

## NAME

RDKitEnumerateCompoundLibrary.py - Enumerate a virtual compound library

## SYNOPSIS

```
RDKitEnumerateCompoundLibrary.py [--compute2DCoords <yes or no>] [--infileParams
<Name,Value,...>] [--mode <RxnByName or RxnBySMIRKS>] [--outfileParams <Name,Value,...>] [
--overwrite] [--prodMolNames <UseReactants or Sequential>] [--rxnName <text>] [--rxnNamesFile
<FileName or auto>] [--smirksRxn <text>] [--sanitize <yes or no>] [-w <dir>] -i <ReactantFile1,...> -o
<outfile>
```

```
RDKitEnumerateCompoundLibrary.py [--rxnNamesFile <FileName or auto>] -l | --list
```

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

## DESCRIPTION

Perform a combinatorial enumeration of a virtual library of molecules for a reaction specified using a reaction name or SMIRKS pattern and reactant input files.

The SMIRKS patterns for supported reactions names [ Ref 134 ] are retrieved from file, ReactionNamesAndSMIRKS.csv, available in MayaChemTools data directory. The current list of supported reaction names is shown below:

'1,2,4-triazole\_acetohydrazide', '1,2,4-triazole\_carboxylic\_acid\_ester', 3\_nitrile\_pyridine, Benzimidazole\_derivatives\_aldehyde, Benzimidazole\_derivatives\_carboxylic\_acid\_ester, Benzofuran, Benzothiazole, Benzothiophene, Benzoxazole\_aromatic\_aldehyde, Benzoxazole\_carboxylic\_acid, Buchwald\_Hartwig, Decarboxylative\_coupling, Fischer\_indole, Friedlaender\_chinoline, Grignard\_alcohol, Grignard\_carbonyl, Heck\_non\_terminal\_vinyl, Heck\_terminal\_vinyl, Heteroaromatic\_nuc\_sub, Huisgen\_Cu\_catalyzed\_1,4\_subst, Huisgen\_disubst\_alkyne, Huisgen\_Ru\_catalyzed\_1,5\_subst, Imidazole, Indole, Mitsunobu\_imide, Mitsunobu\_phenole, Mitsunobu\_sulfonamide, Mitsunobu\_tetrazole\_1, Mitsunobu\_tetrazole\_2, Mitsunobu\_tetrazole\_3, Mitsunobu\_tetrazole\_4, N\_arylation\_heterocycles, Negishi, Niemietowski\_quinazoline, Nucl\_sub\_aromatic\_ortho\_nitro, Nucl\_sub\_aromatic\_para\_nitro, Oxadiazole, Paal\_Knorr\_pyrrole, Phthalazinone, Pictet\_Spengler, Piperidine\_indole, Pyrazole, Reductive\_amination, Schotten\_Baumann\_amide, Sonogashira, Spiro\_chromanone, Stille, Sulfon\_amide, Suzuki, Tetrazole\_connect\_regioisomer\_1, Tetrazole\_connect\_regioisomer\_2, Tetrazole\_terminal, Thiazole, Thiourea, Triaryl\_imidazole, Urea, Williamson\_ether, Wittig

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, --compute2DCoords <yes or no> [default: yes]

Compute 2D coordinates of product molecules before writing them out.

-i, --infile <ReactantFile1, ReactantFile2...>

Comma delimited list of reactant file names for enumerating a compound library using reaction SMIRKS. The number of reactant files must match number of reaction components in reaction SMIRKS. All reactant input files must have the same format.

--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. These parameters apply to all reactant input files, which must have the same file format.

-e, --examples

Print examples.

-h, --help

Print this help message.

-l, --list

List available reaction names along with corresponding SMIRKS patterns without performing any

**-m, --mode <RxnByName or RxnBySMIRKS>** [default: RxnByName]  
 Indicate whether a reaction is specified by a reaction name or a SMIRKS pattern. Possible values: RxnByName or RxnBySMIRKS.

**-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: kekulize,no  
 SMILES: kekulize,no,smilesDelimiter,space, smilesIsomeric,yes,  
 smilesTitleLine,yes

**-p, --prodMolNames <UseReactants or Sequential>** [default: UseReactants]  
 Generate names of product molecules using reactant names or assign names in a sequential order. Possible values: UseReactants or Sequential. Format of molecule names: UseReactants - <ReactName1>\_<ReactName2>...\_Prod<Num>; Sequential - Prod<Num>

**--overwrite**  
 Overwrite existing files.

**-r, --rxnName <text>**  
 Name of a reaction to use for enumerating a compound library. This option is only used during 'RxnByName' value of '-m, --mode' option.

**--rxnNamesFile <FileName or auto>** [default: auto]  
 Specify a file name containing data for names of reactions and SMIRKS patterns or use default file, ReactionNamesAndSMIRKS.csv, available in MayaChemTools data directory.  
 Reactions SMIRKS file format: RxnName,RxnSMIRKS.  
 The format of data in local reaction names file must match format of the reaction SMIRKS file available in MayaChemTools data directory.

**-s, --smirksRxn <text>**  
 SMIRKS pattern of a reaction to use for enumerating a compound library. This option is only used during 'RxnBySMIRKS' value of '-m, --mode' option.

**--sanitize <yes or no>** [default: yes]  
 Sanitize product molecules before writing them out.

**-w, --workingdir <dir>**  
 Location of working directory which defaults to the current directory.

## EXAMPLES

To list all available reaction names along with their SMIRKS pattern, type:

```
% RDKitEnumerateCompoundLibrary.py -l
```

To perform a combinatorial enumeration of a virtual compound library corresponding to named amide reaction, Schotten\_Baumann\_amide and write out a SMILES file type:

```
% RDKitEnumerateCompoundLibrary.py -r Schotten_Baumann_amide  

-i 'SampleAcids.smi,SampleAmines.smi' -o SampleOutCmpdLibrary.smi
```

To perform a combinatorial enumeration of a virtual compound library corresponding to an amide reaction specified using a SMIRKS pattern and write out a SD file containing sanitized molecules, computed 2D coordinates, and generation of molecule names from reactant names, type:

```
% RDKitEnumerateCompoundLibrary.py -m RxnBySMIRKS  

-s '[O:2]=[C:1][OH].[N:3]>>[O:2]=[C:1][N:3]'  

-i 'SampleAcids.smi,SampleAmines.smi' -o SampleOutCmpdLibrary.sdf
```

To perform a combinatorial enumeration of a virtual compound library corresponding to an amide reaction specified using a SMIRKS pattern and write out a SD file containing unsanitized molecules, without generating

2D coordinates, and a sequential generation of molecule names, type:

```
% RDKitEnumerateCompoundLibrary.py -m RxnBySMIRKS -c no -s no
-p Sequential -s '[O:2]=[C:1][OH].[N:3]>>[O:2]=[C:1][N:3]'
-i 'SampleAcids.smi,SampleAmines.smi' -o SampleOutCmpdLibrary.sdf
```

#### AUTHOR

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#### SEE ALSO

RDKitConvertFileFormat.py, RDKitFilterPAINS.py, RDKitSearchFunctionalGroups.py, RDKitSearchSMARTS.py

#### COPYRIGHT

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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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