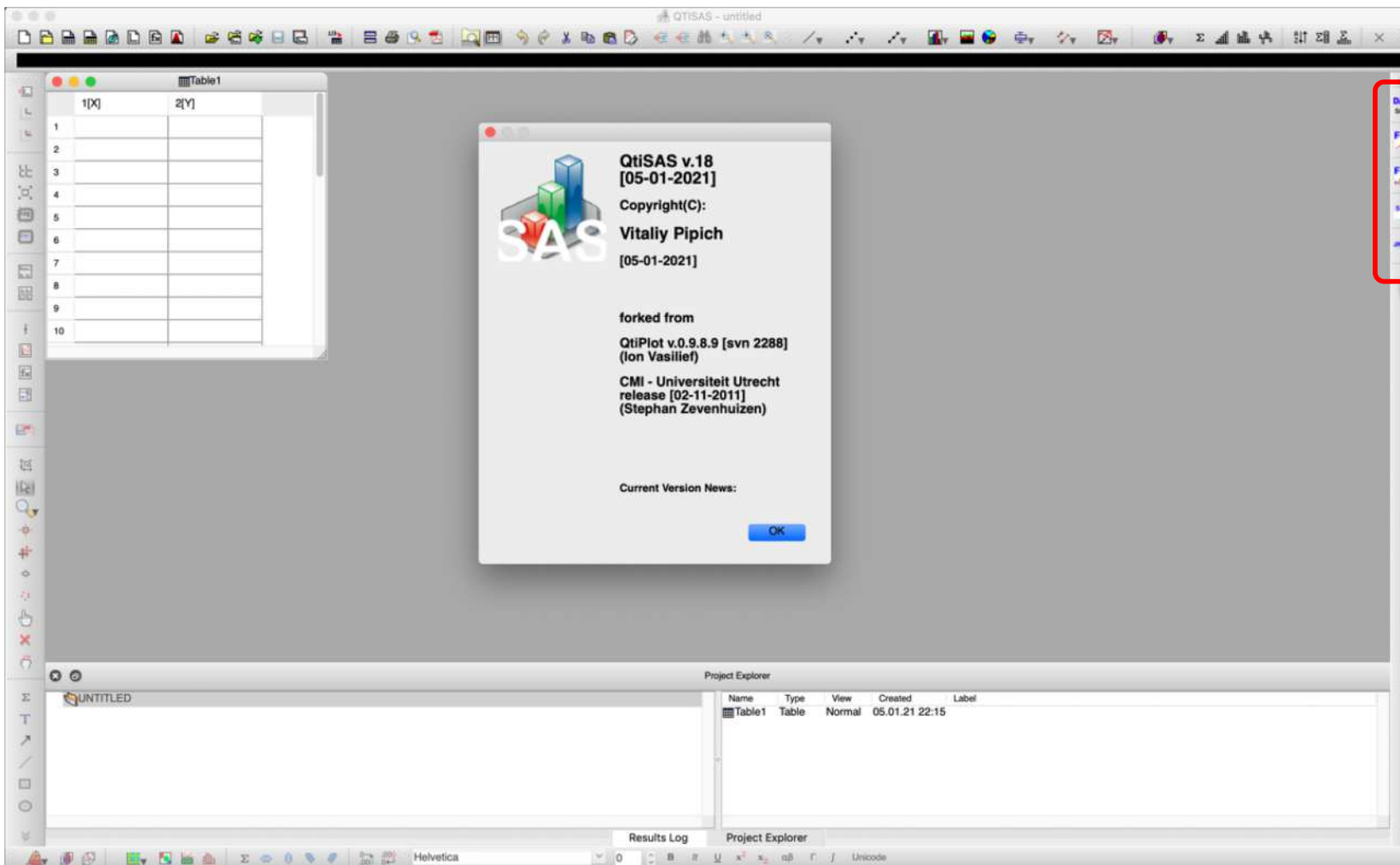




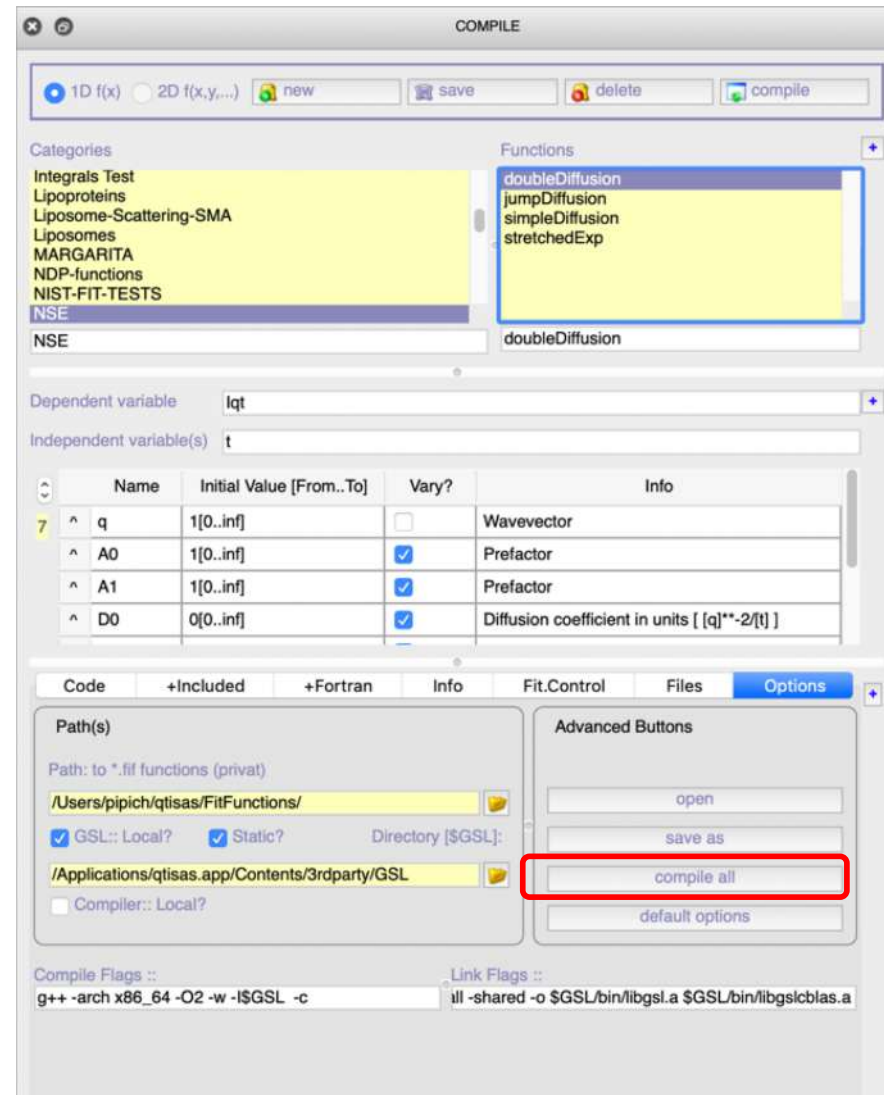
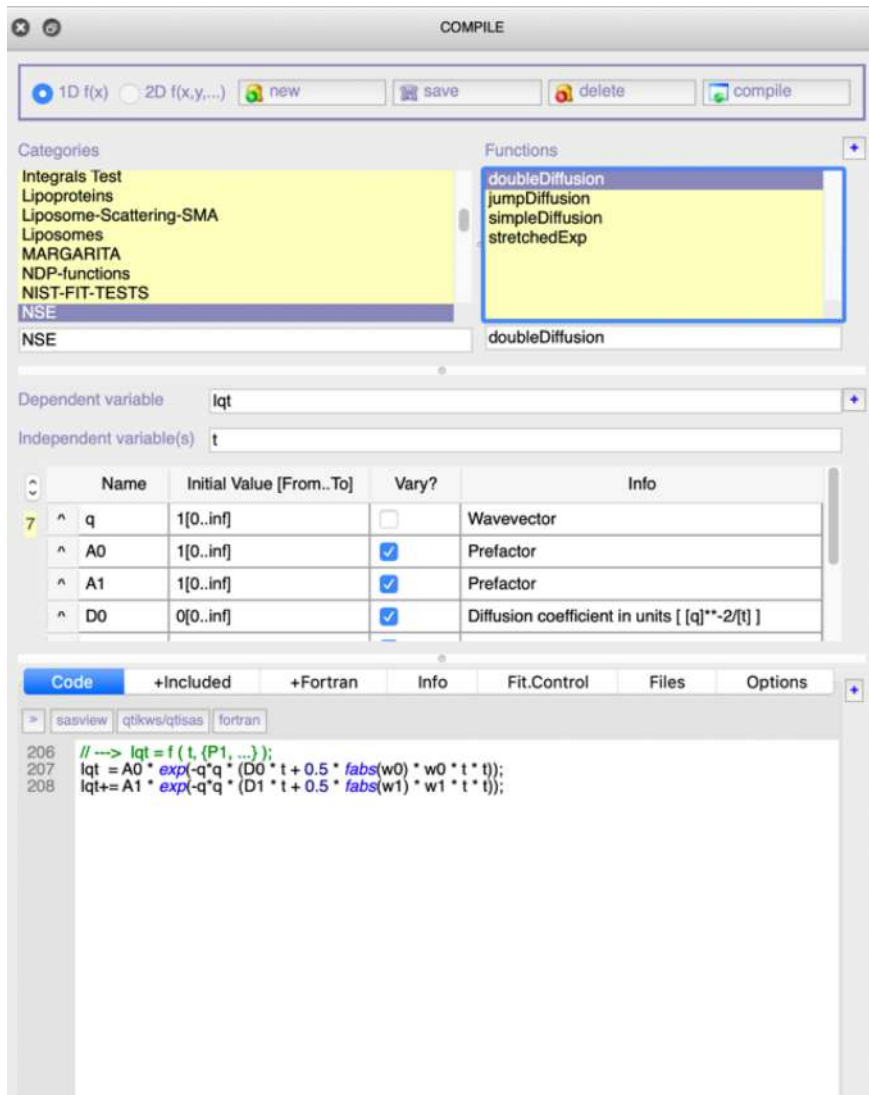
QtISAS | JNSE v.2021-01-05

Implementation (transfer) of J-NSE tools to QtISAS

QtiSAS: version > 01.2021



Compile Fitting Functions

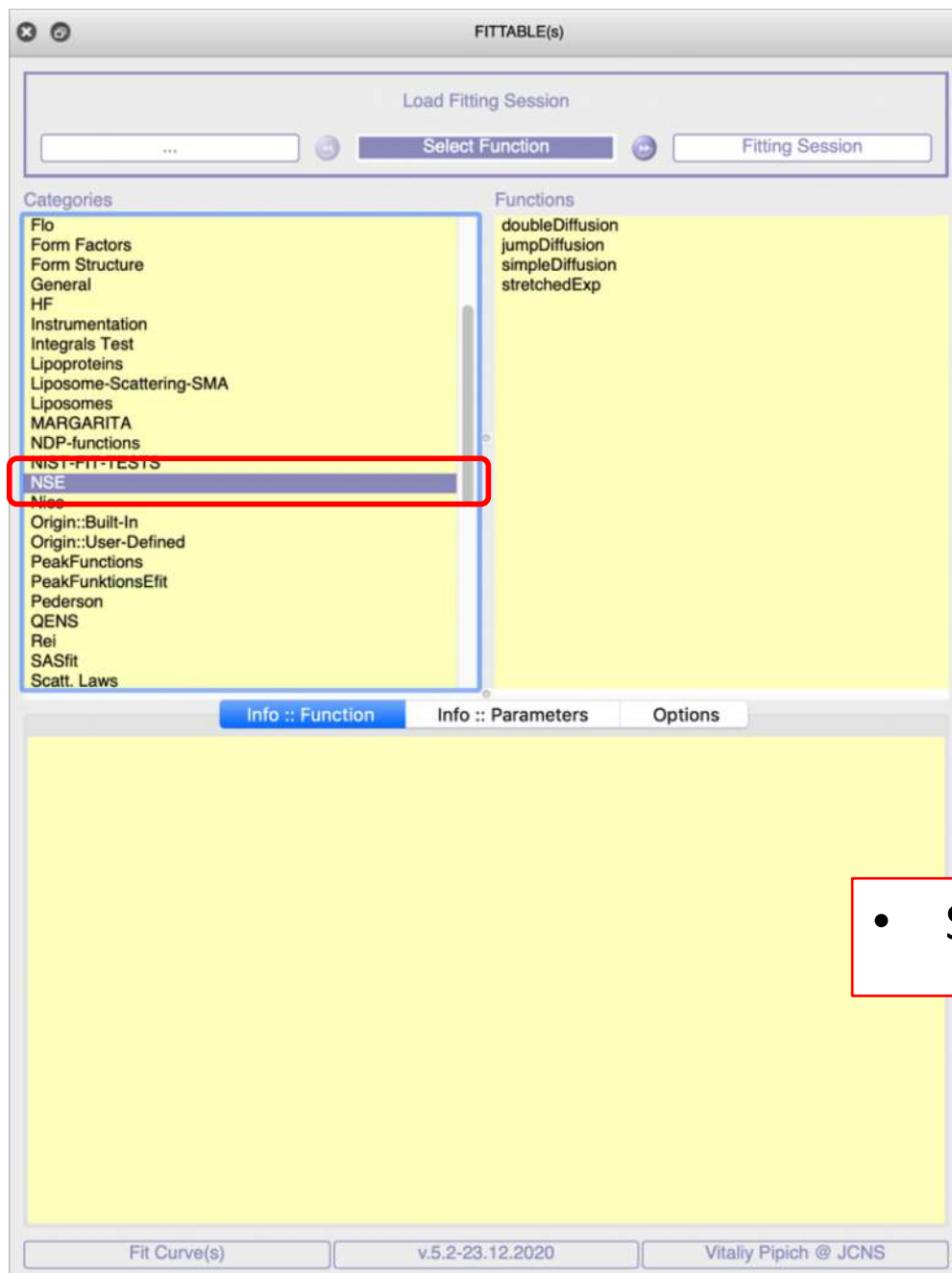


- In “NSE” folder few examples of NSE-related fit functions
- If not inside: download nse.zip file and un-zip it in fitFunctions folder
- Compile all functions: “compile all”

DAN
SANS



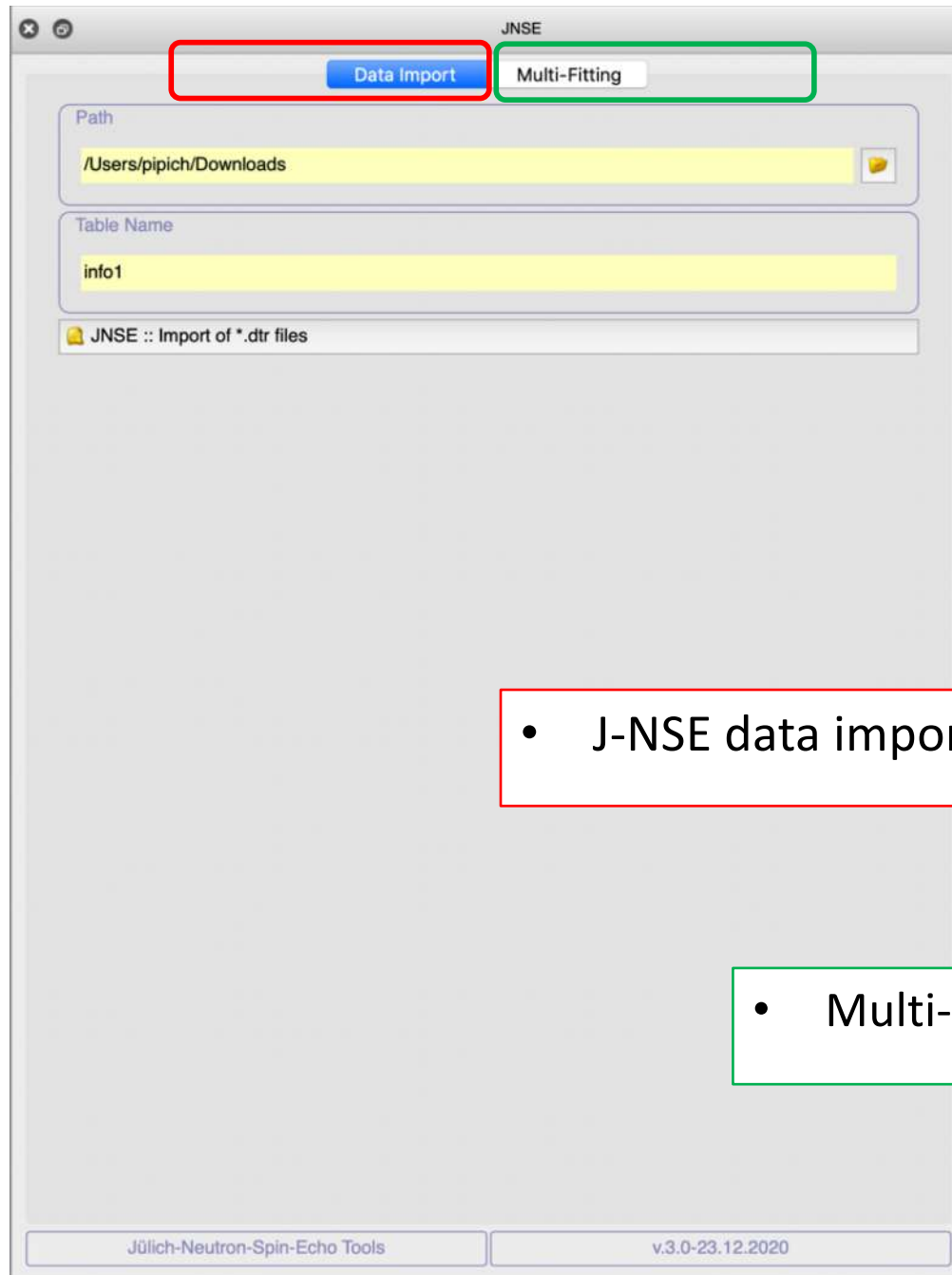
Fitting Interface



- Select “NSE” in Categories

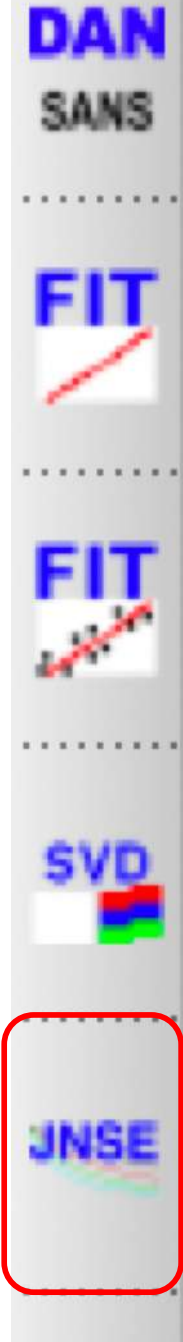


J-NSE interface

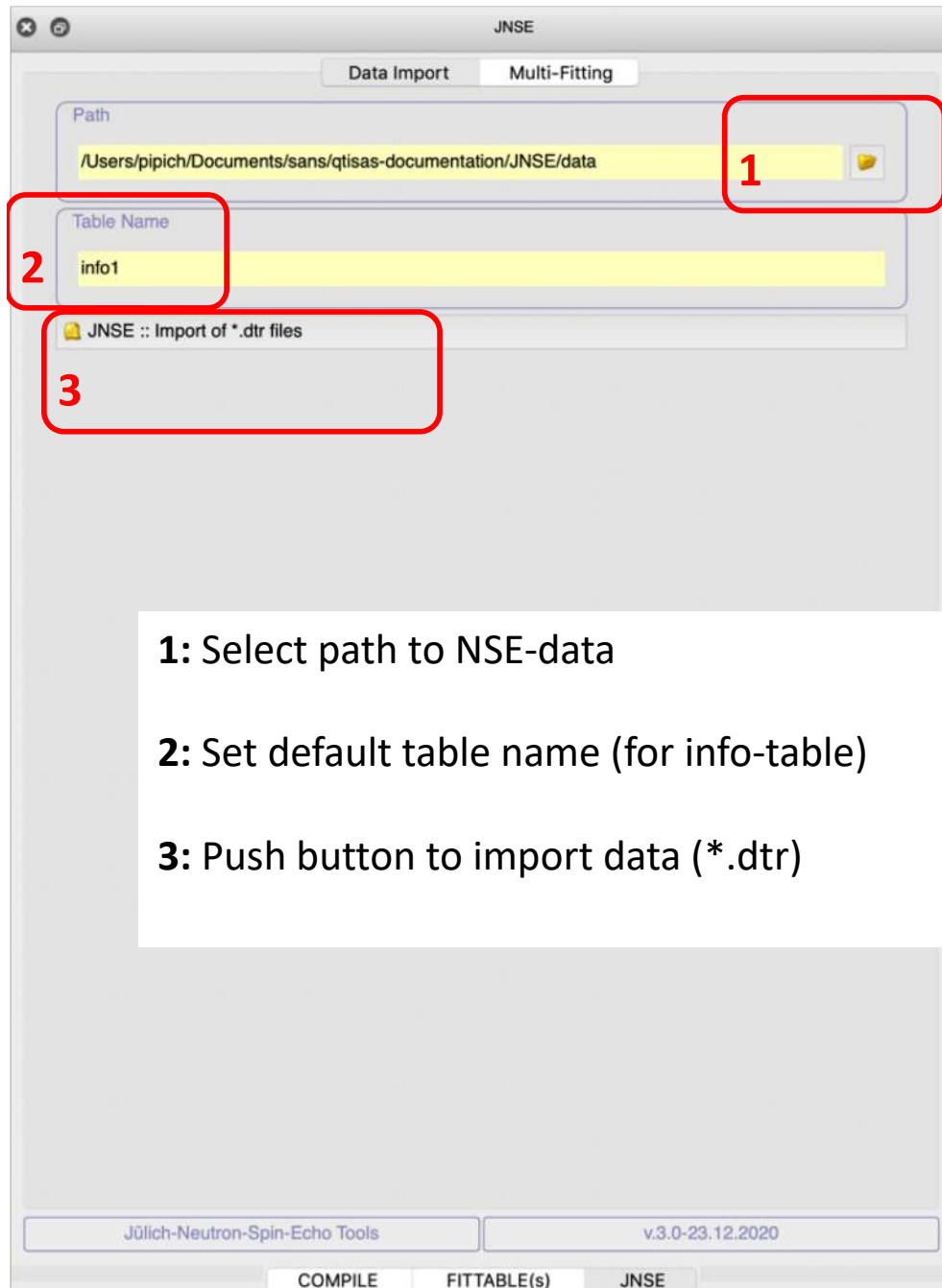


- J-NSE data import tools

- Multi-Fitting initialization tool



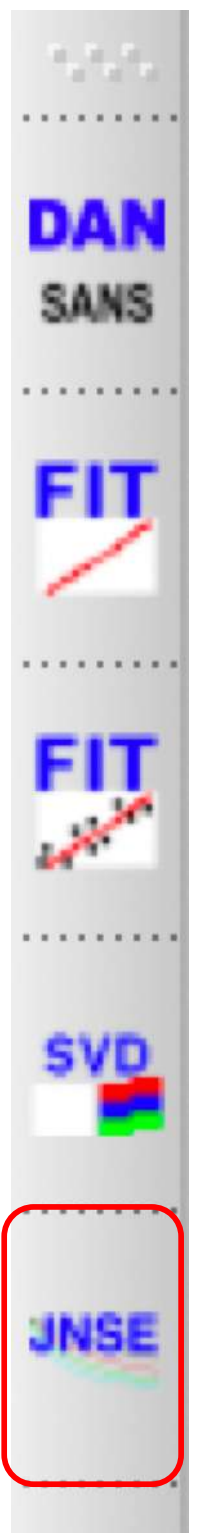
J-NSE interface: data import tools



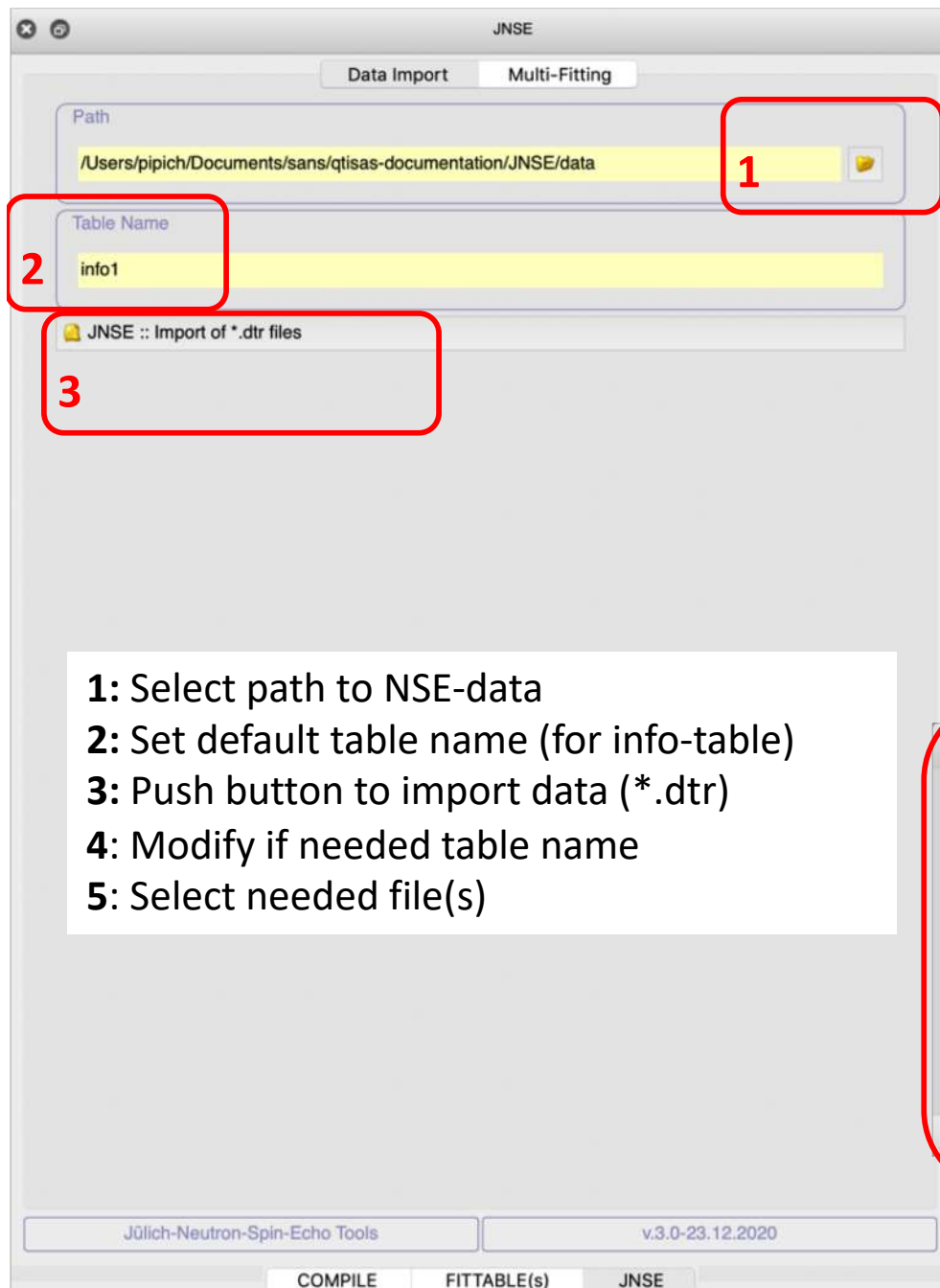
1: Select path to NSE-data

2: Set default table name (for info-table)

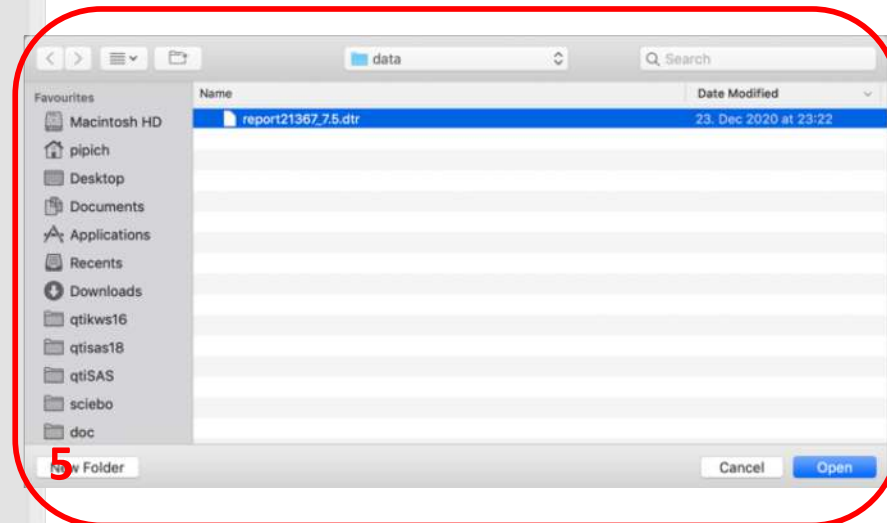
3: Push button to import data (*.dtr)



J-NSE interface: data import tools



- 1: Select path to NSE-data
- 2: Set default table name (for info-table)
- 3: Push button to import data (*.dtr)
- 4: Modify if needed table name
- 5: Select needed file(s)



DAN
SANS

FIT
/

FIT
/

SVD
/

JNSE
/

J-NSE interface:: generated tables

The screenshot displays the J-NSE interface with two main panels. The left panel, titled 'info1 - NSE Headers', shows a table of sample information. The right panel, titled 'JNSE', contains input fields for 'Path' and 'Table Name', and a button for 'Data Import'. Below these, a status bar indicates 'JNSE :: Import of *.dtr files'. At the bottom, a 'Project Explorer' window lists the generated tables.

sample-code	sample-info	mode	run-number	q[X]
1 MBP4MGndCl report21367_7.5	d-MBP pD 7.0 in 4M d-Guanidinium Hydrochlorid, 2mm helima cell, 22 d	fqt	2136701	0.3746068E-01
2 MBP4MGndCl report21367_7.5	d-MBP pD 7.0 in 4M d-Guanidinium Hydrochlorid, 2mm helima cell, 22 d	fqt	2136702	0.4966323E-01
3 MBP4MGndCl report21367_7.5	d-MBP pD 7.0 in 4M d-Guanidinium Hydrochlorid, 2mm helima cell, 22 d	fqt	2136703	0.6261720E-01
4 MBP4MGndCl report21367_7.5	d-MBP pD 7.0 in 4M d-Guanidinium Hydrochlorid, 2mm helima cell, 22 d	fqt	2136704	0.7519690E-01
5 MBP4MGndCl report21367_7.5	d-MBP pD 7.0 in 4M d-Guanidinium Hydrochlorid, 2mm helima cell, 22 d	fqt	2136705	0.8849113E-01
6 MBP4MGndCl report21367_7.5	d-MBP pD 7.0 in 4M d-Guanidinium Hydrochlorid, 2mm helima cell, 22 d	fqt	2136706	0.1013389E+00
7 MBP4MGndCl report21367_7.5	d-MBP pD 7.0 in 4M d-Guanidinium Hydrochlorid, 2mm helima cell, 22 d	fqt	2136707	0.1141266E+00
8 MBP4MGndCl report21367_7.5	d-MBP pD 7.0 in 4M d-Guanidinium Hydrochlorid, 2mm helima cell, 22 d	fqt	2136708	0.1267901E+00
9 MBP4MGndCl report21367_7.5	d-MBP pD 7.0 in 4M d-Guanidinium Hydrochlorid, 2mm helima cell, 22 d	fqt	2136709	0.1396063E+00
10 MBP4MGndCl report21367_7.5	d-MBP pD 7.0 in 4M d-Guanidinium Hydrochlorid, 2mm helima cell, 22 d	fqt	2136710	0.1512649E+00
11 MBP4MGndCl report21367_7.5	d-MBP pD 7.0 in 4M d-Guanidinium Hydrochlorid, 2mm helima cell, 22 d	fqt	2136711	0.1566583E+00

1: All data will be saved in "JCNS:: ..." folder

2: Set default table name (for info-table)

3: I(time) for different q saved as separate tables

The Project Explorer window shows the following table structure:

Name	Type	View	Created	Label
info1	Table	Maximized	05.01.21 23:34	NSE Headers
report21367_7-5-2136701-v-1	Table	Hidden	05.01.21 23:34	NSE Dataset
report21367_7-5-2136702-v-1	Table	Hidden	05.01.21 23:34	NSE Dataset
report21367_7-5-2136703-v-1	Table	Hidden	05.01.21 23:34	NSE Dataset
report21367_7-5-2136704-v-1	Table	Hidden	05.01.21 23:34	NSE Dataset
report21367_7-5-2136705-v-1	Table	Hidden	05.01.21 23:34	NSE Dataset
report21367_7-5-2136706-v-1	Table	Hidden	05.01.21 23:34	NSE Dataset
report21367_7-5-2136707-v-1	Table	Hidden	05.01.21 23:34	NSE Dataset
report21367_7-5-2136708-v-1	Table	Hidden	05.01.21 23:34	NSE Dataset
report21367_7-5-2136709-v-1	Table	Hidden	05.01.21 23:34	NSE Dataset
report21367_7-5-2136710-v-1	Table	Hidden	05.01.21 23:34	NSE Dataset
report21367_7-5-2136711-v-1	Table	Hidden	05.01.21 23:34	NSE Dataset

info-table

```
MBP4MGndCl "d-MBP pD 7.0 in 4M d-Guanidinium Hydrochlorid, 2mm hellma cell, 22 d
MBP4MGnd .fqt vs t/ns 2136701

parameter
q      0.3746068E-01
q_var  0.4899310E-03
q_unit_SI 0.1000000E+11
t_unit_SI 0.1000000E-08
temp   0.0000000E+00
numor1 21367
ref1    21347
bgr1    21392
withbgr 0
tfac_bgr -0.1000000E+01
volfrac 0.1000000E+01
qbins   11
tbins   14
oor_cnt 3510
upd_cnt 51104

values
tau/ns      S(q,t)/S(q)      err(sqrt(sq)      var(sqrt(sq)      var(tau)/ns      nupdates      Qeff/A**-1
0.9724260E-01 0.8832512E+00 0.1828554E-01 0.3411799E+00 0.1319645E-06 96 0.3805328E-01
0.1952923E+00 0.9442981E+00 0.1282973E-01 0.2674864E+00 0.1302189E-02 234 0.3699456E-01
0.4942220E+00 0.9573234E+00 0.1305659E-01 0.2789773E+00 0.1366497E-02 236 0.3686028E-01
0.9922240E+00 0.9528290E+00 0.1323055E-01 0.2257162E+00 0.1325221E-02 234 0.3731082E-01
0.2984534E+01 0.9746612E+00 0.1381281E-01 0.2193089E+00 0.1310810E-02 234 0.3746738E-01
0.4976874E+01 0.9640077E+00 0.1373500E-01 0.2046209E+00 0.1311154E-02 238 0.3724017E-01
0.6970518E+01 0.8906754E+00 0.2010855E-01 0.1852137E+00 0.9155134E-06 94 0.3855767E-01
0.9957600E+01 0.8863031E+00 0.1300164E-01 0.2000779E+00 0.1250521E-02 234 0.3719147E-01
0.1404848E+02 0.9054503E+00 0.1339112E-01 0.1833600E+00 0.9891278E+00 234 0.3729524E-01
0.1841491E+02 0.8363668E+00 0.1099634E-01 0.1843415E+00 0.1680554E+01 336 0.3755998E-01
0.2487222E+02 0.7994278E+00 0.1518850E-01 0.1921554E+00 0.1992017E+01 192 0.3844471E-01
0.3391548E+02 0.7573565E+00 0.9707090E-02 0.2170580E+00 0.4497509E+01 578 0.3738920E-01
0.6060624E+02 0.6604147E+00 0.1049252E-01 0.2508167E+00 0.8374868E+01 610 0.3706229E-01
0.8351547E+02 0.5847356E+00 0.1459630E-01 0.2903003E+00 0.7851879E+01 530 0.3706951E-01
0.1251047E+03 0.4712725E+00 0.1883388E-01 0.4217901E+00 0.1128113E+02 664 0.3741368E-01

#nxt
MBP4MGndCl "d-MBP pD 7.0 in 4M d-Guanidinium Hydrochlorid, 2mm hellma cell, 22 d
MBP4MGnd .fqt vs t/ns 2136702

parameter
q      0.4966323E-01
q_var  0.119059E-03
q_unit_SI 0.1000000E+11
t_unit_SI 0.1000000E-08
temp   0.0000000E+00
numor1 21367
ref1    21347
bgr1    21392
```

File:
report21367_7.5.dtr

Info1 - NSE Headers																				
	sample-code	sample-info	mode	run-number	q[X]	dq[xEr]	q-unit	t-unit	temp	numor	ref	bgr	with-bgr	tfac-bgr	volfrac	qbins	tbins	oor-cnt	upd-cnt	table-name
1	MBP4MGndCl report21367_7.5	d-MBP pD 7.0 in 4M d-C fqt		2136701	0.037461	0.00049	1e+10	1e-09	0	21367	21347	21392	0	-1	1	11	14	3510	51104	report21367_7-5-2136701-v-1
2	MBP4MGndCl report21367_7.5	d-MBP pD 7.0 in 4M d-C fqt		2136702	0.049663	0.000172	1e+10	1e-09	0	21367	21347	21392	0	-1	1	11	14	3510	51104	report21367_7-5-2136702-v-1
3	MBP4MGndCl report21367_7.5	d-MBP pD 7.0 in 4M d-C fqt		2136703	0.062617	0.000193	1e+10	1e-09	0	21367	21347	21392	0	-1	1	11	14	3510	51104	report21367_7-5-2136703-v-1
4	MBP4MGndCl report21367_7.5	d-MBP pD 7.0 in 4M d-C fqt		2136704	0.075197	0.000767	1e+10	1e-09	0	21367	21347	21392	0	-1	1	11	14	3510	51104	report21367_7-5-2136704-v-1
5	MBP4MGndCl report21367_7.5	d-MBP pD 7.0 in 4M d-C fqt		2136705	0.088491	0.000749	1e+10	1e-09	0	21367	21347	21392	0	-1	1	11	14	3510	51104	report21367_7-5-2136705-v-1
6	MBP4MGndCl report21367_7.5	d-MBP pD 7.0 in 4M d-C fqt		2136706	0.101134	0.000241	1e+10	1e-09	0	21367	21347	21392	0	-1	1	11	14	3510	51104	report21367_7-5-2136706-v-1
7	MBP4MGndCl report21367_7.5	d-MBP pD 7.0 in 4M d-C fqt		2136707	0.11413	0.000841	1e+10	1e-09	0	21367	21347	21392	0	-1	1	11	14	3510	51104	report21367_7-5-2136707-v-1
8	MBP4MGndCl report21367_7.5	d-MBP pD 7.0 in 4M d-C fqt		2136708	0.12679	0.00106	1e+10	1e-09	0	21367	21347	21392	0	-1	1	11	14	3510	51104	report21367_7-5-2136708-v-1
9	MBP4MGndCl report21367_7.5	d-MBP pD 7.0 in 4M d-C fqt		2136709	0.13961	0.000246	1e+10	1e-09	0	21367	21347	21392	0	-1	1	11	14	3510	51104	report21367_7-5-2136709-v-1
10	MBP4MGndCl report21367_7.5	d-MBP pD 7.0 in 4M d-C fqt		2136710	0.15126	0.000232	1e+10	1e-09	0	21367	21347	21392	0	-1	1	11	14	3510	51104	report21367_7-5-2136710-v-1
11	MBP4MGndCl report21367_7.5	d-MBP pD 7.0 in 4M d-C fqt		2136711	0.15666	0	1e+10	1e-09	0	21367	21347	21392	0	-1	1	11	14	3510	51104	report21367_7-5-2136711-v-1

I vs time; for different

report21367_7-5-2136701-v-1 - NSE Dataset							
	tau-ns[X]	Sqt-To-Sq[Y]	d-Sqt-To-Sq[yEr]	var-Sqt-To-Sq[yEr]	var-tau-ns[xEr]	nupdates[Y]	Qeff[Y]
1	9.724260E-02	8.832512E-01	1.828554E-02	3.411799E-01	1.319645E-07	9.600000E+01	3.805328E-02
2	1.952923E-01	9.442981E-01	1.282973E-02	2.674864E-01	1.302189E-03	2.340000E+02	3.699456E-02
3	4.942220E-01	9.573234E-01	1.305659E-02	2.789773E-01	1.366497E-03	2.360000E+02	3.686028E-02
4	9.922240E-01	9.528290E-01	1.323055E-02	2.257162E-01	1.325221E-03	2.340000E+02	3.731082E-02
5	2.984534E+00	9.746612E-01	1.381281E-02	2.193089E-01	1.310810E-03	2.340000E+02	3.746738E-02
6	4.976874E+00	9.640077E-01	1.373500E-02	2.046209E-01	1.311154E-03	2.380000E+02	3.724017E-02
7	6.970518E+00	8.906754E-01	2.010855E-02	1.852137E-01	9.155134E-07	9.400000E+01	3.855767E-02
8	9.957600E+00	8.863031E-01	1.300164E-02	2.000779E-01	1.250521E-03	2.340000E+02	3.719147E-02
9	1.404848E+01	9.054503E-01	1.339112E-02	1.833600E-01	9.891278E-01	2.340000E+02	3.729524E-02
10	1.841491E+01	8.363668E-01	1.099634E-02	1.843415E-01	1.680554E+00	3.360000E+02	3.755998E-02
11	2.487222E+01	7.994278E-01	1.518850E-02	1.921554E-01	1.992017E+00	1.920000E+02	3.844471E-02
12	3.391548E+01	7.573565E-01	9.770709E-03	2.170580E-01	4.497509E+00	5.780000E+02	3.738920E-02
13	6.060624E+01	6.604147E-01	1.049252E-02	2.508167E-01	8.374868E+00	6.100000E+02	3.706229E-02
14	8.351547E+01	5.847356E-01	1.459630E-02	2.903003E-01	7.851879E+00	5.300000E+02	3.706951E-02
15	1.251047E+02	4.712725E-01	1.883388E-02	4.217901E-01	1.128113E+01	6.640000E+02	3.741368E-02

```
MBP4MGndCl "d-MBP pD 7.0 in 4M d-Guanidinium Hydrochlorid, 2m helima cell, 22 d
MBP4MGnd. fqt. vs t/ns 2136701

parameter
q      0.3746068E-01
q_var  0.4899310E-03
q_unit_SI  0.1000000E+11
t_unit_SI  0.1000000E-08
temp    0.0000000E+00
numor1  21367
ref1    21347
bgr1    21392
withbgr 0
tfac_bgr -0.1000000E+01
xolfrac  0.1000000E+01
nbins    11
nbins    14
pdr_cnt  3510
upd_cnt  51104

values
tau/ns      S(q,t)/S(q)      err(sq/sq)      var(sq/sq)      var(tau)/ns      nupdates      Qeff/Aw-1
0.9724260E-01  0.8832512E-01  0.1828554E-02  0.3411799E+00  0.1319645E-06  96  0.3805328E-01
0.1952923E+00  0.9442981E-01  0.1282973E-02  0.2674864E+00  0.1302189E-02  234  0.3699456E-01
0.4942220E+00  0.9573234E-01  0.1305659E-02  0.2789773E+00  0.1366497E-02  236  0.3686028E-01
0.9922240E+00  0.9528290E-01  0.1323055E-02  0.2257162E+00  0.1325221E-02  234  0.3731082E-01
0.2984534E+00  0.9746612E-01  0.1381281E-02  0.2193089E+00  0.1310810E-02  234  0.3746738E-01
0.4976874E+00  0.9640077E-01  0.1373500E-02  0.2046209E+00  0.1311154E-02  238  0.3724017E-01
0.6970518E+00  0.8906754E-01  0.2010855E-02  0.1852137E+00  0.9155134E-06  94  0.3855767E-01
0.9957600E+00  0.8863031E-01  0.1300164E-02  0.2000779E+00  0.1250521E-02  234  0.3719147E-01
0.1404848E+01  0.9054503E-01  0.1339112E-02  0.1833600E+00  0.9891278E-02  234  0.3729524E-01
0.1841491E+01  0.8363668E-01  0.1099634E-02  0.1843415E+00  0.1680554E-01  336  0.3755998E-01
0.2487222E+01  0.7994278E-01  0.1518850E-02  0.1921554E+00  0.1992017E+01  192  0.3844471E-01
0.3391548E+01  0.7573565E-01  0.9770709E-03  0.2170580E+00  0.4497509E+01  578  0.3738920E-01
0.6060624E+01  0.6604147E-01  0.1049252E-02  0.2508167E+00  0.8374868E+01  610  0.3706229E-01
0.8351547E+01  0.5847356E-01  0.1459630E-02  0.2903003E+00  0.7851879E+01  530  0.3706951E-01
0.1251047E+02  0.4712725E-01  0.1883388E-02  0.4217901E+00  0.1128113E+02  664  0.3741368E-01

MBP4MGndCl "d-MBP pD 7.0 in 4M d-Guanidinium Hydrochlorid, 2m helima cell, 22 d
MBP4MGnd. fqt. vs t/ns 2136702

parameter
q      0.4966323E-01
q_var  0.1719059E-03
q_unit_SI  0.1000000E+11
t_unit_SI  0.1000000E-08
temp    0.0000000E+00
numor1  21367
ref1    21347
bgr1    21392
```

Project Explorer					
Name	Type	View	Created	Label	
info1	Table	Normal	05.01.21 23:34	NSE Headers	
report21367_7-5-2136701-v-1	Table	Maximized	05.01.21 23:34	NSE Dataset	
report21367_7-5-2136702-v-1	Table	Hidden	05.01.21 23:34	NSE Dataset	
report21367_7-5-2136703-v-1	Table	Hidden	05.01.21 23:34	NSE Dataset	
report21367_7-5-2136704-v-1	Table	Hidden	05.01.21 23:34	NSE Dataset	
report21367_7-5-2136705-v-1	Table	Hidden	05.01.21 23:34	NSE Dataset	
report21367_7-5-2136706-v-1	Table	Hidden	05.01.21 23:34	NSE Dataset	
report21367_7-5-2136707-v-1	Table	Hidden	05.01.21 23:34	NSE Dataset	
report21367_7-5-2136708-v-1	Table	Hidden	05.01.21 23:34	NSE Dataset	
report21367_7-5-2136709-v-1	Table	Hidden	05.01.21 23:34	NSE Dataset	
report21367_7-5-2136710-v-1	Table	Hidden	05.01.21 23:34	NSE Dataset	
report21367_7-5-2136711-v-1	Table	Hidden	05.01.21 23:34	NSE Dataset	

J-NSE interface: Multi-Fitting

JNSE

Data Import Multi-Fitting

1 Select Table of Headers
info1

2 Select Row-range
From: 1 To: 4

3 Select Fitting Function
doubleDiffusion

4 Init Multi-Fit

1: Select needed info-table
2: Select range of rows in the info-table
3: Select Fitting Function
4: Push "Init Multi-Fit"

Jülich-Neutron-Spin-Echo Tools v.3.0-23.12.2020

FITTABLE(s)

Save Current Fitting Session

Select Function Fitting Session Generate Results

Data Function Parameters Global Limits Fit - Control

	Share?	?From	Value #1	Error #1	Vary?From..To	Value #
q	<input type="checkbox"/>	<input type="checkbox"/>	0.037461	---	<input type="checkbox"/> ..	0.049663
A0	<input type="checkbox"/>	<input checked="" type="checkbox"/>	1	---	<input checked="" type="checkbox"/> ..	1
A1	<input type="checkbox"/>	<input checked="" type="checkbox"/>	1	---	<input checked="" type="checkbox"/> ..	1
D0	<input type="checkbox"/>	<input checked="" type="checkbox"/>	0	---	<input checked="" type="checkbox"/> ..	0
D1	<input type="checkbox"/>	<input checked="" type="checkbox"/>	0	---	<input checked="" type="checkbox"/> ..	0
w0	<input type="checkbox"/>	<input type="checkbox"/>	0	---	<input type="checkbox"/> ..	0
w1	<input type="checkbox"/>	<input type="checkbox"/>	0	---	<input type="checkbox"/> ..	0

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

Fit Simulate $\chi^2/\text{dof} = 5.8777688116\text{E}+00$

Script :: Before Fit $R^2 = 3.1819400380\text{E}+05$

Script :: After Fit time = 58 ms - 11 iteration(s)

doubleDiffusion

JNSE FITTABLE(s)

Fitting Interface is ready for global Fit



J-NSE interface: Global-Fit

	Checks #1	Dataset #1	Checks #2	Dataset #2	Checks #3	Dataset #3	Checks #4	Dataset #4
Data Set(s)		report21367_7-5-2136701-v-1_Sqt-To-Sq		report21367_7-5-2136702-v-1_Sqt-To-Sq		report21367_7-5-2136703-v-1_Sqt-To-Sq		report21367_7-5-2136704-v-1_Sqt-To-Sq
N	N	15	N	15	N	15	N	15
First Point	<input type="checkbox"/>	1	<input type="checkbox"/>	1	<input type="checkbox"/>	1	<input type="checkbox"/>	1
Last Point	<input type="checkbox"/>	15	<input type="checkbox"/>	15	<input type="checkbox"/>	15	<input type="checkbox"/>	15
Weighting	<input checked="" type="checkbox"/> on	report21367_7-5-2136701-v-1_d-Sqt-To-Sq	<input checked="" type="checkbox"/> on	report21367_7-5-2136702-v-1_d-Sqt-To-Sq	<input checked="" type="checkbox"/> on	report21367_7-5-2136703-v-1_d-Sqt-To-Sq	<input checked="" type="checkbox"/> on	report21367_7-5-2136704-v-1_d-Sqt-To-Sq

Data
Function
Parameters
Global Limits
Fit - Control

doubleDiffusion

Parameters: 7
Indep. Variables: 1
Dep. Variables: 4

doubleDiffusion

Two exponential decaying functions describing diffusion.

.. math:: I(q,t)=A_1e^{-q^2 (D_{1t} + 0.5w_{1t}^2)} + A_2e^{-q^2 (D_{2t} + 0.5w_{2t}^2)}

q Wavevector
A0 Prefactor
A1 Prefactor
D0 Diffusion coefficient in units [$[q]^{*-2}/[t]$]
D1 Diffusion coefficient in units [$[q]^{*-2}/[t]$]
w0 Width of diffusion coefficient distributions in D unit
w1 Width of diffusion coefficient distributions in D unit

1: q-values moved from info-table

	Share	Vary From: To	Value #1	Error #1	Vary From: To	Value #2	Error #2	Vary From: To	Value #3	Error #3	Vary From: To	Value #4	Error #4
1	<input type="checkbox"/>	<input checked="" type="checkbox"/> ..	0.037461	---	<input type="checkbox"/> ..	0.049663	---	<input type="checkbox"/> ..	0.062617	---	<input checked="" type="checkbox"/> ..	0.075197	---
0	<input type="checkbox"/>	<input checked="" type="checkbox"/> 1	1	---	<input checked="" type="checkbox"/> 1	1	---	<input checked="" type="checkbox"/> 1	1	---	<input checked="" type="checkbox"/> 1	1	---
A1	<input type="checkbox"/>	<input checked="" type="checkbox"/> ..	1	---	<input checked="" type="checkbox"/> ..	1	---	<input checked="" type="checkbox"/> ..	1	---	<input checked="" type="checkbox"/> ..	1	---
D0	<input type="checkbox"/>	<input checked="" type="checkbox"/> ..	0	---	<input checked="" type="checkbox"/> ..	0	---	<input checked="" type="checkbox"/> ..	0	---	<input checked="" type="checkbox"/> ..	0	---
D1	<input type="checkbox"/>	<input checked="" type="checkbox"/> ..	0	---	<input checked="" type="checkbox"/> ..	0	---	<input checked="" type="checkbox"/> ..	0	---	<input checked="" type="checkbox"/> ..	0	---
w0	<input type="checkbox"/>	<input type="checkbox"/> ..	0	---	<input type="checkbox"/> ..	0	---	<input type="checkbox"/> ..	0	---	<input type="checkbox"/> ..	0	---
w1	<input type="checkbox"/>	<input type="checkbox"/> ..	0	---	<input type="checkbox"/> ..	0	---	<input type="checkbox"/> ..	0	---	<input type="checkbox"/> ..	0	---

DAN
SANS

FIT

FIT

SVD

JNSE

NSE: Global Fit

