CEval

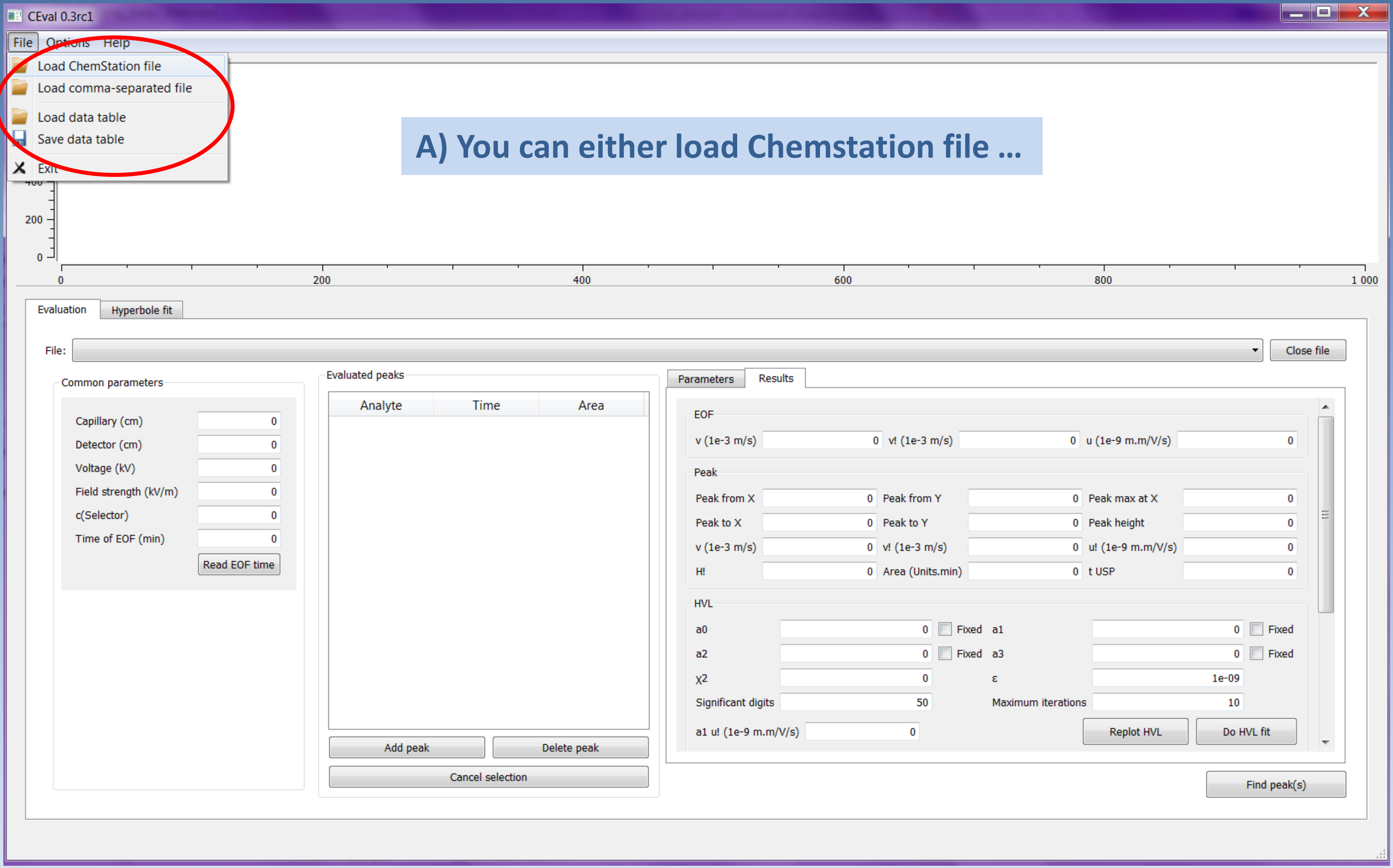
software tool for CE and ACE data evaluation

Step-by-step User Guide

CEval - User Guide

Opening Data

Opening Data



A) You can either load Chemstation file …

File:

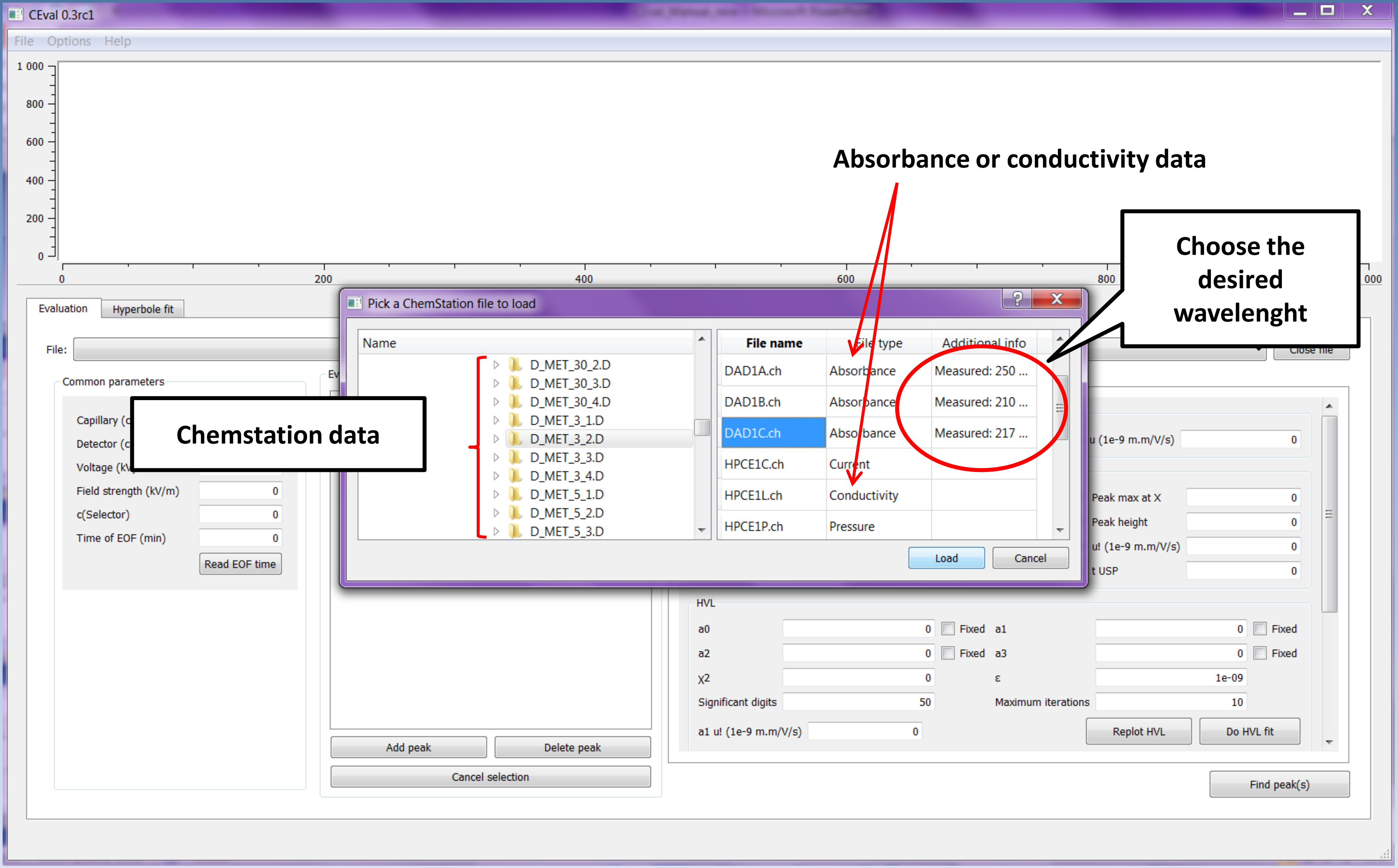
Capillary (cm) 0
Detector (cm) 0
Voltage (kV) 0
Field strength (kV/m) 0
c(Selector) 0
Time of EOF (min) 0

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
χ2 0
ε 1e-09
Significant digits 50
Maximum iterations 10
a1 u! (1e-9 m.m/V/s) 0

Opening Data



Capillary (c
Detector (c
Voltage (kV
Field strength (kV/m) 0
c(Selector) 0
Time of EOF (min) 0

Name
- D_MET_30_2.D
- D_MET_30_3.D
- D_MET_30_4.D
- D_MET_3_1.D
- D_MET_3_2.D
- D_MET_3_3.D
- D_MET_3_4.D
- D_MET_5_1.D
- D_MET_5_2.D
- D_MET_5_3.D

File name	File type	Additional info
DAD1A.ch	Absorbance	Measured: 250 ...
DAD1B.ch	Absorbance	Measured: 210 ...
DAD1C.ch	Absorbance	Measured: 217 ...
HPCE1C.ch	Current	
HPCE1L.ch	Conductivity	
HPCE1P.ch	Pressure	

u (1e-9 m.m/V/s) 0
Peak max at X 0
Peak height 0
u! (1e-9 m.m/V/s) 0
t USP 0

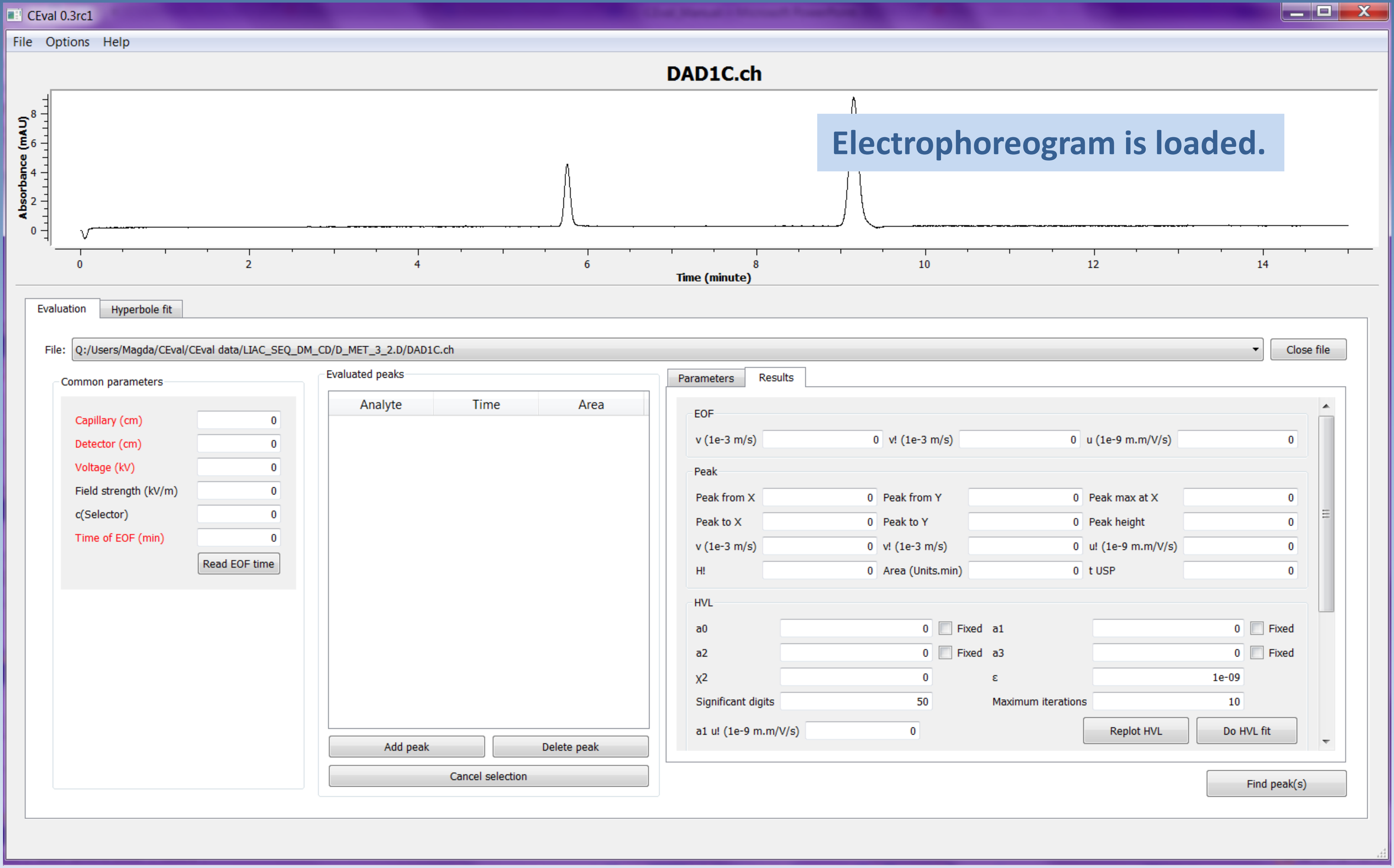
a0 0 ☐ Fixed
a1 0 ☐ Fixed
a2 0 ☐ Fixed
a3 0 ☐ Fixed
χ2 0
ε 1e-09
Significant digits 50
Maximum iterations 10
a1 u! (1e-9 m.m/V/s) 0

Absorbance or conductivity data

Choose the desired wavelenght

Chemstation data

Opening Data



Electrophoreogram is loaded.

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

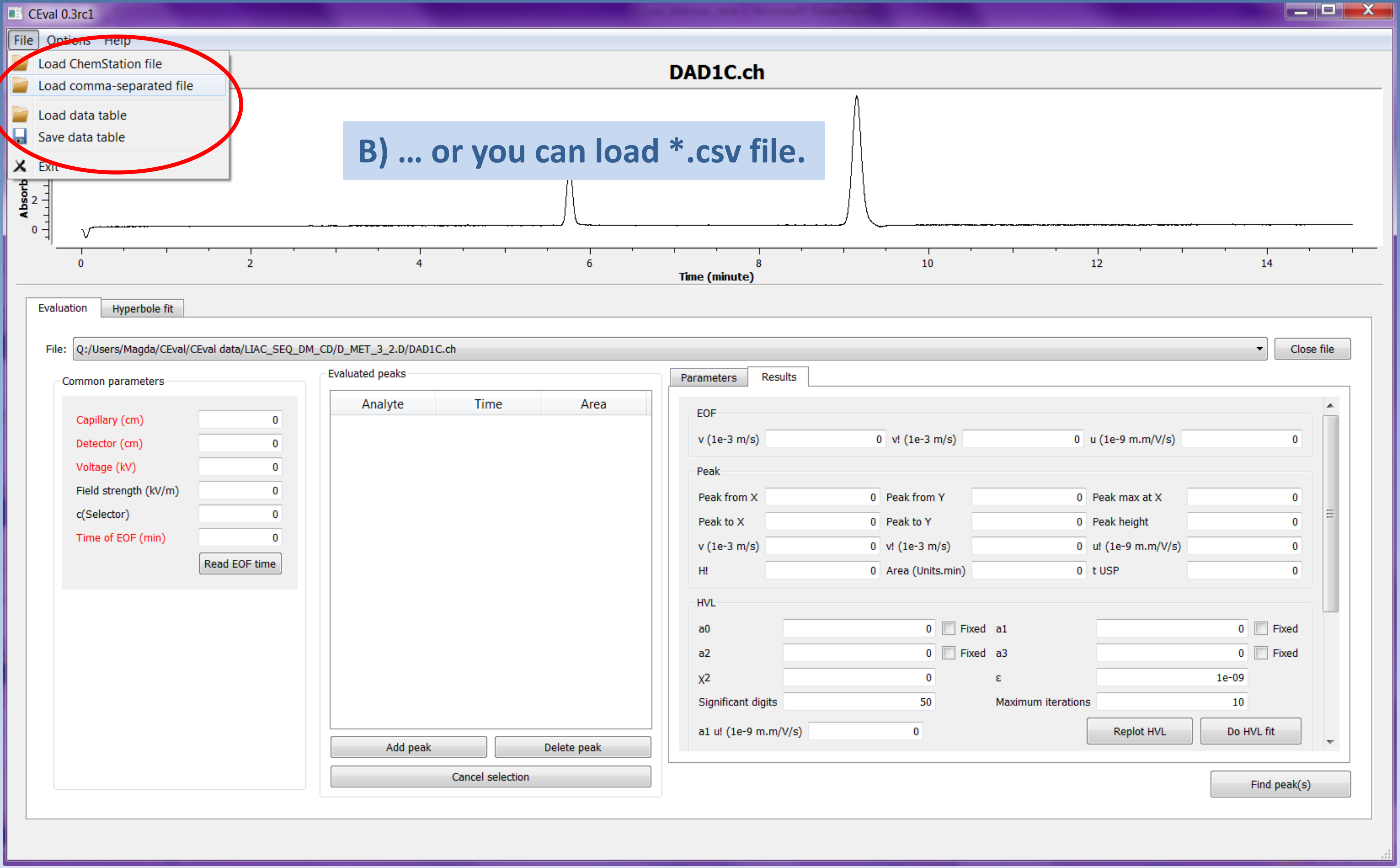
Capillary (cm): 0
Detector (cm): 0
Voltage (kV): 0
Field strength (kV/m): 0
c(Selector): 0
Time of EOF (min): 0

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
χ2: 0
ε: 1e-09
Significant digits: 50
Maximum iterations: 10
a1 u! (1e-9 m.m/V/s): 0

Opening Data



B) … or you can load *.csv file.

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

Evaluated peaks

EOF

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

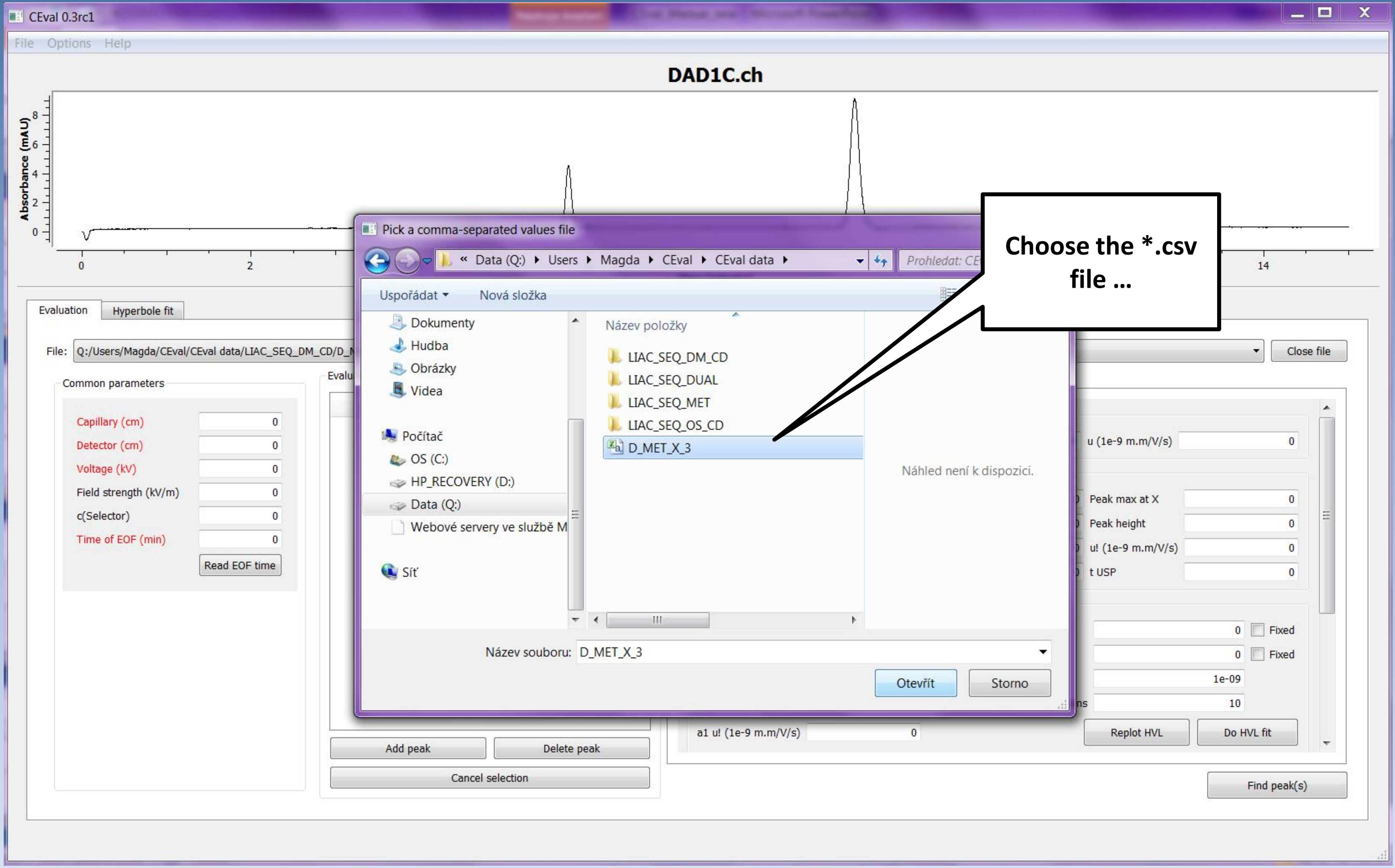
Peak

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
χ2 0
ε 1e-09
Significant digits 50
Maximum iterations 10
a1 u! (1e-9 m.m/V/s) 0

Opening Data



Choose the *.csv file …

File: Q:/Users/Magda/CEval/CEval data/LIAC_SEQ_DM_CD/D_M

Common parameters

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

« Data (Q:) ▸ Users ▸ Magda ▸ CEval ▸ CEval data ▸

Prohledat: CE

- LIAC_SEQ_DM_CD
- LIAC_SEQ_DUAL
- LIAC_SEQ_MET
- LIAC_SEQ_OS_CD
- D_MET_X_3

Náhled není k dispozici.

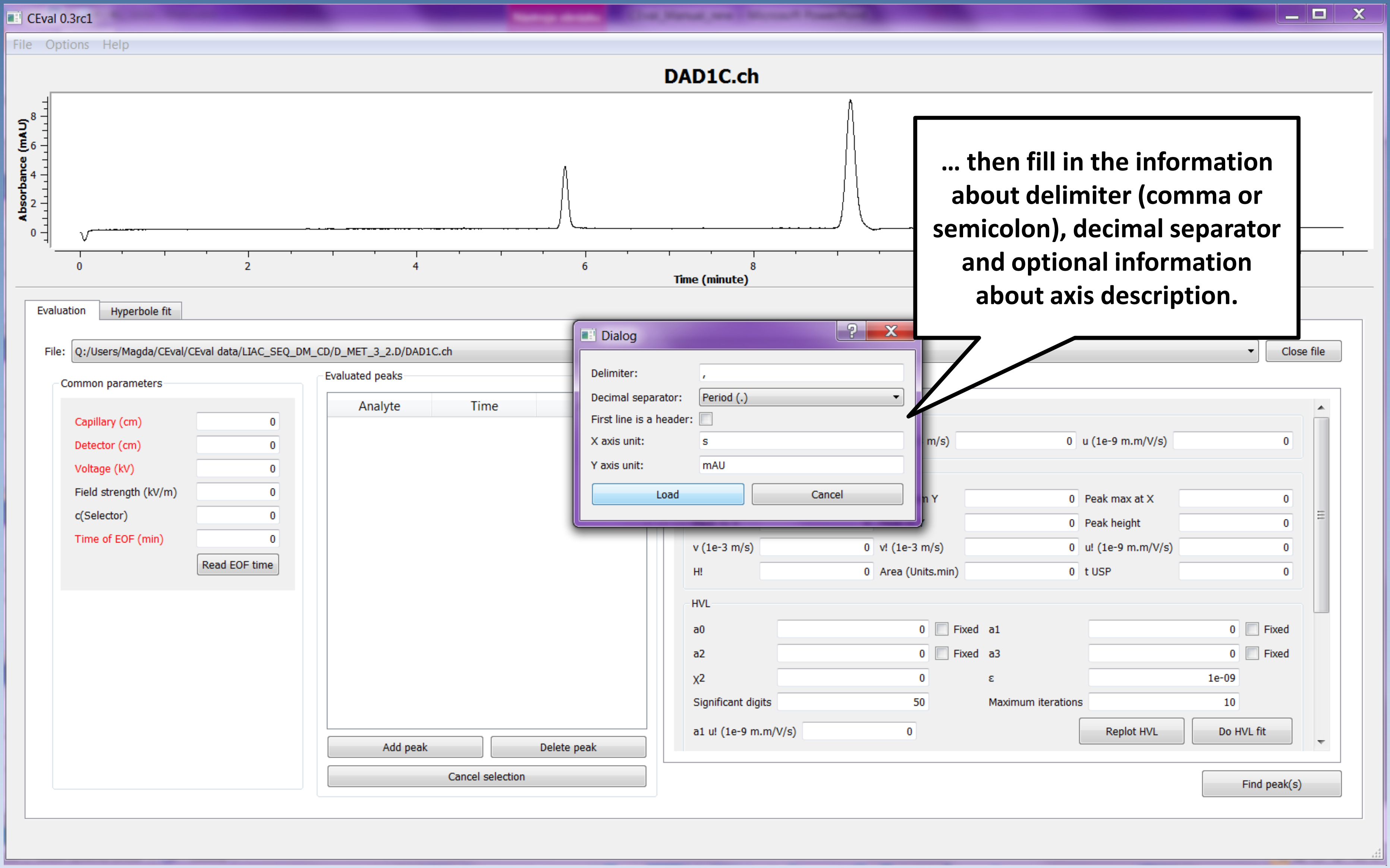
Název souboru: D_MET_X_3

u (1e-9 m.m/V/s)	0
Peak max at X	0
Peak height	0
u! (1e-9 m.m/V/s)	0
t USP	0

0 ☐ Fixed
0 ☐ Fixed
1e-09
10

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

Opening Data



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

Dialog

Delimiter: ,

Decimal separator: Period (.)

First line is a header: ☐

X axis unit: s

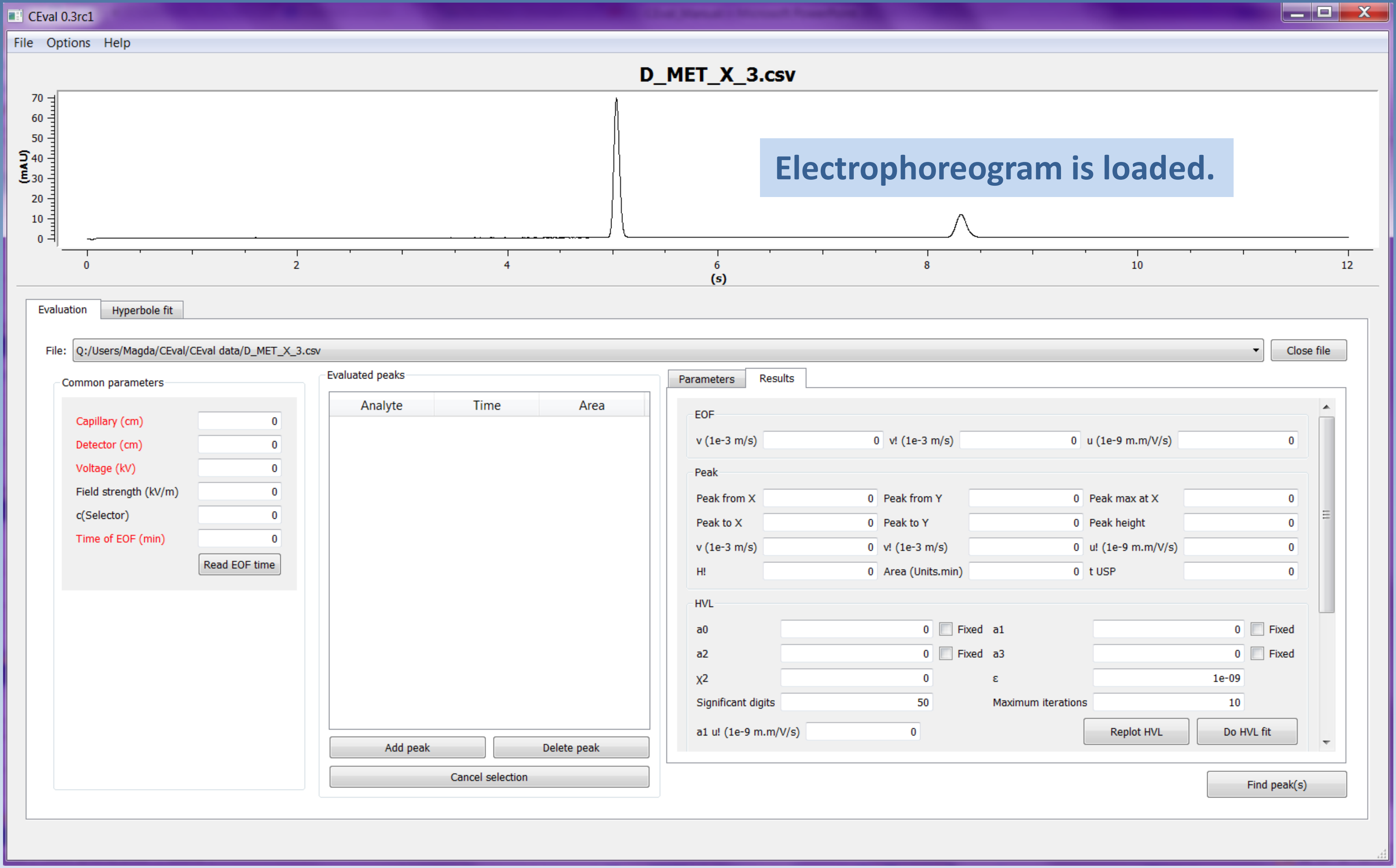
Y axis unit: mAU

Common parameters

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

… then fill in the information about delimiter (comma or semicolon), decimal separator and optional information about axis description.

Opening Data



Electrophoreogram is loaded.

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

Common parameters

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

Evaluated peaks

Analyte	Time	Area

EOF

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

Peak

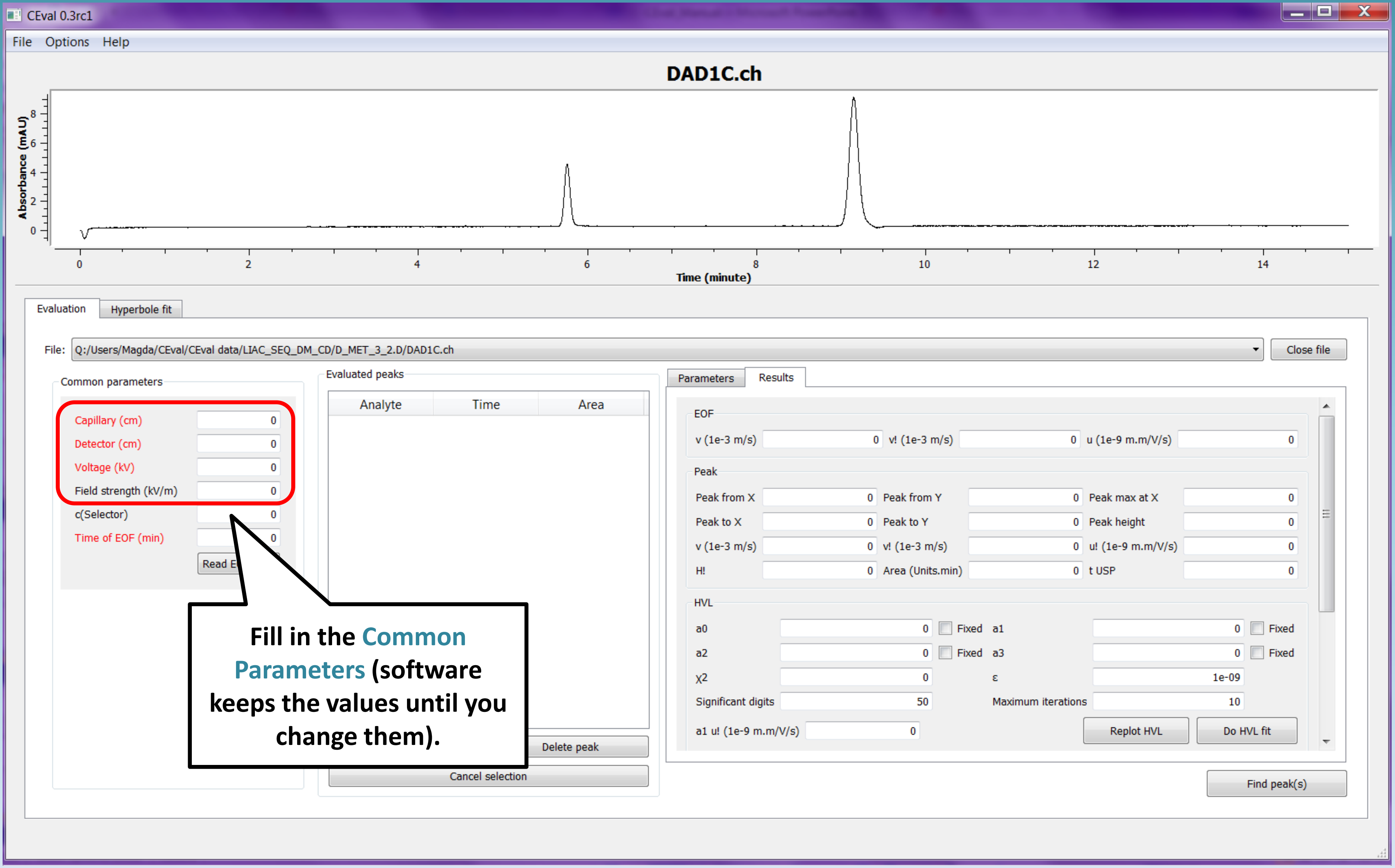
Peak from X: 0
Peak from Y: 0
Peak max at X: 0
Peak to X: 0
Peak to Y: 0
Peak height: 0
v (1e-3 m/s): 0
v! (1e-3 m/s): 0
u! (1e-9 m.m/V/s): 0
H!: 0
Area (Units.min): 0
t USP: 0

HVL

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

Peak Evaluation

Peak Evaluation



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

Evaluated peaks

Analyte	Time	Area

EOF

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

Peak

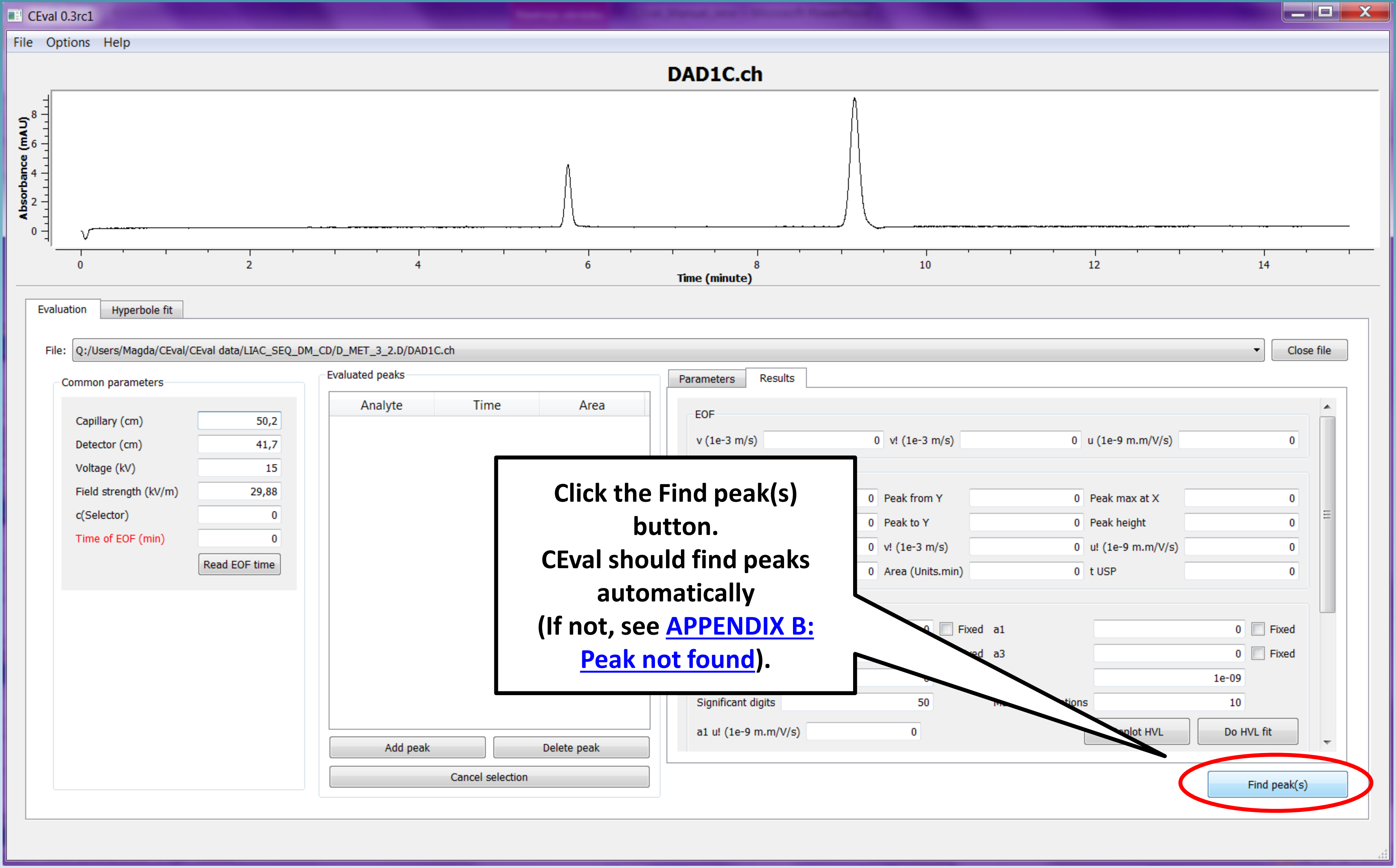
Peak from X 0
Peak from Y 0
Peak max at X 0
Peak to X 0
Peak to Y 0
Peak height 0
v (1e-3 m/s) 0
v! (1e-3 m/s) 0
u! (1e-9 m.m/V/s) 0
H! 0
Area (Units.min) 0
t USP 0

HVL

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

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

Peak Evaluation



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)	0

Evaluated peaks

Analyte	Time	Area

EOF

v (1e-3 m/s)	0	v! (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	v! (1e-3 m/s)	0	u! (1e-9 m.m/V/s)	0
	0	Area (Units.min)	0	t USP	0

a1 0

a3 0

1e-09

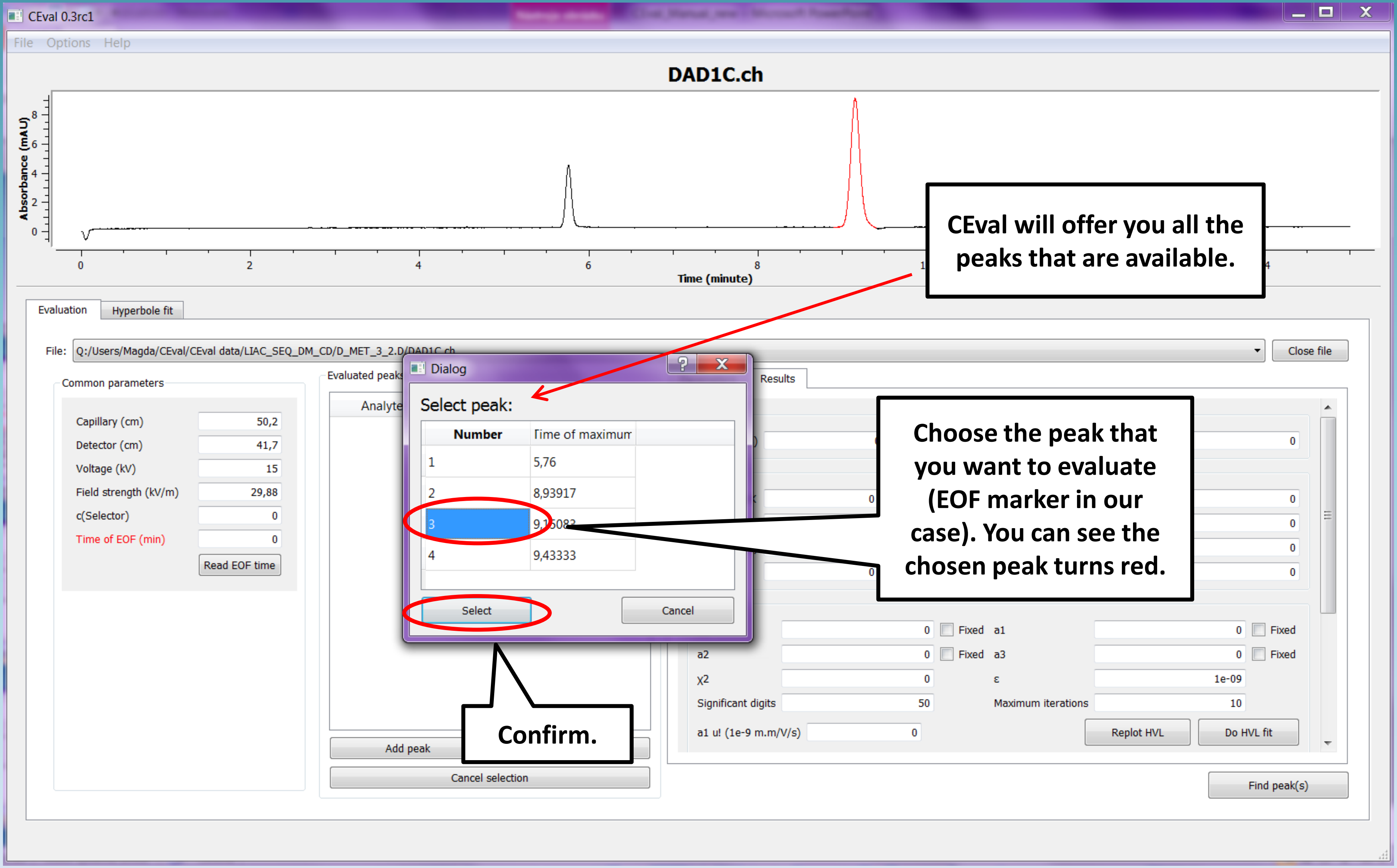
Significant digits 50

10

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

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

Peak Evaluation



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)	0

Read EOF time

Select peak:

Number	Time of maximum
1	5,76
2	8,93917
3	9,15083
4	9,43333

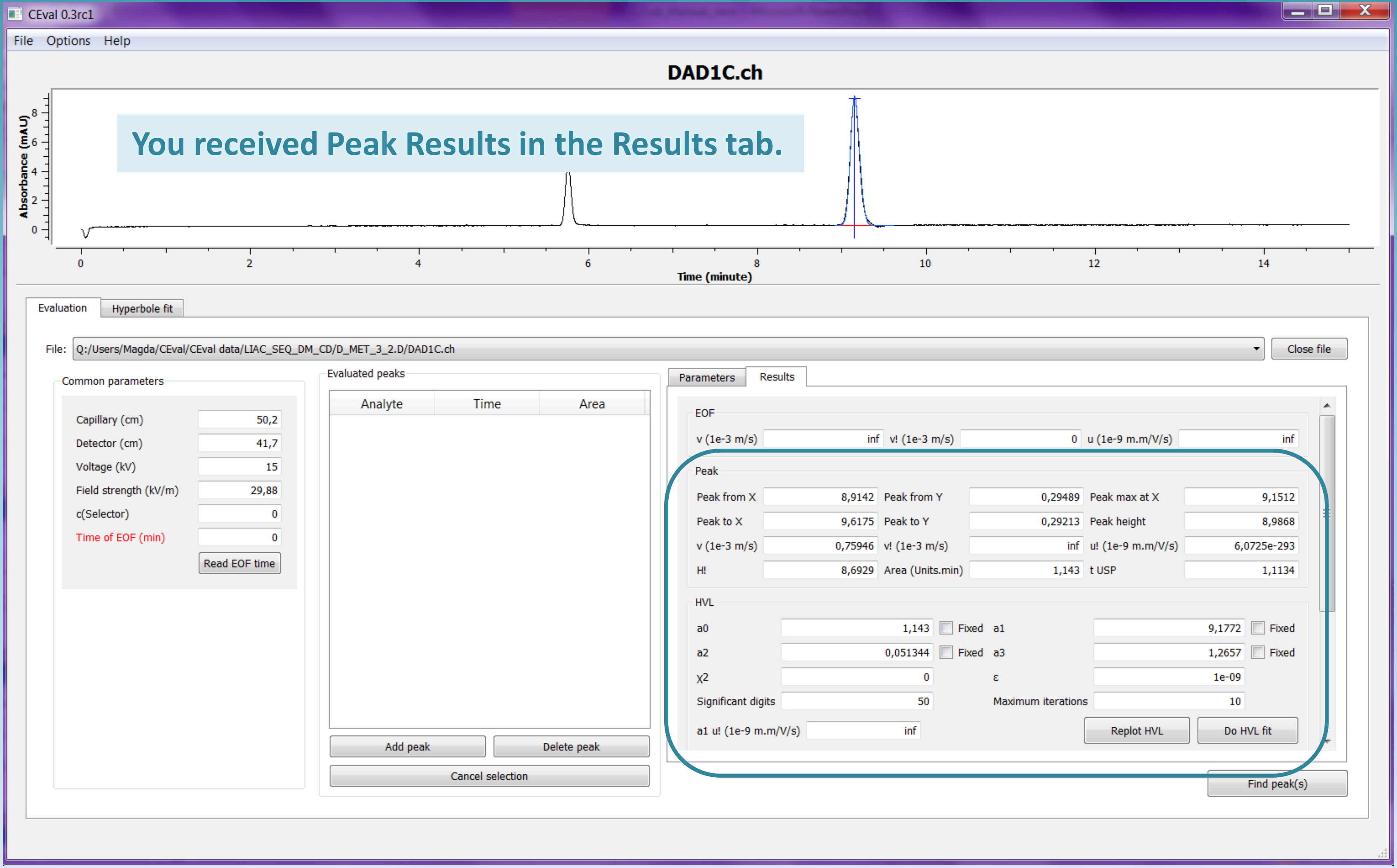
	0	☐ Fixed	a1	0	☐ Fixed
a2	0	☐ Fixed	a3	0	☐ Fixed
χ2	0		ε	1e-09	
Significant digits	50		Maximum iterations	10	
a1 u! (1e-9 m.m/V/s)	0				

CEval will offer you all the peaks that are available.

Choose the peak that you want to evaluate (EOF marker in our case). You can see the chosen peak turns red.

Confirm.

Peak Evaluation



You received Peak Results in the Results tab.

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)	0

Evaluated peaks

EOF

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

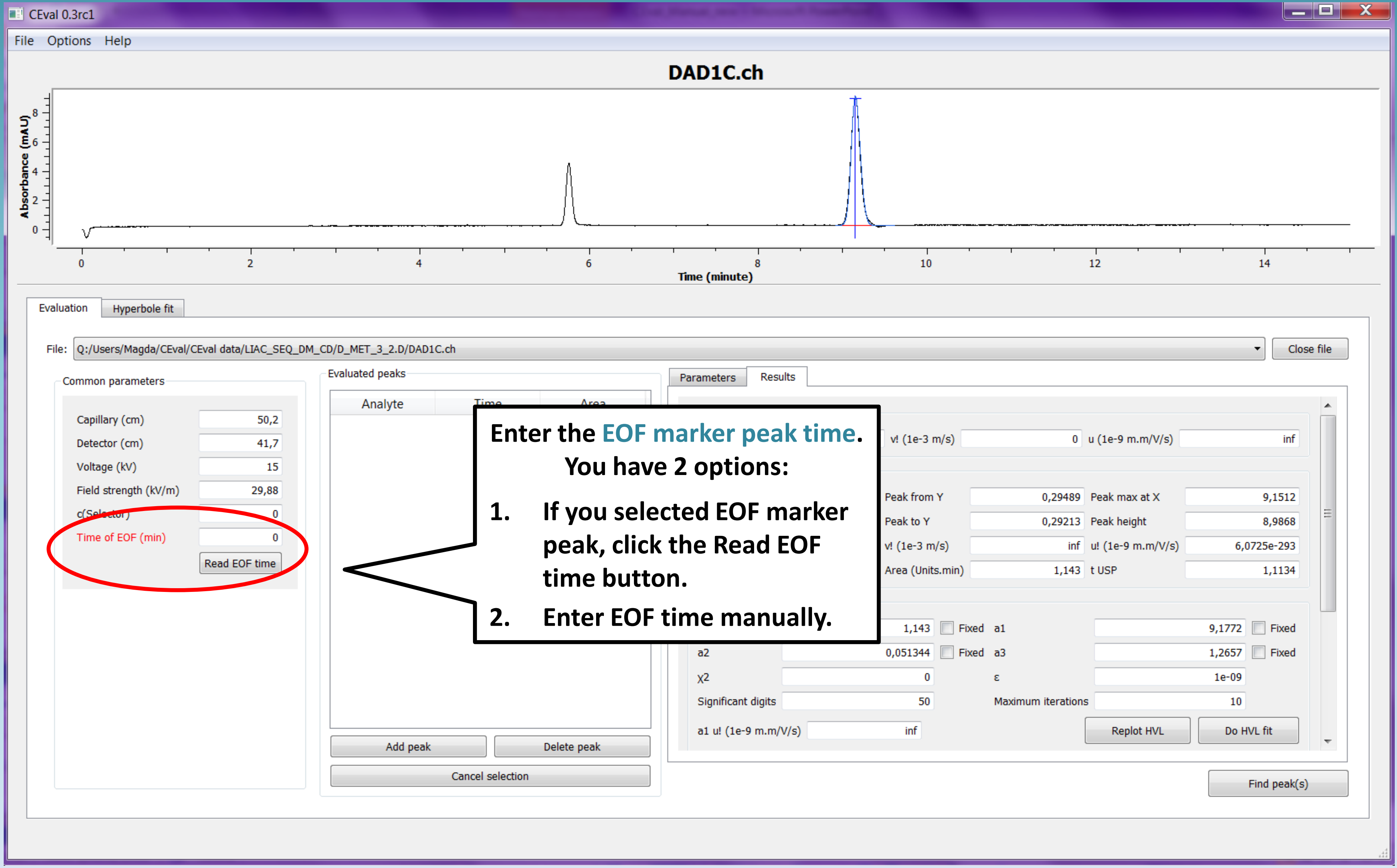
Peak

Peak from X	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	v! (1e-3 m/s)	inf	u! (1e-9 m.m/V/s)	6,0725e-293
H!	8,6929	Area (Units.min)	1,143	t USP	1,1134

HVL

a0	1,143	☐ Fixed	a1	9,1772	☐ Fixed
a2	0,051344	☐ Fixed	a3	1,2657	☐ Fixed
χ2	0		ε	1e-09	
Significant digits	50		Maximum iterations	10	
a1 u! (1e-9 m.m/V/s)	inf				

Peak Evaluation



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

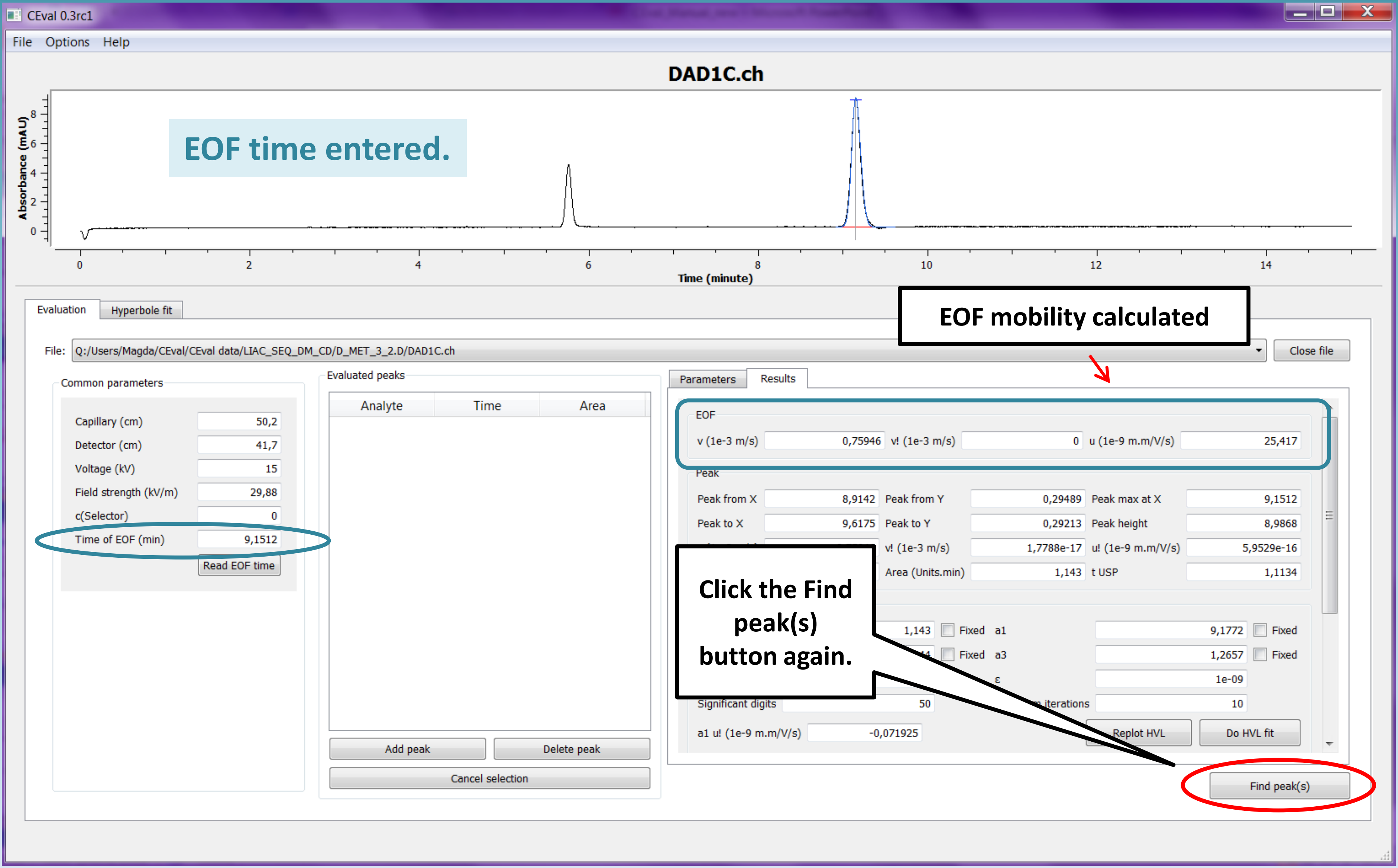
Capillary (cm) 50,2
Detector (cm) 41,7
Voltage (kV) 15
Field strength (kV/m) 29,88
c(Selector) 0
Time of EOF (min) 0

v! (1e-3 m/s) 0
u (1e-9 m.m/V/s) inf
Peak from Y 0,29489
Peak max at X 9,1512
Peak to Y 0,29213
Peak height 8,9868
v! (1e-3 m/s) inf
u! (1e-9 m.m/V/s) 6,0725e-293
Area (Units.min) 1,143
t USP 1,1134
1,143 ☐ Fixed
a1 9,1772 ☐ Fixed
a2 0,051344 ☐ Fixed
a3 1,2657 ☐ Fixed
χ2 0
ε 1e-09
Significant digits 50
Maximum iterations 10
a1 u! (1e-9 m.m/V/s) inf

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



EOF time entered.

EOF mobility calculated

Click the Find peak(s) button again.

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

Evaluated peaks

Analyte	Time	Area

EOF

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

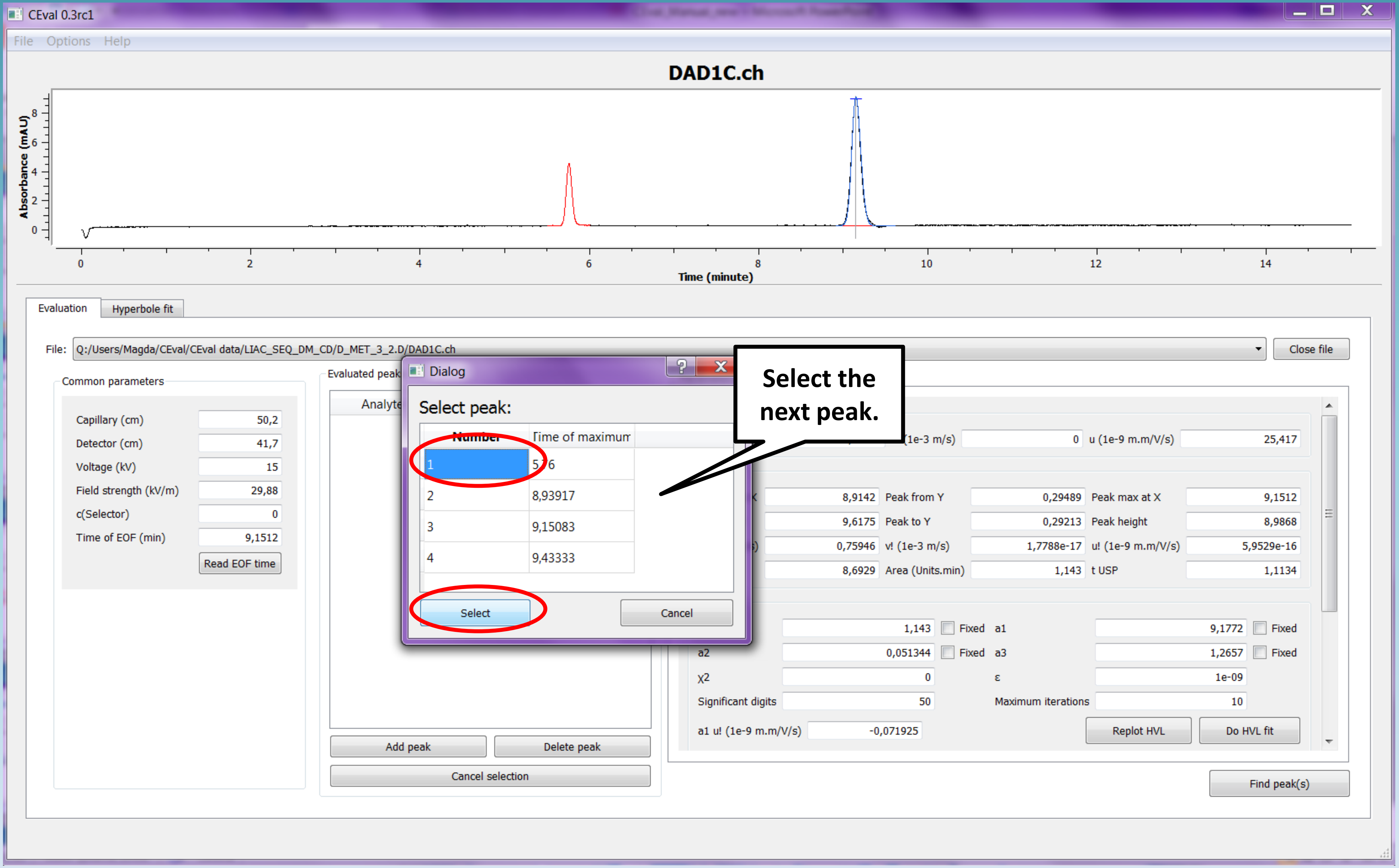
Peak

Peak from X	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)	1,7788e-17	u! (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
	☐ Fixed	a3	1,2657	☐ Fixed
		ε	1e-09	
Significant digits	50	iterations	10	

a1 u! (1e-9 m.m/V/s) -0,071925

Peak Evaluation



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

Evaluated peak

Analyte

Select peak:

Number	Time of maximum
1	5,76
2	8,93917
3	9,15083
4	9,43333

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

8,9142
Peak from Y 0,29489
Peak max at X 9,1512

9,6175
Peak to Y 0,29213
Peak height 8,9868

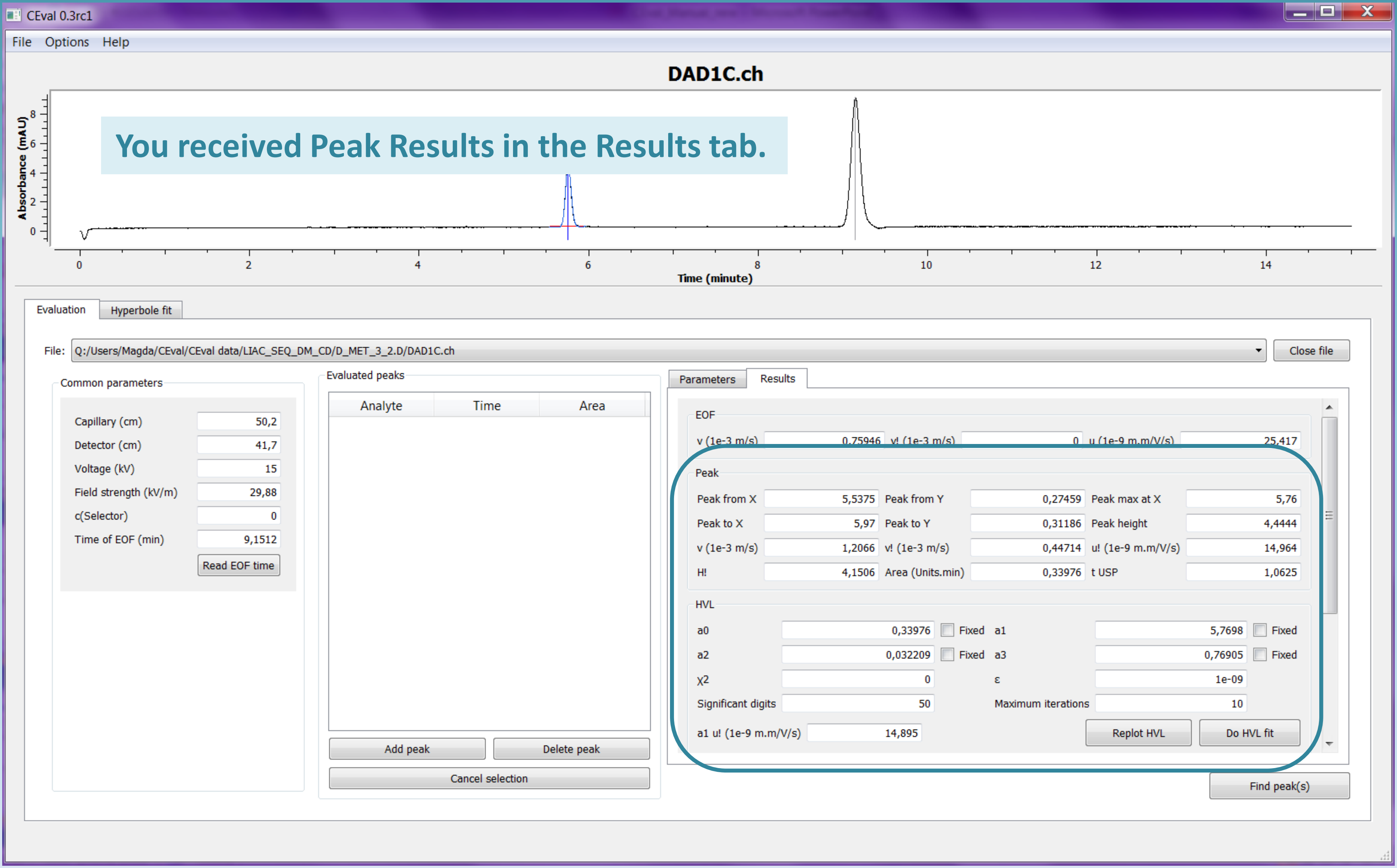
0,75946
v! (1e-3 m/s) 1,7788e-17
u! (1e-9 m.m/V/s) 5,9529e-16

8,6929
Area (Units.min) 1,143
t USP 1,1134

1,143 ☐ Fixed
a1 9,1772 ☐ Fixed
a2 0,051344 ☐ Fixed
a3 1,2657 ☐ Fixed
χ2 0
ε 1e-09
Significant digits 50
Maximum iterations 10
a1 u! (1e-9 m.m/V/s) -0,071925

Select the next peak.

Peak Evaluation



You received Peak Results in the Results tab.

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

Evaluated peaks

Analyte	Time	Area

EOF

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

Peak

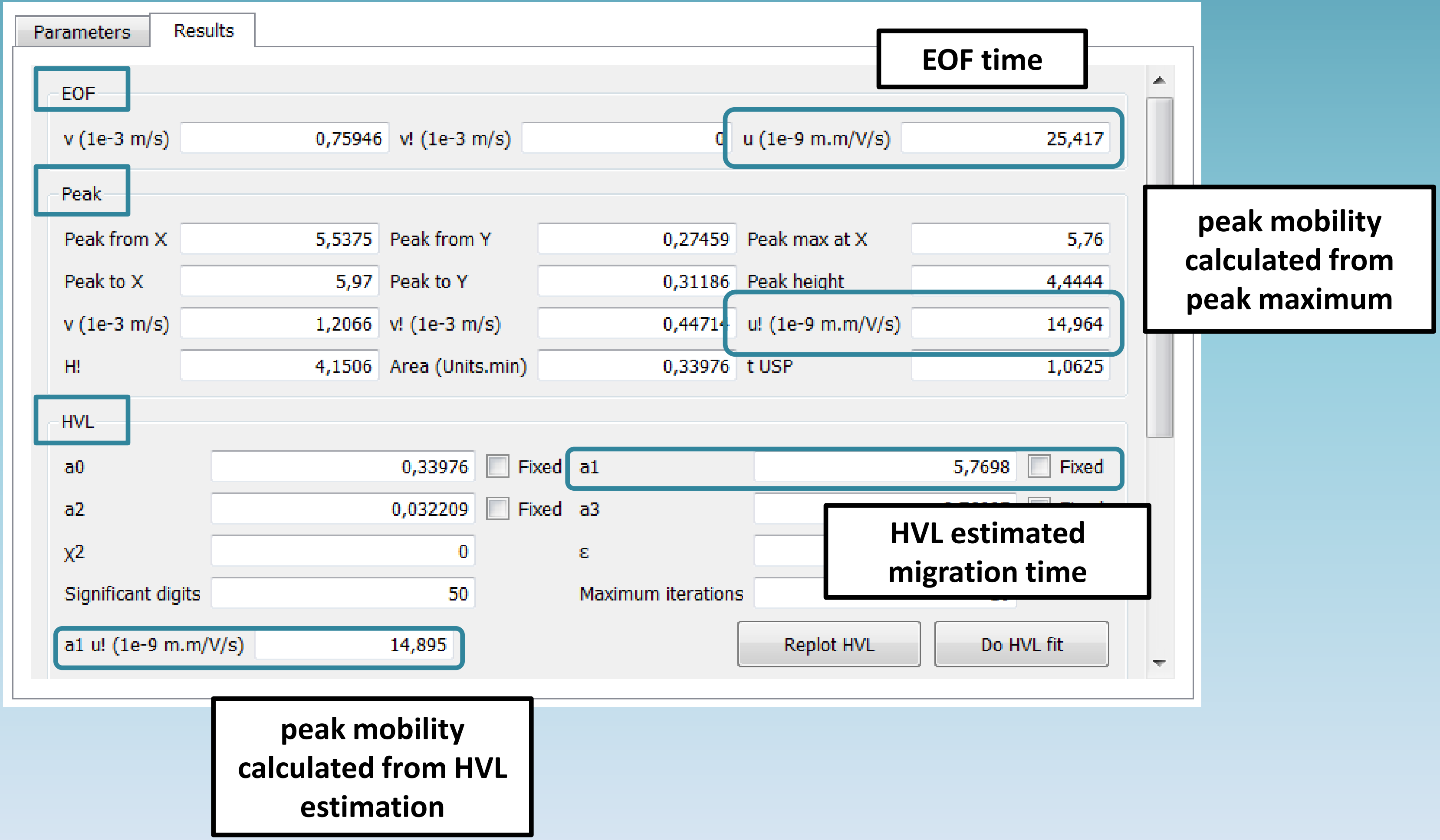
Peak from X: 5,5375
Peak from Y: 0,27459
Peak max at X: 5,76
Peak to X: 5,97
Peak to Y: 0,31186
Peak height: 4,4444
v (1e-3 m/s): 1,2066
v! (1e-3 m/s): 0,44714
u! (1e-9 m.m/V/s): 14,964
H!: 4,1506
Area (Units.min): 0,33976
t USP: 1,0625

HVL

a0: 0,33976 ☐ 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! (1e-9 m.m/V/s): 14,895

Peak Evaluation

You received Peak Results in the Results tab.



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	☐ Fixed	a1	5,7698	☐ Fixed
a2	0,032209	☐ Fixed	a3		☐
χ2	0		ε		
Significant digits	50		Maximum iterations		

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

EOF time

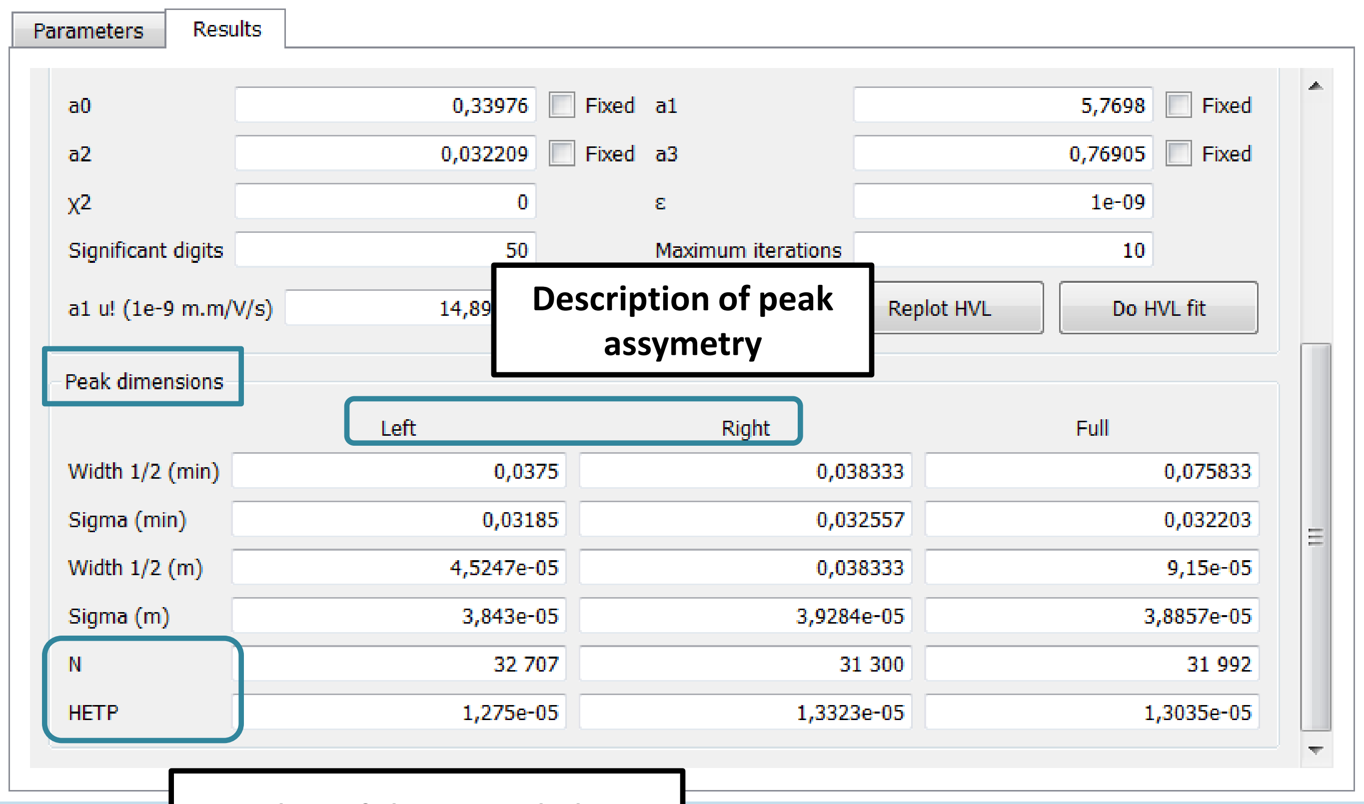
peak mobility calculated from peak maximum

HVL estimated migration time

peak mobility calculated from HVL estimation

Peak Evaluation

You received Peak Results in the Results tab.



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! (1e-9 m.m/V/s) 14,89

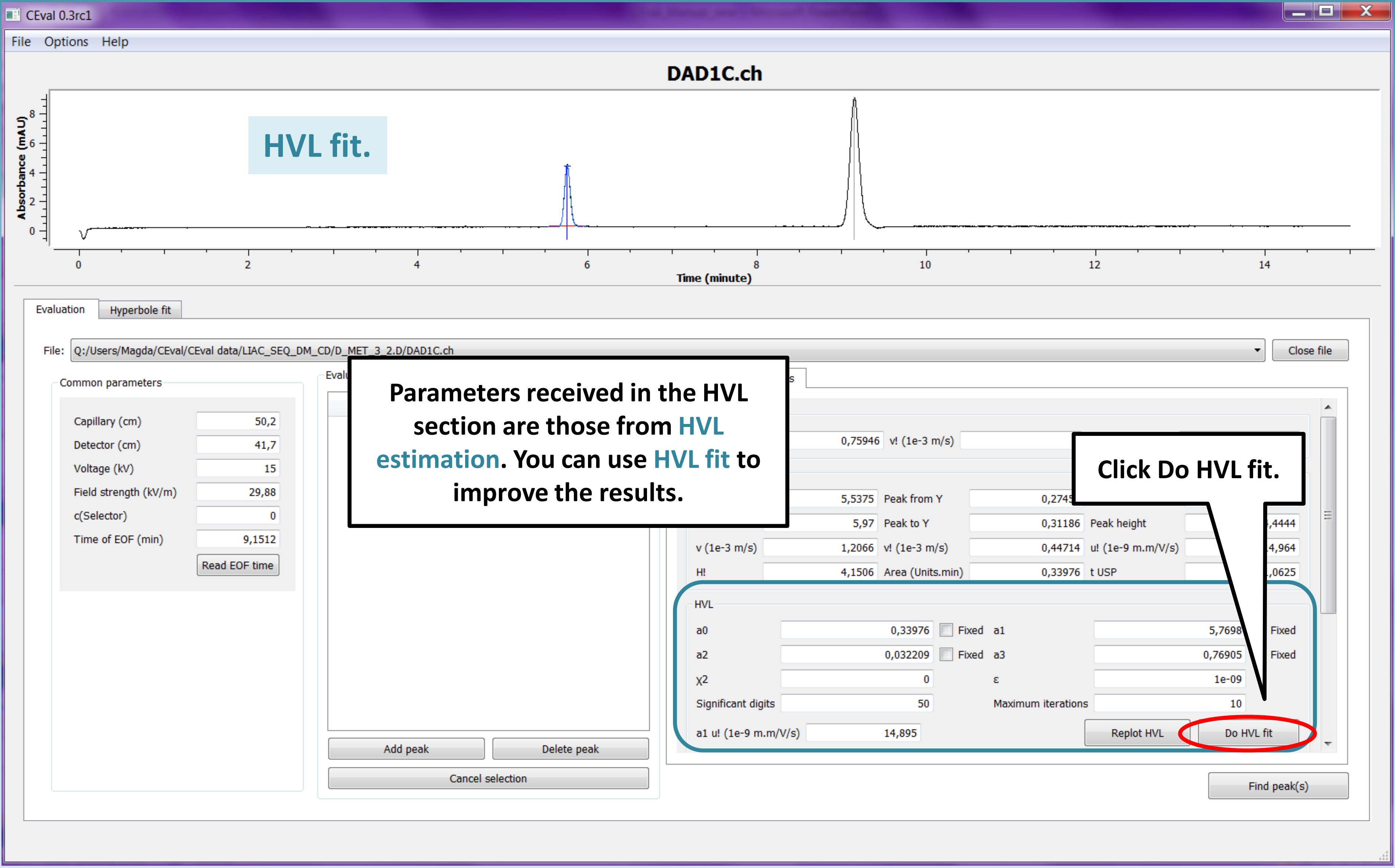
Description of peak assymetry

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



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

	0,75946	v! (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	v! (1e-3 m/s)	0,44714	u! (1e-9 m.m/V/s)	4,964
H!	4,1506	Area (Units.min)	0,33976	t USP	,0625

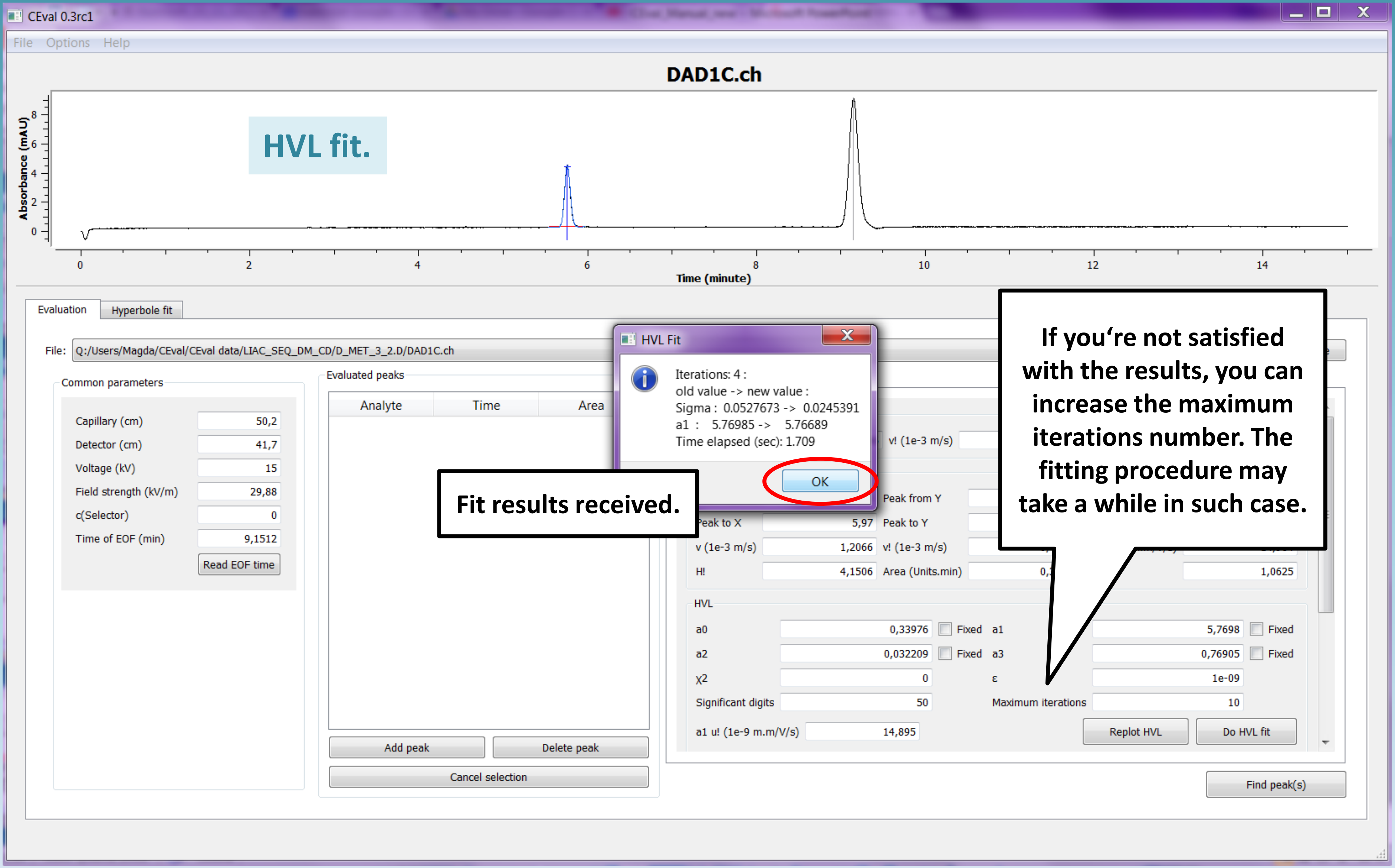
HVL

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

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

Click Do HVL fit.

Peak Evaluation



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

Evaluated peaks

Analyte	Time	Area

HVL Fit

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

v! (1e-3 m/s)

Peak from Y

Peak to X 5,97

Peak to Y

v (1e-3 m/s) 1,2066

v! (1e-3 m/s)

H! 4,1506

Area (Units.min) 0,

1,0625

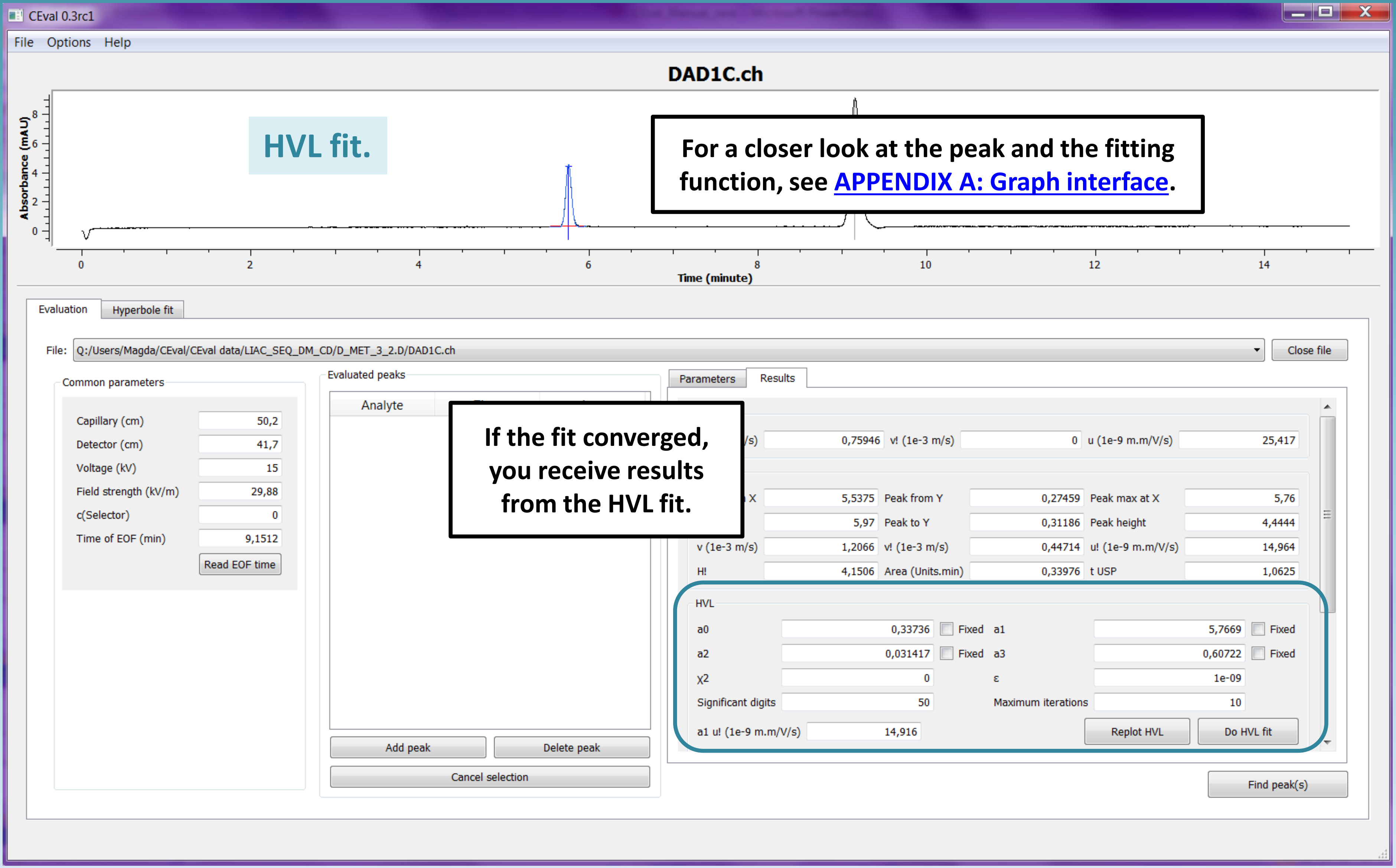
HVL

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

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.

Peak Evaluation



HVL fit.

For a closer look at the peak and the fitting function, see APPENDIX A: Graph interface.

If the fit converged, you receive results from the 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

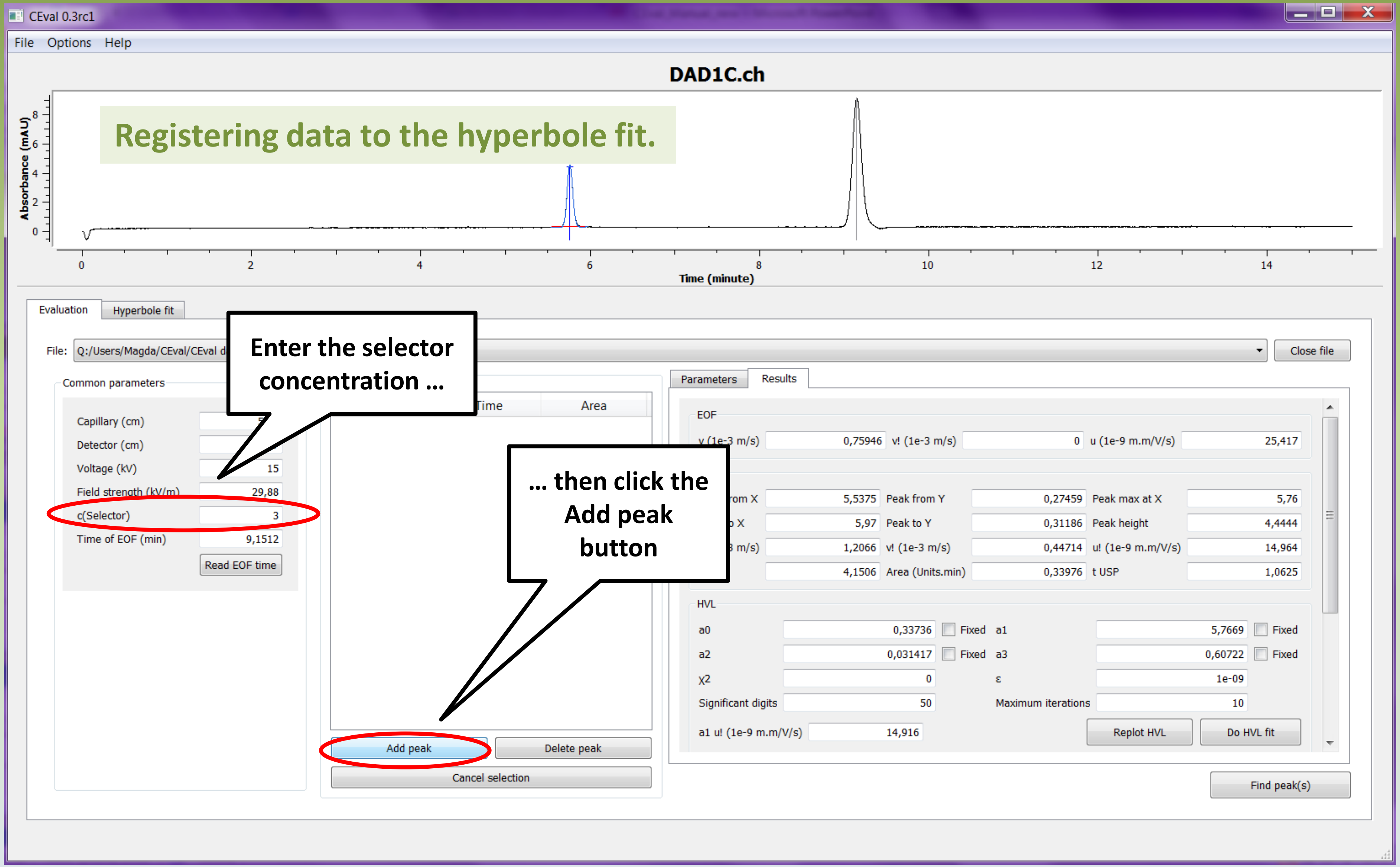
/s)	0,75946	v! (1e-3 m/s)	0	u (1e-9 m.m/V/s)	25,417
X	5,5375	Peak from Y	0,27459	Peak max at X	5,76
	5,97	Peak to Y	0,31186	Peak height	4,4444
v (1e-3 m/s)	1,2066	v! (1e-3 m/s)	0,44714	u! (1e-9 m.m/V/s)	14,964
H!	4,1506	Area (Units.min)	0,33976	t USP	1,0625

HVL

a0	0,33736	☐ Fixed	a1	5,7669	☐ Fixed
a2	0,031417	☐ Fixed	a3	0,60722	☐ Fixed
χ2	0		ε	1e-09	
Significant digits	50		Maximum iterations	10	
a1 u! (1e-9 m.m/V/s)	14,916				

ACE Data Evaluation

ACE Data Evaluation



Registering data to the hyperbole fit.

Enter the selector concentration …

… then click the Add peak button

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

EOF

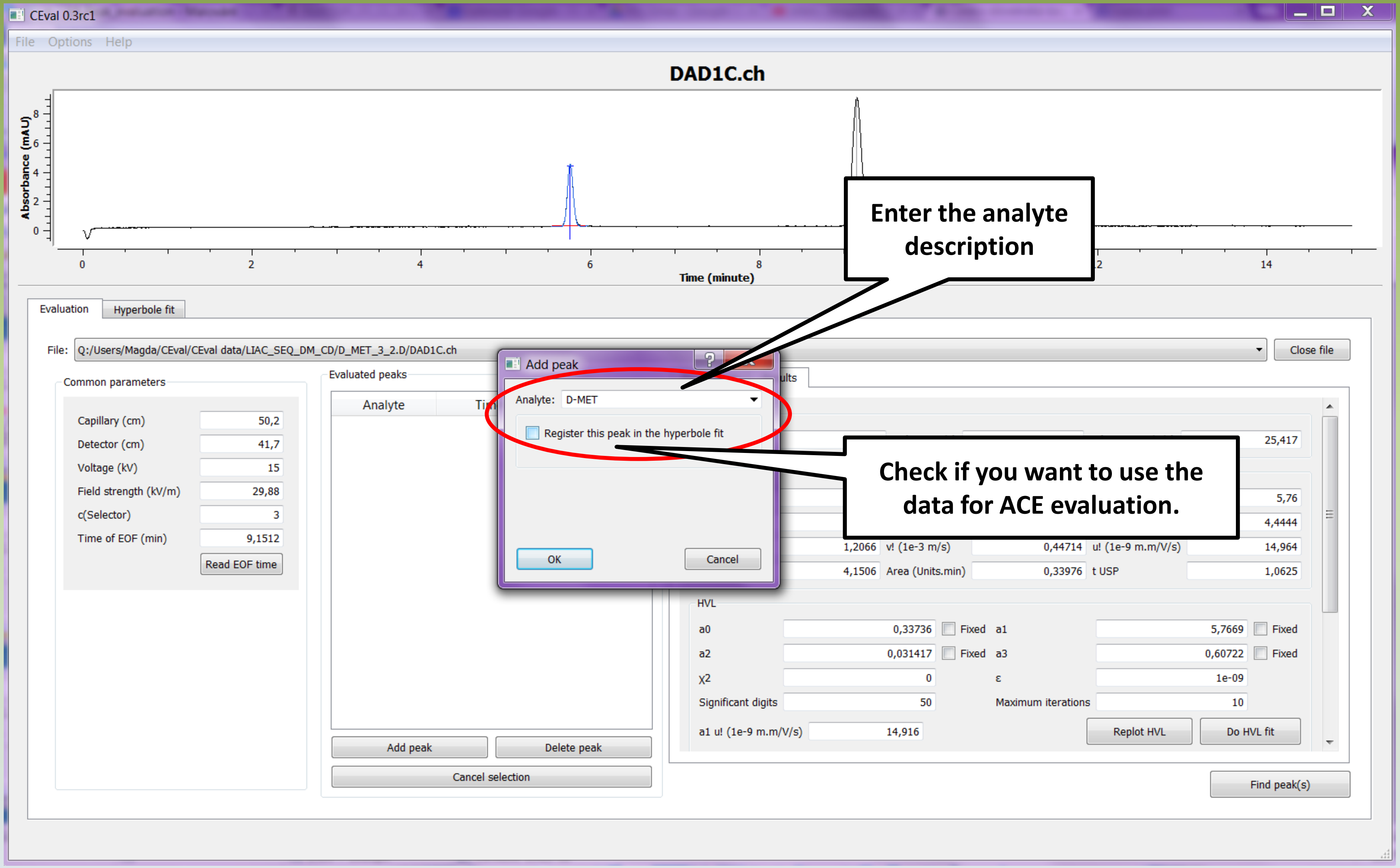
v (1e-3 m/s) 0,75946 v! (1e-3 m/s) 0 u (1e-9 m.m/V/s) 25,417

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

HVL

a0 0,33736 ☐ Fixed a1 5,7669 ☐ Fixed
a2 0,031417 ☐ Fixed a3 0,60722 ☐ Fixed
χ2 0 ε 1e-09
Significant digits 50 Maximum iterations 10
a1 u! (1e-9 m.m/V/s) 14,916

ACE Data Evaluation



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) 3
Time of EOF (min) 9,1512

Evaluated peaks

Analyte	Ti

Add peak

Analyte: D-MET

☐ Register this peak in the hyperbole fit

25,417
5,76
4,4444
1,2066 v! (1e-3 m/s) 0,44714 u! (1e-9 m.m/V/s) 14,964
4,1506 Area (Units.min) 0,33976 t USP 1,0625

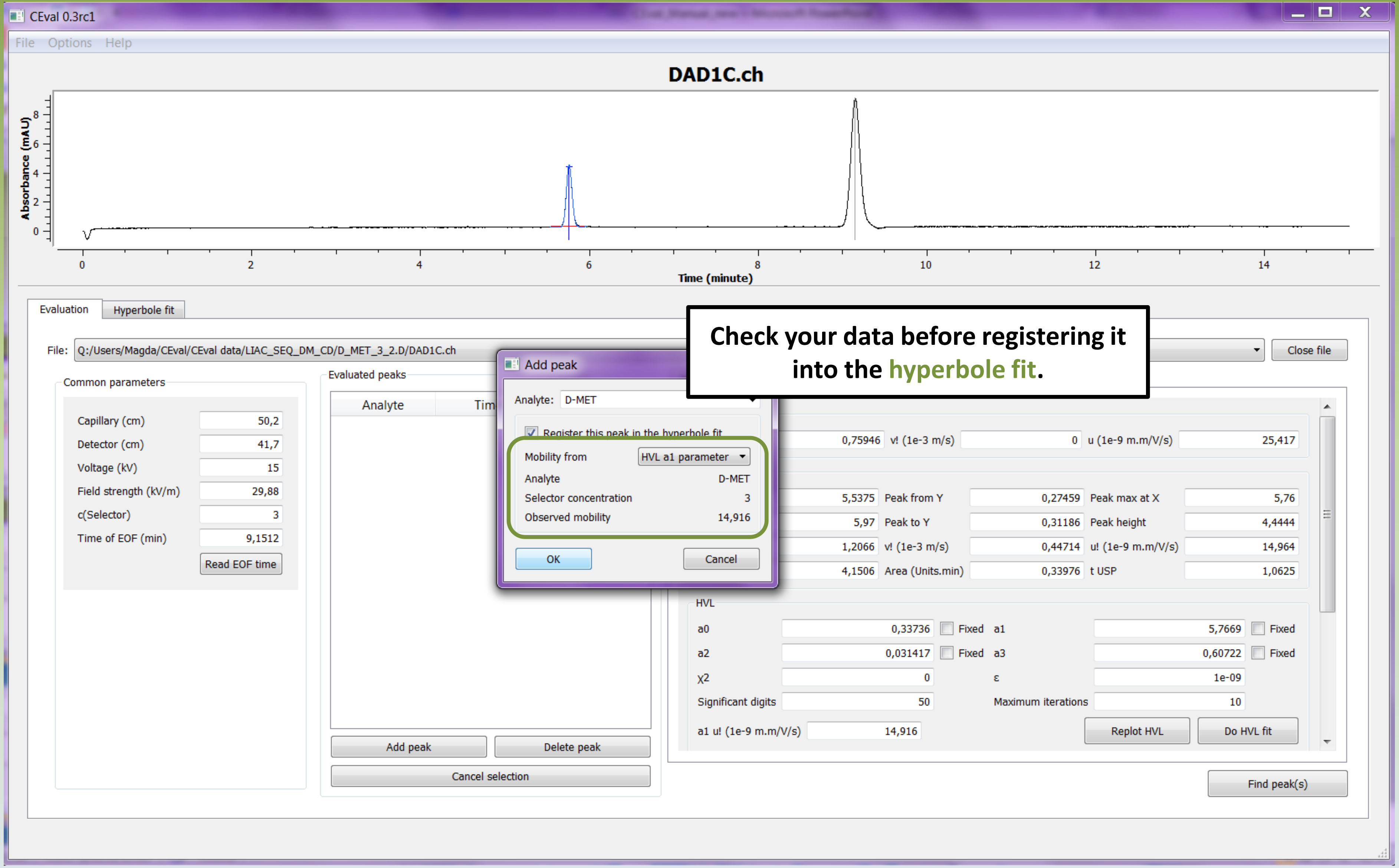
HVL

a0 0,33736 ☐ Fixed a1 5,7669 ☐ Fixed
a2 0,031417 ☐ Fixed a3 0,60722 ☐ Fixed
χ2 0 ε 1e-09
Significant digits 50 Maximum iterations 10
a1 u! (1e-9 m.m/V/s) 14,916

Enter the analyte description

Check if you want to use the data for ACE evaluation.

ACE Data Evaluation



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)	3
Time of EOF (min)	9,1512

Evaluated peaks

Analyte	Tim

Add peak

Analyte: D-MET

☑ Register this peak in the hyperbole fit

Mobility from	HVL a1 parameter
Analyte	D-MET
Selector concentration	3
Observed mobility	14,916

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

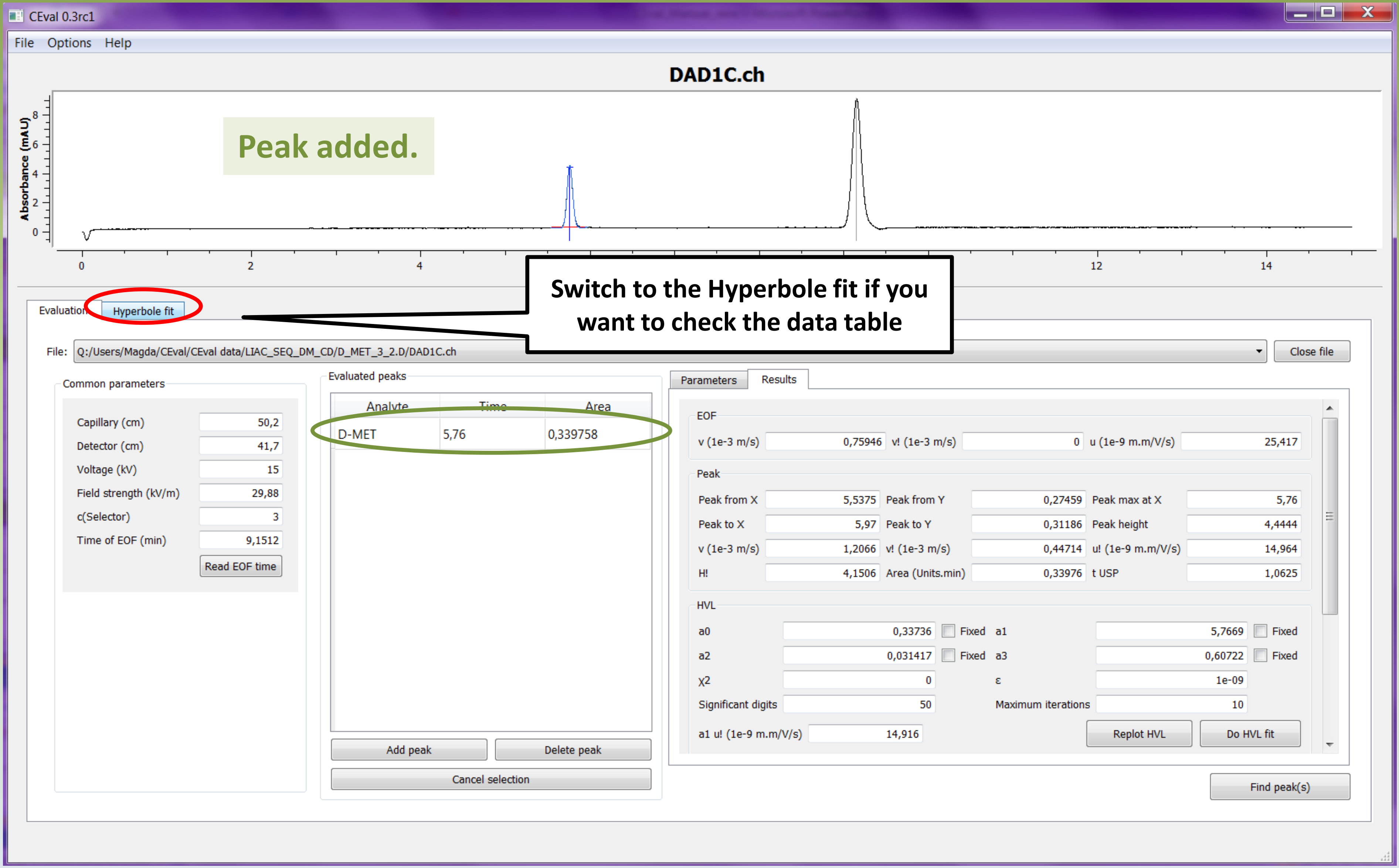
HVL

a0	0,33736	☐ Fixed	a1	5,7669	☐ Fixed
a2	0,031417	☐ Fixed	a3	0,60722	☐ Fixed
χ2	0		ε	1e-09	
Significant digits	50		Maximum iterations	10	

a1 u! (1e-9 m.m/V/s) 14,916

Check your data before registering it into the hyperbole fit.

ACE Data Evaluation



Peak added.

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

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)	3
Time of EOF (min)	9,1512

Evaluated peaks

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

EOF

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

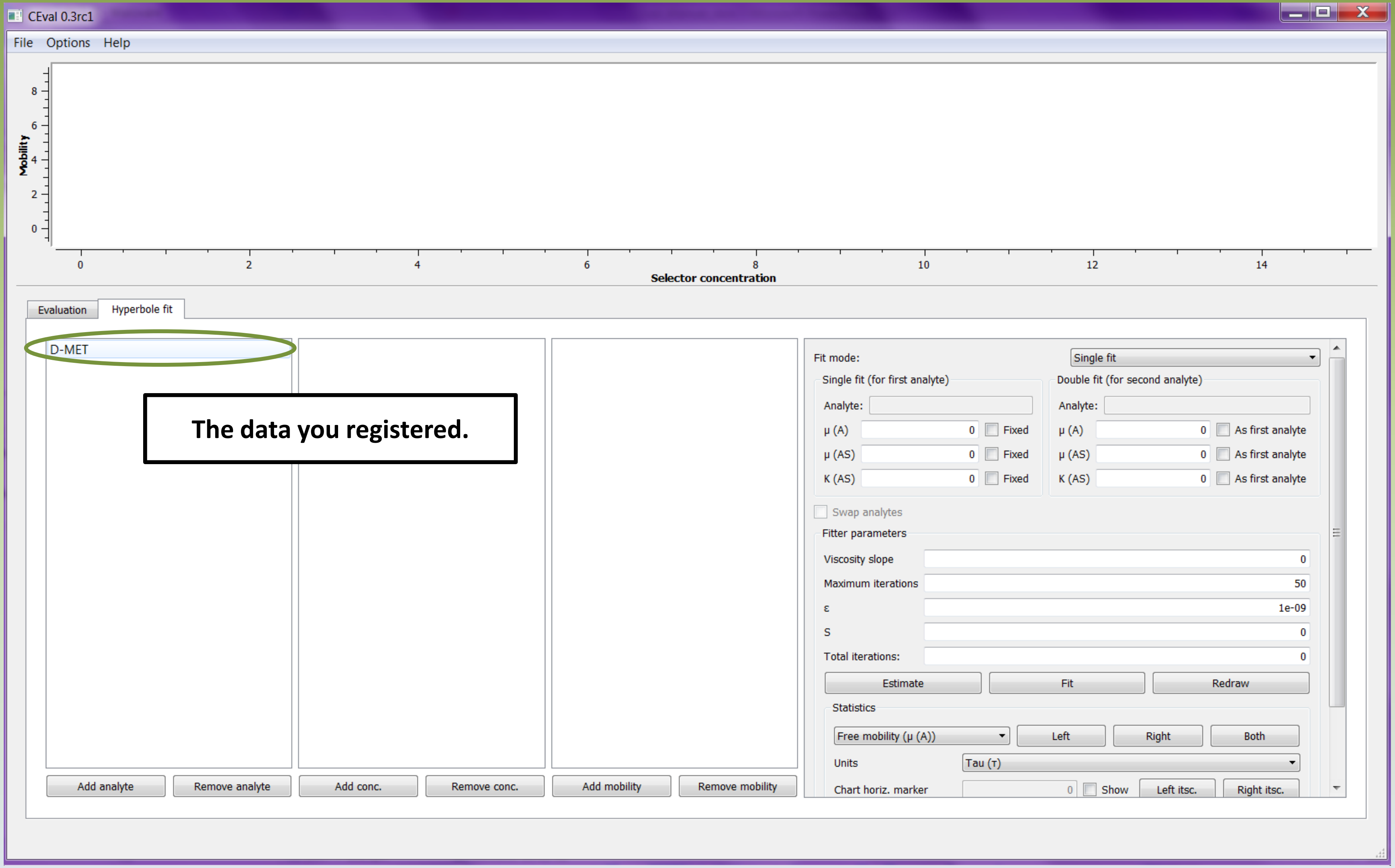
Peak

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	0,33736	☐ Fixed	a1	5,7669	☐ Fixed
a2	0,031417	☐ Fixed	a3	0,60722	☐ Fixed
χ2	0		ε	1e-09	
Significant digits	50		Maximum iterations	10	
a1 u! (1e-9 m.m/V/s)	14,916				

ACE Data Evaluation



D-MET

The data you registered.

Fit mode: Single fit

Single fit (for first analyte)

Analyte:

μ (A) 0 ☐ Fixed

μ (AS) 0 ☐ Fixed

K (AS) 0 ☐ 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

☐ Swap analytes

Fitter parameters

Viscosity slope 0

Maximum iterations 50

ε 1e-09

S 0

Total iterations: 0

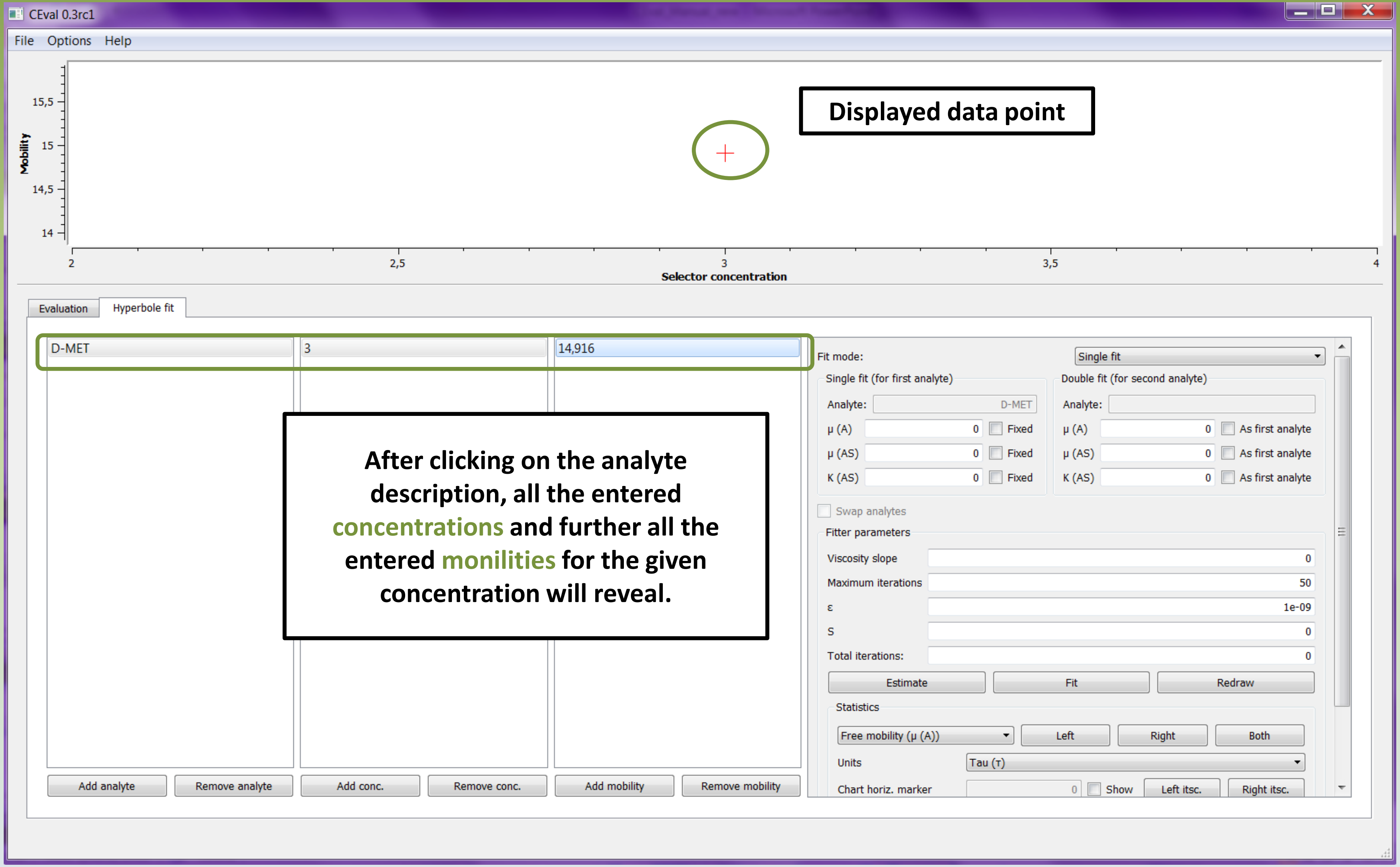
Statistics

Free mobility (μ (A))

Units Tau (τ)

Chart horiz. marker 0 ☐ Show

ACE Data Evaluation



Displayed data point

After clicking on the analyte description, all the entered concentrations and further all the entered monilities for the given concentration will reveal.

D-MET | 3 | 14,916

Fit mode: Single fit

Single fit (for first analyte)

Analyte: D-MET
μ (A) 0 ☐ Fixed
μ (AS) 0 ☐ Fixed
K (AS) 0 ☐ 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

☐ Swap analytes

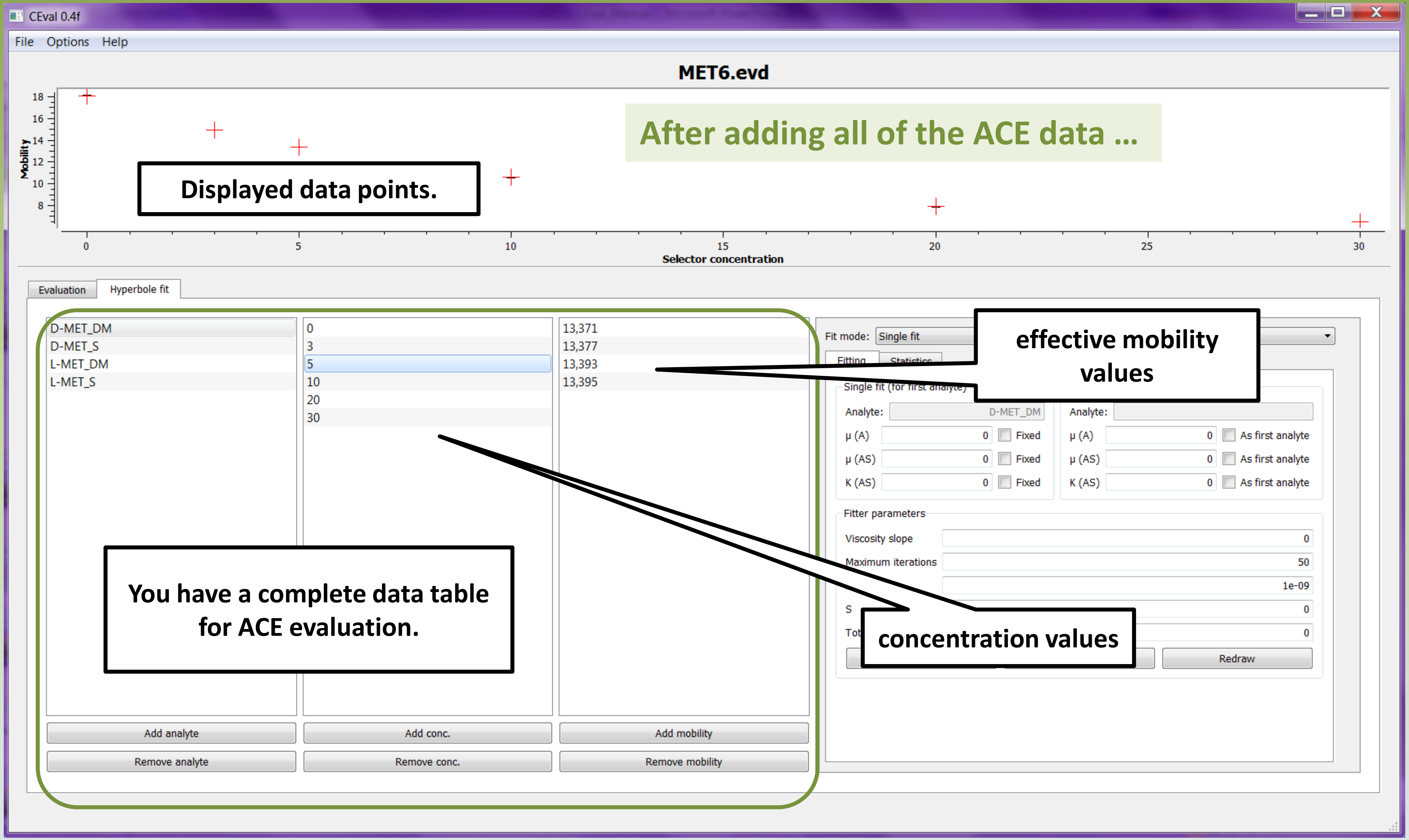
Fitter parameters

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

Statistics

Free mobility (μ (A))
Units Tau (τ)
Chart horiz. marker 0 ☐ Show

ACE Data Evaluation



MET6.evd

After adding all of the ACE data ...

Displayed data points.

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

0
3
5
10
20
30

13,371
13,377
13,393
13,395

effective mobility values

concentration values

You have a complete data table for ACE evaluation.

Fit mode: Single fit

Single fit (for first analyte)

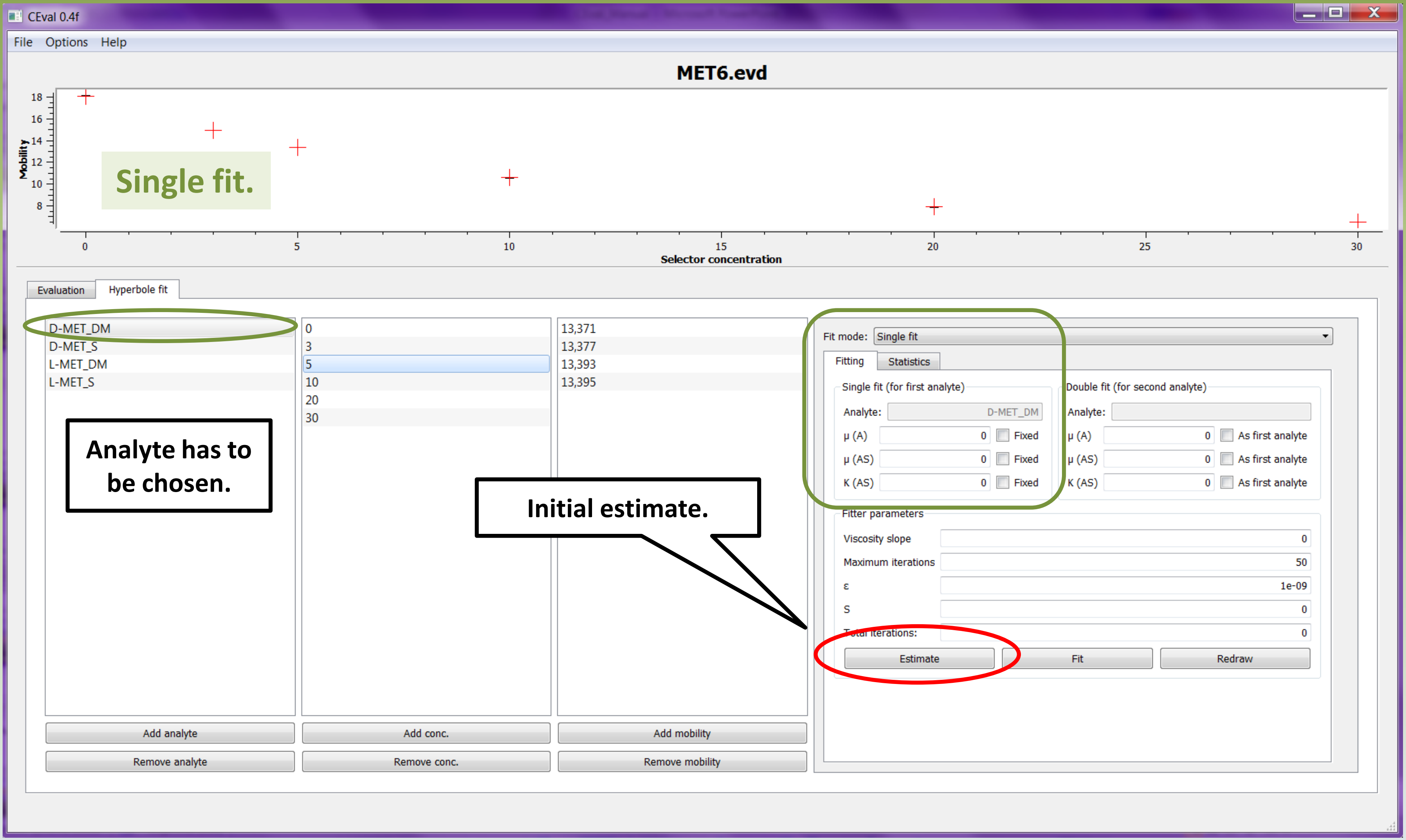
Analyte: D-MET_DM
μ (A) 0 ☐ Fixed
μ (AS) 0 ☐ Fixed
K (AS) 0 ☐ Fixed

Analyte:
μ (A) 0 ☐ As first analyte
μ (AS) 0 ☐ As first analyte
K (AS) 0 ☐ As first analyte

Fitter parameters

Viscosity slope 0
Maximum iterations 50
1e-09
S 0
Tot 0

ACE Data Evaluation



Single fit.

D-MET_DM	0	13,371
D-MET_S	3	13,377
L-MET_DM	5	13,393
L-MET_S	10	13,395
	20	
	30	

Analyte has to be chosen.

Fit mode: Single fit

Single fit (for first analyte)

Analyte: D-MET_DM

μ (A) 0 ☐ Fixed

μ (AS) 0 ☐ Fixed

K (AS) 0 ☐ 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

Fitter parameters

Viscosity slope 0

Maximum iterations 50

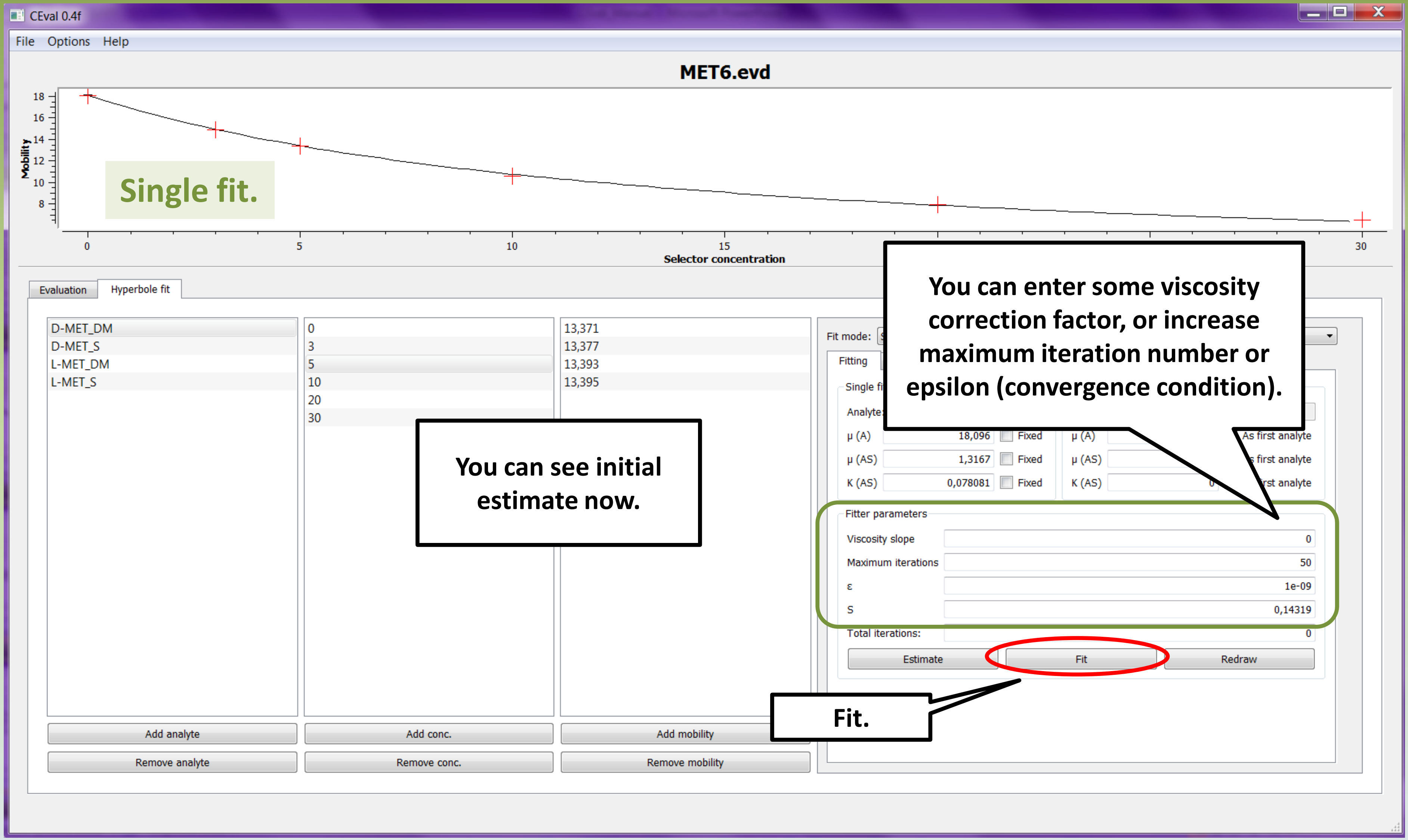
ε 1e-09

S 0

Total iterations: 0

Initial estimate.

ACE Data Evaluation



D-MET_DM	0	13,371
D-MET_S	3	13,377
L-MET_DM	5	13,393
L-MET_S	10	13,395
	20	
	30	

Fit mode:

Analyte:

μ (A)	18,096	☐ Fixed	μ (A)		As first analyte
μ (AS)	1,3167	☐ Fixed	μ (AS)		s first analyte
K (AS)	0,078081	☐ Fixed	K (AS)	0	rst analyte

Fitter parameters

Viscosity slope: 0

Maximum iterations: 50

ε: 1e-09

S: 0,14319

Total iterations: 0

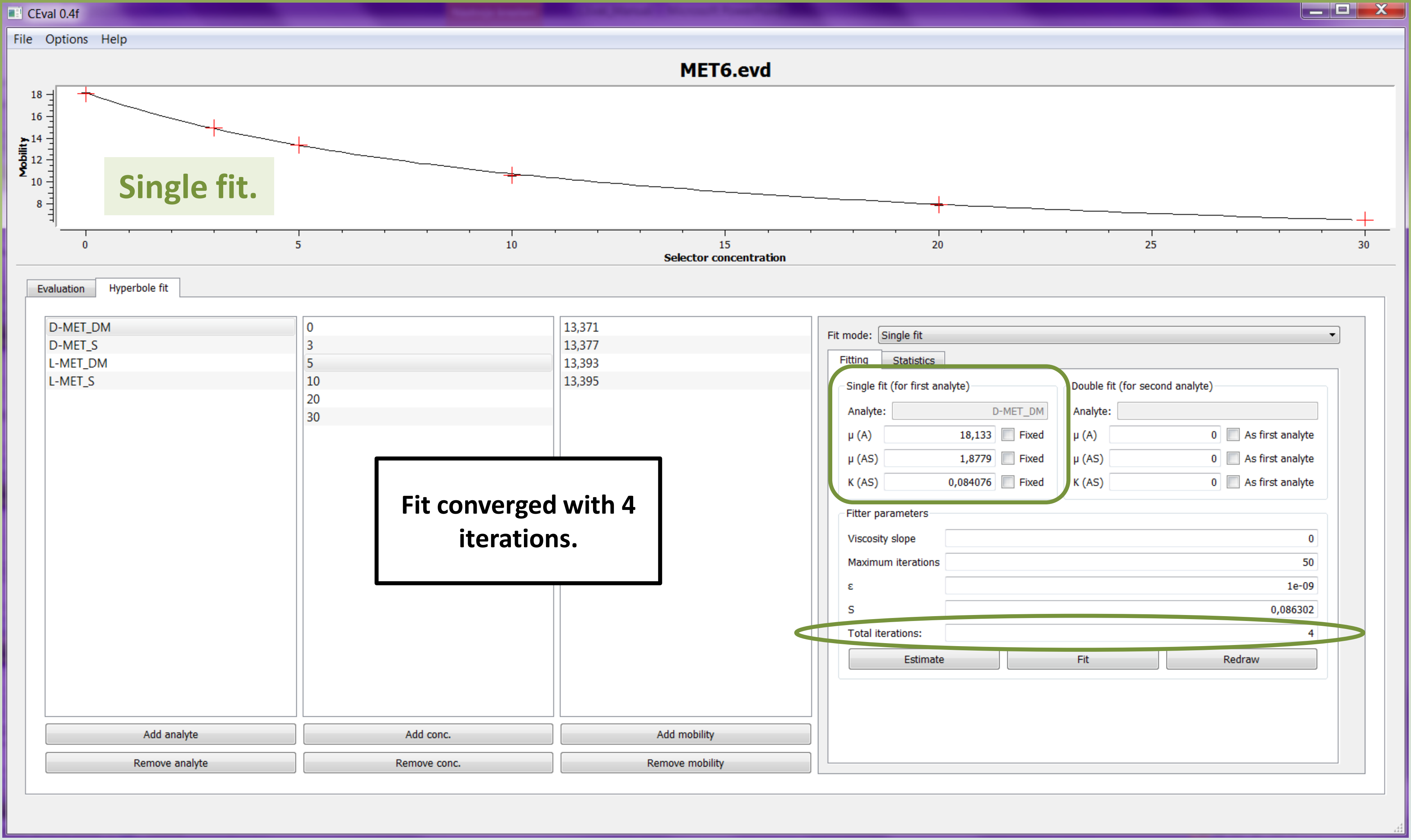
Single fit.

You can see initial estimate now.

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

Fit.

ACE Data Evaluation



Single fit.

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

0
3
5
10
20
30

13,371
13,377
13,393
13,395

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)

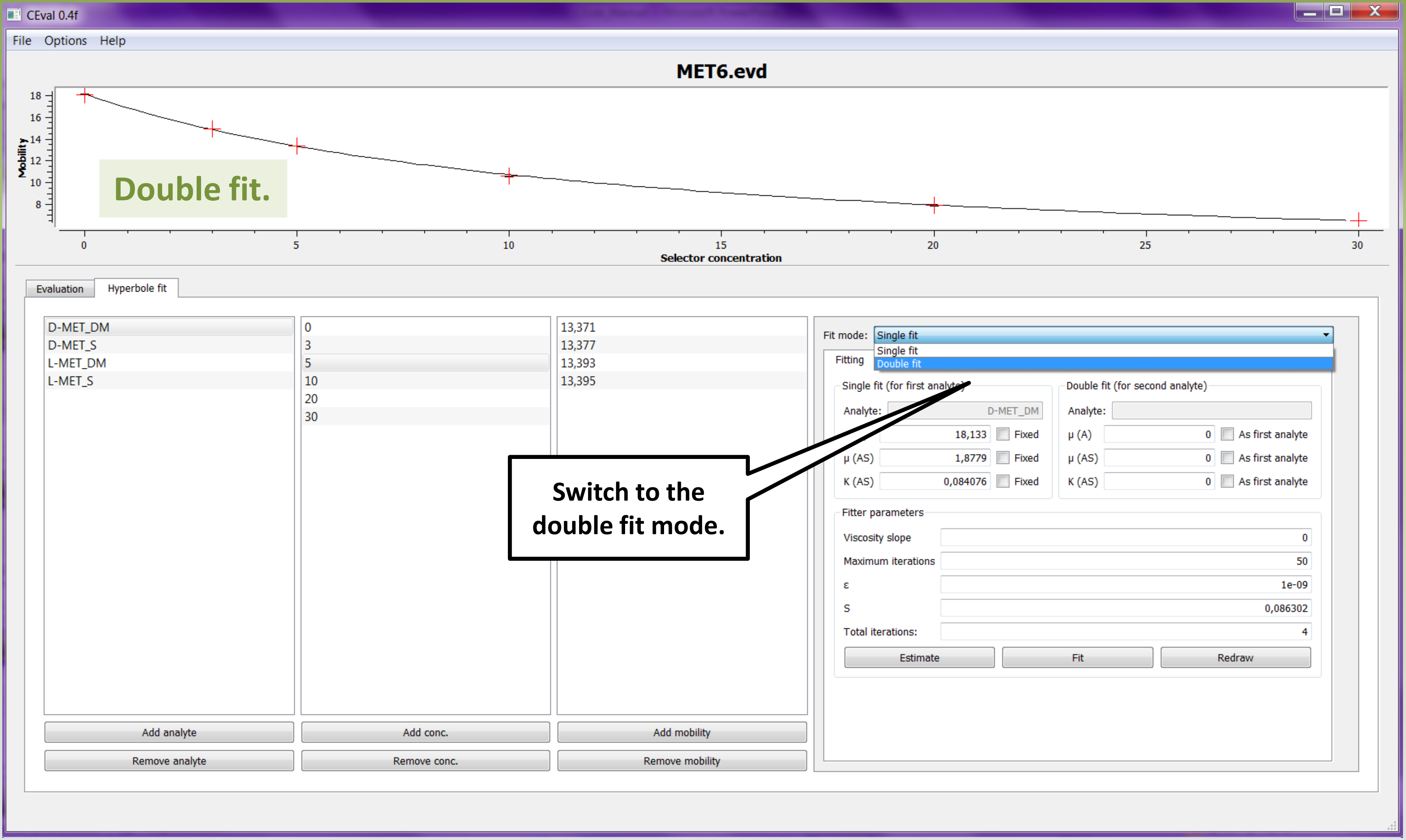
Analyte:
μ (A) 0 ☐ As first analyte
μ (AS) 0 ☐ As first analyte
K (AS) 0 ☐ As first analyte

Fitter parameters

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

Fit converged with 4 iterations.

ACE Data Evaluation



Double fit.

D-MET_DM	0	13,371
D-MET_S	3	13,377
L-MET_DM	5	13,393
L-MET_S	10	13,395
	20	
	30	

Fit mode: Single fit

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

Fitter parameters

Viscosity slope 0

Maximum iterations 50

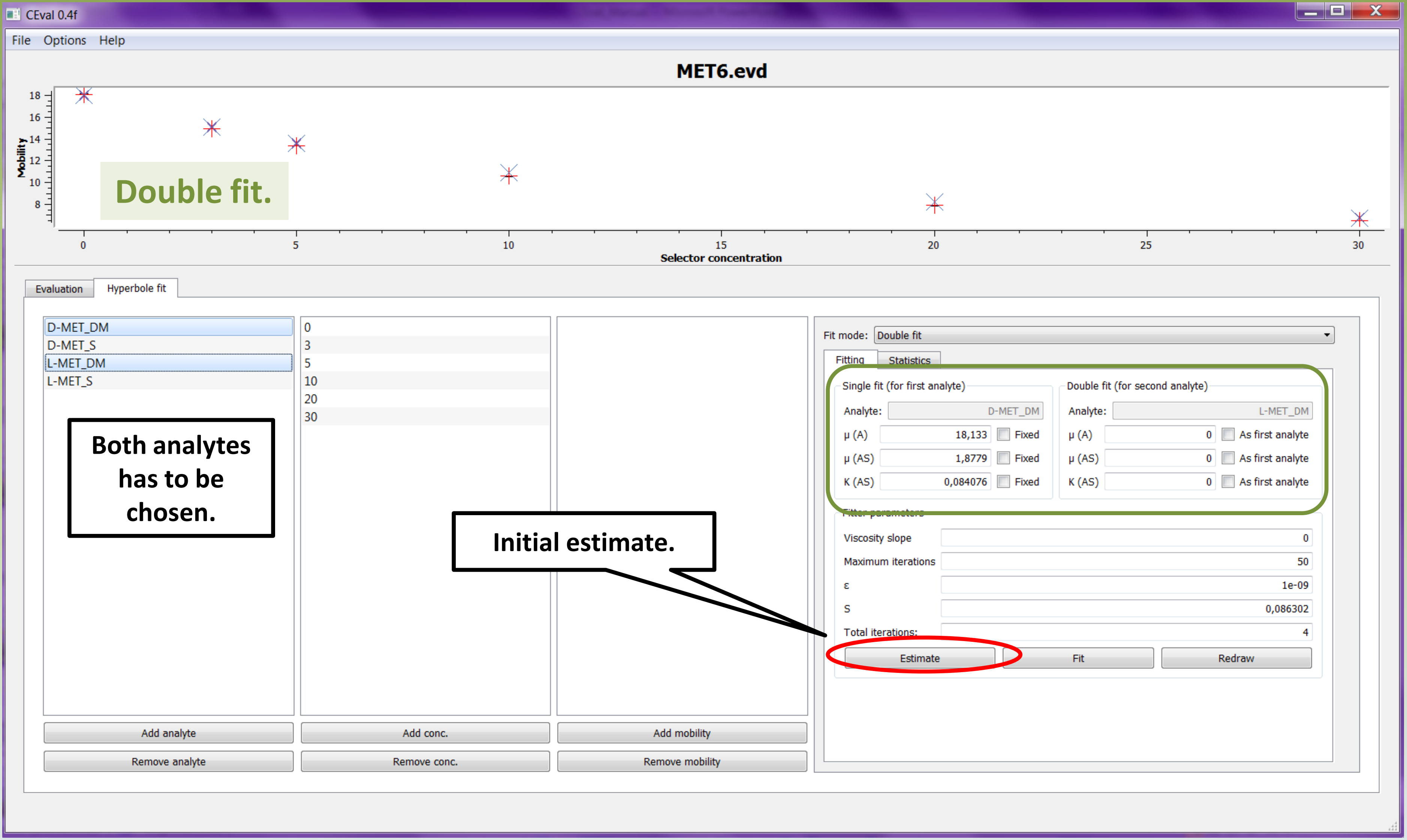
ε 1e-09

S 0,086302

Total iterations: 4

Switch to the double fit mode.

ACE Data Evaluation



Double fit.

Analytes:

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

Concentrations:

- 0
- 3
- 5
- 10
- 20
- 30

Both analytes has to be chosen.

Fit mode: Double fit

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)

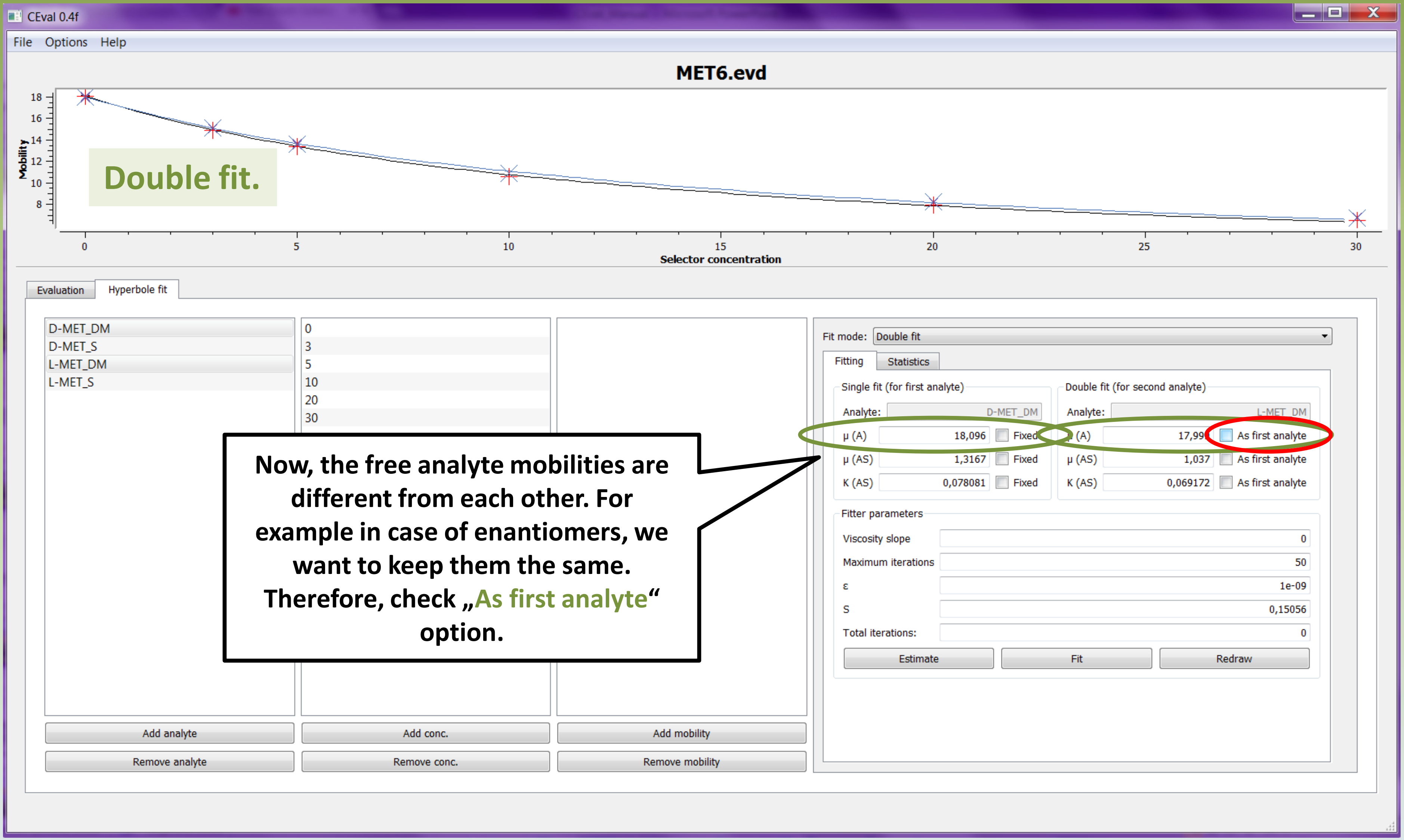
Analyte:	L-MET_DM	
μ (A)	0	☐ As first analyte
μ (AS)	0	☐ As first analyte
K (AS)	0	☐ As first analyte

Fitter parameters

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

Initial estimate.

ACE Data Evaluation



Double fit.

Analytes: D-MET_DM, D-MET_S, L-MET_DM, L-MET_S

Concentrations: 0, 3, 5, 10, 20, 30

Fit mode: Double fit

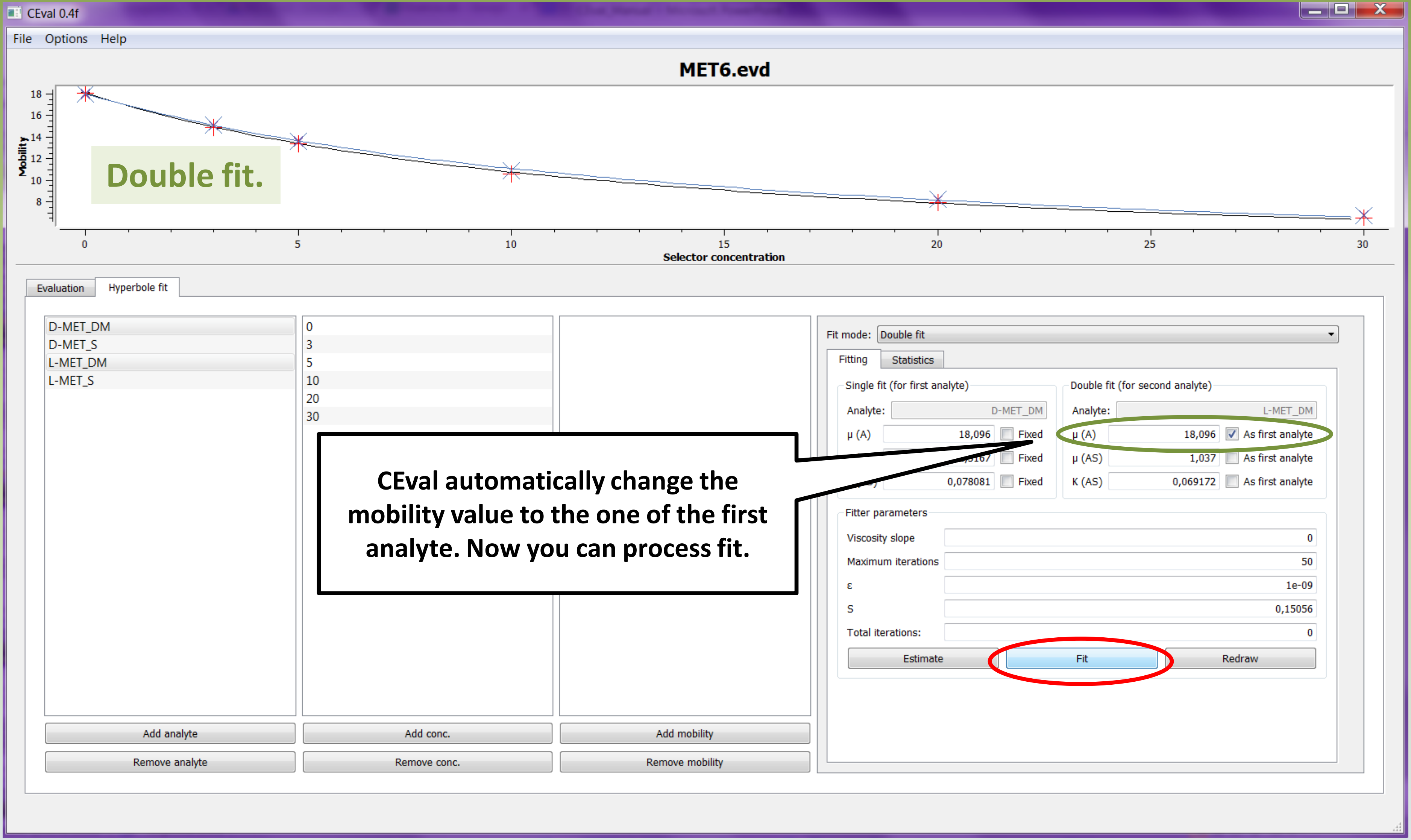
Single fit (for first analyte)
Analyte: D-MET_DM
μ (A): 18,096 ☐ Fixed
μ (AS): 1,3167 ☐ Fixed
K (AS): 0,078081 ☐ Fixed

Double fit (for second analyte)
Analyte: L-MET_DM
μ (A): 17,99 ☐ As first analyte
μ (AS): 1,037 ☐ As first analyte
K (AS): 0,069172 ☐ As first analyte

Fitter parameters
Viscosity slope: 0
Maximum iterations: 50
ε: 1e-09
S: 0,15056
Total iterations: 0

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



Double fit.

Analytes: D-MET_DM, D-MET_S, L-MET_DM, L-MET_S

Concentrations: 0, 3, 5, 10, 20, 30

Fit mode: Double fit

Single fit (for first analyte)

Analyte: D-MET_DM

μ (A): 18,096 ☐ Fixed

,5167 ☐ Fixed

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

Fitter parameters

Viscosity slope: 0

Maximum iterations: 50

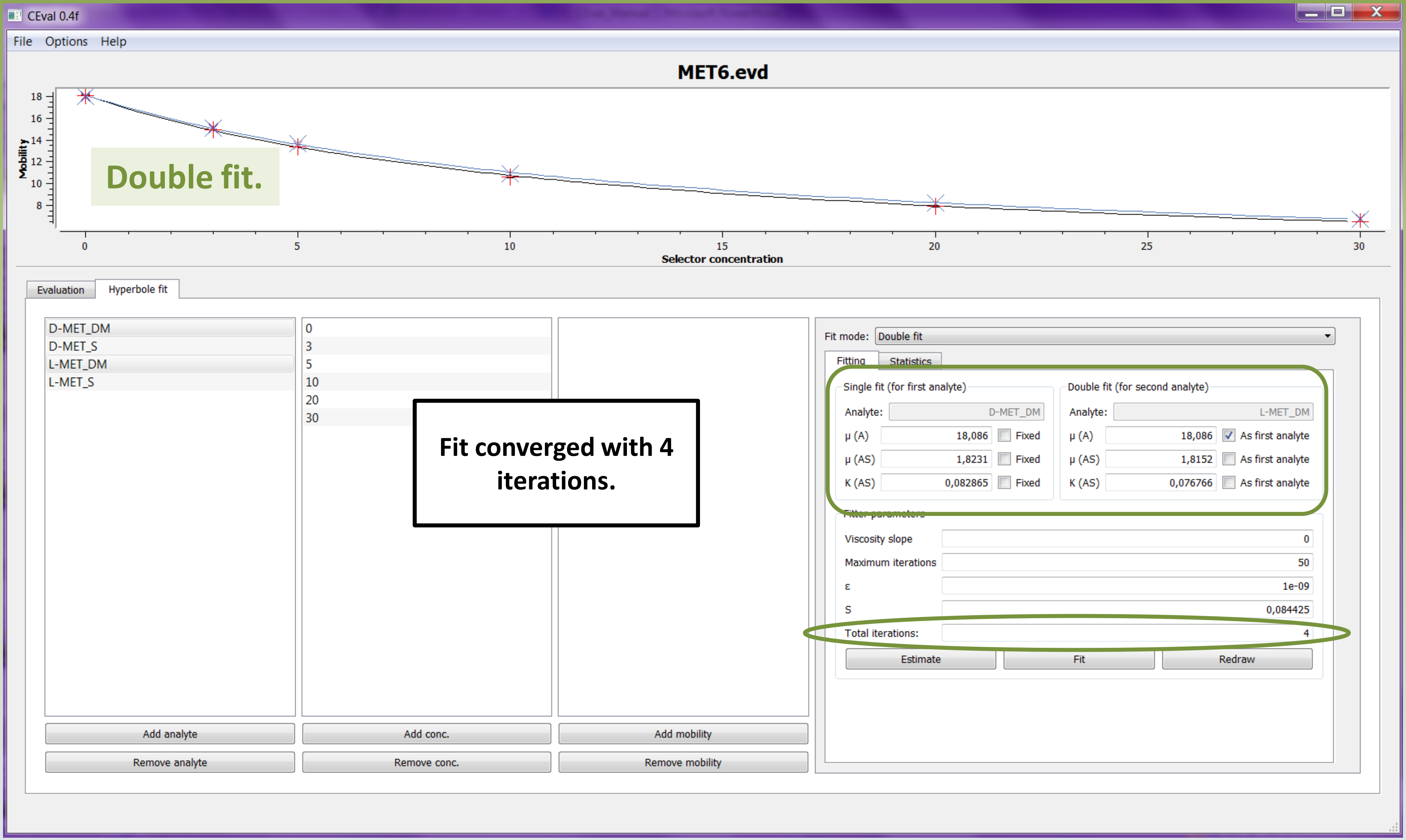
ε: 1e-09

S: 0,15056

Total iterations: 0

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

ACE Data Evaluation



Double fit.

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

0
3
5
10
20
30

Fit converged with 4 iterations.

Fit mode: Double fit

Single fit (for first analyte)

Analyte: D-MET_DM
μ (A): 18,086 ☐ Fixed
μ (AS): 1,8231 ☐ Fixed
K (AS): 0,082865 ☐ Fixed

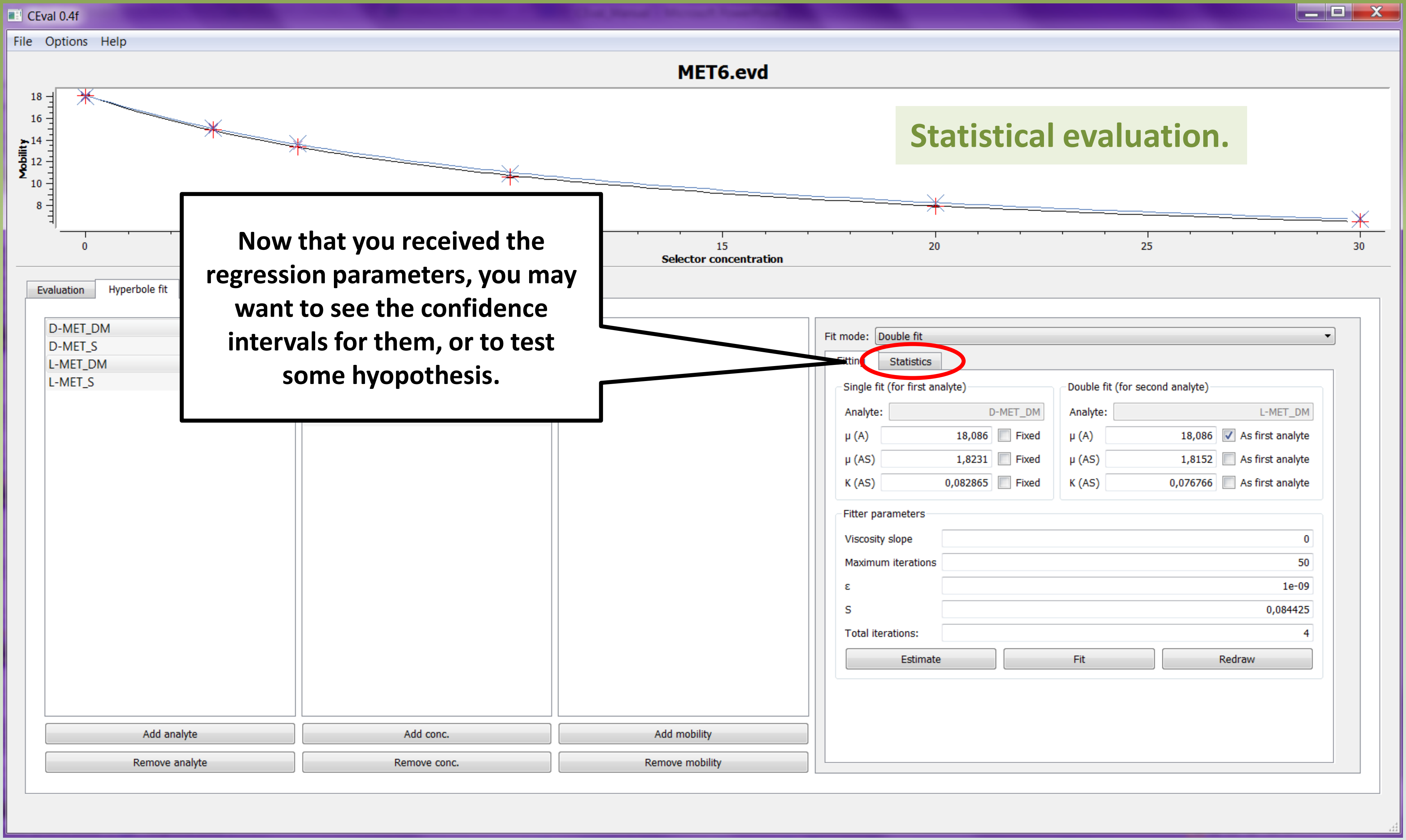
Double fit (for second analyte)

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

ACE Data Evaluation



Statistical evaluation.

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

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

Fit mode: Double fit

Single fit (for first analyte)

Analyte: D-MET_DM
μ (A) 18,086 ☐ Fixed
μ (AS) 1,8231 ☐ Fixed
K (AS) 0,082865 ☐ Fixed

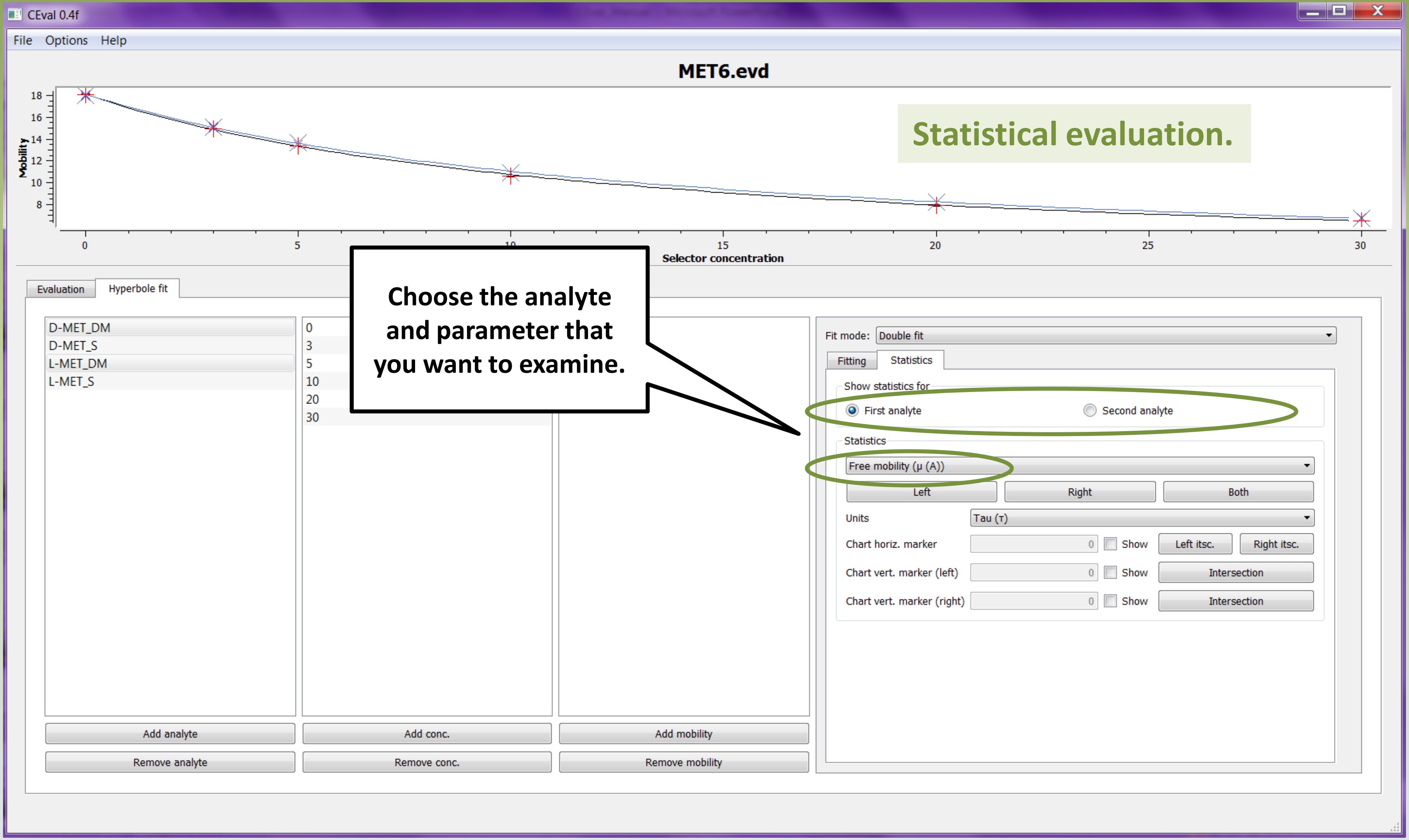
Double fit (for second analyte)

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

ACE Data Evaluation



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

0
3
5
10
20
30

Fit mode: Double fit

Show statistics for
● First analyte ○ Second analyte

Statistics
Free mobility (μ (A))

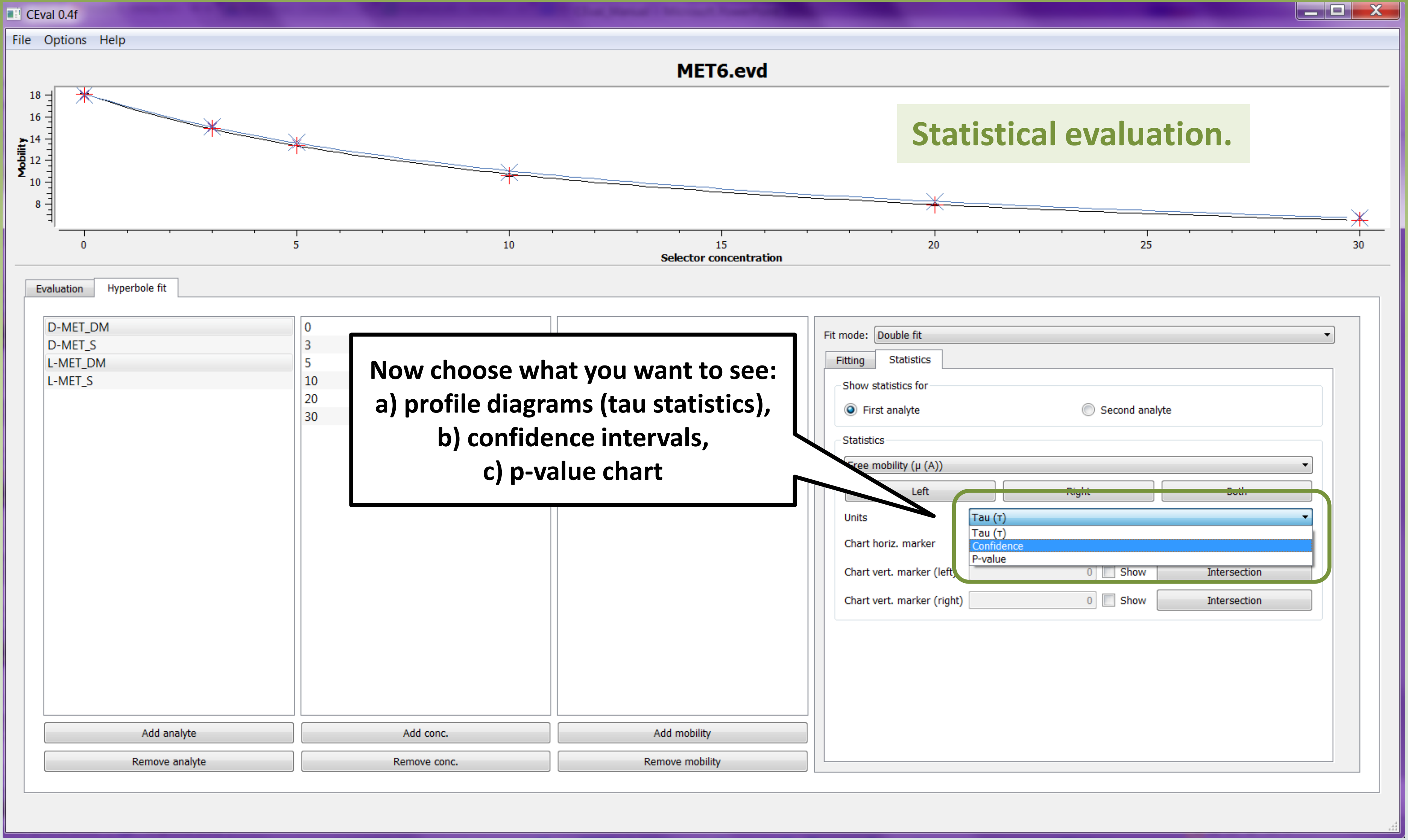
Units: Tau (τ)

Chart horiz. marker: 0 ☐ Show
Chart vert. marker (left): 0 ☐ Show
Chart vert. marker (right): 0 ☐ Show

Statistical evaluation.

Choose the analyte and parameter that you want to examine.

ACE Data Evaluation



Fit mode: Double fit

● First analyte ○ Second analyte

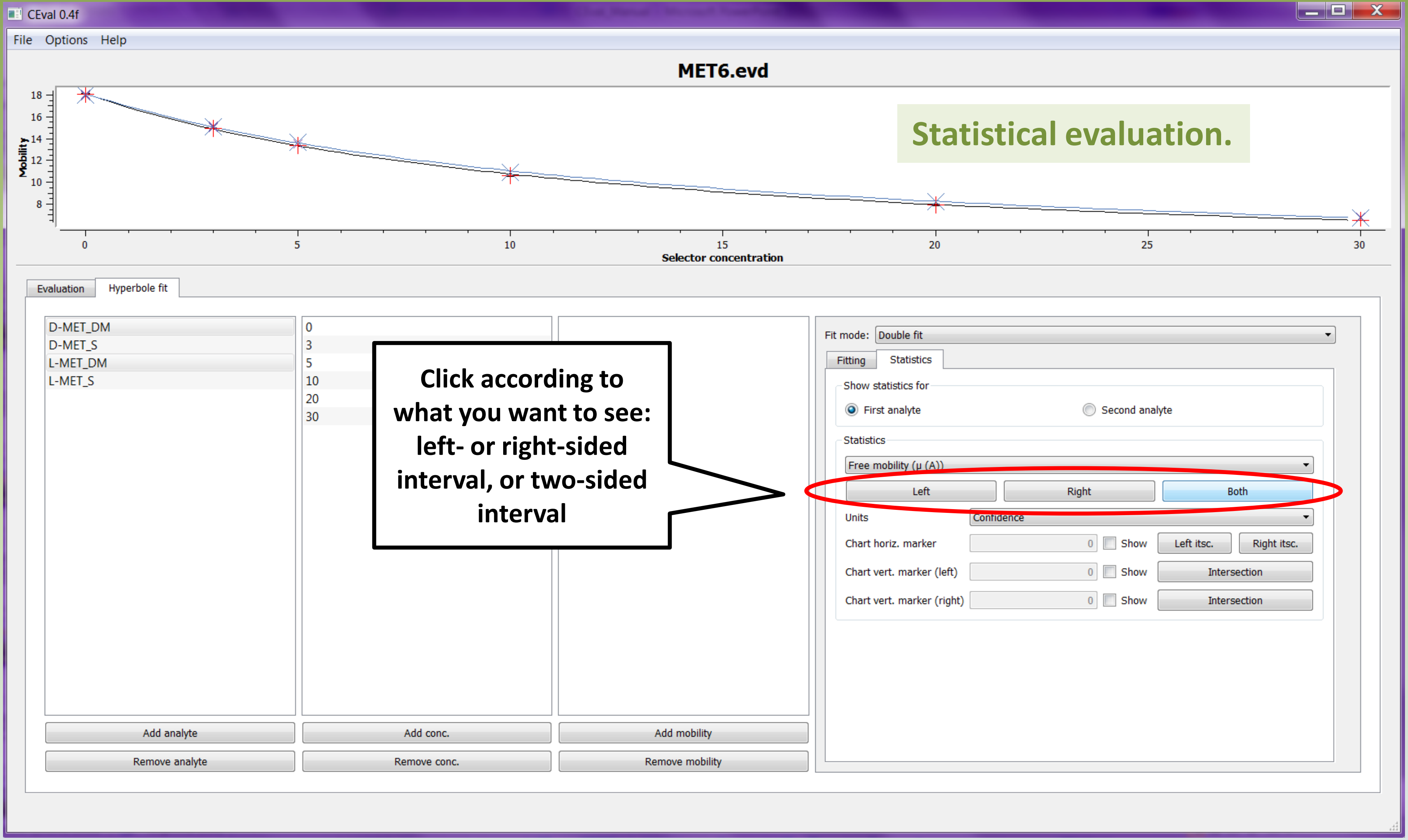
Statistics: Free mobility (μ (A))

Units: Tau (τ)

Statistical evaluation.

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

ACE Data Evaluation



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

0
3
5
10
20
30

Fit mode: Double fit

Show statistics for

● First analyte ○ Second analyte

Statistics: Free mobility (μ (A))

Units: Confidence

Chart horiz. marker 0 ☐ Show

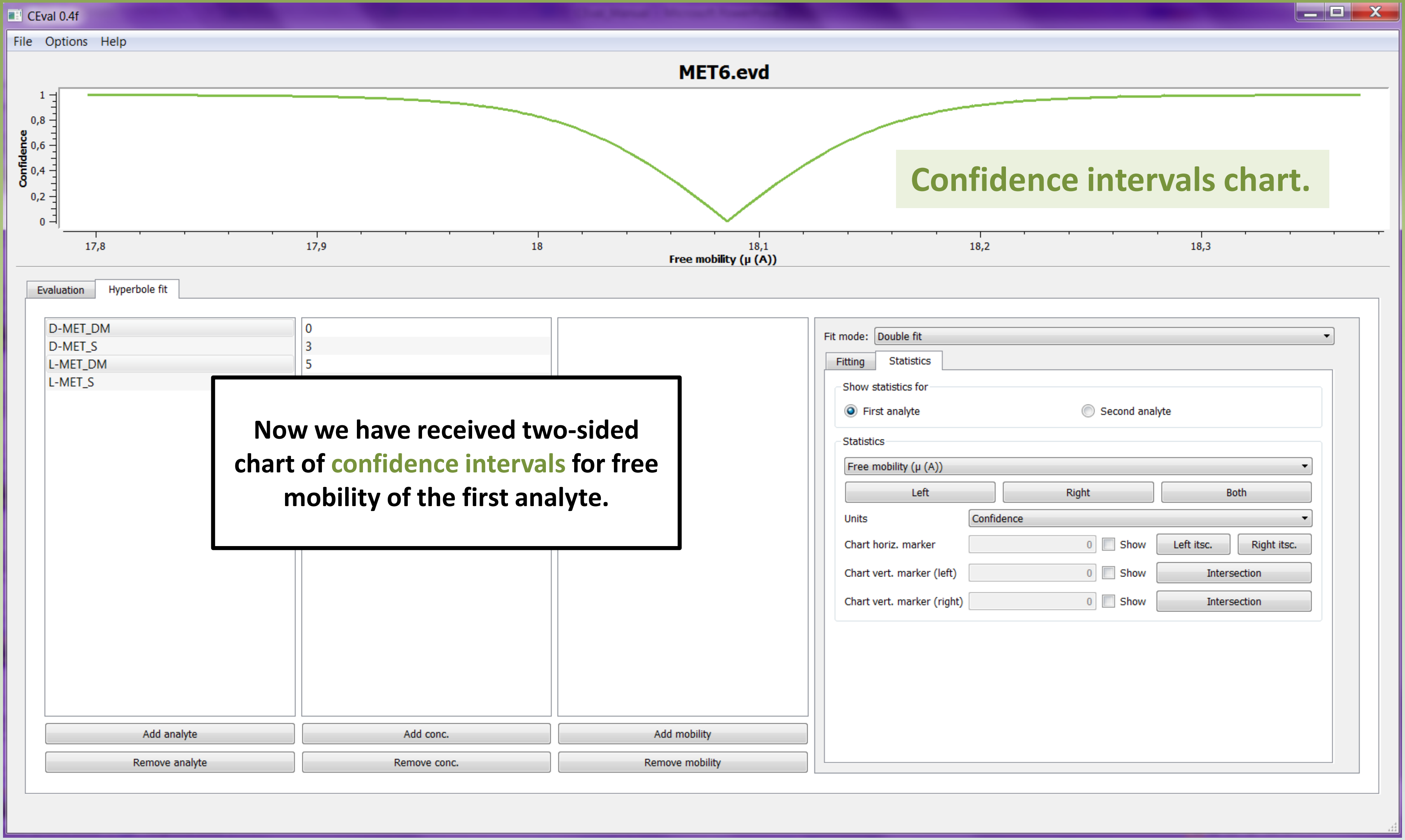
Chart vert. marker (left) 0 ☐ Show

Chart vert. marker (right) 0 ☐ Show

Statistical evaluation.

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

ACE Data Evaluation



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

0
3
5

Fit mode: Double fit

Show statistics for
● First analyte ○ Second analyte

Statistics
Free mobility (μ (A))

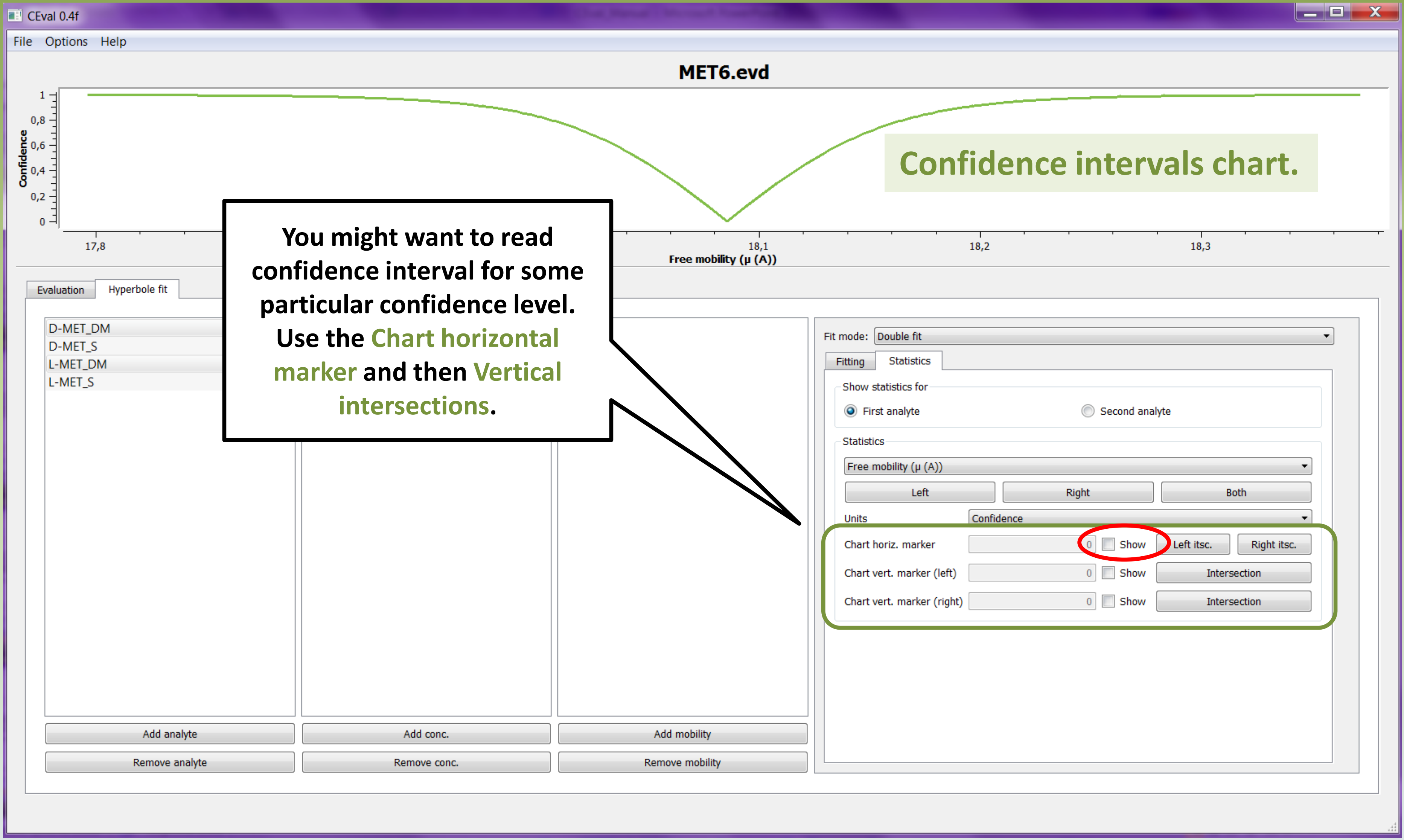
Units: Confidence

Chart horiz. marker: 0 ☐ Show
Chart vert. marker (left): 0 ☐ Show
Chart vert. marker (right): 0 ☐ Show

Confidence intervals chart.

Now we have received two-sided chart of confidence intervals for free mobility of the first analyte.

ACE Data Evaluation



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

Fit mode: Double fit

● First analyte ○ Second analyte

Statistics: Free mobility (μ (A))

Units: Confidence

Chart horiz. marker: 0 ☐ Show

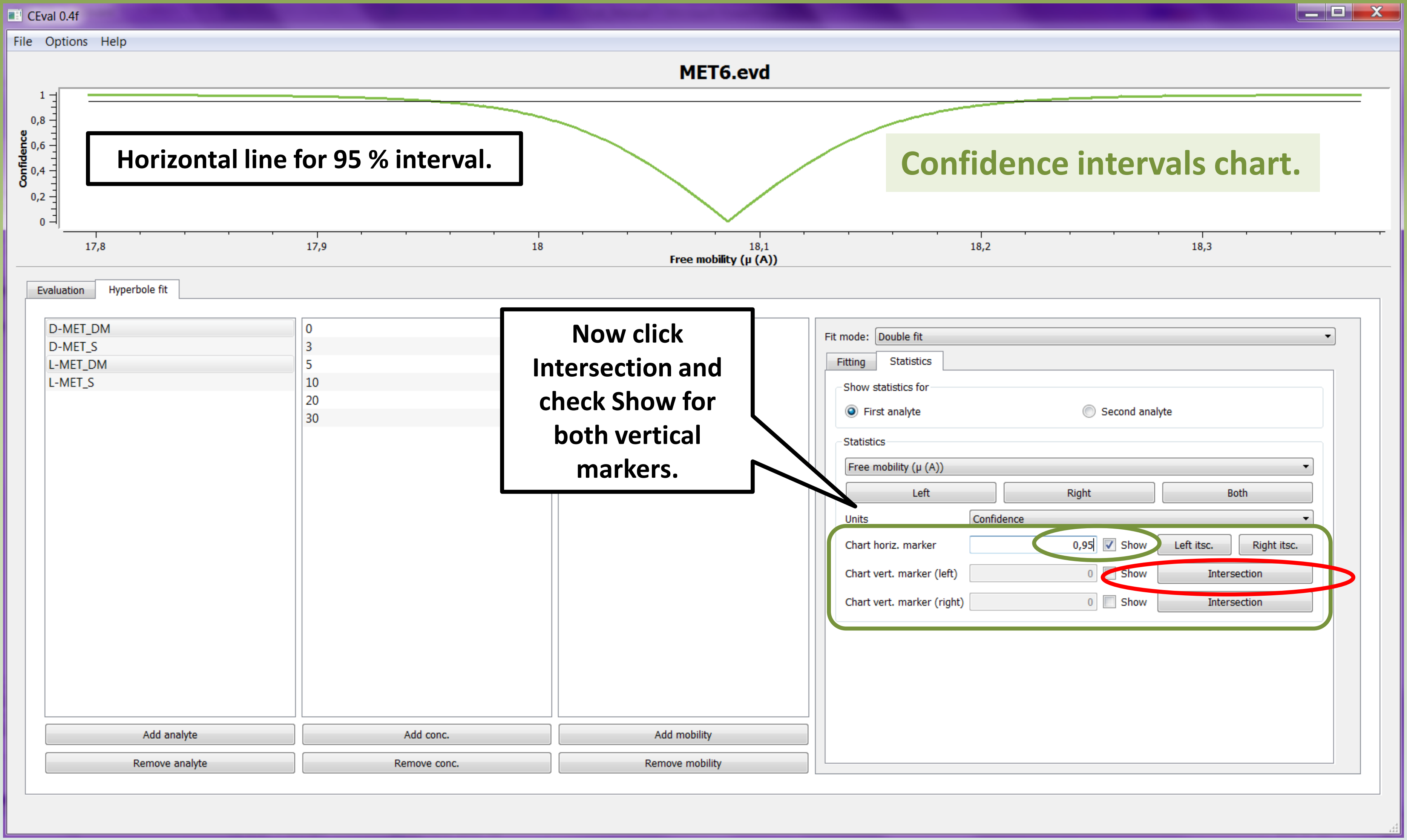
Chart vert. marker (left): 0 ☐ Show

Chart vert. marker (right): 0 ☐ Show

Confidence intervals chart.

You might want to read confidence interval for some particular confidence level. Use the Chart horizontal marker and then Vertical intersections.

ACE Data Evaluation



Fit mode: Double fit

● First analyte ○ Second analyte

Free mobility (μ (A))

Units: Confidence

Chart horiz. marker: 0,95 ☑ Show

Chart vert. marker (left): 0 ☐ Show

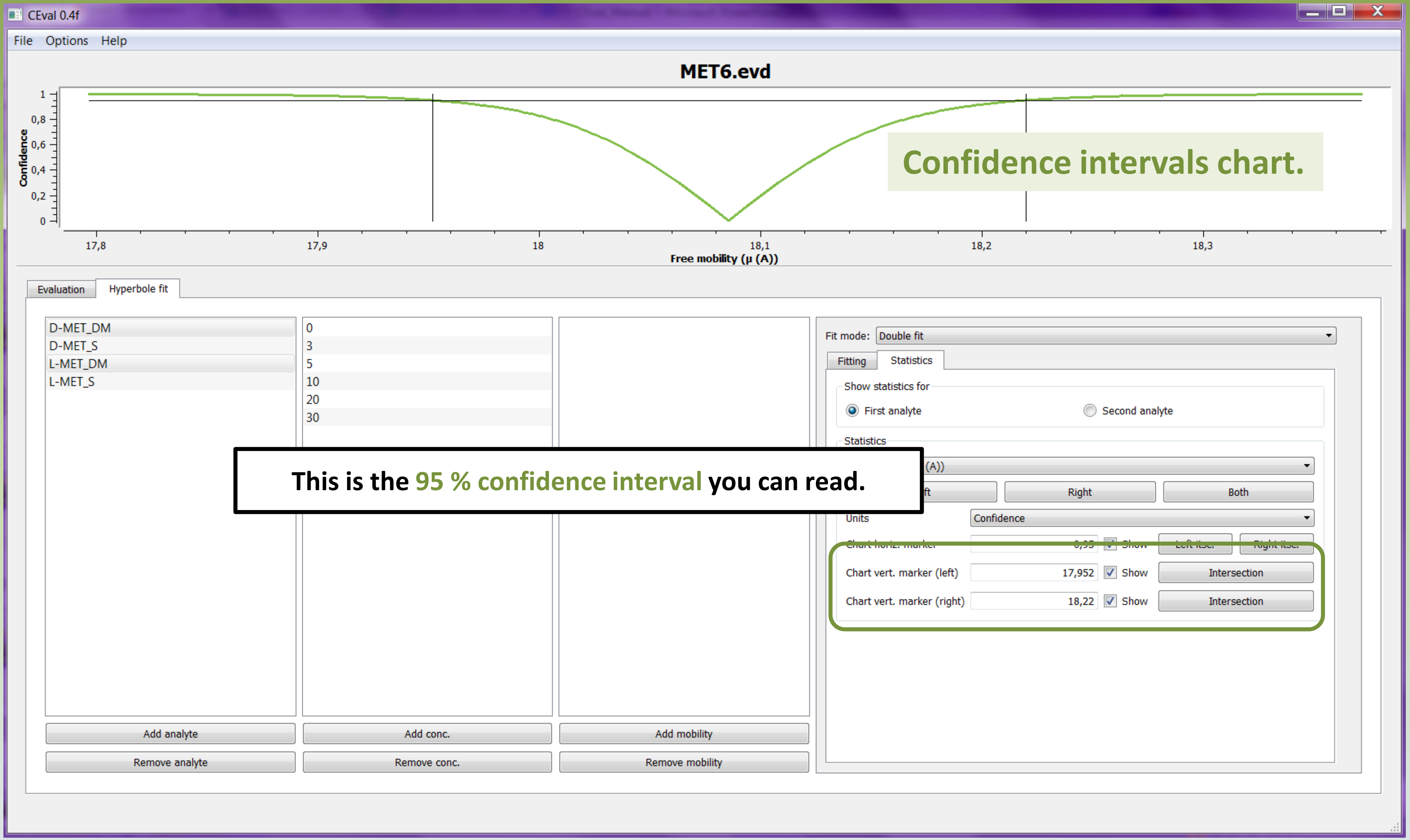
Chart vert. marker (right): 0 ☐ Show

Horizontal line for 95 % interval.

Confidence intervals chart.

Now click Intersection and check Show for both vertical markers.

ACE Data Evaluation



Confidence intervals chart.

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

Fit mode: Double fit

Show statistics for: ● First analyte ○ Second analyte

Units: Confidence

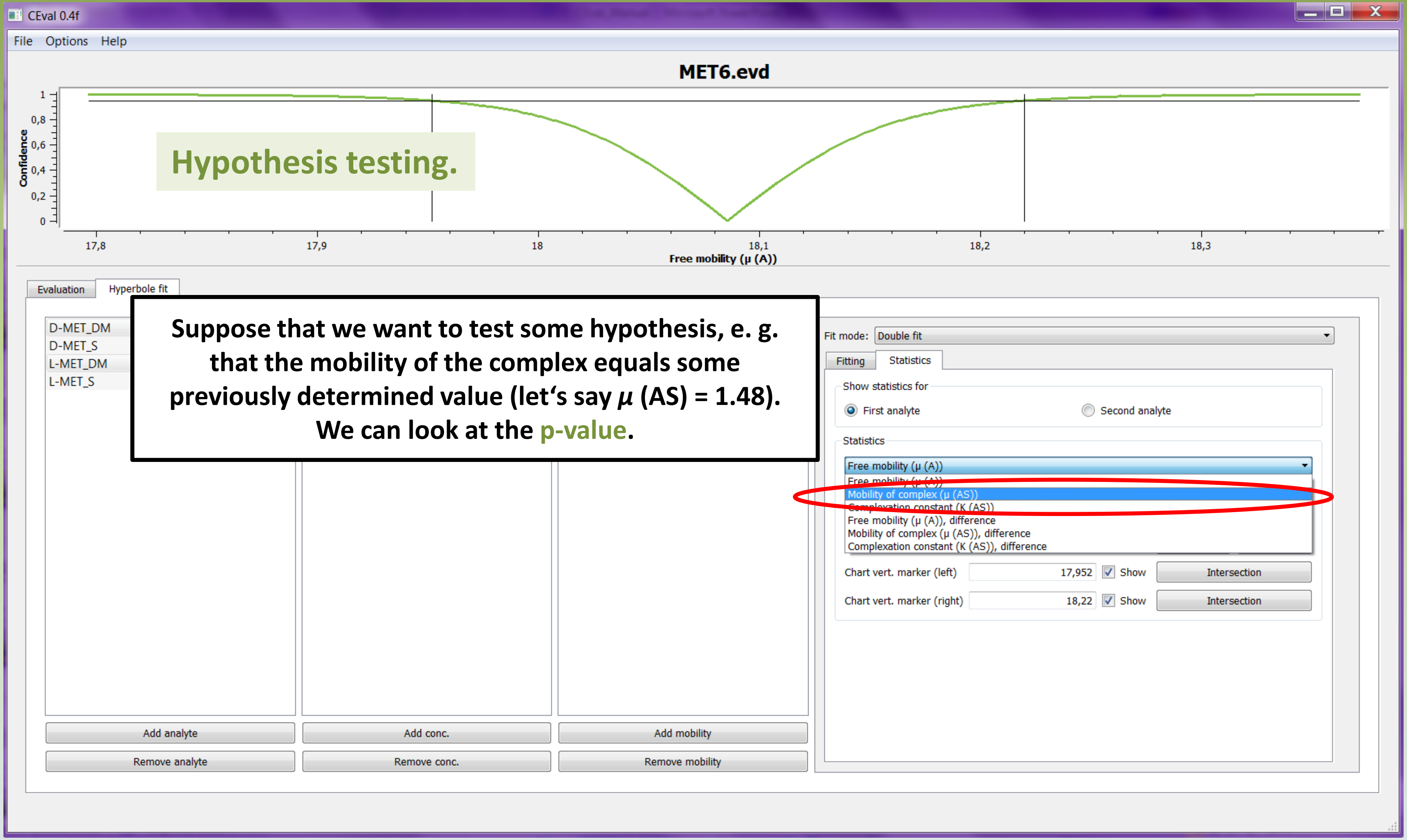
Chart horiz. marker 0,95 ☑ Show

Chart vert. marker (left) 17,952 ☑ Show

Chart vert. marker (right) 18,22 ☑ Show

This is the 95 % confidence interval you can read.

ACE Data Evaluation



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

Fit mode: Double fit

Show statistics for
● First analyte ○ Second analyte

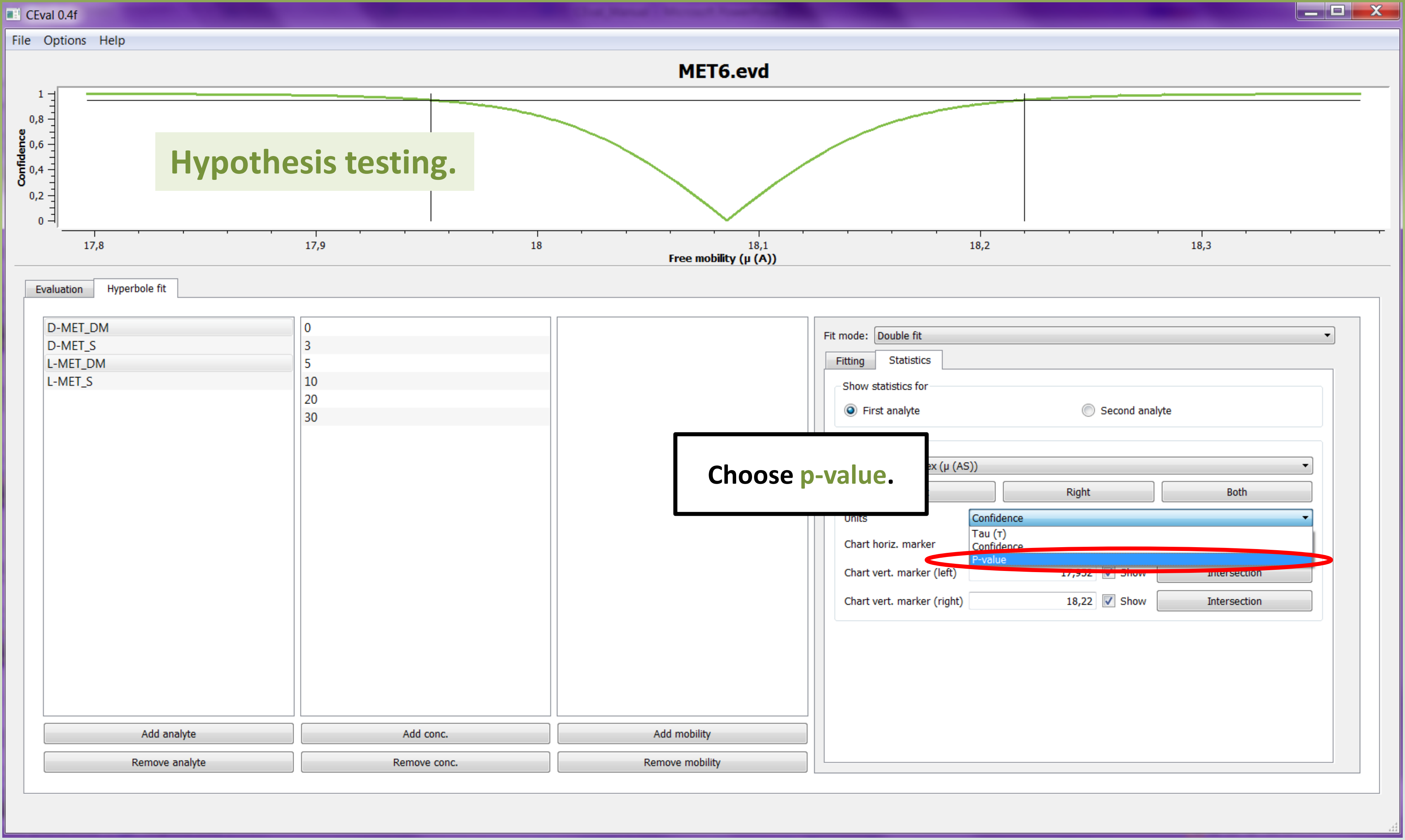
Statistics
Free mobility (μ (A))
- Free mobility (μ (A))
- Mobility of complex (μ (AS))
- Complexation constant (K (AS))
- Free mobility (μ (A)), difference
- Mobility of complex (μ (AS)), difference
- Complexation constant (K (AS)), difference

Chart vert. marker (left) 17,952 ☑ Show
Chart vert. marker (right) 18,22 ☑ Show

Hypothesis testing.

Suppose that we want to test some hypothesis, e. g. that the mobility of the complex equals some previously determined value (let's say μ (AS) = 1.48). We can look at the p-value.

ACE Data Evaluation



Analytes:
- D-MET_DM
- D-MET_S
- L-MET_DM
- L-MET_S

Concentrations:
- 0
- 3
- 5
- 10
- 20
- 30

Fit mode: Double fit

Show statistics for: ● First analyte ○ Second analyte

ex (μ (AS))

Units: Confidence

Chart horiz. marker

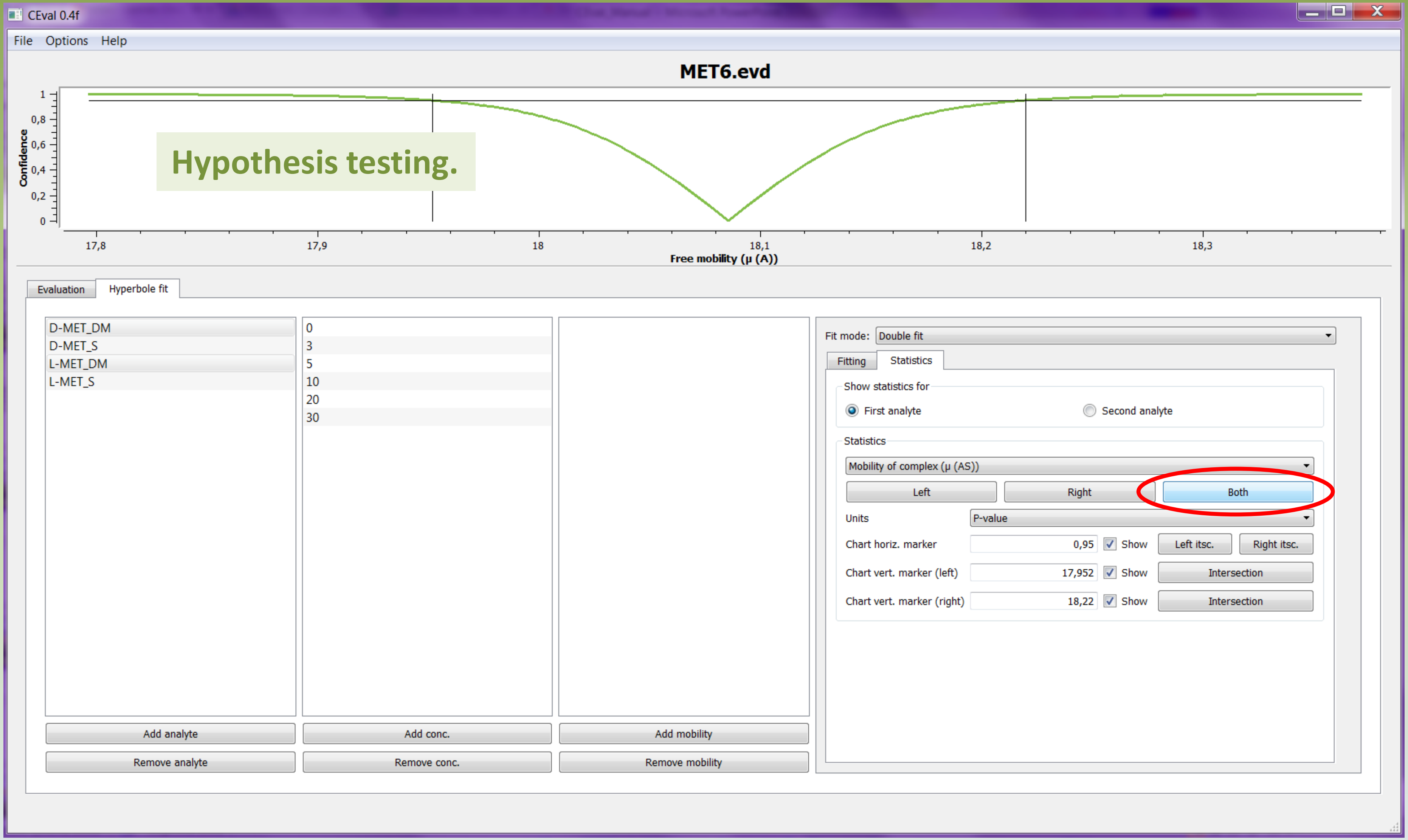
Chart vert. marker (left): 17,952 ☑ Show

Chart vert. marker (right): 18,22 ☑ Show

Hypothesis testing.

Choose p-value.

ACE Data Evaluation



Hypothesis testing.

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

0
3
5
10
20
30

Fit mode: Double fit

Show statistics for
● First analyte ○ Second analyte

Statistics
Mobility of complex (μ (AS))

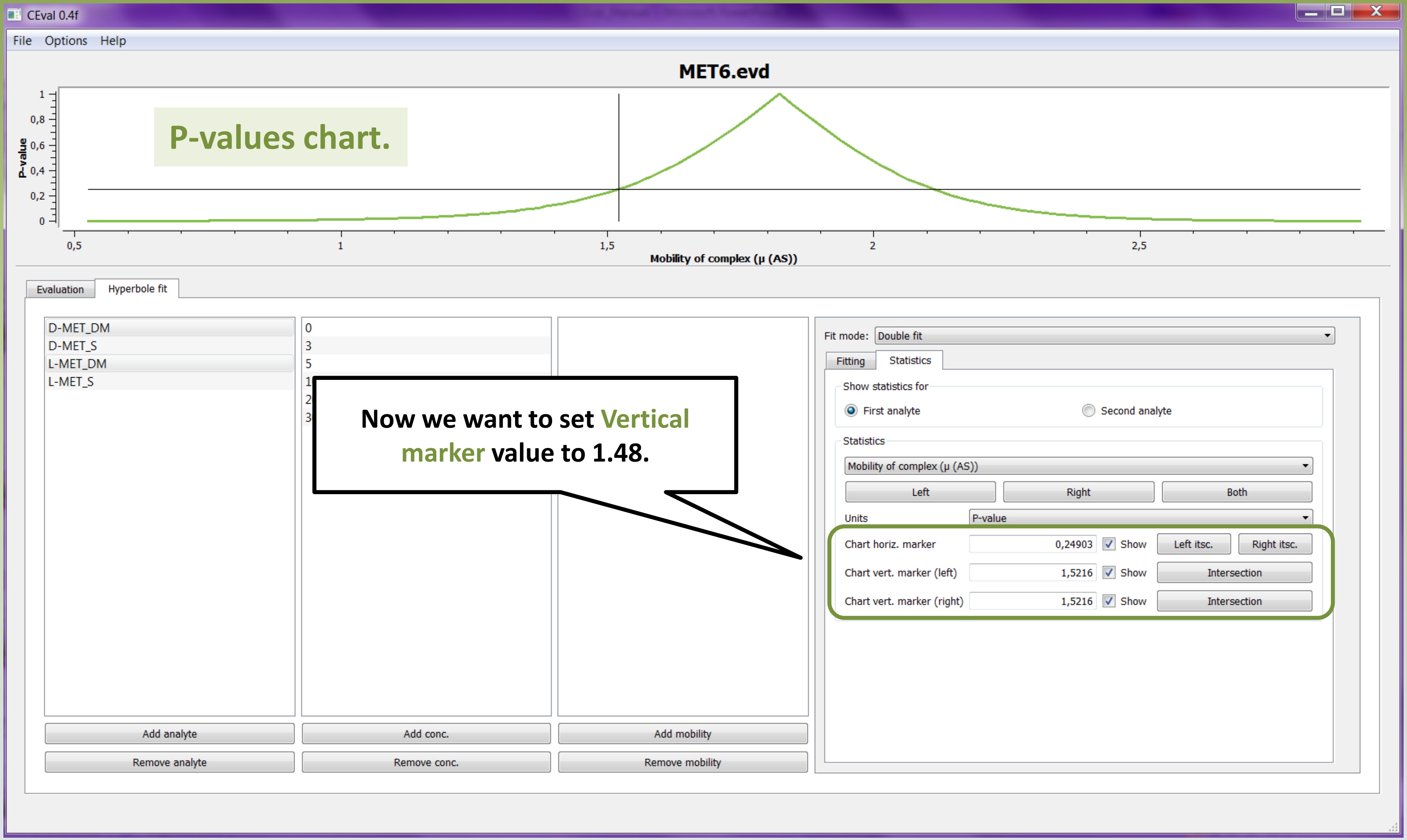
Units: P-value

Chart horiz. marker: 0,95 ☑ Show

Chart vert. marker (left): 17,952 ☑ Show

Chart vert. marker (right): 18,22 ☑ Show

ACE Data Evaluation



P-values chart.

Now we want to set **Vertical marker** value to 1.48.

Fit mode: Double fit

Show statistics for: ● First analyte ○ Second analyte

Statistics: Mobility of complex (μ (AS))

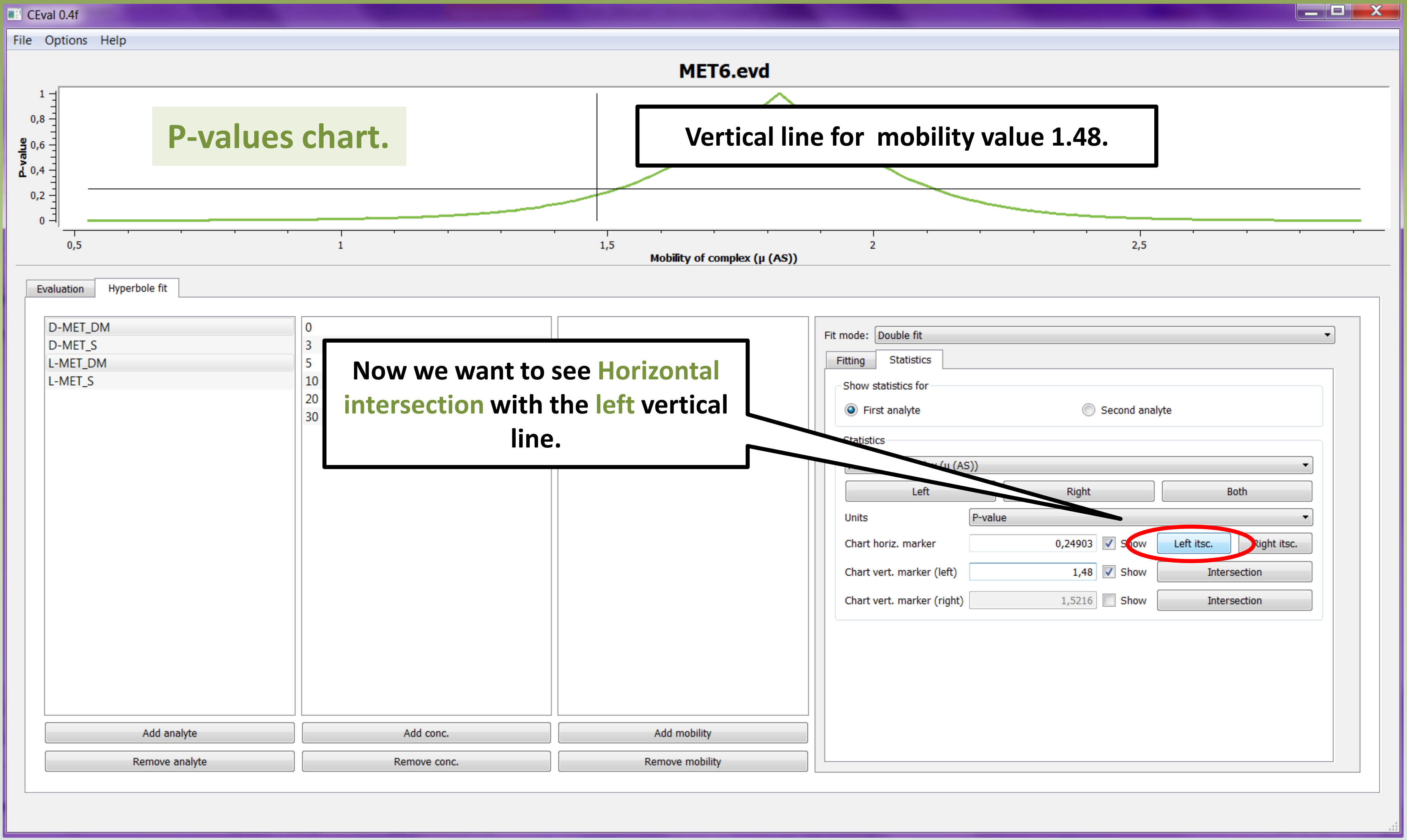
Units: P-value

Chart horiz. marker: 0,24903 ☑ Show

Chart vert. marker (left): 1,5216 ☑ Show

Chart vert. marker (right): 1,5216 ☑ Show

ACE Data Evaluation



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

0
3
5
10
20
30

Fit mode: Double fit

Show statistics for

● First analyte ○ Second analyte

Statistics

(μ (AS))

Units: P-value

Chart horiz. marker: 0,24903 ☑ Show

Chart vert. marker (left): 1,48 ☑ Show

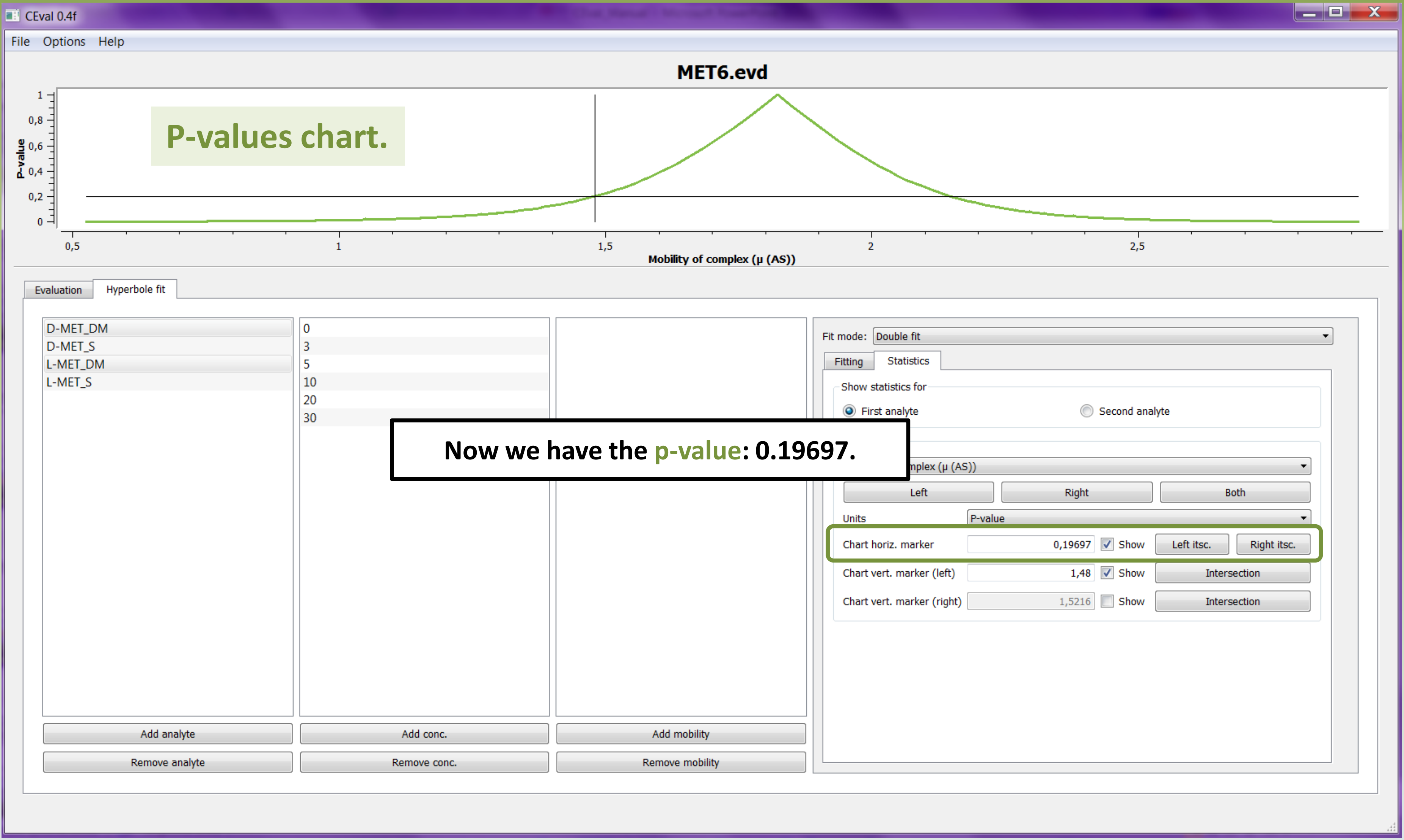
Chart vert. marker (right): 1,5216 ☐ Show

P-values chart.

Vertical line for mobility value 1.48.

Now we want to see Horizontal intersection with the left vertical line.

ACE Data Evaluation



P-values chart.

Now we have the p-value: 0.19697.

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

0
3
5
10
20
30

Fit mode: Double fit

● First analyte ○ Second analyte

Units: P-value

Chart horiz. marker: 0,19697 ☑ Show

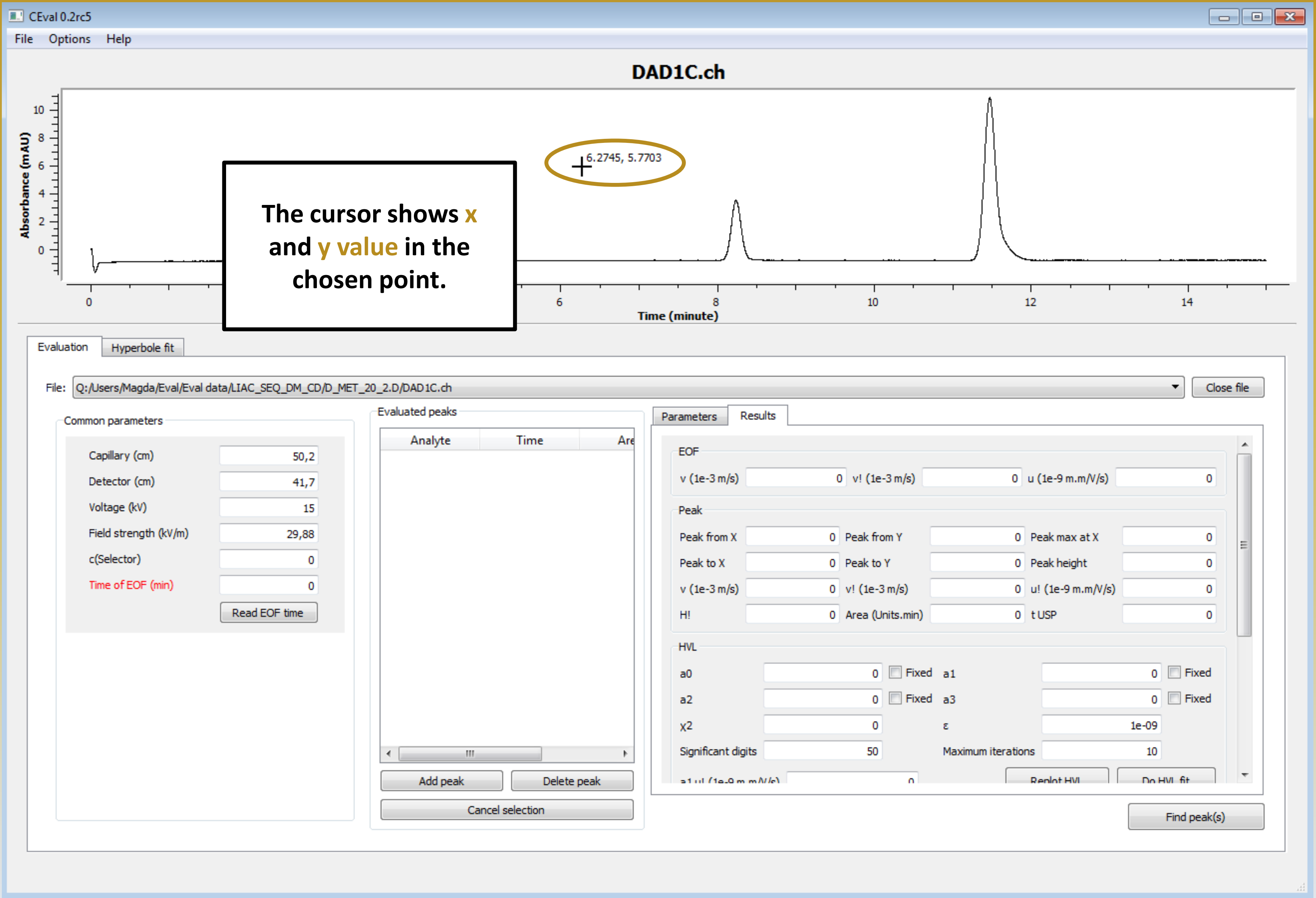
Chart vert. marker (left): 1,48 ☑ Show

Chart vert. marker (right): 1,5216 ☐ Show

Appendix A:

Graph Interface

Appendix A: Graph Interface



The cursor shows **x** and **y value** in the chosen point.

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

EOF

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

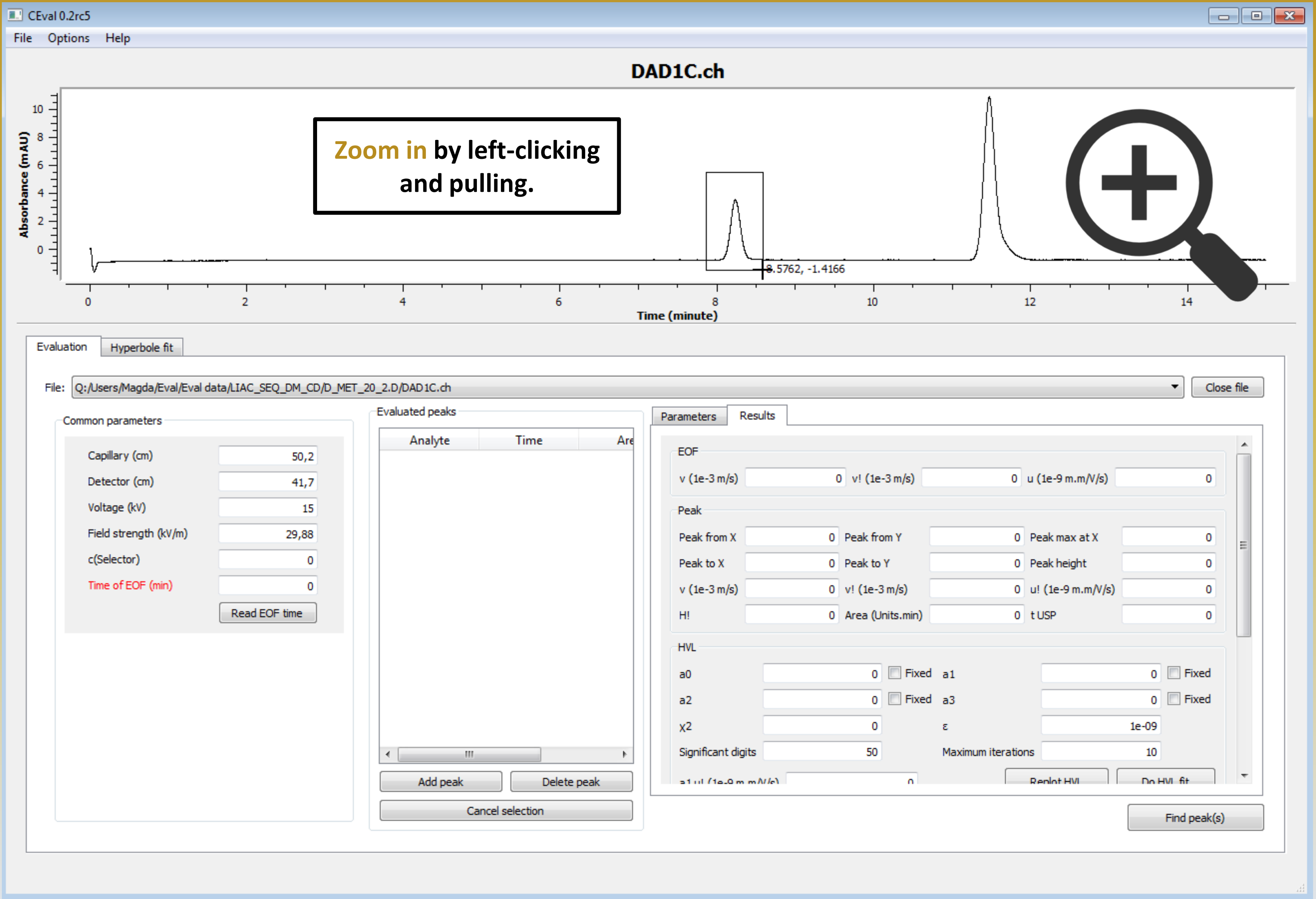
Peak

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
χ2	0		ε	1e-09	
Significant digits	50		Maximum iterations	10	

Appendix A: Graph Interface



Zoom in by left-clicking and pulling.

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

Evaluated peaks

Analyte	Time	Are

EOF

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

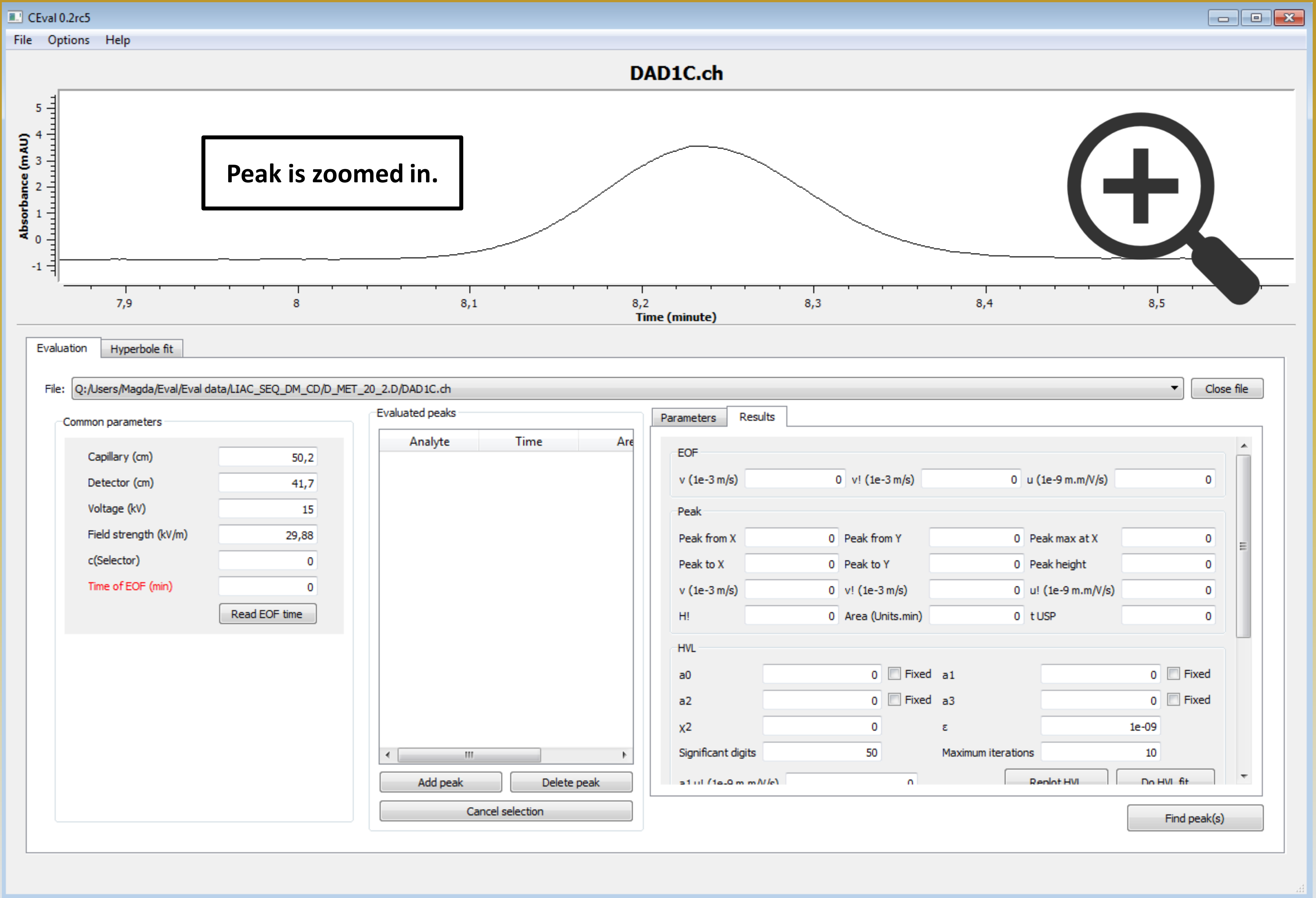
Peak

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
χ2	0		ε	1e-09	
Significant digits	50		Maximum iterations	10	

Appendix A: Graph Interface



Peak is zoomed in.

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

Results

EOF

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

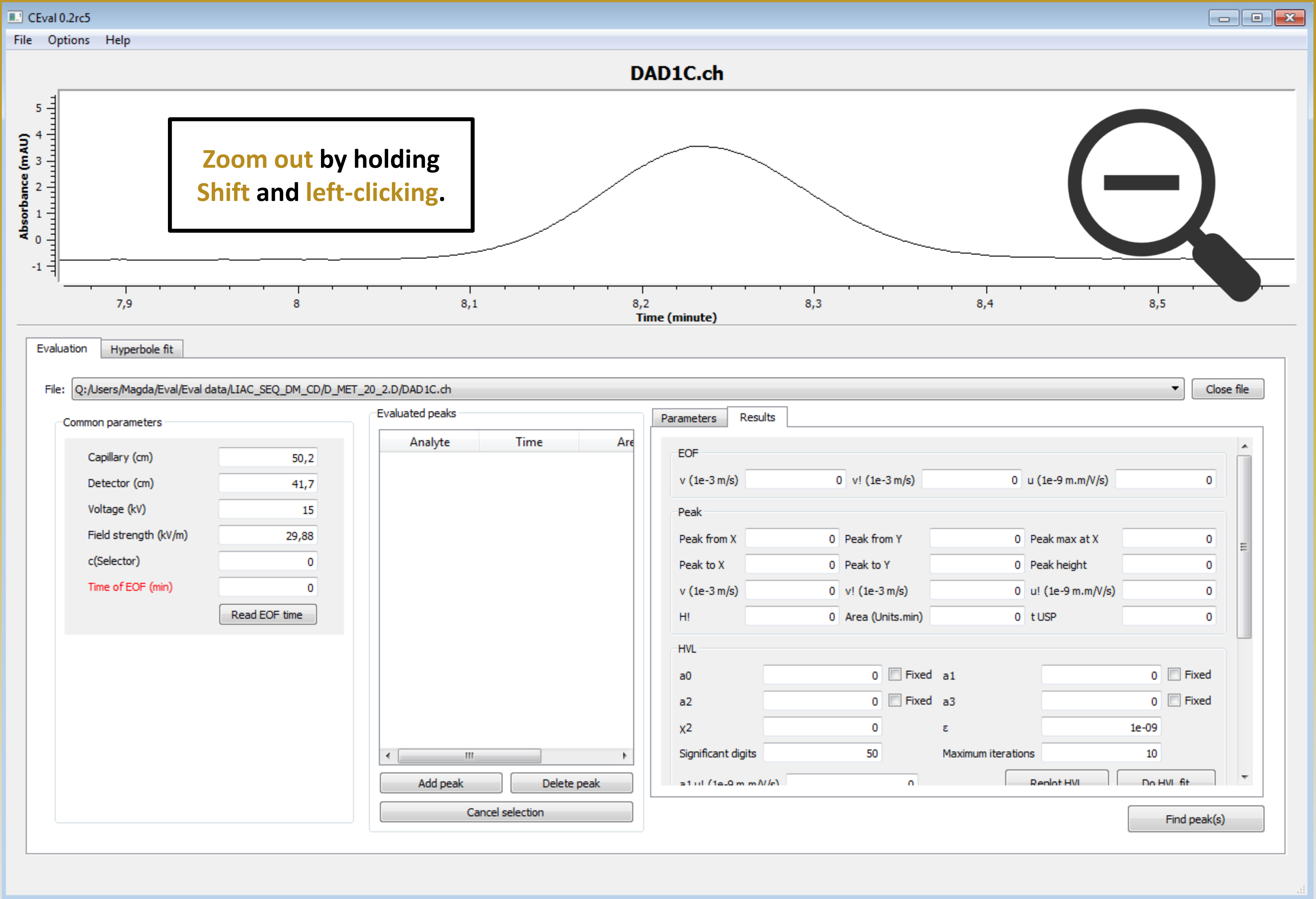
Peak

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
χ2	0		ε	1e-09	
Significant digits	50		Maximum iterations	10	
a1 u! (1e-9 m.m/V/s)	0				

Appendix A: Graph Interface



Zoom out by holding Shift and left-clicking.

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

EOF

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

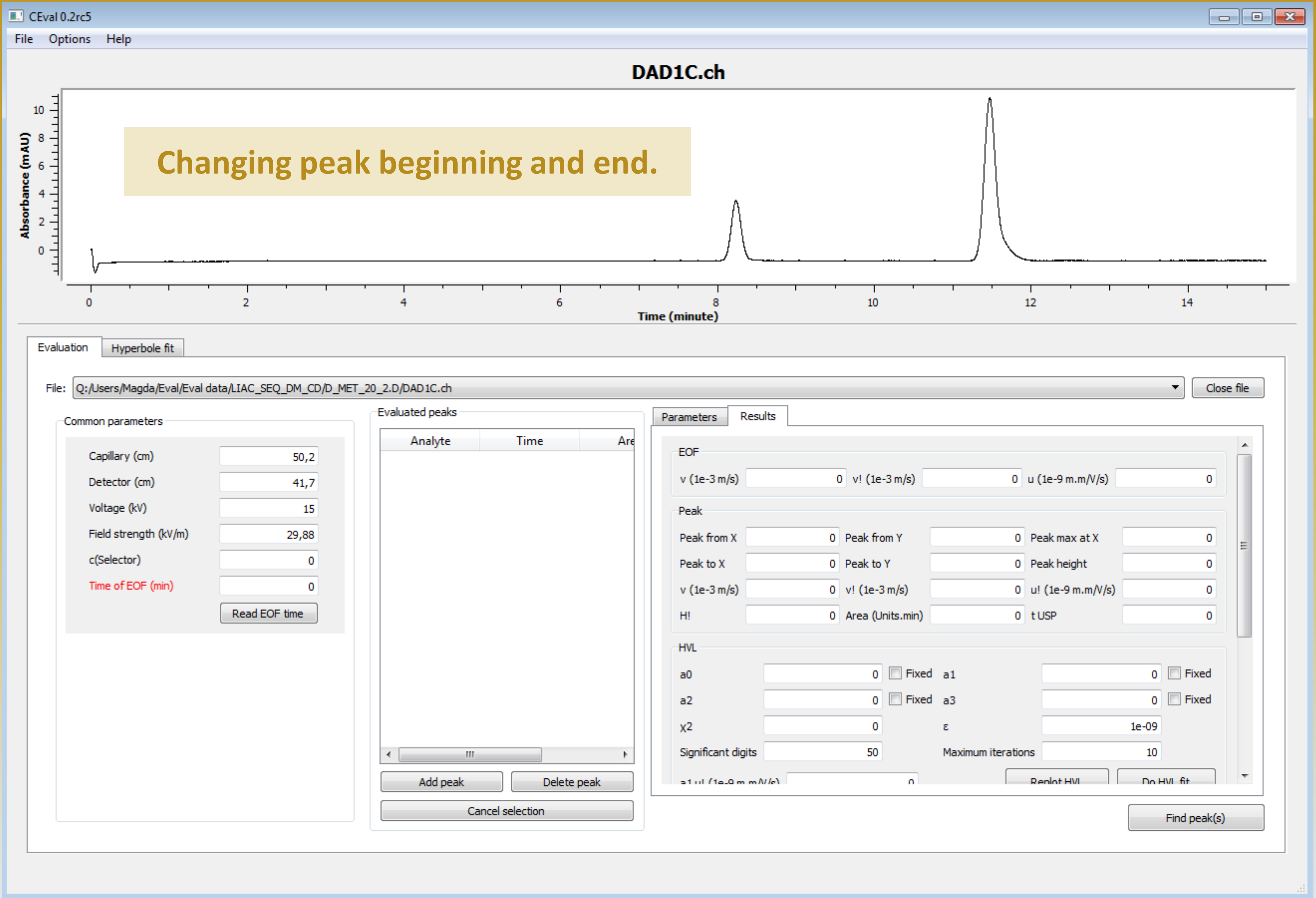
Peak

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
χ2	0		ε	1e-09	
Significant digits	50		Maximum iterations	10	

Appendix A: Graph Interface



Changing peak beginning and end.

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

Evaluated peaks

Analyte	Time	Are

EOF

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

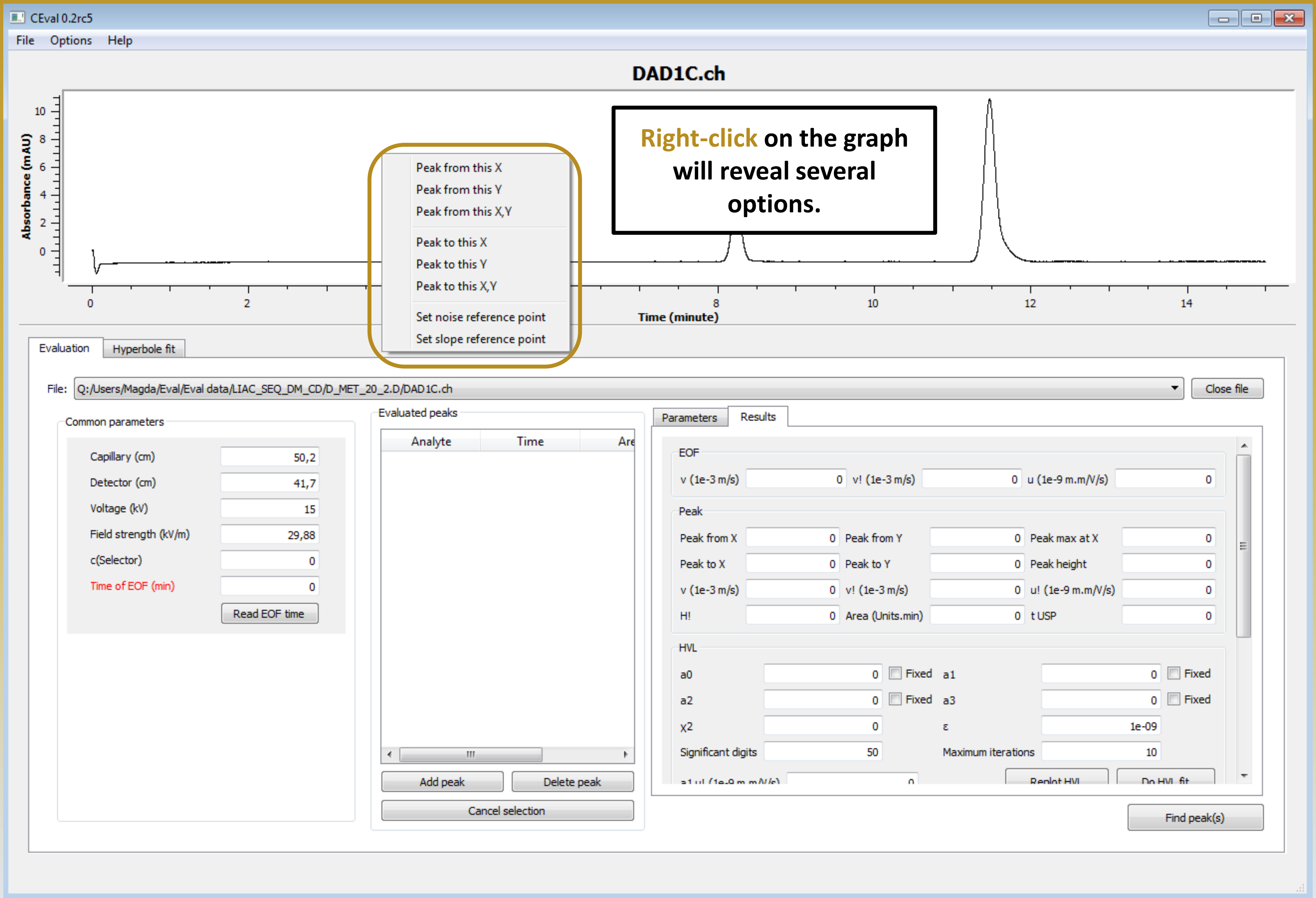
Peak

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
χ2	0		ε	1e-09	
Significant digits	50		Maximum iterations	10	

Appendix A: Graph Interface



Right-click on the graph will reveal several options.

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

Evaluated peaks

EOF

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

Peak

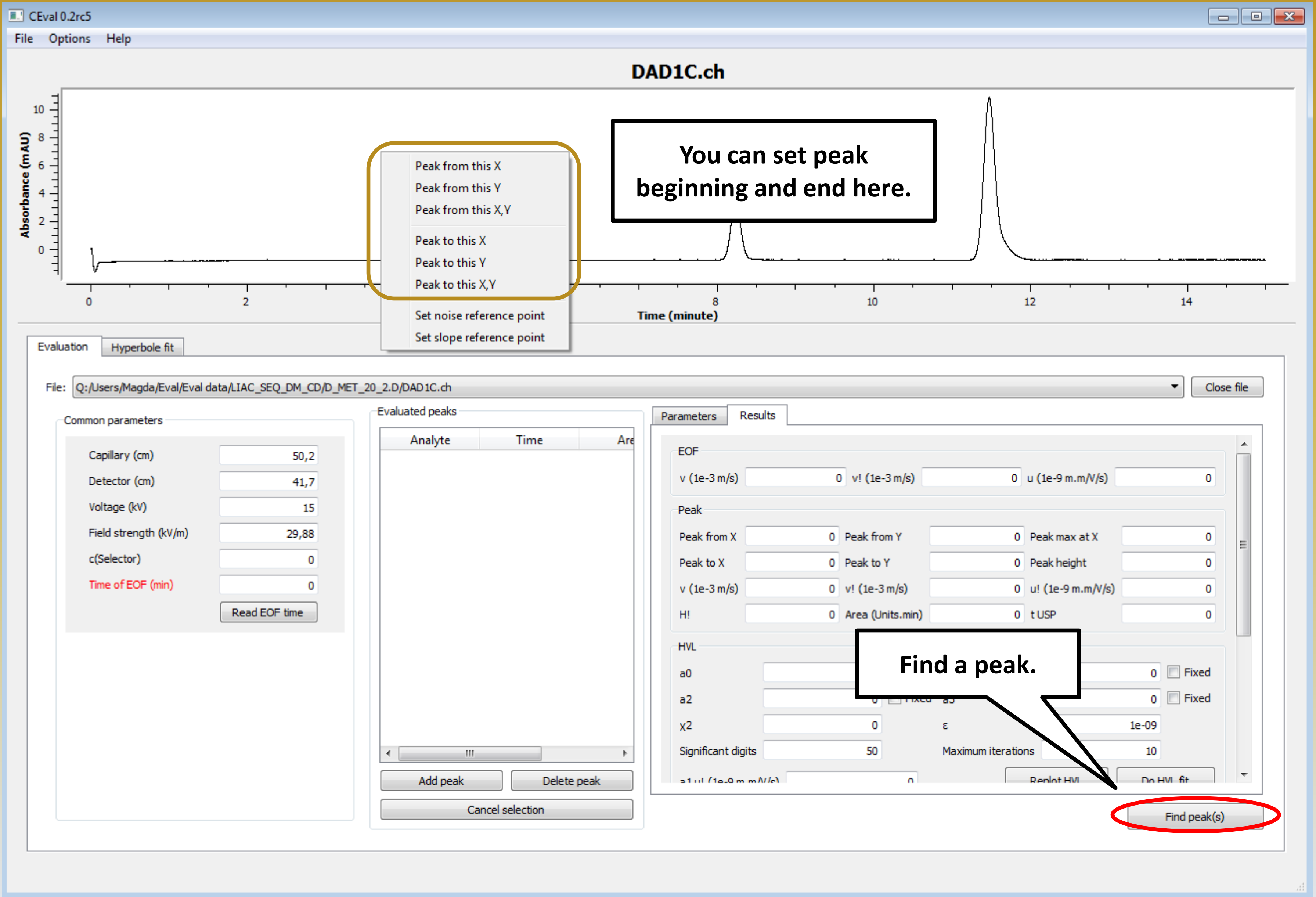
Peak from X	0	Peak from Y	0	Peak max at X	0
Peak to X	0	Peak to Y	0	Peak height	0
v (1e-3 m/s)	0	v! (1e-3 m/s)	0	u! (1e-9 m.m/V/s)	0
H!	0	Area (Units.min)	0	t USP	0

HVL

a0	0	☐ Fixed	a1	0	☐ Fixed
a2	0	☐ Fixed	a3	0	☐ Fixed
χ2	0		ε	1e-09	
Significant digits	50		Maximum iterations	10	

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

Appendix A: Graph Interface



You can set peak beginning and end here.

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

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

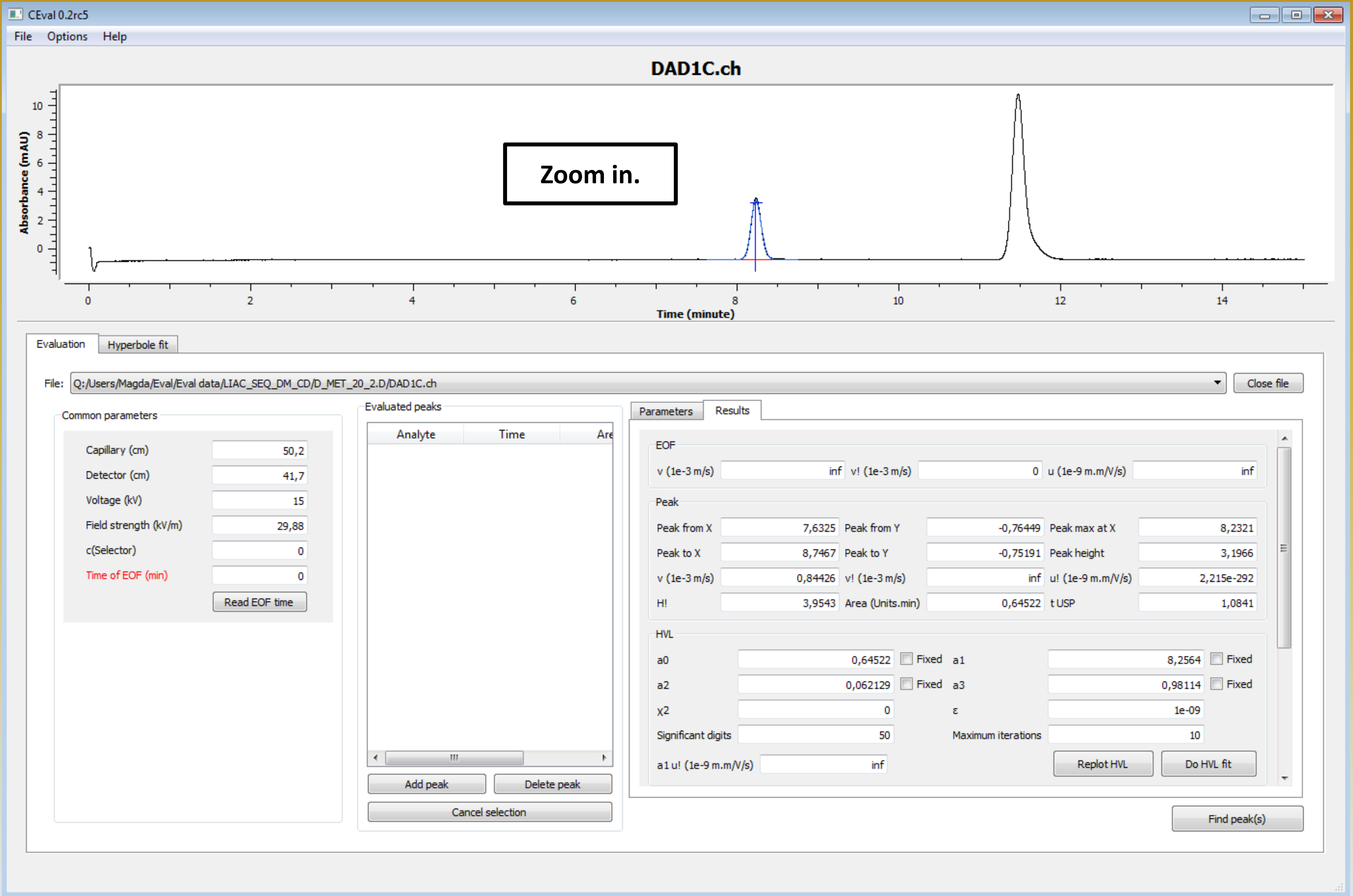
EOF
v (1e-3 m/s) 0
v! (1e-3 m/s) 0
u (1e-9 m.m/V/s) 0

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
a3 0 ☐ Fixed
χ2 0
ε 1e-09
Significant digits 50
Maximum iterations 10
a1 u! (1e-9 m.m/V/s) 0

Find a peak.

Appendix A: Graph Interface



Zoom in.

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

Evaluated peaks

EOF

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

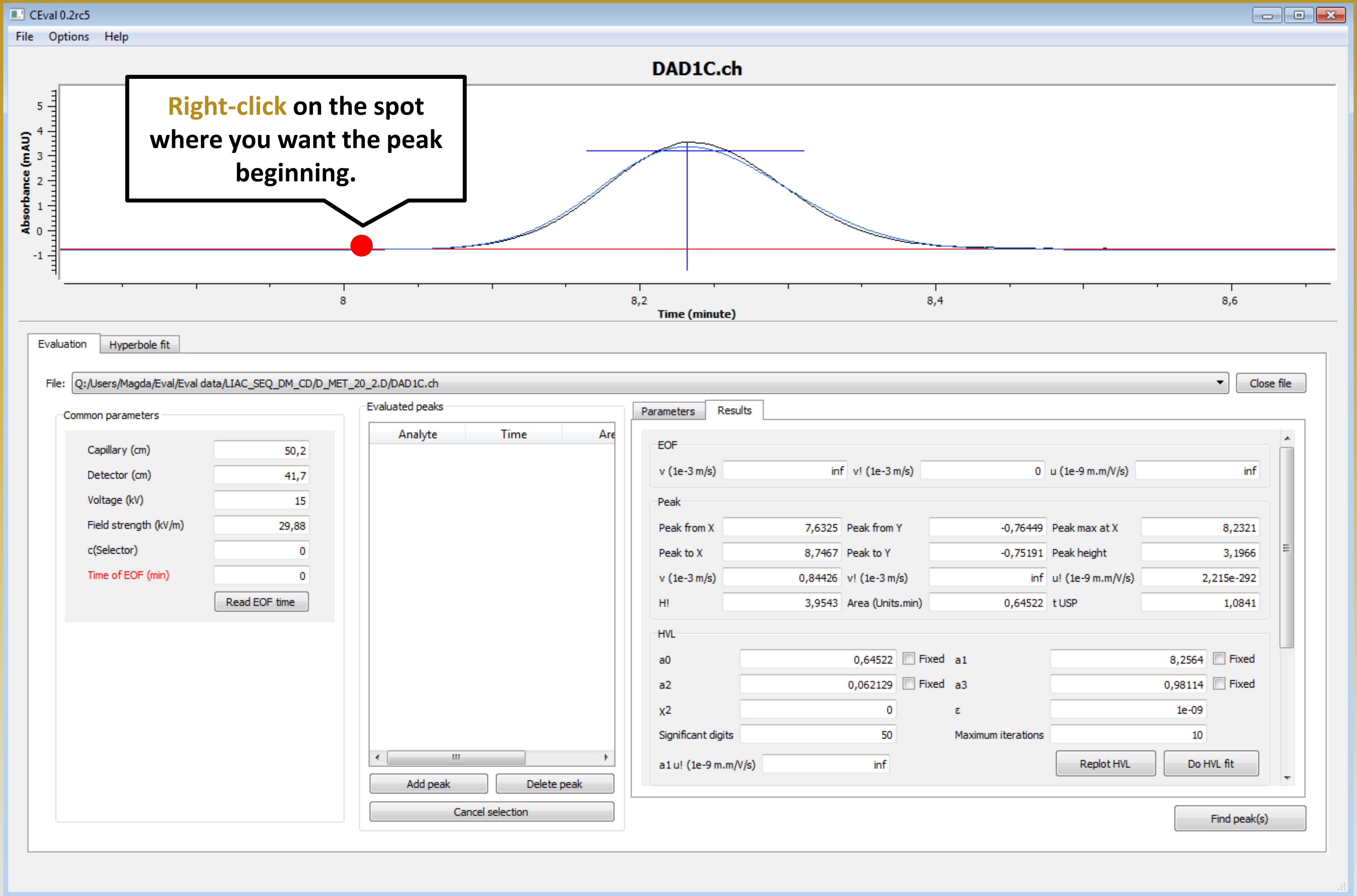
Peak

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 ☐ Fixed
a1: 8,2564 ☐ Fixed
a2: 0,062129 ☐ Fixed
a3: 0,98114 ☐ Fixed
χ2: 0
ε: 1e-09
Significant digits: 50
Maximum iterations: 10
a1 u! (1e-9 m.m/V/s): inf

Appendix A: Graph Interface



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

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

EOF

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

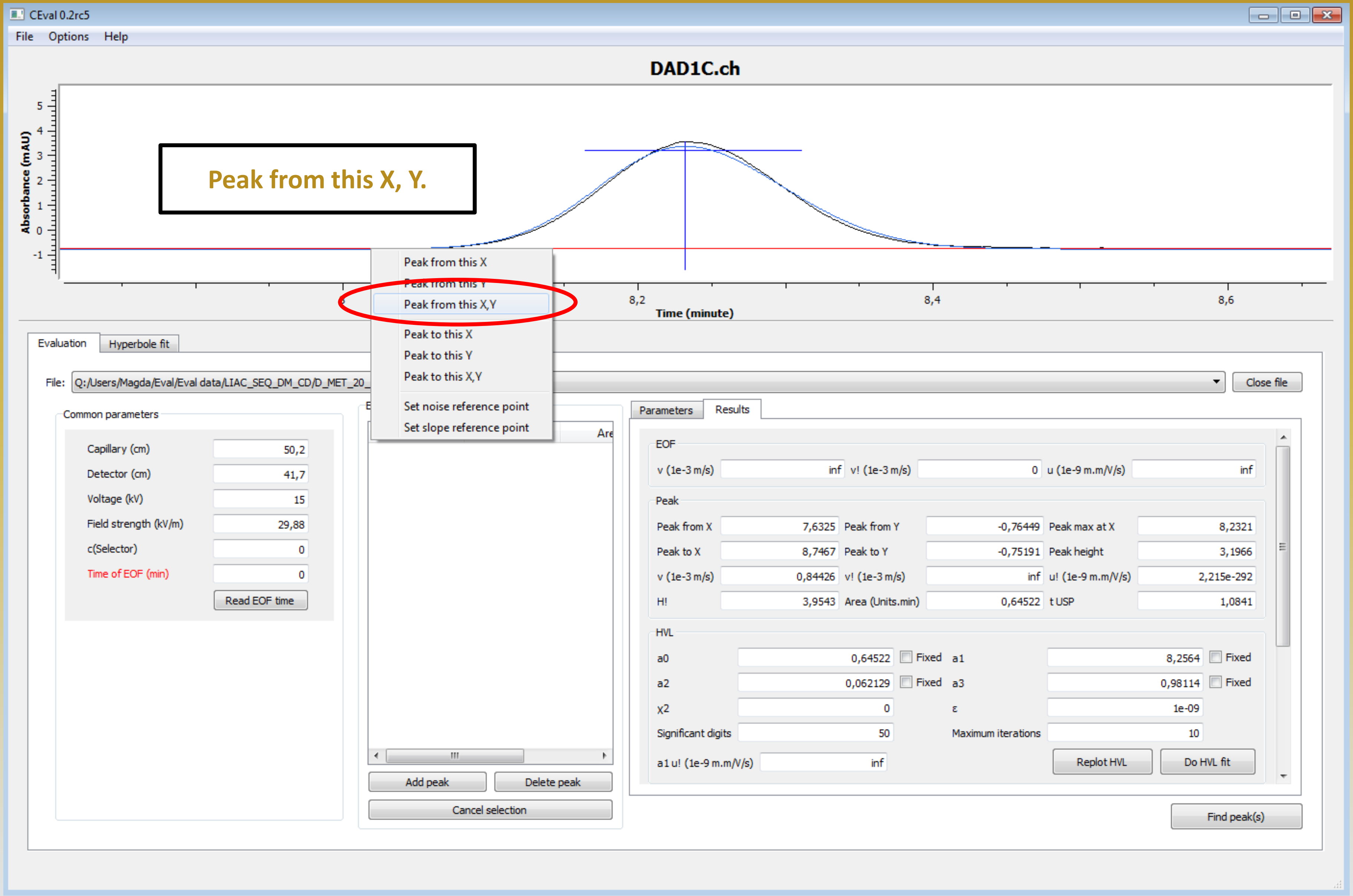
Peak

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	☐ Fixed	a1	8,2564	☐ Fixed
a2	0,062129	☐ Fixed	a3	0,98114	☐ Fixed
χ2	0		ε	1e-09	
Significant digits	50		Maximum iterations	10	
a1 u! (1e-9 m.m/V/s)	inf				

Appendix A: Graph Interface



Peak from this X, Y.

File: Q:/Users/Magda/Eval/Eval data/LIAC_SEQ_DM_CD/D_MET_20_

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

EOF

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

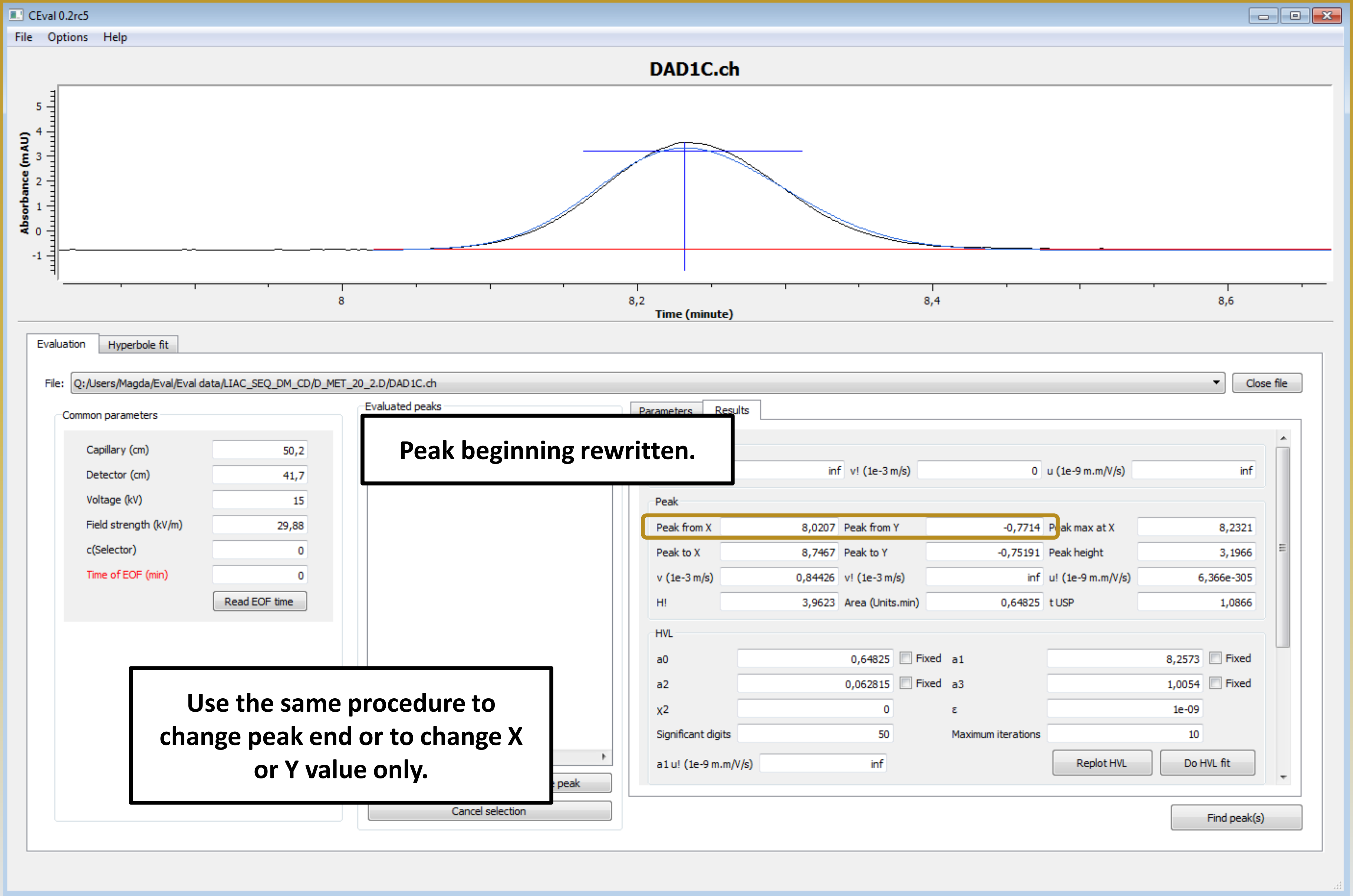
Peak

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	☐ 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				

Appendix A: Graph Interface



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

Evaluated peaks

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

Peak

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

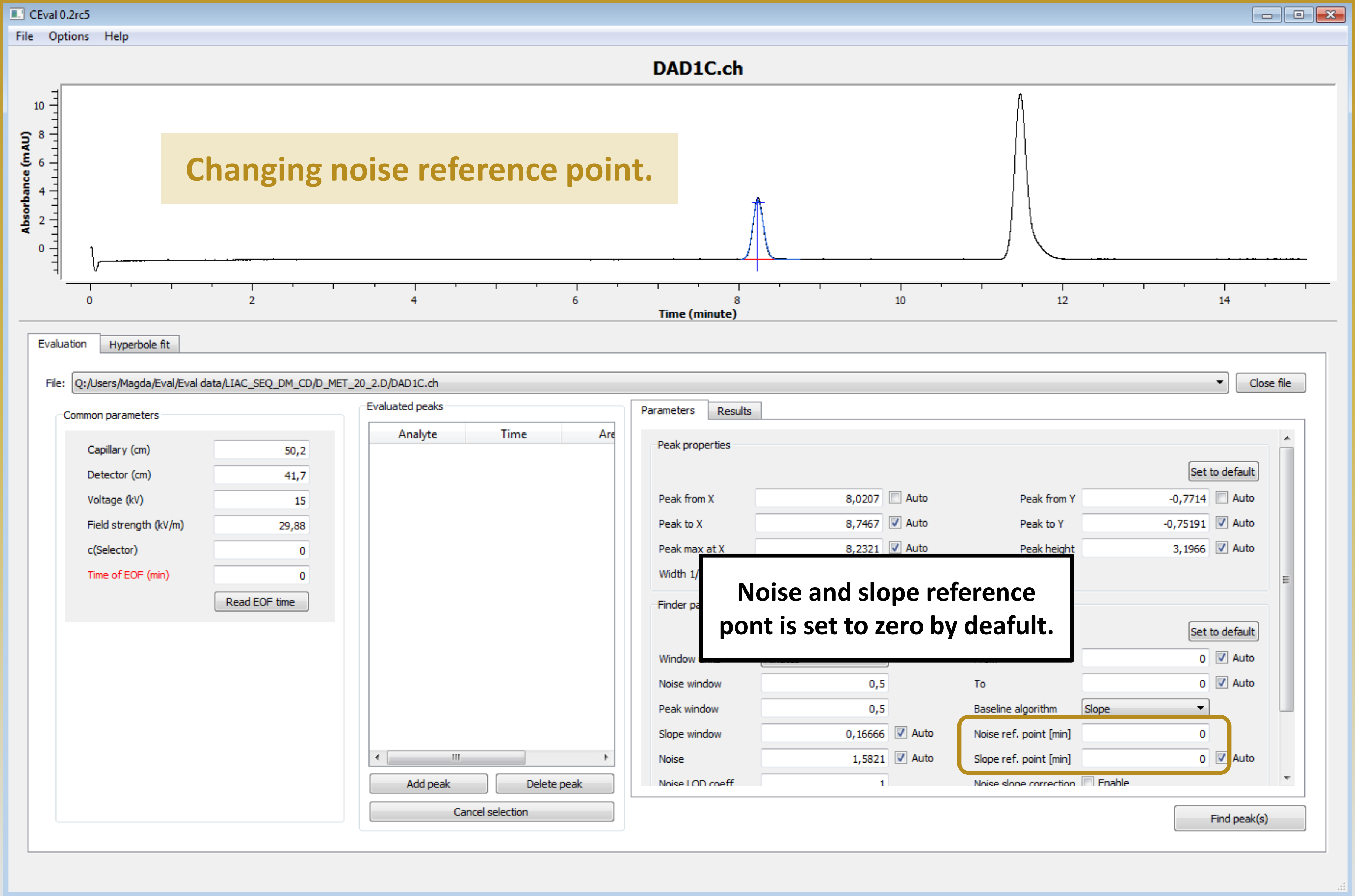
HVL

a0	0,64825	☐ Fixed	a1	8,2573	☐ Fixed
a2	0,062815	☐ Fixed	a3	1,0054	☐ Fixed
x2	0		ε	1e-09	
Significant digits	50		Maximum iterations	10	
a1 u! (1e-9 m.m/V/s)	inf				

Peak beginning rewritten.

Use the same procedure to change peak end or to change X or Y value only.

Appendix A: Graph Interface



Changing noise reference point.

Noise and slope reference pont is set to zero by deafult.

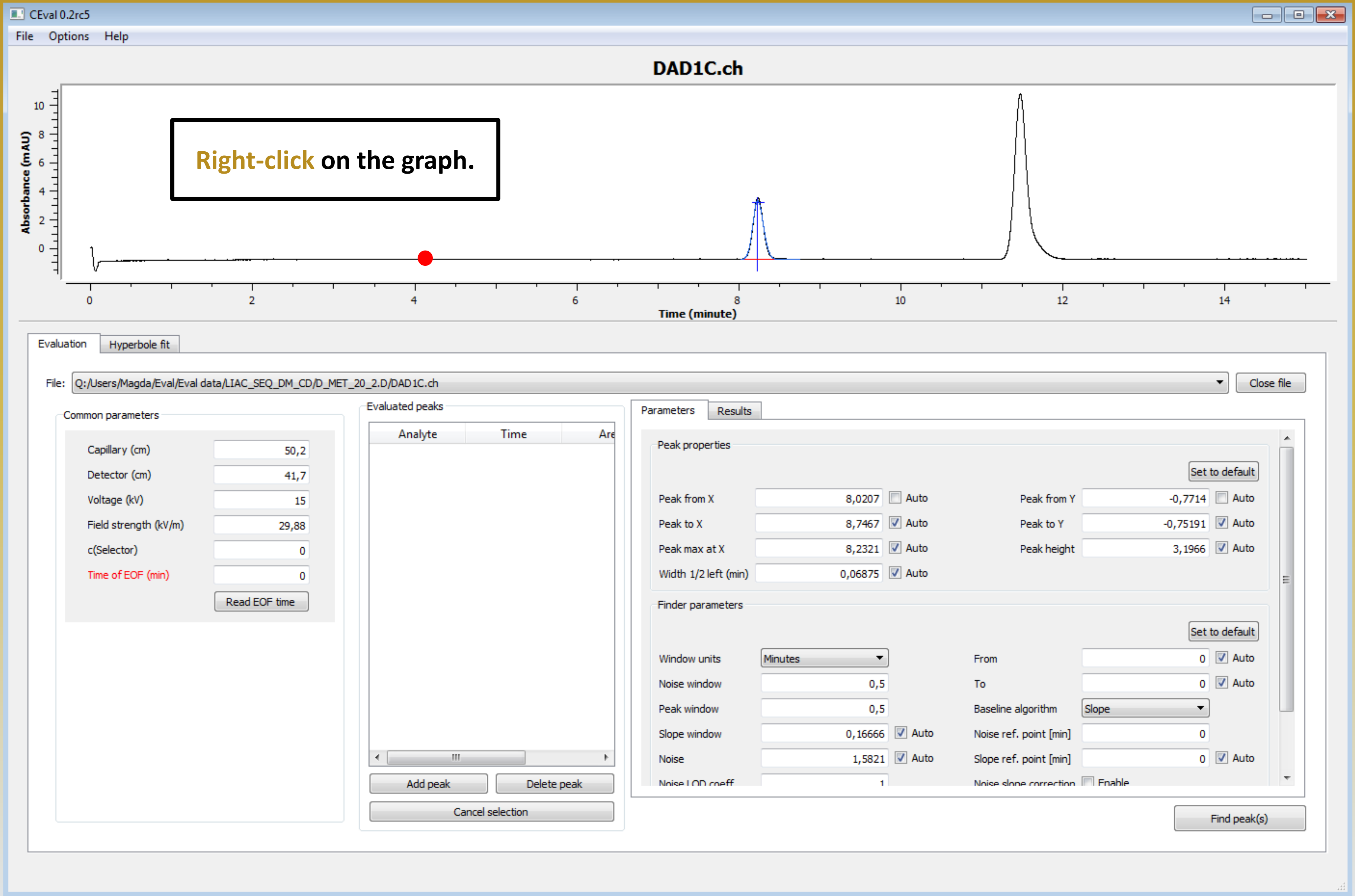
File: Q:/Users/Magda/Eval/Eval data/LIAC_SEQ_DM_CD/D_MET_20_2.D/DAD1C.ch

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

Peak from X 8,0207 ☐ Auto
Peak to X 8,7467 ☑ Auto
Peak max at X 8,2321 ☑ Auto
Width 1/
Peak from Y -0,7714 ☐ Auto
Peak to Y -0,75191 ☑ Auto
Peak height 3,1966 ☑ Auto

Window
Noise window 0,5
Peak window 0,5
Slope window 0,16666 ☑ Auto
Noise 1,5821 ☑ Auto
Noise LOD coeff 1
0 ☑ Auto
To 0 ☑ Auto
Baseline algorithm Slope
Noise ref. point [min] 0
Slope ref. point [min] 0 ☑ Auto
Noise slope correction ☐ Enable

Appendix A: Graph Interface



Right-click on the graph.

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

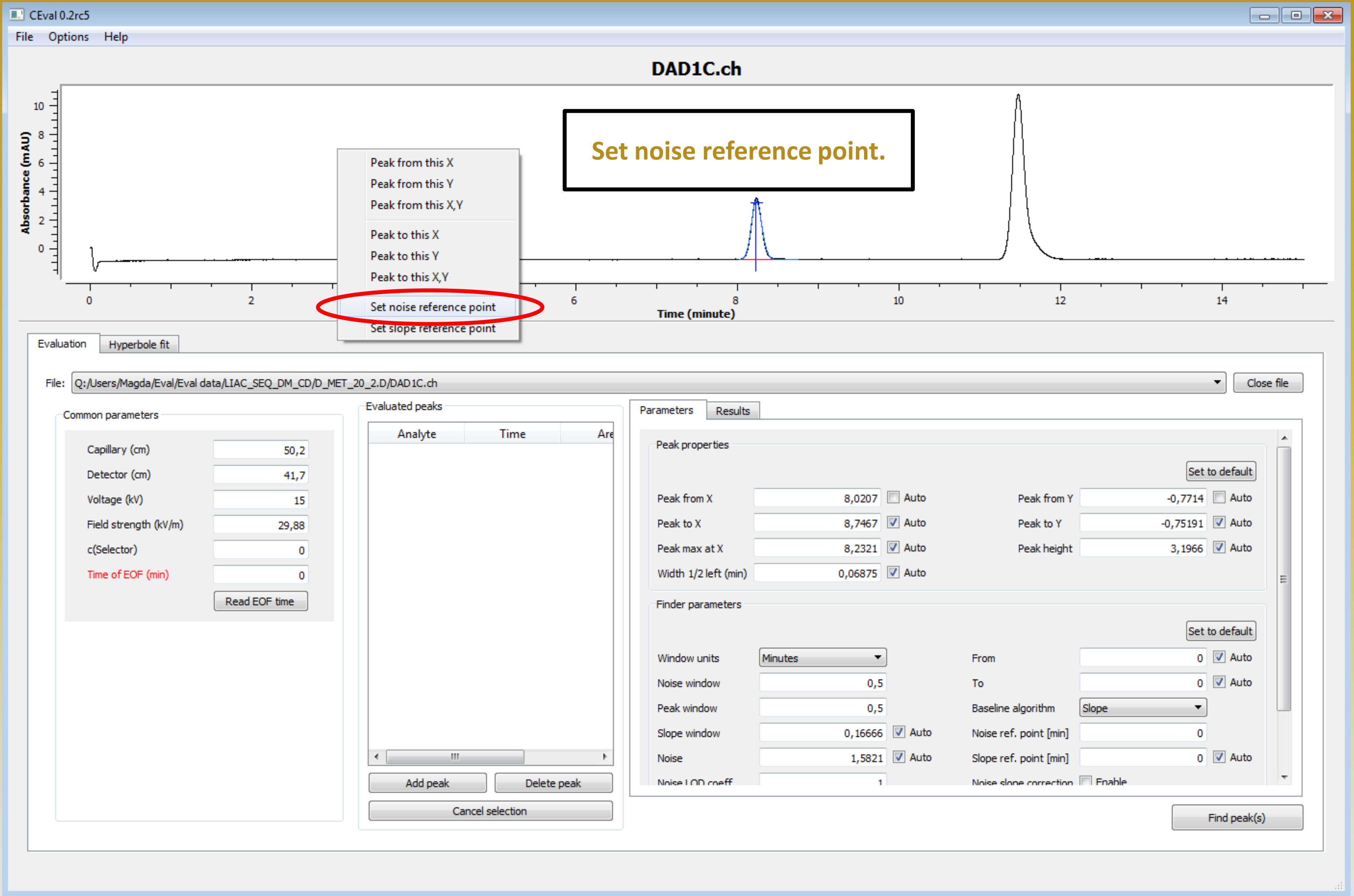
Peak properties

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
Width 1/2 left (min)	0,06875	☑ Auto			

Finder parameters

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

Appendix A: Graph Interface



Set noise reference point.

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

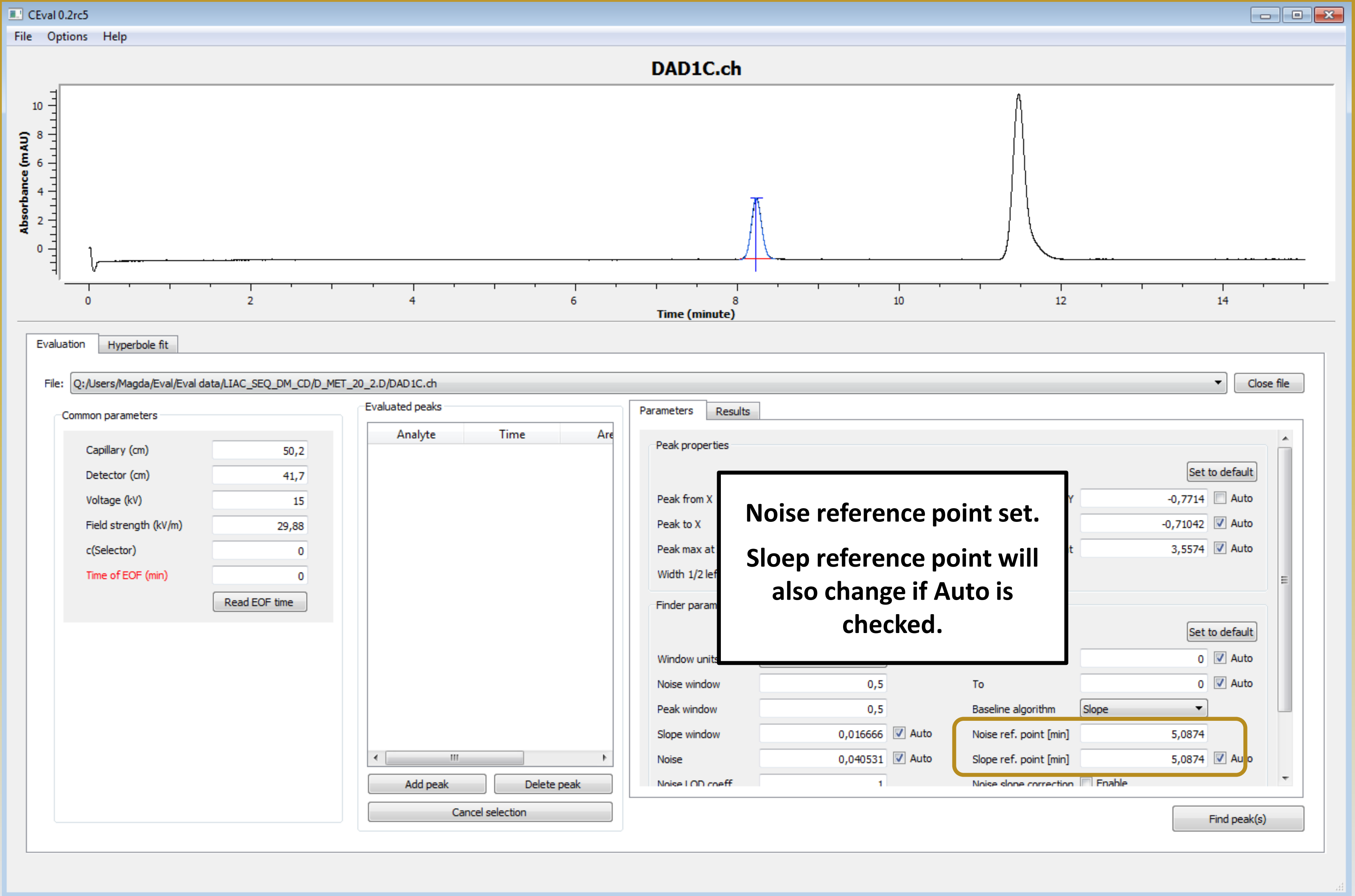
Peak properties

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
Width 1/2 left (min)	0,06875	☑ Auto			

Finder parameters

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

Appendix A: Graph Interface



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

Evaluated peaks

Peak properties

Peak from X		Y	-0,7714	☐ Auto
Peak to X			-0,71042	☑ Auto
Peak max at		t	3,5574	☑ Auto
Width 1/2 lef				

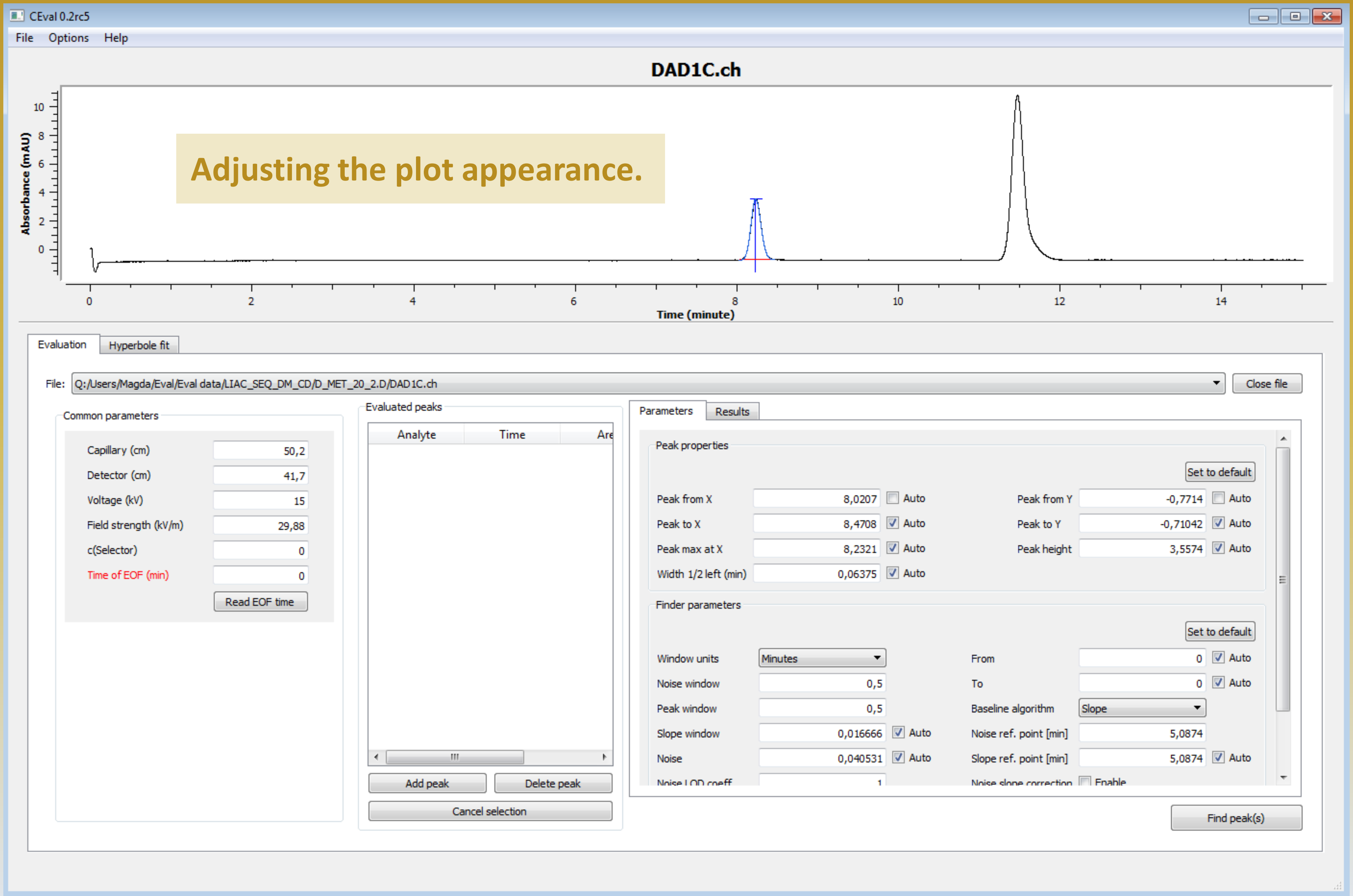
Finder param

Window units			0	☑ Auto
Noise window	0,5	To	0	☑ Auto
Peak window	0,5	Baseline algorithm	Slope	
Slope window	0,016666 ☑ Auto	Noise ref. point [min]	5,0874	
Noise	0,040531 ☑ Auto	Slope ref. point [min]	5,0874	☑ Auto
Noise LOD coeff	1	Noise slope correction	☐ Enable	

Noise reference point set.

Sloep reference point will also change if Auto is checked.

Appendix A: Graph Interface



Adjusting the plot appearance.

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

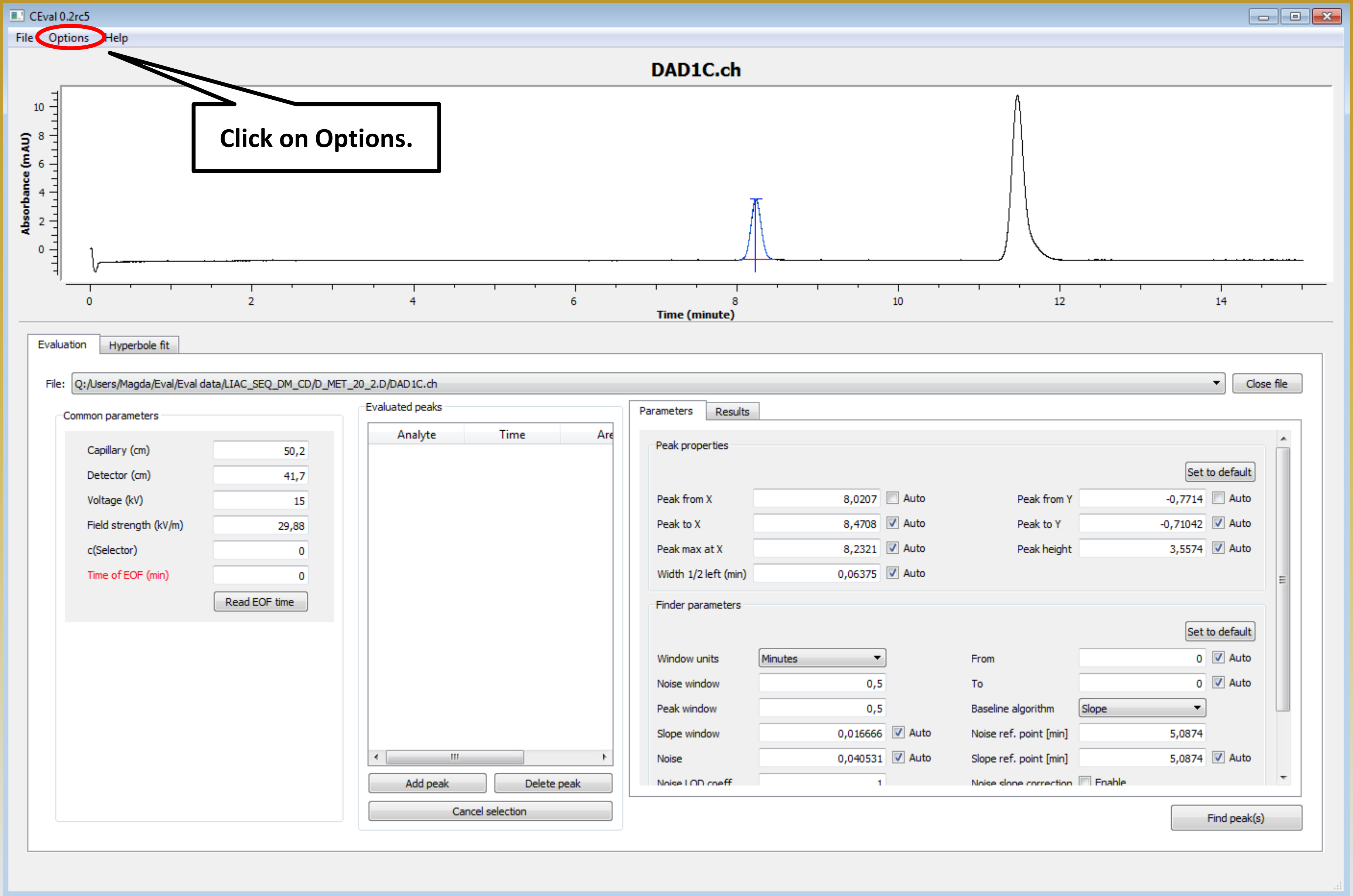
Peak properties

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

Finder parameters

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

Appendix A: Graph Interface



Click on Options.

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

Evaluated peaks

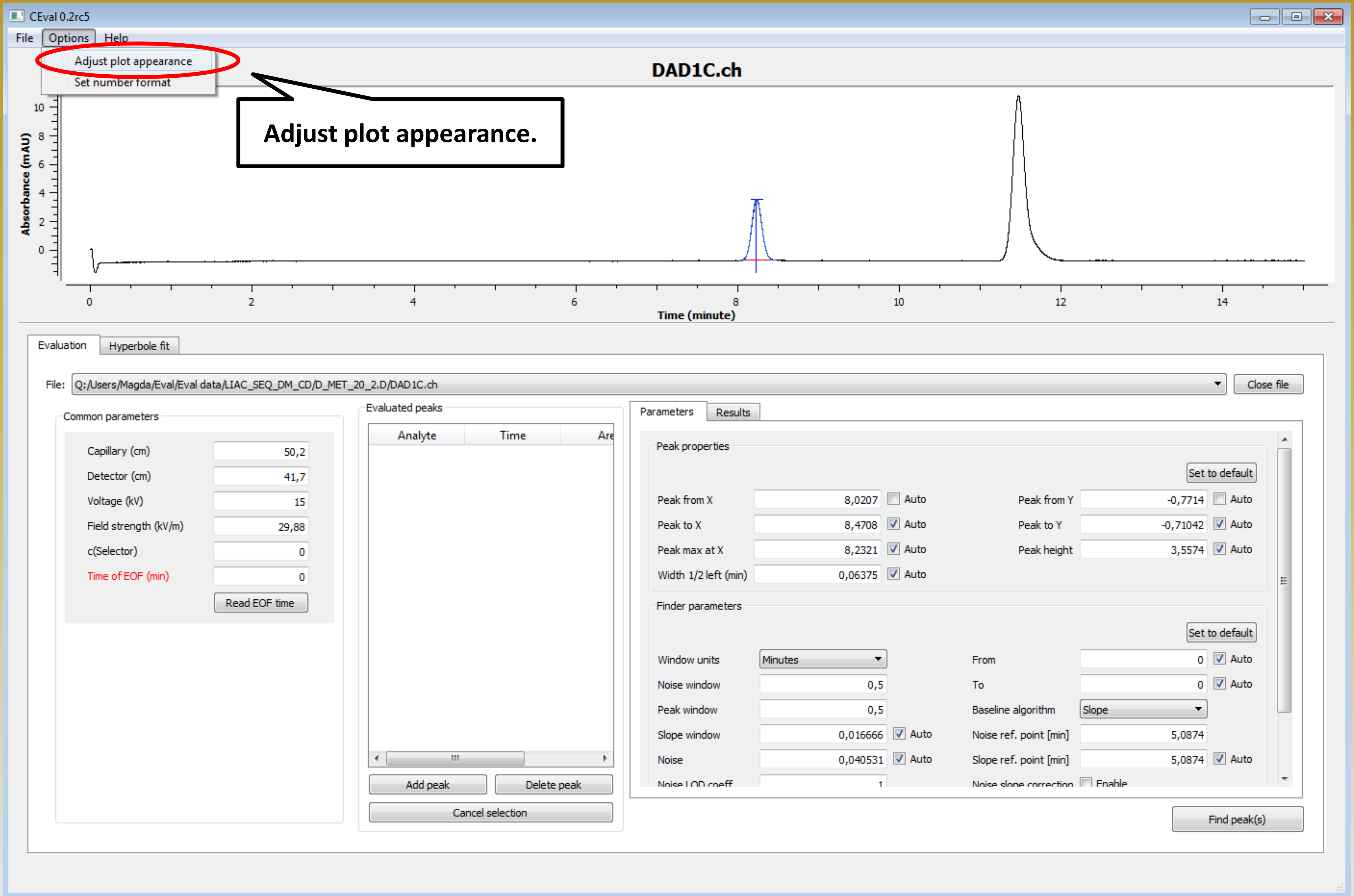
Peak properties

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

Finder parameters

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

Appendix A: Graph Interface



Adjust plot appearance.

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

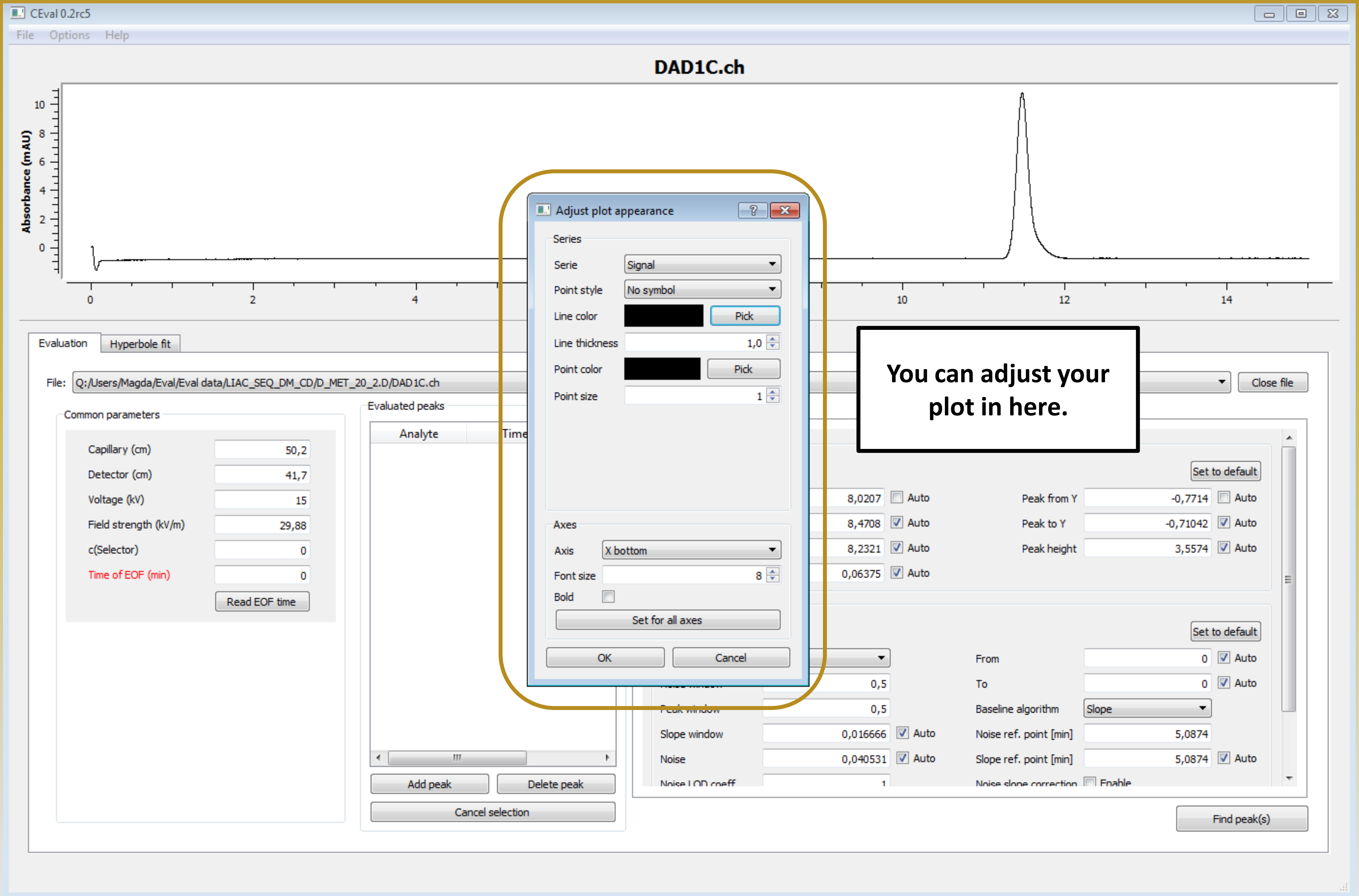
Peak properties

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

Finder parameters

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

Appendix A: Graph Interface



Adjust plot appearance

Series

Serie: Signal

Point style: No symbol

Line color: ■

Line thickness: 1,0

Point color: ■

Point size: 1

Axes

Axis: X bottom

Font size: 8

Bold: ☐

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

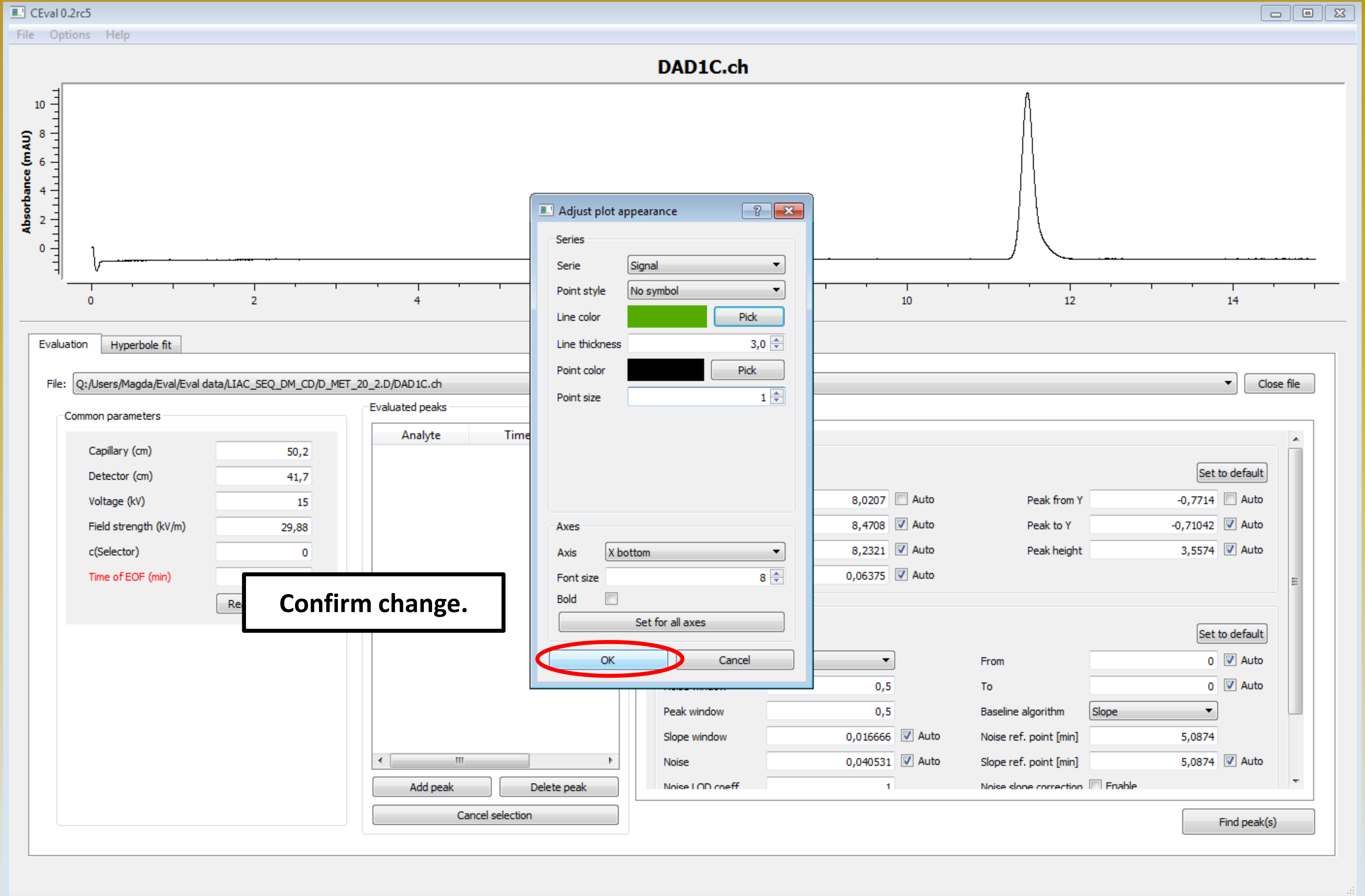
Evaluated peaks

8,0207	☐ Auto	Peak from Y	-0,7714	☐ Auto
8,4708	☑ Auto	Peak to Y	-0,71042	☑ Auto
8,2321	☑ Auto	Peak height	3,5574	☑ Auto
0,06375	☑ Auto			

			From	0	☑ Auto
	0,5		To	0	☑ Auto
	0,5		Baseline algorithm	Slope	
Slope window	0,016666	☑ Auto	Noise ref. point [min]	5,0874	
Noise	0,040531	☑ Auto	Slope ref. point [min]	5,0874	☑ Auto
Noise LOD coeff	1		Noise slope correction	☐ Enable	

You can adjust your plot in here.

Appendix A: Graph Interface



Adjust plot appearance

Series

Serie: Signal

Point style: No symbol

Line color: 🟩 Pick

Line thickness: 3,0

Point color: ■ Pick

Point size: 1

Axes

Axis: X bottom

Font size: 8

Bold ☐

Set for all axes

OK Cancel

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)	

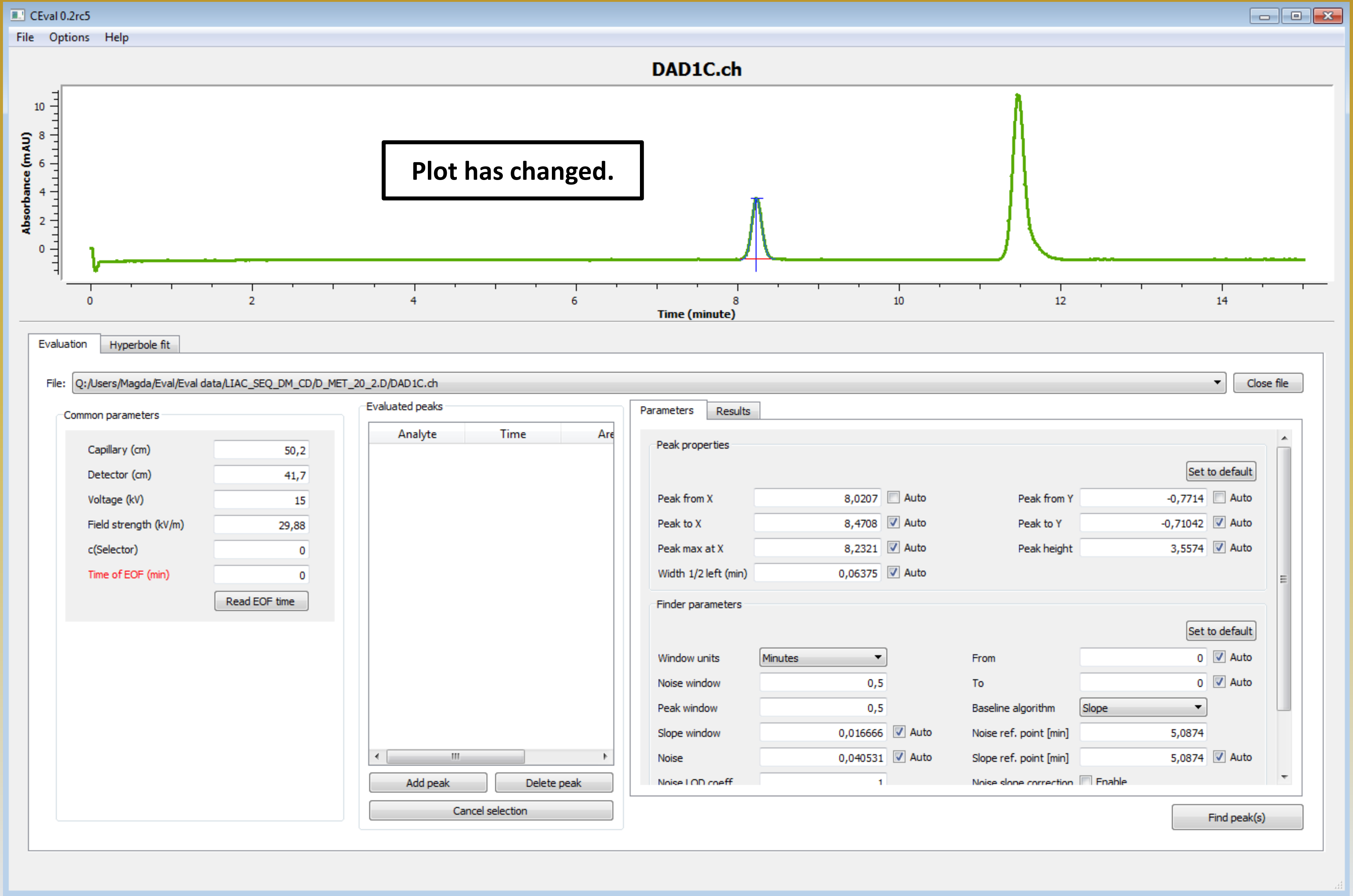
Evaluated peaks

	8,0207	☐ Auto	Peak from Y	-0,7714	☐ Auto
	8,4708	☑ Auto	Peak to Y	-0,71042	☑ Auto
	8,2321	☑ Auto	Peak height	3,5574	☑ Auto
	0,06375	☑ Auto			

			From	0	☑ Auto
	0,5		To	0	☑ Auto
Peak window	0,5		Baseline algorithm	Slope	
Slope window	0,016666	☑ Auto	Noise ref. point [min]	5,0874	
Noise	0,040531	☑ Auto	Slope ref. point [min]	5,0874	☑ Auto
Noise LOD coeff	1		Noise slope correction	☐ Enable	

Confirm change.

Appendix A: Graph Interface



Plot has changed.

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

Peak properties

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

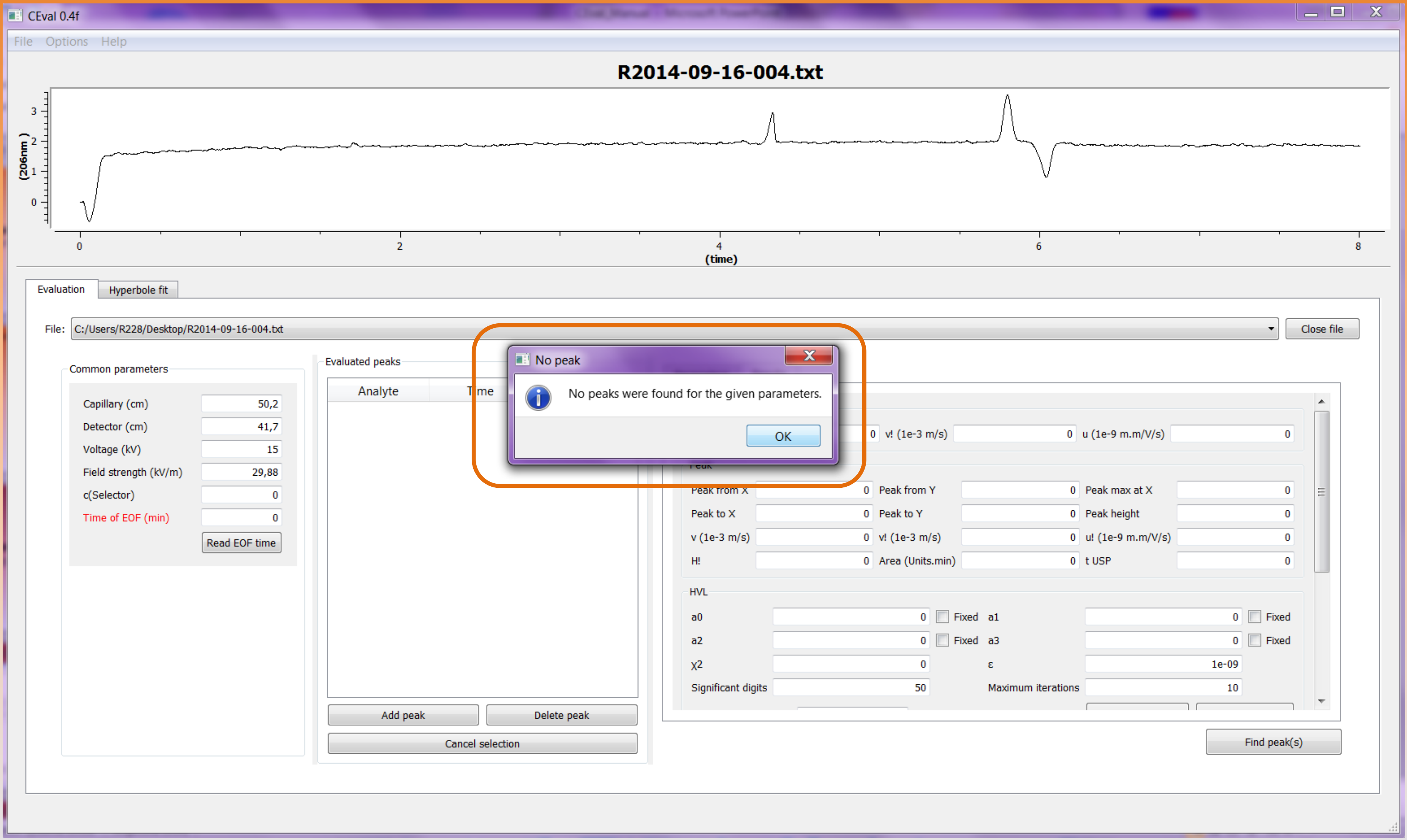
Finder parameters

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

Appendix B:

Peak Not Found

Appendix B: Peak Not Found



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

No peak

No peaks were found for the given parameters.

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

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

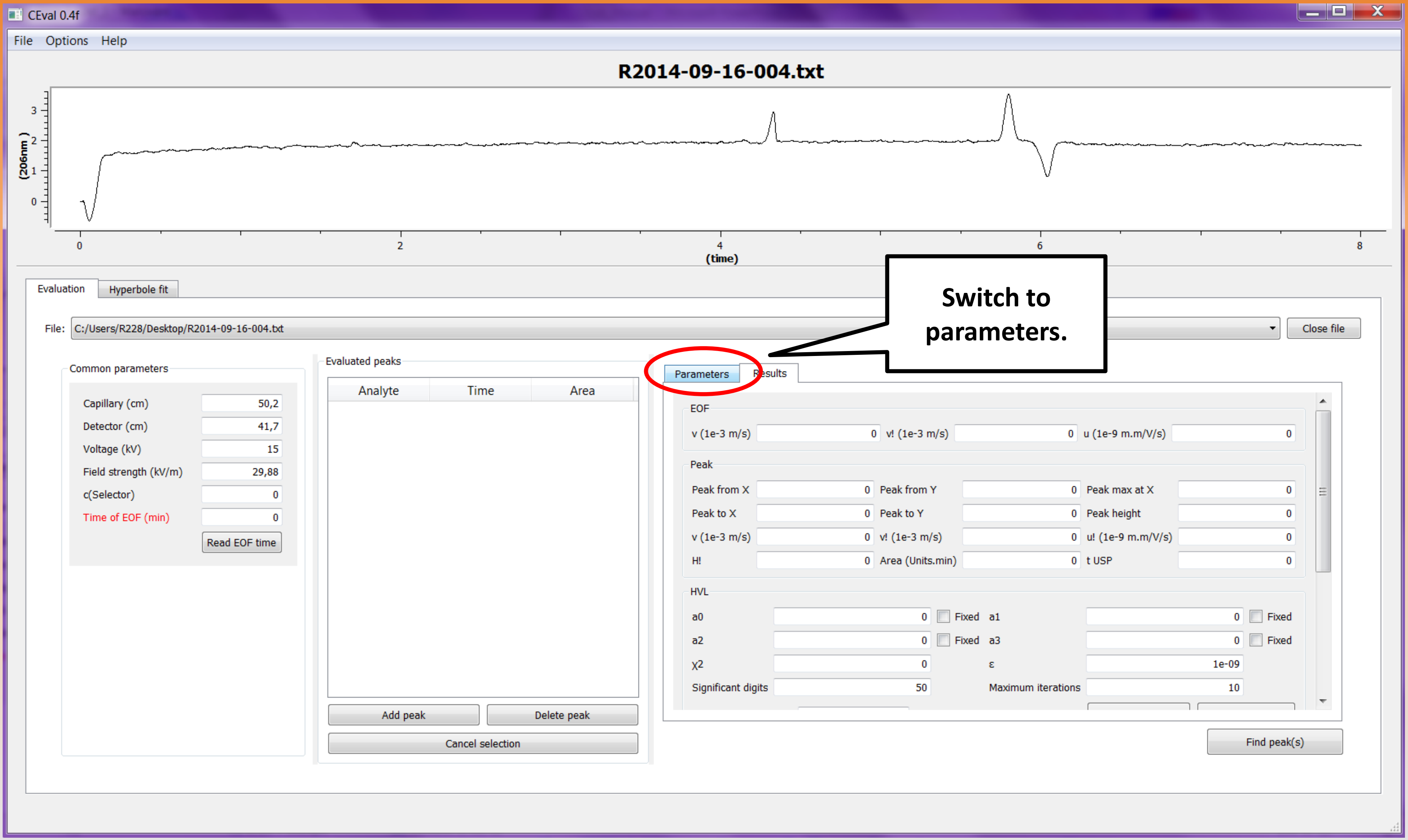
Peak

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
χ2 0 ε 1e-09
Significant digits 50 Maximum iterations 10

Appendix B: Peak Not Found



Switch to parameters.

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

EOF

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

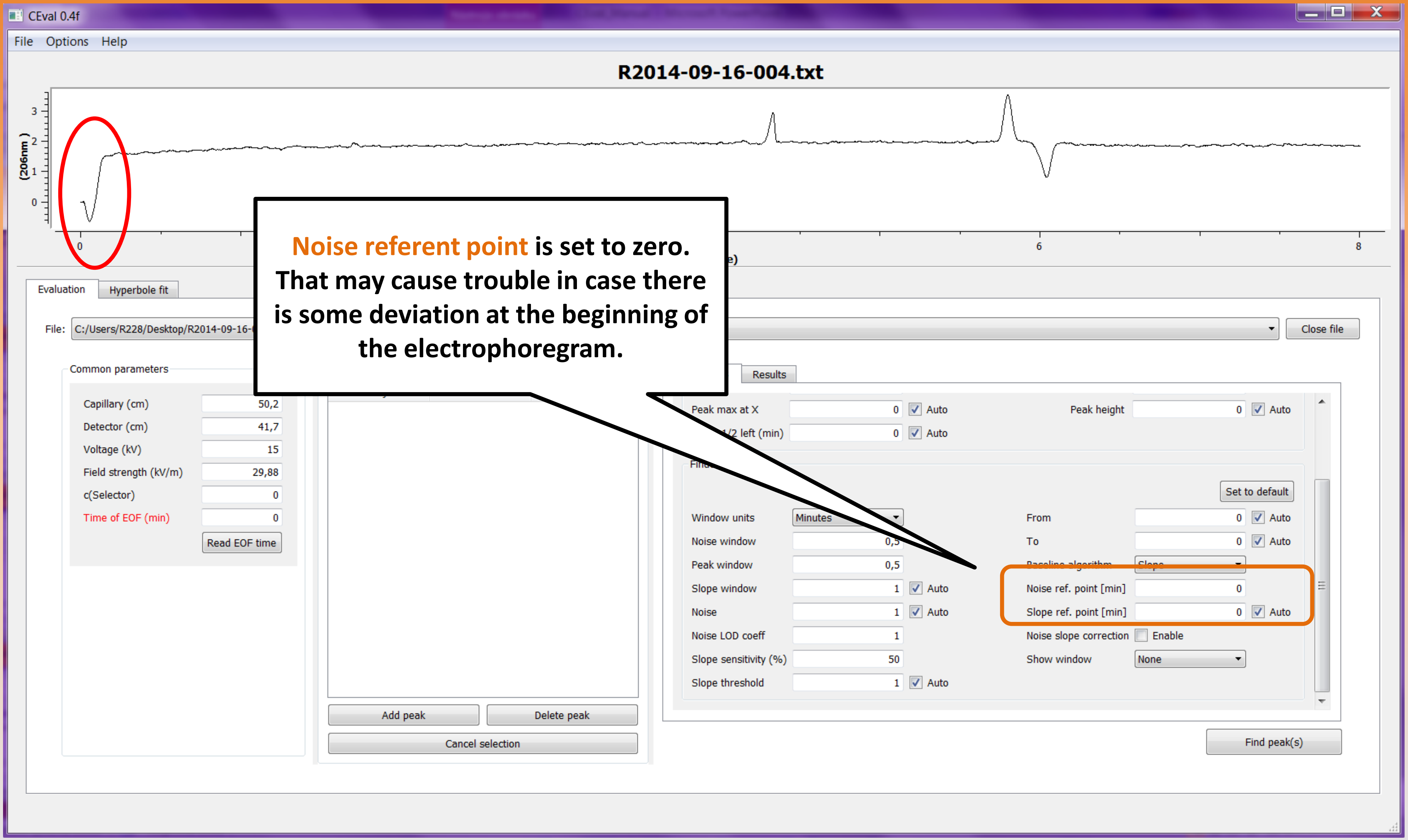
Peak

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
χ2	0		ε	1e-09	
Significant digits	50		Maximum iterations	10	

Appendix B: Peak Not Found



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

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

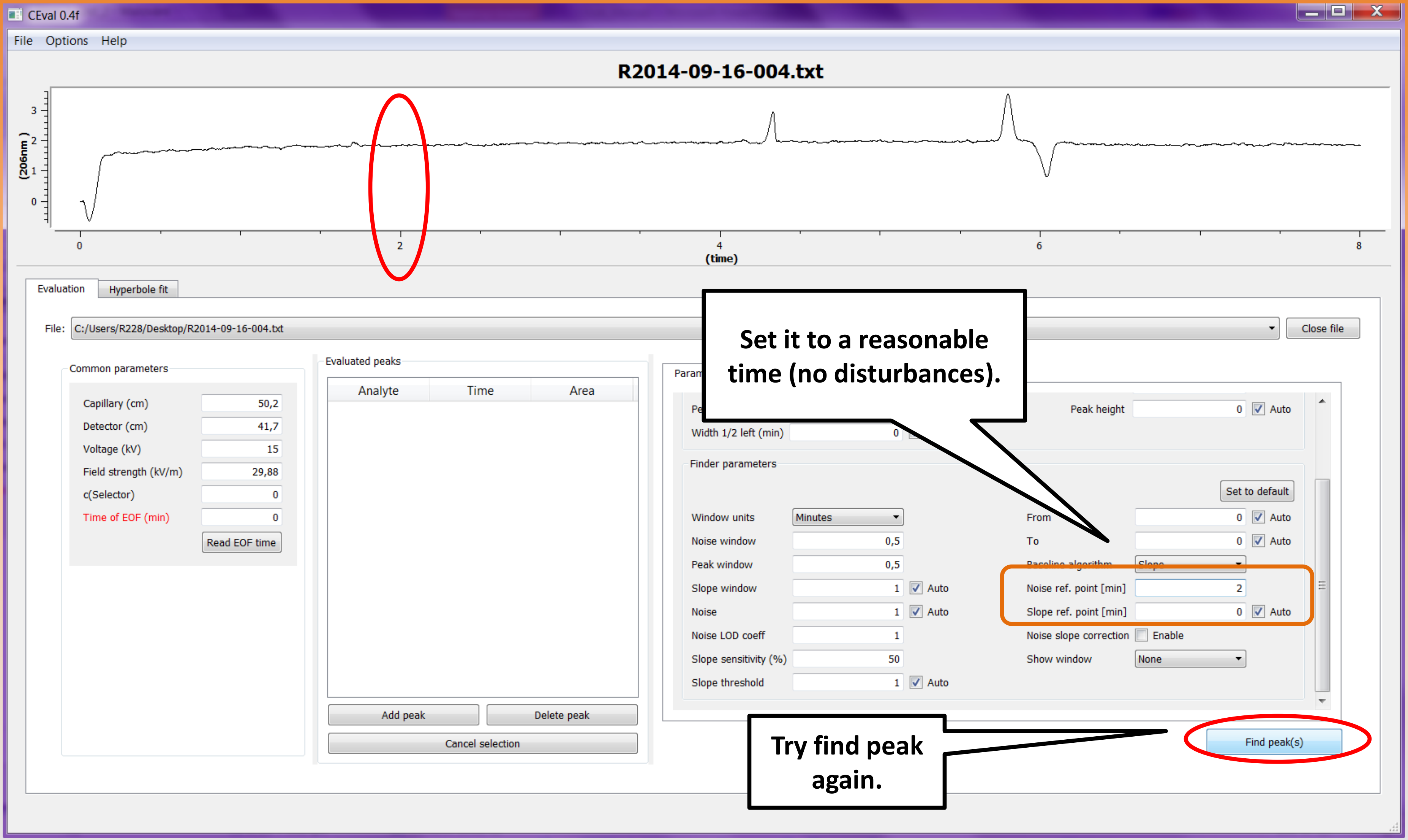
Peak max at X: 0 ☑ Auto
Peak height: 0 ☑ Auto
1/2 left (min): 0 ☑ Auto

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

Noise referent point is set to zero. That may cause trouble in case there is some deviation at the beginning of the electrophoregram.

Appendix B: Peak Not Found



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

Peak height: 0 ☑ Auto
Width 1/2 left (min): 0

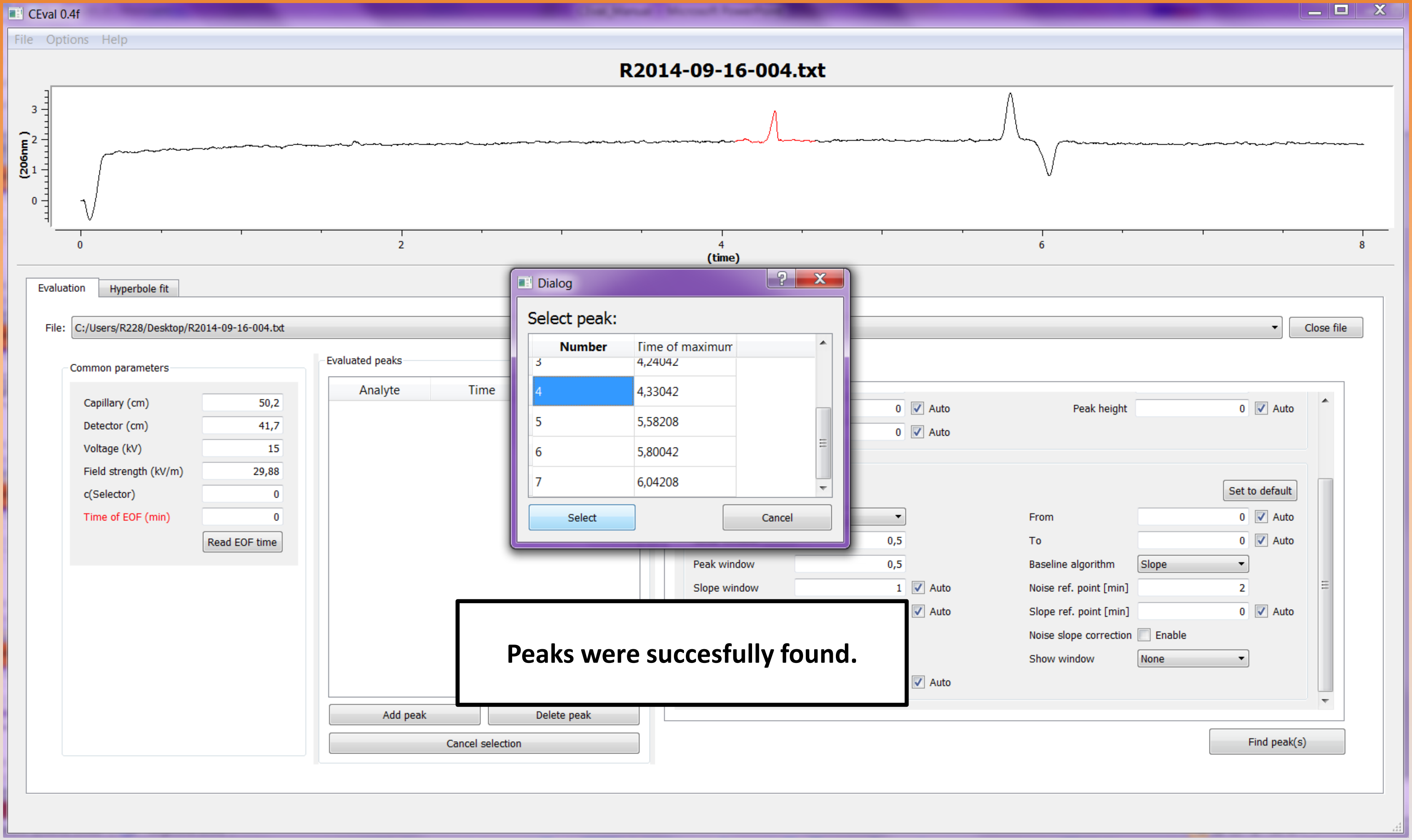
Finder parameters

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
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.

Appendix B: Peak Not Found



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

Select peak:

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

0 ☑ Auto

0 ☑ Auto

Peak height 0 ☑ Auto

0,5

Peak window 0,5

Slope window 1 ☑ Auto

☑ Auto

☑ Auto

From 0 ☑ Auto

To 0 ☑ Auto

Baseline algorithm: Slope

Noise ref. point [min] 2

Slope ref. point [min] 0 ☑ Auto

Noise slope correction ☐ Enable

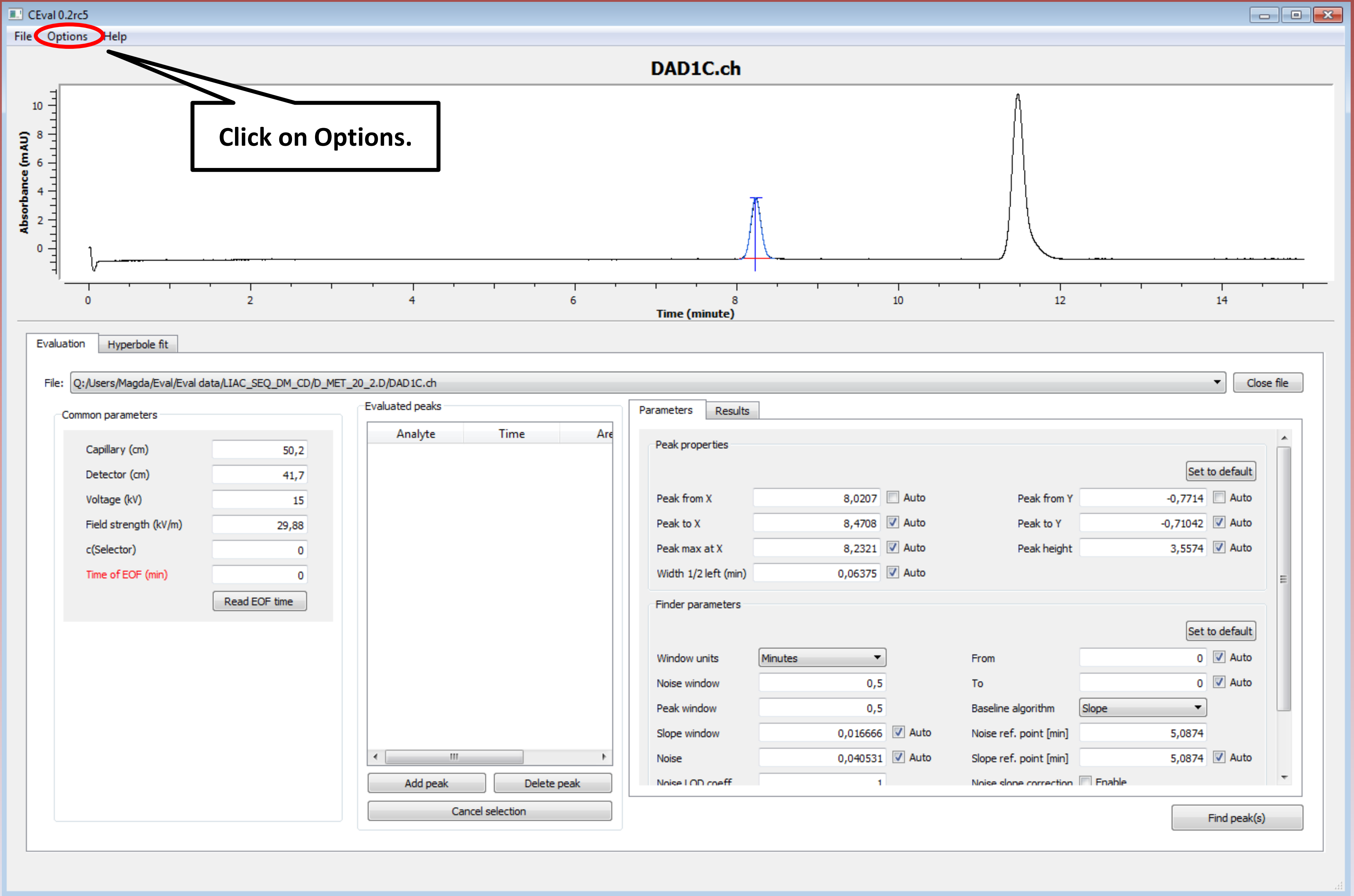
Show window: None

Peaks were succesfully found.

Appendix C:

Changing decimal digits

Appendix C: Changing Decimal Digits



Click on Options.

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

Evaluated peaks

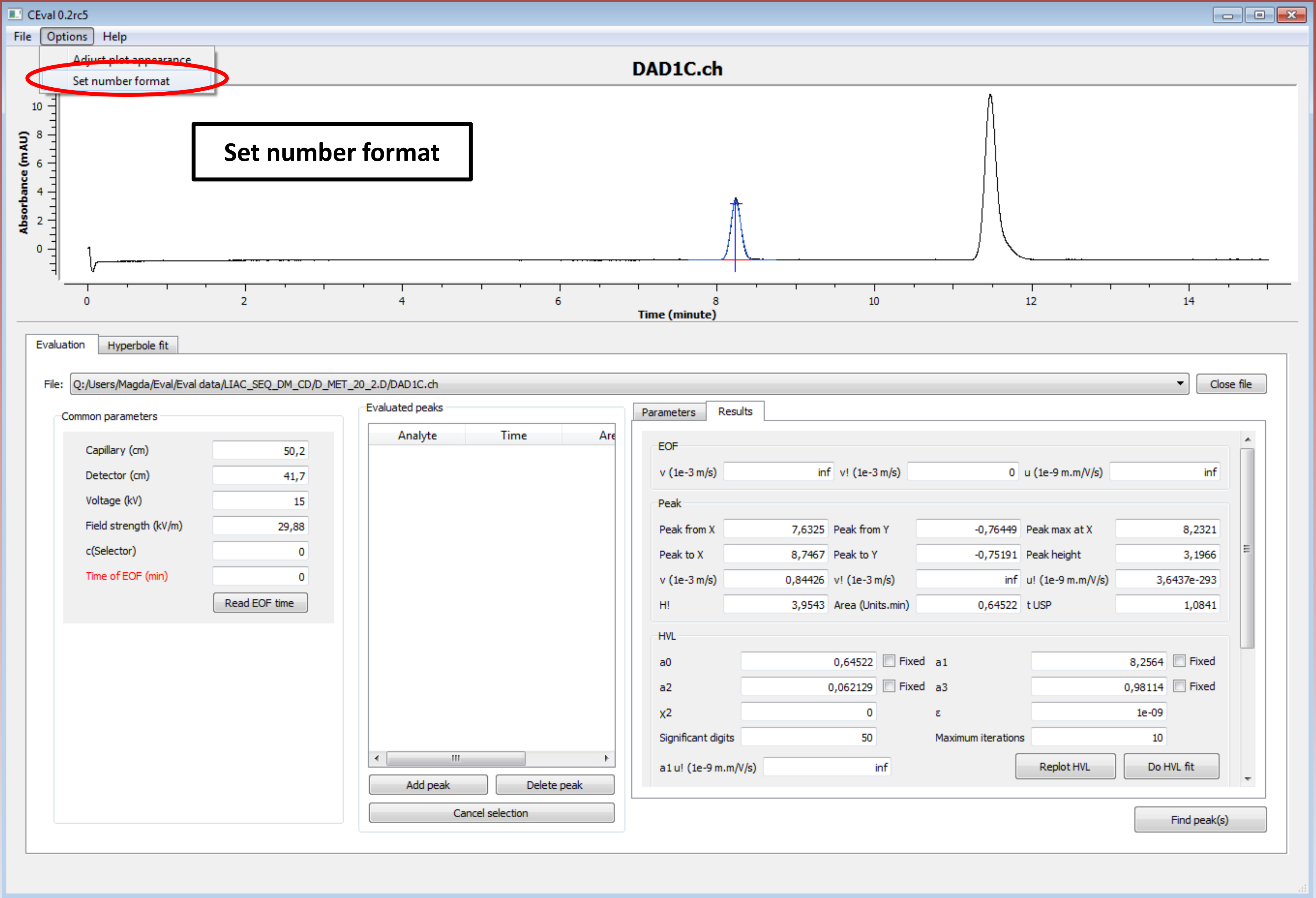
Peak properties

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

Finder parameters

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

Appendix C: Changing Decimal Digits



Set number format

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

EOF

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

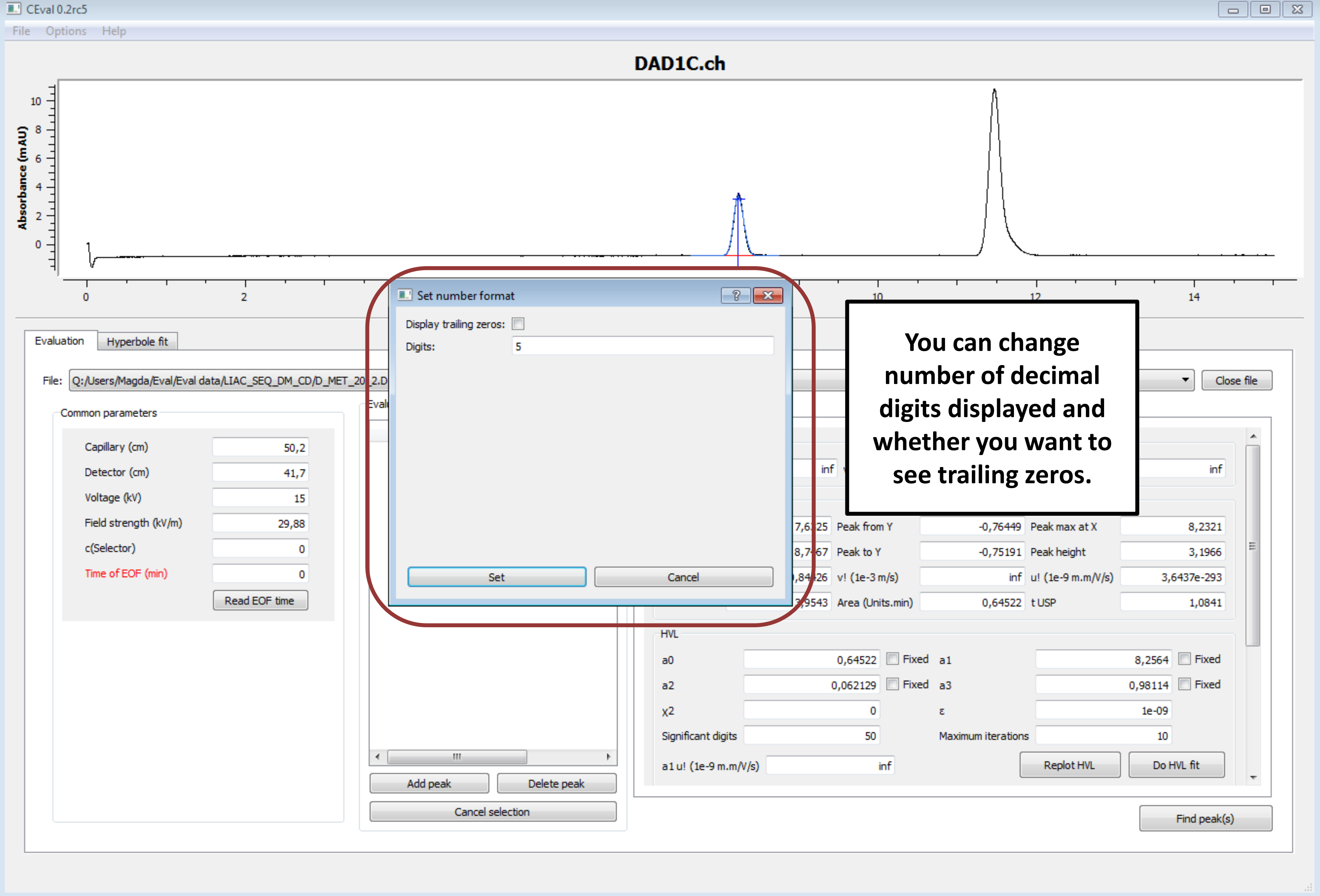
Peak

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 iterations	10	
a1 u! (1e-9 m.m/V/s)	inf				

Appendix C: Changing Decimal Digits



Set number format

Display trailing zeros: ☐

Digits: 5

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

Peak from Y: -0,76449

Peak max at X: 8,2321

Peak to Y: -0,75191

Peak height: 3,1966

v! (1e-3 m/s): inf

u! (1e-9 m.m/V/s): 3,6437e-293

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

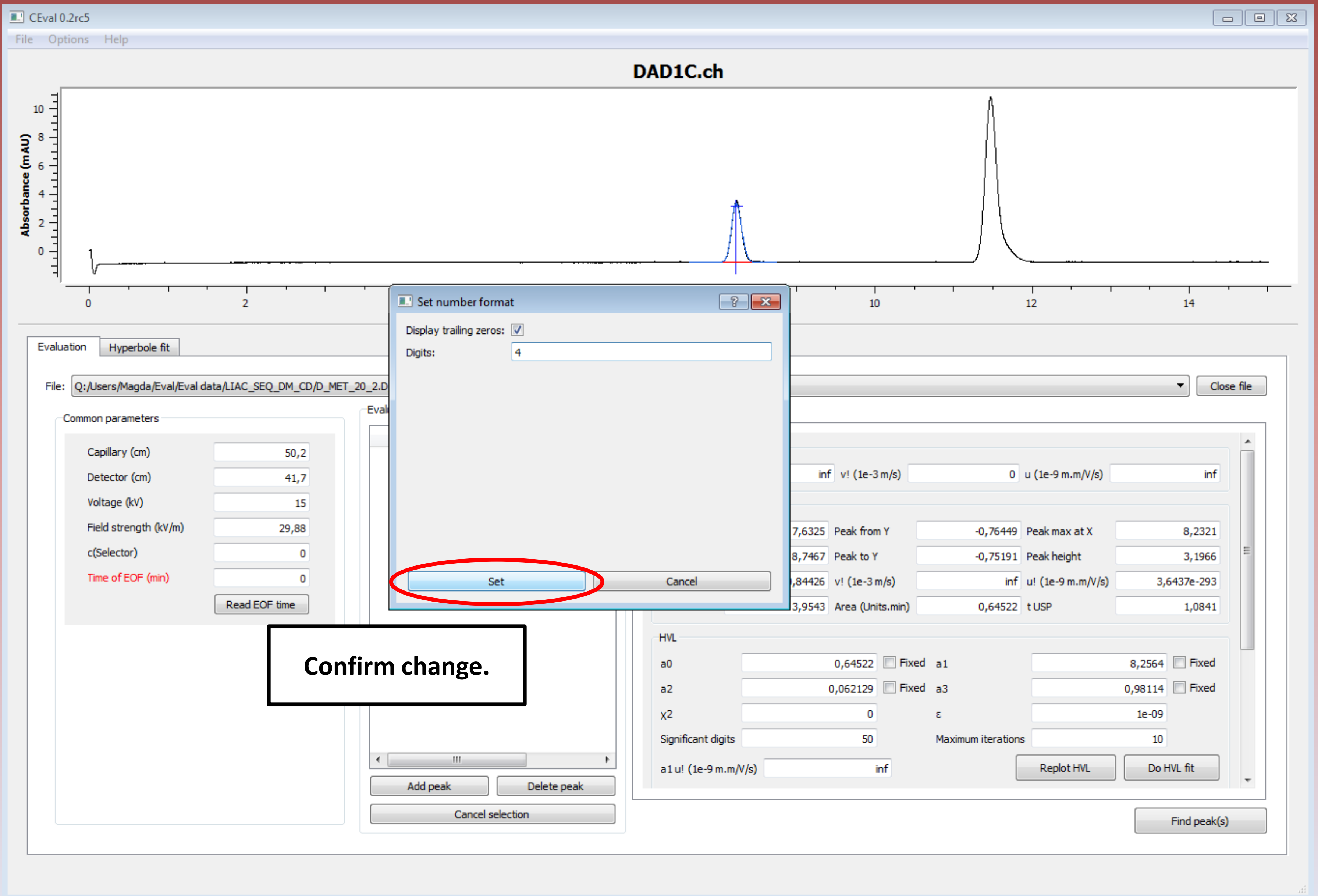
Significant digits: 50

Maximum iterations: 10

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

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

Appendix C: Changing Decimal Digits



Set number format

Display trailing zeros: ☑

Digits: 4

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

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

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

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

,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

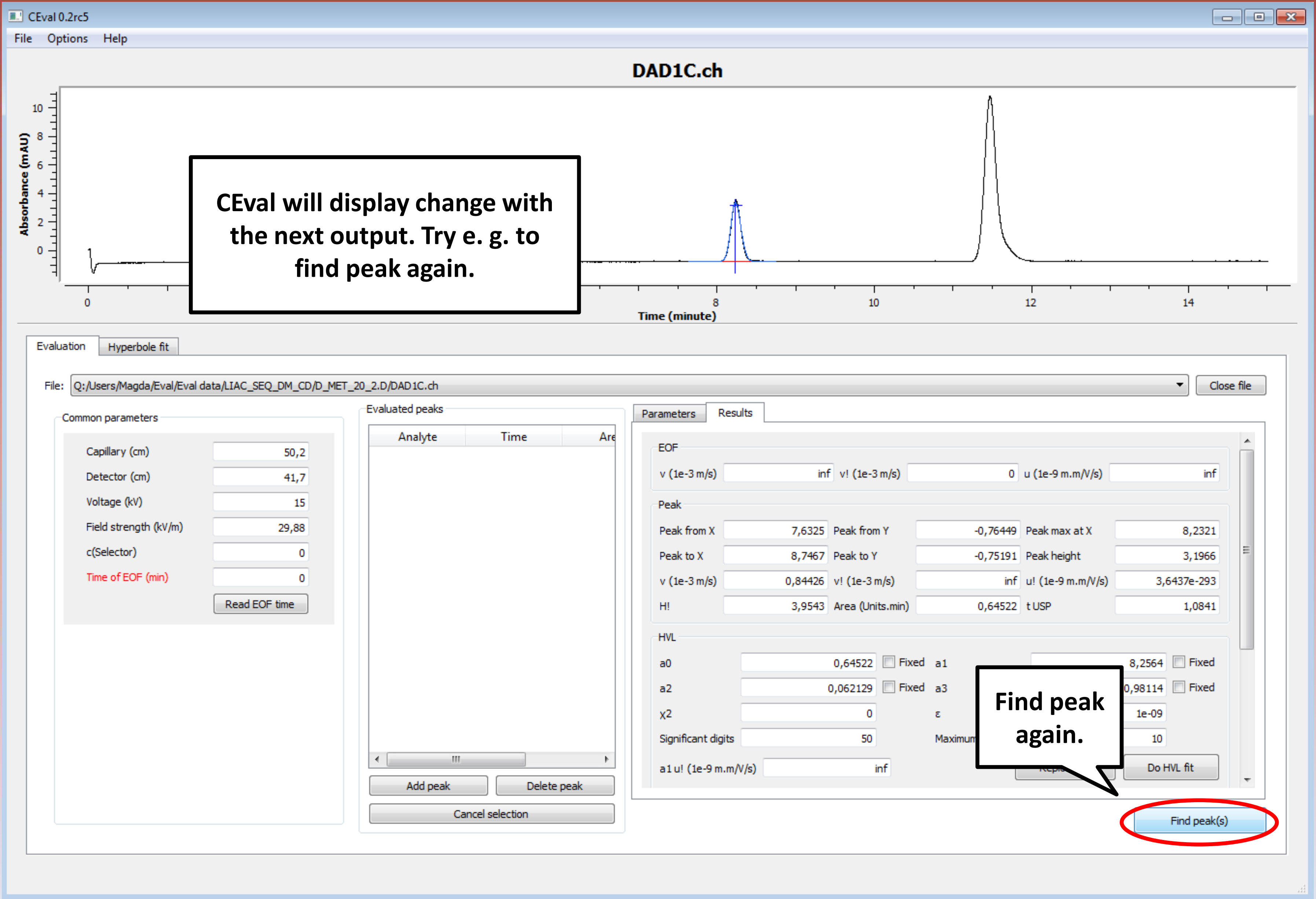
χ2: 0 ε: 1e-09

Significant digits: 50 Maximum iterations: 10

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

Confirm change.

Appendix C: Changing Decimal Digits



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

Evaluated peaks

Analyte	Time	Are

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

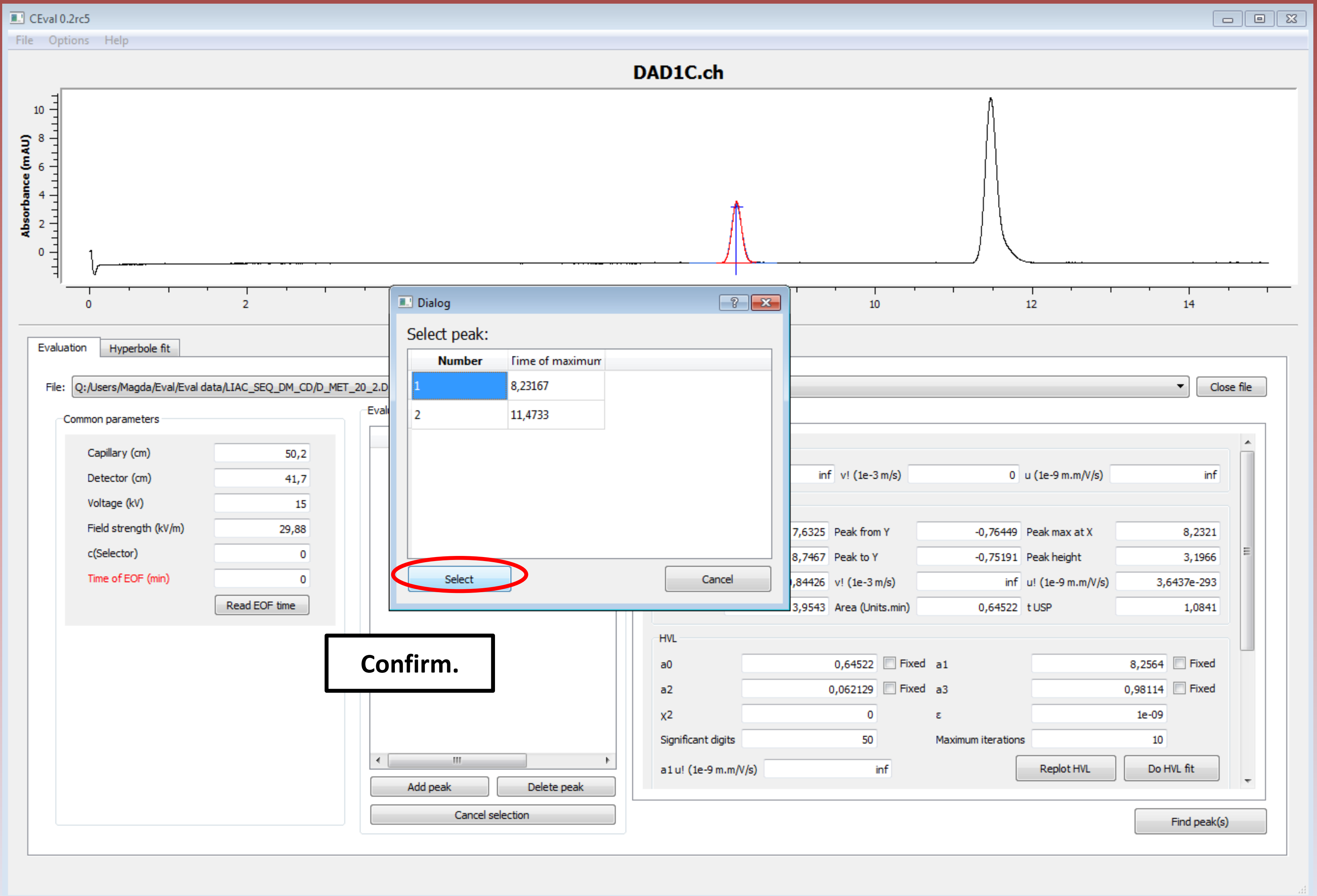
HVL

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	10	
a1 u! (1e-9 m.m/V/s)	inf				

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

Find peak again.

Appendix C: Changing Decimal Digits



Select peak:

Number	Time of maximum
1	8,23167
2	11,4733

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

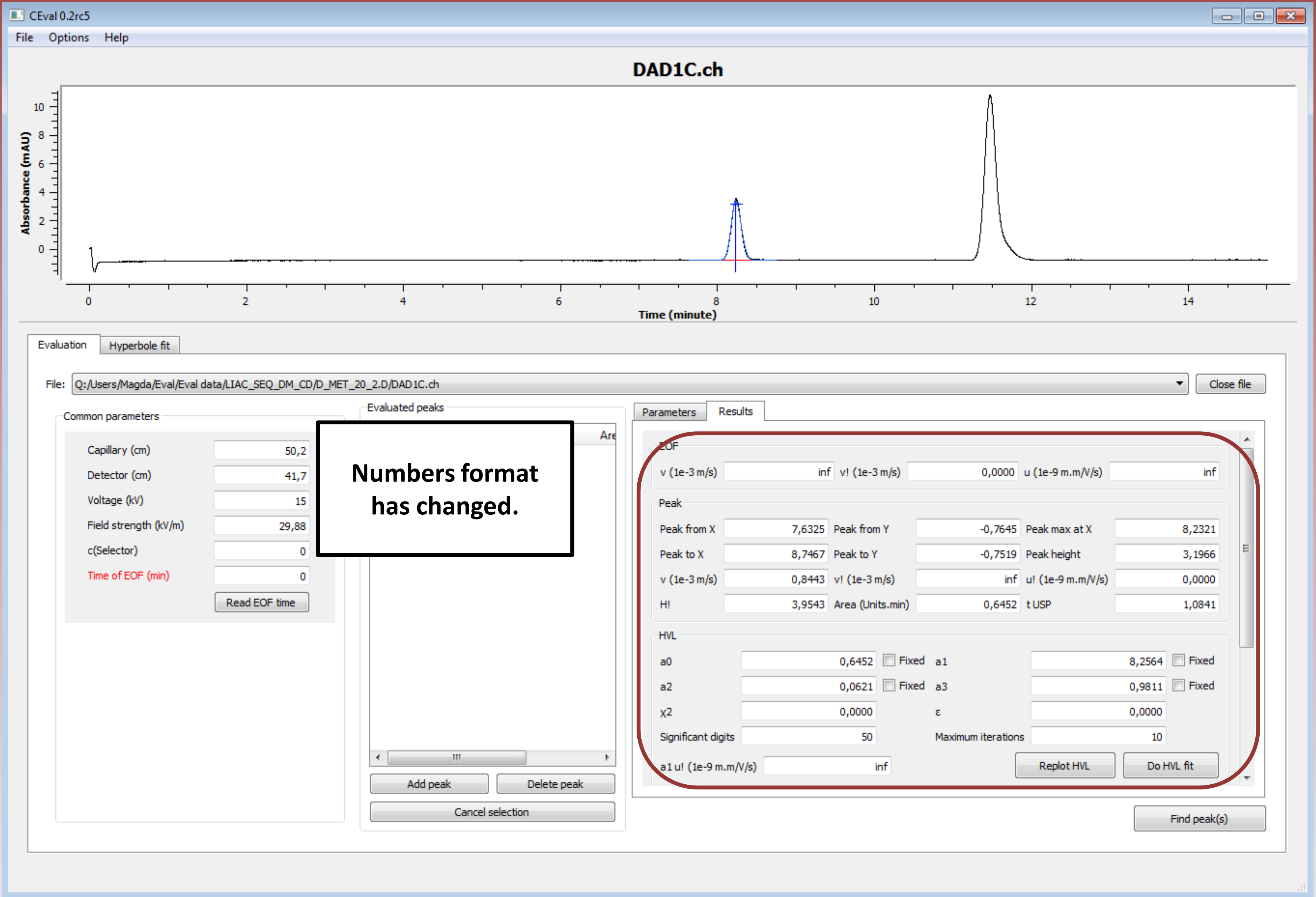
inf v! (1e-3 m/s) 0 u (1e-9 m.m/V/s) inf
7,6325 Peak from Y -0,76449 Peak max at X 8,2321
8,7467 Peak to Y -0,75191 Peak height 3,1966
,84426 v! (1e-3 m/s) inf u! (1e-9 m.m/V/s) 3,6437e-293
3,9543 Area (Units.min) 0,64522 t USP 1,0841

HVL

a0 0,64522 ☐ Fixed a1 8,2564 ☐ Fixed
a2 0,062129 ☐ Fixed a3 0,98114 ☐ Fixed
χ2 0 ε 1e-09
Significant digits 50 Maximum iterations 10
a1 u! (1e-9 m.m/V/s) inf

Confirm.

Appendix C: Changing Decimal Digits



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

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	☐ Fixed	a1	8,2564	☐ Fixed
a2	0,0621	☐ Fixed	a3	0,9811	☐ Fixed
χ2	0,0000		ε	0,0000	
Significant digits	50		Maximum iterations	10	

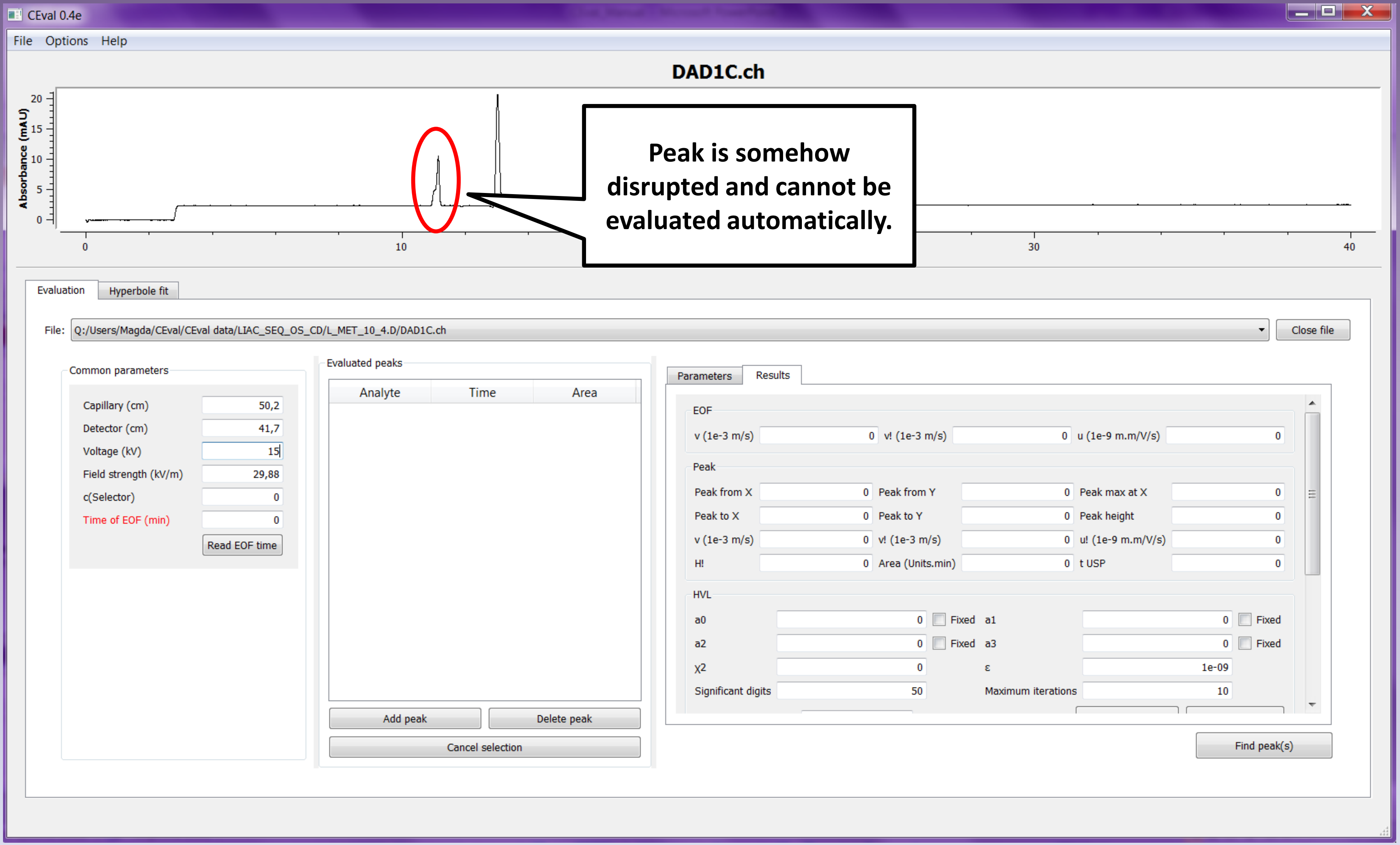
a1 u! (1e-9 m.m/V/s) inf

Numbers format has changed.

Appendix D:

Distorted Peak

Appendix D: Distorted Peak



Peak is somehow disrupted and cannot be evaluated automatically.

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

EOF

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

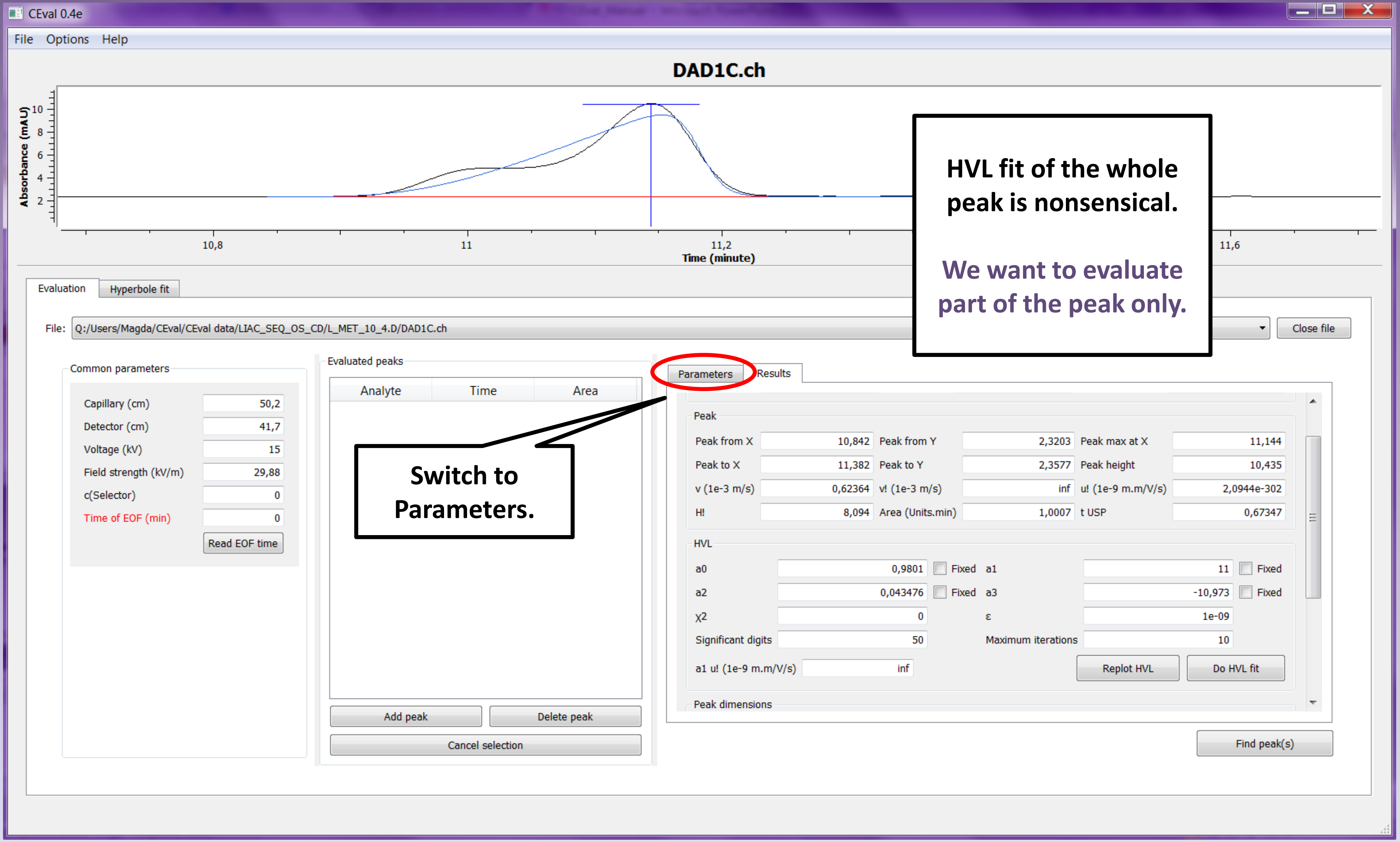
Peak

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
χ2	0		ε	1e-09	
Significant digits	50		Maximum iterations	10	

Appendix D: Distorted Peak



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

Peak

Peak from X	10,842	Peak from Y	2,3203	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	v! (1e-3 m/s)	inf	u! (1e-9 m.m/V/s)	2,0944e-302
H!	8,094	Area (Units.min)	1,0007	t USP	0,67347

HVL

a0	0,9801	☐ Fixed	a1	11	☐ Fixed
a2	0,043476	☐ Fixed	a3	-10,973	☐ Fixed
χ2	0		ε	1e-09	
Significant digits	50		Maximum iterations	10	
a1 u! (1e-9 m.m/V/s)	inf				

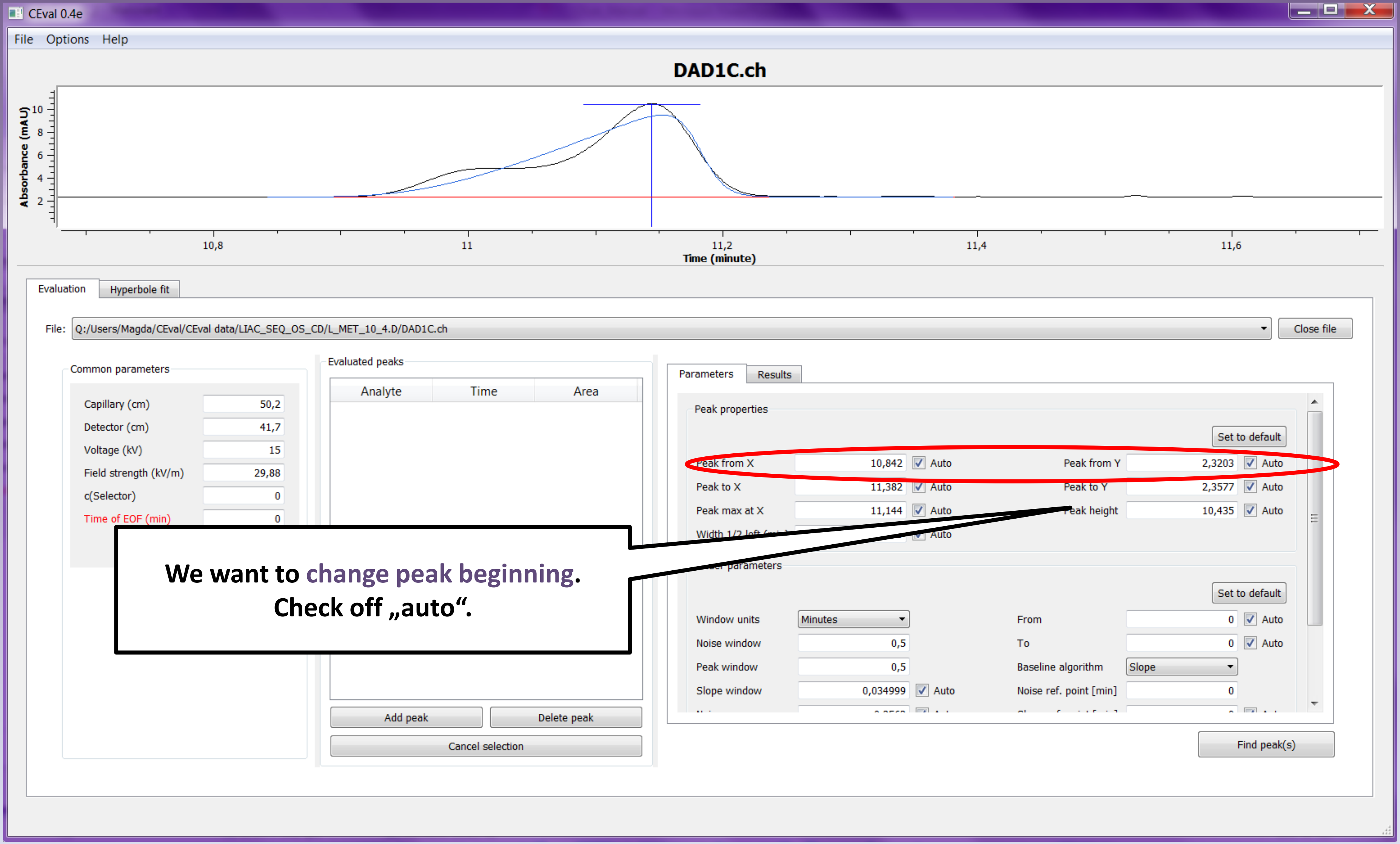
Peak dimensions

HVL fit of the whole peak is nonsensical.

We want to evaluate part of the peak only.

Switch to Parameters.

Appendix D: Distorted Peak



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

Peak properties

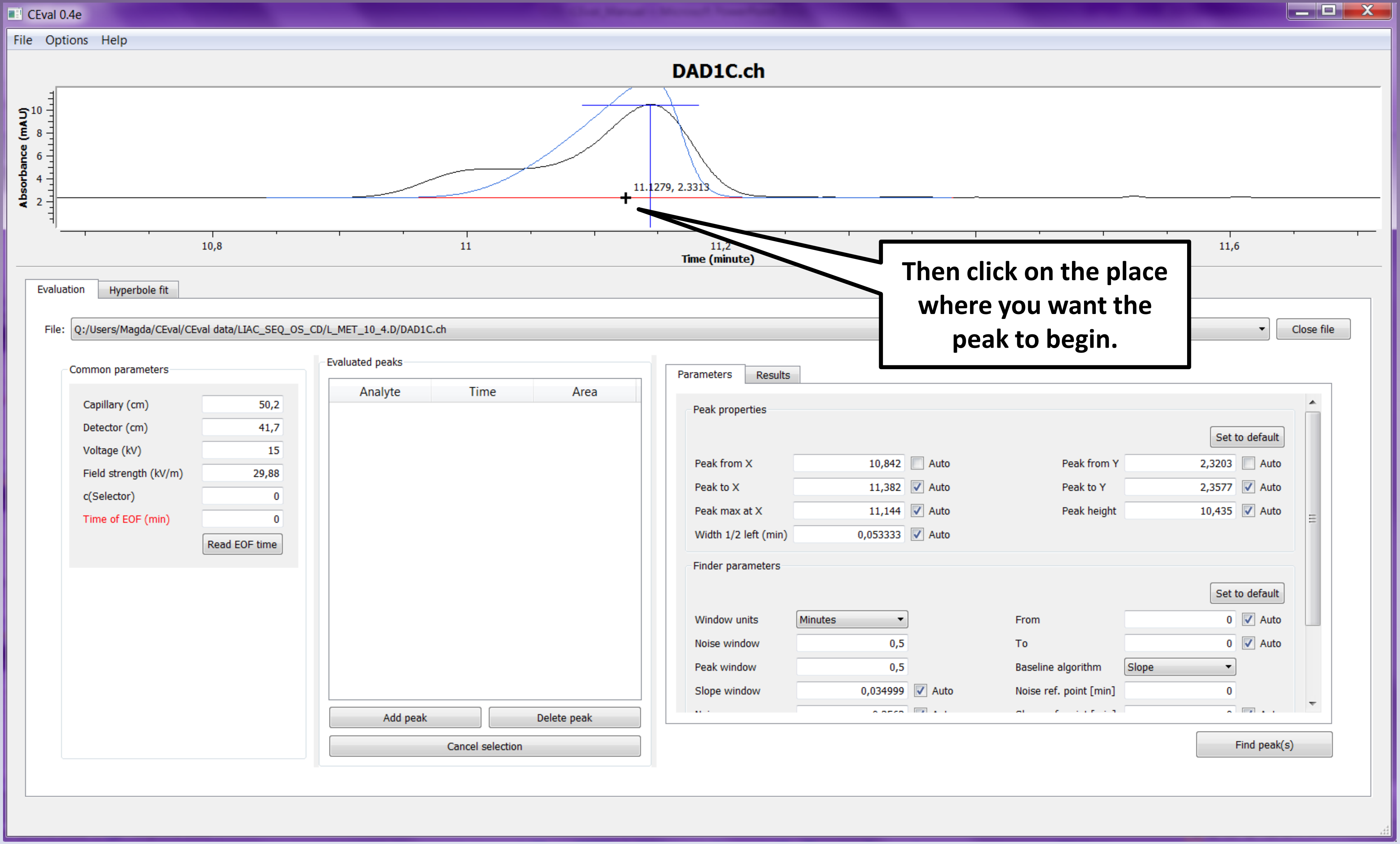
Peak from X	10,842	☑ Auto	Peak from Y	2,3203	☑ Auto
Peak to X	11,382	☑ Auto	Peak to Y	2,3577	☑ Auto
Peak max at X	11,144	☑ Auto	Peak height	10,435	☑ Auto
Width 1/2 left (min)		☑ Auto			

parameters

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

We want to change peak beginning. Check off „auto“.

Appendix D: Distorted Peak



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

Peak properties

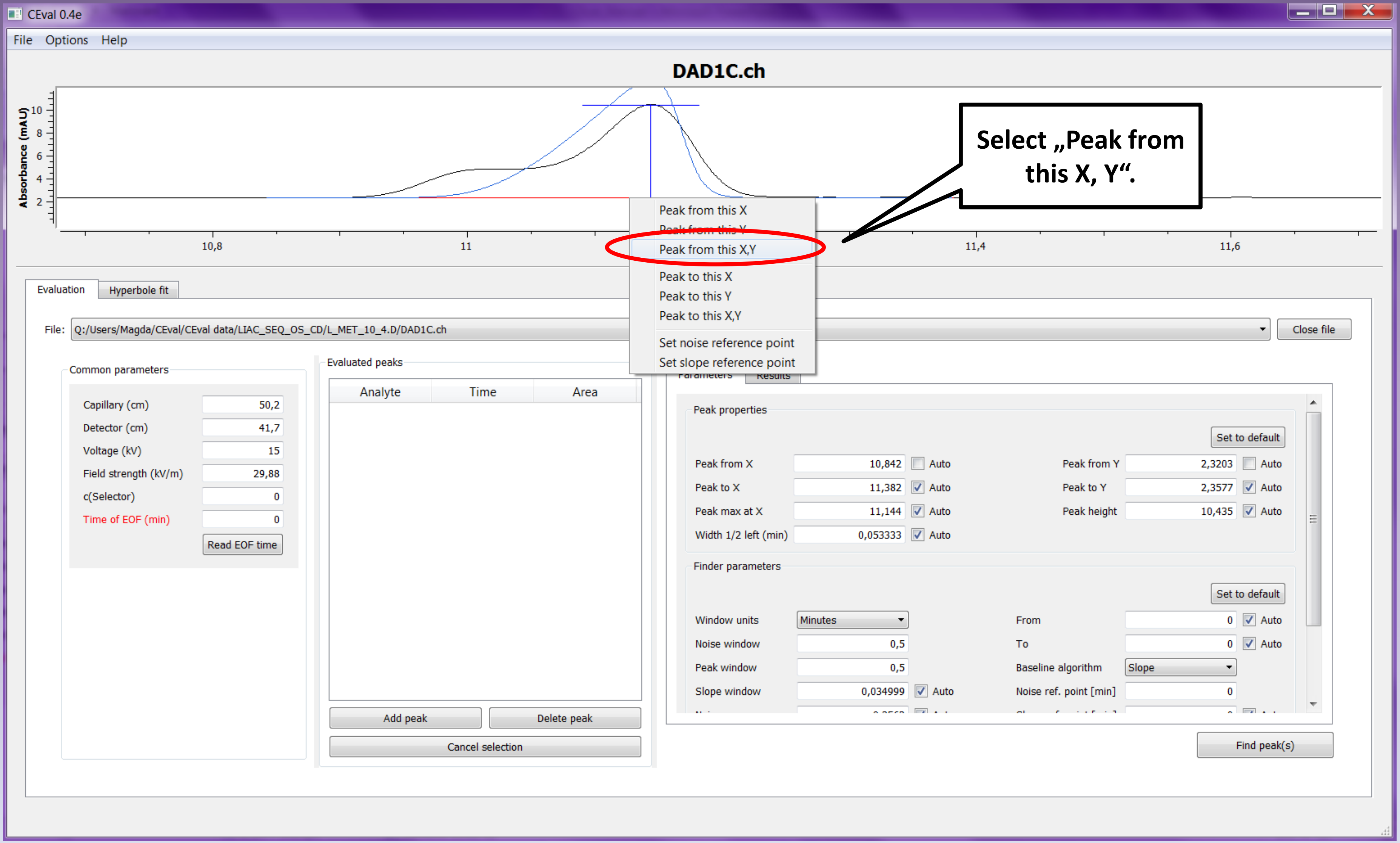
Peak from X	10,842	☐ Auto	Peak from Y	2,3203	☐ Auto
Peak to X	11,382	☑ Auto	Peak to Y	2,3577	☑ Auto
Peak max at X	11,144	☑ Auto	Peak height	10,435	☑ Auto
Width 1/2 left (min)	0,053333	☑ Auto			

Finder parameters

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

Then click on the place where you want the peak to begin.

Appendix D: Distorted Peak



Select „Peak from this X, Y".

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

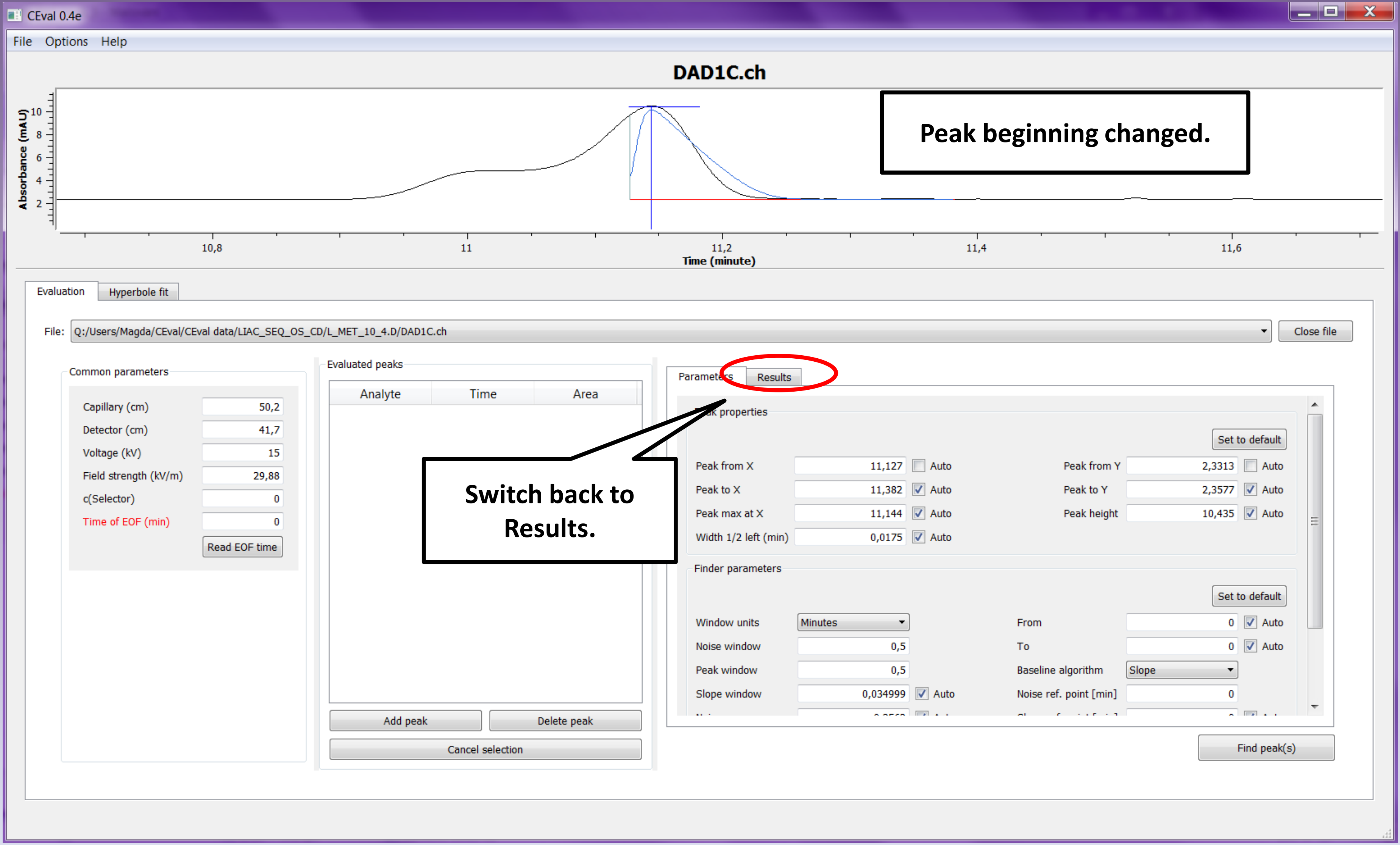
Peak properties

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

Finder parameters

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

Appendix D: Distorted Peak



Peak beginning changed.

Switch back to Results.

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

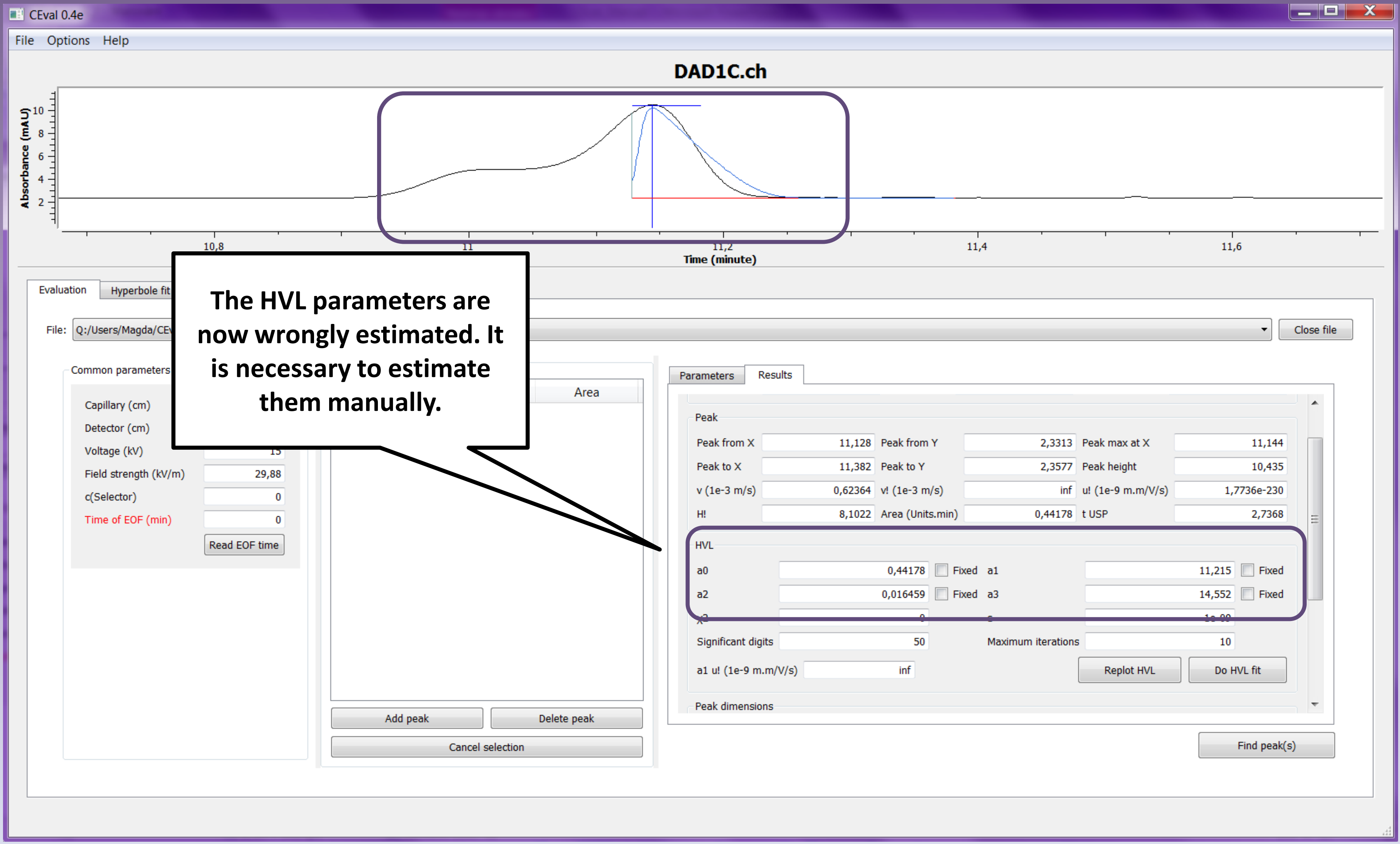
Peak properties

Peak from X	11,127	☐ Auto	Peak from Y	2,3313	☐ Auto
Peak to X	11,382	☑ Auto	Peak to Y	2,3577	☑ Auto
Peak max at X	11,144	☑ Auto	Peak height	10,435	☑ Auto
Width 1/2 left (min)	0,0175	☑ Auto			

Finder parameters

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

Appendix D: Distorted Peak



The HVL parameters are now wrongly estimated. It is necessary to estimate them manually.

File: Q:/Users/Magda/CE

Common parameters

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

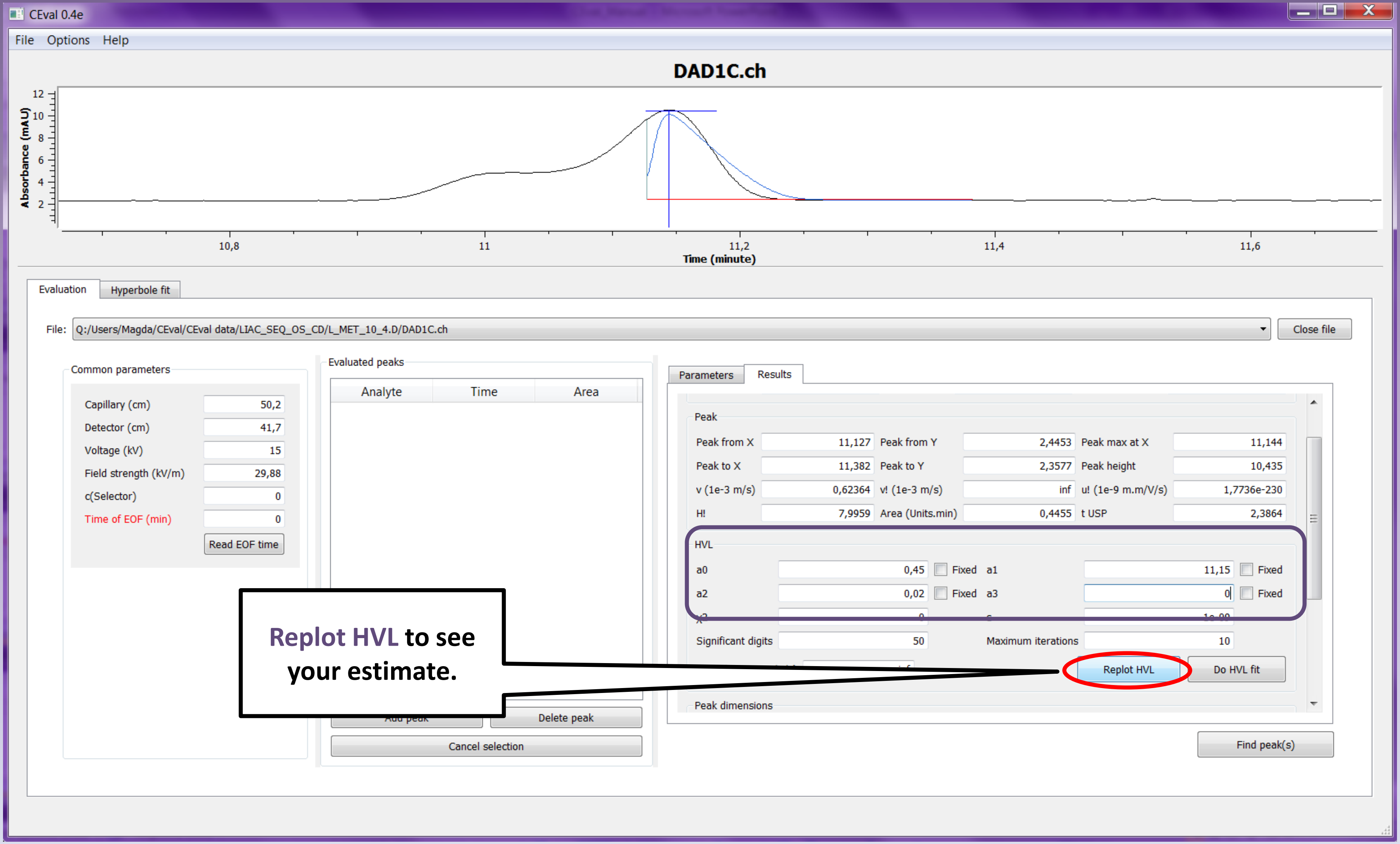
Peak

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	v! (1e-3 m/s)	inf	u! (1e-9 m.m/V/s)	1,7736e-230
H!	8,1022	Area (Units.min)	0,44178	t USP	2,7368

HVL

a0: 0,44178 ☐ Fixed
a1: 11,215 ☐ Fixed
a2: 0,016459 ☐ Fixed
a3: 14,552 ☐ Fixed
χ2: 0
Significant digits: 50
Maximum iterations: 10
a1 u! (1e-9 m.m/V/s): inf

Appendix D: Distorted Peak



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

Peak

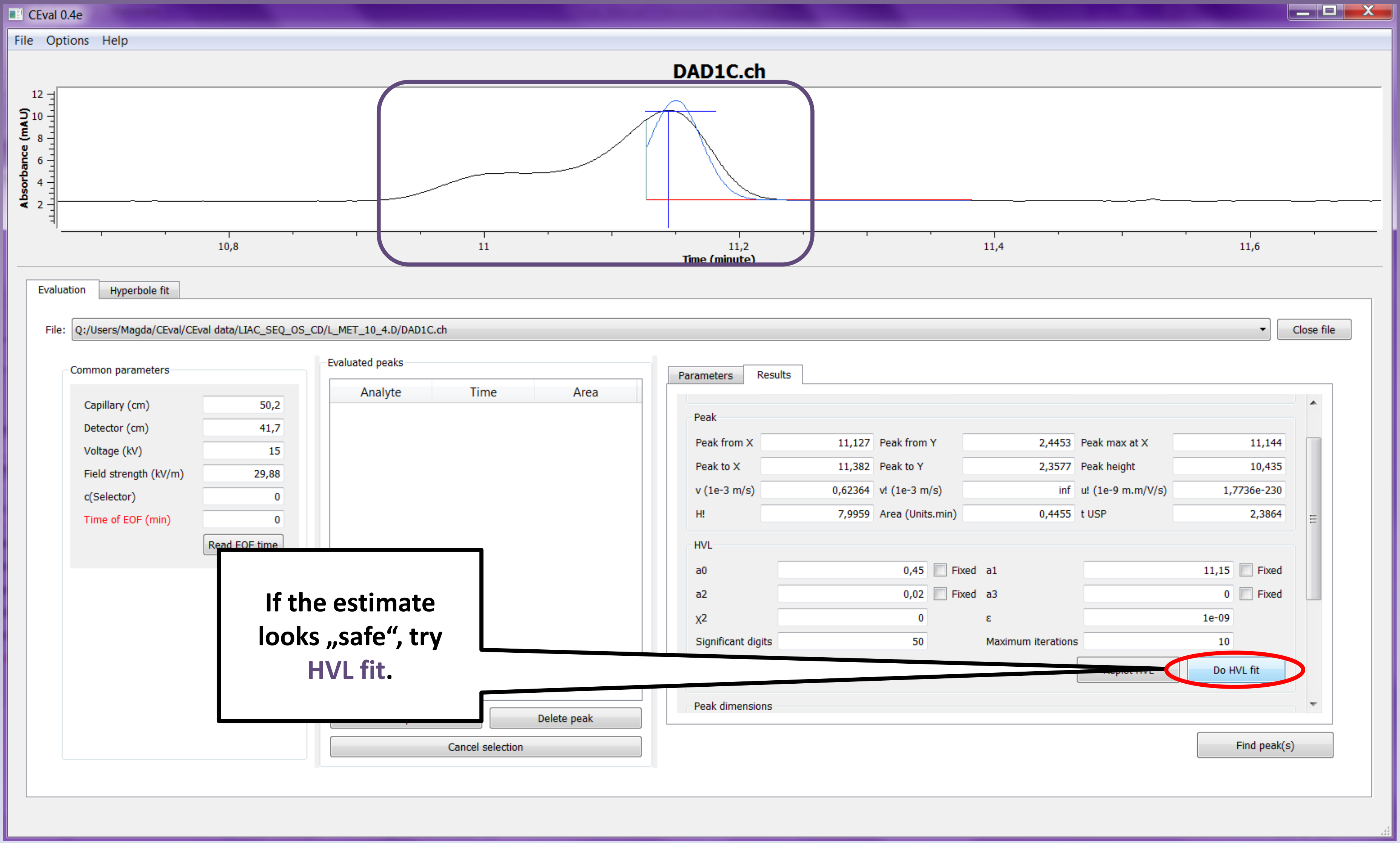
Peak from X: 11,127
Peak from Y: 2,4453
Peak max at X: 11,144
Peak to X: 11,382
Peak to Y: 2,3577
Peak height: 10,435
v (1e-3 m/s): 0,62364
v! (1e-3 m/s): inf
u! (1e-9 m.m/V/s): 1,7736e-230
H!: 7,9959
Area (Units.min): 0,4455
t USP: 2,3864

HVL

a0: 0,45 ☐ Fixed
a1: 11,15 ☐ Fixed
a2: 0,02 ☐ Fixed
a3: 0 ☐ Fixed
Significant digits: 50
Maximum iterations: 10

Replot HVL to see your estimate.

Appendix D: Distorted Peak



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

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	v! (1e-3 m/s)	inf	u! (1e-9 m.m/V/s)	1,7736e-230
H!	7,9959	Area (Units.min)	0,4455	t USP	2,3864

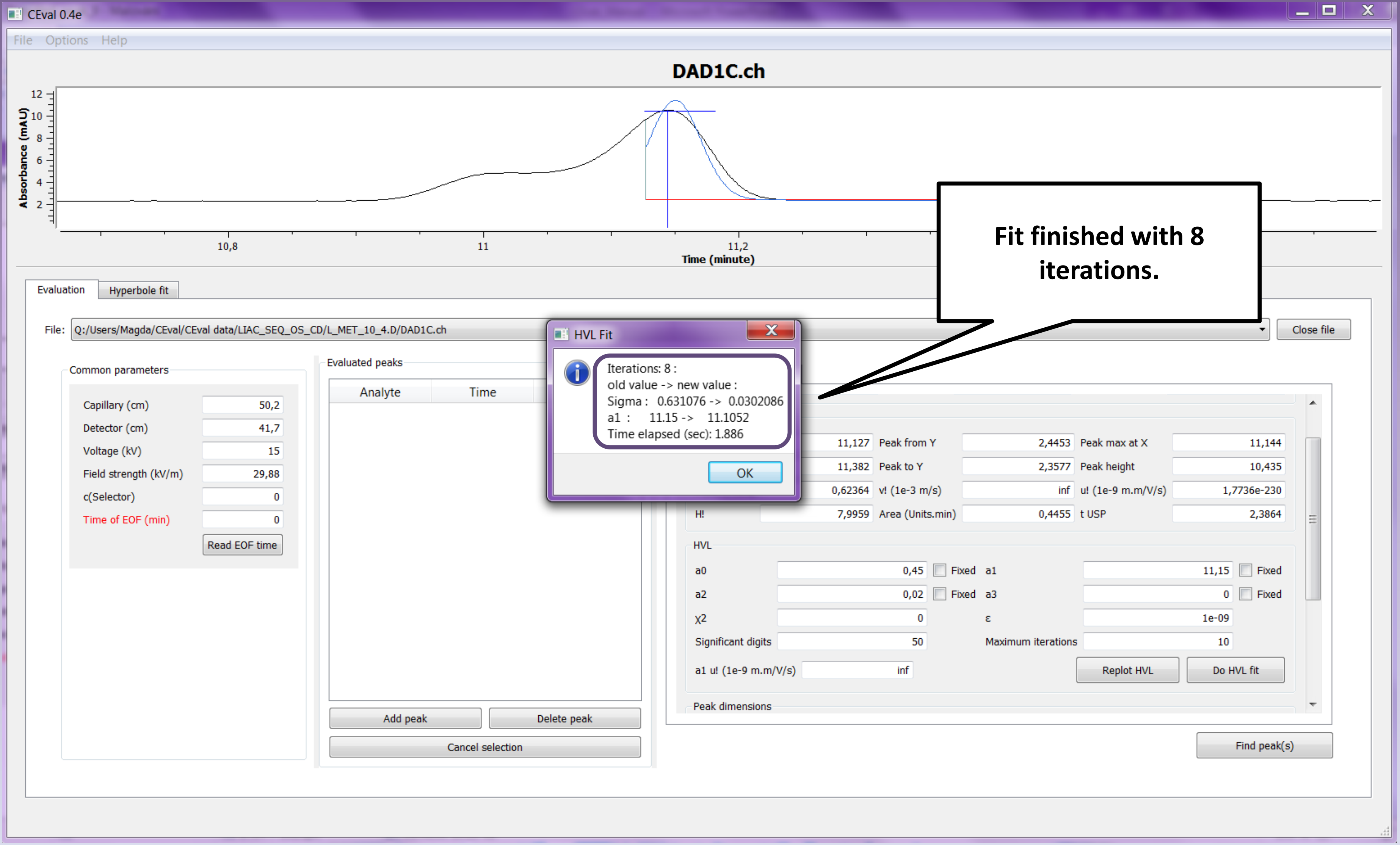
HVL

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	

Peak dimensions

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

Appendix D: Distorted Peak



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

HVL Fit

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

OK

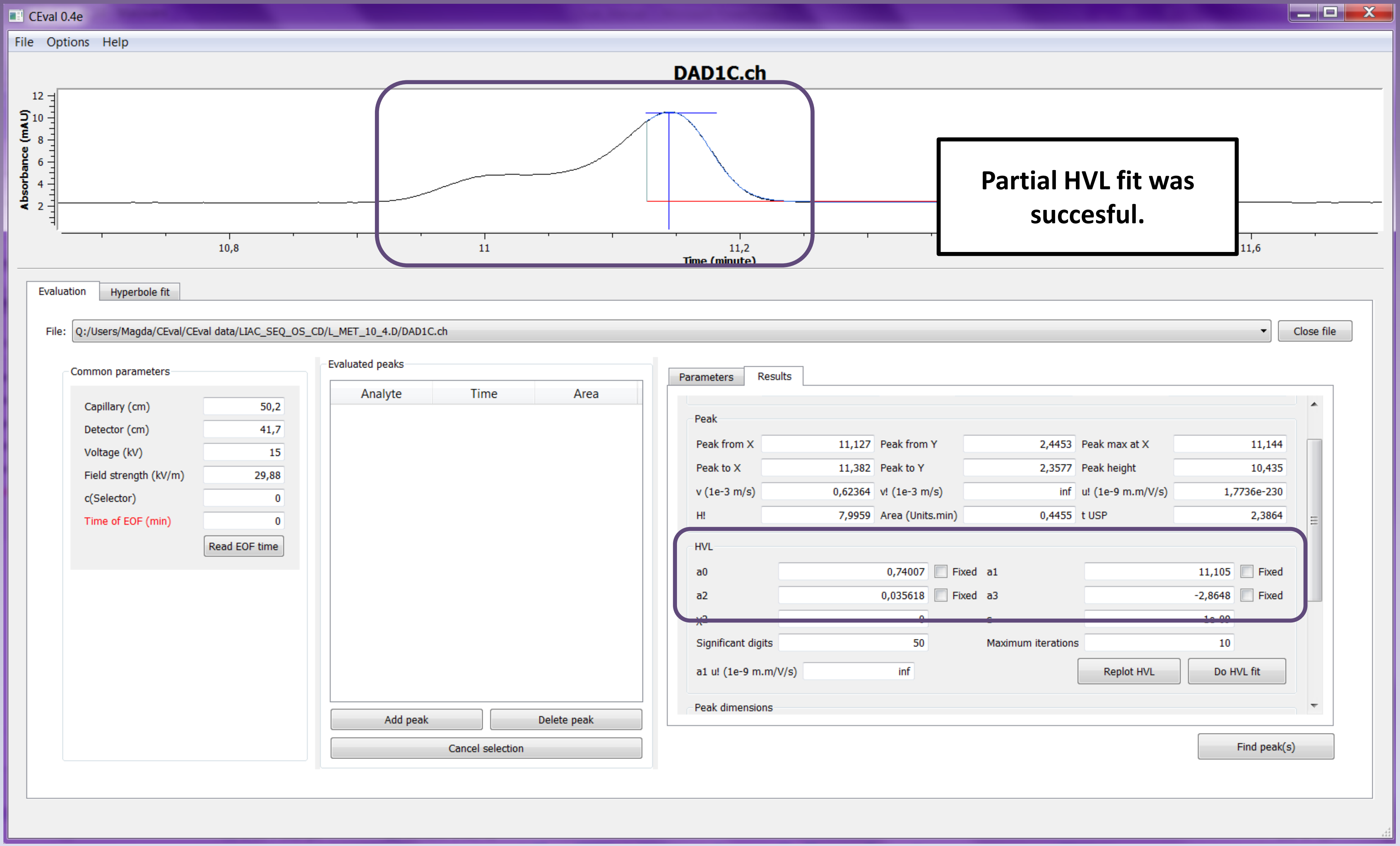
11,127 Peak from Y: 2,4453 Peak max at X: 11,144
11,382 Peak to Y: 2,3577 Peak height: 10,435
0,62364 v! (1e-3 m/s): inf u! (1e-9 m.m/V/s): 1,7736e-230
H!: 7,9959 Area (Units.min): 0,4455 t USP: 2,3864

HVL

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

Fit finished with 8 iterations.

Appendix D: Distorted Peak



Partial HVL fit was succesful.

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

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	v! (1e-3 m/s)	inf	u! (1e-9 m.m/V/s)	1,7736e-230
H!	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
χ2	0		ε	1e-09	
Significant digits	50		Maximum iterations	10	
a1 u! (1e-9 m.m/V/s)	inf				

Peak dimensions