

OpenEye
SCIENTIFIC

FastROCS TK – C#

Release 2026.1.0

Cadence Design Systems, Inc.

August 06, 2026

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> **Note**
>
> **FastROCS TK** is available in Python, Java, and C++ on 64-bit Linux platforms only.

CHAPTER

ONE

INTRODUCTION

FastROCS TK is an extremely fast shape comparison application, based on the idea that molecules have similar shape if their volumes overlay well and any volume mismatch is a measure of dissimilarity. It uses a smooth Gaussian function to represent the molecular volume [Grant-1996], so it is possible to routinely minimize to the best global match. FastROCS will perform millions of these global shape matches every second. See the Molecular Shape section in the **Shape TK** theory documentation for a description of the shape and color theory used in FastROCS TK.

Now, in just seconds, FastROCS TK can perform a virtual screen over an entire multi-conformer representation of a corporate collection to find active compounds with similar shape to a lead compound (a task that could previously take up to a day [Rush-2005]). Recent work suggests that the underlying ligand-based shape similarity approach is competitive with, and often superior to, structure-based approaches in virtual screening [Hawkins-2007] [Venhorst-2008], both in terms of overall performance and consistency [Sheridan-2008]. Alignments to crystallographic conformations have also been useful in pose prediction in the absence of a protein structure [Sutherland-2007].

In addition to virtual screening and lead hopping, FastROCS TK can be used to perform NxN shape comparisons over an entire multiconformer database. A prototype of clustering with FastROCS TK can be found in the SphereExclusionClustering.py example program.

CHAPTER

TWO

FASTROCS VS ROCS

OpenEye makes available two separate shape based virtual screening technologies:

ROCS
: Thousands of conformers per second

FastROCS
: Millions of conformers per second

The ROCS technology is also embodied in the Shape TK. The Shape TK is a very flexible toolkit for experimenting with molecular shape and different ways that it can be applied. FastROCS is also deployed as a toolkit, but with a very different goal in mind: **raw performance**. In order to achieve this raw performance GPU hardware is utilized. The use of GPUs required the complete rewrite of the ROCS algorithm to work well on GPUs. Furthermore, the opportunity was taken to completely rethink all trade-offs the algorithm makes in preference to speed. Therefore, it is expected that ROCS and FastROCS will output slightly different results.

In order for FastROCS to achieve a throughput of millions of conformers per second the entire informatics base of shape comparison had to be reimagined. FastROCS operates on millions of conformers in memory, in parallel, all at once. Whereas, the Shape TK will typically only operate on a single molecule at a time. Therefore, FastROCS is designed as a web service to serve shape queries from a database pre-loaded into memory: ShapeDatabaseServer.py example. The ShapeDatabaseServer.py is the best place for new users to start.

The ShapeDatabaseServer.py example is built around the most important API in FastROCS TK, the *OEShapeDatabase*. The *OEShapeDatabase* class is built to be a natural extension of the OEMolDatabase class in **OEChem TK**. The *OEShapeDatabase* object will manage the storage of conformers in memory and interacting with any GPU in the system. Theoretically, the user of *OEShapeDatabase* should not have to know that their calculation is being performed on a GPU.

> **Note**
>
> For batch processing operations where databases are brought into memory temporarily, the BestShapeOverlay.py is a better first script to read and alter.

CHAPTER

THREE

INSTALLATION

1. Install the OpenEye Toolkits into a virtual environment:

```
$ mkvirtualenv fastrocs
(fastrocs) $ pip install --extra-index-url https://pypi.anaconda.org/OpenEye/simple␣
↪OpenEye-toolkits
```

2. Once installed, follow the instructions in tutorial_basic_usage to get you started.

3.1 Prerequisites

3.1.1 GPU-Related Requirements

The following features are required in order to use GPU-accelerated OpenEye toolkits and applications.

Supported Platforms

CUDA-enabled OpenEye software is only available on supported Linux platforms. For supported Linux platforms see the Platform Support Page.

Supported GPUs

An NVIDIA Tesla, Quadro, or GeForce GPU with a **compute capability of 3.5 or higher** is required on your system. For a comprehensive table of compute capability categories for each GPU, please refer to the CUDA Wikipedia page.

NVIDIA Drivers

- **Minimum NVIDIA Driver version: 450.x**.
- CUDA is **not** required to be installed.

We recommend driver 450.80.02, and we strongly advise manually downloading and installing the appropriate NVIDIA driver for your system as opposed to using a package manager.

To install, root privilege is required. Follow these steps:

1. Download the driver to the machine you are installing it on.
2. `chmod +x` the driver package to make it executable.
3. Ensure you have disabled X-server by killing any running sessions. Reboot may be required if X-server is still running after this step.

> **Warning**
>
> Disabling X-server requires different processes to be killed depending on your Linux distribution. See the NVIDIA installation guide for more details.

> **Warning**
>
> The NVIDIA kernel module can often conflict with the open source Nouveau display drivers, depending on your specific Linux distribution. The NVIDIA documentation is a much more complete and up-to-date source for information on how to work around this issue. See Disabling Nouveau on the NVIDIA website.

4. Install the driver by `sudo ./NVIDIA-Linux-x86_64-450.80.02.run` and follow the step-by-step installation instructions.

For more details on driver installations, see the CUDA Installation Guide

> **Note**
>
> The output of the `nvidia-smi` command is extremely useful when debugging GPU issues. Please include the output from `nvidia-smi` in any request to support@eyesopen.com.

Performance Tuning

To get the most performance out of an NVIDIA graphics card, use the persistence daemon to switch persistence mode across all cards on the system (root privilege required):

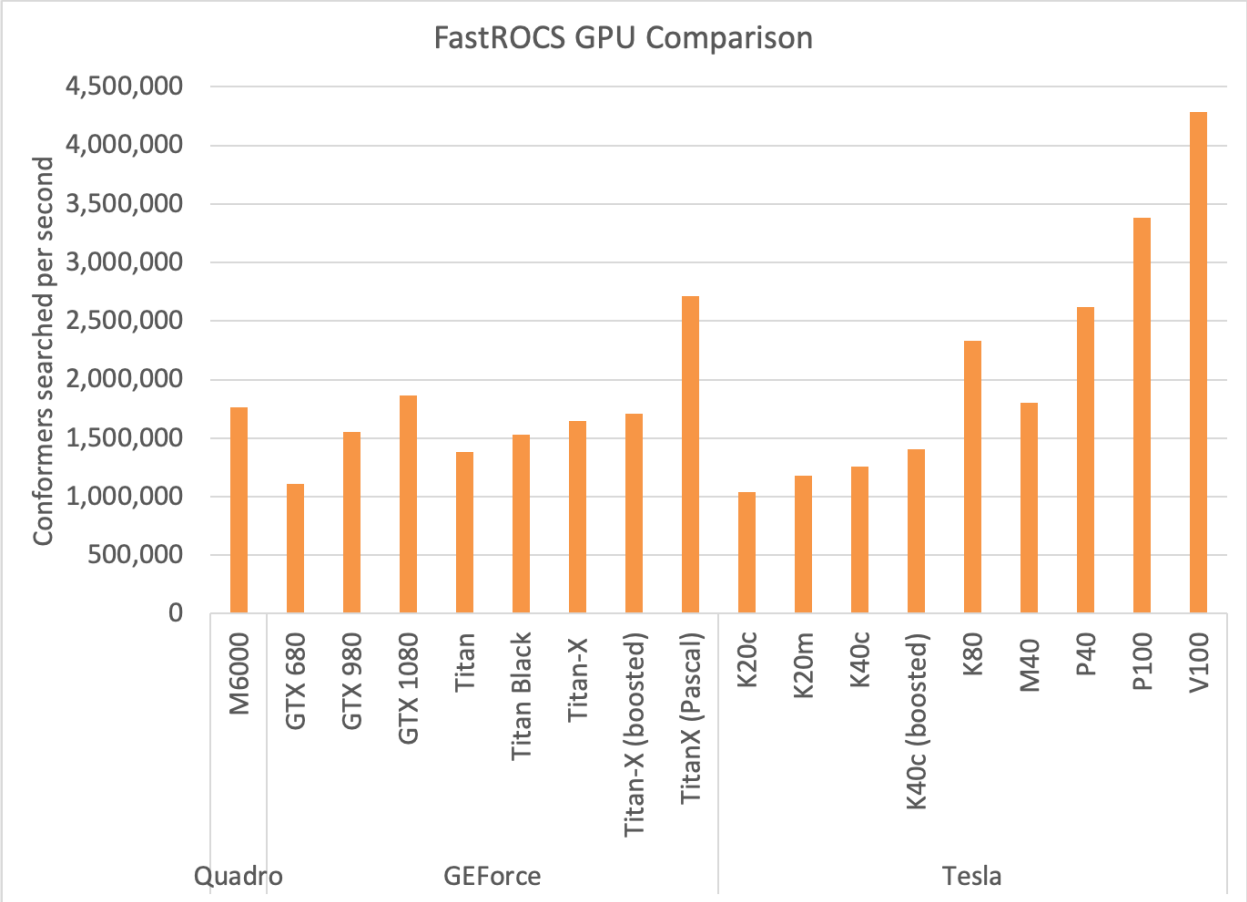
```
sudo nvidia-persistenced --user foo
```

This will automatically enable persistence mode after reboot.

For full instructions on the persistence daemon, see the Persistence daemon section of the NVIDIA docs.

3.2 Hardware Performance Comparison

The following graph shows the performance of **FastROCS TK** on some modern GPU models.



Note

Performance can vary with driver versions and other factors. The above graph is meant as a general guide of what performance customers can expect. It is highly recommended to go with a certified vendor like Exxact to ensure best performance.

CHAPTER

FOUR

FASTROCS ARCHITECTURE

4.1 Memory Usage

A rule of thumb is 1 GB of main memory for every 4 million conformers. The primary variable **FastROCS TK** users need to think about is how many conformers per molecule is needed. The **OMEGA** default of 200 conformers per molecule is much higher than it needs to be due to **OEDocking** vs **ROCS** virtual screening performance. **OEDocking** needs a higher number of conformers than **ROCS** does. **ROCS** can perform quite well with 10-50 conformers per molecule. The number of conformers chosen has a direct linear relationship to **FastROCS** query performance and the amount of memory needed.

Note

The "rule of thumb" is based upon the number of heavy atoms being normally distributed around 25-30 heavy atoms. The number of heavy atoms also has a linear relationship to the memory consumption. So fragment databases will be significantly smaller, but large macro-cycle peptide databases will be significantly larger.

Note

The above "rule of thumb" assumes the default of four inertial starts and no alternative starting points. If you choose to use eight inertial starts, you should assume you'll need about 1.5 as much main memory, i.e. 1.5 GB for every 4 million conformers. If you choose to use alternative starts, you should multiply the amount of main memory by the number of alternative starts / 3.

Color scoring does significantly increase virtual screening performance. As much color information, centroids and self terms, is cached in memory as well. For doing pure *OEShapeDatabaseType.Shape* analysis, color information can be elided allowing for a small percentage in memory size reduction, around 5-10%. For a more complete breakdown of memory usage, use the *OEShapeDatabase.PrintMemoryUsage* method to print statistics on memory usage.

Note

Color atom and self term calculation is a dominating factor in how fast **FastROCS** can load molecules from disk. Therefore, it is heavily recommended to pre-process OEB files with *OEPrepareFastROCSMol*.

It is important to note that **FastROCS** is most sensitive to host main memory, not GPU memory. On board GPU memory size does not heavily affect **FastROCS** performance, so buying the cheaper GPUs with less memory is just fine for **FastROCS**.

> **Note**
>
> This memory overhead will be improved over time. Significant advances were made in version 1.4.0, memory consumption per conformer was cut in half. Then cut in half again for the 1.7.0 release.

4.2 Multi-GPU Scaling

FastROCS will automatically scale across as many GPUs as can be found on the current machine. It is not uncommon or overly expensive to get a machine with 4-8 GPUs in it. As with any parallel program, truly optimal linear scaling is difficult to achieve, but FastROCS gets fairly close as can be seen in the below graph.

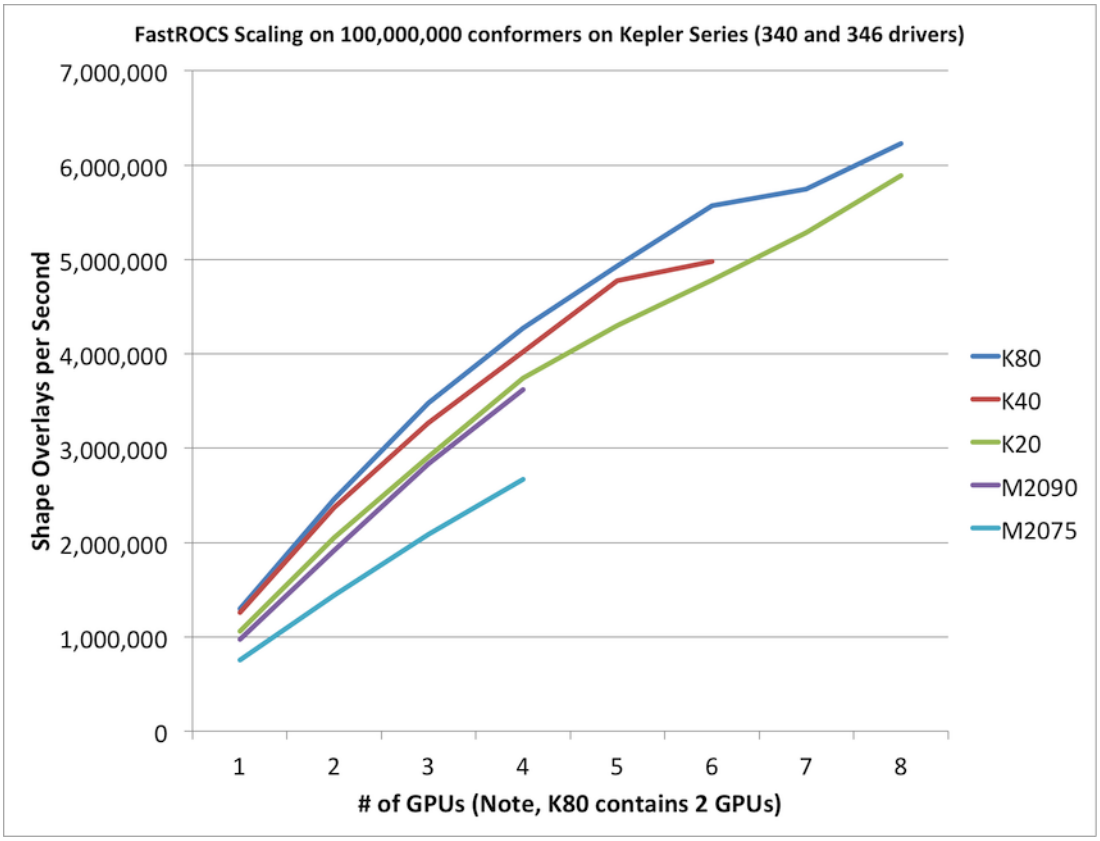


Fig. 1: This graph is a comparison of the various generations of Tesla compute cards produced by NVidia for high performance computing purposes.

> **Note**
>
> Static color calculations are still performed on the CPU. For best performance, a decent mid-range CPU with 2-cores per GPU is recommended.

The *OEShapeDatabase* class will by default automatically scale across all GPUs and CPUs in the system. In this way it can be a very large resource hog for CPU, GPU, and memory. There are some methods provided on the class to control resource utilization, but the current best control is through the CUDA_VISIBLE_DEVICES environment variable.

4.3 Multi-Node Scaling

Scaling FastROCS across multiple nodes is possible with the included `ShapeDatabaseProxy.py` example.

CHAPTER

FIVE

EXAMPLES

5.1 FastROCS Example Suite

FastROCS comes with a variety of scripts for configuring, reporting, and debugging. For more details of how to use these examples please see the *Tutorials* section.

5.1.1 Simple Examples

5.1.2 Alternative Starts

5.1.3 Client-Server

CHAPTER

SIX

TUTORIALS

CHAPTER

SEVEN

API

7.1 OEFastROCS Classes

7.1.1 OEDBTracer

```
class OEDBTracer : public OEDBTracerBase
```

A thread-safe implementation of *OEDBTracerBase* meant for tracking the progress of a *OEShapeDatabase* query.

The following methods are publicly inherited from *OEDBTracerBase*:

SetTotal	*Update*

Constructors

```
OEDBTracer(size_t numBins = 0)
```

Construct a new thread-safe `OEDBTracer` object and initialize the internal synchronization primitives that are required.

The `numBins` argument specifies how many bins the internal *OEFastROCSHistogram* will have. The granularity of each bin is the determined by the range of the score divided by the number of bins. Note, *`OEShapeDatabaseType.Shape`* and *`OEShapeDatabaseType.Color`* have a range of 0.0-1.0, while *`OEShapeDatabaseType.Combo`* has a range of 0.0-2.0.

GetCounts

```
OEULongLong GetCounts(bool blocking = false)
```

Returns the current number of conformers already searched by a *OEShapeDatabase*. This is a thread-safe function for querying the current progress of the database search. *OEShapeDatabase* will update the progress of this tracer through the *`OEDBTracer.Update`* method from multiple threads. This function can be used by another thread to query that total progress.

The optional `blocking` parameter specifies whether the call should wait until there has been an update to the tracer before returning. This can be useful for making progress updates not spin too rapidly reporting the same number every time.

GetHistogram

```
OEFastROCSHistogram GetHistogram()
```

Return a copy of the histogram currently accumulated in this database query as a *OEFastROCSHistogram* object. This histogram will be empty if `numBins` passed to the constructor is `0`.

This is a thread-safe function for querying the current distribution of scores for the molecules already processed. The full histogram of the scores is not available until the value returned by *OEDBTracer.GetCounts* is equal to *OEDBTracer.GetTotal*.

GetNumBins

```
size_t GetNumBins() const
```

Return the number of bins to use for the score histogram during this particular query. Returning '0', the default, will indicate to *OEShapeDatabase.GetScores* or *OEShapeDatabase.GetSortedScores* to skip histogram creation all together.

GetTotal

```
OEULongLong GetTotal()
```

Return the total number of conformers to be processed.

> **Warning**
>
> It is possible for this function to return `0` for a short time after a call to *OEShapeDatabase.GetScores* or *OEShapeDatabase.GetSortedScores*. So a `0` return value should be taken with a grain of salt of that possible race-condition.

SetTotal

```
void SetTotal(OEULongLong total)
```

Called by *OEShapeDatabase.GetScores* and *OEShapeDatabase.GetSortedScores* to set whatever the total number of conformers that will be processed.

Update

```
void Update(OEULongLong step = 1,
            const OEFastROCSHistogram* hist = NULL)
```

Called by *OEShapeDatabase.GetScores* and *OEShapeDatabase.GetSortedScores* from multiple threads to communicate the current progress of the search.

7.1.2 OEDBTracerBase

```
class OEDBTracerBase
```

Abstract base class used by *OEShapeDatabase* to track the progress of an individual search against the database. Users should derive from this class and pass the derived class into *OEShapeDatabaseOptions.SetTracer* for the options object later passed into *OEShapeDatabase.GetScores* or *OEShapeDatabase.GetSortedScores*.

> **Warning**
>
> *OEShapeDatabase.GetScores* and *OEShapeDatabase.GetSortedScores* are multi-threaded functions, so the `Update` method implemented by a derived class should be thread-safe.

The following classes derive from this class and should be used in preference of creating a custom tracer:

- *OEDBTracer*

GetNumBins

```
size_t GetNumBins() const
```

Return the number of bins to use for the score histogram during this particular query. Returning '0', the default, will indicate to *OEShapeDatabase.GetScores* or *OEShapeDatabase.GetSortedScores* to skip histogram creation all together.

SetTotal

```
void SetTotal(OEULongLong total)=0
```

Called once by *OEShapeDatabase.GetScores* or *OEShapeDatabase.GetSortedScores* in a single thread to indicate the total number of conformers that will be searched.

Update

```
void Update(OEULongLong step = 1,
            const OEFastROCSHistogram* hist = NULL)=0
```

Called many times by *OEShapeDatabase.GetScores* or *OEShapeDatabase.GetSortedScores* from many operating system threads so this function should be thread-safe. The *OEShapeDatabase* object will pass in a large `step` size to optimize the number of times this function is called, typically only hundreds of times will this method be called for a database containing millions of conformers. The `step` corresponds to the number of conformers already searched. Even so, this function should be implemented with very efficiently as it is called by the *OEShapeDatabase* search threads, so forward progress can not be made if this function is costly.

The optional `hist` argument is a *OEFastROCSHistogram* to accumulate into a master histogram for the entire query. Typically, *OEShapeDatabase.GetScores* and *OEShapeDatabase.GetSortedScores* will submit will call this method once for very large chunks of the database. This makes the synchronization point of calling this function very minimal to the overall runtime of the query. If a `NULL` pointer is passed, the default, no histogram accumulation will occur.

> **Warning**
>
> The implementer of a sub-class of *OEDBTracerBase* should guarantee the thread-safety of this method.

7.1.3 OEFastROCSHistogram

```
class OEFastROCSHistogram
```

This class is returned from *OEDBTracer.GetHistogram* during and after a query is sent to *OEShapeDatabase.GetScores* or *OEShapeDatabase.GetSortedScores*. It is used to contain a list of frequencies representing the distribution of scores. This same container is used to contain the frequencies of the following 3 score types:

- *OEShapeDatabaseType.Shape*
- *OEShapeDatabaseType.Color*
- *OEShapeDatabaseType.Combo*

Constructors

```
OEFastROCSHistogram(size_t numBins = 200)
```

Construct a new histogram with the specified number of "bins" in which to bin the score distribution. The same number of bins is applied to each score type.

```
OEFastROCSHistogram(const OEFastROCSHistogram& rhs)
```

Copy constructor for moving a *OEFastROCSHistogram* in memory.

GetHistogram

```
void GetHistogram(std::vector<unsigned int>& frequencies,
                  unsigned int scoreType)
```

Initializes the `frequencies` vector to the required size to contain the number of bins for this histogram, then fills it with the number of molecules that falls within each bin for the `scoreType` specified. The `scoreType` should be one of the following:

- *OEShapeDatabaseType.Shape*
- *OEShapeDatabaseType.Color*
- *OEShapeDatabaseType.Combo*

GetNumBins

```
size_t GetNumBins() const
```

Returns the number of bins used for this histogram. The number of bins determines the granularity of the scores.

Update

```
void Update(const OEFastROCSHistogram& rhs)
```

Sum the histogram `rhs` into this histogram. This histogram will then reflect the total of the two histograms. Used for aggregating histograms during the execution of *OEShapeDatabase.GetScores* or *OEShapeDatabase.GetSortedScores*.

```
void Update(const OEShapeDatabaseScore& score)
```

Updates this histogram from an individual *OEShapeDatabaseScore* object usually representing one molecule during the execution of *OEShapeDatabase.GetScores* or *OEShapeDatabase.GetSortedScores*.

7.1.4 OEShapeDatabase

```
class OEShapeDatabase
```

This is the primary class for performing **FastROCS TK** calculations. It is a very heavy-weight object:

- consuming many gigabytes of memory
- managing many host threads
- managing all GPU interaction

The goal is to allow abstracting away the complexities as much as possible to allow writing to a single API, allowing for the improvement of the underlying compute engine over time.

Ideally, this class is initialized once per dataset. There is a fair amount of pre-calculation done on each molecule and conformer while being loaded into memory. Some of this can be alleviated by pre-calculating and caching, but not all of it, as there is a balance between caching and recalculation that is always being tuned.

Constructors

```
OEShapeDatabase(const OEShape::OEColorForceField& cff,
                unsigned int dbtype = OEShapeDatabaseType::Default)
OEShapeDatabase(unsigned int dbtype = OEShapeDatabaseType::Default,
                unsigned int cfftype = OEShape::OEColorFFType::OEDefault)
```

Create a new *OEShapeDatabase* for managing conformers and performing **FastROCS TK** calculations.

Whether the *OEShapeDatabase* can perform color calculations must be chosen at construction. If "shape only" is chosen by passing *OEShapeDatabaseType.Shape*, then there can be significant memory and load-time performance improvements. Color atom assignment can be a significant cost during load and increase memory usage by roughly 2x.

A custom OEColorForceField can be passed to this constructor as well to allow color scoring to be completely customized. Note, in the case of a custom color force field, *OEShapeDatabaseType.Default* is assumed. It is currently not possible to perform a "color only" scoring.

AddMol

```
unsigned int AddMol(const OEChem::OEMCMolBase& mol,
                    const unsigned orient = OEFastROCSOrientation::Inertial)
```

Add a new collection of conformers to this database and return the index used to identify this molecule. This index will start at `0` and monotonically increase by 1 for every multi-conformer molecule added. *OEShapeDatabaseScore.GetMolIdx* will return this index to be able to map **FastROCS** scores to molecules added through this mechanism.

If using alternative start method *OEFastROCSOrientation.AsIs*, this constant needs to be passed as the final argument to the AddMol routine so the database can be loaded without pre-processing conformer coordinates. The final argument is ignored for all other use cases and does not need to be changed from the default argument as all molecules are identically pre-processed for all other starting points.

Warning

Databases must be re-added if using *OEFastROCSOrientation.AsIs*

Note

Even though this method is not `const`, it has been made thread-safe so that it can be called from multiple threads. Furthermore, it has been optimized as much as possible to parallelize the pre-calculation this method performs. This makes it very efficient to use multiple threads to load a database file into memory.

GetColorForceFieldType

```
unsigned int GetColorForceFieldType() const
```

Return a constant from the `OEColorFFType` namespace to indicate the color force field used to construct this database. Returns `OEColorFFType.Custom` if a custom OEColorForceField object was passed to the constructor.

GetColorGridSpacing

```
float GetColorGridSpacing() const
```

Return the grid spacing used to calculate color scores. This defaults to `0.5` for good performance. Lower values will yield answers that agree more closely with the `Exact` analytical calculation, at the expense of performance. Higher values can yield better performance. The default was chosen as a good balance of virtual screening statistical analysis (AUCs) versus raw throughput performance.

GetDatabaseType

```
unsigned int GetDatabaseType() const
```

Returns a constant from the *OEShapeDatabaseType* namespace indicating what type of calculations this database can perform.

GetDeviceToHostStrategy

```
unsigned int GetDeviceToHostStrategy() const
```

GetHostToDeviceStrategy

```
unsigned int GetHostToDeviceStrategy() const
```

GetMaxNumDevices

```
unsigned int GetMaxNumDevices() const
```

Returns the maximum number of GPU devices this database will use for calculations. The only way to restrict the GPUs seen by the database is to use the `CUDA_VISIBLE_DEVICES` environment variable before starting the process.

See also

- *OEShapeDatabase.SetNumDevices*

GetMaxOptIterations

```
unsigned int GetMaxOptIterations() const
```

Return the number of optimizer iterations the **FastROCS** algorithm should use when optimizing the alignment of the database conformer and the query conformer. This currently defaults to `10` based upon analysis of producing good virtual screening statistics (AUCs) without excessive iterations that would cost performance.

GetNumDevices

```
unsigned int GetNumDevices() const
```

Returns the number of GPU devices this database will use for calculation. This will default to all the GPUs that are visible, i.e., the value returned from *OEShapeDatabase.GetMaxNumDevices*.

GetNumThreadsPerDevice

```
unsigned int GetNumThreadsPerDevice() const
```

GetNumOpenThreads

```
unsigned int GetNumOpenThreads() const
```

Return how many CPU threads will be used to read a OEMolDatabase from disk into memory using the *OEShapeDatabase.Open* method. The default, a value of `0`, is to use as many CPUs as can be found on the system with `OEGetNumProcessors`.

GetScores

```
OESystem::OEIterBase<OEShapeDatabaseScore> * GetScores(const OEChem::OEMolBase& query,
                                                       const OEShapeDatabaseOptions&␣
↪options = OEShapeDatabaseOptions()) const
OESystem::OEIterBase<OEShapeDatabaseScore> * GetScores(const OEShape::OEShapeQueryPublic&
↪ shapeQry,
                                                       const OEShapeDatabaseOptions&␣
↪options = OEShapeDatabaseOptions()) const
OESystem::OEIterBase<OEShapeDatabaseScore> * GetScores(const OEShape::OEShapeQuery&␣
↪shapeQry,
                                                       const OEShapeDatabaseOptions&␣
↪options = OEShapeDatabaseOptions()) const
```

Return **ALL** scores of the query against the entire database subject to the options specified in the *OEShapeDatabaseOptions* passed to this method. This is useful for performing larger scale `NxN` clustering type of calculations where all pairs of scores need to be processed.

The query can be either a single conformer OEMolBase, a OEShapeQuery or a OEShapeQueryPublic object read from a `.sq` file. OEShapeQuery or OEShapeQueryPublic objects must contain a molecule. To determine if your OEShapeQuery object is **FastROCS**-friendly see `OEIsFastROCSShapeQuery` in the **Shape TK**.

When passing an OEMolBase query, the molecule must have 3D coordinates assigned and must have been preprocessed with *OEPrepareFastROCSMol* before calling this method.

Warning

The order of the *OEShapeDatabaseScore* returned by the iterator is non-deterministic and will certainly change for each execution due to the multi-threaded nature of this method. However, the values calculated in each *OEShapeDatabaseScore* will be the same. Therefore, users should rely on the return value of *OEShapeDatabaseScore.GetMolIdx* and *OEShapeDatabaseScore.GetConfIdx* to do further processing, not the location within the iterator.

See also

The *OEShapeDatabaseOptions* class is used to control many of the parameters to this method. For example, how many conformers per molecule to return.

GetShapeGridSpacing

```
float GetShapeGridSpacing() const
```

Return the grid spacing used to calculate shape scores and drive the alignment. This defaults to `0.5` for good performance. Lower values will yield answers that agree more closely with the `Exact` analytical calculation, at the expense of performance. Higher values can yield better performance. The default was chosen as a good balance of virtual screening statistical analysis (AUCs) versus raw throughput performance.

GetSortedScores

```
OESystem::OEIterBase<OEShapeDatabaseScore> * GetSortedScores(const OEChem::OEMolBase&␣
↪query,
                                                             unsigned int limit = 0)␣
↪const
OESystem::OEIterBase<OEShapeDatabaseScore> * GetSortedScores(const OEChem::OEMolBase&␣
↪query,
                                                             const␣
↪OEShapeDatabaseOptions& options) const
OESystem::OEIterBase<OEShapeDatabaseScore> * GetSortedScores(const␣
↪OEShape::OEShapeQueryPublic& shapeQry,
                                                             const␣
↪OEShapeDatabaseOptions& options = OEShapeDatabaseOptions()) const
OESystem::OEIterBase<OEShapeDatabaseScore> * GetSortedScores(const OEShape::OEShapeQuery&
↪ shapeQry,
                                                             const␣
↪OEShapeDatabaseOptions& options = OEShapeDatabaseOptions()) const
```

Return a hitlist of the `query` against the database based upon the scoring options of the database and the *OEShapeDatabaseOptions* passed to this method. The *OEShapeDatabaseScore* will be returned in descending order, i.e., the better 'hits' will come first in the iterator.

The query can be either a single conformer OEMolBase, a OEShapeQuery or a OEShapeQueryPublic object read from a `.sq` file. OEShapeQuery or OEShapeQueryPublic objects must contain a molecule. To determine if your OEShapeQuery object is **FastROCS**-friendly see `OEIsFastROCSShapeQuery` in the **Shape TK**.

When passing an OEMolBase query, the molecule must have 3D coordinates assigned and must have been preprocessed with *OEPrepareFastROCSMol* before calling this method.

Note

This method is typically used to select only a subset of the results based upon `limit` or *OEShapeDatabaseOptions.SetLimit*. It is optimized for rapidly constructing relatively small hitlists. If the entire set of scores for the database is desired, it can be faster to use the *OEShapeDatabase.GetScores* to avoid the sorting operation.

See also

The *OEShapeDatabaseOptions* class is used to control many of the parameters to this method. For example, how many conformers per molecule to return.

NumConfs

```
unsigned int NumConfs() const
```

Return the number of conformers the database is currently managing. Useful for getting a ballpark idea of the underlying memory usage.

Note

This value has no relation to the indexes returned by *OEShapeDatabase.AddMol*, except that this value will always be larger than the last index returned.

Open

```
bool Open(const OEChem::OEMolDatabase& moldb,
          const unsigned int orient = OEFastROCSOrientation::Inertial)
bool Open(const OEChem::OEMolDatabase& moldb,
          OESystem::OEThreadedDots& dots,
          const unsigned int orient = OEFastROCSOrientation::Inertial)
```

Initialize the database using a OEMolDatabase. This is the most efficient way to initialize a *OEShapeDatabase* as this method will launch an operating thread for each CPU core available and parallelize all the parsing and pre-calculation. The progress of the loading operation can be tracked through a thread-safe OEThreadedDots object.

If using alternative start method *OEFastROCSOrientation.AsIs*, this constant needs to be passed as the final argument to the Open routine so the database can be loaded without adjusting conformer coordinates. The final argument can be left blank for all other use cases.

Warning

Databases must be re-opened if using *OEFastROCSOrientation.AsIs*

This method will block and return `true` when the database has been successfully loaded into memory.

Note

The indices returned by *OEShapeDatabaseScore.GetMolIdx* are guaranteed to map directly into the OEMolDatabase index space. `OEMolDatabase.GetMolecule` can fail and return no molecule for good reason, i.e., an empty molecule from an SD file. Therefore, the index space used by *OEShapeDatabase* can have "holes" when initialized from a OEMolDatabase.

PrintMemoryUsage

```
void PrintMemoryUsage(OEPlatform::oeostream& os) const
void PrintMemoryUsage() const
```

Print out memory usage statistics for this object. This will break down how much memory is being used to pre-cache various parts of the calculation. By default, the output will be written to `OEPlatform.oeerr`. The output stream can also be passed as an argument. The diagnostic output is meant for human consumption and may change format in future releases.

SetColorGridSpacing

```
bool SetColorGridSpacing(float gridSpacing)
```

Set the grid spacing to use for static color scoring.

See also

- *OEShapeDatabase.GetColorGridSpacing*

SetDeviceToHostStrategy

```
void SetDeviceToHostStrategy(unsigned int strat)
```

SetHostToDeviceStrategy

```
void SetHostToDeviceStrategy(unsigned int strat)
```

SetMaxOptIterations

```
void SetMaxOptIterations(unsigned int maxIter)
```

Set the number of optimizer iterations to use when optimizing the alignment by shape.

See also

- *OEShapeDatabase.GetMaxOptIterations*

SetNumDevices

```
void SetNumDevices(unsigned int ndevices)
```

Set the number of GPU devices this calculation should use. This number should be between 1 and *OEShapeDatabase.GetMaxNumDevices* inclusively. This method is really only useful to efficiently collecting **FastROCS** scalability data across multiple GPUs. To restrict *OEShapeDatabase* to only run on a subset of GPUs on the machine, use the `CUDA_VISIBLE_DEVICES` environment variable instead before the process is launched.

SetNumThreadsPerDevice

```
void SetNumThreadsPerDevice(unsigned int numThrds)
```

SetNumOpenThreads

```
void SetNumOpenThreads(unsigned int numThrds)
```

Set how many CPU threads should be created to read a OEMolDatabase from disk into memory using the *OEShapeDatabase.Open* method. A value of `0` specifies that all CPUs in the system will be used. The value passed to this method should not exceed the value returned by `OEGetNumProcessors`.

SetShapeGridSpacing

```
bool SetShapeGridSpacing(float gridSpacing)
```

Set the grid spacing to use for shape scoring and alignment.

See also

- *OEShapeDatabase.GetShapeGridSpacing*

7.1.5 OEShapeDatabaseOptions

```
class OEShapeDatabaseOptions
```

This class is used to control the behavior of *OEShapeDatabase.GetScores* and *OEShapeDatabase.GetSortedScores*. It allows setting options on a per-search basis.

Note

It is possible for the options selected in this class to not match the settings of the constructed *OEShapeDatabase* causing an error to be thrown.

Constructors

```
OEShapeDatabaseOptions()
OEShapeDatabaseOptions(const OEShapeDatabaseOptions &)
```

Default constructor for creating a new instance with default options. The copy constructor will copy all the options into a new object.

Assignment operator.

ClearCutoff

```
void ClearCutoff()
```

Removes the cutoff from this set of options. The default is to have no cutoff value specified.

See also

- *OEShapeDatabaseOptions.GetCutoff*
- *OEShapeDatabaseOptions.HasCutoff*
- *OEShapeDatabaseOptions.SetCutoff*
- *OEShapeDatabaseOptions.GetCutoffLT*
- *OEShapeDatabaseOptions.HasCutoffLT*
- *OEShapeDatabaseOptions.SetCutoffLT*

ClearTracer

```
void ClearTracer()
```

Removes the progress bar tracer from this set of options.

Note

This does not release the memory of the *OEDBTracerBase* previously passed to *OEShapeDatabaseOptions.SetTracer*.

See also

OEShapeDatabaseOptions.SetTracer

ClearUserStarts

```
void ClearUserStarts()
```

Removes any user inertial starts that have been previously set.

See also

OEShapeDatabaseOptions.SetUserStarts *OEShapeDatabaseOptions.GetUserStarts*
OEShapeDatabaseOptions.GetNumStarts

GetColorForceFieldType

```
unsigned int GetColorForceFieldType() const
```

GetColorOptimization

```
bool GetColorOptimization() const
```

Returns true if color score is being optimized in addition to shape score.

See also

- *OEShapeDatabaseOptions.SetColorOptimization*

GetCutoff

```
float GetCutoff() const
```

Returns the cutoff currently set in this set of options. The default is a cutoff of `0.0`, i.e., no cutoff, all scores will be returned. This is mutually exclusive to *OEShapeDatabaseOptions.GetCutoffLT*.

Note

This cutoff is applied to the final ranking score used. For a *OEShapeDatabaseType.Shape* database, that means only the "shape" score. For the default database type, *OEShapeDatabaseType.Default*, the cutoff is applied to the sum of the shape and color components (*OEShapeDatabaseScore.GetTanimotoCombo*).

See also

- *OEShapeDatabaseOptions.HasCutoff*
- *OEShapeDatabaseOptions.SetCutoff*
- *OEShapeDatabaseOptions.ClearCutoff*

GetCutoffGT

```
float GetCutoffGT() const
```

This method is identical in functionality to *OEShapeDatabaseOptions.GetCutoff* and is mutually exclusive to *OEShapeDatabaseOptions.GetCutoffLT*.

See also

- *OEShapeDatabaseOptions.GetCutoff*

GetCutoffLT

```
float GetCutoffLT() const
```

Returns the cutoff currently set in this set of options. The default is no cutoff, all scores will be returned. This method applies to a cutoff set using *OEShapeDatabaseOptions.SetCutoffLT* to retrieve results less than or equal to the cutoff value.

Note

This cutoff is applied to the final ranking score used. For a *OEShapeDatabaseType.Shape* database, that means only the "shape" score. For the default database type, *OEShapeDatabaseType.Default*, the cutoff is applied to the sum of the shape and color components (*OEShapeDatabaseScore.GetTanimotoCombo*).

See also

- *OEShapeDatabaseOptions.HasCutoffLT*
- *OEShapeDatabaseOptions.SetCutoffLT*
- *OEShapeDatabaseOptions.ClearCutoff*

GetInitialOrientation

```
unsigned int GetInitialOrientation() const
```

Returns the initial orientation to be used for the overlay optimization drawn from the *OEFastROCSOrientation* namespace. The default orientation is *OEFastROCSOrientation.Inertial*

See also

- *OEShapeDatabaseOptions.SetInitialOrientation*
- *OEShapeDatabaseOptions.GetNumStarts* .. oe:method:: GetInitialOrientation

GetFastROCSMode

```
unsigned int GetFastROCSMode() const
```

Returns the calculation mode to be used for the overlay optimization drawn from the *OEFastROCSMode* namespace. The default mode is *OEFastROCSMode.FastROCS*

See also

- *OEShapeDatabaseOptions.SetFastROCSMode*

GetLimit

```
unsigned int GetLimit() const
```

Returns the number of individual molecule "hits" that will be returned from *OEShapeDatabase.GetSortedScores*, i.e., the number of individual *OEShapeDatabaseScore* objects that will be returned.

Note

This method has no effect on the *OEShapeDatabase.GetScores* method.

GetMaxConfs

```
unsigned int GetMaxConfs() const
```

Returns the maximum number of conformers to return per molecule. By default this value is 1 indicating only the best conformer of a molecule that matched the query molecule will be returned as a single *OEShapeDatabaseScore* object. The conformer with the highest score will be indicated by the *OEShapeDatabaseScore.GetConfIdx* method.

GetMaxOverlays

```
unsigned int GetMaxOverlays() const
```

Returns the maximum number of starting points per conformer overlaid. By default this value is 1 indicating only the best of all optimizations performed will be returned.

GetMaxRandomTranslation

```
float GetMaxRandomTranslation() const
```

Returns the maximum allowed translation when using random starting orientations. The default maximum is 2 angstroms.

See also

- *OEShapeDatabaseOptions.SetMaxRandomTranslation*
- *OEShapeDatabaseOptions.SetInitialOrientation*
- *OEShapeDatabaseOptions.GetInitialOrientation*
- *OEShapeDatabaseOptions.SetNumRandomStarts*
- *OEShapeDatabaseOptions.GetNumRandomStarts*
- *OEShapeDatabaseOptions.SetRandomSeed*
- *OEShapeDatabaseOptions.GetRandomSeed*
- *OEFastROCSOrientation*

GetNumInertialStarts

```
unsigned int GetNumInertialStarts() const
```

Returns the number of inertial starts used as starting points for the shape optimization. The default value is 4 starting points oriented along the principle moment of inertia.

GetNumStarts

```
unsigned int GetNumStarts() const
unsigned int GetNumStarts(const OEChem::OEMolBase& query) const
```

Returns the number of alternative starting points set for shape optimization. When using *OEFastROCSOrientation.InertialAtHeavyAtoms* or *OEFastROCSOrientation.InertialAtColorAtoms* the query molecule is required by the method. If alternative starts have **not** been set or *OEFastROCSOrientation.AsIs* is set, these methods will return a value of 1.

See also

- *OEShapeDatabaseOptions.SetInitialOrientation*
- *OEShapeDatabaseOptions.SetUserStarts*
- *OEShapeDatabaseOptions.ClearUserStarts*
- *OEFastROCSOrientation*

GetNumColorAtomStarts

```
unsigned int GetNumColorAtomStarts(const OEChem::OEMolBase& query) const
```

Returns the number of color atom starting points set for shape optimization. This method requires *OEShapeDatabaseOptions.SetInitialOrientation* to be set to *OEFastROCSOrientation.InertialAtColorAtoms* and the query molecule. If the query molecule does not have color atoms the search will throw a warning and default to *OEFastROCSOrientation.Inertial*.

See also

- *OEShapeDatabaseOptions.SetInitialOrientation*
- *OEShapeDatabaseOptions.GetNumStarts*
- *OEFastROCSOrientation*

GetNumHeavyAtomStarts

```
unsigned int GetNumHeavyAtomStarts(const OEChem::OEMolBase& query) const
```

Returns the number of heavy atom starting points set for shape optimization. This method requires *OEShapeDatabaseOptions.SetInitialOrientation* to be set to *OEFastROCSOrientation.InertialAtHeavyAtoms* and the query molecule.

See also

- *OEShapeDatabaseOptions.SetInitialOrientation*
- *OEShapeDatabaseOptions.GetNumStarts*
- *OEFastROCSOrientation*

GetNumRandomStarts

```
unsigned int GetNumRandomStarts() const
```

Returns the number of random starting orientations when using the *OEFastROCSOrientation.Random* alternative start. The default value is 10.

See also

- *OEShapeDatabaseOptions.SetNumRandomStarts*
- *OEFastROCSOrientation*
- *OEShapeDatabaseOptions.SetInitialOrientation*
- *OEShapeDatabaseOptions.GetInitialOrientation*
- *OEShapeDatabaseOptions.SetMaxRandomTranslation*
- *OEShapeDatabaseOptions.GetMaxRandomTranslation*
- *OEShapeDatabaseOptions.SetRandomSeed*
- *OEShapeDatabaseOptions.GetRandomSeed*

GetNumUserStarts

```
unsigned int GetNumUserStarts() const
```

Returns the number of user-defined starting points set for shape optimization. This method requires *OEShapeDatabaseOptions.SetInitialOrientation* to be set to *OEFastROCSOrientation.UserInertialStarts* and user-starts to have been set with *OEShapeDatabaseOptions.SetUserStarts*.

See also

- *OEShapeDatabaseOptions.SetInitialOrientation*
- *OEShapeDatabaseOptions.SetUserStarts*
- *OEShapeDatabaseOptions.ClearUserStarts*
- *OEShapeDatabaseOptions.GetNumStarts*
- *OEFastROCSOrientation*

GetRandomSeed

```
unsigned int GetRandomSeed() const
```

Returns the random seed to be used with *OEFastROCSOrientation.Random*. The default random seed is set based on the time.

See also

- *OEShapeDatabaseOptions.SetRandomSeed*
- *OEFastROCSOrientation*
- *OEShapeDatabaseOptions.SetInitialOrientation*
- *OEShapeDatabaseOptions.GetInitialOrientation*
- *OEShapeDatabaseOptions.SetNumRandomStarts*
- *OEShapeDatabaseOptions.GetNumRandomStarts*
- *OEShapeDatabaseOptions.SetMaxRandomTranslation*
- *OEShapeDatabaseOptions.GetMaxRandomTranslation*

GetScoreType

```
unsigned int GetScoreType() const
```

Returns the score type drawn from the *OEShapeDatabaseType* namespace to be used for the search.

GetSimFunc

```
unsigned int GetSimFunc() const
```

Returns the type of similarity function to be used to score the search results. The constant type returned is either 'Tanimoto' or 'Tversky' which is drawn from the *OEShapeSimFuncType* namespace.

GetTracer

```
OEDBTracerBase* GetTracer() const
```

Returns a pointer to the *OEDBTracerBase* to be used to track the progress of this search. Returns a `NULL` pointer to indicate that no tracer has been registered.

GetTverskyAlpha

```
float GetTverskyAlpha() const
```

Returns the alpha coefficient used in the Tversky similarity calculation. See *OEShapeDatabaseOptions.SetTverskyCoeffs* for details of how to set alpha. The default value is `0.95`.

GetTverskyBeta

```
float GetTverskyBeta() const
```

Returns the beta coefficient used in the Tversky similarity calculation. See *OEShapeDatabaseOptions.SetTverskyCoeffs* for details of how to set beta. The default value is `0.05`.

GetUserStarts

```
bool GetUserStarts(vector<float>& startsCoords) const
```

Fills a float vector of size `number of starts * 3` with the starting coordinates previously set with *OEShapeDatabaseOptions.SetUserStarts*. To ensure vector of the correct size is passed in as an argument, the *OEShapeDatabaseOptions.GetNumStarts* method can be used to retrieve the number of starts set. If successful the return value will be true.

Warning

Code is not available. **FastROCS TK** is supported only in Python.

See also

- *OEShapeDatabaseOptions.ClearUserStarts*
- *OEShapeDatabaseOptions.SetUserStarts*

HasCutoff

```
bool HasCutoff() const
```

Returns a boolean value indicating whether a cutoff value, at which all scores greater than or equal to the value will be saved and all scores less than the value will be discarded, has been previously registered with this set of options. By default this is `false`, no cutoff. If *OEShapeDatabaseOptions.SetCutoff* or *OEShapeDatabaseOptions.SetCutoffGT* has been called already, this will return `true`. *OEShapeDatabaseOptions.ClearCutoff* will set this back to `false` again. This method is mutually exclusive to *OEShapeDatabaseOptions.HasCutoffLT*

See also

- *OEShapeDatabaseOptions.HasCutoffGT*
- *OEShapeDatabaseOptions.GetCutoff*
- *OEShapeDatabaseOptions.SetCutoff*
- *OEShapeDatabaseOptions.ClearCutoff*

HasCutoffGT

```
bool HasCutoffGT() const
```

This method is identical in functionality to *OEShapeDatabaseOptions.HasCutoff* and is mutually exclusive to *OEShapeDatabaseOptions.HasCutoffLT*.

See also

- *OEShapeDatabaseOptions.HasCutoff*
- *OEShapeDatabaseOptions.GetCutoffGT*
- *OEShapeDatabaseOptions.SetCutoffGT*
- *OEShapeDatabaseOptions.ClearCutoff*

HasCutoffLT

```
bool HasCutoffLT() const
```

Returns a boolean value indicating whether a cutoff value, at which all scores less than or equal to the value will be saved and all scores greater than the value will be discarded, has been previously registered with this set of options. By default this is `false`, no cutoffLT. If *OEShapeDatabaseOptions.SetCutoffLT* has been called already, this will return `true`. *OEShapeDatabaseOptions.ClearCutoff* will set this back to `false` again. This method is mutually exclusive to *OEShapeDatabaseOptions.HasCutoffGT*

See also

- *OEShapeDatabaseOptions.GetCutoffLT*
- *OEShapeDatabaseOptions.SetCutoffLT*
- *OEShapeDatabaseOptions.ClearCutoff*

SetColorForceField

```
bool SetColorForceField(const OEShape::OEColorForceField& cff)
```

SetColorForceFieldType

```
bool SetColorForceFieldType(unsigned int type)
```

SetColorOptimization

```
void SetColorOptimization(bool ColorOptimization)
```

Set to true to optimize over color score in addition to shape score. Default is false.

Note

optimizing over color will impact performance. A decrease in 5-20% can be expected.

See also

- *OEShapeDatabaseOptions.GetColorOptimization*

SetCutoff

```
void SetCutoff(float cutoff)
```

Sets the cutoff to use when filtering the results of *OEShapeDatabase.GetScores* and *OEShapeDatabase.GetSortedScores*. Only *OEShapeDatabaseScore* objects greater than or equal to `cutoff` depending on the score type will be returned. This method is mutually exclusive to *OEShapeDatabaseOptions.SetCutoffLT*

Note

This cutoff is applied to the final ranking score used. For a *OEShapeDatabaseType.Shape* database, that means only the "shape" score. For the default database type, *OEShapeDatabaseType.Default*, the cutoff is applied to the sum of the shape and color components (*OEShapeDatabaseScore.GetTanimotoCombo*).

See also

- *OEShapeDatabaseOptions.GetCutoff*
- *OEShapeDatabaseOptions.HasCutoff*
- *OEShapeDatabaseOptions.ClearCutoff*

SetCutoffGT

```
void SetCutoffGT(float cutoff)
```

This method is identical in functionality to *OEShapeDatabaseOptions.SetCutoff* and is mutually exclusive to *OEShapeDatabaseOptions.SetCutoffLT*.

See also

- *OEShapeDatabaseOptions.SetCutoff*

SetCutoffLT

```
void SetCutoffLT(float cutoff)
```

Sets the cutoff to use when filtering the results of *OEShapeDatabase.GetScores* and *OEShapeDatabase.GetSortedScores*. Only *OEShapeDatabaseScore* objects less than or equal to `cutoff` depending on the score type will be returned.

This method is mutually exclusive to *OEShapeDatabaseOptions.SetCutoff*.

Note

This cutoff is applied to the final ranking score used. For a *OEShapeDatabaseType.Shape* database, that means only the "shape" score. For the default database type, *OEShapeDatabaseType.Default*, the cutoff is applied to the sum of the shape and color components (*OEShapeDatabaseScore.GetTanimotoCombo*).

See also

- *OEShapeDatabaseOptions.GetCutoffLT*
- *OEShapeDatabaseOptions.HasCutoffLT*
- *OEShapeDatabaseOptions.ClearCutoff*

SetFastROCSMode

```
void SetFastROCSMode(unsigned int FRMode)
```

Sets the calculation mode to be used for the overlay optimization drawn from the *OEFastROCSMode* namespace. The default mode is *OEFastROCSMode.FastROCS*

See also

- *OEShapeDatabaseOptions.SetFastROCSMode*

SetInitialOrientation

```
bool SetInitialOrientation(unsigned int orient)
```

Set the initial orientation to be used for optimization of the overlap. The options are drawn from the *OEFastROCSOrientation* and the default is *OEFastROCSOrientation.Inertial*. If user-defined inertial starts are to be used then the starting coordinates must be set using the *OEShapeDatabaseOptions.SetUserStarts* method. Returns true if successful.

See also

- *OEShapeDatabaseOptions.SetUserStarts*
- *OEShapeDatabaseOptions.GetInitialOrientation*
- *OEFastROCSOrientation*

SetNumRandomStarts

```
bool SetNumRandomStarts(unsigned int numStarts)
```

Set the number of random starting orientations when using the *OEFastROCSOrientation.Random* alternative start. The default value is 10.

Warning

Search speed and the amount of RAM required are proportional to the number of starting orientations therefore speed & memory degradation are to be expected if searching with a large number of random starting orientations.

See also

- *OEShapeDatabaseOptions.GetNumRandomStarts*
- *OEFastROCSOrientation*
- *OEShapeDatabaseOptions.SetInitialOrientation*
- *OEShapeDatabaseOptions.GetInitialOrientation*
- *OEShapeDatabaseOptions.SetMaxRandomTranslation*
- *OEShapeDatabaseOptions.GetMaxRandomTranslation*
- *OEShapeDatabaseOptions.SetRandomSeed*
- *OEShapeDatabaseOptions.GetRandomSeed*

SetLimit

```
void SetLimit(unsigned int limit)
```

Set the number of individual *OEShapeDatabaseScore* objects that will be returned by *OEShapeDatabase.GetSortedScores*. This is a hard limit regardless of the multiplicative effect of also setting the *OEShapeDatabaseOptions.SetMaxConfs* and *OEShapeDatabaseOptions.SetMaxOverlays* methods to values greater than 1.

Note

This method has no effect on the *OEShapeDatabase.GetScores* method.

SetMaxConfs

```
void SetMaxConfs(unsigned int maxConfs)
```

Set how many conformers per molecule should be returned in the results. The default value is 1, only the best conformer for each database molecule will be returned as an *OEShapeDatabaseScore* object. The conformer with the highest score will be indicated by the *OEShapeDatabaseScore.GetConfIdx* method.

Setting this value to `0` means all database conformers will be returned for every molecule in the database.

SetMaxOverlays

```
void SetMaxOverlays(unsigned int maxOverlaysToReturn)
```

Set how many starting points to return per conformer in the database. The default value is 1, only the best starting point for the conformer will be returned as an *OEShapeDatabaseScore* object.

Setting this value to 0 means all the starting points will be returned, i.e., there will be *OEShapeDatabaseOptions.GetNumInertialStarts* objects returned.

SetMaxRandomTranslation

```
bool SetMaxRandomTranslation(float trans)
```

Set the maximum allowed translation for each random orientation. The default is 2 angstroms. This method requires *OEShapeDatabaseOptions.SetInitialOrientation* to be set to *OEFastROCSOrientation.Random*.

See also

- *OEShapeDatabaseOptions.GetMaxRandomTranslation*
- *OEShapeDatabaseOptions.SetInitialOrientation*
- *OEShapeDatabaseOptions.GetInitialOrientation*
- *OEShapeDatabaseOptions.SetNumRandomStarts*
- *OEShapeDatabaseOptions.GetNumRandomStarts*
- *OEShapeDatabaseOptions.SetRandomSeed*
- *OEShapeDatabaseOptions.GetRandomSeed*
- *OEFastROCSOrientation*

SetNumInertialStarts

```
void SetNumInertialStarts(unsigned int numStarts)
```

Set how many starting points the shape optimization will use. Currently, only values between 1 and 8 inclusive can be set. The default value is 4, i.e., assume there is a dominant moment of inertia for both the query and database conformer. Setting this value higher can yield better global overlays. However, there is a direct linear relation between the performance of **FastROCS TK** and the number of starting points.

SetRandomSeed

```
bool SetRandomSeed(unsigned int seed)
```

Sets the random seed to be used with *OEFastROCSOrientation.Random*. Returns true if successfully set. The default random seed is set based on the time.

See also

- *OEShapeDatabaseOptions.GetRandomSeed*
- *OEFastROCSOrientation*
- *OEShapeDatabaseOptions.SetInitialOrientation*
- *OEShapeDatabaseOptions.GetInitialOrientation*
- *OEShapeDatabaseOptions.SetNumRandomStarts*
- *OEShapeDatabaseOptions.GetNumRandomStarts*

- *OEShapeDatabaseOptions.SetMaxRandomTranslation*
- *OEShapeDatabaseOptions.GetMaxRandomTranslation*

SetScoreType

```
void SetScoreType(unsigned int type)
```

Sets which scores to perform during the search. The constant `type` should be drawn from the *OEShapeDatabaseType* namespace.

> **Note**
>
> The score type must be a proper subset of the score enabled during *OEShapeDatabase construction*. That means if the database was started in "shape only" mode, this value can not include *OEShapeDatabaseType.Color*.

SetSimFunc

```
void SetSimFunc(unsigned int type)
```

Sets which type of similarity function to use to score search results. The constant type should be either "Tanimoto" or "Tversky" and should be drawn from the *OEShapeSimFuncType*.

SetTracer

```
void SetTracer(OEDBTracerBase& tracer)
```

Register a progress bar tracer with this set of options. The `tracer` will be updated with a count as chunks of the database are processed. It is very important that the implementation of *OEDBTracerBase* is thread-safe as it will be updated from multiple threads simultaneously. It is also expected that the consumer of the progress bar will be operating in a separate thread to avoid wasting search thread time on progress update overhead.

> **Warning**
>
> The user must take care to keep the `tracer` in scope during the full duration of the *OEShapeDatabase.GetScores* or *OEShapeDatabase.GetSortedScores* call. The options object will not make a copy of the tracer at all, merely storing a pointer to the `tracer`. If the `tracer` is prematurely `deleted`, this will very likely result in a crash. Probably in a non-deterministic way due to the threading involved.

SetTverskyCoeffs

```
void SetTverskyCoeffs(float alpha, float beta)
```

Sets the alpha and beta coefficients to be used in the Tversky similarity calculation. See the Molecular Shape section in the **Shape TK** theory documentation for a description of how this is calculated. Default values for alpha and beta are 0.95 and 0.05, respectively. Any new values of alpha and beta can be chosen provided they add up to 1.00.

SetUserStarts

```
bool SetUserStarts(vector<float>& startsCoords,
                   unsigned int numStarts)
```

Sets the user-defined starting coordinates. The arguments are a vector of floats of length 3 * the number of starting points (x, y and z coordinates for each start) - `startsCoords` and the number of starting coordinates in an unsigned int variable - `numStarts`.

Warning

Currently, error checking is not performed for user-defined starting coordinates that fall out of scope of the molecule's coordinate range therefore, bad starting coordinates will yield zero shape/color overlap. It is the responsibility of the user to ensure sensible starting coordinates.

The following code snippet shows how to use *OEShapeDatabaseOptions.SetInitialOrientation* and *OEShapeDatabaseOptions.SetUserStarts* in a python example.

Full listing.

See also

- *OEShapeDatabaseOptions.SetInitialOrientation*
- *OEShapeDatabaseOptions.GetInitialOrientation*
- *OEShapeDatabaseOptions.SetUserStarts*
- *OEShapeDatabaseOptions.GetUserStarts*

SetShapeScoreScale

```
void SetShapeScoreScale(float scale)
```

Set a scale factor for the shape component, defaults to 1.0

SetColorScoreScale

```
void SetColorScoreScale(float scale)
```

Set a scale factor for the color component, defaults to 1.0

GetShapeScoreScale

```
float GetShapeScoreScale() const
```

Gets the scale factor for the shape component

GetColorScoreScale

```
void SetColorScoreScale(float scale)
```

Gets the scale factor for the color component

7.1.6 OEShapeDatabaseScore

```
class OEShapeDatabaseScore
```

This object is used to represent the result of a **FastROCS TK** calculation returned by the *OEShapeDatabase.GetSortedScores* and *OEShapeDatabase.GetScores* methods.

It encapsulates the following information:

- Score information:
  - *OEShapeDatabaseScore.GetColorTanimoto*
  - *OEShapeDatabaseScore.GetShapeTanimoto*
  - *OEShapeDatabaseScore.GetTanimotoCombo*
  - *OEShapeDatabaseScore.GetColorTversky*
  - *OEShapeDatabaseScore.GetShapeTversky*
  - *OEShapeDatabaseScore.GetTverskyCombo*
  - *OEShapeDatabaseScore.GetColorScore*
  - *OEShapeDatabaseScore.GetShapeScore*
  - *OEShapeDatabaseScore.GetScore*
- Overlay recreation:
  - *OEShapeDatabaseScore.GetQuat*
  - *OEShapeDatabaseScore.GetRotMatrix*
  - *OEShapeDatabaseScore.GetTranslation*
  - *OEShapeDatabaseScore.Transform*
- Molecule retrieval: * *OEShapeDatabaseScore.GetMolIdx* * *OEShapeDatabaseScore.GetConfIdx*

Warning

The molecular transforms returned by *OEShapeDatabaseScore.GetQuat*, *OEShapeDatabaseScore.GetRotMatrix*, and *OEShapeDatabaseScore.GetTranslation* assume the conformer has already been aligned by *OESetCoordsToInertialFrame*.

While it was definitely in-elegant to require calling *OESetCoordsToInertialFrame* in order to reproduce overlays, this allows *OEShapeDatabase* to not store 28 bytes of memory per conformer, a significant space savings, especially when conformers are stored in rotor-compressed form.

Overlays are usually only required for a small number of conformations, so re-calculating this for only the "hits" is a small price to pay for potentially saving gigabytes of memory on an already memory constrained problem.

Users should prefer to use the *OEShapeDatabaseScore.Transform* directly to avoid having to deal with this subtlety, it will automatically do all the transformations necessary to generate overlays.

Constructors

```
OEShapeDatabaseScore(size_t molIdx, unsigned int confIdx,
                     float shapeScore, float colorScore,
                     const float* quat,
```

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```
                      unsigned int csimFunc = OEShapeSimFuncType::Default,
                      unsigned int orient = OEFastROCSOrientation::Default)
OEShapeDatabaseScore(size_t molIdx, unsigned int confIdx,
                      float shapeScore, float colorScore,
                      const double* quat,
                      unsigned int csimFunc = OEShapeSimFuncType::Default,
                      unsigned int orient = OEFastROCSOrientation::Default)
```

Constructs a new score object with the specified data. Typically only used by the internals of **FastROCS TK** in order to populate the hitlist.

Warning

The constructor has changed in order to support *OEFastROCSOrientation.AsIs*. The constant *OEFastROCSOrientation.Default*, drawn from the *OEFastROCSOrientation* namespace, has been added to the argument list. The default is *OEFastROCSOrientation.Inertial* and the last argument should be left blank unless it is intended to use *OEFastROCSOrientation.AsIs* starts on the database being loaded, in which case `unsigned int orient=OEFastROCSOrientation::AsIs` should be passed to the constructor.

Warning

The constructor has changed in order to support Tversky scoring. The constant "OEShapeSimFuncType::Default", drawn from the *OEShapeSimFuncType* namespace, has been added to the argument list. The default is "Tanimoto". "Tversky" scoring is chosen by passing *OEShapeSimFuncType.Tversky* and setting *OEShapeDatabaseOptions.SetSimFunc* to "Tversky".

GetColorScore

```
float GetColorScore() const
```

Returns the "color" component of the score used for ranking molecules by **FastROCS TK**. See the Molecular Shape section of the **ShapeTK** theory documentation for a description of the calculation. This function should be used in conjunction with *OEShapeDatabaseOptions.GetSimFunc* in order to determine which similarity function ("Tanimoto" or "Tversky") was used to calculate the scores. This function will return `0.0` if the search was requested to be "shape only", i.e., only *OEShapeDatabaseType.Shape* was specified.

GetColorTanimoto

```
float GetColorTanimoto() const
```

Returns the "color" component of the Tanimoto score used for ranking molecules by **FastROCS TK**. See the Color Features section in the **Shape TK** theory documentation for a description of what the "color" term is. This function will return `0.0` if the search was requested to be "shape only", i.e., only *OEShapeDatabaseType.Shape* was specified.

Note

A color tanimoto of `0.0` is also possible if either the query or database molecule does not contain any color atoms. Even more surprising is that this value can sometimes exceed `1.0`, which appears to violate the definition of "tanimoto". This is due to the first-order-gaussian approximation used, i.e, intersection volumes are not actually sub-

tracted out since they have little effect on virtual screening performance and would be significantly more costly to calculate. Typically, these cases are limited to complex cage systems like cubane that have many overlapping "ring" color atoms that heavily overlap. The use of the "ring" color term can be customized by using a custom color field specified through the *OEShapeDatabase constructor*.

GetColorTversky

```
float GetColorTversky() const
```

Returns the "color" component of the Tversky score used for ranking molecules by **FastROCS TK**. See the Color Features section in the **Shape TK** theory documentation for a description of what the "color" term is. This function will return `0.0` if the search was requested to be "shape only", i.e., only *OEShapeDatabaseType.Shape* was specified. If "Tversky" scoring was not set using *OEShapeDatabaseOptions.SetSimFunc* prior to the search this function will return with an error.

GetConfIdx

```
unsigned int GetConfIdx() const
```

Returns the conformer's index of the matching conformer for this particular score. This index will match the index returned by the `OEConfBase.GetIdx` method. This allows retrieving the conformer from the `OEMCMolBase.GetConf` method using the `OEHasConfIdx` predicate like the following:

```
conf = mol.GetConf(OEHasIdx(score.GetConfIdx()))
```

GetMolIdx

```
size_t GetMolIdx() const
```

Returns the molecule index that returned this particular "score". This index maps to the indices used by OEMolDatabase to retrieve molecules assuming the *OEShapeDatabase* was initialized with the *OEShapeDatabase.Open* method. This allows **FastROCS TK** to rely on disk-based storage through OEMolDatabase to retrieve overlays and provide connection tables, a significant memory space savings. However, this does come at the added latency and computational expense of the `OEMolDatabase.GetMolecule` method.

To allow for use cases other than virtual screening where only a small number of "hits" need to be sent on for further processing. This index may map to the index returned by the *OEShapeDatabase.AddMol* method. It is up to the user to decide how to store the OEMCMolBase for later access. Previously versions of **FastROCS TK** used `OEMCMolType.OEDBMCMol` molecules for this purpose.

GetQuat

```
const float* GetQuat() const
```

> **Warning**
>
> It will be easier to use the *OEShapeDatabaseScore.Transform* method than to use figure out how to use the data from this function.

Returns a pointer to a 7-element quaternion that can be used to overlay the database conformer represented by this score with the query conformation. This 7-element quaternion contains both the rotation and translational components: the first 4 elements being the quaternion rotation; the second 3 elements are the translational component.

> **Warning**
>
> Read *FastROCS transforms warning* above about performing overlays with these more advanced methods.

GetRotMatrix

```
bool GetRotMatrix(float* rmat) const
```

> **Warning**
>
> It will be easier to use the *OEShapeDatabaseScore.Transform* method than to use figure out how to use the data from this function.

Fills in the 9-element rotation matrix `rmat` with the rotation component needed to overlay the database conformer represented by this score with the query conformation. Returns `false` if the rotation matrix is ill-defined, i.e., the conversion from the underlying quaternion failed.

> **Warning**
>
> Read *FastROCS transforms warning* above about performing overlays with these more advanced methods.

GetScore

```
float GetScore() const
```

Returns the sum of the "shape" and "color" scores. This function should be used in conjunction with *OEShapeDatabaseOptions.GetSimFunc* in order to determine which similarity function ("Tanimoto" or "Tversky") was used to calculate the scores.

GetShapeScore

```
float GetShapeScore() const
```

Returns the "shape" component of the score used for ranking molecules by **FastROCS TK**. See the Molecular Shape section of the **Shape TK** theory documentation for a description of the calculation. This function should be used in conjunction with *OEShapeDatabaseOptions.GetSimFunc* in order to determine which similarity function ("Tanimoto" or "Tversky") was used to calculate the scores.

Currently, it is not possible to request a "color only" calculation from **FastROCS TK**. Therefore, this function should always be greater than `0.0`. A value of `0.0` would be a molecule with no volume, which is impossible.

GetShapeTanimoto

```
float GetShapeTanimoto() const
```

Returns the "shape" component of the tanimoto score used for ranking molecules by **FastROCS TK**. See the Molecular Shape section in the **Shape TK** theory documentation for a description of how this is calculated.

Currently, it is not possible to request a "color only" calculation from **FastROCS TK**. Therefore, this function should always be greater than `0.0`. A value of `0.0` would be a molecule with no volume, which is impossible.

> **Note**
>
> It is possible, though rare, to see values slightly greater than `1.0` in the 2nd decimal place. This is due to the approximation **FastROCS TK** uses for performance and can be disregarded, especially since they usually only occur whenever a molecule is matched against itself.

GetShapeTversky

```
float GetShapeTversky() const
```

Returns the "shape" component of the tversky score used for ranking molecules by **FastROCS TK**. See the Molecular Shape section in the **Shape TK** theory documentation for a description of how this is calculated. If "Tversky" scoring was not set using *OEShapeDatabaseOptions.SetSimFunc* prior to the search this function will return with an error.

As with the "Tanimoto" scoring option, it is not currently possible to request a "color only" calculation from **FastROCS TK**. Therefore, this function should always be greater than `0.0`. If this is not the case an error has occurred.

> **Note**
>
> It is possible, though rare, to see values slightly greater than `1.0` in the 2nd decimal place. This is due to the approximation **FastROCS TK** uses for performance and can be disregarded, especially since they usually only occur whenever a molecule is matched against itself.

GetSimFunc

```
unsigned int GetSimFunc() const
```

Returns a constant from the *OEShapeSimFuncType* namespace indicating what type of similarity function, "Tanimoto" or "Tversky", is being used for scoring.

GetTanimotoCombo

```
float GetTanimotoCombo() const
```

Returns the sum of the "color" and "shape" tanimotos.

GetTranslation

```
bool GetTranslation(float* trans) const
```

> **Warning**
>
> It will be easier to use the *OEShapeDatabaseScore.Transform* method than to use figure out how to use the data from this function.

Fills in the 3-element vector `trans` with the translation component needed to overlay the database conformer represented by this score with the query conformation. Returns `false` if the translation is ill-defined, i.e., something went horribly wrong.

Warning

Read *FastROCS transforms warning* above about performing overlays with these more advanced methods.

ExtractTransform

```
bool ExtractTransform(OETrans& transform, OEChem::OEMolBase& mol) const
```

Fills in the OETrans object with the translation and rotation matrix necessary to transform mol onto the query. Note that *OEShapeDatabaseScore.Transform* is the preferred method for visualizing overlays. This method is available for the case in which you need to know exactly what transform was performed. For example, when you want to use the same transform on another molecule.

GetTverskyCombo

```
float GetTverskyCombo() const
```

Returns the sum of the "color" and "shape" Tversky scores. If "Tversky" scoring was not set using *OEShapeDatabaseOptions.SetSimFunc* prior to the search this function will return with an error.

Transform

```
bool Transform(OEChem::OEMolBase& mol) const
```

Overlays the conformer represented by `mol` with the query conformation passed as the query to *OEShapeDatabase*. This overlay will be the orientation that was used to calculate the scores returned by the rest of this class.

See also

This is the preferred method for generating overlays with **FastROCS TK**. There is a more complete description of the process and its subtleties above in the *FastROCS transforms warning*.

7.2 OEFastROCS Constants

7.2.1 OEFastROCSOrientation

The **FastROCS TK** search algorithm performs an optimization to maximize the overlap between the query and the database molecule. This namespace defines a set of initial orientations for the optimization that are also referred to as alternative starts. The default orientation is *OEFastROCSOrientation.Inertial*, which can also be accessed via *OEFastROCSOrientation.Default*. As the optimization has a limited number of iterations, it may be beneficial to use alternative starting coordinates for some molecular systems. To set an alternative initial orientation use *OEShapeDatabaseOptions.SetInitialOrientation*.

At present there are 7 initial orientations available:

- *OEFastROCSOrientation.Inertial*
- *OEFastROCSOrientation.UserInertialStarts*
- *OEFastROCSOrientation.InertialAtHeavyAtoms*
- *OEFastROCSOrientation.InertialAtColorAtoms*
- *OEFastROCSOrientation.AsIs*

- *OEFastROCSOrientation.Random*
- *OEFastROCSOrientation.Subrocs*

See also

- *OEShapeDatabaseOptions.SetInitialOrientation*
- *OEShapeDatabaseOptions.GetInitialOrientation*
- *OEShapeDatabaseOptions.SetUserStarts*
- *OEShapeDatabaseOptions.GetUserStarts*
- *OEShapeDatabaseOptions.GetNumStarts*
- *OEShapeDatabaseOptions.GetNumUserStarts*
- *OEShapeDatabaseOptions.GetNumHeavyAtomStarts*
- *OEShapeDatabaseOptions.GetNumColorAtomStarts*

Default

The default orientation is *OEFastROCSOrientation.Inertial*.

Inertial

The query and the database molecule are aligned to the inertial frame and optimizations are performed for 4 inertial orientations of the database molecule, by rotating about its 2 major moments of inertia.

UserInertialStarts

The database molecule is translated to each user-defined starting position and optimizations are performed for 4 inertial starts for each translation. See *OEShapeDatabaseOptions.SetInitialOrientation* and *OEShapeDatabaseOptions.SetUserStarts* for more details on setting the starting coordinates.

Warning

Currently, error checking is not performed for user-defined starting coordinates that fall out of scope of the molecule's coordinate range therefore, bad starting coordinates will yield zero shape/color overlap.

InertialAtHeavyAtoms

The database molecule is translated to each heavy atom of the query molecule and optimizations are performed for 4 inertial starts for each translation. See *OEShapeDatabaseOptions.SetInitialOrientation* and *OEShapeDatabaseOptions.GetInitialOrientation*

InertialAtColorAtoms

The database molecule is translated to each color atom of the query molecule and optimizations are performed for 4 inertial starts for each translation. This method works for combo and shape-only searches. The only requirement is that the query molecule has color atoms. If the query molecule does not have color atoms the search will default to *OEFastROCSOrientation.Inertial*. See *OEShapeDatabaseOptions.SetInitialOrientation*, *OEShapeDatabaseOptions.GetInitialOrientation* and *OEShapeDatabaseOptions.GetNumColorAtomStarts*.

AsIs

The query and database molecules are left `AsIs`. It is presumed that the conformers are already positioned in space (perhaps through docking) therefore they are not centered or set to the inertial frame of reference. This method carries out a single optimization at the query and database molecule's original coordinates. No inertial orientations are optimized.

> **Warning**
>
> In order to use this method on a database the entire database is required to be reloaded with the *OEShapeDatabase.Open* or *OEShapeDatabase.AddMol* routine using `unsigned int orient=OEFastROCSOrientation::AsIs` as the last argument.

> **Warning**
>
> In order to use the *OEShapeDatabaseScore.Constructors* with this method it is required that the final argument to the constructor be `unsigned int orient=OEFastROCSOrientation::AsIs`.

See *OEShapeDatabaseOptions.SetInitialOrientation*, *OEShapeDatabaseOptions.GetInitialOrientation*, *OEShapeDatabase.Open* and *OEShapeDatabaseScore.Constructors*.

Random

N random starts are generated by randomly orientating the database molecule N times. This method includes the ability to set the maximum random translation via the *OEShapeDatabaseOptions.SetMaxRandomTranslation*, option. The default maximum is 2 angstroms. The number of random starts can be set using the *OEShapeDatabaseOptions.SetNumRandomStarts* option. The default number of random starts is `10`. The random seed can be set using the *OEShapeDatabaseOptions.SetRandomSeed*. The default random seed is based on the time.

> **Warning**
>
> The random API point is only deterministic when using the same seed if only one thread is set to open the database using *OEShapeDatabase.SetNumOpenThreads* between calls to GetScores or GetScores is called on the same opened database object.

See *OEShapeDatabaseOptions.SetInitialOrientation* *OEShapeDatabaseOptions.GetInitialOrientation* *OEShapeDatabaseOptions.SetMaxRandomTranslation* *OEShapeDatabaseOptions.GetMaxRandomTranslation* *OEShapeDatabaseOptions.SetNumRandomStarts*

OEShapeDatabaseOptions.GetNumRandomStarts *OEShapeDatabaseOptions.SetRandomSeed* *OEShapeDatabaseOptions.GetRandomSeed*

Subrocs

Optimizations are carried for each inertial orientation at each heavy atom of the molecule with the most heavy atoms regardless of whether it is the query or the database molecule. This method is synonymous with *OEFastROCSOrientation.InertialAtHeavyAtoms*.

See *OEShapeDatabaseOptions.SetInitialOrientation* *OEShapeDatabaseOptions.GetInitialOrientation*

See the Starting positions for optimization section in the **Shape TK** theory documentation for a description of alternative starts.

7.2.2 OEFastROCSReturnCode

This namespace contains constants returned by *OEFastROCSGPUStatus* to indicate the status of the GPU.

See also

- *OEFastROCSGPUStatus*

Success

The API call returned with no errors. The GPU is ready.

InitializationError

The CUDA driver and runtime could not be initialized.

InsufficientDriver

The NVIDIA CUDA driver is older than the CUDA runtime library. This is not a supported configuration. Users should install an updated NVIDIA display driver to allow the application to run.

NoDevice

No CUDA-capable devices were detected by the installed CUDA driver.

NoDeviceDetected

No CUDA-capable devices were detected by the installed CUDA driver.

NotPermitted

The attempted operation is not permitted.

Unknown

Unknown failure.

7.2.3 OEShapeDatabaseType

This namespace is used to control whether a *OEShapeDatabase* object should store the data necessary to calculate the following components of the output score: `OEShapeDatabaseScore.GetShapeTanimoto` and `OEShapeDatabaseScore.GetColorTanimoto`. Each component has an associated memory and calculation overhead that can be avoided is desired. For example, passing `OEShapeDatabaseType.Shape` to the *OEShapeDatabase* constructor will cut memory consumption roughly in half and skip calculating static color scores.

See also

- `OEShapeDatabaseOptions.Constructors`
- `OEShapeDatabaseOptions.SetScoreType`

Color

Instructs *OEShapeDatabase* to cache the necessary color information so that a subsequent search with `OEShapeDatabase.GetScores` or `OEShapeDatabase.GetSortedScores` will yield color scores. It is possible to pass this value into the *OEShapeDatabase* constructor and then turn it off for searches so the same database can be used for shape-only and shape+color searches. To turn off the color term for only a specific search, pass `OEShapeDatabaseType.Shape` into the `OEShapeDatabaseOptions.SetScoreType` method, then pass that options object into either `OEShapeDatabase.GetScores` or `OEShapeDatabase.GetSortedScores`.

Combo

The combination of `OEShapeDatabaseType.Shape` and `OEShapeDatabaseType.Color` as a convenience using the name most often used. This is a synonym of `OEShapeDatabaseType.Default`.

Default

The default setting for *OEShapeDatabase* is to calculate both "Color" and "Shape" scores. The combination of both scores shows very good results for virtual screening performance.

Shape

Must be specified as part of the *OEShapeDatabase* constructor or as a term in the *OEShapeDatabaseOptions* class.

Warning

Color-only functionality is currently not supported.

Sitehopper

Must be specified as part of the *OEShapeDatabase* constructor to run a Sitehopper calculation.

Warning

Sitehopper functionality requires a Sitehopper license in addition to a FastROCS license.

7.2.4 OEShapeSimFuncType

This namespace is used to set which similarity function, 'Tanimoto' or 'Tversky', *OEShapeDatabase* objects use to score search results. The default option is *OEShapeSimFuncType.Tanimoto*. Tversky scoring is set using the *OEShapeDatabaseOptions.SetSimFunc* member function of *OEShapeDatabaseOptions*.

Note

Tanimoto and Tversky scoring options are mutually exclusive therefore, whichever function was previously selected before performing a search will be the one used to calculate the subsequent score. If no function is set the default function is used.

See also

- *OEShapeDatabaseOptions.GetSimFunc*
- *OEShapeDatabaseOptions.SetSimFunc*

Default

Set *OEShapeDatabaseOptions* to instruct *OEShapeDatabaseScore* to calculate scores for search results using the tanimoto similarity function. See *OEShapeSimFuncType.Tanimoto* for more details on usage.

Tanimoto

Set *OEShapeDatabaseOptions* to instruct *OEShapeDatabaseScore* to calculate scores for search results using the tanimoto similarity function. To retrieve the "shape" tanimoto score use either *OEShapeDatabaseScore.GetShapeTanimoto* or *OEShapeDatabaseScore.GetShapeScore*. To retrieve the "color" tanimoto score use either *OEShapeDatabaseScore.GetColorTanimoto* or *OEShapeDatabaseScore.GetColorScore*. To retrieve the combined "shape" and "color" tanimoto scores use either *OEShapeDatabaseScore.GetTanimotoCombo* or *OEShapeDatabaseScore.GetScore*.

Tversky

Set *OEShapeDatabaseOptions* to instruct *OEShapeDatabaseScore* to calculate scores for search results using the tversky similarity function. To retrieve the "shape" tversky score use either *OEShapeDatabaseScore.GetShapeTversky* or *OEShapeDatabaseScore.GetShapeScore*. To retrieve the "color" tversky score use either *OEShapeDatabaseScore.GetColorTversky* or *OEShapeDatabaseScore.GetColorScore*. To retrieve the combined "shape" and "color" tversky scores use either *OEShapeDatabaseScore.GetTverskyCombo* or *OEShapeDatabaseScore.GetScore*.

Warning

If using the *OEShapeDatabaseScore.GetColorScore*, *OEShapeDatabaseScore.GetShapeScore* or *OEShapeDatabaseScore.GetScore* methods to retrieve scores it is advised that the *OEShapeDatabaseOptions.GetSimFunc* method is used to determine which similarity function the scores were calculated with.

Note

See *OEShapeDatabaseType* for details of how to set *OEShapeDatabaseOptions* to store only "shape" scores or both "shape" and "color" scores.

Warning

Color-only functionality is currently not supported.

See Molecular Shape section in the **Shape TK** theory documentation for a description of the Tanimoto and Tversky similarity functions.

7.2.5 OEFastROCSMode

This namespace can be used to activate "ROCS" mode, which will result in scores that are more directly comparable to ROCS. The default option is *OEFastROCSMode.FastROCS*. ROCS mode is set using the *OEShapeDatabaseOptions.SetFastROCSMode* member function of *OEShapeDatabaseOptions*.

See also

- *OEShapeDatabaseOptions.GetFastROCSMode*
- *OEShapeDatabaseOptions.SetFastROCSMode*

Default

The default calculation mode is *OEFastROCSMode.FastROCS*

FastROCS

Set *OEShapeDatabaseOptions* to instruct *OEShapeDatabaseScore* to calculate scores normally.

ROCS

Set *OEShapeDatabaseOptions* to instruct *OEShapeDatabaseScore* to calculate scores for search results more similar to ROCS.

> **Warning**
>
> setting *OEFastROCSMode.ROCS* will impact performance. Between 5-20% performance decrease should be expected.

7.3 OEFastROCS Functions

7.3.1 OEFastROCSCacheStuff

```
bool OEFastROCSCacheStuff(OEChem::OEMCMolBase& mol,
                          const OEShape::OEColorForceField& cff)
```

> **Warning**
>
> This function is deprecated and has been superseded by *OEPrepareFastROCSMol*. Please use *OEPrepareFastROCSMol* to optimize for *OEShapeDatabase.Open* load time performance.

7.3.2 OEFastROCSGetArch

```
const char* OEFastROCSGetArch()
```

Returns the internal build string used by OpenEye, Cadence Molecular Sciences to identify the hardware architecture. The format of these strings may change over time.

7.3.3 OEFastROCSGetLicensee

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

Returns the licensee name from the license file.

7.3.4 OEFastROCSGetNumDevices

```
size_t OEFastROCSGetNumDevices()
```

Returns the number of compatible GPUs available for execution in the system being queried. If no GPUs are visible the function will throw the following warning `Unable to find a suitable device`.

7.3.5 OEFastROCSGetPlatform

```
const char* OEFastROCSGetPlatform()
```

Returns the internal build string used by OpenEye, Cadence Molecular Sciences to identify a platform. The format of these strings may change over time, and future distributions may contain different values even when using the same operating system, compiler and processor. For example, on a `x86_64` Red Hat Enterprise Linux box this would return `redhat-RHEL5-g++4.1-x64`.

7.3.6 OEFastROCSGetRelease

```
const char* OEFastROCSGetRelease()
```

Returns the release name of the *FastROCS* library being used. This returns a value similar to `0.10.0` for production versions of the library, and `0.10.0 debug` for the checking version of the library.

7.3.7 OEFastROCSGetSite

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

Returns the physical site location of the licensee as registered in the license file.

7.3.8 OEFastROCSGetVersion

```
unsigned int OEFastROCSGetVersion()
```

Returns the version number of the library being used. This is an unsigned integer value indicating the date on which the library was built, for example `20141001`, for the 1st of October 2014. This value should be used when reporting problems, and unlike the release string, may be used in comparisons if needed.

7.3.9 OEFastROCSGPUStatus

```
unsigned OEFastROCSGPUStatus()
```

Queries the status of the GPU and returns an *OEFastROCSReturnCode*. Useful for checking whether the machine has an accelerator properly setup and ready to accept FastROCS queries. It is guaranteed that if this function returns *OEFastROCSReturnCode.Success* that all subsequent *OEShapeDatabase* objects can successfully execute queries.

7.3.10 OEFastROCSIsGPUReady

```
bool OEFastROCSIsGPUReady()
```

Returns True if *OEShapeDatabase* can successfully execute queries. Useful for checking whether the machine has an accelerator properly setup and ready to accept FastROCS queries. It is guaranteed that if this function returns 'True' that all subsequent *OEShapeDatabase* object can successfully execute queries. That means that this function will effectively initialize an underlying context that is re-used by *OEShapeDatabase* objects, possibly grabbing an "exclusive process" lock: http://docs.nvidia.com/cuda/cuda-c-programming-guide/#compute-modes

7.3.11 OEFastROCSIsLicensed

```
bool OEFastROCSIsLicensed(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 **FastROCS TK** functionality.

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

See also

- `OEChemIsLicensed` function

7.3.12 OEShapeDatabasePrep

```
bool OEShapeDatabasePrep(std::string filein, std::string fileout,
                         unsigned int cfftype = OEShape::OEColorFFType::OEDefault)
```

Prepares molecules stored in a `OEFormat.OEB` file to improve the performance of loading the molecules into an *OEShapeDatabase* object. This is a **multi-threaded** implementation of the shapedatabaseprep example that takes the input `OEB` filename as the first argument and the output `OEB` filename as the second argument. An optional argument to specify the color force field type can be passed in. The default color force field is Implicit Mills Dean.

Using this function to prep a database will result in as much as 10-fold performance improvement of *`OEShapeDatabase.Open`*. OEShapeDatabasePrep does the following:

- Pre-compresses the output file with `OEPRECompress`, alleviating the need to Gzip the `OEB` and improving the performance of `OEMolDatabase.Open`.
- Sets the energy of each conformer to `0.0` to avoid writing it to `OEB`.
- Suppresses hydrogens and reorders reference conformers for compression.
- Pre-calculates color atoms.
- Pre-calculates self-color and self-shape terms for all conformers.

Note

`OEShapeDatabasePrep` will cache color atoms and self color terms for the `OEColorFFType.ImplicitMillsDean` color force field.

Warning

This function is non-deterministic so molecules will not appear in the same order as the input file.

Warning

This function should not be used to prepare a database intended to be used with a *OEShapeDatabaseType.Sitehopper* database

7.3.13 OEIsDatabasePrepared

```
bool OEIsDatabasePrepared(OEChem::OEMolBase& mol)
bool OEIsDatabasePrepared(OEChem::OEMolDatabase& moldb)
```

Returns True if the database (OEMolDatabase) or molecule (OEMolBase) input has already been prepared with the *OEPrepareFastROCSMol* function and False if preparation is still required.

It is recommended that all sizable databases that are intended to be re-used undergo preparation in order to benefit from significantly faster load times.

7.3.14 OEPrepareFastROCSMol

```
bool OEPrepareFastROCSMol(OEChem::OEMCMolBase& mol)
bool OEPrepareFastROCSMol(OEChem::OEMCMolBase& mol,
                          const OEShape::OEColorForceField& cff)
```

Prepares the molecule `mol` to improve the performance of loading the molecule into memory as an *OEShapeDatabase* object from an `OEFormat.OEB` file. The following steps are taken to improve the performance of *OEShapeDatabase.Open* by as much as 10-fold:

- Sets the energy of each conformer to `0.0` to avoid writing it to OEB.
- Suppresses hydrogens and reorders reference conformers for compression.
- Pre-calculates color atoms.
- Pre-calculates self-color and self-shape terms for all conformers.

It is recommended to call `OEPRECompress` on the oemolostream before writing out to `OEB`. This will store conformers in "PRE-compressed" form therefore alleviating the need to Gzip the `OEB` file and consequently improving the performance of `OEMolDatabase.Open`. In general, calling *OEPrepareFastROCSMol* and `OEPRECompress` will result in a smaller `OEB` file than the default `OEB.GZ` output from OMEGA.

Additionally, if `OEB` file size is of chief concern a further reduction in file size can be achieved by using an `OEMCMolType.HalfFloatCartesian` molecule, which stores reference coordinates and torsions in half floating point precision (16-bit). The following code snippet demonstrates how to cast the resultant molecule from *OEPrepareFastROCSMol* to use half precision:

```
OEPrepareFastROCSMol(mol);
OEMol halfMol(mol, OEMCMolType::HalfFloatCartesian);
OEWriteMolecule(ofs, halfMol);
```

```
OEPrepareFastROCSMol(mol)
halfMol = OEMol(mol, OEMCMolType_HalfFloatCartesian)
OEWriteMolecule(ofs, halfMol)
```

16-bit floating point will give a file size saving of approximately 12% with a tradeoff of about 7% more performance when loading the OEB from disk into memory.

Note

By default, *OEPrepareFastROCSMol* will cache color atoms and self color terms for the `OEColorFFType.ImplicitMillsDean` color force field. The second overload that takes a OEColorForceField can be used to override this default.

7.3.15 OESetCoordsToInertialFrame

```
bool OESetCoordsToInertialFrame(OEChem::OEMolBase& mol)
```

Set the coordinates of `mol` to be aligned by its principle moments of inertia. The transformations returned by *OEShapeDatabaseScore.GetQuat*, *OEShapeDatabaseScore.GetRotMatrix*, and *OEShapeDatabaseScore.GetTranslation* assume the molecule has already been aligned by its principle moment of inertia. Users should prefer to use the *OEShapeDatabaseScore.Transform* directly to avoid having to deal with this subtlety.

See also

OEShapeDatabaseScore

7.4 Using a Custom Color ForceField in FastROCS

Similar to the **Shape Toolkit**, a custom color forcefield can be used to compare color features beyond those captured with the default forcefield. To use a custom color forcefield, specify your forcefield during the initialization of your OEShapeDatabase *OEShapeDatabase*

Custom color forcefields in FastROCS are constructed the same way they are in the OEColorForceField class in the **OEShape TK** but are restricted to the following:

1. Interactions can only be between atoms of the same type
2. Interactions can only be favorable
3. Interactions can only be of type “gaussian”
4. user defined types are not permitted

in the following code example:

a color forcefield is created that will only count interactions between pairs of acceptors and pairs of donors. The -1.0 indicates a favorable interaction, with standard weighting. 2.0 is the range of the color interaction in space.

See also

- OEColorForceField class in the **OEShape TK**

7.5 OEFastROCS ShapeDatabaseServer XMLRPC API

This chapter documents the XMLRPC API that is exposed by the `ShapeDatabaseServer.py` server since the 1.0 release of **FastROCS**. Since that release many users have created internal clients to the server that depend on that XMLRPC API, so **OpenEye** has strived to keep this API stable for pre-existing client code. This chapter should serve as a guide for anyone looking to create a new **FastROCS** server around the toolkit API.

Most users can just use the `ShapeDatabaseClient.py` script directly, without the need to worry about the details of the protocol between the client and server.

Note

The XMLRPC API will be replaced by a RESTful API in a future version of **FastROCS TK**.

7.5.1 GetBestOverlays

```
GetBestOverlays(querymolstr, nhits, iformat = ".oeb", oformat = ".oeb") -> Binary
```

Return the `nhits` results of the database search performed with the query `querymolstr`. The file format of the data in the XML RPC Binary `querymolstr` is specified by the `iformat` argument. Valid `iformat` arguments are any **OEChem** supported molecular file format that `OEIs3DFormat` will return `True` for. This is because **FastROCS TK** requires a 3D conformation to search against.

The returned XML RPC Binary will contain the best `nhits` of query against the database. The returned XML RPC Binary will contain the molecule sorted by the chosen scoring function for the database. `nhits` of `0` specifies that all database molecules should be returned in sorted order, not a very advisable operation as that could move many megabytes to gigabytes of data over the network.

The file format of the returned XML RPC Binary is specified by the `oformat` argument. This can be any **OEChem** supported file format that `OEIsWriteable` will return `True` for. However, scores are only stored as SD data, so only the following file formats will return score information:

- `OEFormat.OEB`
- `OEFormat.SDF`
- `OEFormat.CSV`

Furthermore, the molecules returned will be aligned to the query molecule in 3D. So only formats that can represent 3D information will actually contain the resulting alignment.

See also

The File Formats section of the **OEChem** documentation for a list of valid file formats.

Note

`iformat` and `oformat` default to `.oeb` in order to be compatible with versions of **FastROCS** clients prior to 1.4.0.

Warning

This XML RPC request will block until the search has completed. Since searches can take many seconds to minutes, the underlying network connection for the XML RPC request may time out. This remote procedure call should only be used when the search is known to be short. Using the *`SubmitQuery`* remote procedure call to queue up the query is highly preferred for creating a better user experience.

7.5.2 GetName

```
GetName() -> str
```

Return the name of the database being served from the server. By default, this is the filename the server was started with. However, this can be changed by the *SetName* remote procedure call.

7.5.3 GetVersion

```
GetVersion() -> str
```

Return the version of **FastROCS TK** being run on the server.

7.5.4 IsLoaded

```
IsLoaded(blocking = False) -> bool
```

Returns `True` if the server has finished loading the database into memory and ready to accept queries. Returns `False` if the server is still initializing, causing any queries submitted to wait in a queue before they can be processed.

7.5.5 OEThrowSetLevel

```
OEThrowSetLevel(level)
```

Turns on debugging information for the server, or turning it back off again. The integer `level` should be drawn from the `OEErrorLevel` namespace. **FastROCS TK** uses `OEThrow` to handle all logging information. **FastROCS TK** will throw lots of performance debugging information to the `OEErrorLevel.Debug` level that will not be seen by default. When contacting OpenEye support about **FastROCS** (support@eyesopen.com), including this information would be very beneficial to helping solve the problem.

7.5.6 QueryHistogram

```
QueryHistogram(queryidx) -> [int, ..., int]
```

Return the current distribution of scores for the search specified by the `queryidx`. The distribution is returned as a list of integers. The distribution of scores can be retrieved in 'real-time' during a search as well, though it is recommended to still use `QueryStatus` with the `blocking` parameter set to `True` to avoid spurious requests and load on the server.

The distribution is only guaranteed to be a complete distribution of all the scores once the query has fully completed executing. A query is fully complete when the integers returned by `QueryStatus` are equal and both non-zero.

7.5.7 QueryStatus

```
QueryStatus(queryidx, blocking = False) -> (int, int)
```

Return the current progress of the search specified by the `queryidx`. The progress is returned as a pair of integers. The first integer in the pair is how many conformers have already been searched. The second integer in the pair is how many conformers there are total in the database to be searched. When the two integers are equal, the search has finished, and a call to *QueryResults* will return immediately with the resulting hits.

`queryidx` must be an integer that was previously returned by the *SubmitQuery* remote procedure call. This remote procedure call can be called any number of times with the same `queryidx` between the matching *SubmitQuery* remote procedure call and the finishing *QueryResults* remote procedure call.

The `blocking` parameter specifies whether this remote procedure call should return immediately. If `blocking` is `False`, the remote procedure call will return immediately with the current status. However, this returned value could be identical to a previous call and provide no new information to the end user. If `blocking` is `True`, this remote procedure call will not return until there is new information to return. This will result in less "busy waiting" network traffic constantly pinging the server for an update.

Note

It is possible for both values returned to be `0` even though the search is not complete. There is a very short period of time that the XML RPC service does not know the total number of conformers yet after the query has been submitted. Users can disregard this state and requery the server for a new status.

7.5.8 QueryResults

```
QueryResults(queryidx) -> Binary
```

Return a XML RPC Binary of search results for the specified `queryidx`. The contents of the XML RPC Binary, including file format and size, are controlled by the corresponding call to *SubmitQuery*.

This remote procedure call will block if the search is not completed yet. Use the *QueryStatus* remote procedure call to determine if the results are ready to return.

Warning

This function can only be called once for a particular `queryidx`. Once a query's results are retrieved with this remote procedure call, all record of the search are removed from the server's memory. The reverse is true as well though, if this function is not called, the query's results will stay resident in memory until the server is restarted.

7.5.9 SetName

```
SetName(name)
```

Specify the name of the database this server is serving. Subsequent calls to the *GetName* remote procedure call will return this name.

7.5.10 SubmitQuery

```
SubmitQuery(querymolstr, nhits, iformat = ".oeb", oformat = ".oeb",
            shapeOnly = False) -> int
```

Submit a query 3D molecule to the server and begin processing immediately. If there is already a search in progress, the query will be submitted to a queue. An integer index is returned to allow tracking the progress of the search through the *QueryStatus* function, and then to retrieve the results through the *QueryResults* function. This function will return immediately, unlike the *GetBestOverlays* remote procedure call.

The `shapeOnly` argument specifies that color scoring should not be performed and taken into account when scoring and sorting molecules. This defaults to `False` to be compatible with versions of **FastROCS** prior to 1.5.0.

The file format of the query in the XML RPC Binary `querymolstr` is specified by the `iformat` argument. Valid `iformat` arguments are any **OEChem** supported molecular file format that `OEIs3DFormat` will return `True` for. This is because **FastROCS TK** requires a 3D conformation to search against. In addition to supporting 3D conformations from standard **OEChem** file formats, shape queries from `.sq` files are also supported as queries. `.sq` files are most

easily constructed from within the vROCS GUI. They are usable from the **Shape TK** through the OEShapeQueryPublic APIs.

The `nhits` argument specifies how many hits should be returned by the corresponding *`QueryResults`* remote procedure call. These hits will be returned in the order of the best score first. A value of `0` given to `nhits` specifies that all database molecules should be returned, not a very advisable operation as that can potentially push many megabytes to gigabytes of data over the network.

The file format of the XML RPC Binary to return from *`QueryResults`* is specified by the `oformat` argument. This can be any **OEChem** supported file format that `OEIsWriteable` will return `True` for. However, scores are only stored as SD data, so only the following file formats will return score information:

- `OEFormat.OEB`
- `OEFormat.SDF`
- `OEFormat.CSV`

Furthermore, the molecules returned will be aligned to the query molecule in 3D. So only formats that can represent 3D information will actually contain the resulting alignment.

See also

The File Formats section of the **OEChem** documentation for a list of valid file formats.

Note

`iformat` and `oformat` default to `.oeb` in order to be compatible with versions of **FastROCS** clients prior to 1.4.0.

CHAPTER

EIGHT

RELEASE HISTORY

8.1 FastROCS TK 2.3.2

Minor internal improvements have been made.

8.2 FastROCS TK 2.3.1

Minor internal improvements have been made.

8.3 FastROCS TK 2.3.0

8.3.1 New Features

- **FastROCS TK** now supports shape grids in the input query, analogous to **Shape TK**.

8.3.2 Minor Bug Fixes

- A bug in the overlaid database pose has been fixed in the transformation from the inertial frame to the original one. **FastROCS** scores are unaffected. As a result, the CPU steps on top of **FastROCS** poses are no longer needed in **SiteHopper**.

8.4 FastROCS TK 2.2.7

8.4.1 New features

- New methods have been added to the *OEShapeDatabaseOptions* class that allow the shape and color scales to be modified.
  - *SetShapeScoreScale*
  - *GetShapeScoreScale*
  - *SetColorScoreScale*
  - *GetColorScoreScale*

8.5 FastROCS TK 2.2.6

Minor internal improvements have been made.

8.6 FastROCS TK 2.2.5

Minor internal improvements have been made.

8.7 FastROCS TK 2.2.4

Minor internal improvements have been made.

8.8 FastROCS TK 2.2.3

8.8.1 Major bug fixes

- A memory leak which could cause a crash when calling *OEShapeDatabase.GetScores* or *OEShapeDatabase.GetSortedScores* has bee fixed.

8.9 FastROCS TK 2.2.2

- Minor internal improvements have been made.

8.10 FastROCS TK 2.2.1

- Minor internal improvements have been made.

8.11 FastROCS TK 2.2.0

July 2021

8.11.1 New features

- A new method, *OEShapeDatabaseScore.ExtractTransform*, that extracts an entire transform (not just the post inertial frame transformation) has been added.

8.11.2 Minor bug fixes

- An issue with custom weights in FastROCS *custom color* has been fixed.

8.12 FastROCS TK 2.1.0

Fall 2020

8.12.1 New features

- **FastROCS TK** now requires a minimum NVIDIA Driver version of 450.x. See NVIDIA Drivers for more details.
- **FastROCS TK** now requires a minimum GPU compute capability of 3.5. See Supported GPUs for more details.
- OEShapeQuery objects now have limited support for use as queries with the *OEShapeDatabase.GetScores* and *OEShapeDatabase.GetSortedScores* database searching methods.
- Support has been dropped for database files that are gzipped (e.g. `oeb.gz` in the **FastROCS TK** examples). `.oeb` and `.oez` are still supported.

- A new database type, *OEShapeDatabaseType.Sitehopper*, has been added that runs Sitehopper calculations using fastrocs. Note that a Sitehopper license is required to run a Sitehopper calculation. Please visit https://www.eyesopen.com/contact or your account manager for a license.

8.12.2 Major bug fixes

- Previously, GPU memory limits were being reached for routine searches when using *OEFastROCSOrientation.InertialAtHeavyAtoms* with *OEShapeDatabaseOptions.SetColorOptimization* set to true, causing the color calculation to default to the CPU. The improved alternative starts algorithm handles any number of starts without reaching GPU memory limits.

> **Warning**
>
> Performance will be affected by using large numbers (> 10) of alternative starts.

- Previously, the section_example_fastrocs_shapeclustering example suffered some performance degradation. This has now been fixed thanks to a performance bug fix in `OESelfShape`. The script should now perform at its normal speed, ~10x that of the previous release.

8.12.3 Minor bug fixes

- A warning is now thrown if users attempt to use a custom color forcefield that has either a non-Gaussian functional form or interactions between different color types.

8.12.4 Python specific changes

- `SimplePythonScript.py` has been renamed `SimpleFastROCSSearch.py` in Tutorial 1: Inertial At Heavy Atoms Alternative Starts.
- `OEPreserveRotCompress` has been added to the molecule input stream in the `SimplePrepScript.py` script used in tutorial_database_prep.

8.12.5 Java specific changes

- `SimpleJavaScript.java` has been renamed `SimpleFastROCSSearch.java` in Tutorial 1: Inertial At Heavy Atoms Alternative Starts.
- `OEPreserveRotCompress` has been added to the molecule input stream in the `SimplePrepScript.java` script used in tutorial_database_prep.

8.12.6 C++ specific changes

- `simplecppscript.cpp` has been renamed `simplefastrocssearch.cpp` in Tutorial 1: Inertial At Heavy Atoms Alternative Starts.
- `OEPreserveRotCompress` has been added to the molecule input stream in the `simpleprepscript.cpp` script used in tutorial_database_prep.

8.12.7 Documentation changes

- tutorial_database_prep now has an additional step explaining `OEPreserveRotCompress`.

8.13 FastROCS TK 2.0.0

8.13.1 New features

- Two new options have been added to the *OEShapeDatabase* class:
  - *OEShapeDatabaseOptions.SetColorOptimization* is used for optimization over color overlap in addition to shape overlap during a **FastROCS** overlay calculation.
  - *OEShapeDatabaseOptions.SetFastROCSMode* is used to change several of the options in the *OEShapeDatabase* class to match what they would be in **ROCS** for a closer (though not identical) comparison to **ROCS**.

8.13.2 Minor bug fixes

- A warning regarding Tversky scores greater than 1.0 will now only be thrown if running with the Tversky scoring function.

8.13.3 General Notices

- The C++ **FastROCS TK** is not available on RHEL8 or Ubuntu18 in this release.

8.14 FastROCS TK 1.10.1

8.14.1 New features

- A new function, *OEFastROCSGPUStatus*, has been added that interrogates the status of the GPU and returns a code from the *OEFastROCSReturnCode* namespace. The return codes now allow for more specific error reporting of the GPU system.

8.14.2 Major bug fixes

- An issue that caused *OEFastROCSOrientation.Subrocs* to fail to apply the correct number of starts to the color calculation has been fixed.
- *OEShapeDatabase.SetColorGridSpacing* had been broken after the previous major version change. This has been fixed.
- *OEShapeDatabaseOptions.SetLimit* now returns all `N` overlays of all conformers and orientations when used in conjunction with *OEShapeDatabaseOptions.SetMaxOverlays* set to `0` and *OEShapeDatabaseOptions.SetMaxConfs* set to `0`.
- The default is now to run reference Tversky when running *OEShapeSimFuncType.Tversky*. For more details about Tversky similarity scoring, see the Molecular Shape section of the **Shape TK** theory documentation.

8.14.3 Minor bug fixes

- *OEShapeDatabaseOptions.SetNumInertialStarts* is no longer order-dependent when using alternative starts.
- When running with Tversky similarity scoring, only a single warning about Tversky scores being greater than 1.0 will ever be thrown unless the debug error level is being used.

8.15 FastROCS TK 1.10.0

8.15.1 New features

- **FastROCS TK** has been optimized to yield a further ~2-3x in performance compared to the previous release. The performance improvement will vary from system to system. See more details in the OEToolkits 2019.Apr section.

8.15.2 Minor bug fixes

- GPUs in prohibited mode will now be honored when querying the number of available devices on the system. Previously, a fatal error occurred during the search.

8.15.3 Python-specific changes

- The example in the section_example_fastrocs_shapedatabaseprep section now defaults to a maximum of 10 conformers per molecule and saves the coordinates in half-float precision. A flag is provided to switch to full-float precision coordinates.

8.15.4 Documentation changes

- A new GPU Prerequisites section has been added to the installation guide.

8.16 FastROCS TK 1.9.0

8.16.1 General notices

- **FastROCS TK** no longer supports Nvidia Tesla, GEForce, and Quadro cards with a compute capability of less than 3.0. This includes all GPUs with Fermi architecture (e.g., Tesla C2050 and GEForce GTX 430). If you are running one of these older GPUs and cannot upgrade your hardware, do not update to this version of **FastROCS TK**.

8.16.2 New features

- **FastROCS TK** is now supported for Java and C++. See the new documentation pages for Java and C++ for examples of toolkit usage and syntax.

> **Note**
>
> Java and C++ **FastROCS TK** API points are currently intended to be used only for toolkit functionality and not client-server functionality. The Python API should be used if client-server utilities are needed.

- A new *OEShapeDatabasePrep* function has been added to provide the same functionality as the shape-databaseprep example, except as a multi-threaded function. This should improve performance when prepping databases on systems with multiple cores. This function is non-deterministic, so molecules will not appear in the same order as the input file.

8.16.3 Major bug fixes

- A memory leak that was only detectable when running large numbers of queries in succession against the same database without breaking context has been fixed.
- The *OEShapeDatabase.AddMol* method was previously missing the ability to load molecules for *OEFastROCSOrientation.AsIs* alternative starting points. *OEShapeDatabase.AddMol* now takes the

OEFastROCSOrientation constant as an additional argument. The default is *OEFastROCSOrientation.Inertial*.

8.16.4 Documentation changes

- The examples section of the documentation has been reorganized by type: *Simple Examples*, *Alternative Starts*, and *Client-Server*. All are viewable from the *FastROCS Example Suite*, which includes brief descriptions as well as links to the specific example pages. The example pages now provide more in-depth descriptions of usage and download links to the example code.
- New examples have been added to the *Alternative Starts* section to demonstrate using **FastROCS TK** with alternative starts.
- Documentation for both the Java and C++ versions of **FastROCS TK** has been added.

8.17 FastROCS TK 1.8.4

8.17.1 New features

- A new Python example script, BestShapeOverlayMultiConfQuery.py, has been added to perform a query search for every conformer of the query molecule and save the sorted results sequentially in a single file for each query molecule.

8.17.2 Minor bug fixes

- A small modification has been made to `ShapeDatabaseServer.py` to reduce the number of server-related messages when running a query search via the client/proxy interface.

8.18 FastROCS TK 1.8.3

8.18.1 New features

- Alternative starting points in **FastROCS TK** have been extended to include two additional API points: *OEFastROCSOrientation.Random* and *OEFastROCSOrientation.Subrocs*.
  - *OEFastROCSOrientation.Random* now randomly orients the database molecule N times. By default, N is set to 10 with a maximum allowed translation of 2 angstroms. Random alternative starts can be customized using the *OEShapeDatabaseOptions.SetMaxRandomTranslation*, *OEShapeDatabaseOptions.SetNumRandomStarts*, and *OEShapeDatabaseOptions.SetRandomSeed* methods. The default random seed is time-dependent.
  - *OEFastROCSOrientation.Subrocs* now performs optimizations at every heavy atom of the molecule with the most heavy atoms, regardless of which molecule is the query and which is the database molecule. At each translation, 4 inertial poses are optimized, resulting in a total of [4 * number of heavy atoms of the heaviest molecule] optimizations.

  See *OEFastROCSOrientation* and *OEShapeDatabaseOptions.SetInitialOrientation* for more information.
- The following example scripts have been reworked to enable access to additional features of **FastROCS TK**:
  - `ShapeDatabaseServer.py`
  - `ShapeDatabaseClient.py`
  - `ShapeDatabaseClientHistogram.py`
  - `ShapeDatabaseProxy.py`

Tversky sampling, shape-only searches, and basic alternative starting points can be accessed via the client without having to rerun or modify the server/proxy scripts. Users can submit a query as usual from the client adding the relevant flags. The new flags are:

- `--tversky`
- `--shapeOnly`
- `--alternativeStarts [inertialAtHeavyAtoms|inertialAtColorAtoms|subrocs|random [N]]`

> **Warning**
>
> These scripts are not backwards compatible. The behavior of running server/proxy/client scripts with mismatched versions is undefined. In order to use the new client flags, ensure that the server and proxy scripts are also updated to this version.

- Warnings that are thrown for Tversky and Tanimoto scores greater than 1.0 have been simplified. Messages showing the actual Tversky/Tanimoto calculation are now Debug-level messages.

8.18.2 Minor bug fixes

- *OEDBTracer.GetTotal* now correctly accumulates the total when using the same *OEDBTracer* object for multiple queries.
- *OEShapeDatabaseOptions.SetLimit* now correctly handles the scenario where the limit is greater than the maximum scores available. If the limit is greater than the possible number of scores able to be returned, a warning will be thrown and the limit will fall back to: `number of conformers *` *OEShapeDatabaseOptions.GetMaxOverlays*.

8.18.3 Python-specific changes

- The example script `karma.py` in *FastROCS TK examples* has been renamed to the more descriptive `SphereExclusionClustering.py`.

8.18.4 Documentation changes

- A new tutorial, Tutorial 2, has been created for preparing a database to take advantage of faster *OEShapeDatabase.Open* times.

8.19 FastROCS TK 1.8.2

8.19.1 New features

- Alternative starting points in **FastROCS TK** have been extended to now include *OEFastROCSOrientation.AsIs* and *OEFastROCSOrientation.InertialAtColorAtoms*.
  - *OEFastROCSOrientation.AsIs* presumes that the query and the database molecules are already correctly aligned in space (perhaps through docking), so a single optimization per query-database molecule pair is carried out.
  - *OEFastROCSOrientation.InertialAtColorAtoms* translates each database molecule to each color atom of the query molecule and optimizes for 4 inertial poses at each translation. This method can be used with both shape-only searches and combo searches. The only requirement is that the query molecule must have color atoms; otherwise, the search will throw a warning and default to inertial starts.

See *OEFastROCSOrientation* and *OEShapeDatabaseOptions.SetInitialOrientation* for more information.

- The following new getter methods have been added to *OEShapeDatabaseOptions* for retrieving the number of starts for the relevant method:
  - *OEShapeDatabaseOptions.GetNumUserStarts*
  - *OEShapeDatabaseOptions.GetNumColorAtomStarts*
  - *OEShapeDatabaseOptions.GetNumHeavyAtomStarts*
  - *OEShapeDatabaseOptions.GetNumStarts*

  OEShapeDatabaseOptions.GetNumStarts has also been overloaded for each alternative start option.

- A new argument has been added to *OEShapeDatabase.Open* to ensure that conformers are correctly handled when using *OEFastROCSOrientation.AsIs*.

  When using the new *OEFastROCSOrientation.AsIs* feature, the shape database must be opened with the additional argument set to *OEFastROCSOrientation.AsIs*.

  There is no need to alter existing scripts if the *OEFastROCSOrientation.AsIs* alternative starts feature is not being used since the default argument results in the correct execution path for all other use cases.

  See *OEShapeDatabase.Open* and *OEFastROCSOrientation.AsIs* for more information.

- A new argument has been added to *OEShapeDatabaseScore.Constructors* to correctly transform conformers to their resultant position when using *OEFastROCSOrientation.AsIs*.

  Generally, the constructor is not used in most scripts as the *OEShapeDatabaseScore* object is constructed internally when calling *OEShapeDatabase.GetScores* or *OEShapeDatabase.GetSortedScores*. Therefore, most users will not be affected by this change.

  If the *OEShapeDatabaseScore* constructor is used and *OEFastROCSOrientation.AsIs* is set, the constructor can be modified with the additional argument set to *OEFastROCSOrientation.AsIs*.

  The default value for the additional argument satisfies all other use cases, so no action is required.

  See *OEShapeDatabaseScore.Constructors* for more information.

8.19.2 Major bug fixes

- Previously, GPU memory limits were being reached for routine searches when using *OEFastROCSOrientation.InertialAtHeavyAtoms*, causing searches to default to *OEFastROCSOrientation.Inertial*. The improved alternative starts algorithm handles any number of starts without reaching GPU memory limits.

> **Warning**
>
> Performance will be affected by using large numbers of alternative starts.

- *OEShapeDatabaseOptions.SetMaxOverlays* now sets the number of overlay results to return per conformer. Previously, this was broken and was restricting the number of overlays to 1 per conformer regardless of its setting. *OEShapeDatabaseOptions.SetMaxOverlays* is now fixed and works correctly with *OEShapeDatabaseOptions.SetMaxConfs*, *OEShapeDatabaseOptions.SetNumInertialStarts* and alternative starts for both *OEShapeDatabase.GetScores* and *OEShapeDatabase.GetSortedScores*.

- Tversky calculations no longer overestimate the score of caged systems or conformer pairs where one conformer is much larger than the other.

8.19.3 Minor bug fixes

- A warning is now thrown if *OEFastROCSOrientation.UserInertialStarts* is set with *OEShapeDatabaseOptions.SetInitialOrientation* and *OEShapeDatabase.GetScores* or if *OEShapeDatabase.GetSortedScores* is called before *OEShapeDatabaseOptions.SetUserStarts*.

8.19.4 Documentation changes

- A tutorials page has been created that walks through features of **FastROCS TK** and gives detailed examples. The first tutorial gives step-by-step instructions on how to use alternative starts.

  If you have a specific feature that you would like in a tutorial, please contact support at support@eyesopen.com with the subject header **FastROCS TK Tutorial Request**.

8.20 FastROCS TK 1.8.1

8.20.1 New features

- This release extends the capabilities of **FastROCS TK** to allow for 2 types of alternative starting points: user-defined starts and starts at heavy atoms.

  The **FastROCS TK** algorithm involves optimizing each overlaid query and database molecule by shape. Previously, the optimization had been performed for 4 orientations of each database molecule around its principle axes of inertia.

  User-defined starts allow users to input starting coordinates directly. The database molecule is now translated to each starting position and the 4 inertial poses are optimized.

  Starts at heavy atoms translate each database molecule to each heavy atom plus the center of mass of the query molecule. Again, the 4 inertial poses are optimized at each translation.

  For more information, see *OEShapeDatabaseOptions.SetInitialOrientation* and *OEFastROCSOrientation*.

- A new function, *OEFastROCSGetNumDevices*, has been added that returns the number of GPUs currently visible. Since no **FastROCS TK** objects are required, it can be used to probe a system prior to running any queries.

- A new function, *OEIsDatabasePrepared*, has been added to check whether a database file has already been run through *OEPrepareFastROCSMol*. This is useful for ensuring that a database file has been prepared and also saves time by preventing it from being prepared twice. **OpenEye** recommends preparing all large databases in order to benefit from significantly faster *OEShapeDatabase.Open* times.

- The cutoffs in **FastROCS TK** now support the retrieval of all scores less than or equal to the desired cutoff. See *OEShapeDatabaseOptions.SetCutoffLT*.

8.20.2 Major bug fixes

- Customers using Tesla C2050 cards and GTX cards at compute capability 2.x may have experienced some issues with large databases of very small molecules since compute resources were being over-allocated in some scenarios. This issue has been resolved.

8.20.3 Minor bug fixes

- Warnings had previously been thrown for Tversky scores greater than 1.0 (shape/color). For performance reasons, components of the Tversky/Tanimoto scores can be calculated on either the GPU or CPU. This sometimes results in scores slightly greater than 1.0. Customers should be aware of this possibility when handling scores. A warning is now thrown if a score is greater than 1.2.

- When opening an *OEShapeDatabase* object, the presence of invalid molecules now results in a warning rather than error.
- `karma.py` can now handle databases with molecules that don't have titles. A unique title is given to each untitled molecule.

8.21 FastROCS TK 1.8.0

8.21.1 New features

- **FastROCS TK** has been switched from an OpenCL backend to a CUDA backend. This should have no impact on **FastROCS** usage but may reduce the complexity of the installation process. The installation of CUDA development tools is *not* required to use **FastROCS TK**.
- NVIDIA driver support has been added for driver versions `367.*`. Support has been dropped for `340.*`. A list of currently supported NVIDIA drivers for **FastROCS TK** can be found in the *Installation* section.

8.21.2 Minor bug fixes

- The method *OEShapeDatabase.Open* has been modified to give a warning rather than an error when a file contains some molecules with heavy atoms and some molecules without heavy atoms. This is to prevent an entire database upload from failing if only a handful of molecules are corrupt.
- `ShapeSimilarityMatrix.py` has been renamed `ShapeDistanceMatrix.py` and the resultant matrix has been fixed to accurately reflect distance on the diagonal (i.e., 0.0).

8.21.3 Python-specific changes

- The Python integration tests now check for the presence of a GPU and skip the **FastROCS** test if a GPU is not available. Previously, the integration tests would fail.

8.22 FastROCS TK 1.7.0

8.22.1 New features

- *OEShapeDatabase* now consumes approximately 50% less main memory. This improvement was gained by compressing color information in a more concise way. There should be negligible difference in color Tanimoto scores (only seen in the 4th decimal place).
- Tversky similarity scoring is now available in **FastROCS TK** in addition to the default Tanimoto scoring. The following APIs have been added to support this new scoring:
  - *OEShapeDatabaseOptions.SetSimFunc* and *OEShapeDatabaseOptions.GetSimFunc* methods have been added to set and retrieve the scoring type.
  - *OEShapeDatabaseOptions.SetTverskyCoeffs* method has been included to allow custom tuning of the alpha and beta coefficients. *OEShapeDatabaseOptions.GetTverskyAlpha* and *OEShapeDatabaseOptions.GetTverskyBeta* methods have been added to retrieve the coefficients.
  - *OEShapeDatabaseScore.GetColorTversky*, *OEShapeDatabaseScore.GetShapeTversky*, *OEShapeDatabaseScore.GetTverskyCombo*, *OEShapeDatabaseScore.GetColorScore*, *OEShapeDatabaseScore.GetShapeScore*, and *OEShapeDatabaseScore.GetScore* methods have been provided for retrieving Tversky scores.

  For more details about Tversky similarity scoring, see the Molecular Shape section of the **Shape TK** theory documentation.

- *OEFastROCSIsGPUReady* function has been added to easily determine if the GPU is ready to accept **FastROCS TK** queries. It returns `true` if *OEShapeDatabase* can successfully execute queries on a supported accelerator device, and otherwise returns `false`. This function checks for the presence and status of GPU devices on the system, throwing an error message if the GPU is not ready for use. This function allows for any potential GPU issues to be caught prior to loading large databases.
- *OEShapeDatabase.PrintMemoryUsage* has been added to write out simple statistics about how much memory a particular *OEShapeDatabase* object is using and for what kinds of data.
- Driver support has been extended to include driver `361.*`. A list of currently supported NVIDIA drivers for **FastROCS TK** can be found in the *Installation* section.

8.22.2 Major bug fixes

- *OEShapeDatabase.GetScores* and *OEShapeDatabase.GetSortedScores* will no longer add color atoms to queries passed as OEConfBase objects. Previously, the following code would yield non-deterministic color scores and bugs:

```
for conf in mol.GetConfs():
    for score in shapedb.GetScores(conf):
        ...
```

  Users were previously instructed to make a temporary copy of the conformer into a new OEGraphMol before passing it to the methods that should have been logically `const`. This is no longer necessary.
- *OEShapeDatabaseScore.Transform* will now only change the coordinates of the molecule as the name implies. The method will transform hydrogens and color atoms in the molecule.
- ShapeDatabaseServer.py will now remove hydrogens from hit lists so that results from a cached OEB file (*OEPrepareFastROCSMol*) are identical to when the server is started on a non-cached OEB file.

8.22.3 Minor bug fixes

- *OEShapeDatabase.Open* and *OEShapeDatabase.GetScores* methods now throw an error message if a molecule contains no heavy atoms.

8.22.4 Python-specific changes

- *OEShapeDatabaseScore* methods will no longer release the Python global interpreter lock.

8.22.5 Documentation changes

- ShapeDatabasePrep.py example now has an optional argument to trim to a desired lower number of conformers.
- BestShapeOverlay.py example will now output the proper filenames when a problem occurs while opening them.
- Bugs in ShapeDatabaseServer.py, ShapeDatabaseClient.py, and ShapeDatabaseHistogram.py that were exposed when tested using Python 3.5 have been fixed. Python 3.5 now has a more efficient caching system in which file objects are required to be explicitly closed to ensure data writes are flushed.

8.23 FastROCS TK 1.6.0

8.23.1 New features

- The performance of **FastROCS** when loading a database into memory has been significantly improved when the appropriate caching has been done to the input OEB file. *OEPrepareFastROCSMol* function has been added

to allow preparing a molecule to be written to OEB so that it can be read very quickly by *OEShapeDatabase.Open*. It is highly recommended to pre-process input OEB files with this function to achieve faster load times. This works especially well in combination with `OEPRECompress`, resulting in uncompressed OEB files that are comparable to their gzip-compressed counterparts, even with extra cached information inside them.

> **Warning**
>
> *OEPrepareFastROCSMol* strips out information that **OMEGA** generates (i.e., hydrogen coordinates and conformer energies). Care must be taken when using these OEB files for alternative use cases. Please refer to the *OEPrepareFastROCSMol* documentation for a full accounting of how the molecules are changed.

- `OEFastROCSCacheStuff` was never officially supported and has been replaced by the *OEPrepareFastROCSMol* function. It now throws a deprecation warning and will be removed in a future release.
- **FastROCS TK** should be binary compatible with more NVidia driver versions as of this release. Previously, **FastROCS TK** could only target a single NVidia driver version. Now, several can be targeted in a single toolkit build. This version of **FastROCS TK** will work on the following NVidia driver versions: 340.x, 346.x, and 352.x. This should significantly reduce **FastROCS TK** installation headaches.
- *OEShapeDatabase.SetNumOpenThreads* method has been added to control how many CPU operating-system threads are created when calling *OEShapeDatabase.Open* on an OEMolDatabase object.
- All *OEShapeDatabase* instances now share the same GPU context. Previously, creating many *OEShapeDatabase* instances would result in many operating system threads created per instance. This would often hit resource limits around the number of threads allowed in a single process.

8.23.2 Minor bug fixes

- *OEShapeDatabase.Open* now returns `false` if no molecules are read from the OEMolDatabase object.

8.23.3 Python-specific changes

- All **FastROCS TK** Python examples now use `/usr/bin/env python` to determine the appropriate Python interpreter to use. Previously, some examples were erroneously hardcoded to use `/usr/bin/python`.
- `karma.py` shape clustering example had a minor bug that affected how invalid file names were handled. This has been fixed.

8.23.4 Documentation changes

- The **FastROCS TK** *Installation* section is now more general and defers to the NVidia website for installation instructions. A list of supported NVidia drivers for **FastROCS TK** can also be found in the *Installation* section.

8.24 FastROCS TK 1.5.1

8.24.1 New features

- *OEFastROCSHistogram* has been added to retrieve **FastROCS TK's** score distribution for the entire database, not just the hits, in real-time during a **FastROCS TK** query. The ShapeDatabaseServer.py example was extended with the `OEFastROCS::QueryHistogram` function, as well as the ShapeDatabaseProxy.py. The ShapeDatabase-ClientHistogram.py is an example of a client program to retrieve the histogram from the server in real time and print it to the terminal.

8.24.2 Major bug fixes

- ShapeDatabaseServer.py will now make sure to attach SD data from the parent OEMCMolBase to the output overlaid conformer.
- ShapeDatabaseOEThrowSetLevel.py will now work to effectively turn on additional performance debugging information. The additional operating system threads started by the *OEShapeDatabase* will now inherit the `OEErrorLevel` being used by the thread to execute the query through *`OEShapeDatabase.GetScores`* or *`OEShapeDatabase.GetSortedScores`*.
- **FastROCS TK** will now be compatible with NVidia compute architecture 2.0 cards. **FastROCS TK** beta in 2015.Jun.5 only worked on compute capability 3.x cards. The 2015.Jun.6 release was a bug fix release to fix this oversight. **FastROCS TK** in 2015.Oct should now work with any compute capability 2.0 card (the Fermi architecture) or greater.

8.24.3 Minor bug fixes

- ShapeDatabaseServer.py will now release its port number upon termination more quickly. Previously, the server would sometimes fail because when a new process was started the port number was already reserved by the previous process.

8.24.4 Documentation fixes

- The *Installation* section now recommends installing the NVidia driver with the `--disable-nouveau` flag to ensure that the open source `nouveau` display driver kernel module is turned off. The NVidia CUDA documentation is a much better source of this installation information: http://docs.nvidia.com/cuda/cuda-getting-started-guide-for-linux/#runfile-nouveau

8.24.5 General notices

- This is the last release to support **FastROCS TK** on Ubuntu 12.
- Supported NVIDIA Driver: 352.* (see *Supported NVIDIA Drivers* for alternative **FastROCS TK** releases).

8.25 FastROCS TK 1.5.0

- This is an initial public beta release of **FastROCS TK** as part of the larger **OpenEye Toolkit** suite. Initial support is being limited to 64-bit Linux Python platforms. Please bear with us as we work to bring **FastROCS TK** up to the same level of quality as you should expect from every **OpenEye** toolkit.
- The core suite of *FastROCS TK examples* have been tested and will work in this distribution. Note, the examples are present in the Windows and OSX distributions, but the following examples only work on 64-bit Linux Python platforms:
  - ShapeDatabaseServer.py
  - ShapeDatabaseChunker.py
  - BestShapeOverlay.py
  - karma.py

  As **FastROCS TK** works towards official release, example programs will likely change names and be re-designed. We will keep compatibility with the following core examples many of the current **FastROCS** users depend on:
  - ShapeDatabaseServer.py
  - ShapeDatabaseClient.py

  - ShapeDatabaseIsLoaded.py
  - ShapeDatabaseProxy.py
- ShapeDatabaseServer.py will no longer hang indefinitely whenever the gzipped results are requested by the client.
- ShapeDatabaseServer.py now supports specifying a different color force field, including a custom color force through a .cff file.
- ShapeDatabaseServer.py now supports specifying the hostname to bind to.
- BestShapeOverlay.py optimized by using OEMolDatabase class.
- The name of **FastROCS TK** python module has changed from `oeshapedatabase` to `oefastrocs`. The example scripts have already been updated to account for the name change.
- *OEShapeDatabase* will be much more efficient when the database is in an empty state.
- *OEShapeDatabase* will now co-exist with other GPU processes, including other instances of *OEShapeDatabase* objects. Previously, *OEShapeDatabase* was very aggressive in the amount of GPU memory allocated, even when the data set sizes were very small. *OEShapeDatabase* will now be much more frugal with the amount of GPU memory it allocates making it possible to use many more *OEShapeDatabase* simultaneously, provided each dataset is small.
- *OEShapeDatabase.GetSortedScores* and *OEShapeDatabase.GetScores* will now error more reliably. Previously, an error could occur, like an out-of-memory problem on a GPU, and a partial list of results would be returned. This made it very difficult to notice when something was wrong, requiring someone to notice the error messages in the server log. Now, no results at all will be returned if any problem with the search occurs.
- *OEShapeDatabase.GetSortedScores* and *OEShapeDatabase.GetScores* APIs have changed from strings of shape queries to take actual OEShapeQueryPublic objects.
- *OEShapeDatabase.AddMol* will now throw an error immediately if there are no atoms or conformers in the molecule.

> **Note**
>
> Supported NVIDIA Driver: 346.* (see *Supported NVIDIA Drivers* for alternative **FastROCS TK** releases).

8.26 FastROCS TK 1.4.0

- The structure of the FastROCS tar-ball has changed to mimic an openeye distribution tree usually seen on Linux. All programs can now be found in the openeye/bin directory.
- This version of FastROCS was built with the NVIDIA 310 driver included in this distribution. FastROCS should continue to work with the 295 driver as OpenCL and CUDA have not changed version between these driver versions. However, if problems are experienced during the upgrade, please try upgrading the NVIDIA driver to the 310 version.

8.26.1 Features

- FlaskROCS, an example web page service has been added. See openeye/FlaskROCS/README for more information.
- ShapeDatabaseClient (both Python and Java) no longer requires the OpenEye toolkits to run. This should make client applications a lot more portable and easier to write. Clients written against version 1.3.1 servers and prior versions will still continue to work. The following demonstrates client commands and that their behavior is unchanged when upgrading the server to version 1.4.0.

The 1.3.1 and prior clients: ./ShapeDatabaseClient.py 1_3_1_server_addr query.sdf results.oeb # still works ./ShapeDatabaseClient.py 1_3_1_server_addr query.oeb results.oeb # still works ./ShapeDatabaseClient.py 1_3_1_server_addr query.sdf results.sdf # would never work, results had to be an oeb file

./ShapeDatabaseClient.py 1_4_0_server_addr query.sdf results.oeb # still works ./ShapeDatabaseClient.py 1_4_0_server_addr query.oeb results.oeb # still works ./ShapeDatabaseClient.py 1_4_0_server_addr query.sdf results.sdf # would never work, results had to be an oeb file

The 1.4.0 client will only work with 1.3.1 servers when the input and output format is oeb. However, the results file no longer needs to be oeb when running the 1.4.0 client against a 1.4.0 server. The following demonstrates client commands and that their behavior unchanged when upgrading the server to version 1.4.0.

The 1.4.0 client: ./ShapeDatabaseClient.py 1_3_1_server_addr query.sdf results.oeb # won't work, query is sdf file ./ShapeDatabaseClient.py 1_3_1_server_addr query.oeb results.oeb # still works ./ShapeDatabaseClient.py 1_3_1_server_addr query.sdf results.sdf # would never work, results had to be an oeb file

./ShapeDatabaseClient.py 1_4_0_server_addr query.sdf results.oeb # still works ./ShapeDatabaseClient.py 1_4_0_server_addr query.oeb results.oeb # still works ./ShapeDatabaseClient.py 1_4_0_server_addr query.sdf results.sdf # works now! results can be any file format

Note

The servers (ShapeDatabaseServer.py and ShapeDatabaseProxy.py) still require an OEChem license. Though it is a long term to remove this deficiency in licensing.

The following client scripts still require OEChem: * ShapeDatabaseIsLoaded.py * ShapeDatabaseOEThrowSetLevel.py

This can be coded around upon customer request.

Note

the distribution no longer ships with the OpenEye Java jar files.

- ShapeDatabasePrep multi-threaded program added to replace the CacheStuff.py script to quickly and efficiently prepare OEB database files for faster load times into FastROCS. It is now highly recommended to run this program on your database to save on load time performance by the server.
- The memory footprint of the ShapeDatabaseServer.py has been reduced by about half by making use of new experimental OEChem technology, the OEMolDatabase. This effectively uses the database file itself to serve requests for molecule connection tables. This also improved database load time performance by 2x. Load time is now affected by disk bandwidth, so better load times can be achieved by investing in faster hard drive, e.g., solid state drives.

  Note: it is now highly recommended to pass ShapeDatabaseServer.py an uncompressed .oeb file instead of a .oeb.gz file.
- ShapeDatabaseAddMols.py has been removed from the distribution. ShapeDatabaseServer.py is now a "read-only" database after it finishes loading.
- ShapeDatabaseOEThrowSetLevel.py can now set the server into the "Error" level, that is, warnings are not even printed.
- The ShapeDatabaseServer's XML RPC SubmitQuery method now takes 2 additional optional arguments: iformat='.oeb' and iformat='.oeb'. The *iformat* arguments specifies what file format the query is being sent in at the first argument to SubmitQuery, *querymolstr*. The *oformat* argument specified what file format the results should

be back in from the *QueryResults* method. The default is OEB since clients prior to this version always sent data in the OEB format.

- Added the NumConfs method to the OEShapeDatabase object.
- OEFastROCSGetRelease added to return the version number of the library.
- CustomColorFFPrep.py script added to demonstrate how to cache color atoms on molecules to force the server and client to use a custom color force field.
- Support has been added for custom OEColorForceFields to the OEShapeDatabase and OEShapeDatabaseOptions objects. The color force field given to the OEShapeDatabaseOptions must be a subset of the color force field used to construct the OEShapeDatabase.

8.26.2 Bug Fixes

- Fixed a license check issue that would call sys.exit when no OEChem license was present while importing the oeshapedatabase module.
- Fixed a crash that would be caused by using OESetMemPoolMode after loading the oeshapedatabase module.
- FastROCS results will now be returned in a deterministic order when the scores are identical. The order of hits with identical scores would sometimes appear in a different order upon subsequent runs due to results being sorted in parallel by the server. FastROCS will now break this tie by falling back to the order that the molecules are in the database.

8.27 FastROCS TK 1.3.1

- Adding support for RHEL6-x64 based upon customer request.
- Reducing the size of the FastROCS tar-ball by removing some of the toolkit bloat.

8.28 FastROCS TK 1.3.0

- Major performance improvement in how FastROCS scales to multiple GPUs. The NVidia 275, 285, 295 driver introduced a severe performance regression that hampered FastROCS ability to scale across multiple GPUs. The solution was to use a different strategy to transfer data between the host and the device as well as scaling back the number of host threads launching jobs on the GPUs to only 1 per GPU.
- Many additions to the python interface to allow tweaking how FastROCS is parallelized and memory is moved around in the system: SetNumDevices, SetHostToDeviceStrategy, SetDeviceToHostStrategy, SetNumThreadsPerDevice. The defaults should be reasonable for everyone while using the 295 NVidia driver. They're left here to allow easy tweaking on future drivers, though they may be removed once a toolkit version is released, so don't rely on them.
- Fixed timer restart in OEShapeDatabaseOptions that would cause a reused OEShapeDatabaseOptions object to include time spent on previous searches.
- Only 4 decimal places are stored in the SD data fields for Shape Tanimoto, Color Tanimoto, and Tanimoto Combo.
- Made the NVidia driver install portion of the README easier to follow.
- Removed the restriction to use molecules with less than 3 heavy atoms.

8.29 FastROCS TK 1.2.1

- FastROCS is now built with the 2011.Oct toolkit release. This has some significant performance improvements on the server load time.
- FastROCS is now built against the latest two shipping NVidia drivers: OpenCL 1.1 CUDA 4.1 inside the 285 NVidia driver; and OpenCL 1.0 CUDA 4.0 inside the 275 NVidia driver. These drivers solve some search initialization costs that were seen in some setups.
- The Vida extension is being removed from the FastROCS distribution as a new version is being bundled directly into Vida.
- Significant updates to the README to remove a lot of cruft that had accumulated during development.

8.30 FastROCS TK 1.1.1

- Fixed bug with shape query support that would cause the server to crash when passing an empty shape query.
- Made the client/server interaction more robust in passing errors back from the server to the client.

8.31 FastROCS TK 1.1.0

8.31.1 Major Bug Fixes

- Fixed color bug that was calculating incorrect static color scores. Large errors were caused whenever the shape optimization produced large translations.
- Fixed bug that was causing certain database molecules (usually flat molecules) to be collapsed to a single point during the inertial alignment step of loading the database. This would sometimes manifest as tanimotos being outside the normal 0-1 range.

8.31.2 Minor Bug Fixes

- Fixed incorrect color Gaussian width used in the color score calculation.
- Handle zero division error in the color tanimoto calculation caused whenever a molecule has no color atoms. These tanimotos will now be 0.0.
- In the event an error occurs in the OpenCL driver and a command queue can not be opened to the GPU device only retry a finite amount of time. That is, don't loop infinitely in the event of a lower level error.
- Fixing order dependence problem caused whenever PYTHONPATH was explicitly set overriding the search path explicitly set inside ShapeDatabaseServer.py.
- Fixed bug in ShapeDatabaseServer.py caused by OEHeader objects in OEB files. This will be fixed in a more general sense by the next toolkit release.
- ShapeDatabaseServer.py will only allow one client query to process at a time to ensure that GPU resources are not exhausted. This restriction may be lifted in a future version, but for now this is the best way to keep the server robust in a multi-user environments.
- Cached color in OEB files use compressed color atoms in order to not corrupt the OEB rotor offset compression format. Also use the cached "AllColor" self term as it is closer to how the grid color overlap is calculated.

8.31.3 Major Features

- Added support for Shape Query (.sq) files generated from vROCS. These files can now be passed directly to ShapeDatabaseClient.(py/java).
- Significant performance improvement to post scoring with static color. Post scoring with static color is now essentially "free" as it occurs on the CPU after the shape optimization on the GPU. To achieve this at least 2 CPU cores per Fermi GPU is recommended.

8.31.4 Minor Features

- Significant performance improvement by caching the underlying GPU context more effectively. Some queries were seeing a 1-2 second overhead per GPU device because the GPU context could not be cached. Later versions of the driver seem to support this without crashing. If this version starts giving odd crashing behavior, try updating the NVidia driver first.
- ShapeDatabaseChunker.py is a little more robust in choosing output file names.
- Added ability to use 8 inertial starting points.
- Added the CacheStuff.py script to cache as much as possible to improve database load time. ShapeDatabaseChunker.py updated to cache color stuff as well.
- Totally revamped the output of Debug mode to allow for timing the more asynchronous nature of FastROCS now.

8.32 FastROCS TK 1.0.1

- First version of FastROCS that is designed to only work on a specific hardware and driver configuration. This release will only work on NVidia hardware with the CUDA 3.2 driver. FastROCS will work on any modern NVidia card that reports a compute capability of 1.0 or greater. Typically this is any NVidia card shipped after 2006. For a complete list of cards refer to Appendix A in the CUDA C Programming Guide.

> **Note**
>
> The more stringent requirement is on the driver version, CUDA 3.2. For this reason FastROCS will be shipping with the required associated NVidia Linux driver embedded in the tar-ball: devdriver_3.2_linux_64_260.19.26.run
>
> This requirement is also embedded into the tar-ball name as "OpenCL-1.0-CUDA-3.2" in case we need to support multiple versions or rev'ing to OpenCL 1.1 breaks compatibility. If a driver upgrade needs to occur due to some bug in some other third party software, let OpenEye know and we will see how best we can accommodate you.

- Added ShapeSimilarityMatrix.py example to write out a similarity matrix of an input database into a csv file suitable for feeding to downstream tools like cluster analysis. Note, due to the current slow speed of clCreateContext, the example is not crazy performant on small datasets, but on larger sets it is as the cost of clCreateContext becomes amortized.

8.33 FastROCS TK 1.0.0

- ShapeDatabaseServer.py now has a "-shapeOnly" option to run in a mode where color is not calculated at all. By default this option is off indicated that the server will use color. ShapeDatabaseProxy.py has been updated accordingly to automatically recognize whether to use ComboTanimoto and ShapeTanimoto to resort the results by.
- Fixing BestShapeOverlay.py to work with color.
- karma.py has been updated to work with color.

8.34 FastROCS TK 0.4.0

- An experimental release that includes color support meant for scientific validation with the following implementation caveats:
  - Static color scores are calculated using the alignment generated by a shape driven optimization. Note, a color score is calculated for each of the 4 inertial starting points. Therefore, it is possible for a less favorable shape score to be picked due to a higher tanimoto combo. This is the only part color plays in the optimization.
- Color is calculated using the grid method in order to be fast enough to keep up with the GPU generated alignments.
- Color is calculated on the CPU so there is no increased bus overhead for color, but there is a significant increase in CPU usage. Calculating color on the CPU is a strategic move to see if we can get away with calculating color without any significant increase to the overall search time. This release gets part of the way towards that goal: a single core of a Xeon CPU E5520 at 2.27GHz is about 2 times slower at calculating static colors coming out of a single NVidia C2050. Future releases will spread this over multiple CPU cores to better even out the load.
  - The OEShapeScore object has been renamed to OEShapeDatabaseScore to disambiguate it. Renamed the method GetTanimoto to GetShapeTanimoto. Added GetColorTanimoto and GetTanimotoCombo.
  - Add the OEShapeDatabaseType constants namespace to indicate whether a database should store color information as well and whether a query should use color as well.
  - Added OEShapeDatabaseOptions::SetScoreType to be used with the OEShapeDatabaseType constants to indicate what type of search is being done.
  - Renamed OEShapeDatabase::SetGridSpacing to OEShapeDatabase::SetShapeGridSpacing. Added OEShapeDatabase::SetColorGridSpacing.
  - Load time has been significantly increased due to the calculation of color atoms during load time.

8.35 FastROCS TK 0.3.1

- The server would sometimes crash with a "clCreateContext" error. This is being thrown from the NVidia driver for some unknown reason. This release will continually try to create the worker thread despite all else. Note, if something is truly wrong, this could appear to hang queries as the server will keep retrying to create a context on the GPU, but at least the log will indicate an error code now that may tell us more about what is going on.

8.36 FastROCS TK 0.3.0

- Added ShapeDatabaseAddMols.py script to add molecules to a running ShapeDatabaseServer.
- Added ShapeDatabaseIsLoaded.py script to report whether the initial database load has completed.
- Added argument to ShapeDatabaseClient.py for the number of hits to return, defaults to 100.
- Redesigned how the BestShapeOverlay.py script runs to be more useful for doing evaluations.
- Restricting OEShapeDatabase to only run on one type of device and prefer to run on a GPU, and fall back to a CPU device only if there is no GPU present. Used to be that on OS X the search would run on the GPU and CPU simultaneously, however, the results of the overlay could differ depending on whether they were sent to the GPU or the CPU. Due to dynamic load balancing between the CPU and GPU this could change the rank of the results returned in an apparently non-deterministic manner. It is not pleasant for an end-user to run the same query multiple times and get different results so we restrict searches to either CPU or GPU, not both now. Note, this only would occur on OS X. The NVidia implementation doesn't support a CPU device, so this never occurred there.

8.37 FastROCS TK 0.2.3

- OSX only release to fix obscure bug that occurred when using an NVidia GPU through Apple's OpenCL implementation.

8.38 FastROCS TK 0.2.2

- Fixed a major bug that would cause very high shape tanimotos to be calculated when cached color atoms were present in the input database.
- Added symlink from SLES to SLED to work around OEToolkit issue of not recognizing those as equivalent systems.
- Querying the database with an empty molecule will no longer crash.
- Added BenchmarkDatabaseTransfer.py benchmark to determine the maximum speed being achieved when transferring database chunks across the bus.

8.39 FastROCS TK 0.2.1

- Added support for SUSE 11.
- Added cuda.sh shell script that will create the appropriate nvidia device entries inside /dev/. It is a known issue on SLES11 the nvidia driver will create the /dev/ entries with the wrong permissions. Also, it is known issue that on RHEL5 LDAP users could not launch OpenCL based programs. Running this shell script as root (i.e. during boot) should fix these problems. We should push on NVidia to make this part of their driver installer.
- The PrintOpenCLDevices utility will now print "platform" information about the driver(s) found on the system. This is useful for displaying which version of CUDA is installed, instead of just what version of OpenCL is installed.
- Fixed problem where some systems without SWAP memory would crash with an out of memory error when the OEShapeDatabase object would try to reserve large swaths of memory. The virtual memory size of the process should now track more closely with the resident memory size.

8.40 FastROCS TK 0.2.0

- Added example of a XML RPC client written in Java. (See the javaclient directory.)
- Added example program for doing shape clustering. (See karma.py)
- Refactored benchmarking scripts into the benchmarks directory.
  - Added benchmarks for database size and random access patterns.
- Improved database load time of ShapeDatabaseServer.py by multithreading
  - It is now thread safe to use OEShapeDatabase::AddMol from multiple threads. Note, it is not thread safe to call Get(Sorted)Scores while calling AddMol. Let me know if this is desired.

8.41 FastROCS TK 0.1.1

- Adding the ShapeDatabaseOEThrowSetLevel.py script to adjust the verbosity level of the server without restarting it.

8.42 FastROCS TK 0.1.0

- First public release.

CHAPTER

NINE

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CHAPTER

TEN

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CHAPTER

ELEVEN

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11.2 Orion Floes

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OpenEye Large-Scale Floes 4.2.3. OpenEye, Cadence Molecular Sciences, Santa Fe, NM.␣
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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.

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↪eyesopen.com.
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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.

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

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↪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.

11.4 Publications for Bibliographies

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

11.4.1 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

11.4.2 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

11.4.3 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

11.4.4 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

11.4.5 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

11.5 OpenEye MMDS Web Service

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

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

CHAPTER

TWELVE

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

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

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

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

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

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

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

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

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

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

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

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

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

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

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

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

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

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

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

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

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

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

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

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

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

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

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

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

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

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

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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Table 1 – continued from previous page

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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Table 1 – continued from previous page

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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Table 1 – continued from previous page

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

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Table 1 – continued from previous page

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

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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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Table 1 – continued from previous page

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

12.1 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).

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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.

12.1.1 GCC RUNTIME LIBRARY EXCEPTION

```
Version 3.1, 31 March 2009

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↪notice placed by the copyright holder
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↪files and runtime libraries with
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↪(including proprietary) programs
to use, in this way, the header files and runtime libraries covered by this Exception.

0. Definitions.

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

"GCC" means a version of the GNU Compiler Collection, with or without modifications,␣
↪governed by version 3 (or a specified
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↪subsequent versions published by the FSF.

"GPL-compatible Software" is software whose conditions of propagation, modification and␣
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"Target Code" refers to output from any compiler for a real or virtual target processor␣
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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
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You have permission to propagate a work of Target Code formed by combining the Runtime␣
↪Library with Independent Modules,
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↪Target Code was generated by
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↪your choice, consistent with the
licensing of the Independent Modules.

2. No Weakening of GCC Copyleft.

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

See also

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

12.1.2 GNU GENERAL PUBLIC LICENSE

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

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   The licenses for most software and other practical works are designed
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can do so.  This is fundamentally incompatible with the aim of
protecting users' freedom to change the software.  The systematic
pattern of such abuse occurs in the area of products for individuals to
use, which is precisely where it is most unacceptable.  Therefore, we
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States should not allow patents to restrict development and use of
software on general-purpose computers, but in those that do, we wish to
avoid the special danger that patents applied to a free program could
make it effectively proprietary.  To prevent this, the GPL assures that
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patents cannot be used to render the program non-free.

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

                    TERMS AND CONDITIONS

  0. Definitions.

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

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"recipients" may be individuals or organizations.

  To "modify" a work means to copy from or adapt all or part of the work
in a fashion requiring copyright permission, other than the making of an
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  A "covered work" means either the unmodified Program or a work based
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  To "convey" a work means any kind of propagation that enables other
parties to make or receive copies.  Mere interaction with a user through
a computer network, with no transfer of a copy, is not conveying.

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to the extent that it includes a convenient and prominently visible
feature that (1) displays an appropriate copyright notice, and (2)
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extent that warranties are provided), that licensees may convey the
work under this License, and how to view a copy of this License.  If
the interface presents a list of user commands or options, such as a
menu, a prominent item in the list meets this criterion.

  1. Source Code.

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

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

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

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  5. Conveying Modified Source Versions.

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

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

   b) The work must carry prominent notices stating that it is
   released under this License and any conditions added under section
   7.  This requirement modifies the requirement in section 4 to
   "keep intact all notices".
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    c) You must license the entire work, as a whole, under this
    License to anyone who comes into possession of a copy.  This
    License will therefore apply, along with any applicable section 7
    additional terms, to the whole of the work, and all its parts,
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works, which are not by their nature extensions of the covered work,
and which are not combined with it such as to form a larger program,
in or on a volume of a storage or distribution medium, is called an
"aggregate" if the compilation and its resulting copyright are not
used to limit the access or legal rights of the compilation's users
beyond what the individual works permit.  Inclusion of a covered work
in an aggregate does not cause this License to apply to the other
parts of the aggregate.

  6. Conveying Non-Source Forms.

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

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

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

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

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

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

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

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tangible personal property which is normally used for personal, family,
or household purposes, or (2) anything designed or sold for incorporation
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doubtful cases shall be resolved in favor of coverage.  For a particular
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of the particular user or of the way in which the particular user
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is a consumer product regardless of whether the product has substantial
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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
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protocols for communication across the network.

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