

Recipe 2.9. Shuffling a peptide

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1. Problem

You want to shuffle a peptide.

2. Solution

PeptideResidueManager propose methods to shuffle Peptides:

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

// the peptide to shuffle
Peptide peptide =
    new Peptide.Builder("H_A({128.10})CHUHEUHU({11.90})RHE_OH")
        .build();

// generate 5 peptides
for (int i = 0; i < 5; i++) {
    Peptide shuffled = manager.shuffle(peptide);
    System.out.println(shuffled);
}

// output
H_EHRA({128.10})CHHHUUU({11.90})E_HO
H_HU({11.90})HHREUA({128.10})CHUE_HO
H_HUU({11.90})HREEUCHA({128.10})H_HO
H_CEHU({11.90})A({128.10})HHRHUUE_HO
H_RA({128.10})HHEUEU({11.90})HUHC_HO
```

It is also possible to fixed some positions and while scrambling the others:

```
// the peptide to shuffle
Peptide peptide =
    new Peptide.Builder("H_A({128.10})CHUHEUHU({11.90})RHE_OH")
        .build();

// generate 5 peptides with positions 0 and 8 fixed
for (int i = 0; i < 5; i++) {
    Peptide shuffled =
        manager.shuffle(peptide, new
    HashSet<Integer>(Arrays.asList(0,8)));

    System.out.println(shuffled);
}

// output
H_A({128.10})CHHHUUEU({11.90})RHE_HO
H_A({128.10})HCEEHURU({11.90})HUH_HO
H_A({128.10})ERHHUUHU({11.90})HEC_HO
H_A({128.10})UUCHEEHU({11.90})HRH_HO
H_A({128.10})EHHCURHU({11.90})EUH_HO
```

3. Discussion

4. See Also