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MolProp TK – Java

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CHAPTER

ONE

THEORY

1.1 Filtering Theory

1.1.1 Introduction

Filtering attempts to eliminate inappropriate or undesirable compounds from a large set before beginning to use them in modeling studies. The goal is to remove all of the compounds that should not be suggested to a medicinal chemist as a potential hit. This exercise is obviously case dependent, depending on ease of the assay, intended target, needs of the user, and so on.

To match this need, the default filter encapsulates many of the standard filtering principles, such as removal of unstable, reactive, and toxic moieties. In addition, MolProp TK allows the customization of the filtering criteria to fit specific needs.

The criteria for passing or failing a given molecule fall into three categories.

- Physical properties
  - Molecular weight
  - Topological polar surface area (TPSA)
  - logP
  - Bioavailability
- Atomic and functional group content
  - Absolute and relative content of heteroatoms
  - Limits on a very wide variety of functional groups
- Molecular graph topology
  - Number and size of ring systems
  - Flexibility of the molecule
  - Size and shape of non-ring chains

All of the data generated in filtering molecules can be written to a tab-separated file for easy import into a spreadsheet. This functionality allows for combining the values dynamically for a variety of purposes, including, but not limited to, determining which filter values best fit each project's needs.

History

When OpenEye's work on filtering technology began in 2000, it was designed simply to remove compounds with reactive or otherwise undesirable functional groups. Over the years, the understanding of lead-like and drug-like compound selection has advanced. In addition, with the publication of Lipinski's "Rule of 5" [Lipinski-1997], more and more pharmacokinetic properties have appeared earlier in the virtual screening process.

In addition to providing basic functional group selection, the technology is a one-stop database preparation tool aimed at generating databases suitable for high-throughput virtual screening. The following are some components of this tool.

- Cheminformatics quality control
  - Valence-state validation
  - Aromaticity perception
  - Implicit hydrogen perception
  - Bond-order perception
- Database preparation
  - Setting pKa states
  - Applying normalizations (tautomers and dative or hypervalent states)
- Compound selection
  - Physical properties (see *above*)
  - Assay counter-indicators (aggregators and dyes)
  - Promiscuous actives [Baell-2010]
  - PK ([Martin-2005], [Veber-2002], [Egan-2000], [Lipinski-1997])

Finally, it should be pointed out that in the virtual screening world, time is of the essence. Algorithms for preliminary database preparation should not take large amounts of time. Because of this, all the calculations included are 2D or graph-based algorithms. While this does occasionally limit the technology, it allows for the delivery of a product that is appropriate for the task of virtual-screening database preparation.

A Detailed Examination of False Positives and False Negatives

Nearly every computational tool used in early drug discovery yields statistically predictive, rather than absolutely definitive results. In nearly every case, prudence demands that one consider the causes of false positives and false negatives and make an attempt to optimize the area under the receiver-operator curve (ROC) for the computational tool. However, there are well-known methods for improving statistical predictions of this nature that are independent of the absolute false-positive and false-negative rates. These methods include filtering the population to which a test will be applied. By applying a test to smaller populations that only contain molecules appropriate for the specific application at hand, the negative impact of the false-positive rate on the predictive results can be dramatically improved.

A familiar example from the medical world will serve to illustrate this principle. Assume we have a test for the presence of the new *foo virus* which has an exceptional ROC curve with false-positive and false-negative values (1/1,000 and 1/1,000 respectively). Let us assume that the *foo syndrome*, caused by the *foo virus*, affects 1 person in 20,000. If we gave this test to 100,000 people from the general population, we would expect 5 to actually have the *foo syndrome*. With this test, there is only a 0.05% percent chance that any of them would not be detected (that is, be a false negative). However, we would expect there to be 100 false-positive test results. Thus of the 105 total positive test results, only 4.8% would actually have the *foo syndrome* (positive predictive value = 4.8%).

Table 1: Confusion table for the **unfiltered** *foo virus* test (prevalence 1 in 20,000)

	Actual Positive	Actual Negative	
Predicted Positive	True Positives = 5	False Positives = 100	Positive Predictive Value = 4.8%
Predicted Negative	False Negatives = 0	True Negatives = 99,895	

Alternatively, we could start by using very simple screening before applying the test. We first eliminate people who do not have any risk factors for contracting the *foo virus*. Next, we may eliminate people whose blood is incompatible with the test for the *foo virus*. Further, we may want to eliminate people who acknowledge that they will refuse treatment for the *foo virus* even if we determine that they do have it. By these admittedly simple screens, we apply the test for the *foo virus* to a much smaller group with a decidedly higher prevalence of the virus. For instance, after the filtering, we may be left with a group of only 1,000 people who have a 1 in 200 chance of having the syndrome. Now, we still have the same five people who actually have the disease, but we only expect one false-positive test. Now there are six total positive tests, and 83% of them actually have the syndrome! This is reflected in a much more reasonable (83%) positive predictive value.

Table 2: Confusion table for the **filtered** *foo virus* test (prevalence 1 in 200)

	Actual Positive	Actual Negative	
Predicted Positive	True Positives = 5	False Positives = 1	Positive Predictive Value = 83%
Predicted Negative	False Negatives = 0	True Negatives = 994	

Returning to drug design, in a ligand-based design tool such as **ROCS**, we can posit that the receiver-operator curve may have a false positive rate as low as 1 in 10,000. For this exercise, assume no false negatives. When using that to identify 50 inhibitors from a database of 2.5 million available compounds, we would identify 300 potential inhibitors, and 5 out of every 6 of these would be a false positive (positive predictive value of 17%). However, running `filter` first would eliminate 65% of the 2.5 million compounds, leaving 875,000 compounds to run through **ROCS**. There will be approximately 88 false positives along with the 50 true positives increasing the positive predictive value more than two-fold with relatively little work.

Table 3: Confusion table for the **unfiltered** ROCS virtual screen

	Actual Positive	Actual Negative	
Predicted Positive	True Positives = 50	False Positives = 250	Positive Predictive Value = 17%
Predicted Negative	False Negatives = 0	True Negatives = 2,499,700	

Table 4: Confusion table for the **filtered** ROCS virtual screen

	Actual Positive	Actual Negative	
Predicted Positive	True Positives = 50	False Positives = 88	Positive Predictive Value = 36%
Predicted Negative	False Negatives = 0	True Negatives = 874,862	

Filtering Principles

The same principle of increasing the positive predictive value by removing obvious true negatives applies to screening for lead candidates, regardless of whether it is virtual screening or high-throughput screening (HTS). While both are reasonable screens, each can be plagued by very low positive predictive values (despite low false-positive rates), particularly when applied to all available compounds or large virtual libraries. Simple filtering techniques focus the set of compounds passed on to more computationally intensive screening methods.

The first approach is to filter based on *functional groups*. Generally speaking, there are toxic and reactive functional groups that should be removed from consideration, such as alkyl bromides or metals. There are also functional groups that are not strictly forbidden, but are undesirable in large quantities. For instance, parafluorobenzene or trifluoromethyl have specific purposes, but heavily fluorinated molecules can be eliminated.

Beyond simple functional group filtering, both simple and complex physical properties can be used to characterize the kinds of compounds to keep or to eliminate. These properties attempt to consider drug-like qualities, such as bioavailability, solubility, toxicity, and synthetic accessibility, even before the primary high-throughput or virtual screening, which are primarily geared toward detecting potency alone. The best known physical property filters is *Lipinski's "rule-of-five"*, which focuses on bioavailability [Lipinski-1997]. However, many other physical properties, such as *solubility*, *atomic content*, *ring structures*, and *surface area ratios* can also be considered. MolProp TK provides algorithms for calculating many of these properties and applying them with filters based on literature studies.

Finally, types of compounds that can be troublesome at later stages should be eliminated. For instance, Shoichet's *aggregating compounds* often produce false positives that can waste enormous resources if they are identified by virtual or HTS ([McGovern-2003]; [Seidler-2003]). Similarly, *dyes* can appear to be inhibitors by interfering with colorimetric or fluorometric assays or by nonspecific binding to the target protein.

Variations of Filters

Different types of filters are appropriate under different circumstances. Very early in a project, when little or no information on the structure-activity relationship (SAR) is available, very strict drug-like filters can be applied. This avoids spending chemistry resources to pursue difficult compounds that may not be modifiable for appropriate properties. However, when considering compounds to purchase for HTS, different filters can be applied. Oprea et al. pointed out that the best molecules for initial HTS are smaller and have less functionality than drugs but show some activity [Oprea-2000]. Therefore, strict lead-like filters can be applied to ensure that hits identified from HTS can be investigated for potential leads, especially those that may be larger or more highly functionalized. However, when SAR suggests that particular compounds or series may yield valuable information, filtering criteria can be loosened, because secondary screens can be effective in detecting useful compounds. Circling back to the medical analogy, this is a case where an improved primary screen with a dramatically improved false-positive rate (e.g., 1 in 100,000) can be applied to a larger population without detrimental effects on the positive-predictive value.

MolProp TK provides the following filters:

- **BlockBuster**: The BlockBuster filter is based on 141 best-selling, non-antibiotic prescription drugs. We designed the physical property portion of the filter so that it passes all of the compounds. The physical property values in this filter are quite good. However, the functional group filters in this filter may be too restrictive because 141 compounds will not span all acceptable functionality.
- Drug: The original drug filter is provided as well [Oprea-2000], but has been shown to be very restrictive. The BlockBuster filter was developed as an alternative.
- Fragment: The fragment filter is designed specifically to filter molecules with attachment points. This filter is used inside **CHOMP** to restrict the fragments generated for the **BROOD** database.
- Lead: The Lead filter corresponds to the Oprea lead-like filters that are useful for preparing HTS screening databases.
- PAINS: The PAINS filter is based on work by Baell which describes identification and filtering of promiscuous (nonspecific) actives across a number of screening types and targets [Baell-2010]. Unlike the other filter types,

the PAINS filter consists of only functional group filters; no physical property filters are included. In practice, combination of the PAINS filter with a user-defined set of physical property filters may be desirable.

Hint

We recommend the default BlockBuster filter for most purposes. If you have specific filtering needs or are unsatisfied with the results, please see the *filter file*.

If you modify the *filter file*, the depictions found in the *Functional Group Rules* section can be particularly helpful in determining which functional groups are indicated by each name in the file.

Accumulation of Rules

FILTER contains rules to judge the quality of molecules on various properties. Individually, each of these rules seems quite reasonable and even profitable. However, when each molecule is tested against hundreds of individual filters, the fraction of molecules that pass all the filters can be surprisingly small. Sometimes less than 50% of vendor databases pass the filters. If this is unacceptable, we recommend you examine the predicted aggregator, solubility, and Veber filters. In our experience, these are the most common failures. The best method of investigating failures is looking at the filter log.

The BlockBuster filter addresses these challenges. Sometimes the range needs to be expanded in order to allow more compounds to pass. For each value, its properties extend from the 2.5th percentile to the 97.5th percentile. The differences between the original BlockBuster filter and the adjusted filter are both in reasonable ranges. For instance, the full range of molecular weights for the BlockBuster filter spans 130 to 781, while the 2.5th percentile is 145 and the 97.5th percentile is 570. Surprisingly, when the reduced filter is used, only 75 of the 141 original molecules pass the filter! This demonstrates how slight changes to many filters can lead to a significant reduction in the number of compounds that pass all filters.

The opposite approach of allowing everything to pass can be equally challenging. For example, a filter was designed around the "small molecule drug" file available from the DrugBank website. In order to pass all of these molecules, including some that would no longer be acceptable, many of the individual filters must be set to unreasonable values, such as a molecular weight range from 30 to 1500 and a heteroatom count range from 1 to 60.

Hint

Because every project is different, we recommend that you inspect each *filter file*. The depictions found in the *Functional Group Rules* section can be particularly helpful in discerning what functional groups are desirable and undesirable.

1.2 Filter Preprocessing

Before the application of any *molecular property filters*, a preprocessing step may be used to alter the molecule significantly to fit the criteria needed for most modeling applications. This filter preprocessing step is applied to each molecule in a series of stages in the following order:

1. *Metal Removal*
2. *Salt Removal*
3. *Canonicalization*
4. *pKa Normalization*
5. *Normalization*
6. *Reagent Selection*

7. *Type Checking*
8. *MMFF94 Atom Type Checking*

1.2.1 Metal Removal

Metal removal is the first stage of element-based filtering. This stage removes specified metal complexes from the molecule. It will not reject a molecule with a metal complex. This allows the filter to treat atoms in the counterion portion of a molecule separately from the atoms in the primary portion of the molecular record.

For instance, organic molecules that are complexed with silver can be eliminated based on their metal chelate even though they themselves are acceptable, while at the same time eliminating a sulfate counterion from another molecule before it leads to elimination of the acceptable cationic molecule.

See also

Elemental Filters

1.2.2 Salt Removal

This step deletes all atoms that are not part of the largest connected component of a compound. This effectively eliminates all non-covalently bound portions of the compound.

1.2.3 Canonicalization

This step canonicalizes the atom and bond order of the portion of the molecule that remains after the previous removal steps. This is necessary to avoid different atom orderings producing slightly different normalizations in the following normalization steps.

1.2.4 pKa Normalization

pKa normalization uses a rule-based system to set the ionization state of input molecules. If pKa normalization is turned on, the molecule is set to its most energetically favorable ionization state for pH=7.4. The rule-based nature of this calculation allows it to be very fast. Furthermore, despite being rule-based, this approach takes into account many secondary charge interactions.

While more advanced levels of theory can be found for predicting ionization states, this method is very well suited to virtual-screening database preparation. However, this may not be appropriate for hit-to-lead or lead optimization.

1.2.5 Normalization

In addition to *pKa normalization*, MolProp TK allows any number of additional molecular normalizations. Since normalizations are usually specific to a particular company or site, MolProp TK provides the ability for users to input normalizations, such as the nitro tautomer state, but does not provide default implementations.

1.2.6 Reagent Selection

Reagent selection for small linear library synthesis or large combinatorial library synthesis is usually a necessary task. A user hoping to identify a set of acyl-halide reagents could specify a selection parameter to require each compound to have exactly one acyl-halide. In addition, the filter could be modified to exclude functional groups (such as primary amines) that may be acceptable for typical lead-like molecules, but are not acceptable for the specific reagent the user has in mind.

Therefore, the selection parameter is the reverse of a filtering parameter. The molecule *must include* the given substructure in order to pass the filter.

See also

The *select parameter* in filter files.

1.2.7 Type Checking

This checks the valence state and formal charge of the entire molecule. The check identifies molecules that are poorly specified, or represent nonsensical chemical states, often from corrupt input data. For example, an oxygen with eight hydrogens attached or a carbon with a +9 formal charge would be rejected.

1.2.8 MMFF94 Atom Type Checking

This checks that all atoms in the molecule have valid MMFF94 atom type assignments. The check identifies molecules that will fail downstream processing that depends on MMFF94 atom types (e.g., **Omega**).

1.3 Molecular Properties and Predictors

MolProp TK provides a range of properties to predictors to be used as molecular filters. Molecular properties are distinct physical properties that can be measured, including the following:

- *Structural and Chemical Features*
- *Functional Groups*

There have been several attempts to develop fast-approximate QSAR models for bioavailability. The first of these was *Lipinski's work* [Lipinski-1997], followed by work at Pharmacopia [Egan-2000], Abbott [Martin-2005], and GSK [Veber-2002]. The simplest and probably most trusted work includes studies of *LogP* and *PSA* used by Egan. Martin's Abbott Bioavailability Score (ABS) appears to be a refinement of the first generation models and is designed specifically to categorize a molecule's probability of having a bioavailability >10% in rats.

See also

The *Pharmacokinetic Predictors* section in the Filter Files chapter.

1.3.1 Structural and Chemical Features

A number of important structural and chemical features of molecules should be limited for virtual screening. The following simple measures are provided as filterable properties:

- Molecular weight
- Ring count
- Ring-system size
- Size of non-ring structures
- Length of unbranched chains
- Heteroatom fraction
- Halide fraction
- Formal charges
- Rotatable bonds

MolProp TK also includes slightly more complex algorithms for hydrogen bond donors and acceptors as well as chiral centers.

See also

The *Basic Properties* section in the Filter Files chapter.

1.3.2 Functional Groups

Functional group removal remains at the heart of the **FILTER** algorithm. Functional groups fall into several categories, including:

- Reactive or labile groups
- Undesirable groups
- Generally acceptable groups
- Protecting groups
- User-derived groups

Reasonable defaults are provided for each functional group in the above categories, with the filter files being designed as basic guides. They can be tailored for each user's particular needs. Examining the filter file can provide useful information. Developing a custom filter for a specific task is strongly encouraged.

See also

The filter files contain only functional group names. For clarification of the definitions, please refer to the *Functional Group Rules* section for complete descriptions.

1.3.3 Dyes

In the past, colored molecules interfered with many high-throughput assays. While assay technology continues to advance and this problem has decreased, most dyes are not commonly carried forward in lead development projects. Therefore, a pattern-based filter for dye molecules is included. While these patterns occasionally identify molecules that are considered acceptable by some users, in general, they identify molecules that the majority of chemists would rather not see at the top of their virtual screening hit lists.

1.3.4 LogP

The XLOGP algorithm ([Wang-R-1997]) is provided because its atom type contribution allows calculation of the XLogP contribution of any fragment in a molecule and allows minimal corrections in a simple additive form to calculate the LogP of any molecule made from combinations of fragments. Further, although the method contains many free parameters, its simple linear form allows for ready interpretation of the model, and most of the parameters in the model make rational sense.

Unfortunately, the original algorithm is difficult to implement as published. First, the internal hydrogen bond term was calculated using a single 3D conformation, which was found to be both arbitrary and unnecessary. This arbitrary 3D calculation has been replaced with a 2D approach to recognize common internal hydrogen bonds. In tests, the 2D method worked comparably to the published 3D algorithm. Next, the training set had a few subtle atom-type inconsistencies.

Both of these problems were corrected and refit to the original XLOGP training data. This implementation gives results that are quite similar to the original XLOGP algorithm, so it is called OEXLogP to distinguish it from the original method.

See also

- The *XLogP parameter* in the Filter Files chapter.

1.3.5 LogS

The work of Samuel Yalkowsky [Yalkowsky-1980] at the University of Arizona has resulted in what is now called the "generalized solvation equation." It states that the solubility of a compound can be broken into two steps, first the melting from the pure solid to pure liquid, and second, the phase transfer from pure liquid into water. For many small organic molecules, this second step is somewhat related to LogP.

Because of this relationship, we explored the use of the XLogP atom types in solubility prediction, with the goal of providing an approximate though robust and fast method for calculating solubility. We fit the XLogP atom types to a training set of nearly 1000 public solubility values, then derived a linear model for solubility. The model is extremely fast and can classify compounds as insoluble, poorly soluble, slightly soluble, moderately, soluble, or very soluble. However, it has difficulty in predicting the solubility of compounds with ionizable groups. Furthermore, it is not suitable for the PK predictions that come late in a project. Nevertheless, it can be utilized to eliminate compounds with severe solubility problems early in the virtual screening process.

See also

The *solubility parameter* in the Filter Files chapter.

1.3.6 Polar Surface Area

Topological polar surface area (TPSA) is based on the algorithm developed by Ertl et al [Ertl-2000]. In Ertl's publication, use of TPSA both with and without accounting for phosphorus and sulfur surface area is reported. However, evidence shows that in most PK applications, it is better to avoid counting the contributions of phosphorus and sulfur atoms toward the total TPSA for a molecule. This implementation of TPSA allows either inclusion or exclusion of phosphorus and sulfur surface area, with the default being to exclude it.

See also

Including phosphorus and sulfur surface area:

- The `PSA_USE_SandP` parameter in the *filter file*.

Warning

TPSA values are mildly sensitive to the protonation state of a molecule. If the pKaNorm parameter is false, the TPSA value is calculated using the input structure, and if pKaNorm is true, the TPSA is calculated using the pKa normalized molecular structure.

See also

- The *pKa normalization* section of the Filter Preprocessing chapter.

1.3.7 Lipinski and Hydrogen Bonds

The work of Lipinski [Lipinski-1997] introduced the application of simple filter-like rules to roughly predict late-stage PK properties, in particular oral bioavailability. Unfortunately, Lipinski's rule of five has come into the common vernacular to such a large degree that some of the specific details are often lost. There are two critical examples of this. First, Lipinski used "violation of two rules" to categorize compounds. In the subsequent analysis, a significant difference in the two populations of molecules was detected, however, little analysis of the importance of a single violation was done. However, many now consider a single violation to be bad and two violations to be worse. Second, Lipinski used well-codified and well-understood yet imprecise definitions of "hydrogen bond donors" and "hydrogen bond acceptors" in his classification model. While this makes the algorithm quite understandable and easy to implement, it sometimes causes confusion with those who prefer more refined definitions of hydrogen bond donors and acceptors.

To address the first problem, users are allowed to set the number of Lipinski failures required to reject a molecule. In keeping with the original publication, the default value is 2. To address the second problem, two kinds of hydrogen bond donors and acceptors are calculated. In the Lipinski calculation, the published definitions are used (donor count is the number of nitrogen or oxygen atoms with at least one hydrogen attached and acceptors are the number of nitrogens and oxygens). For calculation of the number of donors and acceptors in the molecule for the sake of chemical properties, a more complex algorithmic approach is taken. This approach identifies the donors and acceptors outlined in the work of Mills and Dean [Mills-Dean-1996] and also in the book by Jeffrey [Jeffrey-1997].

See also

The *Lipinski violations* and *hydrogen-bond acceptors* sections in the Filter Files chapter.

1.3.8 Aggregators

The Shoichet lab ([McGovern-2003]; [Seidler-2003]) has demonstrated the importance of small-molecule aggregation in medium and high-throughput assays. Because these small-molecule aggregates can sequester some proteins, they give the appearance of being active inhibitors. There are now several hundred published aggregators, in addition to a published QSAR model for predicting aggregation propensity. The user can eliminate any of the known aggregators and also eliminate compounds that are predicted to be aggregators using the QSAR model. The published QSAR model for predicting aggregators may be considered quite aggressive, as it occasionally identifies compounds that are known to be genuine small-molecule inhibitors of a specific protein. While in most cases this model can be useful, it is important to gain experience with the model and judge the performance for specific needs.

In some cases, aggregation properties are specific to specific experimental conditions, thus caution should be exercised in the interpretation of these predictions. Nevertheless, aggregation remains an important issue in HTS hit follow-up and, short of experimental validation, this flag may be the best available.

See also

The *aggregators parameter* in the Filter Files chapter.

1.3.9 PAINS

Pan-assay interference compounds (PAINS) filters are a set of functional group filters created to identify and filter promiscuous (nonspecific) actives across a number of screening types and targets [Baell-2010]. The original PAINS paper includes a set of functional group prefilters, created via two iterations of their work, and three sets of structure class filters, called filter sets A, B, and C, which were used to identify and remove promiscuous actives. The OpenEye PAINS filter set is a combination of all four filter sets (the functional group prefilter set plus the three structural class sets) into a single filter set.

There are two distinct use cases for the PAINS filters. The first is the typical prefiltering of structures prior to screening or compound selection to remove undesirable molecules. One can simply eliminate any molecules which fail the PAINS filtering.

The second use case, which may ultimately be more interesting, is to use the PAINS filters retrospectively on a set of data which has been filtered (and tested) using another methodology. In this scenario, the PAINS filters can be used to identify potentially problematic reactive functionality in otherwise reasonable, drug-like structures. By using the table output mode and identifying matches for the A, B, and C filter sets, one can identify fairly specific chemical functionalities that have been known to result in nonspecific activity. This can be useful information for either prioritizing further lead development or for modifying lead structures to mitigate adverse reactivity.

There are approximately 650 SMARTS rules which have been converted from the SLN query strings provided in the supplemental information of the original paper. For the functional group filters, the authors do not provide identifying names for each individual filter, so our PAINS rules are named based on the comments used to describe each functional group class, prefixed with the string `pains_fg_[classname]`. For the structural class filters, the authors provided unique RegID values for each filter. For those cases, our rules are named based on the PAINS group and RegID as `pains_[group]_[RegID]`.

Note that in certain cases, the SLN queries cannot be represented with a single SMARTS, so in those cases the rules have been split out into multiple SMARTS patterns and are named `pains_[group]_[RegID]1`, `pains_[group]_[RegID]2`, etc.

Hint

Unlike the other filter types, the PAINS filter consists only of functional group filters; no physical property filters are included. It may be desirable to combine the PAINS filter with a separate user-defined set of physical property filters. The *filter file* section describes the creation of additional filter rules.

1.4 Filter Files

A user can provide two parameter files if they would like to override or augment the default parameter sets. The first is a *filter file*. It provides acceptable limits for all of the physical properties and functional groups in the default filter. The second is a `NEWRULE` file, which allows you to augment a filter with a set of additional rules.

There are four types of statements that can occur in a filter file:

- Physical property limits
- Rules
- New rules
- Selections

The statements should occur one per line in the filter file.

> **Note**
>
> If the appropriate line is not in the filter file, or the value is false, the respective measure will not be used in filtering and its value will not be included in any table-based output.

1.4.1 Physical Property Limits

There are a large number of physical property limits. They occur as three fields on a line. For example:

```
MIN_HETEROATOMS 2 "Minimum number of heteroatoms"
```

The first field is the property keyword, the second field is the value assigned to that keyword, and the third field is a brief informational message. There are a fixed number of physical property keywords. No additional physical property keywords can be added by the user. The current keywords and brief definitions of each are listed below.

> **Hint**
>
> The values listed below are those found in the default *BlockBuster* filter.

Basic Properties

Molecular Weight

Isotopic molecular weight.

```
MIN_MOLWT 130 "Minimum molecular weight"
MAX_MOLWT 781 "Maximum molecular weight"
```

Heavy Atom Count

Number of non-hydrogen atoms.

```
MIN_NUM_HVY 9 "Minimum number of heavy atoms"
MAX_NUM_HVY 55 "Maximum number of heavy atoms"
```

Carbon Count

Number of carbons.

```
MIN_CARBONS 3 "Minimum number of carbons"
MAX_CARBONS 41 "Maximum number of carbons"
```

Hetero Count

Number of non-carbon and non-hydrogen atoms.

```
MIN_HETEROATOMS 1 "Minimum number of heteroatoms"
MAX_HETEROATOMS 14 "Maximum number of heteroatoms"
```

Heteroatom to Carbon Ratio

Hetero count/carbon count.

```
MIN_Het_C_Ratio 0.04 "Minimum heteroatom to carbon ratio"
MAX_Het_C_Ratio 4.0 "Maximum heteroatom to carbon ratio"
```

Chiral Count

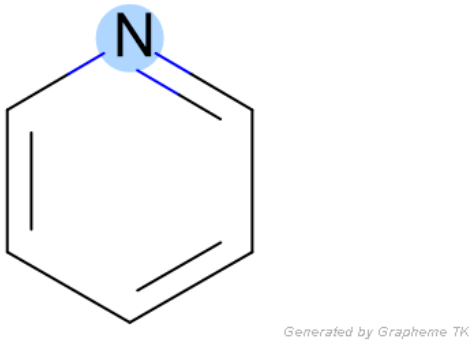
Number of chiral atoms.

```
MIN_CHIRAL_CENTERS 0 "Minimum chiral centers"
MAX_CHIRAL_CENTERS 21 "Maximum chiral centers"
```

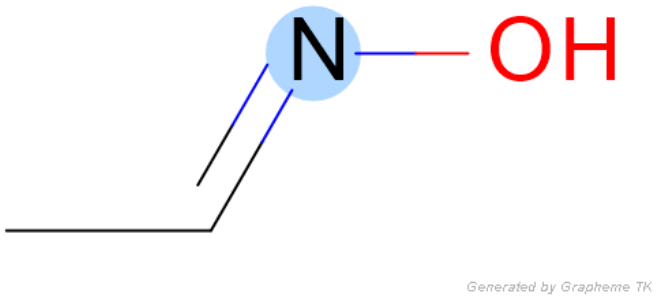
Hydrogen Bond Acceptors

Number of atoms which match any of the following:

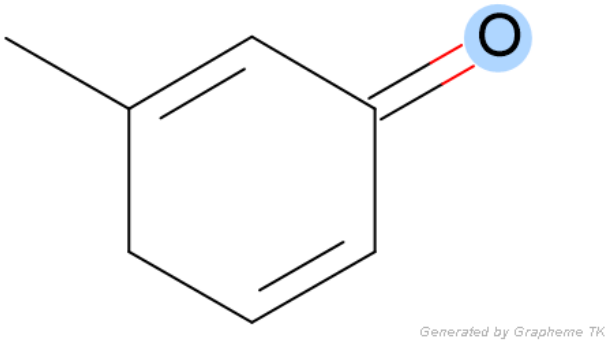
- Degree 2, aromatic, nonpositive nitrogens. An example is shown below.



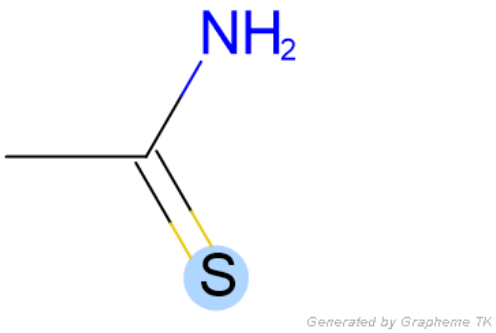
- Electron rich (negative), valence less than 4, nonaromatic nitrogens. An example is shown below.



- Negatively charged (does not withdraw electrons), neutral, nonaromatic oxygens. An example is shown below.



- Degree 1, double bonded, electron rich, nonaromatic sulfur. An example is shown below.



This definition is from the work of Mills and Dean [Mills-Dean-1996] and also by Jeffrey [Jeffrey-1997].

```
MIN_HBOND_ACCEPTORS 0 "Minimum number of hydrogen-bond acceptors"
MAX_HBOND_ACCEPTORS 13 "Maximum number of hydrogen-bond acceptors"
```

See also

- *OEGetHBondAcceptorCount* function
- *Lipinski and Hydrogen Bonds* section

Hydrogen Bond Donors

Number of hydrogen atoms on nitrogen, oxygen, or sulfur atoms. This definition is from the work of Mills and Dean ([Mills-Dean-1996]) and also the book by Jeffrey ([Jeffrey-1997]).

```
MIN_HBOND_DONORS 0 "Minimum number of hydrogen-bond donors"
MAX_HBOND_DONORS 9 "Maximum number of hydrogen-bond donors"
```

See also

- *OEGetHBondDonorCount* function

- *Lipinski and Hydrogen Bonds* section

Lipinski Acceptors

Number of nitrogens or oxygens. This definition is from the work of Lipinski [Lipinski-1997].

```
MIN_LIPINSKI_ACCEPTORS 1 "Minimum number of oxygen & nitrogen atoms"
MAX_LIPINSKI_ACCEPTORS 14 "Maximum number of oxygen & nitrogen atoms"
```

See also

- *OEGetLipinskiAcceptorCount* function
- *Lipinski and Hydrogen Bonds* section

Lipinski Donors

Number of nitrogens and oxygens with at least one hydrogen attached. This definition is from the work of Lipinski [Lipinski-1997].

```
MIN_LIPINSKI_DONORS 0 "Minimum number O & N atoms with hydrogens"
MAX_LIPINSKI_DONORS 6 "Maximum number O & N atoms with hydrogens"
```

See also

- *OEGetLipinskiDonorCount* function
- *Lipinski and Hydrogen Bonds* section

Halide Fraction

Percent of molecular weight from halides.

```
MIN_HALIDE_FRACTION 0.0 "Minimum Halide Fraction"
MAX_HALIDE_FRACTION 0.66 "Maximum Halide Fraction"
```

See also

- *OEGetHalideFraction* function

Formal Count

Number of atoms with a formal charge (excludes dative).

```
MIN_COUNT_FORMAL_CRG 0 "Minimum number formal charges"
MAX_COUNT_FORMAL_CRG 4 "Maximum number of formal charges"
```

Formal Sum

Total formal charge.

```
MIN_SUM_FORMAL_CRG -2 "Minimum sum of formal charges"
MAX_SUM_FORMAL_CRG 2 "Maximum sum of formal charges"
```

Connected Non-Ring

Considers sets of contiguous (bonded) non-ring atoms.

```
MIN_CON_NON_RING 0 "Minimum number of connected non-ring atoms"
MAX_CON_NON_RING 19 "Maximum number of connected non-ring atoms"
```

Unbranched Chains

The size of the longest chain of either heavy atoms or of all carbons. An unbranched atom is an atom with at most two connections to other heavy atoms and is not in a ring. A set of unbranched atoms which are connected together form a chain. A molecule may contain multiple chains which are isolated from each other by non-chain atoms (e.g., ring or branched atoms). The longest chain of heavy atoms and the longest chain of carbons are identified, and the MIN and MAX parameter filters are applied.

```
MIN_UNBRANCHED 1 "Minimum number of connected unbranched non-ring atoms"
MAX_UNBRANCHED 13 "Maximum number of connected unbranched non-ring atoms"
MIN_UNBRANCHED_C 0 "Minimum number of connected unbranched non-ring carbon"
MAX_UNBRANCHED_C 6 "Maximum number of connected unbranched non-ring carbon"
```

See also

- *OEGetLongestUnbranchedHeavyAtomsChain* function
- *OEGetLongestUnbranchedCarbonsChain* function

Total Functional Group Count

Total number of functional groups. Does not count any ring systems as functional groups. Degree 1 heteroatoms, particularly those with double bonds or dative bonds are considered part of ring systems and do not count as functional groups.

```
MIN_FCNGRP 0 "Minimum number of functional groups"
MAX_FCNGRP 7 "Maximum number of functional groups"
```

Note

This is different than the functional group rules.

Ring Systems

Number of ring systems (contiguous systems of ring atoms and bonds).

```
MIN_RING_SYS 0 "Minimum number of ring systems"
MAX_RING_SYS 5 "Maximum number of ring systems"
```

Ring Size

Maximum size of any single ring system.

```
MIN_RING_SIZE 0 "Minimum atoms in any ring system"
MAX_RING_SIZE 20 "Maximum atoms in any ring system"
```

Rotor Count

Number of rotatable bonds. Allows optional adjustment for aliphatic rings following the method of Oprea [Oprea-2000].

```
MIN_ROT_BONDS 0 "Minimum number of rotatable bonds"
MAX_ROT_BONDS 16 "Maximum number of rotatable bonds"
ADJUST_ROT_FOR_RING true "BOOLEAN for whether to estimate degrees of freedom in rings"
```

See also

- OEGetRotatableBondCount function

Rigid Count

Number of rigid bonds (non-rotatable bonds).

```
MIN_RIGID_BONDS 4 "Minimum number of rigid bonds"
MAX_RIGID_BONDS 55 "Maximum number of rigid bonds"
```

Unspecified Atom Stereo

Number of unspecified atom stereos

```
MIN_UNSPECIFIED_ATOM_STEREOS 0 "Minimum number of unspecified atom stereos"
MAX_UNSPECIFIED_ATOM_STEREOS 2 "Maximum number of unspecified atom stereos"
```

Note

`MIN_UNSPECIFIED_ATOM_STEREOS` and `MAX_UNSPECIFIED_ATOM_STEREOS` are not used for filtering in the default filters.

See also

- *OEGetNumUnspecifiedAtomStereos* function
- stereo atom
- Stereochemistry Perception chapter

- `OEAtomBase.HasStereoSpecified`

Unspecified Bond Stereo

Number of unspecified bond stereos

```
MIN_UNSPECIFIED_BOND_STEREOS 0 "Minimum number of unspecified bond stereos"
MAX_UNSPECIFIED_BOND_STEREOS 2 "Maximum number of unspecified bond stereos"
```

Note

`MIN_UNSPECIFIED_BOND_STEREOS` and `MAX_UNSPECIFIED_BOND_STEREOS` are not used for filtering in the default filters.

See also

- *OEGetNumUnspecifiedBondStereos* function
- stereo bond
- Stereochemistry Perception chapter
- `OEBondBase.HasStereoSpecified`

Atom Type Checks

Checks the validity of atom charges, valences or MMFF atom types for the entire molecule.

```
TYPECHECK     false "Screen for unusual valences or charges"
MMFFTYPECHECK false "Screen for atoms with unknown MMFF atom types"
```

See also

- *Type Checking*
- *SetTypeCheck*
- *MMFF94 Atom Type Checking*
- *SetMMFFTypeCheck*

LogP

The logP calculation is a derivative of the published XLOGP algorithm [Wang-R-1997] but is reparameterized without the dependence on 3D coordinates or the SYBYL/Mol2 aromaticity model.

XLogP

Calculated LogP.

```
MIN_XLOGP -3.0 "Minimum XLogP"
MAX_XLOGP 6.85 "Maximum XLogP"
```

Solubility

The solubility predictions are based on the atom types from the XLOGP algorithm (see [Wang-R-1997]) and on reparameterized atom types based on available solubility data. Rather than a quantitative cutoff, the solubility uses six allowable categories:

1. Insoluble
2. Poorly
3. Moderately
4. Soluble
5. Very
6. Highly

These categories are keywords used in the following filter files.

Solubility

Calculated solubility class.

```
MIN_SOLUBILITY insoluble "Minimum solubility"
```

Pharmacokinetic Predictors

Several secondary filters that are built upon published combinations of simpler properties are available.

Note

All of these properties are used for filtering in the default filters.

Anionic Carbon Count

Number of anionic carbons

```
MIN_ANION_C 0 "Minimum number of anionic carbons"
MAX_ANION_C 2 "Maximum number of anionic carbons"
```

Note

`MIN_ANION_C` and `MAX_ANION_C` are not used for filtering in the default filters.

See also

- *OEGetAnionicCarbonCount* function

Lipinski Violations

Number of allowable Lipinski violations. A single Lipinski violation is considered acceptable. The published work allows compounds to pass with a single violation but not multiple violations [Lipinski-1997].

```
MAX_LIPINSKI 3 "Maximum number of Lipinski violations"
```

See also

The *Lipinski theory* section in the Molecular Properties and Predictors chapter.

PSA

Peter Ertl's topological polar surface area (phosphorus and sulfur areas are optional) [Ertl-2000].

```
PSA_USE_SandP false "Count S and P as polar atoms"
MIN_2D_PSA 0.0 "Minimum 2-Dimensional (SMILES) Polar Surface Area"
MAX_2D_PSA 205.0 "Maximum 2-Dimensional (SMILES) Polar Surface Area"
```

See also

The *PSA theory* section in the Molecular Properties and Predictors chapter.

GSK/Veber

Veber's measure of bioavailability (PSA > 140 or Rotatable bonds >10) [Veber-2002].

```
GSK_VEBER false "PSA>140 or >10 rot bonds"
```

Abbott/Martin

Yvonne Martin's Abbott Bioavailability Score [Martin-2005]. This is reported as a probability that F>10% in rats.

```
MIN_ABS 0.11 "Minimum probability F>10% in rats"
```

Pharmacopia/Egan

"Egan egg" measure of bioavailability (LogP >5.88 or PSA > 131.6) [Egan-2000].

```
PHARMACOPIA false "LogP > 5.88 or PSA > 131.6"
```

Aggregators

Aggregators are small molecules that can interfere with assay results by sequestering proteins in an aggregation of small molecules in solution. They appear to have activity in many assays, but in fact are usually not specific inhibitors of the protein in question. This includes two measures of whether a molecule is one of the aggregators defined by Shoichet et al. ([McGovern-2003]; [Seidler-2003]). The first measure, AGGREGATORS, states whether the molecule is an exact match to one of the approximately 400 published aggregators. The second measure, PRED_AGG, states whether the molecule is included in Shoichet's QSAR model for predicting aggregators.

Aggregators

Whether a compound is known or predicted to aggregate in concentrations common in virtual screening.

```
AGGREGATORS true "Eliminate known aggregators"
PRED_AGG false "Eliminate predicted aggregators"
```

Elemental Filters

The elemental filters are applied in this order:

1. Test for the existence of any of the metals in the `ELIMINATE_METALS` filter in the molecule.
2. Remove salts by stripping away all the disconnected components except for the largest.
3. Test to make sure only atoms specified in `ALLOWED_ELEMENTS` filter are in the molecule.

See also

- *Metal Removal*
- *Salt Removal*

The format of the two elemental filter fields is the keyword followed by a comma-delimited list of atomic symbols.

Eliminate Metals

Any molecule with the atoms indicated in `ELIMINATE_METALS` fail to pass the filter.

```
ELIMINATE_METALS Sc,Ti,V,Cr,Mn,Fe,Co,Ni,Cu,Zn,Y,Zr,Nb,Mo,Tc,Ru,Rh,Pd,Ag,Cd
```

Allowed Elements

Molecules with atoms other than those specified by `ALLOWED_ELEMENTS` fail to pass the filter.

```
ALLOWED_ELEMENTS H,C,N,O,F,P,S,Cl,Br,I
```

Aromatic Ring Count

Uses the result of the function OEGetAromaticRingCount (see toolkit docs) to filter molecules based on their number of aromatic rings.

```
MIN_AROMATIC_RING_COUNT 1 "Minimum aromatic ring count"
MAX_AROMATIC_RING_COUNT 6 "Maximum aromatic ring count"
```

CSP3 Carbon Fraction

Uses the result of the *OEGetFractionCsp3* function from MolProp TK to filter molecules based on their CSP3 carbon fraction.

```
MIN_FRACTION_CSP3 0.1 "Minimum fraction CSP3 carbons"
MAX_FRACTION_CSP3 0.5 "Maximum fraction CSP3 carbons"
```

1.4.2 Functional Group Rules

Rules statements set the limits for the maximum number of the specified type of functional group that may be allowed in the molecule.

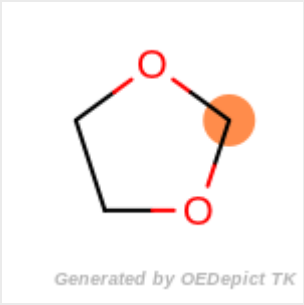
The first field of a rule statement is the word RULE in all capital letters. The second field is a number indicating the maximum number of the group allowed in a molecule. The third field is the functional group keyword. Functional group keywords are case sensitive.

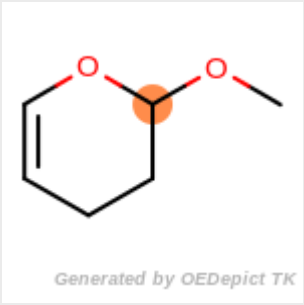
```
RULE 0 acid_halide
```

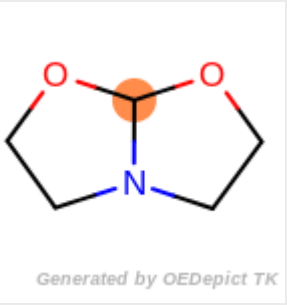
The following is a list of functional groups which the filter recognizes by default. Three example matches are provided with the atoms that correspond to each other highlighted.

> **Note**
>
> Due to the highly complex nature of the patterns, in particular recursive SMARTS, it is not possible to fully highlight every atom that was included as part of the match.

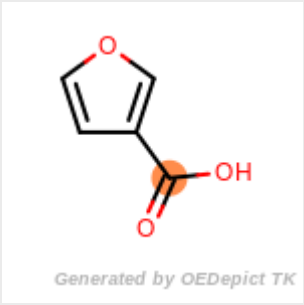
acetal

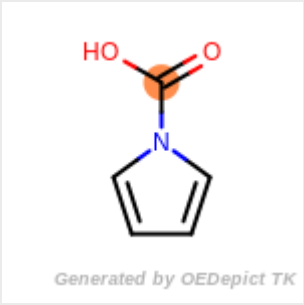


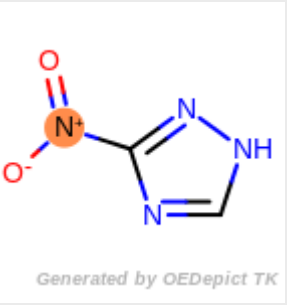




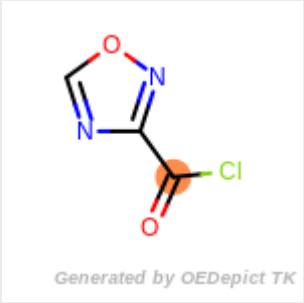
acid

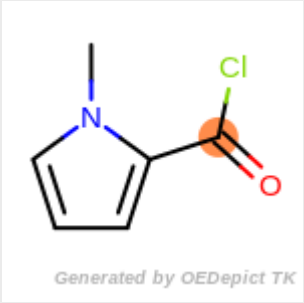


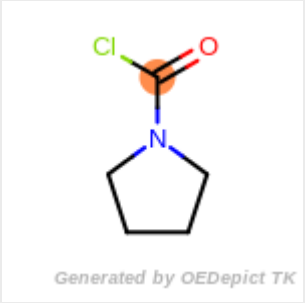




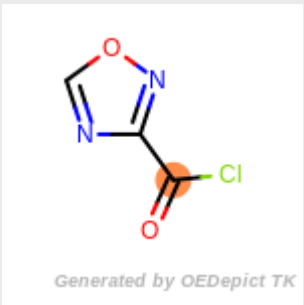
acid_chloride

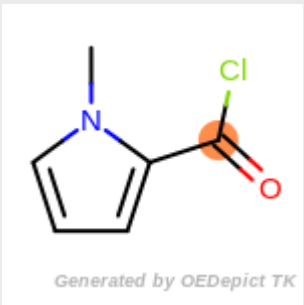


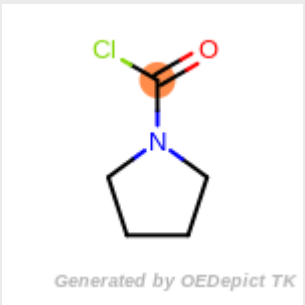




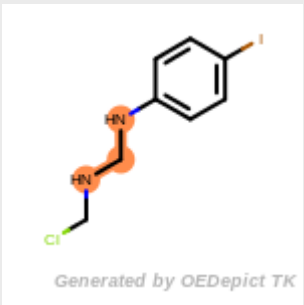
acid_halide

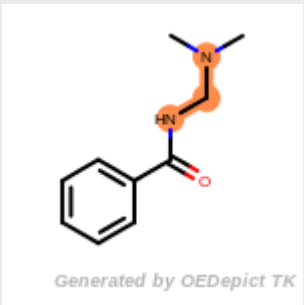


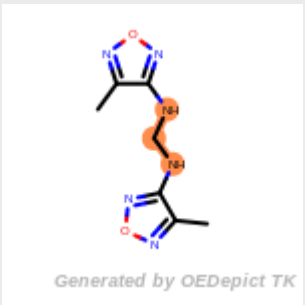




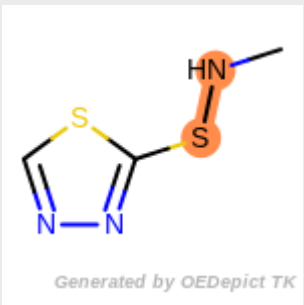
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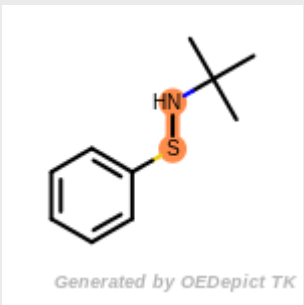


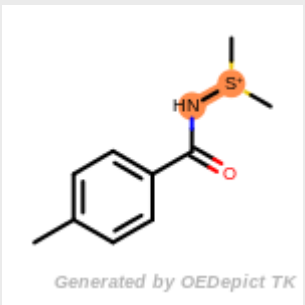




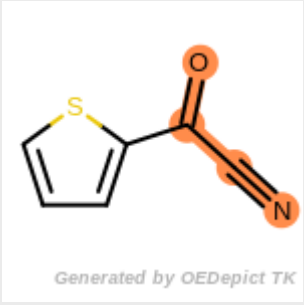
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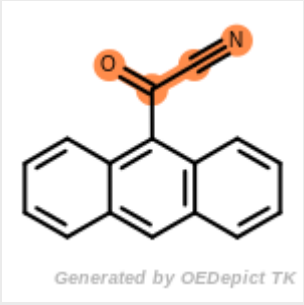


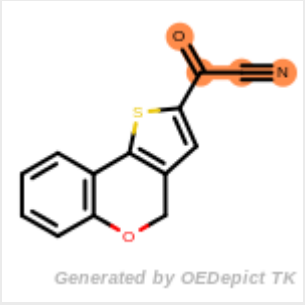




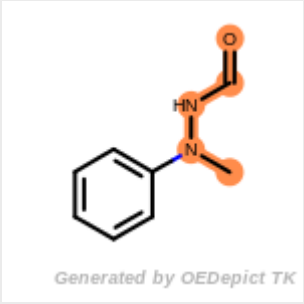
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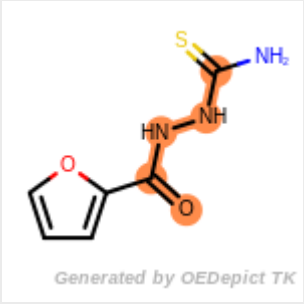


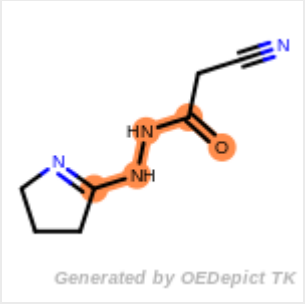




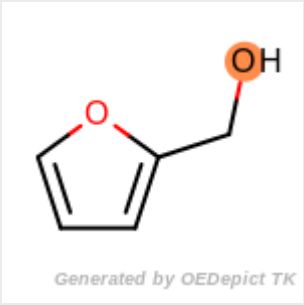
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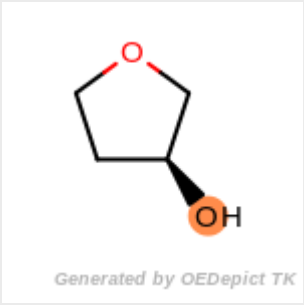


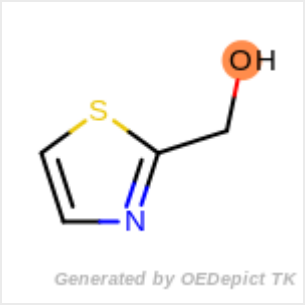




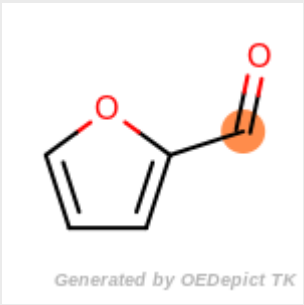
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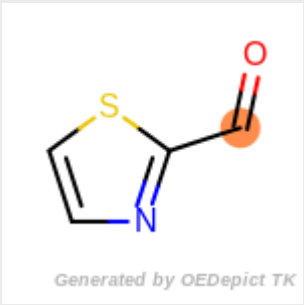


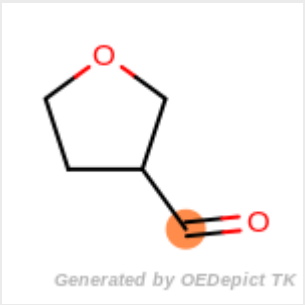




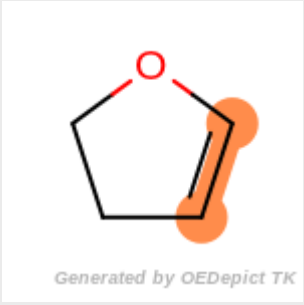
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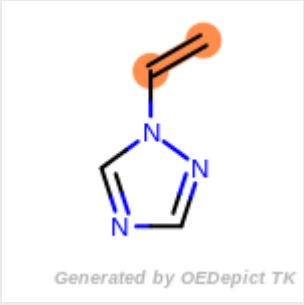


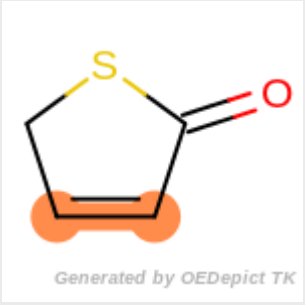




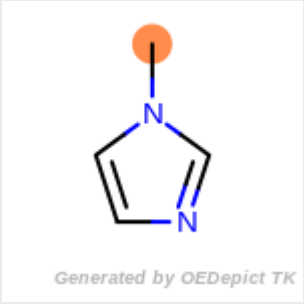
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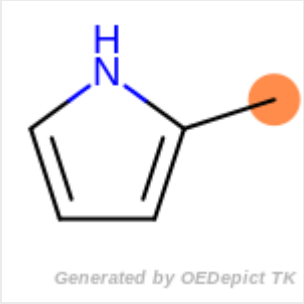


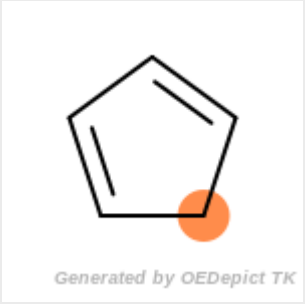




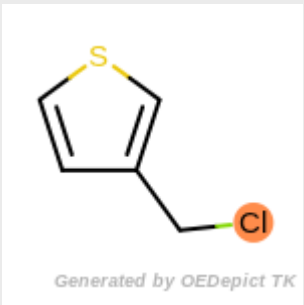
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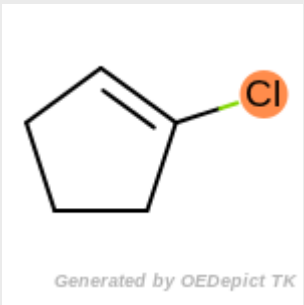


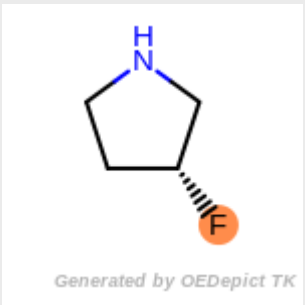




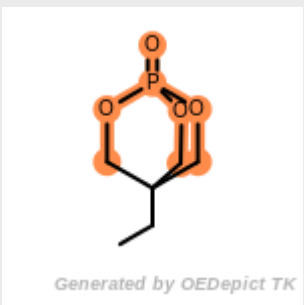
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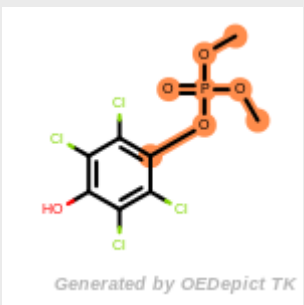


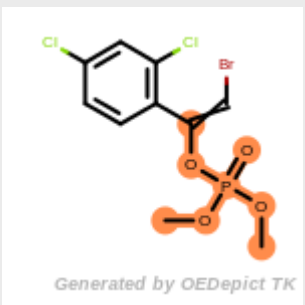




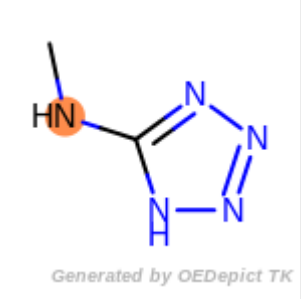
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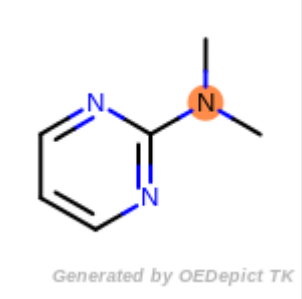


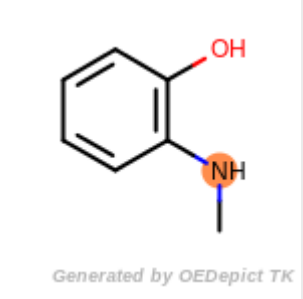




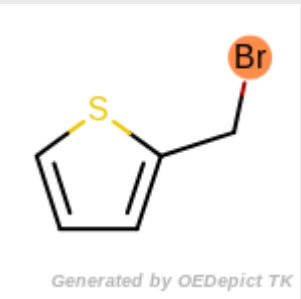
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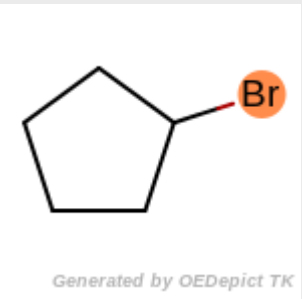


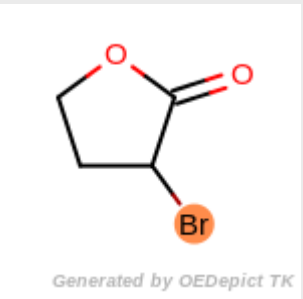




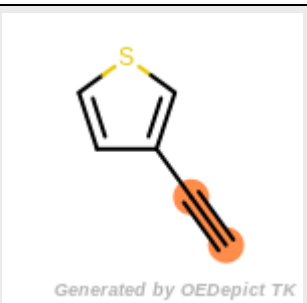
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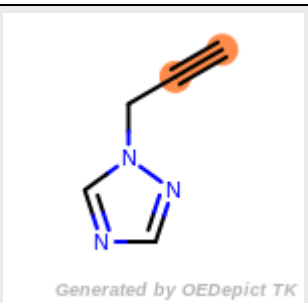


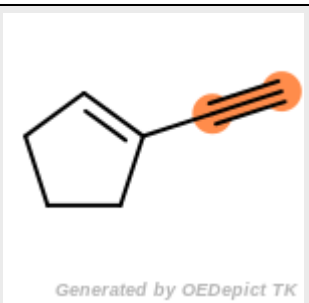




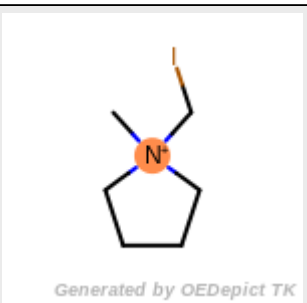
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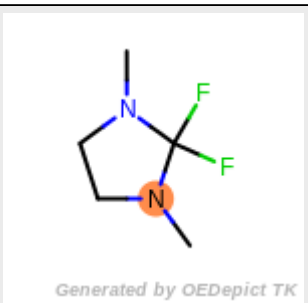


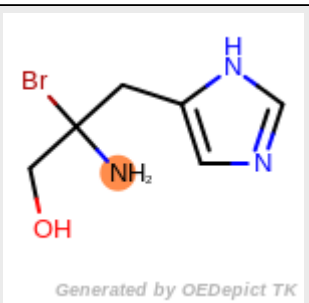




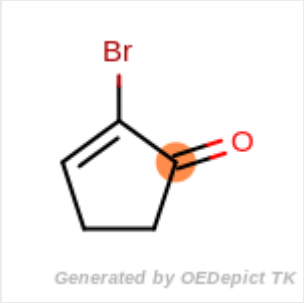
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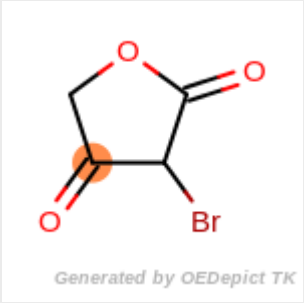


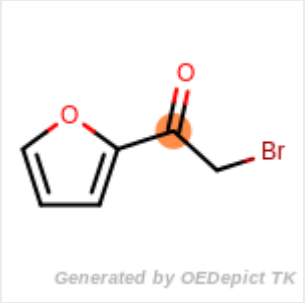




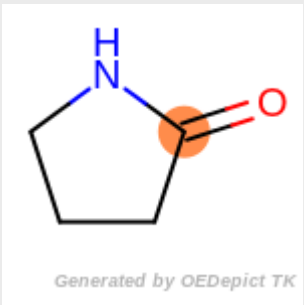
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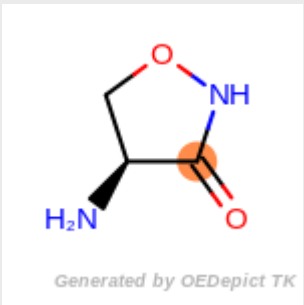


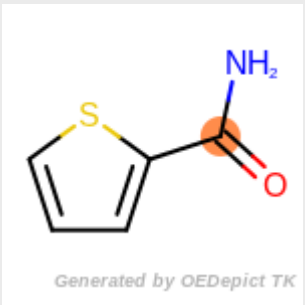




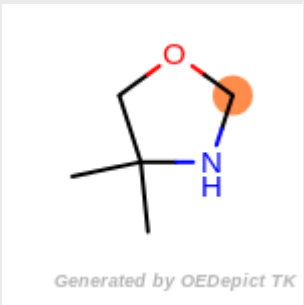
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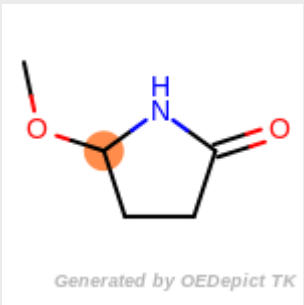


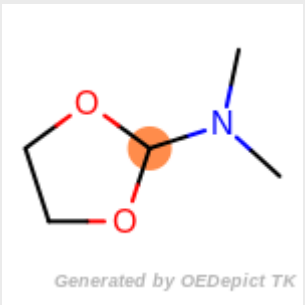




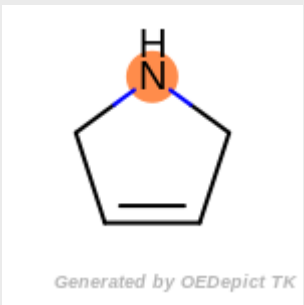
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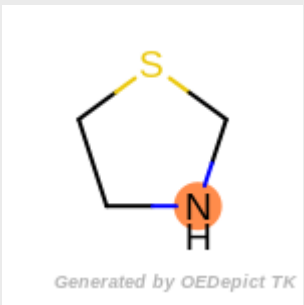


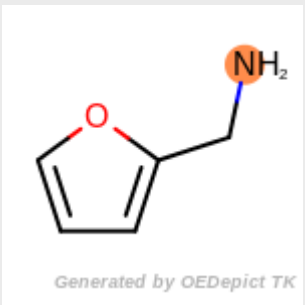




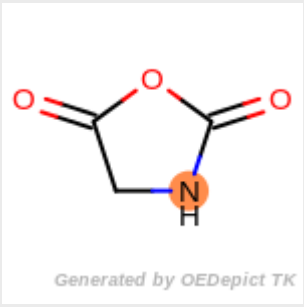
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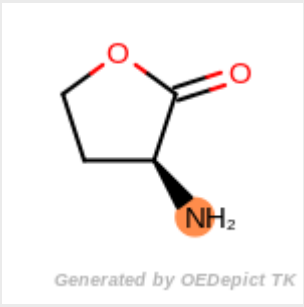


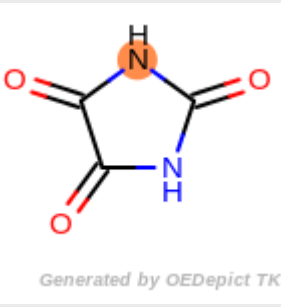




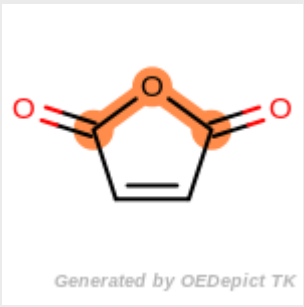
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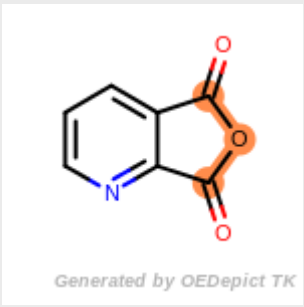


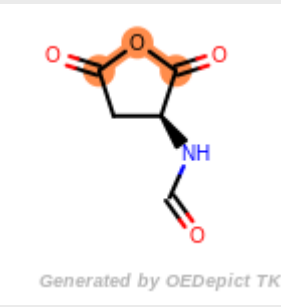




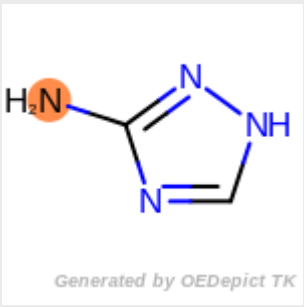
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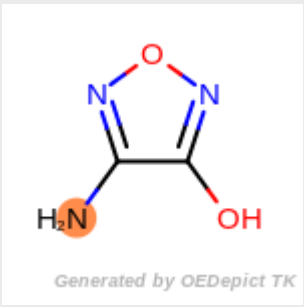


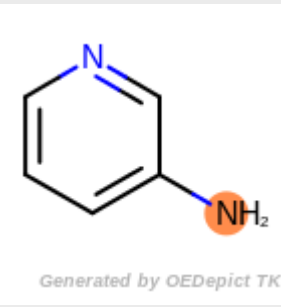




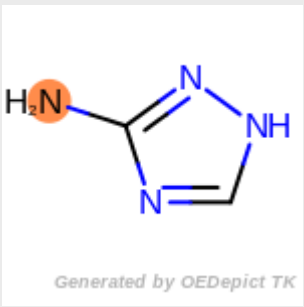
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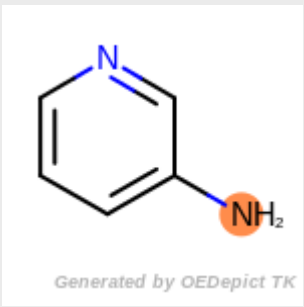


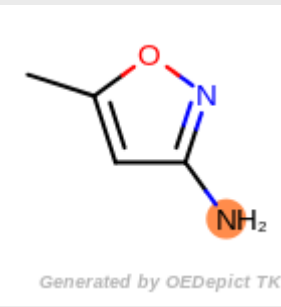




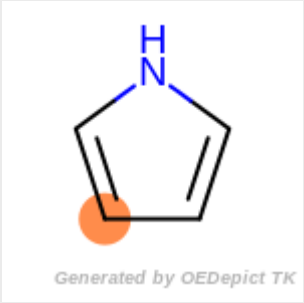
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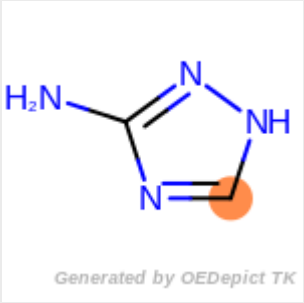


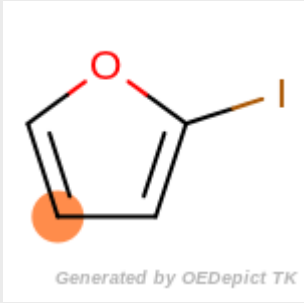




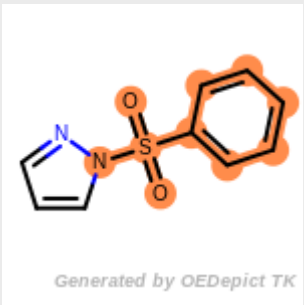
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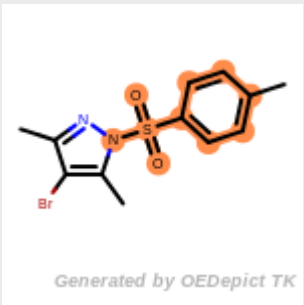


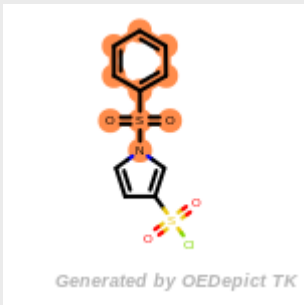




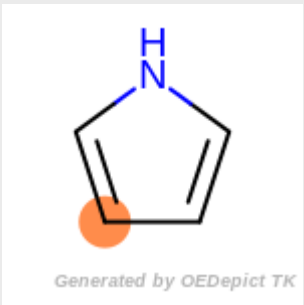
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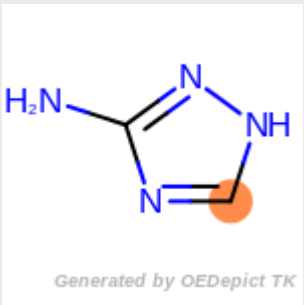


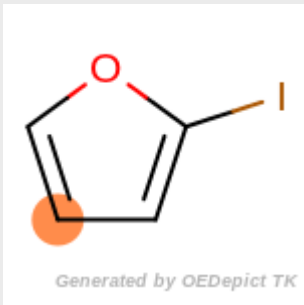




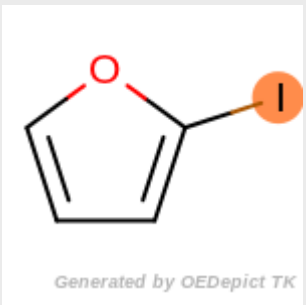
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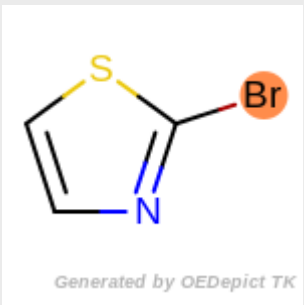


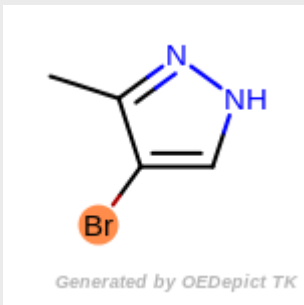




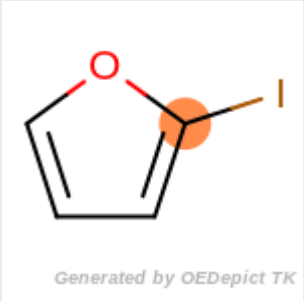
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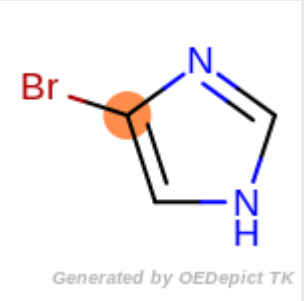


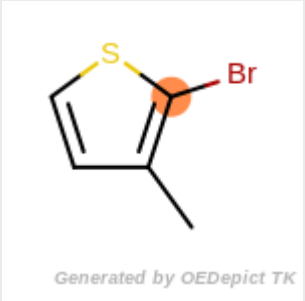




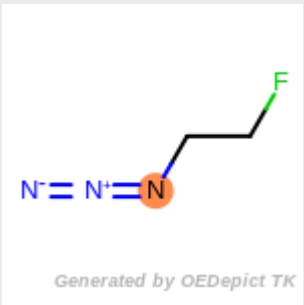
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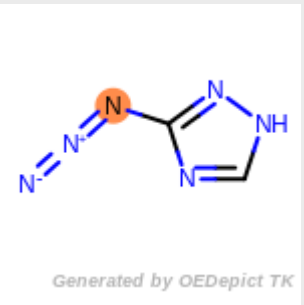


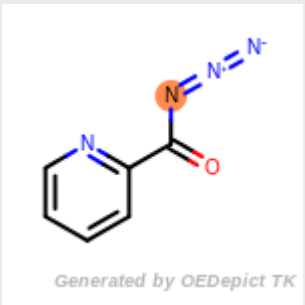




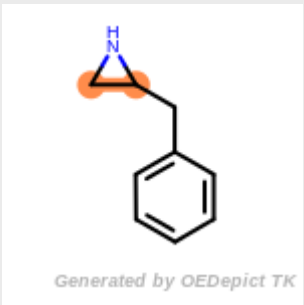
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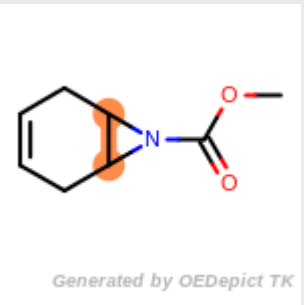


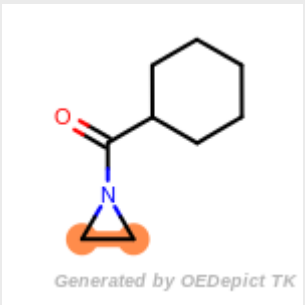




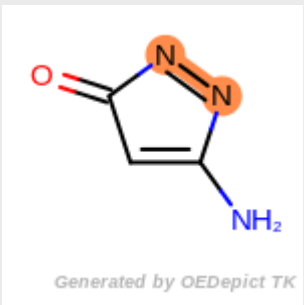
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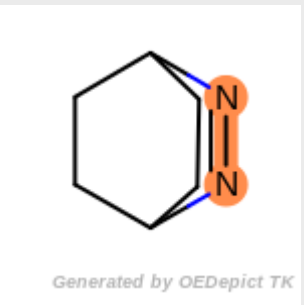


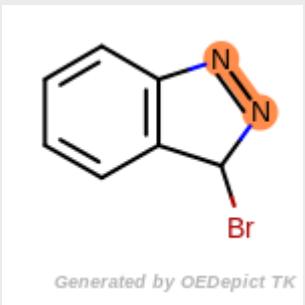




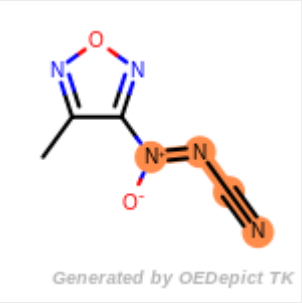
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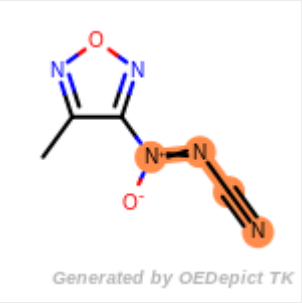


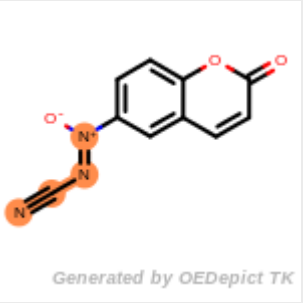




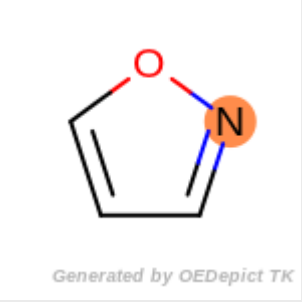
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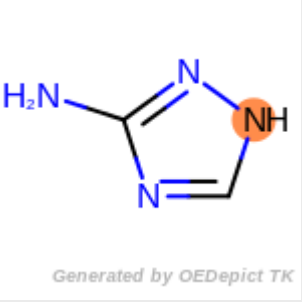


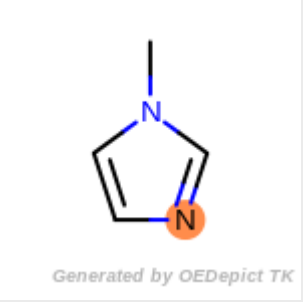




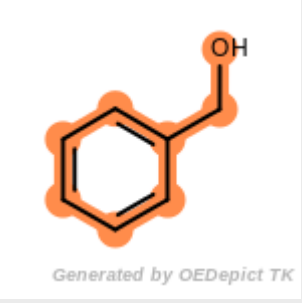
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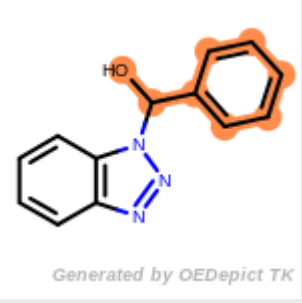


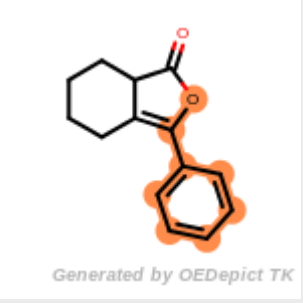




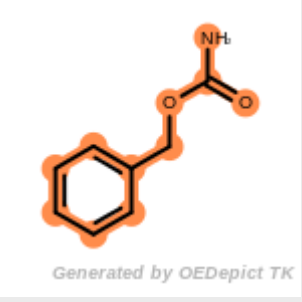
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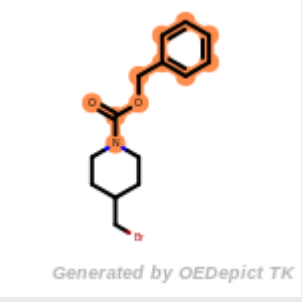


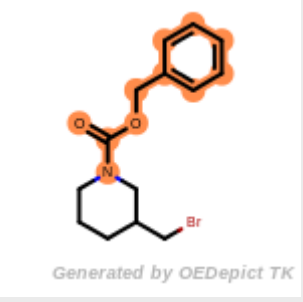




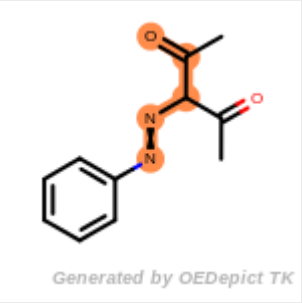
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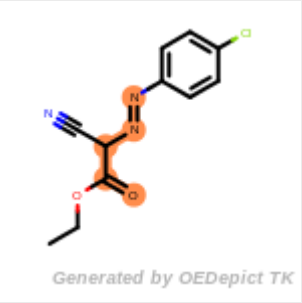


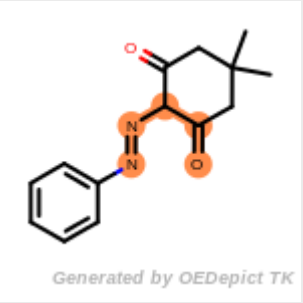




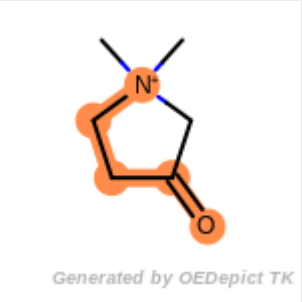
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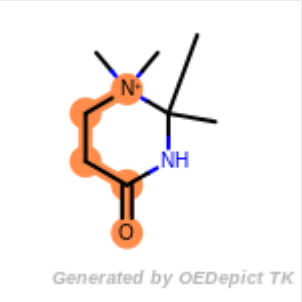


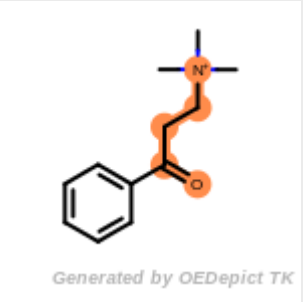




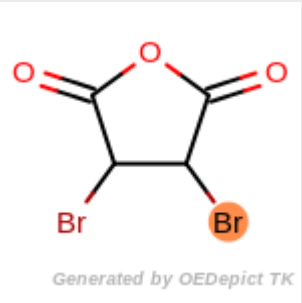
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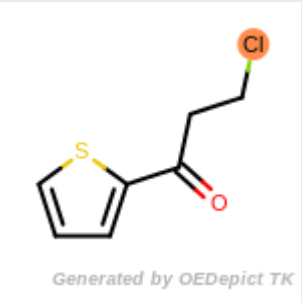


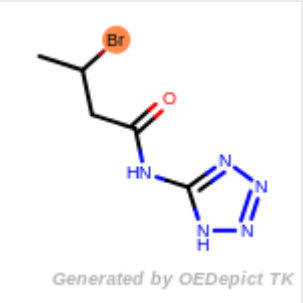




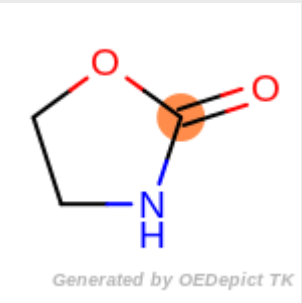
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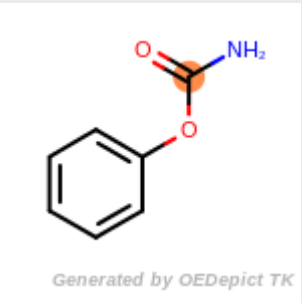


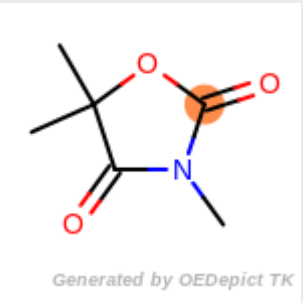




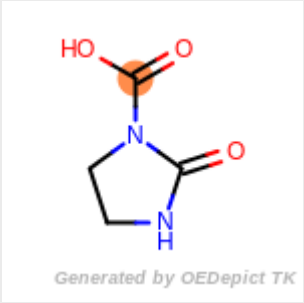
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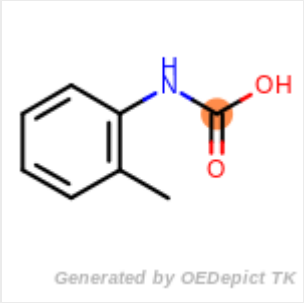


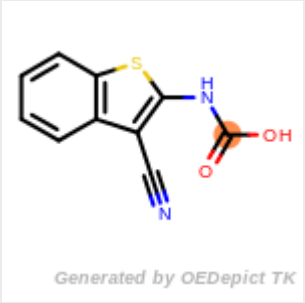




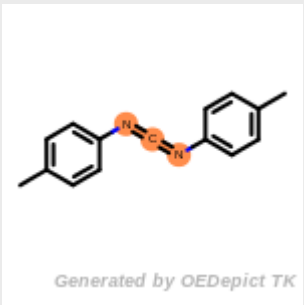
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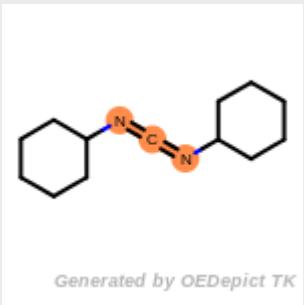


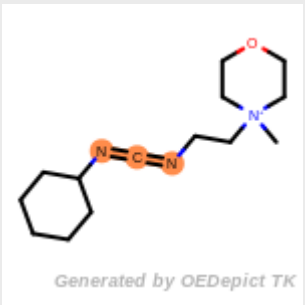




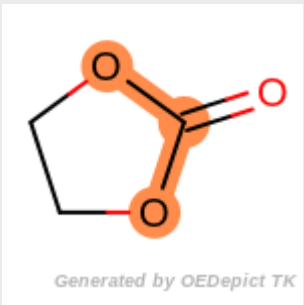
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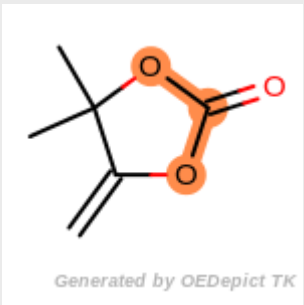


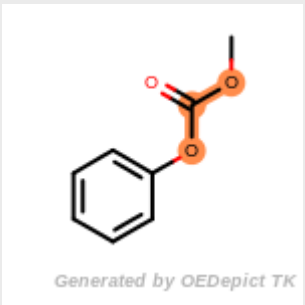




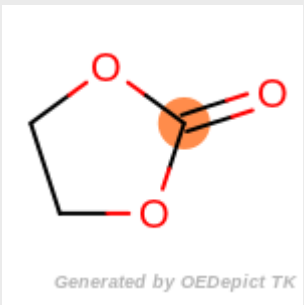
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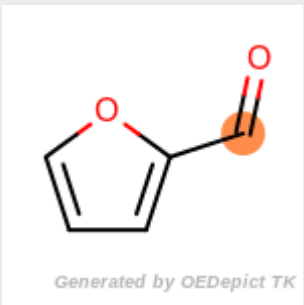


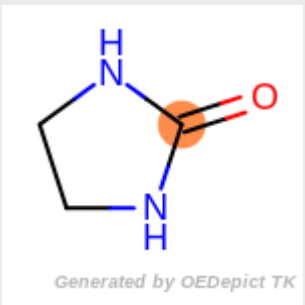




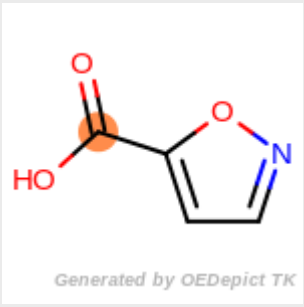
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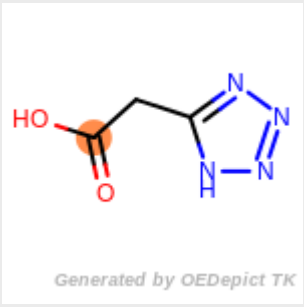


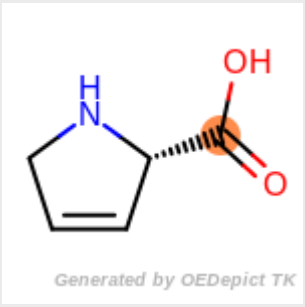




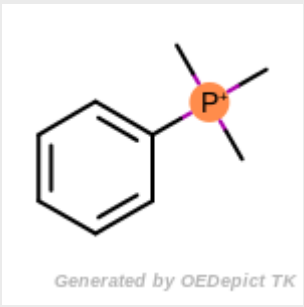
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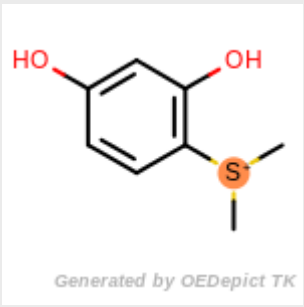


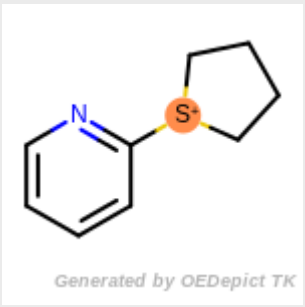




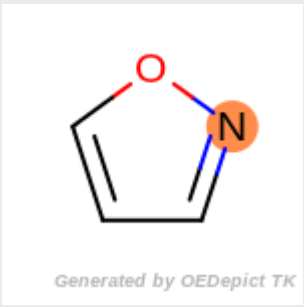
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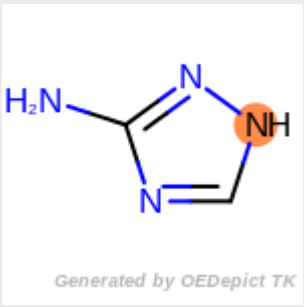


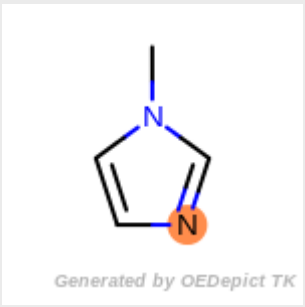




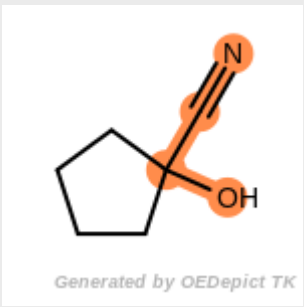
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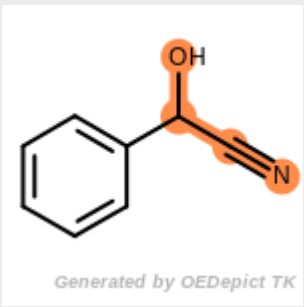


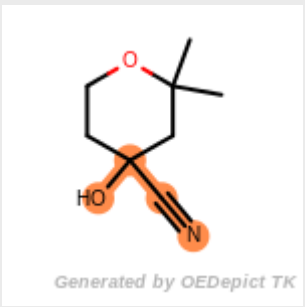




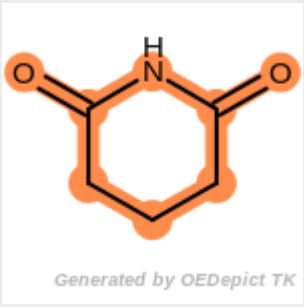
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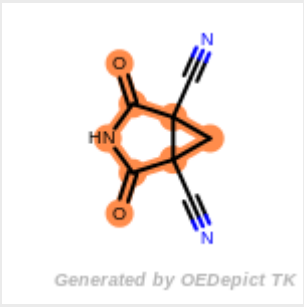


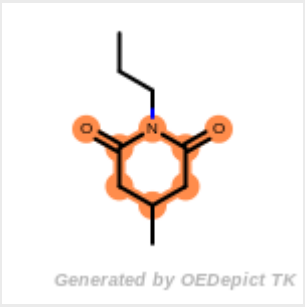




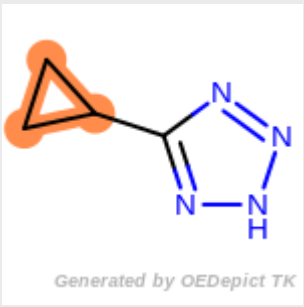
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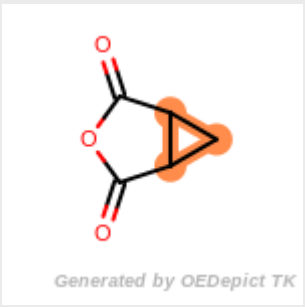




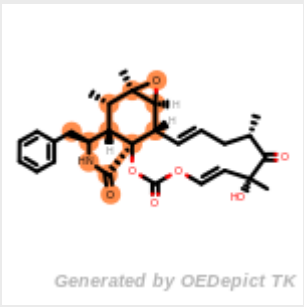
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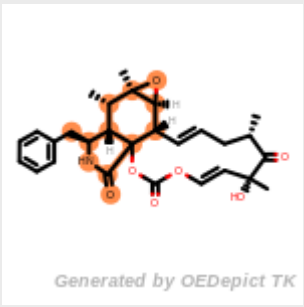


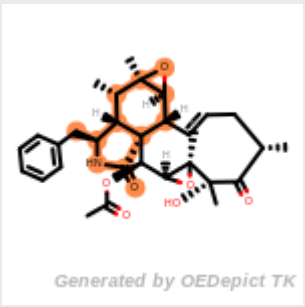




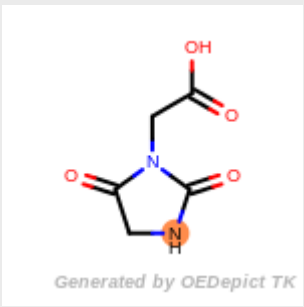
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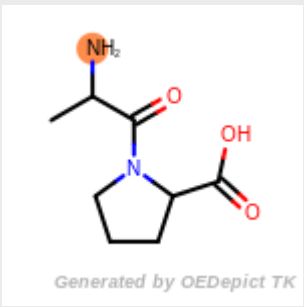


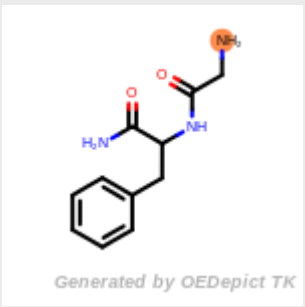




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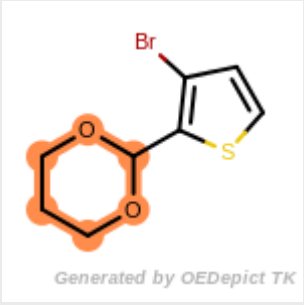


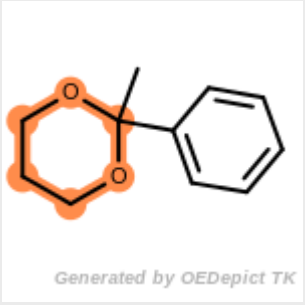




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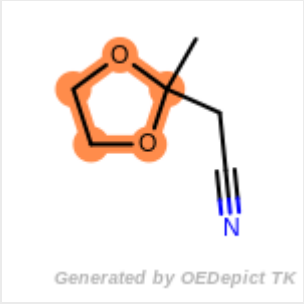


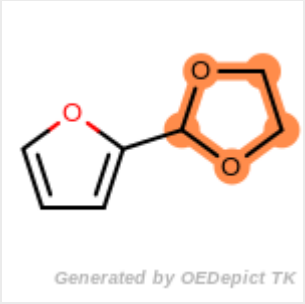




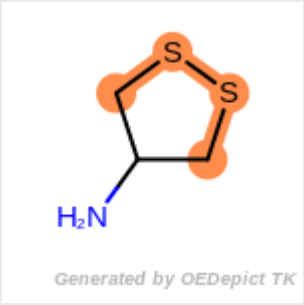
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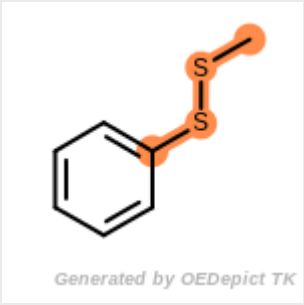


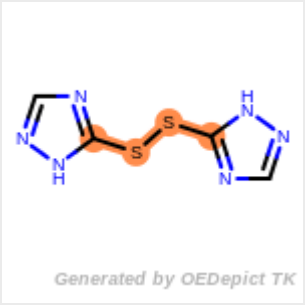




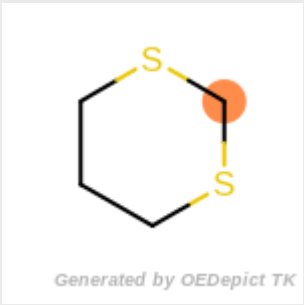
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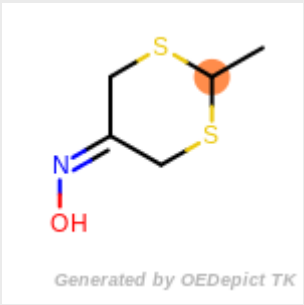


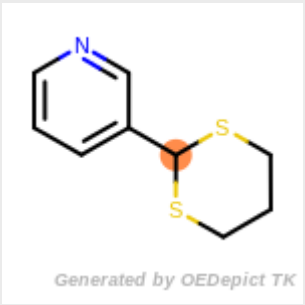




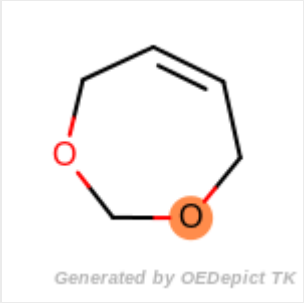
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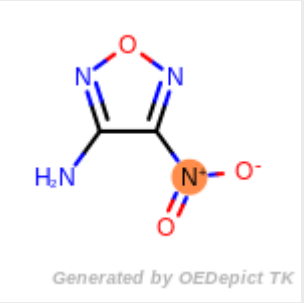


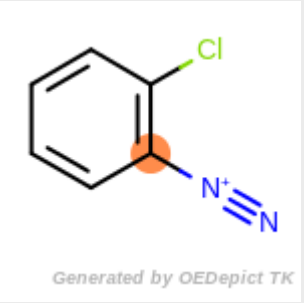




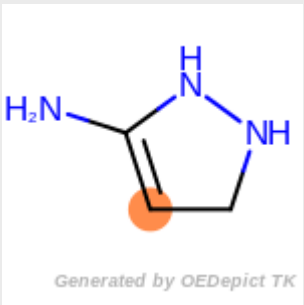
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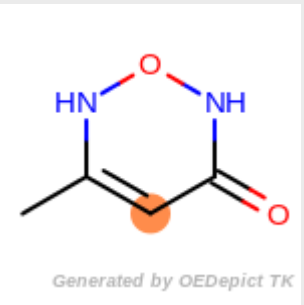


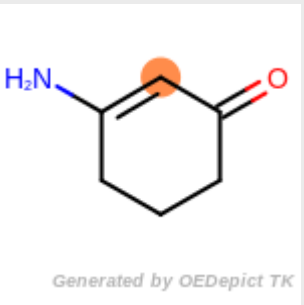




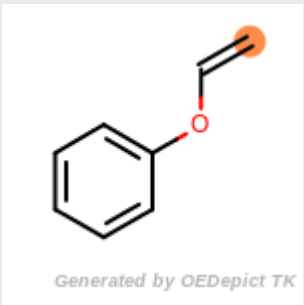
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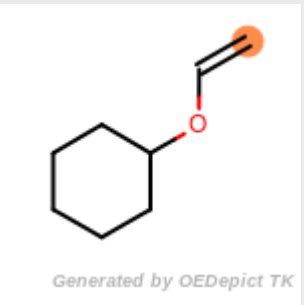


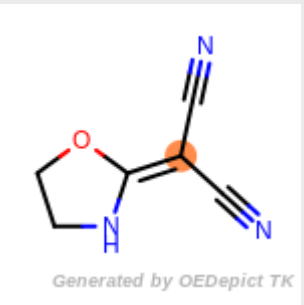




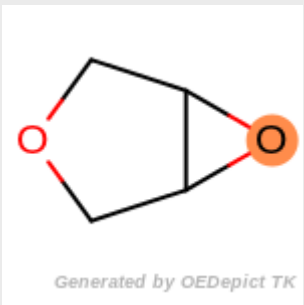
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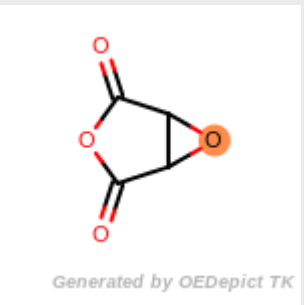


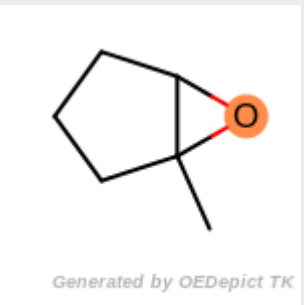




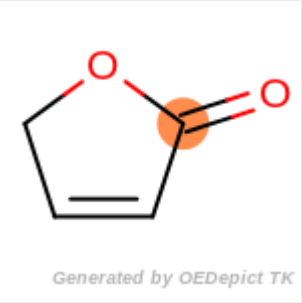
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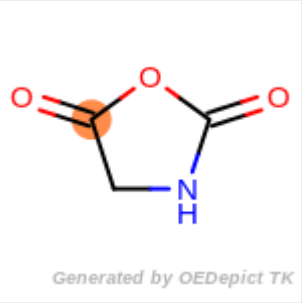


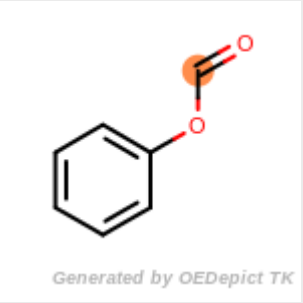




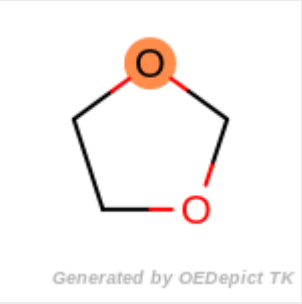
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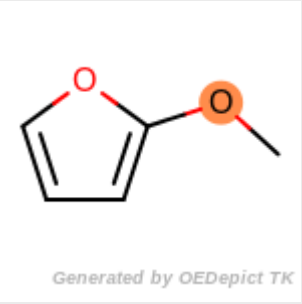


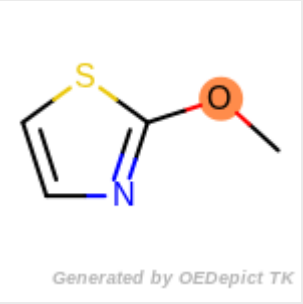




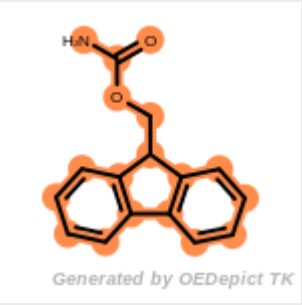
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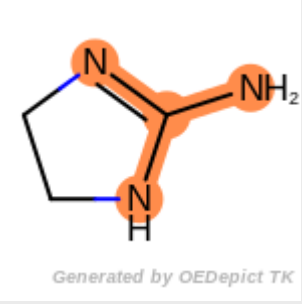


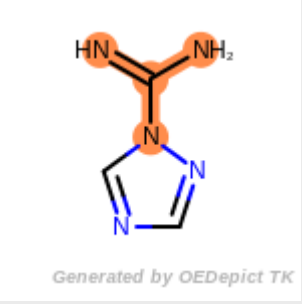


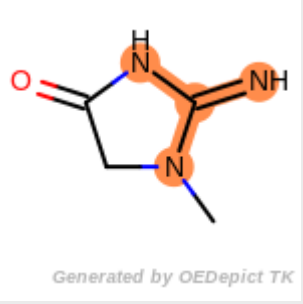
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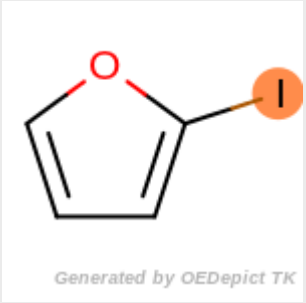
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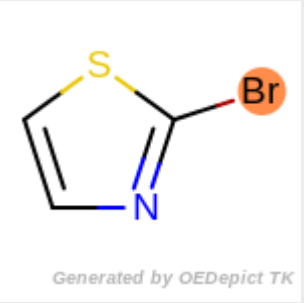


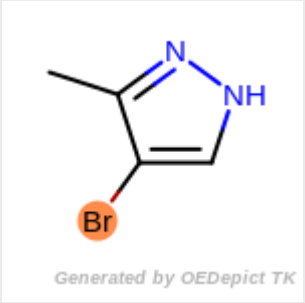




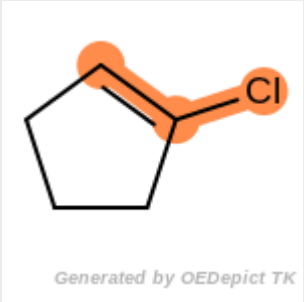
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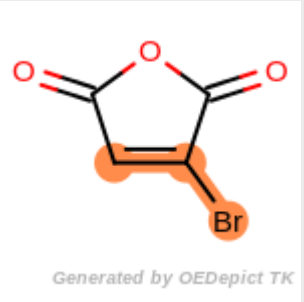


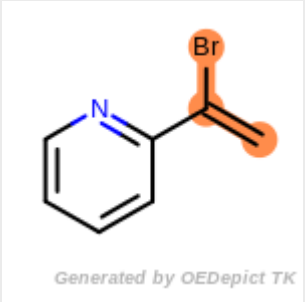




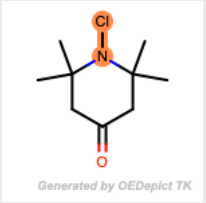
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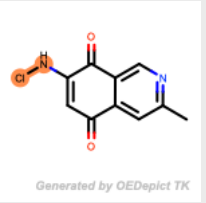


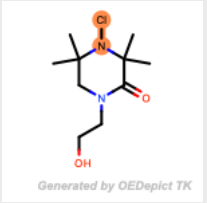




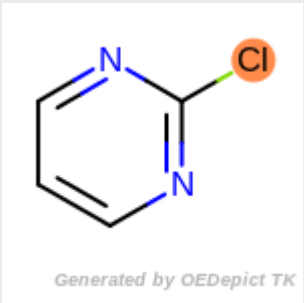
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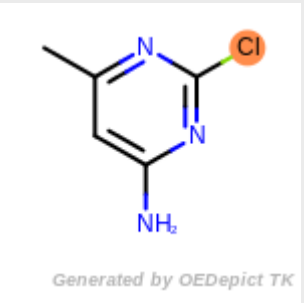


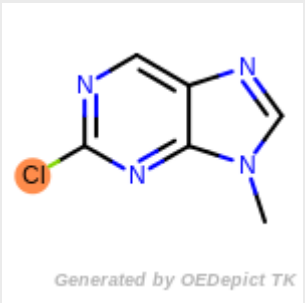




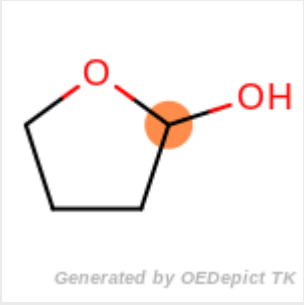
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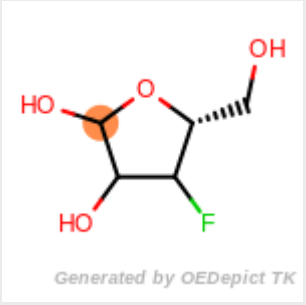


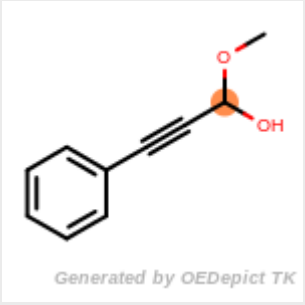




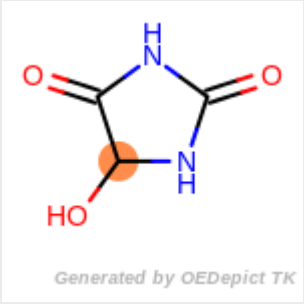
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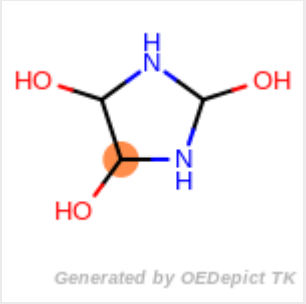


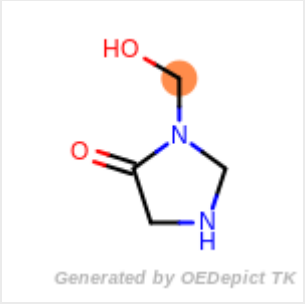




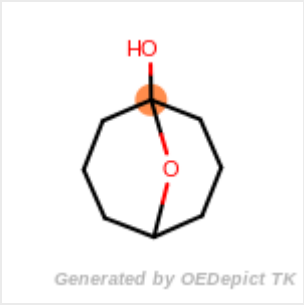
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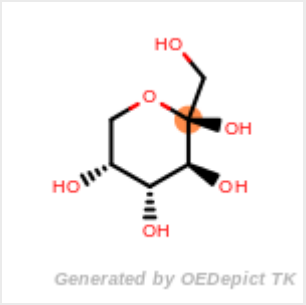


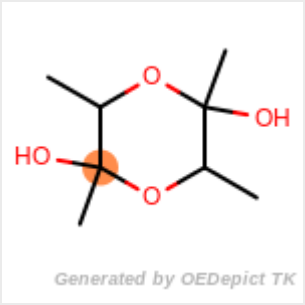




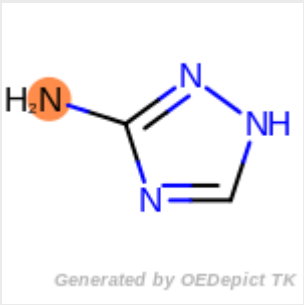
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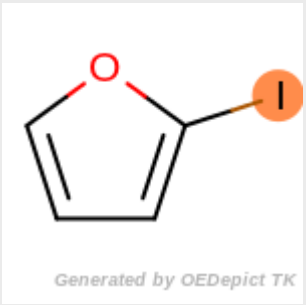


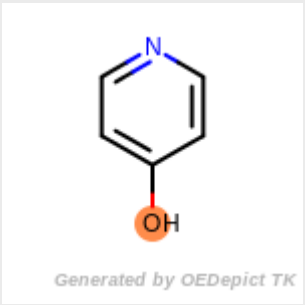




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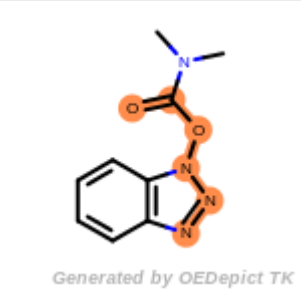


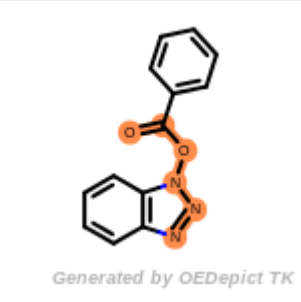




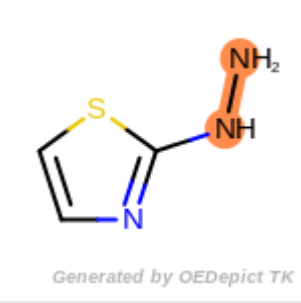
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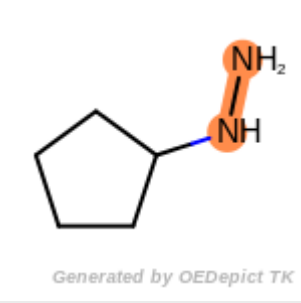
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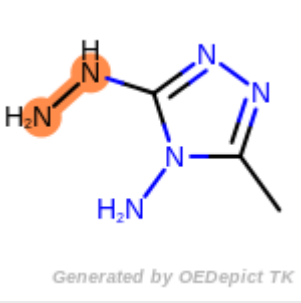




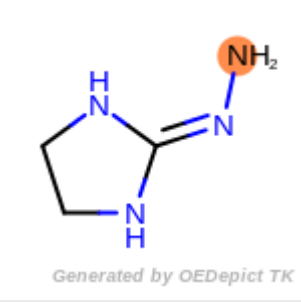
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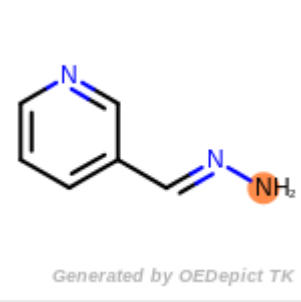


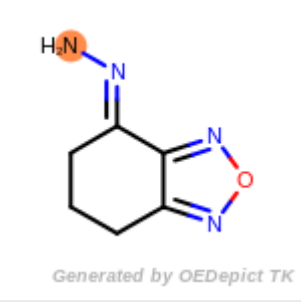




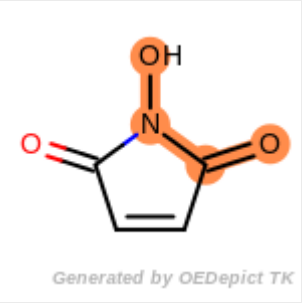
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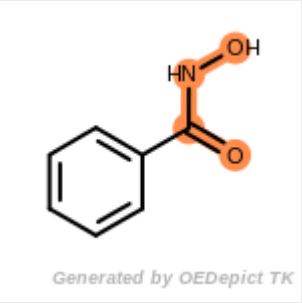


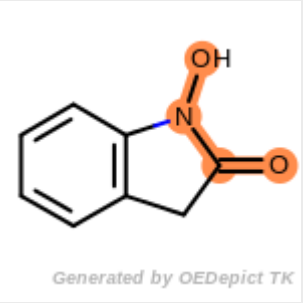




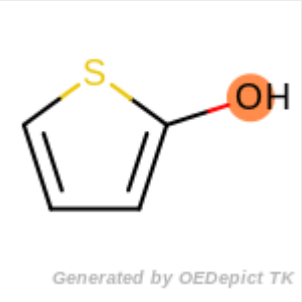
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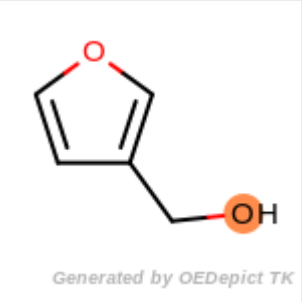


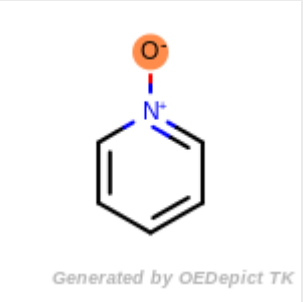




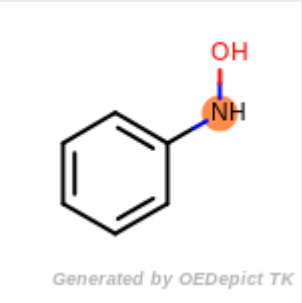
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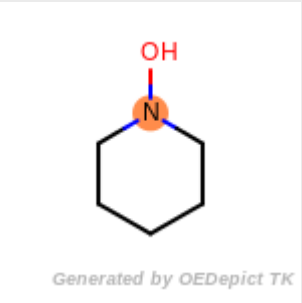


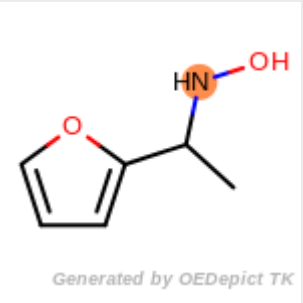




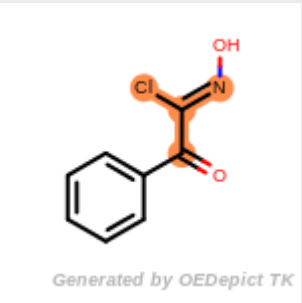
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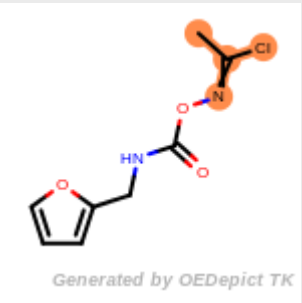


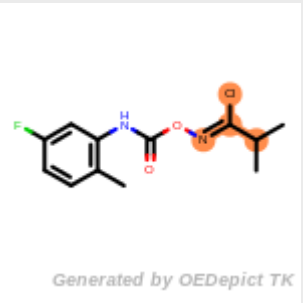




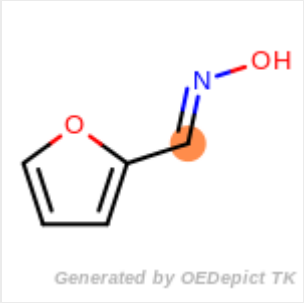
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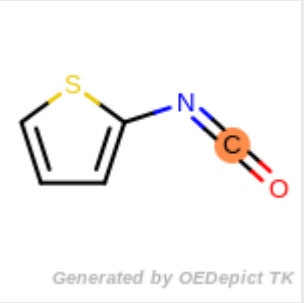


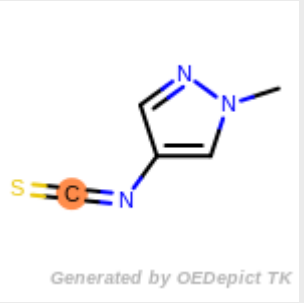




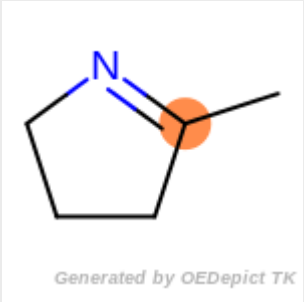
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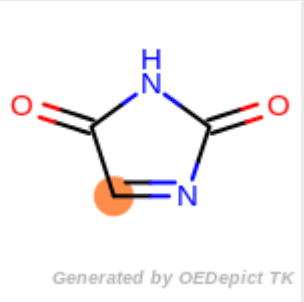


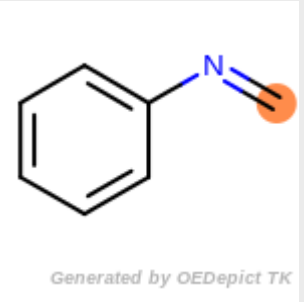




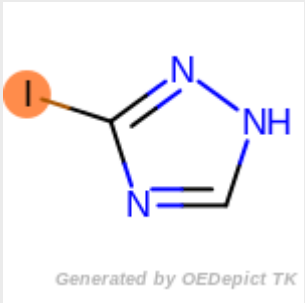
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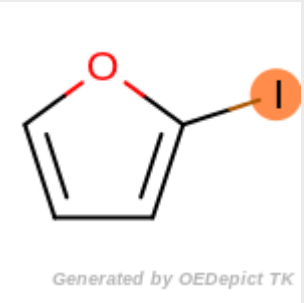


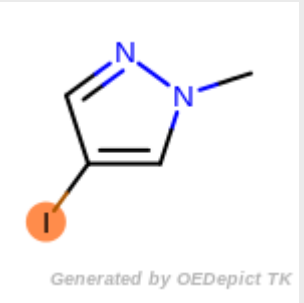




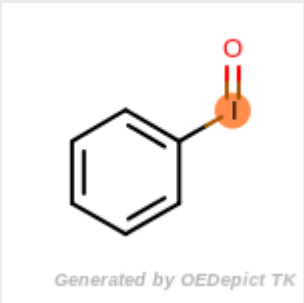
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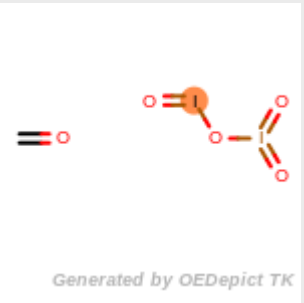


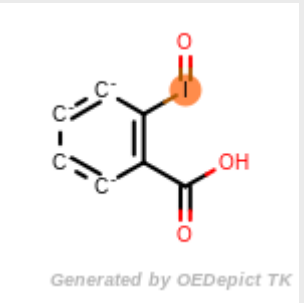




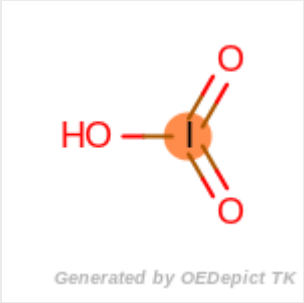
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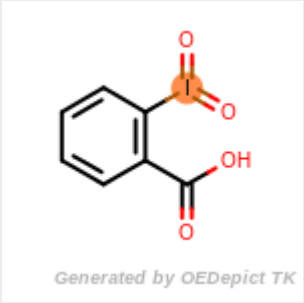


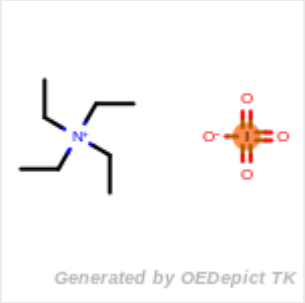




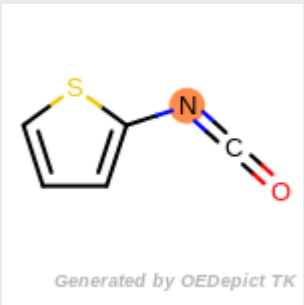
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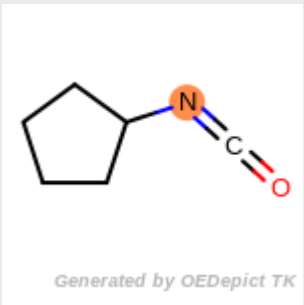


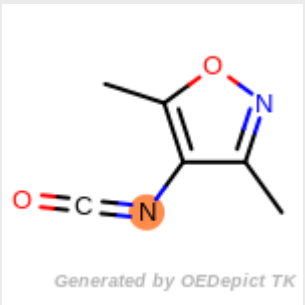




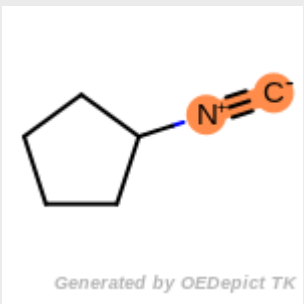
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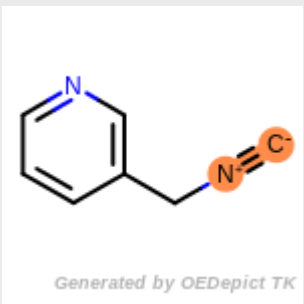


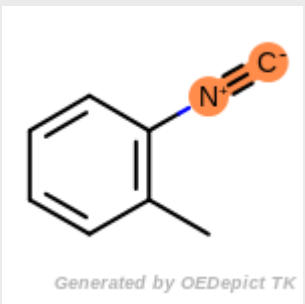




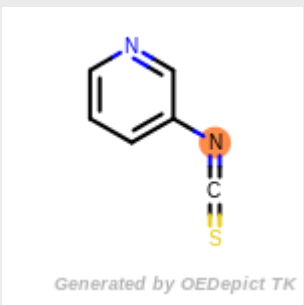
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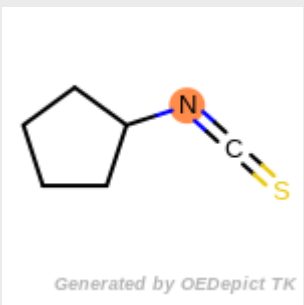


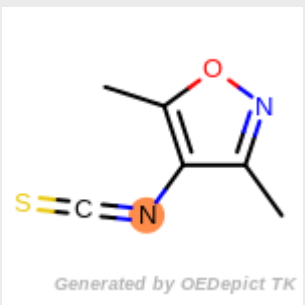




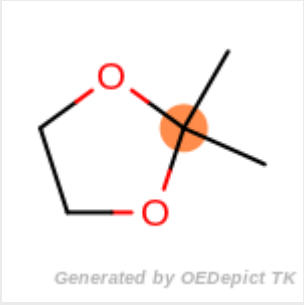
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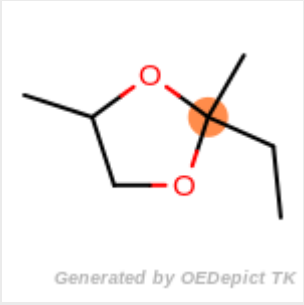


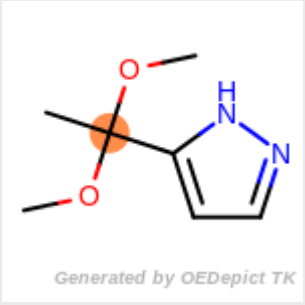




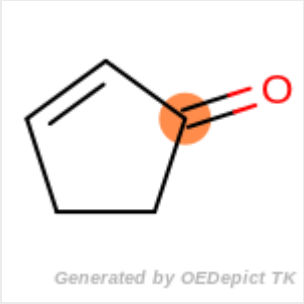
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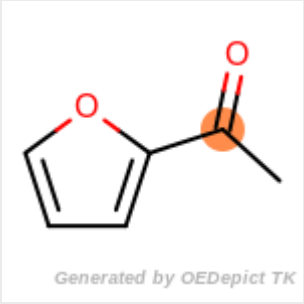


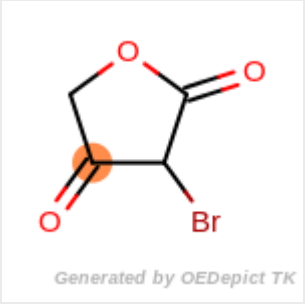




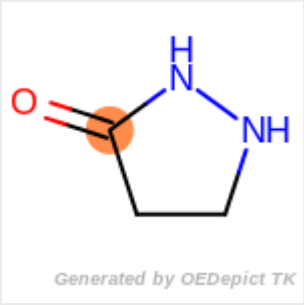
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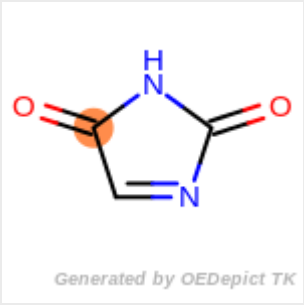


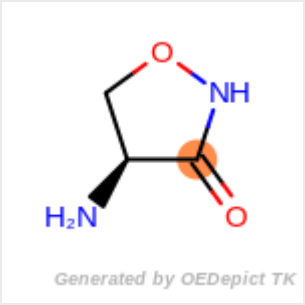




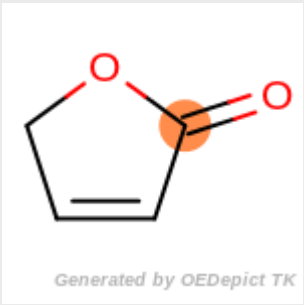
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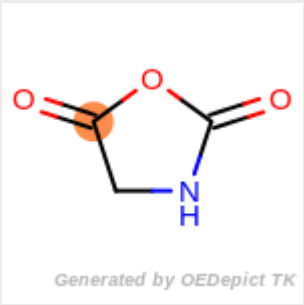


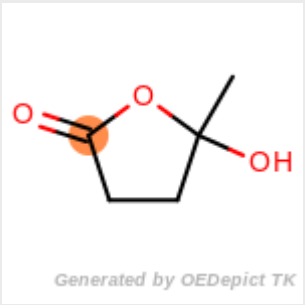




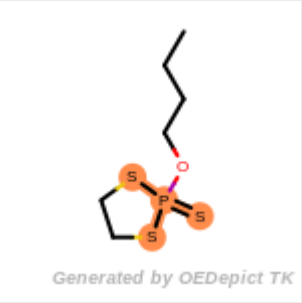
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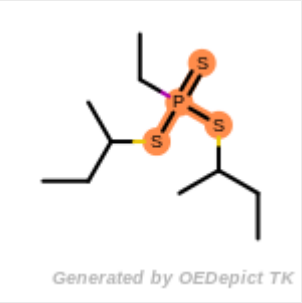


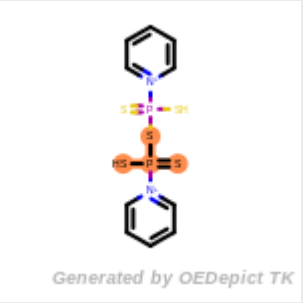




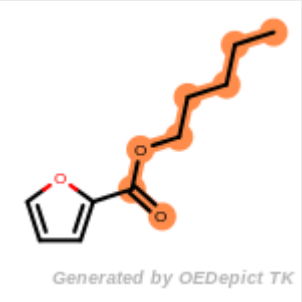
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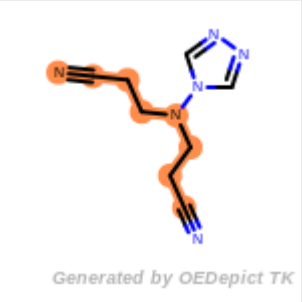


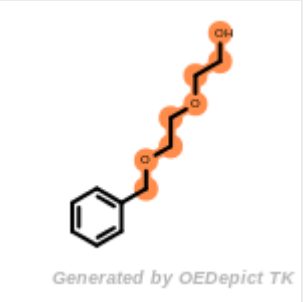




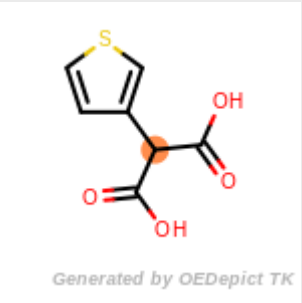
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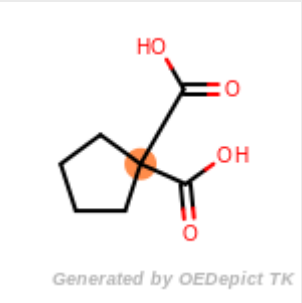


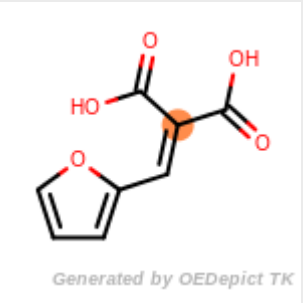




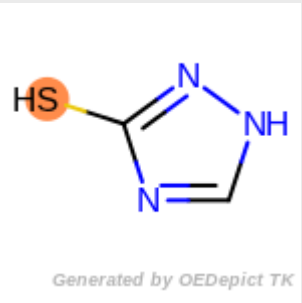
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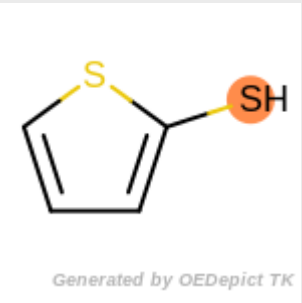


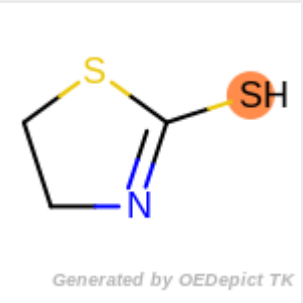




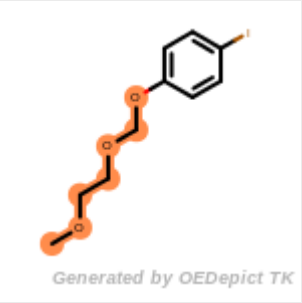
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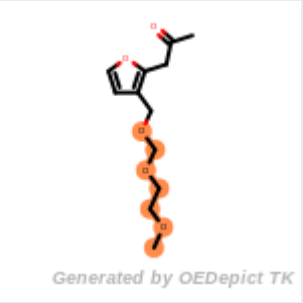




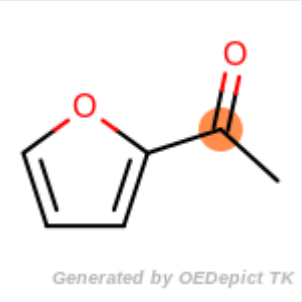
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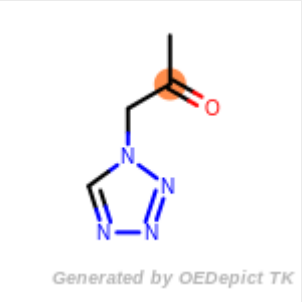


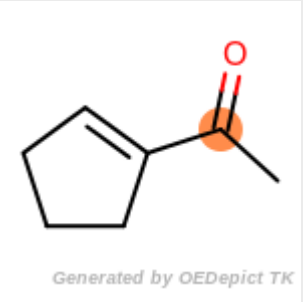




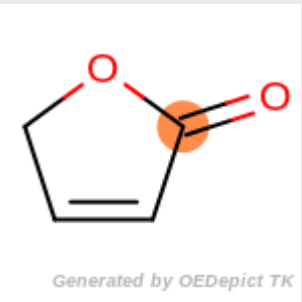
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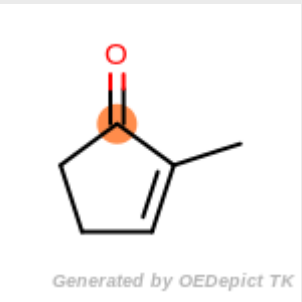


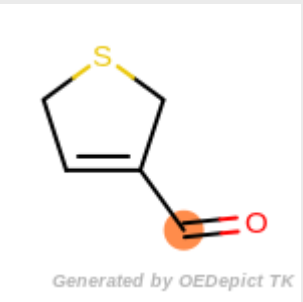




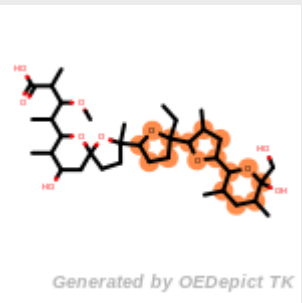
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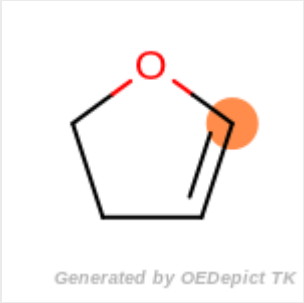


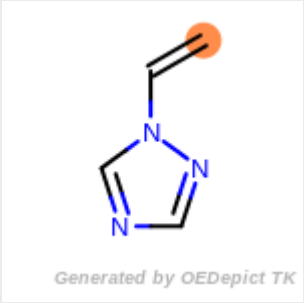


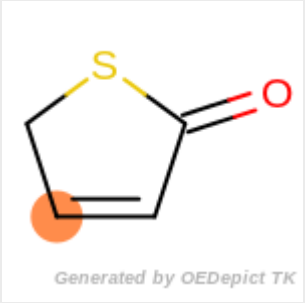
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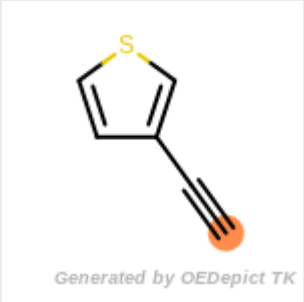
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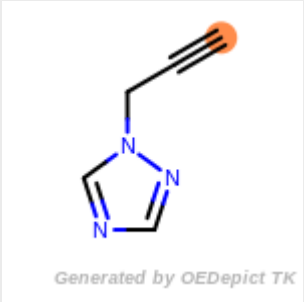


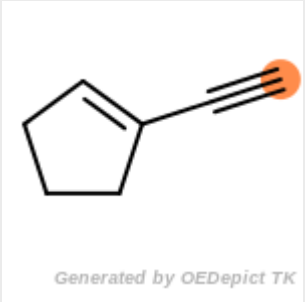




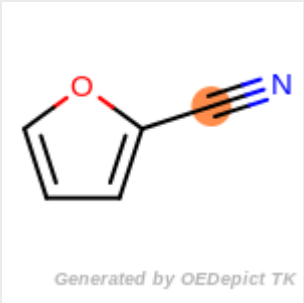
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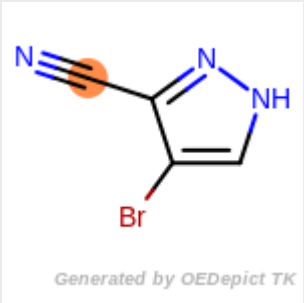


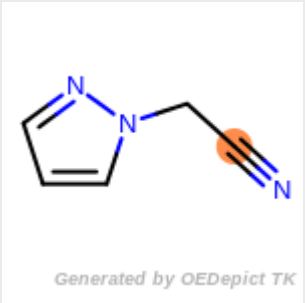




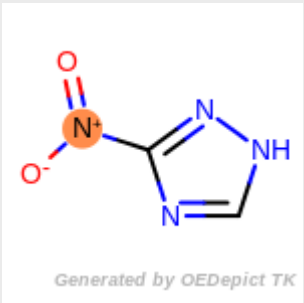
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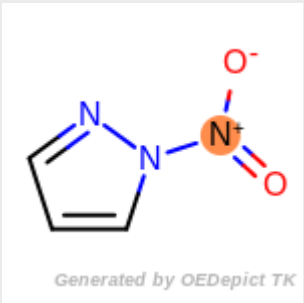


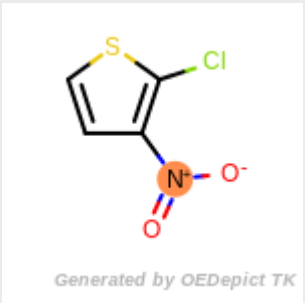




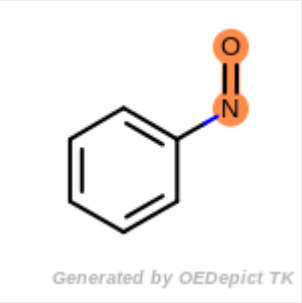
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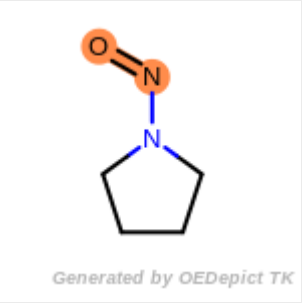


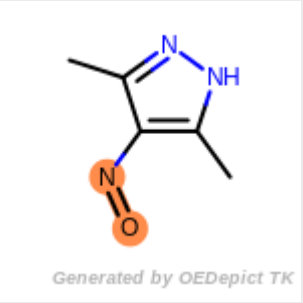




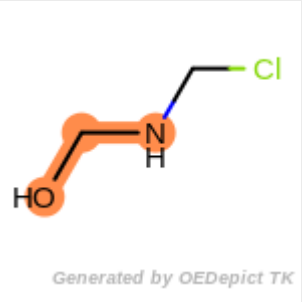
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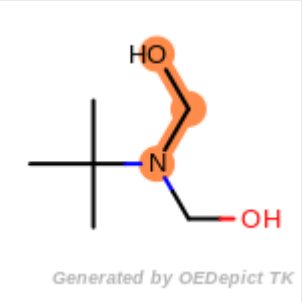


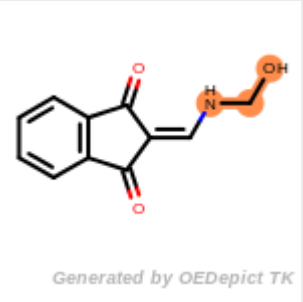




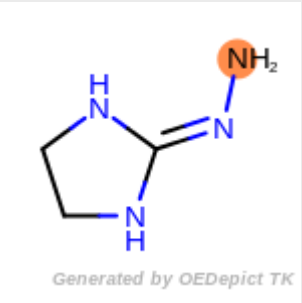
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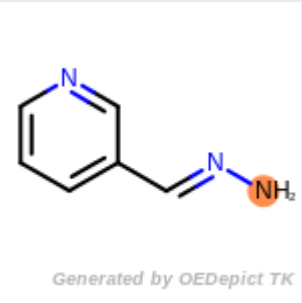


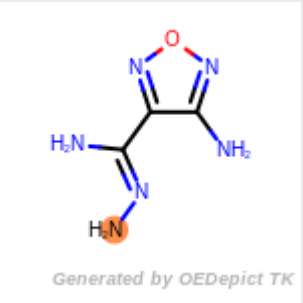




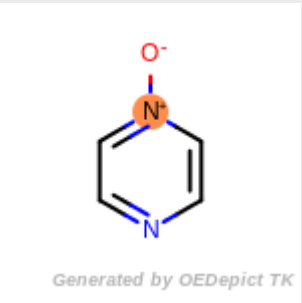
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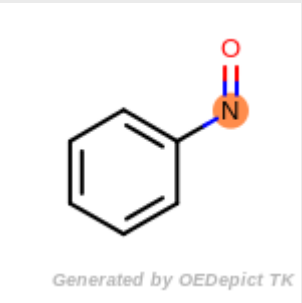


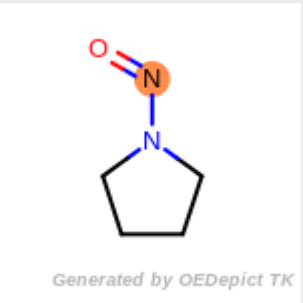




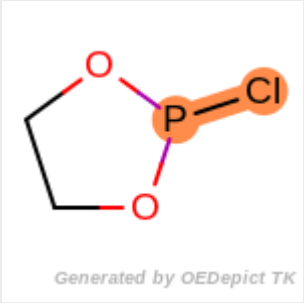
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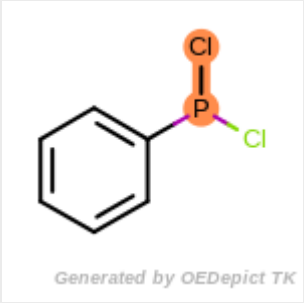


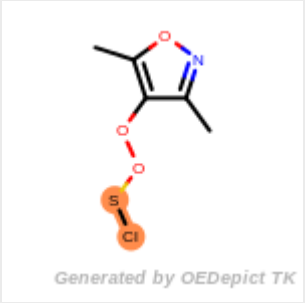




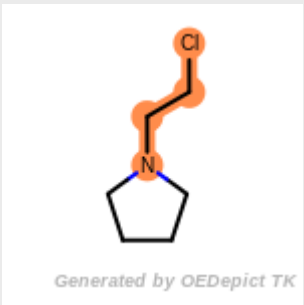
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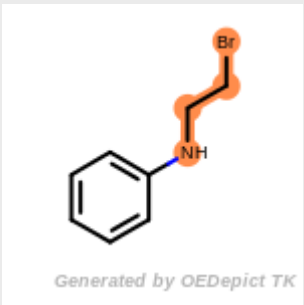


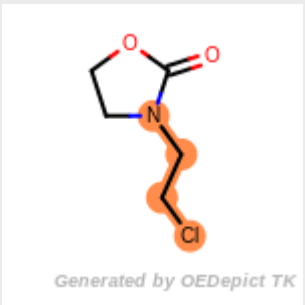




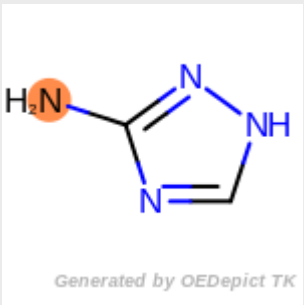
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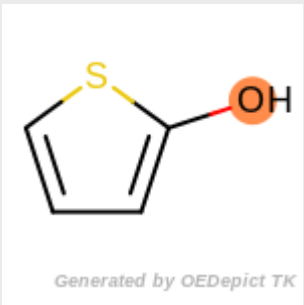


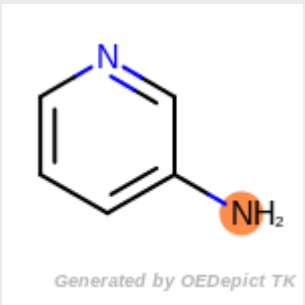




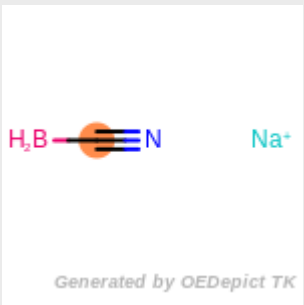
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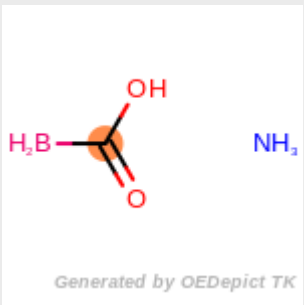


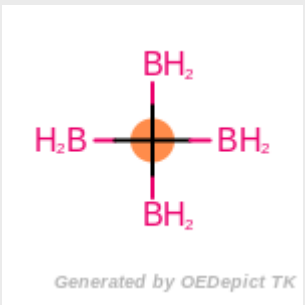




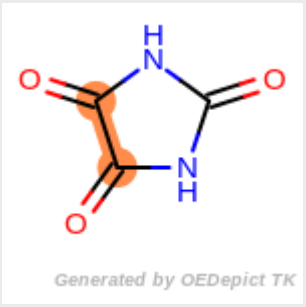
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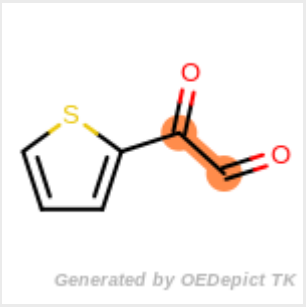


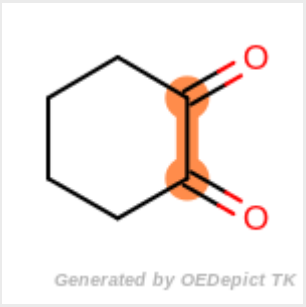




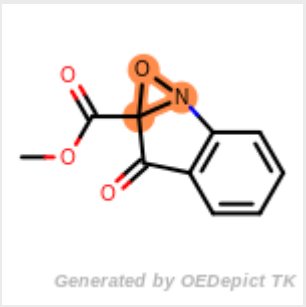
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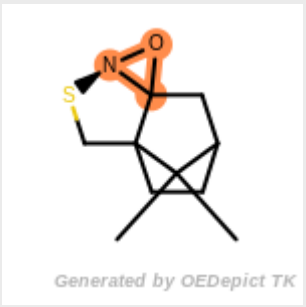


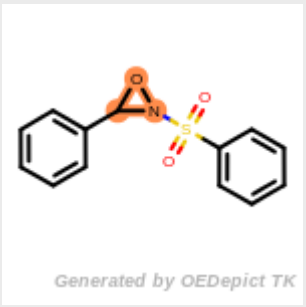




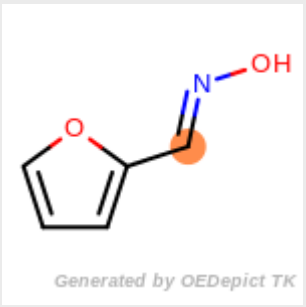
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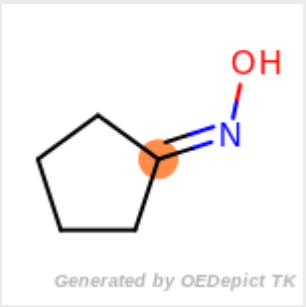


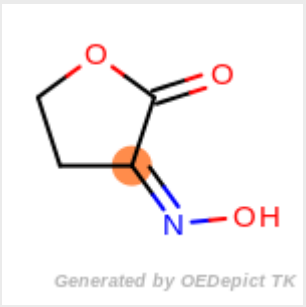




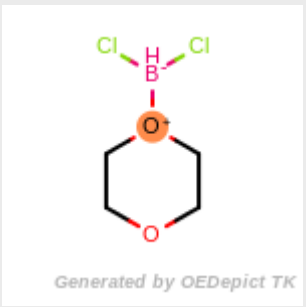
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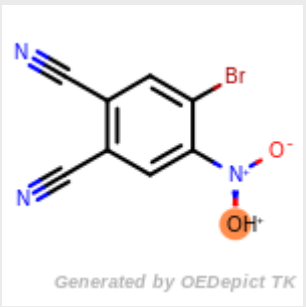


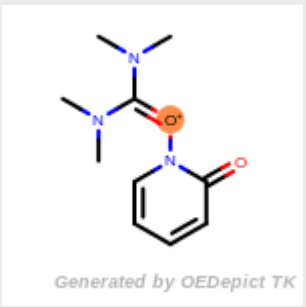




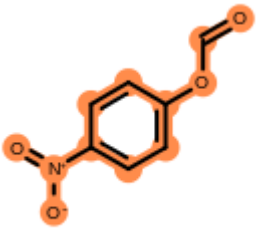
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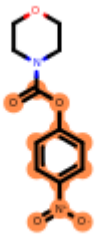


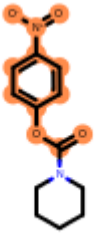




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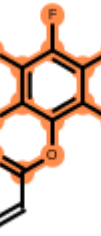


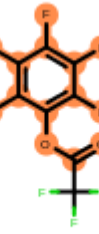




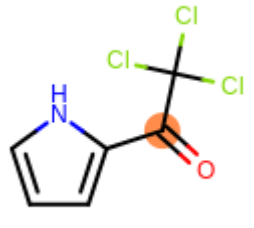
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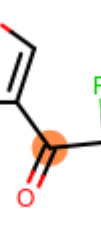


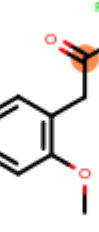




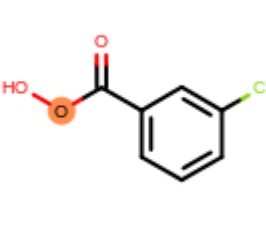
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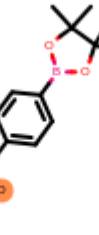




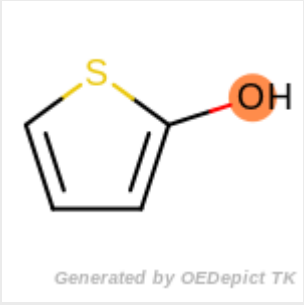
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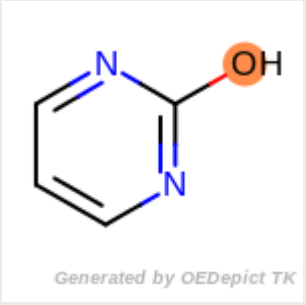


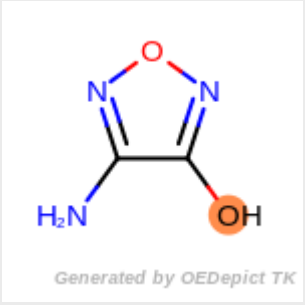




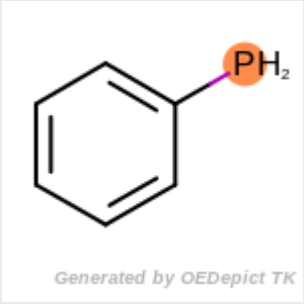
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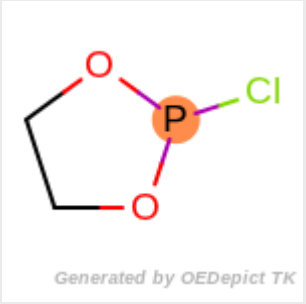


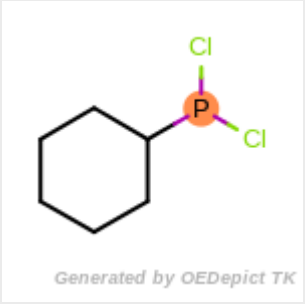




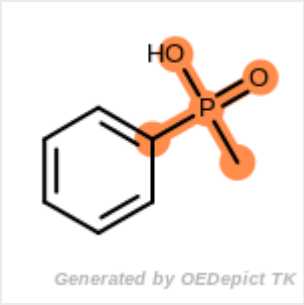
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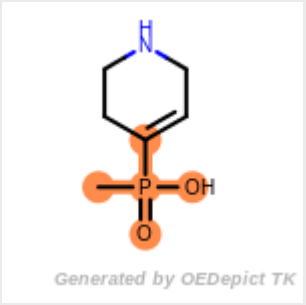


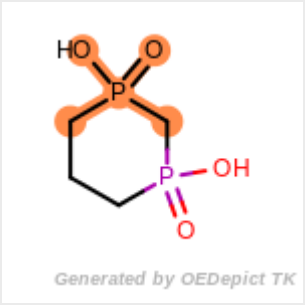




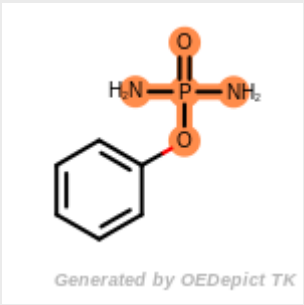
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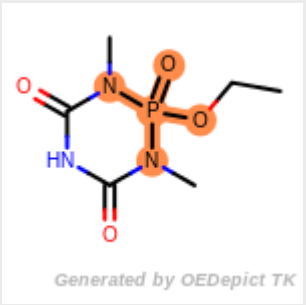


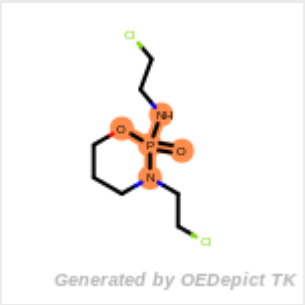




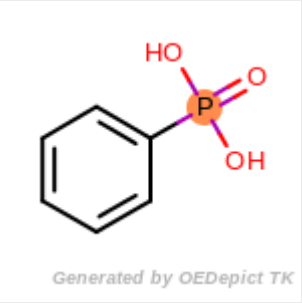
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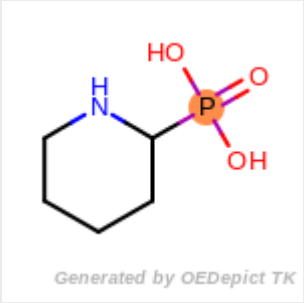


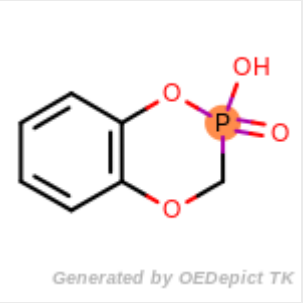




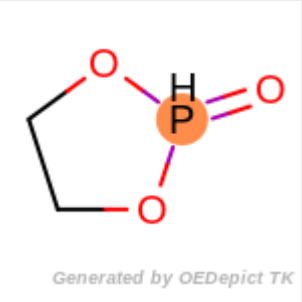
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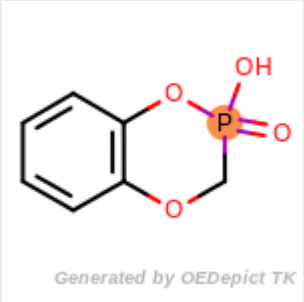


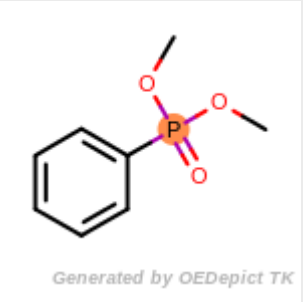




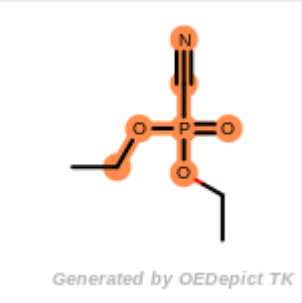
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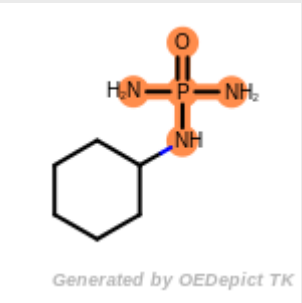


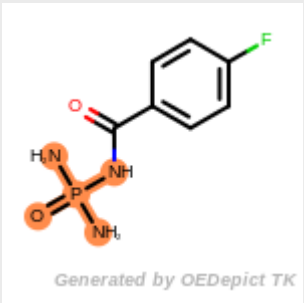


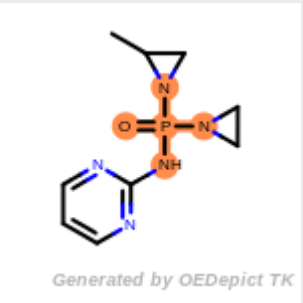
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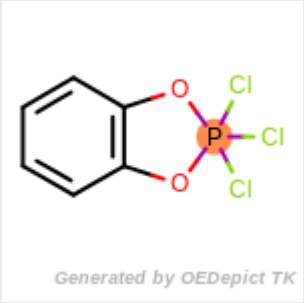
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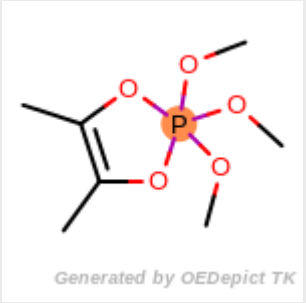


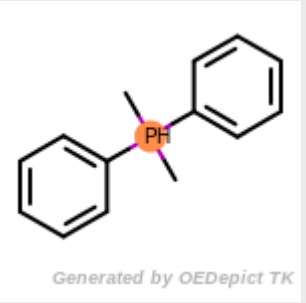




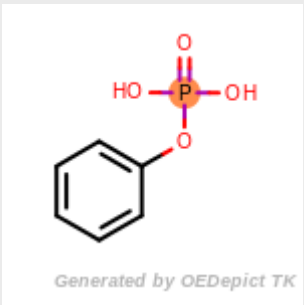
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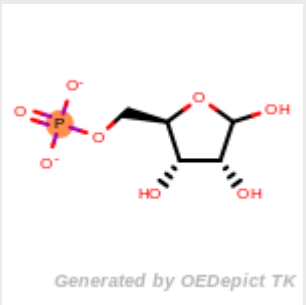


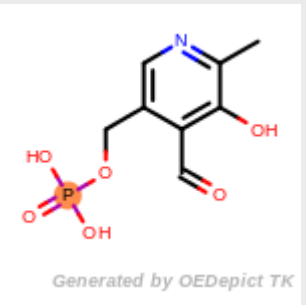




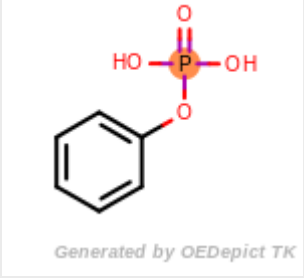
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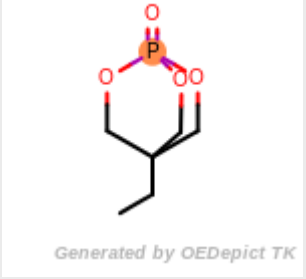


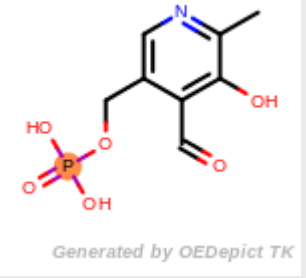




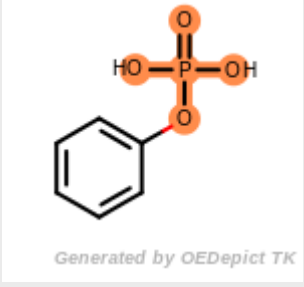
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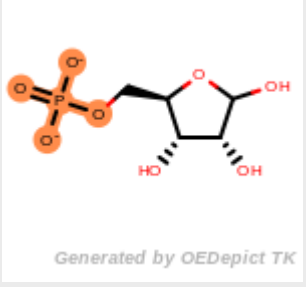


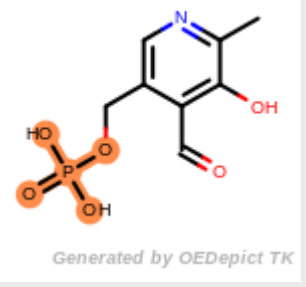




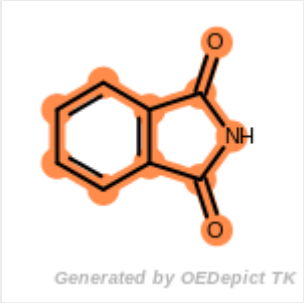
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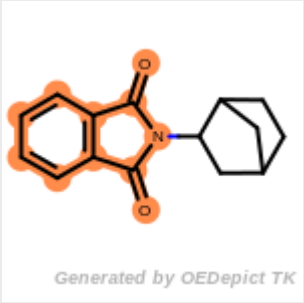


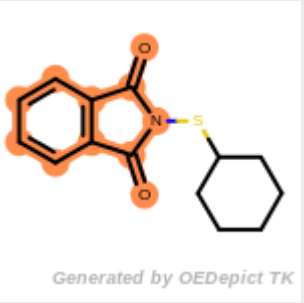




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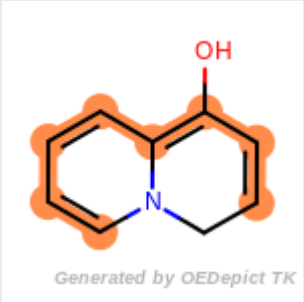


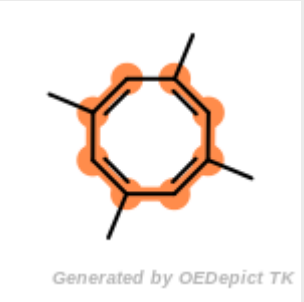




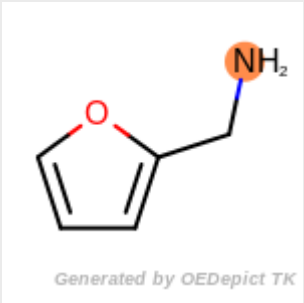
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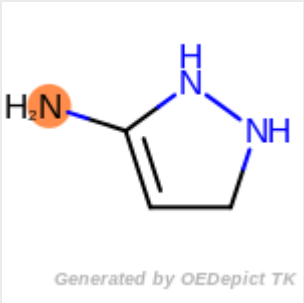


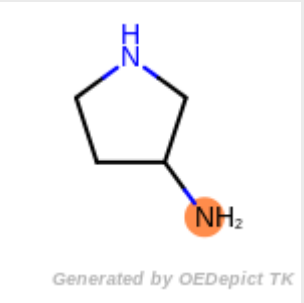




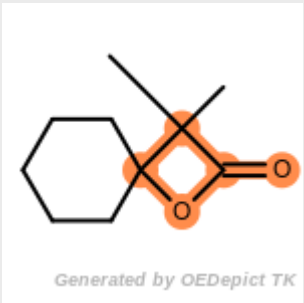
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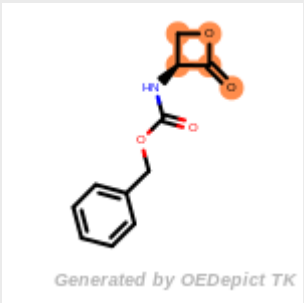


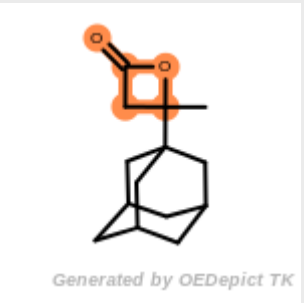




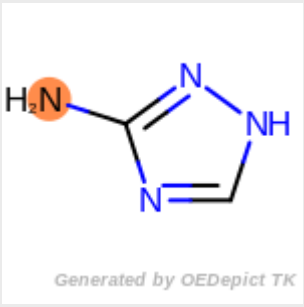
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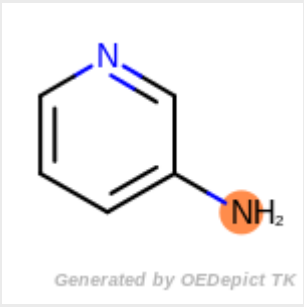


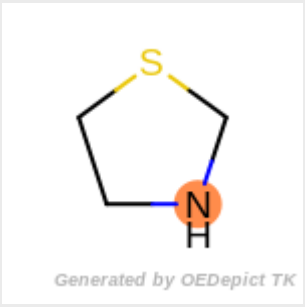




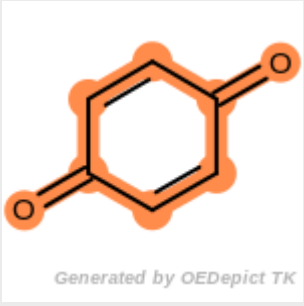
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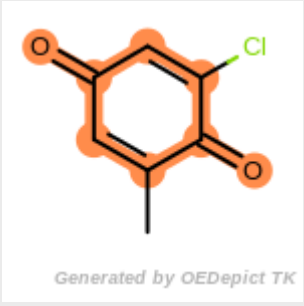


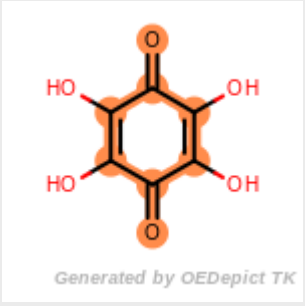




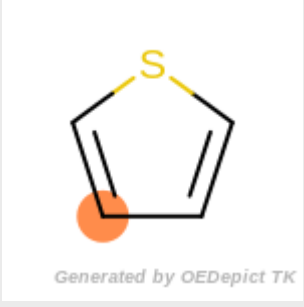
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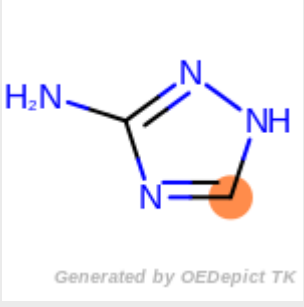


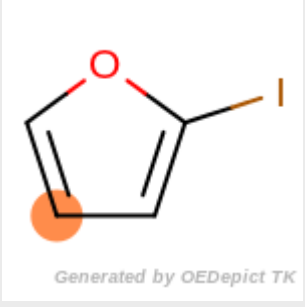




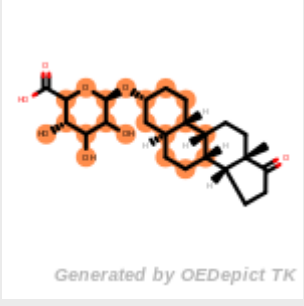
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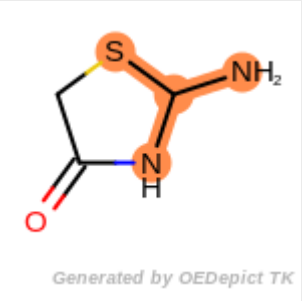


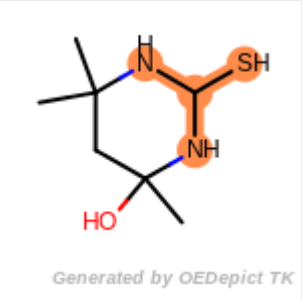


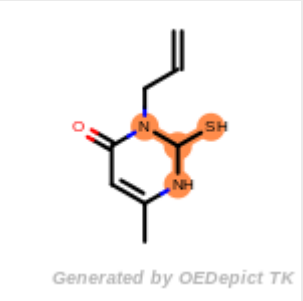
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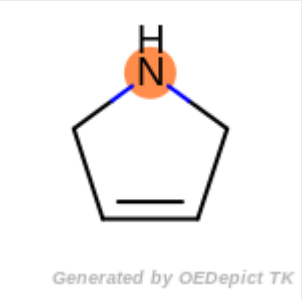
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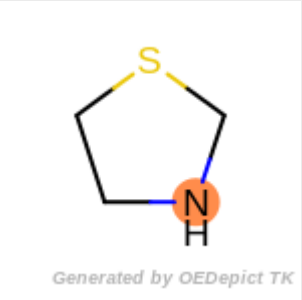


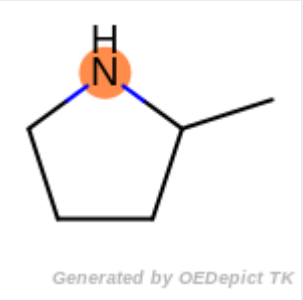




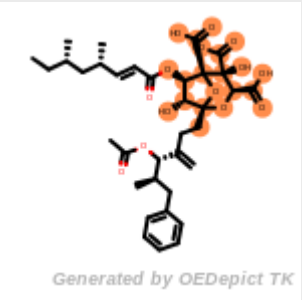
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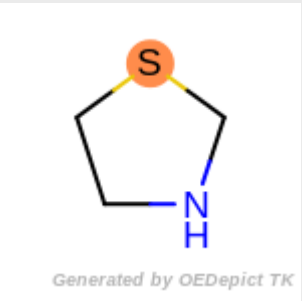


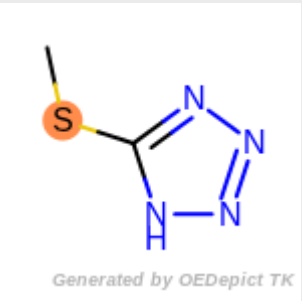


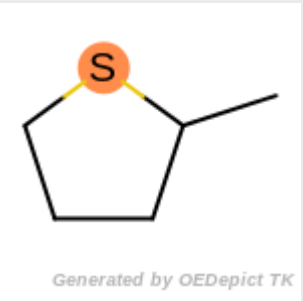
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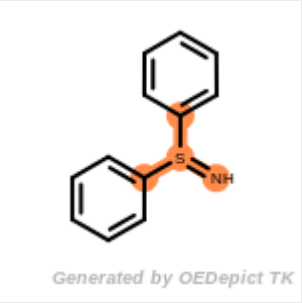
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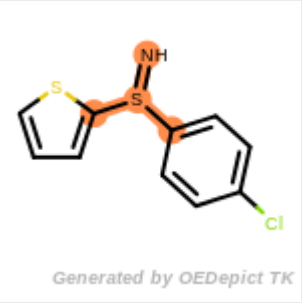


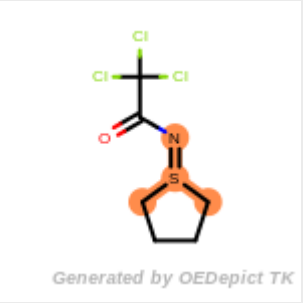




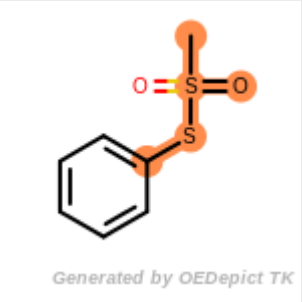
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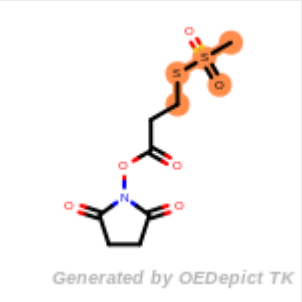


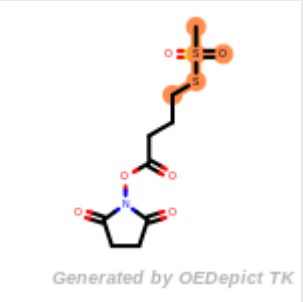




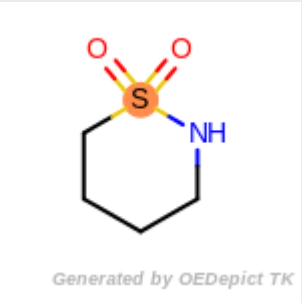
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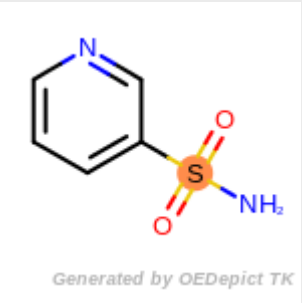


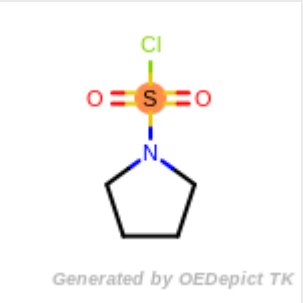




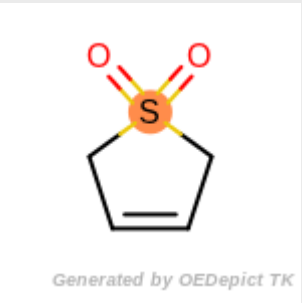
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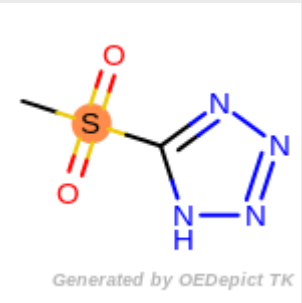


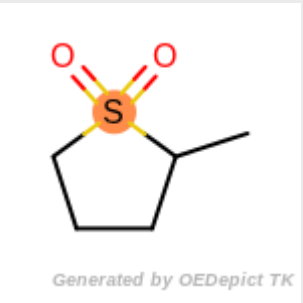




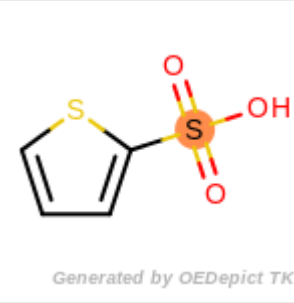
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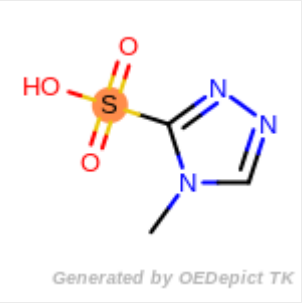


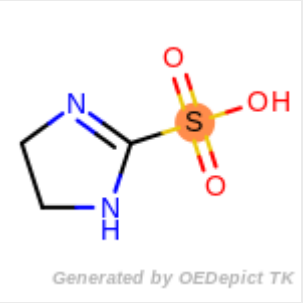




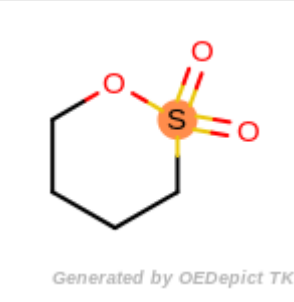
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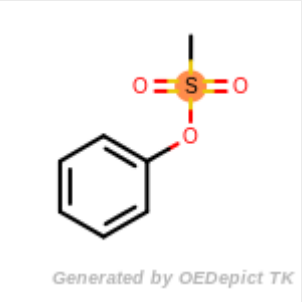


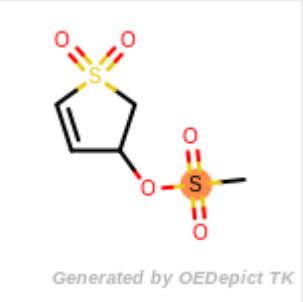




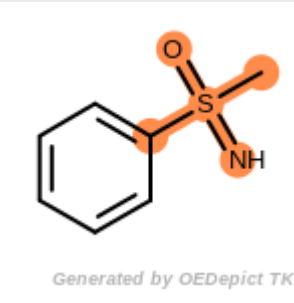
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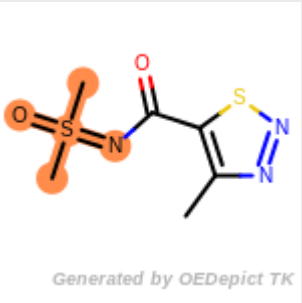


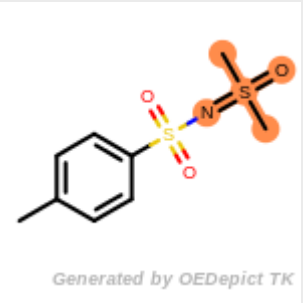




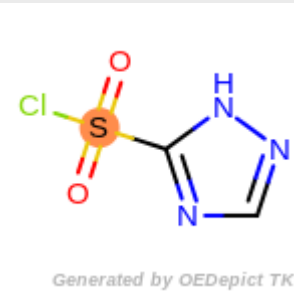
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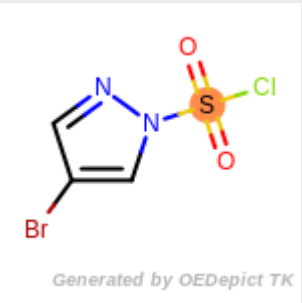


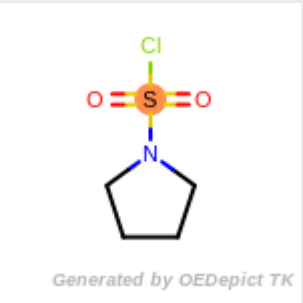




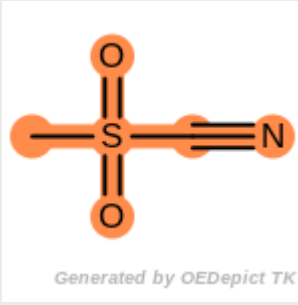
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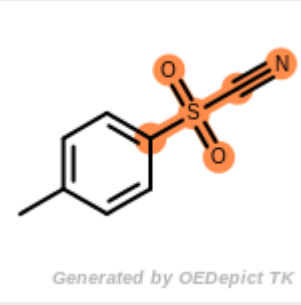


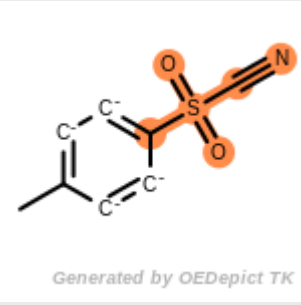




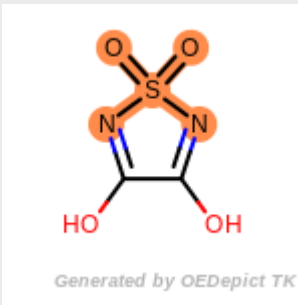
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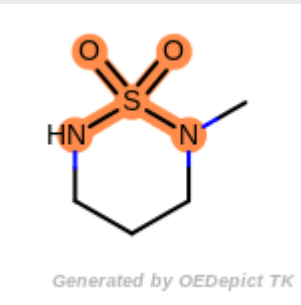


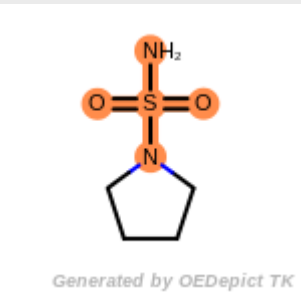




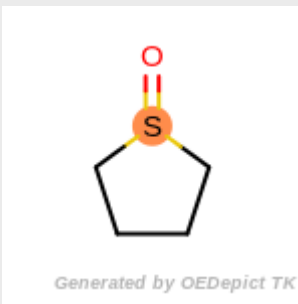
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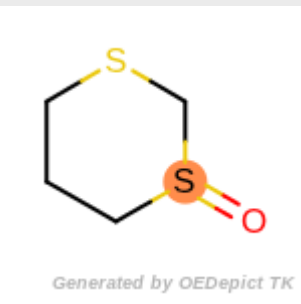


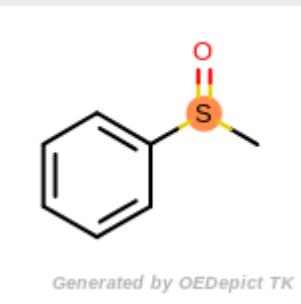




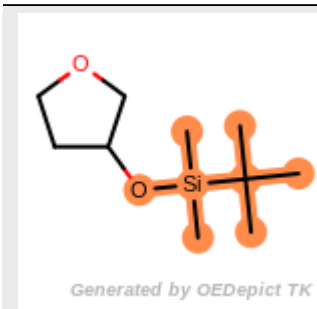
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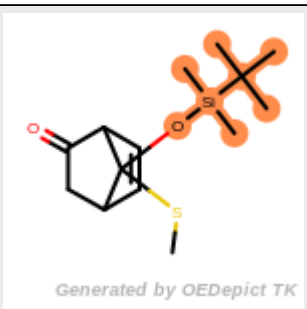


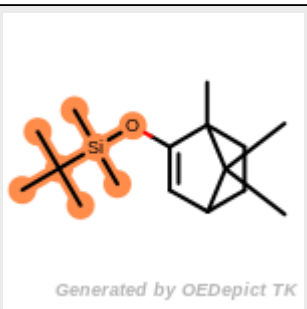




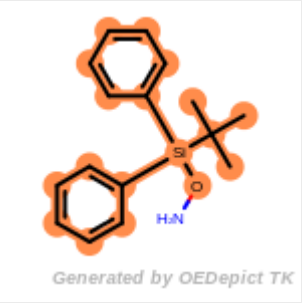
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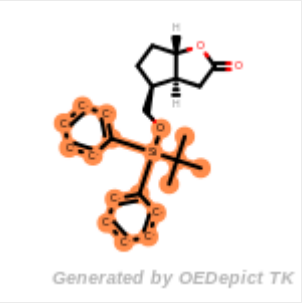




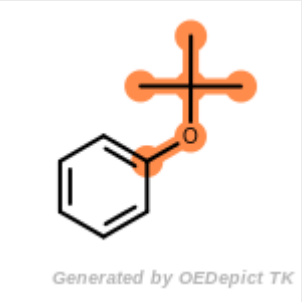


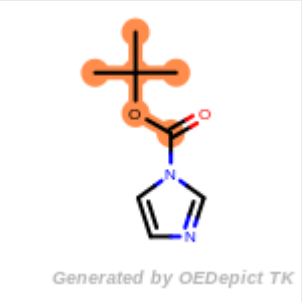
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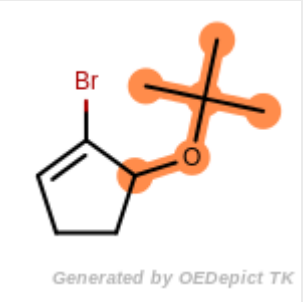




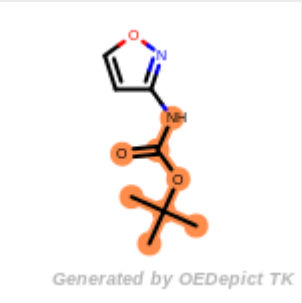
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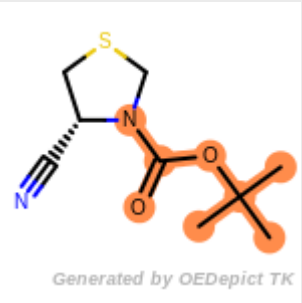


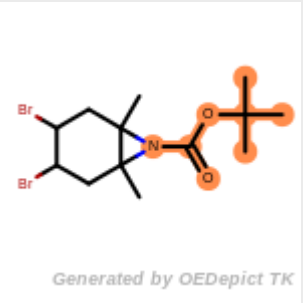




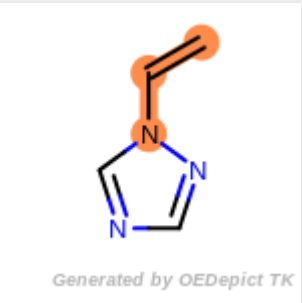
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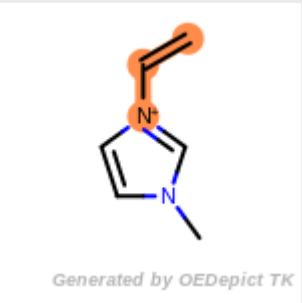


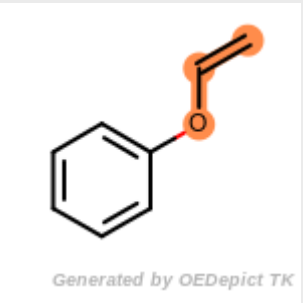




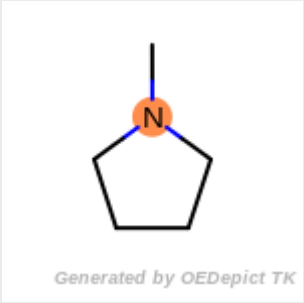
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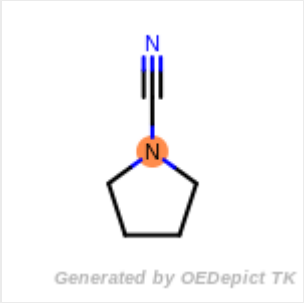


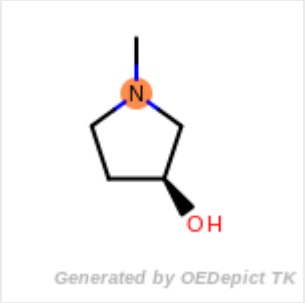




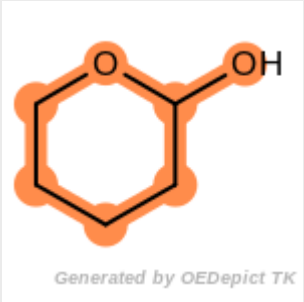
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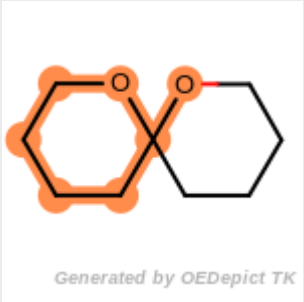


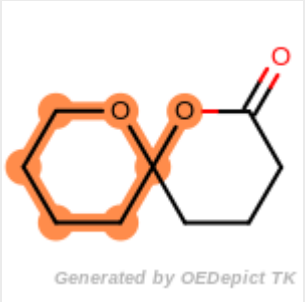




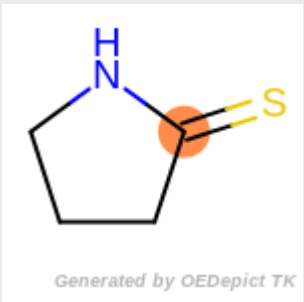
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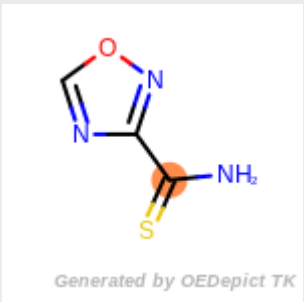


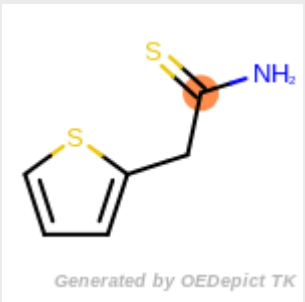




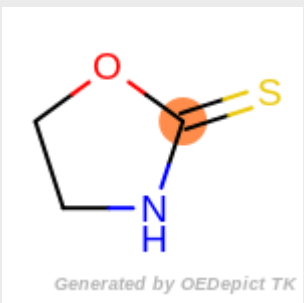
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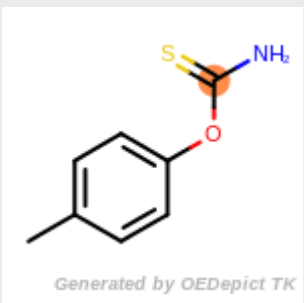


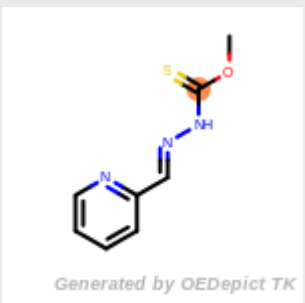




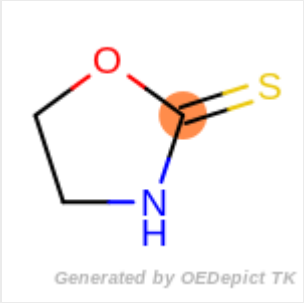
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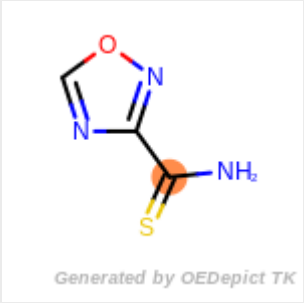


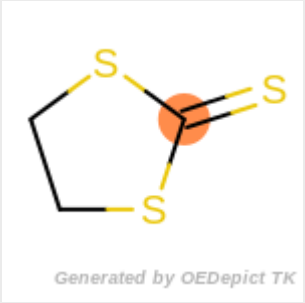




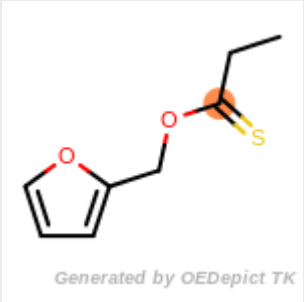
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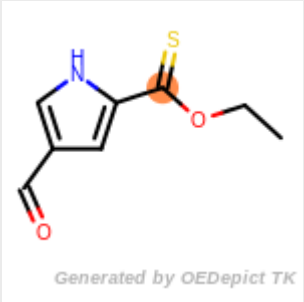


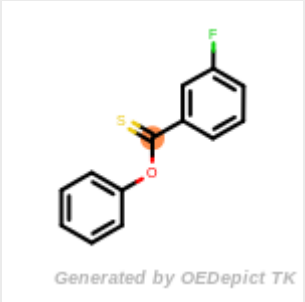




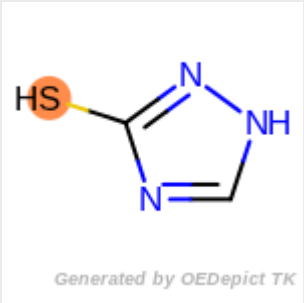
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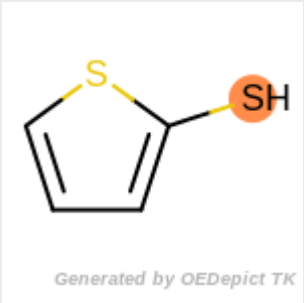


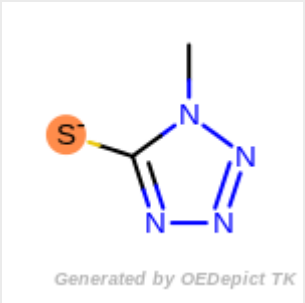




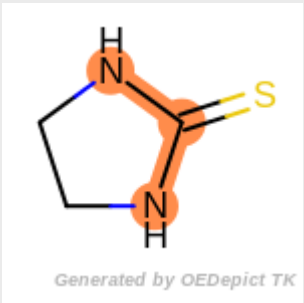
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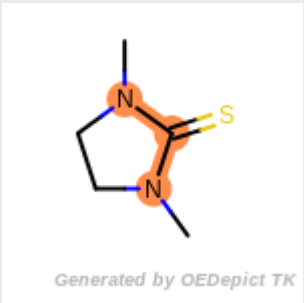


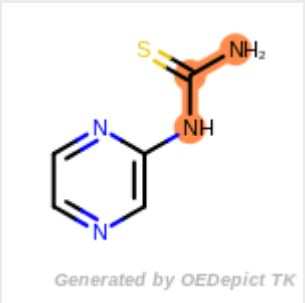




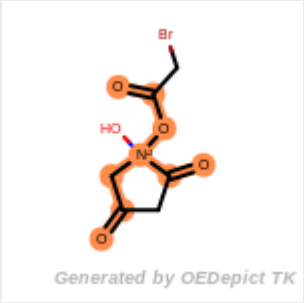
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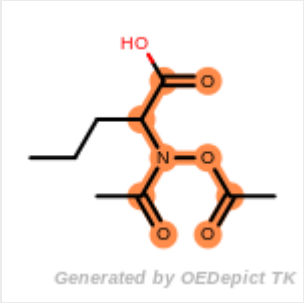


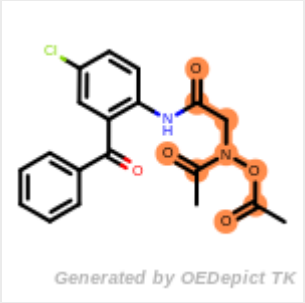




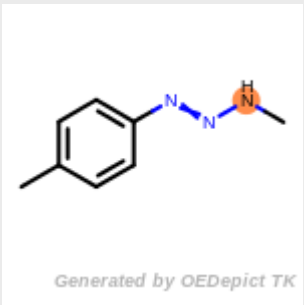
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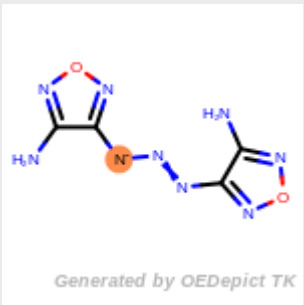


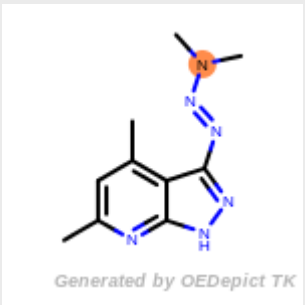




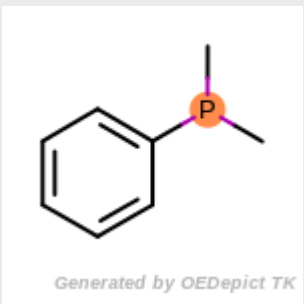
triazine

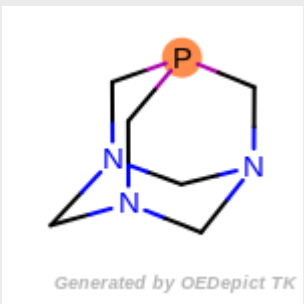


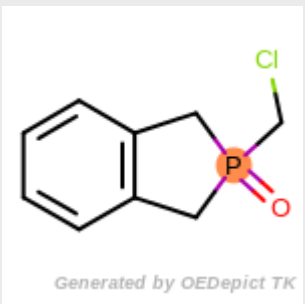




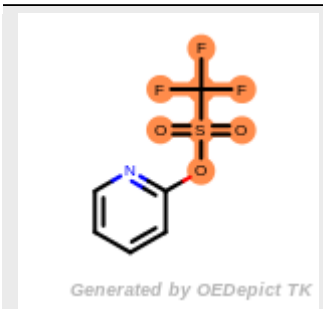
tricarbo_phosphene

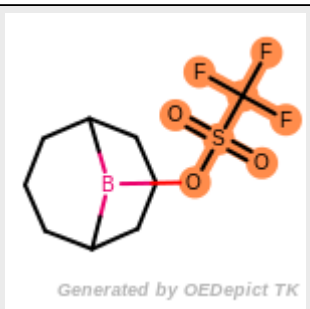


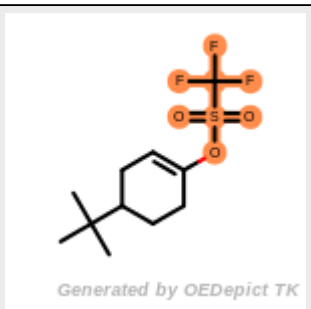




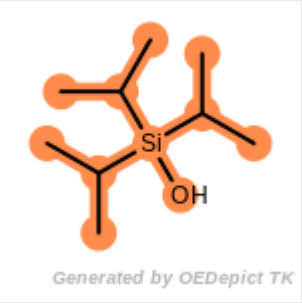
triflates

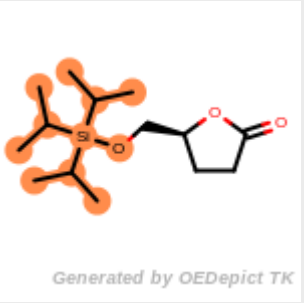


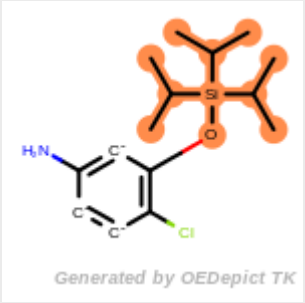




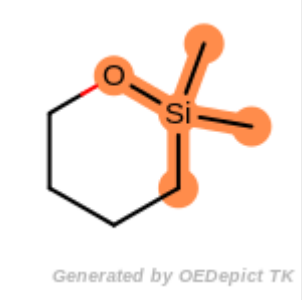
triisopropylsilyl_TIPS

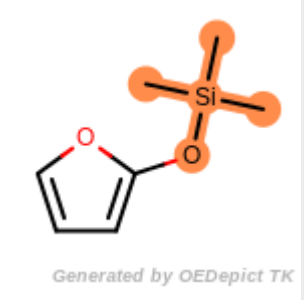


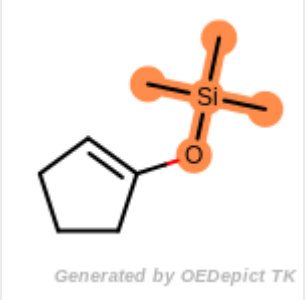




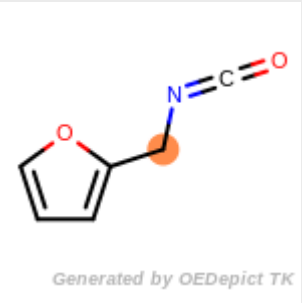
trimethylsilyl_TMS

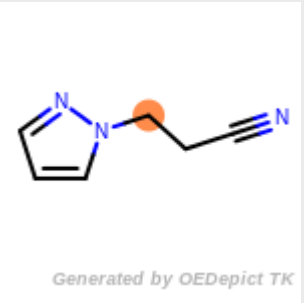


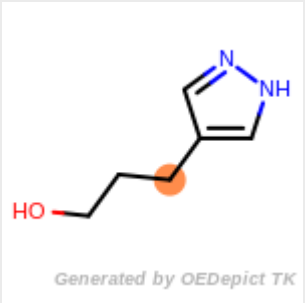




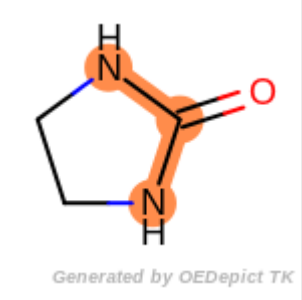
unbranched_chain

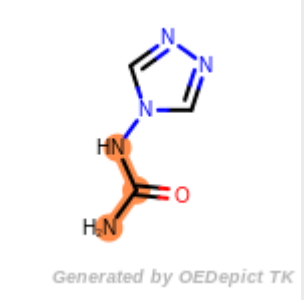


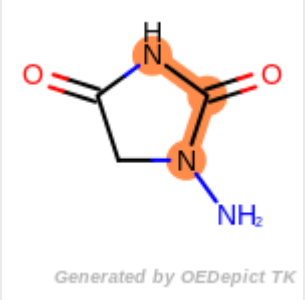




urea







1.4.3 New Rules

New rules specify additional functional groups or substructures that may be used. They must specify a substructure definition in the form of a SMARTS pattern, in addition to the substructure name and maximum limit. For example:

```
NEWRULE norbornane 1 C1CC2CCC1C2
```

The first field is the NEWRULE keyword. The second field defines the name associated with the substructure (primarily for logging purposes). The third field indicates the maximum number of the substructure that can be allowed. The fourth field is the SMARTS string for the substructure, norbornane in this case. This example rule indicates that molecules with a single norbornane substructure would be allowable, but those with two or more norbornanes would be eliminated.

New rules that have a name that is identical with one of the original rules take precedence over the original rule.

1.4.4 Selection Statements

The selection statement allows a filter file to specify the required number of substructures in order to be able to pass the filter. These statements are similar to new rules except that they list a required range for passing the filter rather than the range for failing to pass the filter. For example:

```
SELECT amine 1 1 [N;!$(*-*[!#6;!#1]);!$(*-a);!$(*=,#*)]
```

The first field is the SELECT keyword. The second field indicates the name for the selection (again for logging purposes). The third field is the minimum number of substructures required to be in the molecule. The fourth field is the maximum number of substructures allowed in the molecule. The fifth field is the substructure defined by a SMARTS pattern. The example requires that molecules contain exactly one amine. Only a single SELECT statement is allowed in the filter file. Any complex boolean substructure statements can be incorporated directly into the SMARTS. If multiple SELECT statements occur in a filter file, only the final one will be applied.

CHAPTER

TWO

EXAMPLES

2.1 MolProp TK Examples

The following table lists the currently available **MolProp TK** examples:

Program	Description
MolFilter	basic filtering for a molecule file
QuietFilter	silencing OEFilter logging messages
MolPropTable	generating tabular output of all molecular properties
SpecificMolProp	extract specific property (Lipinski violations) from table output
MolPropSDData	attach molecular properties as SD data
MolPropCSV	Write molecular properties to a CSV file

Examples:

2.1.1 Basic Filtering for a Molecule File

All filtering operations are controlled via the *OEFilter* object. The *OEFilter* object is typically configured with a specified filter and then applied iteratively over a molecule file. This example demonstrates configuring the *OEFilter* object with the *lead-like filter* and then writes out the molecules that pass the filter. The `OEFilter.operator()` method is used to test whether the molecule passes the filter.

> **Note**
>
> The molecule will also be altered by all the specified *Filter Preprocessing* steps.

Command Line Interface

A description of the command line interface can be obtained by executing the program with the –help argument.

```
prompt> java MolFilter --help
```

will generate the following output:

```
Simple parameter list
 filter options :
   -filtertype : filter type

```

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```
 input/output options :
   -in : Input filename
   -out : Output filename
```

```
Usage: ./molfilter <input> <output>
```

Code

```
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*/
package openeye.examples.oemolprop;

import java.net.URL;
import java.util.*;

import openeye.oechem.*;
import openeye.oemolprop.*;

public class MolFilter {

    public static void main(String[] argv) {
        URL fileURL = MolFilter.class.getResource("MolFilter.txt");
        try {
            OEInterface itf = new OEInterface();
            oechem.OEConfigureFromURL(itf, fileURL);
            oemolprop.OEConfigureFilterParams(itf);

            if (!oechem.OEParseCommandLine(itf, argv, "MolFilter")) {
                oechem.OEThrow.Fatal("Unable to interpret command line!");
            }

            String iname = itf.GetString("-in");
            String oname = itf.GetString("-out");

            oemolistream ifs = new oemolistream();
```

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```
            if (!ifs.open(iname)) {
                oechem.OEThrow.Fatal("Cannot open input file!");
            }

            oemolostream ofs = new oemolostream();
            if (!ofs.open(oname)) {
                oechem.OEThrow.Fatal("Cannot create output file!");
            }

            int ftype = oemolprop.OEGetFilterType(itf);
            OEFilter filter = new OEFilter(ftype);

            OEGraphMol mol = new OEGraphMol();
            while (oechem.OEReadMolecule(ifs, mol)) {
                if (filter.call(mol))
                    oechem.OEWriteMolecule(ofs, mol);
            }
            ifs.close();
            ofs.close();
        }
        catch (java.io.IOException e) {
            System.err.println("Unable to open interface file");
        }
    }
}
```

See also

- *OEFilter* class
- *OEConfigureFilterParams* and *OEConfigureFilterType* functions
- *OEGetFilterType* function

Examples

```
prompt> java MolFilter -in mcss.smi.gz -out .smi -filtertype Lead
```

The following is an example of the output:

```
CC1=CC(=O)C=CC1=O    NSC 1,Minimum atom count(10) not reached: 9
c1ccc2c(c1)nc(s2)SSc3nc4ccccc4s3    NSC 2,Maximum disulfide(0) exceeded: 1
c1c(cc(c(c1[N+](=O)[O-])[O-])Cl)[N+](=O)[O-]    NSC 3,Maximum heteroatom to carbon␣
↪ratio(1.10) exceeded: 1.33
c1c(sc(n1)N)[N+](=O)[O-]    NSC 4,Minimum atom count(10) not reached: 9
c1ccc2c(c1)C(=O)c3ccc(cc3C2=O)N    NSC 5,Maximum dye(0) exceeded: 2
c1ccc(c(c1)c2c3ccc(c(c3oc-4c(c(=O)ccc24)Br)Br)O)C(=O)[O-]    NSC 6,Maximum atom␣
↪count(25) exceeded: 27
C[NH+](C)C1=C(C(=O)c2ccccc2C1=O)Cl    NSC 7,Maximum alkyl_halide(0) exceeded: 1
Cc1ccc2c(c1[N+](=O)[O-])C(=O)c3ccccc3C2=O    NSC 8,Maximum nitro(0) exceeded: 1
CC(C)(C)c1cc(c(cc1O)C(C)(C)C)O    NSC 11,Pass
CC1=NN(C(=O)C1)c2ccccc2 NSC    12,Pass
```

By default the *OEFilter.operator()* method will emit information to OEThrow about every molecule passed to it. This example prints that to the screen. The next example, *quietfilter*, shows how to suppress that output. Only the molecules that pass the filter will be written to the output file. The following is the format for what is emitted:

```
[Isomeric SMILES]\t[Title],[Pass|Reason for failure]
```

2.1.2 Quiet Filtering

Log output can be superfluous when using the *OEFilter* object in a more complex program. Since all the log output is written to the OEThrow object, the verbosity level can be lowered by using the OEThrow.SetLevel method. This example demonstrates setting the OEThrow error level to OEErrorLevel.Warning. This will only allow messages at the level of Warning or above to be emitted, thereby silencing the *OEFilter* object's logging output. The -verbose option can be used to change the OEThrow error level.

Command Line Interface

A description of the command line interface can be obtained by executing the program with the –help argument.

```
prompt> java QuietFilter --help
```

will generate the following output:

```
Simple parameter list
 filter options :
   -filtertype : filter type

 input/output options :
   -in : Input filename
   -out : Output filename

 other options :
   -verbose : Error level of messages
```

Code

```
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*/
```

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```
package openeye.examples.oemolprop;

import java.net.URL;
import java.util.*;

import openeye.oechem.*;
import openeye.oemolprop.*;

public class QuietFilter {

    public static void main(String[] argv) {
        URL fileURL = QuietFilter.class.getResource("QuietFilter.txt");
        try {
            OEInterface itf = new OEInterface();
            oechem.OEConfigureFromURL(itf, fileURL);
            oemolprop.OEConfigureFilterParams(itf);

            if (!oechem.OEParseCommandLine(itf, argv, "QuietFilter")) {
                oechem.OEThrow.Fatal("Unable to interpret command line!");
            }

            String iname = itf.GetString("-in");
            String oname = itf.GetString("-out");

            oemolistream ifs = new oemolistream();
            if (!ifs.open(iname)) {
                oechem.OEThrow.Fatal("Cannot open input file!");
            }

            oemolostream ofs = new oemolostream();
            if (!ofs.open(oname)) {
                oechem.OEThrow.Fatal("Cannot create output file!");
            }

            int ftype = oemolprop.OEGetFilterType(itf);
            OEFilter filter = new OEFilter(ftype);

            String ver = itf.GetString("-verbose");
            if (ver.equals("Verbose"))
                oechem.OEThrow.SetLevel(OEErrorLevel.Verbose);
            else if (ver.equals("Info"))
                oechem.OEThrow.SetLevel(OEErrorLevel.Info);
            else if (ver.equals("Warning"))
                oechem.OEThrow.SetLevel(OEErrorLevel.Warning);
            else if (ver.equals("Error"))
                oechem.OEThrow.SetLevel(OEErrorLevel.Error);
            else
                oechem.OEThrow.Fatal("Unrecognized error level!");

            OEGraphMol mol = new OEGraphMol();
            while (oechem.OEReadMolecule(ifs, mol)) {
                if (filter.call(mol))
```

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```
                    oechem.OEWriteMolecule(ofs, mol);
            }
            ofs.close();
            ifs.close();
        }
        catch (java.io.IOException e) {
            System.err.println("Unable to open interface file");
        }
    }
}
```

See also

- *OEFilter* class
- *OEConfigureFilterParams* and *OEConfigureFilterType* functions
- *OEGetFilterType* function
- OEErrorHandler class

Examples

```
prompt> java QuietFilter -in mcss.smi.gz -out .smi -filtertype Lead
```

2.1.3 Molecular Property Table

The *OEFilter* object allows for the calculation of all the molecular properties it uses during the filtering process without actually applying the filter. This may be useful for caching the *OEFilter* object results into a database. The *OEFilter.SetTable* method can be used to specify where to write a tab-delimited table of every property in the associated *filter file*. This example demonstrates how to write the tabular output to standard out.

Note

A tab-delimited file format was chosen to integrate better with Unix commandline utilities. For example, this allows for quick and easy filter experimentation with the awk command line utility. The following snippet will print the number of molecules (plus one for the header) with a molecular weight greater than 200.

```
> java MolPropTable -in drugs.sdf -filtertype Lead > drugs.txt
> cat drugs.txt | awk -F\t '{if ($12 > 200) { print $12 }}' | wc -l
```

Furthermore, all database programs have utilities for importing tab-delimited files. Loading the filter results into a third-party database would provide very speedy filter experimentation since the properties would only have to be calculated once and then cached in the database.

Command Line Interface

A description of the command line interface can be obtained by executing the program with the –help argument.

```
prompt> java MolPropTable --help
```

will generate the following output:

```
Simple parameter list
 filter options :
   -filtertype : filter type

 input/output options :
   -in : Input filename

 other options :
   -verbose : Error level of messages
```

Code

```
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*/
package openeye.examples.oemolprop;

import java.net.URL;
import java.util.*;

import openeye.oechem.*;
import openeye.oemolprop.*;

public class MolPropTable {

    public static void main(String[] argv) {
        URL fileURL = MolPropTable.class.getResource("MolPropTable.txt");
        try{
            OEInterface itf = new OEInterface();
            oechem.OEConfigureFromURL(itf, fileURL);
            oemolprop.OEConfigureFilterParams(itf);

            if (!oechem.OEParseCommandLine(itf, argv, "MolPropTable")) {
                oechem.OEThrow.Fatal("Unable to interpret command line!");
            }

            String iname = itf.GetString("-in");
```

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```
            oemolistream ifs = new oemolistream();
            if (!ifs.open(iname)) {
                oechem.OEThrow.Fatal("Cannot open input file!");
            }

            int ftype = oemolprop.OEGetFilterType(itf);
            OEFilter filter = new OEFilter(ftype);

            int ver = itf.GetInt("-verbose");
            oechem.OEThrow.SetLevel(ver);

            filter.SetTable(oechem.getOeout());

            OEGraphMol mol = new OEGraphMol();
            while (oechem.OEReadMolecule(ifs, mol))
                filter.call(mol);
            ifs.close();
        }
        catch (java.io.IOException e) {
            System.err.println("Unable to open interface file");
        }
    }
}
```

See also

- *OEFilter* class
- *OEConfigureFilterParams* and *OEConfigureFilterType* functions
- *OEGetFilterType* function

Examples

```
prompt> java MolPropTable -in drugs.sdf -filtertype Lead
```

2.1.4 Specific Molecular Properties

The *OEFilter* object table can also be used to retrieve specific molecular properties or filtering terms for which a free function does not exist. The number of molecular properties is large. In addition, some properties are more experimental than others. For these reasons *free functions* are not provided for everything that can be calculated. This example demonstrates how to extract a property, the number of Lipinski violations, from the *OEFilter* object molecular property table by writing the table to a oeosstream.

Warning

The exact number of fields the *OEFilter* object outputs depends on the *filter file* being used. The field will only be output if the filter rule is turned on. That is why this example will search the header line for the position of the "Lipinski violations" field. This key-value lookup is recommended for extracting specific fields from the filter table.

Command Line Interface

A description of the command line interface can be obtained by executing the program with the –help argument.

```
prompt> java SpecificMolProp --help
```

will generate the following output:

```
Simple parameter list
 filter options :
   -filtertype : filter type

 input/output options :
   -in : Input filename
   -out : Output filename
```

Code

```
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*/
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import java.net.URL;
import java.util.*;

import openeye.oechem.*;
import openeye.oemolprop.*;

public class SpecificMolProp {

    public static void main(String[] argv) {
        URL fileURL = SpecificMolProp.class.getResource("SpecificMolProp.txt");
        try {
            OEInterface itf = new OEInterface();
            oechem.OEConfigureFromURL(itf, fileURL);
            oemolprop.OEConfigureFilterParams(itf);

            if (!oechem.OEParseCommandLine(itf, argv, "SpecificMolProp")) {
```

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```
            oechem.OEThrow.Fatal("Unable to interpret command line!");
        }

        String iname = itf.GetString("-in");

        oemolistream ifs = new oemolistream();
        if (!ifs.open(iname)) {
            oechem.OEThrow.Fatal("Cannot open input file!");
        }

        int ftype = oemolprop.OEGetFilterType(itf);
        OEFilter filter = new OEFilter(ftype);

        int ver = itf.GetInt("-verbose");
        oechem.OEThrow.SetLevel(ver);

        oeosstream ostr = new oeosstream();
        filter.SetTable(ostr);

        List<String> fields = Arrays.asList(ostr.str().split("\t"));
        ostr.clear(); // remove the header row from the stream

        int fieldidx = fields.indexOf("Lipinski violations");

        OEGraphMol mol = new OEGraphMol();
        while (oechem.OEReadMolecule(ifs, mol)) {
            filter.call(mol);

            fields = Arrays.asList(ostr.str().split("\t"));
            ostr.clear(); // remove this row from the stream

            System.out.println(mol.GetTitle() + " " + fields.get(fieldidx));
        }
        ostr.close();
        ifs.close();
    }
    catch (java.io.IOException e) {
        System.err.println("Unable to open interface file");
    }
  }
}
```

See also

- *OEFilter* class
- *OEConfigureFilterParams* and *OEConfigureFilterType* functions
- *OEGetFilterType* function

Examples

```
prompt> java SpecificMolProp -in mcss.smi.gz -filtertype Lead
```

2.1.5 Attach Molecular Properties as SD Data

The molecular properties calculated by *OEFilter* can be attached as SD data to the molecule. The *OEFilter.SetSDTag* method is used to attach the calculated molecular properties to molecules passed to the filter object.

SD tag data corresponds to the *tabular data* functionality. The SD data tag names are exactly the same as the names found in the table header. The SD data values are exactly what is output in the data table. The only exceptions are the "SMILES", "Name", and "Filter" columns since this information can be obtained other ways.

This example demonstrates how to set the table output to the `oenul` output stream to allow all properties to be attached as SD data, and write the tabular data to an output in the `OEFormat.SDF`, `OEFormat.OEB`, or the `OEFormat.CSV` format. To specifically write to the `OEFormat.CSV` format, also see the *MolPropCSV* example.

Warning

By default, only the properties up to the failing property will be attached to each molecule. Use *OEFilter.SetTable* to force every property to be attached as SD data. The same rule applies to SD data as *tabular output data*, only the properties specified in the *filter file* will be attached as SD data.

Command Line Interface

A description of the command line interface can be obtained by executing the program with the –help argument.

```
prompt> java MolPropSDData --help
```

will generate the following output:

```
Simple parameter list
 filter options :
   -filtertype : filter type

 input/output options :
   -in : Input filename
   -out : Output filename

 other options :
   -verbose : Error level of messages
```

Code

```
/*
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NOT LIMITED TO, WARRANTIES OF MERCHANTABILITY, FITNESS FOR A
PARTICULAR PURPOSE AND NONINFRINGEMENT. In no event shall Cadence be
liable for any damages or liability in connection with the Sample Code
or its use.
*/
package openeye.examples.oemolprop;

import java.net.URL;
import java.util.*;

import openeye.oechem.*;
import openeye.oemolprop.*;

public class MolPropSDData {

    public static void main(String[] argv) {
        URL fileURL = MolPropSDData.class.getResource("MolPropSDData.txt");
        try {
            OEInterface itf = new OEInterface();
            oechem.OEConfigureFromURL(itf, fileURL);
            oemolprop.OEConfigureFilterParams(itf);

            if (!oechem.OEParseCommandLine(itf, argv, "MolPropSDData")) {
                oechem.OEThrow.Fatal("Unable to interpret command line!");
            }

            String iname = itf.GetString("-in");
            String oname = itf.GetString("-out");

            oemolistream ifs = new oemolistream();
            if (!ifs.open(iname)) {
                oechem.OEThrow.Fatal("Cannot open input file!");
            }

            oemolostream ofs = new oemolostream();
            if (!ofs.open(oname)) {
                oechem.OEThrow.Fatal("Cannot create output file!");
            }
```

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```
            int fmt = ofs.GetFormat();
            if (fmt != OEFormat.SDF && fmt != OEFormat.OEB && fmt != OEFormat.CSV)
                oechem.OEThrow.Fatal("Only SD, OEB, and CSV formats preserve SD data");

            int ftype = oemolprop.OEGetFilterType(itf);
            OEFilter filter = new OEFilter(ftype);

            int ver = itf.GetInt("-verbose");
            oechem.OEThrow.SetLevel(ver);

            filter.SetTable(oechem.getOenul());
            filter.SetSDTag(true);

            OEGraphMol mol = new OEGraphMol();
            while (oechem.OEReadMolecule(ifs, mol)) {
                filter.call(mol);
                oechem.OEWriteMolecule(ofs, mol);
            }
            ifs.close();
            ofs.close();
        }
        catch (java.io.IOException e) {
            System.err.println("Unable to open interface file");
        }
    }
}
```

See also

- *OEFilter* class
- *OEConfigureFilterParams* and *OEConfigureFilterType* functions
- *OEGetFilterType* function

Examples

```
prompt> java MolPropSDData -in drugs.sdf -out out_mpsd.sdf -filtertype Lead
```

2.1.6 Write molecular properties to a CSV file

The molecular properties calculated by *OEFilter* can be written to a file in the `OEFormat.CSV` format as described in the CSV File Format section. Every property specified in the *filter file* will be writtern in the tabular file.

Command Line Interface

A description of the command line interface can be obtained by executing the program with the –help argument.

```
prompt> java MolPropCSV --help
```

will generate the following output:

```
Simple parameter list
 filter options :
   -filtertype : filter type

 input/output options :
   -in : Input filename
   -out : Output filename

 other options :
   -verbose : Error level of messages
```

Code

```
/*
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liable for any damages or liability in connection with the Sample Code
or its use.
*/
/*****************************************************************************
 Write molecular properties to a CSV file
*****************************************************************************/

package openeye.examples.oemolprop;

import java.net.URL;
import java.util.*;

import openeye.oechem.*;
import openeye.oemolprop.*;

public class MolPropCSV {

    public static void main(String[] argv) {
        URL fileURL = MolPropCSV.class.getResource("MolPropCSV.txt");
        try {
            OEInterface itf = new OEInterface();
            oechem.OEConfigureFromURL(itf, fileURL);
            oemolprop.OEConfigureFilterParams(itf);
```

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```
            if (!oechem.OEParseCommandLine(itf, argv, "MolPropCSV")) {
                oechem.OEThrow.Fatal("Unable to interpret command line!");
            }

            String iname = itf.GetString("-in");
            String oname = itf.GetString("-out");

            oemolistream ifs = new oemolistream();
            if (!ifs.open(iname)) {
                oechem.OEThrow.Fatal("Cannot open input file!");
            }

            oemolostream ofs = new oemolostream();
            if (!ofs.open(oname)) {
                oechem.OEThrow.Fatal("Cannot create output file!");
            }

            int ftype = oemolprop.OEGetFilterType(itf);
            OEFilter filter = new OEFilter(ftype);

            int ver = itf.GetInt("-verbose");
            oechem.OEThrow.SetLevel(ver);

            oemolprop.OEWritePropertyDataToCSV(ofs, ifs, filter);

            ifs.close();
            ofs.close();
        }
        catch (java.io.IOException e) {
            System.err.println("Unable to open interface file");
        }
    }
}
```

See also

- *OEFilter* class
- *OEConfigureFilterParams* and *OEConfigureFilterType* functions
- *OEWritePropertyDataToCSV* function

Examples

```
prompt> java MolPropCSV -in drugs.sdf -out out_drugs.csv -filtertype Lead
```

2.2 Python Cookbook Examples

There are large number of code examples available in OpenEye Python Cookbook that use **OpenEye Toolkits** to solve a wide range of cheminformatics and molecular modeling problems.

- 2D Depiction chapter contains examples that illustrate how the **OEDepict TK** and **Grapheme TK** can be utilized to depict molecules and visualize properties calculated with other OpenEye toolkits.
- Visualizing 3D Information chapter contains examples that illustrate how the **Grapheme TK** can be utilized to project complex 3D information into the 2D molecular graph.
- Cheminformatics chapter contains examples that solve various cheminformatics problems such as similarity search, ring perception and manipulating molecular graphs.
- Peptide Informatics chapter contains examples that solve various peptide informatics problems such as generating custom monomer sets, parsing and generating HELM representations, and visualizing peptides.

OpenEye Python Cookbook examples using MolProp TK

- Depicting Atom Contributions of XLogP
- Depicting Fragment Contributions of XLogP
- Depicting Topological Polar Surface Area
- Depicting Molecular Properties

CHAPTER

THREE

APPENDIX: ADDITIONAL EXAMPLES IN PYTHON

These are full listings of programming examples that are excerpted or offered for download, elsewhere in this chapter. For a full list of examples, see *the list in this chapter*.

CHAPTER

FOUR

API

4.1 OEMolProp Classes

4.1.1 OEFilter

```
class OEFilter
```

This class represents a set of filters as initialized from a *filter file*. The primary use of this class is *OEFilter.operator()* method which will return whether the molecule passes or fails the filter.

Constructors

```
OEFilter(unsigned int type = OEFilterType::Default)
```

The *OEFilter* object is usually constructed from an `unsigned integer` from the *OEFilterType* constant namespace. The default constructor will initialize the object to the *OEFilterType.Default* filter. The default filter is an alias for the *OEFilterType.BlockBuster* filter.

> **See also**
>
> The *Variations of Filters* section.

```
OEFilter(OEPlatform::oeistream& filterstr)
```

Fine grained filter control is provided by allowing a custom filter file to be passed to the *OEFilter* object as the `filterstr` argument.

```
OEFilter(const OEFilter& filter)
```

The *OEFilter* object can be copy constructed from another *OEFilter* object.

operator()

```
boolean call(OEMolBase mol)
```

Returns whether the molecule `mol` passes the *OEFilter* object's set of filter rules. This function has been optimized by applying the filter rules in order of how expensive they are to calculate. For example, molecular weight is much easier to calculate than any of the functional group rules.

However, if an output stream has been specified using the *OEFilter.SetTable* method all the filter rules will be checked. This is the only way to ensure that all the fields are filled in the tabular data output to the stream specified in *SetTable* method.

Note

The molecule may be altered by the steps described in the *Filter Preprocessing* chapter.

See also

This method will write logging data to `OEThrow` as described in this *example*.

operator bool

```
boolean IsValid()
```

Returns whether the *OEFilter* object is in a valid state ready to accept molecules to its *OEFilter.operator()* method.

Note

It is nearly impossible for an end user to create an invalid filter. This method is here for future API design to allow for greater programmatic control of the *OEFilter* object.

AddNormalizationRule

```
bool AddNormalizationRule(const OEChem::OEUniMolecularRxn& rxn)
```

Add a OEUniMolecularRxn to apply to the molecule. Special note should be taken about what preprocessing has already occurred on the molecule before generic normalizations are applied as described by the *Filter Preprocessing* chapter.

See also

The *OEChem* manual has a chapter devoted to reactions.

ClearNormalizationRules

```
void ClearNormalizationRules()
```

Remove all normalizations previously added with *OEFilter.AddNormalizationRule*.

GetCanonOrder

```
bool GetCanonOrder() const
```

Returns whether to canonicalize the atom and bond order after salt removal but before the molecule is altered into a neutral pH model.

See also

OEFilter.SetCanonOrder

GetFilterType

```
unsigned int GetFilterType() const
```

Return the `unsigned integer` constant from the *OEFilterType* namespace corresponding to the type of filter used to construct this object.

GetFlagTableFailures

```
bool GetFlagTableFailures() const
```

Return whether values in tabular data output are flagged with an asterisk marking them as outside the valid range for that filter rule. This is useful for figuring out why particular molecules have failed a given filter.

See also

- *Molecular Property Table*
- *OEFilter.SetFlagTableFailures*

GetMessage

```
std::string GetMessage(OEChem::OEMolBase &)
std::string GetMessage(OEChem::OEMCMolBase &)
```

Return a message that is "Pass" if the molecule passes the filter, and a reason for failure if it does not.

GetMMFFTypeCheck

```
bool GetMMFFTypeCheck() const
```

Return whether molecules sent to *OEFilter.operator()* will be *MMFF atom type checked* before any other filtering criteria are applied. The default is `false`.

See also

- *MMFF94 Atom Type Checking*
- *OEFilter.SetMMFFTypeCheck*

GetSDTag

```
bool GetSDTag() const
```

Return whether to attach every molecular property checked by the filter as SD data to the molecule passed to the *OEFilter.operator()* method. By default the the *OEFilter* object will not attach SD data.

See also

OEFilter.SetSDTag

GetTable

```
OEPlatform::oeostream* GetTable() const
```

Return the oeostream object that tabular data is sent to. Will return a zero-pointer, the default, if no output stream has been specified.

See also

- *Molecular Property Table*
- *OEFilter.SetTable*

GetTypeCheck

```
bool GetTypeCheck() const
```

Return whether molecules sent to *OEFilter.operator()* will be *type checked* before any other filtering criteria are applied. The default is `false`.

See also

- *Type Checking*
- *OEFilter.SetTypeCheck*

GetpKaNormalize

```
bool GetpKaNormalize() const
```

Return whether the pKa state of molecules sent to *OEFilter.operator()* will be normalized to a neutral pH. The default is `false`.

See also

- *pKa Normalization*
- *OEFilter.SetpKaNormalize*

ParseNewRules

```
bool ParseNewRules(OEPlatform::oeistream& rulefile)
```

Parse the data from the `rulefile` oeistream as a `NEWRULE` file. These rules will override any rules specified by the *filter file* given to the *OEFilter constructors*.

See also

New Rules

PrintConfig

```
void PrintConfig(OEPlatform::oeostream& log)
```

Print a human readable configuration of the object to the oeostream `log`.

SetCanonOrder

```
void SetCanonOrder(bool b)
```

Specify whether the molecule atom and bond order should be canonicalized after salt removal but before the molecule is altered into a neutral pH model.

See also

OEFilter.GetCanonOrder

SetErrorLevel

```
void SetErrorLevel(unsigned int level)
```

Sets the verbosity of warnings, using a level in the `OEErrorLevel` namespace, that are output when calling the operator *OEFilter.operator()* or the function *GetMessage* on the filter object.

SetFlagTableFailures

```
void SetFlagTableFailures(bool b)
```

Specify whether tabular output data should be marked with an asterisk if that value exceeds the limits specified by the filter.

See also

- *Molecular Property Table*
- *OEFilter.GetFlagTableFailures*

SetMMFFTypeCheck

```
void SetMMFFTypeCheck(bool b)
```

Specify whether molecules sent to *OEFilter.operator()* will be *MMFF atom type checked* before any other filtering criteria are applied.

See also

- *MMFF94 Atom Type Checking*
- *Atom Type Checks* subsection describing filter files
- *OEFilter.GetMMFFTypeCheck*

SetSDTag

```
void SetSDTag(bool b)
```

Specify whether to attach every molecular property checked by the filter as SD data to the molecule passed to the *OEFilter.operator()* method.

Warning

Only the properties up to the failing property will be attached by default. Use *OEFilter.SetTable* to force every property to be attached as SD data. The same rule applies to SD data as tabular output data, only the properties specified in the *filter file* will be attached as SD data.

See also

- *Attach Molecular Properties as SD Data*
- *OEFilter.GetSDTag*

SetTable

```
void SetTable(OEPlatform::oeostream* table, bool owned)
```

Specify the oeostream object that tabular data is sent to. The `owned` parameter specifies whether the *OEFilter* object should take ownership of the `table` pointer. If `owned` is `true` the *OEFilter* destructor will `delete` the `table` pointer, otherwise, it is the user's responsibility.

Specifying a zero-pointer will effectively turn off tabular output data.

Note

The `owned` parameter must always be `false` for extension languages.

See also

- *Molecular Property Table*
- *OEFilter.GetTable*

SetTypeCheck

```
void SetTypeCheck(bool b)
```

Specify whether molecules sent to *OEFilter.operator()* will be *type checked* before any other filtering criteria are applied.

See also

- *Type Checking*
- *Atom Type Checks* subsection describing filter files
- *OEFilter.GetTypeCheck*

SetpKaNormalize

```
void SetpKaNormalize(bool b)
```

Specify whether the pKa state of molecules sent to *OEFilter.operator()* will be normalized to a neutral pH.

See also

- *pKa Normalization*
- *OEFilter.GetpKaNormalize*

4.1.2 OEXLogPResult

```
class OEXLogPResult
```

Used by *OEGetXLogPResult* function to return the computed XLogP and result status.

Constructors

```
OEXLogPResult(bool valid, float value)
```

Constructor. Since this class is mainly used to return values and status from the *OEGetXLogPResult* function, this is generally not used.

IsValid()

```
bool IsValid() const
```

Returns whether the computed value is valid for the molecule. The main reason that the computation fails is that the molecule has one or more atoms that are not parameterized.

GetValue

```
float GetValue() const
```

Returns the computed XLogP value.

4.2 OEMolProp Constants

4.2.1 OEFilterType

This namespace contains built-in filters that can be passed to the *OEFilter constructor*.

> **Warning**
>
> Go look at the *Filter Files* before using any of the following default filters.

> **See also**
>
> *Variations of Filters*

BlockBuster

This is the recommended default filter. We encourage you to use it unless you are familiar with filtering or not satisfied with your initial results.

> **See also**
>
> The development of this filter is described in the *Variations of Filters* section.

Default

An alias for the current default value of *OEFilterType.BlockBuster*.

Drug

Corresponds to the [Oprea-2000] drug-like filters useful for later stage drug development. This is provided as a backwards compatible option. Experience has shown it to be too restrictive, the *OEFilterType.BlockBuster* filter is recommended.

Fragment

Filter for extracting small molecules from a database.

Lead

Corresponds to the [Oprea-2000] lead-like filters useful for preparing HTS databases.

PAINS

Corresponds to the [Baell-2010] filter useful for removing common substructures that interfere with bioassays.

See also

PAINS section

BlockBusterPAINS

Combines the filtering criteria of BlockBuster and PAINS.

Max

Current maximum number of provided built-in filter types.

4.2.2 OEFilterParamName

This namespace contains the default parameter names used when the interface generated by invoking the *OEConfigureFilterParams* function.

See also

- *OEFilterParamSetup* namespace.

The *OEFilterParamName* namespace contains the following constant:

Type

The default name of filter type parameter is **"-filtertype"**.

See also

- *OEFilterParamSetup.Type* constant
- *OEConfigureFilterType* function
- *OEGetFilterType* function

4.2.3 OEFilterParamSetup

This namespace encodes symbolic constants used as bit-masks to indicate which filter interface parameters are being created when invoking the *OEConfigureFilterParams* function.

See also

- *OEFilterParamName* namespace

The *OEFilterParamSetup* namespace contains the following constants:

All

The combination of following constant:

- *OEFilterParamSetup.Type*

Type

Passing this constant to the *OEConfigureFilterParams* function result in generating the following default interface to configure the filter type by invoking the *OEConfigureFilterType* function.

```
Contents of parameter -filtertype
    Aliases : -ftype
    Type : string
    Allow list : false
    Default : BlockBuster
    Simple : true
    Required : false
    Legal values : Lead Drug BlockBuster Fragment PAINS Custom Max
    Brief : filter type
```

See also

- *OEFilterParamName.Type* constant
- *OEConfigureFilterType* function
- *OEGetFilterType* function

4.3 OEMolProp Functions

4.3.1 OECheckXLogXType

```
bool OECheckXLogXType(OEAtomBase atom)
```

Returns true if a given atom or has a valid XLogP type as referenced in the *LogP* section, or if the atom is a hydrogen.

See also

OEGetXLogP function *OECheckXLogXTypes* function *LogP* section

4.3.2 OECheckXLogXTypes

```
bool OECheckXLogXTypes(OEMolBase mol)
```

Returns true if each atom excluding hydrogens in the given molecule has a valid XLogP type as referenced in the *LogP* section. Invalid types for hydrogens are ignored.

See also

OEGetXLogP function *OECheckXLogXType* function *LogP* section

4.3.3 OEConfigureFilterParams

```
bool OEConfigureFilterParams(OESystem::OEInterface& itf,
                             unsigned int config = OEFilterParamSetup::All)
```

Configures the given interface to add filter parameters.

itf
The interface being configured.

config
The option that specifies which parameters will be added to the interface. This value has to be from the *OEFilterParamSetup* namespace.

See also

- OEInterface class in the **OEChem TK** manual
- *OEFilterParamSetup* namespace
- *OEGetFilterType* function

4.3.4 OEConfigureFilterType

```
bool OEConfigureFilterType(OESystem::OEInterface& itf,
                           std::string name = OEFilterParamName::Type,
                           std::string alias = "-ftype")
```

Configures the given interface to add filter type parameter.

itf
The interface being configured.

name
The name of the filter type parameter.

alias
The alternative *i.e.* alias name of the parameter.

See also

- OEInterface class in the **OEChem TK** manual

- *OEGetFilterType* function
- *OEFilterParamSetup* namespace
- *OEFilterParamName* namespace
- *OEFilterType* namespace

4.3.5 OEGet2dPSA

```
float OEGet2dPSA(OEMolBase mol, OEFloatArray atomPSA, boolean SandP)
float OEGet2dPSA(OEMolBase mol, OEFloatArray atomPSA)
float OEGet2dPSA(OEMolBase mol)
```

Returns the topological polar surface area for a given molecule as described in the *Polar Surface Area* section. The SandP parameter controls whether sulfur and phosphorus should be counted towards the total surface area. See example in *Figure: Example of depicting the atom contributions of the polar surface area*.

Note

TPSA values are mildly sensitive to the protonation state of a molecule.

The atomPSA parameter can be used to retrieve the contribution of each atom to the total polar surface area as shown in *Listing 1*.

Listing 1: Example of retrieving individual atom contributions to PSA

```
OEFloatArray atomPSA = new OEFloatArray(mol.GetMaxAtomIdx());
float psa = oemolprop.OEGet2dPSA(mol, atomPSA);

System.out.println("PSA = " + psa);
for (OEAtomBase atom : mol.GetAtoms()) {
    int idx = atom.GetIdx();
    System.out.println(idx + " " + atomPSA.getItem(idx));
}
```

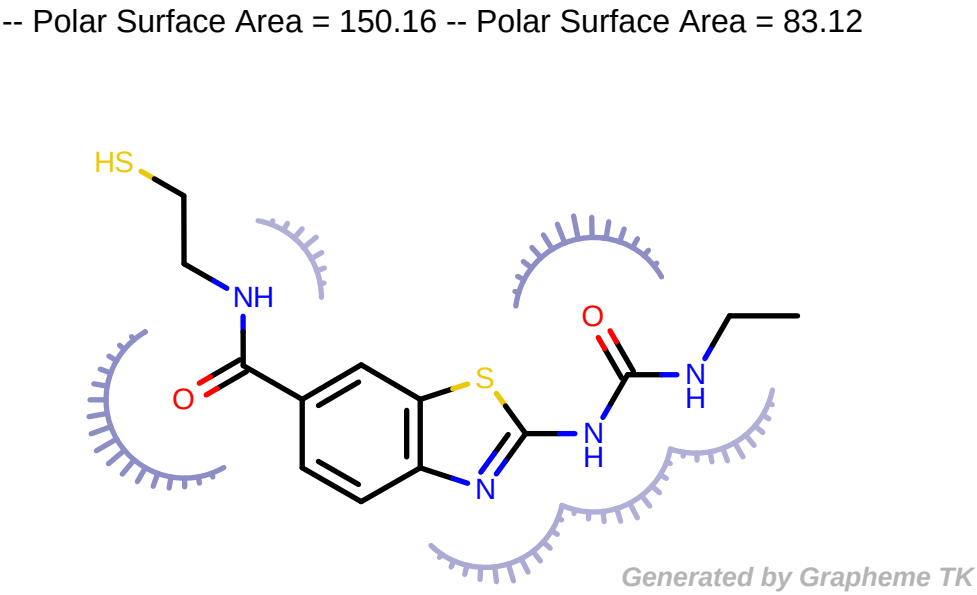


Fig. 1: **Example of depicting the atom contributions of the polar surface area (ignoring S and P atoms)**
(Darker colors and longer spikes indicate larger PSA atom contributions)

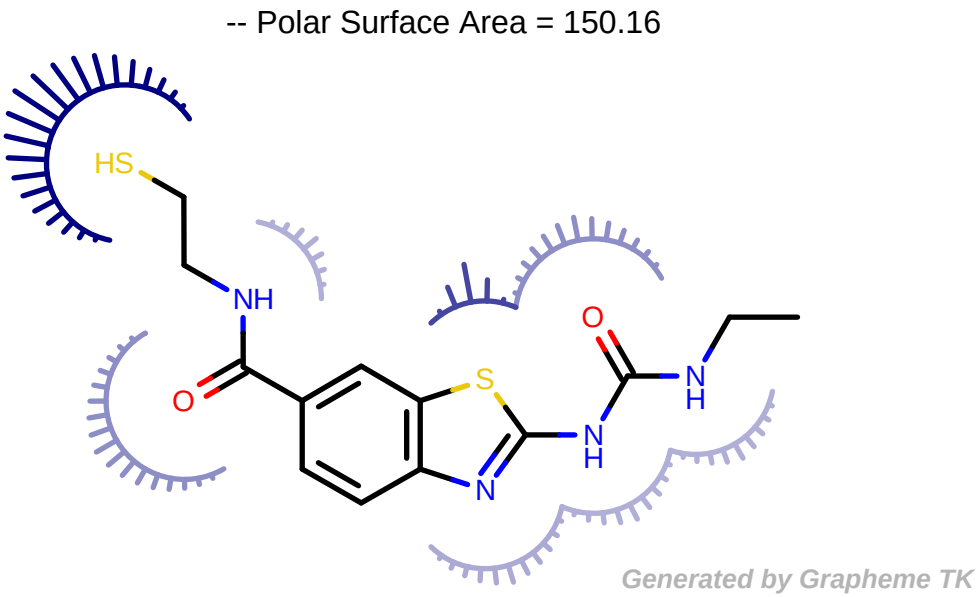


Fig. 2: **Example of depicting the atom contributions of the polar surface area (considering S and P atoms)**
(Darker colors and longer spikes indicate larger PSA atom contributions)

See also

- *Polar Surface Area* section

- OpenEye Python Cookbook — PSA depiction

4.3.6 OEGetAnionicCarbonCount

```
unsigned int OEGetAnionicCarbonCount(const OEChem::OEMolBase& mol)
```

Returns the number of anionic carbons in a molecule. Anionic carbon is defined as an aromatic carbon that has negative 'formal charge'.

See also

- *Anionic Carbon Count* subsection describing filter files
- `OEAtomBase.IsAromatic` and `OEAtomBase.GetFormalCharge` methods in the **OEChem TK** manual

4.3.7 OEGetAromaticRingCount

```
unsigned OEGetAromaticRingCount(const OEChem::OEMolBase& mol)
```

Returns the number of aromatic rings in a molecule as defined in [Ritchie-2009]. The article describes the method as the following:

```
The terminology 'number of aromatic rings' (or aromatic ring
count) is used generically and encompasses both benzenoid
aromatic rings and heteroaromatics (including, e.g. pyridine and
imidazole). ... Each ring in a fused system is counted
individually; thus, indole and naphthalene are each defined as
having two aromatic rings.
```

4.3.8 OEGetFilterType

```
unsigned int OEGetFilterType(const OESystem::OEInterface& itf,
                             std::string name = OEFilterParamName::Type)
```

Returns the filter type initialized in the given interface. The return value is taken from the *OEFilterType* namespace.

itf
The interface in which the parameter is configured.

name
The name of the parameter.

See also

- *OEConfigureFilterParams* function
- *OEConfigureFilterType* function
- *OEFilterType* namespace

4.3.9 OEGetFractionCsp3

```
float OEGetFractionCsp3(const OEChem::OEMolBase& mol)
```

Returns the number of sp^3 carbons divided by the total number of carbons as described by Lovering and coworkers [Lovering-2009].

4.3.10 OEGetHalideFraction

```
double OEGetHalideFraction(const OEChem::OEMolBase& mol,
                           bool isotopic = false)
```

Returns the percent of molecular weight from halides.

isotopic
: This parameter determines whether the isotopic information is taken into account when calculating the molecule weight.

See also

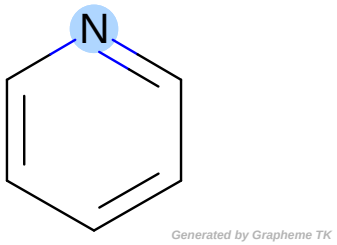
- `OECalculateMolecularWeight` function in the **OEChem TK** manual
- *Halide Fraction* subsection describing filter files

4.3.11 OEGetHBondAcceptorCount

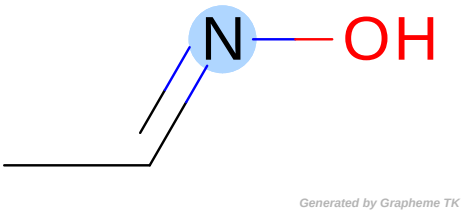
```
unsigned int OEGetHBondAcceptorCount(const OEChem::OEMolBase& mol)
```

Returns the number of hydrogen-bond acceptors in a molecule based on the definition in the work of Mills and Dean ([Mills-Dean-1996]) and also in the book by Jeffrey ([Jeffrey-1997]). It is defined to be the number of atoms which match any of the following:

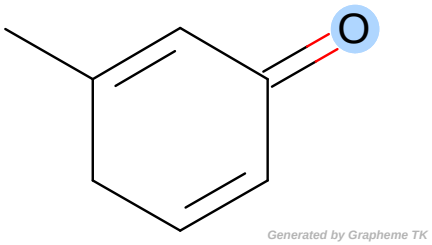
- degree 2, aromatic, non-positive nitrogens. An example is shown below.



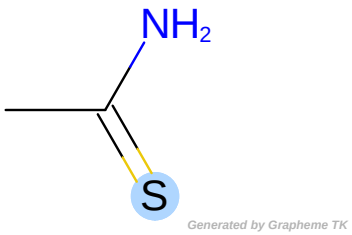
- electron rich or negative, valence less than 4, non-aromatic nitrogens. An example is shown below.



- negatively charged or not electron withdrawn, neutral, non-aromatic oxygens. An example is shown below.



- degree 1, double bonded, electron rich, non-aromatic sulfur. An example is shown below.

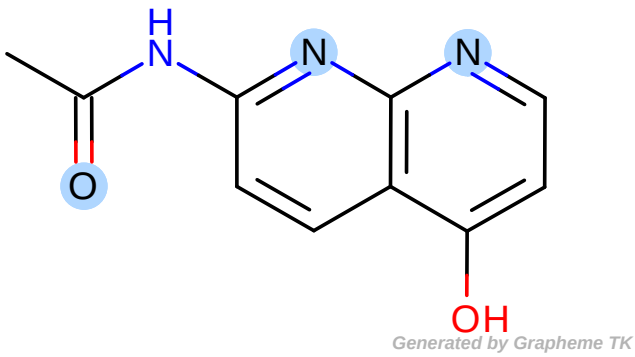


See also

- *OEGetHBondDonorCount* function
- *OEGetLipinskiAcceptorCount* function
- *Lipinski and Hydrogen Bonds* section
- *Hydrogen Bond Acceptors* subsection describing filter files

Example

The *OEGetHBondAcceptorCount* function returns 3 for the molecule below.



4.3.12 OEGetHBondDonorCount

```
unsigned int OEGetHBondDonorCount(const OEChem::OEMolBase& mol)
```

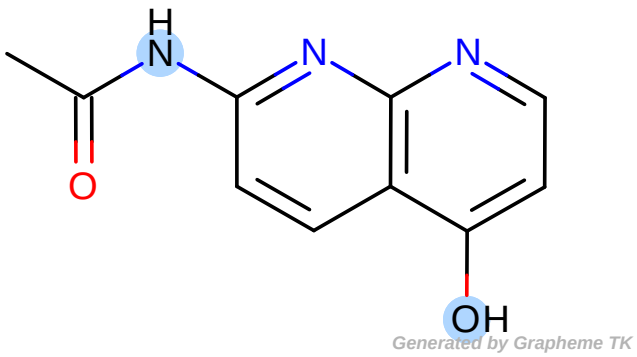
Returns the number of hydrogen-bond donors in a molecule based on the definition in the work of Mills and Dean ([Mills-Dean-1996]) and also in the book by Jeffrey ([Jeffrey-1997]). It is defined to be the number of hydrogen atoms on nitrogen, oxygen, or sulfur atoms.

See also

- *OEGetHBondAcceptorCount* function
- *OEGetLipinskiDonorCount* function
- *Lipinski and Hydrogen Bonds* section
- *Hydrogen Bond Donors* subsection describing filter files

Example

The *OEGetHBondDonorCount* function returns 2 for the molecule below.



4.3.13 OEGetLipinskiAcceptorCount

```
unsigned int OEGetLipinskiAcceptorCount(const OEChem::OEMolBase& mol)
```

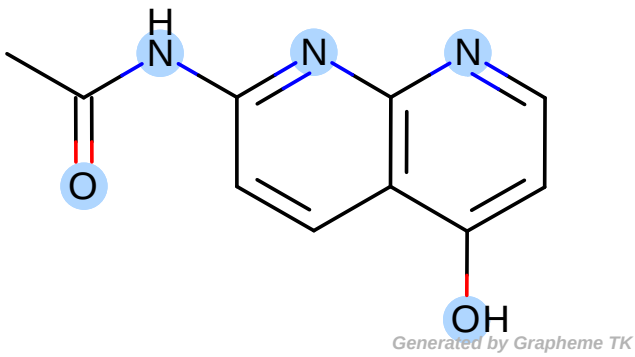
Returns the number of acceptors in a molecule based on the definition from the work of Lipinski ([Lipinski-1997]). It is defined to be the number of nitrogens or oxygens.

See also

- *OEGetLipinskiDonorCount* function
- *OEGetHBondAcceptorCount* function
- *Lipinski and Hydrogen Bonds* section
- *Lipinski Acceptors* subsection describing filter files

Example

The *OEGetLipinskiAcceptorCount* function returns 5 for the molecule below.



4.3.14 OEGetLipinskiDonorCount

```
unsigned int OEGetLipinskiDonorCount(const OEChem::OEMolBase& mol)
```

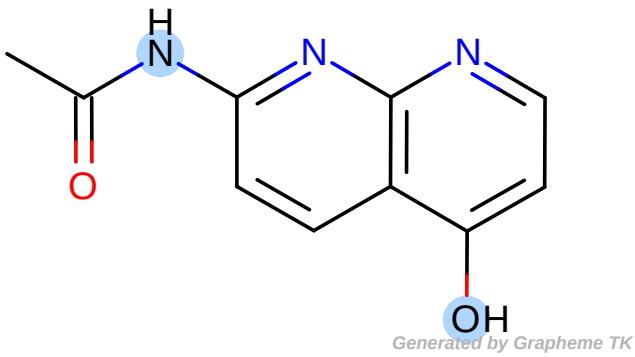
Returns the number of donors in a molecule based on the definition from the work of Lipinski ([Lipinski-1997]). It is defined to be the number of nitrogens and oxygens with at least one hydrogen attached.

See also

- *OEGetLipinskiAcceptorCount* function
- *OEGetHBondDonorCount* function
- *Lipinski and Hydrogen Bonds* section
- *Lipinski Donors* subsection describing filter files

Example

The *OEGetLipinskiDonorCount* function returns 2 for the molecule below.



4.3.15 OEGetLongestUnbranchedHeavyAtomsChain

```
unsigned int OEGetLongestUnbranchedHeavyAtomsChain(const OEChem::OEMolBase& mol)
```

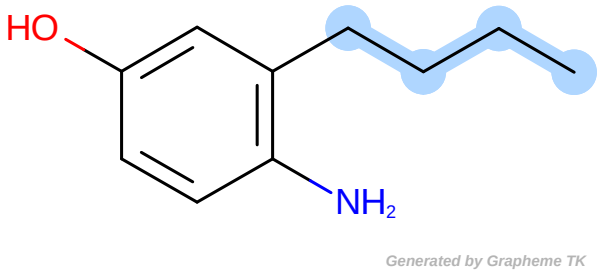
Returns the size of the longest chain of heavy atoms in a molecule. This is defined to be the maximum number of connected, unbranched, and non-ring heavy atoms. An unbranched atom is a chain atom with maximum two connections to other heavy chain atoms. A set of unbranched atoms which are connected together form a chain. A molecule may contain multiple chains which are isolated from each other by non-chain atoms (e.g. ring or branched atoms).

See also

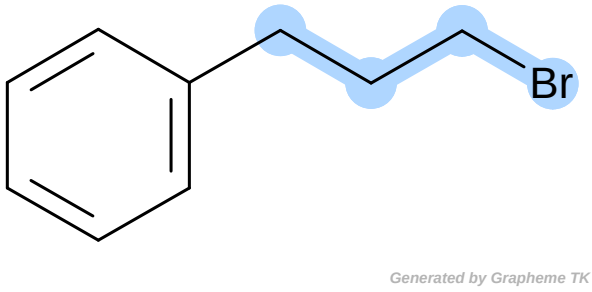
- *OEGetLongestUnbranchedCarbonsChain* function
- *Unbranched Chains* subsection describing filter files

Examples

The *OEGetLongestUnbranchedHeavyAtomsChain* function returns 4 for the molecule below.



The *OEGetLongestUnbranchedHeavyAtomsChain* function returns 4 for the molecule below.



4.3.16 OEGetLongestUnbranchedCarbonsChain

```
unsigned int OEGetLongestUnbranchedCarbonsChain(const OEChem::OEMolBase& mol)
```

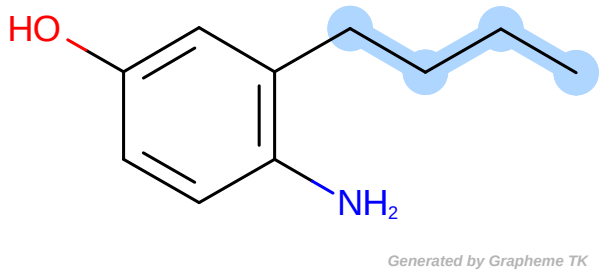
Returns the size of the longest chain of all carbons in a molecule. An unbranched atom is a chain atom with maximum two connections to other heavy chain atoms. A set of unbranched atoms which are connected together form a chain. A molecule may contain multiple chains which are isolated from each other by non-chain atoms (e.g. ring or branched atoms).

See also

- *OEGetLongestUnbranchedHeavyAtomsChain* function
- *Unbranched Chains* subsection describing filter files

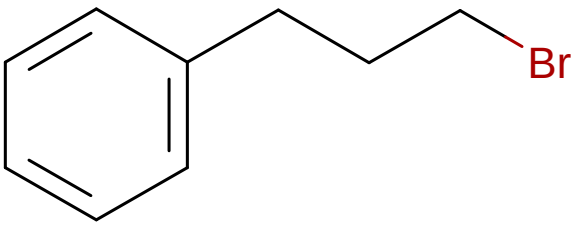
Examples

The *OEGetLongestUnbranchedCarbonsChain* function returns 4 for the molecule below.



Generated by Grapheme TK

The *OEGetLongestUnbranchedCarbonsChain* function returns 0 for the molecule below. It is because the unbranched chain does not contain all carbons.



Generated by Grapheme TK

4.3.17 OEGetNumUnspecifiedAtomStereos

```
unsigned int OEGetNumUnspecifiedAtomStereos(OEChem::OEMolBase& mol)
```

Returns the number of unspecified stereo atoms in a molecule. The OEPerceiveChiral function will be called to perceive chiral atoms in the molecule.

See also

- *Unspecified Atom Stereo* subsection describing filter files
- Stereochemistry Perception chapter in the **OEChem TK** manual
- `OEAtomBase.HasStereoSpecified` method in the **OEChem TK** manual
- *`OEGetNumUnspecifiedBondStereos`* function

4.3.18 OEGetNumUnspecifiedBondStereos

```
unsigned int OEGetNumUnspecifiedBondStereos(OEChem::OEMolBase& mol)
```

Returns the number of unspecified stereo bonds in a molecule. The `OEPerceiveChiral` function will be called to perceive chiral bonds in the molecule.

See also

- *Unspecified Bond Stereo* subsection describing filter files
- Stereochemistry Perception chapter in the **OEChem TK** manual
- `OEBondBase.HasStereoSpecified` method in the **OEChem TK** manual
- *`OEGetNumUnspecifiedAtomStereos`* function

4.3.19 OEGetRotatableBondCount

```
unsigned int OEGetRotatableBondCount(const OEChem::OEMolBase& mol,
                                     bool adjust = false)
```

Returns the number of rotatable bond counts in a molecule. Rotatable bond is defined as any single non-ring bond, bounded to nonterminal heavy (i.e., non-hydrogen) atom. In addition, It considers the carbon-carbon triple bond in acetylene rotatable. The function excludes single bonds observed in a certain groups, such as sulfonamides, esters, and amidine.

adjust
: This parameter allows optional adjustment for aliphatic rings following the method of [Oprea-2000]. In this case, it also estimates the number of flexible bonds in aliphatics rings.

Note

The Oprea's method is individual ring based. Since *Smallest set of smallest rings* perception is not available in **OEChem TK** (see section Smallest Set of Smallest Rings (SSSR) Considered Harmful for more details), we modified Oprea's method to be ring system based (Ring Systems Identification), and implemented the function relatively closed to Oprea's definition. The function works for various complex fused ring-systems and simple bridge ring-systems.

Examples

The number of rotatable bonds calculated for the molecule below is `0`. When considering the flexibility of the aliphatic ring (setting the **adjust** parameter to `true`), the *`OEGetRotatableBondCount`* function returns *3*, based on Oprea's method that considers the amide bonds as non-rotatable.

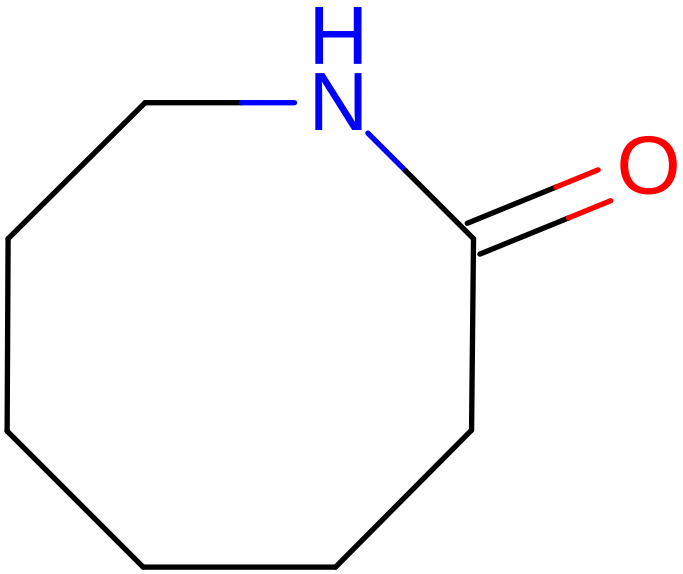


Fig. 3: **Example of aliphatic ring**

The number of rotatable bonds calculated for the molecule below is 7. When considering the flexibility of the aliphatic ring (setting the **adjust** parameter to `true`), the *`OEGetRotatableBondCount`* function returns 11, adjusting the rotatable bond count by 2 from each of the two aliphatic rings.

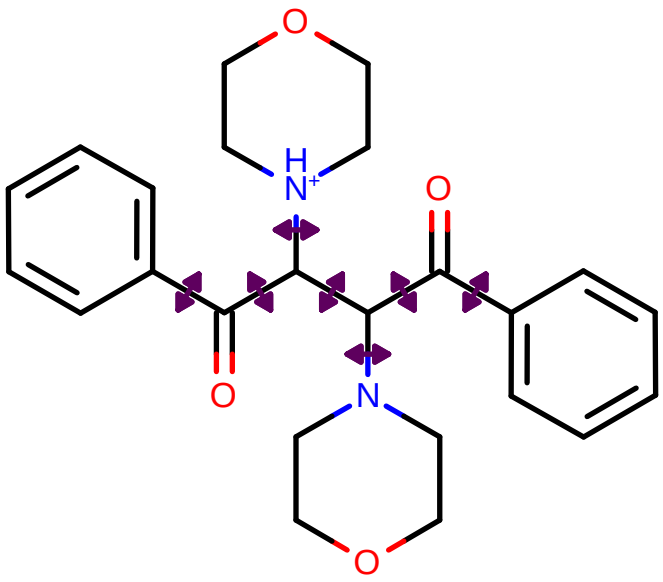


Fig. 4: **Example of rotatable bond count adjustment for aliphatic rings**

See also

- *Rotor Count* subsection describing filter files
- rotatable bond definition in **OEChem TK**
- OEIsRotor functor in **OEChem TK**
- Smallest Set of Smallest Rings (SSSR) Considered Harmful and Ring Systems Identification sections in **OEChem TK**

4.3.20 OEGetXLogP

```
float OEGetXLogP(OEMolBase mol, OEFloatArray atomxlogps)
float OEGetXLogP(OEMolBase mol)
```

Returns the XLogP for a given molecule as described in the *LogP* section. The returned value will be equal to the sum on the individual atom contributions plus the linear regression constant `-0.127`.

Note

The C++ version of this function uses a pointer-to-argument to indicate the success or failure of the computation. This idiom doesn't map directly to the wrapped languages, so the wrapped versions of *OEGetXLogP* use exceptions to signal failure. This is not optimal. Hence, for the wrapped languages, the **preferred method for computing XLogP** is *OEGetXLogPResult*. It does not use exceptions and is much cleaner to use in the wrapped languages.

Note

XLogP should be calculated on the neutral form of the molecule. Therefore, calling the `OERemoveFormalCharge` function of **Quacpac TK** is highly recommended prior to the XLogP calculation.

See also

- *OEGetXLogPResult* function
- *LogP* section

4.3.21 OEGetXLogPResult

```
OEXLogPResult OEGetXLogPResult(OEMolBase mol, OEFloatArray atomxlogps)
OEXLogPResult OEGetXLogPResult(OEMolBase mol)
```

Returns an *OEXLogPResult* object. The object contains the XLogP for the given molecule as described in the *LogP* section and a boolean flag indicating whether or not the computation is valid. The main reason the computation may fail is if one or more atoms are not parameterized. The returned value will be equal to the sum on the individual atom contributions plus the linear regression constant `-0.127`.

Hint

XLogP should be calculated on the neutral form of the molecule. Therefore, calling the `OERemoveFormalCharge` function of **Quacpac TK** is highly recommended prior to the XLogP calculation.

The `atomxlogps` parameter can be used to retrieve the contribution of each atom to the total XLogP as shown in *`Listing 2`*. See example in *Figure: Example of depicting the atom contributions of the XLogP*.

This function exists to make the calling by wrapped languages more convenient. This function should be **preferred over** the original *`OEGetXLogP`* function for wrapped languages.

Listing 2: Example of retrieving individual atom contributions to XLogP

```
OEFloatArray atomXLogP = new OEFloatArray(mol.GetMaxAtomIdx());
OEXLogPResult result = oemolprop.OEGetXLogPResult(mol, atomXLogP);

if (result.IsValid()) {
    System.out.println("XLogP = " + result.GetValue());
    for (OEAtomBase atom : mol.GetAtoms()) {
        int idx = atom.GetIdx();
        System.out.println(idx + " " + atomXLogP.getItem(idx));
    }
}
else
    System.out.println("XLogP failed for molecule");
```

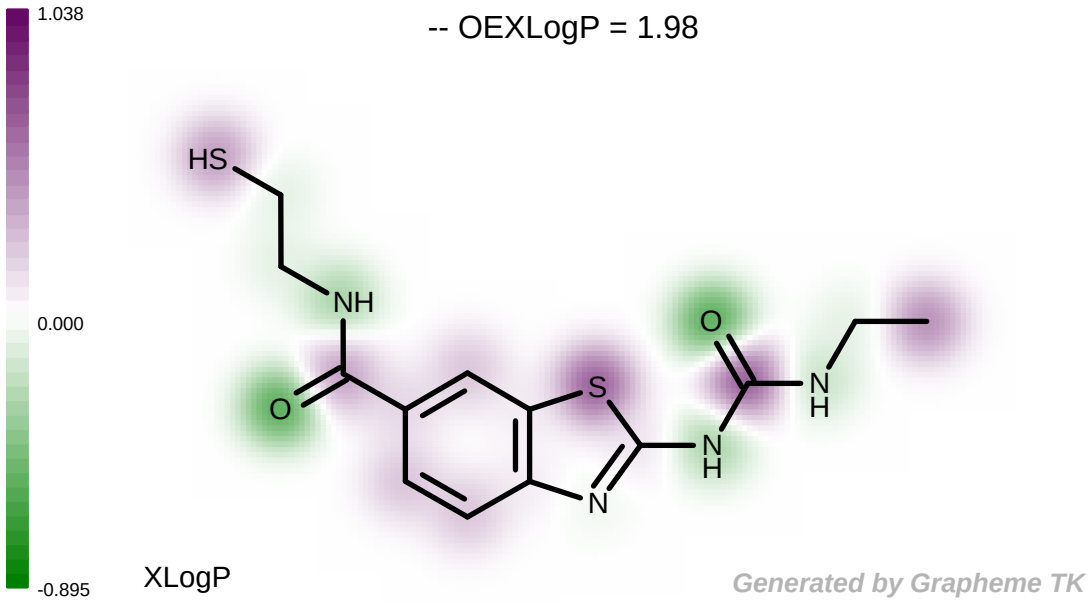


Fig. 5: **Example of depicting the atom contributions of the XLogP**

See also

OEXLogPResult class *LogP* section

Code Example

- Depicting Atom Contributions of XLogP **OpenEye Python Cookbook** recipe
- Depicting Fragment Contributions of XLogP **OpenEye Python Cookbook** recipe

4.3.22 OEGetXLogPVersion

```
std::string OEGetXLogPVersion()
```

Returns the version number for the current XLogP computation as a string.

4.3.23 OEMolPropGetArch

```
const char* OEMolPropGetArch()
```

4.3.24 OEMolPropGetLicensee

```
bool OEMolPropGetLicensee(std::string& licensee)
```

4.3.25 OEMolPropGetPlatform

```
const char* OEMolPropGetPlatform()
```

4.3.26 OEMolPropGetRelease

```
const char* OEMolPropGetRelease()
```

4.3.27 OEMolPropGetSite

```
bool OEMolPropGetSite(std::string& site)
```

4.3.28 OEMolPropGetVersion

```
unsigned int OEMolPropGetVersion()
```

4.3.29 OEMolPropIsLicensed

```
bool OEMolPropIsLicensed(const char* feature = 0,
                         unsigned int* expdate = 0)
```

Determines whether a valid license file is present. This function may be called without a legitimate run-time license to determine whether it is safe to call any **MolProp TK** functionality.

The 'feature' argument can be used to check for a valid license to **MolProp TK** along with the following features: 'python', 'java', or 'clr' (for CSharp).

The 'expdate' argument can be used to obtain the expiration date of the current **MolProp TK** license.

See also

- `OEChemIsLicensed` function

4.3.30 OEWritePropertyDataToCSV

```
bool OEWritePropertyDataToCSV(const std::string& fname,
                              OEChem::oemolistream& ifs,
                              OEMolProp::OEFilter& filter)
bool OEWritePropertyDataToCSV(OEChem::oemolostream& ofs,
                              OEChem::oemolistream& ifs,
                              OEMolProp::OEFilter& filter)
```

Write the molecular properties calculated by *OEFilter* to the output file `fname` or to the stream `ofs` in the `OEFormat.CSV` format. Returns `true` if the output CSV file was successfully written, `false` otherwise.

Molecules are read in from the input stream `ifs`. The output CSV file can be read by the `OEReadCSVFile` function.

See also

- CSV File Format section

Code Example

- *Write molecular properties to a CSV file* example

CHAPTER

FIVE

RELEASE HISTORY

5.1 MolProp TK 2.7.0

5.1.1 Minor Bug Fixes

- The SMARTS pattern of the *halo_amine* functional group has been fixed.

5.2 MolProp TK 2.6.7

Minor internal improvements have been made.

5.3 MolProp TK 2.6.6

Minor internal improvements have been made.

5.4 MolProp TK 2.6.5

Minor internal improvements have been made.

5.5 MolProp TK 2.6.4

Minor internal improvements have been made.

5.6 MolProp TK 2.6.3

Minor internal improvements have been made.

5.7 MolProp TK 2.6.2

Minor internal improvements have been made.

5.8 MolProp TK 2.6.1

5.8.1 New features

- A new free function, *OECheckXLogXType*, that returns `true` if an atom has a valid XLogPType has been added.

- A new free function, *OECheckXLogXTypes*, that returns `true` if all atoms excluding hydrogen in a molecule have valid XLogP types has been added.

5.8.2 Minor bug fixes

- An issue with filter output failure reporting, where failure due to the rules *ALLOWED_ELEMENTS* and *ELIMINATE_METALS* was not included in the output table, has been fixed.

5.9 MolProp TK 2.6.0

5.9.1 New features

- The ability to filter based on aromatic ring count and fraction of CSP3 carbons has been added.

5.10 MolProp TK 2.5.7

Fall 2021

5.10.1 New Features

- A method, *GetMessage*, was added to the *OEFilter* class to be able to retrieve information on whether the filter passed a molecule, or why it failed a specific molecule.
- A method, *SetErrorLevel*, was added to the *OEFilter* class to add explicit control of warnings output by the filter class and the filter application.
- A BlockBusterPAINS filter was added in the *OEFilterType* namespace, which combines filtering criteria for the BlockBuster and PAINS filters .
- Excess warning output that was causing large log files is now suppressed by default, and can be switched on using the new *SetErrorLevel* method. See *OEFilterType*.

5.11 MolProp TK 2.5.6

July 2021

5.11.1 Minor bug fixes

- An issue with OEGetRotatableBondCount counting carbamates and ureas as rotatable has been fixed.

5.12 MolProp TK 2.5.5

Fall 2020

- Minor internal improvements have been made.

5.13 MolProp TK 2.5.4

- Minor internal improvements have been made.

5.14 MolProp TK 2.5.3

5.14.1 New features

- Two new functions, *OEGetHBondDonorCount* and *OEGetHBondAcceptorCount*, have been added that count the number of hydrogen-bond donors and acceptors in a molecule.
- Two new functions, *OEGetLipinskiDonorCount* and *OEGetLipinskiAcceptorCount*, have been added that determine the number of donors and acceptors in a molecule based on the definition from the work of Lipinski ([Lipinski-1997]).
- A new function, *OEGetLongestUnbranchedHeavyAtomsChain*, has been added that determines the size of the longest chain of heavy atoms in a molecule.
- A new function, *OEGetLongestUnbranchedCarbonsChain*, has been added that determines the size of the longest chain of all carbons in a molecule.
- A new function, *OEGetHalideFraction*, has been added that determines the percentage of molecular weight from halides.
- A new function, *OEGetAnionicCarbonCount*, has been added that determines the number of anionic carbons in a molecule. New filter options, `MIN_ANION_C` and `MAX_ANION_C`, have also been added that filter out anionic carbons.
- A new function, *OEWritePropertyDataToCSV*, has been added that writes molecular properties to the output in the `OEFormat.CSV` format.
- Two new functions, *OEGetNumUnspecifiedAtomStereos* and *OEGetNumUnspecifiedBondStereos*, have been added that filter out molecules with unspecified atom and bond stereos. New filter options, `MIN_UNSPECIFIED_ATOM_STEREOS`, `MAX_UNSPECIFIED_ATOM_STEREOS`, `MIN_UNSPECIFIED_BOND_STEREOS`, and `MAX_UNSPECIFIED_BOND_STEREOS`, have also been added.

5.14.2 Minor bug fixes

- The XLogP calculation by the *OEGetXLogPResult* function for molecules with explicit hydrogens has been fixed.

5.14.3 Documentation changes

- A new program, *Write molecular properties to a CSV file*, has been added that demonstrates writing molecular properties to an output file in the `OEFormat.CSV` format.

5.15 MolProp TK 2.5.2

5.15.1 New features

- A new *OEGetRotatableBondCount* function has been added that can calculate either the number of rotatable bonds in the molecule or the molecule flexibility, taking into consideration the flexibility of aliphatic rings.
- New *OEConfigureFilterParams* and *OEConfigureFilterType* functions have been added to configure the given interface.
- A new *OEGetFilterType* function has been added to retrieve the filter type initialized in the given interface.
- New *OEFilterParamSetup*, *OEFilterParamName*, and *OEFilterType* namespaces have been added to provide options for the choice of filter interface parameters, filter parameter names, and filter types, respectively.

5.15.2 Documentation changes

- The following five example programs have been updated to allow switching filter types through the command line option:
  - *Basic Filtering for a Molecule File*
  - *Quiet Filtering*
  - *Molecular Property Table*
  - *Specific Molecular Properties*
  - *Attach Molecular Properties as SD Data*

5.16 MolProp TK 2.5.1

- Minor internal improvements have been made.

5.17 MolProp TK 2.5.0

5.17.1 Bug fixes

- The `aminal` and `hemiaminal` SMARTS rules have been modified to be slightly more general. Both rules now match 1,1-diamines as well as hydroxyl amines.

5.18 MolProp TK 2.4.7

5.18.1 Minor bug fixes

- The `pains_pre_aminal1` rule has been removed from the PAINS filter. The SMARTS for the rule was incorrectly defined and was overly general. The rules `pains_basic_amine1`, `pains_basic_amine2`, and `pains_basic_amine3` cover the same general structural classes in a more precise manner. A SMARTS issue with the `pains_basic_amine3`, uncovered after removing the `pains_pre_aminal1` rule, has also been corrected.

5.19 MolProp TK 2.4.6

- Minor internal improvements have been made.

5.20 MolProp TK 2.4.5

- Minor internal improvements have been made.

5.21 MolProp TK 2.4.4

5.21.1 Minor bug fixes

- The definition for the SMARTS for the CBoring (straight-chain alkane) fragment in the filter fragment set has been changed from `[CR0H2][CH2][CH2][CH2,H3]` to `[CR0H2][CH2][CH2][CH2,CH3]`. Previously, it could erroneously match a heteroatom at the last position.

5.21.2 Documentation changes

- Minor corrections to the bibliography have been made.

5.22 MolProp TK 2.4.3

5.22.1 Major bug fixes

- An issue that affected XLogP values depending on the aromaticity model perception has been repaired. *OEGetXLogP* function now re-perceives the **OpenEye** aromaticity model when necessary before calculating XLogP values.
- A filter with a non-zero MIN_UNBRANCHED_C had previously failed and now is properly calculated.

5.23 MolProp TK 2.4.2

- Minor internal improvements have been made.

5.24 MolProp TK 2.4.1

5.24.1 New features

- A new built-in filter for MMFF atom types has been added that can identify and eliminate molecules that have one or more unknown MMFF atom type assignments. The `MMFFTYPECHECK` directive in rule files controls the behavior. The *OEFilter.SetMMFFTypeCheck* and *OEFilter.GetMMFFTypeCheck* methods control the behavior when using an *OEFilter* object.

5.24.2 Major bug fixes

- *OEFilter.operator()* now handles multi-conformer molecules.

5.24.3 Minor bug fixes

- The pattern for `beta_carbonyl_quat_nitrogen` had previously incorrectly matched tertiary amines as well as quaternary amines. This has been fixed.

5.25 MolProp TK 2.4.0

5.25.1 New features

- *OEFilterType.PAINS* is a new filter for removing substructures that commonly cause problems in bioassays. The SMARTS patterns used in this filter have been adapted from the SLN patterns in the original paper:

  Baell, J.B. and Holloway G.A.,
  New Substructure Filters for Removal of Pan Assay Interference Compounds (PAINS) from Screening Libraries and for Their Exclusion in Bioassays,
  Journal of Medicinal Chemistry, Vol 53, pp. 2719-2740, 2010

  See also

  The *PAINS* section.

5.25.2 Bug fixes

- The displayed precision of the numerical values output in log messages are more realistic and now match the table output precision.
- *OEFilter.operator()* method now skips the calculation of certain physical properties if the filter being used does not require them and a table is not being generated. This quiets erroneous warnings for molecules that could be generated by those property calculations.

5.26 MolProp TK 2.3.0

5.26.1 New features

- A new *OEFilter.GetFilterType* method has been added for retrieving the filter used to construct the *OEFilter* object.

5.26.2 Documentation fixes

- The *Functional Group Rules* section has been updated with much better **OEDepict TK 2.x**-generated images of functional groups. The section should be significantly easier to read with the updated style.
- The example program *Attach Molecular Properties as SD Data* will now allow output to the `.csv` file format.

5.27 MolProp TK 2.2.2

5.27.1 Minor bug fixes

- Typecheck functionality, *OEFilter.SetTypeCheck*, has been changed such that hexavalent sulfur (matching SMARTS [Sv6D6]) will now be an acceptable atom type.

5.27.2 Documentation fixes

- The linear regression constant used by *OEGetXLogP* is now documented.
- PDF documentation should no longer throw warnings about “bad /BBox” in some PDF readers.

5.28 MolProp TK 2.2.1

5.28.1 New features

- *OEGetXLogP* is now thread safe.

5.28.2 Major bug fixes

- *OEGetXLogP* will no longer return garbage data in the per atom data array whenever molecules with deleted atoms are passed to the function.
- *OEFilter* carboxylic acid pattern will now match formic acid, formic esters, and formic thioesters with implicit hydrogens. Previously, explicit hydrogens were required on the molecule.

5.28.3 Minor bug fixes

- Removed unbounded stack allocations.

5.29 MolProp TK 2.2.0

5.29.1 Minor bug fixes

- *OEFilter.SetTable* no longer takes two arguments. The boolean denoting ownership of the oeostream was removed. Setting the ownership argument to true causes a race condition with the garbage collector and therefore crashes.
- Based on new, more reliable pKa data, the "malonic" keyword was refined to identify malonic acid specifically (pKa 2.9, 5.7) rather than generic di-carbonyl carbon acids, which typically have pKa values in the 8.9-11.5 range. This improves the reliability of the "acid" pattern as well, which is dependent on the "malonic" keyword.

5.29.2 Documentation changes

- Lipinski H-Bond donor is now properly described in the documentation. The implementation was already correct.

5.30 MolProp TK 2.1.7

5.30.1 Major bug fixes

- "MIN_*" and "MAX_*" properties filter rules file no longer have to both be specified to work. Previously, if a property filter was specified with "MAX_*", then the corresponding "MIN_*" filter rule had to also be set for the rule to properly function. Now, "MIN_*" and "MAX*" filter rules operate independent of the other.

5.31 MolProp TK 2.1.6

5.31.1 Bug fixes

- *OEFilter.operator()* will now call `OEPrepareSearch` on the molecule to ensure the molecule has all the proper properties initialized for *OEFilter* SMARTS matches.

5.32 MolProp TK 2.1.5

- Minor internal improvements.

5.33 MolProp TK 2.1.4

- The *OEFilter* object will now canonicalize atom and bond order by default. This avoids the problem of the normalization and duplicate removal steps being dependent on input atom order.

5.34 MolProp TK 2.1.3

5.34.1 New features

- Adding pictures to describe *OEGetXLogP* and *OEGet2dPSA* in documentation.
- *OEFilter* through its dependence on Neutral pH model (`OESetNeutralpHModel`) has been refined to reflect feedback from collaborators. In particular isoxazoles and oxadiazoles were added while pyrazoles and aryl sulfonamides were refined. Aryl sulfonamide refinement also incorporated changes based on newly obtained experimental data.

5.34.2 Minor bug fixes

- Through its dependence on `OESetNeutralpHModel` *OEFilter* now correctly addresses beta di-amino groups so that if all other considerations are equivalent, secondary amines are treated as most basic, followed by primary amines, with tertiary amine being treated as least basic.

5.35 MolProp TK 2.1.2

- Minor documentation fixes.

5.36 MolProp TK 2.1.1

5.36.1 New features

- Added several halide that are more strict to the fragment filter.
- Added several rules to remove bad ring systems to the fragment filter.

> **Note**
>
> The proper way to override a `RULE` line is to use a `NEWRULE` line.

5.36.2 Minor bug fixes

- Removing duplicate nitroso and phosphoryl filter file RULES from the default filters.

5.37 MolProp TK 2.1.0

This is the first release of the OEMolProp toolkit. Its version number corresponds to version number of the Filter application.

CHAPTER

SIX

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CHAPTER

SEVEN

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CHAPTER

EIGHT

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- FastROCS TK
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- Lexichem TK
- OEMedChem TK
- MolProp TK
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8.4 Publications for Bibliographies

Please also cite these publications if the corresponding product was used in your research.

8.4.1 Orion

Sørensen, J., Bannan, C.C., Calabrò, G., Jain, V., Ovanesyan, G., Smith, A., Zhang, S., Bayly, C.I., Darden, T.A., Geballe, M.T., LeBard, D.N., McGann, M., Moon, J.B., Muddana, H.S., Shewmaker, A., LaFon, J., Tolbert, R.W., Skillman, A.G., Nicholls, A. Orion® A Cloud-Native Molecular Design Platform. In *Computational Drug Discovery*. V. Poongavanam and V. Ramaswamy, Eds. Wiley-VCH, 2024; pp. 579–615. DOI: 10.1002/9783527840748.ch24

8.4.2 AFITT and FLYNN Applications

Wlodek, S.; Skillman, A.G.; Nicholls, A. Automated Ligand Placement and Refinement with a Combined Force Field and Shape Potential. *Acta Crystallogr., Sect. D: Struct. Biol.* **2006**, *62* (7), 741–749. DOI: 10.1107/s0907444906016076

8.4.3 OEDocking Application and Toolkit

Kelley, B.P.; Brown, S.P.; Warren, G.L.; Muchmore, S.W. POSIT: Flexible Shape-Guided Docking For Pose Prediction. *J. Chem. Inf. Model.* **2015**, *55* (8), 1771-1780. DOI: 10.1021/acs.jcim.5b00142

McGann, M. FRED Pose Prediction and Virtual Screening Accuracy. *J. Chem. Inf. Model.* **2011**, *51* (3), 578-596. DOI: 10.1021/ci100436p

McGann, M. FRED and HYBRID Docking Performance on Standardized Datasets. *J. Comput.-Aided Mol. Des.* **2012**, *26* (8), 897-906. DOI: 10.1007/s10822-012-9584-8

8.4.4 OMEGA Application and Toolkit

If you are using OMEGA in torsion driving mode, please cite the following two publications.

Hawkins, P.C.D.; Skillman, A.G.; Warren, G.L.; Ellingson, B.A.; Stahl, M.T. Conformer Generation with OMEGA: Algorithm and Validation Using High Quality Structures from the Protein Databank and the Cambridge Structural Database. *J. Chem. Inf. Model.* **2010**, *50* (4), 572-584. DOI: 10.1021/ci100031x

Hawkins, P.C.D. and Nicholls, A. Conformer Generation with OMEGA: Learning from the Data Set and the Analysis of Failures. *J. Chem. Inf. Model.* **2012**, *52* (11), 2919–2936. DOI: /10.1021/ci300314k

If you are using OMEGA in macrocyle mode, please cite the following.

Hawkins, P.C.D. and Wlodek, S. Decisions with Confidence: Application to the Conformation Sampling of Molecules in the Solid State. *J. Chem. Inf. Model.* **2020**, *60* (7), 3518–3533. DOI: /10.1021/acs.jcim.0c00358

8.4.5 ROCS Application

Hawkins, P.C.D.; Skillman, A.G.; Nicholls, A. Comparison of Shape-Matching and Docking as Virtual Screening Tools. *J. Med. Chem.* **2007**, *50* (1), 74-82. DOI: 10.1021/jm0603365

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CHAPTER

NINE

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brotli-bin	https://github.com/google/brotli	https://github.com/google/brotli/blob/master/LICENSE
brotli-python	http://python-hyper.org/projects/brotlipy/en/latest/	https://github.com/python-hyper/brotlicffi/blob/main/LICENSE
brotlicffi	https://github.com/python-hyper/brotlicffi	https://github.com/python-hyper/brotlicffi?tab=MIT-1-ov-file#readme
brotlipy	https://github.com/python-hyper/brotlicffi	https://github.com/python-hyper/brotlicffi/blob/main/LICENSE

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Name of Project	Website	License URL
bson	http://github.com/py-bson/bson	https://github.com/py-bson/bson/blob/master/LICENSE_APACHE
bytefmt	https://code.cloudfoundry.org/bytefmt	https://github.com/cloudfoundry/bytefmt/blob/master/LICENSE
bzip2	https://www.bzip.org	https://spdx.org/licenses/bzip2-1.0.6.html
c-ares	https://github.com/c-ares/c-ares	https://github.com/c-ares/c-ares/blob/main/LICENSE.md
ca-certificates	https://github.com/conda-forge/ca-certificates-feedsto	https://wiki.mozilla.org/CA/Included_Certificates
cached-property	https://github.com/pydanny/cached-property	https://github.com/pydanny/cached-property/blob/master/LICENSE
cachetools	https://github.com/tkem/cachetools/	https://github.com/tkem/cachetools/blob/master/LICENSE
cairo	https://pycairo.readthedocs.io/en/latest/	https://github.com/pygobject/pycairo/blob/master/COPYING
canvas	https://github.com/Automattic/node-canvas	https://github.com/Automattic/node-canvas
cctbx	https://github.com/cctbx/cctbx_project	https://github.com/cctbx/cctbx_project/blob/master/cctbx/LICENSE_2_0.txt
celery	https://github.com/celery/celery	https://github.com/celery/celery/blob/master/LICENSE
Cerberus	https://docs.python-cerberus.org/en/stable/	https://docs.python-cerberus.org/en/stable/license.html
certifi	https://certifiio.readthedocs.io/en/latest/	https://wiki.mozilla.org/index.php?title=CA/IncludedCertificates&redirect=no

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Name of Project	Website	License URL
cffi	https://github.com/python-cffi	https://github.com/cffi/cffi/blob/master/COPYRIGHT
cftime	https://pypi.org/project/cftime/	https://github.com/Unidata/cftime/blob/master/LICENSE
chardet	https://github.com/chardet/chardet	https://github.com/chardet/chardet/blob/master/LICENSE
charset-normalizer	https://github.com/ousret/charset_normalizer	https://github.com/Ousret/charset_normalizer/blob/master/LICENSE
ChEMBL Structure Pipeline	https://github.com/chembl/ChEMBL_Structure_Pipeline/tree/master	https://github.com/chembl/ChEMBL_Structure_Pipeline/blob/master/LICENSE
choreographer	https://github.com/mazpie/choreographer	https://github.com/mazpie/choreographer/blob/main/LICENSE
chunkreader	https://github.com/jackc/chunkreader/v2	https://github.com/jackc/chunkreader/blob/master/LICENSE
click	https://palletsprojects.com/p/click/	https://github.com/pallets/click/blob/main/LICENSE.rst
click-completion	https://github.com/click-contrib/click-completion	https://github.com/click-contrib/click-completion/blob/master/LICENSE
click-didyoumean	https://github.com/click-contrib/click-didyoumean	https://github.com/click-contrib/click-didyoumean/blob/master/LICENSE
click-plugins	https://github.com/click-contrib/click-plugins	https://github.com/click-contrib/click-plugins/blob/master/LICENSE.txt

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Name of Project	Website	License URL
click-repl	https://github.com/untitaker/click-repl	https://github.com/click-contrib/click-repl/blob/master/LICENSE
cloudpickle	https://github.com/cloudpipe/cloudpickle	https://github.com/cloudpipe/cloudpickle/blob/master/LICENSE
cmake	https://cmake.org/	https://cmake.org/licensing/
colorama	https://github.com/tartley/colorama	https://github.com/tartley/colorama/blob/master/LICENSE.txt
comm	https://github.com/ipython/comm	https://github.com/ipython/comm/blob/master/LICENSE
compose	https://github.com/docker/compose	https://github.com/docker/compose/blob/v2/LICENSE
conda-content-trust	https://github.com/conda/conda-content-trust	https://github.com/conda/conda-content-trust/blob/main/LICENSE
conda-libmamba-solver	https://github.com/conda/conda-libmamba-solv	https://github.com/conda/conda-libmamba-solv/blob/main/LICENSE
conda-pack	https://conda.github.io/conda-pack/	https://github.com/conda/conda-pack/blob/main/LICENSE.txt
conda-package-handling	https://github.com/conda/conda-package-handli	https://github.com/conda/conda-package-handli/blob/main/LICENSE
conda-package-streaming	https://anaconda.org/conda-forge/conda-package-stream	https://github.com/conda/conda-package-stream/blob/main/LICENSE
conda-token	https://anaconda.org/anaconda/conda-token	https://anaconda.org/anaconda/conda-token

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Name of Project	Website	License URL
conda_package_strear	https://github.com/conda/conda-package-streamtree/main/conda_package_streaming	https://github.com/conda/conda-package-streamtab=License-1-ov-file
confuse	https://github.com/beetbox/confuse	https://github.com/beetbox/confuse/blob/main/LICENSE
contourpy	https://github.com/contourpy/contourpy	https://github.com/contourpy/contourpy/blob/main/LICENSE
cpp-expected	https://github.com/TartanLlama/expected	https://github.com/TartanLlama/expected?tab=CC0-1.0-1-ov-file#readme
cpp-peglib	https://github.com/yhirose/cpp-peglib	https://github.com/yhirose/cpp-peglib/blob/master/LICENSE
cryptography	https://github.com/pyca/cryptography	https://github.com/pyca/cryptography/blob/main/LICENSE
cssselect2	https://github.com/Kozea/cssselect2/	https://github.com/Kozea/cssselect2/blob/master/LICENSE
cuda-bindings	https://nvidia.github.io/cuda-python/cuda-bindings/latest/install.html	https://github.com/NVIDIA/cuda-python/blob/main/cuda_bindings/LICENSE
cuda-pathfinder	https://nvidia.github.io/cuda-python/cuda-pathfinder/latest/	https://nvidia.github.io/cuda-python/cuda-pathfinder/latest/license.html
cudatoolkit	https://developer.nvidia.com/cuda-toolkit	https://docs.nvidia.com/cuda/eula/index.html
cuequivariance-ops-cu12	https://developer.nvidia.com/cuequivariance	https://github.com/NVIDIA/cuEquivariance/blob/main/LICENSES/LICENSE

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Name of Project	Website	License URL
cuequivariance-ops-torch-cu12	https://developer.nvidia.com/cuequivariance	https://github.com/NVIDIA/cuEquivariance/blob/main/LICENSES/LICENSE
cuequivariance-torch	https://docs.nvidia.com/cuda/cuequivariance/	https://github.com/NVIDIA/cuEquivariance/blob/main/LICENSES/LICENSE
cupy-cuda113	https://cupy.dev/	https://github.com/cupy/cupy/blob/main/LICENSE
cupy-cuda11x	https://cupy.dev/	https://github.com/cupy/cupy/?tab=MIT-1-ov-file#readme
curl	https://curl.se	https://curl.se/docs/copyright.html
cycler	https://github.com/matplotlib/cycler	https://github.com/matplotlib/cycler/blob/main/LICENSE
cyrus-sasl	https://github.com/cyrusimap/cyrus-sasl	https://github.com/cyrusimap/cyrus-sasl/blob/master/COPYING
Cython	https://cython.org	https://www.apache.org/licenses/LICENSE-2.0.html
d3	https://github.com/mbostock/d3	https://github.com/mbostock/d3/raw/master/LICENSE
dataclasses	https://github.com/ericvsmith/dataclasses	https://github.com/ericvsmith/dataclasses/blob/master/LICENSE.txt
ddsketch	http://github.com/datadog/sketches-py	https://github.com/DataDog/sketches-py/blob/master/LICENSE
debugpy	https://aka.ms/debugpy	https://github.com/microsoft/debugpy/blob/main/LICENSE

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Name of Project	Website	License URL
decimal	https://github.com/shopspring/decimal	https://github.com/shopspring/decimal/blob/master/LICENSE
decorator	https://github.com/micheles/decorator	https://github.com/micheles/decorator/blob/master/LICENSE.txt
deepdiff	https://github.com/seperman/deepdiff	https://github.com/seperman/deepdiff/blob/master/LICENSE
deeptime	https://github.com/deeptime-ml/deeptime	https://github.com/deeptime-ml/deeptime/blob/main/LICENSE.txt
defusedxml	https://github.com/tiran/defusedxml	https://github.com/tiran/defusedxml/blob/main/LICENSE
dftd3	https://github.com/dftd3/tad-dftd3	https://github.com/dftd3/tad-dftd3/blob/main/LICENSE
dill	https://github.com/uqfoundation/dill	https://github.com/uqfoundation/dill/blob/master/LICENSE
distlib	https://distlib.readthedocs.io/en/latest/	https://github.com/pypa/distlib/blob/master/LICENSE.txt
distro	https://github.com/python-distro/distro	https://github.com/python-distro/distro/blob/master/LICENSE
Django	https://www.djangoproject.com/	https://github.com/django/django/blob/main/LICENSE
django-classy-tags	https://github.com/django-cms/django-classy-tags	https://github.com/django-cms/django-classy-tags/blob/master/LICENSE
django-cors-headers	https://github.com/adamchainz/django-cors-headers	https://github.com/adamchainz/django-cors-headers/blob/main/LICENSE

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Name of Project	Website	License URL
django-csp	https://github.com/mozilla/django-csp	https://github.com/mozilla/django-csp/blob/main/LICENSE
django-extensions	https://github.com/django-extensions/django-extensions	https://github.com/django-extensions/django-extensions/blob/main/LICENSE
django-filter	https://github.com/carltongibson/django-filter/tree/master	https://github.com/carltongibson/django-filter/blob/main/LICENSE
django-redis	https://github.com/jazzband/django-redis	https://github.com/jazzband/django-redis/blob/master/LICENSE
django-taggit	https://github.com/jazzband/django-taggit	https://github.com/jazzband/django-taggit/blob/master/LICENSE
django-taggit-serializer	https://github.com/glemmaPaul/django-taggit-serializ	https://github.com/glemmaPaul/django-taggit-serializ blob/master/LICENSE
django-taggit-templatetags2	https://github.com/fizista/django-taggit-templat	https://github.com/fizista/django-taggit-templat blob/master/LICENSE.txt
djangorestframework	https://www.django-rest-framewor org/	https://github.com/encode/django-rest-framewor blob/master/LICENSE.md
dkh	https://psicode.org/psi4manual/master/dkh.html	https://github.com/psi4/dkh/blob/master/COPYING.LESSER
dm-tree	https://github.com/deepmind/tree	https://github.com/deepmind/tree/blob/master/LICENSE
docker-py	https://github.com/docker/docker-py/	https://github.com/docker/docker-py/blob/master/LICENSE

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Name of Project	Website	License URL
docker-pycreds	https://github.com/shin-/dockerpy-creds	https://github.com/shin-/dockerpy-creds/blob/master/LICENSE
docopt	https://docopt.org	https://github.com/docopt/docopt/blob/master/LICENSE-MIT
docutils	https://docutils.sourceforge.io	https://docutils.sourceforge.io/COPYING.html
drf-dynamic-fields	https://github.com/dbrgn/drf-dynamic-fields	https://github.com/dbrgn/drf-dynamic-fields/blob/master/LICENSE
DuckDB	https://duckdb.org/	https://github.com/duckdb/duckdb?tab=MIT-1-ov-file#readme
edgembar	https://rutgerslbsr.gitlab.io/fe-toolkit/edgembar/index.html	https://gitlab.com/RutgersLBSR/fe-toolkit/-/blob/master/LICENSE
editdistance	https://github.com/roy-ht/editdistance	https://github.com/roy-ht/editdistance/blob/master/LICENSE
eigen	https://eigen.tuxfamily.org/index.php?title=Main_Page	https://eigen.tuxfamily.org/index.php?title=Main_Page#License
einops	https://github.com/arogozhnikov/einops	https://github.com/arogozhnikov/einops/blob/master/LICENSE
einx	https://github.com/fferflo/einx	https://github.com/fferflo/einx/blob/master/LICENSE
entrypoints	https://github.com/takluyver/entrypoints	https://github.com/takluyver/entrypoints/blob/master/LICENSE
errors	https://github.com/pkg/errors	https://github.com/pkg/errors/blob/master/LICENSE

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Name of Project	Website	License URL
eslint-plugin	https://github.com/typescript-eslint/typescript-eslint	https://github.com/typescript-eslint/typescript-eslint/raw/master/LICENSE
et_xmlfile	https://foss.heptapod.net/openpyxl/et_xmlfile	https://foss.heptapod.net/openpyxl/et_xmlfile/-/blob/branch/default/LICENCE.rst
exceptiongroup	https://github.com/agronholm/exceptiongroup	https://github.com/agronholm/exceptiongroup/blob/main/LICENSE
execnet	https://execnet.readthedocs.io/en/latest/	https://github.com/pytest-dev/execnet/blob/master/LICENSE
executing	https://github.com/alexmojaki/executing	https://github.com/alexmojaki/executing/blob/master/LICENSE.txt
expat	https://libexpat.github.io	https://github.com/libexpat/libexpat/blob/master/expat/COPYING
fairscale	https://github.com/facebookresearch/fairscale	https://github.com/facebookresearch/fairscale/blob/main/LICENSE
fairseq	https://github.com/pytorch/fairseq	https://github.com/facebookresearch/fairseq/blob/main/LICENSE
fastjsonschema	https://github.com/horejsek/python-fastjsonschem	https://github.com/horejsek/python-fastjsonschem/blob/master/LICENSE
fastrlock	https://github.com/scoder/fastrlock	https://github.com/scoder/fastrlock/blob/master/LICENSE
fftw	https://www.fftw.org	commercial license

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Name of Project	Website	License URL
filebuffer	https://github.com/mattetti/filebuffer	https://github.com/mattetti/filebuffer/blob/master/LICENSE
filelock	https://py-filelock.readthedocs.io/en/latest/index.html	https://github.com/tox-dev/py-filelock/blob/main/LICENSE
finufft	https://github.com/flatironinstitute/finufft	https://github.com/flatironinstitute/finufft/blob/master/LICENSE
Flask	https://flask.palletsprojects.com/en/2.1.x/	https://flask.palletsprojects.com/en/2.1.x/license/
flatbuffers	https://google.github.io/flatbuffers/	https://github.com/google/flatbuffers/blob/master/LICENSE.txt
flexcache	https://github.com/hgrecco/flexcache	https://github.com/hgrecco/flexcache/blob/main/LICENSE
flexparser	https://github.com/hgrecco/flexparser	https://github.com/hgrecco/flexparser/blob/main/LICENSE
flit-core	https://github.com/pypa/flit	https://github.com/scientific-python/lazy_loader/blob/main/LICENSE.md
FLTK	https://www.fltk.org/index.php	https://www.fltk.org/COPYING.php
fmt	https://fmt.dev/latest/index.html	https://github.com/fmtlib/fmt/blob/master/LICENSE.rst
font-awesome	https://github.com/FortAwesome/Font-Awesome	https://github.com/FortAwesome/Font-Awesome
font-ttf-dejavu-sans-mono	https://dejavu-fonts.github.io	https://dejavu-fonts.github.io/License.html
font-ttf-inconsolata	https://fonts.google.com/specimen/Inconsolata	https://scripts.sil.org/cms/scripts/page.php?site_id=nrsi&id=OFL

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Name of Project	Website	License URL
font-ttf-source-code-pro	https://fonts.google.com/specimen/Source+Code+Pro	https://scripts.sil.org/cms/scripts/page.php?site_id=nrsi&id=OFL
font-ttf-ubuntu	https://fonts.google.com/specimen/Ubuntu	https://ubuntu.com/legal/font-licence
fontconfig	https://www.freedesktop.org/wiki/Software/fontconfig/	https://gitlab.freedesktop.org/fontconfig/fontconfig/-/blob/main/COPYING
fonts-conda-ecosystem	https://anaconda.org/conda-forge/fonts-conda-ecosyster	https://docs.conda.io/en/latest/license.html
fonts-conda-forge	https://anaconda.org/conda-forge/fonts-conda-forge/	https://creativecommons.org/licenses/by/4.0/
fonttools	https://github.com/fonttools/fonttools	https://github.com/fonttools/fonttools/blob/main/LICENSE
forcebalance	https://simtk.org/home/forcebalance OR https://github.com/leeping/forcebalance	https://github.com/leeping/forcebalance/blob/master/LICENSE
fqdn	https://github.com/ypcrts/fqdn	https://github.com/ypcrts/fqdn?tab=MPL-2.0-1-ov-file#readme
freetype	https://freetype.org	https://freetype.org/license.html
freetype-py	https://github.com/rougier/freetype-py	https://github.com/rougier/freetype-py?tab=License-1-ov-file#readme
fribidi	https://github.com/fribidi/fribidi	https://github.com/fribidi/fribidi/blob/master/COPYING
frozendict	https://github.com/Marco-Sulla/python-frozendict	https://github.com/Marco-Sulla/python-frozendict/blob/master/LICENSE.txt
frozenlist	https://github.com/aio-libs/frozenlist	https://github.com/aio-libs/frozenlist/blob/master/LICENSE

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Name of Project	Website	License URL
fsmlite	https://github.com/tkem/fsmlite	https://github.com/tkem/fsmlite/blob/master/LICENSE
fsspec	https://github.com/fsspec/filesystem_spec	https://github.com/fsspec/filesystem_spec/blob/master/LICENSE
funcy	https://github.com/Suor/funcy	https://github.com/Suor/funcy/blob/master/LICENSE
gast	https://github.com/serge-sans-paille/gast/	https://github.com/serge-sans-paille/gast/blob/master/LICENSE
gau2grid	https://github.com/dgasmith/gau2grid	https://github.com/dgasmith/gau2grid/blob/master/LICENSE
gax-go	https://github.com/googleapis/gax-go/v2	https://github.com/googleapis/gax-go/blob/main/LICENSE
gdk-pixbuf	https://gitlab.gnome.org/GNOME/gdk-pixbuf	https://gitlab.gnome.org/GNOME/gdk-pixbuf/-/blob/master/COPYING
gemmi	https://gemmi.readthedocs.io/en/latest/	https://github.com/project-gemmi/gemmi/blob/master/LICENSE.txt
genproto	https://google.golang.org/genproto/googleapis	https://github.com/googleapis/go-genproto/blob/main/LICENSE
geometric	https://openbase.com/python/geometric	https://openbase.com/python/geometric
giflib	https://giflib.sourceforge.net	https://github.com/mirrorer/giflib/blob/master/COPYING
gitdb	https://github.com/gitpython-developers/gitdb	https://github.com/gitpython-developers/gitdb/blob/master/LICENSE
GitPython	https://github.com/gitpython-developers/GitPython	https://github.com/gitpython-developers/GitPython/blob/main/LICENSE

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Name of Project	Website	License URL
glib	https://docs.gtk.org/glib/	https://gitlab.gnome.org/GNOME/glib/-/blob/main/LICENSES/LGPL-2.1-or-later.txt
GLM Library	https://github.com/g-truc/glm	https://github.com/g-truc/glm/blob/master/manual.md#section0
gls	https://github.com/jtolds/gls	https://github.com/jtolds/gls/blob/master/LICENSE
gmpy2	https://github.com/aleaxit/gmpy	https://github.com/gmpy2/gmpy2/blob/master/COPYING.LESSER
go-cleanhttp	https://github.com/hashicorp/go-cleanhttp	https://github.com/hashicorp/go-cleanhttp/blob/master/LICENSE
go-connections	https://github.com/docker/go-connections	https://github.com/docker/go-connections/blob/master/LICENSE
go-cpio	https://github.com/cavaliercoder/go-cpio	https://github.com/cavaliercoder/go-cpio/blob/master/LICENSE
go-getter	https://github.com/hashicorp/go-getter	https://github.com/hashicorp/go-getter/blob/master/LICENSE
go-homedir	https://github.com/mitchellh/go-homedir	https://github.com/mitchellh/go-homedir/blob/master/LICENSE
go-ini	https://github.com/go-ini/ini	https://github.com/go-ini/ini/blob/master/LICENSE
go-jmespath	https://github.com/jmespath/go-jmespath	https://github.com/jmespath/go-jmespath/blob/master/LICENSE

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Name of Project	Website	License URL
go-junit-report	https://github.com/jstemmer/go-junit-report	https://github.com/jstemmer/go-junit-report/blob/master/LICENSE
go-netrc	https://github.com/bgentry/go-netrc/netrc	https://github.com/bgentry/go-netrc/blob/master/LICENSE
go-ole	https://github.com/go-ole/go-ole	https://github.com/go-ole/go-ole/blob/master/LICENSE
go-pg	https://github.com/go-pg/pg	https://github.com/go-pg/pg/blob/master/LICENSE
go-redis	https://github.com/go-redis/redis/v8	https://github.com/go-redis/redis/blob/master/LICENSE
go-rendezvous	https://github.com/dgryski/go-rendezvous	https://github.com/dgryski/go-rendezvous/blob/master/LICENSE
go-safetemp	https://github.com/hashicorp/go-safetemp	https://github.com/hashicorp/go-safetemp/blob/master/LICENSE
go-sysconf	https://github.com/tklauser/go-sysconf	https://github.com/tklauser/go-sysconf/blob/master/LICENSE
go-testing-interface	https://github.com/mitchellh/go-testing-interface	https://github.com/mitchellh/go-testing-interface/blob/master/LICENSE
go-units	https://github.com/docker/go-units	https://github.com/docker/go-units/blob/master/LICENSE
go-version	https://github.com/hashicorp/go-version	https://github.com/hashicorp/go-version/blob/master/LICENSE
go-zglob	https://github.com/mattn/go-zglob	https://github.com/mattn/go-zglob/blob/master/LICENSE

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Name of Project	Website	License URL
go.opencensus	https://go.opencensus.io	https://github.com/census-instrumentatio opencensus-go/blob/master/LICENSE
gobrake.v2	https://gopkg.in/airbrake/gobrake.v2	https://github.com/airbrake/gobrake/blob/v2.0.9/LICENSE
goconvey	https://github.com/smartystreets/goconvey	https://github.com/smartystreets/goconvey/blob/master/LICENSE.md
golden-layout	https://github.com/deepstreamIO/golden-layout	https://github.com/deepstreamIO/golden-layout/raw/master/LICENSE
google-auth	https://google-auth.readthedocs.io/en/master/	https://github.com/GoogleCloudPlatform google-auth-library-p blob/master/LICENSE
google-auth-oauthlib	https://github.com/googleapis/google-auth-library-p	https://github.com/googleapis/google-auth-library-p blob/main/LICENSE
google-cloud-go	https://cloud.google.com/go	https://github.com/googleapis/google-cloud-go/blob/main/LICENSE
google-cloud-go/storage	https://cloud.google.com/go/storage	https://github.com/googleapis/google-cloud-go/blob/main/LICENSE
google-pasta	https://github.com/google/pasta	https://github.com/google/pasta/blob/master/LICENSE
google.golang.org/api	https://google.golang.org/api	https://github.com/googleapis/google-api-go-client/blob/main/LICENSE
gopsutil	https://github.com/shirou/gopsutil	https://github.com/shirou/gopsutil/blob/master/LICENSE

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Name of Project	Website	License URL
gorilla websocket	https://github.com/gorilla/websocket	https://github.com/gorilla/websocket/blob/master/LICENSE
gpytorch	https://gpytorch.ai	https://github.com/cornellius-gp/gpytorch?tab=MIT-1-ov-file#readme
graphite2	https://github.com/silnrsi/graphite	https://github.com/silnrsi/graphite/blob/master/LICENSE
graphviz	https://graphviz.org/	https://graphviz.org/license/
greenlet	https://greenlet.readthedocs.io/en/latest/	https://github.com/python-greenlet/greenlet/blob/master/LICENSE
groupcache	https://github.com/golang/groupcache	https://github.com/golang/groupcache/blob/master/LICENSE
grpc	https://google.golang.org/grpc	https://github.com/grpc/grpc-go/blob/master/LICENSE
grpc-cpp	https://github.com/grpc/grpc	https://github.com/grpc/grpc/blob/master/LICENSE
grpcio	https://github.com/grpc/grpc.io/blob/main/LICENSE	https://github.com/grpc/grpc.io/blob/main/LICENSE
gtk2	https://gitlab.gnome.org/GNOME/gtk	https://gitlab.gnome.org/GNOME/gtk/-/blob/main/COPYING
gts	https://sourceforge.net/projects/gts/	https://www.gnu.org/licenses/lgpl-3.0.html
h11	https://github.com/python-hyper/h11	https://github.com/python-hyper/h11/blob/master/LICENSE.txt
h2	https://github.com/python-hyper/h2	https://github.com/python-hyper/h2?tab=MIT-1-ov-file#readme

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Name of Project	Website	License URL
h5py	https://www.h5py.org	https://docs.h5py.org/en/stable/licenses.html
harfbuzz	https://github.com/harfbuzz/harfbuzz	https://github.com/harfbuzz/harfbuzz/blob/main/COPYING
hdbscan	https://hdbscan.readthedocs.io/en/latest/	https://github.com/scikit-learn-contrib/hdbscan/blob/master/LICENSE
hdf4	https://www.hdfgroup.org/solutions/hdf4/	https://github.com/HDFGroup/hdf4/blob/master/COPYING
hdf5	https://www.hdfgroup.org/solutions/hdf5/	https://github.com/HDFGroup/hdf5/blob/master/COPYING
he	https://github.com/mathiasbynens/he	https://github.com/mathiasbynens/he/raw/master/LICENSE-MIT.txt
hpack	https://github.com/python-hyper/hpack	https://github.com/python-hyper/hpack?tab=MIT-1-ov-file#readme
html-loader	https://github.com/webpack-contrib/html-loader	https://github.com/webpack-contrib/html-loader/raw/master/LICENSE
html5lib	https://github.com/html5lib/html5lib-python	https://github.com/html5lib/html5lib-python/blob/master/LICENSE
htslib	https://www.htslib.org	https://github.com/samtools/htslib/blob/develop/LICENSE
httpcore	https://www.encode.io/httpcore/	https://github.com/encode/httpcore/blob/master/LICENSE.md
httpx	https://github.com/encode/httpx	https://github.com/encode/httpx/blob/master/LICENSE.md

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Name of Project	Website	License URL
humanize	https://github.com/jmoiron/humanize	https://github.com/jmoiron/humanize/blob/master/LICENCE
hydra-core	https://github.com/facebookresearch/hydra	https://github.com/facebookresearch/hydra/blob/main/LICENSE
hyperframe	https://github.com/python-hyper/hyperframe	https://github.com/python-hyper/hyperframe?tab=MIT-1-ov-file#readme
icu	https://github.com/unicode-org/icu	https://github.com/unicode-org/icu/blob/main/icu4c/LICENSE
idna	https://github.com/kjd/idna	https://github.com/kjd/idna/blob/master/LICENSE.md
ihm	https://github.com/ihmwg/python-ihm	https://github.com/ihmwg/python-ihm/blob/main/LICENSE
imageio	https://github.com/imageio/imageio	https://github.com/imageio/imageio/blob/master/LICENSE
imagesize	https://github.com/shibukawa/imagesize_py	https://github.com/shibukawa/imagesize_py/blob/master/LICENSE.rst
ImmuneBuilder	https://github.com/oxpig/ImmuneBuilder/tree/main	https://github.com/oxpig/ImmuneBuilder/blob/main/LICENSE
importlib-metadata	https://github.com/python/importlib_metadata	https://github.com/python/importlib_metadata/blob/main/LICENSE
importlib_metadata	https://github.com/python/importlib_metadata	https://github.com/python/importlib_metadata/blob/main/LICENSE

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Name of Project	Website	License URL
importlib_resources	https://github.com/python/importlib_resources	https://github.com/python/importlib_resources/blob/main/LICENSE
InChI	https://iupac.org/who-we-are/divisions/division-details/inchi/	https://iupac.org/wp-content/uploads/2021/06/iupac-inchi-license_2020.pdf
inflection	https://github.com/jinzhu/inflection	https://github.com/jinzhu/inflection/blob/master/LICENSE
ini.v1	https://gopkg.in/ini.v1	https://github.com/go-ini/ini/blob/v1.66.2/LICENSE
iniconfig	https://github.com/pytest-dev/iniconfig	https://github.com/pytest-dev/iniconfig/blob/main/LICENSE
innersvg-polyfill	https://github.com/dnozay/innersvg-polyfill	https://github.com/dnozay/innersvg-polyfill/raw/master/LICENSE
intel-openmp	https://github.com/hermitcore/libomp_oss	https://github.com/hermitcore/libomp_oss/blob/hermit/LICENSE.txt
ipykernel	https://ipython.org	https://ipython.org
ipython	https://ipython.org	https://github.com/ipython/ipython/blob/master/LICENSE
ipython-genutils	http://ipython.org	https://github.com/ipython/ipython_genutils/blob/master/COPYING.md
ipython_pygments_le	https://github.com/ipython/ipython-pygments-lex	https://github.com/ipython/ipython-pygments-lex blob/main/LICENSE
ipywidgets	http://jupyter.org	https://github.com/jupyter-widgets/ipywidgets/blob/main/LICENSE

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Name of Project	Website	License URL
isodate	https://github.com/gweis/isodate/	https://github.com/gweis/isodate/blob/master/LICENSE
isoduration	https://github.com/bolsote/isoduration	https://github.com/bolsote/isoduration?tab=ISC-1-ov-file#readme
itsdangerous	https://palletsprojects.com/p/itsdangerous/	https://itsdangerous.palletsprojects.com/en/2.1.x/license/
jax	https://github.com/google/jax	https://github.com/google/jax/blob/main/LICENSE
jaxlib	https://github.com/google/jax	https://github.com/google/jax/blob/main/LICENSE
jaxtyping	https://github.com/patrick-kidger/jaxtyping	https://github.com/patrick-kidger/jaxtyping?tab=License-1-ov-file#readme
jedi	https://jedi.readthedocs.io/en/latest/	https://github.com/davidhalter/jedi/blob/master/LICENSE.txt
Jinja2	https://palletsprojects.com/p/jinja/	https://github.com/pallets/jinja/blob/main/LICENSE.rst
jmespath	https://github.com/jmespath/jmespath.py	https://github.com/jmespath/jmespath.py/blob/develop/LICENSE.txt
joblib	https://joblib.readthedocs.io/en/latest/	https://github.com/joblib/joblib/blob/master/LICENSE.txt
jpeg	https://www.ijg.org	https://www.ijg.org/files/README
json5	https://github.com/dpranke/pyjson5	https://github.com/dpranke/pyjson5/blob/main/LICENSE
jsonfield	https://github.com/dmkoch/django-jsonfield/	https://github.com/rpkilby/jsonfield/blob/master/LICENSE

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Name of Project	Website	License URL
jsonpatch	https://github.com/stefankoegl/python-json-patch	https://github.com/stefankoegl/python-json-patch/blob/master/LICENSE
jsonpickle	https://github.com/jsonpickle/jsonpickle	https://github.com/jsonpickle/jsonpickle/blob/main/LICENSE
jsonpointer	https://github.com/stefankoegl/python-json-pointer	https://github.com/stefankoegl/python-json-pointer/blob/master/LICENSE.txt
jsonschema	https://github.com/python-jsonschema/jsonschema	https://github.com/python-jsonschema/jsonschema/blob/master/COPYING
jsonschema-specifications	https://github.com/python-jsonschema/jsonschema-specificat	https://github.com/python-jsonschema/jsonschema-specificat blob/main/COPYING
jstat	https://github.com/jstat/jstat	https://www.opensource.org/licenses/mit-license.php
jupyter-client	https://jupyter.org	https://github.com/jupyter/jupyter_client/blob/main/COPYING.md
jupyter-core	https://jupyter.org	https://github.com/jupyter/jupyter_core/blob/master/COPYING.md
jupyter-events	https://github.com/jupyter/jupyter_events	https://github.com/jupyter/jupyter_events/blob/main/LICENSE
jupyter-lsp	https://github.com/jupyter-lsp/jupyterlab-lsp	https://github.com/jupyter-lsp/jupyterlab-lsp
jupyter-serverhttp://jupyter.or	https://github.com/jupyter-server/jupyter_server/blob/main/LICENSE	
jupyter_client	http://jupyter.org	https://github.com/jupyter/jupyter_client/blob/main/LICENSE

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Name of Project	Website	License URL
jupyter_core	http://jupyter.org	https://github.com/jupyter/jupyter_core/blob/master/LICENSE
jupyter_server	https://github.com/jupyter-server/jupyter_server	https://github.com/jupyter-server/jupyter_server/blob/main/LICENSE
jupyter_server_termin	https://github.com/jupyter-server/jupyter_server_terminals	https://github.com/jupyter-server/jupyter_server_terminals/blob/main/LICENSE
jupyterlab	https://github.com/jupyterlab/jupyterlab	https://github.com/jupyterlab/jupyterlab/blob/main/LICENSE
jupyterlab-pygments	http://jupyter.org	https://github.com/jupyterlab/jupyterlab_pygments/blob/main/LICENSE
jupyterlab-widgets	http://jupyter.org	https://github.com/jupyter-widgets/ipywidgets/blob/master/LICENSE
jupyter-lab_pygments	https://github.com/jupyterlab/jupyterlab_pygments	https://github.com/jupyterlab/jupyterlab_pygments?tab=BSD-3-Clause-1-ov-file#readme
jupyterlab_server	https://github.com/jupyterlab/jupyterlab_server	https://github.com/jupyterlab/jupyterlab_server/blob/main/LICENSE
jupyterlab_widgets	https://github.com/jupyter-widgets/ipywidgets	https://github.com/jupyter-widgets/ipywidgets?tab=BSD-3-Clause-1-ov-file#readme
kaleido	https://github.com/plotly/Kaleido	https://github.com/plotly/Kaleido/blob/master/LICENSE.txt
keras	https://github.com/keras-team/keras	https://github.com/keras-team/keras/blob/master/LICENSE

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Name of Project	Website	License URL
Keras-Preprocessing	https://github.com/keras-team/keras-preprocessing	https://github.com/keras-team/keras-preprocessing/blob/master/LICENSE
keras-tuner	https://github.com/keras-team/keras-tuner	https://github.com/keras-team/keras-tuner/blob/master/LICENSE
keyring	https://github.com/jaraco/keyring	https://github.com/jaraco/keyring/blob/main/LICENSE
keyutils	https://github.com/sassoftware/python-keyutils	https://github.com/sassoftware/python-keyutils/blob/master/LICENSE
kiwisolver	https://kiwisolver.readthedocs.io/en/latest/	https://github.com/nucleic/kiwi/blob/main/LICENSE
kombu	https://kombu.readthedocs.io	https://github.com/celery/kombu/blob/master/LICENSE
krb5	https://web.mit.edu/kerberos/	https://github.com/krb5/krb5/blob/master/src/lib/gssapi/LICENSE
kt-legacy	https://github.com/haifeng-jin/kt-legacy	https://github.com/haifeng-jin/kt-legacy/blob/main/LICENSE
lark	https://github.com/lark-parser/lark	https://github.com/lark-parser/lark?tab=MIT-1-ov-file#readme
lazy_loader	https://github.com/scientific-python/lazy_loader	https://github.com/scientific-python/lazy_loader/blob/main/LICENSE.md
lcms2	https://www.littlecms.com	https://github.com/sk1project/python-lcms2/blob/master/LICENSE
legacy-cgi	https://github.com/jackrosenthal/legacy-cgi	https://github.com/jackrosenthal/legacy-cgi?tab=License-1-ov-file#readme

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Name of Project	Website	License URL
lerc	https://github.com/Esri/lerc	https://github.com/Esri/lerc/blob/master/LICENSE
libarchive	http://www.libarchive.org	https://raw.githubusercontent.com/libarchive/libarchive/master/COPYING
libblas	https://www.netlib.org/blas/	https://www.netlib.org/blas/#_licensing
libbrotlicommon	https://github.com/google/brotli	https://github.com/google/brotli/blob/master/LICENSE
libbrotlidec	https://github.com/google/brotli	https://github.com/google/brotli/blob/master/LICENSE
libbrotlienc	https://github.com/google/brotli	https://github.com/google/brotli/blob/master/LICENSE
libcblas	https://anaconda.org/conda-forge/libcblas	N/A
libclang	https://github.com/sighingnow/libclang	https://github.com/sighingnow/libclang/blob/master/LICENSE.TXT
libcurl	https://curl.se/libcurl/	https://curl.se/docs/copyright.html
libcxx	https://github.com/llvm-mirror/libcxx	https://github.com/llvm-mirror/libcxx/blob/master/LICENSE.TXT
libdb	https://www.oracle.com/technology/software/products/berkeley-db/index.html	https://github.com/berkeleydb/libdb/blob/master/LEGAL
libdeflate	https://github.com/ebiggers/libdeflate	https://github.com/ebiggers/libdeflate/blob/master/COPYING
libedit	https://thrysoee.dk/editline/	http://www.netbsd.org/Goals/redistribution.html
libev	https://software.schmorp.de/pkg/libev.html	https://software.schmorp.de/pkg/libev.html

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Name of Project	Website	License URL
libexpat	https://libexpat.github.io/	https://github.com/libexpat/libexpat?tab=MIT-1-ov-file#readme
libffi	https://github.com/libffi/libffi	https://github.com/libffi/libffi/blob/master/LICENSE
libgcc	https://gcc.gnu.org/onlinedocs/gccint/Libgcc.html	https://gcc.gnu.org/onlinedocs/libstdc++/manual/license.html
libgcrypt	https://gnupg.org/software/index.html	https://git.gnupg.org/cgi-bin/gitweb.cgi?p=libgcrypt.git;a=blob;f=COPYING.LIB;hb=HEAD
libgd	https://libgd.github.io	https://libgd.github.io/manuals/2.2.1/files/license-txt.html
libglib	https://github.com/PolMine/libglib	https://github.com/PolMine/libglib/blob/master/include/glib-2.0/glib.h
libiconv	https://www.gnu.org/software/libiconv/	https://www.gnu.org/software/libiconv/#downloading
libint	https://tinyurl.com/yvw97wbw	https://tinyurl.com/yvw97wbw
liblapack	http://www.netlib.org/lapack/	https://www.netlib.org/lapack/LICENSE.txt
liblapacke	https://anaconda.org/conda-forge/liblapacke	https://www.netlib.org/lapack/LICENSE.txt
liblzma	https://tukaani.org/xz/	https://git.tukaani.org/?p=xz.git;a=blob;f=COPYING.0BSD
libmamba	https://medium.com/@QuantStack/open-software-packag	https://github.com/mamba-org/mamba/blob/main/LICENSE

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Name of Project	Website	License URL
libmambapy	https://www.anaconda.com/blog/a-faster-conda-for-a-g	https://github.com/conda/conda-libmamba-solv blob/main/LICENSE
libnetcdf	https://www.unidata.ucar.edu/software/netcdf/	https://www.unidata.ucar.edu/software/netcdf/copyright.html
libnghttp2	https://github.com/nghttp2/nghttp2	https://github.com/nghttp2/nghttp2/blob/master/COPYING
libnsl	https://github.com/thkukuk/libnsl	https://gcc.gnu.org/onlinedocs/libstdc++/manual/license.html
libopenblas	https://www.openblas.net/	https://github.com/xianyi/OpenBLAS/blob/develop/LICENSE
libpng	https://www.libpng.org/pub/png/libpng.html	https://www.libpng.org/pub/png/src/libpng-LICENSE.txt
libpq	https://www.postgresql.org/	https://www.postgresql.org/about/licence/
librsvg	https://gitlab.gnome.org/GNOME/librsvg	https://gitlab.gnome.org/GNOME/librsvg/-/blob/main/COPYING.LIB
libsolv	https://github.com/openSUSE/libsolv	https://github.com/openSUSE/libsolv/blob/master/LICENSE.BSD
libsqlite	https://github.com/mackyle/sqlite	https://github.com/mackyle/sqlite?tab=License-1-ov-file#readme
libssh2	https://github.com/libssh2/libssh2	https://github.com/libssh2/libssh2/blob/master/COPYING
libstdcxx	https://gcc.gnu.org/	https://gcc.gnu.org/onlinedocs/libstdc++/manual/license.html

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Name of Project	Website	License URL
libtiff	https://www.libtiff.org/	https://www.libtiff.org/misc.html
libtrust	https://github.com/docker/libtrust	https://github.com/docker/libtrust/blob/master/LICENSE
libuuid	https://sourceforge.net/projects/libuuid/	https://sourceforge.net/p/libuuid/code/ci/master/tree/COPYING
libuv	https://github.com/libuv/libuv	https://github.com/libuv/libuv/blob/v1.x/LICENSE
libwebp	https://chromium.googlesource.com/?format=HTML	https://chromium.googlesource.com/chromium/src/third_party/+/refs/heads/main/libwebp/LICENSE
libwebp-base	https://chromium.googlesource.com/?format=HTML	https://chromium.googlesource.com/chromium/src/third_party/+/refs/heads/main/libwebp/LICENSE
libxc	https://www.tddft.org/programs/libxc/	https://gitlab.com/libxc/libxc/-/blob/master/COPYING
libxcb	https://xcb.freedesktop.org	https://github.com/freedesktop/xcb-libxcb/blob/master/COPYING
libxcrypt	https://github.com/besser82/libxcrypt	https://github.com/besser82/libxcrypt?tab=LGPL-2.1-1-ov-file#readme
libxml2	https://git.gnome.org/browse/libxml2/	https://gitlab.gnome.org/GNOME/libxml2/-/blob/master/Copyright
libxmlsec1	https://github.com/lsh123/xmlsec	https://github.com/lsh123/xmlsec/blob/master/README
libxslt	https://gitlab.gnome.org/GNOME/libxslt/-/wikis/home	https://gitlab.gnome.org/GNOME/libxslt/-/blob/master/Copyright

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Name of Project	Website	License URL
libzlib	https://zlib.net	https://zlib.net/zlib_license.html
lightning-utilities	https://github.com/Lightning-AI/utilities	https://github.com/Lightning-AI/utilities?tab=Apache-2.0-1-ov-file#readme
lime	https://github.com/marcotcr/lime	https://github.com/marcotcr/lime/blob/master/LICENSE
linear-operator	https://github.com/cornellius-gp/linear_operator	https://github.com/cornellius-gp/linear_operator?tab=MIT-1-ov-file#readme
lit	http://llvm.org	https://releases.llvm.org/14.0.0/LICENSE.TXT
llvm-openmp	https://github.com/llvm-mirror/openmp	https://github.com/llvm-mirror/openmp/blob/master/LICENSE.txt
llvmlite	http://llvmlite.readthedocs.io	https://github.com/numba/llvmlite/blob/main/LICENSE
loader-utils	https://github.com/webpack/loader-utils	https://github.com/webpack/loader-utils/raw/master/LICENSE
logistro	https://github.com/geopozo/logistro	https://github.com/geopozo/logistro?tab=MIT-1-ov-file#readme
logomaker	https://logomaker.readthedocs.io/en/latest/	https://github.com/jbkinney/logomaker/blob/master/LICENSE
logrus	https://github.com/sirupsen/logrus	https://github.com/sirupsen/logrus/blob/master/LICENSE
logrus-airbrake-hook.v2	https://gopkg.in/gemnasium/logrus-airbrake-hook.v2	https://github.com/gemnasium/logrus-airbrake-hook/blob/v2.1.2/LICENSE
lxml	https://lxml.de	https://lxml.de/index.html#license

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Name of Project	Website	License URL
lz4-c	https://www.lz4.org/	https://github.com/lz4/lz4/blob/dev/LICENSE
lzo	https://www.oberhumer.com/opensource/lzo/	https://www.oberhumer.com/opensource/gpl.html
mamba	https://github.com/mamba-org/mamba	https://github.com/mamba-org/mamba?tab=BSD-3-Clause-1-ov-f readme
markdown	https://github.com/evilstreak/markdown-js	https://www.opensource.org/licenses/mit-license.php
markdown-it-py	https://github.com/executablebooks/markdown-it-py	https://github.com/executablebooks/markdown-it-py/blob/master/LICENSE
markupsafe	https://github.com/pallets/markupsafe/tree/main/src/markupsafe	https://github.com/pallets/markupsafe/tree/main?tab=BSD-3-Clause-1-ov-f
MarkupSafe	https://palletsprojects.com/p/markupsafe/	https://github.com/pallets/markupsafe/blob/main/LICENSE.rst
mashumaro	https://github.com/Fatal1ty/mashumaro	https://github.com/Fatal1ty/mashumaro
matplotlib	https://matplotlib.org	https://matplotlib.org/stable/users/project/license.html
matplotlib-base	https://matplotlib.org	https://matplotlib.org/stable/users/project/license.html
matplotlib-inline	https://github.com/ipython/matplotlib-inline	https://github.com/ipython/matplotlib-inline/blob/master/LICENSE
mda-xdrlib	https://github.com/MDAnalysis/mda-xdrlib	https://github.com/MDAnalysis/mda-xdrlib/blob/main/LICENSE

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Name of Project	Website	License URL
mda_xdrlib	https://github.com/MDAnalysis/mda-xdrlib	https://github.com/MDAnalysis/mda-xdrlib?tab=License-1-ov-file#readme
mdtraj	https://www.mdtraj.org/	https://www.mdtraj.org/1.9.8.dev0/index.html#license
mdurl	https://github.com/markdown-it/mdurl	https://github.com/markdown-it/mdurl/blob/master/LICENSE
menuinst	https://github.com/conda/menuinst	https://github.com/conda/menuinst/blob/main/LICENSE.txt
mergo	https://github.com/imdario/mergo	https://github.com/imdario/mergo/blob/master/LICENSE
mistune	https://github.com/lepture/mistune	https://github.com/lepture/mistune/blob/master/LICENSE
mkl	https://github.com/rust-math/intel-mkl-src	https://github.com/rust-math/intel-mkl-src/blob/master/License.txt
mkl-fft	https://github.com/IntelPython/mkl_fft	https://github.com/IntelPython/mkl_fft/blob/master/LICENSE.txt
mkl-random	https://github.com/IntelPython/mkl_random	https://github.com/IntelPython/mkl_random/blob/master/LICENSE.txt
mkl-service	https://github.com/IntelPython/mkl-service	https://github.com/IntelPython/mkl-service/blob/master/LICENSE.txt
mkl_fft	http://github.com/IntelPython/mkl_fft	https://github.com/IntelPython/mkl_fft?tab=BSD-3-Clause-1-ov-f readme

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Name of Project	Website	License URL
mkl_random	http://github.com/IntelPython/mkl_random	https://github.com/IntelPython/mkl_random?tab=BSD-3-Clause-1-ov-f readme
ml-dtypes	https://github.com/jax-ml/ml_dtypes	https://github.com/jax-ml/ml_dtypes/blob/main/LICENSE
ml_dtypes	https://github.com/jax-ml/ml_dtypes	https://github.com/jax-ml/ml_dtypes/blob/main/LICENSE
modelcif	https://github.com/ihmwg/python-modelcif	https://github.com/ihmwg/python-modelcif/blob/main/LICENSE
molecupy	https://molecupy.readthedocs.io/en/latest/	https://github.com/samirelanduk/atomium/blob/master/LICENSE
moment	https://github.com/moment/moment	https://github.com/moment/moment/raw/master/LICENSE
moment-precise-range-plugin	https://github.com/codebox/moment-precise-range	https://github.com/codebox/moment-precise-range raw/master/LICENSE.md
more-itertools	https://github.com/more-itertools/more-itertools	https://github.com/more-itertools/more-itertools/blob/master/LICENSE
mpiplus	https://github.com/choderalab/mpiplus	https://github.com/choderalab/mpiplus/blob/main/LICENSE
mpmath	http://mpmath.org/	https://github.com/mpmath/mpmath/blob/master/LICENSE
mrcfile	https://github.com/ccpem/mrcfile	https://github.com/ccpem/mrcfile/blob/master/LICENSE.txt

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Name of Project	Website	License URL
msgpack	https://msgpack.org/	https://github.com/msgpack/msgpack-python/blob/main/COPYING
multidict	https://github.com/aio-libs/multidict	https://github.com/aio-libs/multidict/blob/master/LICENSE
multierr	https://go.uber.org/multierr	https://github.com/uber-go/multierr/blob/master/LICENSE.txt
multiprocess	https://github.com/uqfoundation/multiprocess	https://github.com/uqfoundation/multiprocess/blob/master/LICENSE
munkres	https://software.clapper.org/munkres/	https://github.com/bmc/munkres/blob/master/LICENSE.md
myesui uuid	https://github.com/myesui/uuid	https://pkg.go.dev/github.com/myesui/uuid?tab=licenses
namex	https://github.com/bcgov/namex	https://github.com/bcgov/namex/blob/main/LICENSE
narwhals	https://github.com/narwhals-dev/narwhals	https://github.com/narwhals-dev/narwhals?tab=MIT-1-ov-file#readme
nbclassic	http://jupyter.org	https://github.com/jupyter/nbclassic/blob/main/LICENSE
nbclient	https://jupyter.org	https://github.com/jupyter/nbclient/blob/main/LICENSE
nbconvert	https://jupyter.org	https://github.com/jupyter/nbconvert/blob/main/LICENSE
nbformat	http://jupyter.org	https://github.com/jupyter/nbformat/blob/main/LICENSE

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Name of Project	Website	License URL
ncurses	https://invisible-island.net/ncurses/	https://invisible-island.net/ncurses/ncurses-license.html
ndfes	https://rutgerslbsr.gitlab.io/fe-toolkit/	https://gitlab.com/RutgersLBSR/fe-toolkit/-/blob/master/LICENSE
ndindex	https://quansight-labs.github.io/ndindex/	https://github.com/Quansight-Labs/ndindex?tab=MIT-1-ov-file#readme
nest-asyncio	https://github.com/erdewit/nest_asyncio	https://github.com/erdewit/nest_asyncio/blob/master/LICENSE
nest_asyncio	https://github.com/erdewit/nest_asyncio	https://github.com/erdewit/nest_asyncio?tab=BSD-2-Clause-1-ov-f readme
netcdf-fortran	https://www.unidata.ucar.edu/software/netcdf/	https://www.unidata.ucar.edu/software/netcdf/copyright.html
netCDF4	http://github.com/Unidata/netcdf4-python	https://github.com/Unidata/netcdf4-python/blob/master/LICENSE
nettle	https://git.lysator.liu.se/nettle/nettle	https://git.lysator.liu.se/nettle/nettle/-/blob/master/AUTHORS?ref_type=heads
networkx	https://networkx.org	https://github.com/networkx/networkx/blob/main/LICENSE.txt
nfpm	https://github.com/goreleaser/nfpm	https://github.com/goreleaser/nfpm/blob/master/LICENSE.md
ng-tags-input	https://github.com/mbenford/ngTagsInput	https://github.com/mbenford/ngTagsInput
ng-toast	https://github.com/tameraydin/ngToast	https://github.com/tameraydin/ngToast

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Name of Project	Website	License URL
ngdraggable	https://github.com/fatlinesofcode/ngDraggable	https://github.com/fatlinesofcode/ngDraggable/raw/master/LICENSE.txt
ngVue	https://github.com/ngVue/ngVue	https://github.com/ngVue/ngVue/raw/master/LICENSE
nh3	https://nh3.readthedocs.io/en/latest/	https://github.com/messense/nh3/blob/main/LICENSE
nlohmann_json	https://github.com/nlohmann/json	https://github.com/nlohmann/json?tab=MIT-1-ov-file#readme
nlopt	https://nlopt.readthedocs.io/en/latest/NLopt_Python_Reference/	https://nlopt.readthedocs.io/en/latest/NLopt_License_and_Copyright/
nodejs	https://nodejs.org/en/	https://raw.githubusercontent.com/nodejs/node/master/LICENSE
nomkl	https://github.com/conda-forge/nomkl-feedstock	https://github.com/conda-forge/nomkl-feedstock/blob/main/LICENSE.txt
notebook	http://jupyter.org	https://github.com/jupyter/notebook/blob/main/LICENSE
notebook-shim	https://github.com/jupyter/notebook_shim	https://github.com/jupyter/notebook_shim
notebook_shim	http://jupyter.org	https://github.com/jupyter/notebook_shim/blob/main/LICENSE
numba	https://numba.pydata.org	https://github.com/numba/numba/blob/main/LICENSE
numcpus	https://github.com/tklauser/numcpus	https://github.com/tklauser/numcpus/blob/master/LICENSE

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Name of Project	Website	License URL
numexpr	https://github.com/pydata/numexpr	https://github.com/pydata/numexpr/blob/master/LICENSE.txt
numpy	https://numpy.org	https://github.com/numpy/numpy/blob/main/LICENSE.txt
numpy-base	https://numpy.org	https://github.com/numpy/numpy/blob/main/LICENSE.txt
numpydoc	https://numpydoc.readthedocs.io/en/latest/index.html	https://github.com/numpy/numpydoc/blob/main/LICENSE.txt
nvidia-cublas-cu11	https://developer.nvidia.com/cuda-zone	https://docs.nvidia.com/cuda/eula/index.html
nvidia-cublas-cu12	https://developer.nvidia.com/cuda-zone	https://docs.nvidia.com/cuda/eula/index.html
nvidia-cuda-cupti-cu11	https://developer.nvidia.com/cuda-zone	https://docs.nvidia.com/cuda/eula/index.html
nvidia-cuda-cupti-cu12	https://developer.nvidia.com/cuda-zone	https://docs.nvidia.com/cuda/eula/index.html
nvidia-cuda-nvrtc-cu11	https://developer.nvidia.com/cuda-zone	https://docs.nvidia.com/cuda/eula/index.html
nvidia-cuda-nvrtc-cu12	https://developer.nvidia.com/cuda-zone	https://docs.nvidia.com/cuda/eula/index.html
nvidia-cuda-runtime-cu11	https://developer.nvidia.com/cuda-zone	https://docs.nvidia.com/cuda/eula/index.html
nvidia-cuda-runtime-cu12	https://developer.nvidia.com/cuda-zone	https://docs.nvidia.com/cuda/eula/index.html
nvidia-cudnn-cu11	https://developer.nvidia.com/cuda-zone	https://docs.nvidia.com/deeplearning/cudnn/sla/index.html
nvidia-cudnn-cu12	https://developer.nvidia.com/cuda-zone	https://docs.nvidia.com/deeplearning/cudnn/sla/index.html

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Name of Project	Website	License URL
nvidia-cuEquivariance	https://github.com/NVIDIA/cuEquivariance	https://github.com/NVIDIA/cuEquivariance/blob/main/LICENSES/LICENSE
nvidia-cufft-cu11	https://developer.nvidia.com/cuda-zone	https://docs.nvidia.com/cuda/eula/index.html
nvidia-cufft-cu12	https://developer.nvidia.com/cuda-zone	https://docs.nvidia.com/cuda/eula/index.html
nvidia-cufile-cu12	https://developer.nvidia.com/cuda-zone	https://docs.nvidia.com/cuda/eula/index.html#
nvidia-curand-cu11	https://developer.nvidia.com/cuda-zone	https://docs.nvidia.com/cuda/eula/index.html
nvidia-curand-cu12	https://developer.nvidia.com/cuda-zone	https://docs.nvidia.com/cuda/eula/index.html
nvidia-cusolver-cu11	https://developer.nvidia.com/cuda-zone	https://docs.nvidia.com/cuda/eula/index.html
nvidia-cusolver-cu12	https://developer.nvidia.com/cuda-zone	https://docs.nvidia.com/cuda/eula/index.html
nvidia-cusparse-cu11	https://developer.nvidia.com/cuda-zone	https://docs.nvidia.com/cuda/eula/index.html
nvidia-cusparse-cu12	https://developer.nvidia.com/cuda-zone	https://docs.nvidia.com/cuda/eula/index.html
nvidia-cusparselt-cu12	https://docs.nvidia.com/cuda/cusparselt/index.html	https://docs.nvidia.com/cuda/cusparselt/license.html
nvidia-ml-py	https://pypi.org/project/nvidia-ml-py/	https://pypi.org/project/nvidia-ml-py/
nvidia-nccl-cu11	https://developer.nvidia.com/cuda-zone	https://docs.nvidia.com/hpc-sdk/eula/index.html
nvidia-nccl-cu12	https://developer.nvidia.com/cuda-zone	https://docs.nvidia.com/hpc-sdk/eula/index.html
nvidia-nvjitlink-cu12	https://developer.nvidia.com/cuda-zone	https://docs.nvidia.com/cuda/eula/index.html

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Name of Project	Website	License URL
nvidia-nvshmem-cu12	https://developer.nvidia.com/cuda-zone	https://docs.nvidia.com/cuda/eula/index.html
nvidia-nvtx-cu11	https://developer.nvidia.com/cuda-zone	https://docs.nvidia.com/cuda/eula/index.html
nvidia-nvtx-cu12	https://developer.nvidia.com/cuda-zone	https://docs.nvidia.com/cuda/eula/index.html
Oat++	https://oatpp.io/	https://github.com/oatpp/oatpp/blob/master/LICENSE
oauthlib	https://github.com/oauthlib/oauthlib	https://github.com/oauthlib/oauthlib/blob/master/LICENSE
ocl-icd	https://github.com/OCL-dev/ocl-icd	https://github.com/OCL-dev/ocl-icd/blob/master/COPYING
ocl-icd-system	https://github.com/conda-forge/ocl-icd-system-feedst	https://github.com/conda-forge/ocl-icd-system-feedst blob/main/LICENSE.txt
olefile	https://www.decalage.info/python/olefileio	https://olefile.readthedocs.io/en/latest/License.html
omegaconf	https://github.com/omry/omegaconf	https://github.com/omry/omegaconf/blob/master/LICENSE
OmegaFold	https://github.com/HeliXonProtein/OmegaFold/tree/main	https://github.com/HeliXonProtein/OmegaFold/blob/main/LICENSE
omnicanvas	https://omnicanvas.readthedocs.io/en/latest/	https://github.com/samirelanduk/omnicanvas/blob/master/LICENSE
OpenFF	https://openforcefield.org/	https://github.com/openforcefield/openff-forcefields
openff-amber-ff-ports	https://github.com/openforcefield/openff-amber-ff-ports	https://github.com/openforcefield/openff-amber-ff-ports blob/main/LICENSE

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Name of Project	Website	License URL
openff-forcefields	https://openforcefield.org	https://github.com/openforcefield/openff-forcefields/blob/master/LICENSE
openff-fragmenter	https://github.com/openforcefield/openff-fragmenter	https://github.com/openforcefield/openff-fragmenter/blob/main/LICENSE
openff-interchange	https://github.com/openforcefield/openff-interchange	https://github.com/openforcefield/openff-interchange/blob/main/LICENSE
openff-models	https://github.com/openforcefield/openff-models	https://github.com/openforcefield/openff-models/blob/main/LICENSE
openff-nagl	https://docs.openforcefield.org/projects/nagl/en/latest/?badge=latest	https://github.com/openforcefield/openff-nagl/blob/main/LICENSE
openff-nagl-models	https://github.com/openforcefield/openff-nagl-models	https://github.com/openforcefield/openff-nagl-models/blob/main/LICENSE
openff-toolkit	https://openforcefield.org	https://github.com/openforcefield/openff-toolkit/blob/master/LICENSE
openff-toolkit-base	https://openforcefield.org	https://github.com/openforcefield/openff-toolkit/blob/master/LICENSE
openff-units	https://github.com/openforcefield/openff-units	https://github.com/openforcefield/openff-units/blob/main/LICENSE
openff-utilities	https://github.com/openforcefield/openff-utilities	https://github.com/openforcefield/openff-utilities/blob/main/LICENSE
openjpeg	https://github.com/uclouvain/openjpeg	https://github.com/uclouvain/openjpeg/blob/master/LICENSE

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Name of Project	Website	License URL
openldap	https://www.openldap.org/software/repo.html	https://git.openldap.org/openldap/openldap/-/blob/master/LICENSE
OpenMM	https://openmm.org	https://docs.openmm.org/7.1.0/userguide/library.html#license
openmmtools	https://github.com/choderalab/openmmtools	https://github.com/choderalab/openmmtools/blob/main/LICENSE
openmoltools	https://github.com/choderalab/openmoltools	https://github.com/choderalab/openmoltools/blob/master/LICENSE
openpyxl	https://openpyxl.readthedocs.io/en/stable/	https://foss.heptapod.net/openpyxl/openpyxl/-/blob/branch/3.0/LICENCE.rst
openssl	https://www.openssl.org	https://github.com/openssl/openssl/blob/master/LICENSE.txt
opt-einsum	https://github.com/dgasmith/opt_einsum	https://github.com/dgasmith/opt_einsum/blob/master/LICENSE
opt_einsum	https://github.com/dgasmith/opt_einsum	https://github.com/dgasmith/opt_einsum/blob/main/LICENSE
OptKing	https://github.com/psi-rking/optking	https://github.com/psi-rking/optking/blob/master/LICENSE
optree	https://optree.readthedocs.io/en/latest/	https://github.com/metaopt/optree/blob/main/LICENSE
oscrypto	https://github.com/wbond/oscrypto	https://github.com/wbond/oscrypto/blob/master/LICENSE
overrides	https://github.com/mkorpela/overrides	https://github.com/mkorpela/overrides/blob/main/LICENSE

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Name of Project	Website	License URL
packaging	https://github.com/pypa/packaging	https://github.com/pypa/packaging/blob/main/LICENSE
packmol	https://leandro.iqm.unicamp.br/m3g/packmol/home.shtml	https://github.com/m3g/packmol/blob/master/LICENSE
packmol_memgen	http://cpclab.uni-duesseldorf.de/	https://gitlab.com/cbjh/memgen/py-memgen/-/blob/main/LICENSE
pandas	https://pandas.pydata.org	https://github.com/pandas-dev/pandas/blob/main/LICENSE
pandocfilters	http://github.com/jgm/pandocfilters	https://github.com/jgm/pandocfilters/blob/master/LICENSE
panedr	https://github.com/MDAnalysis/panedr	https://github.com/MDAnalysis/panedr/blob/master/LICENSE.txt
pango	https://pango.gnome.org	https://gitlab.gnome.org/GNOME/pango/-/blob/main/COPYING
ParmEd	https://parmed.github.io/ParmEd/html/index.html	https://github.com/ParmEd/ParmEd#license
parser	https://github.com/typescript-eslint/typescript-eslint	https://github.com/typescript-eslint/typescript-eslint/raw/master/LICENSE
parso	https://parso.readthedocs.io/en/latest/	https://github.com/davidhalter/parso/blob/master/LICENSE.txt
pathos	https://github.com/uqfoundation/pathos	https://github.com/uqfoundation/pathos/blob/master/LICENSE
patsy	https://patsy.readthedocs.io/en/latest/	https://github.com/pydata/patsy/blob/master/LICENSE.txt

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Name of Project	Website	License URL
pbkdf2	https://golang.org/x/crypto/pbkdf2	https://cs.opensource.google/go/x/crypto/+/master:LICENSE
pbr	https://docs.openstack.org/pbr/latest/	https://opendev.org/openstack/pbr/src/branch/master/LICENSE
pcmsolver	https://pcmsolver.readthedocs.io/en/stable/	https://github.com/PCMSolver/pcmsolver/blob/master/LICENSE
pcre	https://www.pcre.org	https://www.pcre.org/licence.txt
pcre2	https://www.pcre.org	https://github.com/PCRE2Project/pcre2/blob/master/LICENCE
pdb4amber	https://github.com/Amber-MD/pdb4amber	https://github.com/Amber-MD/pdb4amber/blob/master/LICENSE
pdbfixer	https://github.com/openmm/pdbfixer	https://github.com/openmm/pdbfixer/blob/master/LICENSE
pexpect	https://pexpect.readthedocs.io/	https://github.com/pexpect/pexpect/blob/master/LICENSE
pgconn	https://github.com/jackc/pgconn	https://github.com/jackc/pgconn/blob/master/LICENSE
pgio	https://github.com/jackc/pgio	https://github.com/jackc/pgio/blob/master/LICENSE
pgpassfile	https://github.com/jackc/pgpassfile	https://github.com/jackc/pgpassfile/blob/master/LICENSE
pgproto3	https://github.com/jackc/pgproto3/v2	https://github.com/jackc/pgproto3/blob/master/LICENSE
pgtype	https://github.com/jackc/pgtype	https://github.com/jackc/pgtype/blob/master/LICENSE
pgx	https://github.com/jackc/pgx/v4	https://github.com/jackc/pgx/blob/v4.0.1/LICENSE

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Name of Project	Website	License URL
phonopy	https://github.com/phonopy/phono3py	https://github.com/phonopy/phono3py/blob/develop/LICENSE
pickleshare	https://github.com/pickleshare/pickleshare	https://github.com/pickleshare/pickleshare/blob/master/LICENSE
Pillow	https://python-pillow.org	https://github.com/python-pillow/Pillow/blob/main/LICENSE
Pint	https://pint.readthedocs.io/en/stable/	https://github.com/hgrecco/pint/blob/master/LICENSE
pip	https://pip.pypa.io/	https://github.com/pypa/pip/blob/main/LICENSE.txt
pip-licenses	https://github.com/raimon49/pip-licenses	https://github.com/raimon49/pip-licenses/blob/master/LICENSE
pixman	https://pixman.org	https://cgit.freedesktop.org/pixman/tree/COPYING
pkginfo	https://launchpad.net/pkginfo	https://bazaar.launchpad.net/~tseaver/pkginfo/trunk/view/head:/LICENSE.txt
pkgutil-resolve-name	https://github.com/graingert/pkgutil-resolve-name	https://github.com/graingert/pkgutil-resolve-name?tab=License-1-ov-file#readme
pkgutil_resolve_name	https://github.com/graingert/pkgutil-resolve-name	https://github.com/graingert/pkgutil-resolve-name?tab=License-1-ov-file#readme
platformdirs	https://github.com/platformdirs/platformdirs	https://github.com/platformdirs/platformdirs/blob/main/LICENSE

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Name of Project	Website	License URL
plotly	https://plotly.com/python/	https://github.com/plotly/plotly.py/blob/master/LICENSE.txt
plotly-orca	https://github.com/plotly/orca	https://github.com/plotly/orca/blob/master/LICENSE
plotly.js	https://github.com/plotly/plotly.js	https://github.com/plotly/plotly.js/raw/master/LICENSE
pluggy	https://pluggy.readthedocs.io/en/stable/index.html	https://github.com/pytest-dev/pluggy/blob/main/LICENSE
pooch	https://github.com/fatiando/pooch	https://github.com/fatiando/pooch/blob/main/LICENSE.txt
portalocker	https://github.com/WoLpH/portalocker	https://github.com/wolph/portalocker/blob/develop/LICENSE
pox	https://github.com/uqfoundation/pox	https://github.com/uqfoundation/pox/blob/master/LICENSE
ppft	https://github.com/uqfoundation/ppft	https://github.com/uqfoundation/ppft/blob/master/LICENSE
pq	https://github.com/lib/pq	https://github.com/lib/pq/blob/master/LICENSE.md
ProDy	http://www.csb.pitt.edu/ProDy	https://github.com/prody/ProDy/blob/master/LICENSE.rst
prometheus-client	https://github.com/prometheus/client_python	https://github.com/prometheus/client_python/blob/master/LICENSE
prometheus_client	https://github.com/prometheus/client_python	https://github.com/prometheus/client_python/blob/master/LICENSE
prompt-toolkit	https://python-prompt-toolkit.readthedocs.io/en/stable/	https://github.com/prompt-toolkit/python-prompt-toolkit/blob/master/LICENSE

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Name of Project	Website	License URL
prompt_toolkit	https://github.com/prompt-toolkit/python-prompt-toolki	https://github.com/prompt-toolkit/python-prompt-toolki tab=BSD-3-Clause-1-ov-f readme
propcache	https://github.com/aio-libs/propcache	https://github.com/aio-libs/propcache?tab=Apache-2.0-1-ov-file#readme
protobuf	https://google.golang.org/protobuf	https://github.com/protocolbuffers/protobuf-go/blob/master/LICENSE
psi4	https://psicode.org	https://github.com/psi4/psi4/blob/master/COPYING.LESSER
psutil	https://psutil.readthedocs.io/en/latest/	https://github.com/giampaolo/psutil/blob/master/LICENSE
psycopg2	https://psycopg.org/	https://github.com/psycopg/psycopg2/blob/master/LICENSE
PTable	https://github.com/kxxoling/PTable	https://github.com/kxxoling/PTable/blob/master/COPYING
pthread-stubs	https://xcb.freedesktop.org	https://github.com/freedesktop/xcb-pthread-stubs/blob/master/COPYING
ptyprocess	https://ptyprocess.readthedocs.io/en/latest/	https://github.com/pexpect/ptyprocess/blob/master/LICENSE
pure-eval	http://github.com/alexmojaki/pure_eval	http://github.com/alexmojaki/pure_eval/blob/master/LICENSE.txt
pure_eval	http://github.com/alexmojaki/pure_eval	https://github.com/alexmojaki/pure_eval?tab=MIT-1-ov-file#readme

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Name of Project	Website	License URL
py	https://py.readthedocs.io/en/latest/	https://github.com/pytest-dev/py/blob/master/LICENSE
py-cpuinfo	https://github.com/workhorsy/py-cpuinfo	https://github.com/workhorsy/py-cpuinfo/blob/master/LICENSE
pyasn1	https://github.com/etingof/pyasn1	https://github.com/etingof/pyasn1/blob/master/LICENSE.rst
pyasn1-modules	https://github.com/etingof/pyasn1-modules	https://github.com/etingof/pyasn1-modules/blob/master/LICENSE.txt
pyasn1_modules	https://pyasn1.readthedocs.io/en/latest/contents.html	https://github.com/pyasn1/pyasn1-modules?tab=BSD-2-Clause-1-ov-file#readme
pybind11	http://pybind11.readthedocs.io/en/stable/	https://github.com/pybind/pybind11/blob/master/LICENSE
pybind11-abi	https://github.com/pybind/pybind11	https://github.com/pybind/pybind11/blob/master/LICENSE
pybind11_global	http://pybind11.readthedocs.io/en/stable/	https://github.com/pybind/pybind11/blob/master/LICENSE
pycairo	https://pycairo.readthedocs.io/en/latest/index.html	https://github.com/pygobject/pycairo/blob/master/COPYING
pycosat	https://github.com/conda/pycosat	https://github.com/conda/pycosat/blob/main/LICENSE
pycparser	https://github.com/eliben/pycparser	https://github.com/eliben/pycparser/blob/master/LICENSE
pydantic	https://pydantic-docs.helpmanual.io	https://github.com/samuelcolvin/pydantic/blob/master/LICENSE

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Name of Project	Website	License URL
pydantic-core	https://github.com/pydantic/pydantic-core	https://github.com/pydantic/pydantic-core
pyedr	https://github.com/MDAnalysis/panedr	https://github.com/MDAnalysis/panedr/blob/master/LICENSE.txt
pyEMMA	http://github.com/markovmodel/PyEMMA	https://github.com/markovmodel/PyEMMA/blob/devel/LICENSE.txt
Pygments	https://pygments.org	https://github.com/pygments/pygments/blob/master/LICENSE
pygments	https://pygments.org/	https://github.com/pygments/pygments?tab=BSD-2-Clause-1-ov-file#readme
pygraphviz	https://pygraphviz.github.io	https://github.com/pygraphviz/pygraphviz/blob/main/LICENSE
pygtop	https://pygtop.readthedocs.io/en/latest/	https://github.com/samirelanduk/pygtop/blob/master/LICENSE
pyHanko	https://github.com/MatthiasValvekens/pyHanko	https://github.com/MatthiasValvekens/pyHanko/blob/master/LICENSE
pyhanko-certvalidator	https://github.com/MatthiasValvekens/certvalidator	https://github.com/MatthiasValvekens/certvalidator/blob/master/LICENSE
PyJWT	https://github.com/jpadilla/pyjwt	https://github.com/jpadilla/pyjwt/blob/master/LICENSE
pymbar	https://pymbar.org	https://github.com/choderalab/pymbar/blob/master/LICENSE
pynvml	https://github.com/gpuopenanalytics/pynvml	https://github.com/gpuopenanalytics/pynvml/blob/master/LICENSE.txt

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Name of Project	Website	License URL
pyOpenSSL	https://pyopenssl.org/	https://github.com/pyca/pyopenssl/blob/main/LICENSE
pyparsing	https://pyparsing-docs.readthedocs.io/en/latest/	https://github.com/pyparsing/pyparsing/blob/master/LICENSE
PyPDF3	https://github.com/sfneal/PyPDF3	https://github.com/sfneal/PyPDF3/blob/master/LICENSE
pyrsistent	http://github.com/tobgu/pyrsistent/	https://github.com/tobgu/pyrsistent/blob/master/LICENSE.mit
pysam	https://github.com/pysam-developers/pysam	https://github.com/pysam-developers/pysam/blob/master/COPYING
PySocks	https://github.com/Anorov/PySocks	https://github.com/Anorov/PySocks/blob/master/LICENSE
pytables	https://www.pytables.org	https://github.com/PyTables/PyTables/blob/master/LICENSE.txt
python	https://www.python.org/	https://docs.python.org/3/license.html
python-bidi	https://github.com/MeirKriheli/python-bidi	https://github.com/MeirKriheli/python-bidi/blob/master/COPYING
python-constraint	https://github.com/python-constraint/python-constraint	https://github.com/python-constraint/python-constraint/blob/master/LICENSE
python-dateutil	https://dateutil.readthedocs.io	https://github.com/dateutil/dateutil/blob/master/LICENSE
python-json-logger	http://github.com/madzak/python-json-logger	https://github.com/madzak/python-json-logger/blob/master/LICENSE

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Name of Project	Website	License URL
python-pptx	https://github.com/scanny/python-pptx	https://github.com/scanny/python-pptx/blob/master/LICENSE
python-ldap	https://www.python-ldap.org/	https://github.com/python-ldap/python-ldap/blob/python-ldap-3.4.0/LICENCE
python3-saml	https://github.com/onelogin/python3-saml	https://github.com/onelogin/python3-saml/blob/master/LICENSE
python_abi	https://github.com/conda-forge/python_abi-feedstock	https://github.com/conda-forge/python_abi-feedstock/blob/main/LICENSE.txt
pytorch-lightning	https://github.com/Lightning-AI/pytorch-lightning	https://github.com/Lightning-AI/pytorch-lightning/blob/master/LICENSE
pytz	https://pythonhosted.org/pytz	https://git.launchpad.net/pytz/tree/LICENSE.txt
pytz-deprecation-shim	https://github.com/pganssle/pytz-deprecation-shim	https://github.com/pganssle/pytz-deprecation-shim/blob/master/LICENSE
PyWavelets	https://github.com/PyWavelets/pywt	https://github.com/PyWavelets/pywt/blob/master/LICENSE
PyYAML	https://pyyaml.org/	https://github.com/yaml/pyyaml/blob/master/LICENSE
pyyml	No longer available	No longer available
pyzmq	https://pyzmq.readthedocs.io/en/latest/	https://github.com/zeromq/pyzmq/blob/main/COPYING.BSD
qcelemental	https://github.com/MolSSI/QCElemental	https://github.com/MolSSI/QCElemental/blob/master/LICENSE

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Name of Project	Website	License URL
qcengine	https://github.com/MolSSI/QCEngine	https://github.com/MolSSI/QCEngine/blob/master/LICENSE
qrcode	https://github.com/lincolnloop/python-qrcode	https://github.com/lincolnloop/python-qrcode/blob/main/LICENSE
ramda	https://github.com/ramda/ramda	https://github.com/ramda/ramda/raw/master/LICENSE.txt
rapidjson	https://rapidjson.org/	https://github.com/Tencent/rapidjson/blob/master/license.txt
rdkit	https://www.rdkit.org	https://github.com/rdkit/rdkit/blob/master/license.txt
re2	https://github.com/google/re2	https://github.com/google/re2/blob/main/LICENSE
readme-renderer	https://github.com/pypa/readme_renderer	https://github.com/pypa/readme_renderer/blob/main/LICENSE
redis-py	https://github.com/andymccurdy/redis-py	https://github.com/redis/redis-py/blob/master/LICENSE
referencing	https://github.com/python-jsonschema/referencing	https://github.com/python-jsonschema/referencing
regex	https://github.com/mrabarnett/mrab-regex	https://github.com/mrabarnett/mrab-regex/blob/hg/LICENSE.txt
reportlab	https://www.reportlab.com	https://www.reportlab.com/dev/docs/faq/#1.3
reproc	https://github.com/DaanDeMeyer/reproc	https://github.com/DaanDeMeyer/reproc/blob/main/LICENSE
reproc-cpp	https://github.com/DaanDeMeyer/reproc	https://github.com/DaanDeMeyer/reproc/blob/main/LICENSE

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Name of Project	Website	License URL
requests	https://requests.readthedocs.io	https://github.com/psf/requests/blob/main/LICENSE
requests-oauthlib	https://github.com/requests/requests-oauthlib	https://github.com/requests/requests-oauthlib/blob/master/LICENSE
requests-toolbelt	https://toolbelt.readthedocs.org	https://github.com/requests/toolbelt/blob/master/LICENSE
resumable	https://github.com/stevvooe/resumable	https://github.com/stevvooe/resumable/blob/master/LICENSE
retrying	https://github.com/rholder/retrying	https://github.com/rholder/retrying/blob/master/LICENSE
rfc3339-validator	https://github.com/naimetti/rfc3339-validator	https://github.com/naimetti/rfc3339-validator/blob/master/LICENSE
rfc3339_validator	https://github.com/naimetti/rfc3339-validator	https://github.com/naimetti/rfc3339-validator?tab=MIT-1-ov-file#readme
rfc3986	https://rfc3986.readthedocs.io/en/latest/	https://github.com/python-hyper/rfc3986/blob/main/LICENSE
rfc3986-validator	https://github.com/naimetti/rfc3986-validator	https://github.com/naimetti/rfc3986-validator/blob/master/LICENSE
rfc3987-syntax	https://github.com/willynilly/rfc3987-syntax	https://github.com/willynilly/rfc3987-syntax?tab=MIT-1-ov-file#readme
rich	https://github.com/Textualize/rich	https://github.com/Textualize/rich/blob/master/LICENSE

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Name of Project	Website	License URL
rich-argparse	https://github.com/hamdanal/rich-argparse	https://github.com/hamdanal/rich-argparse/blob/main/LICENSE
rlPyCairo	https://pypi.org/project/rlPyCairo/	https://hg.reportlab.com/hg-public/rlPyCairo/file/tip/rlPyCairo/LICENSE.txt
RocksDict	https://github.com/rocksdict/RocksDict	https://github.com/rocksdict/RocksDict?tab=MIT-1-ov-file#readme
roman-numerals	https://github.com/AA-Turner/roman-numerals	https://github.com/AA-Turner/roman-numerals?tab=License-1-ov-file#readme
roman-numerals-py	https://github.com/AA-Turner/roman-numerals	https://github.com/AA-Turner/roman-numerals?tab=License-1-ov-file#readme
rotary-embedding-torch	https://github.com/lucidrains/rotary-embedding-tor	https://github.com/lucidrains/rotary-embedding-tor blob/main/LICENSE
rpds-py	https://github.com/crate-py/rpds	https://github.com/crate-py/rpds
rpmpack	https://github.com/google/rpmpack	https://github.com/google/rpmpack/blob/master/LICENSE
rsa	https://stuvel.eu/rsa	https://github.com/sybrenstuvel/python-rsa/blob/main/LICENSE
ruamel-yaml	https://sourceforge.net/p/ruamel-yaml/code/ci/default/tree/	https://sourceforge.net/p/ruamel-yaml/code/ci/default/tree/LICENSE
ruamel.yaml.clib	https://sourceforge.net/p/ruamel-yaml-clib/code/ci/default/tree/	https://sourceforge.net/p/ruamel-yaml-clib/code/ci/default/tree/LICENSE

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Name of Project	Website	License URL
s3transfer	https://github.com/boto/s3transfer	https://github.com/boto/s3transfer/blob/develop/LICENSE.txt
sacrebleu	https://github.com/mjpost/sacrebleu	https://github.com/mjpost/sacrebleu/blob/master/LICENSE.txt
sapiens	https://github.com/Merck/Sapiens	https://github.com/Merck/Sapiens/blob/main/LICENSE
sasl	https://mellium.im/sasl	https://github.com/mellium/sasl/blob/main/LICENSE
scikit-gstat	https://mmaelicke.github.io/scikit-gstat/	https://github.com/mmaelicke/scikit-gstat/blob/main/LICENSE
scikit-image	https://scikit-image.org	https://scikit-image.org/docs/dev/license.html
scikit-learn	https://scikit-learn.org/stable/	https://github.com/scikit-learn/scikit-learn/blob/main/COPYING
scikit-learn-extra	https://github.com/scikit-learn-contrib/scikit-learn-extra	https://github.com/scikit-learn-contrib/scikit-learn-extra/blob/main/LICENSE
scikit-network	https://github.com/sknetwork-team/scikit-network	https://github.com/sknetwork-team/scikit-network?tab=License-1-ov-file#readme
scipy	https://scipy.org	https://github.com/scipy/scipy/blob/main/LICENSE.txt
seaborn	https://seaborn.pydata.org	https://github.com/mwaskom/seaborn/blob/master/LICENSE
seaborn-base	https://seaborn.pydata.org	https://github.com/mwaskom/seaborn/blob/master/LICENSE

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Name of Project	Website	License URL
semver	https://github.com/Masterminds/semver/v3	https://github.com/Masterminds/semver/blob/v3.0.3/LICENSE.txt
Send2Trash	https://github.com/arsenetar/send2trash	https://github.com/arsenetar/send2trash/blob/master/LICENSE
sentry-sdk	https://github.com/getsentry/sentry-python	https://github.com/getsentry/sentry-python/blob/master/LICENSE
setproctitle	https://github.com/dvarrazzo/py-setproctitle	https://github.com/dvarrazzo/py-setproctitle/blob/master/LICENSE
setuptools	https://github.com/pypa/setuptools	https://github.com/pypa/setuptools/blob/main/LICENSE
setuptools-scm	https://github.com/pypa/setuptools_scm/	https://github.com/pypa/setuptools_scm/blob/main/LICENSE
sh	https://github.com/amoffat/sh	https://github.com/amoffat/sh/blob/develop/LICENSE.txt
shellingham	https://github.com/sarugaku/shellingham	https://github.com/sarugaku/shellingham/blob/master/LICENSE
simdjson	https://github.com/simdjson/simdjson/tree/master	https://github.com/simdjson/simdjson/blob/master/LICENSE
simint	https://www.bennyp.org/research/simint/	https://github.com/simint-chem/simint-generator/blob/master/LICENSE
simplejson	https://github.com/simplejson/simplejson	https://github.com/simplejson/simplejson/blob/master/LICENSE.txt
six	https://github.com/benjaminp/six	https://github.com/benjaminp/six/blob/master/LICENSE

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Name of Project	Website	License URL
smirnoff99frosst	https://github.com/openforcefield/smirnoff99frosst	https://github.com/openforcefield/smirnoff99Frosst/blob/master/LICENSE
smmap	https://github.com/gitpython-developers/smmap	https://github.com/gitpython-developers/smmap/blob/master/LICENSE
snappy	https://github.com/google/snappy	https://github.com/google/snappy/blob/main/COPYING
sniffio	https://github.com/python-trio/sniffio	https://github.com/python-trio/sniffio/blob/master/LICENSE.MIT
snowballstemmer	https://github.com/snowballstem/snowball	https://github.com/snowballstem/snowball/blob/master/COPYING
soupsieve	https://github.com/facelessuser/soupsieve	https://github.com/facelessuser/soupsieve/blob/main/LICENSE.md
spdlog	https://github.com/gabime/spdlog	https://github.com/gabime/spdlog?tab=License-1-ov-file#readme
spglib	https://spglib.readthedocs.io/	https://github.com/spglib/spglib/blob/develop/COPYING
sphinx	https://github.com/sphinx-doc/sphinx	https://github.com/sphinx-doc/sphinx/blob/5.x/LICENSE
sphinxcontrib-applehelp	https://github.com/sphinx-doc/sphinxcontrib-applehe	https://github.com/sphinx-doc/sphinxcontrib-applehe blob/master/LICENSE
sphinxcontrib-devhelp	https://github.com/sphinx-doc/sphinxcontrib-devhelp	https://github.com/sphinx-doc/sphinxcontrib-devhelp blob/master/LICENSE
sphinxcontrib-htmlhelp	https://github.com/sphinx-doc/sphinxcontrib-htmlhel	https://github.com/sphinx-doc/sphinxcontrib-htmlhel blob/master/LICENSE

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Name of Project	Website	License URL
sphinxcontrib-jsmath	https://github.com/sphinx-doc/sphinxcontrib-jsmath	https://github.com/sphinx-doc/sphinxcontrib-jsmath/blob/master/LICENSE
sphinxcontrib-qthelp	https://github.com/sphinx-doc/sphinxcontrib-qthelp	https://github.com/sphinx-doc/sphinxcontrib-qthelp/blob/master/LICENSE
sphinxcontrib-serializinghtml	https://github.com/sphinx-doc/sphinxcontrib-serializ	https://github.com/sphinx-doc/sphinxcontrib-serializ blob/master/LICENSE
SQLAlchemy	https://www.sqlalchemy.org	https://docs.sqlalchemy.org/en/14/copyright.html
SQLAlchemy	https://www.sqlalchemy.org/	https://github.com/sqlalchemy/sqlalchemy?tab=MIT-1-ov-file#readme
sqlite	https://sqlite.org/index.html	https://sqlite.org/copyright.html
sqlparse	https://github.com/andialbrecht/sqlparse	https://github.com/andialbrecht/sqlparse/blob/master/LICENSE
stack-data	http://github.com/alexmojaki/stack_data	https://github.com/alexmojaki/stack_data/blob/master/LICENSE.txt
stack_data	http://github.com/alexmojaki/stack_data	https://github.com/alexmojaki/stack_data?tab=MIT-1-ov-file#readme
starfile	https://github.com/alisterburt/starfile	https://github.com/teamtomo/starfile/blob/main/LICENSE
statsmodels	https://github.com/statsmodels/statsmodels	https://github.com/statsmodels/statsmodels/blob/main/LICENSE.txt
structlog	https://www.structlog.org/	https://github.com/hynek/structlog/blob/main/LICENSE

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Name of Project	Website	License URL
streamlit	https://github.com/streamlit/streamlit	https://github.com/streamlit/streamlit/blob/develop/LICENSE
svglib	https://github.com/deeplook/svglib	https://github.com/deeplook/svglib/blob/master/LICENSE.txt
sympy	https://sympy.org	https://github.com/sympy/sympy/blob/master/LICENSE
tables	https://www.pytables.org/	https://github.com/PyTables/PyTables/blob/master/LICENSE.txt
tabulate	https://github.com/astanin/python-tabulate	https://github.com/astanin/python-tabulate/blob/master/LICENSE
tbb	https://github.com/oneapi-src/oneTBB	https://github.com/oneapi-src/oneTBB/blob/master/LICENSE.txt
tenacity	https://github.com/jd/tenacity	https://github.com/jd/tenacity/blob/master/LICENSE
tensorboard	https://github.com/tensorflow/tensorboard	https://github.com/tensorflow/tensorboard/blob/master/LICENSE
tensorboard-data-server	https://github.com/tensorflow/tensorboard	https://github.com/tensorflow/tensorboard/blob/master/LICENSE
tensorboard-plugin-wit	https://github.com/pair-code/what-if-tool	https://github.com/PAIR-code/what-if-tool/blob/master/LICENSE
tensorboardX	https://github.com/lanpa/tensorboardX	https://github.com/lanpa/tensorboardX/blob/master/LICENSE
tensorflow	https://github.com/tensorflow/tensorflow	https://github.com/tensorflow/tensorflow/blob/master/LICENSE

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Name of Project	Website	License URL
tensorflow-estimator	https://github.com/tensorflow/estimator	https://github.com/tensorflow/estimator/blob/master/LICENSE
tensorflow-io-gcs-filesystem	https://github.com/tensorflow/io	https://github.com/tensorflow/io/blob/master/LICENSE
tensorflow-probability	https://github.com/tensorflow/probability	https://github.com/tensorflow/probability/blob/main/LICENSE
termcolor	https://github.com/hugovk/termcolor	https://github.com/hugovk/termcolor/blob/main/COPYING.txt
terminado	https://github.com/jupyter/terminado	https://github.com/jupyter/terminado/blob/main/LICENSE
testpath	https://github.com/jupyter/testpath	https://github.com/jupyter/testpath/blob/master/LICENSE
textangular	https://github.com/fraywing/textAngular	https://github.com/fraywing/textAngular
texttable	https://github.com/foutaise/texttable/	https://github.com/foutaise/texttable/?tab=MIT-1-ov-file#readme
tf_keras	https://github.com/keras-team/keras-io	https://github.com/keras-team/keras-io/blob/master/LICENSE
tf_keras	https://github.com/keras-team/keras-io	https://github.com/keras-team/keras-io/blob/master/LICENSE
threadpoolctl	https://github.com/joblib/threadpoolctl	https://github.com/joblib/threadpoolctl/blob/master/LICENSE
three	https://github.com/mrdoob/three.js	https://github.com/mrdoob/three.js/raw/master/LICENSE

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Name of Project	Website	License URL
tifffile	https://github.com/cgohlke/tifffile/	https://github.com/cgohlke/tifffile/blob/master/LICENSE
tinycss2	https://github.com/Kozea/tinycss2/	https://github.com/Kozea/tinycss2/blob/master/LICENSE
tinyxml2	https://github.com/leethomason/tinyxml2	https://github.com/leethomason/tinyxml2/blob/master/LICENSE.txt
tk	https://www.tcl.tk/	https://www.tcl.tk/software/tcltk/license.html
toml	https://github.com/toml-lang/toml	https://github.com/toml-lang/toml/blob/main/LICENSE
tomli	https://github.com/hukkin/tomli	https://github.com/hukkin/tomli/blob/master/LICENSE
toolz	https://github.com/pytoolz/toolz	https://github.com/pytoolz/toolz/blob/master/LICENSE.txt
torch	https://pytorch.org/	https://pypi.org/project/torch/#license
torch-geometric	https://pyg.org/	https://github.com/pyg-team/pytorch_geometric?tab=MIT-1-ov-file#readme
torcheval	https://github.com/pytorch/torcheval	https://github.com/pytorch/torcheval?tab=License-1-ov-file#readme
torchmetrics	https://github.com/Lightning-AI/torchmetrics	https://github.com/Lightning-AI/torchmetrics?tab=Apache-2.0-1-ov-file#readme
tornado	https://www.tornadoweb.org	https://github.com/tornadoweb/tornado/blob/master/LICENSE

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Name of Project	Website	License URL		
tqdm	https://github.com/tqdm/tqdm	https://github.com/tqdm/tqdm/blob/master/LICENCE		
tracy	https://github.com/gear-genomics/tracy	https://github.com/gear-genomics/tracy/blob/main/LICENSE		
traitlets	https://github.com/ipython/traitlets	https://github.com/ipython/traitlets/blob/main/COPYING.md		
triton	https://github.com/openai/triton/	https://github.com/openai/triton/blob/main/LICENSE		
truststore	https://github.com/sethmlarson/trus	https://github.com/sethmlarson/truststore/blob/main/LICENSE		
truststore	https://github.com/sethmlarson/truststore	https://github.com/sethmlarson/truststore/blob/main/LICENSEtruststore	https://github.com/sethmlarson/truststore	https://github.com/sethmlarson/truststore/blob/main/LICENSE
ts-jest	https://github.com/kulshekhar/ts-jest	https://github.com/kulshekhar/ts-jest/raw/master/LICENSE.md		
ts-loader	https://github.com/TypeStrong/ts-loader	https://github.com/TypeStrong/ts-loader/raw/master/LICENSE		
twine	https://github.com/pypa/twine	https://github.com/pypa/twine/blob/main/LICENSE		
twinj uuid	https://github.com/twinj/uuid	https://github.com/twinj/uuid/blob/master/LICENSE		
types	https://github.com/babel/babel	https://github.com/babel/babel/raw/master/LICENSE		
types-python-dateutil	https://github.com/python/typeshed	https://github.com/python/typeshed?tab=License-1-ov-file#readme		
types-requests	https://pypi.org/project/types-requests/	https://github.com/python/typeshed/blob/main/LICENSE		

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Name of Project	Website	License URL
typescript	https://github.com/Microsoft/TypeScript	https://github.com/Microsoft/TypeScript/raw/master/LICENSE.txt
typing-inspection	https://github.com/pydantic/typing-inspection	https://github.com/pydantic/typing-inspection?tab=MIT-1-ov-file#readme
typing-utils	https://github.com/bojiang/typing_utils	https://github.com/bojiang/typing_utils?tab=Apache-2.0-1-ov-file#readme
typing_extensions	https://github.com/python/typing	https://github.com/python/typing/blob/master/LICENSE
typing_utils	https://github.com/bojiang/typing_utils	https://github.com/bojiang/typing_utils?tab=Apache-2.0-1-ov-file#readme
tzdata	https://github.com/python/tzdata	https://github.com/python/tzdata/blob/master/LICENSE
tzlocal	https://github.com/regebro/tzlocal	https://github.com/regebro/tzlocal/blob/master/LICENSE.txt
umf	https://github.com/oneapi-src/unified-memory-fram	https://github.com/oneapi-src/unified-memory-fram tab=License-1-ov-file#readme
umi-tools	https://github.com/CGATOxford/UMI-tools	https://github.com/CGATOxford/UMI-tools/blob/master/LICENSE
unicodedata2	https://github.com/fonttools/unicodedata2	https://github.com/fonttools/unicodedata2/blob/master/LICENSE
uri-template	https://gitlab.linss.com/open-source/python/uri-template	https://gitlab.linss.com/open-source/python/uri-template/-/blob/main/LICENSE
uritools	https://github.com/tkem/uritools/	https://github.com/tkem/uritools/blob/master/LICENSE

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Name of Project	Website	License URL		
urllib3	https://urllib3.readthedocs.io/	https://github.com/urllib3/urllib3/blob/main/LICENSE.txt		
vine	https://github.com/celery/vine	https://github.com/celery/vine/blob/master/LICENSE		
vue	https://github.com/vuejs/vue	https://github.com/vuejs/vue/raw/master/LICENSE		
wadler_lindig	https://github.com/patrick-kidger/wadler_lindig	https://github.com/patrick-kidger/wadler_lindig?tab=Apache-2.0-1-ov-file#readme		
wadler_lindig	https://github.com/patrick-kidger/wadler_lindig	https://github.com/patrick-kidger/wadler_lindig?tab=Apache-2.0-1-ov-file#readmewcwidth	https://github.com/jquast/wcwidth	https://github.com/jquast/wcwidth/blob/master/LICENSE
wandb	https://github.com/wandb/wandb	https://github.com/wandb/wandb/blob/main/LICENSE		
webcolors	https://github.com/ubernostrum/webcolors	https://github.com/ubernostrum/webcolors?tab=BSD-3-Clause-1-ov-file#readme		
webencodings	https://github.com/gsnedders/python-webencodings	https://github.com/gsnedders/python-webencodings/blob/master/LICENSE		
websocket-client	https://github.com/websocket-client/websocket-client.git	https://github.com/websocket-client/websocket-client/blob/master/LICENSE		
Werkzeug	https://palletsprojects.com/p/werkzeug/	https://werkzeug.palletsprojects.com/en/2.1.x/license/		
westpa	http://github.com/westpa/westpa	https://github.com/westpa/westpa/blob/westpa2/LICENSE		
wheel	https://github.com/pypa/wheel	https://github.com/pypa/wheel/blob/main/LICENSE.txt		

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Table 1 – continued from previous page

Name of Project	Website	License URL
widgetsnbextension	https://github.com/jupyter-widgets/ipywidgets#readme	https://github.com/jupyter-widgets/ipywidgets/blob/main/LICENSE
wrapt	https://github.com/GrahamDumpleton/wrapt	https://github.com/GrahamDumpleton/wrapt/blob/develop/LICENSE
wsutil	https://github.com/yhat/wsutil	https://github.com/yhat/wsutil/blob/master/LICENSE
x/lint	https://golang.org/x/lint	https://github.com/golang/lint/blob/master/LICENSE
x/mod	https://golang.org/x/mod/semver	https://cs.opensource.google/go/x/mod/+/master:LICENSE
x/net	https://golang.org/x/net	https://cs.opensource.google/go/x/net/+/master:LICENSE
x/oauth2	https://golang.org/x/oauth2	https://cs.opensource.google/go/x/oauth2/+/master:LICENSE
x/sys	https://golang.org/x/sys	https://cs.opensource.google/go/x/sys/+/master:LICENSE
x/text	https://golang.org/x/text	https://cs.opensource.google/go/x/text/+/master:LICENSE
x/tools	https://golang.org/x/tools	https://cs.opensource.google/go/x/tools/+/master:LICENSE
x/xerrors	https://golang.org/x/xerrors	https://cs.opensource.google/go/x/xerrors/+/master:LICENSE
xgboost	https://github.com/dmlc/xgboost	https://github.com/dmlc/xgboost/blob/master/LICENSE
xhtml2pdf	http://github.com/xhtml2pdf/xhtml2pdf	https://github.com/xhtml2pdf/xhtml2pdf/blob/master/LICENSE.txt

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Table 1 – continued from previous page

Name of Project	Website	License URL
xlrd	https://github.com/python-excel/xlrd	https://github.com/python-excel/xlrd/blob/master/LICENSE
xlsxwriter	https://github.com/jmcnamara/XlsxWriter	https://github.com/jmcnamara/XlsxWriter/blob/main/LICENSE.txt
xmlsec	https://github.com/mehcode/python-xmlsec	https://github.com/mehcode/python-xmlsec/blob/master/LICENSE
xmltodict	https://github.com/martinblech/xmltodict	https://github.com/martinblech/xmltodict/blob/master/LICENSE
xorg-kbproto	https://gitlab.freedesktop.org/xorg/proto/kbproto	https://gitlab.freedesktop.org/xorg/proto/kbproto/-/blob/master/COPYING
xorg-libice	https://gitlab.freedesktop.org/xorg/lib/libice	https://gitlab.freedesktop.org/xorg/lib/libice/-/blob/master/COPYING
xorg-libsm	https://gitlab.freedesktop.org/xorg/lib/libsm	https://gitlab.freedesktop.org/xorg/lib/libsm/-/blob/master/COPYING
xorg-libx11	https://gitlab.freedesktop.org/xorg/lib/libx11	https://gitlab.freedesktop.org/xorg/lib/libx11/-/blob/master/COPYING
xorg-libxau	https://gitlab.freedesktop.org/xorg/lib/libxau	https://gitlab.freedesktop.org/xorg/lib/libxau/-/blob/master/COPYING
xorg-libxdmcp	https://gitlab.freedesktop.org/xorg/lib/libxdmcp	https://gitlab.freedesktop.org/xorg/lib/libxdmcp/-/blob/master/COPYING

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Table 1 – continued from previous page

Name of Project	Website	License URL
xorg-libxext	https://gitlab.freedesktop.org/xorg/lib/libxext	https://gitlab.freedesktop.org/xorg/lib/libxext/-/blob/master/COPYING
xorg-libxrender	https://gitlab.freedesktop.org/xorg/lib/libxrender	https://gitlab.freedesktop.org/xorg/lib/libxrender/-/blob/master/COPYING
xorg-libxt	https://gitlab.freedesktop.org/xorg/lib/libxt	https://gitlab.freedesktop.org/xorg/lib/libxt/-/blob/master/COPYING
xorg-renderproto	https://gitlab.freedesktop.org/xorg/proto/renderproto	https://gitlab.freedesktop.org/xorg/proto/renderproto/-/blob/master/COPYING
xorg-xextproto	https://gitlab.freedesktop.org/xorg/proto/xextproto	https://gitlab.freedesktop.org/xorg/proto/xextproto/-/blob/master/COPYING
xorg-xproto	https://gitlab.freedesktop.org/xorg/proto/xproto	https://gitlab.freedesktop.org/xorg/proto/xproto/-/blob/master/COPYING
xxhash	https://github.com/cespare/xxhash/v2	https://github.com/cespare/xxhash/blob/main/LICENSE.txt
xz	https://github.com/ulikunitz/xz	https://github.com/ulikunitz/xz/blob/master/LICENSE
yaml	https://pyyaml.org/	https://github.com/yaml/pyyaml/blob/master/LICENSE
yaml-cpp	https://github.com/jbeder/yaml-cpp	https://github.com/jbeder/yaml-cpp/blob/master/LICENSE
yaml.v2	https://gopkg.in/yaml.v2	https://github.com/go-yaml/yaml/blob/v2.4.0/LICENSE
yaml.v3	https://gopkg.in/yaml.v3	https://github.com/go-yaml/yaml/blob/v3/LICENSE

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Table 1 – continued from previous page

Name of Project	Website	License URL
yarl	https://github.com/aio-libs/yarl/	https://github.com/aio-libs/yarl/blob/master/LICENSE
yaspin	https://github.com/pavdmyt/yaspin	https://github.com/pavdmyt/yaspin/blob/master/LICENSE
yfiles	https://www.yworks.com/products/yfiles	commercial license
yml	https://pypi.org/project/yml/	N/A
zap	https://go.uber.org/zap	https://github.com/uber-go/zap/blob/master/LICENSE.txt
zipp	https://github.com/jaraco/zipp	https://github.com/jaraco/zipp/blob/main/LICENSE
zlib	https://zlib.net/	https://zlib.net/zlib_license.html
zstandard	https://github.com/indygreg/python-zstandard	https://github.com/indygreg/python-zstandard/blob/main/LICENSE
zstd	https://facebook.github.io/zstd/	https://github.com/facebook/zstd/blob/dev/LICENSE
click-option-group	https://github.com/click-contrib/click-option-group	https://github.com/click-contrib/click-option-group/blob/master/LICENSE

9.1 GCC

On the Linux platform, The OpenEye toolkits are linked with the GCC libraries using an eligible compilation process under the terms of the GCC RUNTIME LIBRARY EXCEPTION (see below).

The OpenEye toolkits are NOT open source software and are NOT governed by GPL or other open source licenses. Your right to use the toolkits are governed by the OpenEye license which is binding to You.

For certain Linux distributions, GCC library components are included as object files. Your rights to use GCC library components (libstdc++, libgcc, and libgomp) included with these distributions are governed by the GPLv3 license as follows:

The components libstdc++, libgcc, and libgomp are part of GCC.

- GCC is free software: you can redistribute it and/or modify it under the terms of the GNU General Public License as published by the Free Software Foundation, either version 3 of the License, or (at your option) any later version.
- GCC is distributed in the hope that it will be useful, but WITHOUT ANY WARRANTY; without even the

implied warranty of MERCHANTABILITY or FITNESS FOR A PARTICULAR PURPOSE. See the GNU General Public License for more details.

You should have received a copy of the GNU General Public License along with GCC (see below). If not, see Licenses GNU Project .

Per GPLv3, section 6d, the source for GCC is available for download from the following location: GNU. The GCC library components included here are from version gcc-4.9.3 and are built using the standard instructions at Installing GCC.

9.1.1 GCC RUNTIME LIBRARY EXCEPTION

```
Version 3.1, 31 March 2009

Copyright © 2009 Free Software Foundation, Inc. http://fsf.org/

Everyone is permitted to copy and distribute verbatim copies of this license document,␣
↪but changing it is not allowed.

This GCC Runtime Library Exception ("Exception") is an additional permission under␣
↪section 7 of the GNU General Public License,
version 3 ("GPLv3"). It applies to a given file (the "Runtime Library") that bears a␣
↪notice placed by the copyright holder
of the file stating that the file is governed by GPLv3 along with this Exception.

When you use GCC to compile a program, GCC may combine portions of certain GCC header␣
↪files and runtime libraries with
the compiled program. The purpose of this Exception is to allow compilation of non-GPL␣
↪(including proprietary) programs
to use, in this way, the header files and runtime libraries covered by this Exception.

0. Definitions.

A file is an "Independent Module" if it either requires the Runtime Library for␣
↪execution after a Compilation Process,
or makes use of an interface provided by the Runtime Library, but is not otherwise based␣
↪on the Runtime Library.

"GCC" means a version of the GNU Compiler Collection, with or without modifications,␣
↪governed by version 3 (or a specified
later version) of the GNU General Public License (GPL) with the option of using any␣
↪subsequent versions published by the FSF.

"GPL-compatible Software" is software whose conditions of propagation, modification and␣
↪use would permit combination with
GCC in accord with the license of GCC.

"Target Code" refers to output from any compiler for a real or virtual target processor␣
↪architecture, in executable
form or suitable for input to an assembler, loader, linker and/or execution phase.␣
↪Notwithstanding that, Target Code
does not include data in any format that is used as a compiler intermediate␣
↪representation, or used for producing a
compiler intermediate representation.
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The "Compilation Process" transforms code entirely represented in non-intermediate␣
↪languages designed for human-written
code, and/or in Java Virtual Machine byte code, into Target Code. Thus, for example, use␣
↪of source code generators and
preprocessors need not be considered part of the Compilation Process, since the␣
↪Compilation Process can be understood
as starting with the output of the generators or preprocessors.

A Compilation Process is "Eligible" if it is done using GCC, alone or with other GPL-
↪compatible software, or if it is
done without using any work based on GCC. For example, using non-GPL-compatible Software␣
↪to optimize any GCC intermediate
representations would not qualify as an Eligible Compilation Process.

1. Grant of Additional Permission.

You have permission to propagate a work of Target Code formed by combining the Runtime␣
↪Library with Independent Modules,
even if such propagation would otherwise violate the terms of GPLv3, provided that all␣
↪Target Code was generated by
Eligible Compilation Processes. You may then convey such a combination under terms of␣
↪your choice, consistent with the
licensing of the Independent Modules.

2. No Weakening of GCC Copyleft.

The availability of this Exception does not imply any general presumption that third-
↪party software is unaffected by
the copyleft requirements of the license of GCC.
```

See also

- http://www.gnu.org/licenses/gcc-exception.html

9.1.2 GNU GENERAL PUBLIC LICENSE

```
                    GNU GENERAL PUBLIC LICENSE
                       Version 3, 29 June 2007

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 Everyone is permitted to copy and distribute verbatim copies
 of this license document, but changing it is not allowed.

                            Preamble

 The GNU General Public License is a free, copyleft license for
 software and other kinds of works.

   The licenses for most software and other practical works are designed
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to take away your freedom to share and change the works.  By contrast,
the GNU General Public License is intended to guarantee your freedom to
share and change all versions of a program--to make sure it remains free
software for all its users.  We, the Free Software Foundation, use the
GNU General Public License for most of our software; it applies also to
any other work released this way by its authors.  You can apply it to
your programs, too.

  When we speak of free software, we are referring to freedom, not
price.  Our General Public Licenses are designed to make sure that you
have the freedom to distribute copies of free software (and charge for
them if you wish), that you receive source code or can get it if you
want it, that you can change the software or use pieces of it in new
free programs, and that you know you can do these things.

  To protect your rights, we need to prevent others from denying you
these rights or asking you to surrender the rights.  Therefore, you have
certain responsibilities if you distribute copies of the software, or if
you modify it: responsibilities to respect the freedom of others.

  For example, if you distribute copies of such a program, whether
gratis or for a fee, you must pass on to the recipients the same
freedoms that you received.  You must make sure that they, too, receive
or can get the source code.  And you must show them these terms so they
know their rights.

  Developers that use the GNU GPL protect your rights with two steps:
(1) assert copyright on the software, and (2) offer you this License
giving you legal permission to copy, distribute and/or modify it.

  For the developers' and authors' protection, the GPL clearly explains
that there is no warranty for this free software.  For both users' and
authors' sake, the GPL requires that modified versions be marked as
changed, so that their problems will not be attributed erroneously to
authors of previous versions.

  Some devices are designed to deny users access to install or run
modified versions of the software inside them, although the manufacturer
can do so.  This is fundamentally incompatible with the aim of
protecting users' freedom to change the software.  The systematic
pattern of such abuse occurs in the area of products for individuals to
use, which is precisely where it is most unacceptable.  Therefore, we
have designed this version of the GPL to prohibit the practice for those
products.  If such problems arise substantially in other domains, we
stand ready to extend this provision to those domains in future versions
of the GPL, as needed to protect the freedom of users.

  Finally, every program is threatened constantly by software patents.
States should not allow patents to restrict development and use of
software on general-purpose computers, but in those that do, we wish to
avoid the special danger that patents applied to a free program could
make it effectively proprietary.  To prevent this, the GPL assures that
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patents cannot be used to render the program non-free.

  The precise terms and conditions for copying, distribution and
modification follow.

                    TERMS AND CONDITIONS

  0. Definitions.

  "This License" refers to version 3 of the GNU General Public License.

  "Copyright" also means copyright-like laws that apply to other kinds of
works, such as semiconductor masks.

  "The Program" refers to any copyrightable work licensed under this
License.  Each licensee is addressed as "you".  "Licensees" and
"recipients" may be individuals or organizations.

  To "modify" a work means to copy from or adapt all or part of the work
in a fashion requiring copyright permission, other than the making of an
exact copy.  The resulting work is called a "modified version" of the
earlier work or a work "based on" the earlier work.

  A "covered work" means either the unmodified Program or a work based
on the Program.

  To "propagate" a work means to do anything with it that, without
permission, would make you directly or secondarily liable for
infringement under applicable copyright law, except executing it on a
computer or modifying a private copy.  Propagation includes copying,
distribution (with or without modification), making available to the
public, and in some countries other activities as well.

  To "convey" a work means any kind of propagation that enables other
parties to make or receive copies.  Mere interaction with a user through
a computer network, with no transfer of a copy, is not conveying.

  An interactive user interface displays "Appropriate Legal Notices"
to the extent that it includes a convenient and prominently visible
feature that (1) displays an appropriate copyright notice, and (2)
tells the user that there is no warranty for the work (except to the
extent that warranties are provided), that licensees may convey the
work under this License, and how to view a copy of this License.  If
the interface presents a list of user commands or options, such as a
menu, a prominent item in the list meets this criterion.

  1. Source Code.

  The "source code" for a work means the preferred form of the work
for making modifications to it.  "Object code" means any non-source
form of a work.
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  A "Standard Interface" means an interface that either is an official
standard defined by a recognized standards body, or, in the case of
interfaces specified for a particular programming language, one that
is widely used among developers working in that language.

  The "System Libraries" of an executable work include anything, other
than the work as a whole, that (a) is included in the normal form of
packaging a Major Component, but which is not part of that Major
Component, and (b) serves only to enable use of the work with that
Major Component, or to implement a Standard Interface for which an
implementation is available to the public in source code form.  A
"Major Component", in this context, means a major essential component
(kernel, window system, and so on) of the specific operating system
(if any) on which the executable work runs, or a compiler used to
produce the work, or an object code interpreter used to run it.

  The "Corresponding Source" for a work in object code form means all
the source code needed to generate, install, and (for an executable
work) run the object code and to modify the work, including scripts to
control those activities.  However, it does not include the work's
System Libraries, or general-purpose tools or generally available free
programs which are used unmodified in performing those activities but
which are not part of the work.  For example, Corresponding Source
includes interface definition files associated with source files for
the work, and the source code for shared libraries and dynamically
linked subprograms that the work is specifically designed to require,
such as by intimate data communication or control flow between those
subprograms and other parts of the work.

  The Corresponding Source need not include anything that users
can regenerate automatically from other parts of the Corresponding
Source.

  The Corresponding Source for a work in source code form is that
same work.

  2. Basic Permissions.

  All rights granted under this License are granted for the term of
copyright on the Program, and are irrevocable provided the stated
conditions are met.  This License explicitly affirms your unlimited
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  You may make, run and propagate covered works that you do not
convey, without conditions so long as your license otherwise remains
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of having them make modifications exclusively for you, or provide you
with facilities for running those works, provided that you comply with
the terms of this License in conveying all material for which you do
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not control copyright.  Those thus making or running the covered works
for you must do so exclusively on your behalf, under your direction
and control, on terms that prohibit them from making any copies of
your copyrighted material outside their relationship with you.

  Conveying under any other circumstances is permitted solely under
the conditions stated below.  Sublicensing is not allowed; section 10
makes it unnecessary.

  3. Protecting Users' Legal Rights From Anti-Circumvention Law.

  No covered work shall be deemed part of an effective technological
measure under any applicable law fulfilling obligations under article
11 of the WIPO copyright treaty adopted on 20 December 1996, or
similar laws prohibiting or restricting circumvention of such
measures.

  When you convey a covered work, you waive any legal power to forbid
circumvention of technological measures to the extent such circumvention
is effected by exercising rights under this License with respect to
the covered work, and you disclaim any intention to limit operation or
modification of the work as a means of enforcing, against the work's
users, your or third parties' legal rights to forbid circumvention of
technological measures.

  4. Conveying Verbatim Copies.

  You may convey verbatim copies of the Program's source code as you
receive it, in any medium, provided that you conspicuously and
appropriately publish on each copy an appropriate copyright notice;
keep intact all notices stating that this License and any
non-permissive terms added in accord with section 7 apply to the code;
keep intact all notices of the absence of any warranty; and give all
recipients a copy of this License along with the Program.


  You may charge any price or no price for each copy that you convey,
and you may offer support or warranty protection for a fee.

  5. Conveying Modified Source Versions.

  You may convey a work based on the Program, or the modifications to
produce it from the Program, in the form of source code under the
terms of section 4, provided that you also meet all of these conditions:

   a) The work must carry prominent notices stating that you modified
   it, and giving a relevant date.

   b) The work must carry prominent notices stating that it is
   released under this License and any conditions added under section
   7.  This requirement modifies the requirement in section 4 to
   "keep intact all notices".
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    c) You must license the entire work, as a whole, under this
    License to anyone who comes into possession of a copy.  This
    License will therefore apply, along with any applicable section 7
    additional terms, to the whole of the work, and all its parts,
    regardless of how they are packaged.  This License gives no
    permission to license the work in any other way, but it does not
    invalidate such permission if you have separately received it.

    d) If the work has interactive user interfaces, each must display
    Appropriate Legal Notices; however, if the Program has interactive
    interfaces that do not display Appropriate Legal Notices, your
    work need not make them do so.

  A compilation of a covered work with other separate and independent
works, which are not by their nature extensions of the covered work,
and which are not combined with it such as to form a larger program,
in or on a volume of a storage or distribution medium, is called an
"aggregate" if the compilation and its resulting copyright are not
used to limit the access or legal rights of the compilation's users
beyond what the individual works permit.  Inclusion of a covered work
in an aggregate does not cause this License to apply to the other
parts of the aggregate.

  6. Conveying Non-Source Forms.

  You may convey a covered work in object code form under the terms
of sections 4 and 5, provided that you also convey the
machine-readable Corresponding Source under the terms of this License,
in one of these ways:

  a) Convey the object code in, or embodied in, a physical product
  (including a physical distribution medium), accompanied by the
  Corresponding Source fixed on a durable physical medium
  customarily used for software interchange.

  b) Convey the object code in, or embodied in, a physical product
  (including a physical distribution medium), accompanied by a
  written offer, valid for at least three years and valid for as
  long as you offer spare parts or customer support for that product
  model, to give anyone who possesses the object code either (1) a
  copy of the Corresponding Source for all the software in the
  product that is covered by this License, on a durable physical
  medium customarily used for software interchange, for a price no
  more than your reasonable cost of physically performing this
  conveying of source, or (2) access to copy the
  Corresponding Source from a network server at no charge.

  c) Convey individual copies of the object code with a copy of the
  written offer to provide the Corresponding Source.  This
  alternative is allowed only occasionally and noncommercially, and
  only if you received the object code with such an offer, in accord
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   with subsection 6b.

   d) Convey the object code by offering access from a designated
   place (gratis or for a charge), and offer equivalent access to the
   Corresponding Source in the same way through the same place at no
   further charge.  You need not require recipients to copy the
   Corresponding Source along with the object code.  If the place to
   copy the object code is a network server, the Corresponding Source
   may be on a different server (operated by you or a third party)
   that supports equivalent copying facilities, provided you maintain
   clear directions next to the object code saying where to find the
   Corresponding Source.  Regardless of what server hosts the
   Corresponding Source, you remain obligated to ensure that it is
   available for as long as needed to satisfy these requirements.

   e) Convey the object code using peer-to-peer transmission, provided
   you inform other peers where the object code and Corresponding
   Source of the work are being offered to the general public at no
   charge under subsection 6d.

  A separable portion of the object code, whose source code is excluded
from the Corresponding Source as a System Library, need not be
included in conveying the object code work.

  A "User Product" is either (1) a "consumer product", which means any
tangible personal property which is normally used for personal, family,
or household purposes, or (2) anything designed or sold for incorporation
into a dwelling.  In determining whether a product is a consumer product,
doubtful cases shall be resolved in favor of coverage.  For a particular
product received by a particular user, "normally used" refers to a
typical or common use of that class of product, regardless of the status
of the particular user or of the way in which the particular user
actually uses, or expects or is expected to use, the product.  A product
is a consumer product regardless of whether the product has substantial
commercial, industrial or non-consumer uses, unless such uses represent
the only significant mode of use of the product.

  "Installation Information" for a User Product means any methods,
procedures, authorization keys, or other information required to install
and execute modified versions of a covered work in that User Product from
a modified version of its Corresponding Source.  The information must
suffice to ensure that the continued functioning of the modified object
code is in no case prevented or interfered with solely because
modification has been made.

  If you convey an object code work under this section in, or with, or
specifically for use in, a User Product, and the conveying occurs as
part of a transaction in which the right of possession and use of the
User Product is transferred to the recipient in perpetuity or for a
fixed term (regardless of how the transaction is characterized), the
Corresponding Source conveyed under this section must be accompanied
by the Installation Information.  But this requirement does not apply
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if neither you nor any third party retains the ability to install
modified object code on the User Product (for example, the work has
been installed in ROM).

  The requirement to provide Installation Information does not include a
requirement to continue to provide support service, warranty, or updates
for a work that has been modified or installed by the recipient, or for
the User Product in which it has been modified or installed.  Access to a
network may be denied when the modification itself materially and
adversely affects the operation of the network or violates the rules and
protocols for communication across the network.

  Corresponding Source conveyed, and Installation Information provided,
in accord with this section must be in a format that is publicly
documented (and with an implementation available to the public in
source code form), and must require no special password or key for
unpacking, reading or copying.

  7. Additional Terms.

  "Additional permissions" are terms that supplement the terms of this
License by making exceptions from one or more of its conditions.
Additional permissions that are applicable to the entire Program shall
be treated as though they were included in this License, to the extent
that they are valid under applicable law.  If additional permissions
apply only to part of the Program, that part may be used separately
under those permissions, but the entire Program remains governed by
this License without regard to the additional permissions.

  When you convey a copy of a covered work, you may at your option
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    author attributions in that material or in the Appropriate Legal
    Notices displayed by works containing it; or

    c) Prohibiting misrepresentation of the origin of that material, or
    requiring that modified versions of such material be marked in
    reasonable ways as different from the original version; or

    d) Limiting the use for publicity purposes of names of licensors or
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