Recipe 3.8. Getting MS annotated peak list from peptide matching a peak list

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1. Problem

You want to compute the alignment between a peak list against theoretical peptide fragments and report annotations in the experimental one.

2. Solution

The object `MSPeptideMatchFactory` is making all the steps for you, from the generation of the theoretical spectrum to the matching:

```
import org.expasy.jpl.msmatch.MSPeptideMatchFactory;

// the experimental peak list that we want to match against the theoretical
fragments
PeakList expPeakList = ...

// the peptide precursor that will be fragmented by the renderer
JPLIonizedPeptide peptide =
        JPLIonizedPeptide.newInstance(new Peptide.Builder(
                "EQVQSC({57})GPPPELLNGNVK").build(), 2);

// The builder defines the settings for:
// 1. the fragmentation of precursor (fragmenter, condition)
// 2. the matching of spectra (tolerance)
MSPeptideMatchFactory factory =
        new MSPeptideMatchFactory.Builder().fragmenter(
                new PeptideFragmenter.Builder(EnumSet.of(
                        FragmentationType.AX, FragmentationType.BY,
                    FragmentationType.CZ)).enableLoss().build())
                    .tolerance(0.1).build();

// process the computation
factory.process(peptide, expPeakList);

// get the updated experimental spectrum (with peak annotations reported)
factory.getUpdatedPeakList();

// get the annotated peaks only
factory.getAnnotatedPeakList();

// get the non-annotated peaks only
factory.getNonAnnotatedPeakList();
```

3. Discussion

See also the recipe about rendering the aligned spectra.

4. See Also

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