

PeakMaster 6

Capillary zone electrophoresis
and affinity capillary electrophoresis
simulator

Step-by-step User Guide



FACULTY OF SCIENCE
Charles University

– ECHMET +

PeakMaster 6 - User Guide

[Input Data](#)

[Complexation](#)

[Results](#)

Input Data

Input Data



PeakMaster 6.0f3

File Export Database Advanced Help

New Load Save Save as Calculate!

Total capillary length (cm)
Effective capillary length (cm)
Driving voltage (V)
Polarity (at inlet)
EOF

Nonideality corrections

pH
Ionic strength (mM)
Conductivity (S/m)
Resistivity (Ohm·m)
Buffer capacity (mM)
EOF marker time (min)
EOF mobility

System eigenzones

Mobility (· 1e-9)	Time (min)
-------------------	------------

Eigenzone details Ionic composition

Background composition:

Complexations	Type	Name	c BGE (mM)	c Sample (mM)	μ Eff (· 1e-9)
---------------	------	------	------------	---------------	--------------------

Analytes:

Complexations	Type	Name	c Sample (mM)	μ Eff (· 1e-9)	Time Max (min)	c Max (mM)	κ Max (S/m)	μ EMD (· 1e-9)
---------------	------	------	---------------	--------------------	----------------	------------	--------------------	--------------------

You have to enter the system parameters first.

Add BGE Remove BGE Add analyte Remove analyte

Profile: Conductivity Plot cutoff (min): Auto Inj. zone length (mm): Replot

Conductivity (S/m)

time (min)

time (min)	Conductivity (S/m)
0	0,0564
1	0,0568
2	0,0572
3	0,0574
4	0,0576

Input Data



The screenshot displays the PeakMaster 6.0f3 software interface. On the left, a panel contains input fields for system parameters: Total capillary length (cm) set to 50, Effective capillary length (cm) set to 41.5, Driving voltage (V) set to 15 000, Polarity (at inlet) set to Positive, EOF Marker time (min) set to 3, and various nonideality correction parameters (pH, Ionic strength, Conductivity, Resistivity, Buffer capacity, EOF marker time, EOF mobility) all set to 0. Below these are System eigenzones and Mobility fields.

The main area features two tables: 'Background composition' and 'Analytes', both with columns for Complexations, Type, Name, c BGE (mM), c Sample (mM), and μ Eff ($\cdot 1e-9$). A central text box with a black border contains the instruction: "Add the components of your system (BGE component or analyte)". Two red arrows point from this box to the 'Add BGE' and 'Add analyte' buttons, which are circled in red. The 'Remove BGE' and 'Remove analyte' buttons are also visible.

At the bottom, a graph shows a 'Conductivity' profile over 'time (min)'. The y-axis ranges from 0 to 1000, and the x-axis ranges from 0 to 1000. A single data point is plotted at 709.1875, 542.0290. The 'Plot cutoff (min)' is set to 60, and 'Auto' is checked. The 'Inj. zone length (mm)' is set to 1. A 'Replot' button is located at the bottom right of the graph area.

Input Data



PeakMaster 6.0f3 - PeakMaster 6.0f3

File Export Database Advanced Help

New Load Save Save as Calculate!

Total capillary length (cm) 50
Effective capillary length (cm) 41,5
Driving voltage (V) 15 000
Polarity (at inlet) Positive
EOF Marker time (min) 3
EOF Marker time (min) 3

Nonideality corrections

pH 0
Ionic strength (mM) 0
Conductivity (S/m) 0
Resistivity (Ohm·m) 0
Buffer capacity (mM) 0
EOF marker time (min) 0
EOF mobility 0

System eigenzones

Mobility (· 1e-9)	Time (min)
-------------------	------------

Background composition:

Complexations	Type	Name	c BGE (mM)	c Sample (mM)	μ Eff (· 1e-9)
---------------	------	------	------------	---------------	----------------

Analytes:

Complexation	Name	μ Eff (· 1e-9)
--------------	------	----------------

Profile: Conductivity

1 000
800
600
400
200
0

0 200 400 600 800 1 000

time (min)

Eigenzone details Ionic composition

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

The screenshot displays the PeakMaster 6.0F3 software interface. On the left, there are input fields for various parameters: Total capillary length (cm) set to 50, Effective capillary length (cm) set to 41,5, Driving voltage (V) set to 15 000, Polarity (at inlet) set to Positive, EOF Marker time (min) set to 3, pH set to 0, Ionic strength (mM) set to 0, Conductivity (S/m) set to 0, Resistivity (Ohm·m) set to 0, Buffer capacity (mM) set to 0, EOF marker time (min) set to 0, and EOF mobility set to 0. Below these are sections for Nonideality corrections and System eigenzones.

The main area shows a plot of Conductivity (S/m) versus time (min). The y-axis ranges from 0,0566 to 0,0574, and the x-axis ranges from 0 to 4. The plot shows a single peak at approximately 1,5 minutes. The profile is labeled 'Conductivity'.

An 'Edit constituent properties' dialog box is open in the center, with a red circle around the 'Pick from database...' button. A callout box with the text 'Pick a component from the database.' points to this button. The dialog box also shows a table with columns 'Mobility' and 'pKa', and buttons for 'Add (1)', 'Remove (0)', 'OK', and 'Cancel'.

At the bottom of the dialog box, there are buttons for 'Add BGE' and 'Remove analyte'.

Input Data



The screenshot displays the PeakMaster 6.0F3 software interface. On the left, there are input fields for various parameters: Total capillary length (cm) set to 50, Effective capillary length (cm) set to 41,5, Driving voltage (V) set to 15 000, Polarity (at inlet) set to Positive, EOF Marker time (min) set to 3, pH set to 0, Ionic strength (mM) set to 0, Conductivity (S/m) set to 0, Resistivity (Ohm·m) set to 0, Buffer capacity (mM) set to 0, EOF marker time (min) set to 0, and EOF mobility set to 0. Below these are system eigenzones and a graph showing Conductivity (S/m) vs. time (min). The graph has a y-axis from 0,0566 to 0,0574 and an x-axis from 0 to 4. A profile for Conductivity is shown above the graph.

Two dialog boxes are overlaid on the interface. The top dialog is 'Edit constituent properties' with fields for Name, Type (set to Ligand), and a 'Pick from database...' button. The bottom dialog is 'Pick constituent from database' with a 'Constituent name:' text box (circled in red), a 'Match type' dropdown (set to 'Name begins with...'), and buttons for 'All compounds', 'OK', and 'Cancel'. A speech bubble points to the 'Constituent name:' text box with the text 'Start typing ...'.

At the bottom of the interface, there are buttons for 'Eigenzone details' and 'Ionic composition'.

Input Data



The screenshot displays the PeakMaster 6.0F3 software interface. On the left, there are input fields for various parameters: Total capillary length (cm) set to 50, Effective capillary length (cm) set to 41,5, Driving voltage (V) set to 15 000, Polarity (at inlet) set to Positive, EOF Marker time (min) set to 3, pH set to 0, Ionic strength (mM) set to 0, Conductivity (S/m) set to 0, Resistivity (Ohm·m) set to 0, Buffer capacity (mM) set to 0, EOF marker time (min) set to 0, and EOF mobility set to 0. Below these are sections for Nonideality corrections and System eigenzones.

In the center, there are two overlapping dialog boxes. The top one is 'Edit constituent properties' with fields for Name, Type (set to Ligand), and a 'Pick from database...' button. The bottom one is 'Pick constituent from database' with a search field containing 'Li' and a 'Match type' dropdown set to 'Name begins with...'. A table in this dialog lists search results:

Constituent name	pKa (+1)	μ (0)	μ (+1)
LITHIUM	13,8	0	40,1
LIDOCAINE	7,85	0	23,6

The 'LITHIUM' row is circled in red. A callout box with a black border and white background points to this row, containing the text 'Pick the desired component.' Below the table are buttons for 'All compounds', 'OK', and 'Cancel'. The 'OK' button is also circled in red.

At the bottom, a plot shows 'Conductivity (S/m)' on the y-axis (ranging from 0,0566 to 0,0574) versus 'time (min)' on the x-axis (ranging from 0 to 4). The plot shows a step-like increase in conductivity starting around 1.5 minutes. At the bottom right, there are buttons for 'Add BGE', 'Remove analyte', and 'Replot'.

Input Data



PeakMaster 6.0F3 - PeakMaster 6.0F3

File Export Database Advanced Help

New Load Save Save as Calculate!

Total capillary length (cm)
Effective capillary length (cm)
Driving voltage (V)
Polarity (at inlet)
EOF
EOF Marker time (min)
Nonideality corrections
pH
Ionic strength (mM)
Conductivity (S/m)
Resistivity (Ohm · m)
Buffer capacity (mM)
EOF marker time (min)
EOF mobility
System eigenzones
Mobility (· 1e-9) Time (min)

Background composition:

Complexations	Type	Name	c BGE (mM)	c Sample (mM)	μ Eff (· 1e-9)
---------------	------	------	------------	---------------	--------------------

Analytes:

Complexations	Type	Name	c Sample (mM)	μ Eff (· 1e-9)	Time Max (min)	c Max (mM)	κ Max (S/m)	μ EMD (· 1e-9)
---------------	------	------	---------------	--------------------	----------------	------------	--------------------	--------------------

Add BGE Remove BGE

Add analyte Remove analyte

Plot cutoff (min): Auto Inj. zone length (mm): Replot

Conductivity (S/m)

time (min)

Eigenzone details Ionic composition

Edit constituent properties

Name: LITHIUM
Type: Ligand
Pick from database...
Add to database

Adjust low charges: Add (-1) Remove (0)

	Mobility	pKa
0	0	-
1	40,1	13,8

Adjust high charges: Add (2) Remove (1)

Confirm.

OK Cancel



Input Data

PeakMaster 6.0F3 - PeakMaster 6.0F3

File Export Database Advanced Help

New Load Save Save as Calculate!

Total capillary length (cm) 50
Effective capillary length (cm) 41,5
Driving voltage (V) 15 000
Polarity (at inlet) Positive
EOF Marker time (min) 3
Nonideality corrections
pH 0
Ionic strength (mM) 0
Conductivity (S/m) 0
Resistivity (Ohm·m) 0
Buffer capacity (mM) 0
EOF marker time (min) 0
EOF mobility 0

System eigenzones

Mobility (· 1e-9) Time (min)

Eigenzone details Ionic composition

Background composition:

Complexation	Type	Name	c BGE (mM)	c Sample (mM)	μ Eff (· 1e-9)
L		LITHIUM	1e-12	1e-12	

Lithium added.

Analytes:

Complexations	Type	Name	c Sample (mM)	μ Eff (· 1e-9)	Time Max (min)	c Max (mM)	κ Max (S/m)	μ EMD (· 1e-9)
---------------	------	------	---------------	--------------------	----------------	------------	--------------------	--------------------

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

Add BGE Remove BGE Add analyte Remove analyte

Profile: Conductivity Plot cutoff (min): 60 Auto Inj. zone length (mm): 1 Replot

Conductivity (S/m)

time (min)

Input Data



PeakMaster 6.0F3 - PeakMaster 6.0F3

File Export Database Advanced Help

New Load Save Save as Calculate!

Total capillary length (cm) 50
Effective capillary length (cm) 41,5
Driving voltage (V) 15 000
Polarity (at inlet) Positive
EOF Marker time (min) 3

Nonideality corrections

pH 0
Ionic strength (mM) 0
Conductivity (S/m) 0
Resistivity (Ohm·m) 0
Buffer capacity (mM) 0
EOF marker time (min) 0
EOF mobility 0

System eigenzones

Mobility (· 1e-9)	Time (min)
-------------------	------------

Eigenzone details Ionic composition

Background composition:

Complexations	Type	Name	c BGE (mM)	c Sample (mM)	μ Eff (· 1e-9)
L		LITHIUM	1e-12	1e-12	

Analytes:

Complexations	Type	Name	c Sample (mM)	μ Eff (· 1e-9)	Time Max (min)	c Max (mM)	κ Max (S/m)	μ EMD (· 1e-9)
---------------	------	------	---------------	----------------	----------------	------------	-------------	----------------

Edit constituent properties

Name:

Type: Nucleus

Pick from database...

Add to database

Adjust low charges: Add (-1) Remove (0)

Mobility	pKa
0	-

Adjust high charges: Add (1) Remove (0)

OK Cancel

Profile: Conductivity

Conductivity (S/m) vs time (min)

0,0574
0,0572
0,057
0,0568
0,0566

0 1 2 3 4

time (min)

Type in the name.

Choose correct type.

Then add the respective ionic form (-1 for anionic, 1 for cationic).

Input Data



The screenshot displays the PeakMaster 6.0F3 software interface. The main window is titled "PeakMaster 6.0F3 - PeakMaster 6.0F3" and features a menu bar (File, Export, Database, Advanced, Help) and a toolbar with buttons for New, Load, Save, Save as, and Calculate!.

On the left side, there are several input fields for system parameters:

- Total capillary length (cm): 50
- Effective capillary length (cm): 41,5
- Driving voltage (V): 15 000
- Polarity (at inlet): Positive
- EOF: Marker time (min)
- EOF Marker time (min): 3
- Nonideality corrections: (button)
- pH: 0
- Ionic strength (mM): 0
- Conductivity (S/m): 0
- Resistivity (Ohm · m): 0
- Buffer capacity (mM): 0
- EOF marker time (min): 0
- EOF mobility: 0

Below these fields is the "System eigenzones" section with a table for "Mobility (· 1e-9)" and "Time (min)".

The main area is divided into "Background composition:" and "Analytes:". The "Background composition:" table has columns for Complexations, Type, Name, c BGE (mM), c Sample (mM), and μ Eff (· 1e-9). It contains one entry: L, LITHIUM, 1e-12, 1e-12.

The "Analytes:" table has columns for Complexations, Type, and Name.

A central dialog box titled "Edit constituent properties" is open, showing the following fields:

- Name: CHES
- Type: Ligand
- Pick from database... (button)
- Add to database (button)
- Adjust low charges: Add (-2) (button), Remove (-1) (button)
- Table with columns "Mobility" and "pKa":

Mobility	pKa
-1,25	9,55
0	0
- Adjust high charges: Add (1) (button), Remove (0) (button)
- OK (button), Cancel (button)

The "OK" button and the "Mobility" and "pKa" values in the table are circled in red.

At the bottom, there is a "Profile:" section set to "Conductivity" and a graph showing "Conductivity (S/m)" on the y-axis (ranging from 0,0566 to 0,0574) and "time (min)" on the x-axis (ranging from 0 to 4). The graph shows a flat line at approximately 0,0568 S/m.

On the right side, there are buttons for "Add analyte" and "Remove analyte", and a "Plot cutoff (min):" field set to 60 with an "Auto" checkbox checked. There is also an "Inj. zone length (mm):" field set to 1 and a "Replot" button.

A callout box on the right contains the following text:

Enter the physico-chemical parameters of the ionic form

- Electrophoretic mobility
- pKa

Input Data



This part is relevant only for complexing systems.

The screenshot shows the PeakMaster 6.0F3 software interface. On the left, there are various input fields for system parameters such as Total capillary length (cm), Effective capillary length (cm), Driving voltage (V), Polarity (at inlet), EOF, EOF Marker time (min), pH, Ionic strength (mM), Conductivity (S/m), Resistivity (Ohm·m), Buffer capacity (mM), EOF marker time (min), and EOF mobility. The 'Background composition' table is highlighted with a blue box and contains the following data:

Complexations	Type	Name	c BGE (mM)	c Sample (mM)	μ Eff ($\cdot 10^{-9}$)
L		LITHIUM	1e-12	1e-12	
L		CHES	1e-12	1e-12	

A black box with the text "CHES added." is placed over the CHES row in the table. Below the table, the "Add BGE" button is circled in red. A black box with the text "Now add the selector – type nucleus." is placed over the "Add BGE" button. At the bottom, a graph shows Conductivity (S/m) on the y-axis (ranging from 0,0566 to 0,0574) versus time (min) on the x-axis (ranging from 0 to 4). A light blue box with the text "If you do NOT deal with complexation, you can ignore the selector." is placed over the graph area.

CHES added.

Now add the selector – type nucleus.

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

Input Data



This part is relevant only for complexing systems.

The screenshot shows the PeakMaster 6.0f3 software interface. On the left, there are various input fields for system parameters such as Total capillary length (50 cm), Effective capillary length (41.5 cm), Driving voltage (15000 V), and EOF Marker time (3 min). The main area contains a 'Background composition' table and an 'Analytes' table. A 'Conductivity' graph is displayed at the bottom, showing a baseline around 0.057 S/m over a 4-minute period.

Complexations	Type	Name	c BGE (mM)	c Sample (mM)	μ Eff ($\cdot 1e-9$)
L		LITHIUM	1e-12	1e-12	
L		CHES	1e-12	1e-12	

Complexations	Type	Name	c Sample (mM)	μ Eff ($\cdot 1e-9$)	Time Max (min)	c Max (mM)	κ Max (S/m)	μ EMD ($\cdot 1e-9$)
---------------	------	------	---------------	----------------------------	----------------	------------	--------------------	----------------------------

Name	Type
Beta-cyclodextrin	Nucleus

Mobility	pKa
0.0	-

Name and type.

If the compound is neutral, you do not need to enter any ionic form.

Input Data



PeakMaster 6.0f3 - PeakMaster 6.0f3

File Export Database Advanced Help

New Load Save Save as Calculate!

Total capillary length (cm)

Effective capillary length (cm)

Driving voltage (V)

Polarity (at inlet)

EOF

EOF Marker time (min)

Nonideality corrections

pH

Ionic strength (mM)

Conductivity (S/m)

Resistivity (Ohm·m)

Buffer capacity (mM)

EOF marker time (min)

EOF mobility

System eigenzones

Mobility (· 1e-9) | Time (min)

Eigenzone details | Ionic composition

Background composition:

Complexations	Type	Name	c BGE (mM)	c Sample (mM)	μ Eff (· 1e-9)
L		LITHIUM	1e-12	1e-12	
L		CHES	1e-12	1e-12	
N		Beta-cyclodextrin	1e-12	1e-12	

Analytes:

Complexations	Type	Name	c Sample (mM)	μ Eff (· 1e-9)	Time Max (min)	c Max (mM)	κ Max (S/m)	μ EMD (· 1e-9)
---------------	------	------	---------------	--------------------	----------------	------------	--------------------	--------------------

Add the analyte(s) in the same way as the BGE components.

Add BGE Remove BGE **Add analyte** Remove analyte

Profile: Conductivity Plot cutoff (min): Auto Inj. zone length (mm): Replot

Conductivity (S/m)

time (min)

Input Data



The screenshot shows the PeakMaster 6.0f3 software interface. The 'Background composition' table is highlighted with a red box, and the 'Analytes' table is also highlighted with a red box. A callout box points to the 'Background composition' table with the following text:

After adding all the components of your system, enter their concentrations (may differ in the BGE zone and in the sample zone).

Complexations	Type	Name	BGE (mM)	Sample (mM)	Eff (· 1e-9)
L	LITHIUM		10	10	
L	CHES		20	20	
N	Beta-cyclodextrin		5	1e-12	

Complexations	Type	Name	Sample (mM)	Eff (· 1e-9)	Time Max (min)	c Max (mM)	κ Max (S/m)	μ EMD (· 1e-9)
L		Flurbiprofen	0,2					

The 'Analytes' table shows a single entry for Flurbiprofen with a concentration of 0,2 mM. The 'Background composition' table shows three entries: LITHIUM (10 mM BGE, 10 mM Sample), CHES (20 mM BGE, 20 mM Sample), and Beta-cyclodextrin (5 mM BGE, 1e-12 mM Sample). The 'Analytes' table shows one entry: Flurbiprofen (0,2 mM Sample).

System eigenzones table:

Mobility (· 1e-9)	Time (min)
0,0574	

Profile: Conductivity

Plot cutoff (min): 60 Auto Inj. zone length (mm): 1 Replot

time (min)

Eigenzone details Ionic composition

0 1 2 3 4

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.

Input Data



PeakMaster 6.0f3 - PeakMaster 6.0f3

File Export Database Advanced Help

New Load Save Save as Calculate!

Total capillary length (cm)

Effective capillary length (cm)

Driving voltage (V)

Polarity (at inlet)

EOF

EOF Marker time (min)

Nonideality corrections

pH

Ionic strength (mM)

Conductivity (S/m)

Resistivity (Ohm·m)

Buffer capacity (mM)

EOF marker time (min)

EOF mobility

System eigenzones

Mobility (· 1e-9) | Time (min)

Eigenzone details | Ionic composition

Background composition:

Complexations	Type	Name	c BGE (mM)	c Sample (mM)	μ Eff (· 1e-9)
L	LITHIUM		10	10	
L	CHES		20	20	
N	Beta-cyclodextrin		5	1e-12	

Analytes:

Complexations	Type	Name	c Sample (mM)	μ Eff (· 1e-9)	Time Max (min)	c Max (mM)	κ Max (S/m)	μ EMD (· 1e-9)
L	Flurbiprofen	0,2						

Add BGE Remove BGE Add analyte Remove analyte

Profile: Conductivity Plot cutoff (min): Auto Inj. zone length (mm): Replot

Conductivity (S/m)

time (min)

0,0574
0,0572
0,057
0,0568
0,0566

0 1 2 3 4

Double-click on the **Name** or **Type** of the constituent to **edit** the parameters.

Input Data



The screenshot displays the PeakMaster 6.0f3 software interface. The 'Calculate!' button in the top toolbar is highlighted with a red box. A central text box contains the instruction: "When the system is complete, let PeakMaster calculate its parameters. Click the Calculate! button or hit F5." A blue-bordered dialog box titled "Calculating..." is open in the center, showing a progress bar and the text "Hang in there, this may take a little while...". The background shows the software's main window with various input fields and tables.

Background composition table:

Complexations	Type	Name	c BGE (mM)	c Sample (mM)	μ Eff ($\cdot 1e-9$)
L	LITHIUM	10	10		
L	CHES	20			
N	Beta-cyclodextrin	5			

Analytes table:

Complexations	Type	Name	c Sample (mM)	μ Eff ($\cdot 1e-9$)	Time Max (min)	c Max (mM)	κ Max (S/m)	μ EMD ($\cdot 1e-9$)
L	Flurbiprofen	0,2						

System eigenzones table:

Mobility ($\cdot 1e-9$)	Time (min)
---------------------------	------------

Conductivity vs. time graph:

Y-axis: Conductivity (S/m) ranging from 0,0566 to 0,0574.
X-axis: time (min) ranging from 0 to 4.

Input Data



PeakMaster 6.0f3 - PeakMaster 6.0f3

File Export Database Advanced Help

New Load Save Save as Calculate!

Total capillary length (cm) 50

Effective capillary length (cm) 41,5

Driving voltage (V) 15 000

Polarity (at inlet) Positive

EOF Marker time (min) 3

EOF Marker time (min) 3

Nonideality corrections

pH 9,50362

Ionic strength (mM) 9,99954

Conductivity (S/m) 0,0569014

Resistivity (Ohm·m) 17,57425

Buffer capacity (mM) 11,59495

EOF marker time (min) 3

EOF mobility 76,85185

System eigenzones

Mobility (· 1e-9)	Time (min)
1 0	3
2 2,6259e-06	3
3 -0,666778	3,02626

Eigenzone details Ionic composition

Background composition:

Complexations	Type	Name	c BGE (mM)	c Sample (mM)	$\mu_{\text{Eff}} (\cdot 1e-9)$
L	LITHIUM	10	10	36,5818	
L	CHES	20	20	-10,855	
N	Beta-cyclodextrin	5	1e-12	0	

Analytes:

Complexations	Type	Name	c Sample (mM)	$\mu_{\text{Eff}} (\cdot 1e-9)$	Time Max (min)	c Max (mM)	$\mu_{\text{Max}} (\text{S/m})$	$\mu_{\text{EMD}} (\cdot 1e-9)$
L	Flurbiprofen	0,2	-17,3267	3,88075	0,140645	0,0566931	-0,185935	

Add BGE Remove BGE Add analyte Remove analyte

Profile Conductivity Plot cutoff (min): 60 Auto Inj. zone length (mm): 1 Replot

Conductivity (S/m)

time (min)

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

Input Data



PeakMaster 6.0f3 - PeakMaster 6.0f3

File Export Database Advanced Help

New Load Save Save as Calculate!

Total capillary length (cm) 50

Effective capillary length (cm) 41,5

Driving voltage (V) 15 000

Polarity (at inlet) Positive

EOF Marker time (min) 3

EOF Marker time (min) 3

Nonideality corrections

pH 9,50362

Ionic strength (mM) 9,99954

Conductivity (S/m) 0,0569014

Resistivity (Ohm·m) 17,57425

Buffer capacity (mM) 11,59495

EOF marker time (min) 3

EOF mobility 76,85185

System eigenzones

Mobility (· 1e-9)	Time (min)
1 0	3
2 2,6259e-06	3
3 -0,666778	3,02626

Eigenzone details Ionic composition

Background composition:

Complexations	Type	Name	c BGE (mM)	c Sample (mM)	μ Eff (· 1e-9)
L	LITHIUM	10	10	10	36,5818
L	CHES	20	20	20	-10,855
N	Beta-cyclodextrin	5	1e-12	0	0

Analyses:

Complexations	Type	Name	c Sample (mM)	μ Eff (· 1e-9)	Time Max (min)	c Max (mM)	κ Max (S/m)	μ EMD (· 1e-9)
L		Flurbiprofen	0,2	-17,3267	3,88075	0,140645	0,0566931	-0,185935

Add BGE Remove BGE Add analyte Remove analyte

Profile: Conductivity Plot cutoff (min): 60 Auto Inj. zone length (mm): 1 Replot

Conductivity (S/m)

time (min)

Input Data



PeakMaster 6.0f3 - PeakMaster 6.0f3

File Export Database Advanced Help

New Load Save Save as Calculate!

Total capillary length (cm)

Effective capillary length (cm)

Driving voltage (V)

Polarity (at inlet)

EOF

EOF Marker time (min)

Nonideality corrections

pH

Ionic strength (mM)

Conductivity (S/m)

Resistivity (Ohm·m)

Buffer capacity (mM)

EOF marker time (min)

EOF mobility

System eigenzones

Mobility (· 1e-9)	Time (min)
1 0	3
2 2,6259e-06	3
3 -0,666778	3,02626

Eigenzone details Ionic composition

Background composition:

Complexations	Type	Name	c BGE (mM)	c Sample (mM)	μ Eff (· 1e-9)
L	LITHIUM	10	10	36,5818	
L	CHES	20	20	-10,855	
N	Beta-cyclodextrin	5	1e-12	0	

Analytes:

Complexations	Type	Name	c Sample (mM)	μ Eff (· 1e-9)	Time Max (min)	c Max (mM)	κ Max (S/m)	μ EMD (· 1e-9)
L		Flurbiprofen	0,2	-17,3267	3,88075	0,140645	0,0566931	-0,185935

Set nonideality corrections

- Debye-Hückel (stability constants)
- Onsager-Fuoss (ionic mobilities)
- Viscosity (ionic mobilities)

OK Cancel

Add BGE Add analyte Remove analyte

Plot cutoff (min): Auto Inj. zone length (mm): Replot

Conductivity (S/m)

time (min)

Correction for ionic effects (Debye-Hückel and Onsager-Fuoss) enabled by default

Correction for viscosity is considered experimental disabled by default

Input Data



PeakMaster 6.0f3 - PeakMaster 6.0f3

File Exp Database Advanced Help

New Load Save Save as Calculate!

Total capillary length (cm) 50
Effective capillary length (cm) 41,5
Driving voltage (V) 15 000
Polarity (at inlet) Positive
EOF Marker time (min) 3
EOF Marker time (min) 3
Nonideality corrections
pH 9,50362
Ionic strength (mM) 9,99954
Conductivity (S/m) 0,0569014
Resistivity (Ohm·m) 17,57425
Buffer capacity (mM) 11,59495
EOF marker time (min) 3
EOF mobility 76,85185

System eigenzones

	Mobility (· 1e-9)	Time (min)
1	0	3
2	2,6259e-06	3
3	-0,666778	3,02626

Eigenzone details Ionic composition

Background composition:

Complexations	Type	Name	c BGE (mM)	c Sample (mM)	μ Eff (· 1e-9)
L	LITHIUM		10	10	36,5818
L	CHES		20	20	-10,855
N	Beta-cyclodextrin		5	1e-12	0

Analyses:

Complexations	Type	Name	c Sample (mM)	μ Eff (· 1e-9)	Time Max (min)	c Max (mM)	κ Max (S/m)	μ EMD (· 1e-9)
L		Flurbiprofen	0,2	-17,3267	3,88075	0,140645	0,0566931	-0,185935

Add BGE Remove BGE Add analyte Remove analyte

Profile: Conductivity Plot cutoff (min): 60 Auto Inj. zone length (mm): 1 Replot

Conductivity (S/m)

time (min)

0,0574
0,0572
0,057
0,0568
0,0566

0 1 2 3 4

Editing the database.

Input Data



PeakMaster 6.0f4 - Manual.json

File Export Database Advanced Help

New Database editor Save as Calculate!

Load another database

Total capillary length (cm) 50
Effective capillary length (cm) 41,5
Driving voltage (V) 15 000
Polarity (at inlet) Positive
EOF Marker time (min) 3

Nonideality corrections

pH 0
Ionic strength (mM) 0
Conductivity (S/m) 0
Resistivity (Ohm · m) 0
Buffer capacity (mM) 0
EOF marker time (min) 0
EOF mobility 0

System eigenzones

Mobility (· 1e-9)	Time (min)
-------------------	------------

Eigenzone details Ionic composition

Background composition:

Complexations	Type	Name	c BGE (mM)	c Sample (mM)	μ Eff (· 1e-9)
	L	CHES	20	20	
	L	LITHIUM	10	10	
	N	Beta-cyclodextrin	5	1e-12	

Analytes:

Complexations	Type	Name	c Sample (mM)	μ Eff (· 1e-9)	Time Max (min)	c Max (mM)	κ Max (S/m)	μ EMD (· 1e-9)
	L	Flurbiprofen	0,2					

Add BGE Remove BGE Add analyte Remove analyte

Profile: Conductivity Plot cutoff (min): 60 Auto Inj. zone length (mm): 1 Replot

Conductivity (S/m)

time (min)

You can edit the existing database ...

Input Data



PeakMaster 6.0f4 - Manual.json

File Export Database Advanced Help

New Database editor Save as Calculate!

Load another database

Total capillary length (cm) 50
Effective capillary length (cm) 41,5
Driving voltage (V) 15 000
Polarity (at inlet) Positive
EOF Marker time (min) 3

Nonideality corrections
pH 0
Ionic strength (mM) 0
Conductivity (S/m) 0
Resistivity (Ohm · m) 0
Buffer capacity (mM) 0
EOF marker time (min) 0
EOF mobility 0

System eigenzones
Mobility (· 1e-9) Time (min)

Background composition:

Complexations	Type	Name	c BGE (mM)	c Sample (mM)	μ Eff (· 1e-9)
	L	CHES	20	20	
	L	LITHIUM	10	10	
	N	Beta-cyclodextrin	5	1e-12	

Analytes:

Complexations	Type	Name	c Sample (mM)	μ Eff (· 1e-9)	Time Max (min)	c Max (mM)	κ Max (S/m)	μ EMD (· 1e-9)
	L	Flurbiprofen	0,2					

... or load a completely different one.

Add BGE Remove BGE Add analyte Remove analyte

Profile: Conductivity Plot cutoff (min): 60 Auto Inj. zone length (mm): 1 Replot

Conductivity (S/m)

time (min)

Eigenzone details Ionic composition

Input Data



PeakMaster 6.0f8

File Export Database Advanced Help

New Load Save Save as Calculate!

Total capillary length (cm)

Effective capillary length (cm)

Driving voltage (V)

Polarity (at inlet)

EOF

Nonideality corrections

Adjust pH

Ionic strength (mM)

Conductivity (S/m)

Resistivity (Ohm · m)

Buffer capacity (mM)

EOF marker time (min)

EOF mobility

System eigenzones

	Mobility (· 1e-9)	Time (min)
1	0	inf
2	2,62686e-06	6,58263e...
3	-0,666778	-

Eigenzone details Ionic composition

Background composition:

Complexations	Type	Name	c BGE (mM)	c Sampl
	N	CHES	20	10
	N	LITHIUM	10	10
	N	Beta-cyclodextrin	5	1e-12

Analytes:

Complexations	Type	Name	c Sample (mM)	μ Eff (· 1e-9)	Time Max (min)
---------------	------	------	---------------	--------------------	----------------

Automatic pH adjustment (since PM6.0f8)

Add BGE Remove BGE Add analyte Remove analyte

Profile: Plot cutoff (min): Auto Inj. zone length (mm): Replot

Conductivity (S/m)

time (min)

Input Data



PeakMaster 6.0f8

File Export Database Advanced Help

New Load Save Save as Calculate!

Total capillary length (cm)

Effective capillary length (cm)

Driving voltage (V)

Polarity (at inlet)

EOF

Nonideality corrections

Adjust pH

Ionic strength (mM)

Conductivity (S/m)

Resistivity (Ohm · m)

Buffer capacity (mM)

EOF marker time (min)

EOF mobility

System eigenzones

	Mobility (· 1e-9)	Time (min)
1	0	inf
2	2,62686e-06	6,58263e...
3	-0,666778	-

Eigenzone details Ionic composition

Background composition:

Complexations	Type	Name	c BGE (mM)	c Sampl
	N	CHES	20	
	N	LITHIUM	10	
	N	Beta-cyclodextrin	5	

Analytes:

Complexations	Type	Name	c Sample (mM)	μ Eff (· 1e-9)	Time Max (min)
---------------	------	------	---------------	----------------	----------------

Adjust BGE pH

Target pH

Current pH

BGE Constituents

Constituent	Concentration (mM)
Beta-cyclodextrin	5
CHES	20
LITHIUM	10

Enter the desired target pH and select a BGE constituent whose concentration shall be adjusted to achieve the target pH.

Adjust Close

Conductivity (S/m)

time (min)

0 10 20 30 40 50

Replot

Remove analyte

Inj. zone length (mm):

Pick a constituent whose concentration you want to adjust to achieve the target pH

Input Data

The screenshot displays the PeakMaster 6.0f8 software interface. On the left, there are input fields for various parameters: Total capillary length (cm) set to 50, Effective capillary length (cm) to 41,5, Driving voltage (V) to 20 000, Polarity (at inlet) set to Positive, EOF set to No EOF, and Nonideality corrections with an Adjust pH button. Below these are fields for Ionic strength (mM) at 9,99954, Conductivity (S/m) at 0,0569014, Resistivity (Ohm · m) at 17,57425, Buffer capacity (mM) at 11,59495, EOF marker time (min) at inf, and EOF mobility at 0. A table for System eigenzones is also present.

The main area shows the Background composition table:

Complexations	Type	Name	c BGE (mM)	c Sampl
	N	CHES	20	10
	N	LITHIUM	10	10
	N	Beta-cyclodextrin	5	1e-12

An Analytes table is also visible but empty.

An 'Adjust BGE pH' dialog box is open in the center. It shows a Target pH of 8,7 and a Current pH of 9,5036. Below this is a table of BGE Constituents:

Constituent	Concentration (mM)
Beta-cyclodextrin	5
CHES	20
LITHIUM	10

The dialog box includes an 'Adjust' button (highlighted with a red box) and a 'Close' button. A callout box points to the Target pH field with the text '1. Enter the desired pH value'. Another callout box points to the Adjust button with the text '2. Click Adjust'.

At the bottom, a graph shows Conductivity (S/m) on the y-axis and time (min) on the x-axis, with a blue line representing the conductivity profile over time.

Input Data



PeakMaster 6.0f8

File Export Database Advanced Help

New Load Save Save as Calculate!

Total capillary length (cm)
Effective capillary length (cm)
Driving voltage (V)
Polarity (at inlet)
EOF

Nonideality corrections

Adjust pH
Ionic strength (mM)
Conductivity (S/m)
Resistivity (Ohm · m)
Buffer capacity (mM)
EOF marker time (min)
EOF mobility

System eigenzones

	Mobility (· 1e-9)	Time (min)
1	0	inf
2	2,62686e-06	6,58263e...
3	-0,666778	-

Eigenzone details Ionic composition

Background composition:

Complexations	Type	Name	c BGE (mM)	c Sampl
	N	CHES	20	10
	N	LITHIUM	10	10
	N	Beta-cyclodextrin	5	1e-12

Analytes:

Complexations	Type	Name	c Sample (mM)	μ Eff (· 1e-9)	Time Max (min)
---------------	------	------	---------------	--------------------	----------------

Adjust BGE pH

Target pH
Current pH

BGE Constituents

Constituent	Concentration (mM)
Beta-cyclodextrin	5
CHES	74,0378
LITHIUM	10

Enter the desired target pH and select a BGE constituent whose concentration shall be adjusted to achieve the target pH.

Adjust Close

Conductivity (S/m)

time (min)

0 10 20 30 40 50

Auto Inj. zone length (mm): Replot

Add analyte Remove analyte

Check the adjusted concentration of the constituent

Input Data

The screenshot displays the PeakMaster 6.0f8 software interface. The main window is titled "PeakMaster 6.0f8" and contains a menu bar (File, Export, Database, Advanced, Help) and a toolbar with buttons for New, Load, Save, Save as, and Calculate!.

On the left side, there are several input fields for system parameters:

- Total capillary length (cm): 50
- Effective capillary length (cm): 41,5
- Driving voltage (V): 20 000
- Polarity (at inlet): Positive
- EOF: No EOF
- Nonideality corrections: Adjust pH (9,50362)
- Ionic strength (mM): 9,99954
- Conductivity (S/m): 0,0569014
- Resistivity (Ohm · m): 17,57425
- Buffer capacity (mM): 11,59495
- EOF marker time (min): inf
- EOF mobility: 0

Below these fields is a table for "System eigenzones":

	Mobility (· 1e-9)	Time (min)
1	0	inf
2	2,62686e-06	6,58263e...
3	-0,666778	-

In the center, the "Background composition" table is visible:

Complexations	Type	Name	c BGE (mM)	c Sampl
	N	CHES	20	10
	N	LITHIUM	10	10
	N	Beta-cyclodextrin	5	1e-12

An "Adjust BGE pH" dialog box is open, displaying an error message:

Failed to adjust pH

Maximum number of iterations exceeded

Note that it may not be possible to achieve the target pH by adjusting the concentration of CHES.

Buttons: OK

Below the dialog box, the "Analytes" table is partially visible:

Complexations	Type	Name	c Sample (mM)	μ Eff (· 1e-9)	Time Max (min)
		LITHIUM	10		

At the bottom of the interface, there is a plot area with the x-axis labeled "time (min)" ranging from 0 to 50. A red box highlights the following text:

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

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 – nucleus, L – ligand, K – ligand*)

✓ **Allowed**

- NL_2
- NL_3K
- NLK_4

! **Not allowed**

- N_2L
- N_4K
- LK

Complexation



PeakMaster 6.0f3 - PeakMaster 6.0f3

File Export Database Advanced Help

New Load Save Save as Calculate!

Total capillary length (cm)

Effective capillary length (cm)

Driving voltage (V)

Polarity (at inlet)

EOF

EOF Marker time (min)

Nonideality corrections

pH

Ionic strength (mM)

Conductivity (S/m)

Resistivity (Ohm · m)

Buffer capacity (mM)

EOF marker time (min)

EOF mobility

System eigenzones

Mobility (· 1e-9)	Time (min)
-------------------	------------

Eigenzone details Ionic composition

Background composition:

Complexations	Type	Name	c BGE (mM)	c Sample (mM)	μ Eff (· 1e-9)
L		LITHIUM	10	10	
L		CHES	20	20	
N		β-cyclodextrin		1e-12	

Analyses:

Complexations	Type	Name	c Sample (mM)	μ Eff (· 1e-9)	Time Max (min)	c Max (mM)	κ Max (S/m)	μ EMD (· 1e-9)
L		Flurbiprofen 0,2						

Add BGE Remove BGE Add analyte Remove analyte

Profile: Conductivity Plot cutoff (min): Auto Inj. zone length (mm): Replot

Conductivity (S/m)

time (min)

0,0574
0,0572
0,057
0,0568
0,0566

0 1 2 3 4

Complexation can be established by dragging the compound and dropping it on the other one.

Complexation



PeakMaster 6.0f3 - Manual.json

File Export Database Advanced Help

New Load Save Save as Calculate!

Total capillary length (cm) 50
Effective capillary length (cm) 41,5
Driving voltage (V) 15 000
Polarity (at inlet) Positive
EOF Marker time (min) 3
EOF Marker time (min) 3

Nonideality corrections

pH 0
Ionic strength (mM) 0
Conductivity (S/m) 0
Resistivity (Ohm·m) 0
Buffer capacity (mM) 0
EOF marker time (min) 0
EOF mobility 0

System eigenzones

Mobility (· 1e-9)	Time (min)
-------------------	------------

Eigenzone details Ionic composition

Background composition:

Complexations	Type	Name	c BGE (mM)	c Sample (mM)	μ Eff (· 1e-9)
L	L	Beta-cyclodextrin	5	1e-12	
L	L	CHES	20	20	
L	L	LITHIUM	10	10	

Analytes:

Complexations	Type	Name	c Sample (mM)	μ Eff (· 1e-9)	Time Max (min)	c Max (mM)	κ Max (S/m)	μ EMD (· 1e-9)
L	L	Flurbiprofen	0,2					

Add BGE Remove BGE Add analyte Remove analyte

Profile: Conductivity Plot cutoff (min): 60 Auto Inj. zone length (mm): 1 Replot

Conductivity (S/m)

time (min)

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

Complexation



PeakMaster 6.0f3 - Manual.json

File Export Database Advanced Help

New Load Save Save as Calculate!

Total capillary length (cm) 50

Effective capillary length (cm) 41,5

Driving voltage (V) 15 000

Polarity (at inlet) Positive

EOF Marker time (min) 3

Nonideality corrections

pH 0

Ionic strength (mM) 0

Conductivity (S/m) 0

Resistivity (Ohm·m) 0

Buffer capacity (mM) 0

EOF marker time (min) 0

EOF mobility 0

System eigenzones

Mobility (· 1e-9) Time (min)

Eigenzone details Ionic composition

Background composition:

Complexations	Type	Name	c BGE (mM)	c Sample (mM)	μ Eff (· 1e-9)
L		Beta-cyclodextrin	5	1e-12	
L		CHES	20	20	
L		LITHIUM	10	10	

Analytes:

Complexations	Type	Name	c Sample (mM)	μ Eff (· 1e-9)	Time Max (min)	c Max (mM)	κ Max (S/m)	μ EMD (· 1e-9)
L		Flurbiprofen	0,2					

Conductivity

Profile: Conductivity

0,022786

0,022784

0,022782

0,02278

0,022778

0,022776

0,022774

0,022772

2 4 6 8

time (min)

Conductivity (S/m)

Constituent types conflict

Constituents have incompatible types to form a complexation relationship. What do you want to do?

Convert "Flurbiprofen" to nucleus

Convert "Beta-cyclodextrin" to nucleus

Cancel

Remove analyte

Auto Inj. zone length (mm): 1 Replot

**Assisted ligand – nucleus conversion:
PeakMaster will ask you which of them
do you wish to convert!**

Complexation



The screenshot displays the PeakMaster 6.0f3 software interface. The main window is titled "PeakMaster 6.0f3 - PeakMaster 6.0f3" and includes a menu bar (File, Export, Database, Advanced, Help) and a toolbar (New, Load, Save, Save as, Calculate!).

On the left, there are input fields for various parameters: Total capillary length (cm) set to 50, Effective capillary length (cm) set to 41,5, Driving voltage (V) set to 15 000, Polarity (at inlet) set to Positive, EOF Marker time (min) set to 3, pH set to 0, Ionic strength (mM) set to 0, Conductivity (S/m) set to 0, Resistivity (Ohm·m) set to 0, Buffer capacity (mM) set to 0, EOF marker time (min) set to 0, and EOF mobility set to 0.

The "Background composition" table lists three complexes:

Complexations	Type	Name	c BGE (mM)	c Sample (mM)	μ Eff (· 1e-9)
	L	LITHIUM	10	10	
	L	CHES	20	20	
	N	Beta-cyclodextrin	5	1e-12	

The "Analytes" table lists one analyte:

Complexations	Type	Name	c Sample (mM)	μ Eff (· 1e-9)	Time Max (min)	c Max (mM)	κ Max (S/m)	μ EMD (· 1e-9)
	L	Flurbiprofen	0,2					

An "Edit complexation" dialog box is open, showing the "Ligands" dropdown set to "Flurbiprofen" and a "Remove ligand" button. The dialog contains a table with the following data:

Nucleus charge	Ligand charge	Mobilities	Kxs
0	-1	10,14	5 000
	0	0	10 000

Below the table, a note states "Mind that the unit of Kxs is M⁻¹". The "OK" button is circled in red.

At the bottom, a "Profile: Conductivity" graph shows Conductivity (S/m) on the y-axis (ranging from 0,0566 to 0,0574) and time (min) on the x-axis (ranging from 0 to 4). The graph shows a step-like increase in conductivity around 2 minutes.

Two callout boxes provide instructions:

- Enter the complexation parameters for each ionic form.
- Complexation constant (Kxs) is related to SI units (M⁻¹).

Complexation



PeakMaster 6.0f3 - PeakMaster 6.0f3

File Export Database Advanced Help

New Load Save Save as Calculate

Total capillary length (cm) 50
Effective capillary length (cm) 41,5
Driving voltage (V) 15 000
Polarity (at inlet) Positive
EOF Marker time (min) 3

Nonideality corrections
pH 0
Ionic strength (mM) 0
Conductivity (S/m) 0
Resistivity (Ohm·m) 0
Buffer capacity (mM) 0
EOF marker time (min) 0
EOF mobility 0

System eigenzones
Mobility (: 1e-9) Time (min)

Background composition:

Complexations	Type	Name	c BGE (mM)	c Sample (mM)	μ Eff (: 1e-9)
	L	LITHIUM	10	10	
	L	CHES	20	20	
	N	Beta-cyclodextrin	5	1e-12	

Analytes:

Complexations	Type	Name	c Sample (mM)	μ Eff (: 1e-9)	Time Max (min)	c Max (mM)	c Max (S/m)	μ EMS (: 1e-9)
	L	Flurbiprofen	0,2					

Add BGE Remove BGE Add analyte Remove analyte

Profile: Conductivity Plot cutoff (min): 60 Auto Inj. zone length (mm): 1 Replot

Conductivity (S/m)

time (min)

Eigenzone details Ionic composition

Complexation between the two compounds established.

Complexation



PeakMaster 6.0f3 - PeakMaster 6.0f3

File Export Database Advanced Help

New Load Save Save as Calculate

Total capillary length (cm) 50
Effective capillary length (cm) 41,5
Driving voltage (V) 15 000
Polarity (at inlet) Positive
EOF Marker time (min) 3

Nonideality corrections
pH 0
Ionic strength (mM) 0
Conductivity (S/m) 0
Resistivity (Ohm·m) 0
Buffer capacity (mM) 0
EOF marker time (min) 0
EOF mobility 0

System eigenzones
Mobility (· 1e-9) Time (min)

Background composition:

Complexations	Type	Name	c BGE (mM)	c Sample (mM)	μ Eff (· 1e-9)
	L	LITHIUM	10	10	
	L	CHES	20	20	
	N	β -cyclodextrin	5	1e-12	

Analytes:

Complexations	Type	Name	c Sample (mM)	μ Eff (· 1e-9)	Time Max (min)	c Max (mM)	κ Max (S/m)	μ EMD (· 1e-9)
	L	Flurbiprofen	0,2					

Adding second complexation with the BGE component (drag and drop again).

Add BGE Remove BGE Add analyte Remove analyte

Profile: Conductivity Plot cutoff (min): 60 Auto Inj. zone length (mm): 1 Replot

Conductivity (S/m)

time (min)

Eigenzone details Ionic composition

Complexation



The screenshot displays the PeakMaster 6.0f3 software interface. On the left, various system parameters are set, including Total capillary length (50 cm), Effective capillary length (41.5 cm), Driving voltage (15 000 V), and EOF Marker time (3 min). The background composition table lists three complexes: LITHIUM, CHES, and Beta-cyclodextrin. The analyte table shows Flurbiprofen. A central 'Edit complexation' dialog box is open, showing parameters for the CHES complex: Nucleus charge (0), Ligand charge (-1), Mobilities (8 and 0), and K_{1s} (460 and 30). A red box highlights these parameters, and a speech bubble points to it with the text 'Enter the parameters of the second complexation.' The bottom of the screen shows a conductivity profile graph with 'Conductivity (S/m)' on the y-axis and 'time (min)' on the x-axis. The graph shows a step-like increase in conductivity around 2 minutes.

Complexations	Type	Name	c BGE (mM)	c Sample (mM)	μ Eff ($\cdot 1e-9$)
	L	LITHIUM	10	10	
	L	CHES	20	20	
	N	Beta-cyclodextrin	5	1e-12	

Complexations	Type	Name	c Sample (mM)	μ Eff ($\cdot 1e-9$)	Time Max (min)	c Max (mM)	κ Max (S/m)	μ EMD ($\cdot 1e-9$)
	L	Flurbiprofen	0,2					

Nucleus charge	Ligand charge	Mobilities	K _{1s}
0	-1	8	460
	0	0	30

Conductivity (S/m) vs time (min) graph showing a step increase around 2 minutes.

Complexation



PeakMaster 6.0f3 - PeakMaster 6.0f3

File Export Database Advanced Help

New Load Save Save as Calculate

Total capillary length (cm) 50
Effective capillary length (cm) 41,5
Driving voltage (V) 15 000
Polarity (at inlet) Positive
EOF Marker time (min) 3

Nonideality corrections
pH 0
Ionic strength (mM) 0
Conductivity (S/m) 0
Resistivity (Ohm·m) 0
Buffer capacity (mM) 0
EOF marker time (min) 0
EOF mobility 0

System eigenzones
Mobility (· 1e-9) Time (min)

Background composition:

Complexations	Type	Name	c BGE (mM)	c Sample (mM)	μ Eff (· 1e-9)
L		LITHIUM	10	10	
L		CHES	20	20	
N		Beta-cyclodextrin	5	1e-12	

Analytes:

Complexations	Type	Name	c Sample (mM)	μ Eff (· 1e-9)	Time Max (min)	c Max (mM)	κ Max (S/m)	μ EMD (· 1e-9)
L		Flurbiprofen	0,2					

Add BGE Remove BGE Add analyte Remove analyte

Profile: Conductivity Plot cutoff (min): 60 Auto Inj. zone length (mm): 1 Replot

Conductivity (S/m)

time (min)

Eigenzone details Ionic composition

New complexation established.

Complexation



PeakMaster 6.0f3 - PeakMaster 6.0f3

File Export Database Advanced Help

New Load Save Save as Calculate

Total capillary length (cm) 50
Effective capillary length (cm) 41,5
Driving voltage (V) 15 000
Polarity (at inlet) Positive
EOF Marker time (min) 3
EOF Marker time (min) 3

Nonideality corrections

pH 0
Ionic strength (mM) 0
Conductivity (S/m) 0
Resistivity (Ohm·m) 0
Buffer capacity (mM) 0
EOF marker time (min) 0
EOF mobility 0

System eigenzones

Mobility (· 1e-9) Time (min)

Eigenzone details Ionic composition

Background composition:

Complexations	Type	Name	c BGE (mM)	c Sample (mM)	μ Eff (· 1e-9)
L	L	LITHIUM	10	10	
L	L	CHES	20	20	
N	N	Beta-cyclodextrin	5	1e-12	
N	N	Heptakis(2,6-di-O-methyl)-beta-cyclodextrin	5	1e-12	

Analytes:

Complexations	Type	Name	c Sample (mM)	μ Eff (· 1e-9)	Time Max (min)	c Max (mM)	κ Max (S/m)	μ EMD (· 1e-9)
L	L	Flurbiprofen	0,2					

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

Profile: Conductivity Plot cutoff (min): 60 Auto Inj. zone length (mm): 1 Replot

Conductivity (S/m)

0,0574
0,0572
0,057
0,0568
0,0566

0 1 2 3 4

time (min)

Complexation



The software interface displays various parameters for a complexation experiment. The 'Background composition' table lists components like LITHIUM, CHES, Beta-cyclodextrin, and Heptakis(2,6-di-O-methyl)-beta-cyclodextrin. The 'Analytes' table shows Flurbiprofen. The 'Edit complexation' dialog box is open, showing the following data:

Ligands	Ligand charge	Mobilities	Kxs
Flurbiprofen	-1	7.4	7.000

Annotations in the image provide context:

- Enter the parameters of this complexation.** (Points to the 'Edit complexation' dialog box)
- Note that if you leave the row empty, it means the respective ionic form does not form a complex.** (Points to the empty row in the dialog box)

The main graph shows Conductivity (S/m) on the y-axis (ranging from 0,0566 to 0,0574) versus time (min) on the x-axis (ranging from 0 to 4). The profile is set to 'Conductivity'.

Complexation



PeakMaster 6.0f3 - PeakMaster 6.0f3

File Export Database Advanced Help

New Load Save Save as Calculate

Total capillary length (cm) 50
Effective capillary length (cm) 41,5
Driving voltage (V) 15 000
Polarity (at inlet) Positive
EOF Marker time (min) 3
EOF Marker time (min) 3

Nonideality corrections

pH 0
Ionic strength (mM) 0
Conductivity (S/m) 0
Resistivity (Ohm·m) 0
Buffer capacity (mM) 0
EOF marker time (min) 0
EOF mobility 0

System eigenzones

Mobility (· 1e-9)	Time (min)
-------------------	------------

Eigenzone details Ionic composition

Background composition:

Complexations	Type	Name	c BGE (mM)	c Sample (mM)	μ Eff (· 1e-9)
	L	LITHIUM	10	10	
	L	CHES	20	20	
	N	Beta-cyclodextrin	5	1e-12	
	N	Heptakis(2,6-di-O-methyl)-beta-cyclodextrin	5	1e-12	

Analytes:

Complexations	Type	Name	c Sample (mM)	μ Eff (· 1e-9)	Time Max (min)	c Max (mM)	k Max (S/m)	μ EMD (· 1e-9)
	L	Flurbiprofen	0,2					

New complexation with a different nucleus established.

Profile: Conductivity Plot cutoff (min): 60 Auto Inj. zone length (mm): 1 Replot

Conductivity (S/m)

time (min)

Complexation



The screenshot displays the PeakMaster 6.0f3 software interface. On the left, there are input fields for various parameters: Total capillary length (cm) set to 50, Effective capillary length (cm) set to 41,5, Driving voltage (V) set to 15 000, Polarity (at inlet) set to Positive, EOF Marker time (min) set to 3, and several other parameters like pH, Ionic strength, Conductivity, Resistivity, Buffer capacity, EOF marker time, and EOF mobility, all set to 0. Below these are 'Nonideality corrections' and 'System eigenzones' sections.

The main area contains two tables: 'Background composition' and 'Analytes'. The 'Background composition' table has columns for Complexations, Type, Name, c BGE (mM), c Sample (mM), and μ Eff ($\cdot 1e-9$). The 'Analytes' table has columns for Complexations, Type, Name, c Sample (mM), μ Eff ($\cdot 1e-9$), Time Max (min), c Max (mM), κ Max (S/m), and μ EMD ($\cdot 1e-9$).

A callout box with a black border and white background points to a yellow field in the 'Background composition' table. The text inside the box reads: "To edit the complexation, double click on the nucleus coloured field." The yellow field is in the 'Complexations' column for the row with Name 'Heptakis(2,6-di-O-methyl)-beta-cyclodextrin'.

At the bottom, there is a 'Profile' dropdown set to 'Conductivity', a 'Plot cutoff (min)' set to 60, a checked 'Auto' checkbox, an 'Inj. zone length (mm)' set to 1, and a 'Replot' button. Below this is a graph with 'Conductivity (S/m)' on the y-axis (ranging from 0,0566 to 0,0574) and 'time (min)' on the x-axis (ranging from 0 to 4). The graph area is currently empty.

Complexation



The screenshot displays the PeakMaster 6.0f3 software interface. The main window is titled "PeakMaster 6.0f3 - PeakMaster 6.0f3". The interface includes a menu bar (File, Export, Database, Advanced, Help) and a toolbar with buttons for New, Load, Save, Save as, and Calculate.

On the left side, there are input fields for various parameters:

- Total capillary length (cm): 50
- Effective capillary length (cm): 41,5
- Driving voltage (V): 15 000
- Polarity (at inlet): Positive
- EOF Marker time (min): 3
- pH: 0
- Ionic strength (mM): 0
- Conductivity (S/m): 0
- Resistivity (Ohm · m): 0
- Buffer capacity (mM): 0
- EOF marker time (min): 0
- EOF mobility: 0

The "Background composition:" table lists the following data:

Complexations	Type	Name	c BGE (mM)	c Sample (mM)	μ Eff (· 1e-9)
	L	LITHIUM	10	10	
	L	CHES	20	20	
	N	Beta-cyclodextrin	5	1e-12	
	N	Heptakis(2,6-di-O-methyl)-beta-cyclodextrin	5	1e-12	

The "Analytes:" table lists the following data:

Complexations	Type	Name	c Sample (mM)	μ Eff (· 1e-9)	Time Max (min)	c Max (mM)	κ Max (S/m)	μ EMD (· 1e-9)
	L	Flurbiprofen	0,2					

An "Edit complexation" dialog box is open, showing the "Ligands" dropdown menu set to "Flurbiprofen". The dialog also displays the following data:

Nucleus charge	Ligand charge	Mobilities	Kxs
0	-1	7,4	7 000
	0		

The "Remove ligand" button is visible next to the "Ligands" dropdown. A red circle highlights the "Ligands" dropdown menu.

At the bottom of the interface, there is a "Profile: Conductivity" plot showing "Conductivity (S/m)" on the y-axis (ranging from 0,0566 to 0,0574) and "time (min)" on the x-axis (ranging from 0 to 4). The plot shows a step-like increase in conductivity over time.

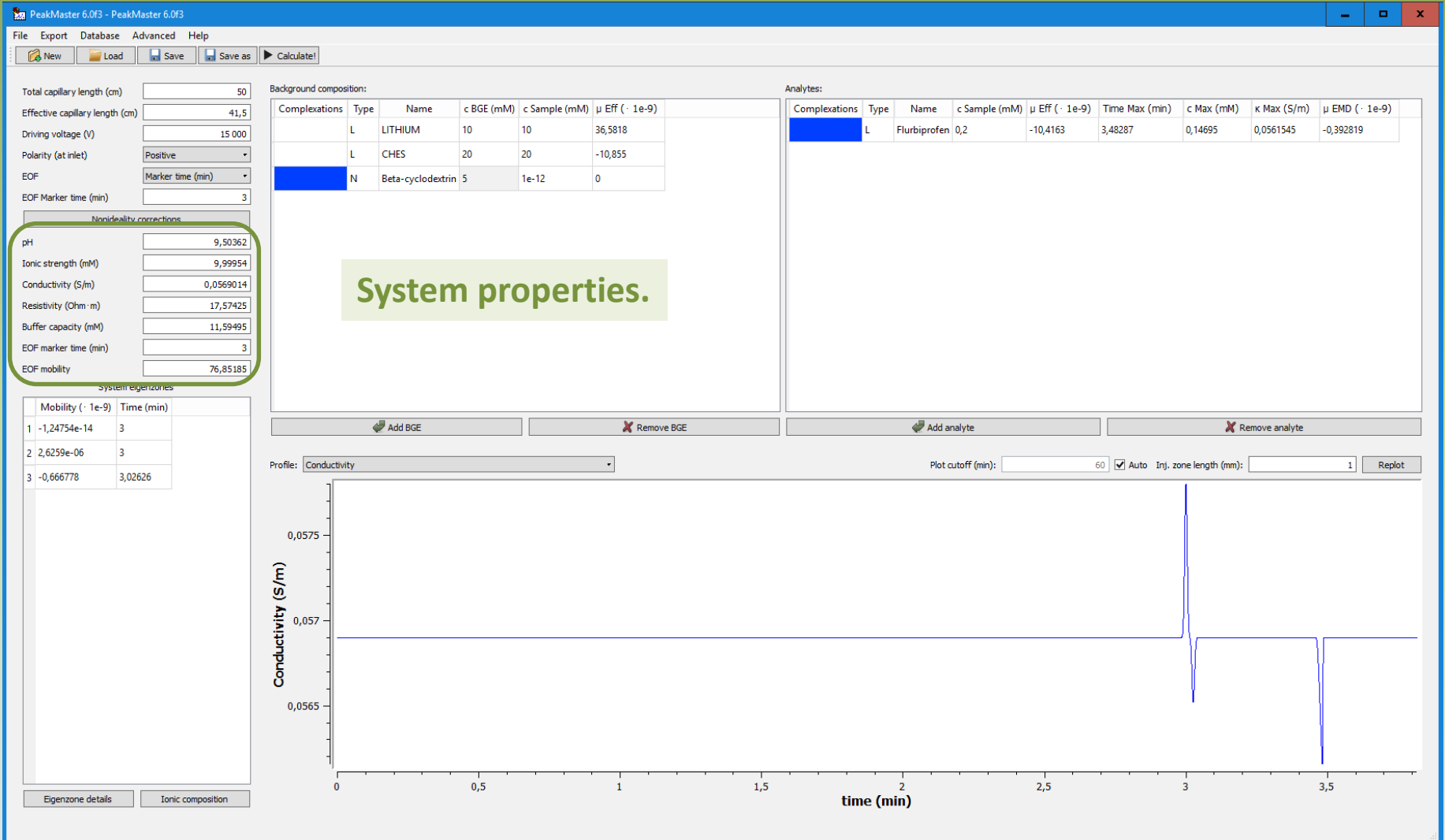
Two callout boxes provide instructions:

- You can choose which ligand interaction you want to edit.**
- By removing the ligand you can remove the complexation.**

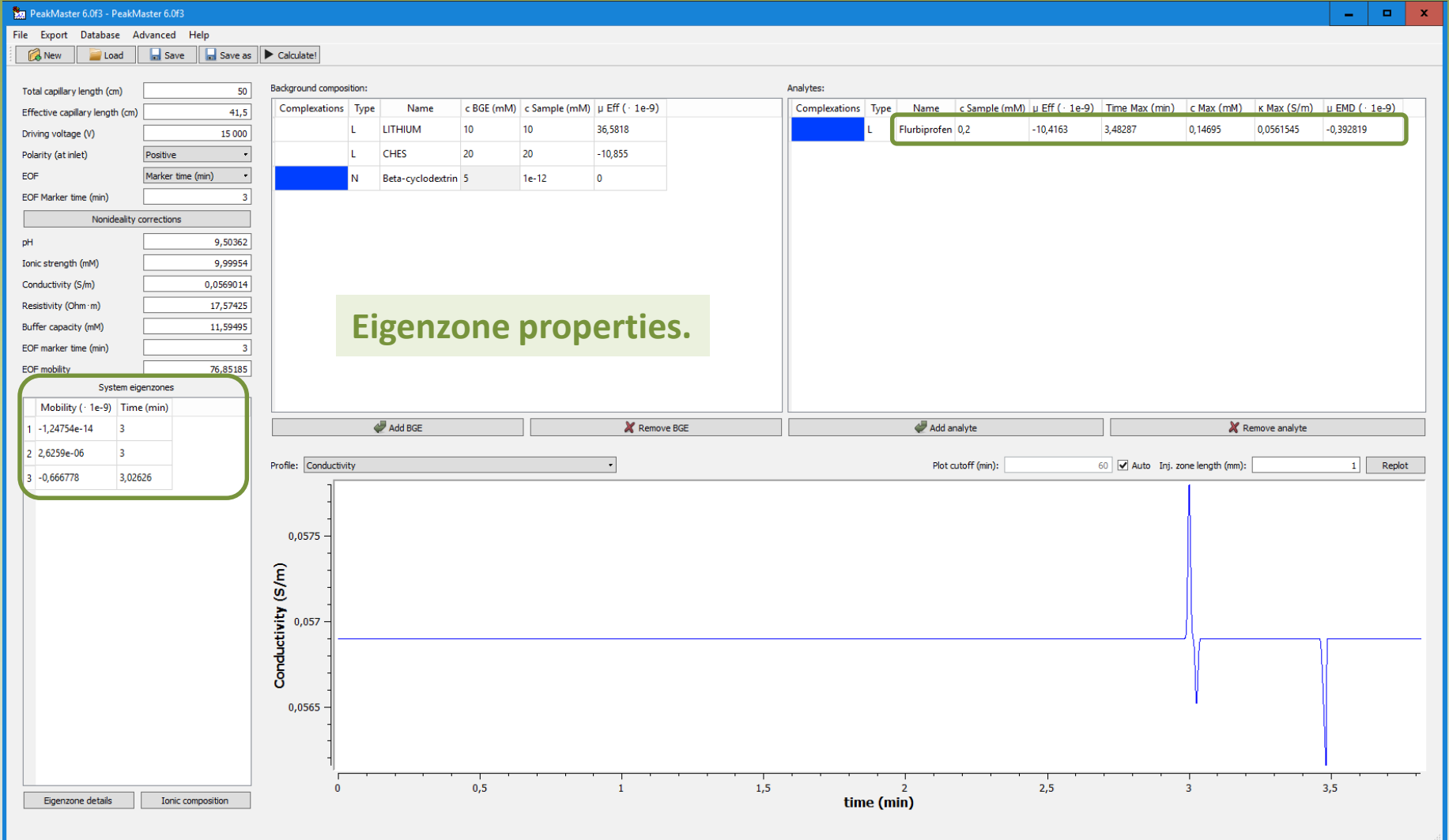


Results

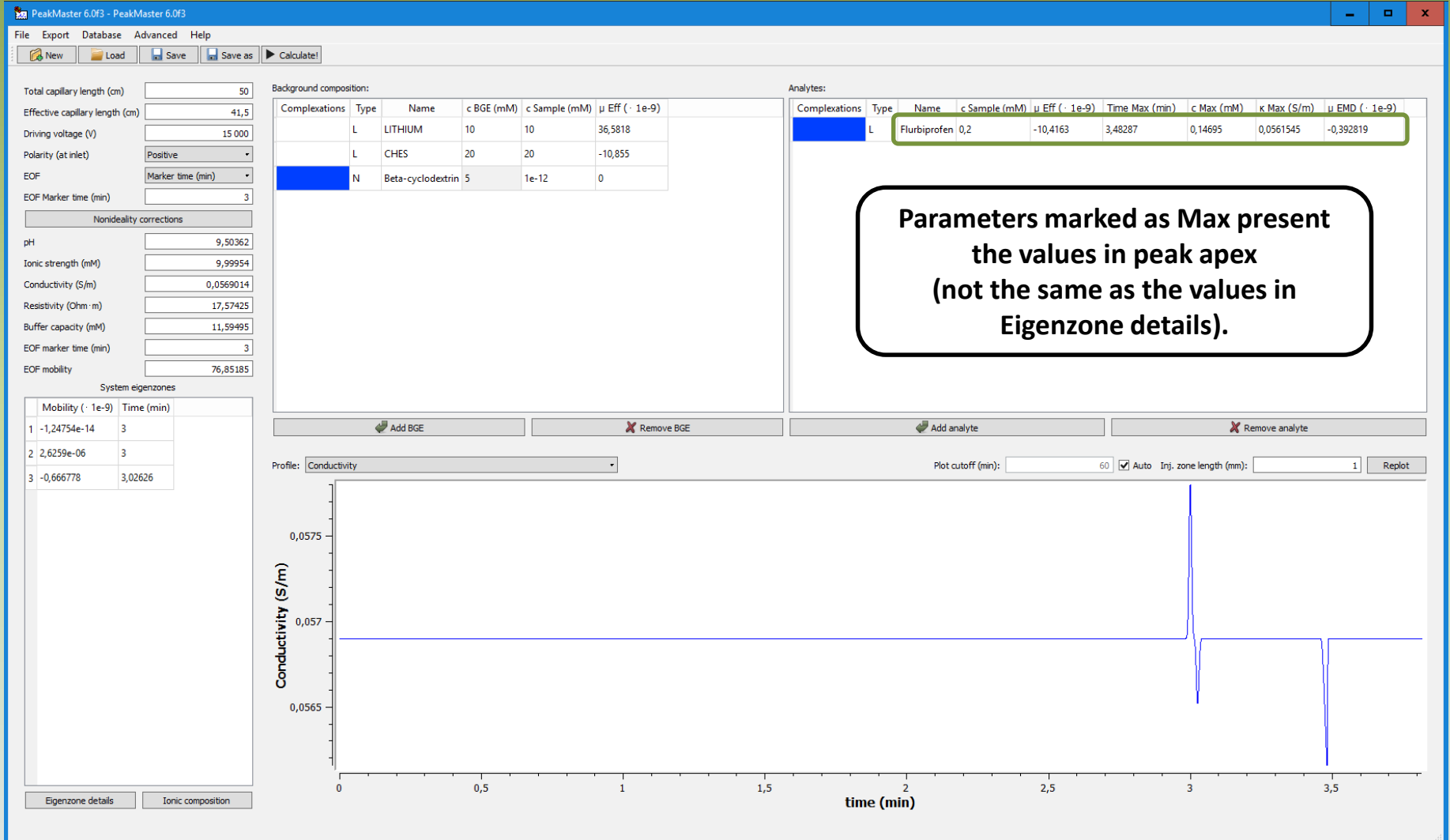
Results



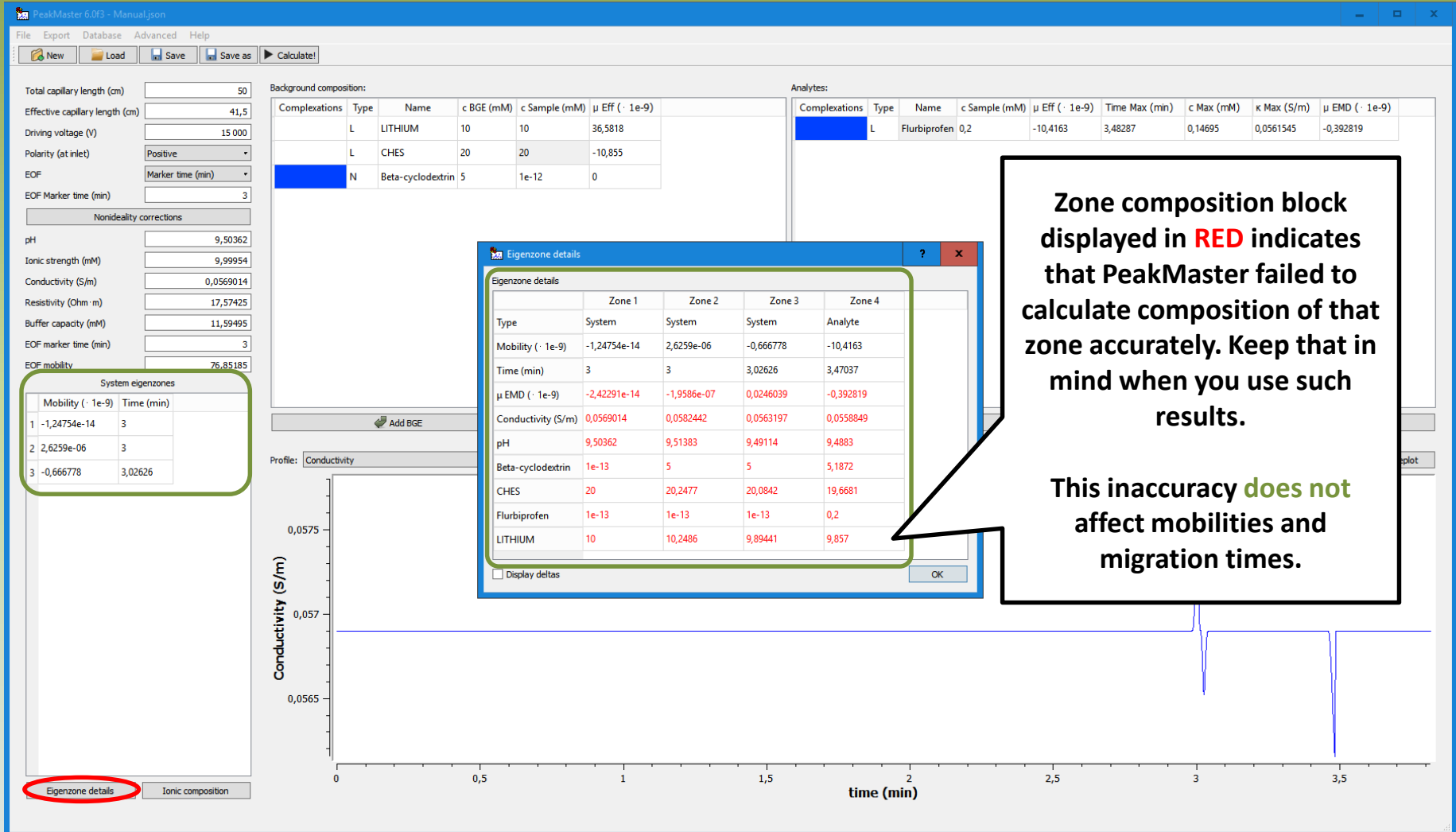
Results



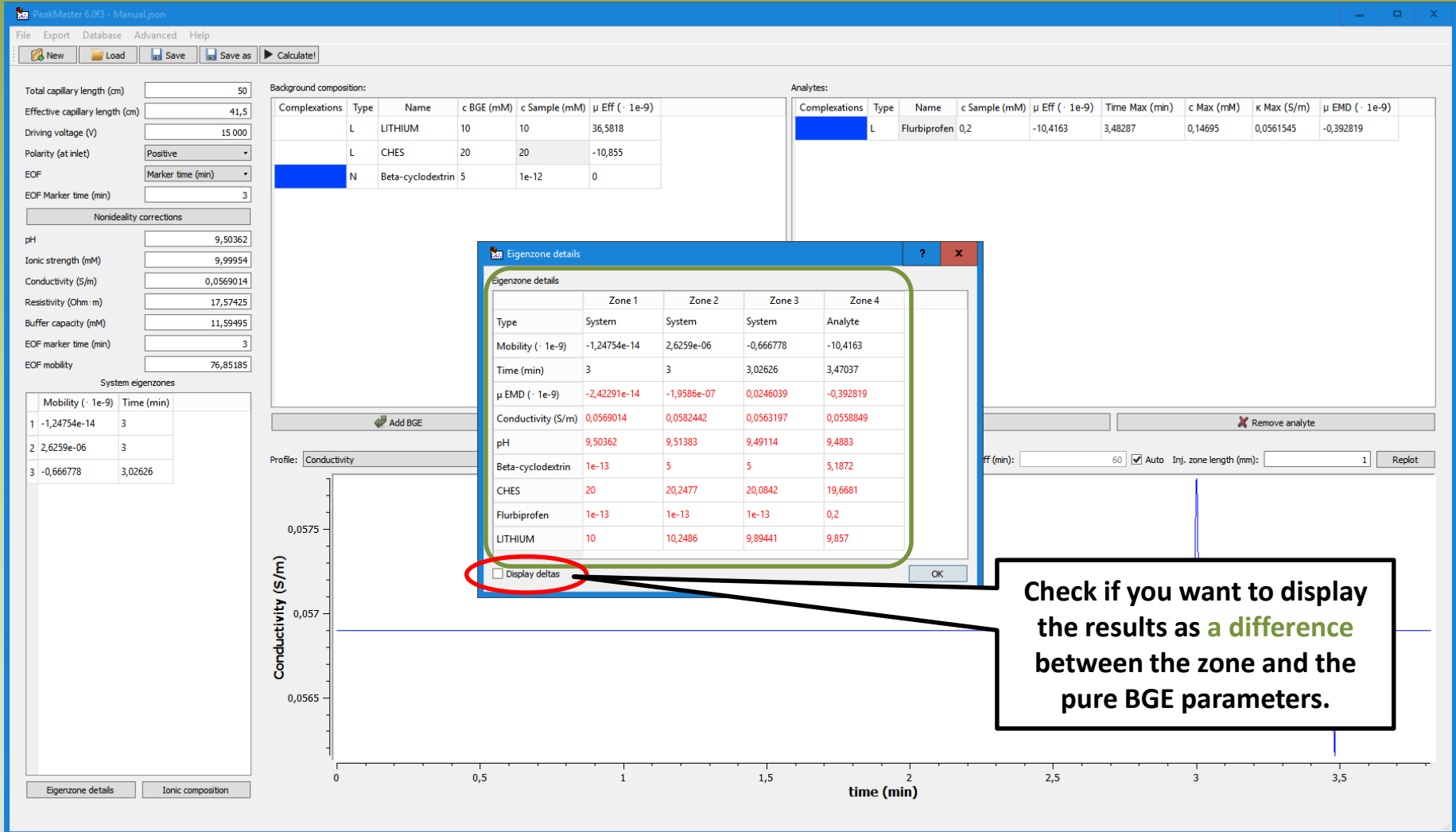
Results



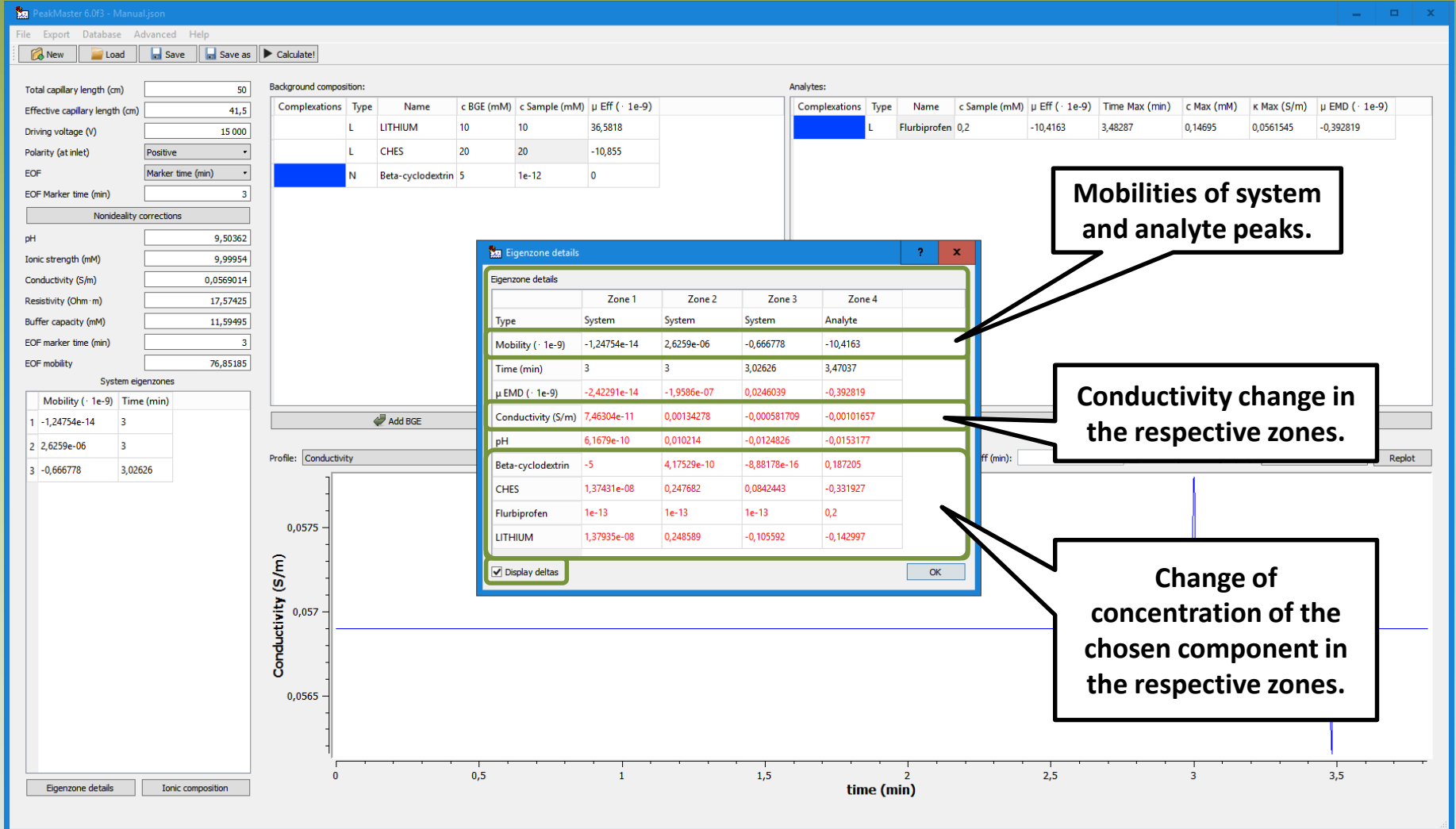
Results



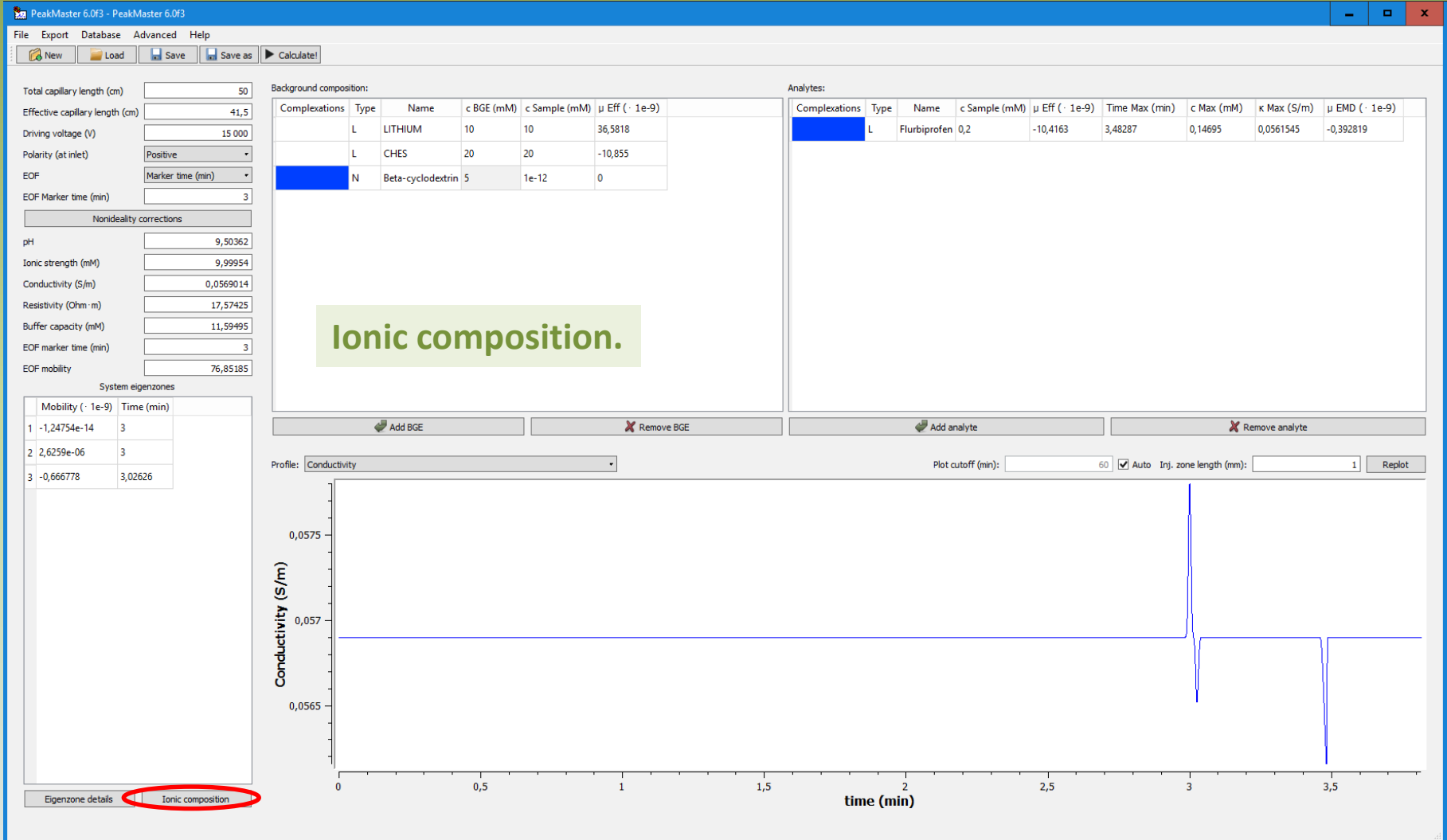
Results



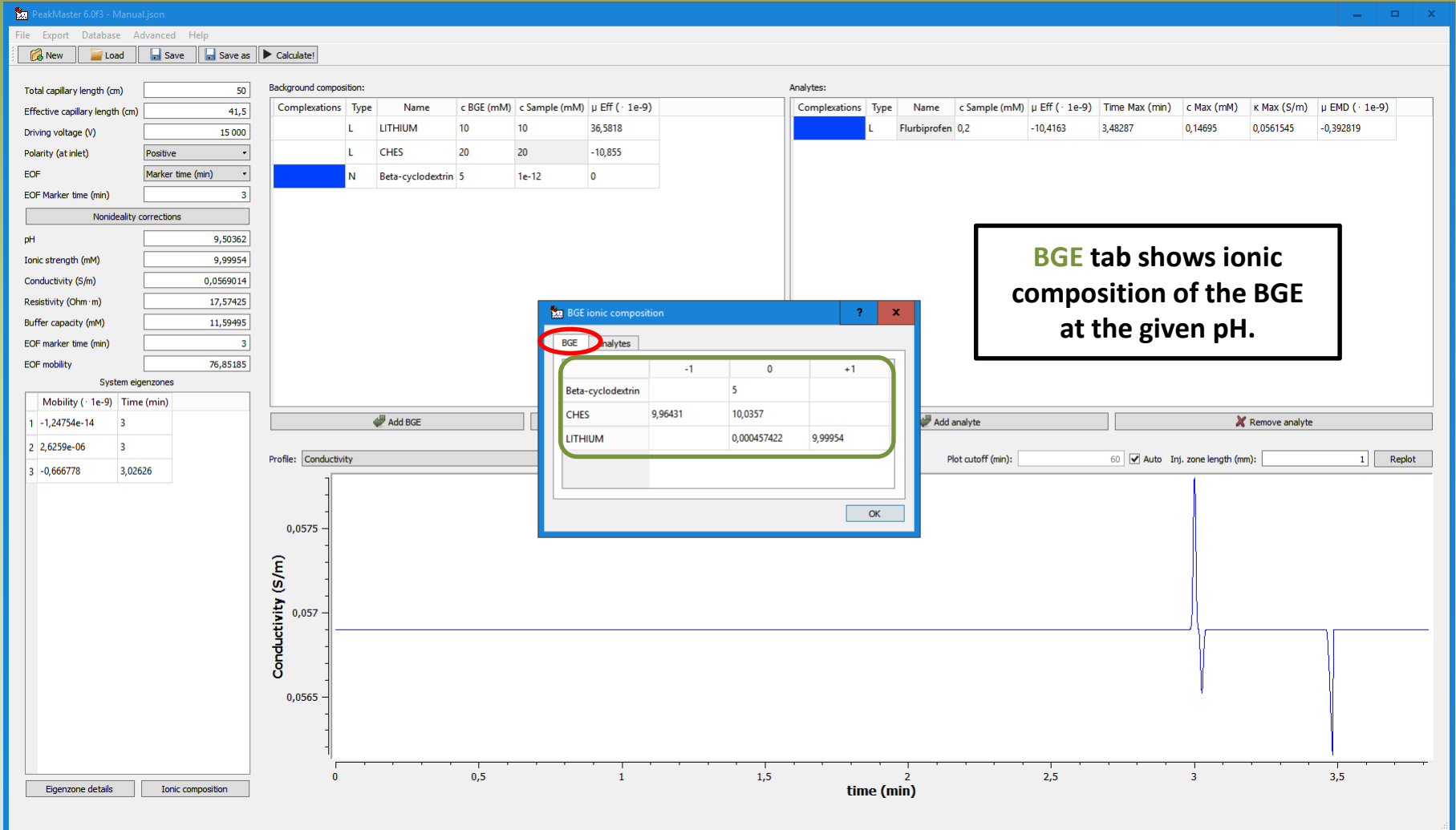
Results



Results



Results



Results



Background composition:

Complexations	Type	Name	c BGE (mM)	c Sample (mM)	μ Eff (· 1e-9)
N		Beta-cyclodextrin	5	1e-12	0
L		CHES	20	20	-10,855
L		LITHIUM	10	10	36,5818

Analytes:

Complexations	Type	Name	c Sample (mM)	μ Eff (· 1e-9)	Time Max (min)	c Max (mM)	κ Max (S/m)	μ EMD (· 1e-9)
L		Flurbiprofen	0,2	-10,4163	3,48287	0,14695	0,0561545	-0,392819

System eigenzones:

Mobility (· 1e-9)	Time (min)
1 -1,24754e-14	3
2 2,6259e-06	3
3 -0,666778	3,02626

Profile: Conductivity

Conductivity (S/m) vs. time (min) plot showing a baseline around 0,057 S/m with a sharp peak at approximately 3,5 minutes.

BGE ionic composition dialog box:

Analyte: Flurbiprofen

WARNING: PeakMaster has detected that dissociation states of this analyte were not calculated correctly. This is a limitation of the current implementation of the computation engine. This miscalculation **does not** have any adverse effects on any other part of the calculation.

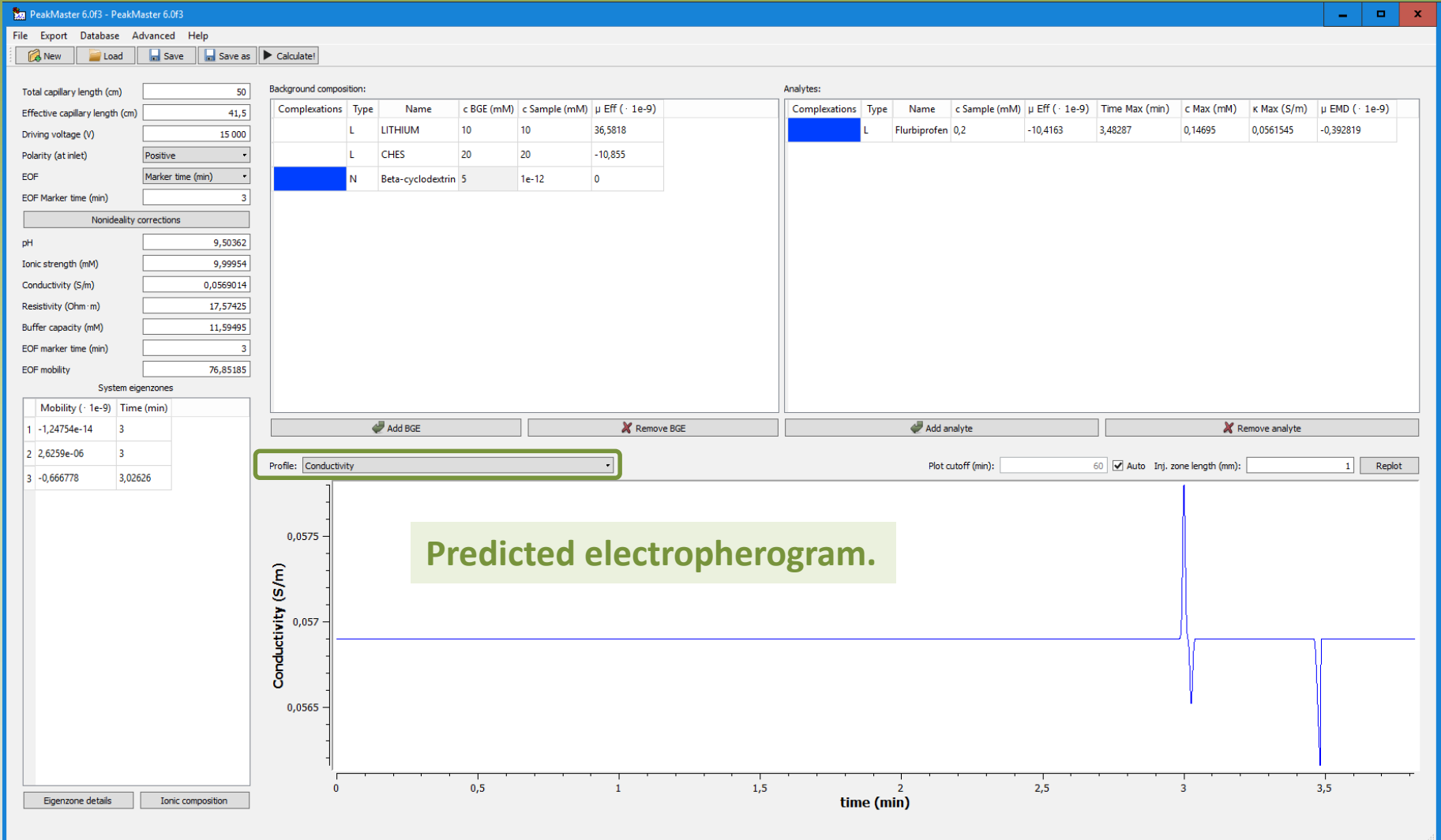
Flurbiprofen(-1)	Flurbiprofen(0)	Beta-cyclodextrin(0)Flurbiprofen(-1)
0,382303	1,68076e-06	9,55756

Note that the dissociation states are computed for analytes at infinite dilution and are expressed as molar fraction.

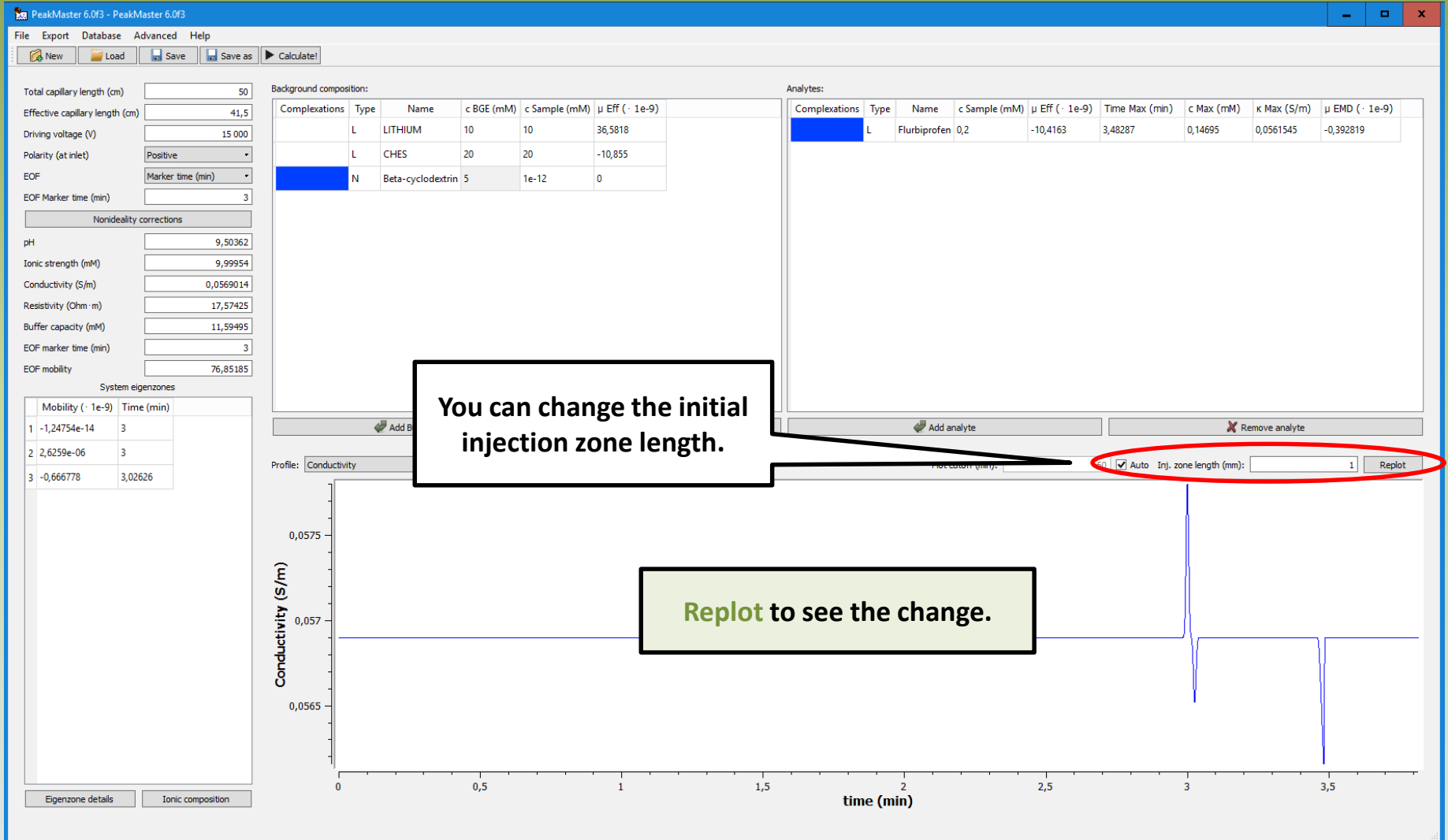
Callout 1: In the **Analytes** tab you can see degree of dissociation of the chosen analyte.

Callout 2: If there is a warning present, the dissociation states may not be correct!

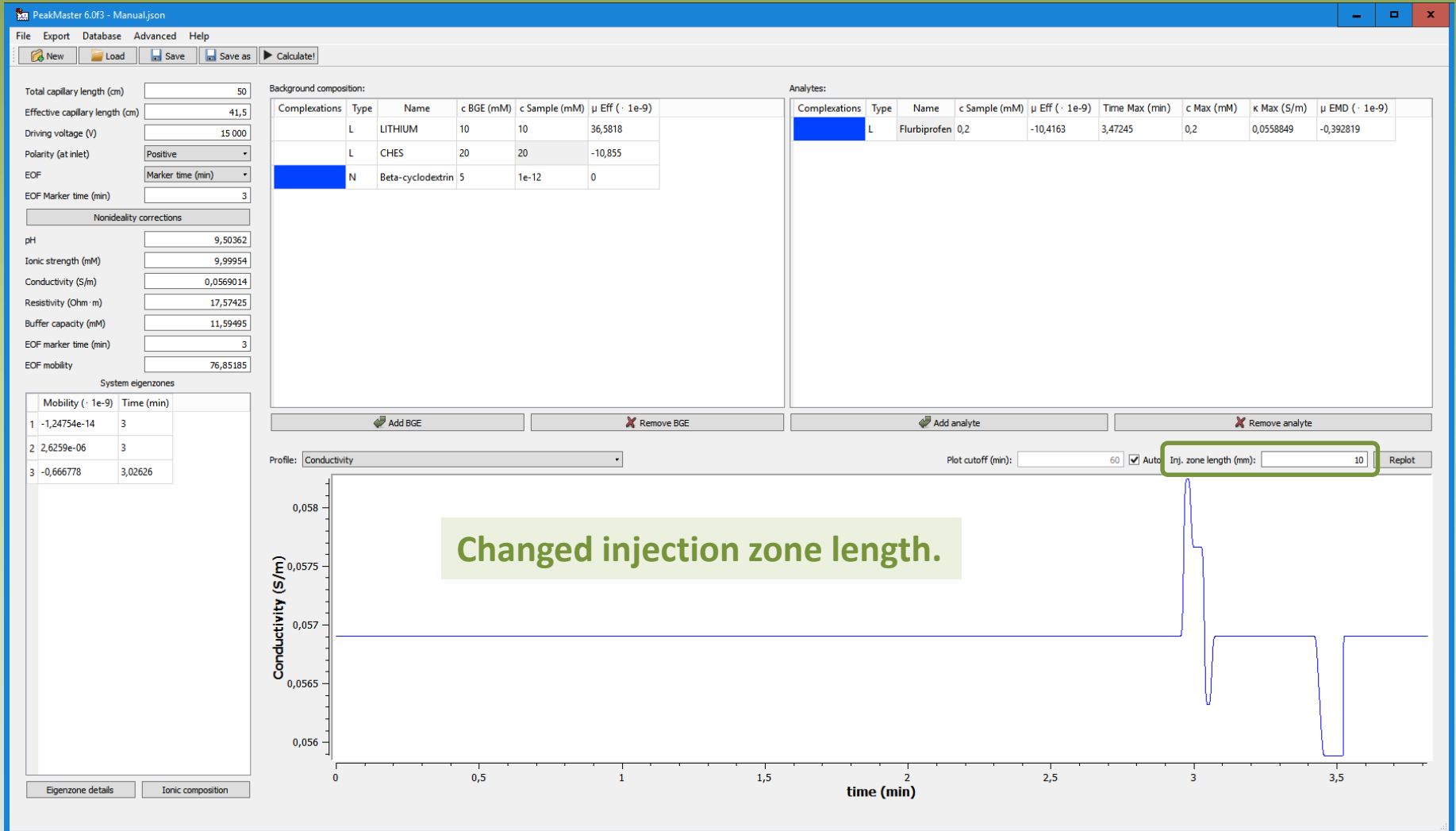
Results



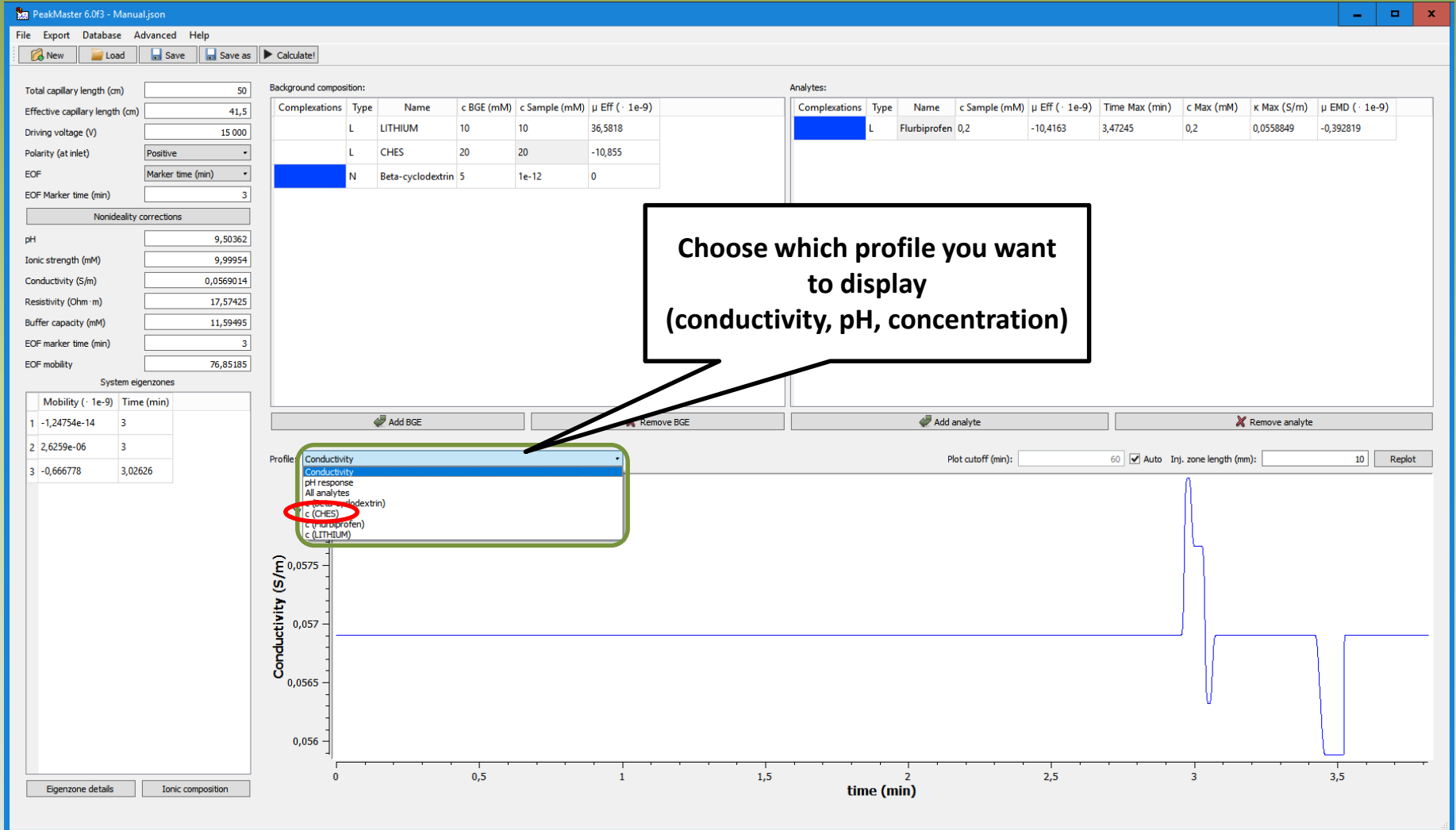
Results



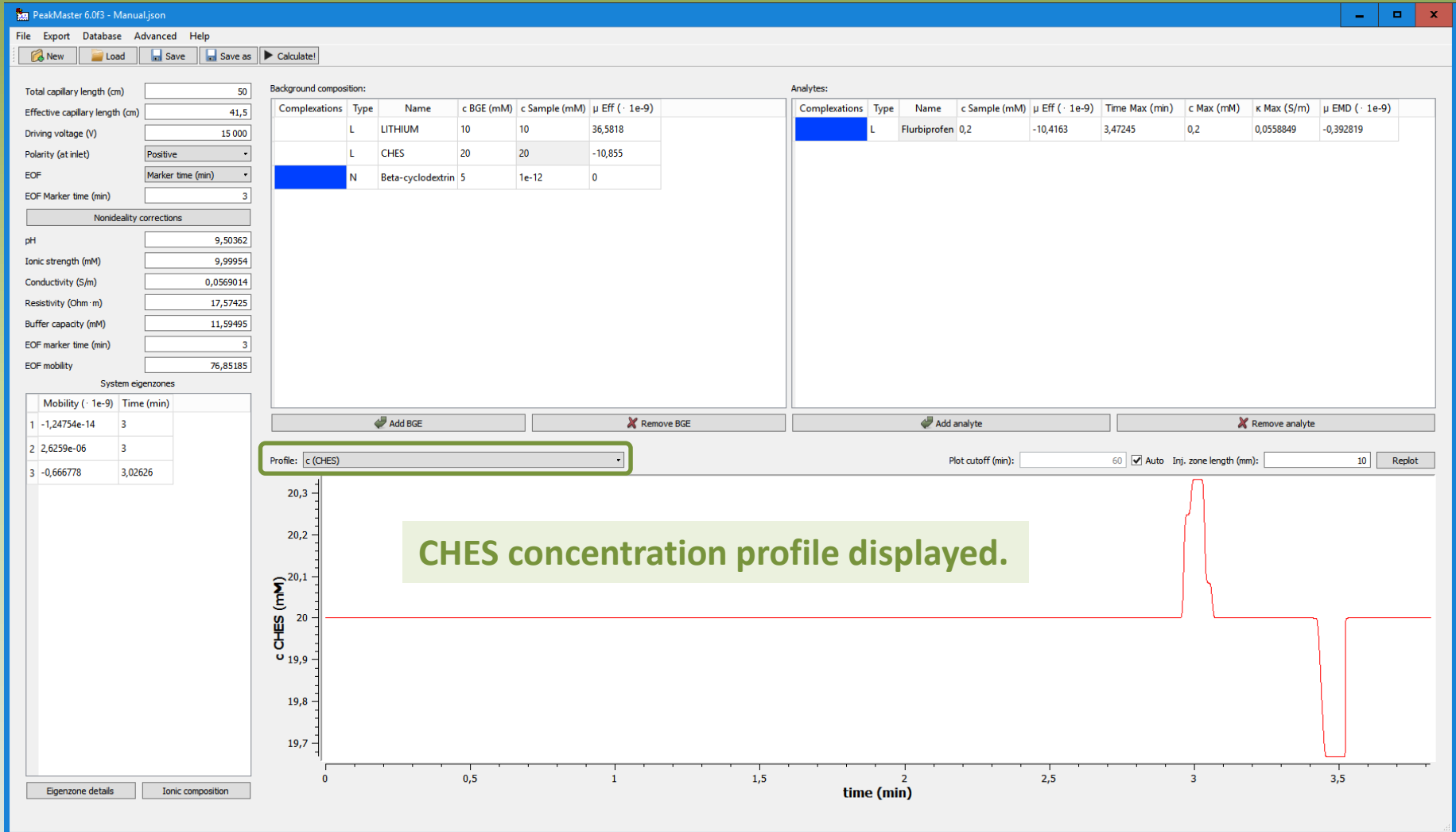
Results



Results



Results



Results



PeakMaster 6.0f3 - Manual.json

File **Export** Database Advanced Help

New Load Save Save as Calculate

Total capillary length (cm) 50
Effective capillary length (cm)
Driving voltage (V) 15 000
Polarity (at inlet) Positive
EOF Marker time (min) 3
EOF Marker time (min) 3

Nonideality corrections

pH 9,50362
Ionic strength (mM) 9,99954
Conductivity (S/m) 0,0569014
Resistivity (Ohm·m) 17,57425
Buffer capacity (mM) 11,59495
EOF marker time (min) 3
EOF mobility 76,85185

System eigenzones

Mobility (· 1e-9)	Time (min)
1 -1,24754e-14	3
2 2,6259e-06	3
3 -0,666778	3,02626

Eigenzone details Ionic composition

Background composition:

Complexations	Type	Name	c BGE (mM)	c Sample (mM)	μ Eff (· 1e-9)
L		LITHIUM	10	10	36,5818
		CHES	20	20	-10,855
		Fluoroxetin	5	1e-12	0

Analytes:

Complexations	Type	Name	c Sample (mM)	μ Eff (· 1e-9)	Time Max (min)	c Max (mM)	κ Max (S/m)	μ EMD (· 1e-9)
L		Flurbiprofen	0,2	-10,4163	3,47245	0,2	0,0558849	-0,392819

Add BGE Remove BGE Add analyte Remove analyte

Profile: c (CHES) Plot cutoff (min): 60 Auto Inj. zone length (mm): 10 Replot

Export the electropherogram.

Results



PeakMaster 6.0f3 - Manual.json

File Export Database Advanced Help

Electrophoregram **As CSV** Calculate

Total capillary length (cm) 50
Effective capillary length (cm) 41,5
Driving voltage (V) 15 000
Polarity (at inlet) Positive
EOF Marker time (min) 3
EOF Marker time (min) 3

Nonideality corrections

pH 9,50362
Ionic strength (mM) 9,99954
Conductivity (S/m) 0,0569014
Resistivity (Ohm·m) 17,57425
Buffer capacity (mM) 11,59495
EOF marker time (min) 3
EOF mobility 76,85185

System eigenzones

Mobility (· 1e-9)	Time (min)
1 -1,24754e-14	3
2 2,6259e-06	3
3 -0,666778	3,02626

Eigenzone details Ionic composition

Background composition:

Complexations	Type	Name	c BGE (mM)	c Sample (mM)	μ Eff (· 1e-9)
L	LITHIUM	10	10	10	36,5818
L	CHES	20	20	20	-10,855
N	Beta-cyclodextrin	5	1e-12	0	0

Analytes:

Complexations	Type	Name	c Sample (mM)	μ Eff (· 1e-9)	Time Max (min)	c Max (mM)	κ Max (S/m)	μ EMD (· 1e-9)
L		Flurbiprofen	0,2	-10,4163	3,47245	0,2	0,0558849	-0,392819

Export graph as *.csv

Add BGE Remove BGE Add analyte Remove analyte

Profile: c (CHES) Plot cutoff (min): 60 Auto Inj. zone length (mm): 10 Replot

c CHES (mM)

time (min)

Results

