

OpenEye
SCIENTIFIC

Lexichem TK – C#

Release 2026.1.0

Cadence Design Systems, Inc.

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CHAPTER

ONE

THEORY

1.1 Input Name Representation

The *oeiupac* library currently processes NULL (zero) terminated ASCII character strings; therefore Greek characters, symbols, fonts and superscripts must be transliterated into the printable subset of ASCII. When parsing compound names, the *oeiupac* library considers both spaces and tab characters as interchangeable, and any number of consecutive 'whitespace' characters are treated as a single space.

Currently, the name parsing is case insensitive, allowing arbitrary mixing of upper and lower case characters, *e.g.* initial letter capitalization.

Greek characters are understood in a number of different representations.

Character	Friendly Code	Decimal Code	Hex Code	Unicode	Addl1	Addl2	Addl3	Addl4
α	α	α	α	\U03B1	.alpha.	$a	${a}	alpha
β	β	β	β	\U03B2	.beta.	$b	${b}	beta
γ	γ	γ	γ	\U03B3	.gamma.	$g	${g}	gamma
δ	δ	δ	δ	\U03B4	.delta.	$d	${d}	delta
ϵ	ε	ε	ε	\U03B5	.epsilon.			epsilon
λ	λ	λ	λ	\U03BB	.lambda.	$l	${l}	lambda
+/-	&PLUSMN	&#177	&#x0B1	\U00B1				

Note: Addl[1-4] are additional identifiers.

For example, the strings '$a', '${a}', 'alpha', '.alpha.', 'α', 'α' and 'α' are all understood to represent the Greek character *alpha*, (α).

1.2 Output Name Representation

Unrecognized functional groups, linkers or ring systems are denoted in the generated name as the string **'BLAH'**. As much of the name as possible is generated resulting in compound names such as 'dichloroBLAHcarboxylic acid'. Generated compound names are entirely lower case, with no initial capitalization. Upper case characters are generated for locants and, as described above, for BLAH.

Names are generated using a set of markup tokens which can be further processed for output to the desired format.

> Greek characters are indicated with the dollar character followed by a single letter. In this formalism, '$a' represents the Greek character alpha, α, '$b' the Greek character beta, β, etc.
>
> Superscripts are indicated by surrounding the superscripted text with caret and curly braces. Hence '$l^{5}' represents the Greek character lambda followed by a superscript five, *i.e.* λ^5. Similarly, 'pentacyclo[4.2.0.0^{2,5}.0^{3,8}.0^{4,7}]octane' would be the von Baeyer system name for cubane.

Subscripts are are indicated by surrounding the superscripted text with underscore and curly braces. Hence 'C_{60} Fullerene' is a generated name for Buckminsterfullerene.

Italics, used for stereochemistry and locants, are indicated with a tilde and curly braces. An example is: '(2~{R})-butan-2-ol'.

The markup tokens are converted into appropriate markup for a particular use during the conversion of the raw name to the desired final character set.

Translation of names to alternate languages may result in characters outside of the default ASCII character set being used. In this case, the characters are encoded as escaped unicode, eg: **'uXXXX'**. The actual output characters are generated in the final character set conversion.

Multiple components in a disconnected molecule, apart from common salts and counter ions, are separated from each other by a semicolon followed by a space. Mixtures containing salts are written ordering the cations before the compound name, followed by anions, followed by any common neutral molecules (*e.g.* hydrate or hydrochloride).

1.2.1 Enhanced Stereochemistry

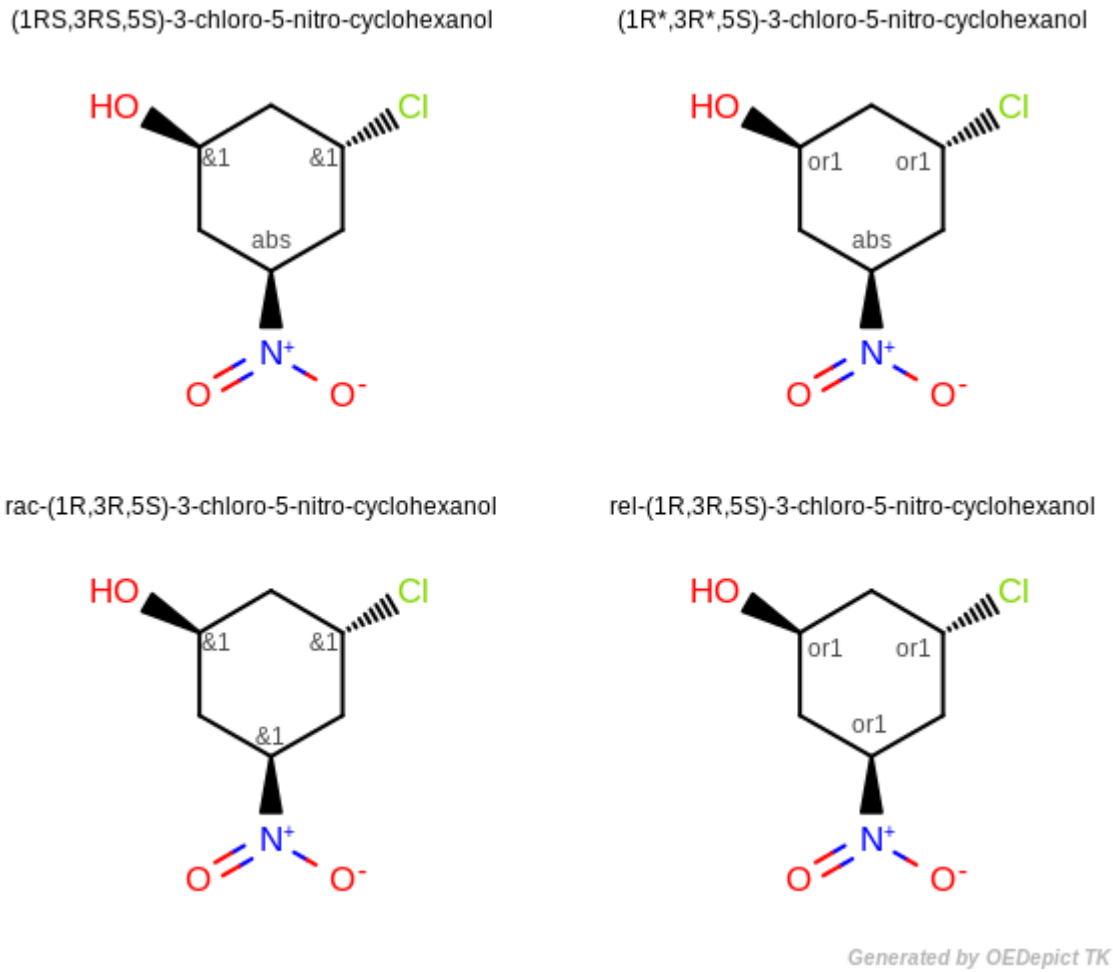


Fig. 1: **Enhanced Stereochemistry**

Note

Enhanced stereochemistry is only supported in for molecules which are represented using MDL V3000 Format.

Naming recognizes enhanced stereochemical features as embodied in the V3000 file format. V3000 allows the specification of **AND** and **OR** stereochemical atom groupings. An **AND** grouping corresponds to a mixture of structures with the center(s) as indicated and their inverse configuration. An **OR** grouping corresponds to either the isomer as indicated or its inverse configuration. Absolute, unspecified, **AND**, and **OR** stereocenters can all be present in single molecule.

Figure: Enhanced Stereochemistry illustrates enhanced stereochemical names generated using the Lexichem TK. Centers in an **AND** grouping are designated with "RS" or "SR". Centers in an **OR** grouping are designated with "R*" or "S*".

For chemical structures with multiple chiral centers where only some are designated as **AND** (see top left image), the descriptors "RS" and "SR" are used to denote **AND** centers.

For a structure where all of the stereocenters are designated as **AND**, the structure represents a molecule and its enantiomer. In that case (even though the V3000 format does not explicitly define the ratio of enantiomers), the molecule is named as a racemate, with a "rac" prefix (see bottom left image).

For chemical structures with multiple chiral centers where only some are designated as **OR** (see top right image), the descriptors "R*" and "S*" are used to denote the **OR** centers.

For a structure where all of the stereocenters are designated as **OR**, the structure represents a molecule or its relative inverse configuration. In that case the molecule is named with a "rel" prefix. (see bottom right image).

The IUPAC standard recommends naming structures so the first **AND** indicator and the first **OR** indicator in the name are "R", "RS", or "R*" as appropriate. When generating a name from a structure, this is easily accomplished by inverting the stereo designation on every center in the stereo grouping. For example, the names "rac-(2R,4R)-4-aminopentan-2-ol" and "rac-(2S,4S)-4-aminopentan-2-ol" are equivalent since they both mean: "a mixture of the (2R,4R) and (2S,4S) isomers". In this case IUPAC conventions recommend using the "rac-(2R,4R)" name.

This choice of recommended name may be a cause for confusion since the atom/bond block of the V3000 molfile indicates a particular configuration and it is possible that the generated name will not appear to correspond to the configuration as found in the atom/bond block. To mitigate the potential for confusion, only the IUPAC and Systematic style of output names perform the inversion. This allows the user to control whether or not the inversion occurs. Comparing the IUPAC and OpenEye style names will give an indication whether or not the inversion is occurring.

For more details please refer to section P-92.1.2 and P-92.1.3 of the Nomenclature of Organic Chemistry [IUPAC-2014].

Note

IUPAC nomenclature currently only allows for a single **AND** group and a single **OR** group on a molecule. The V3000 format allows for multiple independent **AND** and **OR** groups. Names are generated as if all the **AND** centers are in a single **AND** group and all the **OR** centers are in a single **OR** group. This will be remedied when IUPAC defines a naming convention for these more complex cases.

1.2.2 Isotopes

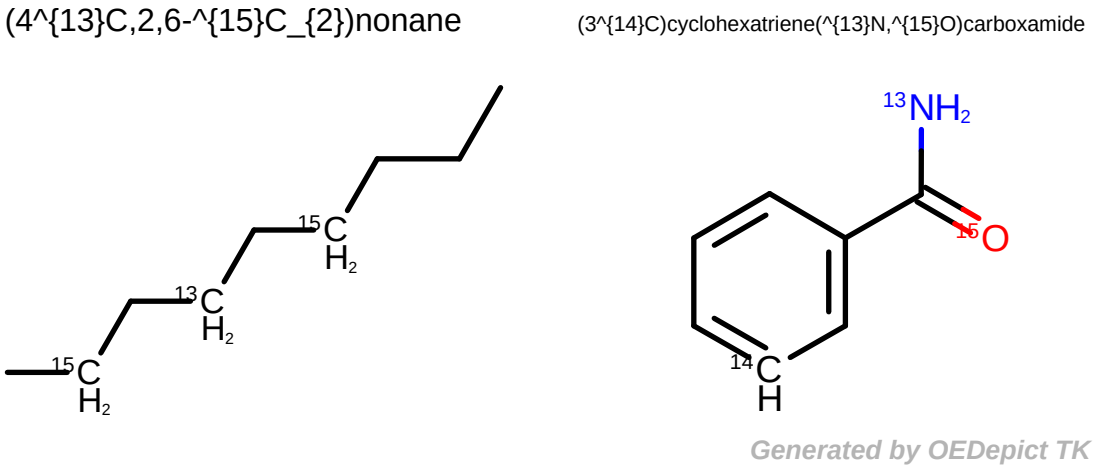


Fig. 2: **Isotopes**

An isotopically substituted compound has a composition such that essentially all the molecules of the compound have only the indicated nuclide at each designated position. For all other positions, the absence of nuclide indication means that the nuclide composition is the natural one [IUPAC-2014].

To name isotopically substituted compounds:

> The name of an isotopically substituted compound is formed by inserting in parentheses the nuclide symbol(s), preceded by any necessary locant(s), letters and/or numerals, before the name or preferably before the denomination of that part of the compound that is isotopically substituted. Immediately after the parentheses there is neither space nor hyphen, except that when the name, or a part of a name, includes a preceding locant, a hyphen is inserted. When polysubstitution is possible, the number of atoms substituted is always specified as a right subscript to the atomic symbol(s), even in case of monosubstitution [IUPAC-2014].

For names composed of two or more words:

> the isotopic descriptor is placed before the appropriate word or part of the word that includes the nuclide(s), unless unambiguous locants are available or are unnecessary [IUPAC-2014].

For more details, please refer to chapter 8 of the IUPAC Nomenclature of Organic Compounds Draft 2004 [IUPAC-2014].

1.3 Output Name Styles

Naming functionality supports the generation of several *styles* of compound names. The currently predefined name styles are *OpenEye* (the default), IUPAC, CAS, Traditional and Systematic. *OpenEye* names loosely correspond to the kinds of names familiar to a medicinal chemist. These names are intended to be a subset of the IUPAC 2005 standard's acceptable names, but not necessarily the PIN (Preferred IUPAC Name). These correspond to the types of names found in a Sigma-Aldrich catalog or a Journal of Medicinal Chemistry article, for example.

IUPAC names are intended to follow the IUPAC 2005 recommendations for the Preferred IUPAC Name (PIN). Future releases may further refine this definition to provide IUPAC2005, IUPAC93 and IUPAC79 name styles that reflect the corresponding standard's preferred name.

The CAS name style is intended to follow the Chemical Abstracts Service's naming conventions, where they differ from IUPAC's.

The Traditional name style corresponds to forms of compound naming that are now no longer acceptable to the IUPAC rules. The boundary between whether a trivial/common name is considered *OpenEye* or Traditional when it is acceptable to IUPAC but not preferred is blurred, with *OpenEye* attempting to follow the more prevalent usage.

Finally, Systematic names correspond to the fully systematic IUPAC names that the IUPAC preferred names are slowly converging towards.

1.4 Examples of Name Style Differences

Some of the concepts explained in the previous section are probably best clarified through some real examples.

1.4.1 Example OpenEye vs. IUPAC vs. Systematic Differences

- The SMILES string `O` is called 'water' by the *OpenEye* name style, but 'oxidane' by the IUPAC and Systematic name styles.
- The SMILES `C#C` is called 'acetylene' by the *OpenEye* and IUPAC name styles, but 'ethyne' by the Systematic name style.
- The SMILES prefix `*Nc1ccccc1` is called 'anilino' by the *OpenEye* and IUPAC name styles, but 'phenylamino' by the Systematic name style.
- The SMILES prefix `*O[N+]#[C-]` is called 'fulminato' by the *OpenEye* name style, but 'isocyanooxy' by the IUPAC and Systematic name styles.
- The SMILES prefix `*C(=O)C` is called 'acetyl' in the *OpenEye* and IUPAC name styles, but 'ethanoyl' in the Systematic name style.
- The SMILES string `CC(=O)C` is called 'acetone" in the *OpenEye* name style, but 'propan-2-one' in the IUPAC and Systematic name styles.
- The SMILES string `C(=O)O` is called 'formic acid' in the *OpenEye* and IUPAC name styles, but 'methanoic acid' in the Systematic name style.

1.4.2 Example OpenEye/IUPAC vs. CAS Differences

- The SMILES string `c1ccccc1CCCCCCC` is named as '1-phenylheptane' by the *OpenEye* and IUPAC name styles, but as 'heptylbenzene' by the CAS name style.
- The SMILES prefix `*[BH2]` is called 'boranyl' by the *OpenEye* and IUPAC name styles, but as 'boryl' by the CAS name style.

1.4.3 Example OpenEye/IUPAC vs. Traditional Differences

- The SMILES prefix `*S` is called ‘sulfanyl’ by the *OpenEye* and IUPAC name styles, but as ‘mercapto’ by the Traditional name style.
- The SMILES string `CCCCCCCCC(=O)O` is called ‘nonanoic acid’ by the *OpenEye* and IUPAC name styles, but as ‘pelargonic acid’ by the Traditional name style.

CHAPTER

TWO

EXAMPLES

2.1 Lexichem TK Examples

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

Program	Description
Mol2Nam_example	convert molecules to names
Nam2Mol_example	convert names to molecules
Translate_example	translate names between languages

Examples:

2.1.1 Converting Molecules to Names

Converts a file of chemical structures (specified by *-in* option) into chemical names (*-out* option), in a choice of language (*-language* option), encodings (*-encoding* option) and styles (*-style* option).

Command Line Interface

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

```
prompt> Mol2Nam_example --help
```

will generate the following output:

```
Simple parameter list

  mol2nam
    I/O
      -in : Input filename
      -out : Output filename

    Lexichem
      -language : Language for output names.
      -style : Style of output names
      -capitalize : Capitalize output names.
      -tag : Set name as SD data with tag
      -delim : Append name to title using "delim"
      -charset : Choose charset/encoding for output names.
```

Code

```
/*
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All rights reserved.
TERMS FOR USE OF SAMPLE CODE The software below ("Sample Code") is
provided to current licensees or subscribers of Cadence products or
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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.
*/
using System;
using OpenEye.OEChem;
using OpenEye.OEIUPAC;

public class Mol2Nam_example
{
  private void Mol2Nam(OEInterface itf)
  {
    oemolistream ifs = new oemolistream();
    if (!ifs.open(itf.GetString("-in")))
      OEChem.OEThrow.Fatal("Unable to open input file: "+itf.GetString("-in"));

    oemolostream ofs = new oemolostream();
    string outname = null;
    if (itf.HasString("-out"))
    {
      outname = itf.GetString("-out");
      if (!ofs.open(outname))
        OEChem.OEThrow.Fatal("Unable to open output file: "+outname);
    }

    uint language = OEIUPAC.OEGetIUPACLanguage(itf.GetString("-language"));
    uint charset  = OEIUPAC.OEGetIUPACCharSet(itf.GetString("-encoding"));
    uint style = OEIUPAC.OEGetIUPACNamStyle(itf.GetString("-style"));

    OEGraphMol mol = new OEGraphMol();
    while (OEChem.OEReadMolecule(ifs, mol))
    {
      if (mol.GetDimension() == 3)
      {
        OEChem.OEPerceiveChiral(mol);
        OEChem.OE3DToAtomStereo(mol);
        OEChem.OE3DToBondStereo(mol);
```

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```
      }

      string name = OEIUPAC.OECreateIUPACName(mol, style);

      if (language > 0)
        name = OEIUPAC.OEToLanguage(name, language);

      if (itf.GetBool("-capitalize"))
        name = OEIUPAC.OECapitalizeName(name);

      if (charset == OECharSet.ASCII)
        name = OEIUPAC.OEToASCII(name);
      else if (charset == OECharSet.UTF8)
        name = OEIUPAC.OEToUTF8(name);
      else if (charset == OECharSet.HTML)
        name = OEIUPAC.OEToHTML(name);
      else if (charset == OECharSet.SJIS)
        name = OEIUPAC.OEToSJIS(name);
      else if (charset == OECharSet.EUCJP)
        name = OEIUPAC.OEToEUCJP(name);

      if (outname != null)
      {
        if (itf.HasString("-delim"))
          name = mol.GetTitle() + itf.GetString("-delim") + name;

        if (itf.HasString("-tag"))
          OEChem.OESetSDData(mol, itf.GetString("-tag"), name);

        mol.SetTitle(name);
        OEChem.OEWriteMolecule(ofs, mol);
      }
      else
        Console.WriteLine(name);
    }
  }

  public static void Main(string[] argv)
  {
    Mol2Nam_example app = new Mol2Nam_example();
    OEInterface itf = new OEInterface(interfaceData, "Mol2Nam_example", argv);
    app.Mol2Nam(itf);
  }

  private static string interfaceData = @"
# mol2nam interface file
!CATEGORY mol2nam

  !CATEGORY I/O
    !PARAMETER -in 1
      !ALIAS -i
      !TYPE string
```

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```
    !REQUIRED true
    !BRIEF Input filename
    !KEYLESS 1
  !END

  !PARAMETER -out 2
    !ALIAS -o
    !TYPE string
    !BRIEF Output filename
    !KEYLESS 2
  !END
!END

!CATEGORY Lexichem Features

  !PARAMETER -language 1
     !ALIAS -lang
     !TYPE string
     !DEFAULT american
     !LEGAL_VALUE american
     !LEGAL_VALUE english
     !LEGAL_VALUE us

     !LEGAL_VALUE british
     !LEGAL_VALUE uk

     !LEGAL_VALUE chinese
     !LEGAL_VALUE zh
     !LEGAL_VALUE cn

     !LEGAL_VALUE danish
     !LEGAL_VALUE dk
     !LEGAL_VALUE da

     !LEGAL_VALUE dutch
     !LEGAL_VALUE nl

     !LEGAL_VALUE french
     !LEGAL_VALUE fr

     !LEGAL_VALUE german
     !LEGAL_VALUE de

     !LEGAL_VALUE greek
     !LEGAL_VALUE el

     !LEGAL_VALUE hungarian
     !LEGAL_VALUE hu

     !LEGAL_VALUE irish
     !LEGAL_VALUE ie
     !LEGAL_VALUE ga
```

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```
    !LEGAL_VALUE italian
    !LEGAL_VALUE it

    !LEGAL_VALUE japanese
    !LEGAL_VALUE jp
    !LEGAL_VALUE ja

    !LEGAL_VALUE polish
    !LEGAL_VALUE pl

    !LEGAL_VALUE portuguese
    !LEGAL_VALUE pt

    !LEGAL_VALUE romanian
    !LEGAL_VALUE ro

    !LEGAL_VALUE russian
    !LEGAL_VALUE ru

    !LEGAL_VALUE slovak
    !LEGAL_VALUE sk

    !LEGAL_VALUE spanish
    !LEGAL_VALUE es

    !LEGAL_VALUE swedish
    !LEGAL_VALUE se
    !LEGAL_VALUE sv

    !LEGAL_VALUE welsh
    !LEGAL_VALUE cy

    !REQUIRED false
    !BRIEF Language for output names.
  !END

  !PARAMETER -style 2
    !ALIAS -namestyle
    !TYPE string
    !DEFAULT openeye
    !LEGAL_VALUE openeye
    !LEGAL_VALUE iupac
    !LEGAL_VALUE cas
    !LEGAL_VALUE traditional
    !LEGAL_VALUE systematic
    !LEGAL_VALUE casindex
    !LEGAL_VALUE casidx
    !LEGAL_VALUE autonom
    !LEGAL_VALUE iupac79
    !LEGAL_VALUE iupac93
    !LEGAL_VALUE acdname
```

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```
      !BRIEF Style of output names
    !END

    !PARAMETER -capitalize 3
       !ALIAS -capitalise
       !TYPE bool
       !DEFAULT false
       !BRIEF Capitalize output names.
    !END

    !PARAMETER -tag 4
       !TYPE string
       !REQUIRED false
       !BRIEF Set name as SD data with tag
    !END

    !PARAMETER -delim 5
       !TYPE string
       !REQUIRED false
       !BRIEF Append name to title using 'delim'
    !END

    !PARAMETER -charset 7
      !ALIAS -encoding
      !TYPE string
      !DEFAULT default
      !REQUIRED false
      !LEGAL_VALUE default
      !LEGAL_VALUE ascii
      !LEGAL_VALUE utf8
      !LEGAL_VALUE html
      !LEGAL_VALUE sjis
      !LEGAL_VALUE eucjp
      !BRIEF Choose charset/encoding for output names.
    !END

  !END

!END
";

}
```

2.1.2 Converting Names to Molecules

Converts a file of chemical names (specified by the *-in* option) of a specific language (*-language* option) into a file of chemical structures (specified by the *-out* option).

Command Line Interface

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

```
prompt> Nam2Mol_example --help
```

will generate the following output:

```
Simple parameter list

  nam2mol
    I/O
      -in : Input filename
      -out : Output filename

    Lexichem
      -language : Language for input names.
      -tag : Set name as SD data with tag
      -empty : Output an empty molecule for unparseable names
      -charset : Choose charset/encoding for input names.
```

Code

```
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or its use.
*/
using System;
using OpenEye.OEChem;
using OpenEye.OEIUPAC;

public class Nam2Mol_example
{
  private void Nam2Mol(OEInterface itf)
  {
    System.IO.StreamReader ifs =
      new System.IO.StreamReader(itf.GetString("-in"));

    oemolostream ofs = new oemolostream();
    if (!ofs.open(itf.GetString("-out")))
```

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```
      OEChem.OEThrow.Fatal("Unable to open output file: " +
                           itf.GetString("-out"));

    uint language = OEIUPAC.OEGetIUPACLanguage(itf.GetString("-language"));
    uint charset = OEIUPAC.OEGetIUPACCharSet(itf.GetString("-charset"));

    OEGraphMol mol = new OEGraphMol();
    string name = "";
    while ((name = ifs.ReadLine()) != null)
    {
      mol.Clear();

      // Speculatively reorder CAS permuted index names
      string str = OEIUPAC.OEReorderIndexName(name);
      if (str.Length == 0)
        str = name;

      if (charset == OECharSet.HTML)
        str = OEIUPAC.OEFromHTML(str);
      else if (charset == OECharSet.UTF8)
        str = OEIUPAC.OEFromUTF8(str);

      str = OEIUPAC.OELowerCaseName(str);

      if (language != OELanguage.AMERICAN)
        str = OEIUPAC.OEFromLanguage(str,language);

      bool done = OEIUPAC.OEParseIUPACName(mol,str);

      if (!done && itf.GetBool("-empty"))
      {
        mol.Clear();
        done = true;
      }

      if (done)
      {
        if (itf.HasString("-tag"))
          OEChem.OESetSDData(mol, itf.GetString("-tag"),name);
        mol.SetTitle(name);
        OEChem.OEWriteMolecule(ofs,mol);
      }
    }
  }

  public static void Main(string[] argv)
  {
    Nam2Mol_example app = new Nam2Mol_example();
    OEInterface itf = new OEInterface(interfaceData, "Nam2Mol_example", argv);
    app.Nam2Mol(itf);
  }
```

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```
  private static string interfaceData = @"
# nam2mol interface file
!CATEGORY nam2mol

  !CATEGORY I/O
    !PARAMETER -in 1
      !ALIAS -i
      !TYPE string
      !REQUIRED true
      !BRIEF Input filename
      !KEYLESS 1
    !END

    !PARAMETER -out 2
      !ALIAS -o
      !TYPE string
      !REQUIRED true
      !BRIEF Output filename
      !KEYLESS 2
    !END
  !END

  !CATEGORY Lexichem Features

    !PARAMETER -language 1
       !ALIAS -lang
       !TYPE string
       !DEFAULT american
       !LEGAL_VALUE american
       !LEGAL_VALUE english
       !LEGAL_VALUE us

       !LEGAL_VALUE chinese
       !LEGAL_VALUE zh
       !LEGAL_VALUE cn

       !LEGAL_VALUE danish
       !LEGAL_VALUE dk
       !LEGAL_VALUE da

       !LEGAL_VALUE dutch
       !LEGAL_VALUE nl

       !LEGAL_VALUE french
       !LEGAL_VALUE fr

       !LEGAL_VALUE german
       !LEGAL_VALUE de

       !LEGAL_VALUE greek
       !LEGAL_VALUE el
```

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```
      !LEGAL_VALUE hungarian
      !LEGAL_VALUE hu

      !LEGAL_VALUE irish
      !LEGAL_VALUE ie
      !LEGAL_VALUE ga

      !LEGAL_VALUE italian
      !LEGAL_VALUE it

      !LEGAL_VALUE japanese
      !LEGAL_VALUE jp
      !LEGAL_VALUE ja

      !LEGAL_VALUE polish
      !LEGAL_VALUE pl

      !LEGAL_VALUE portuguese
      !LEGAL_VALUE pt

      !LEGAL_VALUE romanian
      !LEGAL_VALUE ro

      !LEGAL_VALUE russian
      !LEGAL_VALUE ru

      !LEGAL_VALUE slovak
      !LEGAL_VALUE sk

      !LEGAL_VALUE spanish
      !LEGAL_VALUE es

      !LEGAL_VALUE swedish
      !LEGAL_VALUE se
      !LEGAL_VALUE sv

      !LEGAL_VALUE welsh
      !LEGAL_VALUE cy

      !REQUIRED false
      !BRIEF Language for input names.
   !END

   !PARAMETER -tag 3
      !TYPE string
      !REQUIRED false
      !BRIEF Set name as SD data with tag
   !END

   !PARAMETER -empty 4
      !TYPE bool
      !DEFAULT false
```

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```
      !BRIEF Output an empty molecule for unparseable names
   !END

   !PARAMETER -charset 5
      !ALIAS -encoding
      !TYPE string
      !DEFAULT default
      !REQUIRED false
      !LEGAL_VALUE default
      !LEGAL_VALUE ascii
      !LEGAL_VALUE utf8
      !LEGAL_VALUE html
      !BRIEF Choose charset/encoding for input names.
   !END

  !END
!END
";
}
```

2.1.3 Translating Names Between Languages

Translates a file of chemical names (specified by the *-in* option) in a specific language (*-from* option) into a file of names (specified by the *-out* option) in another language (*-to* option).

Command Line Interface

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

```
prompt> Translate_example --help
```

will generate the following output:

```
Simple parameter list

  translate
    -nobanner : Suppress the program banner.
    -in : Input filename
    -out : Output filename
    -from : Language for input names.
    -to : Language for input names.
    -from_charset : Choose charset/encoding for input names.
    -to_charset : Choose charset/encoding for output names.
```

Code

```
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or its use.
*/

/*****************************************************************************
 Translates between languages.  Internally LexichemTK uses American
 English so it will convert to/from that as an intermediate
 representation.

 By default the program inputs/outputs the internal LexichemTK
 character set representation.  Optionally one can convert the
 input or output to alternate encodings, eg: HTML or UTF8.

 *****************************************************************************/
using System;
using OpenEye.OEChem;
using OpenEye.OEIUPAC;

public class Translate_example
{
  private void Translate(OEInterface itf)
  {
    System.IO.StreamReader ifs =
      new System.IO.StreamReader(itf.GetString("-in"));

    System.IO.StreamWriter sw = null;
    if (itf.HasString("-o"))
    {
      try
      {
        sw = new System.IO.StreamWriter(itf.GetString("-o"));
        Console.SetOut(sw);
      }
      catch
      {
        OEChem.OEThrow.Fatal("Unable to open " + itf.GetString("-o") +
                             " for writing");
      }
    }

    uint to_language =
      OEIUPAC.OEGetIUPACLanguage(itf.GetString("-to_language"));
    uint from_language =
```

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```
    OEIUPAC.OEGetIUPACLanguage(itf.GetString("-from_language"));

  uint from_charset =
    OEIUPAC.OEGetIUPACCharSet(itf.GetString("-from_charset"));
  uint to_charset =
    OEIUPAC.OEGetIUPACCharSet(itf.GetString("-to_charset"));

  string name = "";
  while ((name = ifs.ReadLine()) != null)
  {
    // Convert from charset to internal representation
    if (from_charset == OECharSet.UTF8)
      name = OEIUPAC.OEFromUTF8(name);
    else if (from_charset == OECharSet.HTML)
      name = OEIUPAC.OEFromHTML(name);

    // Translation functions operate on lowercase names
    name = OEIUPAC.OELowerCaseName(name);

    if (from_language != OELanguage.AMERICAN)
      name = OEIUPAC.OEFromLanguage(name, from_language);

    // At this point the name is American English in the
    // LexichemTK default internal character set representation.

    // Convert to output language
    if (to_language != OELanguage.AMERICAN)
      name = OEIUPAC.OEToLanguage(name, to_language);

    // Convert to output charset
    if (to_charset == OECharSet.ASCII)
      name = OEIUPAC.OEToASCII(name);
    else if (to_charset == OECharSet.UTF8)
      name = OEIUPAC.OEToUTF8(name);
    else if (to_charset == OECharSet.HTML)
      name = OEIUPAC.OEToHTML(name);
    else if (to_charset == OECharSet.SJIS)
      name = OEIUPAC.OEToSJIS(name);
    else if (to_charset == OECharSet.EUCJP)
      name = OEIUPAC.OEToEUCJP(name);

    Console.WriteLine(name);
  }

  if (itf.HasString("-o"))
    sw.Close();
}

public static void Main(string[] argv)
{
  Translate_example app = new Translate_example();
  OEInterface itf = new OEInterface(interfaceData,
```

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```
                                        "Translate_example", argv);
    app.Translate(itf);
  }

  private static string interfaceData = @"
# translate interface file
!CATEGORY translate

      !PARAMETER -in 1
        !ALIAS -i
        !TYPE string
        !REQUIRED true
        !BRIEF Input filename
        !KEYLESS 1
      !END

      !PARAMETER -out 2
        !ALIAS -o
        !TYPE string
        !BRIEF Output filename
        !KEYLESS 2
      !END

      !PARAMETER -from 3
         !ALIAS -from_language
         !TYPE string
         !DEFAULT american
         !LEGAL_VALUE american
         !LEGAL_VALUE english
         !LEGAL_VALUE us

         !LEGAL_VALUE chinese
         !LEGAL_VALUE zh
         !LEGAL_VALUE cn

         !LEGAL_VALUE danish
         !LEGAL_VALUE dk
         !LEGAL_VALUE da

         !LEGAL_VALUE dutch
         !LEGAL_VALUE nl

         !LEGAL_VALUE french
         !LEGAL_VALUE fr

         !LEGAL_VALUE german
         !LEGAL_VALUE de

         !LEGAL_VALUE greek
         !LEGAL_VALUE el

         !LEGAL_VALUE hungarian
```

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```
        !LEGAL_VALUE hu

        !LEGAL_VALUE irish
        !LEGAL_VALUE ie
        !LEGAL_VALUE ga

        !LEGAL_VALUE italian
        !LEGAL_VALUE it

        !LEGAL_VALUE japanese
        !LEGAL_VALUE jp
        !LEGAL_VALUE ja

        !LEGAL_VALUE polish
        !LEGAL_VALUE pl

        !LEGAL_VALUE portuguese
        !LEGAL_VALUE pt

        !LEGAL_VALUE romanian
        !LEGAL_VALUE ro

        !LEGAL_VALUE russian
        !LEGAL_VALUE ru

        !LEGAL_VALUE slovak
        !LEGAL_VALUE sk

        !LEGAL_VALUE spanish
        !LEGAL_VALUE es

        !LEGAL_VALUE swedish
        !LEGAL_VALUE se
        !LEGAL_VALUE sv

        !LEGAL_VALUE welsh
        !LEGAL_VALUE cy

        !REQUIRED false
        !BRIEF Language for input names.
    !END

    !PARAMETER -to 4
        !ALIAS -to_language
        !TYPE string
        !DEFAULT american
        !LEGAL_VALUE american
        !LEGAL_VALUE english
        !LEGAL_VALUE us

        !LEGAL_VALUE chinese
        !LEGAL_VALUE zh
```

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```
        !LEGAL_VALUE cn

        !LEGAL_VALUE danish
        !LEGAL_VALUE dk
        !LEGAL_VALUE da

        !LEGAL_VALUE dutch
        !LEGAL_VALUE nl

        !LEGAL_VALUE french
        !LEGAL_VALUE fr

        !LEGAL_VALUE german
        !LEGAL_VALUE de

        !LEGAL_VALUE greek
        !LEGAL_VALUE el

        !LEGAL_VALUE hungarian
        !LEGAL_VALUE hu

        !LEGAL_VALUE irish
        !LEGAL_VALUE ie
        !LEGAL_VALUE ga

        !LEGAL_VALUE italian
        !LEGAL_VALUE it

        !LEGAL_VALUE japanese
        !LEGAL_VALUE jp
        !LEGAL_VALUE ja

        !LEGAL_VALUE polish
        !LEGAL_VALUE pl

        !LEGAL_VALUE portuguese
        !LEGAL_VALUE pt

        !LEGAL_VALUE romanian
        !LEGAL_VALUE ro

        !LEGAL_VALUE russian
        !LEGAL_VALUE ru

        !LEGAL_VALUE slovak
        !LEGAL_VALUE sk

        !LEGAL_VALUE spanish
        !LEGAL_VALUE es

        !LEGAL_VALUE swedish
        !LEGAL_VALUE se
```

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```
        !LEGAL_VALUE sv

        !LEGAL_VALUE welsh
        !LEGAL_VALUE cy

        !REQUIRED false
        !BRIEF Language for input names.
    !END

    !PARAMETER -from_charset 5
        !TYPE string
        !DEFAULT default
        !REQUIRED false
        !LEGAL_VALUE default
        !LEGAL_VALUE ascii
        !LEGAL_VALUE utf8
        !LEGAL_VALUE html
        !LEGAL_VALUE sjis
        !LEGAL_VALUE eucjp
        !BRIEF Choose charset/encoding for input names.
    !END

    !PARAMETER -to_charset 6
        !ALIAS -encoding
        !ALIAS -charset
        !TYPE string
        !DEFAULT default
        !REQUIRED false
        !LEGAL_VALUE default
        !LEGAL_VALUE ascii
        !LEGAL_VALUE utf8
        !LEGAL_VALUE html
        !LEGAL_VALUE sjis
        !LEGAL_VALUE eucjp
        !BRIEF Choose charset/encoding for output names.
    !END

    !PARAMETER -debug
        !TYPE bool
        !DEFAULT false
        !VISIBILITY hidden
    !END

!END
";

}
```

CHAPTER

THREE

API

3.1 OEIUPAC Constants

3.1.1 OECharSet

This namespace contains constants for defining the character set for character conversion.

DEFAULT

No character conversion.

ASCII

See *OEToASCII* for format details.

HTML

See *OEToHTML* for format details.

LATIN1

See *OEToLatin1* for format details.

UTF8

See *OEToUTF8* for format details.

SJIS

See *OEToSJIS* for format details.

EUCJP

See *OEToEUCJP* for format details.

3.1.2 OEIUPAC

This namespace contains constants.

OENamStyleOpenEye

This constant is used to specify the (default) predefined OpenEye name style to the *OECreateIUPACName* function.

OENamStyleTraditional

This constant is used to specify the predefined traditional name style to the *OECreateIUPACName* function.

OENamStyleSystematic

This constant is used to specify the predefined systematic name style to the *OECreateIUPACName* function.

OENamStyleIUPAC

This constant is used to specify the predefined IUPAC 2005 name style to the *OECreateIUPACName* function.

OENamStyleCAS

This constant is used to specify the predefined Chemical Abstracts Service (CAS) name style to the *OECreateIUPACName* function.

OENamStyleCASIndex

This constant is used to specify the predefined Chemical Abstracts Service (CAS) permuted index name style to the *OECreateIUPACName* function.

OENamStyleAutoNom

This constant is used to specify the predefined MDL/Beilstein AutoNom name style to the *OECreateIUPACName* function.

OENamStyleIUPAC79

This constant is used to specify the predefined IUPAC 1979 name style to the *OECreateIUPACName* function.

OENamStyleIUPAC93

This constant is used to specify the predefined IUPAC 1993 name style to the *OECreateIUPACName* function.

OENamStyleACDName

This constant is used to specify the predefined ACD name style to the *OECreateIUPACName* function.

3.1.3 OELanguage

This namespace contains constants for defining which language to translate to/from using *OEFromLanguage* and *OEToLanguage*.

Depending on the language, the translation functions may expect \u escaped Unicode characters. In general the translations only use characters in the Basic Multilingual Plane (BMP). Each language below indicates the range of Unicode characters which are handled. Character set conversion should take into account the range of Unicode expected.

ENGLISH

This constant is used to specify the American dialect of English. This is currently a synonym of the constant *OELanguage.AMERICAN*. Uses only ASCII characters.

AMERICAN

This constant is used to specify the American dialect of English to This is currently a synonym of the constant *OELanguage.ENGLISH*. Uses only ASCII characters.

BRITISH

This constant is used to specify the traditional British dialect of English. Uses only ASCII characters.

INTERNATIONAL

This constant is used to specify the international dialect of English. Uses only ASCII characters.

CHINESE

This constant is used to specify the Chinese language. Uses CJK characters in the Unicode BMP.

DANISH

This constant is used to specify the Danish language. Uses ASCII and Latin-1 Unicode characters in the `\u00a0` to `\u00ff` range.

DUTCH

This constant is used to specify the Dutch language. Uses ASCII and Latin-1 Unicode characters in the `\u00a0` to `\u00ff` range.

FRENCH

This constant is used to specify the French language. Uses ASCII and Latin-1 Unicode characters in the `\u00a0` to `\u00ff` range.

GERMAN

This constant is used to specify the German language. Uses ASCII and Latin-1 Unicode characters in the `\u00a0` to `\u00ff` range.

GREEK

This constant is used to specify the Greek language. Uses ASCII and Greek Unicode characters in the `\u0370` to `\u03ff` range.

HUNGARIAN

This constant is used to specify the Hungarian language. Uses ASCII, Latin-1 Unicode characters in the `\u00a0` to `\u00ff` range and Latin Extended-A Unicode characters in the `\u0100` to `\u017f` range.

IRISH

This constant is used to specify the Irish language. Uses ASCII and Latin-1 Unicode characters in the `\u00a0` to `\u00ff` range.

ITALIAN

This constant is used to specify the Italian language. Uses ASCII and Latin-1 Unicode characters in the `\u00a0` to `\u00ff` range.

JAPANESE

This constant is used to specify the Japanese language. Uses CJK characters in the Unicode BMP.

POLISH

This constant is used to specify the Polish language. Uses ASCII, Latin-1 Unicode characters in the `\u00a0` to `\u00ff` range and Latin Extended-A Unicode characters in the `\u0100` to `\u017f` range.

PORTUGUESE

This constant is used to specify the Portuguese language. Uses ASCII and Latin-1 Unicode characters in the \u00a0 to \u00ff range.

ROMANIAN

This constant is used to specify the Romanian language. Uses ASCII, Latin-1 Unicode characters in the \u00a0 to \u00ff range and Latin Extended-A Unicode characters in the \u0100 to \u017f range.

RUSSIAN

This constant is used to specify the Russian language. Uses ASCII and Cyrillic Unicode characters in the \u0400 to \u04ff range.

SLOVAK

This constant is used to specify the Slovak language. Uses ASCII, Latin-1 Unicode characters in the \u00a0 to \u00ff range and Latin Extended-A Unicode characters in the \u0100 to \u017f range.

SPANISH

This constant is used to specify the Spanish language. Uses ASCII and Latin-1 Unicode characters in the \u00a0 to \u00ff range.

SWEDISH

This constant is used to specify the Swedish language. Uses ASCII and Latin-1 Unicode characters in the \u00a0 to \u00ff range.

WELSH

This constant is used to specify the Welsh language. Uses ASCII, Latin-1 Unicode characters in the \u00a0 to \u00ff range and Latin Extended-A Unicode characters in the \u0100 to \u017f range.

3.2 OEIUPAC Functions

3.2.1 OECapitalizeName

```
std::string OECapitalizeName(const char* ptr)
```

Capitalize the appropriate first letter of a name generated by *OECreateIUPACName*. This function should be called after translating the name to a foreign language, but before converting the character set encoding.

3.2.2 OECreateIUPACName

```
std::string OECreateIUPACName(const OEChem::OEMolBase& mol,
                              const unsigned char* style = OENamStyleOpenEye,
                              const bool warn = true)
```

This function attempts to generate a 'reasonable' IUPAC name for the given molecule, mol, and return the result in a string. These 'reasonable' names attempts to be one of the recommended IUPAC names for a compound, however occasionally this function may fall back to using IUPAC 'systematic' naming for parts of a molecule. Any parts of a molecule that cannot be named result in the substring BLAH appearing in the returned string.

The optional style argument can be used to control and customize the style of the names generated by this function. The nine currently predefined name styles are

- *OEIUPAC.OENamStyleOpenEye* (the default),
- *OEIUPAC.OENamStyleIUPAC*,
- *OEIUPAC.OENamStyleIUPAC79*,
- *OEIUPAC.OENamStyleIUPAC93*,
- *OEIUPAC.OENamStyleTraditional*,
- *OEIUPAC.OENamStyleAutoNom*,
- *OEIUPAC.OENamStyleCAS*,
- *OEIUPAC.OENamStyleCASIndex* and
- *OEIUPAC.OENamStyleSystematic*.

After the name has been generated it may be translated into one of several languages, for example using the *OEToGerman* or *OEToJapanese* functions, then optionally capitalized using *OECapitalizeName*, and finally converted into a final character encoding, for example using *OEToUTF8* or *OEToHTML*.

warn
: If `false`, suppresses warning messages when a name cannot be generated.

3.2.3 OEFromBritish

```
std::string OEFromBritish(const char* ptr)
```

Convert the chemical name specified by 'ptr' from British English to American English.

See *OELanguage* for character set information.

3.2.4 OEFromChinese

```
std::string OEFromChinese(const char* ptr)
```

Convert the chemical name specified by 'ptr' from simplified or traditional Chinese to English.

See *OELanguage* for character set information.

3.2.5 OEFromDanish

```
std::string OEFromDanish(const char* ptr)
```

Convert the chemical name specified by 'ptr' from Danish to English.

See *OELanguage* for character set information.

3.2.6 OEFromDutch

```
std::string OEFromDutch(const char* ptr)
```

Convert the chemical name specified by 'ptr' from Dutch to English.

See *OELanguage* for character set information.

3.2.7 OEFromFrench

```
std::string OEFromFrench(const char* ptr)
```

Convert the chemical name specified by 'ptr' from French to English.

See *OELanguage* for character set information.

3.2.8 OEFromGerman

```
std::string OEFromGerman(const char* ptr)
```

Convert the chemical name specified by 'ptr' from German to English.

See *OELanguage* for character set information.

3.2.9 OEFromGreek

```
std::string OEFromGreek(const char* ptr)
```

Convert the chemical name specified by 'ptr' from Greek to English.

See *OELanguage* for character set information.

3.2.10 OEFromHTML

```
std::string OEFromHTML(const char* ptr)
```

Convert the string 'ptr' from the HTML character encoding to *Lexichem*'s internal encoding, which uses \u escapes to represent non-ASCII characters. Handles conversion of HTML markup to the to internal markup representation.

3.2.11 OEFromHungarian

```
std::string OEFromHungarian(const char* ptr)
```

Convert the chemical name specified by 'ptr' from Hungarian to English.

See *OELanguage* for character set information.

3.2.12 OEFromIrish

```
std::string OEFromIrish(const char* ptr)
```

Convert the chemical name specified by 'ptr' from Irish to English.

See *OELanguage* for character set information.

3.2.13 OEFromItalian

```
std::string OEFromItalian(const char* ptr)
```

Convert the chemical name specified by 'ptr' from Italian to English.

See *OELanguage* for character set information.

3.2.14 OEFromJapanese

```
std::string OEFromJapanese(const char* ptr)
```

Convert the chemical name specified by 'ptr' from Japanese to English.

See *OELanguage* for character set information.

3.2.15 OEFromKOI8R

```
std::string OEFromKOI8R(const char* ptr)
```

Convert the string 'ptr' from the Russian KOI-8 character encoding to the internal string encoding using \u escapes to represent non-ASCII unicode characters.

3.2.16 OEFromLanguage

```
std::string OEFromLanguage(const char* ptr, unsigned int lang)
```

This is a helper wrapper function that can be used to convert the chemical name specified by 'ptr' from the language specified by 'lang' to English. The languages are specified by the constants in the *OELanguage* namespace.

3.2.17 OEFromLatin1

```
std::string OEFromLatin1(const char* ptr)
```

Convert the string 'ptr' from the Latin1 character encoding to *Lexichem*'s internal encoding, which uses \u escapes to represent non-ASCII characters.

> **Note**
>
> This function is not available in Java or Python as those language environments use other character sets.

3.2.18 OEFromPolish

```
std::string OEFromPolish(const char* ptr)
```

Convert the chemical name specified by 'ptr' from Polish to English.

See *OELanguage* for character set information.

3.2.19 OEFromPortuguese

```
std::string OEFromPortuguese(const char* ptr)
```

Convert the chemical name specified by 'ptr' from Portuguese to English.

See *OELanguage* for character set information.

3.2.20 OEFromRomanian

```
std::string OEFromRomanian(const char* ptr)
```

Convert the chemical name specified by 'ptr' from Romanian to English.

See *OELanguage* for character set information.

3.2.21 OEFromRussian

```
std::string OEFromRussian(const char* ptr)
```

Convert the chemical name specified by 'ptr' from Russian to English.

See *OELanguage* for character set information.

3.2.22 OEFromSlovak

```
std::string OEFromSlovak(const char* ptr)
```

Convert the chemical name specified by 'ptr' from Slovak to English.

See *OELanguage* for character set information.

3.2.23 OEFromSpanish

```
std::string OEFromSpanish(const char* ptr)
```

Convert the chemical name specified by 'ptr' from Spanish to English.

See *OELanguage* for character set information.

3.2.24 OEFromSwedish

```
std::string OEFromSwedish(const char* ptr)
```

Convert the chemical name specified by 'ptr' from Swedish to English.

See *OELanguage* for character set information.

3.2.25 OEFromUTF8

```
std::string OEFromUTF8(const char* ptr)
```

Convert the string 'ptr' from the UTF-8 character encoding to *Lexichem*'s internal encoding, which uses \u escapes to represent non-ASCII characters.

3.2.26 OEFromWelsh

```
std::string OEFromWelsh(const char* ptr)
```

Convert the chemical name specified by 'ptr' from simplified or traditional Welsh to English.

See *OELanguage* for character set information.

3.2.27 OEGetCIPStereo

```
char OEGetCIPStereo(const OEChem::OEMolBase& mol,
                    const OEChem::OEAtomBase* atm)
char OEGetCIPStereo(const OEChem::OEMolBase& mol,
                    const OEChem::OEBondBase* bnd)
```

These functions return the Cahn-Ingold-Prelog descriptor for the given atom or bond stereo center, from the stereochemistry set on the OEMolBase. For chiral atom centers, the OEAtomBase form of this function returns either 'R' or 'S' for specified CIP stereo centers, 'N' for CIP stereo centers that don't have stereo specified (*i.e.* `OEAtomBase.HasStereoSpecified` returns `false`), and 'X' for atoms that are not CIP stereo centers. For double bonds, the OEBondBase form of this function returns either 'E' or 'Z' specified CIP stereo centers, 'N' for CIP stereo centers that don't have stereo specified (*i.e.* `OEBondBase.HasStereoSpecified` returns `false`), and 'X' for bonds that are not CIP stereo centers.

3.2.28 OEGetIUPACCharSet

```
unsigned int OEGetIUPACCharSet(const std::string& charset)
```

Returns a constant in the *OECharSet* namespace based on the value of the name.

3.2.29 OEGetIUPACLanguage

```
unsigned int OEGetIUPACLanguage(const std::string& langStr)
```

Returns a constant in the *OELanguage* namespace based on the value of the name. Name can be a language name or two-letter country code.

3.2.30 OEGetIUPACNamStyle

```
const unsigned char* OEGetIUPACNamStyle(const std::string& style)
```

Returns a pointer to the style (*OEIUPAC*) associated with the given name.

3.2.31 OEIUPACGetArch

```
const char* OEIUPACGetArch()
```

Returns the system architecture.

3.2.32 OEIUPACGetLicensee

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

Determines the valid licensee.

3.2.33 OEIUPACGetPlatform

```
const char* OEIUPACGetPlatform()
```

Returns the system platform.

3.2.34 OEIUPACGetRelease

```
const char* OEIUPACGetRelease()
```

Returns the *Lexichem* toolkit release number.

3.2.35 OEIUPACGetSite

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

Determines whether a valid site is present.

3.2.36 OEIUPACGetVersion

```
unsigned int OEIUPACGetVersion()
```

Returns *Lexichem* toolkit build date.

3.2.37 OEIUPACIsLicensed

```
bool OEIUPACIsLicensed(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 **Lexichem TK** functionality.

The 'feature' argument can be used to check for a valid license to **Lexichem 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 **Lexichem TK** license.

See also

- `OEChemIsLicensed` function

3.2.38 OELowerCaseName

```
std::string OELowerCaseName(const char* ptr)
```

Convert the specified compound name to lower-case. This function understands chemical nomenclature and foreign alphabets. This function should be called prior to translating a name from a foreign language, as the language translation routines assume that the name is lower-case.

3.2.39 OENameLocant

```
std::string OENameLocant(unsigned int loc, bool iupac = false)
```

Generate the lexical form of a *Lexichem* locant index. The molecules created by the function *OEParseIUPACName* are annotated with locant information in each atom's integer atom type field. These locant indices may be retrieved using *OEChem*'s `GetIntType` method.

3.2.40 OEParseIUPACName

```
bool OEParseIUPACName(OEChem::OEMolBase& mol, const char* name)
```

This function parses the compound name (not necessarily a systematic or preferred IUPAC name) from the NULL-terminated string given by name, and places the processed molecule in mol. This function returns `true` if the name could be parsed without problems and false otherwise. If the function returns `false`, the mol will contain as much of the name as could be processed.

3.2.41 OEReorderIndexName

```
std::string OEReorderIndexName(const char* ptr)
```

Attempt to reorder the specified permuted index name. This permute strings such as "benzene, chloro-" into the form "chloro-benzene" which can then be processed by the *OEParseIUPACName* function.

This function returns an empty string (or the original input string) if its argument is not recognized as a permuted index name.

3.2.42 OESetCIPStereo

```
bool OESetCIPStereo(OEChem::OEMolBase& mol, OEChem::OEAtomBase* atm,
                    char s)
bool OESetCIPStereo(OEChem::OEMolBase& mol, OEChem::OEBondBase* bnd,
                    char s)
```

Set the internal *OEChem* stereochemistry from the given CIP stereo descriptor. For OEAtomBase the descriptor must be either 'R' or 'S', and for OEBondBase the descriptor must be either 'E' or 'Z'. Returns `true` if the stereochemistry was successfully set, and `false` otherwise: *i.e.* the descriptor was invalid or the specified atom or bond was not a CIP stereo center.

3.2.43 OEToASCII

```
std::string OEToASCII(const char* ptr, const bool remove_markup = true)
```

Convert the string 'ptr', typically the output of the function *OECreateIUPACName* optionally post-processed by a language translation function, from the internal encoding, which uses \u escapes to represent non-ASCII characters, into a reduced 7-bit ASCII representation by mapping accented 8-bit characters into their ASCII counterparts.

The 'remove_markup' flag controls the disposition of italics, superscript, and subscript markup. If the value is `true` (the default), the markup is removed. If `false`, the markup is left in the output string, which should be post-processed.

3.2.44 OEToBritish

```
std::string OEToBritish(const char* ptr, bool sulph)
```

Convert the string 'ptr', typically the output of the function *OECreateIUPACName*, from the default American output, to either British spelling (when 'sulph' is `true`) or IUPAC international spelling (when 'sulph' is `false`).

See *OELanguage* for character set information.

3.2.45 OEToChinese

```
std::string OEToChinese(const char* ptr)
```

Convert the string 'ptr', typically the output of the function *OECreateIUPACName*, from English to simplified Chinese.

See *OELanguage* for character set information.

3.2.46 OEToDanish

```
std::string OEToDanish(const char* ptr)
```

Convert the string 'ptr', typically the output of the function *OECreateIUPACName*, from English to Danish.

See *OELanguage* for character set information.

3.2.47 OEToDutch

```
std::string OEToDutch(const char* ptr)
```

Convert the string 'ptr', typically the output of the function *OECreateIUPACName*, from English to Dutch.

See *OELanguage* for character set information.

3.2.48 OEToEUCJP

```
std::string OEToEUCJP(const char* ptr)
```

Convert the string 'ptr', typically the output of the function *OECreateIUPACName* post-processed by a call to *OEToJapanese*, from the default encoding which uses \u escapes to represent unicode characters to instead use the EUC-JP character encoding for Japanese characters.

3.2.49 OEToFrench

```
std::string OEToFrench(const char* ptr)
```

Convert the string 'ptr', typically the output of the function *OECreateIUPACName*, from English to French.

See *OELanguage* for character set information.

3.2.50 OEToGerman

```
std::string OEToGerman(const char* ptr)
```

Convert the string 'ptr', typically the output of the function *OECreateIUPACName*, from English to German.

See *OELanguage* for character set information.

3.2.51 OEToGreek

```
std::string OEToGreek(const char* ptr)
```

Convert the string 'ptr', typically the output of the function *OECreateIUPACName*, from English to Greek.

See *OELanguage* for character set information.

3.2.52 OEToHTML

```
std::string OEToHTML(const char* ptr)
```

Convert the string 'ptr', typically the output of the function *OECreateIUPACName* optionally post-processed by a language translation function, from the default internal encoding, which uses \u escapes to represent non-ASCII characters, to use HTML mark-up to represent Latin1 characters, unicode characters, italics, superscripts, and subscripts.

3.2.53 OEToHungarian

```
std::string OEToHungarian(const char* ptr)
```

Convert the string 'ptr', typically the output of the function *OECreateIUPACName*, from English to Hungarian.

See *OELanguage* for character set information.

3.2.54 OEToIrish

```
std::string OEToIrish(const char* ptr)
```

Convert the string 'ptr', typically the output of the function *OECreateIUPACName*, from English to Irish.

See *OELanguage* for character set information.

3.2.55 OEToItalian

```
std::string OEToItalian(const char* ptr)
```

Convert the string 'ptr', typically the output of the function *OECreateIUPACName*, from English to Italian.

See *OELanguage* for character set information.

3.2.56 OEToJapanese

```
std::string OEToJapanese(const char* ptr)
```

Convert the string 'ptr', typically the output of the function *OECreateIUPACName*, from English to Japanese.

See *OELanguage* for character set information.

3.2.57 OEToLanguage

```
std::string OEToLanguage(const char* ptr, unsigned int lang)
```

This is a helper wrapper function that can be used to convert the chemical name specified by 'ptr' from English to the language specified by 'lang'. The languages are specified by the constants in the *OELanguage* namespace.

3.2.58 OEToLatin1

```
std::string OEToLatin1(const char* ptr, const bool remove_markup = true)
```

Convert the string 'ptr', typically the output of the function *OECreateIUPACName* optionally post-processed by a language translation function, from the internal encoding, which uses \u escapes to represent non-ASCII characters, to Latin1 character encoding.

the 'remove_markup' flag controls the disposition of italics, superscript, and subscript markup. If the value is 'true' (the default), the markup is removed. If 'false', the markup is left in the output string, which should be post-processed.

Note

This function is not available in Java or Python as those language environments use other character sets.

3.2.59 OEToPolish

```
std::string OEToPolish(const char* ptr)
```

Convert the string 'ptr', typically the output of the function *OECreateIUPACName*, from English to Polish.

See *OELanguage* for character set information.

3.2.60 OEToPortuguese

```
std::string OEToPortuguese(const char* ptr)
```

Convert the string 'ptr', typically the output of the function *OECreateIUPACName*, from English to Portuguese.

See *OELanguage* for character set information.

3.2.61 OEToRomanian

```
std::string OEToRomanian(const char* ptr)
```

Convert the string 'ptr', typically the output of the function *OECreateIUPACName*, from English to Romanian.

See *OELanguage* for character set information.

3.2.62 OEToRussian

```
std::string OEToRussian(const char* ptr)
```

Convert the string 'ptr', typically the output of the function *OECreateIUPACName*, from English to Russian.

See *OELanguage* for character set information.

3.2.63 OEToSJIS

```
std::string OEToSJIS(const char* ptr)
```

Convert the string 'ptr', typically the output of the function *OECreateIUPACName* post-processed by a call to *OEToJapanese*, from the default encoding which uses \u escapes to represent unicode characters to instead use the Shift-JIS character encoding for Japanese characters.

3.2.64 OEToSlovak

```
std::string OEToSlovak(const char* ptr)
```

Convert the string 'ptr', typically the output of the function *OECreateIUPACName*, from English to Slovak.

See *OELanguage* for character set information.

3.2.65 OEToSpanish

```
std::string OEToSpanish(const char* ptr)
```

Convert the string 'ptr', typically the output of the function *OECreateIUPACName*, from English to Spanish.

See *OELanguage* for character set information.

3.2.66 OEToSwedish

```
std::string OEToSwedish(const char* ptr)
```

Convert the string 'ptr', typically the output of the function *OECreateIUPACName*, from English to Swedish.

See *OELanguage* for character set information.

3.2.67 OEToUTF8

```
std::string OEToUTF8(const char* ptr, const bool remove_markup = true)
```

Convert the string 'ptr', typically the output of the function *OECreateIUPACName* optionally post-processed by a language translation function, from the internal encoding, which uses \u escapes to represent non-ASCII characters, to UTF-8 character encoding.

The 'remove_markup' flag controls the disposition of italics, superscript, and subscript markup. If the value is 'true' (the default), the markup is removed. If 'false', the markup is left in the output string, which should be post-processed.

3.2.68 OEToWelsh

```
std::string OEToWelsh(const char* ptr)
```

Convert the string 'ptr', typically the output of the function *OECreateIUPACName*, from English to Welsh.

See *OELanguage* for character set information.

CHAPTER

FOUR

RELEASE HISTORY

4.1 Lexichem TK 2.9.5

Minor internal improvements have been made.

4.2 Lexichem TK 2.9.4

4.2.1 Minor Bug Fixes

- An issue has been fixed relating to IUPAC name generation where the term `substituted` was incorrectly inserted in certain cases.
- A round-trip conversion issue between SMILES and IUPAC names has been resolved for cases where a SMILES string contained a single asterisk.

4.3 Lexichem TK 2.9.3

Minor internal improvements have been made.

4.4 Lexichem TK 2.9.2

Minor internal improvements have been made.

4.5 Lexichem TK 2.9.1

Minor internal improvements have been made.

4.6 Lexichem TK 2.9.0

4.6.1 Minor bug fixes

- Custom polymer naming was added in the molecule-to-name workflow to avoid memory overflow when reading in large polymers.
- Kekulization was added in the molecule-to-name workflow to ensure that the same aromatic structures produce the same names.
- Support was added for some cases of complex (bis-, tris-, tetrakis-, etc.) multipliers in the molecule-to-name and name-to-molecule workflows.

4.7 Lexichem TK 2.8.1

Minor internal improvements have been made.

4.8 Lexichem TK 2.8.0

4.8.1 New features

- Many conventional names for inorganic salts have been added to the name parser.
- Parsing for some non-IUPAC names, including DMF and beta-alanine, have been added.

4.8.2 Major bug fixes

- Parsing of many common conventional inorganic salt names, such as calcium chloride, was corrected to include the correct number of anions in the resulting salt.
- Simple salt names no longer include a semicolon between parts of the name.

4.8.3 Minor bug fixes

- An issue with ketone oxime stereochemistry naming has been fixed.
- An issue in cycloalkane stereochemistry naming has been fixed.
- An issue in parsing of carbonate salt names has been fixed.

4.9 Lexichem TK 2.7.5

4.9.1 New features

- Some new antiviral drug names are now supported in the name to molecule workflow.

4.9.2 Minor bug fixes

- A bug with IUPAC naming of pyridine ring substitution has been fixed.

4.10 Lexichem TK 2.7.4

Fall 2021

4.10.1 New features

- Support for common alkaloid name conversion to `SMILES` was added.

4.10.2 Major bug fixes

- A bug where isotopes were not labeled on certain ring substituents when naming molecules or `SMILES` has been fixed.

4.10.3 Minor bug fixes

- A bug where pyrazole ring substituents were not numbered correctly has been fixed.
- A bug where reaction input was incorrectly parsed into a single molecule has been fixed so that reaction input is now rejected as invalid in the name to molecule workflow.

- A bug where primary amines with non-IUPAC names, such as methylethylamine, were incorrectly parsed into SMILES has been fixed.

4.11 Lexichem TK 2.7.3

July 2021

4.11.1 New features

- Support for input of many common drug names has been added.
- Support for SMILES input of disubstituted alkenes when unknown subsituents are marked as * has been added. For example, SMILES input of *CCC* is now parsed and named as 1,3-disubstitutedpropylene.

4.11.2 Major bug fixes

- An issue with naming of highly branched carbons structures has been fixed.

4.12 Lexichem TK 2.7.2

Fall 2020

4.12.1 Minor bug fixes

- An issue that caused the function *OEParseIUPACName* to incorrectly interpret elemental halogens as aromatic molecules due to their suffix "ine" has been fixed. Previously, the function failed to kekulize the halogens and therefore failed to parse them.
- An issue that caused the function *OEParseIUPACName* to fail to parse non-IUPAC names of carboxamide derivatives, such as benzimidazole-5-carboxylic acid, due to a failure to kekulize the benzimidazole rings has been fixed. 1H hydrogen is now added by default to benzimidazole if a prefix is not included to specify hydrogen locations.
- An issue that caused the function *OEParseIUPACName* to fail to parse names, such as carboxylic acid methyl amide, where methyl amide is used as a suffix has been fixed.

4.13 Lexichem TK 2.7.1

- Minor internal improvements have been made.

4.14 Lexichem TK 2.7.0

- Minor internal improvements have been made.

4.15 Lexichem TK 2.6.7

- Minor internal improvements have been made.

4.16 Lexichem TK 2.6.6

- Minor internal improvements have been made.

4.17 Lexichem TK 2.6.5

4.17.1 Minor bug fixes

- The name-to-structure conversion for amino acids has been improved.
- Recognition of several additional unnatural amino acids has been added.
- Problems with stereo handling and substituent numbering of some unnatural amino acids have been corrected.

4.17.2 Documentation changes

- Example documentation has been updated and a `-debug` flag has been added to the `mol2nam` and `nam2mol` examples.

4.18 Lexichem TK 2.6.4

- Minor internal improvements have been made.

4.19 Lexichem TK 2.6.3

4.19.1 Minor bug fixes

- Previously, redundant cis-trans stereochemistry for certain multi-ring aromatic systems was not suppressed, resulting in names with erroneous E-Z specifications. The stereo perception for these systems has been fixed.

4.20 Lexichem TK 2.6.2

4.20.1 New features

- The template-based Von Baeyer ring-naming scheme has been replaced with an algorithmic approach. This significantly improves the naming of complex ring systems.

4.21 Lexichem TK 2.6.1

4.21.1 Minor bug fixes

- A number of new high-frequency von Baeyer ring templates have been added.

4.22 Lexichem TK 2.6.0

4.22.1 New features

- *OEFromBritish* function has been added for completeness. The name perception code already handled British-style input names without this conversion function; however, it is useful to have the function available for use by higher-level APIs that dispatch based on input language.

4.22.2 Major bug fixes

- Handling of character sets for non-English language names has been improved. The internal string representation of all non-ASCII characters is now their \u escaped Unicode codepoints. Previously, Latin-1 characters (e.g., the output of the *OEToFrench*) were encoded as their Latin-1 bytes (0x80 - 0xff). Now they are encoded as escaped unicode. This eliminates character encoding problems for the Java and Python language wrappers that

occurred when intermediate name strings were being processed. Now, only the following final character set encoding/decoding functions need to handle non-ASCII bytes: *OEFromHTML*, *OEFromKOI8R*, *OEFromLatin1*, *OEFromUTF8*, *OEToEUCJP*, *OEToHTML*, *OEToSJIS*, *OEToLatin1*, and *OEToUTF8*.

4.22.3 Minor bug fixes

- Name-to-structure conversions for certain uncommon functional groups (nitramide, nitrile oxide, oxycyano) previously resulted in structures with 5-valent nitrogen. These now result in charge-separated N(III) structures, consistent with other nitrogen functional groups.

4.22.4 Documentation changes

- The documentation has been updated to indicate the range of Unicode codepoints that are handled for each of the language translation functions. This allows users to determine the appropriate output character set conversion. For example, the Chinese language translation results in CJK characters in the Unicode Basic Multilingual Plane (BMP). Therefore, it is only appropriate to convert Chinese language names to UTF8 or HTML, which can handle the full Unicode BMP. Since the French language translation results in ASCII and Latin-1 characters, it is reasonable to use Latin1, UTF8, or HTML as the output character set.
- The example programs have been updated to better illustrate character set conversions.

4.23 Lexichem TK 2.5.2

4.23.1 Major bug fixes

- The perception of certain complex ring systems has been changed. Ring systems with three separate fused components are now named using VonBaeyer nomenclature rather than fusion nomenclature. In all but a few cases, these are more closely aligned with the IUPAC preferred names, and the resulting names round trip correctly.

4.23.2 Minor bug fixes

- A bug affecting several specific VonBaeyer ring system numberings has been fixed.

4.24 Lexichem TK 2.5.1

4.24.1 New features

- Approximately 150 additional dictionary entries, including 2014 FDA small-molecule NDA approvals and some isotopic fragments for name suffixes, have been added.

4.24.2 Major bug fixes

- The naming of Von Baeyer ring systems has been reworked to fix the numbering assignment. Previously, the substituent ordering was sometimes incorrectly perceived, resulting in names with non-preferred numberings of substituents on rings.
- The naming of Von Baeyer polycyclic systems has been improved.

4.24.3 Minor bug fixes

- The handling of vowel elision for certain complex ring systems has been fixed.
- The naming of sulfur stereochemistry has been improved. Instances in which the sulfur stereo is in the suffix of the name (*e.g.*, “methyl (S)-methansulfinate”) are now correctly handled.

4.24.4 Documentation changes

- All examples have been rewritten (see the *Examples* chapter).
- The *translate* examples have been restructured to better handle the input and output character sets.
- Missing documentation for functions *OEGetIUPACCharSet*, *OEGetIUPACLanguage*, *OEGetIUPACNamStyle*, and constants *OECharSet* has been added. Documentation for other constants has been reworked.

4.25 Lexichem TK 2.5.0

4.25.1 New features

- Support for text markup (italics, superscripts, subscripts, special characters) has been improved and unified.
  - *OECreateIUPACName* function now generates names with the appropriate new text markup tokens (inspired by LaTeX):
    - Italics as: ~{}
    - Subscript as: _{}
    - Superscript as: ^{}
  - *OEToHTML* and *OEToUTF8* functions now properly handle the new markup tokens. *OEToUTF8* function has a new optional Boolean parameter that controls markup annotations. Set the new parameter to `false` in order to get the old behavior.
  - *OEFromHTML* function has been created to properly convert the markup to HTML tags.

4.25.2 Bug fixes

- The handling of molecules with relative stereochemistry has been improved. Relative stereochemistry is a feature of the V3000 file format encapsulated in the **OEChem TK**. See the OEGroupBase class.
- Name generation for molecules with stereochemistry is better due to improvements to the Cahn-Ingold-Prelog stereochemistry perception in **OEChem TK**.

4.26 Lexichem TK 2.4.2

4.26.1 Important note

- Custom dictionary entry points added in version 2.4.0 (but not documented) have been removed pending redesign/reimplementation.

4.26.2 New features

- New translate examples have been added for all languages (C++, C#, Java, Python).

4.26.3 Minor bug fixes

- A memory leak that occurred when naming certain structures with Von Baeyer rings has been fixed.
- String length overflows in language translation code have been fixed. These overflows were functionally benign but did show up with certain sanitizing compilers.
- The internal name dictionary has been cleaned up:
  - The dictionary lookup for names for which one entry is a strict substring of another(eg: AZT and AZTREONAM) has been fixed.

  - All nitro groups are now charge-separated (4-valent).
  - Dash vs. space separators are now handled gracefully. Dictionary entries with spaces now also match input names containing dashes.

- Warnings for name conversion failures have been modified. When a name cannot be converted, the warning is now "Failed to parse name: BADNAME". Additional developer-oriented messages about "unexpected tokens" are now debug-level messages and are not seen by default.

4.26.4 Documentation fixes

- PDF documentation will no longer throw a warning about "Arial-Bold bad BBox" in some PDF readers.

4.27 Lexichem TK 2.4.1

4.27.1 Minor bug fixes

- Tramadol removed from the dictionary since it is actually a racemic structure that was previously being returned as an absolute enantiomer.

4.28 Lexichem TK 2.4.0

4.28.1 New features

- Support for racemates and enhanced stereochemical name parsing.

4.28.2 Minor bug fixes

- Removed unbounded stack allocations.
- Corrected the form of metformin in the dictionary.
- Fixed an issue with names like p/m/o-bis(trifluoromethyl)benzene that were defaulting to the ortho form.
- Fixed parsing of (R,S)-3-ethyl 5-methyl 2-[(2-aminoethoxy)methyl]-4-(2-chlorophenyl)-6-methyl-1,4-dihydropyridine-3,5-dicarboxylate.
- Fixed an issue with an unnecessary isotopic prefix in the suffix for peroxycarboxylic acid esters.
- Added a number of ring templates.
- Fixed English to French translations that move the suffixes acetate, chloride, sulfate, and trisulfate to be prefixes connected with the "de" particle.

4.29 Lexichem TK 2.3.2

4.29.1 New features

- Added phosphorous oxychloride, and gleevec to the dictionary.
- Added a number of additional ring templates.
- Added support for isotopes in naming metal linking groups.
- Added structure to name support for deuterated water and phosphoryl trichloride.

4.29.2 Major bug fixes

- Fixed a memory leak in structure to name generation for simple tricyclic fused ring systems.

4.29.3 Minor bug fixes

- Reverted a regression in names like (R)-2-(1H-indol-1-yl)propanoic acid, where the locant position for the CIP stereo center was previously automatically determined.
- Updated the dictionary entry for lipitor to have two atorvastatin molecules and the water of crystallization.
- Updated anthramycin's representation to be canonical and isomeric.
- Tweaked the parser to correctly parse cyclosporin A without a warning.

4.30 Lexichem TK 2.3.0

4.30.1 New features

- Name generation for racemic structures when the 'MDL AND' group is present in the MDL V3000 format. Stereodescriptors 'rac', 'RS' and 'SR'. (Section P-92.1.3 of the IUPAC Nomenclature of Organic Compounds, Draft 2004 - Racemates and meso compounds). Racemic stereogenic centers are labeled with 'RS' if the CIP stereo descriptor is 'R' and has the MDL AND group present, else 'SR' if the stereogenic center has the CIP stereo descriptor 'S' and an MDL AND group present. The prefix 'rac' is used in front of a set of descriptors or locants, if all stereogenic centers in the molecule are racemic.

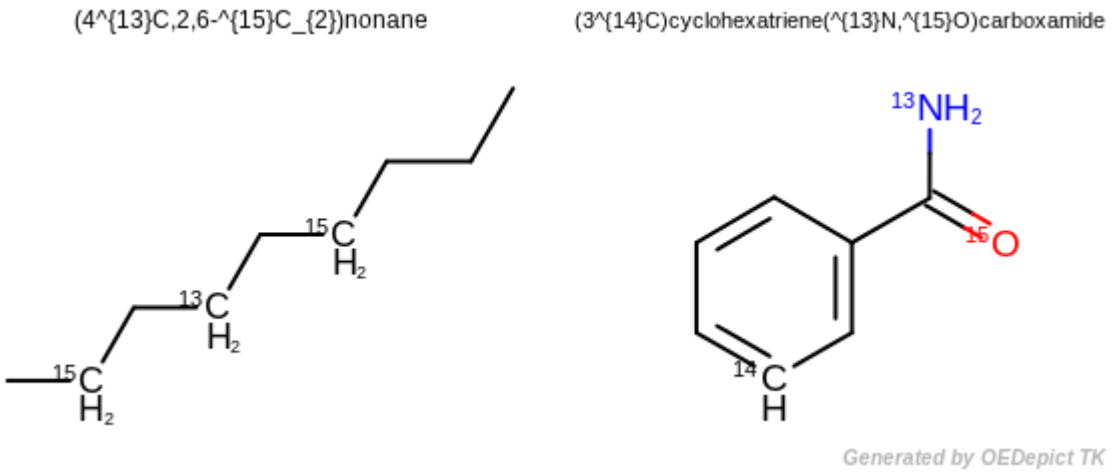


Fig. 1: **Isotope Example Depictions**

- Support has been added for name generation for isotopic carbon atoms in chains (e.g. the SMILES: `C[15CH2]C[13CH2]C[15CH2]CCC` will generate the name `(4^{13}C,2,6-^{15}C_{2})nonane`), simple rings and simple suffixes (e.g. the SMILES: `[13NH2]C(=[15O])C1=C[14CH]=CC=C1` will generate the name `(3^{14}C)cyclohexatriene(^{13}N,^{15}O)carboxamide`). The chemical structures generated from parsing the example SMILES strings into a molecule object are depicted in *Figure: Isotope Example Depictions*.
- Support for simple rings and simple suffixes in isotopic name generation e.g. the SMILES: `[13NH2]C(=[15O])C1=C[14CH]=CC=C1` will generate the name `(3^{14}C)cyclohexatriene(^{13}N,^{15}O)carboxamide`

4.30.2 Minor bug fixes

- Fixed Lexichem's thread safety. A global variable in Lexichem that has persisted since its first release in 2005, has been removed. This global variable affected the function *OEParseIUPACName*, used in name to structure conversion. Two thread safety issues used in structure to name conversion, namely: double bond (E/Z) CIP stereo (thread safety broken in the June 2012TK release) and enhanced relative stereochemistry (thread safety broken in the June 2013TK release), that affected the function *OECreateIUPACName*, have been resolved.
- *OEParseIUPACName* will no longer access invalid memory for names of the form '(di/tri/tetra)BLAH (ester/hydrazone/oxime/selenoxime/telluroxime/thioxime)'.

4.31 Lexichem TK 2.2.3

4.31.1 New features

- Added support for relative configuration (P-92.1.2 of IUPAC Nomenclature of Organic Compounds, Draft 2004). The stereodescriptors "rel", "R*" and "S*".

4.31.2 Minor bug fixes

- The synonym "english" now returns OELanguage::AMERICAN.

4.32 Lexichem TK 2.2.2

4.32.1 Bug fixes

- Fixed a number of dictionary entries: arestin, klinomycin, minocin, tetrodotoxin and vectrin.
- Added ring template. For a tetracyclic triaza ring system.
- Added support for automatically determining R/S stereo center position for molecules with 1 stereo center e.g. (R)-2-(1H-indol-1-yl)propanoic acid would set the R on position 2.
- Added the ability to parse names with benzylamide in.

4.33 Lexichem TK 2.2.0

4.33.1 Feature Requests

- Added an OEThrow.Warning, warning that names generated with BLAH are incorrect.
- Added support for the token BOC (tert-Butyloxycarbonyl).
- 'OEIUPAC::OEMatchDictionaryNames' added to extract names from Lexichem's dictionary.

4.33.2 Bug fixes

- Fixed a number of name failures concerning acenaphthoquinone derivatives.
- Added a number of ring templates and fixed an issue regarding loss of stereochemistry for the name N-[(E)-(1,3-dimethyl-4-piperidylidene)amino]-1,3-dimethyl-piperidin-4-imine on round-tripping.
- Added support for the name 7-chloro-1,3-dihydro-1-methyl-5-phenyl-1,4-benzodiazepin-2(3H)-one.
- Fixed a problem with locant numbering of bicyclic ring systems of the form bicyclo[3.1.0]hexane.
- Fixed rendering of cisplatin.
- Fixed a number of hydrazone entries.

- Removed all duplicates in dictionary.
- Fixed an issue with the name dicyclopentynyl acrylate.
- Fixed crashes on a number of malformed von Baeyer names.
- Fixed bug with sunitinib and triprolidine dictionary entries.
- Fixed 12H-benzo[g]pyrido[2,1-b]quinazoline ring system.

4.34 Lexichem TK 2.1.2

4.34.1 Bug fixes

- 4-methylimidazole now explicitly adds a hydrogen atom to the nitrogen atom in position 1.
- Added imidazole ring template.
- Added explicit hydrogen to 6 dictionary entries: arestin, klinomycin, minocin, parsalmide, tetrodotoxin and vectrin.
- Fixed crash with name bis(methacryloyloxymethyl)tricyclo[5.2,1,0^{2,6}.
- Fixed crash in name tetraethyn.
- Added ring template: iindeno[7,1-de:1',7'-fg][1,3,2]dioxaphosphocine.
- Corrected dictionary entry: O-orsellinic acid, o-phenanthroline and syrosingopine.

4.35 Lexichem TK 2.1.1

4.35.1 Bug fixes

- Fixed a bug with structure generation for tetramethylammonium pyrrolidine-2-carboxylate trihydrate.
- Components of salts are now separated by semi-colons.
- Added numerous dictionary entries.
- Added additional ring templates.
- Fixed a bug with names including benzene) or benzene}, the appropriate substitution should have been phenyl.
- Fixed an issue when incorrect von Baeyer names are parsed to Lexichem, Lexichem now fails silently.
- Fixed dictionary lookup algorithm.
- Fixed a crash in Mol2Nam when a H-atom was part of the main ring system in simple spiro compounds.
- Fixed a bug in names like sulfuric acid mono(x) ester.

4.36 Lexichem TK 2.1.0

- Performance benchmark results: conversion of canonical isomeric smiles to names and back to the same canonical isomeric smiles. Size of the databases are given in brackets after the name.

	v2.0.2	v2.1.0
Database	Round Tripping	Round Tripping
Maybridge (63872)	88.94%	98.69%
MDDR (111171)	48.69%	88.54%
NCI (250251)	84.54%	92.32%
Wombat (53214)	52.80%	89.54%

4.36.1 New features

- Added support for converting von Baeyer names to structures e.g. tricyclo[5.2.2.0^{3,5}]undecane is converted to :C1CC2CCC1CC3CC3C2.
- Added basic support for a number of steroid, alkaloid and terpene parent structures.
- Added support for L/D-amino acids.
- Added support for R-groups for name to structure conversion.
- Added support for both linear and branched polyspiro alicyclic hydrocarbons.
- Activated stereochemistry support for name to structure.
- Added a number of dictionary entries.
- Added a number of ring templates.
- Added partial support for von Baeyer name generation from structures.

4.36.2 Bug fixes

- Added support for names: 2H-imidazol-4-thiol and 1,2-dihydroimidazole-5-imine.
- Added support for barium(2+), sodium(1+).
- *LEXICHEM* now understands trifluoroneodymium.
- Added support for dihydrides e.g. calcium dihydride, magnesium dihydride.
- *LEXICHEM* now supports multi-ammonium salts and multi-derivative ethynyl pyridines.
- Added support for oxoarsinite based compounds.
- Added support for a number of additional metal linking groups e.g. Mg, K, La, Dy, Er, V, Ni etc.
- Fixed a bug in the name: 3-acetyl-8-bromo-1,2,3,6-tetrahydro-azepino[4,5-b]indole-2,5-dicarboxylic acid diethyl ester.
- Corrected unicode conversion for: acetate, glycinate, nitrite and iodide.

4.37 Lexichem TK 2.0.2

- Updated ring numbering templates that catch a significant fraction of ring naming failures in the NCBI's PubChem database.
- Updated the rules we use for naming the prefix "2-carboxyethyl" and friends, which we'd previously name "3-hydroxy-3-oxopropyl" (or similar).
- Added parsing support for the traditional prefix "phenethoxy".

- Removed the insertion of a single explicit space after a semi-colon. We now prefer to preserve the original input string, rather than beautify it. This also plays nicer with HTML style input, where "λ" really doesn't need an explicit space character after it.
- Added several minor tweaks to AutoNom-style naming, such as "isophthalic acid" and "benzene-1,2-carbaldehyde".
- Updated some erroneous SMILES in the dictionary including sulfamethoxazole and tinidazole.

4.38 Lexichem TK 2.0.0

- The applications have a new, standardized command line interface. Please have a look at the updated documentation for *mol2nam*, *nam2mol* and *translate*.
- This release includes the ability to parse stereo on input names. Previously it was read and ignored.
- Fixed a bug where, in rare cases, the output name depended on input atom ordering.
- Fixed a crash in determining CIP stereo for very large, pathological molecules.

4.39 Lexichem TK 1.9

- On a benchmark of 250251 compounds in the NCI00 database, `mol2nam` is able to convert 234297 structures (93.62%) to names without BLAH. Of these 234297 names, `nam2mol` is able to convert 231566 (98.83%) back into structures.
- This release includes a significant number of improvements to both name generation and name parsing. Several bugs have also been fixed. The name parsing conversion rate for the 71367 compound names in the 2003 Maybridge catalog is now up to 95.24%.
- Several improvements have been made to the specification of CIP stereochemistry during name generation. For example, previously linking groups such as `amidino`, `carbamimidoyl` and `diazenyl` would forget to specify E/Z descriptors if they contained a chiral double bond with specified stereochemistry. We would also fail to place some chiral prefixes such as `(E)-styrl` and `(Z)-cinnamyl` in brackets which can lead to ambiguity when interpreting the generated name.

4.40 Lexichem TK 1.8

- On a benchmark of 250251 compounds in the NCI00 database, `mol2nam` is able to convert 234296 structures (93.62%) to names without BLAH. Of these 234296 names, `nam2mol` is able to convert 228102 (97.36%) back into structures.
- This release includes a significant number of improvements to both name generation and name parsing. Several bugs have also been fixed. The name parsing conversion rate for the 71367 compound names in the 2003 Maybridge catalog is now up to 95.12%.
- One of the major parsing improvements in this release is the much improved support for handling von Baeyer ring nomenclature. We can now parse names such as:
  - '`1,4-dithioniabicyclo[2.2.2]octane`',
  - '`bicyclo[4.2.0]octa-1(6),2,4-triene`' and
  - '`2,4-diazaspiro[4.4]nonane-1,3-dione`'.

4.41 Lexichem TK 1.7

- On a benchmark of 250251 compounds in the NCI00 database, `mol2nam` is able to convert 234155 structures (93.57%) to names without BLAH. Of these 234155 names, `nam2mol` is able to convert 223246 (95.34%) back into structures.
- This release includes a significant number of improvements to both name generation and name parsing. Several bugs have also been fixed. The name parsing conversion rate for the 71367 compound names in the 2003 Maybridge catalog is now up to 93.81%.
- A new *OELowerCaseName* function has been added to the *Lexichem* toolkit API. This function converts the input chemical name to lower-case, whilst preserving the case sensitive aspects of IUPAC names. This functionality allows uppercase and mixed case names to be translated into English, as the `OEFrom<Foo>` functions assume their input is lowercase. For example, this feature allows `AGUA` to be recognized via *OEFromSpanish*.
- A new *OEReorderIndexName* function has been added to the *Lexichem* toolkit API. This function attempts to reorder the given permuted index name into a form that can be handled by the *OEParseIUPACName* function. For example, this will convert the string '`benzene, chloro-`' into '`chloro-benzene`'.
- A number of improvements and bug fixes have been made to *Lexichem*'s naming styles. For example, AutoNom and CAS permuted index styles are now far more AutoNom-like and CAS-like respectively. Naming of metallocenes and fullerenes is much improved.
- Some dramatic improvements have been made with foreign language support. On the 250251 compounds in the NCI00 database mentioned above, we now round-trip 100% to German and back without any differences. Japanese, Spanish and Swedish rates are all currently above 99%. Support for Hungarian and Polish has been dramatically improved.

4.42 Lexichem TK 1.6

- On a benchmark of 250251 compounds in the NCI00 database, `mol2nam` is able to convert 233010 structures (93.11%) to names without BLAH. Of these 233010 names, `nam2mol` is able to convert 221331 (94.99%) back into structures.
- This release includes a significant number of improvements to both name generation and name parsing. For example, both name generation and parsing now do a much better job on ring fusion nomenclature, for names like '`5,6,7,8-tetrahydro[1,2,4]triazolo[4,3-a]pyridine`'. There's also much improved handling of charged ring systems. The name parsing conversion rate for the 71367 compound names in the 2003 Maybridge catalog is now 93.25% in v1.6, up from 80.80% in v1.5.
- In name generation, new naming styles have been added for MDL/Beilstein AutoNom style names, for CAS permuted index style names (and there are new placeholder styles for IUPAC79 and IUPAC93 naming). A large number of improvements have been made to names generated using the 'traditional' naming style. A new *OECapitalizeName* API function is available to capitalizing the appropriate first letter of a generated name, such as '`p-tert-Butylbenzoic acid`'.
- Several bug fixes have been made to the Cahn-Ingold-Prelog (CIP) chirality perception implementation.
- The *OEParseIUPACName* function is now able return supplementary locant annotations for each atom. This function now stores an integer locant code/identifier in the integer atom type field of each atom, which may be retrieved using the `OEAtomBase.GetIntType` method and converted into a readable/displayable string using the recently exposed *OENameLocant* function. This functionality is a recent addition (obviously), and most but not all supported ring systems and parents have locant annotations in this initial release.
- Finally, for the adventurous, new APIs for translating compound names from foreign languages into English are available as the experimental *OEFromJapanese*, *OEFromSwedish* and *OEFromSpanish* functions. Additionally, a *OEFromUTF8* function is available for converting UTF-8 encoded strings into the escaped sequences expected by these functions (effectively the inverse of *OEToUTF8*).

4.43 Lexichem TK 1.5

- On a benchmark of 250251 compounds in the NCI00 database, `mol2nam` is able to convert 223066 structures (89.14%) to names without BLAH. Of these 223066 names, `nam2mol` is able to convert 192487 (86.29%) back into structures.
- This release includes a significant number of improvements to both name generation and name parsing. For example, `nam2mol` now supports more numbered locants, such as '`N1-methylaniline`' and for 'Maybridge-style' locant names such as `N'1` (interpreted as the more common `N1'`). These and similar changes have increased the conversion rate for the 71367 compound names in the 2003 Maybridge catalog, from 69.51% in v1.4 to 80.80% in v1.5.
- This release includes the ability to generate compound names in Japanese, and much improved Spanish and Polish naming support. In order to better support internationalization, APIs are now available to map from the default ISO-8859-1 output to either 7-bit ASCII, UTF-8, HTML and for Japanese locales, Shift-JIS or EUC-JP.
- Although impossible in the general case, several improvements have been made to *Lexichem*'s compound naming such that the assigned names are now more stable under arbitrary input ordering of atoms and bonds.

4.44 Lexichem TK 1.4

- On a benchmark of 250251 compounds in the NCI00 database, `mol2nam` is able to convert 221254 structures (88.41%) to names without BLAH. Of these 221254 names, `nam2mol` is able to convert 192345 (86.93%) back into structures.
- *Lexichem* v1.4 is predominantly a maintenance to provide a version of the *oeiupac* library that is compatible with *OEChem* v1.4. However, there have been a number of significant improvements to name parsing, and minor improvements to name generation since last month's v1.3 release.
- This release also includes the ability to generate compound names in several languages. In addition, to British spellings, *Lexichem* can now generate German, Italian, French, Spanish, Swedish, Dutch and Polish names. Whilst the translations for German, Italian, Swedish and Polish are quite comprehensive, those for French, Spanish and Dutch are less complete.
- A potential ambiguity with the ring names '`oxazole`' and '`thiazole`' has also been resolved. The IUPAC documentation states that it is permissible to omit locants from Hantzsch-Widman names when the locants are consecutive, *i.e.* '`1,2,3,4-tetrazole`' may be written as '`tetrazole`', and '`1,2-oxazirene`' is preferred as '`oxazirene`'. Unfortunately, this conflicts with the traditional interpretations of '`oxazole`' as meaning '`1,3-oxazole`' and '`thiazole`' as '`1,3-thiazole`'. Instead the traditional names '`isoxazole`' and '`isothiazole`' denote the '`1,2-`' forms. This ambiguity, that affected IUPAC-style (but not OpenEye-style) names, has been resolved by preserving the locants, so that the IUPAC names '`1,2-oxazole`', '`1,3-oxazole`', '`1,2-thiazole`' and '`1,3-thiazole`' are now generated for '`isoxazole`', '`oxazole`', '`isothiazole`' and '`thiazole`' respectively.

4.45 Lexichem TK 1.3

- On a benchmark of 250251 compounds in the NCI00 database, `mol2nam` is able to convert 221205 structures (88.39%) to names without BLAH. Of these 221205 names, `nam2mol` is able to convert 183444 (82.93%) back into structures.
- The major announcement of this release is the support for stereochemistry in compound naming. The CIP rules for assigning R/S descriptors to tetrahedral chiral centers, and E/Z descriptors to double bonds are used during name generation.

4.46 Lexichem TK 1.2

On a benchmark of 250251 compounds in the NCI00 database, `mol2nam` is able to convert 220949 structures (88.29%) to names without BLAH. Of these 220949 names, `nam2mol` is able to convert 182438 (82.57%) back into structures.

4.47 Lexichem TK 1.1

- On a benchmark of 250251 compounds in the NCI00 database, `mol2nam` is able to convert 220924 structures (88.28%) to names without BLAH. Of these 220924 names, `nam2mol` is able to convert 177145 (80.18%) back into structures.
- A new *OEIUPACIsLicensed* API has been added so allow applications to check whether *Lexichem*'s parsing and naming functionality can safely be used.

4.47.1 OEParseIUPACName Improvements

The *Lexichem* name parsing routines now handle a small number of structural abbreviations when parsing names. For example, it can now handle names like '`3-CF3-5-NO2-benzoic acid`'. The usual improvements in name parsing, including more entries for common names in the Lexichem dictionary. Support for names containing multiple explicit hydrogen locants, such as '`pyrimidine-2,4(1H,3H)-dione`' and '`2,4(1H,3H)-pyrimidinedione`'.

4.47.2 OECreateIUPACName Improvements

A serious bug that could cause a core dump when naming thioperoxoic acids has been fixed. The performance of compound naming has been improved. The usual improvements in the names generated (following the IUPAC standards more closely).

4.48 Lexichem TK 1.0

On a benchmark of 250251 compounds in the NCI00 database, `mol2nam` is able to convert 220922 structures (88.28%) to names without BLAH. Of these 220922 names, `nam2mol` is able to convert 177032 (80.13%) back into structures.

4.48.1 OEParseIUPACName Improvements

In addition to a great many other improvements to the name parsing code, the *Lexichem* parser now contains an internal dictionary allowing the recognition of common non-systematic names, such as 'ranitidine' and 'zantac'.

4.48.2 OECreateIUPACName Improvements

In addition to a great many improvements to the name generation code, the *Lexichem* naming functionality now allows the specification of a naming style, allowing the compound to be named in either a traditional, OpenEye, IUPAC, CAS or systematic naming style.

CHAPTER

FIVE

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CHAPTER

SIX

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CHAPTER

SEVEN

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↪http://www.eyesopen.com.
```

The version number for a floe package is displayed on the first page of the package's release notes. For example: https://docs.eyesopen.com/floe/modules/large_scale_floes/docs/source/releasenotes_2025_1.html.

7.3 Toolkits and Applications

To cite OpenEye toolkits or applications used in your work, please use the following:

```
OpenEye Toolkits [or Applications] <version-number>. OpenEye, Cadence Molecular Sciences,
↪ Santa Fe, NM. http://www.eyesopen.com.
```

For example:

```
OpenEye Toolkits 2024.2.1. OpenEye, Cadence Molecular Sciences, Santa Fe, NM. http://www.
↪eyesopen.com.
```

The Applications and Toolkits are released as a package, multiple times per year. The first part of the version number designates the calendar year. The version number appears on the summary document for the package.

If you want to cite an individual application or toolkit, you can use the syntax:

```
<product name> <version-number>. OpenEye, Cadence Molecular Sciences, Santa Fe, NM.␣
↪http://www.eyesopen.com.
```

where <*product name*> is:

- Bioisostere TK
- OEChem TK
- OEDepict TK
- OEDocking TK
- OEFF TK
- Eon TK
- FastROCS TK
- Grapheme TK
- GraphSim TK
- Lexichem TK
- OEMedChem TK
- MolProp TK
- Omega TK
- Quacpac TK
- Shape TK
- Spicoli TK
- Spruce TK
- Szmap TK
- Szybki TK
- Zap TK
- AFITT Application
- BROOD Application
- OEDocking Application
- EON Application
- OMEGA Application
- PICTO Application
- pKa-Prospector Application
- QUACPAC Application

- ROCS Application
- SiteHopper Application
- SPRUCE Application
- SZMAP Application
- SZYBKI Application
- VIDA Application

You can use the version number of the individual Application or Toolkit. For example:

```
SZYBKI Application 2.8.0.1. OpenEye, Cadence Molecular Sciences, Santa Fe, NM. http://
↪www.eyesopen.com.

Szybki TK 2.8.0.1. OpenEye, Cadence Molecular Sciences, Santa Fe, NM. http://www.
↪eyesopen.com.
```

The first documentation pages give the product names and version numbers, as in https://docs.eyesopen.com/applications/szybki/index.html and https://docs.eyesopen.com/toolkits/python/szybkitk/index.html.

7.4 Publications for Bibliographies

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

7.4.1 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

7.4.2 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

7.4.3 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

7.4.4 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

7.4.5 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

7.5 OpenEye MMDS Web Service

To cite use of the Macromolecular Data Service (MMDS) web service, please use the syntax:

```
Macromolecular Data Service <version-number>. OpenEye, Cadence Molecular Sciences, Santa␣
↪Fe, NM. http://www.eyesopen.com.
```

For example:

```
Macromolecular Data Service 1.1. OpenEye, Cadence Molecular Sciences, Santa Fe, NM.␣
↪http://www.eyesopen.com.
```

The MMDS version number appears on the web service's release notes.

CHAPTER

EIGHT

TECHNOLOGY LICENSING

OpenEye products use the following technology under license.

Some of the open source technologies we use are licensed under the GNU Public License (GPL) version 2 or 3. In all instances, these technologies are communicated with using the "at arms length" principle, using pipes and command line arguments.

While the software is in some instances assembled into a container, that assembly does not invoke the GPL copyleft scope. For each Floe package where these are used, the environment log clearly details the installed programs and their version numbers. With the links below for each technology, the source for each of those programs is available.

Table 1: Licensed Technology

Name of Project	Website	License URL
_libgcc_mutex	https://github.com/conda-forge/_libgcc_mutex-feedstock	https://github.com/conda-forge/_libgcc_mutex-feedstock/blob/master/LICENSE.txt
_openmp_mutex	https://github.com/conda-forge/_openmp_mutex-feedstock	https://github.com/conda-forge/_openmp_mutex-feedstock/blob/main/LICENSE.txt
ablang2	https://github.com/TobiasHeOl/AbLang2	https://github.com/TobiasHeOl/AbLang2/blob/main/LICENSE
abseil-cpp	https://github.com/abseil/abseil-cpp	https://github.com/abseil/abseil-cpp/blob/master/LICENSE
absl-py	https://github.com/abseil/abseil-py	https://github.com/abseil/abseil-py/blob/main/LICENSE

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Table 1 – continued from previous page

Name of Project	Website	License URL
aiohappyeyeballs	https://github.com/aio-libs/aiohappyeyeballs	https://github.com/aio-libs/aiohappyeyeballs/blob/main/LICENSE
aiohttp	https://docs.aiohttp.org/en/stable/	https://github.com/aio-libs/aiohttp/blob/master/LICENSE.txt
aiosignal	https://github.com/aio-libs/aiosignal	https://github.com/aio-libs/aiosignal/blob/master/LICENSE
Amazon Linux 2	https://aws.amazon.com/amazon-linux-2	N/A
AmberUtils	http://ambermd.org	N/A
ambit	https://github.com/khimaros/ambit	https://github.com/khimaros/ambit/blob/master/LICENSE
amqp	https://github.com/celery/py-amqp	https://github.com/celery/py-amqp/blob/master/LICENSE
anaconda-anon-usage	https://github.com/anaconda/anaconda-anon-usage	https://github.com/anaconda/anaconda-anon-usage/blob/main/LICENSE
angular	https://github.com/angular/angular.js	https://github.com/angular/angular.js/raw/master/LICENSE.md
angular-animate	https://github.com/angular/angular.js	https://github.com/angular/angular.js/raw/master/LICENSE.md
angular-cache	https://github.com/jmdobry/angular-cache	https://github.com/jmdobry/angular-cache/raw/master/LICENSE
angular-cookies	https://github.com/angular/angular.js	https://github.com/angular/angular.js/raw/master/LICENSE.md

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Table 1 – continued from previous page

Name of Project	Website	License URL
angular-loggly-logger	https://github.com/ajbrown/angular-loggly-logger	https://github.com/ajbrown/angular-loggly-logger/raw/master/LICENSE.md
angular-mocks	https://github.com/angular/angular.js	https://raw.githubusercontent.com/angular/angular.js/master/LICENSE
angular-resource	https://github.com/angular/angular.js	https://raw.githubusercontent.com/angular/angular.js/master/LICENSE
angular-toggle-switch	https://github.com/cgarvis/angular-toggle-switch	https://github.com/cgarvis/angular-toggle-switch/blob/master/LICENSE
angular-ui-grid	https://github.com/angular-ui/ui-grid	https://github.com/angular-ui/ui-grid
angular-ui-router	https://github.com/angular-ui/ui-router	https://github.com/angular-ui/ui-router/raw/master/LICENSE
angular-ui-tree	https://github.com/angular-ui-tree/angular-ui-tree	https://github.com/angular-ui-tree/angular-ui-tree/raw/master/LICENSE
angular-vs-repeat	https://github.com/kamilkp/angular-vs-repeat	https://raw.githubusercontent.com/kamilkp/angular-vs-repeat/master/LICENSE
aniso8601	https://bitbucket.org/nielsenb/aniso8601	https://bitbucket.org/nielsenb/aniso8601/src/master/LICENSE
annotated-types	https://github.com/annotated-types/annotated-types	https://github.com/annotated-types/annotated-types/blob/main/LICENSE
antlr4-python3-runtime	http://www.antlr.org OR https://pypi.org/project/antlr4-python3-runtin	https://github.com/conda-forge/antlr4-python3-runtin/blob/master/LICENSE.txt

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Table 1 – continued from previous page

Name of Project	Website	License URL
anyio	https://github.com/agronholm/anyio	https://github.com/agronholm/anyio/blob/master/LICENSE
appdirs	http://github.com/ActiveState/appdirs	http://github.com/ActiveState/appdirs/blob/master/LICENSE.txt
appengine	https://google.golang.org/appengine	https://github.com/golang/appengine/blob/master/LICENSE
arabic-reshaper	https://github.com/mpcabd/python-arabic-reshape	https://github.com/mpcabd/python-arabic-reshape/blob/master/LICENSE
archspec	https://github.com/archspec/archspec/blob/master/README.md	https://github.com/archspec/archspec/blob/master/COPYRIGHT
argon2-cffi	https://github.com/hynek/argon2-cffi	https://github.com/hynek/argon2-cffi/blob/master/LICENSE
argon2-cffi-bindings	https://github.com/hynek/argon2-cffi-bindings	https://github.com/hynek/argon2-cffi-bindings/blob/master/LICENSE
arpack	https://www.caam.rice.edu/software/ARPACK/	https://www.caam.rice.edu/software/ARPACK/
arrow	https://github.com/arrow-py/arrow	https://github.com/arrow-py/arrow?tab=Apache-2.0-1-ov-file#readme
ascii85	https://github.com/huandu/node-ascii85	https://github.com/huandu/node-ascii85/raw/master/LICENSE
ase	https://wiki.fysik.dtu.dk/ase/	https://wiki.fysik.dtu.dk/ase/development/licenseinfo.html#license-info
asgiref	https://github.com/django/asgiref/	https://github.com/django/asgiref/blob/main/LICENSE

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Table 1 – continued from previous page

Name of Project	Website	License URL
asn1crypto	https://github.com/wbond/asn1crypto	https://github.com/wbond/asn1crypto/blob/master/LICENSE
assertions go-render	https://github.com/smartystreets/assertions/internal/go-render/render	https://github.com/smartystreets/assertions/blob/master/internal/go-render/LICENSE
assertions oglmatchers	https://github.com/smartystreets/assertions/internal/oglematchers	https://github.com/smartystreets/assertions/blob/master/internal/oglematchers/LICENSE
assertions	https://github.com/smartystreets/assertions	https://github.com/smartystreets/assertions/blob/master/LICENSE.md
asttokens	https://github.com/gristlabs/asttokens	https://github.com/gristlabs/asttokens/blob/master/LICENSE
astunparse	https://github.com/simonpercivall/astunparse	https://github.com/simonpercivall/astunparse/blob/master/LICENSE
async-lru	https://github.com/aio-libs/async-lru	https://github.com/aio-libs/async-lru/blob/master/LICENSE
async-timeout	https://github.com/aio-libs/async-timeout	https://github.com/aio-libs/async-timeout/blob/master/LICENSE
atk-1.0	https://docs.gtk.org/atk/	https://gitlab.gnome.org/GNOME/atk/-/blob/master/COPYING
atomic	https://github.com/uber-go/atomic	https://github.com/uber-go/atomic/blob/master/LICENSE.txt

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Table 1 – continued from previous page

Name of Project	Website	License URL
atomicwrites	https://github.com/untitaker/python-atomicwrites	https://github.com/untitaker/python-atomicwrites/blob/master/LICENSE
attrs	https://www.attrs.org/	https://github.com/python-attrs/attrs/blob/main/LICENSE
aws-sdk-go	https://github.com/aws/aws-sdk-go	https://github.com/aws/aws-sdk-go/blob/master/LICENSE.txt
babel	https://babel.pocoo.org/ OR https://github.com/python-babel/babel	https://github.com/python-babel/babel/blob/master/LICENSE OR https://babel.pocoo.org/en/latest/license.html#babel-license
Babel	https://github.com/python-babel/babel	https://github.com/python-babel/babel/blob/master/LICENSE
backcall	https://github.com/takluyver/backcall	https://github.com/takluyver/backcall/blob/master/LICENSE
backports	https://github.com/brandon-rhodes/backports	https://github.com/brandon-rhodes/backports/blob/master/LICENSE.TXT
backports.functools-lru-cache	https://github.com/jaraco/backports.functools_lru_cache	https://github.com/jaraco/backports.functools_lru_cache/blob/main/LICENSE
backports.zstd	https://github.com/rogdham/backports.zstd	https://github.com/rogdham/backports.zstd?tab=License-1-ov-file#readme
base62	https://github.com/kare/base62	https://github.com/kare/base62/blob/main/LICENSE
beautifulsoup4	https://www.crummy.com/software/BeautifulSoup/	https://www.crummy.com/software/BeautifulSoup/

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Table 1 – continued from previous page

Name of Project	Website	License URL
billiard	https://github.com/celery/billiard	https://github.com/celery/billiard/blob/master/LICENSE.txt
biopython	https://biopython.org	https://github.com/biopython/biopython/blob/master/LICENSE.rst
biotite	https://github.com/biotite-dev/biotite/blob/master/README.rst	https://github.com/biotite-dev/biotite/blob/master/LICENSE.rst
bitarray	https://github.com/ilanschnell/bitarray	https://github.com/ilanschnell/bitarray/blob/master/LICENSE
bitset	https://github.com/willf/bitset	https://github.com/willf/bitset/blob/master/LICENSE
blas	https://www.netlib.org/blas/	https://www.netlib.org/blas/#_licensing
bleach	https://github.com/mozilla/bleach	https://github.com/mozilla/bleach/blob/main/LICENSE
blessings	https://github.com/erikrose/blessings	https://github.com/erikrose/blessings/blob/master/LICENSE
blinker	https://pythonhosted.org/blinker/	https://github.com/pallets-eco/blinker/blob/master/LICENSE
bokeh	https://github.com/bokeh/bokeh	https://github.com/bokeh/bokeh/blob/branch-4.0/LICENSE.txt
blosc	https://github.com/Blosc/python-blosc	https://github.com/Blosc/python-blosc/blob/master/LICENSE.txt
blosc2	https://github.com/Blosc/python-blosc2	https://github.com/Blosc/c-blosc2/blob/main/LICENSE.txt

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Table 1 – continued from previous page

Name of Project	Website	License URL
boltons	https://github.com/mahmoud/boltons	https://github.com/mahmoud/boltons/blob/master/LICENSE
Boltz	https://boltz.bio	https://github.com/jwohlwend/boltz/blob/main/LICENSE
boost	https://www.boost.org/doc/libs/1_71_0/libs/python/doc/html/index.html	https://www.boost.org/LICENSE_1_0.txt
boost-cpp	https://www.boost.org/doc/libs/1_71_0/libs/python/doc/html/index.html	https://www.boost.org/LICENSE_1_0.txt
bootstrap-vue	https://github.com/bootstrap-vue/bootstrap-vue	https://github.com/bootstrap-vue/bootstrap-vue/raw/master/LICENSE
boto3	https://github.com/boto/boto3	https://github.com/boto/boto3/blob/develop/LICENSE
botocore	https://github.com/boto/botocore	https://github.com/boto/botocore/blob/develop/LICENSE.txt
Bottleneck	https://bottleneck.readthedocs.io/en/latest/index.html	https://bottleneck.readthedocs.io/en/latest/license.html
Brotli	https://github.com/google/brotli	https://github.com/google/brotli/blob/master/LICENSE
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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Table 1 – continued from previous page

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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Table 1 – continued from previous page

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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Table 1 – continued from previous page

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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Table 1 – continued from previous page

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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Table 1 – continued from previous page

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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Table 1 – continued from previous page

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-file#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
tiffile	https://github.com/cgohlke/tiffile/	https://github.com/cgohlke/tiffile/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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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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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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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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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

8.1 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.

8.1.1 GCC RUNTIME LIBRARY EXCEPTION

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Version 3.1, 31 March 2009

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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,␣
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↪subsequent versions published by the FSF.

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

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

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The availability of this Exception does not imply any general presumption that third-
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See also

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

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  Some devices are designed to deny users access to install or run
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pattern of such abuse occurs in the area of products for individuals to
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stand ready to extend this provision to those domains in future versions
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  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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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
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Component, and (b) serves only to enable use of the work with that
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"Major Component", in this context, means a major essential component
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  The "Corresponding Source" for a work in object code form means all
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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,
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   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,
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works, which are not by their nature extensions of the covered work,
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"aggregate" if the compilation and its resulting copyright are not
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beyond what the individual works permit.  Inclusion of a covered work
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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,
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