

# Recipe 2.1.3. Getting molecular mass

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## 1. Problem

You want to compute molecular mass given an accuracy.

## 2. Solution

The dedicated object `MassCalculator` makes the computation. It just need a `Molecule` or a `BioPolymer`:

```
// monoisotopic mass calculator
MassCalculator monoMassCalc =
    MassCalculator.getMonoAccuracyInstance();

// average mass calculator
MassCalculator avgMassCalc =
    MassCalculator.getAvgAccuracyInstance();

Molecule methane = ChemicalFacade.getMolecule("CH4");

// compute mass of a molecule
Assert.assertEquals(16.0313, monoMassCalc.getMass(methane));
Assert.assertEquals(16.0429, avgMassCalc.getMass(methane));

// compute mass of polymer
Peptide peptide =
    new Peptide.Builder("MQRSTA({133.0})TGCFKL").build();
Assert.assertEquals(1474.6533, monoMassCalc.getMass(peptide));
```

## 3. Discussion

## 4. See Also