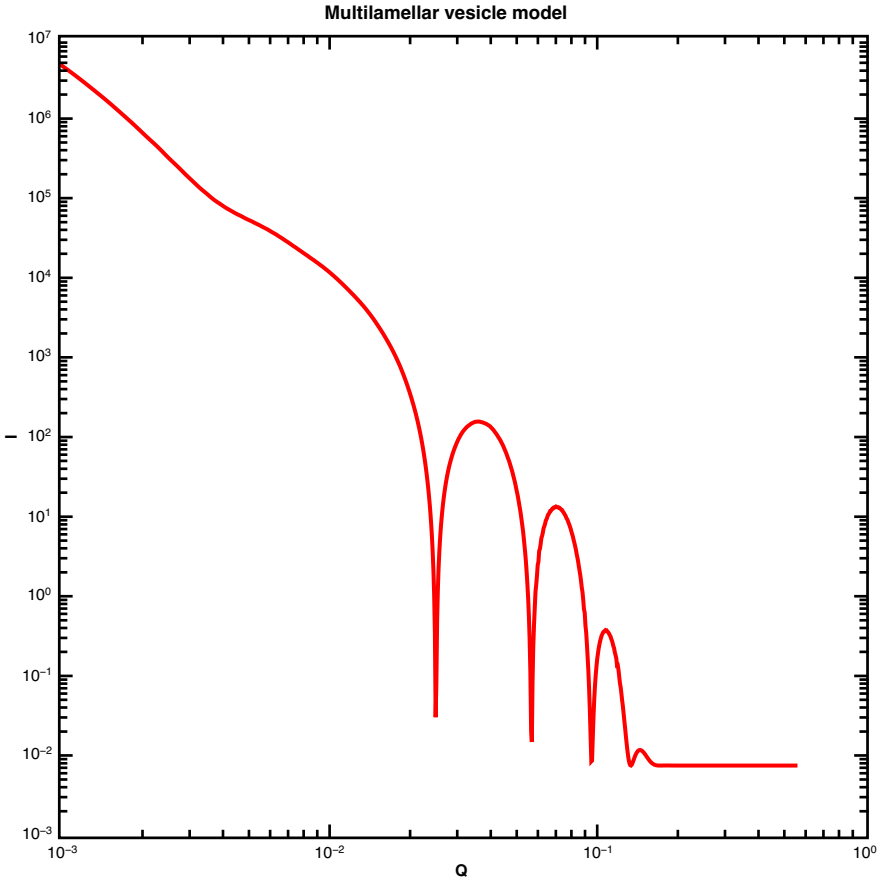
Using Fortran code in Fitting Functions



Multilamellar Vesicle Model

Model author: Henrich Frielinghaus

Fortran code author: Henrich Frielinghaus

QtiKWS/QtiSAS integration: Vitaliy Pipich

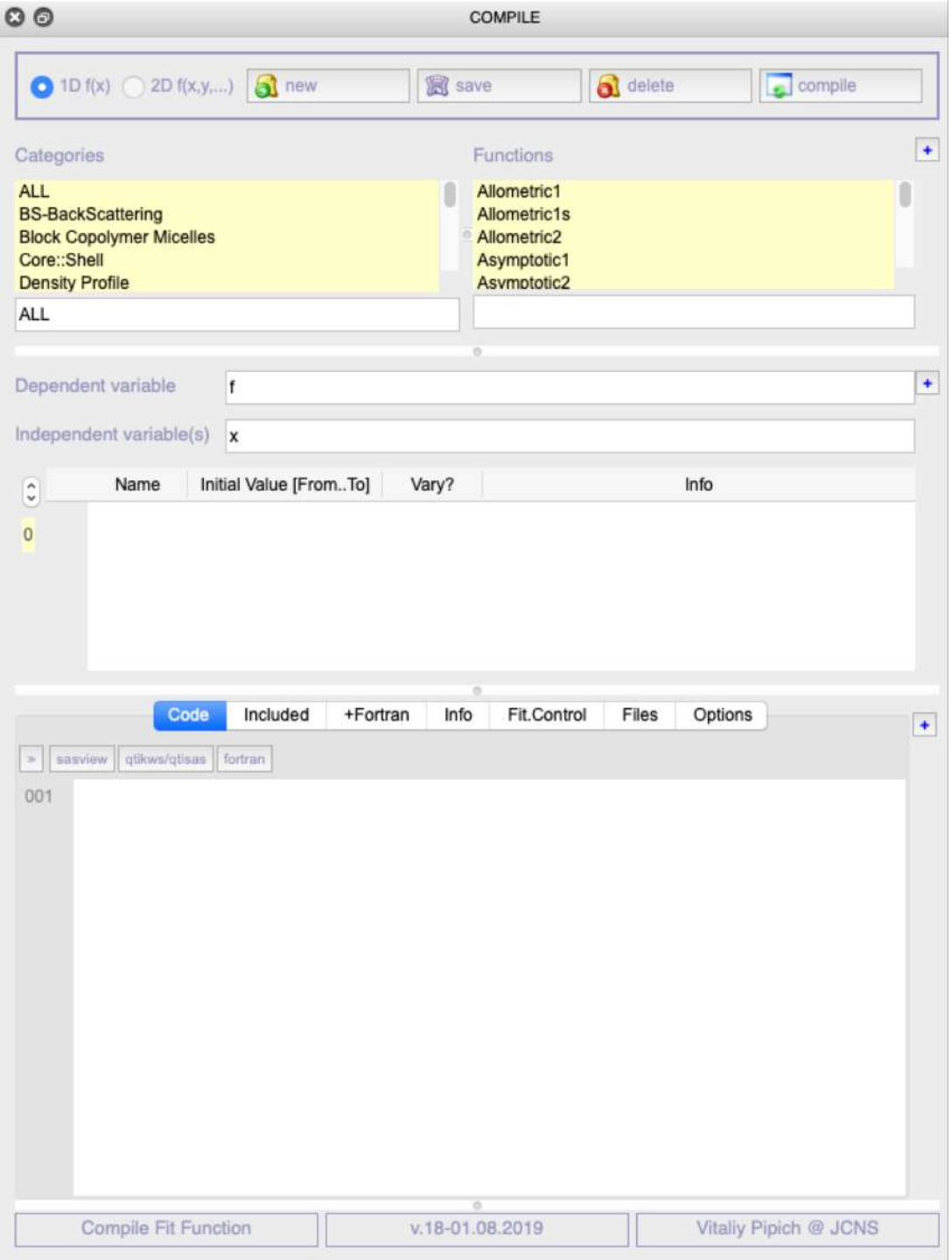
Reference:
https://journals.aps.org/pre/abstract/10.1103/PhysRevE.76.051603

Fortran code: fortran-sphere-vesicle-mlv.f
[move to ”FitFunctions/IncludedFunctions”]

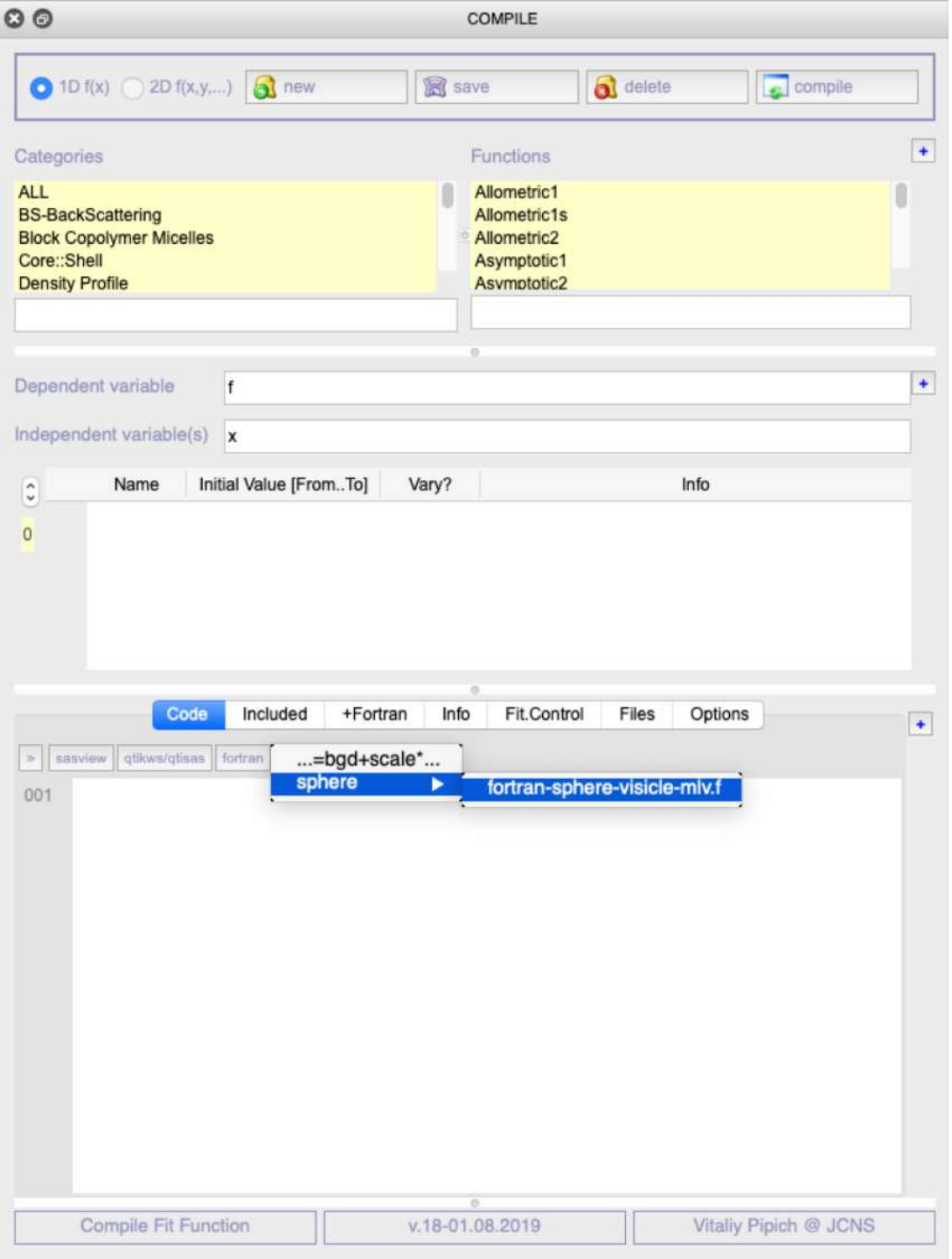
FIF-file: multilamellar-vesicle-model-hf.fif
[move to ”FitFunctions”]

Example: **Multilamellar Vesicle Model**

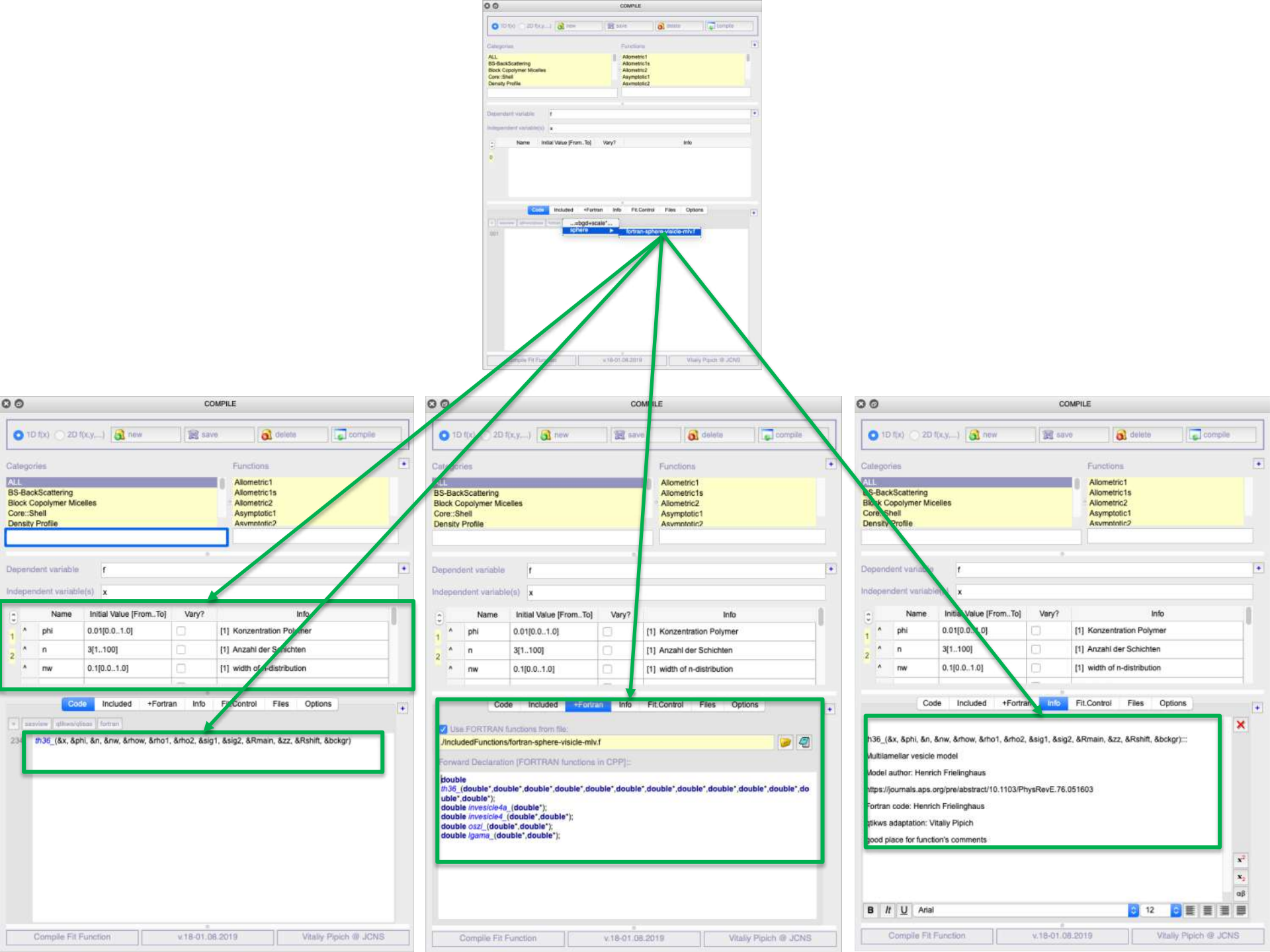
th36_(&Q, &phi, &n, &nw, &rhow, &rho1, &rho2, &sig1, &sig2, &Rmain, &zz, &Rshift, &bckgr)

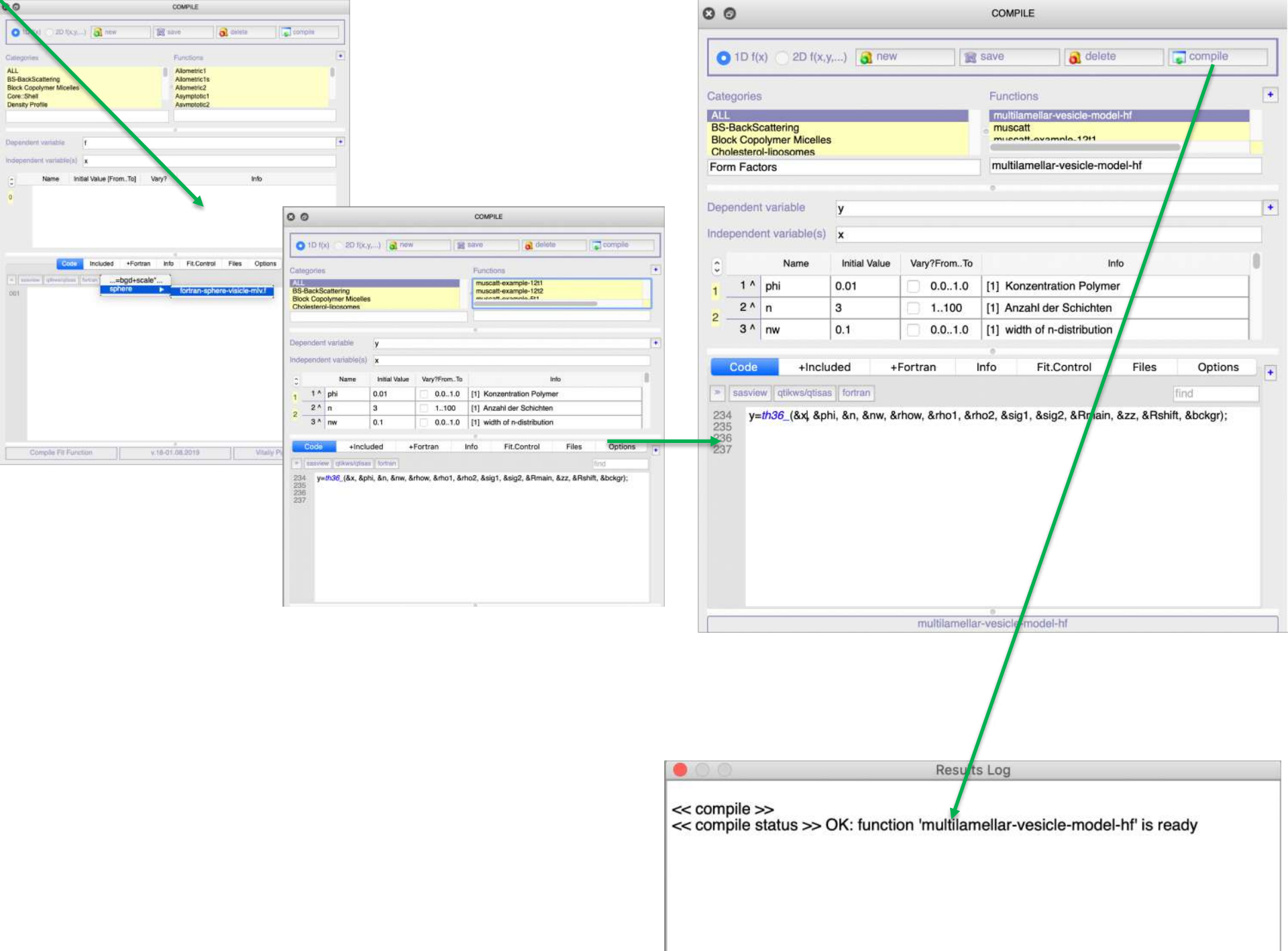


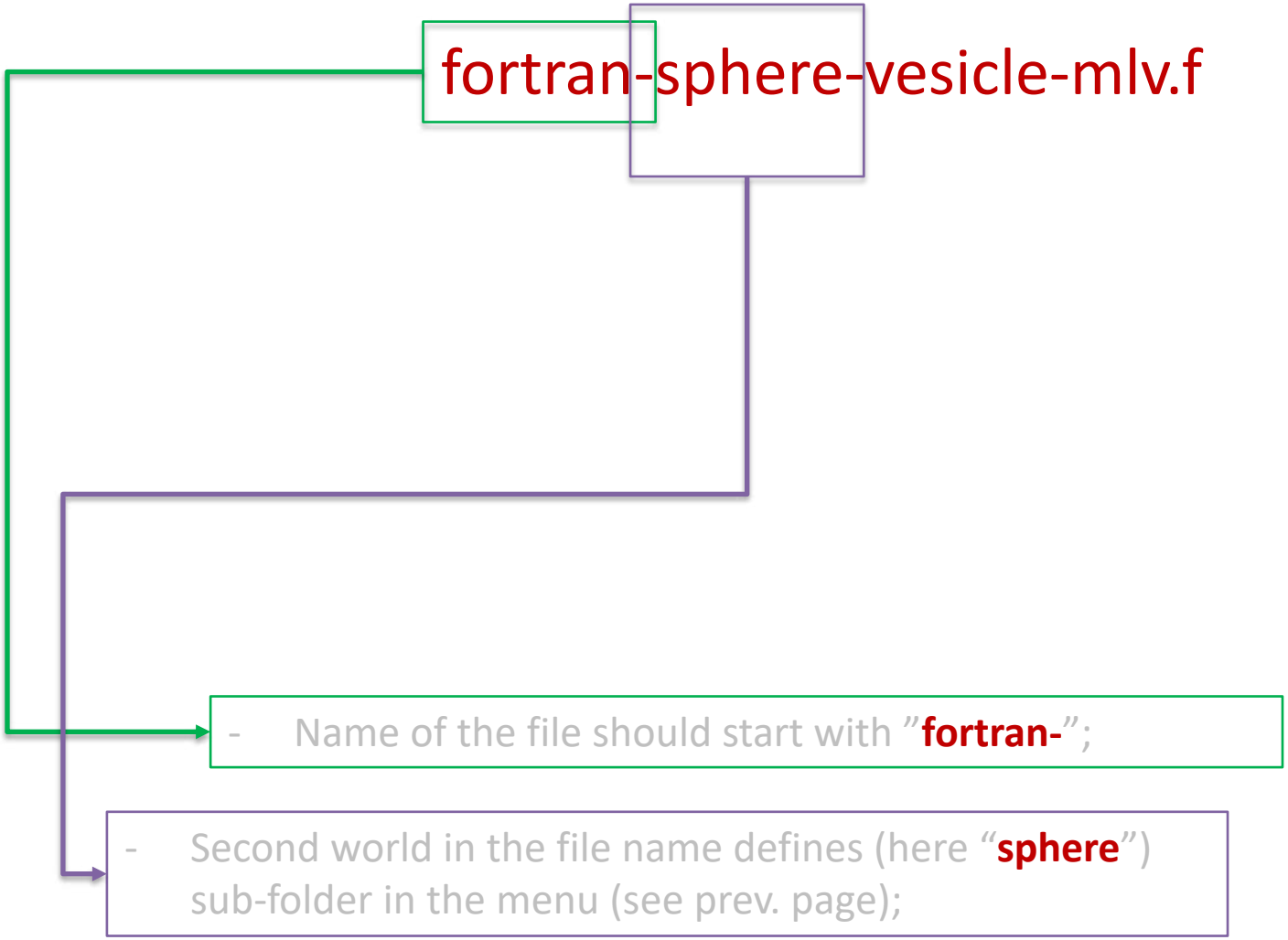
Push „new“ button



- push „fortran“ button;
- select from menu needed Fortran file;
- to use Fortran file from ”fortran” menu file should be prepared (see next pages);
- In example we selected “fortran-sphere-vesicle-mlv.f”


COMPILE
1D f(x)
2D f(x,y,...)
new
save
delete
compile
Categories
Functions
ALL
BS-BackScattering
Block Copolymer Micelles
Core::Shell
Density Profile
Allometric1
Allometric1s
Allometric2
Asymptotic1
Asymptotic2
Dependent variable
f
Independent variable(s)
x
Name
Initial Value [From..To]
Vary?
Info
phi
0.01[0.0..1.0]
[1] Konzentration Polymer
n
3[1..100]
[1] Anzahl der Schichten
nw
0.1[0.0..1.0]
[1] width of n-distribution
Code
Included
+Fortran
Info
Fit.Control
Files
Options
th36_(&x, &phi, &n, &nw, &rhow, &rho1, &rho2, &sig1, &sig2, &Rmain, &zz, &Rshift, &bckgr)
Use FORTRAN functions from file:
./IncludedFunctions/fortran-sphere-visicle-mlv.f
Forward Declaration [FORTRAN functions in CPP]:
double th36_(double*,double*,double*,double*,double*,double*,double*,double*,double*,double*,double*,double*,double*);
double invesicle4a_(double*);
double invesicle4_(double*,double*);
double oszi_(double*,double*);
double lgama_(double*,double*);
th36_(&x, &phi, &n, &nw, &rhow, &rho1, &rho2, &sig1, &sig2, &Rmain, &zz, &Rshift, &bckgr):::
Multilamellar vesicle model
Model author: Henrich Frielinghaus
https://journals.aps.org/pre/abstract/10.1103/PhysRevE.76.051603
Fortran code: Henrich Frielinghaus
qtikws adaptation: Vitally Pipich
good place for function's comments
Arial
12
Compile Fit Function
v.18-01.08.2019
Vitally Pipich @ JCNS


COMPILE
1D f(x)
2D f(x,y,...)
new
save
delete
compile
Categories
Functions
ALL
BS-BackScattering
Block Copolymer Micelles
Cholesterol-liposomes
Form Factors
multilamellar-vesicle-model-hf
muscatt
Dependent variable
y
Independent variable(s)
x
Name
Initial Value
Vary?From..To
Info
1 ^ phi 0.01 0.0..1.0 [1] Konzentration Polymer
2 ^ n 3 1..100 [1] Anzahl der Schichten
3 ^ nw 0.1 0.0..1.0 [1] width of n-distribution
Code
+Included
+Fortran
Info
Fit.Control
Files
Options
sasview
qtikws/qtisas
fortran
find
y=th36_(&x, &phi, &n, &nw, &rhow, &rho1, &rho2, &sig1, &sig2, &Rmain, &zz, &Rshift, &bckgr);
multilamellar-vesicle-model-hf
Results Log
<< compile >>
<< compile status >> OK: function 'multilamellar-vesicle-model-hf' is ready



- File should be located in ”**FitFunctions/IncludedFunctions**” folder;

Fortran file is “decorated“ with 7 lines of comments in the header (see below first 7 lines)

```
1  C[name] th36
2  C[parameter_names]  phi, n, nw, rhow, rho1, rho2, sig1, sig2, Rmain, zz, Rshift, bckgr
3  C[parameter_init_values] 0.01, 3, 0.1, -0.56e10, 2e10, 3e10, 50.0, 20.0, 800.0, 0.2, 10.0, 0.01
4  C[parameter_init_range] [0.0..1.0], [1..100], [0.0..1.0], [-1e10..10e10], [-1e10..10e10], [-1e10..10e10], [0.0..10000.0], [0.0..10000], [0.0..100000.0], [0.0..10000], [0.0..10000.0], [0.0..1.0]
5  C[parameter_units] [1], [1], [1], [1/cm^2], [1/cm^2], [1/cm^2], [1/cm^2], [A], [A], [A], [?1], [A], [1/cm]
6  C[parameter_info]  [Konzentration Polymer], [Anzahl der Schichten], [width of n-distribution], [SLD Wasser], [SLD der zentralen Schicht (1)], [SLD der Dekoration (2)], [Dicke der zentralen Schicht (1)], [Dicke der Dekoration (2)]
7  C[info]  "Multilamellar vesicle model",, "Model author: Henrich Frielinghaus",, "https://journals.aps.org/pre/abstract/10.1103/PhysRevE.76.051603",, "Fortran code: Henrich Frielinghaus",, "qtikws adaptation: Vitaliy Pipich"
8
9      function th36(x,xphi,xn,xnw,xrhow,xrho1,xrho2,xsig1,xsig2,
10     *            xRmain,xzz,xRshift,xbckgr)
11 C
12     implicit none
13 C
14     double precision th36
15     double precision x
16 C
17     double precision Pi
18     parameter (Pi = 3.14159265358979323846264338328d0)
19 C
20     double precision xphi       ! Konzentration Polymer
21     double precision xn         ! Anzahl der Schichten
22     double precision xnw        ! width of n-distribution
23     double precision xrhoW      ! SLD   Wasser
24     double precision xrho1,xrho2 ! SLD   der zentralen Schicht (1) und Dekoration (2)
25     double precision xsig1,xsig2 ! Dicke der zentralen Schicht (1) und Dekoration (2)
26     double precision xRmain     ! Main Radius
27     double precision xzz        ! Z - Schultz distribution
28     double precision xRshift    ! Maximum possible shift
29     double precision xbckgr     ! background
30 c
31     double precision q          ! Q-Vektor
32     double precision phi        ! Konzentration Polymer
33     double precision n          ! Anzahl der Schichten
34     double precision nw         ! width of n-distribution
35     double precision rhoW       ! SLD   Wasser
36     double precision rho1,rho2  ! SLD   der zentralen Schicht (1) und Dekoration (2)
37     double precision sig1,sig2  ! Dicke der zentralen Schicht (1) und Dekoration (2)
38     double precision Rmain      ! Main Radius
39     double precision zz         ! Z - Schultz distribution
40     double precision Rshift     ! Maximum possible shift
41     double precision bckgr      ! background
42 C
43     double precision drho1,drho2 ! Kontrast der zentralen Schicht (1) und Dekoration (2) zum L"osungsmittel
44 C
45     double precision bmin,bmax  ! Integrationsgrenzen
46     double precision eps        ! Fehler
47     integer          maxit      ! Maximale Iterationen
```

Line #1 starts with **C[name]** and comtains “main“ Fortran function will be called from c-code of fitting function

```
1   C[name] th36
2   C[parameter_names]  phi, n, nw, rhow, rho1, rho2, sig1, sig2, Rmain, zz, Rshift, bckgr
3   C[parameter_init_values] 0.01, 3, 0.1, -0.56e10, 2e10, 3e10, 50.0, 20.0, 800.0, 0.2, 10.0, 0.01
4   C[parameter_init_range] [0.0..1.0], [1..100], [0.0..1.0], [-1e10..10e10], [-1e10..10e10], [-1e10..10e10], [0.0..10000.0], [0.0..10000], [0.0..100000.0], [0.0..10000], [0.0..10000.0], [0.0..1.0]
5   C[parameter_units] [1], [1], [1], [1/cm^2], [1/cm^2], [1/cm^2], [A], [A], [A], [?1], [A], [1/cm]
6   C[parameter_info]  [Konzentration Polymer], [Anzahl der Schichten], [width of n-distribution], [SLD Wasser], [SLD der zentralen Schicht (1)], [SLD der Dekoration (2)], [Dicke der zentralen Schicht (1)], [Dicke der Dekoration (2)]
7   C[info]  "Multilamellar vesicle model",, "Model author: Henrich Frielinghaus",, "https://journals.aps.org/pre/abstract/10.1103/PhysRevE.76.051603",, "Fortran code: Henrich Frielinghaus",, "qtikws adaptation: Vitaliy Pipich"
8
9       function th36(x,xphi,xn,xnw,xrhow,xrho1,xrho2,xsig1,xsig2,
10      *              xRmain,xzz,xRshift,xbckgr)
11  C
12      implicit none
13  C
14      double precision th36
15      double precision x
16  C
17      double precision Pi
18      parameter (Pi = 3.14159265358979323846264338328d0)
19  C
20      double precision xphi       ! Konzentration Polymer
21      double precision xn         ! Anzahl der Schichten
22      double precision xnw        ! width of n-distribution
23      double precision xrhoW      ! SLD   Wasser
24      double precision xrho1,xrho2 ! SLD   der zentralen Schicht (1) und Dekoration (2)
25      double precision xsig1,xsig2 ! Dicke der zentralen Schicht (1) und Dekoration (2)
26      double precision xRmain     ! Main Radius
27      double precision xzz        ! Z - Schultz distribution
28      double precision xRshift    ! Maximum possible shift
29      double precision xbckgr     ! background
30  c
31      double precision q          ! Q-Vektor
32      double precision phi        ! Konzentration Polymer
33      double precision n          ! Anzahl der Schichten
34      double precision nw         ! width of n-distribution
35      double precision rhoW       ! SLD   Wasser
36      double precision rho1,rho2  ! SLD   der zentralen Schicht (1) und Dekoration (2)
37      double precision sig1,sig2  ! Dicke der zentralen Schicht (1) und Dekoration (2)
38      double precision Rmain      ! Main Radius
39      double precision zz         ! Z - Schultz distribution
40      double precision Rshift     ! Maximum possible shift
41      double precision bckgr      ! background
42  C
43      double precision drho1,drho2 ! Kontrast der zentralen Schicht (1) und Dekoration (2) zum L"osungsmittel
44  C
45      double precision bmin,bmax   ! Integrationsgrenzen
46      double precision eps        ! Fehler
47      integer          maxit      ! Maximale Iterationen
```

Code | Included | +Fortran | Info | Fit.Control | Files | Options

» | sasview | qtikws/qtisas | fortran

```
234  // ---> f = f ( x, {P1, ...} );
235  th36_(&x, &phi, &n, &nw, &rhow, &rho1, &rho2, &sig1, &sig2, &Rmain, &zz, &Rshift, &bckgr)
```

Line #2 starts with **C[parameter_name]** and contains list of parameter names separates by **,**

```
C[name] th36
C[parameter_names] phi, n, nw, rhow, rho1, rho2, sig1, sig2, Rmain, zz, Rshift, bckgr
C[parameter_init_values] 0.01, 3, 0.1, -0.56e10, 2e10, 3e10, 50.0, 20.0, 800.0, 0.2, 10.0, 0.01
C[parameter_init_range] [0.0..1.0], [1..100], [0.0..1.0], [-1e10..10e10], [-1e10..10e10], [-1e10..10e10], [0.0..10000.0], [0.0..10000], [0.0..100000.0], [0.0..10000], [0.0..10000.0], [0.0..1.0]
C[parameter_units] [1], [1], [1], [1/cm^2], [1/cm^2], [1/cm^2], [A], [A], [A], [?1], [A], [1/cm]
C[parameter_info] [Konzentration Polymer], [Anzahl der Schichten], [width of n-distribution], [SLD Wasser], [SLD der zentralen Schicht (1)], [SLD der Dekoration (2)], [Dicke der zentralen Schicht (1)], [Dicke der Dekoration (2)]
C[info] "Multilamellar vesicle model",, "Model author: Henrich Frielinghaus",, "https://journals.aps.org/pre/abstract/10.1103/PhysRevE.76.051603",, "Fortran code: Henrich Frielinghaus",, "qtikws adaptation: Vitaliy Pipich"

      function th36(x,xphi,xn,xnw,xrhow,xrho1,xrho2,xsig1,xsig2,
     *              xRmain,xzz,xRshift,xbckgr)
C
      implicit none
C
      double precision th36
      double precision x
C
      double precision Pi
      parameter (Pi = 3.14159265358979323846264338328d0)
C
      double precision xphi       ! Konzentration Polymer
      double precision xn         ! Anzahl der Schichten
      double precision xnw        ! width of n-distribution
      double precision xrhoW      ! SLD   Wasser
      double precision xrho1,xrho2 ! SLD   der zentralen Schicht (1) und Dekoration (2)
      double precision xsig1,xsig2 ! Dicke der zentralen Schicht (1) und Dekoration (2)
      double precision xRmain     ! Main Radius
      double precision xzz        ! Z - Schultz distribution
      double precision xRshift    ! Maximum possible shift
      double precision xbckgr     ! background
c
      double precision q          ! Q-Vektor
      double precision phi        ! Konzentration Polymer
      double precision n          ! Anzahl der Schichten
      double precision nw         ! width of n-distribution
      double precision rhoW       ! SLD   Wasser
      double precision rho1,rho2  ! SLD   der zentralen Schicht (1) und Dekoration (2)
      double precision sig1,sig2  ! Dicke der zentralen Schicht (1) und Dekoration (2)
      double precision Rmain      ! Main Radius
      double precision zz         ! Z - Schultz distribution
      double precision Rshift     ! Maximum possible shift
      double precision bckgr      ! background
C
      double precision drho1,drho2 ! Kontrast der zentralen Schicht (1) und Dekoration (2) zum L"osungsmittel
C
      double precision bmin,bmax  ! Integrationsgrenzen
      double precision eps        ! Fehler
      integer          maxit      ! Maximale Iterationen
```

Code | Included | +Fortran | Info | Fit.Control | Files | Options

sasview | qtikws/qtisas | fortran

```
// ---> f = f ( x, {P1, ...} );
th36 (&x, &phi, &n, &nw, &rhow, &rho1, &rho2, &sig1, &sig2, &Rmain, &zz, &Rshift, &bckgr);
```

Dependent variable: y

Independent variable(s): x

	Name	Initial Value	Vary?From..To	Info
1 ^	phi	0.01	0.0..1.0	[1] Konzentration Polymer
2 ^	n	3	1..100	[1] Anzahl der Schichten
3 ^	nw	0.1	0.0..1.0	[1] width of n-distribution
4 ^	rhow	-5.6e+09	-1e10..10e10	[1/cm^2] SLD Wasser
5 ^	rho1	2e+10	-1e10..10e10	[1/cm^2] SLD der zentralen Schicht (1)
6 ^	rho2	3e+10	-1e10..10e10	[1/cm^2] SLD der Dekoration (2)
7 ^	sig1	50	0.0..10000.0	[A] Dicke der zentralen Schicht (1)
8 ^	sig2	20	0.0..10000	[A] Dicke der Dekoration (2)
9 ^	Rmain	800	0.0..100000.0	[A] Main Radius
10 ^	zz	0.2	0.0..10000	[?1] Z - Schultz distribution
11 ^	Rshift	10	0.0..10000.0	[A] Maximum possible shift
12 ^	bckgr	0.01	..	[1/cm] background

Line #3 starts with **C[parameter_init_values]** and contains list of initial values of parameters separates by **,**

```
1  C[name] th36
2  C[parameter_names] phi, n, nw, rhow, rho1, rho2, sig1, sig2, Rmain, zz, Rshift, bckgr
3  C[parameter_init_values] 0.01, 3, 0.1, -0.56e10, 2e10, 3e10, 50.0, 20.0, 800.0, 0.2, 10.0, 0.01
4  C[parameter_init_range] [0.0..1.0], [1..100], [0.0..1.0], [-1e10..10e10], [-1e10..10e10], [-1e10..10e10], [0.0..10000.0], [0.0..10000], [0.0..100000.0], [0.0..10000], [0.0..10000.0], [0.0..1.0]
5  C[parameter_units] [1], [1], [1], [1/cm^2], [1/cm^2], [1/cm^2], [A], [A], [A], [?1], [A], [1/cm]
6  C[parameter_info] [Konzentration Polymer], [Anzahl der Schichten], [width of n-distribution], [SLD Wasser], [SLD der zentralen Schicht (1)], [SLD der Dekoration (2)], [Dicke der zentralen Schicht (1)], [Dicke der Dekoration (2)]
7  C[info] "Multilamellar vesicle model",, "Model author: Henrich Frielinghaus",, "https://journals.aps.org/pre/abstract/10.1103/PhysRevE.76.051603",, "Fortran code: Henrich Frielinghaus",, "qtikws adaptation: Vitaliy Pipich"
8
9      function th36(x,xphi,xn,xnw,xrhow,xrho1,xrho2,xsig1,xsig2,
10     *           xRmain,xzz,xRshift,xbckgr)
11 C
12     implicit none
13 C
14     double precision th36
15     double precision x
16 C
17     double precision Pi
18     parameter (Pi = 3.14159265358979323846264338328d0)
19 C
20     double precision xphi       ! Konzentration Polymer
21     double precision xn         ! Anzahl der Schichten
22     double precision xnw        ! width of n-distribution
23     double precision xrhoW      ! SLD   Wasser
24     double precision xrho1,xrho2 ! SLD   der zentralen Schicht (1) und Dekoration (2)
25     double precision xsig1,xsig2 ! Dicke der zentralen Schicht (1) und Dekoration (2)
26     double precision xRmain     ! Main Radius
27     double precision xzz        ! Z - Schultz distribution
28     double precision xRshift    ! Maximum possible shift
29     double precision xbckgr     ! background
30 c
31     double precision q          ! Q-Vektor
32     double precision phi        ! Konzentration Polymer
33     double precision n          ! Anzahl der Schichten
34     double precision nw         ! width of n-distribution
35     double precision rhoW       ! SLD   Wasser
36     double precision rho1,rho2  ! SLD   der zentralen Schicht (1) und Dekoration (2)
37     double precision sig1,sig2  ! Dicke der zentralen Schicht (1) und Dekoration (2)
38     double precision Rmain      ! Main Radius
39     double precision zz         ! Z - Schultz distribution
40     double precision Rshift     ! Maximum possible shift
41     double precision bckgr      ! background
42 C
43     double precision drho1,drho2 ! Kontrast der zentralen Schicht (1) und Dekoration (2) zum L"osungsmittel
44 C
45     double precision bmin,bmax  ! Integrationsgrenzen
46     double precision eps        ! Fehler
47     integer          maxit      ! Maximale Iterationen
```

Dependent variable: y

Independent variable(s): x

	Name	Initial Value	Vary?From..To	Info
1 ^	phi	0.01	0.0..1.0	[1] Konzentration Polymer
2 ^	n	3	1..100	[1] Anzahl der Schichten
3 ^	nw	0.1	0.0..1.0	[1] width of n-distribution
4 ^	rhow	-5.6e+09	-1e10..10e10	[1/cm^2] SLD Wasser
5 ^	rho1	2e+10	-1e10..10e10	[1/cm^2] SLD der zentralen Schicht (1)
6 ^	rho2	3e+10	-1e10..10e10	[1/cm^2] SLD der Dekoration (2)
7 ^	sig1	50	0.0..10000.0	[A] Dicke der zentralen Schicht (1)
8 ^	sig2	20	0.0..10000	[A] Dicke der Dekoration (2)
9 ^	Rmain	800	0.0..100000.0	[A] Main Radius
10 ^	zz	0.2	0.0..10000	[?1] Z - Schultz distribution
11 ^	Rshift	10	0.0..10000.0	[A] Maximum possible shift
12 ^	bckgr	0.01	..	[1/cm] background

Line #4 starts with **C[parameter_init_range]** and contains list of ranges of initial values of parameters separates by **,**
In format "**[left..right]**"

```
1  C[name] th36
2  C[parameter_names]  phi, n, nw, rhow, rho1, rho2, sig1, sig2, Rmain, zz, Rshift, bckgr
3  C[parameter_init_values] 0.01, 3, 0.1, -0.56e10, 2e10, 3e10, 50.0, 20.0, 800.0, 0.2, 10.0, 0.01
4  C[parameter_init_range] [0.0..1.0], [1..100], [0.0..1.0], [-1e10..10e10], [-1e10..10e10], [-1e10..10e10], [0.0..10000.0], [0.0..10000], [0.0..100000.0], [0.0..10000], [0.0..10000.0], [0.0..1.0]
5  C[parameter_units] [1], [1], [1], [1/cm^2], [1/cm^2], [1/cm^2], [A], [A], [A], [?1], [A], [1/cm]
6  C[parameter_info]  [Konzentration Polymer], [Anzahl der Schichten], [width of n-distribution], [SLD Wasser], [SLD der zentralen Schicht (1)], [SLD der Dekoration (2)], [Dicke der zentralen Schicht (1)], [Dicke der Dekoration (2)]
7  C[info]  "Multilamellar vesicle model",, "Model author: Henrich Frielinghaus",, "https://journals.aps.org/pre/abstract/10.1103/PhysRevE.76.051603",, "Fortran code: Henrich Frielinghaus",, "qtikws adaptation: Vitaliy Pipich"
8
9      function th36(x,xphi,xn,xnw,xrhow,xrho1,xrho2,xsig1,xsig2,
10     *           xRmain,xzz,xRshift,xbckgr)
11 C
12     implicit none
13 C
14     double precision th36
15     double precision x
16 C
17     double precision Pi
18     parameter (Pi = 3.14159265358979323846264338328d0)
19 C
20     double precision xphi       ! Konzentration Polymer
21     double precision xn         ! Anzahl der Schichten
22     double precision xnw        ! width of n-distribution
23     double precision xrhoW      ! SLD   Wasser
24     double precision xrho1,xrho2 ! SLD   der zentralen Schicht (1) und Dekoration (2)
25     double precision xsig1,xsig2 ! Dicke der zentralen Schicht (1) und Dekoration (2)
26     double precision xRmain     ! Main Radius
27     double precision xzz        ! Z - Schultz distribution
28     double precision xRshift    ! Maximum possible shift
29     double precision xbckgr     ! background
30 c
31     double precision q          ! Q-Vektor
32     double precision phi        ! Konzentration Polymer
33     double precision n          ! Anzahl der Schichten
34     double precision nw         ! width of n-distribution
35     double precision rhoW       ! SLD   Wasser
36     double precision rho1,rho2  ! SLD   der zentralen Schicht (1) und Dekoration (2)
37     double precision sig1,sig2  ! Dicke der zentralen Schicht (1) und Dekoration (2)
38     double precision Rmain      ! Main Radius
39     double precision zz         ! Z - Schultz distribution
40     double precision Rshift     ! Maximum possible shift
41     double precision bckgr      ! background
42 C
43     double precision drho1,drho2 ! Kontrast der zentralen Schicht (1) und Dekoration (2) zum L"osungsmittel
44 C
45     double precision bmin,bmax   ! Integrationsgrenzen
46     double precision eps        ! Fehler
47     integer          maxit      ! Maximale Iterationen
```

Dependent variable: y

Independent variable(s): x

	Name	Initial Value	Vary?	From..To	Info
1 ^	phi	0.01	☐	0.0..1.0	[1] Konzentration Polymer
2 ^	n	3	☐	1..100	[1] Anzahl der Schichten
3 ^	nw	0.1	☐	0.0..1.0	[1] width of n-distribution
4 ^	rhow	-5.6e+09	☐	-1e10..10e10	[1/cm^2] SLD Wasser
5 ^	rho1	2e+10	☐	-1e10..10e10	[1/cm^2] SLD der zentralen Schicht (1)
6 ^	rho2	3e+10	☐	-1e10..10e10	[1/cm^2] SLD der Dekoration (2)
7 ^	sig1	50	☐	0.0..10000.0	[A] Dicke der zentralen Schicht (1)
8 ^	sig2	20	☐	0.0..10000	[A] Dicke der Dekoration (2)
9 ^	Rmain	800	☐	0.0..100000.0	[A] Main Radius
10 ^	zz	0.2	☐	0.0..10000	[?1] Z - Schultz distribution
11 ^	Rshift	10	☐	0.0..10000.0	[A] Maximum possible shift
12 ^	bckgr	0.01	☐	..	[1/cm] background

Line #5 starts with **C[parameter_units]** and contains list of units of parameters separates by **,**
In format "**[UNITS]**"

```
1  C[name] th36
2  C[parameter_names] phi, n, nw, rhow, rho1, rho2, sig1, sig2, Rmain, zz, Rshift, bckgr
3  C[parameter_init_values] 0.01, 3, 0.1, -0.56e10, 2e10, 3e10, 50.0, 20.0, 800.0, 0.2, 10.0, 0.01
4  C[parameter_init_range] [0.0..1.0], [1..100], [0.0..1.0], [-1e10..10e10], [-1e10..10e10], [-1e10..10e10], [0.0..10000.0], [0.0..10000], [0.0..100000.0], [0.0..10000], [0.0..10000.0], [0.0..1.0]
5  C[parameter_units] [1], [1], [1], [1/cm^2], [1/cm^2], [1/cm^2], [A], [A], [A], [?1], [A], [1/cm]
6  C[parameter_info] [Konzentration Polymer], [Anzahl der Schichten], [width of n-distribution], [SLD Wasser], [SLD der zentralen Schicht (1)], [SLD der Dekoration (2)], [Dicke der zentralen Schicht (1)], [Dicke der Dekoration (2)]
7  C[info] "Multilamellar vesicle model",, "Model author: Henrich Frielinghaus",, "https://journals.aps.org/pre/abstract/10.1103/PhysRevE.76.051603",, "Fortran code: Henrich Frielinghaus",, "qtikws adaptation: Vitaliy Pipich"
8
9      function th36(x,xphi,xn,xnw,xrhow,xrho1,xrho2,xsig1,xsig2,
10     *           xRmain,xzz,xRshift,xbckgr)
11 C
12     implicit none
13 C
14     double precision th36
15     double precision x
16 C
17     double precision Pi
18     parameter (Pi = 3.14159265358979323846264338328d0)
19 C
20     double precision xphi       ! Konzentration Polymer
21     double precision xn         ! Anzahl der Schichten
22     double precision xnw        ! width of n-distribution
23     double precision xrhoW      ! SLD   Wasser
24     double precision xrho1,xrho2 ! SLD   der zentralen Schicht (1) und Dekoration (2)
25     double precision xsig1,xsig2 ! Dicke der zentralen Schicht (1) und Dekoration (2)
26     double precision xRmain     ! Main Radius
27     double precision xzz        ! Z - Schultz distribution
28     double precision xRshift    ! Maximum possible shift
29     double precision xbckgr     ! background
30 c
31     double precision q          ! Q-Vektor
32     double precision phi        ! Konzentration Polymer
33     double precision n          ! Anzahl der Schichten
34     double precision nw         ! width of n-distribution
35     double precision rhoW       ! SLD   Wasser
36     double precision rho1,rho2  ! SLD   der zentralen Schicht (1) und Dekoration (2)
37     double precision sig1,sig2  ! Dicke der zentralen Schicht (1) und Dekoration (2)
38     double precision Rmain      ! Main Radius
39     double precision zz         ! Z - Schultz distribution
40     double precision Rshift     ! Maximum possible shift
41     double precision bckgr      ! background
42 C
43     double precision drho1,drho2 ! Kontrast der zentralen Schicht (1) und Dekoration (2) zum L"osungsmittel
44 C
45     double precision bmin,bmax  ! Integrationsgrenzen
46     double precision eps        ! Fehler
47     integer          maxit      ! Maximale Iterationen
```

Dependent variable: y

Independent variable(s): x

	Name	Initial Value	Vary?From..To	Info
1 ^	phi	0.01	0.0..1.0	[1] Konzentration Polymer
2 ^	n	3	1..100	[1] Anzahl der Schichten
3 ^	nw	0.1	0.0..1.0	[1] width of n-distribution
4 ^	rhow	-5.6e+09	-1e10..10e10	[1/cm^2] SLD Wasser
5 ^	rho1	2e+10	-1e10..10e10	[1/cm^2] SLD der zentralen Schicht (1)
6 ^	rho2	3e+10	-1e10..10e10	[1/cm^2] SLD der Dekoration (2)
7 ^	sig1	50	0.0..10000.0	[A] Dicke der zentralen Schicht (1)
8 ^	sig2	20	0.0..10000	[A] Dicke der Dekoration (2)
9 ^	Rmain	800	0.0..100000.0	[A] Main Radius
10 ^	zz	0.2	0.0..10000	[?1] Z - Schultz distribution
11 ^	Rshift	10	0.0..10000.0	[A] Maximum possible shift
12 ^	bckgr	0.01	..	[1/cm] background

Line #6 starts with **C[parameter_info]** and contains list of descriptions of parameters separates by **,**
In format "**[INFO…]**"

```
1  C[name] th36
2  C[parameter_names]  phi, n, nw, rhow, rho1, rho2, sig1, sig2, Rmain, zz, Rshift, bckgr
3  C[parameter_init_values] 0.01, 3, 0.1, -0.56e10, 2e10, 3e10, 50.0, 20.0, 800.0, 0.2, 10.0, 0.01
4  C[parameter_init_range] [0.0..1.0], [1..100], [0.0..1.0], [-1e10..10e10], [-1e10..10e10], [-1e10..10e10], [0.0..10000.0], [0.0..10000], [0.0..100000.0], [0.0..10000], [0.0..10000.0], [0.0..1.0]
5  C[parameter_units] [1], [1], [1], [1/cm^2], [1/cm^2], [1/cm^2], [A], [A], [A], [?1], [A], [1/cm]
6  C[parameter_info]  [Konzentration Polymer], [Anzahl der Schichten], [width of n-distribution], [SLD Wasser], [SLD der zentralen Schicht (1)], [SLD der Dekoration (2)], [Dicke der zentralen Schicht (1)], [Dicke der Dekoration (2)]
7  C[info]  "Multilamellar vesicle model",, "Model author: Henrich Frielinghaus",, "https://journals.aps.org/pre/abstract/10.1103/PhysRevE.76.051603",, "Fortran code: Henrich Frielinghaus",, "qtikws adaptation: Vitaliy Pipich"
8
9      function th36(x,xphi,xn,xnw,xrhow,xrho1,xrho2,xsig1,xsig2,
10     *           xRmain,xzz,xRshift,xbckgr)
11 C
12     implicit none
13 C
14     double precision th36
15     double precision x
16 C
17     double precision Pi
18     parameter (Pi = 3.14159265358979323846264338328d0)
19 C
20     double precision xphi       ! Konzentration Polymer
21     double precision xn         ! Anzahl der Schichten
22     double precision xnw        ! width of n-distribution
23     double precision xrhoW      ! SLD   Wasser
24     double precision xrho1,xrho2 ! SLD   der zentralen Schicht (1) und Dekoration (2)
25     double precision xsig1,xsig2 ! Dicke der zentralen Schicht (1) und Dekoration (2)
26     double precision xRmain     ! Main Radius
27     double precision xzz        ! Z - Schultz distribution
28     double precision xRshift    ! Maximum possible shift
29     double precision xbckgr     ! background
30 c
31     double precision q          ! Q-Vektor
32     double precision phi        ! Konzentration Polymer
33     double precision n          ! Anzahl der Schichten
34     double precision nw         ! width of n-distribution
35     double precision rhoW       ! SLD   Wasser
36     double precision rho1,rho2  ! SLD   der zentralen Schicht (1) und Dekoration (2)
37     double precision sig1,sig2  ! Dicke der zentralen Schicht (1) und Dekoration (2)
38     double precision Rmain      ! Main Radius
39     double precision zz         ! Z - Schultz distribution
40     double precision Rshift     ! Maximum possible shift
41     double precision bckgr      ! background
42 C
43     double precision drho1,drho2 ! Kontrast der zentralen Schicht (1) und Dekoration (2) zum L"osungsmittel
44 C
45     double precision bmin,bmax   ! Integrationsgrenzen
46     double precision eps        ! Fehler
47     integer          maxit      ! Maximale Iterationen
```

Dependent variable: y
Independent variable(s): x

	Name	Initial Value	Vary?From..To		Info
1 ^	phi	0.01	0.0..1.0	[1]	Konzentration Polymer
2 ^	n	3	1..100	[1]	Anzahl der Schichten
3 ^	nw	0.1	0.0..1.0	[1]	width of n-distribution
4 ^	rhow	-5.6e+09	-1e10..10e10	[1/cm^2]	SLD Wasser
5 ^	rho1	2e+10	-1e10..10e10	[1/cm^2]	SLD der zentralen Schicht (1)
6 ^	rho2	3e+10	-1e10..10e10	[1/cm^2]	SLD der Dekoration (2)
7 ^	sig1	50	0.0..10000.0	[A]	Dicke der zentralen Schicht (1)
8 ^	sig2	20	0.0..10000	[A]	Dicke der Dekoration (2)
9 ^	Rmain	800	0.0..100000.0	[A]	Main Radius
10 ^	zz	0.2	0.0..10000	[?1]	Z - Schultz distribution
11 ^	Rshift	10	0.0..10000.0	[A]	Maximum possible shift
12 ^	bckgr	0.01	..	[1/cm]	background

Line #7 starts with **C[info]** and contains information about function. Every line is separated by **„**

```
1  C[name] th36
2  C[parameter_names]  phi, n, nw, rhow, rho1, rho2, sig1, sig2, Rmain, zz, Rshift, bckgr
3  C[parameter_init_values] 0.01, 3, 0.1, -0.56e10, 2e10, 3e10, 50.0, 20.0, 800.0, 0.2, 10.0, 0.01
4  C[parameter_init_range] [0.0..1.0], [1..100], [0.0..1.0], [-1e10..10e10], [-1e10..10e10], [-1e10..10e10], [0.0..10000.0], [0.0..10000], [0.0..100000.0], [0.0..10000], [0.0..10000.0], [0.0..1.0]
5  C[parameter_units] [1], [1], [1], [1/cm^2], [1/cm^2], [1/cm^2], [A], [A], [A], [?1], [A], [1/cm]
6  C[parameter_info]  [Konzentration Polymer], [Anzahl der Schichten], [width of n-distribution], [SLD Wasser], [SLD der zentralen Schicht (1)], [SLD der Dekoration (2)], [Dicke der zentralen Schicht (1)], [Dicke der Dekoration (2)]
7  C[info]  "Multilamellar vesicle model",, "Model author: Henrich Frielinghaus",, "https://journals.aps.org/pre/abstract/10.1103/PhysRevE.76.051603",, "Fortran code: Henrich Frielinghaus",, "qtikws adaptation: Vitaliy Pipich"
8
9      function th36(x,xphi,xn,xnw,xrhow,xrho1,xrho2,xsig1,xsig2,
10     *           xRmain,xzz,xRshift,xbckgr)
11 C
12     implicit none
13 C
14     double precision th36
15     double precision x
16 C
17     double precision Pi
18     parameter (Pi = 3.14159265358979323846264338328d0)
19 C
20     double precision xphi       ! Konzentration Polymer
21     double precision xn         ! Anzahl der Schichten
22     double precision xnw        ! width of n-distribution
23     double precision xrhoW      ! SLD   Wasser
24     double precision xrho1,xrho2 ! SLD   der zentralen Schicht (1) und Dekoration (2)
25     double precision xsig1,xsig2 ! Dicke der zentralen Schicht (1) und Dekoration (2)
26     double precision xRmain     ! Main Radius
27     double precision xzz        ! Z - Schultz distribution
28     double precision xRshift    ! Maximum possible shift
29     double precision xbckgr     ! background
30 c
31     double precision q          ! Q-Vektor
32     double precision phi        ! Konzentration Polymer
33     double precision n          ! Anzahl der Schichten
34     double precision nw         ! width of n-distribution
35     double precision rhoW       ! SLD   Wasser
36     double precision rho1,rho2  ! SLD   der zentralen Schicht (1) und Dekoration (2)
37     double precision sig1,sig2  ! Dicke der zentralen Schicht (1) und Dekoration (2)
38     double precision Rmain      ! Main Radius
39     double precision zz         ! Z - Schultz distribution
40     double precision Rshift     ! Maximum possible shift
41     double precision bckgr      ! background
42 C
43     double precision drho1,drho2 ! Kontrast der zentralen Schicht (1) und Dekoration (2) zu
44 C
45     double precision bmin,bmax  ! Integrationsgrenzen
46     double precision eps        ! Fehler
47     integer          maxit      ! Maximale Iterationen
```