PeakMaster 6

Capillary zone electrophoresis and affinity capillary electrophoresis simulator

Step-by-step User Guide
Input Data
You have to enter the system parameters first.
Add the components of your system (BGE component or analyte).
Input Data

You can skip this step unless you want to work with complexing systems.

Type of the component: NUCLEUS or LIGAND

This is explained in detail in the Complexation part.

In this example, we will add all the components as ligands and then the selector (β-cyclodextrin) as nucleus.
Input Data

Pick a component from the database.
Input Data

Start typing ...
Input Data

Pick the desired component.
Input Data

Add the components of your system (BGE component or analyte). Confirm.
Lithium added.

If you cannot find the component in the database ...
Input Data

- Type in the name.
- Choose correct type.
- Then add the respective ionic form (-1 for anionic, 1 for cationic).
Input Data

Enter the physico-chemical parameters of the ionic form:
- Electrophoretic mobility
- pKa
Add the components of your system (BGE component or analyte). Now add the selector – type nucleus.

If you do NOT deal with complexation, you can ignore the selector.

This part is relevant only for complexing systems.
Input Data

This part is relevant only for complexing systems.

Name and type.

If the compound is neutral, you do not need to enter any ionic form.
Add the analyte(s) in the same way as the BGE components.
After adding all the components of your system, enter their concentrations (may differ in the BGE zone and in the sample zone).

**Zero concentration:**
PM 6 cannot operate with zero concentrations.

If you enter concentration whose value is lower than the allowed limit, it will be changed automatically to the lowest acceptable concentration.
Double-click on the **Name** or **Type** of the constituent to edit the parameters.
Input Data

When the system is complete, let PeakMaster calculate its parameters.

Click the **Calculate!** button or hit **F5**.
Input Data

PeakMaster 6 has calculated the system parameters and shows the conductivity electropherogram.
Input Data

Nonideality corrections (ionic effects, viscosity)
Correction for ionic effects (Debye-Hückel and Onsager-Fuoss) enabled by default.

Correction for viscosity is considered experimental disabled by default.
Input Data

Editing the database.
You can edit the existing database...
Input Data

... or load a completely different one.
Automatic pH adjustment (since PM6.0f8)
Input Data

Pick a constituent whose concentration you want to adjust to achieve the target pH.
1. Enter the desired pH value

2. Click Adjust
Check the adjusted concentration of the constituent.
Keep in mind that it may not be always possible to achieve the desired pH by adjusting the concentration of the selected constituent. If that happens, you will receive an error message.

Additionally, automatic pH adjuster may not work reliably with highly concentrated solutions (IS of 1000mM or above).
Complexation
There are few basic rules for describing complexation in the PeakMaster 6.

- **NUCLEUS** – any ionic form of a nucleus can interact with an arbitrary number of ionic forms of ligands
  - each complex **MUST** contain ONE AND ONLY ONE nucleus

- **LIGAND** – any ionic form of a ligand can interact with any ionic form of nuclei

- Ligands can **NOT** interact with other ligands and the same goes for nuclei.

- **A FEW EXAMPLES:**
  
  \((N – \text{nucleus}, L – \text{ligand}, K – \text{ligand})\)

- **Allowed**
  - \(NL_2\)
  - \(NL_3K\)
  - \(NLK_4\)

- **Not allowed**
  - \(N_2L\)
  - \(N_4K\)
  - \(LK\)
Complexation can be established by dragging the compound and dropping it on the other one.
Complexation

Assisted ligand – nucleus conversion:
In case you forget to change the type ...
Complexation

Assisted ligand – nucleus conversion: PeakMaster will ask you which of them do you wish to convert!
Enter the complexation parameters for each ionic form.

**Complexation constant (Kxs)** is related to SI units (M⁻¹) .
Complexation

Complexation between the two compounds established.
Adding second complexation with the BGE component (drag and drop again).
Enter the parameters of the second complexation.

### Complexation Parameters

<table>
<thead>
<tr>
<th>Complexation</th>
<th>Type</th>
<th>Name</th>
<th>c BGE (mM)</th>
<th>c Sample (mM)</th>
<th>u EFF (14-9)</th>
</tr>
</thead>
<tbody>
<tr>
<td>L</td>
<td>LITHIUM</td>
<td>10</td>
<td>10</td>
<td></td>
<td></td>
</tr>
<tr>
<td>L</td>
<td>CHES</td>
<td>20</td>
<td>20</td>
<td></td>
<td></td>
</tr>
<tr>
<td>N</td>
<td>Beta-cyclooctxine</td>
<td>5</td>
<td>1e-12</td>
<td></td>
<td></td>
</tr>
</tbody>
</table>
Complexation

New complexation established.
Complexation

New selector (nucleus type) added – establishing **new complexation** (drag and drop).
Complexation

Enter the parameters of this complexation.

Note that if you leave the row empty, it means the respective ionic form does not form a complex.
Complexation

New complexation with a different nucleus established.
Complexation

To edit the complexation, double click on the nucleus coloured field.
You can choose which ligand interaction you want to edit.

By removing the ligand you can remove the complexation.
Results
System properties.
### Results

Eigenzone properties:

<table>
<thead>
<tr>
<th>Name</th>
<th>c Sample (mM)</th>
<th>c BEGE (mM)</th>
<th>ε Eff (× 10⁻⁶)</th>
</tr>
</thead>
<tbody>
<tr>
<td>Lithium</td>
<td>10</td>
<td>10</td>
<td>36.5818</td>
</tr>
<tr>
<td>CHES</td>
<td>20</td>
<td>20</td>
<td>-10.0155</td>
</tr>
<tr>
<td>Beta-cyclodextrin</td>
<td>5e-12</td>
<td>0</td>
<td>0</td>
</tr>
</tbody>
</table>

**Flurbiprofen**

<table>
<thead>
<tr>
<th>Name</th>
<th>c Sample (mM)</th>
<th>c BEGE (mM)</th>
<th>ε Eff (× 10⁻⁶)</th>
</tr>
</thead>
<tbody>
<tr>
<td>Flurbiprofen</td>
<td>0.2</td>
<td>-10.0165</td>
<td>3.40287</td>
</tr>
</tbody>
</table>

**System eigenzone**

<table>
<thead>
<tr>
<th>Mobility (-10⁻⁹)</th>
<th>Time (min)</th>
</tr>
</thead>
<tbody>
<tr>
<td>1</td>
<td>1.2475e-14</td>
</tr>
<tr>
<td>2</td>
<td>2.6296e-05</td>
</tr>
<tr>
<td>3</td>
<td>3.66678</td>
</tr>
</tbody>
</table>
Parameters marked as Max present the values in peak apex (not the same as the values in Eigenzone details).
Zone composition block displayed in RED indicates that PeakMaster failed to calculate composition of that zone accurately. Keep that in mind when you use such results.

This inaccuracy **does not** affect mobilities and migration times.
Check if you want to display the results as a difference between the zone and the pure BGE parameters.
Results

- Change of concentration of the chosen component in the respective zones.
- Conductivity change in the respective zones.
- Mobilities of system and analyte peaks.
Results

Ionic composition.
Results

BGE tab shows ionic composition of the BGE at the given pH.
In the **Analytes** tab you can see the degree of dissociation of the chosen analyte.

If there is a warning present, the dissociation states may not be correct!
Results

Predicted electropherogram.
Results

You can change the initial injection zone length.

Replot to see the change.
Results

Changed injection zone length.
Results

Choose which profile you want to display (conductivity, pH, concentration)
Results

CHES concentration profile displayed.
Results

Export the electropherogram.
Results

Export graph as *.csv.
You can also save the whole PeakMaster setup and load it later.

(Setup saves as *.json file.)