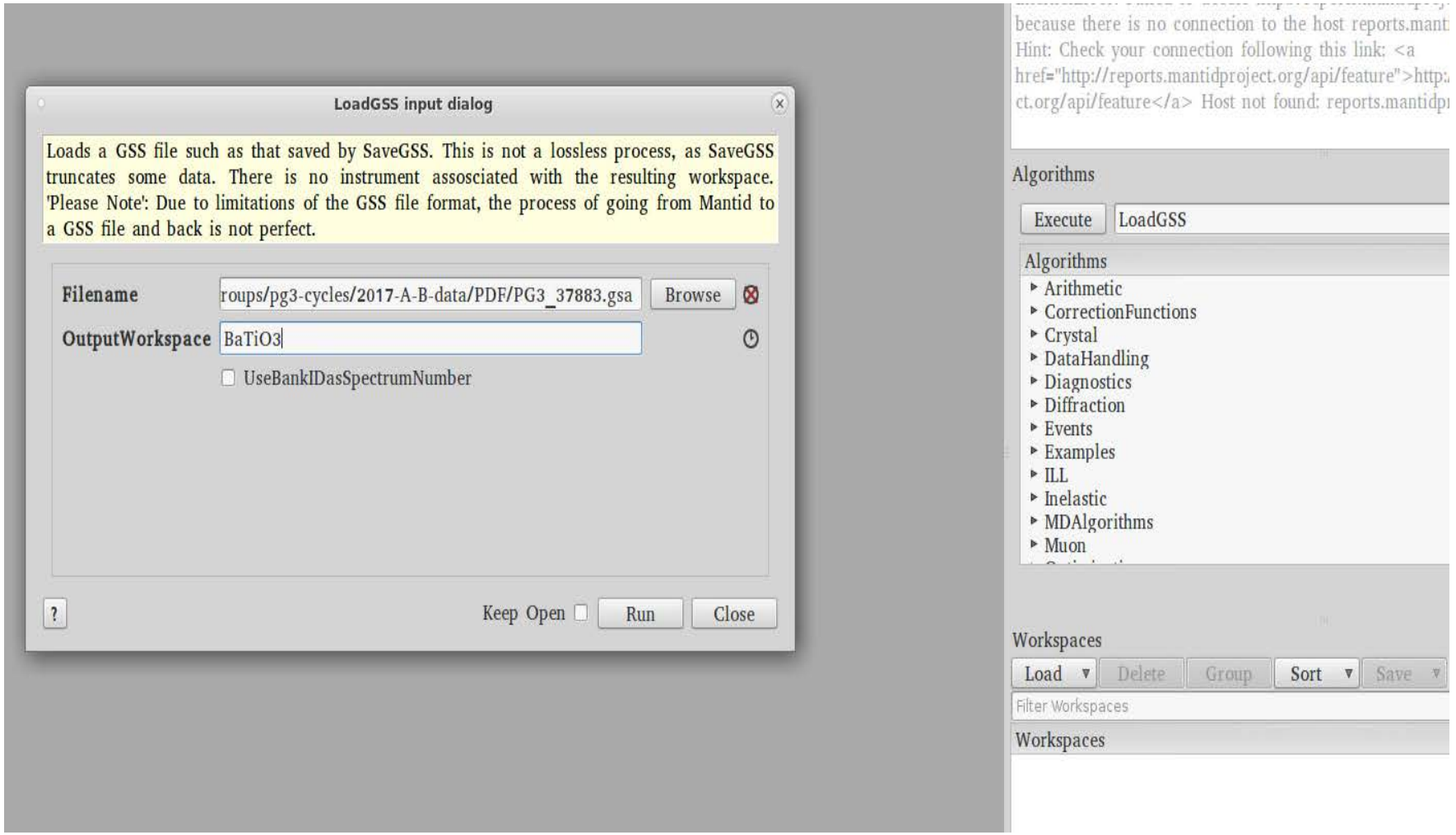
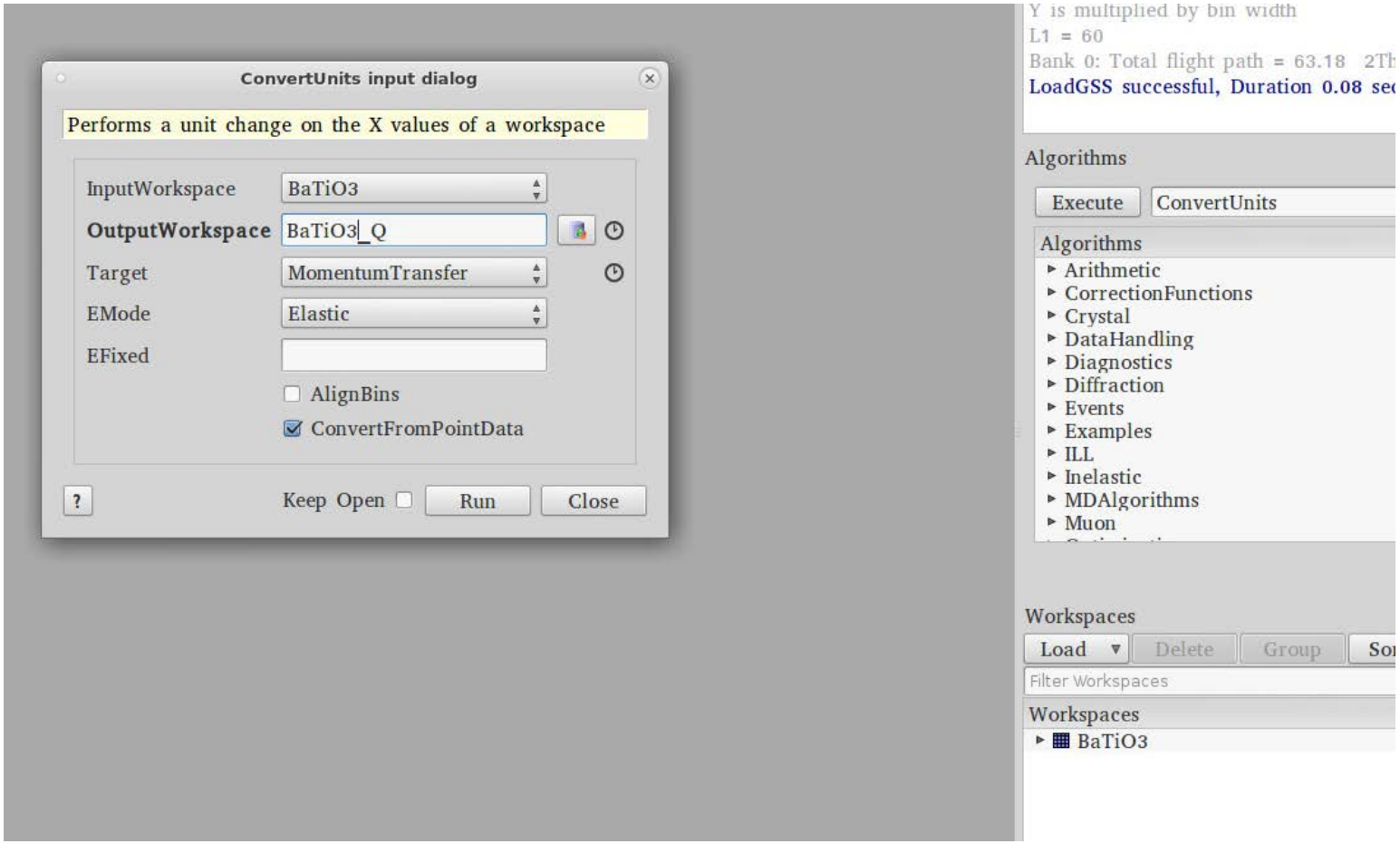
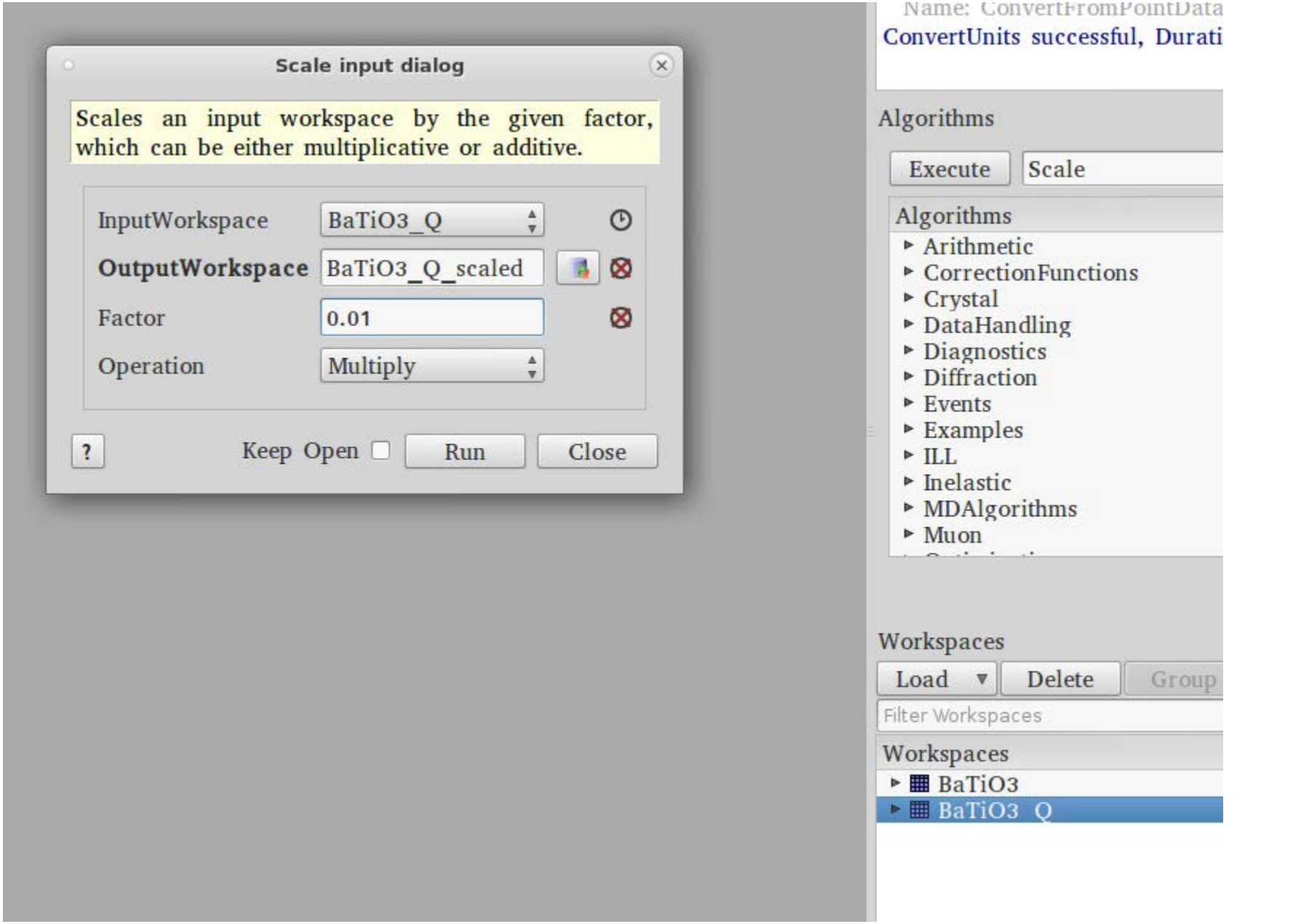
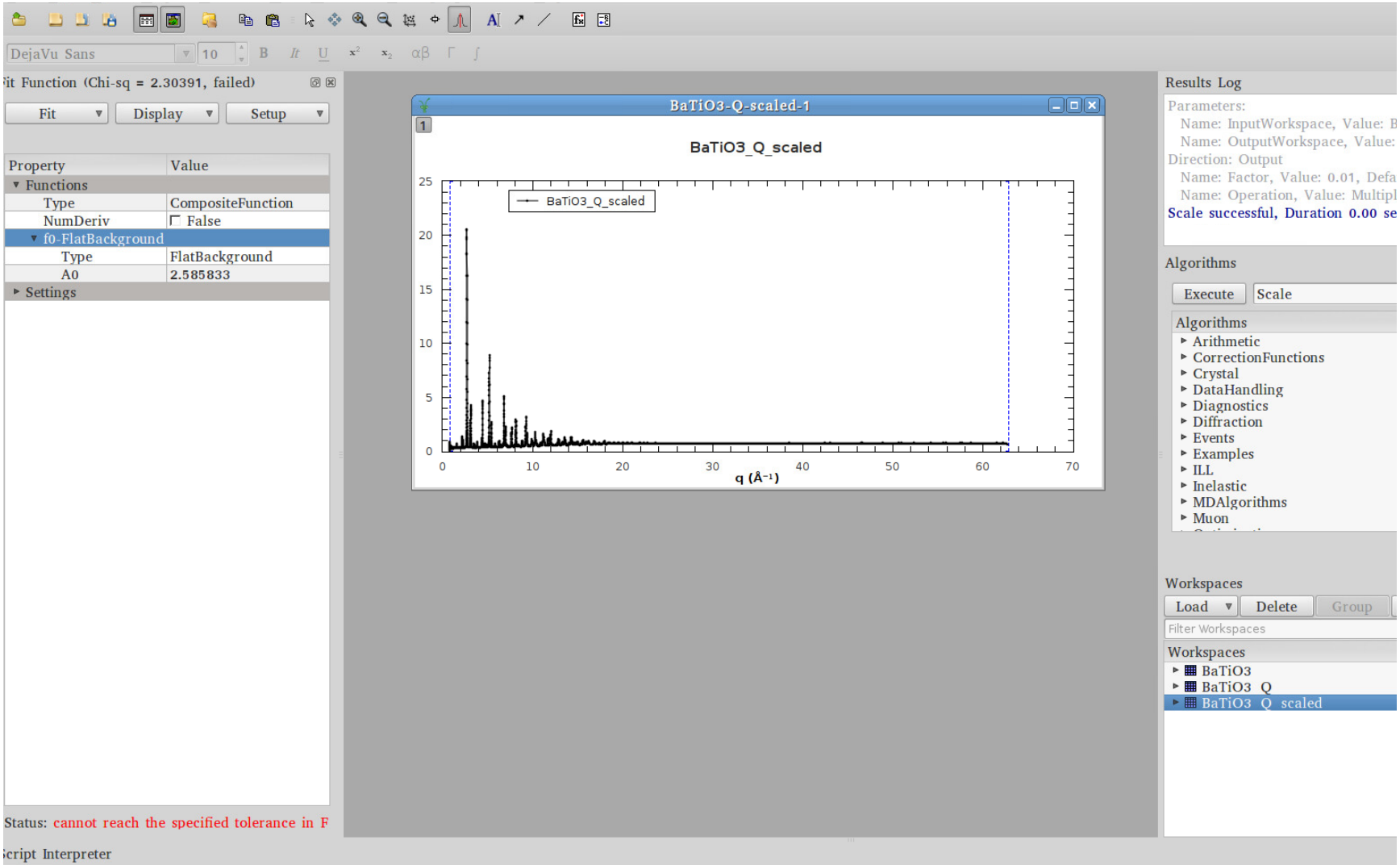
PDF reduction
(no inelastic, absorption or multiple scattering correction for sample, correction is done for V rod)

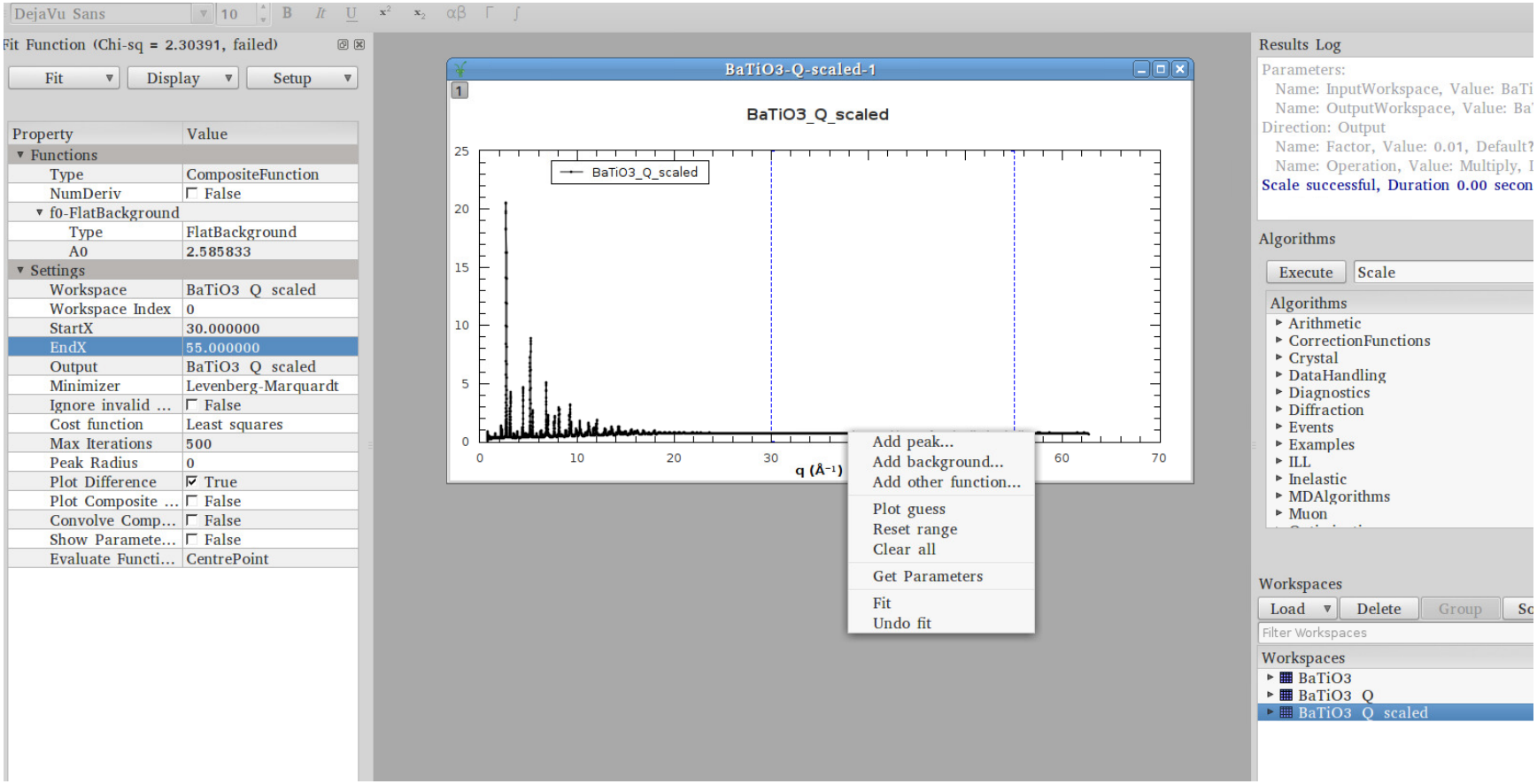
1. In mantidplotnightly use ‘LoadGSS’ to load autoreduced gsas file
2. ‘ConvertUnits’ to momentum transfer
3. ‘Scale’ by Multiplying the data by 0.01
4. Plot Spectrum
5. Fit Q space from 30 – 50 using a flat background
6. Divide the spectrum by the flat background coefficient A0 so that the q data →1 using scale command. This is your arbitrarily normalized S(Q)
7. Now use ‘PDFFourierTransform’ to chose Qmin, Qmax etc. to produce G(r)
8. SavePDFGui to generate Gr for PDFGui which generates relevant header for neutron.

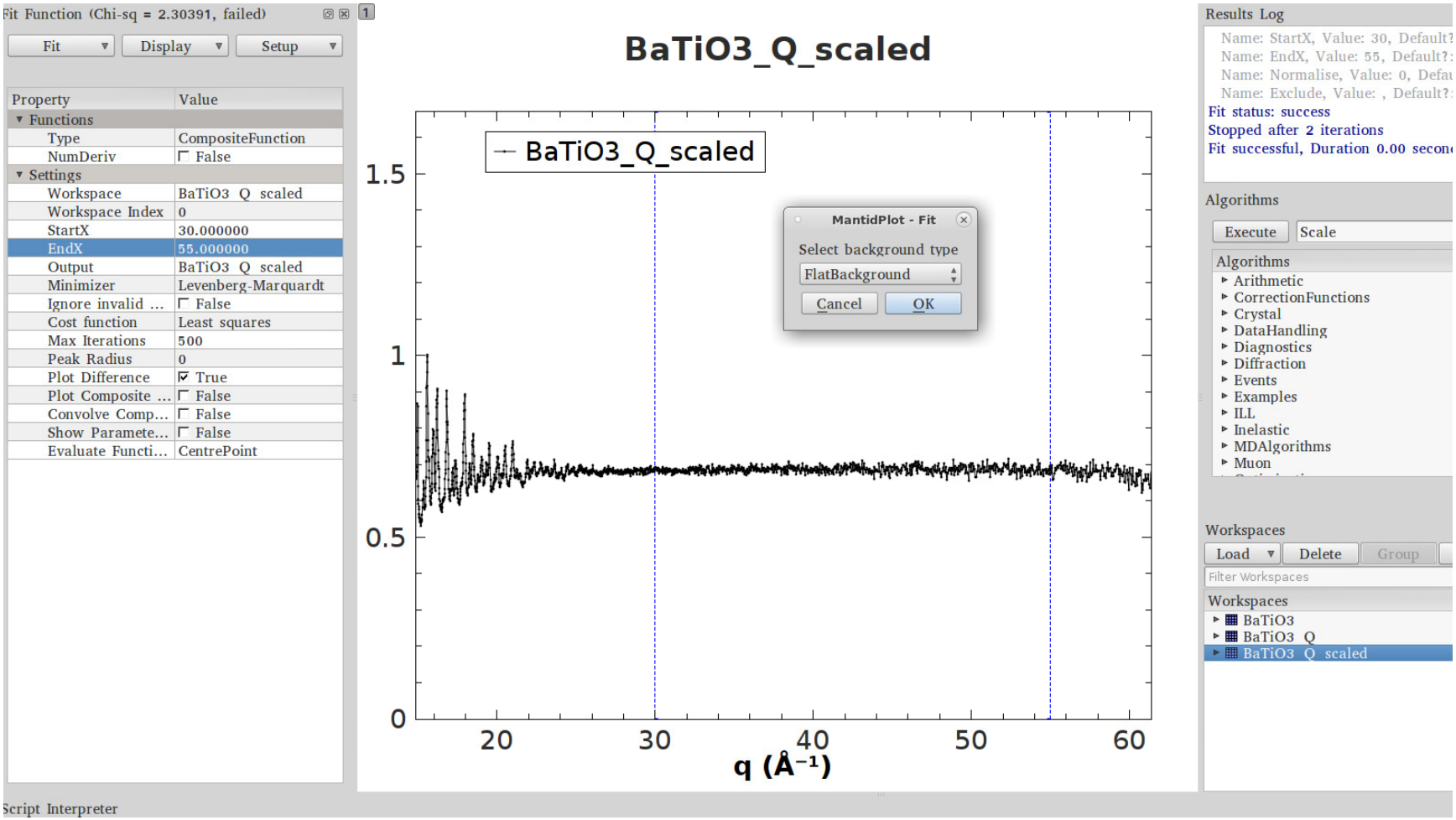

LoadGSS input dialog
Loads a GSS file such as that saved by SaveGSS. This is not a lossless process, as SaveGSS truncates some data. There is no instrument assosciated with the resulting workspace. 'Please Note': Due to limitations of the GSS file format, the process of going from Mantid to a GSS file and back is not perfect.
Filename
roups/pg3-cycles/2017-A-B-data/PDF/PG3_37883.gsa
Browse
OutputWorkspace
BaTiO3
UseBankIDasSpectrumNumber
?
Keep Open
Run
Close
because there is no connection to the host reports.mant
Hint: Check your connection following this link: <a
href="http://reports.mantidproject.org/api/feature">http:
ct.org/api/feature Host not found: reports.mantidp
Algorithms
Execute
LoadGSS
Algorithms
Arithmetic
CorrectionFunctions
Crystal
DataHandling
Diagnostics
Diffraction
Events
Examples
ILL
Inelastic
MDAlgorithms
Muon
Workspaces
Load
Delete
Group
Sort
Save
Filter Workspaces
Workspaces

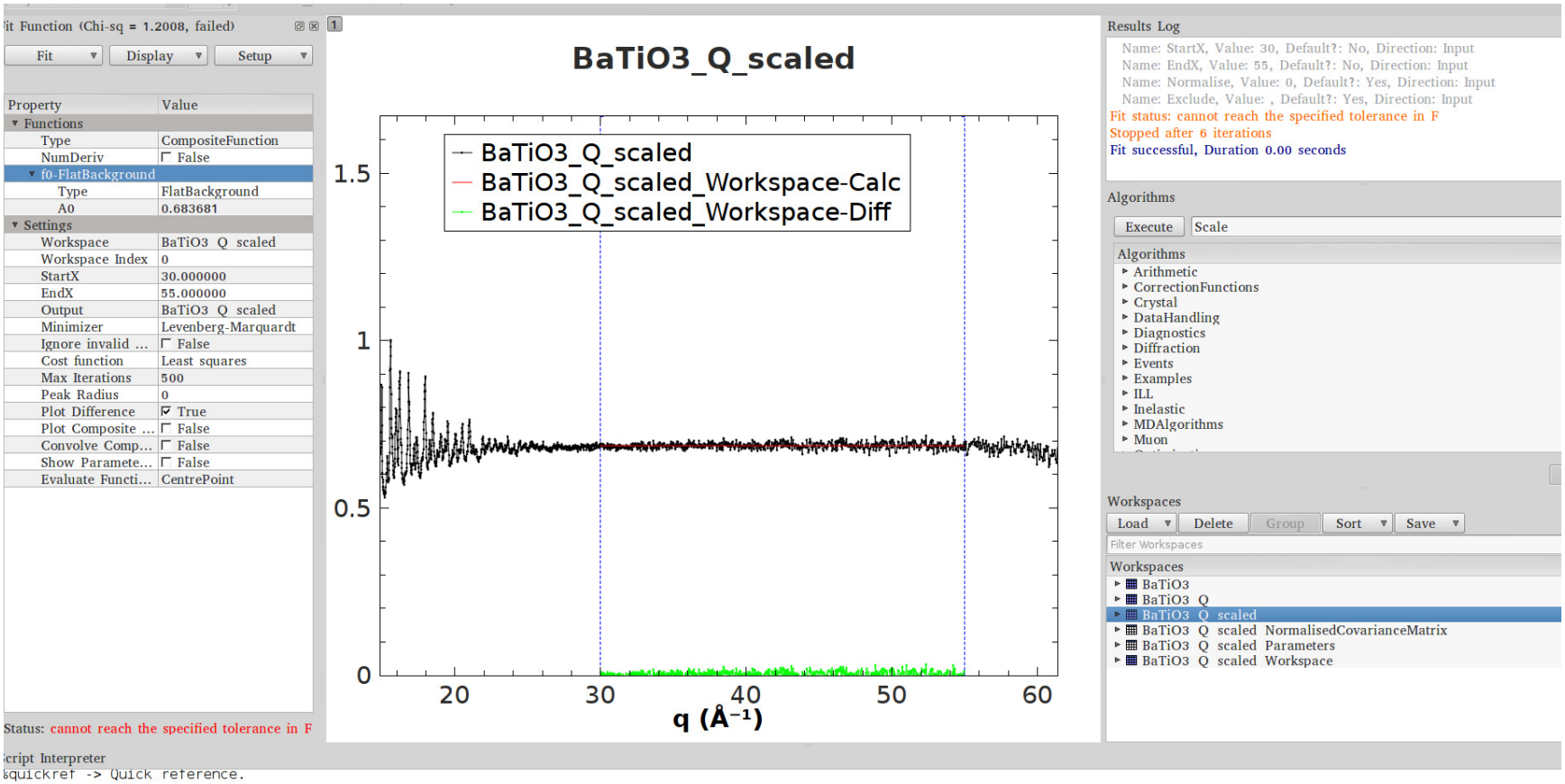

ConvertUnits input dialog
Performs a unit change on the X values of a workspace
InputWorkspace
BaTiO3
OutputWorkspace
BaTiO3_Q
Target
MomentumTransfer
EMode
Elastic
EFixed
AlignBins
ConvertFromPointData
?
Keep Open
Run
Close
Y is multiplied by bin width
L1 = 60
Bank 0: Total flight path = 63.18 2Th
LoadGSS successful, Duration 0.08 sec
Algorithms
Execute
ConvertUnits
Algorithms
Arithmetic
CorrectionFunctions
Crystal
DataHandling
Diagnostics
Diffraction
Events
Examples
ILL
Inelastic
MDAlgorithms
Muon
Workspaces
Load
Delete
Group
Filter Workspaces
Workspaces
BaTiO3

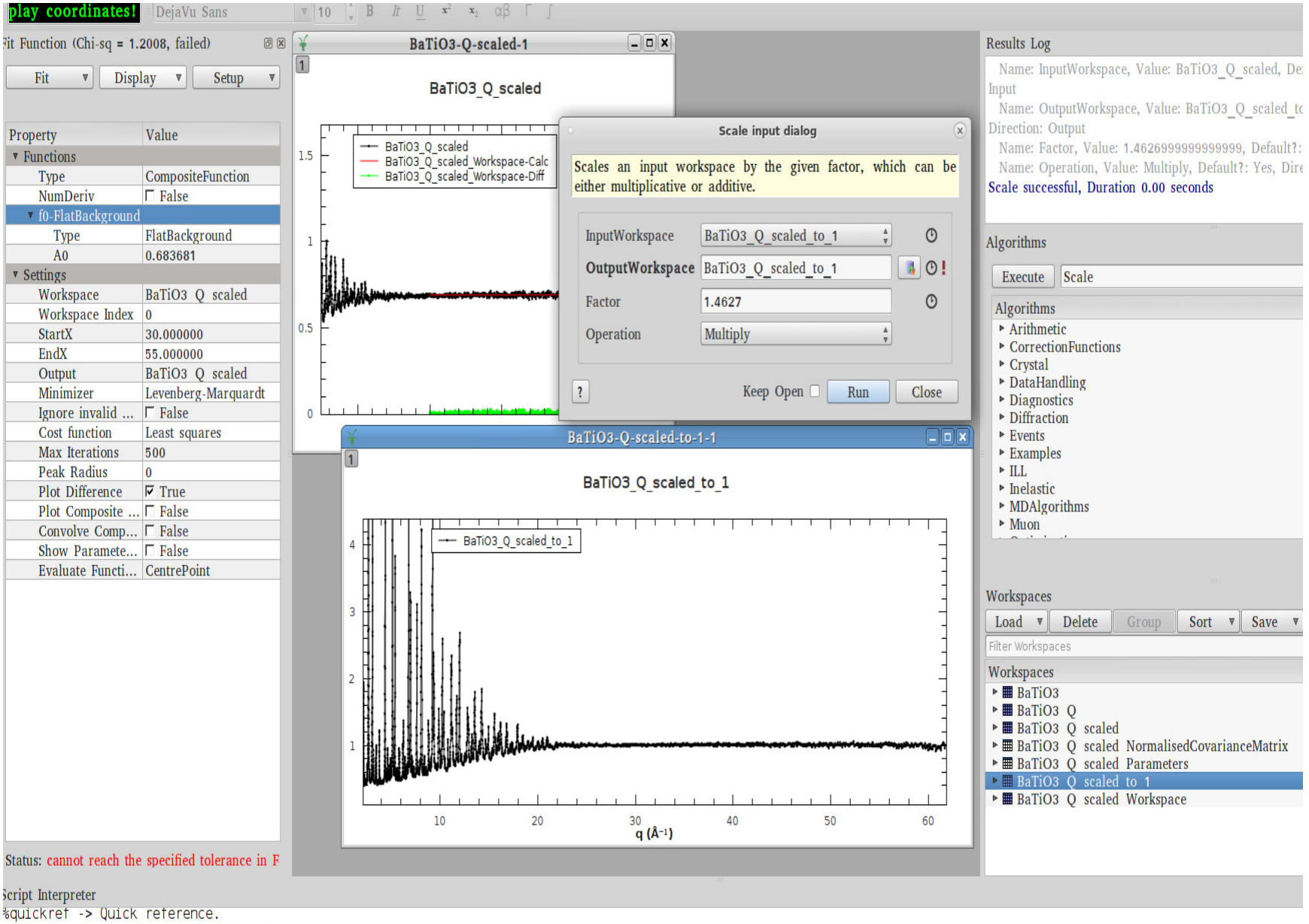

Scale input dialog
Scales an input workspace by the given factor, which can be either multiplicative or additive.
InputWorkspace
BaTiO3_Q
OutputWorkspace
BaTiO3_Q_scaled
Factor
0.01
Operation
Multiply
?
Keep Open
Run
Close
Name: ConvertFromPointData
ConvertUnits successful, Durati
Algorithms
Execute
Scale
Algorithms
Arithmetic
CorrectionFunctions
Crystal
DataHandling
Diagnostics
Diffraction
Events
Examples
ILL
Inelastic
MDAlgorithms
Muon
Workspaces
Load
Delete
Group
Filter Workspaces
Workspaces
BaTiO3
BaTiO3_Q

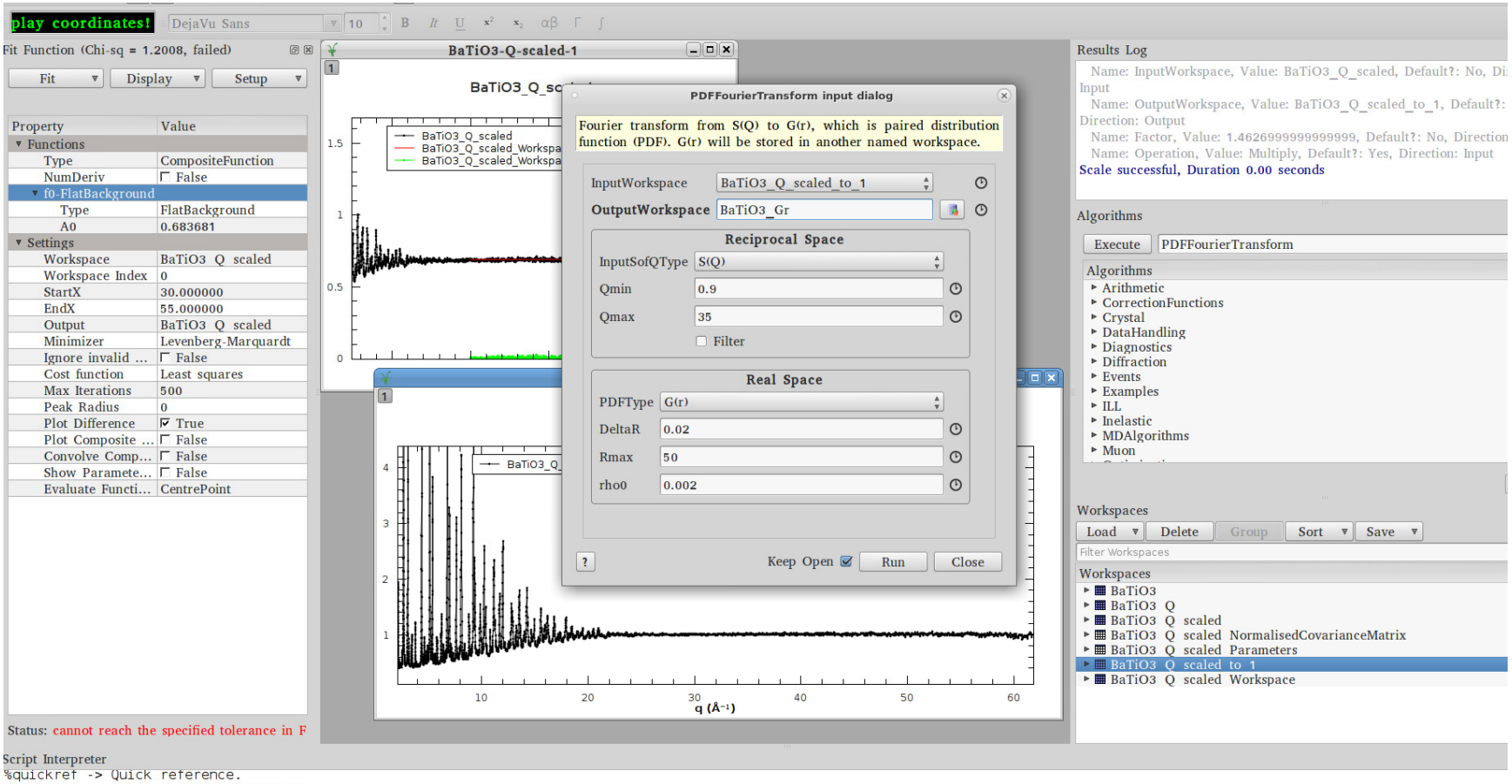

DejaVu Sans
10
Fit Function (Chi-sq = 2.30391, failed)
Fit
Display
Setup
Property
Value
Functions
Type
CompositeFunction
NumDeriv
False
f0-FlatBackground
Type
FlatBackground
A0
2.585833
Settings
Status: cannot reach the specified tolerance in F
Script Interpreter
BaTiO3-Q-scaled-1
BaTiO3_Q_scaled
BaTiO3_Q_scaled
q (Å⁻¹)
Results Log
Parameters:
Name: InputWorkspace, Value: B
Name: OutputWorkspace, Value:
Direction: Output
Name: Factor, Value: 0.01, Defa
Name: Operation, Value: Multipl
Scale successful, Duration 0.00 se
Algorithms
Execute
Scale
Algorithms
Arithmetic
CorrectionFunctions
Crystal
DataHandling
Diagnostics
Diffraction
Events
Examples
ILL
Inelastic
MDAlgorithms
Muon
Workspaces
Load
Delete
Group
Filter Workspaces
Workspaces
BaTiO3
BaTiO3_Q
BaTiO3_Q_scaled

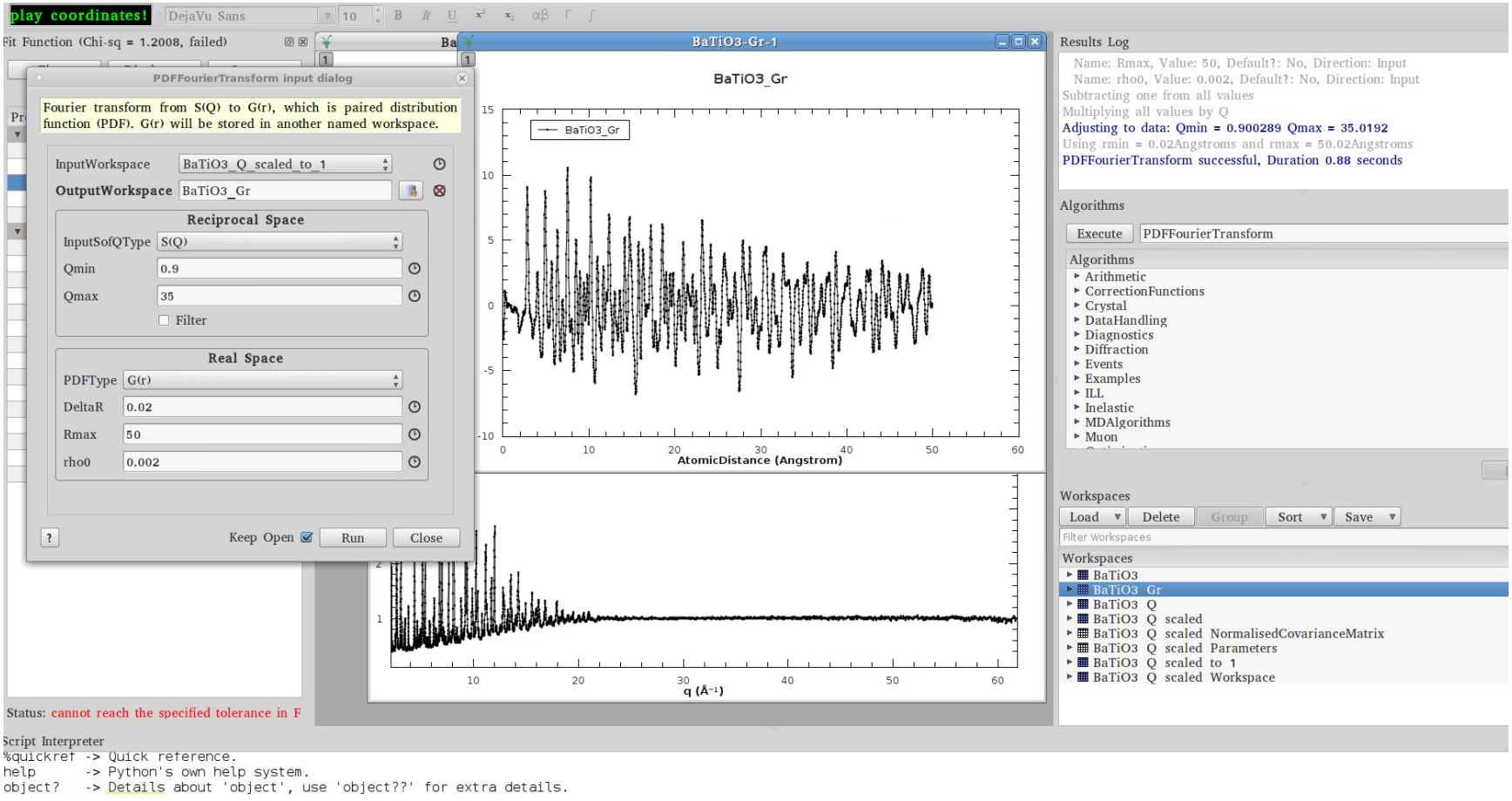

DejaVu Sans
10
Fit Function (Chi-sq = 2.30391, failed)
Fit
Display
Setup
Property
Value
Functions
Type
CompositeFunction
NumDeriv
False
f0-FlatBackground
Type
FlatBackground
A0
2.585833
Settings
Workspace
BaTiO3_Q_scaled
Workspace Index
0
StartX
30.000000
EndX
55.000000
Output
BaTiO3_Q_scaled
Minimizer
Levenberg-Marquardt
Ignore invalid ...
False
Cost function
Least squares
Max Iterations
500
Peak Radius
0
Plot Difference
True
Plot Composite ...
False
Convolve Comp...
False
Show Paramete...
False
Evaluate Functi...
CentrePoint
BaTiO3-Q-scaled-1
BaTiO3_Q_scaled
BaTiO3_Q_scaled
q (Å⁻¹)
Add peak...
Add background...
Add other function...
Plot guess
Reset range
Clear all
Get Parameters
Fit
Undo fit
Results Log
Parameters:
Name: InputWorkspace, Value: BaTi
Name: OutputWorkspace, Value: Ba
Direction: Output
Name: Factor, Value: 0.01, Default?
Name: Operation, Value: Multiply, I
Scale successful, Duration 0.00 secon
Algorithms
Execute
Scale
Algorithms
Arithmetic
CorrectionFunctions
Crystal
DataHandling
Diagnostics
Diffraction
Events
Examples
ILL
Inelastic
MDAlgorithms
Muon
Workspaces
Load
Delete
Group
Filter Workspaces
Workspaces
BaTiO3
BaTiO3_Q
BaTiO3_Q_scaled

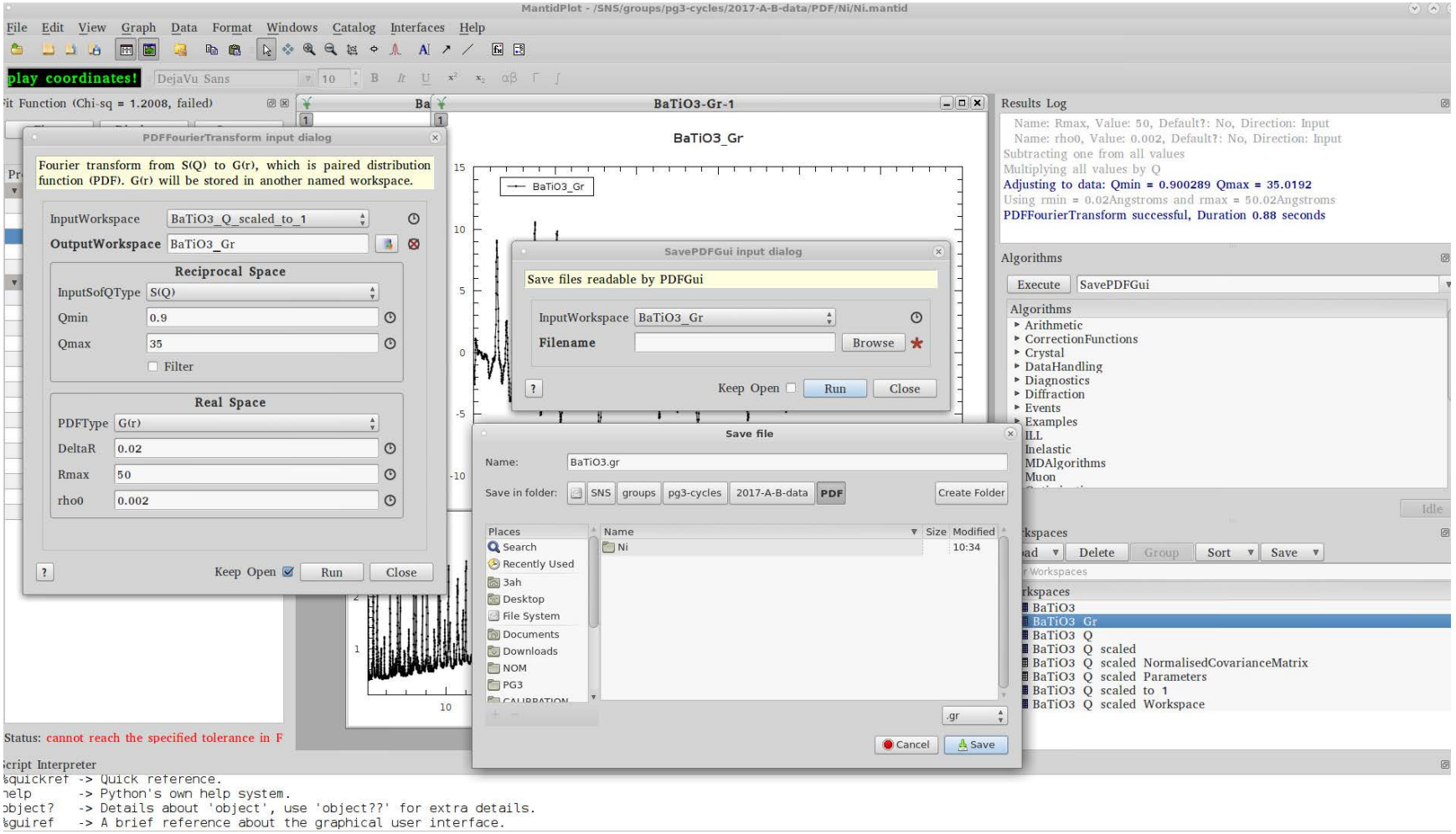

Fit Function (Chi-sq = 2.30391, failed)
Fit
Display
Setup
Property
Value
Functions
Type
CompositeFunction
NumDeriv
False
Settings
Workspace
BaTiO3_Q_scaled
Workspace Index
0
StartX
30.000000
EndX
55.000000
Output
BaTiO3_Q_scaled
Minimizer
Levenberg-Marquardt
Ignore invalid ...
False
Cost function
Least squares
Max Iterations
500
Peak Radius
0
Plot Difference
True
Plot Composite ...
False
Convolve Comp...
False
Show Paramete...
False
Evaluate Functi...
CentrePoint
BaTiO3_Q_scaled
BaTiO3_Q_scaled
MantidPlot - Fit
Select background type
FlatBackground
Cancel
OK
1.5
1
0.5
0
20
30
40
50
60
q (Å⁻¹)
Results Log
Name: StartX, Value: 30, Default?
Name: EndX, Value: 55, Default?
Name: Normalise, Value: 0, Defau
Name: Exclude, Value: , Default?
Fit status: success
Stopped after 2 iterations
Fit successful, Duration 0.00 secon
Algorithms
Execute
Scale
Algorithms
Arithmetic
CorrectionFunctions
Crystal
DataHandling
Diagnostics
Diffraction
Events
Examples
ILL
Inelastic
MDAlgorithms
Muon
Workspaces
Load
Delete
Group
Filter Workspaces
Workspaces
BaTiO3
BaTiO3_Q
BaTiO3_Q_scaled
Script Interpreter


it Function (Chi-sq = 1.2008, failed)
Fit
Display
Setup
Property
Value
Functions
Type
CompositeFunction
NumDeriv
False
f0-FlatBackground
Type
FlatBackground
A0
0.683681
Settings
Workspace
BaTiO3_Q_scaled
Workspace Index
0
StartX
30.000000
EndX
55.000000
Output
BaTiO3_Q_scaled
Minimizer
Levenberg-Marquardt
Ignore invalid ...
False
Cost function
Least squares
Max Iterations
500
Peak Radius
0
Plot Difference
True
Plot Composite ...
False
Convolve Comp...
False
Show Paramete...
False
Evaluate Functi...
CentrePoint
Status: cannot reach the specified tolerance in F
BaTiO3_Q_scaled
BaTiO3_Q_scaled
BaTiO3_Q_scaled_Workspace-Calc
BaTiO3_Q_scaled_Workspace-Diff
1.5
1
0.5
0
20
30
40
50
60
q (Å⁻¹)
Results Log
Name: StartX, Value: 30, Default?: No, Direction: Input
Name: EndX, Value: 55, Default?: No, Direction: Input
Name: Normalise, Value: 0, Default?: Yes, Direction: Input
Name: Exclude, Value: , Default?: Yes, Direction: Input
Fit status: cannot reach the specified tolerance in F
Stopped after 6 iterations
Fit successful, Duration 0.00 seconds
Algorithms
Execute
Scale
Algorithms
Arithmetic
CorrectionFunctions
Crystal
DataHandling
Diagnostics
Diffraction
Events
Examples
ILL
Inelastic
MDAlgorithms
Muon
Workspaces
Load
Delete
Group
Sort
Save
Filter Workspaces
Workspaces
BaTiO3
BaTiO3_Q
BaTiO3_Q_scaled
BaTiO3_Q_scaled_NormalisedCovarianceMatrix
BaTiO3_Q_scaled_Parameters
BaTiO3_Q_scaled_Workspace
cript Interpreter
squickref -> Quick reference.


play coordinates!
DejaVu Sans
10
Fit Function (Chi-sq = 1.2008, failed)
Fit
Display
Setup
Property
Value
Functions
Type
CompositeFunction
NumDeriv
False
f0-FlatBackground
Type
FlatBackground
A0
0.683681
Settings
Workspace
BaTiO3_Q_scaled
Workspace Index
0
StartX
30.000000
EndX
55.000000
Output
BaTiO3_Q_scaled
Minimizer
Levenberg-Marquardt
Ignore invalid ...
False
Cost function
Least squares
Max Iterations
500
Peak Radius
0
Plot Difference
True
Plot Composite ...
False
Convolve Comp...
False
Show Paramete...
False
Evaluate Functi...
CentrePoint
Status: cannot reach the specified tolerance in F
BaTiO3-Q-scaled-1
BaTiO3_Q_scaled
BaTiO3_Q_scaled
BaTiO3_Q_scaled_Workspace-Calc
BaTiO3_Q_scaled_Workspace-Diff
Scale input dialog
Scales an input workspace by the given factor, which can be either multiplicative or additive.
InputWorkspace
BaTiO3_Q_scaled_to_1
OutputWorkspace
BaTiO3_Q_scaled_to_1
Factor
1.4627
Operation
Multiply
?
Keep Open
Run
Close
BaTiO3-Q-scaled-to-1-1
BaTiO3_Q_scaled_to_1
BaTiO3_Q_scaled_to_1
q (Å⁻¹)
Results Log
Name: InputWorkspace, Value: BaTiO3_Q_scaled, De
Input
Name: OutputWorkspace, Value: BaTiO3_Q_scaled_to
Direction: Output
Name: Factor, Value: 1.4626999999999999, Default?:
Name: Operation, Value: Multiply, Default?: Yes, Dire
Scale successful, Duration 0.00 seconds
Algorithms
Execute
Scale
Algorithms
Arithmetic
CorrectionFunctions
Crystal
DataHandling
Diagnostics
Diffraction
Events
Examples
ILL
Inelastic
MDAlgorithms
Muon
Workspaces
Load
Delete
Group
Sort
Save
Filter Workspaces
Workspaces
BaTiO3
BaTiO3_Q
BaTiO3_Q_scaled
BaTiO3_Q_scaled_NormalisedCovarianceMatrix
BaTiO3_Q_scaled_Parameters
BaTiO3_Q_scaled_to_1
BaTiO3_Q_scaled_Workspace
Script Interpreter
%quickref -> Quick reference.
help -> Python's own help system.
object? -> Details about 'object', use 'object??' for extra details.
%guiref -> A brief reference about the graphical user interface


play coordinates!
DejaVu Sans
10
Fit Function (Chi-sq = 1.2008, failed)
Fit
Display
Setup
Property
Value
Functions
Type
CompositeFunction
NumDeriv
False
f0-FlatBackground
Type
FlatBackground
A0
0.683681
Settings
Workspace
BaTiO3_Q_scaled
Workspace Index
0
StartX
30.000000
EndX
55.000000
Output
BaTiO3_Q_scaled
Minimizer
Levenberg-Marquardt
Ignore invalid ...
False
Cost function
Least squares
Max Iterations
500
Peak Radius
0
Plot Difference
True
Plot Composite ...
False
Convolve Comp...
False
Show Paramete...
False
Evaluate Functi...
CentrePoint
Status: cannot reach the specified tolerance in F
BaTiO3-Q-scaled-1
BaTiO3_Q_scaled
BaTiO3_Q_scaled_Workspa
BaTiO3_Q_scaled_Workspa
PDFFourierTransform input dialog
Fourier transform from S(Q) to G(r), which is paired distribution function (PDF). G(r) will be stored in another named workspace.
InputWorkspace
BaTiO3_Q_scaled_to_1
OutputWorkspace
BaTiO3_Gr
Reciprocal Space
InputSofQType
S(Q)
Qmin
0.9
Qmax
35
Filter
Real Space
PDFType
G(r)
DeltaR
0.02
Rmax
50
rho0
0.002
?
Keep Open
Run
Close
q (Å⁻¹)
Results Log
Name: InputWorkspace, Value: BaTiO3_Q_scaled, Default?: No, Di
Input
Name: OutputWorkspace, Value: BaTiO3_Q_scaled_to_1, Default?:
Direction: Output
Name: Factor, Value: 1.4626999999999999, Default?: No, Direction
Name: Operation, Value: Multiply, Default?: Yes, Direction: Input
Scale successful, Duration 0.00 seconds
Algorithms
Execute
PDFFourierTransform
Algorithms
Arithmetic
CorrectionFunctions
Crystal
DataHandling
Diagnostics
Diffraction
Events
Examples
ILL
Inelastic
MDAlgorithms
Muon
Workspaces
Load
Delete
Group
Sort
Save
Filter Workspaces
Workspaces
BaTiO3
BaTiO3_Q
BaTiO3_Q_scaled
BaTiO3_Q_scaled_NormalisedCovarianceMatrix
BaTiO3_Q_scaled_Parameters
BaTiO3_Q_scaled_to_1
BaTiO3_Q_scaled_Workspace
Script Interpreter
%quickref -> Quick reference.
help -> Python's own help system.


play coordinates!
DejaVu Sans
Fit Function (Chi-sq = 1.2008, failed)
PDFFourierTransform input dialog
Fourier transform from S(Q) to G(r), which is paired distribution function (PDF). G(r) will be stored in another named workspace.
InputWorkspace
BaTiO3_Q_scaled_to_1
OutputWorkspace
BaTiO3_Gr
Reciprocal Space
InputSofQType
S(Q)
Qmin
0.9
Qmax
35
Filter
Real Space
PDFType
G(r)
DeltaR
0.02
Rmax
50
rho0
0.002
Keep Open
Run
Close
BaTiO3-Gr-1
BaTiO3_Gr
AtomicDistance (Angstrom)
q (Å⁻¹)
Results Log
Name: Rmax, Value: 50, Default?: No, Direction: Input
Name: rho0, Value: 0.002, Default?: No, Direction: Input
Subtracting one from all values
Multiplying all values by Q
Adjusting to data: Qmin = 0.900289 Qmax = 35.0192
Using rmin = 0.02Angstroms and rmax = 50.02Angstroms
PDFFourierTransform successful, Duration 0.88 seconds
Algorithms
Execute
PDFFourierTransform
Algorithms
Arithmetic
CorrectionFunctions
Crystal
DataHandling
Diagnostics
Diffraction
Events
Examples
ILL
Inelastic
MDAlgorithms
Muon
Workspaces
Load
Delete
Group
Sort
Save
Filter Workspaces
Workspaces
BaTiO3
BaTiO3_Gr
BaTiO3_Q
BaTiO3_Q_scaled
BaTiO3_Q_scaled_NormalisedCovarianceMatrix
BaTiO3_Q_scaled_Parameters
BaTiO3_Q_scaled_to_1
BaTiO3_Q_scaled_Workspace
Status: cannot reach the specified tolerance in F
Script Interpreter
%quickref -> Quick reference.
help -> Python's own help system.
object? -> Details about 'object', use 'object??' for extra details.


MantidPlot - /SNS/groups/pg3-cycles/2017-A-B-data/PDF/Ni/Ni.mantid
File Edit View Graph Data Format Windows Catalog Interfaces Help
PDFFourierTransform input dialog
Fourier transform from S(Q) to G(r), which is paired distribution function (PDF). G(r) will be stored in another named workspace.
InputWorkspace BaTiO3_Q_scaled_to_1
OutputWorkspace BaTiO3_Gr
Reciprocal Space
InputSofQType S(Q)
Qmin 0.9
Qmax 35
Filter
Real Space
PDFType G(r)
DeltaR 0.02
Rmax 50
rho0 0.002
Keep Open
Run
Close
BaTiO3-Gr-1
BaTiO3_Gr
SavePDFGui input dialog
Save files readable by PDFGui
InputWorkspace BaTiO3_Gr
Filename
Browse
Keep Open
Run
Close
Save file
Name: BaTiO3.gr
Save in folder: SNS groups pg3-cycles 2017-A-B-data PDF
Create Folder
Places
Search
Recently Used
3ah
Desktop
File System
Documents
Downloads
NOM
PG3
Name
Size
Modified
Ni
10:34
.gr
Cancel
Save
Results Log
Name: Rmax, Value: 50, Default?: No, Direction: Input
Name: rho0, Value: 0.002, Default?: No, Direction: Input
Subtracting one from all values
Multiplying all values by Q
Adjusting to data: Qmin = 0.900289 Qmax = 35.0192
Using rmin = 0.02Angstroms and rmax = 50.02Angstroms
PDFFourierTransform successful, Duration 0.88 seconds
Algorithms
Execute
SavePDFGui
Algorithms
Arithmetic
CorrectionFunctions
Crystal
DataHandling
Diagnostics
Diffraction
Events
Examples
ILL
Inelastic
MDAlgorithms
Muon
Idle
Delete
Group
Sort
Save
BaTiO3
BaTiO3_Gr
BaTiO3_Q
BaTiO3_Q_scaled
BaTiO3_Q_scaled_NormalisedCovarianceMatrix
BaTiO3_Q_scaled_Parameters
BaTiO3_Q_scaled_to_1
BaTiO3_Q_scaled_Workspace
Status: cannot reach the specified tolerance in F
Script Interpreter
&quickref -> Quick reference.
help -> Python's own help system.
object? -> Details about 'object', use 'object??' for extra details.
&guiref -> A brief reference about the graphical user interface.