

IsoSpec

1.95

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Chapter 1

Namespace Index

1.1 Namespace List

Here is a list of all documented namespaces with brief descriptions:

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Chapter 2

Hierarchical Index

2.1 Class Hierarchy

This inheritance list is sorted roughly, but not completely, alphabetically:

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IsoSpec::IsoSpec::ReverseOrder< T >	24
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IsoSpec::Tabulator< T >	25
IsoSpec::ThreadSumimator	25
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Chapter 3

Class Index

3.1 Class List

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Chapter 4

Namespace Documentation

4.1 IsoSpec Namespace Reference

Classes

- class [Allocator](#)
- class [ConfEqual](#)
- class [ConfOrder](#)
- class [ConfOrderMarginal](#)
- class [ConfOrderMarginalDescending](#)
- class [DirtyAllocator](#)
- class [Iso](#)

The [Iso](#) class for the calculation of the isotopic distribution.

- class [IsoGenerator](#)

The generator of isotopologues.

- class [IsoLayeredGenerator](#)
- class [IsoOrderedGenerator](#)

The generator of isotopologues sorted by their probability of occurrence.

- class [IsoThresholdGenerator](#)
- class [KeyHasher](#)
- class [Marginal](#)
- class [MarginalTrek](#)
- class [PrecalculatedMarginal](#)
- class [ReverseOrder](#)
- class [SSummator](#)
- class [Summator](#)
- class [TableOrder](#)
- class [Tabulator](#)
- class [ThreadSummator](#)
- class [TSummator](#)

Typedefs

- typedef int * **Conf**

Functions

- `template<typename T >`
`void copyConf (const T *source, T *destination, int dim)`
- `double RationalApproximation (double t)`
- `double NormalCDFInverse (double p)`
- `double NormalCDFInverse (double p, double mean, double stdev)`
- `double NormalCDF (double x, double mean, double stdev)`
- `double NormalPDF (double x, double mean, double stdev)`
- `int str_to_int (const string &s)`
- `unsigned int parse_formula (const char *formula, std::vector< const double *> &isotope_masses, std::vector< const double *> &isotope_probabilities, int **isotopeNumbers, int **atomCounts, unsigned int *confSize)`
- `void printConfigurations (const std::tuple< double *, double *, int *, int > &results, int dimNumber, int *isotopeNumbers)`
- `Conf initialConfigure (const int atomCnt, const int isotopeNo, const double *probs, const double *lprobs)`
- `void printMarginal (const std::tuple< double *, double *, int *, int > &results, int dim)`
- `double * getMLogProbs (const double *probs, int isoNo)`
- `double get_loggamma_nominator (int x)`
- `Conf initialConfigure (int atomCnt, int isotopeNo, const double *probs)`
- `double combinedSum (const int *conf, const std::vector< double > **valuesContainer, int dimNumber)`
- `int * getConf (void *conf)`
- `double getLProb (void *conf)`
- `double unnormalized_logProb (const int *conf, const double *logProbs, int dim)`
- `double mass (const int *conf, const double *masses, int dim)`
- `bool tupleCmp (std::tuple< double, double, int *> t1, std::tuple< double, double, int *> t2)`
- `template<typename T >`
`void printArray (const T *array, int size)`
- `template<typename T >`
`void printVector (const std::vector< T > &vec)`
- `template<typename T >`
`void printNestedArray (const T **array, const int *shape, int size)`
- `template<typename T >`
`void dealloc_table (T *tbl, int dim)`
- `void reallocate (double **array, int new_size)`

Variables

- `const int elem_table_atomicNo [ISOSPEC_NUMBER_OF_ISOTOPIC_ENTRIES]`
- `const double elem_table_mass [ISOSPEC_NUMBER_OF_ISOTOPIC_ENTRIES]`
- `const int elem_table_massNo [ISOSPEC_NUMBER_OF_ISOTOPIC_ENTRIES]`
- `const int elem_table_extraNeutrons [ISOSPEC_NUMBER_OF_ISOTOPIC_ENTRIES]`
- `const char * elem_table_element [ISOSPEC_NUMBER_OF_ISOTOPIC_ENTRIES]`
- `const char * elem_table_symbol [ISOSPEC_NUMBER_OF_ISOTOPIC_ENTRIES]`
- `const bool elem_table_Radioactive [ISOSPEC_NUMBER_OF_ISOTOPIC_ENTRIES]`
- `const double elem_table_probability [ISOSPEC_NUMBER_OF_ISOTOPIC_ENTRIES]`
- `const double elem_table_log_probability [ISOSPEC_NUMBER_OF_ISOTOPIC_ENTRIES]`
- `const double pi = 3.14159265358979323846264338328`
- `double * g_ifact_table = reinterpret_cast<double*>(calloc(ISOSPEC_G_FACT_TABLE_SIZE, sizeof(double)))`

4.1.1 Detailed Description

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4.1.2 Function Documentation

4.1.2.1 `getMLogProbs()`

```
double* IsoSpec::getMLogProbs (
    const double * probs,
    int isoNo )
```

Here we order the processor to round the numbers up rather than down. Rounding down could result in the algorithm falling in an infinite loop because of the numerical instability of summing.

4.1.2.2 `initialConfigure()`

```
Conf IsoSpec::initialConfigure (
    const int atomCnt,
    const int isotopeNo,
    const double * probs,
    const double * lprobs )
```

Here we perform hill climbing to the mode of the marginal distribution (the subisotopologue distribution). We start from the point close to the mean of the underlying multinomial distribution.

Chapter 5

Class Documentation

5.1 `IsoSpec::Allocator< T >` Class Template Reference

Public Member Functions

- **Allocator** (const int dim, const int tabSize=10000)
- void **shiftTables** ()
- T * **newConf** ()
- T * **makeCopy** (const T *conf)
- T * **makeExternalCopy** (const T *conf)

The documentation for this class was generated from the following files:

- /Users/matteo/Projects/isospec/IsoSpec/IsoSpec++/allocator.h
- /Users/matteo/Projects/isospec/IsoSpec/IsoSpec++/allocator.cpp

5.2 `IsoSpec::ConfEqual` Class Reference

Public Member Functions

- **ConfEqual** (int dim)
- bool **operator()** (const int *conf1, const int *conf2) const

The documentation for this class was generated from the following file:

- /Users/matteo/Projects/isospec/IsoSpec/IsoSpec++/operators.h

5.3 `IsoSpec::IsoSpec::ConfEqual` Class Reference

Public Member Functions

- **ConfEqual** (int dim)
- bool **operator()** (const int *conf1, const int *conf2) const

The documentation for this class was generated from the following file:

- /Users/matteo/Projects/isospec/IsoSpec/IsoSpec++/operators.cpp

5.4 IsoSpec::ConfOrder Class Reference

Public Member Functions

- **bool operator()** (void *conf1, void *conf2) const

The documentation for this class was generated from the following file:

- /Users/matteo/Projects/isospec/IsoSpec/IsoSpec++/operators.h

5.5 IsoSpec::IsoSpec::ConfOrder Class Reference

Public Member Functions

- **bool operator()** (void *conf1, void *conf2) const

The documentation for this class was generated from the following file:

- /Users/matteo/Projects/isospec/IsoSpec/IsoSpec++/operators.cpp

5.6 IsoSpec::ConfOrderMarginal Class Reference

Public Member Functions

- **ConfOrderMarginal** (const double *logProbs, int dim)
- **bool operator()** (const Conf conf1, const Conf conf2)

The documentation for this class was generated from the following file:

- /Users/matteo/Projects/isospec/IsoSpec/IsoSpec++/operators.h

5.7 IsoSpec::IsoSpec::ConfOrderMarginal Class Reference

Public Member Functions

- **ConfOrderMarginal** (const double *logProbs, int dim)
- **bool operator()** (const Conf conf1, const Conf conf2)

The documentation for this class was generated from the following file:

- /Users/matteo/Projects/isospec/IsoSpec/IsoSpec++/operators.cpp

5.8 IsoSpec::ConfOrderMarginalDescending Class Reference

Public Member Functions

- **ConfOrderMarginalDescending** (const double *logProbs, int dim)
- bool **operator()** (const Conf conf1, const Conf conf2)

The documentation for this class was generated from the following file:

- /Users/matteo/Projects/isospec/IsoSpec/IsoSpec++/operators.h

5.9 IsoSpec::IsoSpec::ConfOrderMarginalDescending Class Reference

Public Member Functions

- **ConfOrderMarginalDescending** (const double *logProbs, int dim)
- bool **operator()** (const Conf conf1, const Conf conf2)

The documentation for this class was generated from the following file:

- /Users/matteo/Projects/isospec/IsoSpec/IsoSpec++/operators.cpp

5.10 IsoSpec::DirtyAllocator Class Reference

Public Member Functions

- **DirtyAllocator** (const int dim, const int tabSize=10000)
- void **shiftTables** ()
- void * **newConf** ()
- void * **makeCopy** (const void *conf)
- void * **makeExternalCopy** (const void *conf)

The documentation for this class was generated from the following files:

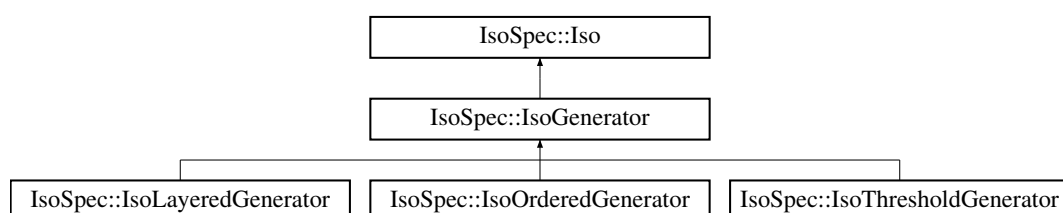
- /Users/matteo/Projects/isospec/IsoSpec/IsoSpec++/dirtyAllocator.h
- /Users/matteo/Projects/isospec/IsoSpec/IsoSpec++/dirtyAllocator.cpp

5.11 IsoSpec::Iso Class Reference

The **Iso** class for the calculation of the isotopic distribution.

```
#include <isoSpec++.h>
```

Inheritance diagram for IsoSpec::Iso:



Public Member Functions

- [Iso](#) (int `_dimNumber`, const int * `_isotopeNumbers`, const int * `_atomCounts`, const double *const * `_isotopeMasses`, const double *const * `_isotopeProbabilities`)
General constructor.
- [Iso](#) (const char * `formula`)
Constructor from the formula object.
- **Iso** ([Iso](#) && `other`)
- **Iso** (const [Iso](#) & `other`, bool `fullcopy`)
- double [getLightestPeakMass](#) () const
Get the mass of the lightest peak in the isotopic distribution.
- double [getHeaviestPeakMass](#) () const
Get the mass of the heaviest peak in the isotopic distribution.
- double [getModelProb](#) () const
Get the log-probability of the mode-configuration (if there are many modes, they share this value).
- int [getDimNumber](#) () const
Get the number of elements in the chemical formula of the molecule.
- int [getAllDim](#) () const
Get the total number of isotopes of elements present in a chemical formula.
- [PrecalculatedMarginal](#) ** [get_MT_marginal_set](#) (double `Lcutoff`, bool `absolute`, int `tabSize`, int `hashSize`)
Get the marginal distributions of subisotopologues.

Public Attributes

- bool [disowned](#)

Protected Attributes

- int [dimNumber](#)
- int * [isotopeNumbers](#)
- int * [atomCounts](#)
- unsigned int [confSize](#)
- int [allDim](#)
- [Marginal](#) ** [marginals](#)
- double [modelProb](#)

5.11.1 Detailed Description

The [Iso](#) class for the calculation of the isotopic distribution.

It contains full description of the molecule for which one would like to calculate the isotopic distribution.

5.11.2 Constructor & Destructor Documentation

5.11.2.1 Iso()

```

IsoSpec::Iso::Iso (
    int _dimNumber,
    const int * _isotopeNumbers,
    const int * _atomCounts,
    const double *const * _isotopeMasses,
    const double *const * _isotopeProbabilities )

```

General constructor.

Parameters

<i>_dimNumber</i>	The number of elements in the formula, e.g. for C100H202 it would be 2, as there are only carbon and hydrogen atoms.
<i>_isotopeNumbers</i>	A table with numbers of isotopes for each element, e.g. for C100H202 it would be {2, 2}, because both C and H have two stable isotopes.
<i>_atomCounts</i>	Number of atoms of each element in the formula, e.g. for C100H202 corresponds to {100, 202}.
<i>_isotopeMasses</i>	A table of masses of isotopes of the elements in the chemical formula, e.g. {12.0, 13.003355, 1.007825, 2.014102} for C100H202.
<i>_isotopeProbabilities</i>	A table of isotope frequencies of the elements in the chemical formula, e.g. {.989212, .010788, .999885, .000115} for C100H202.

5.11.3 Member Function Documentation

5.11.3.1 get_MT_marginal_set()

```
PrecalculatedMarginal** IsoSpec::Iso::get_MT_marginal_set (
    double Lcutoff,
    bool absolute,
    int tabSize,
    int hashSize )
```

Get the marginal distributions of subisotopologues.

Parameters

<i>Lcutoff</i>	The logarithm of the cut off value.
<i>absolute</i>	Should the cutoff be in terms of absolute height of the peak, or relative to the height/probability of the mode.
<i>tabSize</i>	The size of the extension of the table with configurations.
<i>hashSize</i>	The size of the hash-table used to store subisotopologues and check if they have been already calculated.

5.11.4 Member Data Documentation

5.11.4.1 allDim

```
int IsoSpec::Iso::allDim [protected]
```

The total number of isotopes of elements present in a chemical formula, e.g. for H2O it is 2+3=5.

5.11.4.2 atomCounts

```
int* IsoSpec::Iso::atomCounts [protected]
```

A table with numbers of isotopes for each element.

5.11.4.3 confSize

```
unsigned int IsoSpec::Iso::confSize [protected]
```

The number of bytes needed to represent the counts of isotopes present in the extended chemical formula.

5.11.4.4 dimNumber

```
int IsoSpec::Iso::dimNumber [protected]
```

The number of elements in the chemical formula of the molecule.

5.11.4.5 disowned

```
bool IsoSpec::Iso::disowned
```

A variable showing if the [Iso](#) class was specialized by its child-class. If so, then the description of the molecules has been transferred there and [Iso](#) is a carcass class, dead as a dodo, an ex-class if you will.

5.11.4.6 isotopeNumbers

```
int* IsoSpec::Iso::isotopeNumbers [protected]
```

A table with numbers of isotopes for each element.

5.11.4.7 marginals

```
Marginal** IsoSpec::Iso::marginals [protected]
```

The table of pointers to the distributions of individual subisotopologues.

5.11.4.8 modeLProb

```
double IsoSpec::Iso::modeLProb [protected]
```

The log-probability of the mode of the isotopic distribution.

The documentation for this class was generated from the following files:

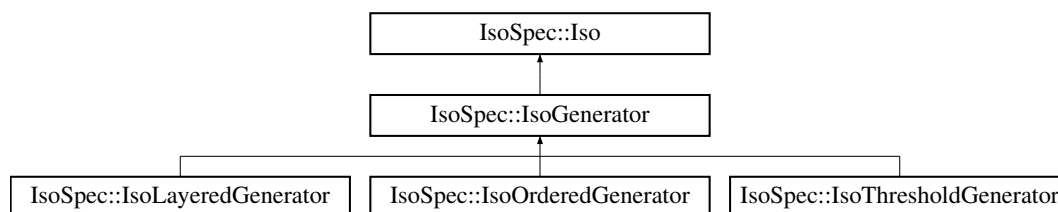
- /Users/matteo/Projects/isospec/IsoSpec/IsoSpec++/isoSpec++.h
- /Users/matteo/Projects/isospec/IsoSpec/IsoSpec++/isoSpec++.cpp

5.12 IsoSpec::IsoGenerator Class Reference

The generator of isotopologues.

```
#include <isoSpec++.h>
```

Inheritance diagram for IsoSpec::IsoGenerator:



Public Member Functions

- virtual bool [advanceToNextConfiguration](#) ()=0
- double **lprob** () const
- double **mass** () const
- double **eprob** () const
- virtual void **get_conf_signature** (int *space) const =0
- **IsoGenerator** ([Iso](#) &&iso)

Protected Attributes

- double * **partialLProbs**
- double * [partialMasses](#)
- double * [partialExpProbs](#)

Additional Inherited Members

5.12.1 Detailed Description

The generator of isotopologues.

This class provides the common interface for all isotopic generators.

5.12.2 Member Function Documentation

5.12.2.1 [advanceToNextConfiguration\(\)](#)

```
virtual bool IsoSpec::IsoGenerator::advanceToNextConfiguration ( ) [pure virtual]
```

The prefix product of the probabilities of the current isotopologue.

Implemented in [IsoSpec::IsoLayeredGenerator](#), [IsoSpec::IsoThresholdGenerator](#), and [IsoSpec::IsoOrderedGenerator](#).

5.12.3 Member Data Documentation

5.12.3.1 partialExpProbs

```
double* IsoSpec::IsoGenerator::partialExpProbs [protected]
```

The prefix sum of the masses of the current isotopologue.

5.12.3.2 partialMasses

```
double* IsoSpec::IsoGenerator::partialMasses [protected]
```

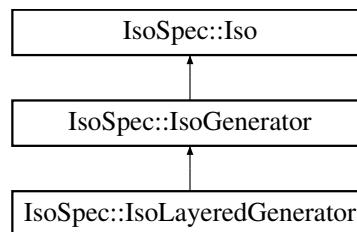
The prefix sum of the log-probabilities of the current isotopologue.

The documentation for this class was generated from the following files:

- /Users/matteo/Projects/isospec/IsoSpec/IsoSpec++/isoSpec++.h
- /Users/matteo/Projects/isospec/IsoSpec/IsoSpec++/isoSpec++.cpp

5.13 IsoSpec::IsoLayeredGenerator Class Reference

Inheritance diagram for IsoSpec::IsoLayeredGenerator:



Public Member Functions

- bool **advanceToNextConfiguration_internal** ()
- void **setup_delta** (double new_delta)
- bool **advanceToNextConfiguration** () override final
- bool **nextLayer** (double logCutoff_delta)
- **IsoLayeredGenerator** (**Iso** &&iso, double _delta=-3.0, int _tabSize=1000, int _hashSize=1000)
- void **get_conf_signature** (int *space) const override final
- void **terminate_search** ()

Additional Inherited Members

5.13.1 Member Function Documentation

5.13.1.1 advanceToNextConfiguration()

```
bool IsoSpec::IsoLayeredGenerator::advanceToNextConfiguration ( ) [inline], [final], [override],
[virtual]
```

The prefix product of the probabilities of the current isotopologue.

Implements [IsoSpec::IsoGenerator](#).

The documentation for this class was generated from the following file:

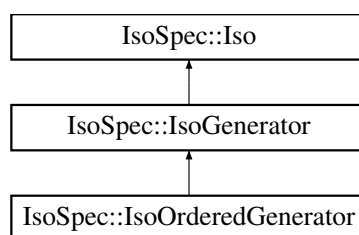
- /Users/matteo/Projects/isospec/IsoSpec/IsoSpec++/isoSpec++.h

5.14 IsoSpec::IsoOrderedGenerator Class Reference

The generator of isotopologues sorted by their probability of occurrence.

```
#include <isoSpec++.h>
```

Inheritance diagram for IsoSpec::IsoOrderedGenerator:



Public Member Functions

- bool [advanceToNextConfiguration](#) () override final
- void **get_conf_signature** (int *space) const override final
- **IsoOrderedGenerator** ([Iso](#) &&iso, int _tabSize=1000, int _hashSize=1000)

Additional Inherited Members

5.14.1 Detailed Description

The generator of isotopologues sorted by their probability of occurrence.

The subsequent isotopologues are generated with diminishing probability, starting from the mode. This algorithm take $O(N \cdot \log(N))$ to compute the N isotopologues because of using the Priority Queue data structure. Obtaining the N isotopologues can be achieved in $O(N)$ if they are not required to be spit out in the descending order.

5.14.2 Member Function Documentation

5.14.2.1 advanceToNextConfiguration()

```
bool IsoSpec::IsoOrderedGenerator::advanceToNextConfiguration ( ) [final], [override], [virtual]
```

The prefix product of the probabilities of the current isotopologue.

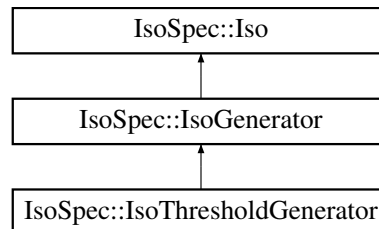
Implements [IsoSpec::IsoGenerator](#).

The documentation for this class was generated from the following files:

- /Users/matteo/Projects/isospec/IsoSpec/IsoSpec++/isoSpec++.h
- /Users/matteo/Projects/isospec/IsoSpec/IsoSpec++/isoSpec++.cpp

5.15 IsoSpec::IsoThresholdGenerator Class Reference

Inheritance diagram for IsoSpec::IsoThresholdGenerator:



Public Member Functions

- bool [advanceToNextConfiguration](#) () override final
- void **get_conf_signature** (int *space) const override final
- **IsoThresholdGenerator** ([Iso](#) &&iso, double _threshold, bool _absolute=true, int _tabSize=1000, int _hash↔Size=1000)
- void **terminate_search** ()

Additional Inherited Members

5.15.1 Member Function Documentation

5.15.1.1 advanceToNextConfiguration()

```
bool IsoSpec::IsoThresholdGenerator::advanceToNextConfiguration ( ) [final], [override], [virtual]
```

The prefix product of the probabilities of the current isotopologue.

Implements [IsoSpec::IsoGenerator](#).

The documentation for this class was generated from the following files:

- /Users/matteo/Projects/isospec/IsoSpec/IsoSpec++/isoSpec++.h
- /Users/matteo/Projects/isospec/IsoSpec/IsoSpec++/isoSpec++.cpp

5.16 IsoSpec::KeyHasher Class Reference

Public Member Functions

- **KeyHasher** (int dim)
- `std::size_t operator()` (const int *conf) const

The documentation for this class was generated from the following file:

- /Users/matteo/Projects/isospec/IsoSpec/IsoSpec++/operators.h

5.17 IsoSpec::IsoSpec::KeyHasher Class Reference

Public Member Functions

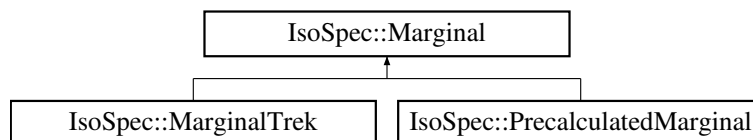
- **KeyHasher** (int dim)
- `std::size_t operator()` (const int *conf) const

The documentation for this class was generated from the following file:

- /Users/matteo/Projects/isospec/IsoSpec/IsoSpec++/operators.cpp

5.18 IsoSpec::Marginal Class Reference

Inheritance diagram for IsoSpec::Marginal:



Public Member Functions

- **Marginal** (const double *_masses, const double *_probs, int _isotopeNo, int _atomCnt)
- **Marginal** ([Marginal](#) &other)=delete
- [Marginal](#) & **operator=** (const [Marginal](#) &other)=delete
- **Marginal** ([Marginal](#) &&other)
- int **get_isotopeNo** () const
- double **getLightestConfMass** () const
- double **getHeaviestConfMass** () const
- double **getModelProb** () const
- double **getModelMass** () const
- double **getModelEProb** () const
- double **getSmallestLProb** () const
- double **logProb** (Conf conf) const

Protected Attributes

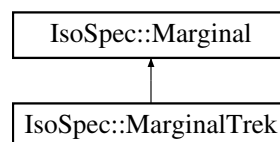
- const unsigned int **isotopeNo**
- const unsigned int **atomCnt**
- const double *const **atom_masses**
- const double *const **atom_lProbs**
- const double **loggamma_nominator**
- const Conf **mode_conf**
- const double **mode_lprob**
- const double **mode_mass**
- const double **mode_eprob**
- const double **smallest_lprob**

The documentation for this class was generated from the following files:

- /Users/matteo/Projects/isospec/IsoSpec/IsoSpec++/marginalTrek++.h
- /Users/matteo/Projects/isospec/IsoSpec/IsoSpec++/marginalTrek++.cpp

5.19 IsoSpec::MarginalTrek Class Reference

Inheritance diagram for IsoSpec::MarginalTrek:



Public Member Functions

- **MarginalTrek** ([Marginal](#) &&m, int tabSize=1000, int hashSize=1000)
- bool **probeConfigurationIdx** (int idx)
- int **processUntilCutoff** (double cutoff)
- const std::vector< double > & **conf_probs** () const
- const std::vector< double > & **conf_masses** () const
- const std::vector< int * > & **confs** () const

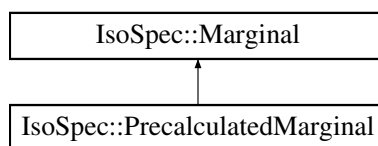
Additional Inherited Members

The documentation for this class was generated from the following files:

- /Users/matteo/Projects/isospec/IsoSpec/IsoSpec++/marginalTrek++.h
- /Users/matteo/Projects/isospec/IsoSpec/IsoSpec++/marginalTrek++.cpp

5.20 IsoSpec::PrecalculatedMarginal Class Reference

Inheritance diagram for IsoSpec::PrecalculatedMarginal:



Public Member Functions

- **PrecalculatedMarginal** ([Marginal](#) &&m, double lCutOff, bool sort=true, int tabSize=1000, int hashSize=1000)
- bool **inRange** (unsigned int idx) const
- const double & **get_IProb** (int idx) const
- const double & **get_eProb** (int idx) const
- const double & **get_mass** (int idx) const
- const double * **get_IProbs_ptr** () const
- const double * **get_masses_ptr** () const
- const Conf & **get_conf** (int idx) const
- unsigned int **get_no_confs** () const

Protected Attributes

- std::vector< Conf > [configurations](#)
- Conf * **confs**
- unsigned int **no_confs**
- double * **masses**
- double * **IProbs**
- double * **eProbs**
- [Allocator](#)< int > **allocator**

5.20.1 Member Data Documentation

5.20.1.1 configurations

```
std::vector<Conf> IsoSpec::PrecalculatedMarginal::configurations [protected]
```

This class serves to calculate a set of isotopologues that is defined by the minimal probability threshold.

This works faster than if you did not know the threshold. If you have no idea about the threshold, you would need to call us, to change encode the layered version of the marginal.

The documentation for this class was generated from the following files:

- /Users/matteo/Projects/isospec/IsoSpec/IsoSpec++/marginalTrek++.h
- /Users/matteo/Projects/isospec/IsoSpec/IsoSpec++/marginalTrek++.cpp

5.21 IsoSpec::IsoSpec::ReverseOrder< T > Class Template Reference

Public Member Functions

- bool **operator()** (const T a, const T b) const

The documentation for this class was generated from the following file:

- /Users/matteo/Projects/isospec/IsoSpec/IsoSpec++/operators.cpp

5.22 IsoSpec::ReverseOrder< T > Class Template Reference

Public Member Functions

- bool **operator()** (const T a, const T b) const

The documentation for this class was generated from the following file:

- /Users/matteo/Projects/isospec/IsoSpec/IsoSpec++/operators.h

5.23 IsoSpec::SSumlator Class Reference

Public Member Functions

- **SSumlator** ([SSumlator](#) &other)
- void **add** (double x)
- double **get** ()

The documentation for this class was generated from the following file:

- /Users/matteo/Projects/isospec/IsoSpec/IsoSpec++/sumlator.h

5.24 IsoSpec::Sumlator Class Reference

Public Member Functions

- void **add** (double what)
- double **get** ()

The documentation for this class was generated from the following file:

- /Users/matteo/Projects/isospec/IsoSpec/IsoSpec++/sumlator.h

5.25 IsoSpec::TableOrder< T > Class Template Reference

Public Member Functions

- **TableOrder** (const T * _tbl)
- bool **operator()** (unsigned int i, unsigned int j)

The documentation for this class was generated from the following file:

- /Users/matteo/Projects/isospec/IsoSpec/IsoSpec++/operators.h

5.26 IsoSpec::IsoSpec::TableOrder< T > Class Template Reference

Public Member Functions

- **TableOrder** (const T * _tbl)
- bool **operator()** (unsigned int i, unsigned int j)

The documentation for this class was generated from the following file:

- /Users/matteo/Projects/isospec/IsoSpec/IsoSpec++/operators.cpp

5.27 IsoSpec::Tabulator< T > Class Template Reference

Public Member Functions

- **Tabulator** (T *generator, bool get_masses, bool get_probs, bool get_lprobs, bool get_confs)
- double * **masses** ()
- double * **lprobs** ()
- double * **probs** ()
- int * **confs** ()
- size_t **confs_no** ()

The documentation for this class was generated from the following file:

- /Users/matteo/Projects/isospec/IsoSpec/IsoSpec++/tabulator.h

5.28 IsoSpec::ThreadSummator Class Reference

Public Member Functions

- void **add** (double what)
- double **get** ()

The documentation for this class was generated from the following file:

- /Users/matteo/Projects/isospec/IsoSpec/IsoSpec++/summator.h

5.29 IsoSpec::TSummator Class Reference

Public Member Functions

- void **add** (double what)
- double **get** ()

The documentation for this class was generated from the following file:

- /Users/matteo/Projects/isospec/IsoSpec/IsoSpec++/summator.h

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