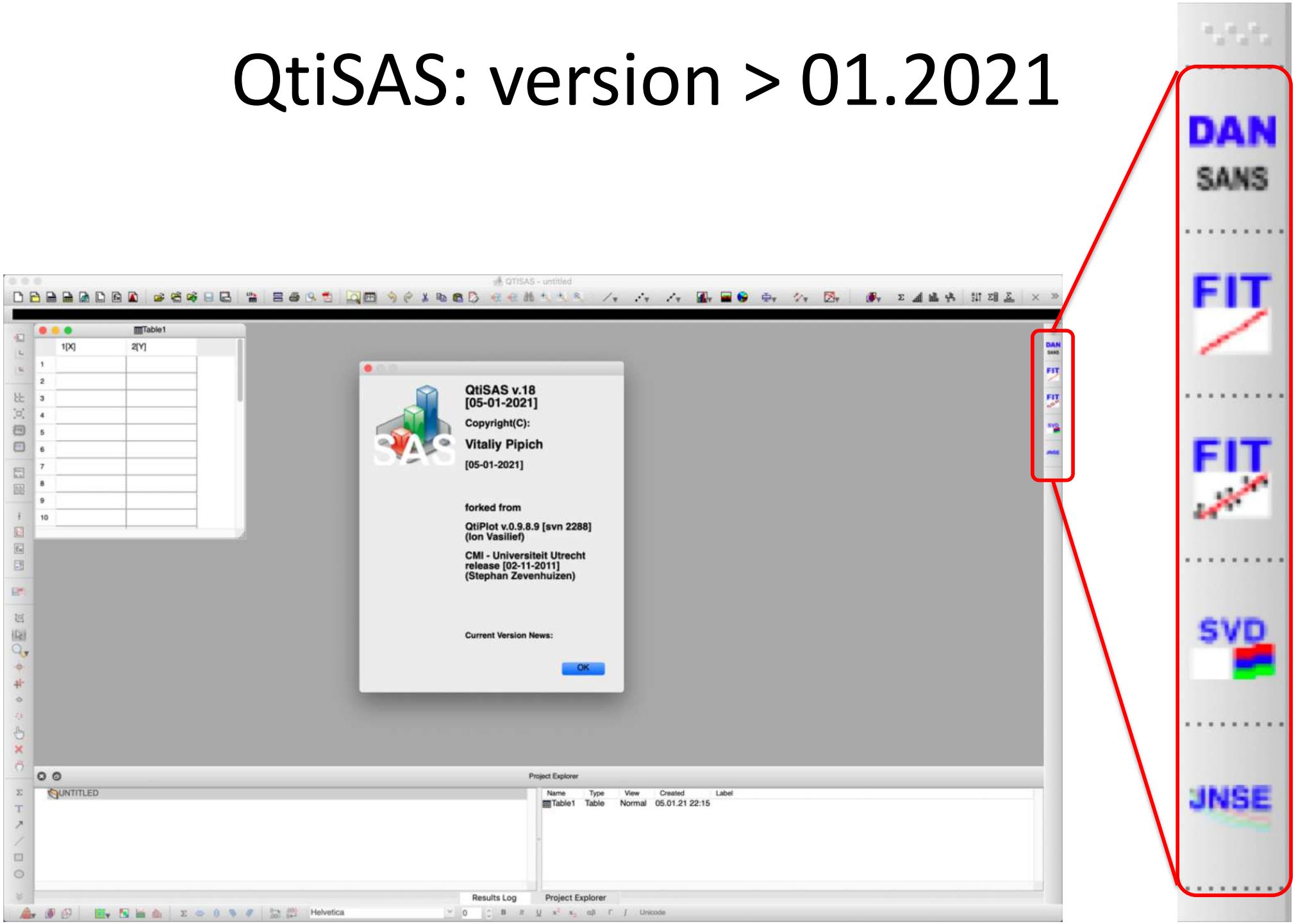
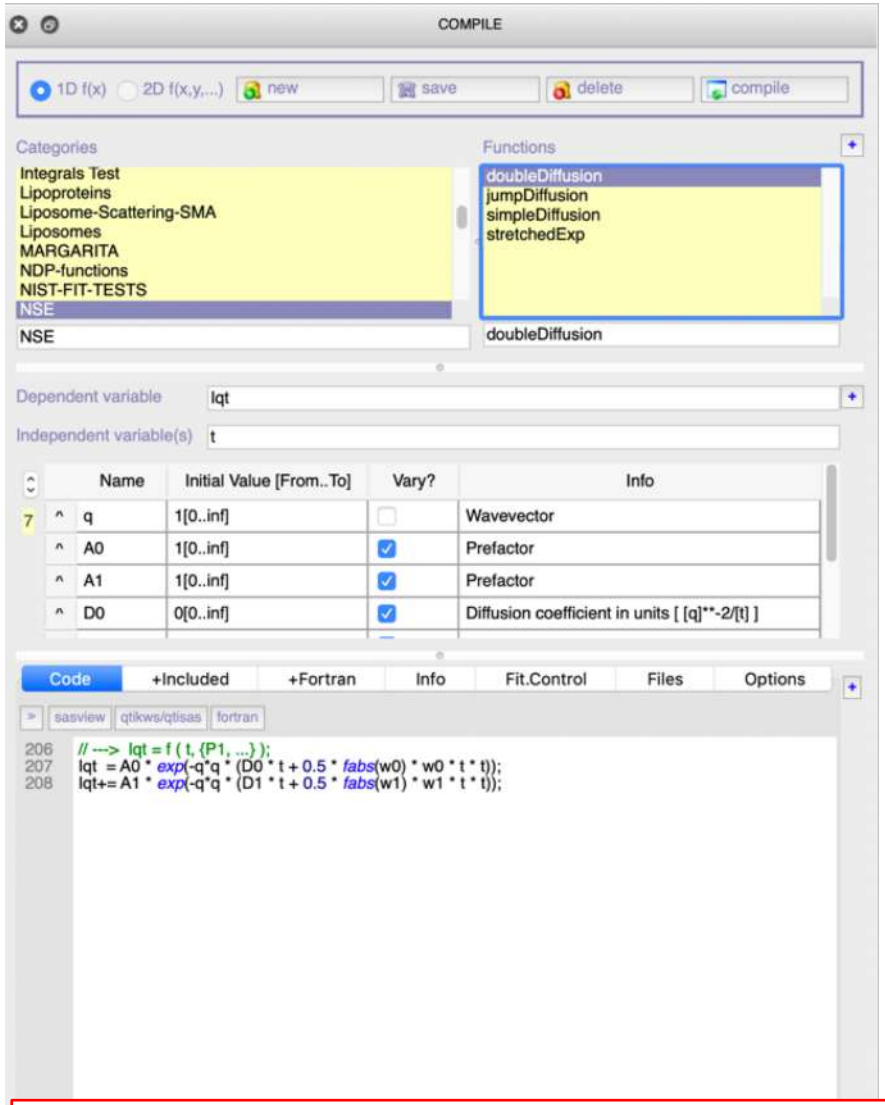
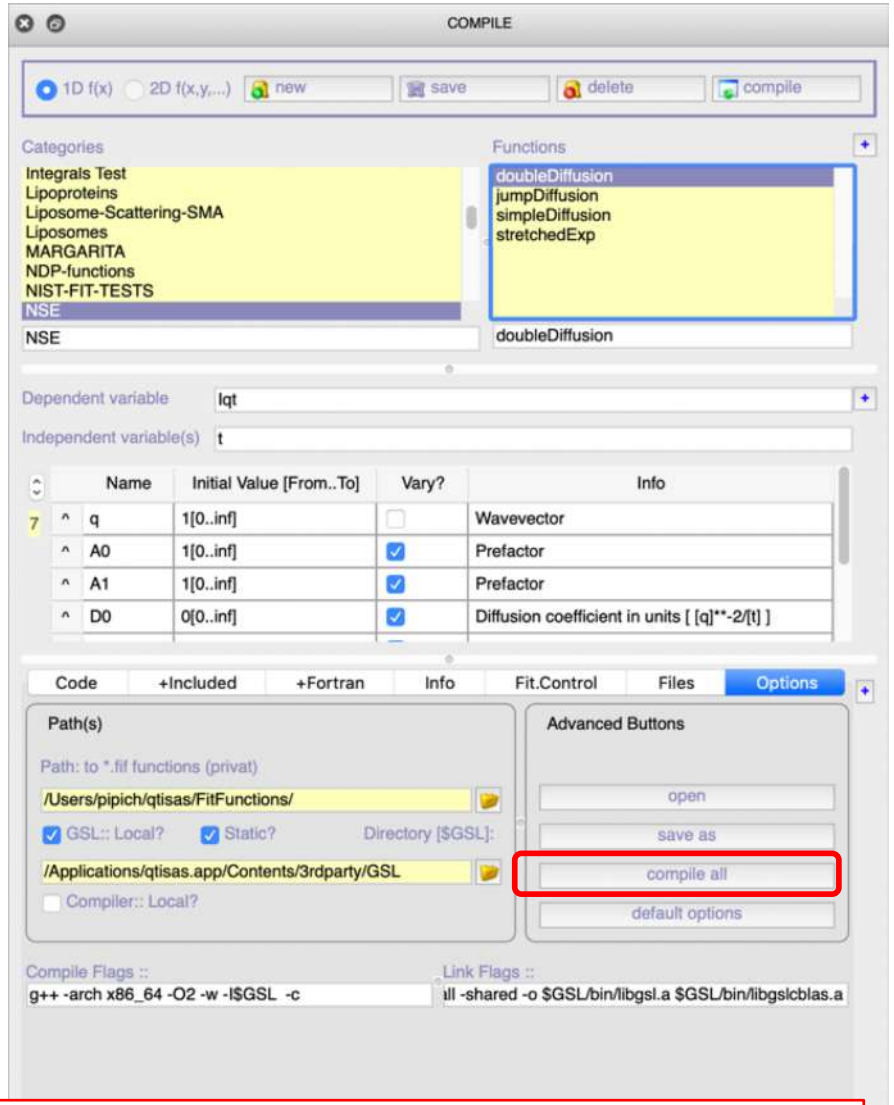
Implementation (transfer) of J-NSE tools to QtiSAS

QtiSAS: version > 01.2021



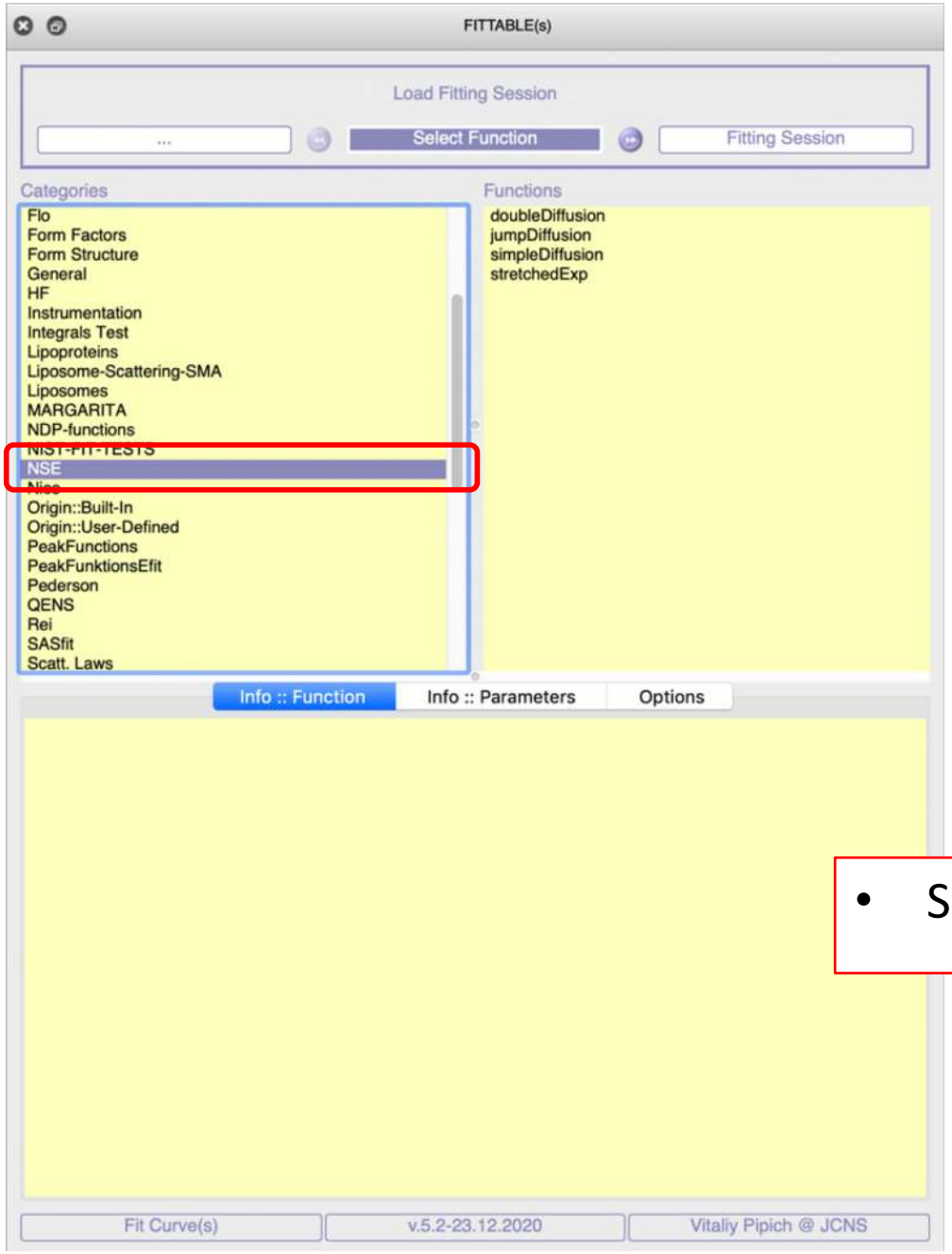
Compile Fitting Functions





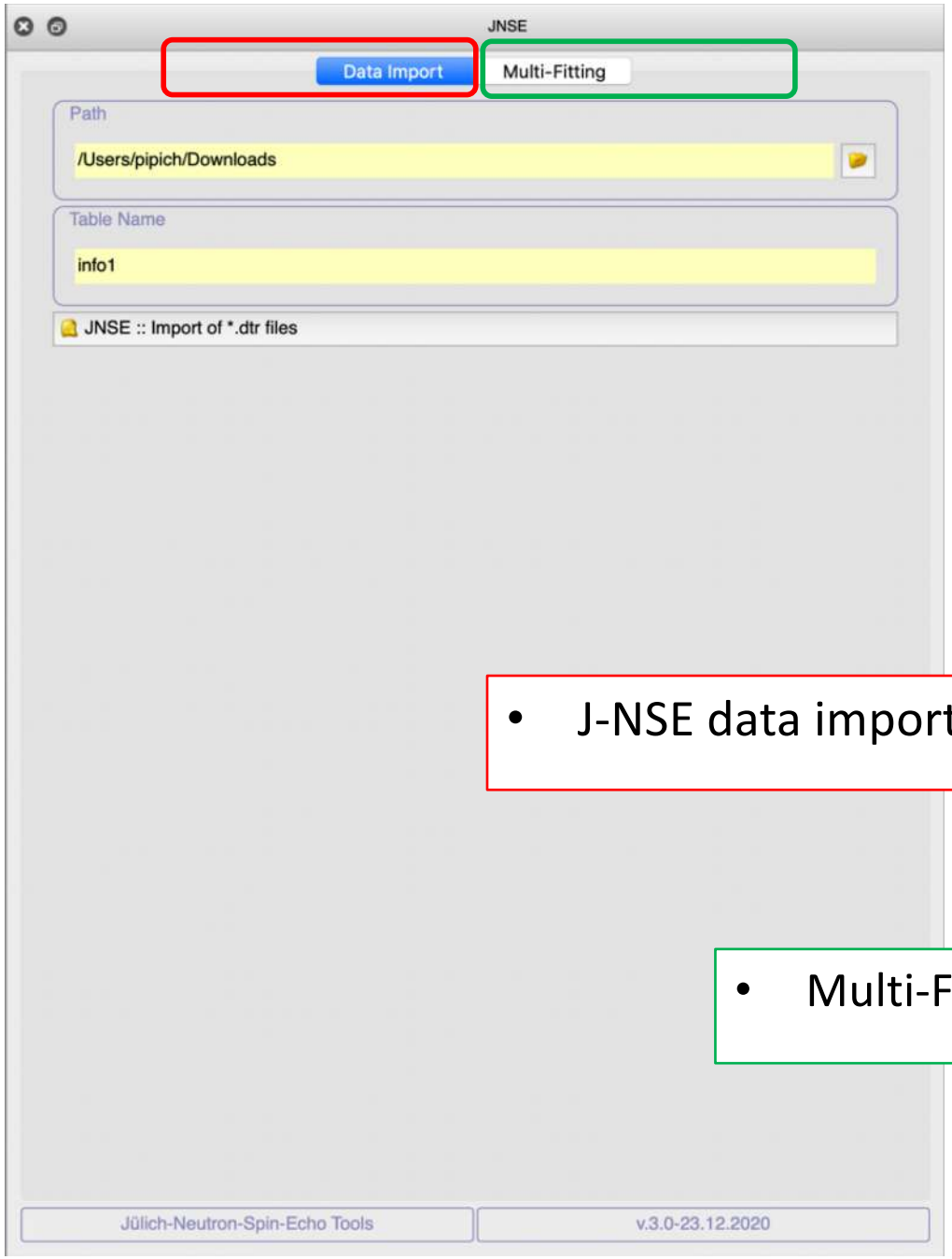
- In “NSE” folder few examples of NSE-related fit functions
- If not inside: download nse.zip file and un-zip it in fitFunctions folder
- Compile all functions: “compile all”

Fitting Interface



- Select “NSE” in Categories

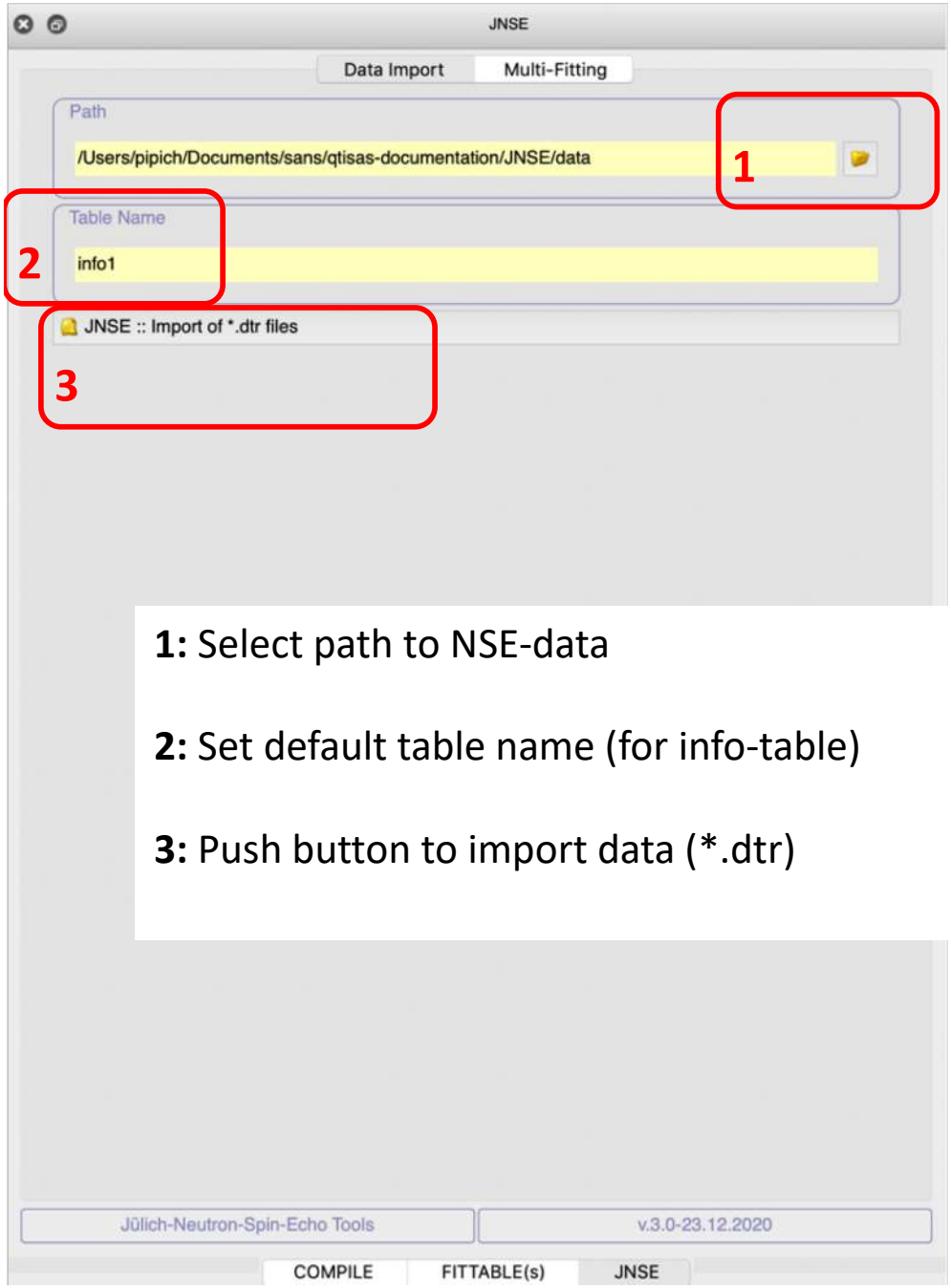
J-NSE interface



- J-NSE data import tools

- Multi-Fitting initialization tool

J-NSE interface: data import tools

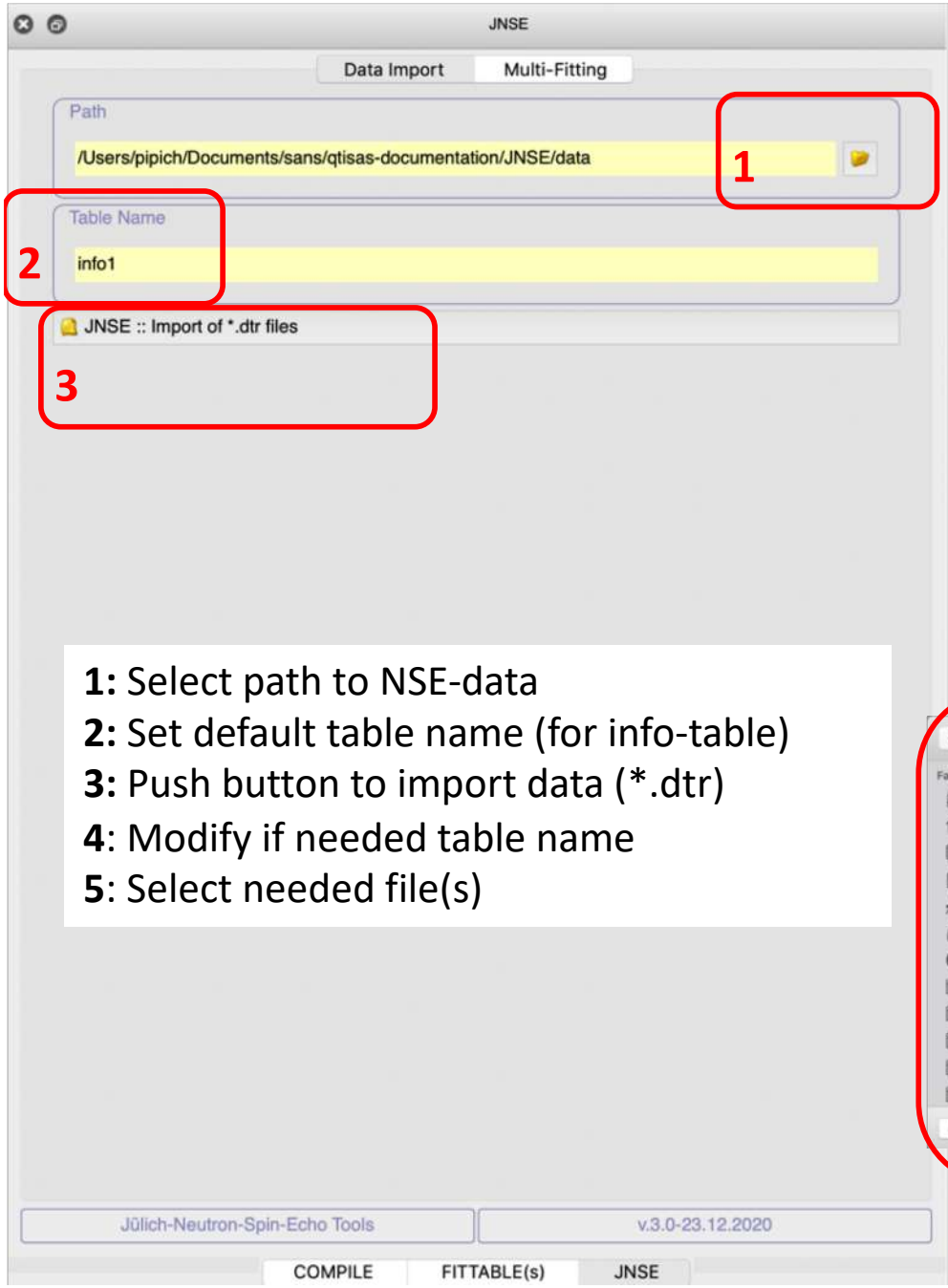


1: Select path to NSE-data

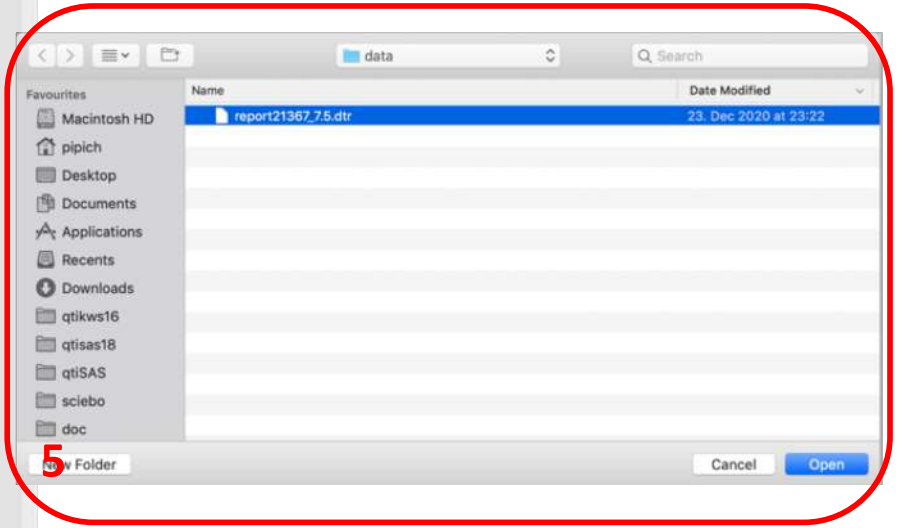
2: Set default table name (for info-table)

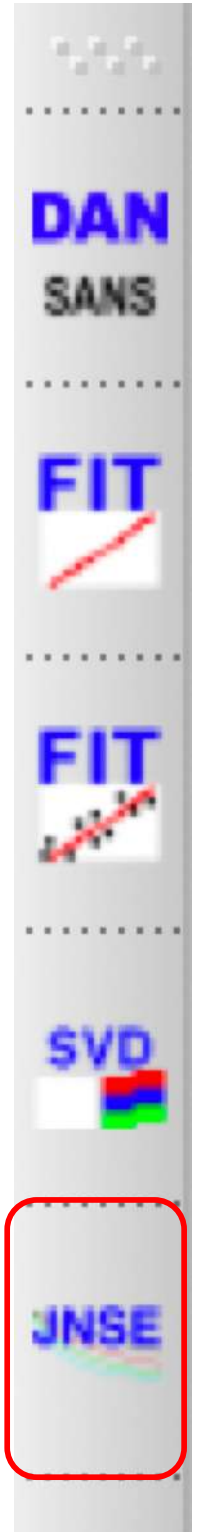
3: Push button to import data (*.dtr)

J-NSE interface: data import tools

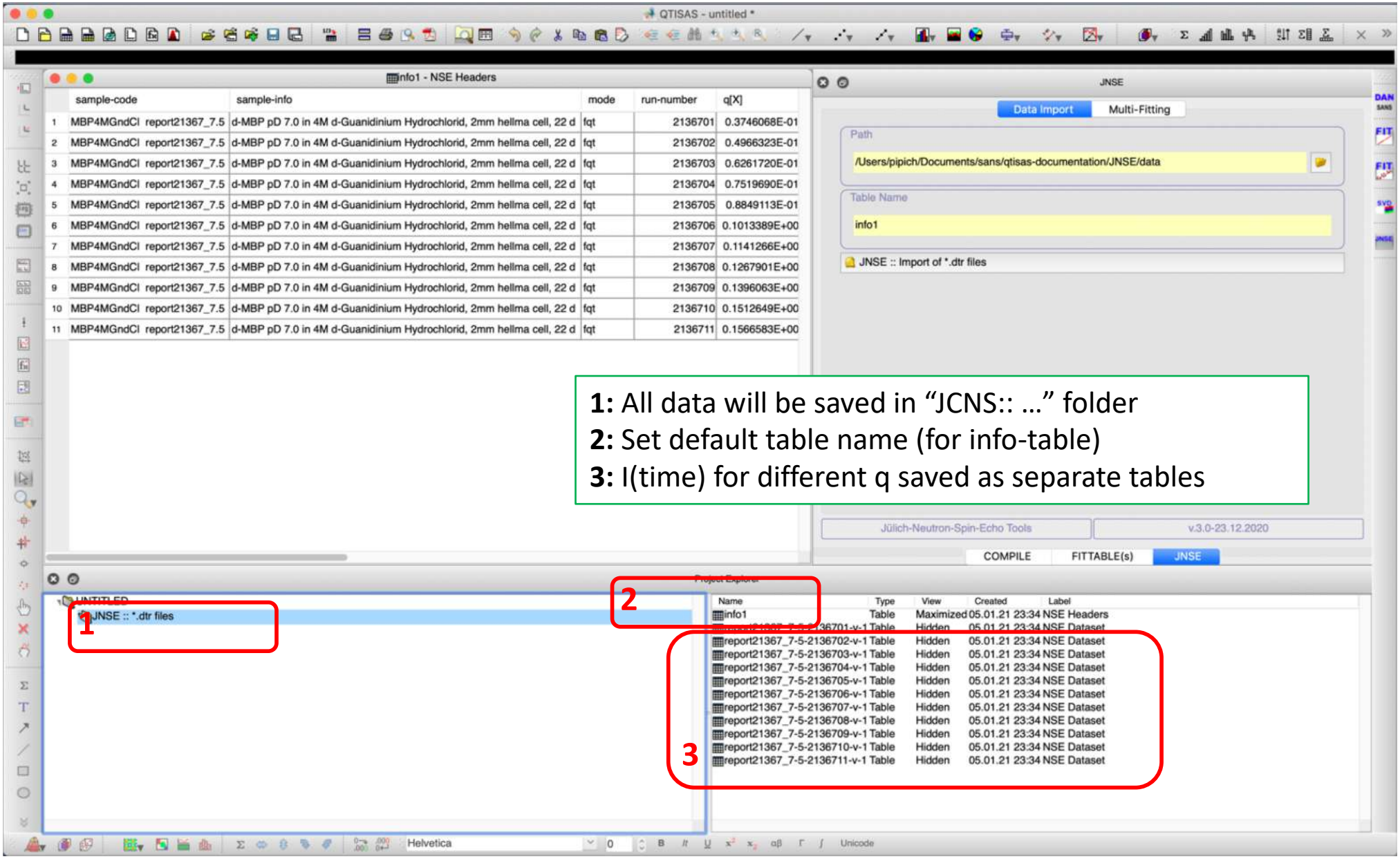


1: Select path to NSE-data
2: Set default table name (for info-table)
3: Push button to import data (*.dtr)
4: Modify if needed table name
5: Select needed file(s)





J-NSE interface:: generated tables



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

info-table

File:
report21367_7.5.dtr

```
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(sqt/sq)     var(sqt/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       0.1719059E-03
q_unit_SI   0.1000000E+11
t_unit_SI   0.1000000E-08
temp        0.0000000E+00
numor1        21367
ref1          21347
bgr1          21392
```

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	0.10134	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	9.707090E-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

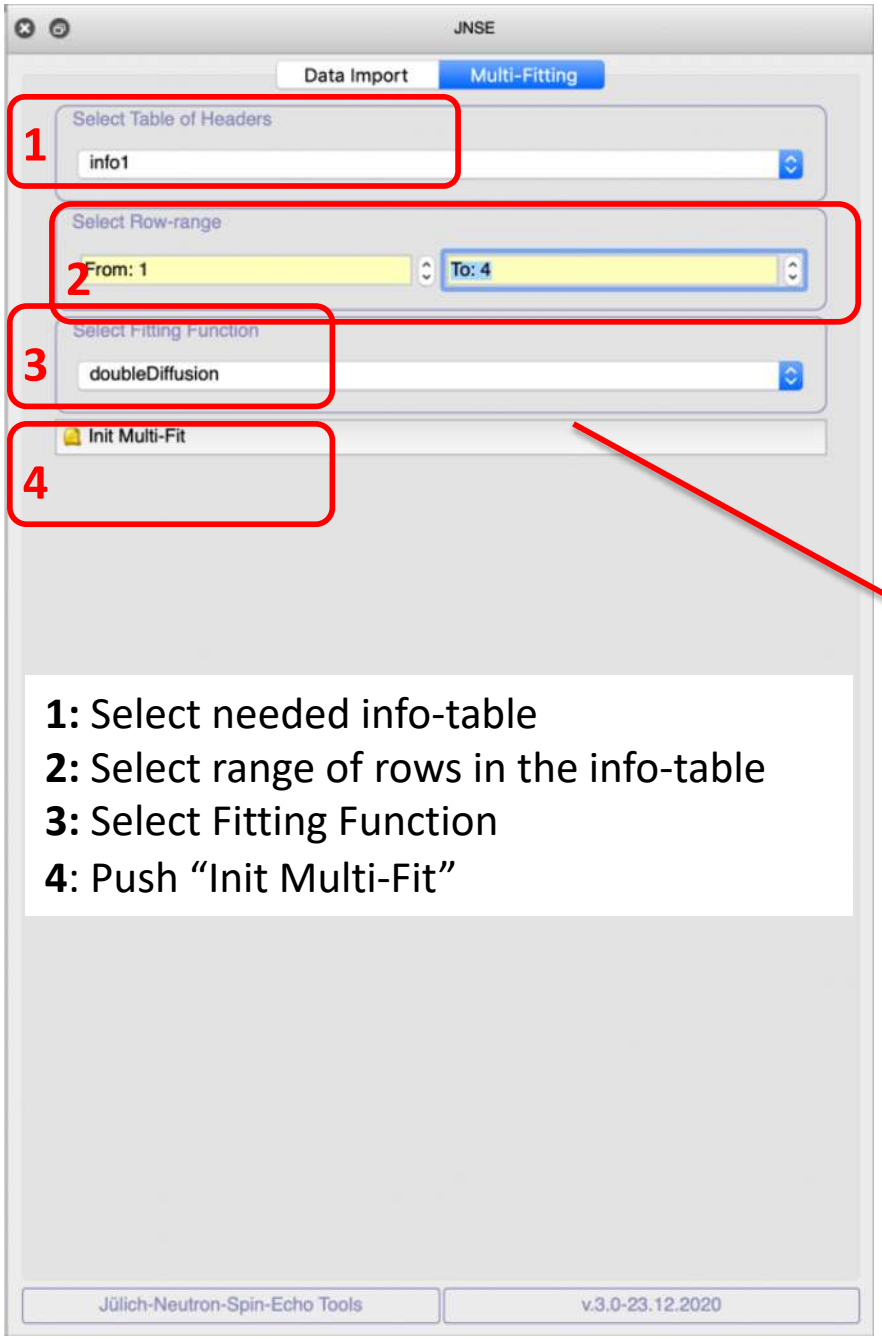
```
MBP4MGndCl "d-MBP pD 7.0 in 4M d-Guanidinium Hydrochlorid, 2mm hellma cell, 22 d
MBP4MGnd  fqt   vs   t/ns  2136701

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
xslfrac     0.1000000E+01
qbins            11
tbins            14
qgr_cnt        3510
upd_cnt       51104

values
        tau/ns    S(q,t)/S(q)    err(sqt/sq)    var(sqt/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

text
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       0.1719059E-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

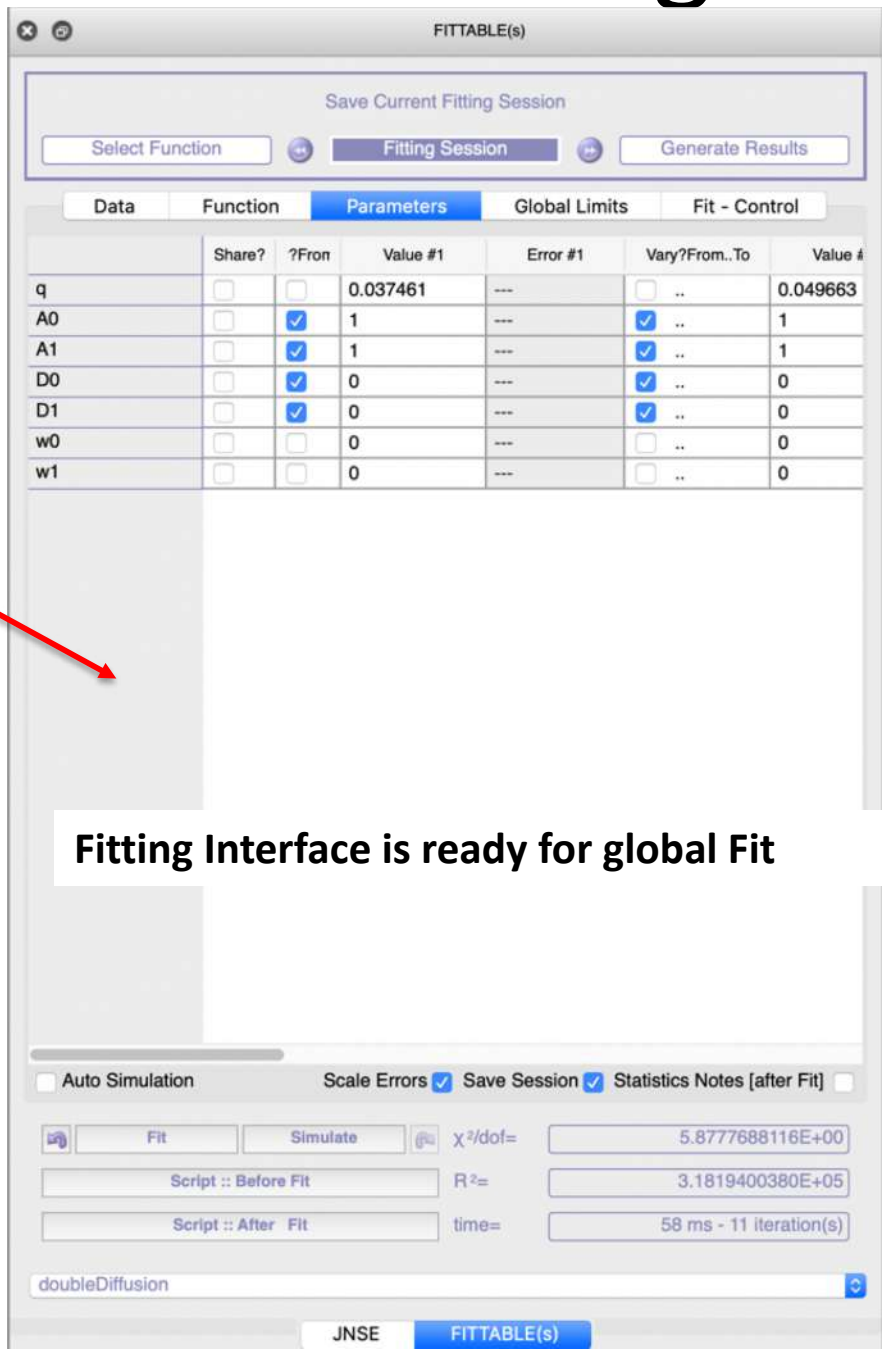
UNTITLED
JNSE :: *.dtr files

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



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



Fitting Interface is ready for global Fit

J-NSE interface: Global-Fit

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

	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		1		1		1		1
Last Point		15		15		15		15
Weighting	☑ on	report21367_7-5-2136701-v-1_d-Sqt-To-Sq	☑ on	report21367_7-5-2136702-v-1_d-Sqt-To-Sq	☑ on	report21367_7-5-2136703-v-1_d-Sqt-To-Sq	☑ 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_1^2t^2)} + A_2e^{-q^2 (D_2t + 0.5w_2^2t^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

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

	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
q		..	0.037461	---	..	0.049663	---	..	0.062617	---	..	0.075197	---
A0		☑ ..	1	---	☑ ..	1	---	☑ ..	1	---	☑ ..	1	---
A1		☑ ..	1	---	☑ ..	1	---	☑ ..	1	---	☑ ..	1	---
D0		☑ ..	0	---	☑ ..	0	---	☑ ..	0	---	☑ ..	0	---
D1		☑ ..	0	---	☑ ..	0	---	☑ ..	0	---	☑ ..	0	---
w0		..	0	---	..	0	---	..	0	---	..	0	---
w1		..	0	---	..	0	---	..	0	---	..	0	---

1

NSE: Global Fit