

Recipe 2.3. Computing biochemical properties in peptides

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1. Problem

You want to estimate the isoelectric point or the partial charge in peptides.

2. Solution

The `BioPolymerUtils` class provides methods to estimate biochemical properties in peptide or proteins:

```
String seq =
    new String("mvhltpeeksavtalwgvnvdvgealgrllvypwtq"
        + "rffesfgdlstpdavmgnpkvkahgkklvlgafsdglahld"
        + "nlkgtfatlsehcdklhvdpenfrllgnvlvcvpahhfg"
        + "keftppvqaayqkvvagvanalahkyh").toUpperCase();

Peptide peptide = new Peptide.Builder(seq).build();

// default gravy method
float score = BioPolymerUtils.getGravyScore(sequence);
Assert.assertEquals(-0.023, score, 0.001);

// gravy "kyledoolittle" method
score = BioPolymerUtils.getGravyScore(sequence,
    AAHydropathyManager.newInstance("kyledoolittle"));
Assert.assertEquals(-0.023, score, 0.001);

peptide = new Peptide.Builder("QEAYEGK").build();
Assert.assertEquals(4.54, BioPolymerUtils.getIsoelectricPoint(peptide),
    0.01);

final float score = BioPolymerUtils.getGravyScore(peptide);
Assert.assertEquals(-0.023, score, 0.001);
```

3. Discussion

4. See Also