

# MuScatt@QtiSAS

MuScatt: Multiple Scattering Program for Small Angle Scattering [Henrich Frielinghaus]

Integration of MuScatt c-code to Fitting interface of QtiSAS

(Fit-Compile & Fit-Table)

**Vitaliy Pipich**

<https://jugit.fz-juelich.de/sans/muscatt>

SANS > MuScatt > Details

**MuScatt** Project ID: 425

☆ Star 0 Clone

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Multiple Scattering Program for Small Angle Scattering Data

master muscatt History Find file

**README.md and paper.md changed**  
Frielinghaus, Henrich authored 6 months ago adeb7c79

README

Name	Last commit	Last update
.DS_Store	Initial commit	6 months ago
Makefile	Initial commit	6 months ago
MakefileSP	Initial commit	6 months ago
MuScatt.c	Initial commit	6 months ago
README.md	README.md and paper.md changed	6 months ago
alloc.c	Initial commit	6 months ago
alloc.h	Initial commit	6 months ago
data12t1.DAT	Initial commit	6 months ago
data12t2.DAT	Initial commit	6 months ago

MuScatt

<https://www.qtisas.com/download>

Trace: • compile • **downloads**

installation instructions: [Windows](#) [MacOS](#) [Linux](#) [Windows-no-installation](#)

Read installation instructions

## QtISAS: Download Page

Binary for MAC, WINDOWS, LINUX plus SOURCE

>= 29.10.2019

[17 FEB 2021] Binaries	
Windows	<a href="#">win</a> <a href="#">win-no-installation-needed</a>
MacOS	<a href="#">mac</a>
Linux	<a href="#">linux</a>
Source	<a href="#">source</a>

Download Executable Binary of QtISAS

# MuScatt: Input files

## “Control” File:

```
parPolyRes.dat.txt
dataPolyRes.dat filename of data file
1 switch for lowQ extrapolation: 0 automatic, 1 guinier, 2 power law, 3 constant
-1 switch for incoherent background subtraction: -1 none, 0 automatic, (real)value>0
gives exact level to be subtracted
5.0 lambda (Angstrom), negative or zero will set lambda to 5.0
0.1 d, sample thickness in cm, negative or zero will set d to 0.1
0.900 experimental transmission as measured
0.001 sigma due to incoherent scattering and absorption, calculated from table (will be
divided by 4pi for full 3d angle)
0 high q extrapolation (0 for off, 1 for on)
0.0689 q range from which pure power law is achieved
0 resolution mode #n (-1 is off, 0 for no combination), combines with DEMUX/MUX
calculation of type #n (1-6)
0.1 fraction of lambda resolution at fwhm, i.e. delta lambda / lambda
8.0 detector distance [m] for lowest Q measurements
0.01 sample aperture [m]
8.0 collimation distance [m] for lowest Q measurements, negative values if not
specified (symmetric setting)
0.03 entrance aperture [m], negative values if not specified (symmetric setting)
2.0 resolution cutoff (in terms of multiples of sigma)
0 thickness correction mode #n (<=0 is off, combines with DEMUX/MUX calculation of
type #n (1-6) and (7-12) for (1-6) with resolution correction
```

## “data” File [Q I dI]:

```
dataPolyRes.dat.txt
0.00775 441.15 4.4115
0.00861 428.668 4.28668
0.00947 415.23 4.1523
0.01033 400.932 4.00932
0.01119 385.878 3.85878
0.01205 370.172 3.70172
0.01291 353.922 3.53922
0.01377 337.236 3.37236
0.01463 320.224 3.20224
0.01549 302.995 3.02995
0.01635 285.655 2.85655
0.01721 268.309 2.68309
0.01807 251.056 2.51056
0.01893 233.992 2.33992
0.01979 217.207 2.17207
0.02066 200.783 2.00783
0.02152 184.799 1.84799
0.02238 169.326 1.69326
0.02324 154.422 1.54422
0.0241 140.145 1.40145
```

$N_Q$



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# MuScatt: Output file

outPolyRes.txt

7.7500e-03	4.3412e+02	4.3145e+00	6.0344e+02	4.2775e+00	4.3209e+02	4.2775e+00	4.4481e+02	4.5130e+00	6.2426e+02	4.5541e+00	4.4699e+02	4.5541e+00	4.4457e+02	1.2965e+01	0.0000e+00	0.0000e+00
8.6100e-03	4.2163e+02	4.1924e+00	5.8604e+02	4.1565e+00	4.1963e+02	4.1565e+00	4.3214e+02	4.3853e+00	6.0651e+02	4.4252e+00	4.3429e+02	4.4252e+00	4.3178e+02	1.6524e+01	0.0000e+00	0.0000e+00
9.4700e-03	4.0822e+02	4.0610e+00	5.6737e+02	4.0262e+00	4.0626e+02	4.0262e+00	4.1854e+02	4.2478e+00	5.8746e+02	4.2865e+00	4.2065e+02	4.2865e+00	4.1805e+02	1.8835e+01	0.0000e+00	0.0000e+00
1.0330e-02	3.9394e+02	3.9211e+00	5.4748e+02	3.8876e+00	3.9202e+02	3.8876e+00	4.0406e+02	4.1015e+00	5.6718e+02	4.1389e+00	4.0612e+02	4.1389e+00	4.0341e+02	1.9854e+01	0.0000e+00	0.0000e+00
1.1190e-02	3.7894e+02	3.7739e+00	5.2659e+02	3.7416e+00	3.7706e+02	3.7416e+00	3.8884e+02	3.9475e+00	5.4587e+02	3.9835e+00	3.9086e+02	3.9835e+00	3.8802e+02	1.9943e+01	0.0000e+00	0.0000e+00
1.2050e-02	3.6330e+02	3.6203e+00	5.0482e+02	3.5893e+00	3.6147e+02	3.5893e+00	3.7297e+02	3.7869e+00	5.2364e+02	3.8214e+00	3.7495e+02	3.8214e+00	3.7196e+02	1.9221e+01	0.0000e+00	0.0000e+00
1.2910e-02	3.4715e+02	3.4614e+00	4.8233e+02	3.4317e+00	3.4537e+02	3.4317e+00	3.5658e+02	3.6206e+00	5.0068e+02	3.6536e+00	3.5851e+02	3.6536e+00	3.5537e+02	1.8469e+01	0.0000e+00	0.0000e+00
1.3770e-02	3.3058e+02	3.2982e+00	4.5925e+02	3.2700e+00	3.2884e+02	3.2700e+00	3.3976e+02	3.4499e+00	4.7711e+02	3.4814e+00	3.4163e+02	3.4814e+00	3.3835e+02	1.7691e+01	0.0000e+00	0.0000e+00
1.4630e-02	3.1370e+02	3.1318e+00	4.3574e+02	3.1050e+00	3.1201e+02	3.1050e+00	3.2261e+02	3.2759e+00	4.5309e+02	3.3057e+00	3.2443e+02	3.3057e+00	3.2100e+02	1.6891e+01	0.0000e+00	0.0000e+00
1.5490e-02	2.9662e+02	2.9633e+00	4.1196e+02	2.9379e+00	2.9498e+02	2.9379e+00	3.0526e+02	3.0996e+00	4.2879e+02	3.1279e+00	3.0703e+02	3.1279e+00	3.0345e+02	1.6075e+01	0.0000e+00	0.0000e+00
1.6350e-02	2.7944e+02	2.7937e+00	3.8804e+02	2.7698e+00	2.7785e+02	2.7698e+00	2.8780e+02	2.9223e+00	4.0433e+02	2.9489e+00	2.8951e+02	2.9489e+00	2.8579e+02	1.5247e+01	0.0000e+00	0.0000e+00
1.7210e-02	2.6227e+02	2.6241e+00	3.6414e+02	2.6016e+00	2.6074e+02	2.6016e+00	2.7035e+02	2.7448e+00	3.7988e+02	2.7698e+00	2.7201e+02	2.7698e+00	2.6811e+02	1.4407e+01	0.0000e+00	0.0000e+00
1.8070e-02	2.4520e+02	2.4553e+00	3.4038e+02	2.4343e+00	2.4373e+02	2.4343e+00	2.5300e+02	2.5683e+00	3.5557e+02	2.5917e+00	2.5460e+02	2.5917e+00	2.5052e+02	1.3563e+01	0.0000e+00	0.0000e+00
1.8930e-02	2.2833e+02	2.2885e+00	3.1690e+02	2.2689e+00	2.2691e+02	2.2689e+00	2.3584e+02	2.3937e+00	3.3152e+02	2.4155e+00	2.3738e+02	2.4155e+00	2.3315e+02	1.2720e+01	0.0000e+00	0.0000e+00
1.9790e-02	2.1180e+02	2.1243e+00	2.9389e+02	2.1061e+00	2.1044e+02	2.1061e+00	2.1902e+02	2.2220e+00	3.0794e+02	2.2423e+00	2.2050e+02	2.2423e+00	2.1620e+02	1.1887e+01	0.0000e+00	0.0000e+00
2.0660e-02	1.9555e+02	1.9637e+00	2.7127e+02	1.9469e+00	1.9424e+02	1.9469e+00	2.0247e+02	2.0540e+00	2.8474e+02	2.0727e+00	2.0389e+02	2.0727e+00	1.9958e+02	1.1060e+01	0.0000e+00	0.0000e+00
2.1520e-02	1.7980e+02	1.8073e+00	2.4936e+02	1.7919e+00	1.7855e+02	1.7919e+00	1.8643e+02	1.8905e+00	2.6226e+02	1.9077e+00	1.8779e+02	1.9077e+00	1.8342e+02	1.0259e+01	0.0000e+00	0.0000e+00
2.2380e-02	1.6456e+02	1.6560e+00	2.2815e+02	1.6418e+00	1.6336e+02	1.6418e+00	1.7089e+02	1.7322e+00	2.4047e+02	1.7480e+00	1.7219e+02	1.7480e+00	1.6771e+02	9.4781e+00	0.0000e+00	0.0000e+00
2.3240e-02	1.4988e+02	1.5103e+00	2.0773e+02	1.4973e+00	1.4875e+02	1.4973e+00	1.5593e+02	1.5797e+00	2.1949e+02	1.5941e+00	1.5717e+02	1.5941e+00	1.5258e+02	8.7174e+00	0.0000e+00	0.0000e+00
2.4100e-02	1.3585e+02	1.3706e+00	1.8820e+02	1.3589e+00	1.3476e+02	1.3589e+00	1.4160e+02	1.4337e+00	1.9940e+02	1.4467e+00	1.4278e+02	1.4467e+00	1.3812e+02	7.9794e+00	0.0000e+00	0.0000e+00
2.4960e-02	1.2248e+02	1.2376e+00	1.6961e+02	1.2270e+00	1.2145e+02	1.2270e+00	1.2794e+02	1.2945e+00	1.8025e+02	1.3063e+00	1.2907e+02	1.3063e+00	1.2436e+02	7.2647e+00	0.0000e+00	0.0000e+00
2.5820e-02	1.0982e+02	1.1115e+00	1.5200e+02	1.1020e+00	1.0884e+02	1.1020e+00	1.1500e+02	1.1626e+00	1.6210e+02	1.1732e+00	1.1607e+02	1.1732e+00	1.1135e+02	6.5803e+00	0.0000e+00	0.0000e+00
2.6680e-02	9.7895e+01	9.9260e-01	1.3543e+02	9.8410e-01	9.6974e+01	9.8410e-01	1.0281e+02	1.0383e+00	1.4499e+02	1.0477e+00	1.0382e+02	1.0477e+00	9.9100e+01	5.9284e+00	0.0000e+00	0.0000e+00
2.7540e-02	8.6730e+01	8.8116e-01	1.1991e+02	8.7362e-01	8.5860e+01	8.7362e-01	9.1010e+01	9.1010e+01	1.2894e+02	9.3010e-01	9.2327e+01	9.3010e-01	8.7632e+01	5.3108e+00	0.0000e+00	0.0000e+00
2.8400e-02	7.6336e+01	7.7733e-01	1.0546e+02	7.7067e-01	7.5516e+01	7.7067e-01	8.0010e+01	8.0010e+01	1.1398e+02	8.2050e-01	8.1616e+01	8.2050e-01	7.6961e+01	4.7291e+00	0.0000e+00	0.0000e+00
2.9260e-02	6.6720e+01	6.8112e-01	9.2102e+01	6.7529e-01	6.5949e+01	6.7529e-01	7.0010e+01	7.0010e+01	1.0012e+02	7.1895e-01	7.1691e+01	7.1895e-01	6.7094e+01	4.4067e+00	0.0000e+00	0.0000e+00
3.0120e-02	5.7874e+01	5.9255e-01	7.9815e+01	5.8748e-01	5.7151e+01	5.8748e-01	6.1010e+01	6.1010e+01	8.7350e+01	6.2546e-01	6.2547e+01	6.2546e-01	5.8025e+01	3.8816e+00	0.0000e+00	0.0000e+00
3.0980e-02	4.9795e+01	5.1154e-01	6.8595e+01	5.0716e-01	4.9117e+01	5.0716e-01	5.3010e+01	5.3010e+01	7.5663e+01	5.3994e-01	5.4178e+01	5.3994e-01	4.9750e+01	3.3948e+00	0.0000e+00	0.0000e+00
3.1840e-02	4.2468e+01	4.3794e-01	5.8425e+01	4.3419e-01	4.1834e+01	4.3419e-01	4.5010e+01	4.5010e+01	6.5040e+01	4.6226e-01	4.6571e+01	4.6226e-01	4.2255e+01	2.9466e+00	0.0000e+00	0.0000e+00

N<sub>Q</sub>

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MuScatt Web-page: <https://jugit.fz-juelich.de/sans/muscatt/blob/master/readme.pdf>

# MuScatt@QtiSAS integration : input

- Instead of „Control“ file  
-> parameters of function

	Name	Initial Value	Vary?From..To	Info
1 ^	lowQ	0	<input type="checkbox"/> ..	switch for lowQ extrapolation: 0 automatic 1 guinier 2 power l...
2 ^	bgksub	0	<input type="checkbox"/> ..	incoherent background subtraction: -1 none 0 automatic (rea...
3 ^	lambda	5	<input type="checkbox"/> ..	lambda (Angstroem)
4 ^	d	0.1	<input type="checkbox"/> ..	sample thickness in cm
5 ^	transm	0.554	<input type="checkbox"/> ..	experimental transmission as measured
6 ^	sigmia	3.6442	<input type="checkbox"/> ..	sigma due to incoherent scattering and absorption calculate...
7 ^	hgqmod	0	<input type="checkbox"/> ..	high q extrapolation (0 for off 1 for on)
8 ^	hgqcut	0.0689	<input type="checkbox"/> ..	q range from which pure power law is achieved
9 ^	resmod	0	<input type="checkbox"/> ..	resolution mode #n (-1 is off;; 0 for no combination);; combin...
10 ^	dlfwhm	0.1	<input type="checkbox"/> ..	fraction of lambda resolution at fwhm;; i.e. delta lambda / la...
11 ^	detlen	20	<input type="checkbox"/> ..	detector distance [m] for lowest Q measurements
12 ^	sampap	0.01	<input type="checkbox"/> ..	sample aperture [m]
13 ^	collen	20	<input type="checkbox"/> ..	collimation distance [m] for lowest Q measurements;; negati...
14 ^	entrap	0.03	<input type="checkbox"/> ..	enttance aperture [m];; negative values if not specified (sym...
15 ^	reswdt	2	<input type="checkbox"/> ..	resolution cutoff (in terms of multiples of sigma)
16 ^	thkmod	0	<input type="checkbox"/> ..	thickness correction mode #n (<=0 is off;; combines with DE...
17 ^	activeOutput	1	<input type="checkbox"/> ..	0..8: 0 input data;; 1 Eq.1;; 2 Eq. 3;; 3 Eq. 2...

COMPILE

1D f(x) 2D f(x,y,...) new save delete compile

Categories: HF, Instrumentation, Integrals Test, Lipoproteins, Liposome-Scattering-SMA, Liposomes, MARGARITA

Functions: muscatt, muscatt-example-12t1, muscatt-example-12t2, muscatt-example-5t1, muscatt-example-5t2, muscatt-example-kugel, muscatt

Dependent variable: I

Independent variable(s): Q

	Name	Initial Value	Vary?From..To	Info
1 ^	lowQ	0	<input type="checkbox"/> ..	switch for lowQ extrapolation: 0 automatic 1 guinier 2 pow...
2 ^	bgksub	0	<input type="checkbox"/> ..	incoherent background subtraction: -1 none 0 automatic (r...
3 ^	lambda	5	<input type="checkbox"/> ..	lambda (Angstroem)
4 ^	d	0.1	<input type="checkbox"/> ..	sample thickness in cm
5 ^	transm	0.554	<input type="checkbox"/> ..	experimental transmission as measured
6 ^	sigmia	3.6442	<input type="checkbox"/> ..	sigma due to incoherent scattering and absorption calculat...
7 ^	hgmod	0	<input type="checkbox"/> ..	high q extrapolation (0 for off 1 for on)

Code +Included +Fortran Info Fit.Control Files Options

```

290 /* qtisas initial part: start */
291
292 int activeCol=Int(activeOutput*2-2); // what to show after pressing "Simulate"
293 int numberPointsReal=currentLastPoint-currentFirstPoint+1;
294
295 if ( !beforeFit && !afterFit && !beforeIter && !afterIter ) if (calculated)
296 {
297   if (activeCol>=0 && activeCol<15) return ln[orderQ[currentPoint-currentFirstPoint]][activeCol];
298   else return YYY[currentPoint];
299 }
300
301 if ( afterIter ) { calculated = false; return 1.0;};
302 if ( currentInt!=0 ) { calculated = false; return 1.0;};
303
304 if (afterFit && calculated ) { saveToTable(numberPointsReal, ParaM ); return 1.0;};
305
306 /* qtisas initial part: finish */
307
308
309 if (numberPointsReal>300) numberPointsReal=300;
    
```

muscatt

# MuScatt@QtiSAS integration: input

- Instead of “data file” [Q I dI] -> „data table“ in qtisas project: Q[X], I[Y], dI[yErr]

The screenshot displays the QtiSAS software interface. A purple box highlights a data table with the following columns: Q[X], I[Y], and dI[yErr]. A purple arrow points from the text '„data table“' in the bullet point above to this table. The table contains 27 rows of data. To the right, the 'COMPILE' panel is visible, showing a list of functions and a table of parameters.

Q[X]	I[Y]	dI[yErr]
1	0.00775	441.15
2	0.00861	428.668
3	0.00947	415.23
4	0.01033	400.932
5	0.01119	385.878
6	0.01205	370.172
7	0.01291	353.922
8	0.01377	337.236
9	0.01463	320.224
10	0.01549	302.995
11	0.01635	285.655
12	0.01721	268.309
13	0.01807	251.056
14	0.01893	233.992
15	0.01979	217.207
16	0.02066	200.783
17	0.02152	184.799
18	0.02238	169.326
19	0.02324	154.422
20	0.0241	140.145
21	0.02496	126.541
22	0.02582	113.647
23	0.02668	101.492
24	0.02754	90.0983
25	0.0284	79.4807
26	0.02926	69.6441
27	0.03012	60.5877

The 'COMPILE' panel shows a table of parameters:

Name	Initial Value [From..To]	Vary?	Info
lowQ	0	<input type="checkbox"/>	switch for lowQ extrapolation: 0 automatic 1 ...
bgksub	0	<input type="checkbox"/>	incoherent background subtraction: -1 none ...
lambda	5	<input type="checkbox"/>	lambda (Angstrom)
d	0.1	<input type="checkbox"/>	sample thickness in cm

The 'Code' panel shows the following Fortran code:

```
301 /* qtisas initial part: start */
302
303 int activeCol=Int(activeOutput*2-2); // what to show after pressing "Simulate"
304 int numberPointsReal=currentLastPoint-currentFirstPoint+1;
305
306 if ( lbeforeFit && lafterFit && lbeforeIter && lafterIter ) if (calculated)
307 {
308 if (activeCob=0 && activeCol<15) return In[orderQ[currentPoint-currentFirstPoint]][activeCol];
309 else return YYY[currentPoint];
310 }
311
312 if ( afterIter ) { calculated = false; return 1.0;};
313 if ( currentInt=0 ) { calculated = false; return 1.0;};
314
315 if ( afterFit && calculated ) { saveToTable(numberPointsReal, ParaM ); return 1.0;};
316
317 /* qtisas initial part: finish */
318
```

# MuScatt@QtiSAS integration: output

- Instead Output file -> output Table „muscott”
- 1-3 column: input data; 1,4-19 columns == “Output File”
- “muscott” table generated after pushing button “**Script: After Fit**”

The screenshot displays the QtiSAS software interface. The main window shows a table titled "muscott - Matrix Fit :: Matrix-to-Table" with 27 rows and 11 columns. The columns are labeled: Q(x), f(y), dEq1(yEr), Eq1(y), dEq1(yEr), Eq1(y), dEq2(yEr), Eq2(y), dEq2(yEr), Eq2(y), and Eqreverse(y). The data in the table consists of numerical values for each row.

On the right side of the interface, there is a "COMPILER" panel. It shows a list of functions, including "muscott-example-512", "muscott-example-kugel", "muscott-example-polyres", and "muscott". Below this, there is a "Code" panel with a script titled "qisas initial part: start". The script contains Fortran code for handling the output of the fit, including variables like "activeCol", "numberPointsReal", and "currentPoint".

At the bottom of the interface, there is a "Project Explorer" panel showing a list of files and tables. The "muscott" table is highlighted, indicating it is the current active table.

# MuScatt@QtiSAS: how to use

- Download [muscatt.fif](#) and place it in ./qtisas/FitFunctions/ folder;
- Download [muscatt-included-h-files.zip](#) archive and unzip it in ./qtisas/FitFunctions/IncludedFunctions/ folder
- Compile „muscatt“ function in QtiSAS | Compile interface
- In QtiSAS | FitTable: select function „muscatt“
- In QtiSAS | FitTable | Data: select table with SA(N)S data
- In QtiSAS | FitTable | Parameters: input correct parameters values
- In QtiSAS: activate plot with SA(N)S data
- In QtiSAS | FitTable: push button "Simulate" -> in active plot you will see output curve [parameter "activeOutput" control dataset to show]
- In QtiSAS | FitTable: push button "Script: After Fit" -> "muscatt" table will be generated with all output data; "muscatt" table will be overwritten if you will push "Script: After Fit" second time

Categories

Functions

muscatl-example-011  
muscatl-example-012  
muscatl-example-lupel  
muscatl-example-polyres  
muscatl

Dependent variable

Independent variables

Name	Initial Value (From To)	Vary?	Info
lowQ	0	<input type="checkbox"/>	switch for lowQ extrapolation: 0 automatic 1 guinier 2 power law 3 constant
bgsub	0	<input type="checkbox"/>	incoherent background subtraction: -1 none 0 automatic (real)value=0 gives exact level to be subtracted
lambda	5	<input type="checkbox"/>	lambda (Angstroms)
d	0.1	<input type="checkbox"/>	sample thickness in cm
transm	0.554	<input type="checkbox"/>	experimental transmission as measured
sigma	3.6442	<input type="checkbox"/>	sigma due to incoherent scattering and absorption calculated from table (will be divided by 4pi for full 3d angle)
hgmod	0	<input type="checkbox"/>	high q extrapolation (0 for off 1 for on)
hgcut	0.0089	<input type="checkbox"/>	q range from which pure power law is achieved
resmod	0	<input type="checkbox"/>	resolution mode #n (-1 is off; 0 for no combination); combines with DEMONEX calculation of type #n (1-5)
dthrm	0.1	<input type="checkbox"/>	fraction of lambda resolution at thrm; i.e. delta lambda / lambda
dellen	20	<input type="checkbox"/>	detector distance [m] for lowest Q measurements
sampap	0.01	<input type="checkbox"/>	sample aperture [m]
colen	20	<input type="checkbox"/>	collimation distance [m] for lowest Q measurements; negative values if not specified (symmetric setting)
entrap	0.03	<input type="checkbox"/>	entrance aperture [m]; negative values if not specified (symmetric setting)
reswdt	2	<input type="checkbox"/>	resolution cutoff (in terms of multiples of sigma)

Code

```

int activeCol: int(ActiveOutput*2);
int numberPoints: currentLastPoint-currentFirstPoint+1;
if ( beforeFit && !afterFit && beforeRes && !afterRes ) if (calculated)
if ( activeCol==0 && activeCol!=1 ) return I[orderQ[currentPoint-currentFirstPoint+activeCol];
else return I[orderPoint];
if ( afterFit ) ( calculated = false; return 1.0; );
if ( currentRes!=0 ) ( calculated = false; return 1.0; );
if ( afterFit && calculated ) ( saveToTable(numberPointsReal, Param); return 1.0; );
glsas initial part: finish;
if (numberPointsReal>300) numberPointsReal=300;
  
```

COMPILE FITTABLE(s)

Load Fitting Session

Select Function Fitting Session

Categories

Functions

muscatl  
muscatl-example-1211  
muscatl-example-1212  
muscatl-example-511  
muscatl-example-512  
muscatl-example-lupel  
muscatl-example-polyres

good place for function's comments

Info :: Function Info :: Parameters Options

Fit Curve [1D fit] v.18-29.10.2019 Vitaliy Pipich @ JCMS

COMPILE FITTABLE(s)

Save Current Fitting Session

Select Function Fitting Session Generate Results

Data Function Parameters Global Limits Fit - Control

Dataset #1 Dataset #1

outPolyRes\_Eq1

N 172

First Point 1

Last Point 172

Weighting outPolyRes\_dEq1

Fit Simulate  $\chi^2/\text{dof}$

Script :: Before Fit R<sup>2</sup> time

Script :: After Fit time

muscatl

COMPILE FITTABLE(s)

Save Current Fitting Session

Select Function Fitting Session Generate Results

	Vary/From To	Value #1	Error #1
lowQ	<input type="checkbox"/>	1	---
bgsub	<input type="checkbox"/>	-1	---
lambda	<input type="checkbox"/>	5	---
d	<input type="checkbox"/>	0.1	---
transm	<input type="checkbox"/>	0.9	---
sigma	<input type="checkbox"/>	0.001	---
hgmod	<input type="checkbox"/>	0	---
hgcut	<input type="checkbox"/>	0.0689	---
resmod	<input type="checkbox"/>	0	---
dthrm	<input type="checkbox"/>	0.1	---
dellen	<input type="checkbox"/>	8	---
sampap	<input type="checkbox"/>	0.01	---
colen	<input type="checkbox"/>	8	---
entrap	<input type="checkbox"/>	0.03	---
reswdt	<input type="checkbox"/>	2	---
thkmod	<input type="checkbox"/>	0	---
activeOutput	<input type="checkbox"/>	7	---

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

Fit Simulate  $\chi^2/\text{dof}$

Script :: Before Fit R<sup>2</sup> time

Script :: After Fit time

# MuScatt@QtiSAS: how to use [in figures]

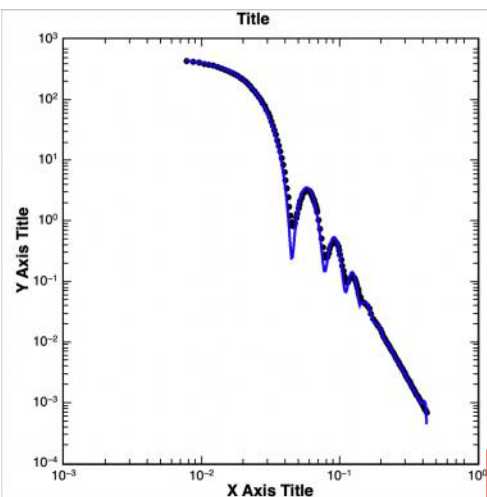
transm	<input type="checkbox"/>	0.9	---
sigma	<input type="checkbox"/>	0.001	---
hgmod	<input type="checkbox"/>	0	---
hgcut	<input type="checkbox"/>	0.0689	---
resmod	<input type="checkbox"/>	0	---
dthrm	<input type="checkbox"/>	0.1	---
dellen	<input type="checkbox"/>	8	---
sampap	<input type="checkbox"/>	0.01	---
colen	<input type="checkbox"/>	8	---
entrap	<input type="checkbox"/>	0.03	---
reswdt	<input type="checkbox"/>	2	---
thkmod	<input type="checkbox"/>	0	---
activeOutput	<input type="checkbox"/>	7	---

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

Fit Simulate  $\chi^2/\text{dof}$

Script :: Before Fit R<sup>2</sup> time

Script :: After Fit time



transm	<input type="checkbox"/>	0.9	---
sigma	<input type="checkbox"/>	0.001	---
hgmod	<input type="checkbox"/>	0	---
hgcut	<input type="checkbox"/>	0.0689	---
resmod	<input type="checkbox"/>	0	---
dthrm	<input type="checkbox"/>	0.1	---
dellen	<input type="checkbox"/>	8	---
sampap	<input type="checkbox"/>	0.01	---
colen	<input type="checkbox"/>	8	---
entrap	<input type="checkbox"/>	0.03	---
reswdt	<input type="checkbox"/>	2	---
thkmod	<input type="checkbox"/>	0	---
activeOutput	<input type="checkbox"/>	7	---

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

Fit Simulate  $\chi^2/\text{dof}$

Script :: Before Fit R<sup>2</sup> time

Script :: After Fit time

MuScatt - Matrix Fit: Matrix-Table

Q21	Q11	Q12	Q13	Q14	Q15	Q16	Q17	Q18	Q19	Q20
0.00775	441.15	4.4115	434.125	4.31447	803.445	4.27754	432.092	4.27754	44	44
0.00661	428.666	4.28666	421.629	4.1924	588.043	4.15651	419.631	4.15651	43	43
0.00647	415.25	4.1525	408.219	4.06907	567.388	4.02821	406.236	4.02821	41	41
0.01033	400.932	4.00932	393.34	3.90114	547.481	3.85977	392.016	3.85977	40	40
0.01116	386.676	3.86676	379.343	3.77391	528.395	3.7416	377.054	3.7416	38	38
0.01205	373.172	3.73172	365.346	3.65031	509.309	3.61817	367.981	3.61817	37	37
0.01291	359.302	3.59302	347.153	3.48138	482.235	3.43174	345.365	3.43174	35	35
0.01377	347.238	3.47238	330.884	3.35819	458.233	3.29959	328.844	3.29959	33	33
0.01463	335.234	3.35234	313.637	3.13181	435.730	3.105	312.008	3.105	32	32
0.01548	323.965	3.23965	296.618	2.93331	411.952	2.93794	294.96	2.93794	30	30
0.01633	285.655	2.85655	279.435	2.79372	388.037	2.78681	277.85	2.78681	28	28
0.01721	268.309	2.68309	262.287	2.63406	364.136	2.61011	260.737	2.61011	27	27
0.01807	251.056	2.51056	245.204	2.45334	340.383	2.43432	243.729	2.43432	25	25
0.01893	233.993	2.33993	228.333	2.28845	316.696	2.26886	226.912	2.26886	23	23
0.01979	217.207	2.17207	211.801	2.1243	293.088	2.10611	210.437	2.10611	21	21
0.02066	200.793	2.00793	195.547	1.96037	271.268	1.94886	194.24	1.94886	20	20
0.02152	184.790	1.84790	179.803	1.80734	249.361	1.79187	178.553	1.79187	1	1
0.02238	169.326	1.69326	164.567	1.60926	228.147	1.61484	163.383	1.61484	1	1
0.02324	154.422	1.54422	149.884	1.51026	207.733	1.49733	148.746	1.49733	15	15
0.0241	140.145	1.40145	135.845	1.37693	188.204	1.35889	134.762	1.35889	14	14
0.02496	126.541	1.26541	122.477	1.23758	169.611	1.22698	121.449	1.22698	12	12
0.02582	113.647	1.13647	109.816	1.11147	152.004	1.10196	108.841	1.10196	11	11
0.02668	101.482	1.01482	97.8855	0.952937	135.43	0.9841	95.9736	0.9841	10	10
0.02754	90.0883	0.900883	86.7301	0.881183	119.909	0.87382	85.8938	0.87382	9	9
0.0284	79.4807	0.794807	76.3356	0.777328	105.483	0.770674	75.1537	0.770674	8	8
0.02926	69.6441	0.696441	66.7198	0.651122	92.1018	0.675291	65.3487	0.675291	7	7
0.03012	60.5877	0.605888	57.6742	0.532554	79.8146	0.587481	57.1006	0.587481	6	6

Project Explorer

Sample Polyres

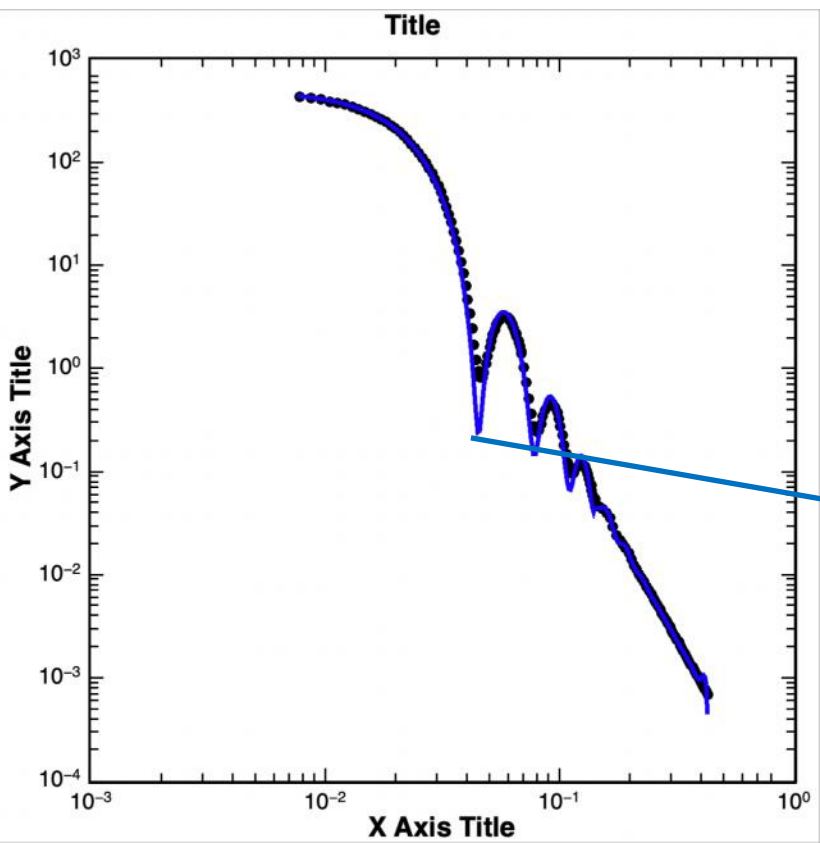
Name Table None

Graph None

Table None

muScattContWithPleas Table None

# Parameter “activeOutput” selection of dataset to show



	2
	0

Scale Error

Simulate

Script :: Before Fit

FITTABLE(s)

Save Current Fitting Session

Select Function   Fitting Session   Generate Results

Data   Function   Parameters   Global Limits   Fit - Control

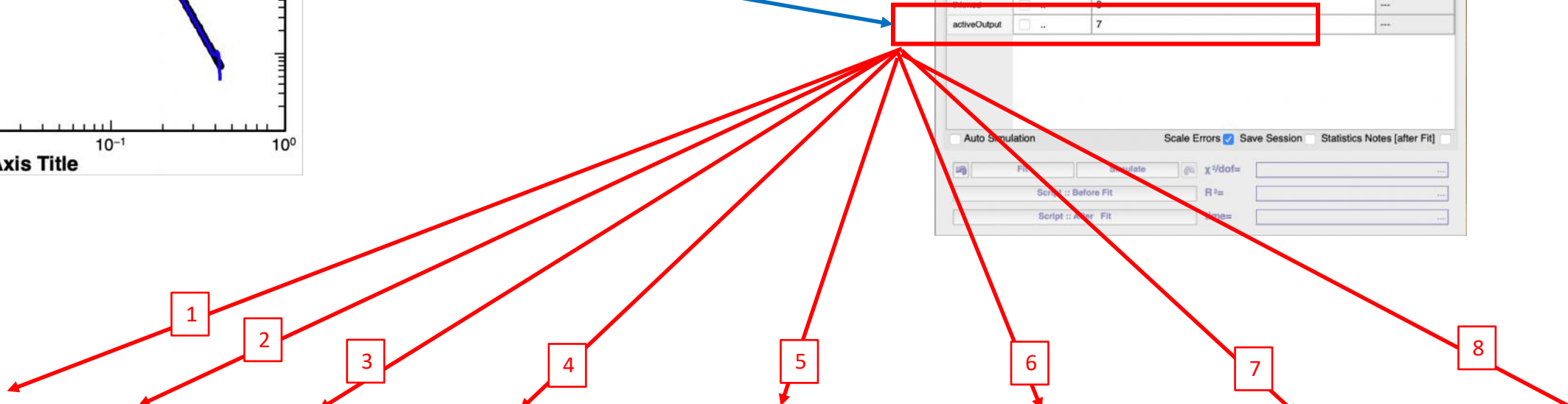
	Vary?From..To	Value #1	Error #1
lowQ	<input type="checkbox"/> .. 1		---
bgksub	<input type="checkbox"/> .. -1		---
lambda	<input type="checkbox"/> .. 5		---
d	<input type="checkbox"/> .. 0.1		---
transn	<input type="checkbox"/> .. 0.9		---
sigma	<input type="checkbox"/> .. 0.001		---
hgqmod	<input type="checkbox"/> .. 0		---
hgqcut	<input type="checkbox"/> .. 0.0689		---
resmod	<input type="checkbox"/> .. 0		---
dltwhm	<input type="checkbox"/> .. 0.1		---
detlen	<input type="checkbox"/> .. 8		---
sampap	<input type="checkbox"/> .. 0.01		---
collen	<input type="checkbox"/> .. 8		---
entrap	<input type="checkbox"/> .. 0.03		---
reswdt	<input type="checkbox"/> .. 2		---
activeOutput	<input type="checkbox"/> .. 7		---

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

Fit   Simulate   x<sup>2</sup>/dof=

Script :: Before Fit   R<sup>2</sup>=

Script :: After Fit   Error



[X]	I[Y]	dI[yEr]	Eq1[Y]	dEq1[yEr]	Eq3[Y]	dEq3[yEr]	Eq2[Y]	dEq2[yEr]	Eq1reversal[Y]	dEq1reversal[yEr]	Eq3reversal[Y]	dEq3reversal[yEr]	Eq2reversal[Y]	dEq2reversal[yEr]	CorrIntWithReso[Y]	dCorrIntWithReso[yEr]
-----	------	---------	--------	-----------	--------	-----------	--------	-----------	----------------	-------------------	----------------	-------------------	----------------	-------------------	--------------------	-----------------------

# MuScatt@QtiSAS vs MuScatt

„MuScatt“ Sample Name	MuScatt@QtiSAS results	Fitting Function in QtiSAS with correct parameters ( <u>eFit</u> ready)	MuScatt Output File [generated by H. Frielinghaus]
5t1	<a href="#">sample-5t1.zip</a>	<a href="#">muscatt-example-5t1.fif</a>	<a href="#">out5t1.txt</a>
5t2	<a href="#">sample-5t2.zip</a>	<a href="#">muscatt-example-5t2.fif</a>	<a href="#">out5t2.txt</a>
12t1	<a href="#">sample-12t1.zip</a>	<a href="#">muscatt-example-12t1.fif</a>	<a href="#">out12t1.txt</a>
12t2	<a href="#">sample-12t2.zip</a>	<a href="#">muscatt-example-12t2.fif</a>	<a href="#">out12t2.txt</a>
Kugel	<a href="#">sample-kugel.zip</a>	<a href="#">muscatt-example-kugel.fif</a>	<a href="#">outKugel.txt</a>
PolyRes	<a href="#">sample-polyres.zip</a>	<a href="#">muscatt-example-polyres.fif</a>	<a href="#">outPolyRes.txt</a>

Sample Name  
[in MuScatt manual ]

Results of comparison in QtiSAS.  
Zip files contain:  
example-XXX.qti.  
example-XXX-res.qti

This example will be shown in next pages

Download [muscatt-included-h-files.zip](#) archive  
and unzip it in `./qtisas/FitFunctions/IncludedFunctions/` folder

MuScatt@QtiSAS: sample 12t1

Q[X]	I[Y]	dI[yEr]	dI[yEr]
1	0.00287	530.63148	4.22951
2	0.00323	485.14237	3.38612
3	0.00359	471.82243	3.02934
4	0.00394	471.68147	2.86387
5	0.0043	468.25718	2.70481
6	0.00466	465.63931	2.59009
7	0.00502	467.40911	2.46438
8	0.00538	457.18124	2.3459
9	0.00574	452.44218	2.2323
10	0.0061	451.20202	2.1819
11	0.00645	448.37428	2.11513
12	0.00681	450.39613	2.05879
13	0.00717	443.36823	1.96855
14	0.00753	449.74399	1.9133
15	0.00789	450.84629	1.87523
16	0.00825	438.71047	1.78848
17	0.00861	443.38668	1.77892
18	0.00896	441.35361	1.73094
19	0.00932	442.54104	1.69348
20	0.00968	441.45071	1.68109
21	0.01004	439.32075	1.71162
22	0.0104	438.89106	1.73804
23	0.01076	440.1547	1.67613
24	0.01112	440.47305	1.62208
25	0.01147	436.57979	1.5653
26	0.01183	437.13712	1.54912
27	0.01219	436.80166	1.52772
28	0.01255	439.05832	1.49588
29	0.01291	448.10408	1.48278
30	0.01327	455.36849	1.46628
31	0.01362	448.88984	1.44355
32	0.01398	453.11756	1.43637
33	0.01434	450.11613	1.41356
34	0.0147	453.64761	1.40556
35	0.01506	451.95006	1.37633
36	0.01542	459.82567	1.37092
37	0.01577	466.78454	1.35181
38	0.01613	469.60157	1.33583
39	0.01649	469.16981	1.32567
40	0.01685	472.76421	1.33999
41	0.01721	473.19098	1.34761
42	0.01757	483.02506	1.36054
43	0.01792	486.80214	1.37755
44	0.01828	492.60371	1.37596
45	0.01864	498.12925	1.37445
46	0.019	504.86167	1.36563
47	0.01936	514.22251	1.3531

1. SANS data: table data12t1

COMPILE

1D f(x) 2D f(x,y,...) new save delete compile

Categories: ALL, BS-BackScattering, Block Copolymer Micelles, Core::Shell, Density Profile

Functions: [Empty]

Dependent variable: f

Independent variable(s): x

Name	Initial Value [From..To]	Vary?	Info
0			

Code +Included +Fortran Info Fit.Control Files Options

```

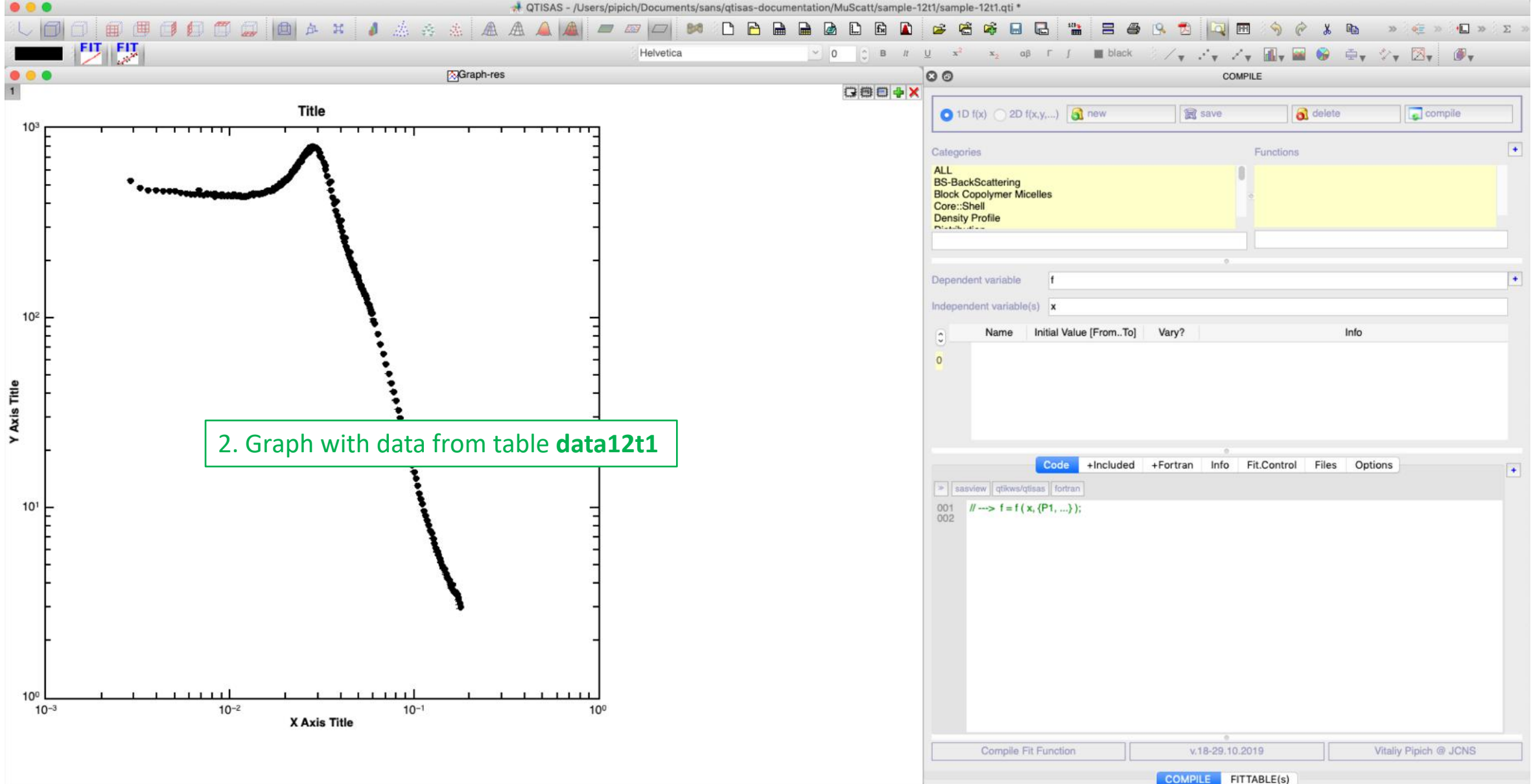
sasview qtikws/qtisas fortran
001 // --> f = f ( x, {P1, ...} );
002
    
```

Compile Fit Function v.18-29.10.2019 Vitaliy Pipich @ JCNS

COMPILE FITTABLE(s)

Project Explorer

Name	Type	View	Created	Label
data12t1	Table	Maximized	29.10.19 17:35	/Users/pipich/Documents/sans/qtisas-documentation/MuScatt/sample-12t1/data12t1.DAT.txt
Graph-res	Graph	Normal	29.10.19 17:36	
out12t1	Table	Normal	29.10.19 11:54	/Users/pipich/Documents/sans/qtisas-documentation/MuScatt/sample-12t1/out12t1.txt



2. Graph with data from table data12t1

```
Code +Included +Fortran Info Fit.Control Files Options
sasview qtkws/qtisas fortran
001 // --> f = f ( x, {P1, ...} );
002
```

Compile Fit Function v.18-29.10.2019 Vitaliy Pipich @ JCNS

COMPILE FITTABLE(s)

Project Explorer

Name	Type	View	Created	Label
data12t1	Table	Normal	29.10.19 17:35	/Users/pipich/Documents/sans/qtisas-documentation/MuScatt/sample-12t1/data12t1.DAT.txt
Graph-res	Graph	Maximized	29.10.19 17:36	
out12t1	Table	Normal	29.10.19 11:54	/Users/pipich/Documents/sans/qtisas-documentation/MuScatt/sample-12t1/out12t1.txt

The screenshot shows the QtISAS software interface. On the left, a log-log plot titled "Title" displays experimental data points (black dots) and a fitted curve (black line). The y-axis is labeled "Y Axis Title" and ranges from  $10^0$  to  $10^3$ . The x-axis is labeled "X Axis Title" and ranges from  $10^{-3}$  to  $10^0$ . A green box highlights the "FIT" buttons in the top-left corner. On the right, the "COMPILE" panel is active, showing a list of functions under the "Functions" category. A green box highlights the "muscott-example-121" function. Below the function list, the "Dependent variable" is set to "I" and the "Independent variable(s)" is set to "Q". A table of fit parameters is visible, with the parameter "d" checked for varying. At the bottom of the compile panel, there are buttons for "Code", "+Included", "+Fortran", "Info", "Fit.Control", "Files", and "Options". The "Code" tab is selected, showing Fortran code for the fit function. At the bottom of the compile panel, there are buttons for "Compile Fit Function", "v.18-29.10.2019", and "Vitaliy Pipich @ JCNS". A "COMPILE" button and "FITTABLE(s)" label are also present.

3. QtISAS:Compile: select function muscott-example-121

Project Explorer

Name	Type	View	Created	Label
data1211	Table	Normal	29.10.19 17:35	/Users/pipich/Documents/sans/qtisas-documentation/MuScatt/sample-1211/data1211.DAT.txt
Graph-res	Graph	Maximized	29.10.19 17:36	
out1211	Table	Normal	29.10.19 11:54	/Users/pipich/Documents/sans/qtisas-documentation/MuScatt/sample-1211/out1211.txt

QTISAS - /Users/pipich/Documents/sans/qtisas-documentation/MuScatt/sample-1211/sample-1211.qti \*

Graph-res

COMPILE

1D f(x) 2D f(x,y,...) new save delete **compile**

Categories: General, Instrumentation, Integrals Test, Liposomes

Functions: muscatt-example-1211, muscatt-example-1212, muscatt-example-511, muscatt-example-512, muscatt-example-kugel, muscatt-example-1211

Dependent variable: I

Independent variable(s): Q

Name	Initial Value [From..To]	Vary?	Info
lowQ	0	<input type="checkbox"/>	switch for lowQ extrapolation: 0 automatic 1 guinier 2 power law 3 constant
bgksub	2.7	<input type="checkbox"/>	incoherent background subtraction: -1 none 0 automatic (real)value>0 gives exact level to be subtracted
lambda	12	<input type="checkbox"/>	lambda (Angstrom)
d	0.1	<input checked="" type="checkbox"/>	sample thickness in cm

Code +Included +Fortran Info Fit.Control Files Options

```

301 /* qtisas initial part: start */
302
303 int activeCol=int(activeOutput*2-2); // what to show after pressing "Simulate"
304 int numberPointsReal=currentLastPoint-currentFirstPoint+1;
305
306 if ( !beforeFit && !afterFit && !beforeIter && !afterIter ) if (calculated)
307 {
308   if (activeCol>=0 && activeCol<15) return ln[orderQ[currentPoint-currentFirstPoint]][activeCol];
309   else return YYY[currentPoint];
310 }
311
312 if ( afterIter ) { calculated = false; return 1.0;};
313 if ( currentInt!=0 ) { calculated = false; return 1.0;};
314
315 if ( afterFit && calculated ) { saveToTable(numberPointsReal, Param ); return 1.0;};
316
317 /* qtisas initial part: finish */
318
319
320 if (numberPointsReal>300) numberPointsReal=300;
321
322 int orderQtmo[300];
  
```

Compile Fit Function v.18-29.10.2019 Vitaliy Pipich @ JCNS

**COMPILE** FITTABLE(s)

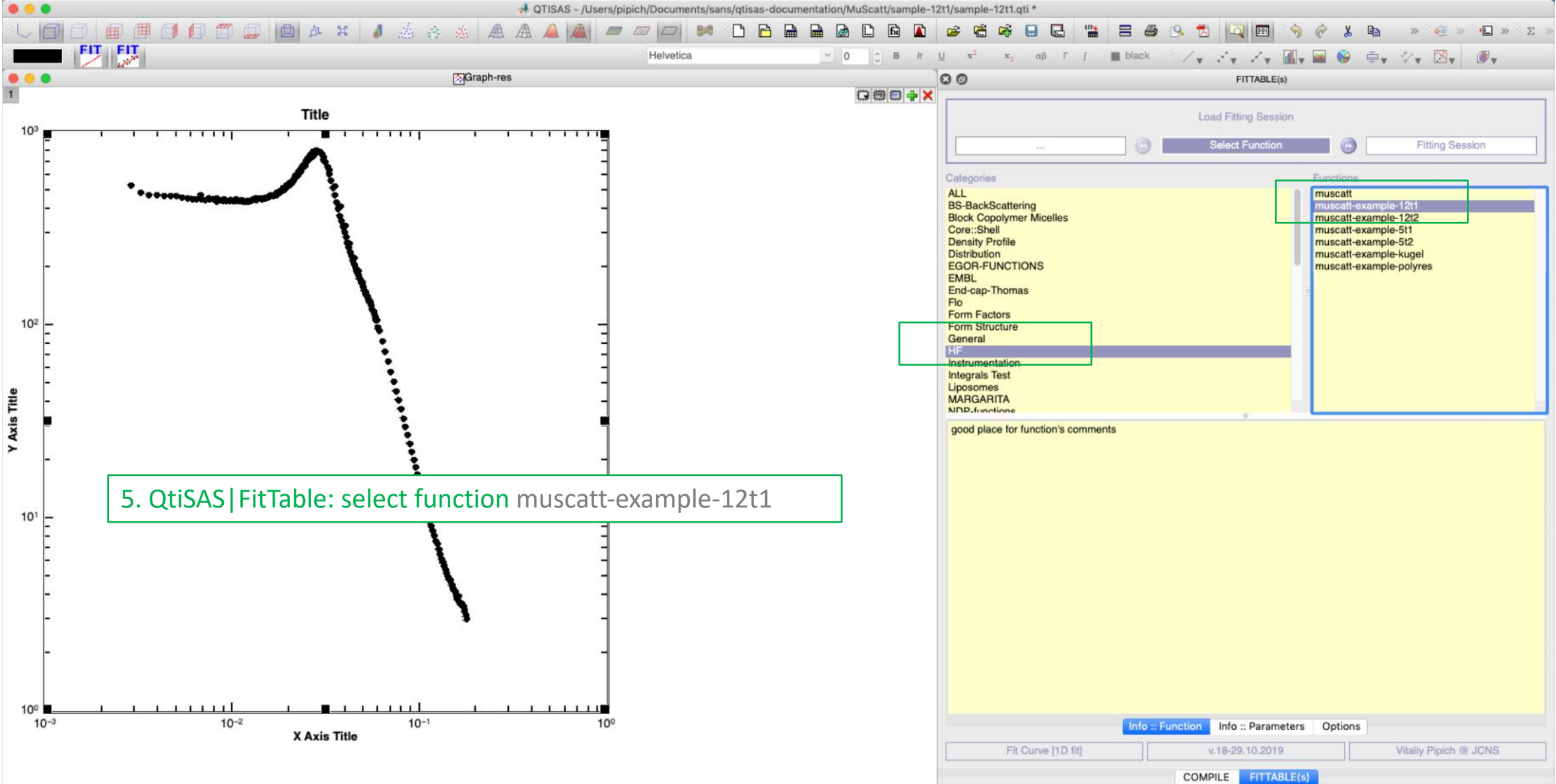
4. QtiSAS:Compile: push "compile" button

Results Log

```

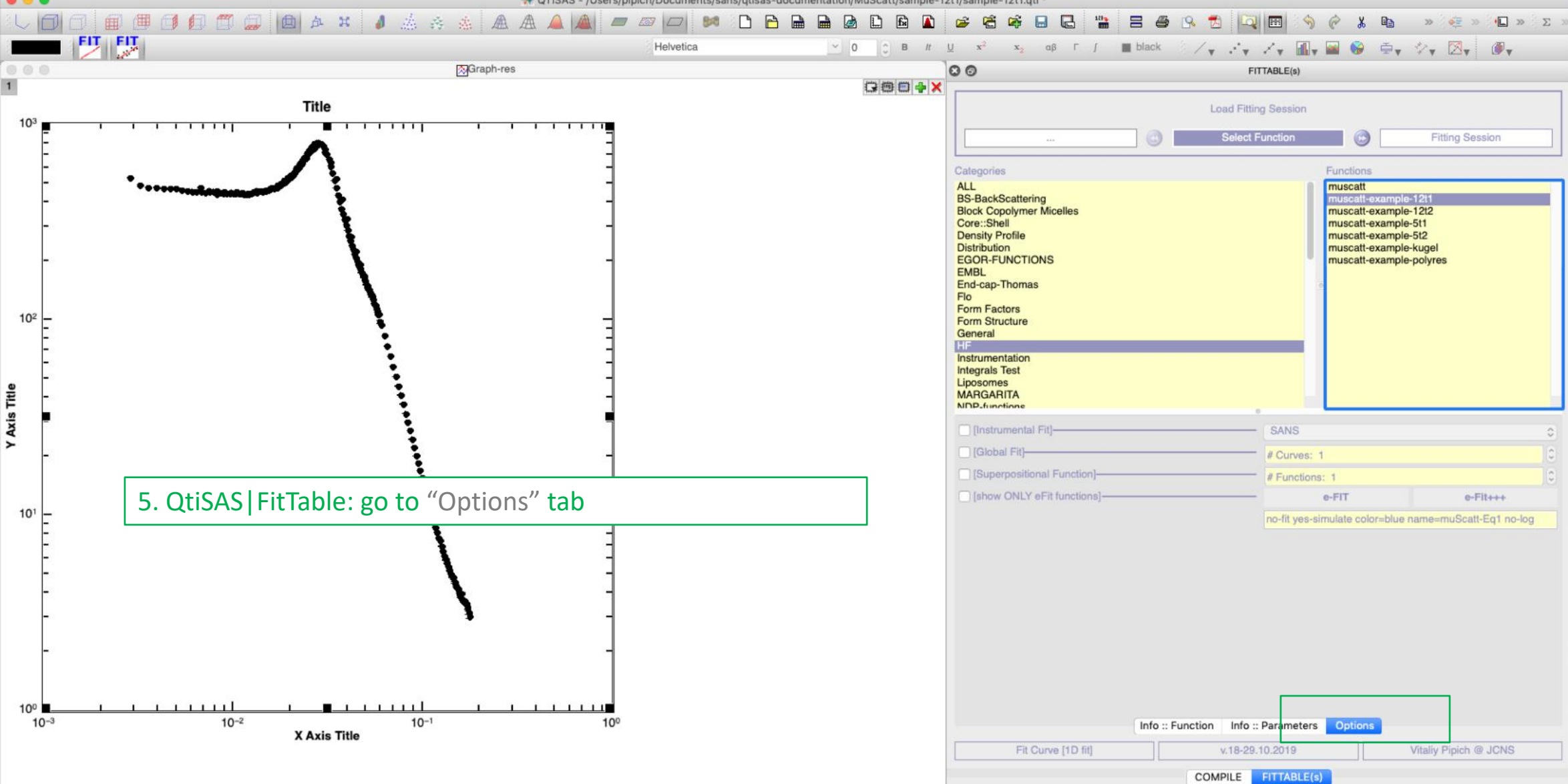
<< compile >>
<< compile status >> OK: function 'muscatt' is ready

<< compile >>
<< compile status >> OK: function 'muscatt-example-1211' is ready
  
```



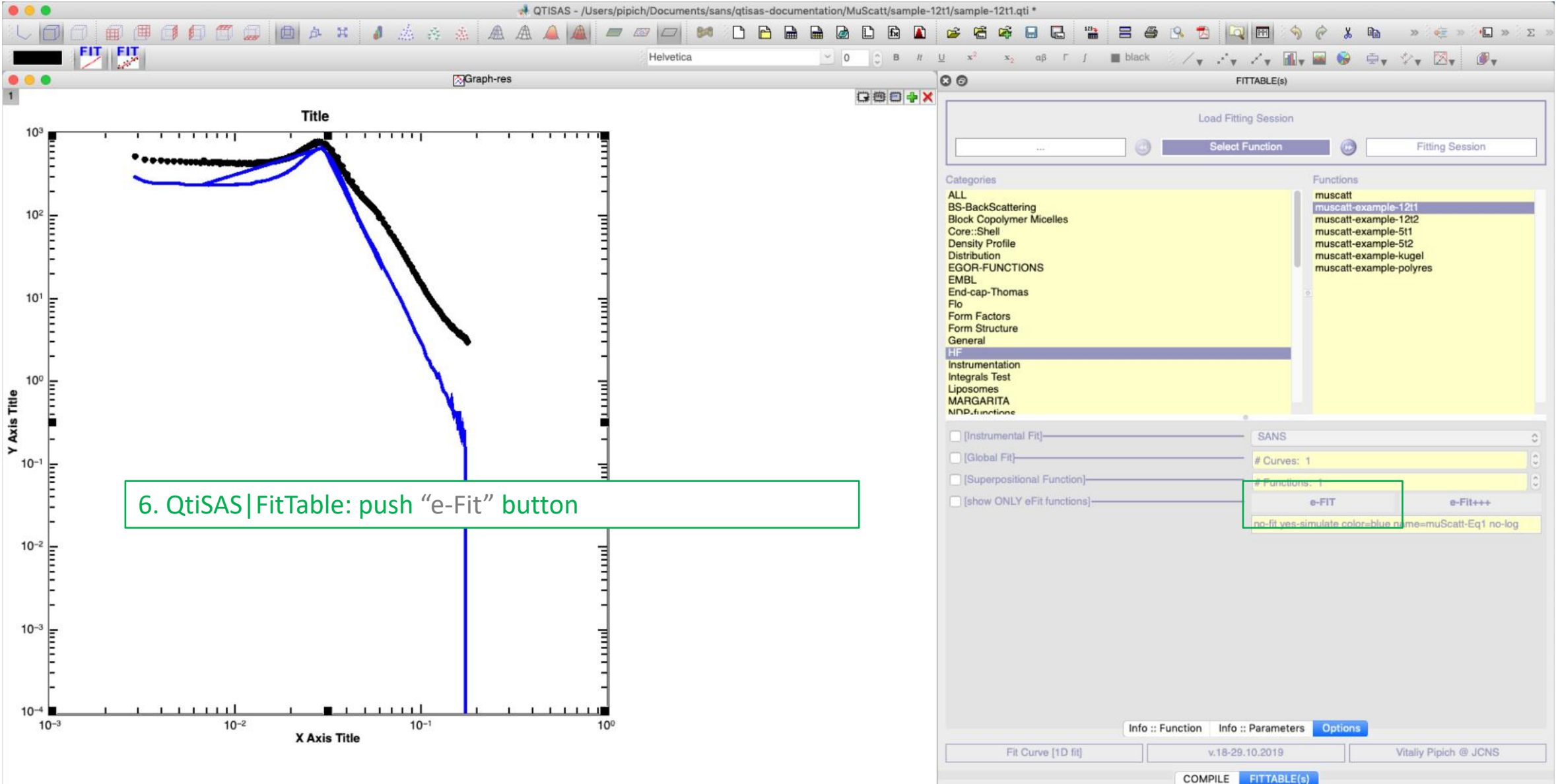
Project Explorer

Name	Type	View	Created	Label
data12t1	Table	Normal	29.10.19 17:35	/Users/pipich/Documents/sans/qtisas-documentation/MuScatt/sample-12t1/data12t1.DAT.txt
Graph-res	Graph	Maximized	29.10.19 17:36	
out12t1	Table	Normal	29.10.19 11:54	/Users/pipich/Documents/sans/qtisas-documentation/MuScatt/sample-12t1/out12t1.txt



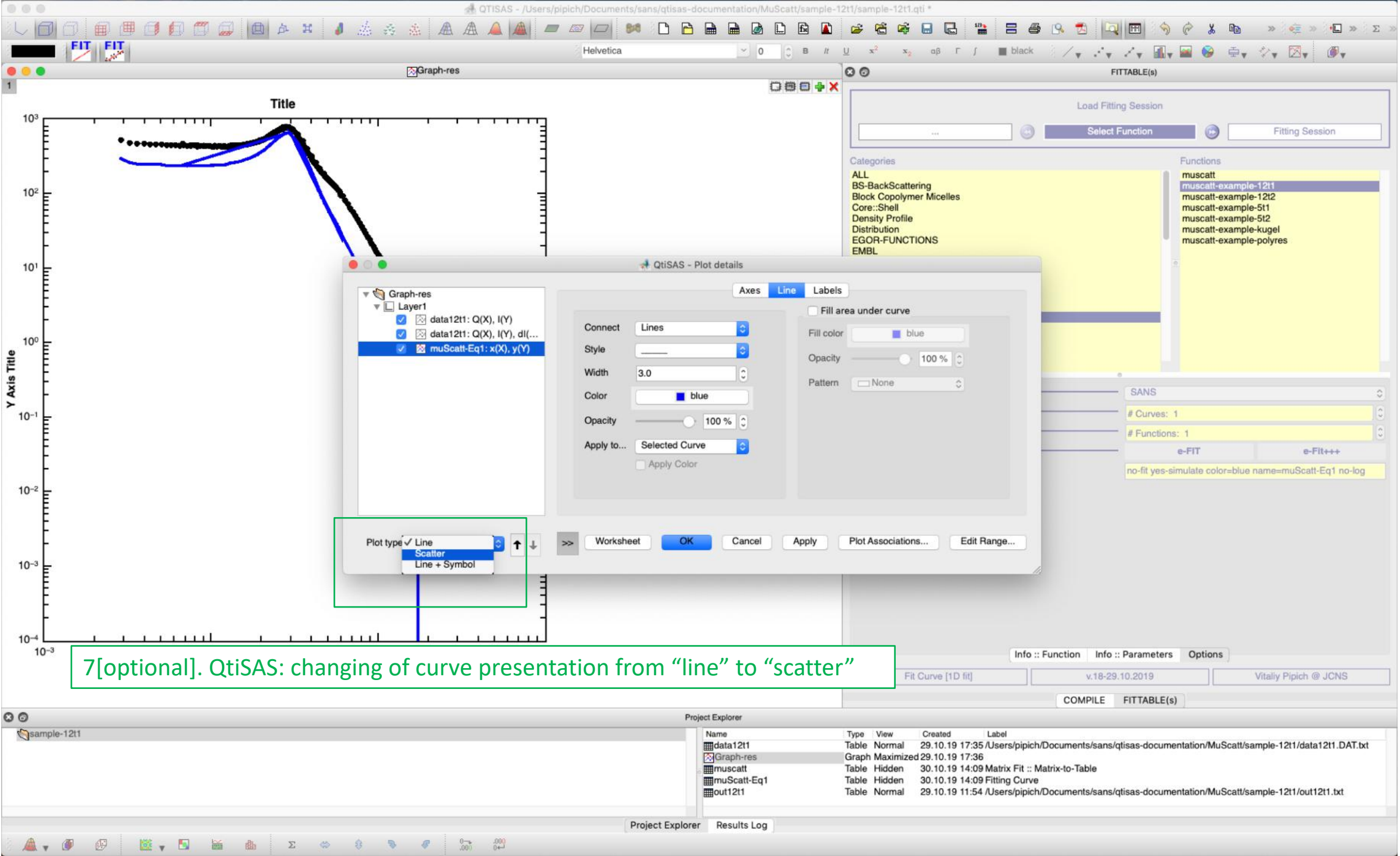
Project Explorer

Name	Type	View	Created	Label
data12t1	Table	Normal	29.10.19 17:35	/Users/pipich/Documents/sans/qtiSAS-documentation/MuScatt/sample-12t1/data12t1.DAT.txt
Graph-res	Graph	Maximized	29.10.19 17:36	
out12t1	Table	Normal	29.10.19 11:54	/Users/pipich/Documents/sans/qtiSAS-documentation/MuScatt/sample-12t1/out12t1.txt



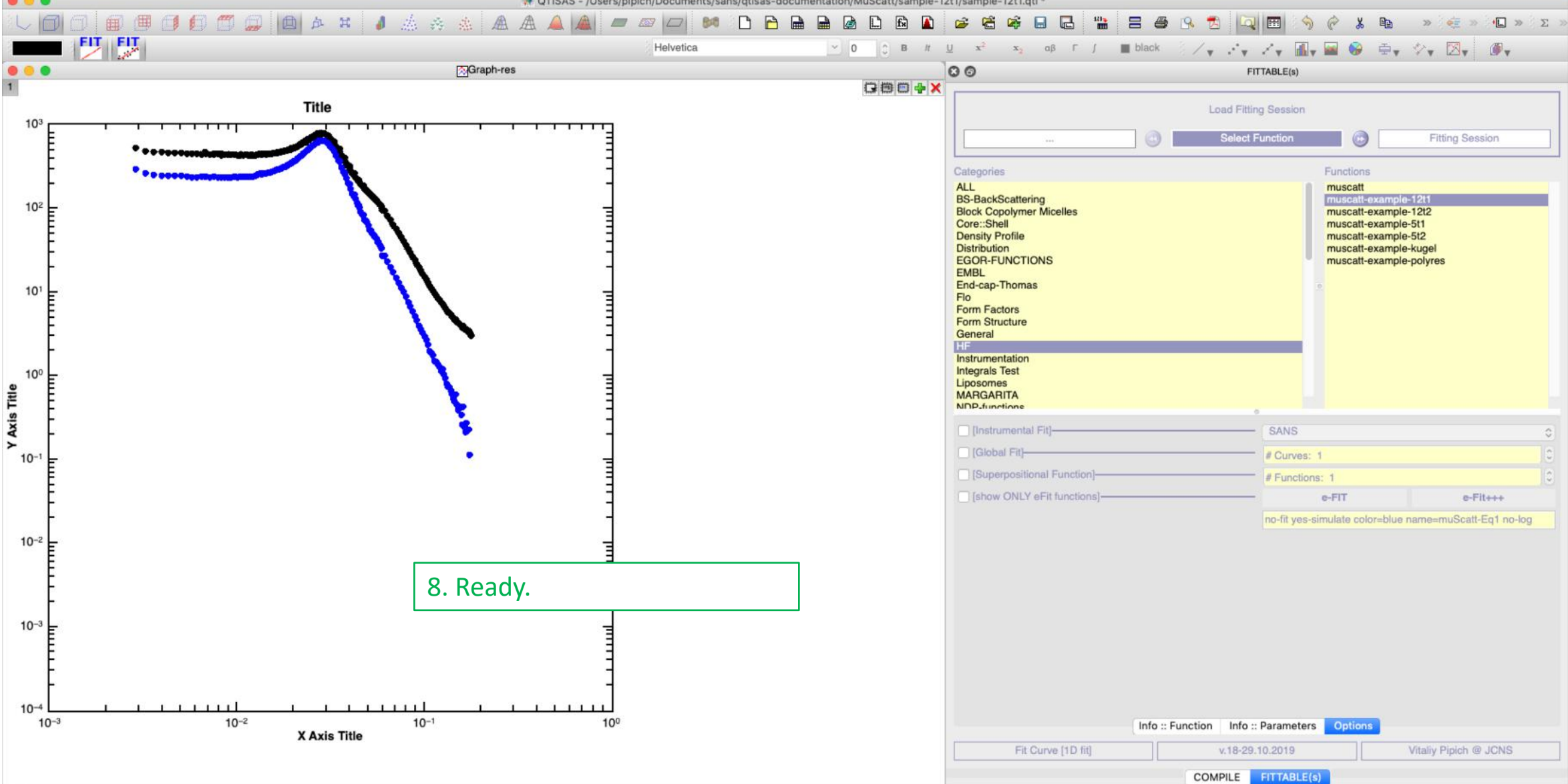
Project Explorer

Name	Type	View	Created	Label
data12t1	Table	Normal	29.10.19 17:35	/Users/pipich/Documents/sans/qtisas-documentation/MuScatt/sample-12t1/data12t1.DAT.txt
Graph-res	Graph	Maximized	29.10.19 17:36	
muscatt	Table	Hidden	30.10.19 14:09	Matrix Fit :: Matrix-to-Table
muScatt-Eq1	Table	Hidden	30.10.19 14:09	Fitting Curve
out12t1	Table	Normal	29.10.19 11:54	/Users/pipich/Documents/sans/qtisas-documentation/MuScatt/sample-12t1/out12t1.txt



#### Project Explorer

Name	Type	View	Created	Label
data12t1	Table	Normal	29.10.19 17:35	/Users/pipich/Documents/sans/qtiSAS-documentation/MuScatt/sample-12t1/data12t1.DAT.txt
Graph-res	Graph	Maximized	29.10.19 17:36	
muscatt	Table	Hidden	30.10.19 14:09	Matrix Fit :: Matrix-to-Table
muScatt-Eq1	Table	Hidden	30.10.19 14:09	Fitting Curve
out12t1	Table	Normal	29.10.19 11:54	/Users/pipich/Documents/sans/qtiSAS-documentation/MuScatt/sample-12t1/out12t1.txt



Project Explorer

Name	Type	View	Created	Label
data12t1	Table	Normal	29.10.19 17:35	/Users/pipich/Documents/sans/qtisas-documentation/MuScatt/sample-12t1/data12t1.DAT.txt
Graph-res	Graph	Maximized	29.10.19 17:36	
muscatt	Table	Hidden	30.10.19 14:09	Matrix Fit :: Matrix-to-Table
muScatt-Eq1	Table	Hidden	30.10.19 14:09	Fitting Curve
out12t1	Table	Normal	29.10.19 11:54	/Users/pipich/Documents/sans/qtisas-documentation/MuScatt/sample-12t1/out12t1.txt

Info :: Function Info :: Parameters Options

Fit Curve [1D fit] v.18-29.10.2019 Vitaliy Pipich @ JCNS

COMPILE FITTABLE(s)

Project Explorer

Name	Type	View	Created	Label
data12t1	Table	Normal	29.10.19 17:35	/Users/pipich/Documents/sans/qtisas-documentation/MuScatt/sample-12t1/data12t1.DAT.txt
Graph-res	Graph	Maximized	29.10.19 17:36	
muscatt	Table	Hidden	30.10.19 14:09	Matrix Fit :: Matrix-to-Table
muScatt-Eq1	Table	Hidden	30.10.19 14:09	Fitting Curve
out12t1	Table	Normal	29.10.19 11:54	/Users/pipich/Documents/sans/qtisas-documentation/MuScatt/sample-12t1/out12t1.txt

Project Explorer Results Log

„muScatt-Eq1“ -> „active“ dataset

“out12t1”: dataset generated by Muscatt Program [H. Frielinghaus]; for comparison

„muscatt“ table, generated in QtiSAS

QtISAS - /Users/pipich/Documents/sans-qtisas-documentation/MuScatt/sample-121/sample-121.qti\*

muscatt - Matrix Fit :: Matrix-to-Table

	Q[X]	I[Y]	dI[yEr]	Eq1[Y]	dEq1[yEr]	Eq3[Y]	dEq3[yEr]	Eq2[Y]	dEq2[yEr]	Eq1reversal[Y]	dEq1reversal[yEr]	Eq3revers	
1	2.87000E-03	5.30631E+02	4.22951E+00	2.97342E+02	2.42774E+00	2.99687E+02	2.41291E+00	2.94835E+02	2.41291E+00	1.03409E+03	1.17395E+01	1.0631	
2	3.23000E-03	4.85142E+02	3.38612E+00	2.63190E+02	1.94364E+00	2.64985E+02	1.93176E+00	2.60694E+02	1.93176E+00	9.98439E+02	9.39859E+00	1.0271	
3	3.59000E-03	4.71822E+02	3.02934E+00	2.51045E+02	1.73884E+00	2.52653E+02	1.72822E+00	2.48562E+02	1.72822E+00	9.84661E+02	8.40831E+00	1.0131	
4	3.94000E-03	4.71681E+02	2.86387E+00	2.50033E+02	1.64386E+00	2.51637E+02	1.63382E+00	2.47562E+02	1.63382E+00	9.81928E+02	7.94902E+00	1.0101	
5	4.30000E-03	4.68257E+02	2.70481E+00	2.47913E+02	1.55256E+00	2.49496E+02	1.54308E+00	2.45457E+02	1.54308E+00	9.77922E+02	7.50753E+00	1.0061	
6	4.66000E-03	4.65639E+02	2.59009E+00	2.47262E+02	1.48671E+00	2.48850E+02	1.47763E+00	2.44821E+02	1.47763E+00	9.75261E+02	7.18911E+00	1.0044	
7	5.02000E-03	4.67409E+02	2.46438E+00	2.46772E+02	1.41456E+00	2.48367E+02	1.40591E+00	2.44346E+02	1.40591E+00	9.72619E+02	6.84019E+00	1.0011	
8	5.38000E-03	4.57181E+02	2.34590E+00	2.39922E+02	1.34655E+00	2.41422E+02	1.33832E+00	2.37513E+02	1.33832E+00	9.63516E+02	6.51133E+00	9.9201	
9	5.74000E-03	4.52442E+02	2.23230E+00	2.36643E+02	1.28134E+00	2.38106E+02	1.27351E+00	2.34251E+02	1.27351E+00	9.57886E+02	6.19602E+00	9.8621	
10	6.10000E-03	4.51202E+02	2.18190E+00	2.35962E+02	1.25241E+00	2.37433E+02	1.24476E+00	2.33589E+02	1.24476E+00	9.54764E+02	6.05613E+00	9.8301	
11	6.45000E-03	4.48374E+02	2.11513E+00	2.40658E+02	1.21409E+00	2.42224E+02	1.20667E+00	2.38302E+02	1.20667E+00	9.57004E+02	5.87080E+00	9.8531	
12	6.75000E-03	4.72536E+02	1.63254E+00	2.42560E+02	9.37080E-01	2.44174E+02	9.31354E-01	2.40220E+02	9.31354E-01	9.56749E+02	4.53132E+00	9.8501	
13	6.81000E-03	4.50396E+02	2.05879E+00	2.40582E+02	1.18175E+00	2.42167E+02	1.17453E+00	2.38246E+02	1.17453E+00	9.54333E+02	5.71442E+00	9.8261	
14	7.17000E-03	4.43368E+02	1.96855E+00	2.35607E+02	1.12995E+00	2.37129E+02	1.12305E+00	2.32320E+02	1.12305E+00	9.46678E+02	5.46395E+00	9.7471	
15	7.50000E-03	4.55588E+02	1.43665E+00	2.41138E+02	8.24639E-01	2.42769E+02	8.19600E-01	2.38839E+02	8.19600E-01	9.49695E+02	3.98760E+00	9.7781	
16	7.53000E-03	4.49744E+02	1.91330E+00	2.41195E+02	1.09824E+00	2.42829E+02	1.09153E+00	2.38897E+02	1.09153E+00	9.49521E+02	5.31060E+00	9.7761	
17	7.89000E-03	4.50846E+02	1.87523E+00	2.39746E+02	1.07638E+00	2.41377E+02	1.06981E+00	2.37469E+02	1.06981E+00	9.45273E+02	5.20493E+00	9.7331	
18	8.25000E-03	4.38710E+02	1.78848E+00	2.39632E+02	1.02659E+00	2.41282E+02	1.02032E+00	2.37376E+02	1.02032E+00	9.42312E+02	4.96415E+00	9.7021	
19	8.25000E-03	4.53416E+02	1.34031E+00	2.39632E+02	7.69339E-01	2.41282E+02	7.64639E-01	2.37376E+02	7.64639E-01	9.42312E+02	3.72020E+00	9.7021	
20	8.61000E-03	4.43387E+02	1.77892E+00	2.37969E+02	1.02110E+00	2.39613E+02	1.01486E+00	2.35733E+02	1.01486E+00	9.37756E+02	4.93761E+00	9.6561	
21	8.96000E-03	4.41354E+02	1.73094E+00	2.39221E+02	9.93562E-01	2.40906E+02	9.87491E-01	2.37006E+02	9.87491E-01	9.36162E+02	4.80444E+00	9.6391	
22	9.00000E-03	4.48674E+02	1.28465E+00	2.39644E+02	7.37391E-01	2.41339E+02	7.32885E-01	2.37431E+02	7.32885E-01	9.36258E+02	3.56570E+00	9.6401	
23	9.32000E-03	4.42541E+02	1.69348E+00	2.38675E+02	9.72059E-01	2.40372E+02	9.66120E-01	2.36481E+02	9.66120E-01	9.32656E+02	4.70046E+00	9.6031	
24	9.68000E-03	4.41451E+02	1.68109E+00	2.40227E+02	9.64948E-01	2.41971E+02	9.59052E-01	2.38054E+02	9.59052E-01	9.31213E+02	4.66607E+00	9.5881	
25	9.75000E-03	4.46555E+02	1.22714E+00	2.40623E+02	7.04380E-01	2.42379E+02	7.00076E-01	2.38454E+02	7.00076E-01	9.31025E+02	3.40608E+00	9.5861	
26	1.00400E-02	4.39321E+02	1.71162E+00	2.38318E+02	9.82472E-01	2.40053E+02	9.76469E-01	2.36166E+02	9.76469E-01	9.26291E+02	4.75081E+00	9.5381	
27	1.04000E-02	4.38891E+02	1.73804E+00	2.41743E+02	9.97637E-01	2.43555E+02	9.91542E-01	2.39612E+02	9.91542E-01	9.26685E+02	4.82414E+00	9.5421	
28	1.05000E-02	4.47934E+02	1.17414E+00	2.43437E+02	6.73958E-01	2.45283E+02	6.69840E-01	2.41312E+02	6.69840E-01	9.27534E+02	3.25897E+00	9.5501	
29	1.07600E-02	4.40155E+02	1.67613E+00	2.42759E+02	9.62101E-01	2.44610E+02	9.56222E-01	2.40650E+02	9.56222E-01	9.24657E+02	4.65230E+00	9.5211	
30	1.11200E-02	4.40473E+02	1.62208E+00	2.44141E+02	9.31076E-01	2.46037E+02	9.25387E-01	2.42053E+02	9.25387E-01	9.22984E+02	4.50228E+00	9.5031	
31	1.12500E-02	4.44850E+02	1.12660E+00	2.44514E+02	6.46670E-01	2.46423E+02	6.42719E-01	2.42433E+02	6.42719E-01	9.22252E+02	3.12702E+00	9.4961	
32	1.14700E-02	4.36580E+02	1.56530E+00	2.42291E+02	8.98484E-01	2.44177E+02	8.92994E-01	2.40223E+02	8.92994E-01	9.18160E+02	4.34468E+00	9.4541	
33	1.1												
34	1.2												
35	1.2												
36	1.25500E-02	4.39058E+02	1.49588E+00	2.49041E+02	8.58637E-01	2.51102E+02	8.53391E-01	2.47036E+02	8.53391E-01	9.15716E+02	4.15200E+00	9.4281	
37	1.27500E-02	4.43650E+02	1.04775E+00	2.54443E+02	8.91410E-01	2.56604E+02	8.87335E-01	2.52449E+02	8.87335E-01	9.19417E+02	2.90816E+00	9.4661	
38	1.29100E-02	4.48104E+02	1.48278E+00	2.59477E+02	8.51117E-01	2.61730E+02	8.45917E-01	2.57492E+02	8.45917E-01	9.23093E+02	4.11564E+00	9.5031	
39	1.32700E-02	4.55368E+02	1.46628E+00	2.63347E+02	8.41646E-01	2.65685E+02	8.36504E-01	2.61383E+02	8.36504E-01	9.23912E+02	4.06984E+00	9.5111	
40	1.35000E-02	4.45342E+02	1.01401E+00	2.61260E+02	8.2043E-01	2.63576E+02	8.18487E-01	2.59308E+02	8.18487E-01	9.19879E+02	2.81451E+00	9.4701	
41	1.36200E-02	4.48890E+02	1.44355E+00	2.62417E+02	8.28599E-01	2.64759E+02	8.23537E-01	2.60473E+02	8.23537E-01	9.20023E+02	4.00675E+00	9.4711	
42	1.39800E-02	4.53118E+02	1.43637E+00	2.66903E+02	8.24478E-01	2.69339E+02	8.19441E-01	2.64978E+02	8.19441E-01	9.21476E+02	3.98682E+00	9.4851	
43	1.42500E-02	4.52466E+02	1.00461E+00	2.67035E+02	8.11385E-01	2.69488E+02	8.06428E-01	2.65125E+02	8.06428E-01	9.19340E+02	2.78842E+00	9.4631	
44	1.43400E-02	4.50116E+02	1.41356E+00	2.67113E+02	8.11385E-01	2.69572E+02	8.06428E-01	2.65205E+02	8.06428E-01	9.18663E+02	3.92351E+00	9.4561	
45	1.47000E-02	4.53648E+02	1.40556E+00	2.70570E+02	8.06793E-01	2.73107E+02	8.01864E-01	2.68685E+02	8.01864E-01	9.19110E+02	3.90130E+00	9.4611	
46	1.50000E-02	4.56915E+02	9.75160E-01	2.72621E+02	5.59743E-01	2.75207E+02	5.56323E-01	2.70751E+02	5.56323E-01	9.18661E+02	2.70668E+00	9.4561	

„muscatt“ table, generated in QtISAS

FITTABLE(s)

Load Fitting Session

Select Function

Fitting Session

Categories

- ALL
- BS-BackScattering
- Block Copolymer Micelles
- Core::Shell
- Density Profile
- Distribution
- EGOR-FUNCTIONS
- EMBL
- End-cap-Thomas
- Flo
- Form Factors
- Form Structure
- General
- HF
- Instrumentation
- Integrals Test
- Liposomes
- MARGARITA
- NRP.functions

Functions

- muscatt
- muscatt-example-1211
- muscatt-example-1212
- muscatt-example-511
- muscatt-example-512
- muscatt-example-kugel
- muscatt-example-polyres

[Instrumental Fit]

[Global Fit]

[Superpositional Function]

[show ONLY eFit functions]

SANS

# Curves: 1

# Functions: 1

e-FIT

e-Fit+++

no-fit yes-simulate color=blue name=muScatt-Eq1 no-log

Info :: Function

Info :: Parameters

Options

Fit Curve [1D fit]

v.18-29.10.2019

Vitaliy Pipich @ JCNS

COMPILE

FITTABLE(s)

Project Explorer

Name	Type	View	Created	Label
data-1211	Table	Normal	29.10.19 17:35	/Users/pipich/Documents/sans/qtisas-documentation/MuScatt/sample-1211/data1211.DAT.txt
Graph-1211	Graph	Normal	29.10.19 17:36	
muscatt	Table	Maximized	30.10.19 14:09	Matrix Fit :: Matrix-to-Table
muScatt-Eq1	Table	Hidden	30.10.19 14:09	Fitting Curve
out1211	Table	Normal	29.10.19 11:54	/Users/pipich/Documents/sans/qtisas-documentation/MuScatt/sample-1211/out1211.txt

Project Explorer

Results Log

Q[X]	Eq1[Y]	dEq1[yEr]	Eq3[Y]	dEq3[yEr]	Eq2[Y]	dEq2[yEr]	Eq1reversal[Y]	dEq1reversal[Y]
1	0.00287	297.34	2.4277	299.69	2.4129	294.84	2.4129	1034.1
2	0.00323	263.19	1.9436	264.99	1.9318	260.69	1.9318	998.44
3	0.00359	251.05	1.7388	252.65	1.7282	248.56	1.7282	984.66
4	0.00394	250.03	1.6439	251.64	1.6338	247.56	1.6338	981.93
5	0.0043	247.91	1.5526	249.5	1.5431	245.46	1.5431	977.92
6	0.00466	247.26	1.4867	248.85	1.4776	244.82	1.4776	975.26
7	0.00502	246.77	1.4146	248.37	1.4059	244.35	1.4059	972.62
8	0.00538	239.92	1.3465	241.42	1.3383	237.51	1.3383	963.52
9	0.00574	236.64	1.2813	238.11	1.2735	234.25	1.2735	957.89
10	0.0061	235.96	1.2524	237.43	1.2448	233.59	1.2448	954.76
11	0.00645	240.66	1.2141	242.22	1.2067	238.3	1.2067	957
12	0.00675	242.56	0.93708	244.17	0.93135	240.22	0.93135	956.75
13	0.00681	240.58	1.1817	242.17	1.1745	238.25	1.1745	954.33
14	0.00717	235.61	1.1299	237.13	1.123	233.29	1.123	946.68
15	0.0075	241.14	0.82464	242.77	0.8196	238.84	0.8196	949.69
16	0.00753	241.19	1.0982	242.83	1.0915	238.9	1.0915	949.52
17							1.0698	945.27
18							1.0203	942.31
19							0.76464	942.31
20							1.0149	937.76
21							0.98749	936.16
22	0.009	239.04	0.73739	241.34	0.73289	237.43	0.73289	936.26
23	0.00932	238.67	0.97206	240.37	0.96612	236.48	0.96612	932.66
24	0.00968	240.23	0.96495	241.97	0.95905	238.05	0.95905	931.21
25	0.00975	240.62	0.70438	242.38	0.70008	238.45	0.70008	931.02
26	0.01004	238.32	0.98247	240.05	0.97647	236.17	0.97647	926.29
27	0.0104	241.74	0.99764	243.56	0.99154	239.61	0.99154	926.68
28	0.0105	243.44	0.67396	245.28	0.66984	241.31	0.66984	927.53
29	0.01076	242.76	0.9621	244.61	0.95622	240.65	0.95622	924.66
30	0.01112	244.14	0.93108	246.04	0.92539	242.05	0.92539	922.98
31	0.01125	244.51	0.64667	246.42	0.64272	242.43	0.64272	922.25
32	0.01147	242.29	0.89848	244.18	0.89299	240.22	0.89299	918.16
33	0.01183	243.75	0.8892	245.68	0.88376	241.71	0.88376	916.56
34	0.012	245.25	0.61722	247.21	0.61345	243.21	0.61345	916.6
35	0.01219	245.09	0.87691	247.07	0.87156	243.07	0.87156	914.83
36	0.01255	249.04	0.85864	251.1	0.85339	247.04	0.85339	915.72
37	0.01275	254.44	0.60141	256.6	0.59774	252.45	0.59774	919.42
38	0.01291	259.48	0.85112	261.73	0.84592	257.49	0.84592	923.09
39	0.01327	263.35	0.84165	265.69	0.8365	261.38	0.8365	923.91
40	0.0135	261.26	0.58204	263.58	0.57849	259.91	0.57849	919.88
41	0.01362	262.42	0.8286	264.76	0.82354	260.47	0.82354	920.02
42	0.01398	266.9	0.82448	269.34	0.81944	264.98	0.81944	921.48
43	0.01425	267.03	0.57665	269.49	0.57312	265.13	0.57312	919.34
44	0.01434	267.11	0.81139	269.57	0.80643	265.21	0.80643	918.66
45	0.0147	270.57	0.80679	273.11	0.80186	268.68	0.80186	919.11
46	0.015	272.62	0.55974	275.21	0.55632	270.75	0.55632	918.66

“out12t1”: dataset generated by Muscatt Program [H. Frielinghaus]; for comparison

FITTABLE(s)

Load Fitting Session

Select Function

Fitting Session

Categories

- ALL
- BS-BackScattering
- Block Copolymer Micelles
- Core::Shell
- Density Profile
- Distribution
- EGOR-FUNCTIONS
- EMBL
- End-cap-Thomas
- Flo
- Form Factors
- Form Structure
- General
- HF
- Instrumentation
- Integrals Test
- Liposomes
- MARGARITA
- NPD.functions

Functions

- muscatt
- muscatt-example-12t1
- muscatt-example-12t2
- muscatt-example-5t1
- muscatt-example-5t2
- muscatt-example-kugel
- muscatt-example-polyres

[Instrumental Fit]

[Global Fit]

[Superpositional Function]

[show ONLY eFit functions]

SANS

# Curves: 1

# Functions: 1

e-FIT e-Fit+++

no-fit yes-simulate color=blue name=muScatt-Eq1 no-log

Info :: Function Info :: Parameters Options

Fit Curve [1D fit] v.18-29.10.2019 Vitaliy Pipich @ JCNS

COMPILE FITTABLE(s)

Project Explorer

Name	Type	View	Created	Label
data12t1	Table	Normal	29.10.19 17:35	/Users/pipich/Documents/sans/qtisas-documentation/MuScatt/sample-12t1/data12t1.DAT.txt
Graph-res	Graph	Normal	29.10.19 17:36	
muScatt	Table	Normal	30.10.19 14:09	Matrix Fit :: Matrix-to-Table
muScatt-Eq1	Table	Hidden	30.10.19 14:09	Fitting Curve
out12t1	Table	Maximized	29.10.19 11:54	/Users/pipich/Documents/sans/qtisas-documentation/MuScatt/sample-12t1/out12t1.txt

x[X]	y[Y]	weight[yEr]	sigma[xEr]	residues[Y]	Characteristics	Conditions	Parameters	Values	Errors[Y]
1	2.870000E-03	2.973418E+02	1.000000E+00	0.000000E+00	2.332892E+02	Fitting Function	-> muscatt-example-12t1	lowQ	0 ---
2	3.230000E-03	2.631898E+02	1.000000E+00	0.000000E+00	2.219522E+02	Number of Parameters	-> 17	bgksub	2.7 ---
3	3.590000E-03	2.510454E+02	1.000000E+00	0.000000E+00	2.207766E+02	Time of Simulation	-> 60 ms	lambda	12 ---
4	3.940000E-03	2.500328E+02	1.000000E+00	0.000000E+00	2.216482E+02	x-Range Source	-> Same x as Fitting Data	d	0.1 ---
5	4.300000E-03	2.479130E+02	1.000000E+00	0.000000E+00	2.203440E+02	x-min	-> 0.00287	transm	0.179 ---
6	4.660000E-03	2.472624E+02	1.000000E+00	0.000000E+00	2.183766E+02	x-max	-> 0.17821	sigmia	3.6442 ---
7	5.020000E-03	2.467716E+02	1.000000E+00	0.000000E+00	2.206374E+02	Number Points	-> 211	hgqmod	1 ---
8	5.380000E-03	2.399218E+02	1.000000E+00	0.000000E+00	2.172592E+02	Logarithmic Step	-> Yes	hgqcut	0.0689 ---
9	5.740000E-03	2.366429E+02	1.000000E+00	0.000000E+00	2.157991E+02	Dataset	-> data12t1_I	resmod	-1 ---
10	6.100000E-03	2.359625E+02	1.000000E+00	0.000000E+00	2.152395E+02	SANS mode	-> No	difwhm	0.1 ---
11	6.450000E-03	2.406579E+02	1.000000E+00	0.000000E+00	2.077161E+02	N	-> 211	detlen	20 ---
12	6.810000E-03	2.405824E+02	1.000000E+00	0.000000E+00	2.098136E+02	np	-> 1	sampap	0.01 ---
13	7.170000E-03	2.356072E+02	1.000000E+00	0.000000E+00	2.077608E+02	DoF=N-np	-> 210	collen	20 ---
14	7.530000E-03	2.411947E+02	1.000000E+00	0.000000E+00	2.085493E+02	chi^2	-> 4.0622074087E+06	entrap	0.03 ---
15	7.890000E-03	2.397456E+02	1.000000E+00	0.000000E+00	2.111004E+02	chi^2/DoF	-> 1.9343844803E+04	reswdt	2 ---
16	8.250000E-03	2.396323E+02	1.000000E+00	0.000000E+00	1.990777E+02	TSS	-> 1.3292282506E+07	thkmod	0 ---
17	8.610000E-03	2.379691E+02	1.000000E+00	0.000000E+00	2.054179E+02	R^2=1-chi^2/TSS	-> 6.9439353949E-01	activeOutput	1 ---
18	8.960000E-03	2.392214E+02	1.000000E+00	0.000000E+00	2.021326E+02	R=1-sqrt(chi^2/TSS)	-> 4.4718315826E-01		
19	9.320000E-03	2.386750E+02	1.000000E+00	0.000000E+00	2.038660E+02				
20	9.680000E-03	2.402268E+02	1.000000E+00	0.000000E+00	2.012242E+02				
21	1.004000E-02	2.383182E+02	1.000000E+00	0.000000E+00	2.010028E+02				
22	1.040000E-02	2.417426E+02	1.000000E+00	0.000000E+00	1.971484E+02				
23	1.076000E-02	2.427592E+02	1.000000E+00	0.000000E+00	1.955397E+02				
24	1.112000E-02	2.441411E+02	1.000000E+00	0.000000E+00	1.917103E+02				
25	1.147000E-02	2.422908E+02	1.000000E+00	0.000000E+00	1.900169E+02				
26	1.183000E-02	2.437523E+02	1.000000E+00	0.000000E+00	1.886274E+02				
27	1.219000E-02	2.450917E+02	1.000000E+00	0.000000E+00	1.864728E+02				
28	1.255000E-02	2.490411E+02	1.000000E+00	0.000000E+00	1.862152E+02				
29	1.291000E-02	2.594766E+02	1.000000E+00	0.000000E+00	1.830033E+02				
30	1.327000E-02	2.633474E+02	1.000000E+00	0.000000E+00	1.830033E+02				
31	1.362000E-02	2.624172E+02	1.000000E+00	0.000000E+00	1.808680E+02				
32	1.398000E-02	2.669028E+02	1.000000E+00	0.000000E+00	1.790065E+02				
33	1.434000E-02	2.671127E+02	1.000000E+00	0.000000E+00	1.811510E+02				
34	1.470000E-02	2.705703E+02	1.000000E+00	0.000000E+00	1.808680E+02				
35	1.506000E-02	2.729435E+02	1.000000E+00	0.000000E+00	1.788202E+02				
36	1.542000E-02	2.786750E+02	1.000000E+00	0.000000E+00	1.749405E+02				
37	1.577000E-02	2.859170E+02	1.000000E+00	0.000000E+00	1.758185E+02				
38	1.613000E-02	2.907818E+02	1.000000E+00	0.000000E+00	1.683504E+02				
39	1.649000E-02	2.942295E+02	1.000000E+00	0.000000E+00	1.725545E+02				
40	1.685000E-02	2.969455E+02	1.000000E+00	0.000000E+00	1.682376E+02				
41	1.721000E-02	3.048406E+02	1.000000E+00	0.000000E+00	1.712782E+02				
42	1.757000E-02	3.104705E+02	1.000000E+00	0.000000E+00	1.664065E+02				
43	1.792000E-02	3.185644E+02	1.000000E+00	0.000000E+00	1.675499E+02				
44	1.828000E-02	3.213258E+02	1.000000E+00	0.000000E+00					
45	1.864000E-02	3.317225E+02	1.000000E+00	0.000000E+00					
46	1.900000E-02	3.373121E+02	1.000000E+00	0.000000E+00					

„muScatt-Eq1“ -> „active“ dataset

FITTABLE(s)

Load Fitting Session

Select Function

Fitting Session

Categories

- ALL
- BS-BackScattering
- Block Copolymer Micelles
- Core::Shell
- Density Profile
- Distribution
- EGOR-FUNCTIONS
- EMBL
- End-cap-Thomas
- Flo
- Form Factors
- Form Structure
- General
- HF
- Instrumentation
- Integrals Test
- Liposomes
- MARGARITA
- NRP.functions

Functions

- muscatt
- muscatt-example-12t1
- muscatt-example-12t2
- muscatt-example-5t1
- muscatt-example-5t2
- muscatt-example-kugel
- muscatt-example-polyres

[Instrumental Fit]

[Global Fit]

[Superpositional Function]

[show ONLY eFit functions]

SANS

# Curves: 1

# Functions: 1

e-FIT

e-Fit+++

no-fit yes-simulate color=blue name=muScatt-Eq1 no-log

Info :: Function

Info :: Parameters

Options

Fit Curve [1D fit]

v.18-29.10.2019

Vitaliy Pipich @ JCNS

COMPILE

FITTABLE(s)

Project Explorer

Name	Type	View	Created	Label
data12t1	Table	Normal	29.10.19 17:35	/Users/pipich/Documents/sans/qtisas-documentation/MuScatt/sample-12t1/data12t1.DAT.txt
Graph-res	Graph	Normal	29.10.19 17:36	
muscatt	Table	Normal	30.10.19 14:09	Matrix Fit :: Matrix-to-Table
muScatt-Eq1	Table	Maximized	30.10.19 14:09	Fitting Curve
out12t1	Table	Normal	29.10.19 11:54	/Users/pipich/Documents/sans/qtisas-documentation/MuScatt/sample-12t1/out12t1.txt

# E-Fit mode explanation



## e-Fit Options:

- „no-fit“ : we use just Fitting interface for calculations;
- “yes-simulate“: we calculate & plot active dataset;
- „color=blue“: just selection of color;
- „name=miScatt-Eq1“: instead of classical name of fitting curve we use given name;
- “no-log“: we show no output in log window

The image shows the 'FITTABLE(s)' software interface. The 'Select Function' dialog box is open, showing a list of functions on the left and a list of selected functions on the right. The 'e-FIT' and 'e-Fit+++' tabs are visible, with 'e-Fit+++' selected. A green box highlights the 'e-Fit Options' section, which contains a list of options and their descriptions:

- [1] Script :: Before Fit
- "Before Fit"; to skip it: write here "no-before"
- [2] Fit
- "Fit"; to skip it: write here "no-fit"
- "color=color\_name"; select color of the fitting curve
- [3] Script :: After Fit
- "After Fit"; to skip it: write here "no-after"
- [4] Simulate
- "Simulate"; by default after fit fitting curve is calculated and plotted in the plot;
- name of the default table "fitCurve-FUNCTION-NAME";
- if you want to have "unique" name write here "name=TABLE-NAME"
- in case of "no-fit": if you want just to simulate data select option "yes-simulate"
- [5] Results of the fit is shown in Res-Log: Main-Table
- "no-reslog"; to skip it
- "yes-res-in-plot"; to show results in graph

A green arrow points from the 'E-Fit options' label to the highlighted section. The label 'E-Fit options' is enclosed in a green box.