

CEval

software tool for CE and ACE data
evaluation

Step-by-step User Guide



CEval - User Guide

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Opening Data

Opening Data



The screenshot displays the CEval 0.3rc1 software interface. The 'File' menu is open, with options: 'Load ChemStation file', 'Load comma-separated file', 'Load data table', 'Save data table', and 'Exit'. A red circle highlights the first three options. A blue callout box contains the text: 'A) You can either load Chemstation file ...'. The main window shows a plot area with axes from 0 to 1000. Below the plot is the 'Evaluation' section with a 'Hyperbole fit' tab. It includes a 'File:' field, 'Common parameters' (Capillary, Detector, Voltage, Field strength, c(Selector), Time of EOF), 'Evaluated peaks' table, and 'Parameters' (EOF, Peak, HVL) with various input fields and checkboxes. Buttons for 'Add peak', 'Delete peak', 'Cancel selection', 'Replot HVL', 'Do HVL fit', and 'Find peak(s)' are visible.

File: Close file

Common parameters

Capillary (cm)
Detector (cm)
Voltage (kV)
Field strength (kV/m)
c(Selector)
Time of EOF (min)
Read EOF time

Evaluated peaks

Analyte	Time	Area
---------	------	------

Add peak Delete peak
Cancel selection

Parameters **Results**

EOF

v (1e-3 m/s) v! (1e-3 m/s) u (1e-9 m.m/V/s)

Peak

Peak from X Peak from Y Peak max at X
Peak to X Peak to Y Peak height
v (1e-3 m/s) v! (1e-3 m/s) u! (1e-9 m.m/V/s)
Ht Area (Units.min) t USP

HVL

a0 Fixed a1 Fixed
a2 Fixed a3 Fixed
 χ^2 ϵ
Significant digits Maximum iterations
a1 u! (1e-9 m.m/V/s)

Replot HVL Do HVL fit
Find peak(s)

Opening Data



The screenshot displays the CEval 0.3rc1 software interface. At the top, a graph shows a plot with a y-axis from 0 to 1000 and an x-axis from 0 to 1000. Below the graph, the 'Evaluation' section is active, showing 'Hyperbole fit' and various parameters like 'Capillary (d)', 'Detector (d)', 'Voltage (kV)', 'Field strength (kV/m)', 'c(Selector)', and 'Time of EOF (min)'. A 'Read EOF time' button is present. A 'Pick a ChemStation file to load' dialog box is open in the center, showing a list of files and folders. A red box highlights the 'D_MET_3_2.D' folder, and a red arrow points to the 'DAD1C.ch' file. A callout box labeled 'Absorbance or conductivity data' points to the 'Absorbance' file type. Another callout box labeled 'Choose the desired wavelength' points to the 'Measured: 217 ...' value in the 'Additional info' column. The 'DAD1C.ch' file is selected, and the 'Load' button is visible. Below the dialog, there are 'Add peak', 'Delete peak', and 'Cancel selection' buttons. At the bottom right, there are 'Replot HVL', 'Do HVL fit', and 'Find peak(s)' buttons. The 'HVL' section includes input fields for 'a0', 'a1', 'a2', 'a3', 'χ²', 'Significant digits', 'a1 ul (1e-9 m.m/V/s)', 'ε', and 'Maximum iterations', along with 'Fixed' checkboxes and '0' values.

Chemstation data

Absorbance or conductivity data

Choose the desired wavelength

Name	File name	File type	Additional info
▶ D_MET_30_2.D	DAD1A.ch	Absorbance	Measured: 250 ...
▶ D_MET_30_3.D	DAD1B.ch	Absorbance	Measured: 210 ...
▶ D_MET_30_4.D	DAD1C.ch	Absorbance	Measured: 217 ...
▶ D_MET_3_1.D	HPCE1C.ch	Current	
▶ D_MET_3_2.D	HPCE1L.ch	Conductivity	
▶ D_MET_3_3.D	HPCE1P.ch	Pressure	
▶ D_MET_3_4.D			
▶ D_MET_5_1.D			
▶ D_MET_5_2.D			
▶ D_MET_5_3.D			

Opening Data



CEval 0.3rc1

File Options Help

DAD1C.ch

Absorbance (mAU)

Time (minute)

Electrophoreogram is loaded.

Evaluation Hyperbole fit

File: Q:/Users/Magda/CEval/CEval data/LIAC_SEQ_DM_CD/D_MET_3_2.D/DAD1C.ch Close file

Common parameters

- Capillary (cm)
- Detector (cm)
- Voltage (kV)
- Field strength (kV/m)
- c(Selector)
- Time of EOF (min)

Evaluated peaks

Analyte	Time	Area
---------	------	------

Parameters Results

EOF

- v (1e-3 m/s) v_t (1e-3 m/s) u (1e-9 m.m/V/s)

Peak

- Peak from X Peak from Y Peak max at X
- Peak to X Peak to Y Peak height
- v (1e-3 m/s) v_t (1e-3 m/s) u_t (1e-9 m.m/V/s)
- H_t Area (Units.min) t USP

HVL

- a₀ Fixed a₁ Fixed
- a₂ Fixed a₃ Fixed
- χ² ε
- Significant digits Maximum iterations
- a₁ u_t (1e-9 m.m/V/s)

Opening Data



The screenshot displays the CEval 0.3rc1 software interface. At the top, the menu bar includes File, Options, and Help. The File menu is open, with options: Load ChemStation file, Load comma-separated file, Load data table, Save data table, and Exit. A red circle highlights the 'Load comma-separated file' option. The main window shows a chromatogram titled 'DAD1C.ch' with 'Absorb' on the y-axis and 'Time (minute)' on the x-axis. A blue text box overlaid on the chromatogram reads: 'B) ... or you can load *.csv file.' Below the chromatogram, the 'Evaluation' section is active, showing 'Hyperbole fit' as the selected method. The file path is 'Q:/Users/Magda/CEval/CEval data/LIAC_SEQ_DM_CD/D_MET_3_2.D/DAD1C.ch'. The interface is divided into three main panels: 'Common parameters' on the left, 'Evaluated peaks' in the center, and 'Parameters' on the right. The 'Parameters' panel is further divided into 'EOF', 'Peak', and 'HVL' sections, each with various input fields and checkboxes. A 'Find peak(s)' button is located at the bottom right of the interface.

File: Q:/Users/Magda/CEval/CEval data/LIAC_SEQ_DM_CD/D_MET_3_2.D/DAD1C.ch

Common parameters:

- Capillary (cm): 0
- Detector (cm): 0
- Voltage (kV): 0
- Field strength (kV/m): 0
- c(Selector): 0
- Time of EOF (min): 0
- Read EOF time

Evaluated peaks:

Analyte	Time	Area
---------	------	------

Parameters:

EOF

- v (1e-3 m/s): 0
- vI (1e-3 m/s): 0
- u (1e-9 m.m/V/s): 0

Peak

- Peak from X: 0
- Peak from Y: 0
- Peak max at X: 0
- Peak to X: 0
- Peak to Y: 0
- Peak height: 0
- v (1e-3 m/s): 0
- vI (1e-3 m/s): 0
- uI (1e-9 m.m/V/s): 0
- H!: 0
- Area (Units.min): 0
- t USP: 0

HVL

- a0: 0
- a1: 0
- a2: 0
- a3: 0
- χ²: 0
- ε: 1e-09
- Significant digits: 50
- Maximum iterations: 10
- a1 uI (1e-9 m.m/V/s): 0

Buttons: Add peak, Delete peak, Cancel selection, Replot HVL, Do HVL fit, Find peak(s)

Opening Data



The screenshot shows the CEval 0.3rc1 software interface. At the top, the window title is "CEval 0.3rc1" and the menu bar includes "File", "Options", and "Help". The main window displays a chromatogram titled "DAD1C.ch" with "Absorbance (mAU)" on the y-axis (0 to 8) and time on the x-axis (0 to 14). Two peaks are visible. Below the plot is an "Evaluation" section with a "Hyperbole fit" button and a "File:" field showing the path "Q:/Users/Magda/CEval/CEval data/LIAC_SEQ_DM_CD/D...".

A file selection dialog box is open in the foreground, titled "Pick a comma-separated values file". The path is "Data (Q:) > Users > Magda > CEval > CEval data". The file list shows folders for "LIAC_SEQ_DM_CD", "LIAC_SEQ_DUAL", "LIAC_SEQ_MET", and "LIAC_SEQ_OS_CD", and a file named "D_MET_X_3" which is selected. The dialog has "Otevřít" (Open) and "Storno" (Cancel) buttons. A callout box with a black border and white background points to the selected file, containing the text "Choose the *.csv file ...".

At the bottom of the software interface, there are buttons for "Add peak", "Delete peak", "Cancel selection", and "Find peak(s)". On the right side, there are various input fields and buttons like "Replot HVL" and "Do HVL fit".

Opening Data



The screenshot displays the CEval 0.3rc1 software interface. At the top, a menu bar includes 'File', 'Options', and 'Help'. The main window title is 'DAD1C.ch'. Below the title is a chromatogram plot with 'Absorbance (mAU)' on the y-axis (0 to 8) and 'Time (minute)' on the x-axis (0 to 8). Two peaks are visible: a smaller one at approximately 5.5 minutes and a larger one at approximately 9.5 minutes.

Below the plot is an 'Evaluation' section with a 'Hyperbole fit' tab. It shows the file path: 'Q:/Users/Magda/CEval/CEval data/LIAC_SEQ_DM_CD/D_MET_3_2_D/DAD1C.ch'. On the left, 'Common parameters' are listed with input fields: Capillary (cm), Detector (cm), Voltage (kV), Field strength (kV/m), c(Selector), and Time of EOF (min). A 'Read EOF time' button is at the bottom of this section. In the center, an 'Evaluated peaks' table has columns for 'Analyte' and 'Time'. Below the table are 'Add peak', 'Delete peak', and 'Cancel selection' buttons.

On the right, there are various numerical input fields for peak parameters, including 'v (1e-3 m/s)', 'Ht', 'Area (Units.min)', 't USP', and 'Peak max at X'. There are also 'Replot HVL' and 'Do HVL fit' buttons.

A 'Dialog' box is overlaid in the center, containing the following settings:

- Delimiter: ,
- Decimal separator: Period (.)
- First line is a header:
- X axis unit: s
- Y axis unit: mAU

'Load' and 'Cancel' buttons are at the bottom of the dialog.

A callout box with a black border and white background points to the dialog box, containing the text: **... then fill in the information about delimiter (comma or semicolon), decimal separator and optional information about axis description.**

Opening Data



CEval 0.3rc1

File Options Help

D_MET_X_3.csv

Electrophoreogram is loaded.

70
60
50
40
30
20
10
0

0 2 4 6 8 10 12

(s)

Evaluation **Hyperbole fit**

File: Q:/Users/Magda/CEval/CEval data/D_MET_X_3.csv Close file

Common parameters

Capillary (cm)

Detector (cm)

Voltage (kV)

Field strength (kV/m)

c(Selector)

Time of EOF (min) Read EOF time

Evaluated peaks

Analyte	Time	Area
---------	------	------

Add peak Delete peak

Cancel selection

Parameters Results

EOF

v (1e-3 m/s) v! (1e-3 m/s) u (1e-9 m.m/V/s)

Peak

Peak from X Peak from Y Peak max at X

Peak to X Peak to Y Peak height

v (1e-3 m/s) v! (1e-3 m/s) u! (1e-9 m.m/V/s)

H! Area (Units.min) t USP

HVL

a0 Fixed a1 Fixed

a2 Fixed a3 Fixed

χ^2 ϵ

Significant digits Maximum iterations

a1 u! (1e-9 m.m/V/s) Replot HVL Do HVL fit

Find peak(s)



Peak Evaluation

Peak Evaluation



CEval 0.3rc1

File Options Help

DAD1C.ch

Y-axis: Absorbance (mAU) (0 to 8)
X-axis: Time (minute) (0 to 14)

Evaluation Hyperbole fit

File: Q:/Users/Magda/CEval/CEval data/LIAC_SEQ_DM_CD/D_MET_3_2.0/DAD1C.ch Close file

Common parameters

- Capillary (cm)
- Detector (cm)
- Voltage (kV)
- Field strength (kV/m)
- c(Selector)
- Time of EOF (min)

Read E

Analyte	Time	Area
---------	------	------

Delete peak

Cancel selection

Parameters Results

EOF

v (1e-3 m/s) vI (1e-3 m/s) u (1e-9 m.m/V/s)

Peak

Peak from X Peak from Y Peak max at X

Peak to X Peak to Y Peak height

v (1e-3 m/s) vI (1e-3 m/s) uI (1e-9 m.m/V/s)

HI Area (Units.min) t USP

HVL

a0 Fixed a1 Fixed

a2 Fixed a3 Fixed

χ^2 ϵ

Significant digits Maximum iterations

a1 uI (1e-9 m.m/V/s)

Replot HVL Do HVL fit

Fill in the **Common Parameters** (software keeps the values until you change them).

Peak Evaluation



CEval 0.3rc1

File Options Help

DAD1C.ch

Absorbance (mAU)

Time (minute)

Evaluation Hyperbole fit

File: Q:/Users/Magda/CEval/CEval data/LIAC_SEQ_DM_CD/D_MET_3_2.D/DAD1C.ch Close file

Common parameters

- Capillary (cm) 50,2
- Detector (cm) 41,7
- Voltage (kV) 15
- Field strength (kV/m) 29,88
- c(Selector) 0
- Time of EOF (min) 0

Read EOF time

Evaluated peaks

Analyte	Time	Area
---------	------	------

Add peak Delete peak Cancel selection

Parameters Results

EOF

v (1e-3 m/s) 0 vt (1e-3 m/s) 0 u (1e-9 m.m/V/s) 0

0 Peak from Y 0 Peak max at X 0

0 Peak to Y 0 Peak height 0

0 vt (1e-3 m/s) 0 ut (1e-9 m.m/V/s) 0

0 Area (Units.min) 0 t USP 0

0 Fixed a1 0 Fixed

0 Fixed a3 0 Fixed

1e-09

Significant digits 50

a1 ut (1e-9 m.m/V/s) 0

Plot HVL Do HVL fit

Find peak(s)

Click the Find peak(s) button.
CEval should find peaks automatically
(If not, see [APPENDIX B: Peak not found](#)).

Peak Evaluation



The screenshot displays the CEval 0.3rc1 software interface. At the top, a chromatogram titled "DAD1C.ch" shows Absorbance (mAU) on the y-axis (0 to 8) and Time (minute) on the x-axis (0 to 10). Three peaks are visible: a small peak at approximately 5.76 minutes, a medium peak at 8.93917 minutes, and a large, sharp peak at 9.25082 minutes. The large peak is highlighted in red.

Below the chromatogram, the "Evaluation" tab is active, showing "Hyperbole fit" as the selected method. A "Dialog" window titled "Select peak:" is open, displaying a table of detected peaks. The third peak is selected, and the "Select" button is highlighted.

Number	Time of maximum
1	5,76
2	8,93917
3	9,25082
4	9,43333

Annotations include:

- A red arrow pointing from the text box "CEval will offer you all the peaks that are available." to the list of peaks in the dialog box.
- A black callout box pointing to the selected peak in the dialog box with the text: "Choose the peak that you want to evaluate (EOF marker in our case). You can see the chosen peak turns red."
- A black callout box pointing to the "Select" button with the text: "Confirm."

Other interface elements include a "Common parameters" section with fields for Capillary (cm), Detector (cm), Voltage (kV), Field strength (kV/m), c(Selector), and Time of EOF (min). A "Results" section contains various fit parameters like a1, a2, x2, Significant digits, and Maximum iterations, along with "Replot HVL" and "Do HVL fit" buttons. A "Find peak(s)" button is located at the bottom right.

Peak Evaluation



CEval 0.3rc1

File Options Help

DAD1C.ch

You received Peak Results in the Results tab.

Time (minute)

Evaluation Hyperbole fit

File: Q:/Users/Magda/CEval data/LIAC_SEQ_DM_CD/D_MET_3_2.D/DAD1C.ch Close file

Common parameters

Capillary (cm) 50,2
Detector (cm) 41,7
Voltage (kV) 15
Field strength (kV/m) 29,88
c(Selector) 0
Time of EOF (min) 0
Read EOF time

Evaluated peaks

Analyte	Time	Area
---------	------	------

Add peak Delete peak Cancel selection

Parameters Results

EOF
v (1e-3 m/s) inf vt (1e-3 m/s) 0 u (1e-9 m.m/V/s) inf

Peak

Peak from X	8,9142	Peak from Y	0,29489	Peak max at X	9,1512
Peak to X	9,6175	Peak to Y	0,29213	Peak height	8,9868
v (1e-3 m/s)	0,75946	vt (1e-3 m/s)	inf	u! (1e-9 m.m/V/s)	6,0725e-293
Ht	8,6929	Area (Units.min)	1,143	t USP	1,1134

HVL

a0	1,143	<input type="checkbox"/> Fixed	a1	9,1772	<input type="checkbox"/> Fixed
a2	0,051344	<input type="checkbox"/> Fixed	a3	1,2657	<input type="checkbox"/> Fixed
χ^2	0		ϵ	1e-09	
Significant digits	50		Maximum iterations	10	
a1 u! (1e-9 m.m/V/s)	inf				

Replot HVL Do HVL fit

Find peak(s)

Peak Evaluation



The screenshot displays the CEval 0.3rc1 software interface. At the top, a chromatogram titled "DAD1C.ch" shows Absorbance (mAU) on the y-axis (0 to 8) and Time (minute) on the x-axis (0 to 14). Two peaks are visible: a smaller one at approximately 5.5 minutes and a larger one at approximately 9.2 minutes. The larger peak is highlighted with a blue fit curve and a vertical red line indicating its retention time.

Below the chromatogram is the "Evaluation" section, which includes a "Hyperbole fit" tab. The "Common parameters" section on the left contains several input fields: Capillary (cm) 50,2, Detector (cm) 41,7, Voltage (kV) 15, Field strength (kV/m) 29,88, c(Sector) 0, and Time of EOF (min) 0. The "Time of EOF (min)" field is circled in red, and a "Read EOF time" button is located below it.

The "Evaluated peaks" section in the center features a table with columns for Analyte, Time, and Area. Below the table are buttons for "Add peak", "Delete peak", and "Cancel selection".

On the right side, the "Parameters" and "Results" tabs are visible. The "Parameters" tab shows various input fields for peak evaluation, including "Peak from Y", "Peak to Y", "Area (Units.min)", and "t USP". The "Results" tab displays the calculated values for the selected peak, such as "Peak max at X" (9,1512) and "Peak height" (8,9868).

A callout box with a black border and white background is overlaid on the interface, containing the following text:

Enter the EOF marker peak time.
You have 2 options:

- 1. If you selected EOF marker peak, click the Read EOF time button.**
- 2. Enter EOF time manually.**

Peak Evaluation



CEval 0.3rc1

File Options Help

DAD1C.ch

EOF time entered.

Evaluation Hyperbole fit

File: Q:/Users/Magda/CEval/CEval data/LIAC_SEQ_DM_CD/D_MET_3_2.D/DAD1C.ch

Close file

EOF mobility calculated

Common parameters

- Capillary (cm): 50,2
- Detector (cm): 41,7
- Voltage (kV): 15
- Field strength (kV/m): 29,88
- c(Selector): 0
- Time of EOF (min): 9,1512

Read EOF time

Evaluated peaks

Analyte	Time	Area
---------	------	------

Add peak Delete peak Cancel selection

Parameters Results

EOF

- v (1e-3 m/s): 0,75946
- vI (1e-3 m/s): 0
- u (1e-9 m.m/V/s): 25,417

Peak

- Peak from X: 8,9142
- Peak from Y: 0,29489
- Peak max at X: 9,1512
- Peak to X: 9,6175
- Peak to Y: 0,29213
- Peak height: 8,9868
- vI (1e-3 m/s): 1,7788e-17
- uI (1e-9 m.m/V/s): 5,9529e-16
- Area (Units.min): 1,143
- t USP: 1,1134

1,143 Fixed a1: 9,1772 Fixed

1,143 Fixed a3: 1,2657 Fixed

ε: 1e-09

Significant digits: 50 Iterations: 10

a1 uI (1e-9 m.m/V/s): -0,071925

Replot HVL Do HVL fit

Click the Find peak(s) button again.

Find peak(s)

Peak Evaluation



The screenshot displays the CEval 0.3rc1 software interface. At the top, a chromatogram titled "DAD1C.ch" shows Absorbance (mAU) on the y-axis (0 to 8) and Time (minute) on the x-axis (0 to 14). Two peaks are visible: a smaller red peak at approximately 5.6 minutes and a larger blue peak at approximately 9.15 minutes.

Below the chromatogram, the "Evaluation" panel is active, showing "Hyperbole fit" as the selected method. A "Dialog" window titled "Select peak:" is overlaid on the interface. This dialog contains a table with the following data:

Number	Time of maximum
1	5,6
2	8,93917
3	9,15083
4	9,43333

The "Number" column in the table is highlighted in blue, and the "Select" button at the bottom of the dialog is also highlighted in blue. A callout box with a black border and white background contains the text "Select the next peak." with an arrow pointing to the "Select" button.

The background interface includes a "Common parameters" section with fields for Capillary (cm), Detector (cm), Voltage (kV), Field strength (kV/m), c(Selector), and Time of EOF (min). The "Time of EOF (min)" field is set to 9,1512. There are also buttons for "Read EOF time", "Add peak", "Delete peak", and "Cancel selection".

Peak Evaluation



CEval 0.3rc1

File Options Help

DAD1C.ch

You received Peak Results in the Results tab.

Absorbance (mAU)

Time (minute)

Evaluation **Hyperbole fit**

File: Q:/Users/Magda/CEval/CEval data/LIAC_SEQ_DM_CD/D_MET_3_2.D/DAD1C.ch Close file

Common parameters

Capillary (cm) 50,2
Detector (cm) 41,7
Voltage (kV) 15
Field strength (kV/m) 29,88
c(Selector) 0
Time of EOF (min) 9,1512 Read EOF time

Evaluated peaks

Analyte	Time	Area
---------	------	------

Add peak Delete peak
Cancel selection

Parameters **Results**

EOF
v (1e-3 m/s) 0,75946 v_f (1e-3 m/s) 0 u (1e-9 m.m/V/s) 25,417

Peak

Peak from X 5,5375 Peak from Y 0,27459 Peak max at X 5,76
Peak to X 5,97 Peak to Y 0,31186 Peak height 4,4444
v (1e-3 m/s) 1,2066 v_f (1e-3 m/s) 0,44714 u_f (1e-9 m.m/V/s) 14,964
H_f 4,1506 Area (Units.min) 0,33976 t USP 1,0625

HVL

a0 0,33976 Fixed a1 5,7698 Fixed
a2 0,032209 Fixed a3 0,76905 Fixed
χ² 0 ε 1e-09
Significant digits 50 Maximum iterations 10
a1 u_f (1e-9 m.m/V/s) 14,895 Replot HVL Do HVL fit

Find peak(s)

Peak Evaluation



You received Peak Results in the Results tab.

Parameters Results

EOF

v (1e-3 m/s) 0,75946 v! (1e-3 m/s) 0 u (1e-9 m.m/V/s) 25,417

Peak

Peak from X	5,5375	Peak from Y	0,27459	Peak max at X	5,76
Peak to X	5,97	Peak to Y	0,31186	Peak height	4,4444
v (1e-3 m/s)	1,2066	v! (1e-3 m/s)	0,44714	u! (1e-9 m.m/V/s)	14,964
H!	4,1506	Area (Units.min)	0,33976	t USP	1,0625

HVL

a0	0,33976	<input type="checkbox"/> Fixed	a1	5,7698	<input type="checkbox"/> Fixed
a2	0,032209	<input type="checkbox"/> Fixed	a3		
χ^2	0		ϵ		
Significant digits	50		Maximum iterations		

a1 u! (1e-9 m.m/V/s) 14,895

Replot HVL Do HVL fit

EOF time

peak mobility calculated from peak maximum

HVL estimated migration time

peak mobility calculated from HVL estimation

Peak Evaluation

You received Peak Results in the Results tab.

Parameters Results

a0 0,33976 Fixed a1 5,7698 Fixed
a2 0,032209 Fixed a3 0,76905 Fixed
 χ^2 0 ϵ 1e-09
Significant digits 50 Maximum iterations 10
a1 u! (1e-9 m.m/V/s) 14,89 **Description of peak assymetry** Replot HVL Do HVL fit

Peak dimensions

	Left	Right	Full
Width 1/2 (min)	0,0375	0,038333	0,075833
Sigma (min)	0,03185	0,032557	0,032203
Width 1/2 (m)	4,5247e-05	0,038333	9,15e-05
Sigma (m)	3,843e-05	3,9284e-05	3,8857e-05
N	32 707	31 300	31 992
HETP	1,275e-05	1,3323e-05	1,3035e-05

number of theoretical plates and its height equivalent

Peak Evaluation



DAD1C.ch

Absorbance (mAU)

Time (minute)

HVL fit.

File: Q:/Users/Magda/CEval/CEval data/LIAC_SEQ_DM_CD/D_MET_3_2/D/DAD1C.ch

Common parameters

Capillary (cm)	50,2
Detector (cm)	41,7
Voltage (kV)	15
Field strength (kV/m)	29,88
c(Selector)	0
Time of EOF (min)	9,1512

Read EOF time

Parameters received in the HVL section are those from HVL estimation. You can use HVL fit to improve the results.

0,75946	v1 (1e-3 m/s)		
5,5375	Peak from Y	0,2745	
5,97	Peak to Y	0,31186	Peak height
			,4444
v (1e-3 m/s)	1,2066	v1 (1e-3 m/s)	0,44714
		u1 (1e-9 m.m/V/s)	4,964
HI	4,1506	Area (Units.min)	0,33976
		t USP	,0625

HVL

a0	0,33976	<input type="checkbox"/> Fixed	a1	5,7698	Fixed
a2	0,032209	<input type="checkbox"/> Fixed	a3	0,76905	Fixed
χ^2	0		ϵ	1e-09	
Significant digits	50		Maximum iterations	10	
a1 u1 (1e-9 m.m/V/s)	14,895				

Replot HVL

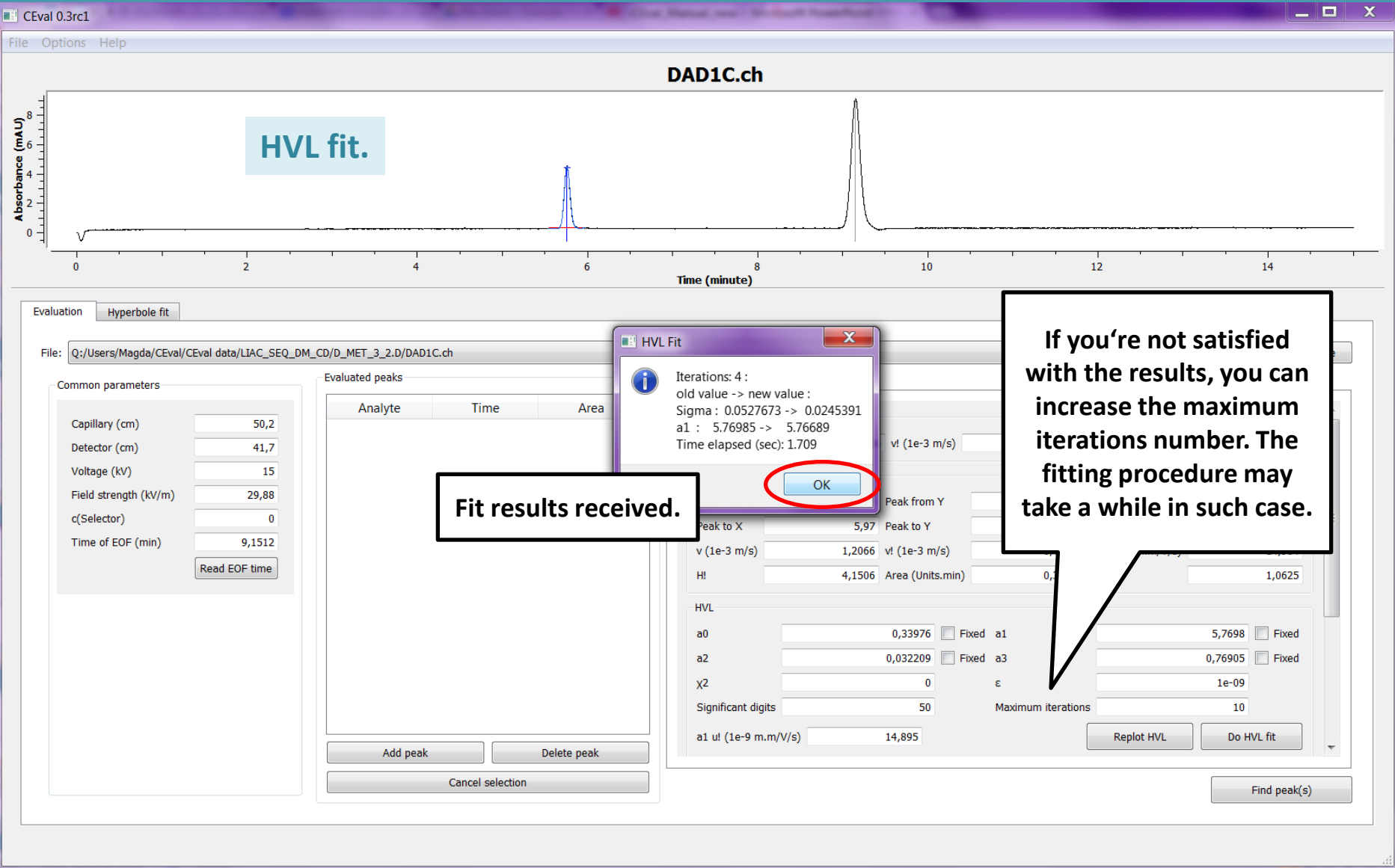
Do HVL fit

Find peak(s)

Peak Evaluation



HVL fit.



Fit results received.

If you're not satisfied with the results, you can increase the maximum iterations number. The fitting procedure may take a while in such case.

HVL Fit
Iterations: 4 :
old value -> new value :
Sigma : 0.0527673 -> 0.0245391
a1 : 5.76985 -> 5.76689
Time elapsed (sec): 1.709

OK

Analyte	Time	Area

Add peak Delete peak

Cancel selection

Common parameters

Capillary (cm)

Detector (cm)

Voltage (kV)

Field strength (kV/m)

c(Selector)

Time of EOF (min)

Read EOF time

Peak to X Peak to Y

v (1e-3 m/s) vt (1e-3 m/s)

Hl Area (Units.min)

HVL

a0 Fixed a1 Fixed

a2 Fixed a3 Fixed

χ² ε

Significant digits Maximum iterations

a1 u! (1e-9 m.m/V/s)

Replot HVL Do HVL fit

Find peak(s)

Peak Evaluation



CEval 0.3rc1

File Options Help

DAD1C.ch

Absorbance (mAU)

Time (minute)

HVL fit.

For a closer look at the peak and the fitting function, see [APPENDIX A: Graph interface.](#)

Evaluation Hyperbole fit

File: Q:/Users/Magda/CEval/CEval data/LIAC_SEQ_DM_CD/D_MET_3_2.D/DAD1C.ch Close file

Common parameters

Capillary (cm)	50,2
Detector (cm)	41,7
Voltage (kV)	15
Field strength (kV/m)	29,88
c(Selector)	0
Time of EOF (min)	9,1512

Read EOF time

Evaluated peaks

Analyte	Parameters	Results			
	v (1e-3 m/s)	0,75946			
	v _t (1e-3 m/s)	0			
	u (1e-9 m.m/V/s)	25,417			
X	5,5375	Peak from Y	0,27459	Peak max at X	5,76
	5,97	Peak to Y	0,31186	Peak height	4,4444
v (1e-3 m/s)	1,2066	v _t (1e-3 m/s)	0,44714	u _t (1e-9 m.m/V/s)	14,964
H _t	4,1506	Area (Units.min)	0,33976	t USP	1,0625

If the fit converged, you receive results from the HVL fit.

HVL

a0	0,33736	<input type="checkbox"/> Fixed	a1	5,7669	<input type="checkbox"/> Fixed
a2	0,031417	<input type="checkbox"/> Fixed	a3	0,60722	<input type="checkbox"/> Fixed
χ ²	0		ε	1e-09	
Significant digits	50		Maximum iterations	10	
a1 u _t (1e-9 m.m/V/s)	14,916				

Replot HVL Do HVL fit

Find peak(s)

Add peak Delete peak Cancel selection



ACE Data Evaluation

ACE Data Evaluation



CEval 0.3rc1

File Options Help

DAD1C.ch

Registering data to the hyperbole fit.

Y-axis: Absorbance (mAU) (0 to 8)
X-axis: Time (minute) (0 to 14)

File: Q:/Users/Magda/CEval/CEval d

Common parameters

Capillary (cm)	
Detector (cm)	
Voltage (kV)	15
Field strength (kV/m)	29,88
c(Selector)	3
Time of EOF (min)	9,1512

Read EOF time

Parameters Results

EOF

y (1e-3 m/s)	0,75946	vt (1e-3 m/s)	0	u (1e-9 m.m/V/s)	25,417
--------------	---------	---------------	---	------------------	--------

from X	5,5375	Peak from Y	0,27459	Peak max at X	5,76
to X	5,97	Peak to Y	0,31186	Peak height	4,4444
from Y	1,2066	vt (1e-3 m/s)	0,44714	u! (1e-9 m.m/V/s)	14,964
to Y	4,1506	Area (Units.min)	0,33976	t USP	1,0625

HVL

a0	0,33736	<input type="checkbox"/> Fixed	a1	5,7669	<input type="checkbox"/> Fixed
a2	0,031417	<input type="checkbox"/> Fixed	a3	0,60722	<input type="checkbox"/> Fixed
χ ²	0		ε	1e-09	
Significant digits	50		Maximum iterations	10	
a1 u! (1e-9 m.m/V/s)	14,916				

Buttons: Add peak, Delete peak, Cancel selection, Replot HVL, Do HVL fit, Find peak(s)

Enter the selector concentration ...

... then click the Add peak button

ACE Data Evaluation



The screenshot displays the CEval 0.3rc1 software interface. At the top, a chromatogram titled "DAD1C.ch" shows Absorbance (mAU) on the y-axis (0 to 8) and Time (minute) on the x-axis (0 to 14). Two peaks are visible: a smaller one at approximately 5.5 minutes and a larger one at approximately 14.9 minutes.

Below the chromatogram is the "Evaluation" section, which includes a "Hyperbole fit" tab. The "Common parameters" section contains the following values:

- Capillary (cm): 50,2
- Detector (cm): 41,7
- Voltage (kV): 15
- Field strength (kV/m): 29,88
- c(Selector): 3
- Time of EOF (min): 9,1512

The "Evaluated peaks" table is partially visible, showing columns for Analyte, Time, and other parameters. A dialog box titled "Add peak" is overlaid on the interface, with the following details:

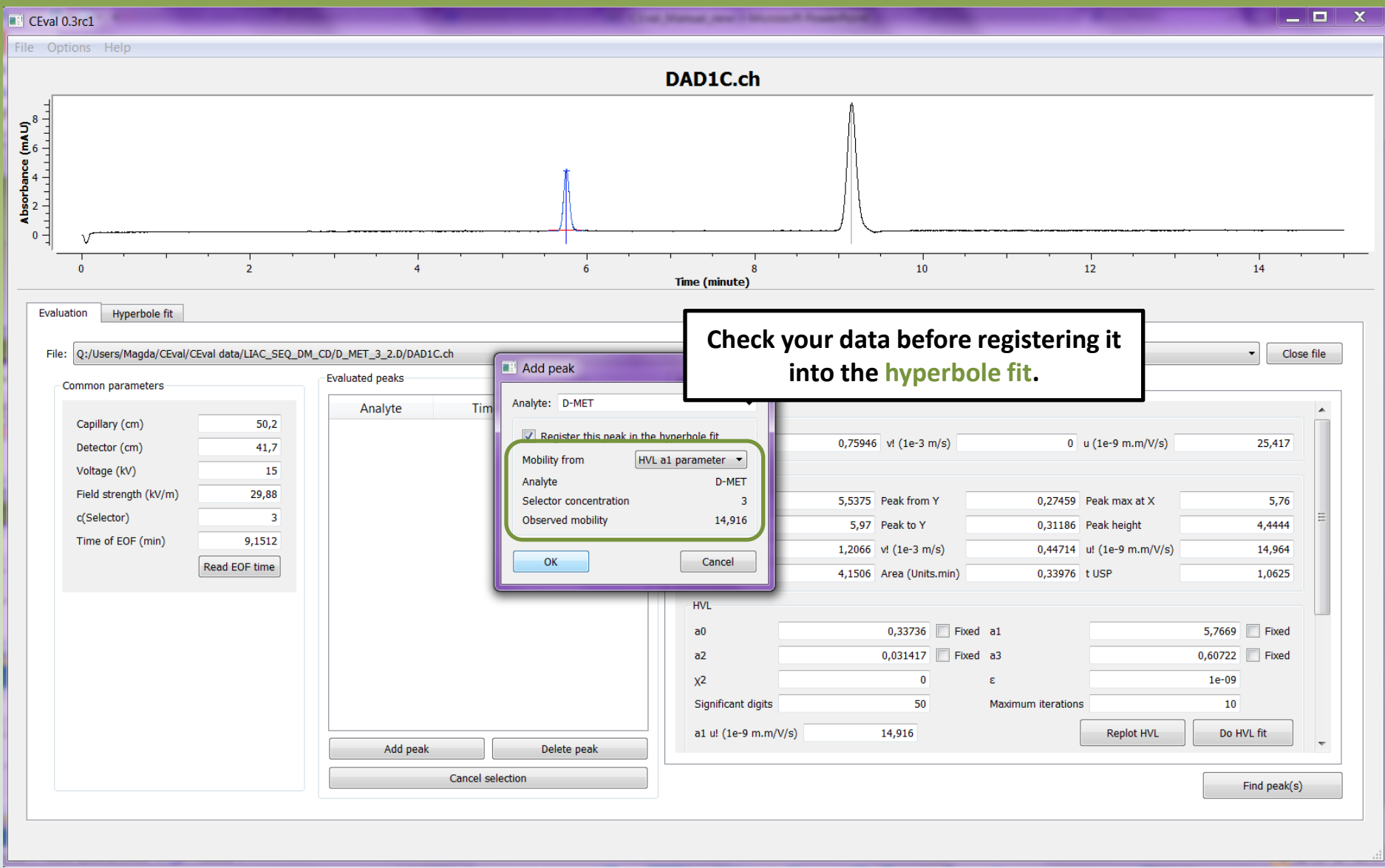
- Analyte: D-MET
- Register this peak in the hyperbole fit

Two callout boxes provide instructions:

- One points to the "Analyte" dropdown in the dialog box with the text: "Enter the analyte description".
- Another points to the "Register this peak in the hyperbole fit" checkbox with the text: "Check if you want to use the data for ACE evaluation."

At the bottom of the interface, there are buttons for "Add peak", "Delete peak", "Cancel selection", "Replot HVL", "Do HVL fit", and "Find peak(s)".

ACE Data Evaluation



ACE Data Evaluation



Peak added.

Switch to the Hyperbole fit if you want to check the data table

The screenshot displays the CEval 0.3rc1 software interface. At the top, the window title is "CEval 0.3rc1" and the menu bar includes "File", "Options", and "Help". The main plot area, titled "DAD1C.ch", shows a chromatogram with Absorbance (mAU) on the y-axis (0 to 8) and time on the x-axis (0 to 14). A peak is visible at approximately 5.76 minutes, highlighted with a blue fit line. A green box with the text "Peak added." is overlaid on the plot. Below the plot, the "Evaluation" section is active, with the "Hyperbole fit" button circled in red. A callout box with a black border and white background contains the text "Switch to the Hyperbole fit if you want to check the data table". The "Common parameters" section on the left includes fields for Capillary (cm), Detector (cm), Voltage (kV), Field strength (kV/m), c(Selector), and Time of EOF (min), along with a "Read EOF time" button. The "Evaluated peaks" table is circled in green and contains the following data:

Analyte	Time	Area
D-MET	5,76	0,339758

Below the table are buttons for "Add peak", "Delete peak", and "Cancel selection". The "Parameters" and "Results" tabs are visible. The "Parameters" tab shows EOF parameters (v, v!, u), Peak parameters (Peak from X, Peak to X, Peak from Y, Peak to Y, Peak height, v, v!, u!, H!, Area, t USP), and HVL parameters (a0, a1, a2, a3, x2, c, Significant digits, Maximum iterations, a1 u!). The "Results" tab shows the "Find peak(s)" button.

ACE Data Evaluation



The screenshot displays the CEval 0.3rc1 software interface. At the top, a menu bar includes 'File', 'Options', and 'Help'. Below this is a large graph area with a vertical axis labeled 'Mobility' (ranging from 0 to 8) and a horizontal axis labeled 'Selector concentration' (ranging from 0 to 14). The graph is currently empty.

Below the graph, there are two tabs: 'Evaluation' and 'Hyperbole fit'. The 'Evaluation' tab is active and contains a list of analytes, with 'D-MET' highlighted and circled in green. A text box with a black border and white background is overlaid on the list, containing the text 'The data you registered.'

To the right of the analyte list is a control panel with the following sections:

- Fit mode:** A dropdown menu set to 'Single fit'.
- Single fit (for first analyte):** Includes an 'Analyte:' field and three rows of input fields for μ (A), μ (AS), and K (AS), each with a value of 0 and a 'Fixed' checkbox.
- Double fit (for second analyte):** Includes an 'Analyte:' field and three rows of input fields for μ (A), μ (AS), and K (AS), each with a value of 0 and an 'As first analyte' checkbox.
- Swap analytes:** A checkbox that is currently unchecked.
- Filter parameters:** Includes input fields for 'Viscosity slope' (0), 'Maximum iterations' (50), ' ϵ ' (1e-09), and 'S' (0). A 'Total iterations:' field shows 0.
- Buttons:** 'Estimate', 'Fit', and 'Redraw' buttons.
- Statistics:** A dropdown menu set to 'Free mobility (μ (A))' and buttons for 'Left', 'Right', and 'Both'.
- Units:** A dropdown menu set to 'Tau (τ)'.
- Chart horiz. marker:** An input field with 0, a 'Show' checkbox, and buttons for 'Left itsc.' and 'Right itsc.'

ACE Data Evaluation



The screenshot displays the CEval 0.3rc1 software interface. At the top, there is a menu bar with 'File', 'Options', and 'Help'. Below the menu is a graph with 'Mobility' on the y-axis (ranging from 14 to 15.5) and 'Selector concentration' on the x-axis (ranging from 2 to 4). A single data point is plotted at a concentration of 3 and a mobility of approximately 14.916, highlighted with a green circle and a red cross. A black-bordered box with white text points to this data point, stating 'Displayed data point'.

Below the graph is a table with three columns: 'Analyte', 'Concentration', and 'Mobility'. The first row is highlighted with a green border and contains the following data:

Analyte	Concentration	Mobility
D-MET	3	14,916

A black-bordered box with white text is overlaid on the table, stating: 'After clicking on the analyte description, all the entered concentrations and further all the entered monilities for the given concentration will reveal.'

At the bottom of the interface, there are several control buttons: 'Add analyte', 'Remove analyte', 'Add conc.', 'Remove conc.', 'Add mobility', and 'Remove mobility'. To the right of the table is a 'Fit mode' section with a dropdown menu set to 'Single fit'. Below this are two columns of fit parameters for 'Single fit (for first analyte)' and 'Double fit (for second analyte)'. Each column has input fields for μ (A), μ (AS), and K (AS), each with a 'Fixed' checkbox. Below these are 'Filter parameters' including 'Viscosity slope', 'Maximum iterations', ϵ , and S. At the bottom of the fit section are buttons for 'Estimate', 'Fit', and 'Redraw'. A 'Statistics' section includes a dropdown for 'Free mobility (μ (A))' and buttons for 'Left', 'Right', and 'Both'. The 'Units' section has a dropdown set to 'Tau (τ)'. At the very bottom, there is a 'Chart horiz. marker' section with a value of 0 and a 'Show' checkbox, along with 'Left itsc.' and 'Right itsc.' buttons.

ACE Data Evaluation



CEval 0.4f

File Options Help

MET6.evd

After adding all of the ACE data ...

Displayed data points.

Selector concentration	Mobility
0	18
3	15
5	13
10	10
20	8

Effective mobility values

Analyte	Concentration	Effective Mobility
D-MET_DM	0	13,371
D-MET_S	3	13,377
L-MET_DM	5	13,393
L-MET_S	10	13,395

You have a complete data table for ACE evaluation.

concentration values

Fit mode: Single fit

Single fit (for first analyte)

Analyte: D-MET_DM

μ (A) 0 Fixed As first analyte

μ (AS) 0 Fixed As first analyte

K (AS) 0 Fixed As first analyte

Filter parameters

Viscosity slope 0

Maximum iterations 50

S 1e-09

S 0

Tot 0

Redraw

ACE Data Evaluation



The screenshot displays the CEval 0.4f software interface. At the top, a plot titled "MET6.evd" shows "Mobility" on the y-axis (ranging from 8 to 18) and "Selector concentration" on the x-axis (ranging from 0 to 30). Five red '+' markers represent data points at approximately (0, 17.5), (3, 15), (5, 13.5), (10, 10.5), and (20, 8.5). A green box with the text "Single fit." is overlaid on the plot.

Below the plot, the "Evaluation" panel is active, showing a "Hyperbole fit" configuration. On the left, a list of analytes includes "D-MET_DM", "D-MET_S", "L-MET_DM", and "L-MET_S". The "D-MET_DM" entry is circled in green. A callout box with the text "Analyte has to be chosen." points to this entry. In the center, a table lists selector concentrations: 0, 3, 5, 10, 20, and 30. The value "5" is highlighted in blue. A callout box with the text "Initial estimate." points to this value. On the right, a "Fitting" panel is open, showing "Fit mode: Single fit". It contains two sections: "Single fit (for first analyte)" and "Double fit (for second analyte)". Both sections have "Analyte:" dropdowns set to "D-MET_DM" and three parameter rows for μ (A), μ (AS), and K (AS), each with a value of 0 and a "Fixed" checkbox. The "Fitter parameters" section includes fields for "Viscosity slope" (0), "Maximum iterations" (50), " ϵ " (1e-09), "S" (0), and "Total iterations" (0). The "Estimate" button is circled in red.

Selector concentration	Mobility
0	17.5
3	15.0
5	13.5
10	10.5
20	8.5

ACE Data Evaluation



Single fit.

MET6.evd

You can see initial estimate now.

You can enter some viscosity correction factor, or increase maximum iteration number or epsilon (convergence condition).

Fit.

Analyte	Concentration	Mobility
D-MET_DM	0	13,371
D-MET_S	3	13,377
L-MET_DM	5	13,393
L-MET_S	10	13,395

Fit mode: Single fit

Analyte: μ (A) 18,096 Fixed μ (AS) Fixed

μ (AS) 1,3167 Fixed μ (AS) Fixed

K (AS) 0,078081 Fixed K (AS) Fixed

Filter parameters

Viscosity slope: 0

Maximum iterations: 50

ϵ : 1e-09

S: 0,14319

Total iterations: 0

Estimate **Fit** Redraw

ACE Data Evaluation



CEval 0.4f

File Options Help

MET6.evd

Single fit.

Selector concentration	Mobility
0	18,133
3	13,377
5	13,393
10	13,395
20	8,084
30	7,084

Evaluation Hyperbole fit

Analyte	Concentration	Mobility
D-MET_DM	0	13,371
D-MET_S	3	13,377
L-MET_DM	5	13,393
L-MET_S	10	13,395

Fit converged with 4 iterations.

Fit mode: Single fit

Fitting Statistics

Single fit (for first analyte)

Analyte: D-MET_DM

μ (A) 18,133 Fixed

μ (AS) 1,8779 Fixed

K (AS) 0,084076 Fixed

Double fit (for second analyte)

Analyte:

μ (A) 0 As first analyte

μ (AS) 0 As first analyte

K (AS) 0 As first analyte

Filter parameters

Viscosity slope 0

Maximum iterations 50

ϵ 1e-09

S 0,086302

Total iterations: 4

Estimate Fit Redraw

Add analyte Add conc. Add mobility

Remove analyte Remove conc. Remove mobility

ACE Data Evaluation



CEval 0.4f

File Options Help

MET6.evd

Double fit.

Selector concentration	Mobility
0	18,133
3	15,000
5	13,993
10	11,000
20	8,000
30	7,000

Evaluation Hyperbole fit

Analyte	Concentration	Mobility
D-MET_DM	0	13,371
D-MET_S	3	13,377
L-MET_DM	5	13,393
L-MET_S	10	13,395

Fit mode: **Double fit**

Fitting: **Double fit**

Single fit (for first analyte):
Analyte: D-MET_DM
 μ : 18,133 Fixed
 μ (AS): 1,8779 Fixed
K (AS): 0,084076 Fixed

Double fit (for second analyte):
Analyte:
 μ (A): 0 As first analyte
 μ (AS): 0 As first analyte
K (AS): 0 As first analyte

Filter parameters:
Viscosity slope: 0
Maximum iterations: 50
 ϵ : 1e-09
S: 0,086302
Total iterations: 4

Estimate Fit Redraw

Switch to the double fit mode.

Add analyte Add conc. Add mobility
Remove analyte Remove conc. Remove mobility

ACE Data Evaluation



CEval 0.4f

File Options Help

MET6.evd

Selector concentration	Mobility
0	18
3	15
5	14
10	11
20	8
30	7

Both analytes has to be chosen.

Initial estimate.

Fit mode: Double fit

Fitting Statistics

Single fit (for first analyte)		Double fit (for second analyte)	
Analyte:	D-MET_DM	Analyte:	L-MET_DM
μ (A)	18,133 <input type="checkbox"/> Fixed	μ (A)	0 <input type="checkbox"/> As first analyte
μ (AS)	1,8779 <input type="checkbox"/> Fixed	μ (AS)	0 <input type="checkbox"/> As first analyte
K (AS)	0,084076 <input type="checkbox"/> Fixed	K (AS)	0 <input type="checkbox"/> As first analyte

Fitter parameters:

Viscosity slope	0
Maximum iterations	50
ϵ	1e-09
S	0,086302
Total iterations:	4

Estimate Fit Redraw

Add analyte Add conc. Add mobility

Remove analyte Remove conc. Remove mobility

ACE Data Evaluation



CEval 0.4f

File Options Help

MET6.evd

Mobility

Selector concentration

Double fit.

Evaluation Hyperbole fit

D-MET_DM	0
D-MET_S	3
L-MET_DM	5
L-MET_S	10
	20
	30

Add analyte Add conc. Add mobility

Remove analyte Remove conc. Remove mobility

Fit mode: Double fit

Fitting Statistics

Single fit (for first analyte) Double fit (for second analyte)

Analyte: D-MET_DM Analyte: L-MET_DM

μ (A) 18,096 Fixed μ (A) 17,99 As first analyte

μ (AS) 1,3167 Fixed μ (AS) 1,037 As first analyte

K (AS) 0,078081 Fixed K (AS) 0,069172 As first analyte

Fitter parameters

Viscosity slope 0

Maximum iterations 50

ϵ 1e-09

S 0,15056

Total iterations: 0

Estimate Fit Redraw

Now, the free analyte mobilities are different from each other. For example in case of enantiomers, we want to keep them the same. Therefore, check „As first analyte“ option.

ACE Data Evaluation



CEval 0.4f

File Options Help

MET6.evd

Mobility

Selector concentration

Double fit.

Evaluation Hyperbole fit

D-MET_DM	0	
D-MET_S	3	
L-MET_DM	5	
L-MET_S	10	
	20	
	30	

Add analyte Add conc. Add mobility

Remove analyte Remove conc. Remove mobility

Fit mode: Double fit

Fitting Statistics

Single fit (for first analyte)

Analyte: D-MET_DM

μ (A) 18,096 Fixed

μ (AS) 1,037 Fixed

K (AS) 0,078081 Fixed

Double fit (for second analyte)

Analyte: L-MET_DM

μ (A) 18,096 As first analyte

μ (AS) 1,037 As first analyte

K (AS) 0,069172 As first analyte

Filter parameters

Viscosity slope 0

Maximum iterations 50

ϵ 1e-09

S 0,15056

Total iterations: 0

Estimate **Fit** Redraw

CEval automatically change the mobility value to the one of the first analyte. Now you can process fit.

ACE Data Evaluation



CEval 0.4f

File Options Help

MET6.evd

Mobility

Selector concentration

Double fit.

Evaluation Hyperbole fit

D-MET_DM	0
D-MET_S	3
L-MET_DM	5
L-MET_S	10
	20
	30

Fit converged with 4 iterations.

Fit mode: Double fit

Fitting Statistics

Single fit (for first analyte)

Analyte: D-MET_DM

μ (A) 18,086 Fixed

μ (AS) 1,8231 Fixed

K (AS) 0,082865 Fixed

Double fit (for second analyte)

Analyte: L-MET_DM

μ (A) 18,086 As first analyte

μ (AS) 1,8152 As first analyte

K (AS) 0,076766 As first analyte

Fitter parameters

Viscosity slope 0

Maximum iterations 50

ϵ 1e-09

S 0,084425

Total iterations: 4

Estimate Fit Redraw

ACE Data Evaluation



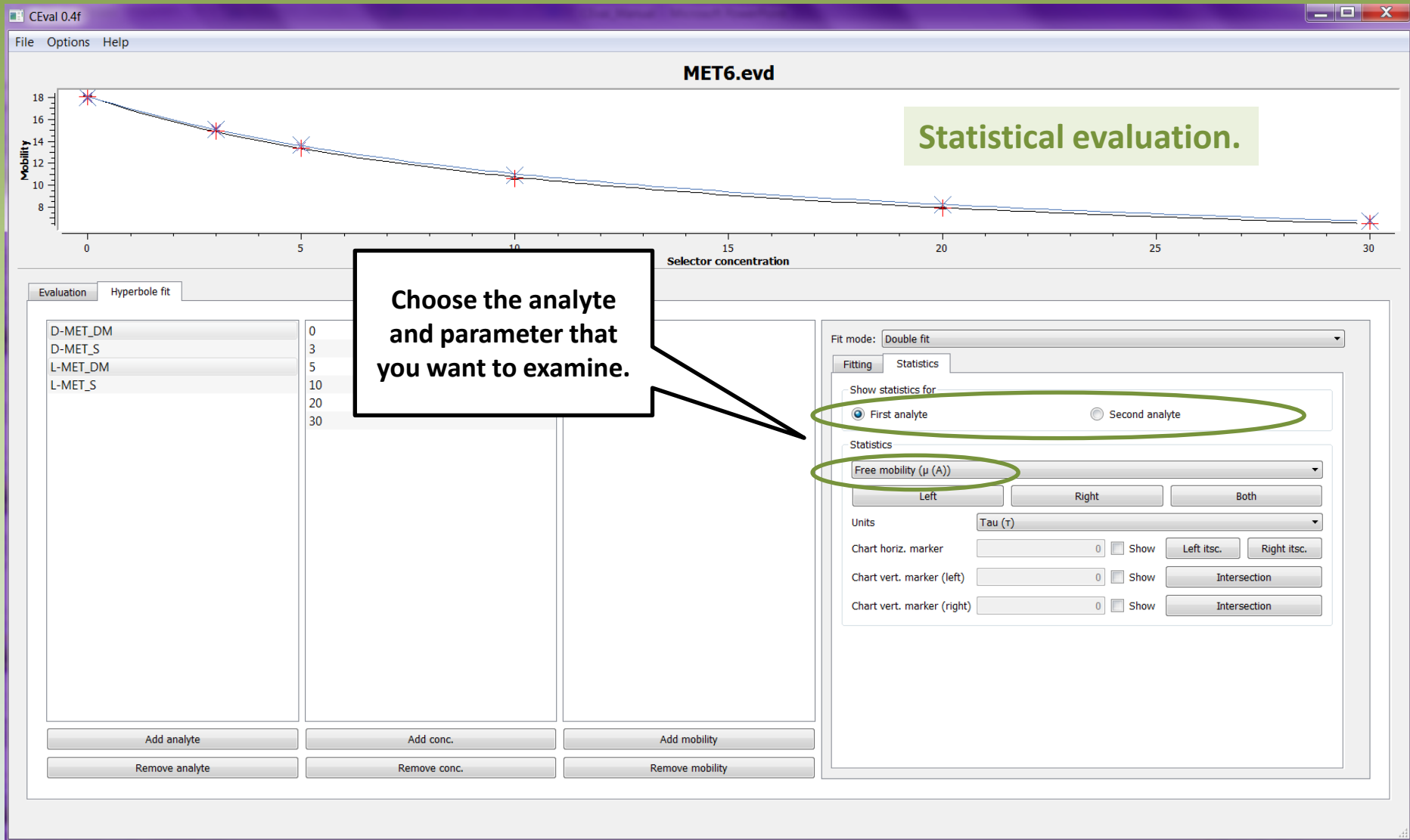
The screenshot displays the CEval 0.4f software interface. At the top, the window title is "CEval 0.4f" and the file name is "MET6.evd". The main graph shows "Mobility" on the y-axis (ranging from 8 to 18) and "Selector concentration" on the x-axis (ranging from 0 to 30). Five data points are plotted with red asterisks, and a blue curve represents the fit. A green box with the text "Statistical evaluation." is overlaid on the graph. Below the graph, there is a list of analytes: D-MET_DM, D-MET_S, L-MET_DM, and L-MET_S. A callout box points to the "Statistics" button in the "Fitting" panel, which is circled in red. The "Fitting" panel shows "Fit mode: Double fit" and "Fitting: Statistics". It contains two columns of parameters for "Single fit (for first analyte)" and "Double fit (for second analyte)". The "Single fit" parameters are: μ (A) = 18,086 (Fixed), μ (AS) = 1,8231 (Fixed), and K (AS) = 0,082865 (Fixed). The "Double fit" parameters are: μ (A) = 18,086 (As first analyte), μ (AS) = 1,8152 (As first analyte), and K (AS) = 0,076766 (As first analyte). Below these are "Filter parameters": Viscosity slope = 0, Maximum iterations = 50, ϵ = 1e-09, S = 0,084425, and Total iterations = 4. At the bottom of the panel are buttons for "Estimate", "Fit", and "Redraw".

Statistical evaluation.

Now that you received the regression parameters, you may want to see the confidence intervals for them, or to test some hypothesis.

Parameter	Value	Fixed	As first analyte
μ (A)	18,086	<input type="checkbox"/>	<input type="checkbox"/>
μ (AS)	1,8231	<input type="checkbox"/>	<input type="checkbox"/>
K (AS)	0,082865	<input type="checkbox"/>	<input type="checkbox"/>
μ (A)	18,086	<input checked="" type="checkbox"/>	<input checked="" type="checkbox"/>
μ (AS)	1,8152	<input type="checkbox"/>	<input type="checkbox"/>
K (AS)	0,076766	<input type="checkbox"/>	<input type="checkbox"/>

ACE Data Evaluation



ACE Data Evaluation



CEval 0.4f

File Options Help

MET6.evd

Statistical evaluation.

Selector concentration	Mobility
0	18
3	15
5	14
10	11
20	8
30	7

Evaluation Hyperbole fit

D-MET_DM
D-MET_S
L-MET_DM
L-MET_S

0
3
5
10
20
30

**Now choose what you want to see:
a) profile diagrams (tau statistics),
b) confidence intervals,
c) p-value chart**

Fit mode: Double fit

Fitting Statistics

Show statistics for
 First analyte Second analyte

Statistics
Free mobility (μ (A))

Left Right Both

Units
Tau (τ)
Tau (τ)
Confidence
P-value

Chart horiz. marker

Chart vert. marker (left) 0 Show Intersection

Chart vert. marker (right) 0 Show Intersection

Add analyte Add conc. Add mobility
Remove analyte Remove conc. Remove mobility

ACE Data Evaluation



CEval 0.4f

File Options Help

MET6.evd

Statistical evaluation.

Selector concentration	Mobility
0	18
3	15
5	14
10	11
20	8
30	7

Evaluation Hyperbole fit

D-MET_DM 0
D-MET_S 3
L-MET_DM 5
L-MET_S 10
20
30

Click according to what you want to see: left- or right-sided interval, or two-sided interval

Fit mode: Double fit

Fitting Statistics

Show statistics for
 First analyte Second analyte

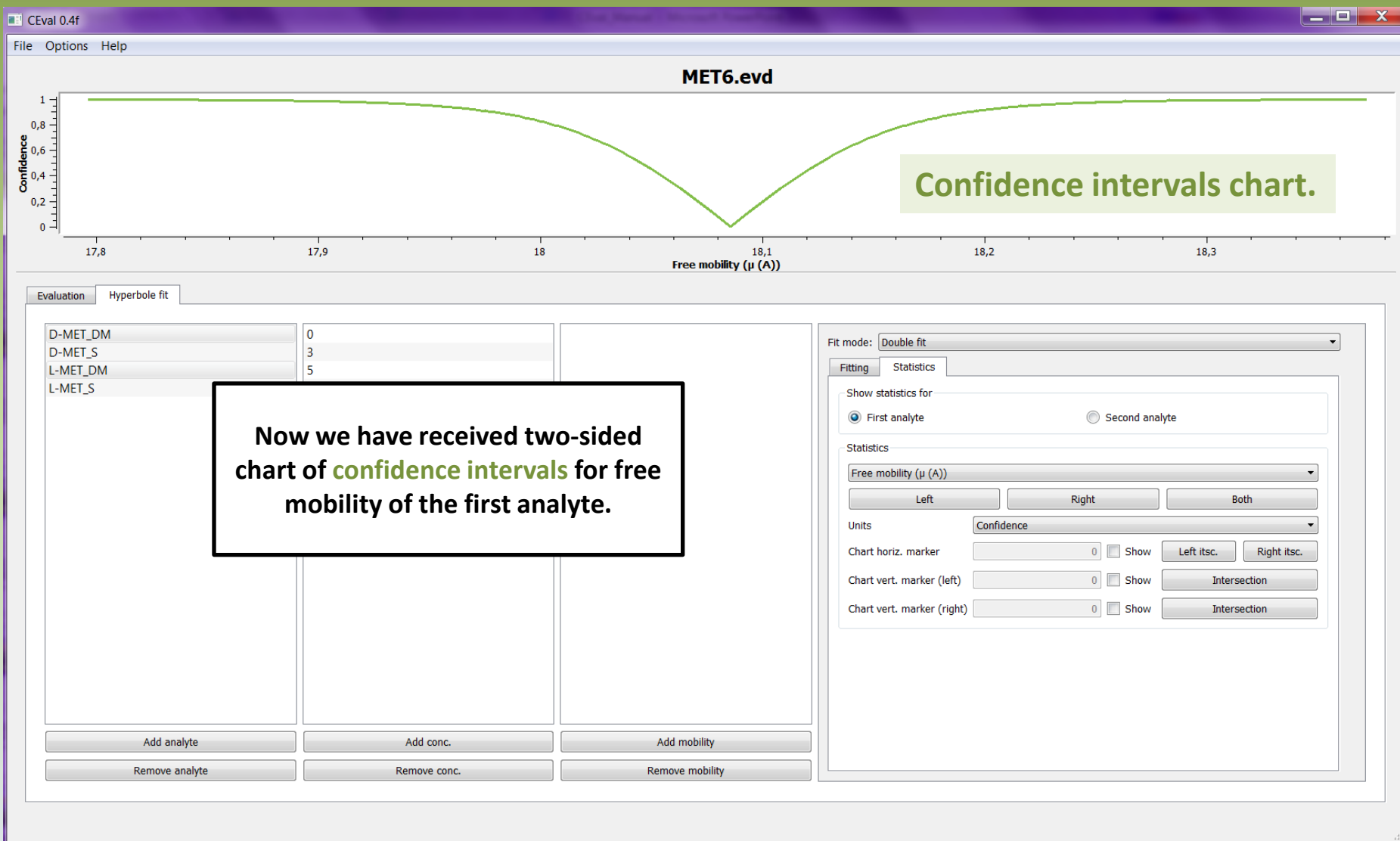
Statistics
Free mobility (μ (A))

Units Confidence

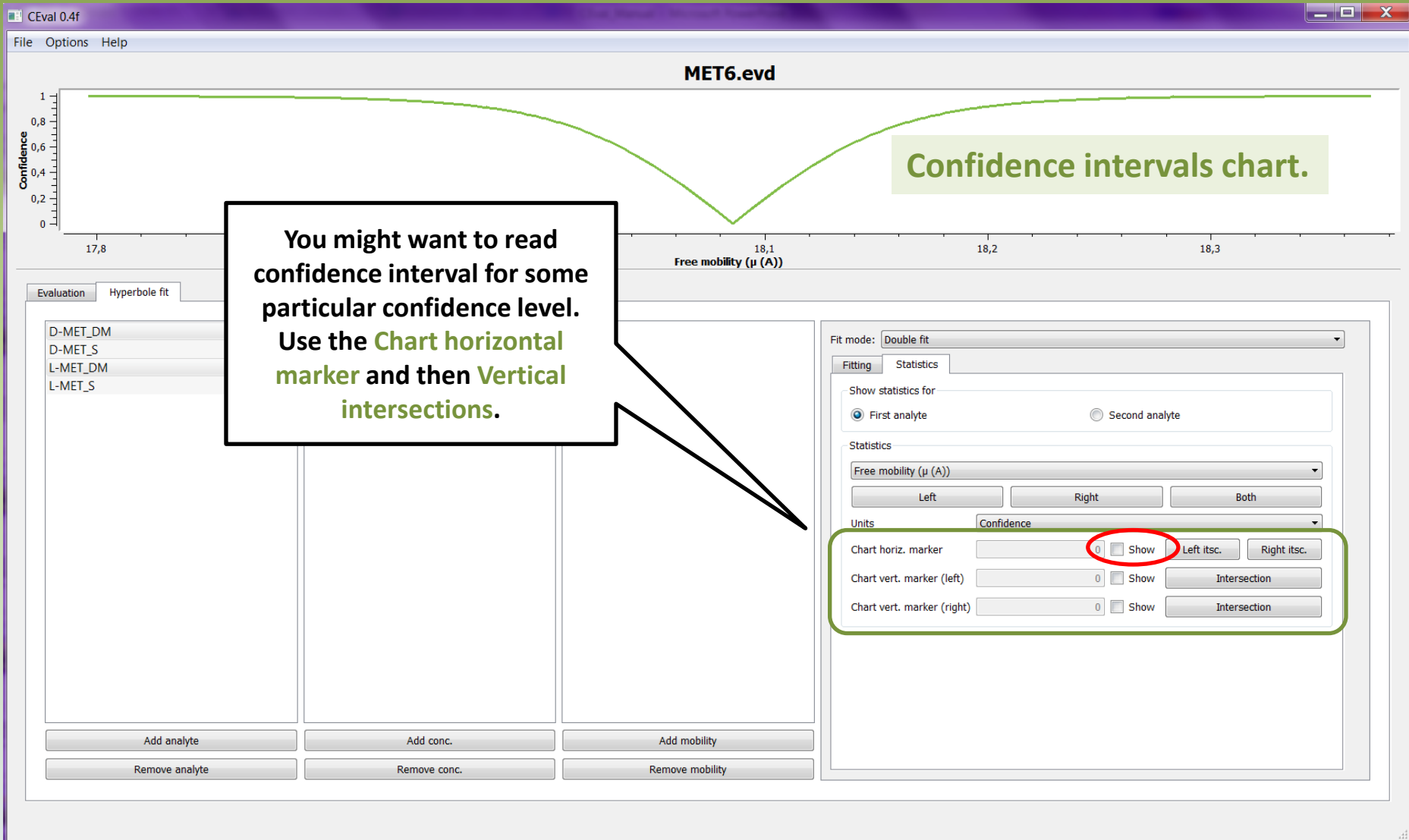
Chart horiz. marker Show
Chart vert. marker (left) Show
Chart vert. marker (right) Show

Add analyte Add conc. Add mobility
Remove analyte Remove conc. Remove mobility

ACE Data Evaluation



ACE Data Evaluation



ACE Data Evaluation

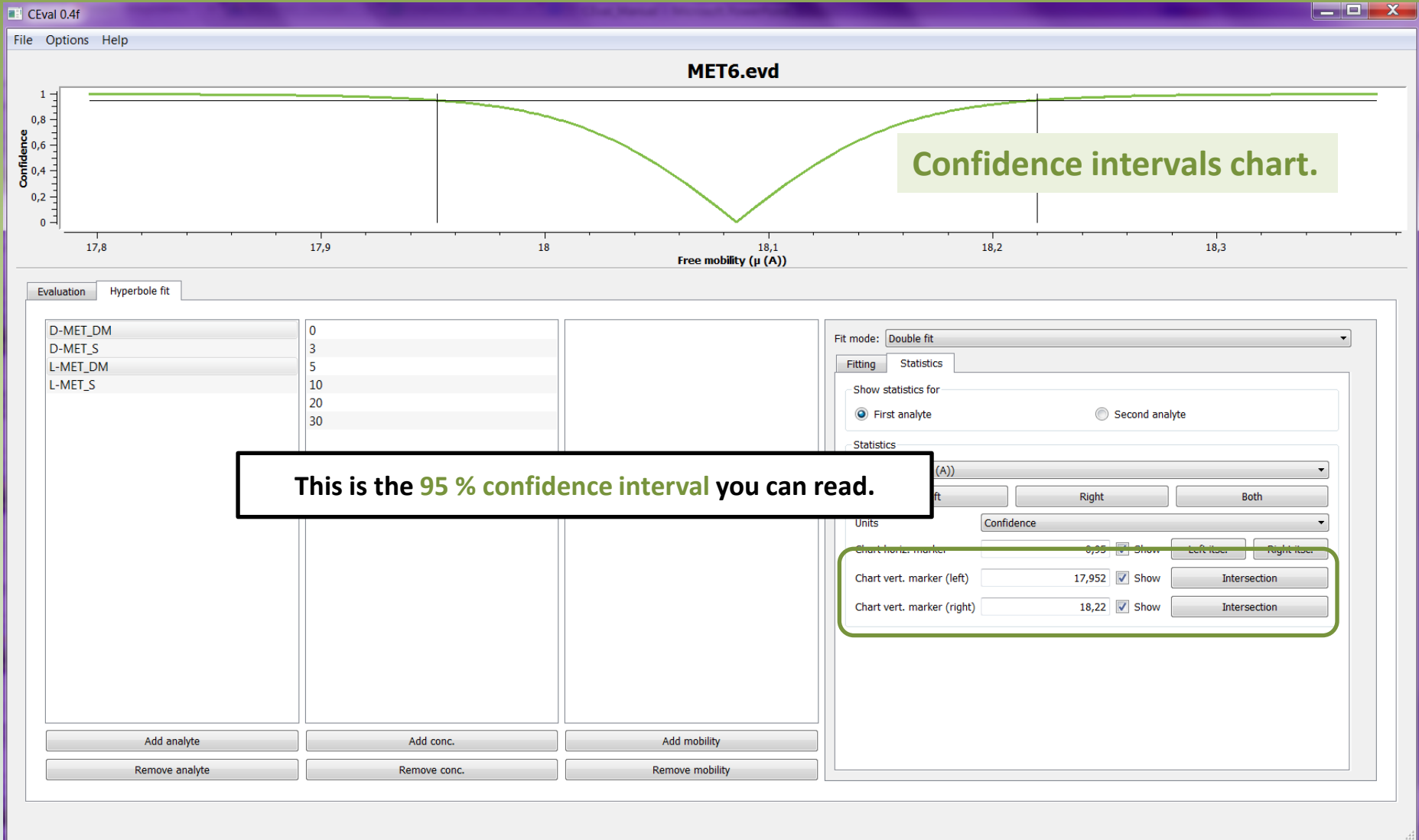


The screenshot displays the CEval 0.4f software interface. At the top, a window titled "MET6.evd" shows a plot of Confidence (y-axis, 0 to 1) versus Free mobility (μ (A)) (x-axis, 17,8 to 18,3). A horizontal line is drawn at a confidence level of 0,95, labeled "Horizontal line for 95 % interval." The plot shows a dip in confidence around 18,1, with a shaded area representing the confidence interval. A callout box points to the settings panel on the right, stating "Now click Intersection and check Show for both vertical markers." The settings panel includes a "Confidence" section with the following options:

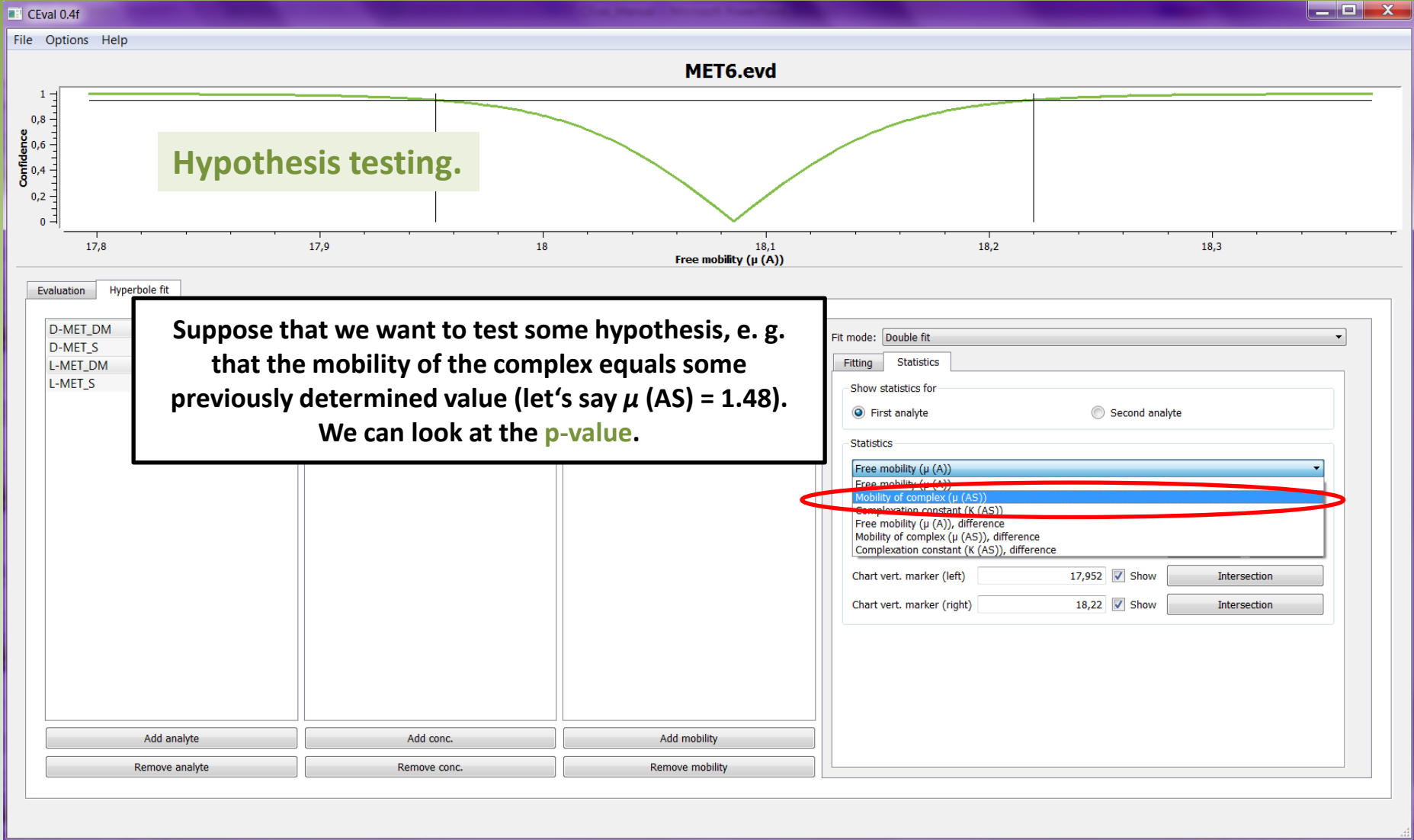
Parameter	Value	Show	Intersection
Chart horiz. marker	0,95	<input checked="" type="checkbox"/>	Left itsc. / Right itsc.
Chart vert. marker (left)	0	<input checked="" type="checkbox"/>	Intersection
Chart vert. marker (right)	0	<input checked="" type="checkbox"/>	Intersection

Buttons for "Add analyte", "Remove analyte", "Add conc.", "Remove conc.", "Add mobility", and "Remove mobility" are located at the bottom of the interface.

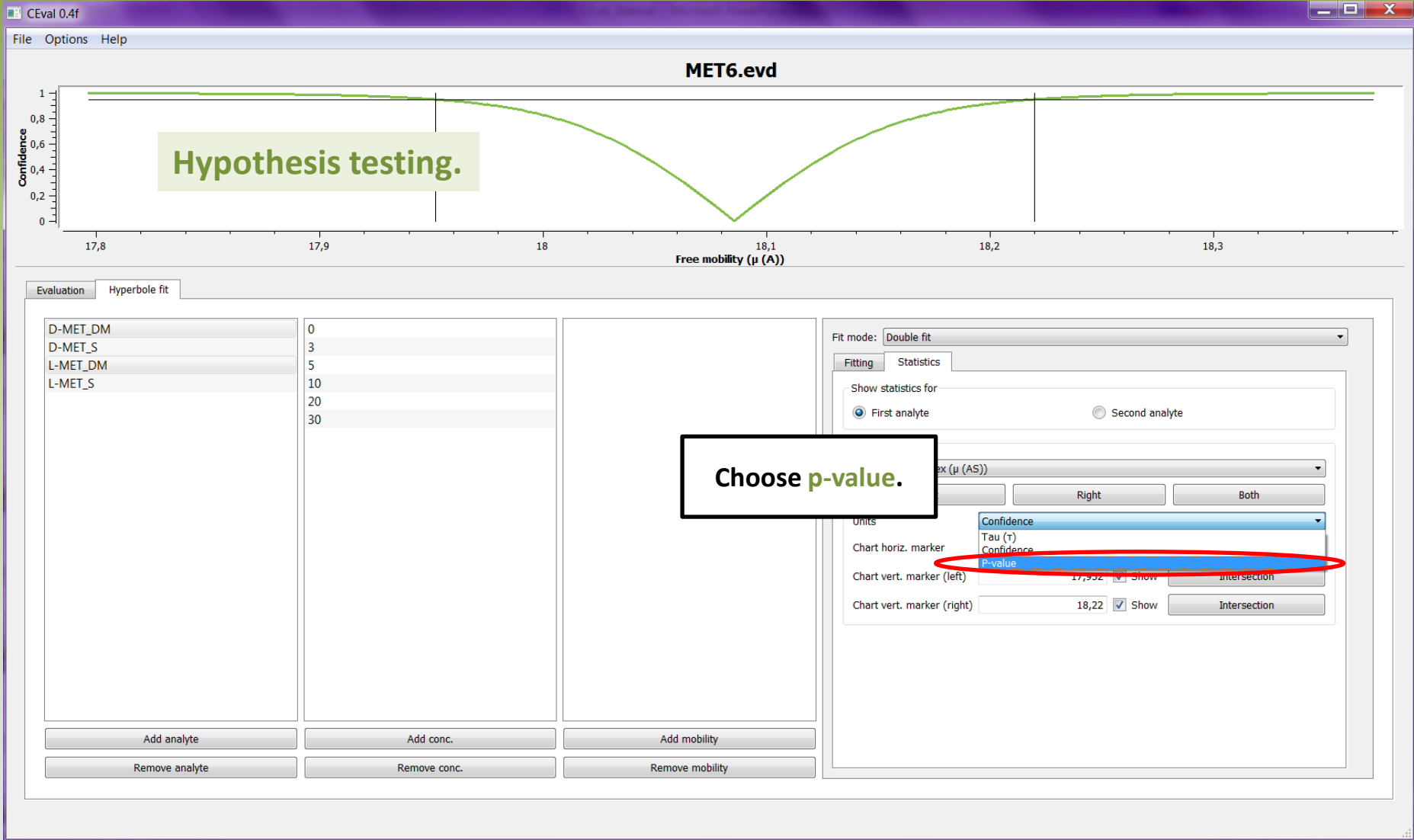
ACE Data Evaluation



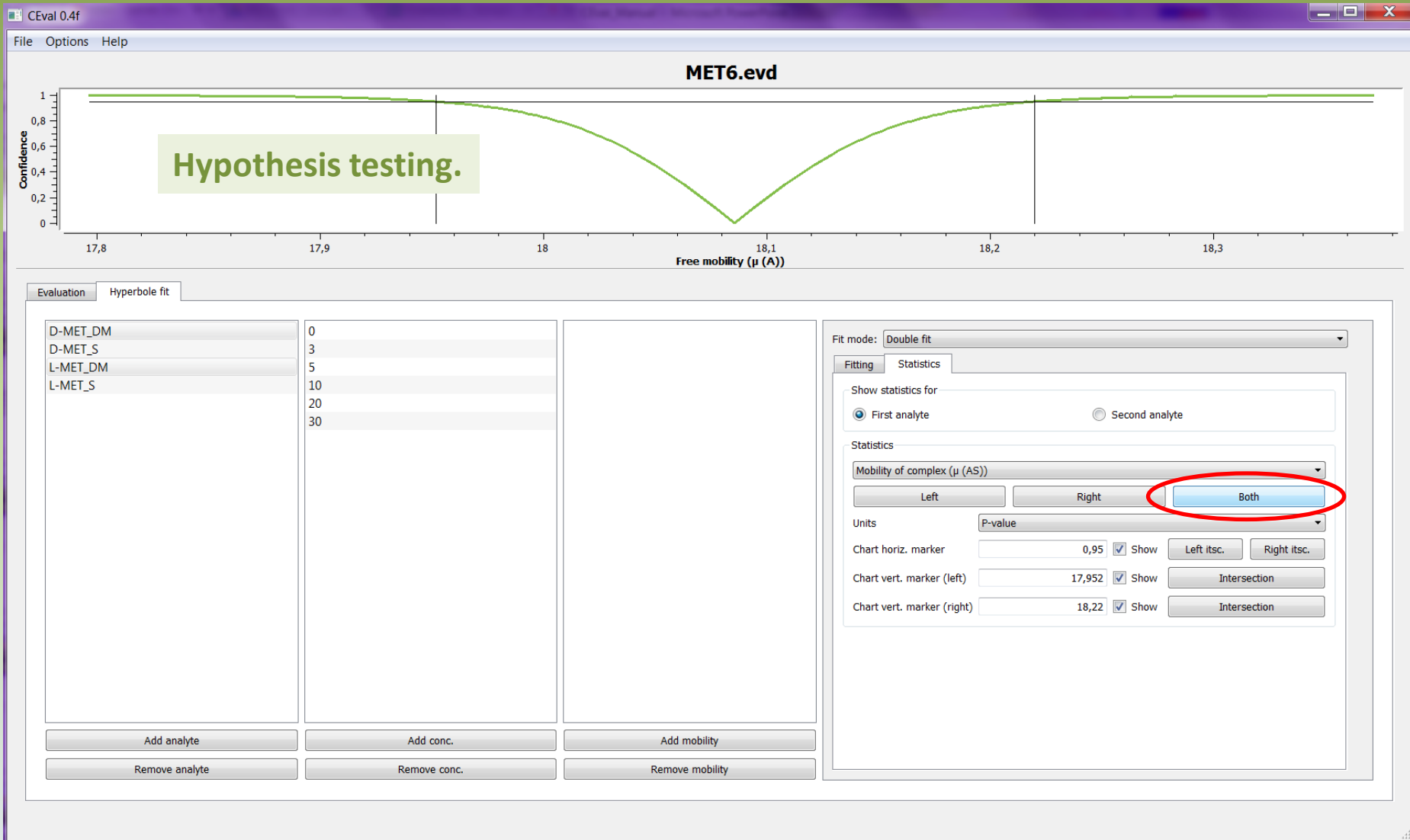
ACE Data Evaluation



ACE Data Evaluation



ACE Data Evaluation



ACE Data Evaluation



CEval 0.4f

File Options Help

MET6.evd

P-values chart.

Mobility of complex (μ (AS))

Evaluation Hyperbole fit

D-MET_DM
D-MET_S
L-MET_DM
L-MET_S

0
3
5
1
2
3

Now we want to set Vertical marker value to 1.48.

Fit mode: Double fit

Fitting Statistics

Show statistics for
 First analyte Second analyte

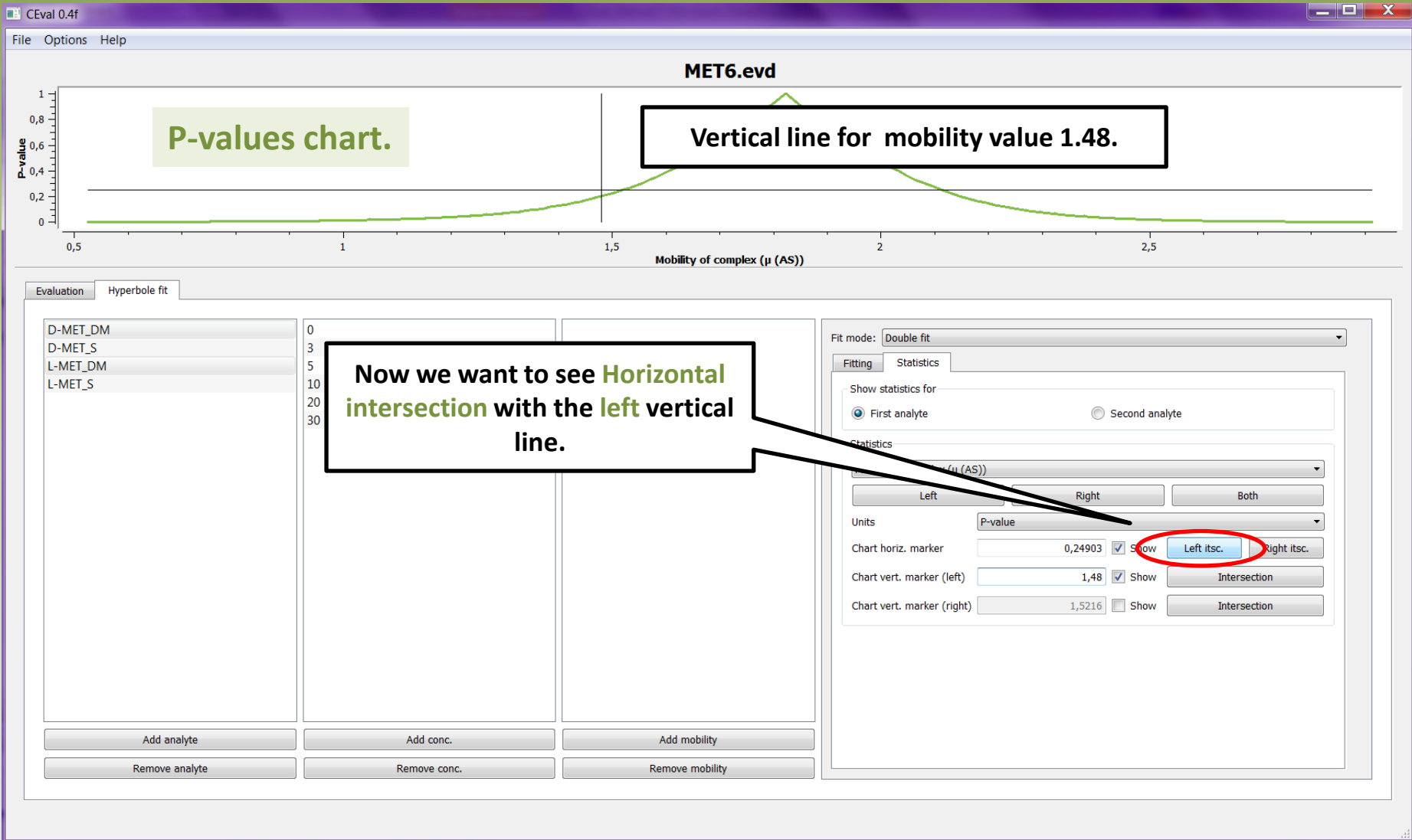
Statistics
Mobility of complex (μ (AS))
Left Right Both

Units P-value

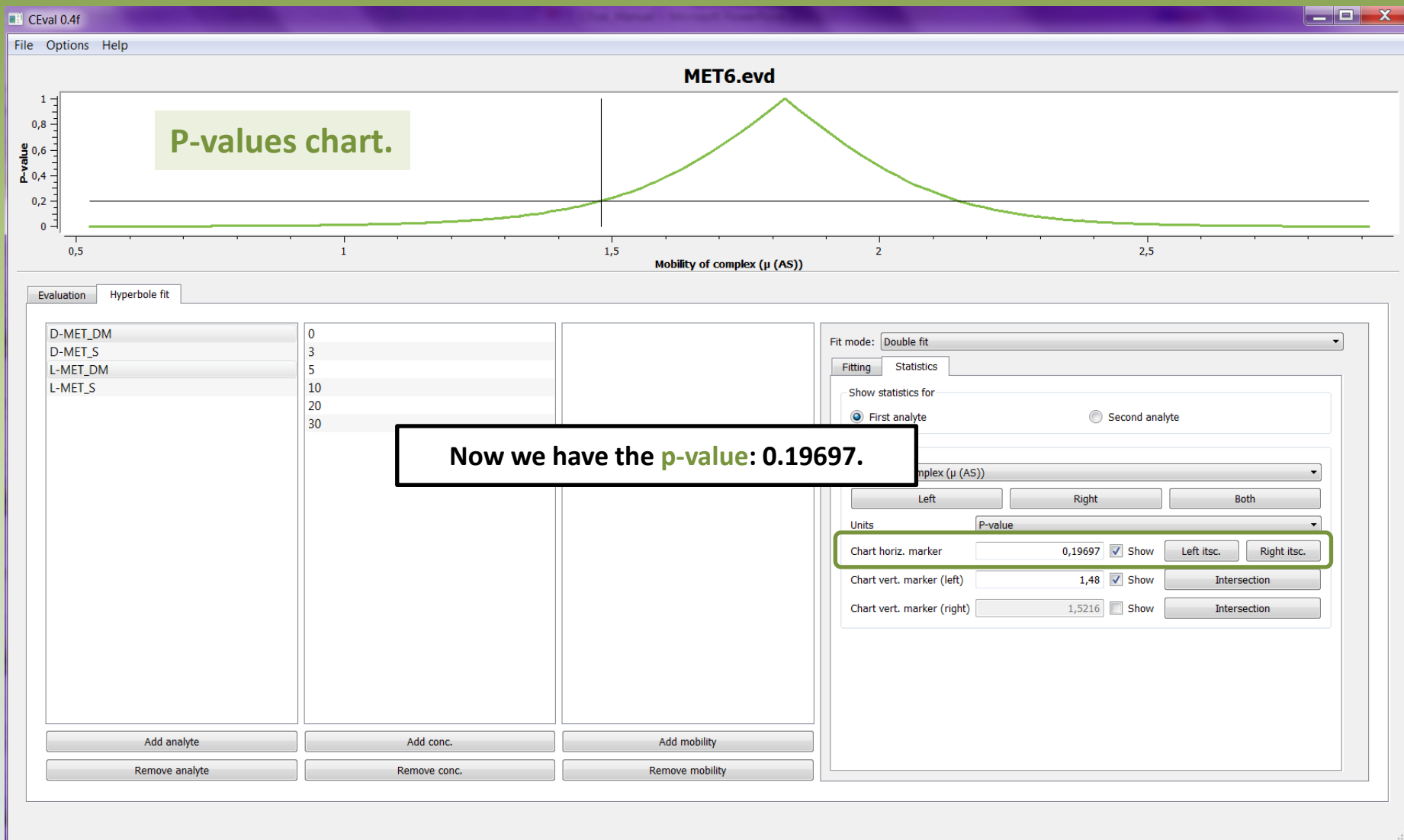
Chart horiz. marker	0,24903	<input checked="" type="checkbox"/> Show	Left itsc. Right itsc.
Chart vert. marker (left)	1,5216	<input checked="" type="checkbox"/> Show	Intersection
Chart vert. marker (right)	1,5216	<input checked="" type="checkbox"/> Show	Intersection

Add analyte Add conc. Add mobility
Remove analyte Remove conc. Remove mobility

ACE Data Evaluation



ACE Data Evaluation





Appendix A: Graph Interface

Appendix A: Graph Interface

The screenshot displays the CEval 0.2rc5 software interface. At the top, the window title is "CEval 0.2rc5" and the menu bar includes "File", "Options", and "Help". The main plot area is titled "DAD1C.ch" and shows a chromatogram with Absorbance (mAU) on the y-axis (0 to 10) and Time (minute) on the x-axis (0 to 14). A peak is highlighted with a cursor at coordinates (6.2745, 5.7703), which are circled in yellow. A text box with a black border and white background contains the text: "The cursor shows **x** and **y** value in the chosen point."

Below the plot, the "Evaluation" section is active, showing a "Hyperbole fit" tab. The file path is "Q:/Users/Magda/Eval/Eval data/LIAC_SEQ_DM_CD/D_MET_20_2.D/DAD1C.ch". The interface is divided into several panels:

- Common parameters:** Capillary (cm) 50,2; Detector (cm) 41,7; Voltage (kV) 15; Field strength (kV/m) 29,88; c(Selector) 0; Time of EOF (min) 0. A "Read EOF time" button is present.
- Evaluated peaks:** A table with columns "Analyte", "Time", and "Area". Below the table are "Add peak", "Delete peak", and "Cancel selection" buttons.
- Parameters / Results:** EOF parameters: v (1e-3 m/s) 0, v! (1e-3 m/s) 0, u (1e-9 m.m/V/s) 0. Peak parameters: Peak from X 0, Peak from Y 0, Peak max at X 0, Peak to X 0, Peak to Y 0, Peak height 0, v (1e-3 m/s) 0, v! (1e-3 m/s) 0, u! (1e-9 m.m/V/s) 0, HI 0, Area (Units.min) 0, t USP 0. HVL parameters: a0 0, a1 0, a2 0, a3 0, x2 0, ε 1e-09, Significant digits 50, Maximum iterations 10. Buttons for "Print HVL" and "Do HVL fit" are present.

A "Find peak(s)" button is located at the bottom right of the interface.

Appendix A: Graph Interface



CEval 0.2rc5

File Options Help

DAD1C.ch

Zoom in by left-clicking and pulling.

8.5762, -1.4166

Time (minute)

Evaluation Hyperbole fit

File: Q:/Users/Magda/Eval/Eval data/LIAC_SEQ_DM_CD/D_MET_20_2/D/DAD1C.ch Close file

Common parameters

Capillary (cm) 50,2
Detector (cm) 41,7
Voltage (kV) 15
Field strength (kV/m) 29,88
c(Selector) 0
Time of EOF (min) 0
Read EOF time

Evaluated peaks

Analyte	Time	Area
---------	------	------

Add peak Delete peak Cancel selection

Parameters Results

EOF

v (1e-3 m/s) 0 v! (1e-3 m/s) 0 u (1e-9 m.m/V/s) 0

Peak

Peak from X 0 Peak from Y 0 Peak max at X 0
Peak to X 0 Peak to Y 0 Peak height 0
v (1e-3 m/s) 0 v! (1e-3 m/s) 0 u! (1e-9 m.m/V/s) 0
H! 0 Area (Units.min) 0 t USP 0

HVL

a0 0 Fixed a1 0 Fixed
a2 0 Fixed a3 0 Fixed
x2 0 ε 1e-09
Significant digits 50 Maximum iterations 10
a1 u! (1e-9 m.m/V/s) 0 Replnt HVL Do HVL fit

Find peak(s)

Appendix A: Graph Interface



CEval 0.2rc5

File Options Help

DAD1C.ch

Peak is zoomed in.

Y-axis: Absorbance (mAU) from -1 to 5
X-axis: Time (minute) from 7,9 to 8,5

Buttons:

Evaluation **Hyperbole fit**

File: Q:/Users/Magda/Eval/Eval data/LIAC_SEQ_DM_CD/D_MET_20_2.D/DAD1C.ch Close file

Common parameters

Capillary (cm)
Detector (cm)
Voltage (kV)
Field strength (kV/m)
c(Selector)
Time of EOF (min)
Read EOF time

Evaluated peaks

Analyte	Time	Area
---------	------	------

Add peak Delete peak
Cancel selection

Parameters Results

EOF
v (1e-3 m/s) v! (1e-3 m/s) u (1e-9 m.m/V/s)

Peak
Peak from X Peak from Y Peak max at X
Peak to X Peak to Y Peak height
v (1e-3 m/s) v! (1e-3 m/s) u! (1e-9 m.m/V/s)
H! Area (Units.min) t USP

HVL
a0 Fixed a1 Fixed
a2 Fixed a3 Fixed
X2 ε
Significant digits Maximum iterations
Print HVL Do HVL fit

Find peak(s)

Appendix A: Graph Interface



CEval 0.2rc5

File Options Help

DAD1C.ch

Zoom out by holding Shift and left-clicking.

Y-axis: Absorbance (mAU) from -1 to 5
X-axis: Time (minute) from 7,9 to 8,5

Evaluation Hyperbole fit

File: Q:/Users/Magda/Eval/Eval data/LIAC_SEQ_DM_CD/D_MET_20_2.D/DAD1C.ch Close file

Common parameters

Capillary (cm)
Detector (cm)
Voltage (kV)
Field strength (kV/m)
c(Selector)
Time of EOF (min)
Read EOF time

Evaluated peaks

Analyte	Time	Area
---------	------	------

Add peak Delete peak
Cancel selection

Parameters Results

EOF
v (1e-3 m/s) v! (1e-3 m/s) u (1e-9 m.m/V/s)

Peak
Peak from X Peak from Y Peak max at X
Peak to X Peak to Y Peak height
v (1e-3 m/s) v! (1e-3 m/s) u! (1e-9 m.m/V/s)
H! Area (Units.min) t USP

HVL
a0 Fixed a1 Fixed
a2 Fixed a3 Fixed
X2 ε
Significant digits Maximum iterations
Replot HVL Do HVL fit

Find peak(s)

Appendix A: Graph Interface



CEval 0.2rc5

File Options Help

DAD1C.ch

Changing peak beginning and end.

Absorbance (mAU)

Time (minute)

Evaluation **Hyperbole fit**

File: Q:\Users\Magda\Eval\Eval data\LIAC_SEQ_DM_CD\D_MET_20_2.D\DAD1C.ch Close file

Common parameters

Capillary (cm)

Detector (cm)

Voltage (kV)

Field strength (kV/m)

c(Selector)

Time of EOF (min) Read EOF time

Evaluated peaks

Analyte	Time	Area
---------	------	------

Add peak Delete peak

Cancel selection

Parameters Results

EOF

v (1e-3 m/s) $v!$ (1e-3 m/s) u (1e-9 m.m/V/s)

Peak

Peak from X Peak from Y Peak max at X

Peak to X Peak to Y Peak height

v (1e-3 m/s) $v!$ (1e-3 m/s) $u!$ (1e-9 m.m/V/s)

H1 Area (Units.min) t USP

HVL

a_0 Fixed a_1 Fixed

a_2 Fixed a_3 Fixed

χ^2 ϵ

Significant digits Maximum iterations

$a_1!$ (1e-9 m.m/V/s) Print HVL Do HVL fit

Find peak(s)

Appendix A: Graph Interface

The screenshot displays the CEval 0.2rc5 software interface. At the top, the window title is "CEval 0.2rc5" and the menu bar includes "File", "Options", and "Help". The main plot area is titled "DAD1C.ch" and shows a chromatogram with "Absorbance (mAU)" on the y-axis (0 to 10) and "Time (minute)" on the x-axis (0 to 14). A prominent peak is visible at approximately 11.5 minutes. A yellow box highlights a context menu that appears when right-clicking on the graph, containing the following options: "Peak from this X", "Peak from this Y", "Peak from this X,Y", "Peak to this X", "Peak to this Y", "Peak to this X,Y", "Set noise reference point", and "Set slope reference point". A text box with a black border and yellow text states: "Right-click on the graph will reveal several options." Below the graph, the "Evaluation" tab is active, showing a "Hyperbole fit" button. The "File" field contains the path "Q:\Users\Magda\Eval\Eval data\LIAC_SEQ_DM_CD\MET_20_2_D\DAD1C.ch" and a "Close file" button. The interface is divided into several panels: "Common parameters" (Capillary: 50,2; Detector: 41,7; Voltage: 15; Field strength: 29,88; c(Selector): 0; Time of EOF: 0), "Evaluated peaks" (empty table with columns for Analyte, Time, and Area), and "Parameters" (EOF, Peak, and HVL settings). The "Parameters" panel includes fields for EOF (v, v!, u), Peak (Peak from X/Y, Peak to X/Y, Peak height, v, v!, u, H!, Area, t USP), and HVL (a0, a1, a2, a3, x2, ε, Significant digits, Maximum iterations). A "Find peak(s)" button is located at the bottom right.

CEval 0.2rc5

File Options Help

DAD1C.ch

Absorbance (mAU)

Time (minute)

Peak from this X
Peak from this Y
Peak from this X,Y
Peak to this X
Peak to this Y
Peak to this X,Y
Set noise reference point
Set slope reference point

Right-click on the graph will reveal several options.

Evaluation Hyperbole fit

File: Q:\Users\Magda\Eval\Eval data\LIAC_SEQ_DM_CD\MET_20_2_D\DAD1C.ch Close file

Common parameters

Capillary (cm) 50,2
Detector (cm) 41,7
Voltage (kV) 15
Field strength (kV/m) 29,88
c(Selector) 0
Time of EOF (min) 0
Read EOF time

Evaluated peaks

Analyte	Time	Area
---------	------	------

Add peak Delete peak Cancel selection

Parameters Results

EOF
v (1e-3 m/s) 0 v! (1e-3 m/s) 0 u (1e-9 m.m/V/s) 0

Peak
Peak from X 0 Peak from Y 0 Peak max at X 0
Peak to X 0 Peak to Y 0 Peak height 0
v (1e-3 m/s) 0 v! (1e-3 m/s) 0 u! (1e-9 m.m/V/s) 0
H! 0 Area (Units.min) 0 t USP 0

HVL
a0 0 Fixed a1 0 Fixed
a2 0 Fixed a3 0 Fixed
x2 0 ε 1e-09
Significant digits 50 Maximum iterations 10
Print HVL Do HVL fit

Find peak(s)

Appendix A: Graph Interface

The screenshot displays the CEval 0.2rc5 software interface. At the top, the window title is "CEval 0.2rc5" and the menu bar includes "File", "Options", and "Help". The main plot area, titled "DAD1C.ch", shows a chromatogram with "Absorbance (mAU)" on the y-axis (0 to 10) and "Time (minute)" on the x-axis (0 to 14). A prominent peak is visible at approximately 11.5 minutes. A yellow-bordered box highlights a context menu with options: "Peak from this X", "Peak from this Y", "Peak from this X,Y", "Peak to this X", "Peak to this Y", "Peak to this X,Y", "Set noise reference point", and "Set slope reference point". A black-bordered box with white text says "You can set peak beginning and end here." pointing to the peak. Below the plot is an "Evaluation" section with a "Hyperbole fit" tab. The "File" field shows the path "Q:\Users\Magda\Eval\Eval data\LIAC_SEQ_DM_CD\MET_20_2\D\DAD1C.ch" and a "Close file" button. The interface is divided into three main panels: "Common parameters" (with fields for Capillary, Detector, Voltage, Field strength, c(Selector), and Time of EOF), "Evaluated peaks" (with a table for Analyte, Time, and Area, and buttons for Add peak, Delete peak, and Cancel selection), and "Parameters" (with sub-tabs for EOF, Peak, and HVL, and various numerical input fields). A black-bordered box with white text says "Find a peak." pointing to the "Find peak(s)" button, which is circled in red.

CEval 0.2rc5

File Options Help

DAD1C.ch

Absorbance (mAU)

Time (minute)

Peak from this X
Peak from this Y
Peak from this X,Y
Peak to this X
Peak to this Y
Peak to this X,Y
Set noise reference point
Set slope reference point

You can set peak beginning and end here.

Evaluation Hyperbole fit

File: Q:\Users\Magda\Eval\Eval data\LIAC_SEQ_DM_CD\MET_20_2\D\DAD1C.ch Close file

Common parameters

Capillary (cm) 50,2
Detector (cm) 41,7
Voltage (kV) 15
Field strength (kV/m) 29,88
c(Selector) 0
Time of EOF (min) 0
Read EOF time

Evaluated peaks

Analyte	Time	Area
---------	------	------

Add peak Delete peak Cancel selection

Parameters Results

EOF
v (1e-3 m/s) 0 v! (1e-3 m/s) 0 u (1e-9 m.m/V/s) 0

Peak
Peak from X 0 Peak from Y 0 Peak max at X 0
Peak to X 0 Peak to Y 0 Peak height 0
v (1e-3 m/s) 0 v! (1e-3 m/s) 0 u! (1e-9 m.m/V/s) 0
H! 0 Area (Units.min) 0 t USP 0

HVL
a0 0 Fixed
a2 0 Fixed
χ2 0 ε 1e-09
Significant digits 50 Maximum iterations 10
Print HVL On HVL fit

Find a peak.

Find peak(s)

Appendix A: Graph Interface



CEval 0.2rc5

File Options Help

DAD1C.ch

Zoom in.

Y-axis: Absorbance (mAU)

X-axis: Time (minute)

Evaluation: Hyperbole fit

File: Q:/Users/Magda/Eval/Eval data/LIAC_SEQ_DM_CD/D_MET_20_2-D/DAD1C.ch

Common parameters:

- Capillary (cm): 50,2
- Detector (cm): 41,7
- Voltage (kV): 15
- Field strength (kV/m): 29,88
- c(Selector): 0
- Time of EOF (min): 0

Read EOF time

Evaluated peaks:

Analyte	Time	Area
---------	------	------

Parameters Results

EOF

v (1e-3 m/s): inf v1 (1e-3 m/s): 0 u (1e-9 m.m/V/s): inf

Peak

Peak from X: 7,6325 Peak from Y: -0,76449 Peak max at X: 8,2321

Peak to X: 8,7467 Peak to Y: -0,75191 Peak height: 3,1966

v (1e-3 m/s): 0,84426 v1 (1e-3 m/s): inf u1 (1e-9 m.m/V/s): 2,215e-292

H1: 3,9543 Area (Units.min): 0,64522 t USP: 1,0841

HVL

a0: 0,64522 Fixed a1: 8,2564 Fixed

a2: 0,062129 Fixed a3: 0,98114 Fixed

x2: 0 ε: 1e-09

Significant digits: 50 Maximum iterations: 10

a1 u1 (1e-9 m.m/V/s): inf

Replot HVL Do HVL fit

Find peak(s)

Appendix A: Graph Interface



CEval 0.2rc5

File Options Help

DAD1C.ch

Right-click on the spot where you want the peak beginning.

Absorbance (mAU)

Time (minute)

Evaluation Hyperbole fit

File: Q:\Users\Magda\Eval\Eval data\LIAC_SEQ_DM_CD\D_MET_20_2.D\DAD1C.ch Close file

Common parameters

- Capillary (cm): 50,2
- Detector (cm): 41,7
- Voltage (kV): 15
- Field strength (kV/m): 29,88
- c(Selector): 0
- Time of EOF (min): 0

Read EOF time

Evaluated peaks

Analyte	Time	Area
---------	------	------

Add peak Delete peak Cancel selection

Parameters Results

EOF

v (1e-3 m/s) inf $v!$ (1e-3 m/s) 0 u (1e-9 m.m/V/s) inf

Peak

Peak from X	7,6325	Peak from Y	-0,76449	Peak max at X	8,2321
Peak to X	8,7467	Peak to Y	-0,75191	Peak height	3,1966
v (1e-3 m/s)	0,84426	$v!$ (1e-3 m/s)	inf	$u!$ (1e-9 m.m/V/s)	2,215e-292
H!	3,9543	Area (Units.min)	0,64522	t USP	1,0841

HVL

a0	0,64522	<input type="checkbox"/> Fixed	a1	8,2564	<input type="checkbox"/> Fixed
a2	0,062129	<input type="checkbox"/> Fixed	a3	0,98114	<input type="checkbox"/> Fixed
χ^2	0		ϵ	1e-09	
Significant digits	50		Maximum iterations	10	
a1 u! (1e-9 m.m/V/s)	inf				

Replot HVL Do HVL fit

Find peak(s)

Appendix A: Graph Interface



The screenshot displays the CEval 0.2rc5 software interface. At the top, the window title is "CEval 0.2rc5" and the menu bar includes "File", "Options", and "Help". The main plot area is titled "DAD1C.ch" and shows a chromatogram with "Absorbance (mAU)" on the y-axis (ranging from -1 to 5) and "Time (minute)" on the x-axis (ranging from approximately 8.0 to 8.6). A single peak is visible, centered around 8.25 minutes. A blue vertical line marks the peak's position, and a blue horizontal line indicates its height. A red horizontal line is drawn at the baseline. A black box with the text "Peak from this X, Y." is positioned above the peak. A context menu is open over the peak, with the option "Peak from this X,Y" highlighted in blue and circled in red. Other menu options include "Peak from this X", "Peak from this Y", "Peak to this X", "Peak to this Y", "Set noise reference point", and "Set slope reference point".

Below the plot, the "Evaluation" tab is active, showing "Hyperbole fit" as the selected method. The file path is "Q:/Users/Magda/Eval/Eval data/LIAC_SEQ_DM_CD/D_MET_20...". The "Common parameters" section includes:

- Capillary (cm): 50,2
- Detector (cm): 41,7
- Voltage (kV): 15
- Field strength (kV/m): 29,88
- c(Selector): 0
- Time of EOF (min): 0

A "Read EOF time" button is located below these parameters. The "Parameters" tab is also visible, showing the following data:

Parameter	Value
Peak from X	7,6325
Peak from Y	-0,76449
Peak max at X	8,2321
Peak to X	8,7467
Peak to Y	-0,75191
Peak height	3,1966
v (1e-3 m/s)	0,84426
v! (1e-3 m/s)	inf
u! (1e-9 m.m/V/s)	2,215e-292
H!	3,9543
Area (Units.min)	0,64522
t USP	1,0841

The "HVL" section includes parameters for fitting: a0 (0,64522), a1 (8,2564), a2 (0,062129), a3 (0,98114), x2 (0), ε (1e-09), Significant digits (50), and Maximum iterations (10). Buttons for "Replot HVL" and "Do HVL fit" are present. At the bottom right, a "Find peak(s)" button is visible.

Appendix A: Graph Interface



The screenshot displays the CEval 0.2rc5 software interface. At the top, a window titled "DAD1C.ch" shows a chromatogram with Absorbance (mAU) on the y-axis (ranging from -1 to 5) and Time (minute) on the x-axis (ranging from 8 to 8.6). A single peak is visible, centered around 8.25 minutes, with a blue fit curve overlaid. A vertical blue line marks the peak maximum at approximately 8.2321 minutes. A horizontal blue line is drawn across the peak at approximately 3.1966 mAU. A red horizontal line is drawn at the baseline level, approximately -0.7714 mAU.

Below the graph, the "Evaluation" window is open, showing a "Hyperbole fit" model. The file path is "Q:/Users/Magda/Eval/Eval data/LIAC_SEQ_DM_CD/D_MET_20_2.D/DAD1C.ch". The "Evaluated peaks" tab is active, displaying the following parameters:

Parameter	Value
Peak from X	8,0207
Peak from Y	-0,7714
Peak max at X	8,2321
Peak to X	8,7467
Peak to Y	-0,75191
Peak height	3,1966
v (1e-3 m/s)	0,84426
v! (1e-3 m/s)	inf
u! (1e-9 m.m/V/s)	6,366e-305
H!	3,9623
Area (Units.min)	0,64825
t USP	1,0866

The "HVL" section contains the following parameters:

Parameter	Value	Fixed
a0	0,64825	<input type="checkbox"/>
a1	8,2573	<input type="checkbox"/>
a2	0,062815	<input type="checkbox"/>
a3	1,0054	<input type="checkbox"/>
χ^2	0	
ϵ	1e-09	
Significant digits	50	
Maximum iterations	10	
a1 u! (1e-9 m.m/V/s)	inf	

Buttons for "Replot HVL" and "Do HVL fit" are present. A "Find peak(s)" button is at the bottom right.

Two callout boxes provide instructions:

- Peak beginning rewritten.** (A black box with white text pointing to the "Peak from X" field)
- Use the same procedure to change peak end or to change X or Y value only.** (A black box with white text pointing to the "Peak to X" and "Peak to Y" fields)

Appendix A: Graph Interface



CEval 0.2rc5

File Options Help

DAD1C.ch

Absorbance (mAU)

Time (minute)

Changing noise reference point.

Evaluation Hyperbole fit

File: Q:/Users/Magda/Eval/Eval data/LIAC_SEQ_DM_CD/D_MET_20_2.D/DAD1C.ch

Common parameters

- Capillary (cm): 50,2
- Detector (cm): 41,7
- Voltage (kV): 15
- Field strength (kV/m): 29,88
- c(Selector): 0
- Time of EOF (min): 0

Read EOF time

Evaluated peaks

Analyte	Time	Area
---------	------	------

Parameters Results

Peak properties

- Peak from X: 8,0207 Auto
- Peak from Y: -0,7714 Auto
- Peak to X: 8,7467 Auto
- Peak to Y: -0,75191 Auto
- Peak max at X: 8,2321 Auto
- Peak height: 3,1966 Auto

Finder parameters

- Noise window: 0,5
- Peak window: 0,5
- Slope window: 0,16666 Auto
- Noise: 1,5821 Auto
- Noise LOD coeff: 1

Window

- To: 0 Auto
- To: 0 Auto

Baseline algorithm: Slope

- Noise ref. point [min]: 0
- Slope ref. point [min]: 0 Auto

Find peak(s)

Noise and slope reference point is set to zero by default.

Appendix A: Graph Interface



CEval 0.2rc5

File Options Help

DAD1C.ch

Right-click on the graph.

Y-axis: Absorbance (mAU) (0 to 10)
X-axis: Time (minute) (0 to 14)

File: Q:/Users/Magda/Eval/Eval data/LIAC_SEQ_DM_CD/D_MET_20_2.D/DAD1C.ch

Common parameters

- Capillary (cm): 50,2
- Detector (cm): 41,7
- Voltage (kV): 15
- Field strength (kV/m): 29,88
- c(Selector): 0
- Time of EOF (min): 0

Read EOF time

Evaluated peaks

Analyte	Time	Area
	8,2321	

Parameters Results

Peak properties

- Peak from X: 8,0207 Auto
- Peak to X: 8,7467 Auto
- Peak max at X: 8,2321 Auto
- Width 1/2 left (min): 0,06875 Auto
- Peak from Y: -0,7714 Auto
- Peak to Y: -0,75191 Auto
- Peak height: 3,1966 Auto

Finder parameters

- Window units: Minutes
- Noise window: 0,5
- Peak window: 0,5
- Slope window: 0,16666 Auto
- Noise: 1,5821 Auto
- Noise LOD coeff: 1
- From: 0 Auto
- To: 0 Auto
- Baseline algorithm: Slope
- Noise ref. point [min]: 0
- Slope ref. point [min]: 0 Auto
- Noise slope correction: Enable

Find peak(s)

Appendix A: Graph Interface



CEval 0.2rc5

File Options Help

DAD1C.ch

Absorbance (mAU)

Time (minute)

Set noise reference point.

- Peak from this X
- Peak from this Y
- Peak from this X,Y
- Peak to this X
- Peak to this Y
- Peak to this X,Y
- Set noise reference point**
- Set slope reference point

Evaluation Hyperbole fit

File: Q:/Users/Magda/Eval/Eval data/LIAC_SEQ_DM_CD/D_MET_20_2.D/DAD1C.ch Close file

Common parameters		
Capillary (cm)	50,2	
Detector (cm)	41,7	
Voltage (kV)	15	
Field strength (kV/m)	29,88	
c(Selector)	0	
Time of EOF (min)	0	

Evaluated peaks		
Analyte	Time	Area

Add peak Delete peak Cancel selection

Parameters		Results			
Peak properties					
Peak from X	8,0207	<input type="checkbox"/> Auto	Peak from Y	-0,7714	<input type="checkbox"/> Auto
Peak to X	8,7467	<input checked="" type="checkbox"/> Auto	Peak to Y	-0,75191	<input checked="" type="checkbox"/> Auto
Peak max at X	8,2321	<input checked="" type="checkbox"/> Auto	Peak height	3,1966	<input checked="" type="checkbox"/> Auto
Width 1/2 left (min)	0,06875	<input checked="" type="checkbox"/> Auto			
Finder parameters					
Window units	Minutes	From	0	<input checked="" type="checkbox"/> Auto	
Noise window	0,5	To	0	<input checked="" type="checkbox"/> Auto	
Peak window	0,5	Baseline algorithm	Slope		
Slope window	0,16666	<input checked="" type="checkbox"/> Auto	Noise ref. point [min]	0	
Noise	1,5821	<input checked="" type="checkbox"/> Auto	Slope ref. point [min]	0	<input checked="" type="checkbox"/> Auto
Noise LOD coeff	1	Noise slope correction	<input type="checkbox"/> Enable		

Set to default

Set to default

Find peak(s)

Appendix A: Graph Interface



CEval 0.2rc5

File Options Help

DAD1C.ch

Absorbance (mAU)

Time (minute)

Evaluation Hyperbole fit

File: Q:\Users\Magda\Eval\Eval data\LIAC_SEQ_DM_CD\D_MET_20_2.D\DAD1C.ch Close file

Common parameters

- Capillary (cm): 50,2
- Detector (cm): 41,7
- Voltage (kV): 15
- Field strength (kV/m): 29,88
- c(Selector): 0
- Time of EOF (min): 0
- Read EOF time

Evaluated peaks

Analyte	Time	Area
---------	------	------

Add peak Delete peak Cancel selection

Parameters Results

Peak properties

Peak from X: -0,7714 Auto

Peak to X: -0,71042 Auto

Peak max at: 3,5574 Auto

Width 1/2 left: Auto

Finder param: Auto

Window units: Auto

Noise window: 0,5 To: Auto

Peak window: 0,5

Slope window: 0,016666 Auto

Noise: 0,040531 Auto

Noise LOD coeff: 1

Baseline algorithm: Slope

Noise ref. point [min]: 5,0874

Slope ref. point [min]: 5,0874 Auto

Noise slope correction Enable

Find peak(s)

**Noise reference point set.
Slope reference point will also change if Auto is checked.**

Appendix A: Graph Interface



CEval 0.2rc5

File Options Help

DAD1C.ch

Absorbance (mAU)

Adjusting the plot appearance.

Time (minute)

Evaluation Hyperbole fit

File: Q:\Users\Magda\Eval\Eval data\LIAC_SEQ_DM_CD\D_MET_20_2\D\DAD1C.ch Close file

Common parameters

Capillary (cm)	50,2
Detector (cm)	41,7
Voltage (kV)	15
Field strength (kV/m)	29,88
c(Selector)	0
Time of EOF (min)	0

Read EOF time

Evaluated peaks

Analyte	Time	Area
---------	------	------

Add peak Delete peak Cancel selection

Parameters Results

Peak properties

Peak from X	8,0207	<input type="checkbox"/> Auto	Peak from Y	-0,7714	<input type="checkbox"/> Auto
Peak to X	8,4708	<input checked="" type="checkbox"/> Auto	Peak to Y	-0,71042	<input checked="" type="checkbox"/> Auto
Peak max at X	8,2321	<input checked="" type="checkbox"/> Auto	Peak height	3,5574	<input checked="" type="checkbox"/> Auto
Width 1/2 left (min)	0,06375	<input checked="" type="checkbox"/> Auto			

Set to default

Finder parameters

Window units	Minutes	From	0	<input checked="" type="checkbox"/> Auto
Noise window	0,5	To	0	<input checked="" type="checkbox"/> Auto
Peak window	0,5	Baseline algorithm	Slope	
Slope window	0,016666	Noise ref. point [min]	5,0874	
Noise	0,040531	Slope ref. point [min]	5,0874	<input checked="" type="checkbox"/> Auto
Noise LOD coeff	1	Noise slope correction	<input type="checkbox"/> Enable	

Set to default

Find peak(s)

Appendix A: Graph Interface



CEval 0.2rc5

File **Options** Help

DAD1C.ch

Absorbance (mAU)

Time (minute)

Click on Options.

Evaluation **Hyperbole fit**

File: Q:\Users\Magda\Eval\Eval data\LIAC_SEQ_DM_CD\D_MET_20_2\D\DAD1C.ch Close file

Common parameters

Capillary (cm)	50,2
Detector (cm)	41,7
Voltage (kV)	15
Field strength (kV/m)	29,88
c(Selector)	0
Time of EOF (min)	0

Read EOF time

Evaluated peaks

Analyte	Time	Area
---------	------	------

Add peak Delete peak
Cancel selection

Parameters **Results**

Peak properties

Peak from X	8,0207	<input type="checkbox"/> Auto	Peak from Y	-0,7714	<input type="checkbox"/> Auto
Peak to X	8,4708	<input checked="" type="checkbox"/> Auto	Peak to Y	-0,71042	<input checked="" type="checkbox"/> Auto
Peak max at X	8,2321	<input checked="" type="checkbox"/> Auto	Peak height	3,5574	<input checked="" type="checkbox"/> Auto
Width 1/2 left (min)	0,06375	<input checked="" type="checkbox"/> Auto			

Set to default

Finder parameters

Window units	Minutes	From	0	<input checked="" type="checkbox"/> Auto
Noise window	0,5	To	0	<input checked="" type="checkbox"/> Auto
Peak window	0,5	Baseline algorithm	Slope	
Slope window	0,016666	Noise ref. point [min]	5,0874	
Noise	0,040531	Slope ref. point [min]	5,0874	<input checked="" type="checkbox"/> Auto
Noise LOD coeff	1	Noise slope correction	<input type="checkbox"/> Enable	

Set to default

Find peak(s)

Appendix A: Graph Interface



The screenshot displays the CEval 0.2rc5 software interface. At the top, the menu bar includes 'File', 'Options', and 'Help'. The 'Options' menu is open, with 'Adjust plot appearance' and 'Set number format' visible. A red circle highlights the 'Adjust plot appearance' option, and a callout box points to it with the text 'Adjust plot appearance.'.

The main window shows a chromatogram titled 'DAD1C.ch'. The y-axis is labeled 'Absorbance (mAU)' and ranges from 0 to 10. The x-axis is labeled 'Time (minute)' and ranges from 0 to 14. Two peaks are visible: a small peak at approximately 8.2 minutes and a larger peak at approximately 11.5 minutes. The smaller peak is highlighted with a blue fit curve and a red vertical line.

Below the chromatogram, the 'Evaluation' section is active, showing 'Hyperbole fit'. The file path is 'Q:/Users/Magda/Eval/Eval data/LIAC_SEQ_DM_CD/D_MET_20_2.D/DAD1C.ch'. The interface is divided into several panels:

- Common parameters:** Includes input fields for Capillary (cm) 50,2, Detector (cm) 41,7, Voltage (kV) 15, Field strength (kV/m) 29,88, c(Selector) 0, and Time of EOF (min) 0. A 'Read EOF time' button is present.
- Evaluated peaks:** A table with columns 'Analyte', 'Time', and 'Area'. It contains one entry for the peak at 8.207 minutes. Buttons for 'Add peak', 'Delete peak', and 'Cancel selection' are at the bottom.
- Parameters / Results:** Contains two sub-sections:
 - Peak properties:** Includes fields for Peak from X (8,0207), Peak to X (8,4708), Peak max at X (8,2321), Width 1/2 left (min) (0,06375), Peak from Y (-0,7714), Peak to Y (-0,71042), and Peak height (3,5574). Each field has an 'Auto' checkbox and a 'Set to default' button.
 - Finder parameters:** Includes 'Window units' (Minutes), 'Noise window' (0,5), 'Peak window' (0,5), 'Slope window' (0,016666), 'Noise' (0,040531), 'Noise 1/2 coeff' (1), 'From' (0), 'To' (0), 'Baseline algorithm' (Slope), 'Noise ref. point [min]' (5,0874), and 'Slope ref. point [min]' (5,0874). It also has 'Auto' checkboxes and 'Set to default' buttons.

A 'Find peak(s)' button is located at the bottom right of the Parameters/Results section.

Appendix A: Graph Interface



The screenshot displays the CEval 0.2rc5 software interface. At the top, the window title is "CEval 0.2rc5" and the menu bar includes "File", "Options", and "Help". The main plot area is titled "DAD1C.ch" and shows a chromatogram with "Absorbance (mAU)" on the y-axis (ranging from 0 to 10) and time on the x-axis (ranging from 0 to 14). A single sharp peak is visible at approximately 11.5 minutes.

An "Adjust plot appearance" dialog box is open in the center, highlighted with a yellow border. It contains the following settings:

- Series: Signal
- Point style: No symbol
- Line color: Black (with a "Pick" button)
- Line thickness: 1,0
- Point color: Black (with a "Pick" button)
- Point size: 1
- Axis: X bottom
- Font size: 8
- Bold:
- Buttons: "Set for all axes", "OK", "Cancel"

A white text box with a black border is overlaid on the right side of the dialog box, containing the text: "You can adjust your plot in here."

The background interface includes an "Evaluation" section with a "Hyperbole fit" tab, a file path "Q:/Users/Magda/Eval/Eval data/LIAC_SEQ_DM_CD/D_MET_20_2.D/DAD1C.ch", and a "Common parameters" panel with fields for Capillary (cm), Detector (cm), Voltage (kV), Field strength (kV/m), c(Selector), and Time of EOF (min). Below this is a table for "Evaluated peaks" with columns for "Analyte" and "Time".

At the bottom right, there are several numerical input fields with "Auto" checkboxes, including "Peak from Y", "Peak to Y", "Peak height", "From", "To", "Baseline algorithm" (set to "Slope"), "Noise ref. point [min]", "Slope ref. point [min]", and "Noise LOD coeff". A "Find peak(s)" button is located at the bottom right corner.

Appendix A: Graph Interface



The screenshot displays the CEval 0.2rc5 software interface. The main window, titled "DAD1C.ch", shows a chromatogram with Absorbance (mAU) on the y-axis (0 to 10) and Time (min) on the x-axis (0 to 14). A single sharp peak is visible at approximately 11.5 minutes. An "Adjust plot appearance" dialog box is open in the center, with the "OK" button circled in red. A black box with white text "Confirm change." is overlaid on the dialog box. The background interface includes an "Evaluation" section with a "Hyperbole fit" tab, a "Common parameters" section with input fields for Capillary (cm), Detector (cm), Voltage (kV), Field strength (kV/m), and c(Selector), and an "Evaluated peaks" table. The table has columns for "Analyte" and "Time" and contains several rows of peak data with checkboxes for "Auto" and "Peak from Y". Other settings like "Peak window", "Slope window", "Noise", and "Baseline algorithm" are also visible.

Analyte	Time	Auto	Peak from Y
	8,0207	<input type="checkbox"/>	-0,7714 <input type="checkbox"/>
	8,4708	<input checked="" type="checkbox"/>	-0,71042 <input checked="" type="checkbox"/>
	8,2321	<input checked="" type="checkbox"/>	3,5574 <input checked="" type="checkbox"/>
	0,06375	<input checked="" type="checkbox"/>	

Appendix A: Graph Interface



CEval 0.2rc5

File Options Help

DAD1C.ch

Plot has changed.

Absorbance (mAU)

Time (minute)

Evaluation Hyperbole fit

File: Q:/Users/Magda/Eval/Eval data/LIAC_SEQ_DM_CD/D_MET_20_2.D/DAD1C.ch Close file

Common parameters

- Capillary (cm): 50,2
- Detector (cm): 41,7
- Voltage (kV): 15
- Field strength (kV/m): 29,88
- c(Selector): 0
- Time of EOF (min): 0

Read EOF time

Evaluated peaks

Analyte	Time	Area
---------	------	------

Add peak Delete peak

Cancel selection

Parameters Results

Peak properties Set to default

- Peak from X: 8,0207 Auto
- Peak to X: 8,4708 Auto
- Peak max at X: 8,2321 Auto
- Width 1/2 left (min): 0,06375 Auto
- Peak from Y: -0,7714 Auto
- Peak to Y: -0,71042 Auto
- Peak height: 3,5574 Auto

Finder parameters Set to default

- Window units: Minutes
- Noise window: 0,5
- Peak window: 0,5
- Slope window: 0,016666 Auto
- Noise: 0,040531 Auto
- Noise 1/3 coeff: 1
- From: 0 Auto
- To: 0 Auto
- Baseline algorithm: Slope
- Noise ref. point [min]: 5,0874
- Slope ref. point [min]: 5,0874 Auto
- Noise slope correction: Enable

Find peak(s)



Appendix B: Peak Not Found

Appendix B: Peak Not Found



The screenshot displays the CEval 0.4f software interface. At the top, the window title is "R2014-09-16-004.txt". Below the title bar is a menu with "File", "Options", and "Help". The main area shows a chromatogram with the y-axis labeled "(206nm)" ranging from 0 to 3 and the x-axis labeled "(time)" ranging from 0 to 8. The chromatogram shows a noisy baseline with two distinct peaks around 4.5 and 5.5 minutes.

Below the chromatogram is the "Evaluation" section, currently set to "Hyperbole fit". The file path is "C:/Users/R228/Desktop/R2014-09-16-004.txt".

On the left, the "Common parameters" section includes:

- Capillary (cm): 50,2
- Detector (cm): 41,7
- Voltage (kV): 15
- Field strength (kV/m): 29,88
- c(Selector): 0
- Time of EOF (min): 0

A "Read EOF time" button is located below these parameters.

In the center, a dialog box titled "No peak" is displayed, containing the message: "No peaks were found for the given parameters." and an "OK" button. This dialog box is highlighted with an orange border.

On the right, the "Evaluated peaks" table is empty. Below it are buttons for "Add peak", "Delete peak", and "Cancel selection".

At the bottom right, there are various input fields for peak parameters (Peak from X, Peak from Y, Peak max at X, Peak to X, Peak to Y, Peak height, v (1e-3 m/s), v (1e-3 m/s), u (1e-9 m.m/V/s), u (1e-9 m.m/V/s), Ht, Area (Units.min), t USP) and HVL parameters (a0, a1, a2, a3, x2, ε, Significant digits, Maximum iterations). A "Find peak(s)" button is located at the bottom right of the interface.

Appendix B: Peak Not Found



The screenshot displays the CEval 0.4f software interface. At the top, a menu bar includes 'File', 'Options', and 'Help'. The main window title is 'R2014-09-16-004.txt'. Below this is a chromatogram plot with 'COF(mm)' on the y-axis (ranging from -1 to 3) and 'time' on the x-axis (ranging from 0 to 8). The plot shows a baseline with two distinct peaks around 4.5 and 6 minutes.

Below the plot, the 'Evaluation' section is active, showing 'Hyperbole fit'. The file path is 'C:/Users/R228/Desktop/R2014-09-16-004.txt'. On the left, 'Common parameters' are listed: Capillary (cm) 50,2; Detector (cm) 41,7; Voltage (kV) 15; Field strength (kV/m) 29,88; c(Selector) 0; Time of EOF (min) 0. A 'Read EOF time' button is present.

In the center, the 'Evaluated peaks' section contains a table with columns 'Analyte', 'Time', and 'Area'. Below the table are buttons for 'Add peak', 'Delete peak', and 'Cancel selection'. A red circle highlights the 'Parameters' tab, which is also pointed to by a callout box containing the text 'Switch to parameters.'

On the right, the 'Parameters' tab is active, showing various input fields for EOF, Peak, and HVL. The EOF section includes v (1e-3 m/s), vt (1e-3 m/s), and u (1e-9 m.m/V/s), all set to 0. The Peak section includes Peak from X, Peak from Y, Peak max at X, Peak to X, Peak to Y, Peak height, v (1e-3 m/s), vt (1e-3 m/s), ut (1e-9 m.m/V/s), HI, Area (Units.min), and t USP, all set to 0. The HVL section includes a0, a1, a2, a3, x2, ε, Significant digits (50), and Maximum iterations (10). A 'Find peak(s)' button is located at the bottom right.

Appendix B: Peak Not Found



The screenshot displays the CEval 0.4f software interface. At the top, the file name is "R2014-09-16-004.txt". The main window shows an electropherogram with a y-axis labeled "(206nm)" and an x-axis labeled "min". A red circle highlights the initial baseline deviation at approximately 0.5 minutes. A text box with a pointer indicates: "Noise referent point is set to zero. That may cause trouble in case there is some deviation at the beginning of the electropherogram." The "Evaluation" tab is active, showing "Hyperbole fit" and the file path "C:/Users/R228/Desktop/R2014-09-16-...". The "Common parameters" section includes: Capillary (cm) 50,2; Detector (cm) 41,7; Voltage (kV) 15; Field strength (kV/m) 29,88; c(Selector) 0; Time of EOF (min) 0. The "Results" section shows various parameters: Peak max at X (0, Auto), Peak height (0, Auto), Peak width at 1/2 left (min) (0, Auto), Window units (Minutes), Noise window (0,5), Peak window (0,5), Slope window (1, Auto), Noise (1, Auto), Noise LOD coeff (1), Slope sensitivity (%) (50), Slope threshold (1, Auto), From (0, Auto), To (0, Auto), Baseline algorithm (Slope), Noise ref. point [min] (0), Slope ref. point [min] (0, Auto), Noise slope correction (Disable), and Show window (None). A "Find peak(s)" button is at the bottom right.

CEval 0.4f

File Options Help

R2014-09-16-004.txt

(206nm)

0 3

0 6 8

File: C:/Users/R228/Desktop/R2014-09-16-...

Evaluation Hyperbole fit

Common parameters

Capillary (cm) 50,2

Detector (cm) 41,7

Voltage (kV) 15

Field strength (kV/m) 29,88

c(Selector) 0

Time of EOF (min) 0

Read EOF time

Results

Peak max at X 0 Auto

Peak height 0 Auto

Peak width at 1/2 left (min) 0 Auto

Window units Minutes

Noise window 0,5

Peak window 0,5

Slope window 1 Auto

Noise 1 Auto

Noise LOD coeff 1

Slope sensitivity (%) 50

Slope threshold 1 Auto

From 0 Auto

To 0 Auto

Baseline algorithm Slope

Noise ref. point [min] 0

Slope ref. point [min] 0 Auto

Noise slope correction Enable

Show window None

Add peak Delete peak Cancel selection

Find peak(s)

Appendix B: Peak Not Found



The screenshot displays the CEval 0.4f software interface. At the top, a menu bar includes 'File', 'Options', and 'Help'. The main window title is 'R2014-09-16-004.txt'. Below this is a chromatogram plot with 'Abundance' on the y-axis (0 to 3) and 'time' on the x-axis (0 to 8). A red oval highlights a region on the baseline at approximately 2 minutes. The 'Evaluation' section is active, showing 'Hyperbole fit' as the method. The 'File' field contains 'C:/Users/R228/Desktop/R2014-09-16-004.txt'. The 'Common parameters' section includes: Capillary (cm) 50,2; Detector (cm) 41,7; Voltage (kV) 15; Field strength (kV/m) 29,88; c(Selector) 0; Time of EOF (min) 0. The 'Evaluated peaks' table is empty. The 'Finder parameters' section includes: Window units (Minutes), Noise window (0,5), Peak window (0,5), Slope window (1, Auto), Noise (1, Auto), Noise LOD coeff (1), Slope sensitivity (%) (50), Slope threshold (1, Auto), Peak height (0, Auto), Width 1/2 left (min) (0), From (0, Auto), To (0, Auto), Baseline algorithm (Slope), Noise ref. point [min] (2), Slope ref. point [min] (0, Auto), Noise slope correction (None), and Show window (None). A red oval highlights the 'Find peak(s)' button. Two callout boxes provide instructions: 'Set it to a reasonable time (no disturbances).' pointing to the 'Noise ref. point [min]' field, and 'Try find peak again.' pointing to the 'Find peak(s)' button.

File: C:/Users/R228/Desktop/R2014-09-16-004.txt

Common parameters

- Capillary (cm): 50,2
- Detector (cm): 41,7
- Voltage (kV): 15
- Field strength (kV/m): 29,88
- c(Selector): 0
- Time of EOF (min): 0

Evaluated peaks

Analyte	Time	Area
---------	------	------

Finder parameters

- Window units: Minutes
- Noise window: 0,5
- Peak window: 0,5
- Slope window: 1 Auto
- Noise: 1 Auto
- Noise LOD coeff: 1
- Slope sensitivity (%): 50
- Slope threshold: 1 Auto
- Peak height: 0 Auto
- Width 1/2 left (min): 0
- From: 0 Auto
- To: 0 Auto
- Baseline algorithm: Slope
- Noise ref. point [min]: 2
- Slope ref. point [min]: 0 Auto
- Noise slope correction: Enable
- Show window: None

Set it to a reasonable time (no disturbances).

Try find peak again.

Find peak(s)

Appendix B: Peak Not Found



The screenshot displays the CEval 0.4f software interface. At the top, the file name is R2014-09-16-004.txt. The main window shows a chromatogram with a y-axis labeled 'C(06mm)' ranging from 0 to 3 and an x-axis labeled '(time)' ranging from 0 to 8. Two peaks are visible: a small peak at approximately 4.3 minutes and a larger peak at approximately 5.8 minutes. A dialog box titled 'Dialog' is open in the center, with the title 'Select peak:'. It contains a table with the following data:

Number	Time of maximum
3	4,24042
4	4,33042
5	5,58208
6	5,80042
7	6,04208

The dialog box has 'Select' and 'Cancel' buttons. Below the dialog box, a white box with a black border contains the text 'Peaks were succesfully found.' (Note the spelling error in the original image). The software interface also shows various settings panels, including 'Common parameters' (Capillary, Detector, Voltage, Field strength, c(Selector), Time of EOF) and 'Evaluated peaks' (Analyte, Time). The 'Find peak(s)' button is visible at the bottom right.



Appendix C: Changing decimal digits

Appendix C: Changing Decimal Digits



CEval 0.2rc5

File **Options** Help

DAD1C.ch

Absorbance (mAU)

Time (minute)

Click on Options.

Evaluation: Hyperbole fit

File: Q:\Users\Magda\Eval\Eval data\LIAC_SEQ_DM_CD\D_MET_20_2.D\DAD1C.ch

Common parameters

Capillary (cm)	50,2
Detector (cm)	41,7
Voltage (kV)	15
Field strength (kV/m)	29,88
c(Selector)	0
Time of EOF (min)	0

Read EOF time

Evaluated peaks

Analyte	Time	Area
---------	------	------

Add peak Delete peak Cancel selection

Parameters Results

Peak properties

Peak from X	8,0207	<input type="checkbox"/> Auto	Peak from Y	-0,7714	<input type="checkbox"/> Auto
Peak to X	8,4708	<input checked="" type="checkbox"/> Auto	Peak to Y	-0,71042	<input checked="" type="checkbox"/> Auto
Peak max at X	8,2321	<input checked="" type="checkbox"/> Auto	Peak height	3,5574	<input checked="" type="checkbox"/> Auto
Width 1/2 left (min)	0,06375	<input checked="" type="checkbox"/> Auto			

Finder parameters

Window units	Minutes	From	0	<input checked="" type="checkbox"/> Auto
Noise window	0,5	To	0	<input checked="" type="checkbox"/> Auto
Peak window	0,5	Baseline algorithm	Slope	
Slope window	0,016666	Noise ref. point [min]	5,0874	
Noise	0,040531	Slope ref. point [min]	5,0874	<input checked="" type="checkbox"/> Auto
Noise LOD coeff	1	Noise slope correction	<input type="checkbox"/> Enable	

Find peak(s)

Appendix C: Changing Decimal Digits



The screenshot displays the CEval 0.2rc5 software interface. At the top, the menu bar includes 'File', 'Options', and 'Help'. The 'Options' menu is open, with 'Set number format' highlighted by a red oval. The main window shows a chromatogram titled 'DAD1C.ch' with 'Absorbance (mAU)' on the y-axis and 'Time (minute)' on the x-axis. A peak at approximately 8.7 minutes is highlighted with a blue dashed line and a vertical red line. A black box with the text 'Set number format' is overlaid on the plot area.

Below the plot, the 'Evaluation' section is active, showing 'Hyperbole fit' as the selected method. The file path is 'Q:\Users\Magda\Eval\Eval data\LIAC_SEQ_DM_CD\D_MET_20_2.D\DAD1C.ch'. The interface is divided into several panels:

- Common parameters:** Capillary (cm) 50,2; Detector (cm) 41,7; Voltage (kV) 15; Field strength (kV/m) 29,88; c(Selector) 0; Time of EOF (min) 0. A 'Read EOF time' button is present.
- Evaluated peaks:** A table with columns 'Analyte', 'Time', and 'Area'. Buttons for 'Add peak', 'Delete peak', and 'Cancel selection' are at the bottom.
- Parameters / Results:** A detailed parameter list for the fit, including EOF parameters (v, u), Peak parameters (Peak from X, Peak to X, Peak height, etc.), HVL parameters (a0, a1, a2, a3, X2, Significant digits, Maximum iterations), and a1 u1. Buttons for 'Replot HVL' and 'Do HVL fit' are included.

A 'Find peak(s)' button is located at the bottom right of the evaluation section.

Appendix C: Changing Decimal Digits



The screenshot displays the CEval 0.2rc5 software interface. At the top, the window title is 'CEval 0.2rc5' and the file name is 'DAD1C.ch'. The main plot shows 'Absorbance (mAU)' on the y-axis (0 to 10) versus time on the x-axis (0 to 14). Two peaks are visible: a small peak at approximately 7.6 minutes and a larger peak at approximately 11.8 minutes. A 'Set number format' dialog box is open in the center, with a red circle around it. The dialog box has the following fields:

- Display trailing zeros:
- Digits:
- Buttons: Set, Cancel

To the right of the dialog box, a white text box contains the following text:

You can change number of decimal digits displayed and whether you want to see trailing zeros.

The software interface also includes a 'Common parameters' section on the left with the following values:

- Capillary (cm): 50,2
- Detector (cm): 41,7
- Voltage (kV): 15
- Field strength (kV/m): 29,88
- c(Selector): 0
- Time of EOF (min): 0

At the bottom, there are buttons for 'Add peak', 'Delete peak', 'Cancel selection', and 'Find peak(s)'. The 'HVL' section at the bottom right shows various parameters like a0, a1, a2, a3, x2, and Maximum iterations.

Appendix C: Changing Decimal Digits



The screenshot shows the CEval 0.2rc5 software interface. At the top, the window title is "DAD1C.ch". Below the title bar is a menu with "File", "Options", and "Help". The main area displays a chromatogram with "Absorbance (mAU)" on the y-axis (0 to 10) and time on the x-axis (0 to 14). Two peaks are visible: a smaller one at approximately 8.7 minutes and a larger one at approximately 11.5 minutes. A blue fit line is overlaid on the smaller peak.

In the foreground, a "Set number format" dialog box is open. It has a "Display trailing zeros:" checkbox which is checked, and a "Digits:" input field containing the number "4". The "Set" button is circled in red. Below the dialog box, a white callout box with a black border contains the text "Confirm change."

The background interface includes an "Evaluation" section with a "Hyperbole fit" tab. Below this is a "File:" field with the path "Q:/Users/Magda/Eval/Eval data/LIAC_SEQ_DM_CD/D_MET_20_2.D". There are several input fields for "Common parameters":
Capillary (cm): 50,2
Detector (cm): 41,7
Voltage (kV): 15
Field strength (kV/m): 29,88
c(Selector): 0
Time of EOF (min): 0
A "Read EOF time" button is located below these fields.

On the right side, there are several data fields and buttons:
- "Close file" button
- A table of peak data:
 7,6325 Peak from Y: -0,76449 Peak max at X: 8,2321
 8,7467 Peak to Y: -0,75191 Peak height: 3,1966
 8,8426 v! (1e-3 m/s): inf u! (1e-9 m.m/V/s): 3,6437e-293
 3,9543 Area (Units.min): 0,64522 t USP: 1,0841
- "HVL" section with fields for a0 (0,64522), a1 (8,2564), a2 (0,062129), a3 (0,98114), x2 (0), and epsilon (1e-09). There are checkboxes for "Fixed" and a "Maximum iterations" field set to 10.
- "Replot HVL" and "Do HVL fit" buttons.
- "Add peak", "Delete peak", and "Cancel selection" buttons at the bottom.

Appendix C: Changing Decimal Digits



CEval 0.2rc5
File Options Help

DAD1C.ch

Absorbance (mAU)

Time (minute)

CEval will display change with the next output. Try e. g. to find peak again.

Evaluation Hyperbole fit

File: Q:/Users/Magda/Eval/Eval data/LIAC_SEQ_DM_CD/D_MET_20_2.D/DAD1C.ch Close file

Common parameters

Capillary (cm) 50,2
Detector (cm) 41,7
Voltage (kV) 15
Field strength (kV/m) 29,88
c(Selector) 0
Time of EOF (min) 0
Read EOF time

Evaluated peaks

Analyte	Time	Area
---------	------	------

Add peak Delete peak Cancel selection

Parameters Results

EOF
v (1e-3 m/s) inf v! (1e-3 m/s) 0 u (1e-9 m.m/V/s) inf

Peak
Peak from X 7,6325 Peak from Y -0,76449 Peak max at X 8,2321
Peak to X 8,7467 Peak to Y -0,75191 Peak height 3,1966
v (1e-3 m/s) 0,84426 v! (1e-3 m/s) inf u! (1e-9 m.m/V/s) 3,6437e-293
H! 3,9543 Area (Units.min) 0,64522 t USP 1,0841

HVL
a0 0,64522 Fixed a1 8,2564 Fixed
a2 0,062129 Fixed a3 0,98114 Fixed
χ2 0 ε 1e-09
Significant digits 50 Maximum
a1 u! (1e-9 m.m/V/s) inf

Find peak again.

Find peak(s)

Appendix C: Changing Decimal Digits



CEval 0.2rc5

DAD1C.ch

Absorbance (mAU)

10
8
6
4
2
0

0 2 10 12 14

File Options Help

Hyperbole fit

File: Q:/Users/Magda/Eval/Eval data/LIAC_SEQ_DM_CD/D_MET_20_2.D

Common parameters

Capillary (cm) 50,2
Detector (cm) 41,7
Voltage (kV) 15
Field strength (kV/m) 29,88
c(Selector) 0
Time of EOF (min) 0

Read EOF time

Dialog

Select peak:

Number	Time of maximum
1	8,231.67
2	11,473.3

Select Cancel

7,6325 Peak from Y -0,76449 Peak max at X 8,2321
8,7467 Peak to Y -0,75191 Peak height 3,1966
1,84426 v! (1e-3 m/s) inf u! (1e-9 m.m/V/s) 3,6437e-293
3,9543 Area (Units.min) 0,64522 t USP 1,0841

HVL

a0 0,64522 Fixed a1 8,2564 Fixed
a2 0,062129 Fixed a3 0,98114 Fixed
x2 0 ε 1e-09
Significant digits 50 Maximum iterations 10

a1 u! (1e-9 m.m/V/s) inf

Replot HVL Do HVL fit

Find peak(s)

Confirm.

Appendix C: Changing Decimal Digits



CEval 0.2rc5

File Options Help

DAD1C.ch

Y-axis: Absorbance (mAU)
X-axis: Time (minute)

File: Q:/Users/Magda/Eval/Eval data/LIAC_SEQ_DM_CD/D_MET_20_2.D/DAD1C.ch

Common parameters

Capillary (cm)	50,2
Detector (cm)	41,7
Voltage (kV)	15
Field strength (kV/m)	29,88
c(Selector)	0
Time of EOF (min)	0

Read EOF time

Evaluated peaks

Add peak Delete peak Cancel selection

Parameters Results

Parameters

EOF

v (1e-3 m/s)	inf	v! (1e-3 m/s)	0,0000	u (1e-9 m.m/V/s)	inf
--------------	-----	---------------	--------	------------------	-----

Peak

Peak from X	7,6325	Peak from Y	-0,7645	Peak max at X	8,2321
Peak to X	8,7467	Peak to Y	-0,7519	Peak height	3,1966
v (1e-3 m/s)	0,8443	v! (1e-3 m/s)	inf	u! (1e-9 m.m/V/s)	0,0000
H!	3,9543	Area (Units.min)	0,6452	t USP	1,0841

HVL

a0	0,6452	<input type="checkbox"/> Fixed	a1	8,2564	<input type="checkbox"/> Fixed
a2	0,0621	<input type="checkbox"/> Fixed	a3	0,9811	<input type="checkbox"/> Fixed
x2	0,0000		ε	0,0000	
Significant digits	50		Maximum iterations	10	
a1 u! (1e-9 m.m/V/s)	inf				

Replot HVL Do HVL fit

Find peak(s)

Numbers format has changed.



Appendix D: Distorted Peak

Appendix D: Distorted Peak



CEval 0.4e

File Options Help

DAD1C.ch

Peak is somehow disrupted and cannot be evaluated automatically.

Evaluation Hyperbole fit

File: Q:/Users/Magda/CEval/CEval data/LIAC_SEQ_OS_CD/L_MET_10_4.D/DAD1C.ch Close file

Common parameters

- Capillary (cm) 50,2
- Detector (cm) 41,7
- Voltage (kV) 15
- Field strength (kV/m) 29,88
- c(Selector) 0
- Time of EOF (min) 0 Read EOF time

Evaluated peaks

Analyte	Time	Area
---------	------	------

Add peak Delete peak
Cancel selection

Parameters Results

EOF

- v (1e-3 m/s) 0 vI (1e-3 m/s) 0 u (1e-9 m.m/V/s) 0

Peak

- Peak from X 0 Peak from Y 0 Peak max at X 0
- Peak to X 0 Peak to Y 0 Peak height 0
- v (1e-3 m/s) 0 vI (1e-3 m/s) 0 uI (1e-9 m.m/V/s) 0
- H! 0 Area (Units.min) 0 t USP 0

HVL

- a0 0 Fixed a1 0 Fixed
- a2 0 Fixed a3 0 Fixed
- X2 0 e 1e-09
- Significant digits 50 Maximum iterations 10

Find peak(s)

Appendix D: Distorted Peak



The screenshot displays the CEval 0.4e software interface. At the top, a chromatogram titled "DAD1C.ch" plots Absorbance (mAU) on the y-axis (ranging from 0 to 10) against Time (minute) on the x-axis (ranging from 10,8 to 11,6). A peak is visible around 11,2 minutes, with a blue curve representing the fit and a red horizontal line indicating the baseline. A callout box on the right states: "HVL fit of the whole peak is nonsensical. We want to evaluate part of the peak only."

Below the chromatogram, the "Evaluation" section is active, showing "Hyperbole fit" as the selected method. The file path is "Q:/Users/Magda/CEval data/LIAC_SEQ_OS_CD/L_MET_10_4.D/DAD1C.ch".

The "Evaluated peaks" section contains a table with columns for "Analyte", "Time", and "Area". A callout box points to the "Parameters" tab, stating: "Switch to Parameters." The "Parameters" tab is currently selected and circled in red. It displays the following data:

Peak			
Peak from X	10,842	Peak from Y	2,3203
Peak to X	11,382	Peak to Y	2,3577
v (1e-3 m/s)	0,62364	vf (1e-3 m/s)	inf
H!	8,094	Area (Units.min)	1,0007
Peak max at X	11,144	Peak height	10,435
u! (1e-9 m.m/V/s)	2,0944e-302	t USP	0,67347

Below the peak data, the "HVL" section contains the following parameters:

HVL					
a0	0,9801	<input type="checkbox"/> Fixed	a1	11	<input type="checkbox"/> Fixed
a2	0,043476	<input type="checkbox"/> Fixed	a3	-10,973	<input type="checkbox"/> Fixed
χ ²	0	ε	1e-09		
Significant digits	50	Maximum iterations	10		
a1 u! (1e-9 m.m/V/s)	inf				

Buttons for "Replot HVL" and "Do HVL fit" are located below the HVL parameters. At the bottom right, a "Find peak(s)" button is visible.

Appendix D: Distorted Peak



The screenshot displays the CEval 0.4e software interface. At the top, a chromatogram titled "DAD1C.ch" shows Absorbance (mAU) on the y-axis (ranging from 0 to 10) and Time (minute) on the x-axis (ranging from 10,8 to 11,6). A peak is visible around 11,2 minutes, with a blue vertical line indicating its position and a red horizontal line indicating the baseline. Below the chromatogram, the "Evaluation" tab is active, showing a "Hyperbole fit" model. The "Common parameters" section includes fields for Capillary (cm), Detector (cm), Voltage (kV), Field strength (kV/m), c(Selector), and Time of EOF (min). The "Evaluated peaks" table is empty. The "Parameters" section is expanded to show "Peak properties" and "Window parameters". The "Peak properties" section includes fields for Peak from X, Peak to X, Peak max at X, Width 1/2 IeB, Peak from Y, Peak to Y, and Peak height. The "Peak from X" and "Peak from Y" fields are circled in red. The "Window parameters" section includes fields for Window units, Noise window, Peak window, Slope window, From, To, Baseline algorithm, and Noise ref. point [min]. A callout box with a black border and white background points to the "Peak from X" and "Peak from Y" fields with the text: "We want to change peak beginning. Check off „auto“."

File: Q:/Users/Magda/CEval/CEval data/LIAC_SEQ_OS_CD/L_MET_10_4.D/DAD1C.ch

Common parameters

Capillary (cm)	50,2
Detector (cm)	41,7
Voltage (kV)	15
Field strength (kV/m)	29,88
c(Selector)	0
Time of EOF (min)	0

Evaluated peaks

Analyte	Time	Area
---------	------	------

Parameters

Peak properties

Peak from X	10,842	<input checked="" type="checkbox"/> Auto	Peak from Y	2,3203	<input checked="" type="checkbox"/> Auto
Peak to X	11,382	<input checked="" type="checkbox"/> Auto	Peak to Y	2,3577	<input checked="" type="checkbox"/> Auto
Peak max at X	11,144	<input checked="" type="checkbox"/> Auto	Peak height	10,435	<input checked="" type="checkbox"/> Auto
Width 1/2 IeB		<input checked="" type="checkbox"/> Auto			

Window parameters

Window units	Minutes	From	0	<input checked="" type="checkbox"/> Auto
Noise window	0,5	To	0	<input checked="" type="checkbox"/> Auto
Peak window	0,5	Baseline algorithm	Slope	
Slope window	0,034999	<input checked="" type="checkbox"/> Auto	Noise ref. point [min]	0

Buttons: Add peak, Delete peak, Cancel selection, Find peak(s)

Appendix D: Distorted Peak



The screenshot displays the CEval 0.4e software interface. At the top, a menu bar includes 'File', 'Options', and 'Help'. The main window title is 'DAD1C.ch'. The central plot shows 'Absorbance (mAU)' on the y-axis (ranging from 0 to 10) and 'Time (minute)' on the x-axis (ranging from 10,8 to 11,6). A peak is visible, with a red vertical line at 11,1279 and a blue vertical line at 2,3313. A callout box with a black border and white background points to the red line, containing the text: "Then click on the place where you want the peak to begin." Below the plot, the 'Evaluation' tab is active, showing 'Hyperbole fit'. The 'File' field contains the path: 'Q:/Users/Magda/CEval data/LIAC_SEQ_OS_CD/L_MET_10_4.D/DAD1C.ch'. On the left, the 'Common parameters' section includes input fields for 'Capillary (cm)' (50,2), 'Detector (cm)' (41,7), 'Voltage (kV)' (15), 'Field strength (kV/m)' (29,88), 'c(Selector)' (0), and 'Time of EOF (min)' (0), with a 'Read EOF time' button. The 'Evaluated peaks' section contains a table with columns 'Analyte', 'Time', and 'Area', and buttons for 'Add peak', 'Delete peak', and 'Cancel selection'. On the right, the 'Parameters' and 'Results' tabs are visible. The 'Peak properties' section includes fields for 'Peak from X' (10,842), 'Peak to X' (11,382), 'Peak max at X' (11,144), 'Width 1/2 left (min)' (0,053333), 'Peak from Y' (2,3203), 'Peak to Y' (2,3577), and 'Peak height' (10,435). The 'Finder parameters' section includes 'Window units' (Minutes), 'Noise window' (0,5), 'Peak window' (0,5), 'Slope window' (0,034999), 'From' (0), 'To' (0), and 'Baseline algorithm' (Slope). A 'Find peak(s)' button is located at the bottom right.

Appendix D: Distorted Peak



The screenshot displays the CEval 0.4e software interface. At the top, a chromatogram titled "DAD1C.ch" shows Absorbance (mAU) on the y-axis (0 to 10) and time on the x-axis (10.8 to 11.6). A peak is visible around 11.144 minutes, with a blue vertical line indicating its position. A context menu is open over the peak, listing several options. The option "Peak from this X,Y" is circled in red. A callout box with a black border and white background points to this option, containing the text "Select „Peak from this X, Y“".

Below the chromatogram, the "Evaluation" section is active, showing "Hyperbole fit" as the selected method. The file path is "Q:/Users/Magda/CEval/CEval data/LIAC_SEQ_OS_CD/L_MET_10_4.D/DAD1C.ch".

The "Common parameters" section includes:

- Capillary (cm): 50,2
- Detector (cm): 41,7
- Voltage (kV): 15
- Field strength (kV/m): 29,88
- c(Selector): 0
- Time of EOF (min): 0

The "Evaluated peaks" table is empty, with columns for "Analyte", "Time", and "Area".

The "Peak properties" section includes:

- Peak from X: 10,842 Auto
- Peak to X: 11,382 Auto
- Peak max at X: 11,144 Auto
- Width 1/2 left (min): 0,053333 Auto
- Peak from Y: 2,3203 Auto
- Peak to Y: 2,3577 Auto
- Peak height: 10,435 Auto

The "Finder parameters" section includes:

- Window units: Minutes
- Noise window: 0,5
- Peak window: 0,5
- Slope window: 0,034999 Auto
- From: 0 Auto
- To: 0 Auto
- Baseline algorithm: Slope
- Noise ref. point [min]: 0

Buttons for "Add peak", "Delete peak", "Cancel selection", and "Find peak(s)" are visible at the bottom.

Appendix D: Distorted Peak



The screenshot displays the CEval 0.4e software interface. At the top, a chromatogram titled "DAD1C.ch" shows Absorbance (mAU) on the y-axis (ranging from 0 to 10) and Time (minute) on the x-axis (ranging from 10,8 to 11,6). A peak is visible around 11,2 minutes, with a blue curve representing the fit and a red curve representing the baseline. A black box with white text "Peak beginning changed." is positioned to the right of the peak.

Below the chromatogram, the "Evaluation" section is active, showing a "Hyperbole fit" tab. The file path is "Q:/Users/Magda/CEval/CEval data/LIAC_SEQ_OS_CD/L_MET_10_4.D/DAD1C.ch".

The "Common parameters" section includes:

- Capillary (cm): 50,2
- Detector (cm): 41,7
- Voltage (kV): 15
- Field strength (kV/m): 29,88
- c(Selector): 0
- Time of EOF (min): 0

The "Evaluated peaks" section contains a table with columns for Analyte, Time, and Area. Below the table are buttons for "Add peak", "Delete peak", and "Cancel selection".

The "Parameters" section is currently selected, but a red circle highlights the "Results" tab. A callout box with a black border and white text "Switch back to Results." points to the "Results" tab. The "Parameters" section includes:

- Peak properties: Peak from X (11,127), Peak to X (11,382), Peak max at X (11,144), Width 1/2 left (min) (0,0175), Peak from Y (2,3313), Peak to Y (2,3577), Peak height (10,435).
- Finder parameters: Window units (Minutes), Noise window (0,5), Peak window (0,5), Slope window (0,034999), From (0), To (0), Baseline algorithm (Slope), Noise ref. point [min] (0).

Buttons for "Set to default" and "Find peak(s)" are also visible.

Appendix D: Distorted Peak



The screenshot displays the CEval 0.4e software interface. At the top, a plot titled "DAD1C.ch" shows Absorbance (mAU) on the y-axis (ranging from 0 to 10) and Time (minute) on the x-axis (ranging from 10.8 to 11.6). A peak is visible around 11.15 minutes, which is highlighted by a purple rounded rectangle. The peak is distorted, with a blue curve representing the fit and a red curve representing the actual data. A vertical blue line marks the peak maximum at approximately 11.144 minutes.

A callout box with a black border and white background contains the text: "The HVL parameters are now wrongly estimated. It is necessary to estimate them manually." This box is connected to the HVL parameters section of the software interface.

The software interface includes a menu bar (File, Options, Help) and a toolbar. The main window is divided into several panels:

- Common parameters:** Includes fields for Capillary (cm), Detector (cm), Voltage (kV) (set to 15), Field strength (kV/m) (set to 29,88), c(Selector) (set to 0), and Time of EOF (min) (set to 0). A "Read EOF time" button is present.
- Parameters:** Contains a table of peak data and HVL parameters.
- Results:** Contains a table of peak data.

The **Parameters** panel shows the following data:

Parameter	Value	Fixed
Peak from X	11,128	
Peak from Y	2,3313	
Peak max at X	11,144	
Peak to X	11,382	
Peak to Y	2,3577	
Peak height	10,435	
v (1e-3 m/s)	0,62364	
vf (1e-3 m/s)	inf	
ul (1e-9 m.m/V/s)	1,7736e-230	
Hl	8,1022	
Area (Units.min)	0,44178	
t USP	2,7368	

The **HVL** parameters are listed below:

Parameter	Value	Fixed
a0	0,44178	<input type="checkbox"/>
a1	11,215	<input type="checkbox"/>
a2	0,016459	<input type="checkbox"/>
a3	14,552	<input type="checkbox"/>

Other parameters include Significant digits (50) and Maximum iterations (10). Buttons for "Replot HVL" and "Do HVL fit" are available. The "Peak dimensions" section is currently empty.

Appendix D: Distorted Peak



The screenshot displays the CEval 0.4e software interface. At the top, a chromatogram titled "DAD1C.ch" shows Absorbance (mAU) on the y-axis (ranging from 0 to 12) and Time (minute) on the x-axis (ranging from 10,8 to 11,6). A peak is visible at approximately 11,15 minutes, with a blue curve representing the fit and a red curve representing the baseline. The peak is annotated with a vertical blue line at its maximum and a horizontal red line at its baseline.

Below the chromatogram, the "Evaluation" section is active, showing a "Hyperbole fit" model. The file path is "Q:/Users/Magda/CEval/CEval data/LIAC_SEQ_OS_CD/L_MET_10_4.0/DAD1C.ch".

The "Common parameters" section includes:

- Capillary (cm): 50,2
- Detector (cm): 41,7
- Voltage (kV): 15
- Field strength (kV/m): 29,88
- c(Selector): 0
- Time of EOF (min): 0

The "Evaluated peaks" table is empty.

The "Parameters" section shows the following values:

Parameter	Value	Unit/Note
Peak from X	11,127	
Peak from Y	2,4453	
Peak max at X	11,144	
Peak to X	11,382	
Peak to Y	2,3577	
Peak height	10,435	
v (1e-3 m/s)	0,62364	
vt (1e-3 m/s)	inf	
ut (1e-9 m.m/V/s)	1,7736e-230	
Hl	7,9959	
Area (Units.min)	0,4455	
t USP	2,3864	

The "HVL" section includes parameters a0, a1, a2, a3, and a4, with values 0,45, 11,15, 0,02, 0, and 1e-00 respectively. The "Significant digits" is set to 50 and "Maximum iterations" is 10.

A callout box with a black border and white background contains the text: "Replot HVL to see your estimate." A black arrow points from this box to a blue button labeled "Replot HVL" in the "HVL" section, which is circled in red. Another black arrow points from the callout box to the "Do HVL fit" button.

Buttons for "Add peak", "Delete peak", "Cancel selection", and "Find peak(s)" are also visible.

Appendix D: Distorted Peak



The screenshot displays the CEval 0.4e software interface. At the top, a chromatogram titled "DAD1C.ch" shows Absorbance (mAU) on the y-axis (ranging from 0 to 12) and Time (minute) on the x-axis (ranging from 10,8 to 11,6). A peak is visible around 11,15 minutes, which is highlighted by a purple rounded rectangle. A blue curve represents the fit to this peak, and a red horizontal line indicates the baseline. Below the chromatogram, the "Evaluation" tab is active, showing a "Hyperbole fit" method. The file path is "Q:/Users/Magda/CEval/CEval data/LIAC_SEQ_OS_CD/L_MET_10_4.D/DAD1C.ch".

The "Parameters" window is open, showing the following data:

Common parameters	
Capillary (cm)	50,2
Detector (cm)	41,7
Voltage (kV)	15
Field strength (kV/m)	29,88
c(Selector)	0
Time of EOF (min)	0

Evaluated peaks		
Analyte	Time	Area

Parameters		Results	
Peak			
Peak from X	11,127	Peak from Y	2,4453
Peak to X	11,382	Peak to Y	2,3577
v (1e-3 m/s)	0,62364	vt (1e-3 m/s)	inf
H!	7,9959	Area (Units.min)	0,4455
HVL		Peak max at X	11,144
a0	0,45	Peak height	10,435
a2	0,02	ul (1e-9 m.m/V/s)	1,7736e-230
x2	0	t USP	2,3864
Significant digits	50	a1	11,15
		a3	0
		ε	1e-09
		Maximum iterations	10

Buttons: "Delete peak", "Cancel selection", "Do HVL fit" (circled in red), "Find peak(s)".

If the estimate looks „safe“, try HVL fit.

Appendix D: Distorted Peak



The screenshot shows the CEval 0.4e software interface. At the top, a plot titled "DAD1C.ch" displays Absorbance (mAU) on the y-axis (ranging from 0 to 12) and Time (minute) on the x-axis (ranging from 10,8 to 11,2). A peak is visible around 11,15 minutes, with a fitted curve overlaid. A callout box points to the peak with the text "Fit finished with 8 iterations."

The software interface includes several panels:

- Evaluation:** Hyperbole fit
- File:** Q:/Users/Magda/CEval/CEval data/LIAC_SEQ_OS_CD/L_MET_10_4.D/DAD1C.ch
- Common parameters:**
 - Capillary (cm): 50,2
 - Detector (cm): 41,7
 - Voltage (kV): 15
 - Field strength (kV/m): 29,88
 - c(Selector): 0
 - Time of EOF (min): 0
 - Read EOF time button
- Evaluated peaks:** A table with columns for Analyte and Time. Buttons for "Add peak", "Delete peak", and "Cancel selection" are present.
- Fit Parameters:**
 - 11,127 Peak from Y: 2,4453
 - 11,382 Peak to Y: 2,3577
 - 0,62364 v_f (1e-3 m/s): inf
 - 7,9959 H_l: Area (Units.min): 0,4455
 - Peak max at X: 11,144
 - Peak height: 10,435
 - u_l (1e-9 m.m/V/s): 1,7736e-230
 - t USP: 2,3864
- HVL Parameters:**
 - a0: 0,45 (Fixed)
 - a1: 11,15 (Fixed)
 - a2: 0,02 (Fixed)
 - a3: 0 (Fixed)
 - χ²: 0
 - ε: 1e-09
 - Significant digits: 50
 - Maximum iterations: 10
 - a1 u_l (1e-9 m.m/V/s): inf
 - Buttons: Replot HVL, Do HVL fit
- Peak dimensions:** Find peak(s) button

The "HVL Fit" dialog box displays the following information:

- Iterations: 8
- old value -> new value:
- Sigma: 0.631076 -> 0.0302086
- a1: 11.15 -> 11.1052
- Time elapsed (sec): 1.886
- OK button

Appendix D: Distorted Peak



CEval 0.4e

File Options Help

DAD1C.ch

Partial HVL fit was successful.

Evaluation Hyperbole fit

File: Q:/Users/Magda/CEval/CEval data/LIAC_SEQ_OS_CD/L_MET_10_4.D/DAD1C.ch Close file

Common parameters

Capillary (cm) 50,2
Detector (cm) 41,7
Voltage (kV) 15
Field strength (kV/m) 29,88
c(Selector) 0
Time of EOF (min) 0
Read EOF time

Evaluated peaks

Analyte	Time	Area
---------	------	------

Add peak Delete peak Cancel selection

Parameters Results

Peak

Peak from X 11,127 Peak from Y 2,4453 Peak max at X 11,144
Peak to X 11,382 Peak to Y 2,3577 Peak height 10,435
v (1e-3 m/s) 0,62364 vt (1e-3 m/s) inf ul (1e-9 m.m/V/s) 1,7736e-230
Hl 7,9959 Area (Units.min) 0,4455 t USP 2,3864

HVL

a0 0,74007 Fixed a1 11,105 Fixed
a2 0,035618 Fixed a3 -2,8648 Fixed
b0 0 b1 1e-09
Significant digits 50 Maximum iterations 10
a1 ul (1e-9 m.m/V/s) inf Replot HVL Do HVL fit

Peak dimensions Find peak(s)