Recipe 2.8. Creating a peptide from molecules

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1. Problem

You want to create a peptide from a list of molecules.

2. Solution

`PeptideResidueManager` can join a list of bio-elements such as N/C termini and its residues in a `Peptide`:

```
import org.expasy.jpl.core.mol.polymer.pept.PeptideResidueManager;

// get the manager unique instance
PeptideResidueManager manager =
        PeptideResidueManager.getInstance();

// a list of molecules
List<Molecule> molecules =
        new ArrayList<Molecule>();

// add bio elements
molecules.add(AminoAcid.RAD_P);
molecules.add(AminoAcid.RAD_E);
molecules.add(AminoAcid.RAD_P);
molecules.add(new ModifiedMolecule.Builder(AminoAcid.RAD_T,
        ModificationFactory.valueOf(21.)).build());
molecules.add(AminoAcid.RAD_I);
molecules.add(AminoAcid.RAD_D);
molecules.add(AminoAcid.RAD_E);
molecules.add(new ModifiedMolecule.Builder(CTerminus.PEP_C,
        ModificationFactory.valueOf(17.)).build());

// make the join and create a new instance of Peptide
Peptide pept = manager.join(l);

Assert.assertEquals("H_PEPT({21.00})IDE_HO({17.00})", pept.toString());
```

3. Discussion

4. See Also

See also <u>how to create a `ModifiedMolecule`</u> when modified amino-acids have to be inserted in the peptide.