

NAME

RDKitSearchFunctionalGroups.py - Search for functional groups using SMARTS patterns

SYNOPSIS

```
RDKitSearchFunctionalGroups.py [--combineMatches <yes or no>] [--combineOperator <and or or>] [--groupNamesFile
<FileName or auto>] [--infileParams <Name,Value,...>] [--mode <retrieve or count>] [--negate <yes or no>] [
--outfileParams <Name,Value,...>] [--overwrite] [--useChirality <yes or no>] [-w <dir>] [-o <outfile>] -i <infile> -f
<Name1,Name2,Name3... or All>
```

```
RDKitSearchFunctionalGroups.py [--groupNamesFile <FileName or auto>] -l | --list
```

```
RDKitSearchFunctionalGroups.py -h | --help | -e | --examples
```

DESCRIPTION

Perform a substructure search in an input file using SMARTS patterns for functional groups and write out the matched molecules to an output file or simply count the number of matches.

The SMARTS patterns for specified functional group(s) are retrieved from file, Functional_Group_Hierarchy.txt, available in RDKit data directory.

The names of valid functional groups and hierarchies are dynamically retrieved from the functional groups hierarchy file and are shown below:

```
AcidChloride, AcidChloride.Aromatic, AcidChloride.Aliphatic
Alcohol, Alcohol.Aromatic, Alcohol.Aliphatic
Aldehyde, Aldehyde.Aromatic, Aldehyde.Aliphatic
Amine, Amine.Primary, Amine.Primary.Aromatic, Amine.Primary.Aliphatic,
Amine.Secondary, Amine.Secondary.Aromatic, Amine.Secondary.Aliphatic
Amine.Tertiary, Amine.Tertiary.Aromatic, Amine.Tertiary.Aliphatic
Amine.Aromatic, Amine.Aliphatic, Amine.Cyclic
Azide, Azide.Aromatic, Azide.Aliphatic
BoronicAcid, BoronicAcid.Aromatic, BoronicAcid.Aliphatic
CarboxylicAcid, CarboxylicAcid.Aromatic, CarboxylicAcid.Aliphatic,
CarboxylicAcid.AlphaAmino
Halogen, Halogen.Aromatic, Halogen.Aliphatic
Halogen.NotFluorine, Halogen.NotFluorine.Aliphatic,
Halogen.NotFluorine.Aromatic
Halogen.Bromine, Halogen.Bromine.Aliphatic, Halogen.Bromine.Aromatic,
Halogen.Bromine.BromoKetone
Isocyanate, Isocyanate.Aromatic, Isocyanate.Aliphatic
Nitro, Nitro.Aromatic, Nitro.Aliphatic,
SulfonylChloride, SulfonylChloride.Aromatic, SulfonylChloride.Aliphatic
TerminalAlkyne
```

The supported input file formats are: SD (.sdf, .sd), SMILES (.smi, .csv, .tsv, .txt)

The supported output file formats are: SD (.sdf, .sd), SMILES (.smi)

OPTIONS

-c, --combineMatches <yes or no> [default: yes]

Combine search results for matching SMARTS patterns of specified functional groups against a molecule. Possible values: yes or no.

The matched molecules are written to a single output file for "yes" value. Otherwise, multiple output files are generated, one for each functional group. The names of these files correspond to a combination of the basename of the specified output file and the name of the functional group.

No output files are generated during "count" value of "-m, --mode" option.

--combineOperator <and or or> [default: and]

Logical operator to use for combining match results corresponding to specified functional group names before writing out a single file. This option is ignored during "No" value of "-c, --combineMatches" option.

-e, --examples

Print examples.

-g, --groupNamesFile <FileName or auto> [default: auto]

Specify a file name containing data for functional groups hierarchy or use functional group hierarchy file, Functional_Group_Hierarchy.txt, available in RDKit data directory.

RDKit data format: Name<tab>Smarts<tab>Label<tab>RemovalReaction (optional)

The format of data in local functional group hierarchy must match format of the data in functional group file available in

RDKit data directory.

-f, --functionalGroups <Name1,Name2,Name3... or All> [default: none]

Functional group names for performing substructure SMARTS search. Possible values: Comma delimited list of valid functional group names or All. The current set of valid functional group names are listed in the description section.

The match results for multiple functional group names are combined using 'and' operator before writing them out to single file. No merging of match results takes place during generation of individual result files corresponding to fictional group names.

The functional group name may be started with an exclamation mark to negate the match result for that fictional group.

-h, --help

Print this help message.

-i, --infile <infile>

Input file name.

--infileParams <Name,Value,...> [default: auto]

A comma delimited list of parameter name and value pairs for reading molecules from files. The supported parameter names for different file formats, along with their default values, are shown below:

```
SD:  MOL:  removeHydrogens,yes,sanitize,yes,strictParsing,yes
SMILES: smilesColumn,1,smilesNameColumn,2,smilesDelimiter,space,
        smilesTitleLine,auto,sanitize,yes
```

Possible values for smilesDelimiter: space, comma or tab.

-l, --list

List functional groups information without performing any search.

-m, --mode <retrieve or count> [default: retrieve]

Specify whether to retrieve and write out matched molecules to an output file or simply count the number of matches.

-o, --outfile <outfile>

Output file name.

--outfileParams <Name,Value,...> [default: auto]

A comma delimited list of parameter name and value pairs for writing molecules to files. The supported parameter names for different file formats, along with their default values, are shown below:

```
SD:  compute2DCoords,auto,kekulize,no
SMILES: kekulize,no,smilesDelimiter,space, smilesIsomeric,yes,
        smilesTitleLine,yes
```

Default value for compute2DCoords: yes for SMILES input file; no for all other file types.

--overwrite

Overwrite existing files.

-u, --useChirality <yes or no> [default: no]

Use stereochemistry information for SMARTS search.

-w, --workingdir <dir>

Location of working directory which defaults to the current directory.

EXAMPLES

To list names of all available functional groups along with their SMARTS patterns, type:

```
% RDKitSearchFunctionalGroups.py -l
```

To retrieve molecule containing amine functional group and write out a SMILES file, type:

```
% RDKitSearchFunctionalGroups.py -f Amine -i Sample.smi -o SampleOut.smi
```

To retrieve molecules containing amine functional group but not halogens and carboxylic acid functional groups and write out a SMILES file, type:

```
% RDKitSearchFunctionalGroups.py -f 'Amine,!Halogen,!CarboxylicAcid'
-i Sample.smi -o SampleOut.smi
```

To retrieve molecules containing amine, halogens or carboxylic acid functional groups and write out a SMILES file, type:

```
% RDKitSearchFunctionalGroups.py -f 'Amine, Halogen, CarboxylicAcid'
--combineOperator or -i Sample.smi -o SampleOut.smi
```

To retrieve molecules containing amine and carboxylic acid functional groups defined in a local functional groups hierarchy file and write out individual SD files for each functional group, type:

```
% RDKitSearchFunctionalGroups.py -f 'Amine, CarboxylicAcid' -i Sample.sdf
-g Custom_Functional_Group_Hierarchy.txt --combineMatches No -o SampleOut.sdf
```

To count number of all functional groups in molecules without writing out an output files, type:

```
% RDKitSearchFunctionalGroups.py -m count -f All --combineMatches no -i Sample.smi
```

To retrieve molecule not containing aromatic alcohol and aromatic halogen functional group along with the use of chirality during substructure search and write out individual SMILES files for each functional group, type:

```
% RDKitSearchFunctionalGroups.py --combineMatches no -u yes
-f '!Alcohol.Aromatic,!Halogen.Aromatic' -i Sample.smi -o SampleOut.smi
```

To retrieve molecule containing amine functional group from a CSV SMILES file, SMILES strings in column 1, name in column 2, and write out a SD file, type:

```
% RDKitSearchFunctionalGroups.py -f Amine --infileParams
"smilesDelimiter,comma,smilesTitleLine,yes,smilesColumn,1,
smilesNameColumn,2" --outfileParams "compute2DCoords,yes"
-i SampleSMILES.csv -o SampleOut.sdf
```

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SEE ALSO

RDKitConvertFileFormat.py, RDKitFilterPAINS.py, RDKitSearchSMARTS.py

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The functionality available in this script is implemented using RDKit, an open source toolkit for cheminformatics developed by Greg Landrum.

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