

Recipe 2.4. Adding modifications in polypeptide

Table of contents

1 Problem.....	2
2 Solution.....	2
3 Discussion.....	3
4 See Also.....	3

1. Problem

You want to add modifications on peptides.

2. Solution

You need a manager to add modifications on peptides:

```
// a simple peptide (peptide type by default)
Peptide peptide =
    new Peptide.Builder("MQRSTATGCFKL").build();

// get the modif manager
ModifContainerManager modifManager =
    ModifContainerManager.getInstance();

// add modifications
modifManager.addModifAt(peptide, ModificationFactory.valueOf(134), 5);
modifManager.addCtModif(peptide, ModificationFactory.valueOf(16));

Assert.assertEquals("H_MQRSTA({134.00})TGCFKL_HO({16.00})",
    peptide.toString());
```

As some amino-acids are ionizable as some modifications:

```
import org.expasy.jpl.core.mol.modif.*;

// a new ionizable modification
IonizableModification phospho =
    IonizableModification.newInstance(
        ModificationFactory.withLabel("phosphorylation",
            ChemicalFacade.getMolecule("H2PO3")),
        new IonizableGroup.Builder(7.21,
            NeutralMoleculeType.ACID)
            .addPKa(12.67).build());

// a simple peptide
Peptide peptide = new Peptide.Builder("QEAYEGK").build();

// the modif manager
ModifContainerManager manager =
    ModifContainerManager.getInstance();

// add ionizable modif
manager.addModifAt(peptide, phospho, 3);

// toString() modif format
// 1. default display is contextual (phospho is based on a formula):
// => "H_QEAY(H2O3P)EGK_HO"
System.out.println(peptide);
```

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```
// 2a. format can be defined at building time:
peptide =
    new Peptide.Builder("QEAYEGK").doubleDisplayPrecision(2)
        .forceModifDoubleDisplay().build();

// 2b. ... or after building peptide:
peptide.setModifFormatDisplay(new ModifFormat.Builder().decimal(2)
    .format(Format.DOUBLE).build());

// add ionizable modif
manager.addModifAt(peptide, phospho, 3);

// => "H_QEAY({80.97})EGK_HO"
System.out.println(peptide);

// display "partial charge at pH 7 = -1.6189328858092091"
System.out.println("partial charge at pH 7 = "+
    + BioPolymerUtils.getPartialCharges(peptide, 7));
```

3. Discussion

4. See Also

See also [this recipe](#) to create a modified peptide at building time or [this one](#) to create modifications.