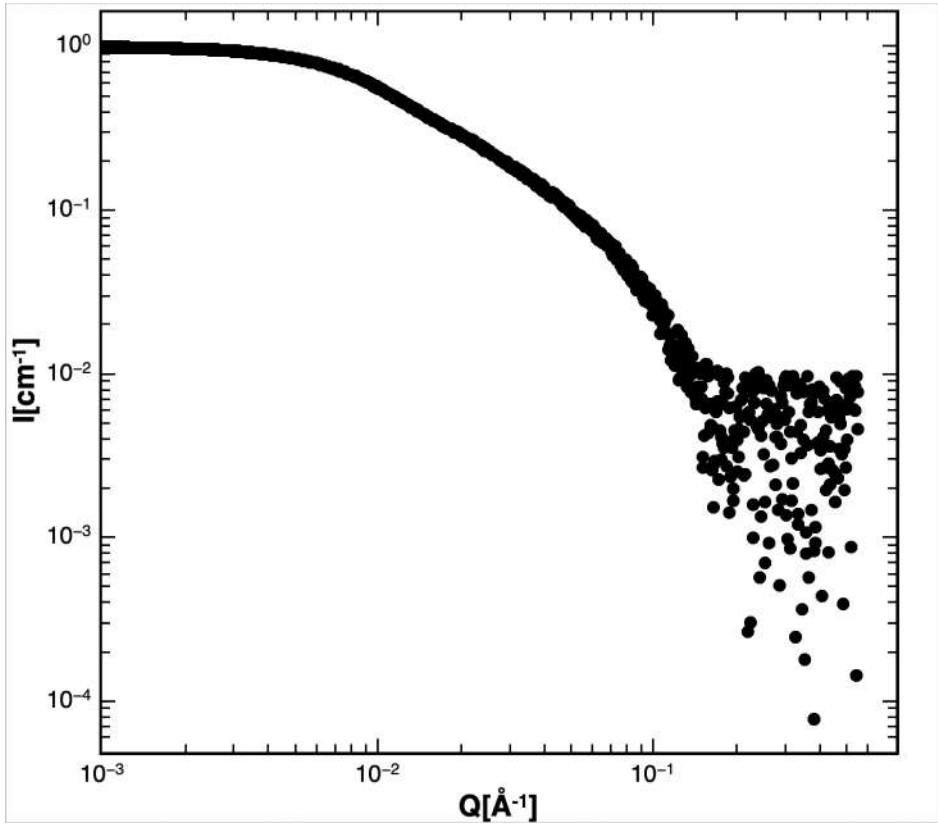
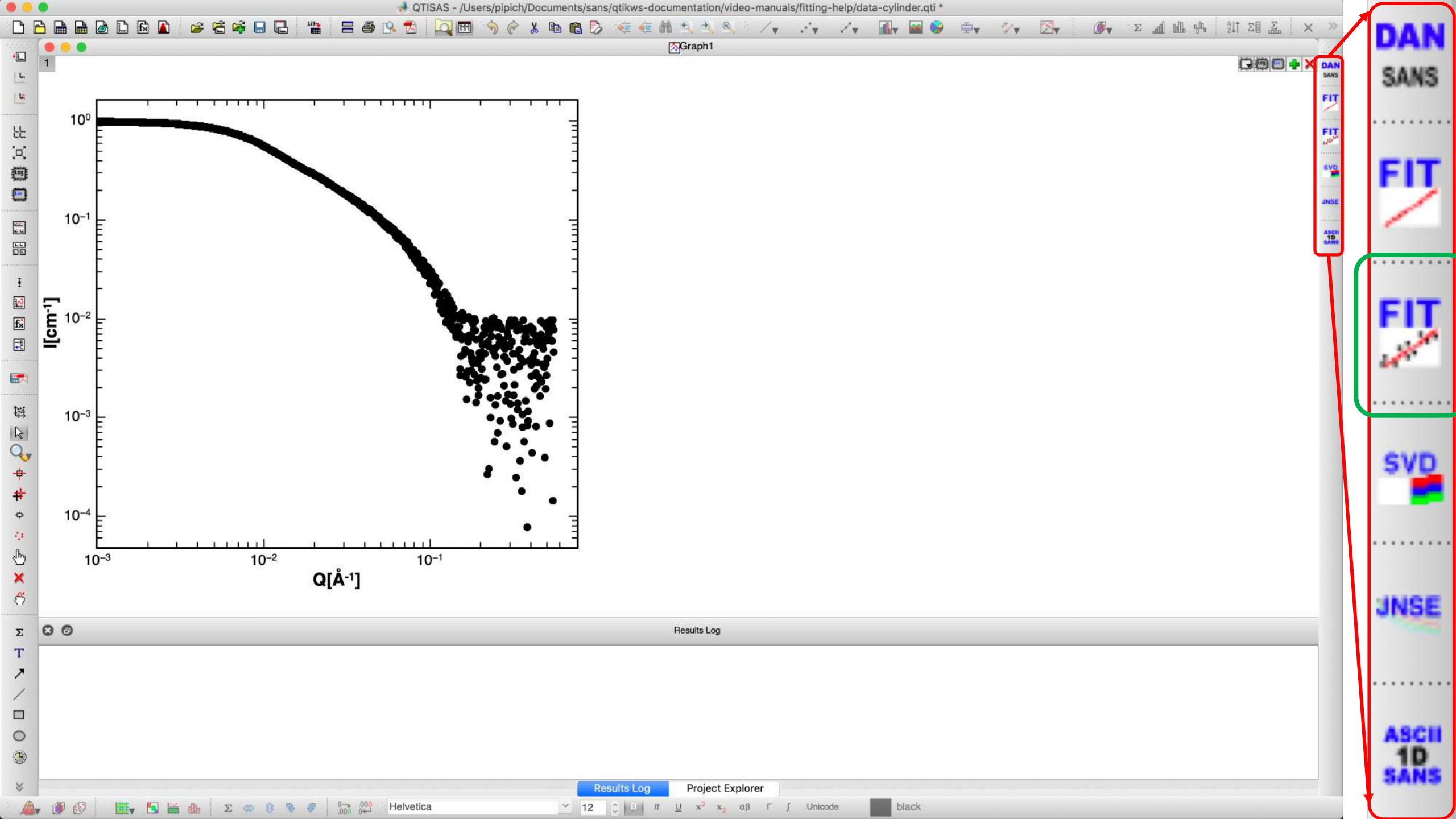
Fit.Curve(s): Standard Fit Mode

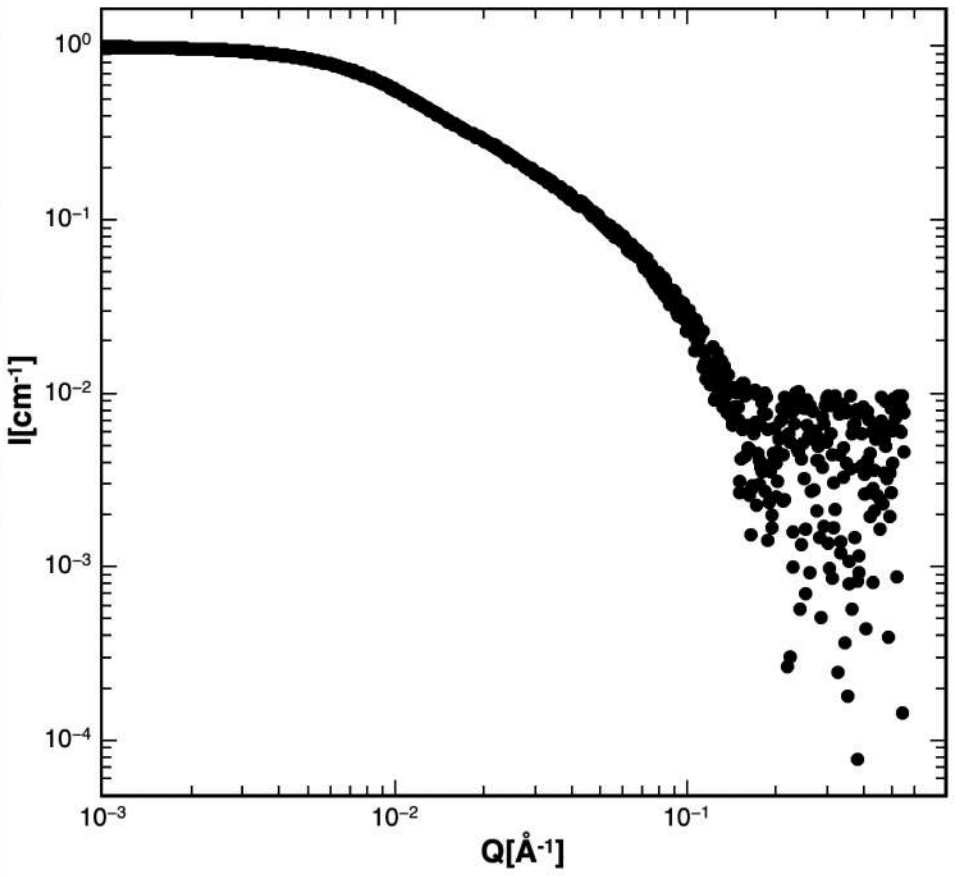


Function: Cylinder Form Factor


QTISAS - /Users/pipich/Documents/sans/qtikws-documentation/video-manuals/fitting-help/data-cylinder.qti *
Graph1
I[cm⁻¹]
Q[Å⁻¹]
Results Log
Project Explorer
Helvetica
12
Unicode
black
DAN
SANS
FIT
FIT
FIT
SVD
JNSE
ASCII
1D
SANS

QTISAS - /Users/pipich/Documents/sans/qtikws-documentation/video-manuals/fitting-help/data-cylinder.qti *

Graph1



FITTABLE(s)

Load Fitting Session

... | Select Function | Fitting Session

Categories

ALL
BS-BackScattering
Block Copolymer Micelles
Cholesterol-liposomes
Core::Shell
Density Profile
Distribution
EGOR-FUNCTIONS
EMBL
End-cap-Thomas
Flo
Form Factors
Form Structure
General
HF
Instrumentation
Integrals Test
Lipoproteins

Functions

FlexCylExv-sourcecode-SASview-simulated-in-QTI
Gauss-Coil
HammodaTwoLevels
HammodaTwoLevelsPlusGuinier
KholodenkoWorm
WormLikeCylinder-NEW
cylinder-efit
mass-fractal-aggregate
mass-fractal-aggregate-GuinierAgg
mass-fractal-aggregate-sphAgg
membrane-HF
pearl-necklace-chain
pearl-necklace-rod
spherical-core-shell
symmetricBilayer
symmetricBilayerDMPSSchultz
testmicelle-ohne-kern-vorfatkrowiestefan-andersintegrier

Info :: Function | Info :: Parameters | Options

Form Factor of Cylinder with Radius R and Length L:

$I(Q) = I0 \times P(Q)$;

$P(Q) = \int [0..\pi/2]\ F^2(Q,R,L,\alpha)\ sin(\alpha)d\alpha$;

$F(Q,R,L,a) \Rightarrow 2J_1[QRsin(\alpha)] / [QRsin(\alpha)] \times sin(QLcos(\alpha)/2) / (QLcos(\alpha)/2)$;

$J_1(x)$ - the regular cylindrical Bessel function of first order .

efit-ready

v. 2019-10-09

Project Explorer

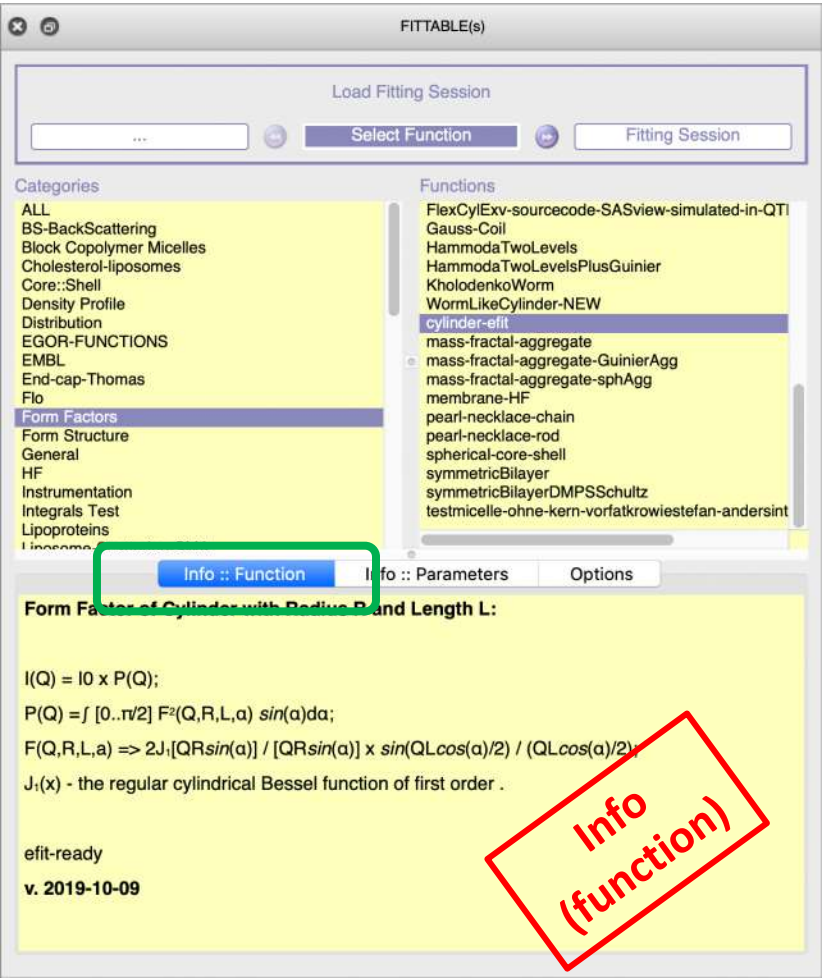
data-cylinder

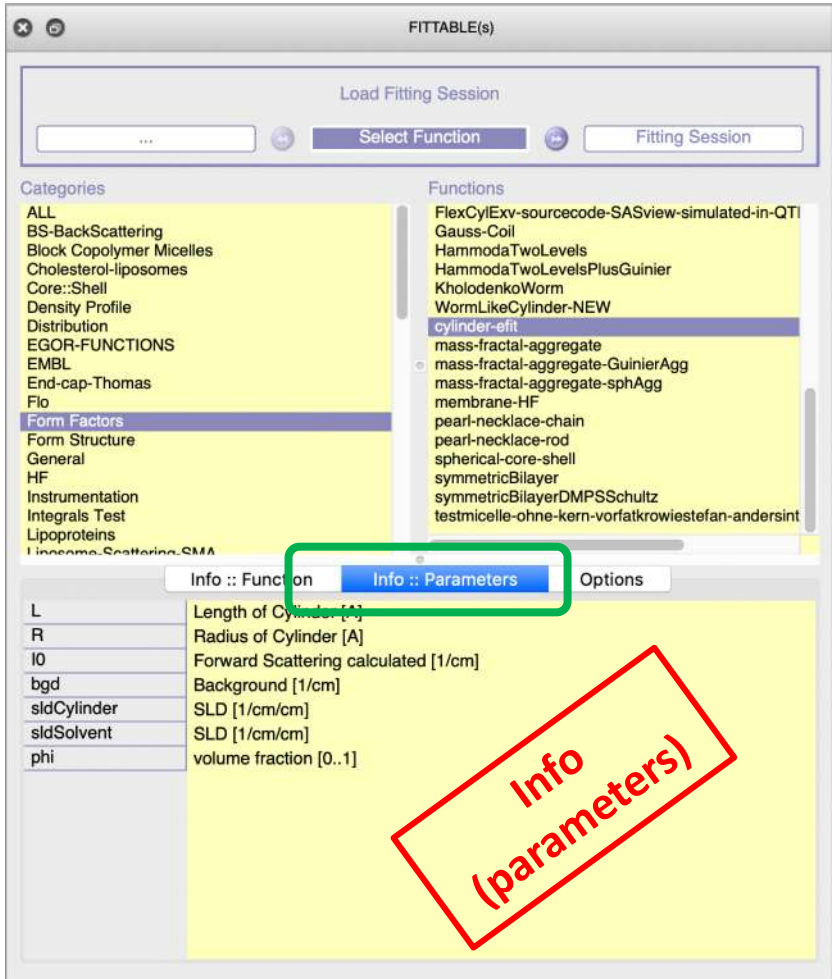
Name	Type	View	Created	Label
data	Table	Normal	11/11/15 00:11:19	Simulated Curve
Graph1	Graph	Maximized	25.02.21 10:29	

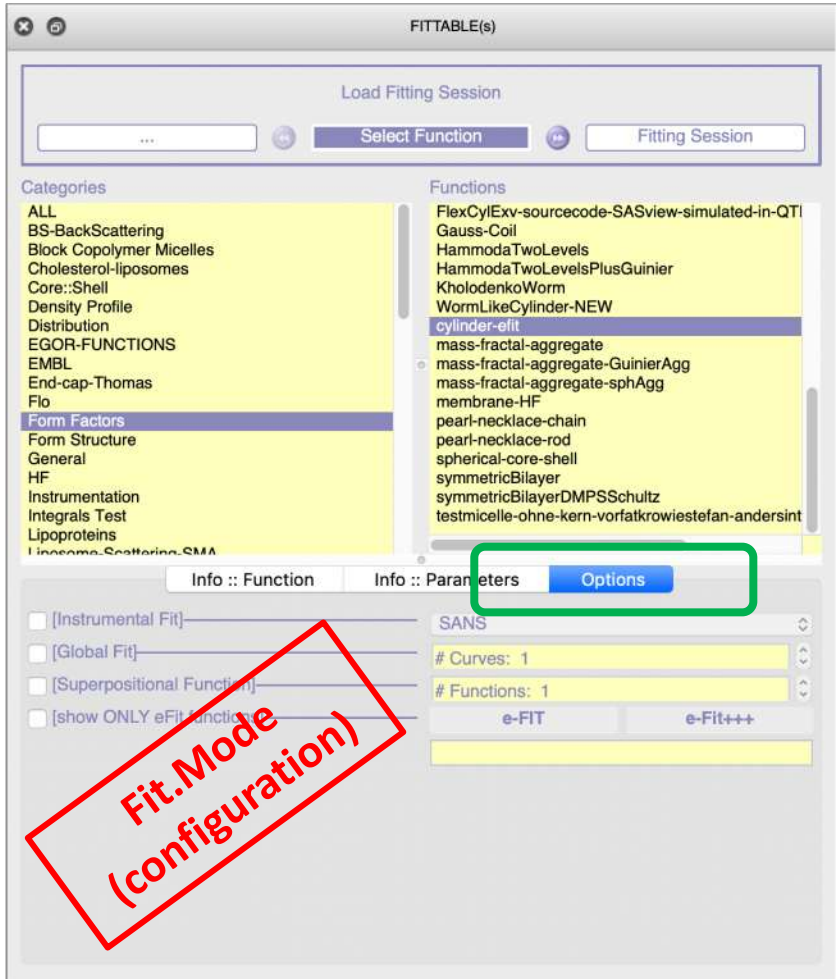
Results Log | Project Explorer

Helvetica 12 Unicode black

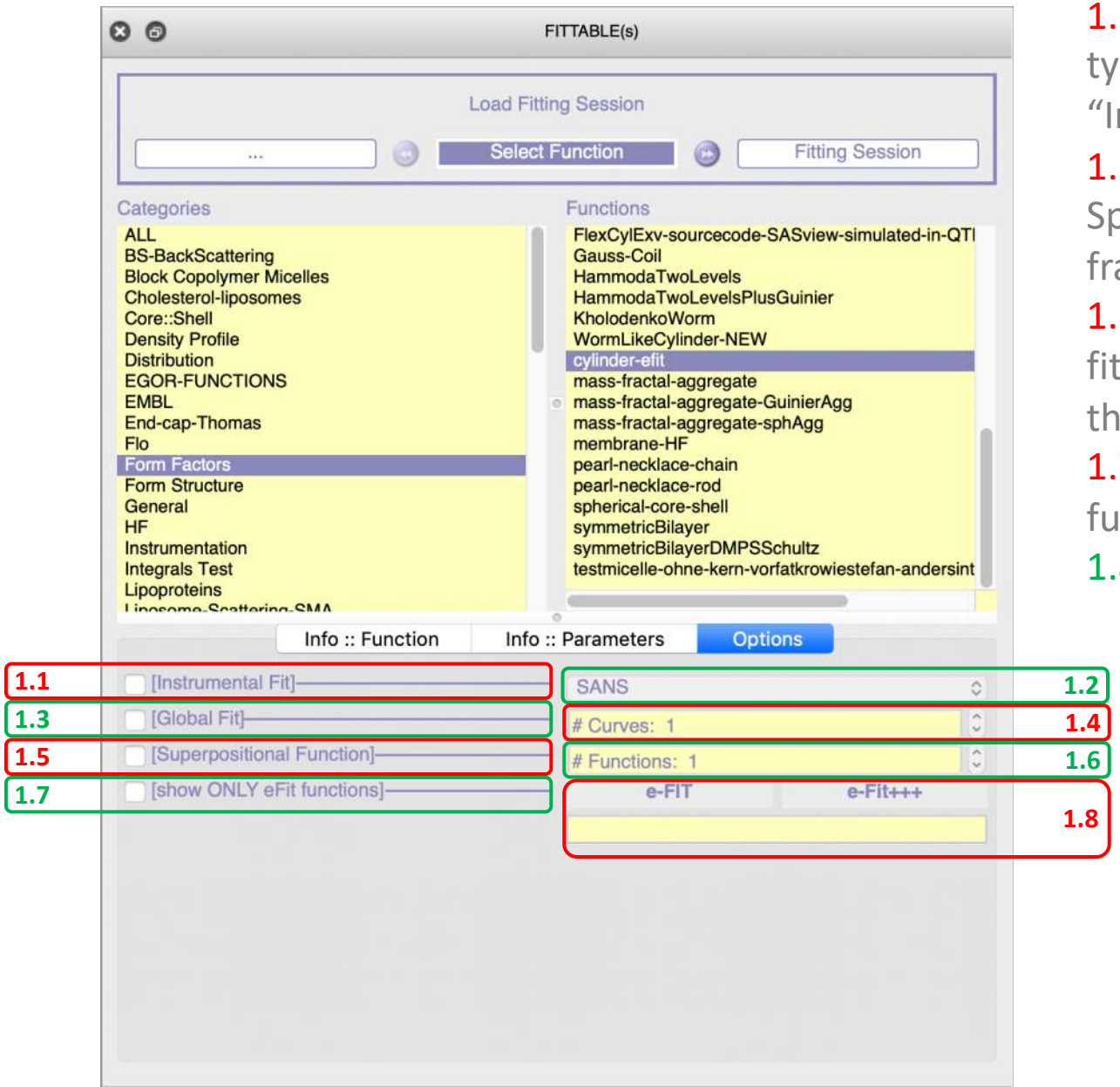
Step 1: Select Function and **Fit.Mode** Options







Fit.Mode Options



1.1 **CheckBox [Instrumental Fit]**: if checked, you could select type of instrumental fit (in 1.2 ComboBox) within "Instumental.Fit.Mode"

1.3 **CheckBox [Global Fit]**: if checked you could set (in 1.4 SpinBox) number of curves to be fitted simultaneously in the frame of "Global.Fit.Mode"

1.5 **CheckBox [Superpositional Function]**: if checked the fitting function contains several sub-functions, and number of the sub-functions is defined in 1.6 SpinBox.

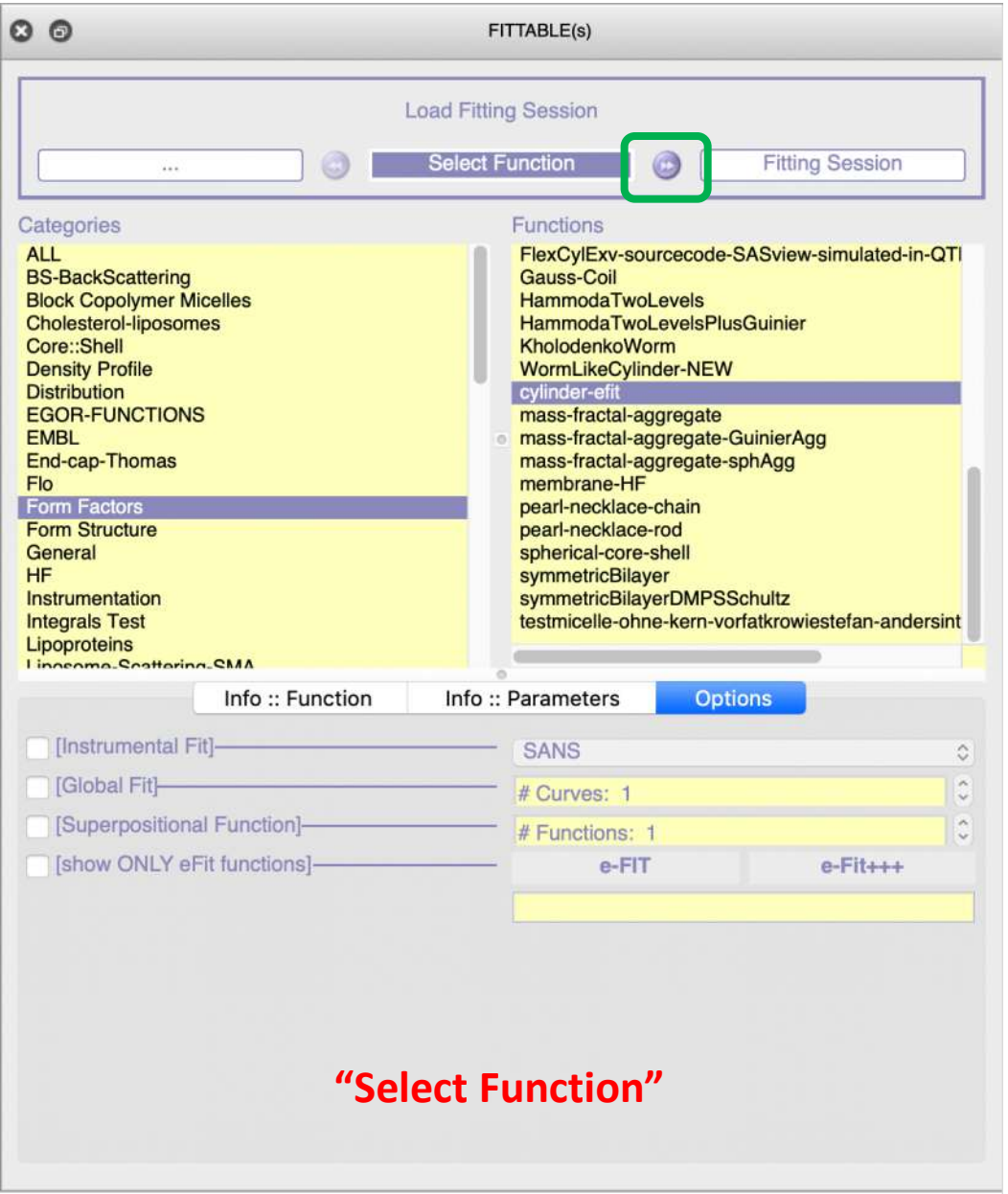
1.7 **CheckBox [show only eFit Functions]**: if checked, in the function explorer will be shown only "eFit ready" functions

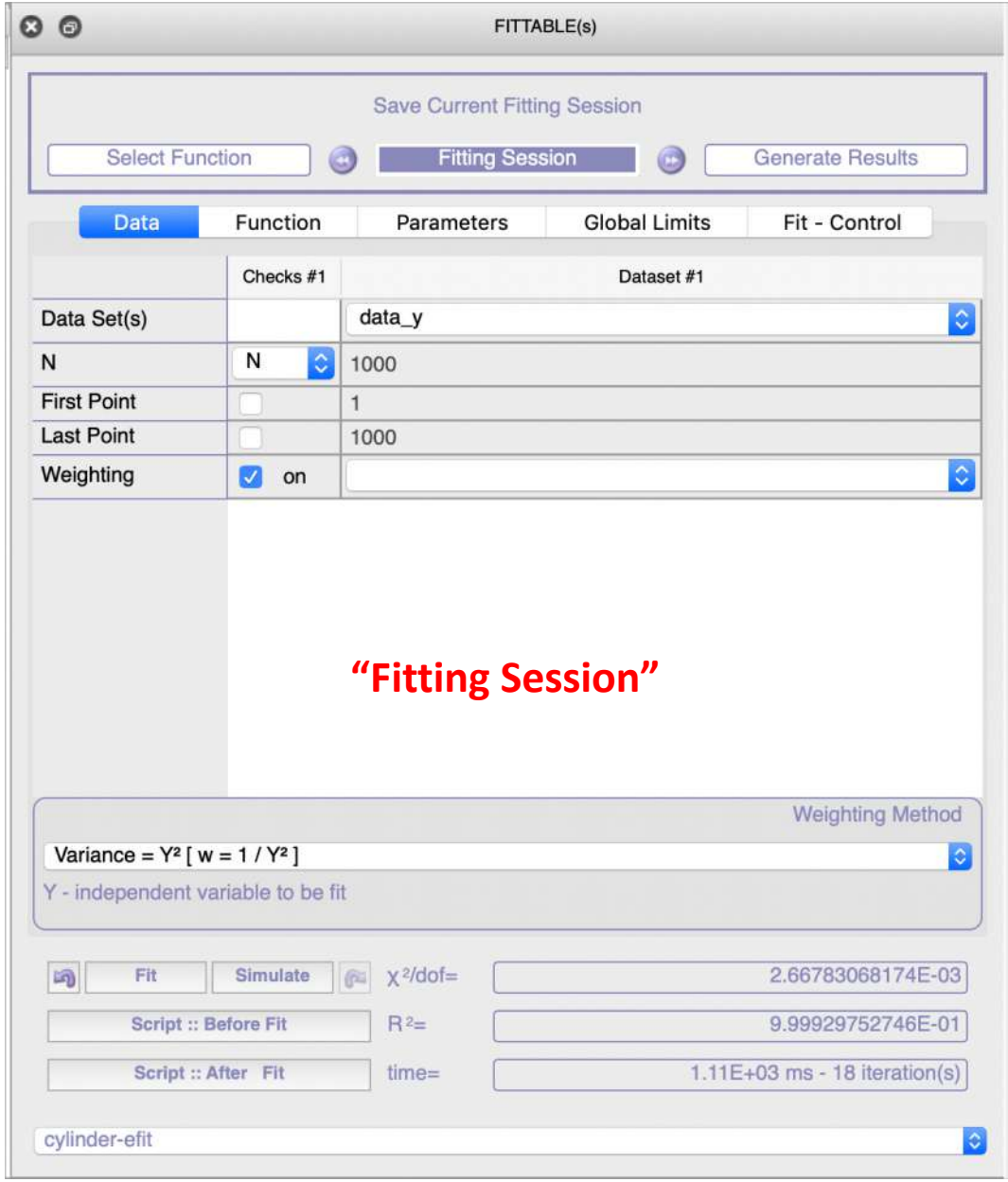
1.8 eFit buttons and options

In this example, we use:

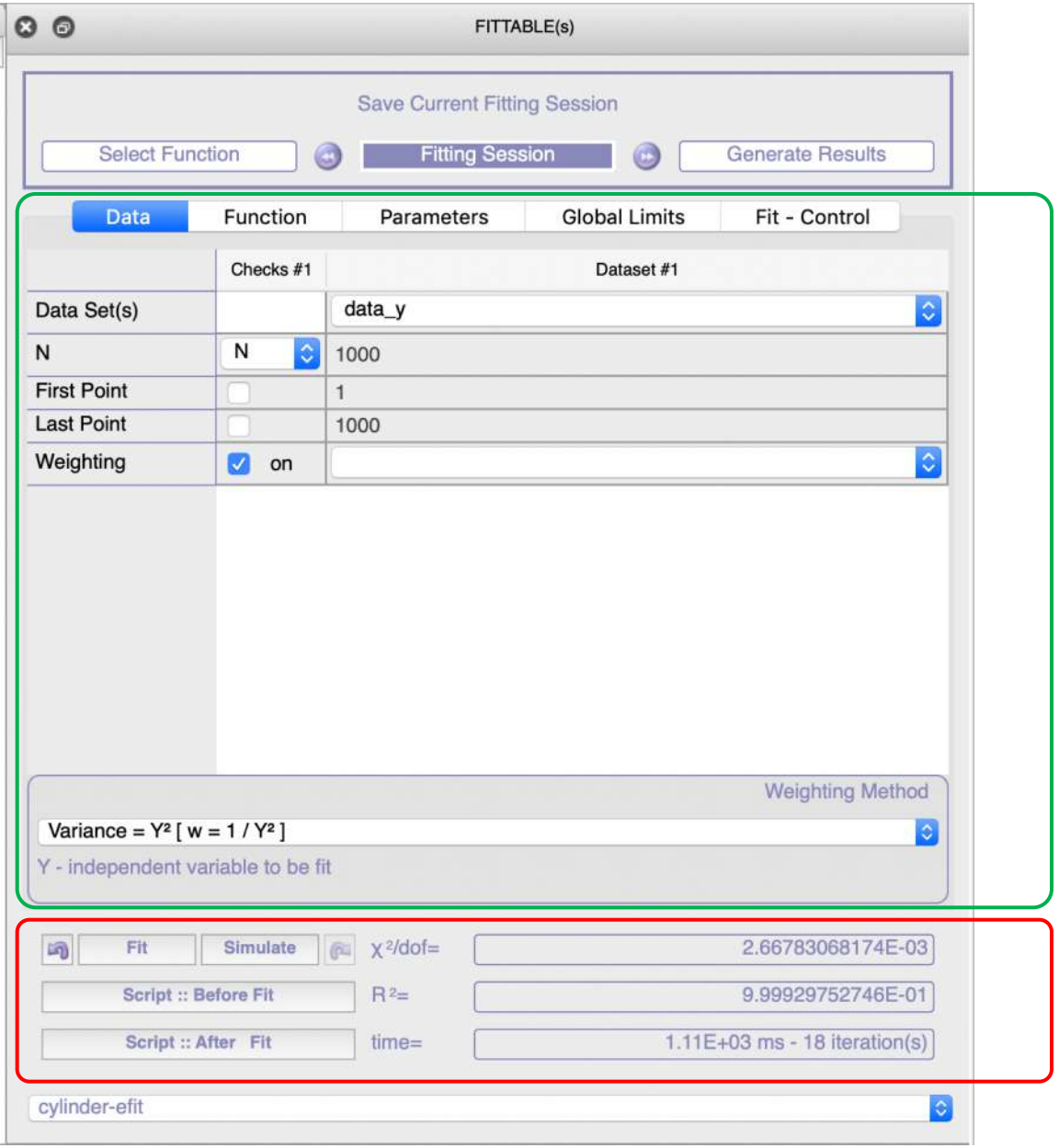
Standard Fit Mode

Step 2: Push Button “next” to “Fitting Session”





“Fitting Session” interface has “Tab-Widget” and “Fit Buttons”



“Tab-Widgets”

Data | Function | Parameters | Global Limits | Fit - Control

	Checks #1	Dataset #1
Data Set(s)		data_y
N	N	1000
First Point		1
Last Point		1000
Weighting	on	

Weighting Method

Variance = Y² [w = 1 / Y²]

Y - independent variable to be fit

Data

Weighting

Data | Function | Parameters | Global Limits | Fit - Control

cylinder-efit

Parameters: 7 | # Indep. Variables: 1 | # Dep. Variables: 1

Form Factor of Cylinder with Radius R and Length L:

I(Q) = I0 x P(Q);

P(Q) =∫ [0..π/2] F²(Q,R,L,α) *sin*(α)dα;

F(Q,R,L,a) => 2J₁[QR*sin*(α)] / [QR*sin*(α)] x *sin*(QL*cos*(α)/2) / (QL*cos*(α)/2);

$J_1(x)$ - the regular cylindrical Bessel function of first order .

L	Length of Cylinder [A]
R	Radius of Cylinder [A]
I0	Forward Scattering calculated [1/cm]
bgd	Background [1/cm]
sldCylinder	SLD [1/cm/cm]
sldSolvent	SLD [1/cm/cm]
phi	volume fraction [0..1]

Function Info

Data | Function | Parameters | Global Limits | Fit - Control

	Vary?From..To	Value #1	Error #1
L	..	500	---
R	..	20	---
I0		1	---
bgd	..	0	---
sldCylinder	..	3E+10	---
sldSolvent	..	-5.6E+09	---
phi		0.01	---

Auto Simulation | Scale Errors | Save Session | Statistics Notes [after Fit]

Fit?
Local Limits

Parameters
Init.Values

Data | Function | Parameters | Global Limits | Fit - Control

Global Limits for Parameters [FROM .. TO] ::

1	=<	L	=<	10000
1	=<	R	=<	1000
0	=<	I0	=<	1e+06
0	=<	bgd	=<	10
-inf	=<	sldCylinder	=<	inf
-inf	=<	sldSolvent	=<	inf
0.001	=<	phi	=<	1

Reset

Global
Limits

Data | Function | Parameters | Global Limits | Fit - Control

Algorithm: Levenberg-Marquardt

Significant Digits: 9

Levenberg-Marquardt Options

Levenberg Mode: [delta, scaled]

Derivative Step Size: 1e-4

Stopping Criteria:

Maximal # Iterations: 1000

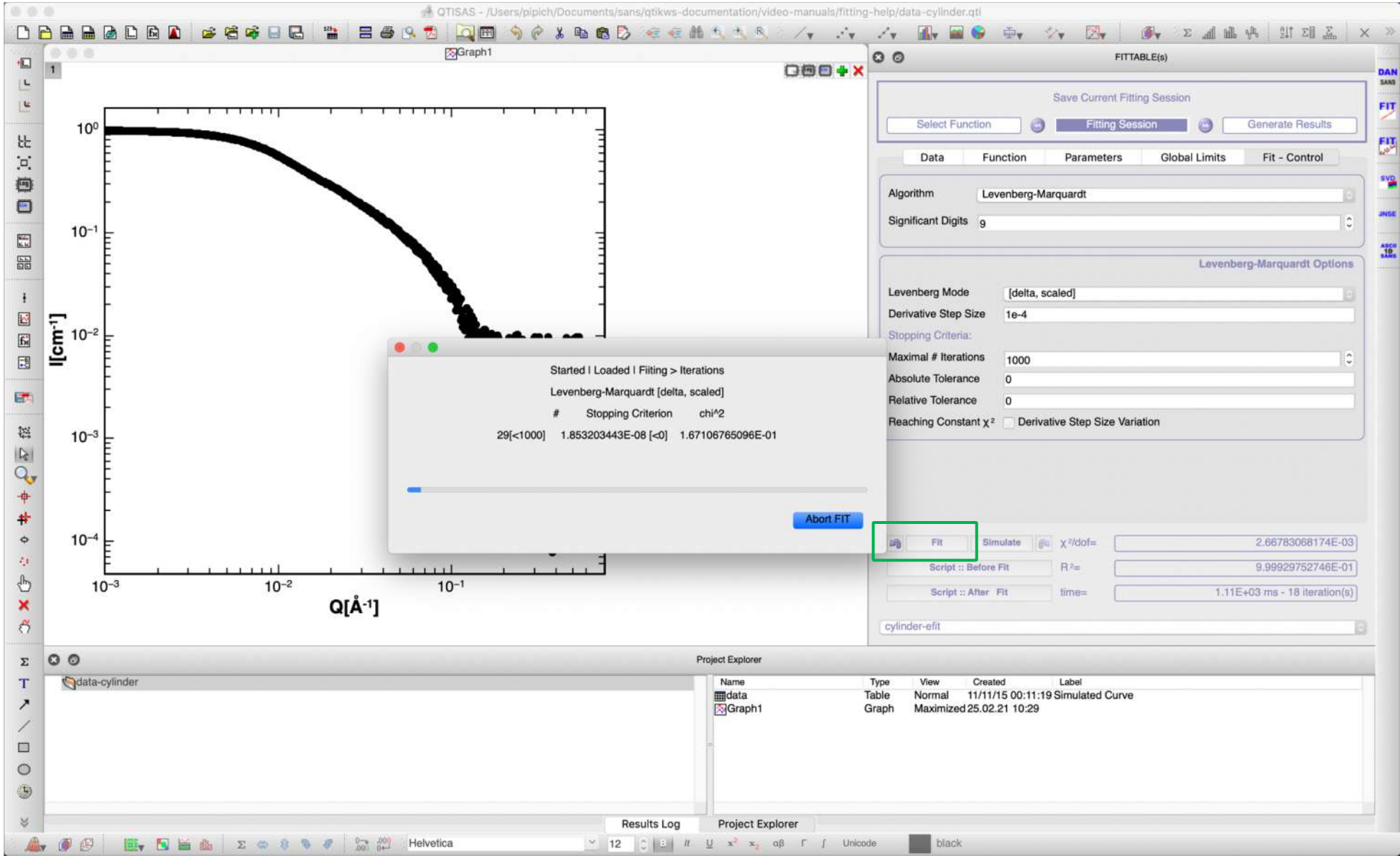
Absolute Tolerance: 0

Relative Tolerance: 0

Reaching Constant χ² | Derivative Step Size Variation

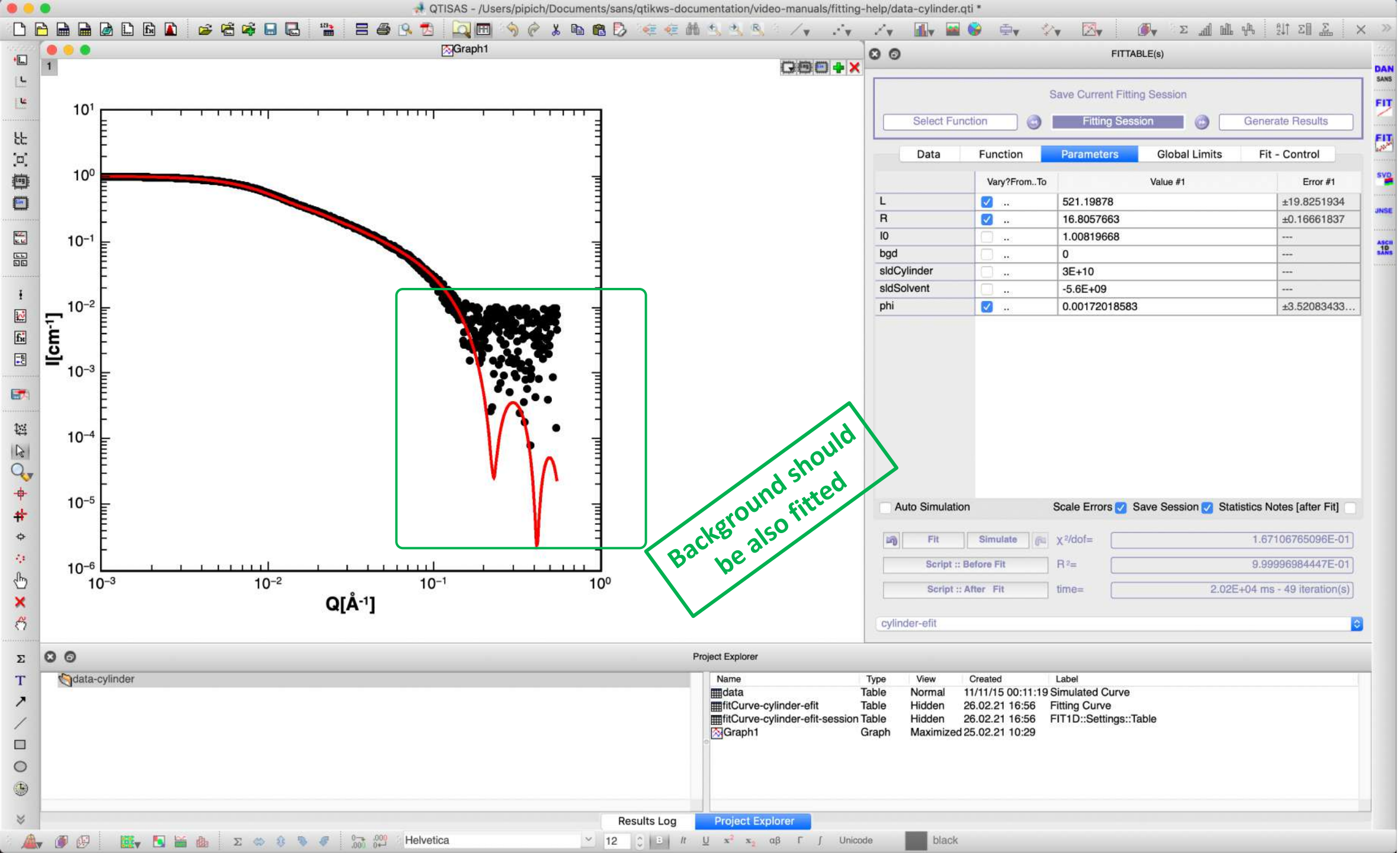
Fitting
Algorithm

Step 3: Push Button “Fit”



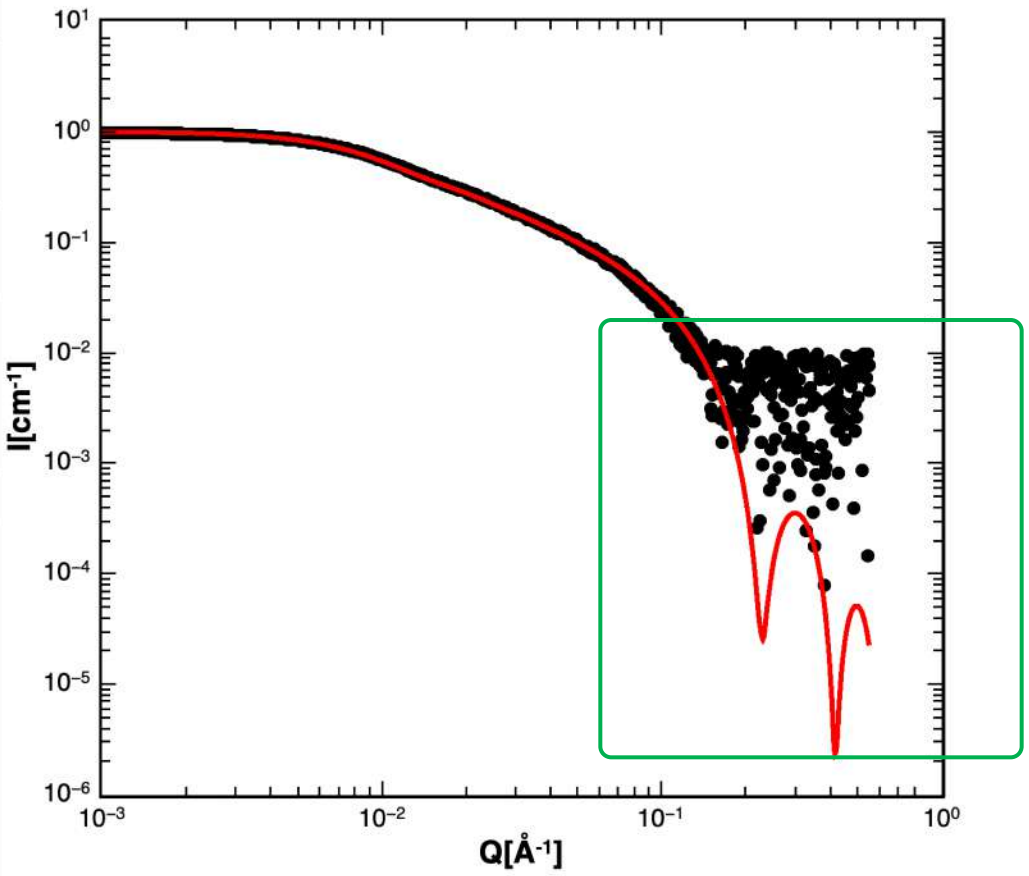
```
Fit|Init:                                0.014sec
Fit|Started|Data Loading:                0.289sec
Fit|Started|Loaded|Fit Preparation:      0.356sec
Fit|Started|Loaded|Prepared|Iterations:
# (levenberg)    1[<1000]     3.3968 [<         0] chi^2     0.202428326 [  496.603  19.7662 0.00154453  ] 1 [x const chi] 0.351sec
# (levenberg)    2[<1000]     19.225 [<         0] chi^2    0.1734698122 [  477.378  18.3574 0.0015594  ] 0.672sec
# (levenberg)    3[<1000]     17.232 [<         0] chi^2    0.1686691554 [   494.61  17.4949 0.00164753  ] 0.326sec
# (levenberg)    4[<1000]     17.003 [<         0] chi^2    0.1673645813 [  511.613  17.0773 0.00169125  ] 0.328sec
# (levenberg)    5[<1000]     6.2538 [<         0] chi^2      0.16714799 [  517.867  16.9101 0.0017092  ] 0.341sec
# (levenberg)    6[<1000]     2.6768 [<         0] chi^2    0.1671124956 [  520.544  16.8436 0.00171567  ] 0.345sec
# (levenberg)    7[<1000]    0.37847 [<         0] chi^2    0.1671075469 [  520.922  16.8196 0.00171858  ] 0.339sec
# (levenberg)    8[<1000]    0.19798 [<         0] chi^2    0.1671068698 [   521.12  16.8108 0.00171959  ]  0.34sec
# (levenberg)    9[<1000]   0.040531 [<         0] chi^2    0.1671067793 [  521.161  16.8075 0.00171999  ] 0.334sec
# (levenberg)   10[<1000]    0.03074 [<         0] chi^2     0.167106767 [  521.192  16.8063 0.00172012  ]  0.33sec
# (levenberg)   11[<1000]  0.0035503 [<         0] chi^2    0.1671067653 [  521.195  16.8059 0.00172017  ] 0.339sec
# (levenberg)   12[<1000]  0.0024742 [<         0] chi^2    0.1671067651 [  521.198  16.8058 0.00172018  ] 0.357sec
# (levenberg)   13[<1000]  0.0003871 [<         0] chi^2    0.1671067651 [  521.198  16.8058 0.00172018  ] 0.359sec
# (levenberg)   14[<1000] 8.1353e-05 [<         0] chi^2    0.1671067651 [  521.198  16.8058 0.00172018  ] 0.354sec
# (levenberg)   15[<1000] 0.00018307 [<         0] chi^2    0.1671067651 [  521.198  16.8058 0.00172018  ] 0.342sec
# (levenberg)   16[<1000] 3.7324e-05 [<         0] chi^2    0.1671067651 [  521.198  16.8058 0.00172018  ] 0.348sec
# (levenberg)   17[<1000] 7.7269e-05 [<         0] chi^2    0.1671067651 [  521.199  16.8058 0.00172018  ] 0.334sec
# (levenberg)   18[<1000] 0.00015815 [<         0] chi^2    0.1671067651 [  521.199  16.8058 0.00172019  ] 0.338sec
# (levenberg)   19[<1000] 3.1621e-05 [<         0] chi^2    0.1671067651 [  521.199  16.8058 0.00172019  ] 0.351sec
# (levenberg)   20[<1000] 6.3738e-05 [<         0] chi^2    0.1671067651 [  521.199  16.8058 0.00172019  ] 0.395sec
# (levenberg)   21[<1000] 1.2586e-05 [<         0] chi^2    0.1671067651 [  521.199  16.8058 0.00172019  ] 0.359sec
# (levenberg)   22[<1000] 2.5108e-06 [<         0] chi^2    0.1671067651 [  521.199  16.8058 0.00172019  ] 0.361sec
# (levenberg)   23[<1000] 5.0257e-06 [<         0] chi^2    0.1671067651 [  521.199  16.8058 0.00172019  ] 0.337sec
# (levenberg)   24[<1000] 7.4687e-08 [<         0] chi^2    0.1671067651 [  521.199  16.8058 0.00172019  ] 1 [x const chi] 0.167sec
# (levenberg)   25[<1000] 9.7877e-05 [<         0] chi^2    0.1671067651 [  521.199  16.8058 0.00172019  ] 2 [x const chi] 0.498sec
# (levenberg)   26[<1000] 3.0901e-07 [<         0] chi^2    0.1671067651 [  521.199  16.8058 0.00172019  ] 0.736sec
# (levenberg)   27[<1000] 6.1768e-07 [<         0] chi^2    0.1671067651 [  521.199  16.8058 0.00172019  ] 0.343sec
# (levenberg)   28[<1000] 1.2339e-06 [<         0] chi^2    0.1671067651 [  521.199  16.8058 0.00172019  ] 0.344sec
# (levenberg)   29[<1000] 1.8532e-08 [<         0] chi^2    0.1671067651 [  521.199  16.8058 0.00172019  ] 0.376sec
# (levenberg)   30[<1000] 3.7065e-08 [<         0] chi^2    0.1671067651 [  521.199  16.8058 0.00172019  ]  0.34sec
# (levenberg)   31[<1000] 3.7065e-08 [<         0] chi^2    0.1671067651 [  521.199  16.8058 0.00172019  ] 0.344sec
# (levenberg)   32[<1000] 3.7064e-08 [<         0] chi^2    0.1671067651 [  521.199  16.8058 0.00172019  ] 0.337sec
# (levenberg)   33[<1000] 3.7066e-09 [<         0] chi^2    0.1671067651 [  521.199  16.8058 0.00172019  ] 0.356sec
# (levenberg)   34[<1000] 3.7065e-09 [<         0] chi^2    0.1671067651 [  521.199  16.8058 0.00172019  ] 0.347sec
# (levenberg)   35[<1000] 7.4131e-09 [<         0] chi^2    0.1671067651 [  521.199  16.8058 0.00172019  ] 0.335sec
# (levenberg)   36[<1000]  7.413e-09 [<         0] chi^2    0.1671067651 [  521.199  16.8058 0.00172019  ]  0.34sec
# (levenberg)   37[<1000] 7.4131e-10 [<         0] chi^2    0.1671067651 [  521.199  16.8058 0.00172019  ] 0.368sec
# (levenberg)   38[<1000] 1.4826e-09 [<         0] chi^2    0.1671067651 [  521.199  16.8058 0.00172019  ]  0.34sec
# (levenberg)   39[<1000] 1.4826e-09 [<         0] chi^2    0.1671067651 [  521.199  16.8058 0.00172019  ] 0.337sec
# (levenberg)   40[<1000] 1.0919e-10 [<         0] chi^2    0.1671067651 [  521.199  16.8058 0.00172019  ] 1 [x const chi] 0.072sec
# (levenberg)   41[<1000] 3.0684e-09 [<         0] chi^2    0.1671067651 [  521.199  16.8058 0.00172019  ] 0.768sec
# (levenberg)   42[<1000] 6.1369e-13 [<         0] chi^2    0.1671067651 [  521.199  16.8058 0.00172019  ] 1 [x const chi] 0.086sec
# (levenberg)   43[<1000] 3.0684e-12 [<         0] chi^2    0.1671067651 [  521.199  16.8058 0.00172019  ] 2 [x const chi] 0.509sec
# (levenberg)   44[<1000] 3.0684e-12 [<         0] chi^2    0.1671067651 [  521.199  16.8058 0.00172019  ] 3 [x const chi]   0.5sec
# (levenberg)   45[<1000] 3.0684e-12 [<         0] chi^2    0.1671067651 [  521.199  16.8058 0.00172019  ] 4 [x const chi] 0.501sec
# (levenberg)   46[<1000] 8.5611e-05 [<         0] chi^2    0.1671067651 [  521.199  16.8058 0.00172019  ] 5 [x const chi] 0.496sec
# (levenberg)   47[<1000] 3.9178e-09 [<         0] chi^2    0.1671067651 [  521.199  16.8058 0.00172019  ] 6 [x const chi] 0.502sec
# (levenberg)   48[<1000] 3.9178e-09 [<         0] chi^2    0.1671067651 [  521.199  16.8058 0.00172019  ] 7 [x const chi] 0.499sec
# (levenberg)   49[<1000] 8.5611e-05 [<         0] chi^2    0.1671067651 [  521.199  16.8058 0.00172019  ] 8 [x const chi]   0.5sec
Fit|Finished
Fit|Finished|Jacobian Matrix:            0.344sec
Fit|Finished|Covariant Matrix:               0sec
Fit|Finished|Parameter Transfer:             0sec
```

In terminal:
Iterations information


QTISAS - /Users/pipich/Documents/sans/qtikws-documentation/video-manuals/fitting-help/data-cylinder.qti *
Graph1
I[cm⁻¹]
Q[Å⁻¹]
Background should be also fitted
FITTABLE(s)
Save Current Fitting Session
Select Function
Fitting Session
Generate Results
Data
Function
Parameters
Global Limits
Fit - Control
Vary?From..To
Value #1
Error #1
L .. 521.19878 ±19.8251934
R .. 16.8057663 ±0.16661837
I0 .. 1.00819668 ---
bgd .. 0 ---
sldCylinder .. 3E+10 ---
sldSolvent .. -5.6E+09 ---
phi .. 0.00172018583 ±3.52083433...
Auto Simulation
Scale Errors
Save Session
Statistics Notes [after Fit]
Fit
Simulate
χ²/dof= 1.67106765096E-01
Script :: Before Fit
R²= 9.99996984447E-01
Script :: After Fit
time= 2.02E+04 ms - 49 iteration(s)
cylinder-efit
Project Explorer
data-cylinder
Name Type View Created Label
data Table Normal 11/11/15 00:11:19 Simulated Curve
fitCurve-cylinder-efit Table Hidden 26.02.21 16:56 Fitting Curve
fitCurve-cylinder-efit-session Table Hidden 26.02.21 16:56 FIT1D::Settings::Table
Graph1 Graph Maximized 25.02.21 10:29
Results Log
Project Explorer
Helvetica
12
Unicode
black

QTISAS - /Users/pipich/Documents/sans/qtikws-documentation/video-manuals/fitting-help/data-cylinder.qti *

Graph1



FITTABLE(s)

Save Current Fitting Session

Select Function | Fitting Session | Generate Results

Data | Function | Parameters | Global Limits | Fit - Control

	Vary?From..To	Value #1	Error #1
L	..	521.19878	±19.8251934
R	..	16.8057663	±0.16661837
I0	..	1.00813668	---
bgd	..	0	---
sldCylinder	..	3E+10	---
sldSolvent	..	-5.6E+09	---
phi	..	0.00172018583	±3.52083433...

Auto Simulation | Scale Errors | Save Session | Statistics Notes [after Fit]

Fit | Simulate | χ²/dof= 1.67106765096E-01

Script :: Before Fit | R²= 9.99996984447E-01

Script :: After Fit | time= 2.02E+04 ms - 49 iteration(s)

cylinder-efit

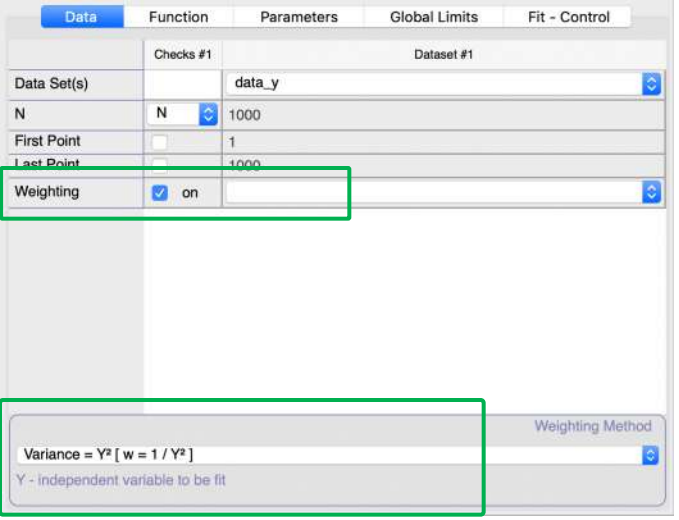
Project Explorer

data-cylinder

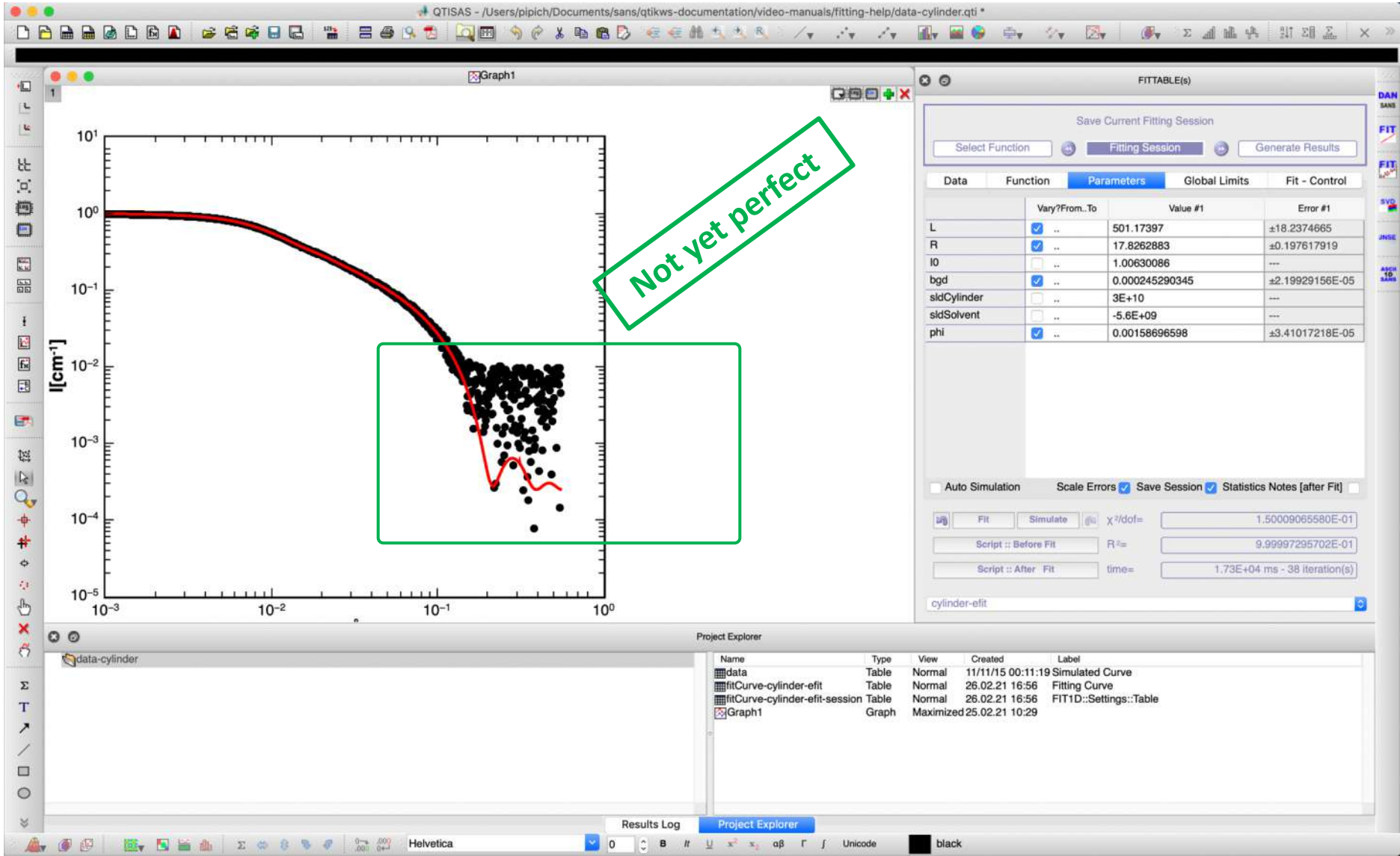
Name	Type	View	Created	Label
data	Table	Normal	11/11/15 00:11:19	Simulated Curve
fitCurve-cylinder-efit	Table	Hidden	26.02.21 16:56	Fitting Curve
fitCurve-cylinder-efit-session	Table	Hidden	26.02.21 16:56	FIT1D::Settings::Table
Graph1	Graph	Maximized	25.02.21 10:29	

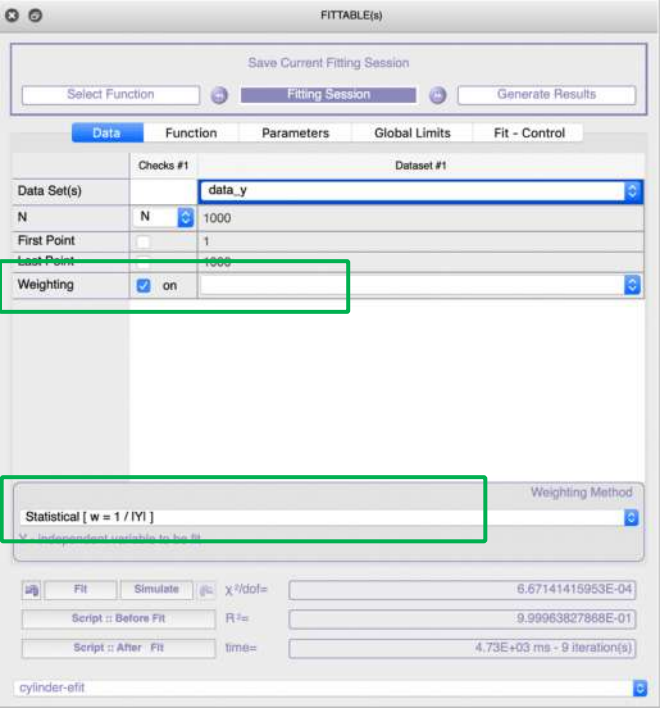
Results Log | Project Explorer

Helvetica 12 Unicode black

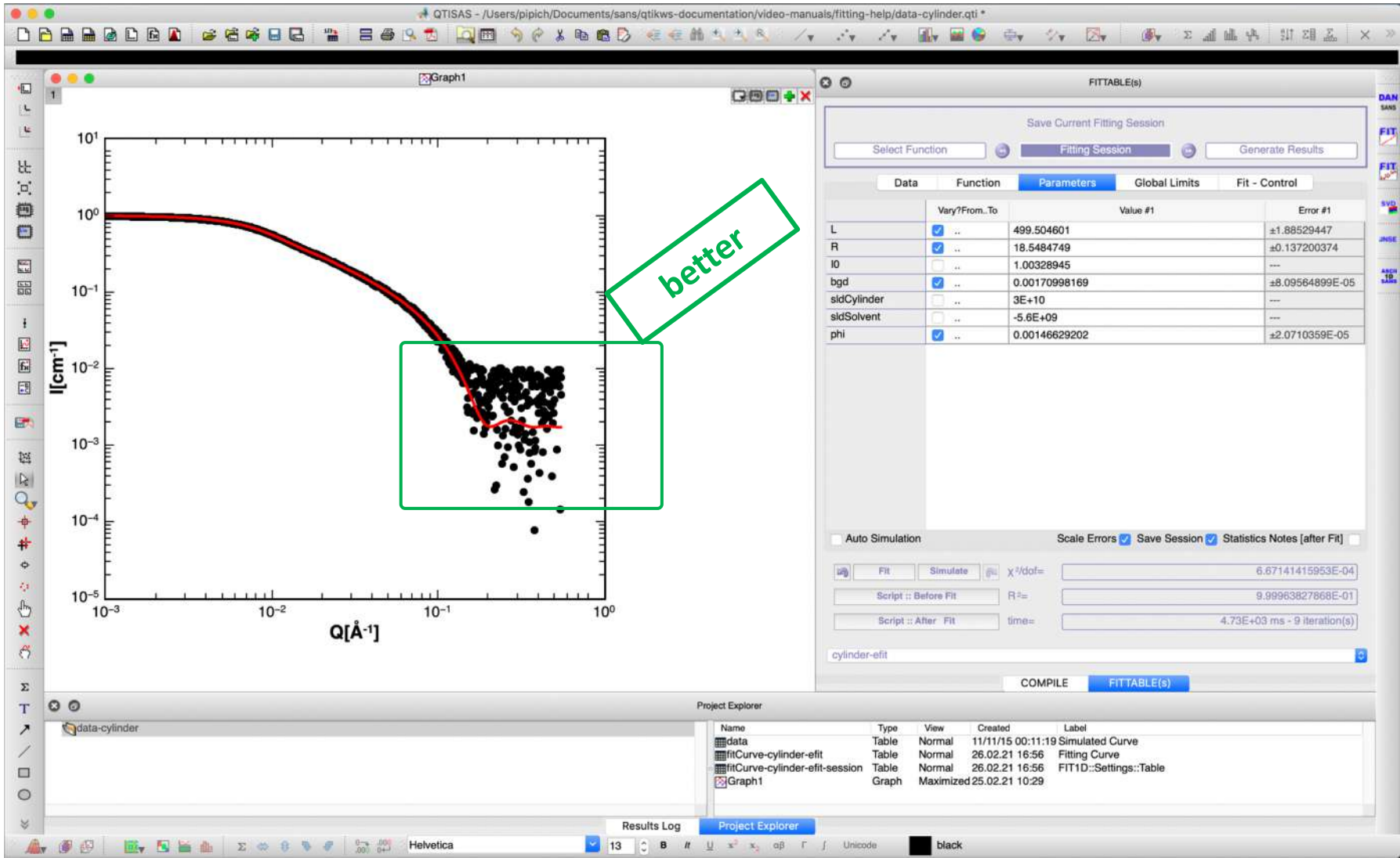

Data
Function
Parameters
Global Limits
Fit - Control
Checks #1
Dataset #1
Data Set(s)
data_y
N
1000
First Point
1
Last Point
1000
Weighting
on
Weighting Method
Variance = Y² [w = 1 / Y²]
Y - independent variable to be fit

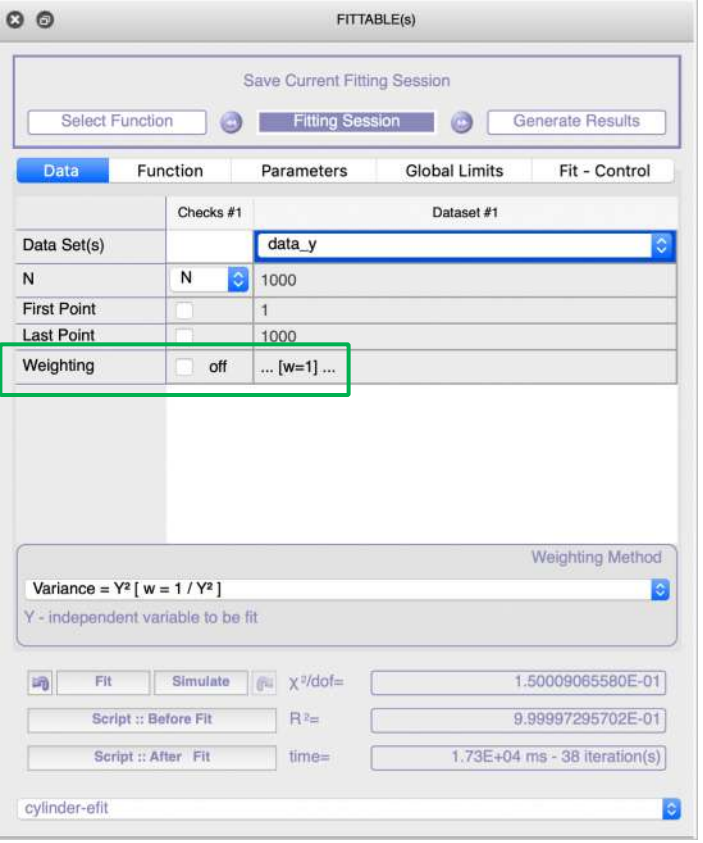

Weighting Method
Variance = Y² [w = 1 / Y²]
Y - independent variable to be fit


QTISAS - /Users/pipich/Documents/sans/qtikws-documentation/video-manuals/fitting-help/data-cylinder.qti *
Graph1
I[cm⁻¹]
Not yet perfect
FITTABLE(s)
Save Current Fitting Session
Select Function
Fitting Session
Generate Results
Data
Function
Parameters
Global Limits
Fit - Control
Vary?From..To
Value #1
Error #1
L
501.17397
±18.2374665
R
17.8262883
±0.197617919
I0
1.00630086
bgd
0.000245290345
±2.19929156E-05
sldCylinder
3E+10
sldSolvent
-5.6E+09
phi
0.00158696598
±3.41017218E-05
Auto Simulation
Scale Errors
Save Session
Statistics Notes [after Fit]
Fit
Simulate
Script :: Before Fit
Script :: After Fit
1.50009065580E-01
9.99997295702E-01
1.73E+04 ms - 38 iteration(s)
cylinder-efit
Project Explorer
data-cylinder
Name
Type
View
Created
Label
data
Table
Normal
11/11/15 00:11:19
Simulated Curve
fitCurve-cylinder-efit
Table
Normal
26.02.21 16:56
Fitting Curve
fitCurve-cylinder-efit-session
Table
Normal
26.02.21 16:56
FIT1D::Settings::Table
Graph1
Graph
Maximized
25.02.21 10:29
Results Log
Project Explorer
Helvetica
Unicode
black

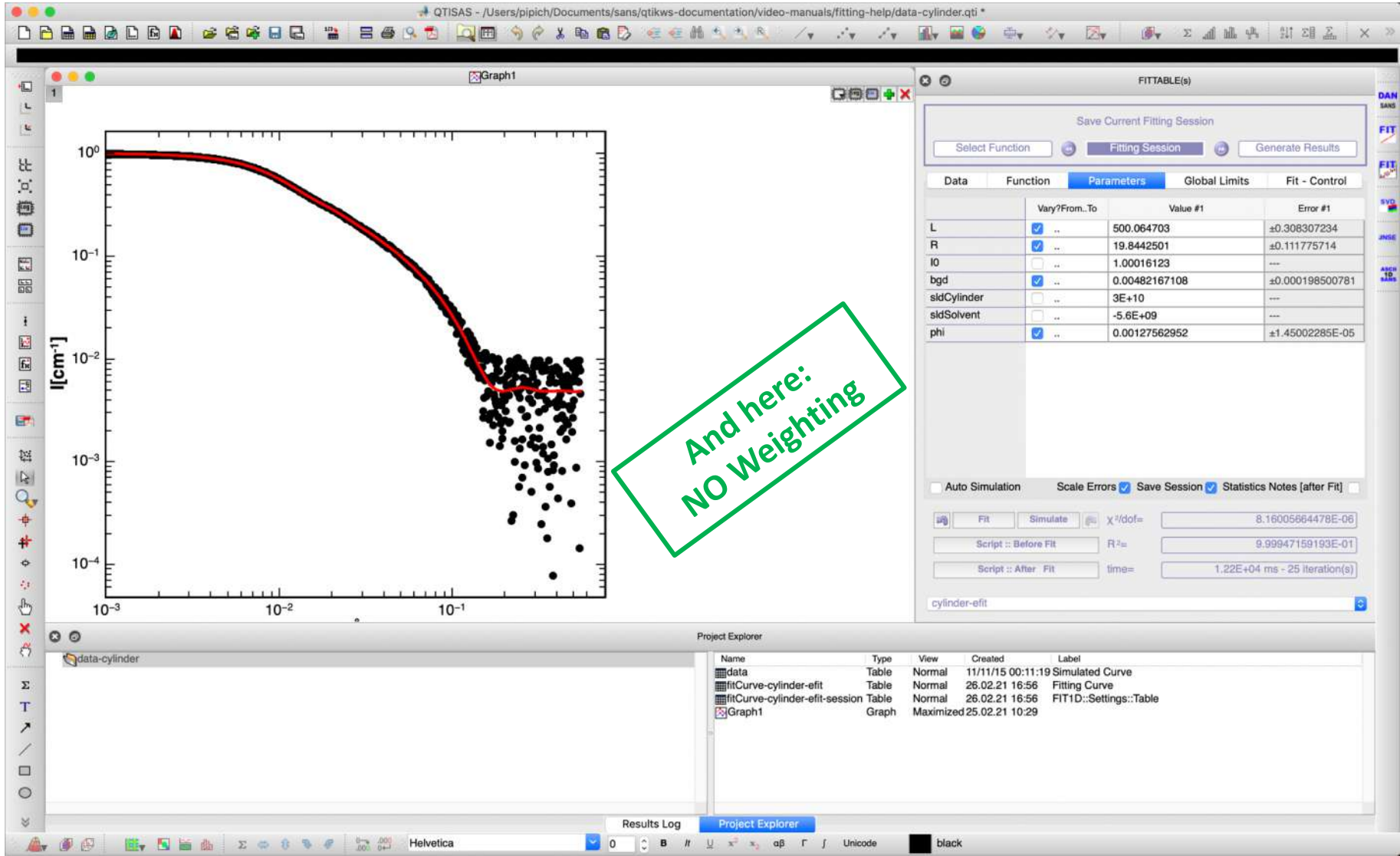

FITTABLE(s)
Save Current Fitting Session
Select Function
Fitting Session
Generate Results
Data
Function
Parameters
Global Limits
Fit - Control
Checks #1
Dataset #1
Data Set(s)
data_y
N
1000
First Point
1
Weighting
on
Weighting Method
Statistical [w = 1 / |Y|]
Fit
Simulate
Script :: Before Fit
Script :: After Fit
6.67141415953E-04
9.99963827868E-01
4.73E+03 ms - 9 iteration(s)
cylinder-efit


Weighting Method
Statistical [w = 1 / |Y|]
Y - independent variable to be fit


QTISAS - /Users/pipich/Documents/sans/qtikws-documentation/video-manuals/fitting-help/data-cylinder.qti *
Graph1
I[cm⁻¹]
Q[Å⁻¹]
better
FITTABLE(s)
Save Current Fitting Session
Select Function
Fitting Session
Generate Results
Data
Function
Parameters
Global Limits
Fit - Control
Vary?From..To
Value #1
Error #1
L
499.504601
±1.88529447
R
18.5484749
±0.137200374
I0
1.00328945
bgd
0.00170998169
±8.09564899E-05
sldCylinder
3E+10
sldSolvent
-5.6E+09
phi
0.00146629202
±2.0710359E-05
Auto Simulation
Scale Errors
Save Session
Statistics Notes [after Fit]
Fit
Simulate
Script :: Before Fit
Script :: After Fit
6.67141415953E-04
9.99963827868E-01
4.73E+03 ms - 9 iteration(s)
cylinder-efit
COMPILE
FITTABLE(s)
Project Explorer
data-cylinder
Name
Type
View
Created
Label
data
Table
Normal
11/11/15 00:11:19
Simulated Curve
fitCurve-cylinder-efit
Table
Normal
26.02.21 16:56
Fitting Curve
fitCurve-cylinder-efit-session
Table
Normal
26.02.21 16:56
FIT1D::Settings::Table
Graph1
Graph
Maximized
25.02.21 10:29
Results Log
Project Explorer
Helvetica
13
black



Weighting	off	... [w=1] ...



QTISAS - /Users/pipich/Documents/sans/qtikws-documentation/video-manuals/fitting-help/data-cylinder.qti *

fitCurve-cylinder-efit - Fitting Curve

	x[X]	y[Y]	weight[yEr]	sigma[xEr]	residues[Y]	Characteristics	Conditions
1	1.000000000E-03	9.980047983E-01	1.000000000E+00	000000000E+00	3.905201662E-03	Fitting Function	-> cylinder-efit
2	1.006340000E-03	9.979164839E-01	1.000000000E+00	000000000E+00	2.123516134E-03	Number of Parameters	-> 7
3	1.012710000E-03	9.978272008E-01	1.000000000E+00	000000000E+00	1.699799198E-03	Time of Simulation	-> 16 ms
4	1.019130000E-03	9.977366586E-01	1.000000000E+00	000000000E+00	-3.422658631E-03	x-Range Source	-> Same x as Fitting Data
5	1.025590000E-03	9.976449868E-01	1.000000000E+00	000000000E+00	3.805013173E-03	x-min	-> 0.001
6	1.032090000E-03	9.975521751E-01	1.000000000E+00	000000000E+00	-3.548175085E-03	x-max	-> 0.55
7	1.038620000E-03	9.974583572E-01	1.000000000E+00	000000000E+00	-9.413571576E-04	Number Points	-> 1000
8	1.045210000E-03	9.973630903E-01	1.000000000E+00	000000000E+00	-2.322090278E-03	Logarithmic Step	-> Yes
9	1.051830000E-03	9.972667963E-01	1.000000000E+00	000000000E+00	-3.044796323E-03	y-min	-> 0
10	1.058490000E-03	9.971693206E-01	1.000000000E+00	000000000E+00	2.581679352E-03	Dataset	-> data_y
11	1.065200000E-03	9.970705050E-01	1.000000000E+00	000000000E+00	1.957495048E-03	N	-> 1000
12	1.071950000E-03	9.969704845E-01	1.000000000E+00	000000000E+00	4.769515508E-03	np	-> 4
13	1.078740000E-03	9.968692486E-01	1.000000000E+00	000000000E+00	-4.542485626E-04	DoF=N-np	-> 996
14	1.085580000E-03	9.967666359E-01	1.000000000E+00	000000000E+00	-1.454635925E-03	chi^2	-> 8.12741641820E-03
15	1.092450000E-03	9.966629358E-01	1.000000000E+00	000000000E+00	4.727064200E-03	chi^2/DoF	-> 8.16005664478E-06
16	1.099380000E-03	9.965576831E-01	1.000000000E+00	000000000E+00	2.614316929E-03	TSS	-> 1.53809468408E+02
17	1.106340000E-03	9.964513210E-01	1.000000000E+00	000000000E+00	3.638678957E-03	R^2=1-chi^2/TSS	-> 9.99947159193E-01
18	1.113350000E-03	9.963435331E-01	1.000000000E+00	000000000E+00	-3.803533081E-03	R=1-sqrt(chi^2/TSS)	-> 9.92730831761E-01
19	1.120410000E-03	9.962343053E-01	1.000000000E+00	000000000E+00	-4.639305291E-03		
20	1.127510000E-03	9.961237798E-01	1.000000000E+00	000000000E+00	4.176220157E-03		
21	1.134650000E-03	9.960119456E-01	1.000000000E+00	000000000E+00	-1.926945567E-03		
22	1.141840000E-03	9.958986332E-01	1.000000000E+00	000000000E+00	1.039366843E-03		
23	1.149070000E-03	9.957839875E-01	1.000000000E+00	000000000E+00	2.217012526E-03		
24	1.156360000E-03	9.956676771E-01	1.000000000E+00	000000000E+00	-2.536771046E-04		
25	1.163680000E-03	9.955501678E-01	1.000000000E+00	000000000E+00	-2.529167815E-03		

Parameters	Values	Errors
L	500.064703	±0.308307234
R	19.8442501	±0.111775714
I0	1.0048088	---
bgd	0.00482167108	±0.000198500781
sldCylinder	3E+10	---
sldSolvent	-5.6E+09	---
phi	0.00127562952	±1.45002285E-05

Structure of “Fitted Curve Table”

Project Explorer

data-cylinder

Fitted Curve:

Name	Type	View	Created	Label
data	Table	Normal	11/11/15 00:11:19	Simulated Curve
fitCurve-cylinder-efit	Table	Maximized	26.02.21 16:56	Fitting Curve
fitCurve-cylinder-efit-session	Table	Normal	26.02.21 16:56	FIT1D::Settings::Table
fitCurve-cylinder-efit-statistics	Note	Normal	01.03.21 15:25	TableFit :: statistics info
Graph1	Graph	Normal	25.02.21 10:29	

Results Log | Project Explorer

Helvetica 13 Unicode

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fitCurve-cylinder-efit-statistics - TableFit :: statistics info

untitled

[01.03.21 15:26]

Using Function: cylinder-efit

The Variance-Covariance Matrix *cov*(i,i):

L	R	bgd	phi	
1.164861404E+04	-4.389593306E+02	1.553618937E+00	3.116928952E-02	l L
-4.389593306E+02	1.531093556E+03	1.921605572E+00	-1.983609284E-01	l R
1.553618937E+00	1.921605572E+00	4.828711602E-03	-2.569529733E-04	l bgd
3.116928952E-02	-1.983609284E-01	-2.569529733E-04	2.576656442E-05	l phi

Values, Errors and Dependences:

Value	Error[$\sqrt{\chi^2/(N-p)} \cdot cov(i,i)$]	Error[$\sqrt{cov(i,i)}$]	Dependency [1-1/*cov*(i,i)/cov'(i,i)]	Name
5.00064703E+02	± 3.08307234E-01	± 1.07928745E+02	8.95476570E-01	l L
1.98442501E+01	± 1.11775714E-01	± 3.91291906E+01	9.99792823E-01	l R
4.82167108E-03	± 1.98500781E-04	± 6.94889315E-02	7.92905420E-01	l bgd
1.27562952E-03	± 1.45002285E-05	± 5.07607766E-03	9.99797988E-01	l phi

χ^2 = 8.12741641820E-03 $\chi^2/(N-p)$ = 8.16005664478E-06 $\chi^2/(N-p)$/Weight = 8.16005664478E-06

Generated "**Statistical Note**"

FITTABLE(s)

Save Current Fitting Session

Select Function | Fitting Session | Generate Results

Data | Function | Parameters | Global Limits | Fit - Control

	Vary?From..To	Value #1	Error #1
L	..	500.064703	±0.308307234
R	..	19.8442501	±0.111775714
I0	..	1.00016123	---
bgd	..	0.00482167108	±0.000198500781
sldCylinder	..	3E+10	---
sldSolvent	..	-5.6E+09	---
phi	..	0.00127562952	±1.45002285E-05

Auto Simulation | Scale Errors | Save Session | Statistics Notes [after Fit]

Fit | Simulate | χ^2/dof= 8.16005664478E-06

Script :: Before Fit | R^2= 9.99947159193E-01

Script :: After Fit | time= 1.23E+04 ms - 26 iteration(s)

cylinder-efit

Project Explorer

data-cylinder

Name	Type	View	Created	Label
data	Table	Normal	11/11/15 00:11:19	Simulated Curve
fitCurve-cylinder-efit	Table	Normal	26.02.21 16:56	Fitting Curve
fitCurve-cylinder-efit-session	Table	Normal	26.02.21 16:56	FIT1D::Settings::Table
fitCurve-cylinder-efit-statistics	Note	Maximized	01.03.21 15:25	TableFit :: statistics info
Graph1	Graph	Normal	25.02.21 10:29	

Results Log | Project Explorer

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QTISAS - /Users/pipich/Documents/sans/qtikws-documentation/video-manuals/fitting-help/data-cylinder.qti *

fitCurve-cylinder-efit-session - FIT1D::Settings::Table

	Parameter	Parameter-Value
27	Session::Parameters::Use::3	0 <
28	Session::Parameters::Values::3	1.00016123 <
29	Session::Parameters::Ranges::3	.. <
30	Session::Parameters::Use::4	1 <
31	Session::Parameters::Values::4	0.00482167108 <
32	Session::Parameters::Ranges::4	.. <
33	Session::Parameters::Use::5	0 <
34	Session::Parameters::Values::5	3E+10 <
35	Session::Parameters::Ranges::5	.. <
36	Session::Parameters::Use::6	0 <
37	Session::Parameters::Values::6	-5.6E+09 <
38	Session::Parameters::Ranges::6	.. <
39	Session::Parameters::Use::7	1 <
40	Session::Parameters::Values::7	0.00127562952 <
41	Session::Parameters::Ranges::7	.. <
42	Session::Parameters::Errors	±0.308307234 ±0.111775714 --- ±0.000198500781 --- --- ±1.45002285E-05 <
43	Session::Fit::SaveSession	yes <
44	Session::Chi2	1.27989808882E-05 <
45	Session::R2	9.99917036421E-01 <
46	Session::Time	1.23E+04 ms - 26 iteration(s) <
47	Simulate::Color	0 <
48	Simulate::Color::Indexing	yes <
49	Simulate::Statistics	yes <
50	S	
51	S	
52	S	
53	Simulate::Uniform::Parameters	0.001 0.55 1000 1 0 <

Automatically saved "**Fitting Session**"

FITTABLE(s)

Save Current Fitting Session

Select Function | Fitting Session | Generate Results

Data | Function | Parameters | Global Limits | Fit - Control

	Vary?From..To	Value #1	Error #1
L	☑ ..	500.064703	±0.308307234
R	☑ ..	19.8442501	±0.111775714
I0	☐ ..	1.00016123	---
bgd	☑ ..	0.00482167108	±0.000198500781
sldCylinder	☐ ..	3E+10	---
sldSolvent	☐ ..	-5.6E+09	---
phi	☑ ..	0.00127562952	±1.45002285E-05

Auto Simulation | Scale Errors ☑ | Save Session ☑ | Statistics Notes [after Fit] ☑

Fit | Simulate | χ^2/dof= 8.16005664478E-06

Script :: Before Fit | R= 9.99947159193E-01

Script :: After Fit | time= 1.23E+04 ms - 26 iteration(s)

cylinder-efit

Project Explorer

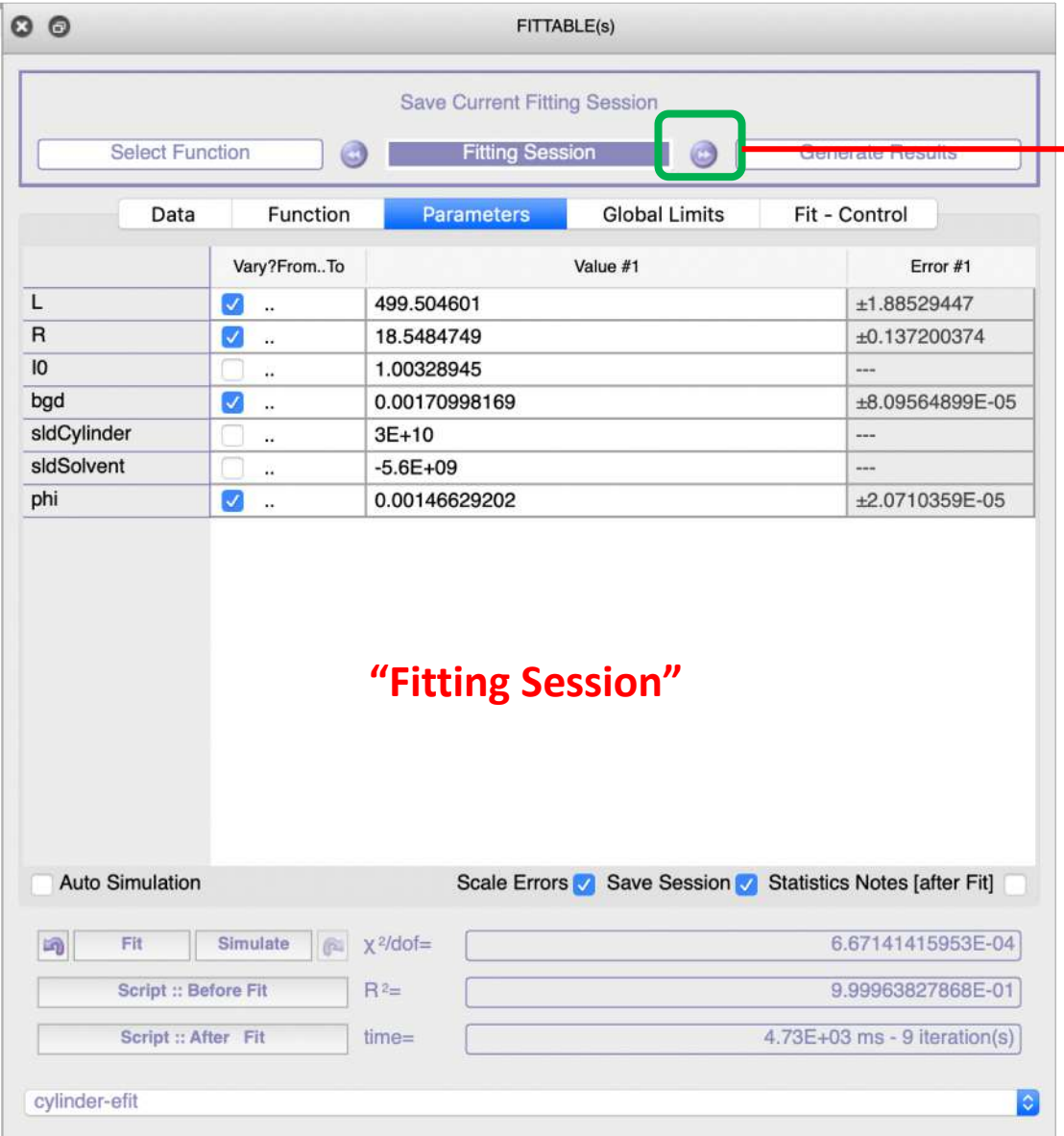
data-cylinder

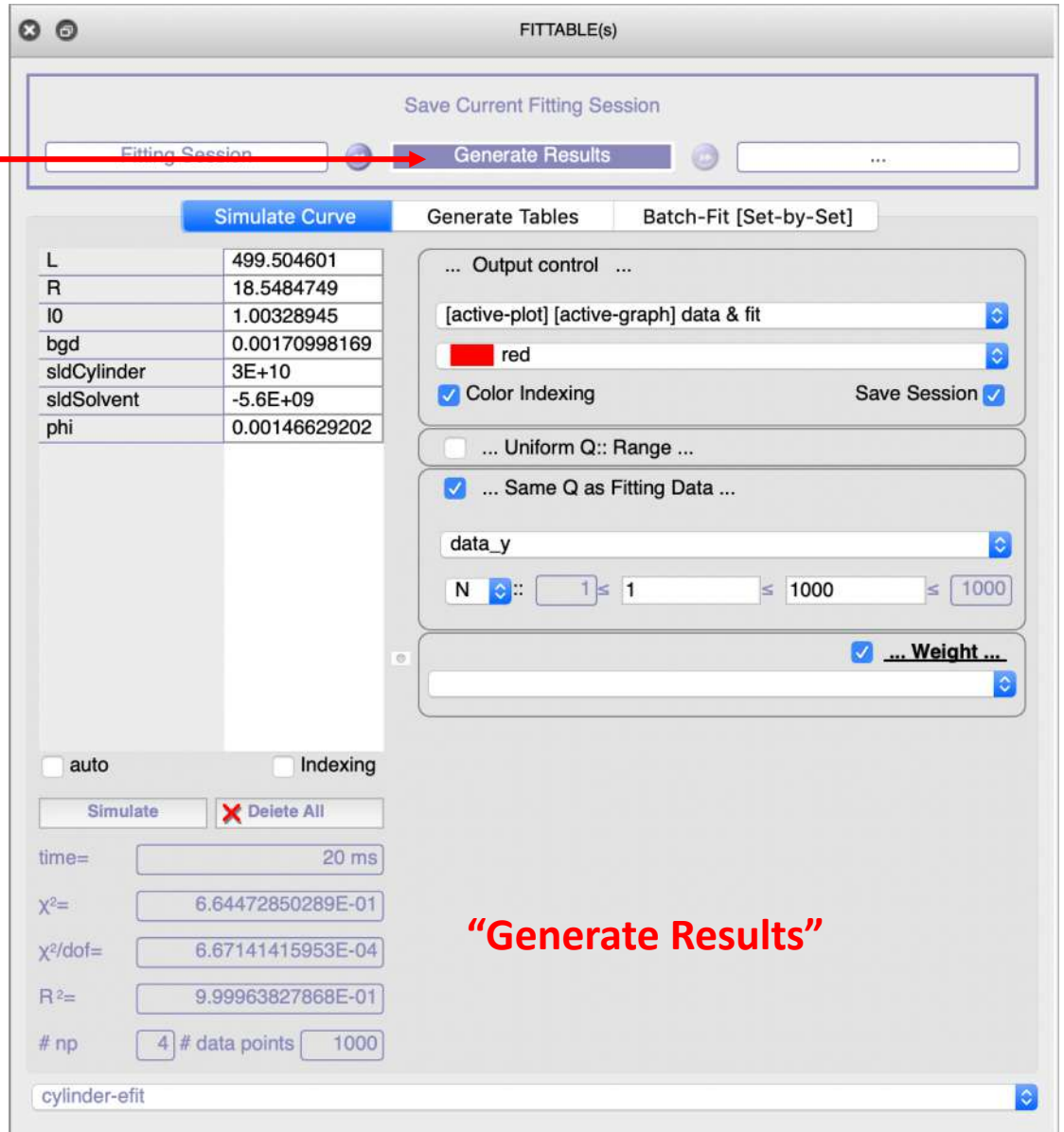
Name	Type	View	Created	Label
data	Table	Normal	11/11/15 00:11:19	Simulated Curve
fitCurve-cylinder-efit	Table	Normal	26.02.21 16:56	Fitting Curve
fitCurve-cylinder-efit-session	Table	Maximized	26.02.21 16:56	FIT1D::Settings::Table
fitCurve-cylinder-efit-statistics	Note	Normal	01.03.21 15:25	TableFit :: statistics info
Graph1	Graph	Normal	25.02.21 10:29	

Results Log | Project Explorer

Helvetica 13 Unicode

Step 4 [optional]: Push Button “next” to go to “**Generate Results**”

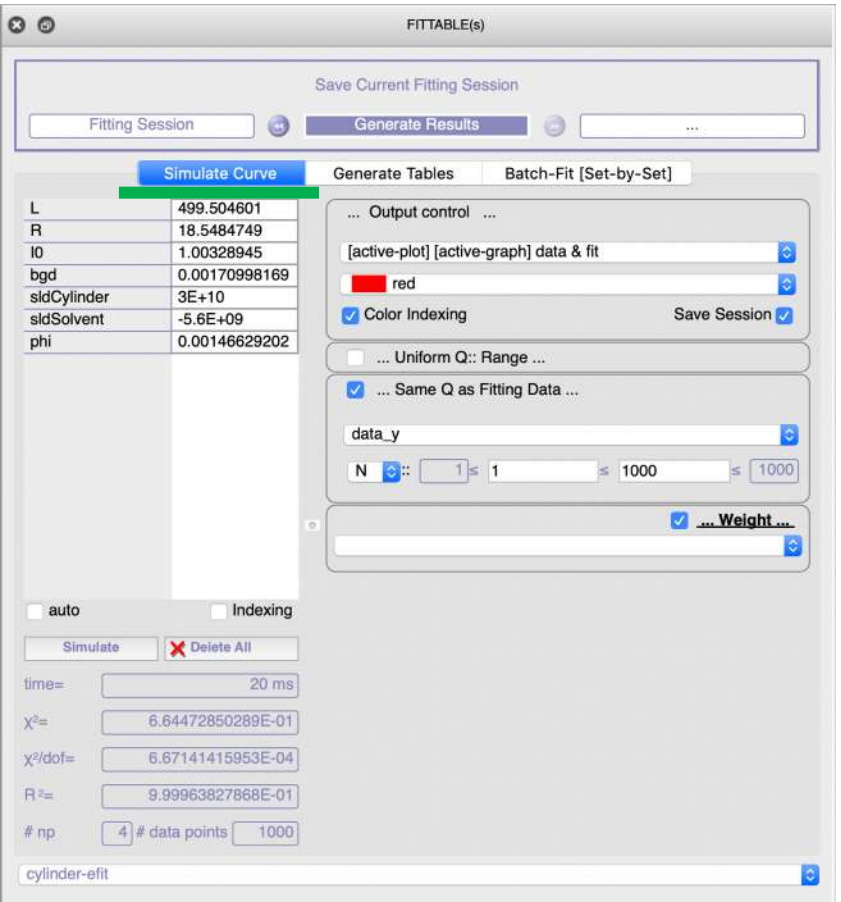


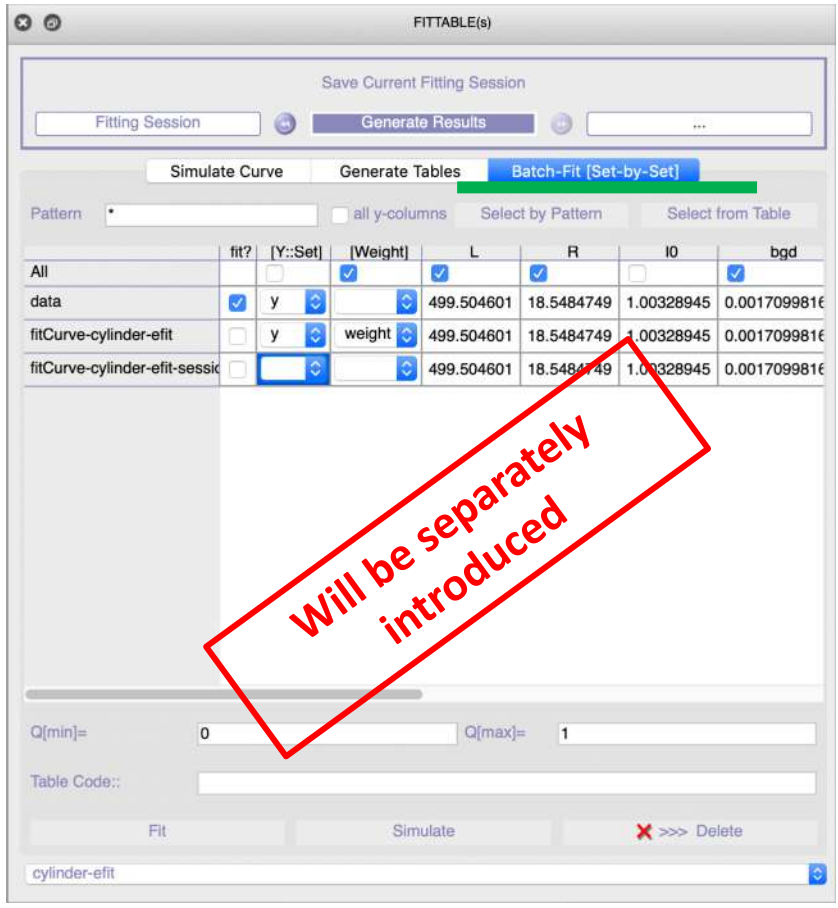


1. “**Simulate Curve**” interface

2. “**Generate Tables**” interface

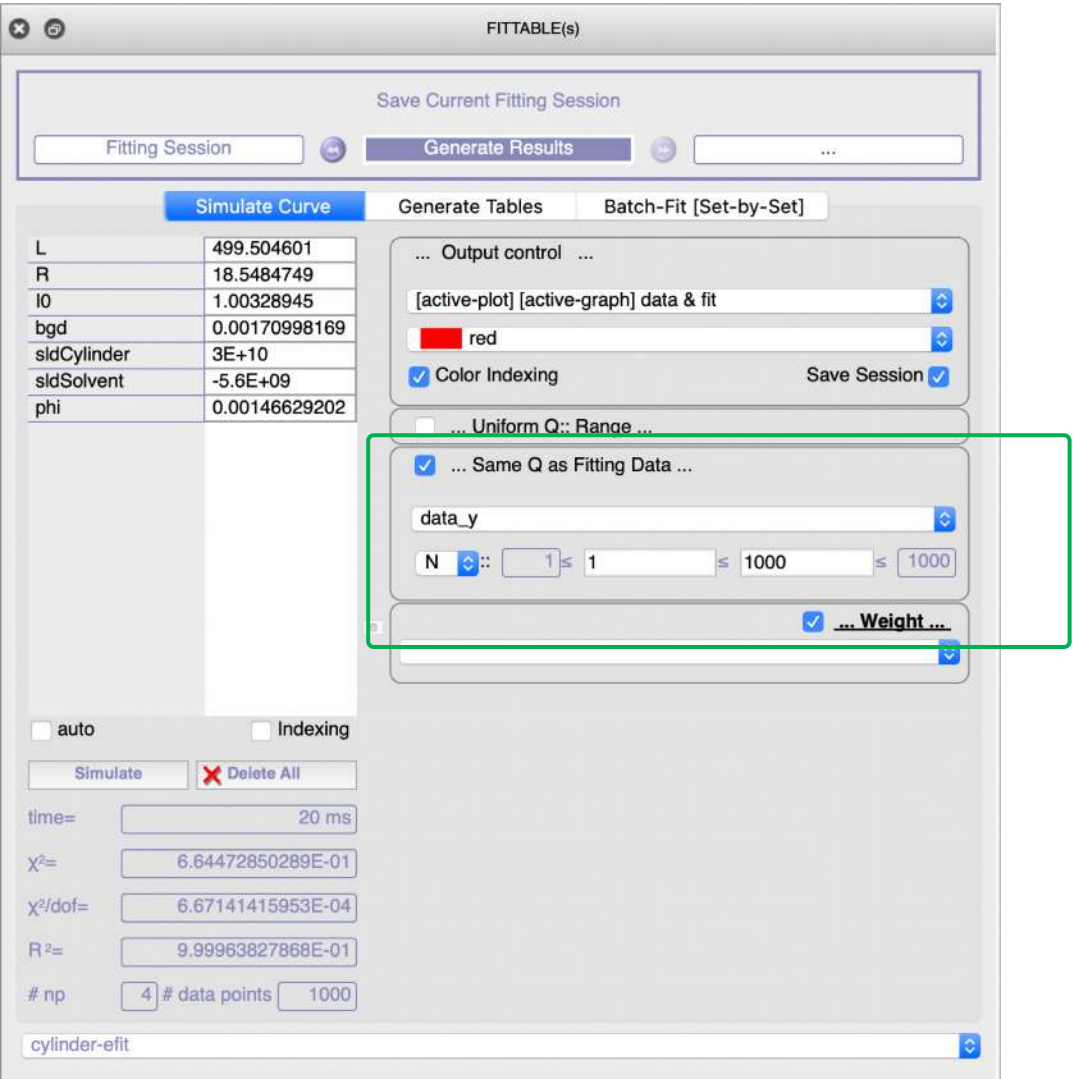
3. “**Batch-Fit**” interface



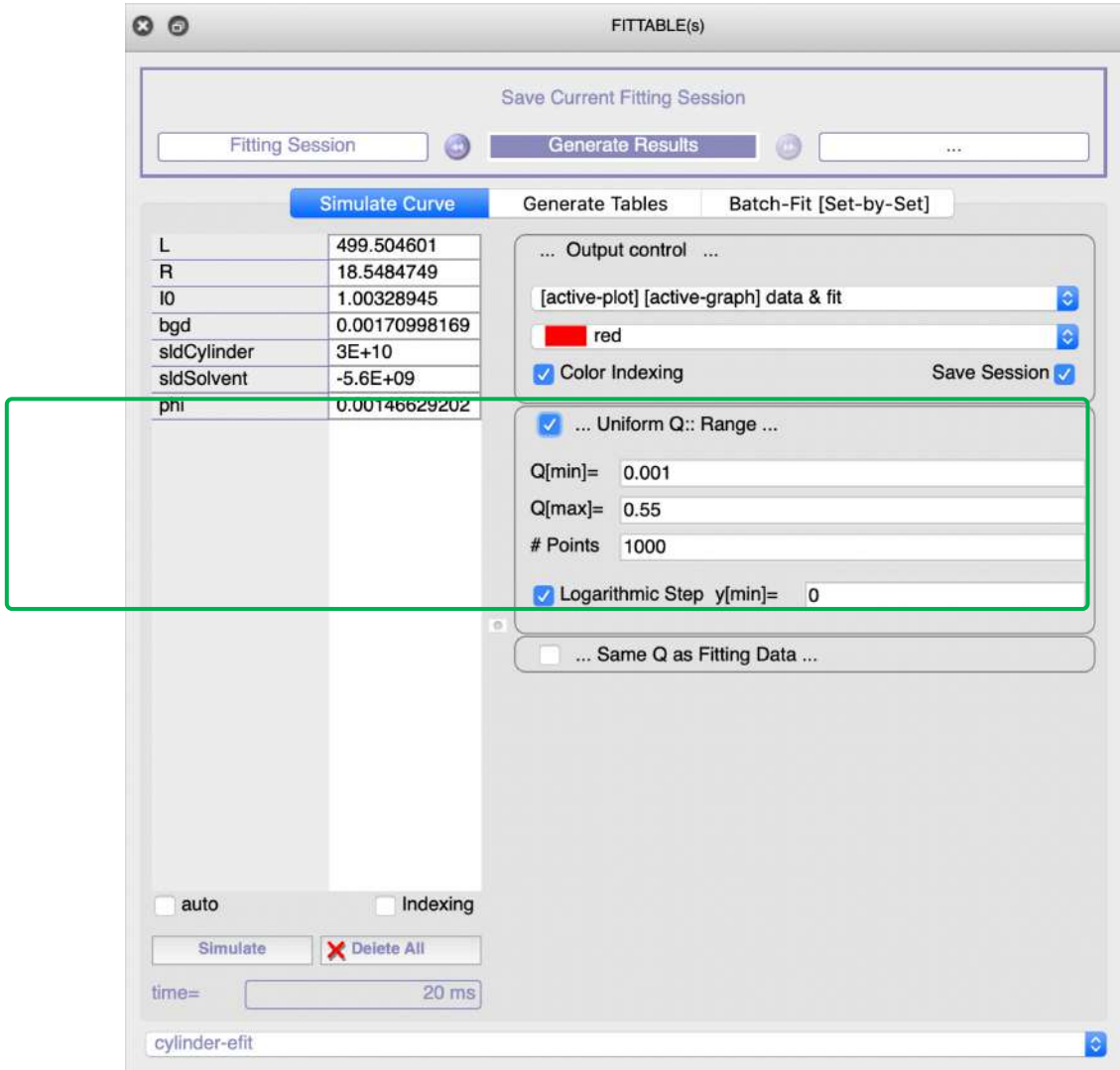


1. “**Simulate Curve**” interface

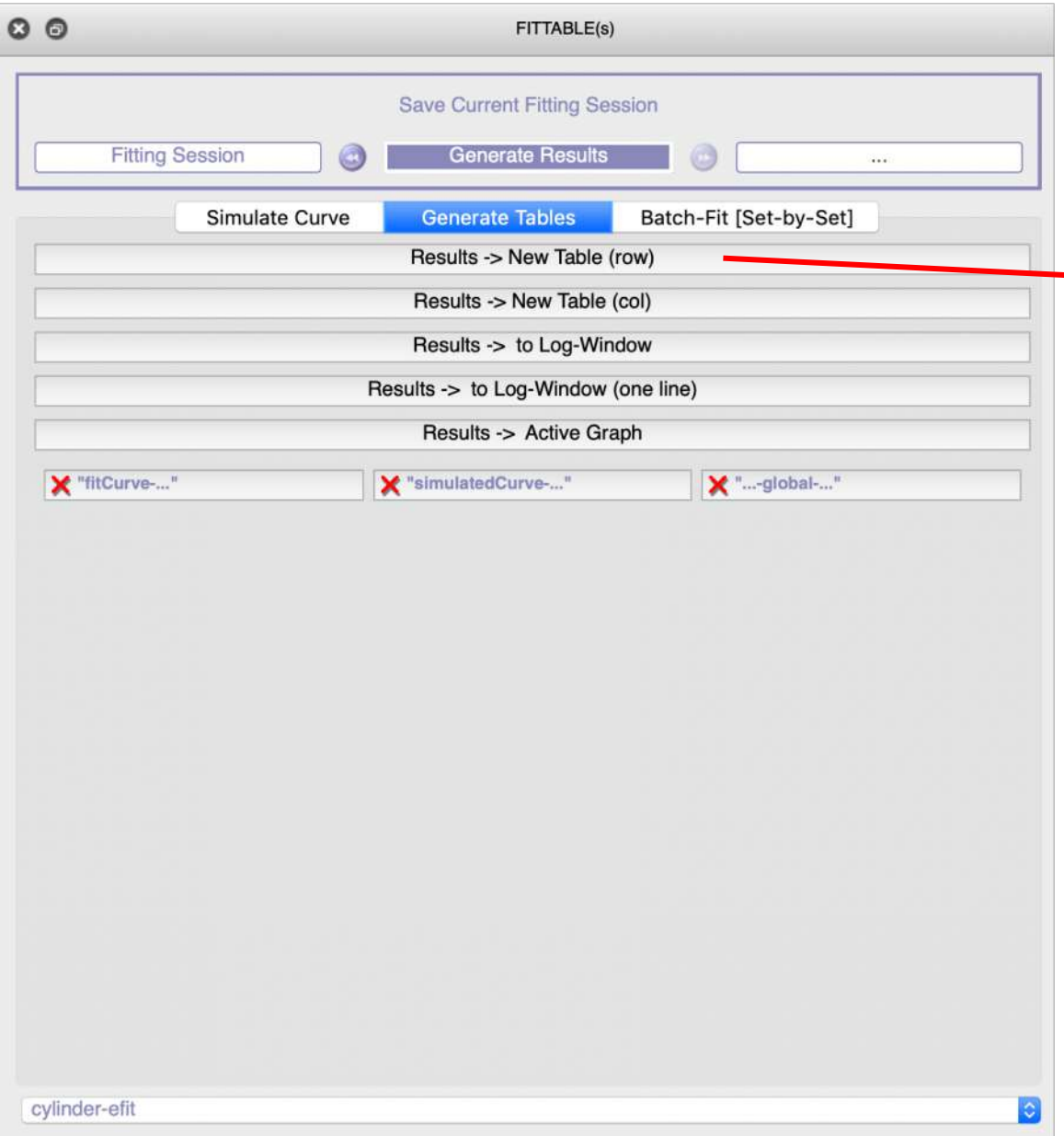
1.1 “**… Same Q/x :: Range …**”



1.2 “**… Uniform Q/x :: Range …**”



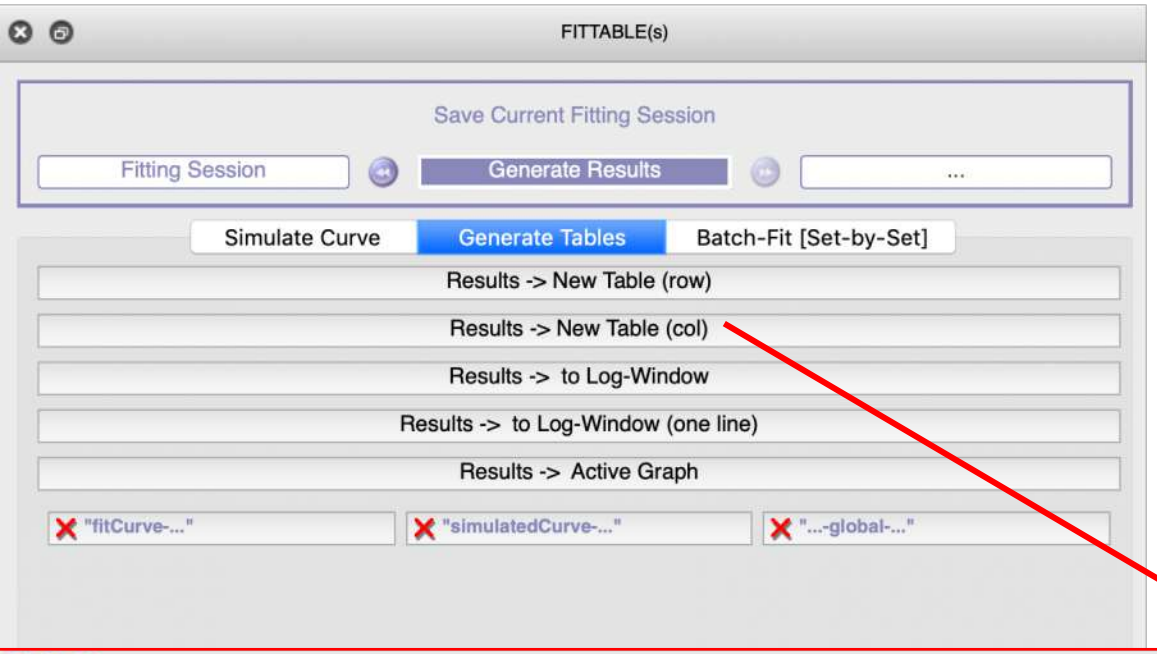
2. “**Generate Tables**” interface



newFitTableRowcylinder-efit1

	Characteristics[X]	Conditions[Y]	Parameters[Y]	Value01[Y]	Error01[Y]
1	Fitting Function	-> cylinder-efit	L	499.504601	1.88529447
2	Number of Parameters	-> 7	R	18.5484749	0.137200374
3	Number of data sets M	-> 1	I0	1.00328945	---
4	chi^2	-> 6.67141415953E-04	bgd	0.00170998169	8.09564899E-05
5	R^2	-> 9.99963827868E-01	sldCylinder	3E+10	---
6	Time of Fit	-> 4.73E+03 ms - 9 iteration(s)	sldSolvent	-5.6E+09	---
7			phi	0.00146629202	2.0710359E-05

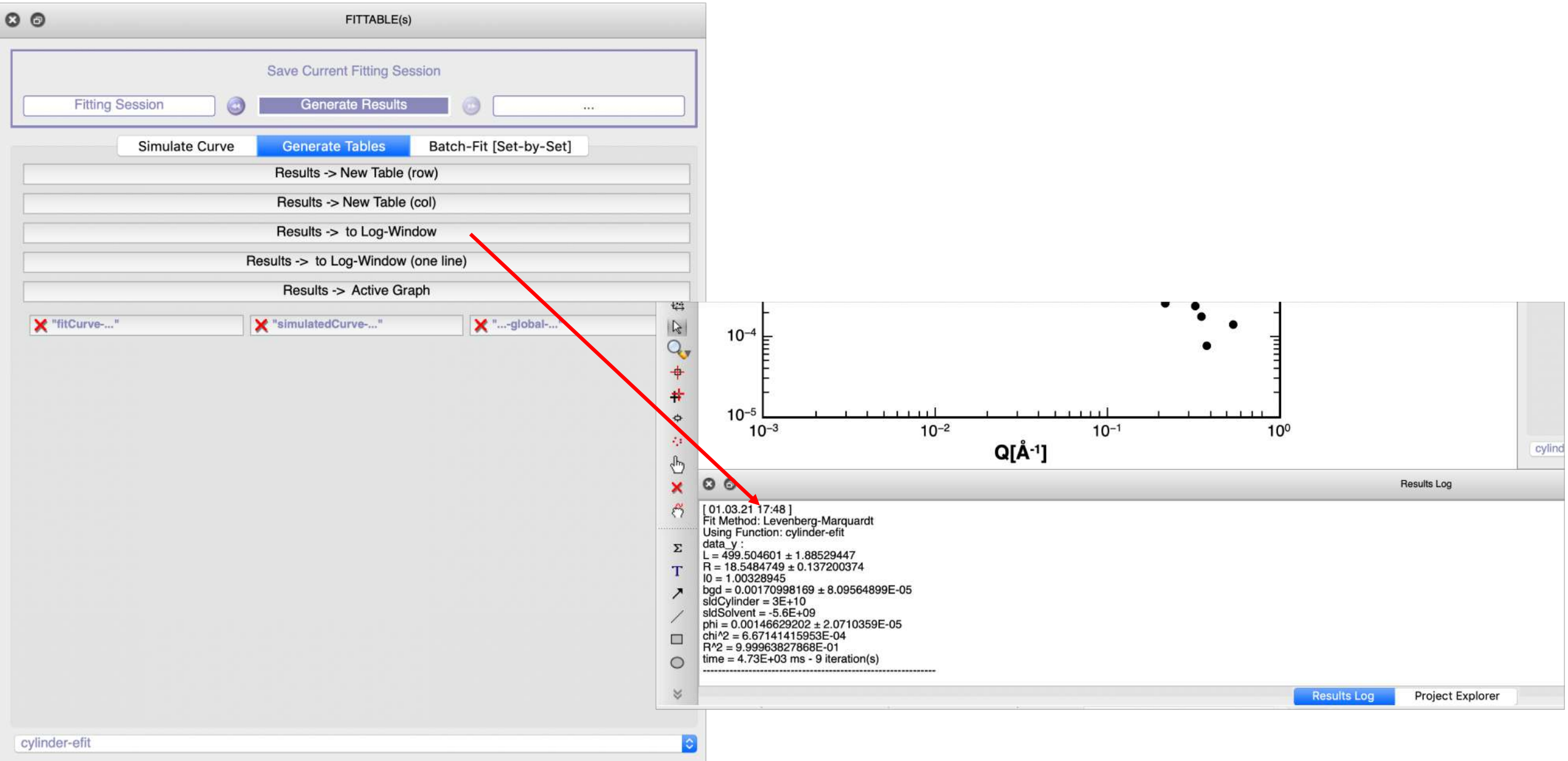
2. “**Generate Tables**” interface



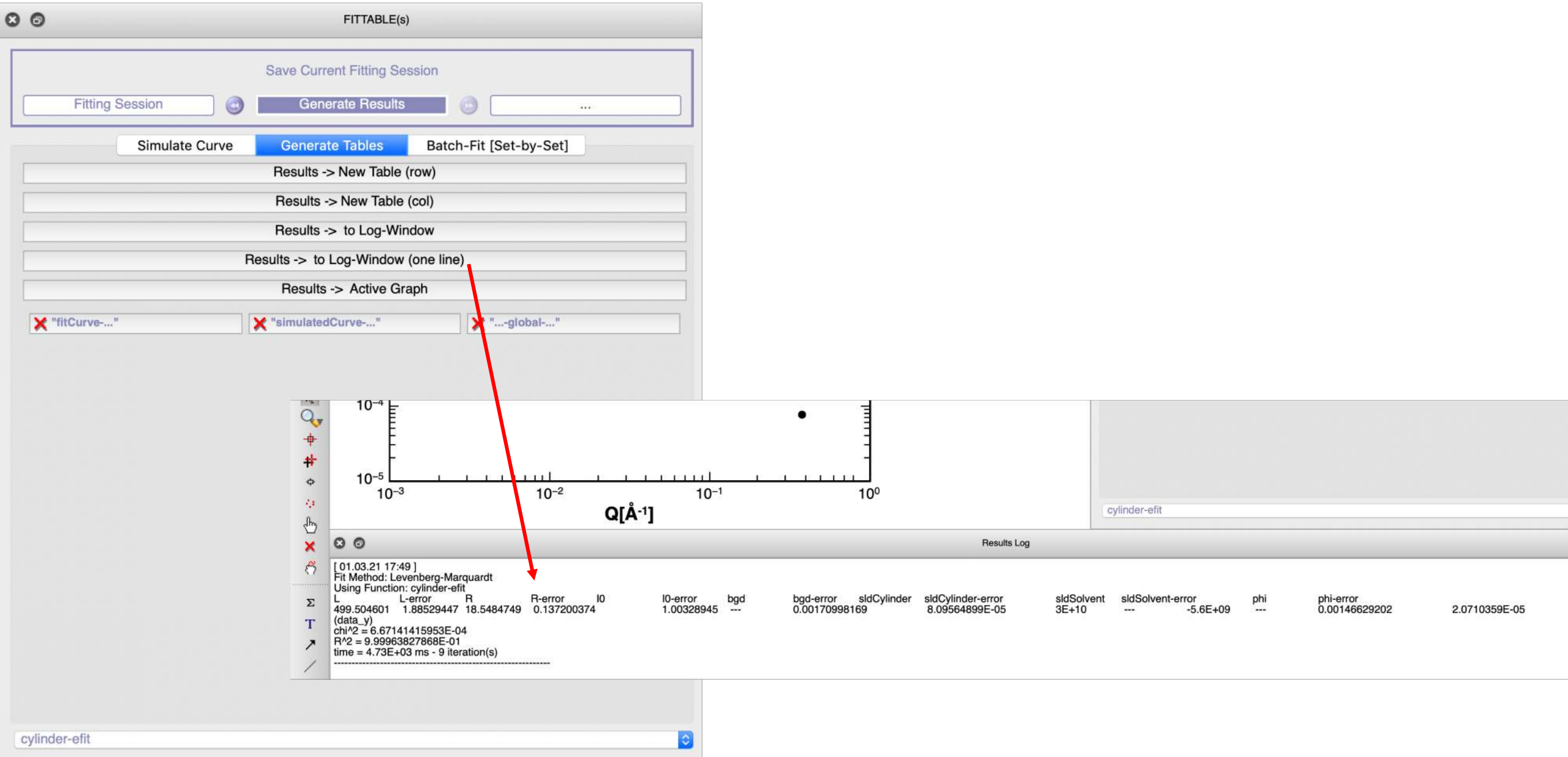
newFitTableColcylinder-efit1

	Characteristics	Conditions	Nr[X]	L[Y]	LError[yEr]	R[Y]	RError[yEr]	I0[Y]	I0Error[yEr]	bgd[Y]	bgdError[yEr]	sldCylinder[Y]	sldCylinderError[yEr]
1	Fitting Function	-> cylinder-efit	1	499.504601	1.88529447	18.5484749	0.137200374	1.00328945	---	0.00170998169	8.09564899E-05	3E+10	---
2	Number of Parameters	-> 7											
3	Number of data sets M	-> 1											
4	chi^2	-> 6.67141415953E-04											
5	R^2	-> 9.99963827868E-01											
6	Time of Fit	-> 4.73E+03 ms - 9 iteration(s)											

2. “**Generate Tables**” interface



2. “**Generate Tables**” interface



2. “**Generate Tables**” interface