
KRFP4820	KRFPC4820	<chem>OCCc1ccccc1</chem>
KRFP4821	KRFPC4821	<chem>OCCCC=O</chem>
KRFP4822	KRFPC4822	<chem>OCCCl</chem>
KRFP4823	KRFPC4823	<chem>OCCCNc=O</chem>
KRFP4824	KRFPC4824	<chem>OCCF</chem>
KRFP4825	KRFPC4825	<chem>OCCN(CCO)S(=O)=O</chem>
KRFP4826	KRFPC4826	<chem>OCCNc=O</chem>
KRFP4827	KRFPC4827	<chem>OCCNCCO</chem>
KRFP4828	KRFPC4828	<chem>OCCNS(=O)=O</chem>
KRFP4829	KRFPC4829	<chem>OCCO</chem>
KRFP4830	KRFPC4830	<chem>OCCOC=O</chem>
KRFP4831	KRFPC4831	<chem>OCCS</chem>
KRFP4832	KRFPC4832	<chem>OCCS(=O)=O</chem>
KRFP4833	KRFPC4833	<chem>ON(=O)c1ccccc1</chem>
KRFP4834	KRFPC4834	<chem>ON=C</chem>
KRFP4835	KRFPC4835	<chem>ONC=O</chem>
KRFP4836	KRFPC4836	<chem>OP(=O)(O)O</chem>
KRFP4837	KRFPC4837	<chem>OS(=O)(=O)c1ccc(NN=C(C=O)C=O)cc1</chem>
KRFP4838	KRFPC4838	<chem>OS(=O)(=O)c1ccc(NN=Cc2ccccc2)cc1</chem>
KRFP4839	KRFPC4839	<chem>OS(=O)(=O)c1ccccc1</chem>
KRFP4840	KRFPC4840	<chem>OS(=O)(=O)CCCS</chem>
KRFP4841	KRFPC4841	<chem>OS(=O)(=O)CCS</chem>
KRFP4842	KRFPC4842	<chem>OS(=O)=O</chem>
KRFP4843	KRFPC4843	<chem>S</chem>
KRFP4844	KRFPC4844	<chem>S=C(Nc1ccccc1)Nc2ccccc2</chem>
KRFP4845	KRFPC4845	<chem>S=c1[nH]c2ccccc2[nH]1</chem>
KRFP4846	KRFPC4846	<chem>S=c1[nH]c2ccccc2o1</chem>
KRFP4847	KRFPC4847	<chem>S=c1[nH]c2ccccc2s1</chem>

Name	Count name	Pattern
KRFP4848	KRFPC4848	<chem>S=C1NC=CC(N1)c2ccccc2</chem>
KRFP4849	KRFPC4849	<chem>SC(=N)NN=C</chem>
KRFP4850	KRFPC4850	<chem>SC(=O)c1ccccc1</chem>
KRFP4851	KRFPC4851	<chem>SC(NC=O)C(Cl)(Cl)Cl</chem>
KRFP4852	KRFPC4852	<chem>SC=O</chem>
KRFP4853	KRFPC4853	<chem>S(c1ccccc1)</chem>
KRFP4854	KRFPC4854	<chem>S(c1nc2ccccc2s1)</chem>
KRFP4855	KRFPC4855	<chem>SCC(=O)NN=C</chem>
KRFP4856	KRFPC4856	<chem>SCC=O</chem>
KRFP4857	KRFPC4857	<chem>SCc1ccccc1</chem>
KRFP4858	KRFPC4858	<chem>SCCC=O</chem>
KRFP4859	KRFPC4859	<chem>SCCS</chem>
KRFP4860	KRFPC4860	<chem>SCCS(=O)=O</chem>

6.4 Substructure

The following table is adapted from PaDEL-Descriptor v2.21 documentation.

Name	Count name	Description	Pattern
SubFP1	SubFPC1	Primary carbon	<chem>[CX4H3][#6]</chem>
SubFP2	SubFPC2	Secondary carbon	<chem>[CX4H2]([#6])[#6]</chem>
SubFP3	SubFPC3	Tertiary carbon	<chem>[CX4H1]([#6])([#6])[#6]</chem>
SubFP4	SubFPC4	Quaternary carbon	<chem>[CX4]([#6])([#6])([#6])[#6]</chem>
SubFP5	SubFPC5	Alkene	<chem>[CX3;\$([H2]),\$([H1][#6]),\$(C([#6][#6])=[CX3;\$([H2]),\$([H1][#6]),\$(C([#6])[#6])]</chem>
SubFP6	SubFPC6	Alkyne	<chem>[CX2]#[CX2]</chem>
SubFP7	SubFPC7	Allene	<chem>[CX3]=[CX2]=[CX3]</chem>
SubFP8	SubFPC8	Alkylchloride	<chem>[ClX1][CX4]</chem>
SubFP9	SubFPC9	Alkylfluoride	<chem>[FX1][CX4]</chem>
SubFP10	SubFPC10	Alkylbromide	<chem>[BrX1][CX4]</chem>
SubFP11	SubFPC11	Alkyliodide	<chem>[IX1][CX4]</chem>
SubFP12	SubFPC12	Alcohol	<chem>[OX2H][CX4;!\$(C([OX2H])[O,S,#7,#15])]</chem>
SubFP13	SubFPC13	Primary alcohol	<chem>[OX2H][CX4H2;!\$(C([OX2H])[O,S,#7,#15])]</chem>
SubFP14	SubFPC14	Secondary alcohol	<chem>[OX2H][CX4H;!\$(C([OX2H])[O,S,#7,#15])]</chem>
SubFP15	SubFPC15	Tertiary alcohol	<chem>[OX2H][CX4D4;!\$(C([OX2H])[O,S,#7,#15])]</chem>
SubFP16	SubFPC16	Dialkylether	<chem>[OX2]([CX4;!\$(C([OX2])[O,S,#7,#15,F,Cl,Br,I])])[CX4;!\$(C([OX2])[O,S,#7,#15])]</chem>
SubFP17	SubFPC17	Dialkylthioether	<chem>[SX2]([CX4;!\$(C([OX2])[O,S,#7,#15,F,Cl,Br,I])])[CX4;!\$(C([OX2])[O,S,#7,#15])]</chem>
SubFP18	SubFPC18	Alkylarylether	<chem>[OX2](c)[CX4;!\$(C([OX2])[O,S,#7,#15,F,Cl,Br,I])]</chem>
SubFP19	SubFPC19	Diarylether	<chem>[c][OX2][c]</chem>

Name	Count name	Description	Pattern
SubFP20	SubFPC20	Alkylarylthioether	[SX2](c)[CX4;!\$(C([OX2])[O,S,#7,#15,F,Cl,Br,I])]
SubFP21	SubFPC21	Diarylthioether	[c][SX2][c]
SubFP22	SubFPC22	Oxonium	[O+;!\$([O]~[!#6]);!\$([S]*~[#7,#8,#15,#16])]
SubFP23	SubFPC23	Amine	[NX3+0,NX4+;!\$([N]~[!#6]);!\$([N]*~[#7,#8,#15,#16])]
SubFP24	SubFPC24	Primary aliph amine	[NX3H2+0,NX4H3+;!\$([N][!C]);!\$([N]*~[#7,#8,#15,#16])]
SubFP25	SubFPC25	Secondary aliph amine	[NX3H1+0,NX4H2+;!\$([N][!C]);!\$([N]*~[#7,#8,#15,#16])]
SubFP26	SubFPC26	Tertiary aliph amine	[NX3H0+0,NX4H1+;!\$([N][!C]);!\$([N]*~[#7,#8,#15,#16])]
SubFP27	SubFPC27	Quaternary aliph ammonium	[NX4H0+;!\$([N][!C]);!\$([N]*~[#7,#8,#15,#16])]
SubFP28	SubFPC28	Primary arom amine	[NX3H2+0,NX4H3+]c
SubFP29	SubFPC29	Secondary arom amine	[NX3H1+0,NX4H2+;!\$([N][!c]);!\$([N]*~[#7,#8,#15,#16])]
SubFP30	SubFPC30	Tertiary arom amine	[NX3H0+0,NX4H1+;!\$([N][!c]);!\$([N]*~[#7,#8,#15,#16])]
SubFP31	SubFPC31	Quaternary arom ammonium	[NX4H0+;!\$([N][!c]);!\$([N]*~[#7,#8,#15,#16])]
SubFP32	SubFPC32	Secondary mixed amine	[NX3H1+0,NX4H2+;\$([N]([c])[C]);!\$([N]*~[#7,#8,#15,#16])]
SubFP33	SubFPC33	Tertiary mixed amine	[NX3H0+0,NX4H1+;\$([N]([c])([C])[#6]);!\$([N]*~[#7,#8,#15,#16])]
SubFP34	SubFPC34	Quaternary mixed ammonium	[NX4H0+;\$([N]([c])([C])[#6])[#6];!\$([N]*~[#7,#8,#15,#16])]
SubFP35	SubFPC35	Ammonium	[N+;!\$([N]~[!#6]);!\$(N=*);!\$([N]*~[#7,#8,#15,#16])]
SubFP36	SubFPC36	Alkylthiol	[SX2H][CX4;!\$(C([SX2H])~[O,S,#7,#15])]
SubFP37	SubFPC37	Dialkylthioether	[SX2]([CX4;!\$(C([SX2])[O,S,#7,#15,F,Cl,Br,I])])[CX4;!\$(C([SX2])[O,S,#7,#15])]
SubFP38	SubFPC38	Alkylarylthioether	[SX2](c)[CX4;!\$(C([SX2])[O,S,#7,#15])]
SubFP39	SubFPC39	Disulfide	[SX2D2][SX2D2]
SubFP40	SubFPC40	1,2-Aminoalcohol	[OX2H][CX4;!\$(C([OX2H])[O,S,#7,#15,F,Cl,Br,I])][CX4;!\$(C([N])[O,S,#7,#15])] [NX3;!\$(NC=[O,S,N])]
SubFP41	SubFPC41	1,2-Diol	[OX2H][CX4;!\$(C([OX2H])[O,S,#7,#15])] [CX4;!\$(C([OX2H])[O,S,#7,#15])][OX2H]
SubFP42	SubFPC42	1,1-Diol	[OX2H][CX4;!\$(C([OX2H])([OX2H])[O,S,#7,#15])][OX2H]

Name	Count name	Description	Pattern
SubFP43	SubFPC43	Hydroperoxide	[OX2H][OX2]
SubFP44	SubFPC44	Peroxo	[OX2D2][OX2D2]
SubFP45	SubFPC45	Organolithium compounds	[LiX1][#6,#14]
SubFP46	SubFPC46	Organomagnesium compounds	[MgX2][#6,#14]
SubFP47	SubFPC47	Organometallic compounds	[!#1;!#5;!#6;!#7;!#8;!#9;!#14; !#15;!#16;!#17;!#33;!#34;!#35; !#52;!#53;!#85]~[#6;-]
SubFP48	SubFPC48	Aldehyde	[\$([CX3H][#6]),\$([CX3H2])]=[OX1]
SubFP49	SubFPC49	Ketone	[#6][CX3](=[OX1])[#6]
SubFP50	SubFPC50	Thioaldehyde	[\$([CX3H][#6]),\$([CX3H2])]=[SX1]
SubFP51	SubFPC51	Thioketone	[#6][CX3](=[SX1])[#6]
SubFP52	SubFPC52	Imine	[NX2;\$([N][#6]),\$([NH]);!\$([N] [CX3]=[#7,#8,#15,#16])]=[CX3;\$([CH2]), \$([CH][#6]),\$([C]([#6])[#6])]
SubFP53	SubFPC53	Immonium	[NX3+;!\$([N][!#6]);!\$([N][CX3]=[#7, #8,#15,#16])]
SubFP54	SubFPC54	Oxime	[NX2](=[CX3;\$([CH2]),\$([CH][#6]), \$([C]([#6])[#6]))[OX2H]
SubFP55	SubFPC55	Oximether	[NX2](=[CX3;\$([CH2]),\$([CH][#6]), \$([C]([#6])[#6]))[OX2][#6;!\$(C=[#7,#8])]
SubFP56	SubFPC56	Acetal	[OX2]([#6;!\$(C=[O,S,N]))[CX4;!\$(C(O) (O)[!#6])][OX2][#6;!\$(C=[O,S,N])]
SubFP57	SubFPC57	Hemiacetal	[OX2H][CX4;!\$(C(O)(O)[!#6])][OX2] [#6;!\$(C=[O,S,N])]
SubFP58	SubFPC58	Aminal	[NX3v3;!\$(NC=[#7,#8,#15,#16])] ([#6])[CX4;!\$(C(N)(N)[!#6])][NX3v3; !\$(NC=[#7,#8,#15,#16])][#6]
SubFP59	SubFPC59	Hemiaminal	[NX3v3;!\$(NC=[#7,#8,#15,#16])] ([#6])[CX4;!\$(C(N)(N)[!#6])][OX2H]
SubFP60	SubFPC60	Thioacetal	[SX2]([#6;!\$(C=[O,S,N]))[CX4;!\$(C(S) (S)[!#6])][SX2][#6;!\$(C=[O,S,N])]
SubFP61	SubFPC61	Thiohemiacetal	[SX2]([#6;!\$(C=[O,S,N]))[CX4;!\$(C(S) (S)[!#6])][OX2H]
SubFP62	SubFPC62	Halogen acetal like	[NX3v3,SX2,OX2;!\$(C=[#7,#8,#15, #16])][CX4;!\$(C([N,S,O])([N,S,O])[!#6])] [FX1,CIX1,BrX1,IX1]
SubFP63	SubFPC63	Acetal like	[NX3v3,SX2,OX2;!\$(C=[#7,#8,#15, #16])][CX4;!\$(C([N,S,O])([N,S,O])[!#6])] [FX1,CIX1,BrX1,IX1,NX3v3,SX2,OX2; !\$(C=[#7,#8,#15,#16])]
SubFP64	SubFPC64	Halogenmethylen ester and similar	[NX3v3,SX2,OX2;\$(**=[#7,#8,#15, #16])][CX4;!\$(C([N,S,O])([N,S,O]) [!#6])][FX1,CIX1,BrX1,IX1]

Name	Count name	Description	Pattern
SubFP65	SubFPC65	NOS methylen ester andsimilar	[NX3v3,SX2,OX2;\$(**=[#7,#8,#15,#16]))[CX4;!\$(C([N,S,O])([N,S,O])([#6]))] [NX3v3,SX2,OX2;!\$(C=[#7,#8,#15,#16]))]
SubFP66	SubFPC66	Hetero methylen esterand similar	[NX3v3,SX2,OX2;\$(**=[#7,#8,#15,#16]))[CX4;!\$(C([N,S,O])([N,S,O])([#6]))] [FX1,CIX1,BrX1,IX1,NX3v3,SX2,OX2; !\$(C=[#7,#8,#15,#16]))]
SubFP67	SubFPC67	Cyanhydrine	[NX1]#[CX2][CX4;\$([CH2]),\$([CH] ([CX2])([#6]),\$(C([CX2])([#6])([#6]))][OX2H]
SubFP68	SubFPC68	Chloroalkene	[CIX1][CX3]=[CX3]
SubFP69	SubFPC69	Fluoroalkene	[FX1][CX3]=[CX3]
SubFP70	SubFPC70	Bromoalkene	[BrX1][CX3]=[CX3]
SubFP71	SubFPC71	Iodoalkene	[IX1][CX3]=[CX3]
SubFP72	SubFPC72	Enol	[OX2H][CX3;\$([H1]),\$(C[#6])]=[CX3]
SubFP73	SubFPC73	Endiol	[OX2H][CX3;\$([H1]),\$(C[#6])]=[CX3; \$([H1]),\$(C[#6]))][OX2H]
SubFP74	SubFPC74	Enolether	[OX2]([#6;!\$(C=[N,O,S]))][CX3;\$([H0] [#6]),\$([H1]))]=[CX3]
SubFP75	SubFPC75	Enolester	[OX2]([CX3]=[OX1])([#6X3;\$([#6][#6]), \$([H1]))=[#6X3;\$([C[OX2H]])]
SubFP76	SubFPC76	Enamine	[NX3;\$([NH2][CX3]),\$([NH1])([CX3]) [#6]),\$([N])([CX3])([#6])([#6]); !\$(N)*=[#7,#8,#15,#16]))[CX3; \$([CH]),\$([C][#6])]=[CX3]
SubFP77	SubFPC77	Thioenol	[SX2H][CX3;\$([H1]),\$(C[#6])]=[CX3]
SubFP78	SubFPC78	Thioenolether	[SX2]([#6;!\$(C=[N,O,S]))][CX3; \$(C[#6]),\$([CH]))]=[CX3]
SubFP79	SubFPC79	Acylchloride	[CX3;\$([R0][#6]),\$([H1R0]))(=[OX1]) [CIX1]
SubFP80	SubFPC80	Acylfluoride	[CX3;\$([R0][#6]),\$([H1R0]))(=[OX1]) [FX1]
SubFP81	SubFPC81	Acylbromide	[CX3;\$([R0][#6]),\$([H1R0]))(=[OX1]) [BrX1]
SubFP82	SubFPC82	Acyl iodide	[CX3;\$([R0][#6]),\$([H1R0]))(=[OX1]) [IX1]
SubFP83	SubFPC83	Acylhalide	[CX3;\$([R0][#6]),\$([H1R0]))(=[OX1]) [FX1,CIX1,BrX1,IX1]
SubFP84	SubFPC84	Carboxylic acid	[CX3;\$([R0][#6]),\$([H1R0]))(=[OX1]) \$([OX2H]),\$([OX1-])]
SubFP85	SubFPC85	Carboxylic ester	[CX3;\$([R0][#6]),\$([H1R0]))(=[OX1]) [OX2][#6;!\$(C=[O,N,S])]
SubFP86	SubFPC86	Lactone	[#6][#6X3R])(=[OX1])([#8X2][#6;!\$(C= [O,N,S])]
SubFP87	SubFPC87	Carboxylic anhydride	[CX3;\$([H0][#6]),\$([H1]))(=[OX1]) [#8X2][CX3;\$([H0][#6]),\$([H1]))(=[OX1])]

Name	Count name	Description	Pattern
SubFP88	SubFPC88	Carboxylic acid derivative	<chem>[\$([#6X3H0][#6]),\$([#6X3H])](=[!#6])[!#6]</chem>
SubFP89	SubFPC89	Carbothioic acid	<chem>[CX3;!R;\$([C][#6]),\$([CH]);\$([C](=[OX1])[\$([SX2H]),\$([SX1-])]),\$([C](=[SX1])[\$([OX2H]),\$([OX1-])])]</chem>
SubFP90	SubFPC90	Carbothioic S ester	<chem>[CX3;\$([R0][#6]),\$([H1R0])(=[OX1])[SX2][#6;!\$(C=[O,N,S])]</chem>
SubFP91	SubFPC91	Carbothioic S lactone	<chem>[#6][#6X3R](=[OX1])[#16X2][#6;!\$(C=[O,N,S])]</chem>
SubFP92	SubFPC92	Carbothioic O ester	<chem>[CX3;\$([H0][#6]),\$([H1])(=[SX1])[OX2][#6;!\$(C=[O,N,S])]</chem>
SubFP93	SubFPC93	Carbothioic O lactone	<chem>[#6][#6X3R](=[SX1])[#8X2][#6;!\$(C=[O,N,S])]</chem>
SubFP94	SubFPC94	Carbothioic halide	<chem>[CX3;\$([H0][#6]),\$([H1])(=[SX1])[FX1,CIX1,BrX1,IX1]</chem>
SubFP95	SubFPC95	Carbodithioic acid	<chem>[CX3;!R;\$([C][#6]),\$([CH]);\$([C](=[SX1])[SX2H])]</chem>
SubFP96	SubFPC96	Carbodithioic ester	<chem>[CX3;!R;\$([C][#6]),\$([CH]);\$([C](=[SX1])[SX2][#6;!\$(C=[O,N,S])])]</chem>
SubFP97	SubFPC97	Carbodithiolactone	<chem>[#6][#6X3R](=[SX1])[#16X2][#6;!\$(C=[O,N,S])]</chem>
SubFP98	SubFPC98	Amide	<chem>[CX3;\$([R0][#6]),\$([H1R0])(=[OX1])[#7X3;\$([H2]),\$([H1][#6;!\$(C=[O,N,S])])],\$([#7]([#6;!\$(C=[O,N,S])])[#6;!\$(C=[O,N,S])])]</chem>
SubFP99	SubFPC99	Primary amide	<chem>[CX3;\$([R0][#6]),\$([H1R0])(=[OX1])[NX3H2]</chem>
SubFP100	SubFPC100	Secondary amide	<chem>[CX3;\$([R0][#6]),\$([H1R0])(=[OX1])[#7X3H1][#6;!\$(C=[O,N,S])]</chem>
SubFP101	SubFPC101	Tertiary amide	<chem>[CX3;\$([R0][#6]),\$([H1R0])(=[OX1])[#7X3H0]([#6;!\$(C=[O,N,S])])[#6;!\$(C=[O,N,S])]</chem>
SubFP102	SubFPC102	Lactam	<chem>[#6R][#6X3R](=[OX1])[#7X3;\$([H1][#6;!\$(C=[O,N,S])]),\$([H0]([#6;!\$(C=[O,N,S])])[#6;!\$(C=[O,N,S])])]</chem>
SubFP103	SubFPC103	Alkyl imide	<chem>[#6X3;\$([H0][#6]),\$([H1])(=[OX1])[#7X3H0]([#6])[#6X3;\$([H0][#6]),\$([H1])(=[OX1])]</chem>
SubFP104	SubFPC104	N hetero imide	<chem>[#6X3;\$([H0][#6]),\$([H1])(=[OX1])[#7X3H0]([!#6])[#6X3;\$([H0][#6]),\$([H1])(=[OX1])]</chem>
SubFP105	SubFPC105	Imide acidic	<chem>[#6X3;\$([H0][#6]),\$([H1])(=[OX1])[#7X3H1][#6X3;\$([H0][#6]),\$([H1])(=[OX1])]</chem>

Name	Count name	Description	Pattern
SubFP106	SubFPC106	Thioamide	$[\$(CX3;R)[\#6]),\$(CX3H;R)](=[SX1])$ $[\#7X3;\$(H2)],\$(H1)[\#6;!\$(C=[O,N,S])],$ $\$([\#7])([\#6;!\$(C=[O,N,S])])$ $[\#6;!\$(C=[O,N,S])])$
SubFP107	SubFPC107	Thiolactam	$[\#6R][\#6X3R](=[SX1])[\#7X3;\$(H1)$ $[\#6;!\$(C=[O,N,S])],\$(H0)([\#6;$ $!\$(C=[O,N,S])][\#6;!\$(C=[O,N,S])])$
SubFP108	SubFPC108	Oximester	$[\#6X3;\$(H0)[\#6]),\$(H1)](=[OX1])$ $[\#8X2][\#7X2]=,:[\#6X3;\$(H0)([\#6][\#6])$ $,\$(H1)[\#6]),\$(H2)]$
SubFP109	SubFPC109	Amidine	$[NX3;!\$(NC=[O,S])][CX3;\$(CH)],\$(C$ $[\#6])]=[NX2;!\$(NC=[O,S])]$
SubFP110	SubFPC110	Hydroxamic acid	$[CX3;\$(H0)[\#6]),\$(H1)](=[OX1])$ $[\#7X3;\$(H1)],\$(H0)[\#6;!\$(C=[O,N,S])])$ $[\$(OX2H)],\$(OX1-)]$
SubFP111	SubFPC111	Hydroxamic acid ester	$[CX3;\$(H0)[\#6]),\$(H1)](=[OX1])$ $[\#7X3;\$(H1)],\$(H0)[\#6;!\$(C=[O,N,S])])$ $[OX2][\#6;!\$(C=[O,N,S])]$
SubFP112	SubFPC112	Imidoacid	$[CX3R0;\$(H0)[\#6]),\$(H1)]$ $(=[NX2;\$(H1)],\$(H0)[\#6;!\$(C=[O,N,S])])$ $[\$(OX2H)],\$(OX1-)]$
SubFP113	SubFPC113	Imidoacid cyclic	$[\#6R][\#6X3R](=,:[\#7X2;\$(H1),$ $\$(H0)[\#6;!\$(C=[O,N,S])])][\$(OX2H),$ $\$(OX1-)]$
SubFP114	SubFPC114	Imidoester	$[CX3R0;\$(H0)[\#6]),\$(H1)](=[NX2;$ $\$(H1)],\$(H0)[\#6;!\$(C=[O,N,S])])][OX2]$ $[\#6;!\$(C=[O,N,S])]$
SubFP115	SubFPC115	Imidolactone	$[\#6R][\#6X3R](=,:[\#7X2;\$(H1),$ $\$(H0)[\#6;!\$(C=[O,N,S])])][OX2]$ $[\#6;!\$(C=[O,N,S])]$
SubFP116	SubFPC116	Imidothioacid	$[CX3R0;\$(H0)[\#6]),\$(H1)](=[NX2;$ $\$(H1)],\$(H0)[\#6;!\$(C=[O,N,S])])$ $[\$(SX2H)],\$(SX1-)]$
SubFP117	SubFPC117	Imidothioacid cyclic	$[\#6R][\#6X3R](=,:[\#7X2;\$(H1),$ $\$(H0)[\#6;!\$(C=[O,N,S])])$ $[\$(SX2H)],\$(SX1-)]$
SubFP118	SubFPC118	Imidothioester	$[CX3R0;\$(H0)[\#6]),\$(H1)](=[NX2;$ $\$(H1)],\$(H0)[\#6;!\$(C=[O,N,S])])][SX2]$ $[\#6;!\$(C=[O,N,S])]$
SubFP119	SubFPC119	Imidothiolactone	$[\#6R][\#6X3R](=,:[\#7X2;\$(H1),$ $\$(H0)[\#6;!\$(C=[O,N,S])])][SX2][\#6;$ $!\$(C=[O,N,S])]$
SubFP120	SubFPC120	Amidine	$[\#7X3v3;!\$(N([\#6X3]=[\#7X2])$ $C=[O,S])][CX3R0;\$(H1)],\$(H0)[\#6)]$ $=[NX2v3;!\$(N([\#6X3][\#7X3])C=[O,S])]$

Name	Count name	Description	Pattern
SubFP121	SubFPC121	Imidolactam	[#6][#6X3R;\$([H0])(=[NX2;!\$(N(=[#6X3][#7X3])C=[O,S]))[#7X3;!\$(N([#6X3]=[#7X2])C=[O,S])),\$([H0](-[NX3;!\$(N([#6X3]=[#7X2])C=[O,S]))=,:[#7X2;!\$(N(=[#6X3][#7X3])C=[O,S])))]
SubFP122	SubFPC122	Imidoylhalide	[CX3R0;\$([H0][#6]),\$([H1]))(=[NX2;\$([H1]),\$([H0][#6;!\$(C=[O,N,S])))]([FX1,ClX1,BrX1,IX1]
SubFP123	SubFPC123	Imidoylhalide cyclic	[#6R][#6X3R](=,:[#7X2;\$([H1]),\$([H0][#6;!\$(C=[O,N,S])))]([FX1,ClX1,BrX1,IX1]
SubFP124	SubFPC124	Amidrazone	[\$([#6X3][#6]),\$([#6X3H])](=[#7X2v3][#7X3v3][#7X3v3]),\$([#6X3][#6]),\$([#6X3H])([#7X3v3])=[#7X2v3][#7X3v3]]
SubFP125	SubFPC125	Alpha aminoacid	[NX3,NX4+;!\$([N]~[!#6]);!\$([N]*~[#7,#8,#15,#16])[C][CX3](=[OX1])[OX2H,OX1-]
SubFP126	SubFPC126	Alpha hydroxyacid	[OX2H][C][CX3](=[OX1])[OX2H,OX1-]
SubFP127	SubFPC127	Peptide middle	[NX3;\$([N][CX3](=[OX1])[C][NX3,NX4+))][C][CX3](=[OX1])[NX3;\$([N][C][CX3](=[OX1])[NX3,OX2,OX1-])]
SubFP128	SubFPC128	Peptide C term	[NX3;\$([N][CX3](=[OX1])[C][NX3,NX4+))][C][CX3](=[OX1])[OX2H,OX1-]
SubFP129	SubFPC129	Peptide N term	[NX3,NX4+;!\$([N]~[!#6]);!\$([N]*~[#7,#8,#15,#16])[C][CX3](=[OX1])[NX3;\$([N][C][CX3](=[OX1])[NX3,OX2,OX1-])]
SubFP130	SubFPC130	Carboxylic orthoester	[#6][OX2][CX4;\$([C][#6]),\$([CH])](=[OX2][#6])[OX2][#6]
SubFP131	SubFPC131	Ketene	[CX3]=[CX2]=[OX1]
SubFP132	SubFPC132	Ketenacetal	[#7X2,#8X3,#16X2;\$(*[#6,#14])][#6X3]([#7X2,#8X3,#16X2;\$(*[#6,#14]))=[#6X3]
SubFP133	SubFPC133	Nitrile	[NX1]#[CX2]
SubFP134	SubFPC134	Isonitrile	[CX1-]#[NX2+]
SubFP135	SubFPC135	Vinylogous carbonyl or carboxyl derivative	[#6X3](=[OX1])[#6X3]=,:[#6X3][#7,#8,#16,F,Cl,Br,I]
SubFP136	SubFPC136	Vinylogous acid	[#6X3](=[OX1])[#6X3]=,:[#6X3]([\$([OX2H]),\$([OX1-])]
SubFP137	SubFPC137	Vinylogous ester	[#6X3](=[OX1])[#6X3]=,:[#6X3][#6;!\$(C=[O,N,S])]

Name	Count name	Description	Pattern
SubFP138	SubFPC138	Vinylogous amide	[#6X3](=[OX1])[#6X3]=,:[#6X3] [#7X3;\$([H2]),\$([H1][#6;!\$(C=[O,N,S]))], \$([#7]([#6;!\$(C=[O,N,S])) [#6;!\$(C=[O,N,S]))])]
SubFP139	SubFPC139	Vinylogous halide	[#6X3](=[OX1])[#6X3]=,:[#6X3][FX1, ClX1,BrX1,Ix1]
SubFP140	SubFPC140	Carbonic acid dieester	[#6;!\$(C=[O,N,S]))[#8X2][#6X3] (=[OX1])[#8X2][#6;!\$(C=[O,N,S]))]
SubFP141	SubFPC141	Carbonic acid esterhalide	[#6;!\$(C=[O,N,S]))[OX2;!R][CX3] (=[OX1])[OX2][FX1,ClX1,BrX1,Ix1]
SubFP142	SubFPC142	Carbonic acid monoester	[#6;!\$(C=[O,N,S]))[OX2;!R][CX3] (=[OX1])\$([OX2H]),\$([OX1-])]
SubFP143	SubFPC143	Carbonic acid derivatives	[!#6][#6X3](=[!#6])[!#6]
SubFP144	SubFPC144	Thiocarbonic acid dieester	[#6;!\$(C=[O,N,S]))[#8X2][#6X3] (=[SX1])[#8X2][#6;!\$(C=[O,N,S]))]
SubFP145	SubFPC145	Thiocarbonic acid esterhalide	[#6;!\$(C=[O,N,S]))[OX2;!R][CX3] (=[SX1])[OX2][FX1,ClX1,BrX1,Ix1]
SubFP146	SubFPC146	Thiocarbonic acid monoester	[#6;!\$(C=[O,N,S]))[OX2;!R][CX3] (=[SX1])\$([OX2H]),\$([OX1-])]
SubFP147	SubFPC147	Urea	[#7X3;\$([#7][!#6]))[#6X3](=[OX1]) [#7X3;\$([#7][!#6]))]
SubFP148	SubFPC148	Thiourea	[#7X3;\$([#7][!#6]))[#6X3](=[SX1]) [#7X3;\$([#7][!#6]))]
SubFP149	SubFPC149	Isourea	[#7X2;\$([#7][!#6]))=,:[#6X3] ([#8X2&\$([#8][!#6]),OX1-])[#7X3;\$([#7][!#6]))]
SubFP150	SubFPC150	Isothiourea	[#7X2;\$([#7][!#6]))=,:[#6X3] ([#16X2&\$([#16][!#6]),SX1-])[#7X3;\$([#7][!#6]))]
SubFP151	SubFPC151	Guanidine	[N;v3X3,v4X4+][CX3](=[N;v3X2,v4X3+]) [N;v3X3,v4X4+]
SubFP152	SubFPC152	Carbaminic acid	[NX3]C(=[OX1])[O;X2H,X1-]
SubFP153	SubFPC153	Urethan	[#7X3][#6](=[OX1])[#8X2][#6]
SubFP154	SubFPC154	Biuret	[#7X3][#6](=[OX1])[#7X3][#6](=[OX1]) [#7X3]
SubFP155	SubFPC155	Semicarbazide	[#7X3][#7X3][#6X3]([#7X3;!\$([#7 [#7]))]=[OX1]
SubFP156	SubFPC156	Carbazide	[#7X3][#7X3][#6X3]([#7X3][#7X3]) =[OX1]

Name	Count name	Description	Pattern
SubFP157	SubFPC157	Semicarbazone	[#7X2](=[#6])[#7X3][#6X3]([#7X3;! \$([#7][#7]))=[OX1]
SubFP158	SubFPC158	Carbazone	[#7X2](=[#6])[#7X3][#6X3]([#7X3] [#7X3])=[OX1]
SubFP159	SubFPC159	Thiosemicarbazide	[#7X3][#7X3][#6X3]([#7X3;! \$([#7][#7]))=[SX1]
SubFP160	SubFPC160	Thiocarbazide	[#7X3][#7X3][#6X3]([#7X3][#7X3]) =[SX1]
SubFP161	SubFPC161	Thiosemicarbazone	[#7X2](=[#6])[#7X3][#6X3]([#7X3; ! \$([#7][#7]))=[SX1]
SubFP162	SubFPC162	Thiocarbazone	[#7X2](=[#6])[#7X3][#6X3]([#7X3] [#7X3])=[SX1]
SubFP163	SubFPC163	Isocyanate	[NX2]=[CX2]=[OX1]
SubFP164	SubFPC164	Cyanate	[OX2][CX2]#[NX1]
SubFP165	SubFPC165	Isothiocyanate	[NX2]=[CX2]=[SX1]
SubFP166	SubFPC166	Thiocyanate	[SX2][CX2]#[NX1]
SubFP167	SubFPC167	Carbodiimide	[NX2]=[CX2]=[NX2]
SubFP168	SubFPC168	Orthocarbonic derivatives	[CX4H0]([O,S,#7])([O,S,#7])([O,S,#7]) [O,S,#7,F,Cl,Br,I]
SubFP169	SubFPC169	Phenol	[OX2H][c]
SubFP170	SubFPC170	1,2-Diphenol	[OX2H][c][c][OX2H]
SubFP171	SubFPC171	Arylchloride	[Cl][c]
SubFP172	SubFPC172	Arylfluoride	[F][c]
SubFP173	SubFPC173	Arylbromide	[Br][c]
SubFP174	SubFPC174	Aryliodide	[I][c]
SubFP175	SubFPC175	Arylthiol	[SX2H][c]
SubFP176	SubFPC176	Iminoarene	[c]=[NX2;\$([H1]),\$([H0][#6;! \$([C]=[N,S,O]))]
SubFP177	SubFPC177	Oxoarene	[c]=[OX1]
SubFP178	SubFPC178	Thioarene	[c]=[SX1]
SubFP179	SubFPC179	Hetero N basic H	[nX3H1+0]
SubFP180	SubFPC180	Hetero N basic no H	[nX3H0+0]
SubFP181	SubFPC181	Hetero N nonbasic	[nX2,nX3+]
SubFP182	SubFPC182	Hetero O	[o]
SubFP183	SubFPC183	Hetero S	[sX2]
SubFP184	SubFPC184	Heteroaromatic	[a;!c]
SubFP185	SubFPC185	Nitrite	[NX2](=[OX1])[O;\$([X2]),\$([X1-])]
SubFP186	SubFPC186	Thionitrite	[SX2][NX2]=[OX1]

Name	Count name	Description	Pattern
SubFP187	SubFPC187	Nitrate	<chem>[\$(NX3)(=[OX1])(=[OX1])[O;\$([X2]),\$([X1-])]),\$(NX3+)([OX1-])(=[OX1])[O;\$([X2]),\$([X1-])])]</chem>
SubFP188	SubFPC188	Nitro	<chem>[\$(NX3)(=O)=O,\$(NX3+)(=O)[O-]] [!#8]</chem>
SubFP189	SubFPC189	Nitroso	<chem>[NX2](=[OX1])[!#7;!#8]</chem>
SubFP190	SubFPC190	Azide	<chem>[NX1]~[NX2]~[NX2,NX1]</chem>
SubFP191	SubFPC191	Acylazide	<chem>[CX3](=[OX1])[NX2]~[NX2]~[NX1]</chem>
SubFP192	SubFPC192	Diazo	<chem>[\$([#6]=[NX2+]=[NX1-]),\$([#6-].[NX2+]#[NX1])]</chem>
SubFP193	SubFPC193	Diazonium	<chem>[#6][NX2+]#[NX1]</chem>
SubFP194	SubFPC194	Nitrosamine	<chem>[#7;!\$(N*=O)][NX2]=[OX1]</chem>
SubFP195	SubFPC195	Nitrosamide	<chem>[NX2](=[OX1])N-*=O</chem>
SubFP196	SubFPC196	N-Oxide	<chem>[\$([#7+][OX1-]),\$([#7v5]=[OX1]);!\$([#7](~[O])~[O]);!\$([#7]=[#7])]</chem>
SubFP197	SubFPC197	Hydrazine	<chem>[NX3,\$([H2]),\$([H1][#6]),\$([H0]([#6])[#6]);!\$(NC=[O,N,S])[NX3,\$([H2]),\$([H1][#6]),\$([H0]([#6])[#6]);!\$(NC=[O,N,S])]</chem>
SubFP198	SubFPC198	Hydrazone	<chem>[NX3,\$([H2]),\$([H1][#6]),\$([H0]([#6])[#6]);!\$(NC=[O,N,S])[NX2]=[#6]</chem>
SubFP199	SubFPC199	Hydroxylamine	<chem>[NX3,\$([H2]),\$([H1][#6]),\$([H0]([#6])[#6]);!\$(NC=[O,N,S])[OX2,\$([H1]),\$([O][#6;!\$(C=[N,O,S])])]</chem>
SubFP200	SubFPC200	Sulfon	<chem>[\$([SX4](=[OX1])(=[OX1])([#6])[#6]),\$([SX4+2]([OX1-])([OX1-])([#6])[#6])]</chem>
SubFP201	SubFPC201	Sulfoxide	<chem>[\$([SX3](=[OX1])([#6])[#6]),\$([SX3+](OX1-)([#6])[#6])]</chem>
SubFP202	SubFPC202	Sulfonium	<chem>[S+;!\$(S)~[!#6]);!\$(S)*~[#7,#8,#15,#16])]</chem>
SubFP203	SubFPC203	Sulfuric acid	<chem>[SX4](=[OX1])(=[OX1])([\$([OX2H]),\$([OX1-])])[\$([OX2H]),\$([OX1-])]</chem>
SubFP204	SubFPC204	Sulfuric monoester	<chem>[SX4](=[OX1])(=[OX1])([\$([OX2H]),\$([OX1-])])][OX2][#6;!\$(C=[O,N,S])]</chem>
SubFP205	SubFPC205	Sulfuric diester	<chem>[SX4](=[OX1])(=[OX1])([OX2][#6;!\$(C=[O,N,S])])[OX2][#6;!\$(C=[O,N,S])]</chem>
SubFP206	SubFPC206	Sulfuric monoamide	<chem>[SX4](=[OX1])(=[OX1])([#7X3,\$([H2]),\$([H1][#6;!\$(C=[O,N,S])]),\$([#7]([#6;!\$(C=[O,N,S])])[#6;!\$(C=[O,N,S])])])[\$([OX2H]),\$([OX1-])]</chem>

Name	Count name	Description	Pattern
SubFP207	SubFPC207	Sulfuric diamide	[SX4](=[OX1])(=[OX1])([#7X3;\$([H2]), \$([H1])[#6;!\$(C=[O,N,S])])\$([#7 ([#6;!\$(C=[O,N,S])])[#6;!\$(C=[O,N,S])])) [#7X3;\$([H2]),\$([H1])[#6;!\$(C=[O,N,S])]), \$([#7])([#6;!\$(C=[O,N,S])])[#6; !\$(C=[O,N,S])])]
SubFP208	SubFPC208	Sulfuric esteramide	[SX4](=[OX1])(=[OX1])([#7X3][#6; !\$(C=[O,N,S])])[OX2][#6;!\$(C=[O,N,S])]
SubFP209	SubFPC209	Sulfuric derivative	[SX4D4](=[!#6])(=[!#6])([!#6])[!#6]
SubFP210	SubFPC210	Sulfonic acid	[SX4;\$([H1]),\$([H0][#6]))(=[OX1]) (=[OX1])\$([OX2H]),\$([OX1-])]
SubFP211	SubFPC211	Sulfonamide	[SX4;\$([H1]),\$([H0][#6]))(=[OX1]) (=[OX1])[#7X3;\$([H2]),\$([H1])[#6; !\$(C=[O,N,S])]),\$([#7])([#6; !\$(C=[O,N,S])])[#6;!\$(C=[O,N,S])])]
SubFP212	SubFPC212	Sulfonic ester	[SX4;\$([H1]),\$([H0][#6]))(=[OX1]) (=[OX1])[OX2][#6;!\$(C=[O,N,S])]
SubFP213	SubFPC213	Sulfonic halide	[SX4;\$([H1]),\$([H0][#6]))(=[OX1]) (=[OX1])[FX1,CIX1,BrX1,IX1]
SubFP214	SubFPC214	Sulfonic derivative	[SX4;\$([H1]),\$([H0][#6]))(=[!#6]) (=[!#6])[!#6]
SubFP215	SubFPC215	Sulfinic acid	[SX3;\$([H1]),\$([H0][#6]))(=[OX1]) \$([OX2H]),\$([OX1-])]
SubFP216	SubFPC216	Sulfinic amide	[SX3;\$([H1]),\$([H0][#6]))(=[OX1]) [#7X3;\$([H2]),\$([H1])[#6; !\$(C=[O,N,S])]),\$([#7])([#6;!\$(C=[O,N,S])]) [#6;!\$(C=[O,N,S])])]
SubFP217	SubFPC217	Sulfinic ester	[SX3;\$([H1]),\$([H0][#6]))(=[OX1]) [OX2][#6;!\$(C=[O,N,S])]
SubFP218	SubFPC218	Sulfinic halide	[SX3;\$([H1]),\$([H0][#6]))(=[OX1]) [FX1,CIX1,BrX1,IX1]
SubFP219	SubFPC219	Sulfinic derivative	[SX3;\$([H1]),\$([H0][#6]))(=[!#6]) [!#6]
SubFP220	SubFPC220	Sulfenic acid	[SX2;\$([H1]),\$([H0][#6])) \$([OX2H]),\$([OX1-])]
SubFP221	SubFPC221	Sulfenic amide	[SX2;\$([H1]),\$([H0][#6]))[#7X3; \$([H2]),\$([H1])[#6;!\$(C=[O,N,S])]), \$([#7])([#6;!\$(C=[O,N,S])]) [#6;!\$(C=[O,N,S])])]
SubFP222	SubFPC222	Sulfenic ester	[SX2;\$([H1]),\$([H0][#6]))[OX2] [#6;!\$(C=[O,N,S])]
SubFP223	SubFPC223	Sulfenic halide	[SX2;\$([H1]),\$([H0][#6])) [FX1,CIX1,BrX1,IX1]
SubFP224	SubFPC224	Sulfenic derivative	[SX2;\$([H1]),\$([H0][#6]))[!#6]

Name	Count name	Description	Pattern
SubFP225	SubFPC225	Phosphine	[PX3;\$([H3]),\$([H2][#6]),\$([H1][#6])[#6]),\$([H0]([#6])([#6])[#6])]
SubFP226	SubFPC226	Phosphine oxide	[PX4;\$([H3]=[OX1]),\$([H2](=[OX1])[#6]),\$([H1](=[OX1])([#6])[#6]),\$([H0](=[OX1])([#6])([#6])[#6])]
SubFP227	SubFPC227	Phosphonium	[P+;!\$([P]~[!#6]);!\$([P]*~[#7,#8,#15,#16])]
SubFP228	SubFPC228	Phosphorylen	[PX4;\$([H3]=[CX3]),\$([H2](=[CX3])[#6]),\$([H1](=[CX3])([#6])[#6]),\$([H0](=[CX3])([#6])([#6])[#6])]
SubFP229	SubFPC229	Phosphonic acid	[PX4;\$([H1]),\$([H0][#6])(=[OX1])([\$([OX2H]),\$([OX1-])])[\$([OX2H]),\$([OX1-])])]
SubFP230	SubFPC230	Phosphonic monoester	[PX4;\$([H1]),\$([H0][#6])(=[OX1])([\$([OX2H]),\$([OX1-])])][OX2][#6;!\$(C=[O,N,S])]
SubFP231	SubFPC231	Phosphonic diester	[PX4;\$([H1]),\$([H0][#6])(=[OX1])([OX2][#6;!\$(C=[O,N,S])])[OX2][#6;!\$(C=[O,N,S])]
SubFP232	SubFPC232	Phosphonic monoamide	[PX4;\$([H1]),\$([H0][#6])(=[OX1])([\$([OX2H]),\$([OX1-])])[#7X3;\$([H2]),\$([H1][#6;!\$(C=[O,N,S])]),\$([#7]([#6;!\$(C=[O,N,S])])[#6;!\$(C=[O,N,S])])]
SubFP233	SubFPC233	Phosphonic diamide	[PX4;\$([H1]),\$([H0][#6])(=[OX1])([#7X3;\$([H2]),\$([H1][#6;!\$(C=[O,N,S])]),\$([#7]([#6;!\$(C=[O,N,S])])][#6;!\$(C=[O,N,S])])][#7X3;\$([H2]),\$([H1][#6;!\$(C=[O,N,S])]),\$([#7]([#6;!\$(C=[O,N,S])])[#6;!\$(C=[O,N,S])])]
SubFP234	SubFPC234	Phosphonic esteramide	[PX4;\$([H1]),\$([H0][#6])(=[OX1])([OX2][#6;!\$(C=[O,N,S])])[#7X3;\$([H2]),\$([H1][#6;!\$(C=[O,N,S])]),\$([#7]([#6;!\$(C=[O,N,S])])[#6;!\$(C=[O,N,S])])]
SubFP235	SubFPC235	Phosphonic acid derivative	[PX4;\$([H1]),\$([H0][#6])(=[!#6])([!#6])[!#6]
SubFP236	SubFPC236	Phosphoric acid	[PX4D4](=[OX1])([\$([OX2H]),\$([OX1-])])(\$([OX2H]),\$([OX1-]))(\$([OX2H]),\$([OX1-]))
SubFP237	SubFPC237	Phosphoric monoester	[PX4D4](=[OX1])([\$([OX2H]),\$([OX1-])])(\$([OX2H]),\$([OX1-]))[OX2][#6;!\$(C=[O,N,S])]
SubFP238	SubFPC238	Phosphoric diester	[PX4D4](=[OX1])([\$([OX2H]),\$([OX1-])])([OX2][#6;!\$(C=[O,N,S])])[OX2][#6;!\$(C=[O,N,S])]

Name	Count name	Description	Pattern
SubFP239	SubFPC239	Phosphoric triester	[PX4D4](=[OX1])([OX2][#6;!\$(C=[O,N,S])])([OX2][#6;!\$(C=[O,N,S])]) [OX2][#6;!\$(C=[O,N,S])]
SubFP240	SubFPC240	Phosphoric monoamide	[PX4D4](=[OX1])([OX2H]),\$([OX1-])) ([OX2H]),\$([OX1-]))[#7X3;\$([H2]), \$([H1][#6;!\$(C=[O,N,S])]),\$([#7]([#6; !\$(C=[O,N,S])])[#6;!\$(C=[O,N,S])])]
SubFP241	SubFPC241	Phosphoric diamide	[PX4D4](=[OX1])([OX2H]),\$([OX1-])) ([#7X3;\$([H2]),\$([H1][#6;!\$(C=[O,N,S])]), \$([#7]([#6;!\$(C=[O,N,S])]) [#6;!\$(C=[O,N,S])])])[#7X3;\$([H2]),\$([H1] [#6;!\$(C=[O,N,S])]),\$([#7] ([#6;!\$(C=[O,N,S])])[#6;!\$(C=[O,N,S])])]
SubFP242	SubFPC242	Phosphoric triamide	[PX4D4](=[OX1])([#7X3;\$([H2]),\$([H1] [#6;!\$(C=[O,N,S])]),\$([#7]([#6; !\$(C=[O,N,S])])[#6;!\$(C=[O,N,S])])]) ([#7X3;\$([H2]),\$([H1][#6;!\$(C=[O,N,S])]), \$([#7]([#6;!\$(C=[O,N,S])])[#6; !\$(C=[O,N,S])])])[#7X3;\$([H2]),\$([H1][#6; !\$(C=[O,N,S])]),\$([#7]([#6;!\$(C=[O,N,S])]) [#6;!\$(C=[O,N,S])])]
SubFP243	SubFPC243	Phosphoric monoestermonoamide	[PX4D4](=[OX1])([OX2H]),\$([OX1-])) ([OX2][#6;!\$(C=[O,N,S])])[#7X3;\$([H2]), \$([H1][#6;!\$(C=[O,N,S])]),\$([#7]([#6; !\$(C=[O,N,S])])[#6;!\$(C=[O,N,S])])]
SubFP244	SubFPC244	Phosphoric diestermonoamide	[PX4D4](=[OX1])([OX2][#6;!\$(C=[O,N,S])]) ([OX2][#6;!\$(C=[O,N,S])])[#7X3;\$([H2]), \$([H1][#6;!\$(C=[O,N,S])]),\$([#7] ([#6;!\$(C=[O,N,S])])[#6;!\$(C=[O,N,S])])]
SubFP245	SubFPC245	Phosphoric monoesterdiamide	[PX4D4](=[OX1])([OX2][#6;!\$(C=[O,N,S])]) ([#7X3;\$([H2]),\$([H1][#6;!\$(C=[O,N,S])]), \$([#7]([#6;!\$(C=[O,N,S])])[#6; !\$(C=[O,N,S])])])[#7X3;\$([H2]),\$([H1][#6; !\$(C=[O,N,S])]),\$([#7]([#6;!\$(C=[O,N,S])]) [#6;!\$(C=[O,N,S])])]
SubFP246	SubFPC246	Phosphoric acid derivative	[PX4D4](=[!#6])([!#6])([!#6])[!#6]
SubFP247	SubFPC247	Phosphinic acid	[PX4;\$([H2]),\$([H1][#6]),\$([H0] ([#6])[#6])](=[OX1])\$([OX2H]),\$([OX1-])]
SubFP248	SubFPC248	Phosphinic ester	[PX4;\$([H2]),\$([H1][#6]),\$([H0] ([#6])[#6])](=[OX1])[OX2][#6; !\$(C=[O,N,S])]
SubFP249	SubFPC249	Phosphinic amide	[PX4;\$([H2]),\$([H1][#6]),\$([H0] ([#6])[#6])](=[OX1])[#7X3;\$([H2]), \$([H1][#6;!\$(C=[O,N,S])]),\$([#7] ([#6;!\$(C=[O,N,S])])[#6;!\$(C=[O,N,S])])]

Name	Count name	Description	Pattern
SubFP250	SubFPC250	Phosphinic acid derivative	[PX4;\$([H2]),\$([H1][#6]),\$([H0][#6])[#6])](=[!#6])[!#6]
SubFP251	SubFPC251	Phosphonous acid	[PX3;\$([H1]),\$([H0][#6]))(\$([OX2H]),\$([OX1-]))]\$([OX2H]),\$([OX1-])]
SubFP252	SubFPC252	Phosphonous monoester	[PX3;\$([H1]),\$([H0][#6]))(\$([OX2H]),\$([OX1-]))[OX2][#6;!\$(C=[O,N,S])]
SubFP253	SubFPC253	Phosphonous diester	[PX3;\$([H1]),\$([H0][#6]))([OX2][#6;!\$(C=[O,N,S])])[OX2][#6;!\$(C=[O,N,S])]
SubFP254	SubFPC254	Phosphonous monoamide	[PX3;\$([H1]),\$([H0][#6]))(\$([OX2H]),\$([OX1-]))[#7X3;\$([H2]),\$([H1][#6;!\$(C=[O,N,S])]),\$([#7][#6;!\$(C=[O,N,S])])[#6;!\$(C=[O,N,S])]
SubFP255	SubFPC255	Phosphonous diamide	[PX3;\$([H1]),\$([H0][#6]))([#7X3;\$([H2]),\$([H1][#6;!\$(C=[O,N,S])]),\$([#7][#6;!\$(C=[O,N,S])])[#6;!\$(C=[O,N,S])])[#7X3;\$([H2]),\$([H1][#6;!\$(C=[O,N,S])]),\$([#7][#6;!\$(C=[O,N,S])])[#6;!\$(C=[O,N,S])]
SubFP256	SubFPC256	Phosphonous esteramide	[PX3;\$([H1]),\$([H0][#6]))([OX2][#6;!\$(C=[O,N,S])])[#7X3;\$([H2]),\$([H1][#6;!\$(C=[O,N,S])]),\$([#7][#6;!\$(C=[O,N,S])])[#6;!\$(C=[O,N,S])]
SubFP257	SubFPC257	Phosphonous derivatives	[PX3;\$([D2]),\$([D3][#6]))([!#6]) [!#6]
SubFP258	SubFPC258	Phosphinous acid	[PX3;\$([H2]),\$([H1][#6]),\$([H0][#6])[#6])[\$([OX2H]),\$([OX1-])]
SubFP259	SubFPC259	Phosphinous ester	[PX3;\$([H2]),\$([H1][#6]),\$([H0][#6])[#6])[OX2][#6;!\$(C=[O,N,S])]
SubFP260	SubFPC260	Phosphinous amide	[PX3;\$([H2]),\$([H1][#6]),\$([H0][#6])[#6])[#7X3;\$([H2]),\$([H1][#6;!\$(C=[O,N,S])]),\$([#7][#6;!\$(C=[O,N,S])])[#6;!\$(C=[O,N,S])]
SubFP261	SubFPC261	Phosphinous derivatives	[PX3;\$([H2]),\$([H1][#6]),\$([H0][#6])[#6])[!#6]
SubFP262	SubFPC262	Quart silane	[SiX4]([#6])([#6])([#6])[#6]
SubFP263	SubFPC263	Non-quart silane	[SiX4;\$([H1])([#6])([#6])[#6]),\$([H2])([#6])([#6]),\$([H3][#6]),\$([H4])]
SubFP264	SubFPC264	Silylmonohalide	[SiX4]([FX1,CIX1,BrX1,IX1])([#6])([#6])[#6]
SubFP265	SubFPC265	Het trialkylsilane	[SiX4]([!#6])([#6])([#6])[#6]
SubFP266	SubFPC266	Dihet dialkylsilane	[SiX4]([!#6])([!#6])([#6])[#6]
SubFP267	SubFPC267	Trihet alkylsilane	[SiX4]([!#6])([!#6])([!#6])[#6]
SubFP268	SubFPC268	Silicic acid derivative	[SiX4]([!#6])([!#6])([!#6])[!#6]
SubFP269	SubFPC269	Trialkylborane	[BX3]([#6])([#6])[#6]

Name	Count name	Description	Pattern
SubFP270	SubFPC270	Boric acid derivatives	[BX3]([!#6])([!#6])[!#6]
SubFP271	SubFPC271	Boronic acid derivative	[BX3]([!#6])([!#6])[!#6]
SubFP272	SubFPC272	Borohydride	[BH1,BH2,BH3,BH4]
SubFP273	SubFPC273	Quaternary boron	[BX4]
SubFP274	SubFPC274	Aromatic	a
SubFP275	SubFPC275	Heterocyclic	[!#6;!R0]
SubFP276	SubFPC276	Epoxide	[OX2r3]1[#6r3][#6r3]1
SubFP277	SubFPC277	NH aziridine	[NX3H1r3]1[#6r3][#6r3]1
SubFP278	SubFPC278	Spiro	[D4R;\$(*(@*)(@*)(@*)@*)]
SubFP279	SubFPC279	Annelated rings	[R;\$(*(@*)(@*)@*);!\$([R2;\$(*(@*)(@*)(@*)@*)])@R;\$(*(@*)(@*)@*);!\$([R2;\$(*(@*)(@*)(@*)@*)])]
SubFP280	SubFPC280	Bridged rings	[R;\$(*(@*)(@*)@*);!\$([D4R;\$(*(@*)(@*)(@*)@*)])!\$([R;\$(*(@*)(@*)(@*)@*)];!\$([R2;\$(*(@*)(@*)(@*)@*)])@R;\$(*(@*)(@*)(@*)(@*)@*);!\$([R2;\$(*(@*)(@*)(@*)(@*)@*)])]
SubFP281	SubFPC281	Sugar pattern 1	[OX2;\$([r5]1@C@C@C(O)@C1),\$([r6]1@C@C@C(O)@C(O)@C1)]
SubFP282	SubFPC282	Sugar pattern 2	[OX2;\$([r5]1@C(!@OX2,NX3,SX2,FX1,CIX1,BrX1,IX1))@C@C@C1),\$([r6]1@C(!@OX2,NX3,SX2,FX1,CIX1,BrX1,IX1))@C@C@C@C1)]
SubFP283	SubFPC283	Sugar pattern combi	[OX2;\$([r5]1@C(!@OX2,NX3,SX2,FX1,CIX1,BrX1,IX1))@C@C(O)@C1),\$([r6]1@C(!@OX2,NX3,SX2,FX1,CIX1,BrX1,IX1))@C@C(O)@C(O)@C1)]
SubFP284	SubFPC284	Sugar pattern 2 reducing	[OX2;\$([r5]1@C(!@OX2H1))@C@C@C1),\$([r6]1@C(!@OX2H1))@C@C@C@C1)]
SubFP285	SubFPC285	Sugar pattern 2 alpha	[OX2;\$([r5]1@C@C@C(!@OX2,NX3,SX2,FX1,CIX1,BrX1,IX1))@C@C@C1),\$([r6]1@C@C@C(!@OX2,NX3,SX2,FX1,CIX1,BrX1,IX1))@C@C@C@C1)]
SubFP286	SubFPC286	Sugar pattern 2 beta	[OX2;\$([r5]1@C@C@C(!@OX2,NX3,SX2,FX1,CIX1,BrX1,IX1))@C@C@C1),\$([r6]1@C@C@C(!@OX2,NX3,SX2,FX1,CIX1,BrX1,IX1))@C@C@C@C1)]
SubFP287	SubFPC287	Conjugated double bond	*=[*]=,#,:[*]
SubFP288	SubFPC288	Conjugated tripple bond	*#[*]=,#,:[*]
SubFP289	SubFPC289	Cis double bond	*/[D2]=[D2]/*
SubFP290	SubFPC290	Trans double bond	*/[D2]=[D2]/*
SubFP291	SubFPC291	Mixed anhydrides	[\$(*=O),\$([#16,#14,#5]),\$([#7]([#6]=[OX1]))][#8X2][\$(*=O),\$([#16,#14,#5]),\$([#7]([#6]=[OX1]))]

Name	Count name	Description	Pattern
SubFP292	SubFPC292	Halogen on hetero	[FX1,CIX1,BrX1,IX1][!#6]
SubFP293	SubFPC293	Halogen multi subst	[F,Cl,Br,I;!\$([X1]);!\$([X0-])]
SubFP294	SubFPC294	Trifluoromethyl	[FX1][CX4;!\$([H0][Cl,Br,I]);!\$([F][C]([F])([F])[F]))([FX1])([FX1])]
SubFP295	SubFPC295	C ONS bond	[#6]~[#7,#8,#16]
SubFP296	SubFPC296	Charged	[!+0]
SubFP297	SubFPC297	Anion	[-1,-2,-3,-4,-5,-6,-7]
SubFP298	SubFPC298	Kation	[+1,+2,+3,+4,+5,+6,+7]
SubFP299	SubFPC299	Salt	([-1,-2,-3,-4,-5,-6,-7]).([+1,+2,+3,+4,+5,+6,+7])
SubFP300	SubFPC300	1,3-Tautomerizable	[\$([#7X2,OX1,SX1]=*!H0;!\$([a;!n]))], \$([#7X3,OX2,SX2;!H0]*=*), \$([#7X3,OX2,SX2;!H0]*:n)]
SubFP301	SubFPC301	1,5-Tautomerizable	[\$([#7X2,OX1,SX1]=,::*=,*!H0;!\$([a;!n]))], \$([#7X3,OX2,SX2;!H0]*=**=*), \$([#7X3,OX2,SX2;!H0]*=,::*:n)]
SubFP302	SubFPC302	Rotatable bond	[!\$(*#*)&!D1]-!@!\$(*#*)&!D1]
SubFP303	SubFPC303	Michael acceptor	[CX3]=[CX3][!\$([CX3]=[O,N,S]),\$(C#[N]),\$([S,P]=[OX1]),\$([NX3]=O),\$([NX3+](=O)[O-]))]
SubFP304	SubFPC304	Dicarbodiazene	[CX3](=[OX1])[NX2]=[NX2][CX3](=[OX1])
SubFP305	SubFPC305	CH-acidic	[\$([CX4;!\$([H0]);!\$([C]!#6;!\$([P,S]=O);!\$([N(~O)~O]))][!\$([CX3]=[O,N,S]),\$(C#[N]),\$([S,P]=[OX1]),\$([NX3]=O),\$([NX3+](=O)[O-]);!\$(*[S,O,N;H1,H2]);!\$(*+0)[S,O;X1-])]), \$([CX4;!\$([H0]))1[CX3]=[CX3][CX3]=[CX3]1)]
SubFP306	SubFPC306	CH-acidic strong	[CX4;!\$([H0]);!\$([C]!#6;!\$([P,S]=O);!\$([N(~O)~O]))][!\$([CX3]=[O,N,S]),\$(C#[N]),\$([S,P]=[OX1]),\$([NX3]=O),\$([NX3+](=O)[O-]);!\$(*[S,O,N;H1,H2]);!\$(*+0)[S,O;X1-])][!\$([CX3]=[O,N,S]),\$(C#[N]),\$([S,P]=[OX1]),\$([NX3]=O),\$([NX3+](=O)[O-]);!\$(*[S,O,N;H1,H2]);!\$(*+0)[S,O;X1-])]
SubFP307	SubFPC307	Chiral center specified	[\$([*@](~*)(~*)(*)*),\$([*@H](*)(*)(*)*),\$([*@](~*)(~*)(*)*),\$([*@H](~*)(~*)(*)*)]