

# Recipe 2.2. Creating modifications

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## 1. Problem

You want to create new modifications.

## 2. Solution

Modifications can be created mainly from molecular formulae or from masses. Some molecular groups may be ionizable.

Here is a list of examples:

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

// create a modification from a formula
ModificationFactory.valueOf("CH3");

// create a modification from a double
ModificationFactory.valueOf("15.0349");

// with a label and a molecule
ModificationFactory.withLabel("MSO",
    ChemicalFacade.getMolecule("O2"));

// also exists loss modification
LossModification.valueOf(ModificationFactory.valueOf(-23)
    .valueOf(ChemicalFacade.getMolecule("C-1H-4")));

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