Frequently Asked Questions

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Overview

Here are the JPL Frequently Asked Questions organized in different themes that follows a "How to ...?" type approach where each question is linked to some precise explanations and associated cookbooks (see table of contents of cookbooks).

0. Setting Up

How to install JPL ?

First, read downloading instructions where you have all explanation to get the good package jpl-PACKAGENAME-VERSION.jar and add this compiled jar and all its dependencies in your classpath.

How to get distribution ?

The last releases for jpl distributions are available there, unzip and untar the compressed file and open README.txt for more informations.

How to get sources ?

You have to download the distribution (see dist) first. After unzipping and untarring your distribution, you will access the sources from the src/ directory.

How to make sources jar ?

You have to download the distribution (see dist) first. After unzipping and untarring your distribution, you will have to execute "ant src" and get the jpl-PACKNAME-VERSION-src.jar in the jar/ directory.

How to run tests ?

You have to download the distribution (see dist) first. After unzipping and untarring your distribution, you will have to execute "ant test".

How to make html doc locally ?

You have to download the distribution (see dist) first. After unzipping and untarring your distribution, you will have to execute "ant doc".

1. Symbols and Sequences

How to define a custom symbol ?

See Recipe 1.1. Creating a custom symbol.

How to define a symbol manager ?

See Recipe 1.2. Creating a symbol manager.

How to make a new sequence ?

See Recipe 1.3. Creating a sequence of symbols.

How to make a (sub-)sequence from another sequence ?

See Recipe 1.4. Creating a sequence of symbols from another sequence.

How to merge sequences ?

See Recipe 1.5. Merging sequences of symbols.

How to create a motif matcher on sequence ?

Counts and Distributions

How to count the symbols in a sequence ?

How to calculate the frequency of a symbol in a sequence ?

How can I generate a random sequence from a distribution?

not yet available

2. Bio Data

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2.1 Chemicals

How to get atoms and molecules ...

... from a chemical formula ?

A call to method ChemicalFacade.getMolecule(String formula) simply returns the molecule.

All instanciations of molecules are controlled there. For more explanations.

... from a molecular symbol ?

You need to call MolecularSymbolFacade.getMolecule(String managerName, String symbolName) given the correct molecular symbol manager.

How to build a molecular expression ?

See Recipe 2.1.1.

How to define a molecule with a modification ?

See Recipe 2.1.2.

How to get the mass of any molecule ?

See Recipe 2.1.3.

How to define a molecule with ionized groups and compute average charge ?

See Recipe 2.1.4.

2.2. Monomers and Polymers (Sequences of bio-Symbols)

How to create a new modification ?

See Recipe 2.2

How to create peptide and protein sequence ?

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See Recipe 2.3.

How to compute gravy score, pI, partial charge on peptides and proteins ?

See Recipe 2.3.

How to create a motif matcher on polymer ?

How to define a custom peptidase ?

How to add a modification in a peptide ?

See Recipe 2.4

How to digest a protein ?

See Recipe 2.5

How to calculate a polymer mass ?

See Recipe 2.1.3.

How to fragment a peptide in MS2 spectrum ?

See Recipe 2.6.

How to split a peptide in amino-acids ?

See Recipe 2.7

How to create a peptide from a list of amino-acids ?

See Recipe 2.8

How to shuffle a peptide ?

See Recipe 2.9

How to generate modified peptides given rules ?

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See Recipe 2.10

How to randomly generate a polymer (w/wo modifications)?

See Recipe 2.11

3. MS Data

How to make a peak list ?

See Recipe 3.1.

How to modify peak lists ?

See Recipe 3.2.

How to make a binned peak list ?

See Recipe 3.3.

How to compute simple stats on collection of peak lists ?

How to make a MS peak annotation ?

How to fragment a peptide and generate an MS2 spectrum ?

See Recipe 2.6.

How to create a peak list editor for processing peak lists?

How to export peak list graph charts ?

See Recipe 3.5.

How to compare MS peak lists ?

See Recipe 3.6.

How to create a peak list filter for processing peak lists ?

See Recipe 3.7.

How to compute the alignment between an experimental versus a theoretical spectrum coming from a fragmented peptide (and report annotations from the later to the former) ?

See Recipe 3.8.

How to render MS peak list versus theoretical fragments (see previous question) ?

See Recipe 3.9.

How to cluster MS spectra ?

How to report annotations from a theoretical spectrum that match an experimental one ?

4. Readers/Writers

How to setup and read a Fasta file ?

How do I write Polymers in Fasta format ?

How to extract information from parsed results ?

How to read MS data from available formats ?

Follow this link.

0. Utils

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How to create a domain of definition ?

See Recipe 0.0.

How to create an interval ?

See Recipe 0.1.

How to create a sequence of integers ?

See Recipe 0.2.

See Recipe 0.3.

How to handle and generate tuples ?

See Recipe 0.4.

How to handle and generate combinations ?

See Recipe 0.5.

How to create a condition on any object to test ?

See Recipe 0.6 and Recipe 0.7 for building conditions and conditional expressions.

How to create a terminal progress bar ?

See Recipe 0.8.

How to create a counter ?

How to create a data table with typed fields ?