



QtiSAS | Fit-Compile

v. 2021-02-17

Fit-Compile : Introduction . Screenshots . Example

Fit-Compile :: GUI to compile fitting functions

# Fit-Compile :: how to open

The screenshot displays the QTISAS software interface. On the left, a 'Table1' window shows a table with two columns: '1[X]' and '2[Y]'. The main window is titled 'COMPILER' and contains the following elements:

- Buttons: 'new', 'save', 'delete', 'compile'.
- Categories list: ALL, BS-BackScattering, Block Copolymer Micelles, Cholesterol-liposomes, Core::Shell.
- Functions list: 3-shell-model-adv-SQ2-qtisas, 3-shell-model-adv-SQ3-qtisas, Allometric1, Allometric2.
- Dependent variable: f
- Independent variable(s): x
- Table with columns: Name, Initial Value, Vary?From..To, Info.
- Code editor with tabs: Code, +Included, +Fortran, Info, Fit.Control, Files, Options.
- Code editor content: '213'.
- Buttons at the bottom: 'COMPILE', 'FITTABLE(s)', 'ASCII.SANS.1D'.

At the bottom of the interface, the 'Project Explorer' shows a table with the following data:

Name	Type	View	Created	Label
Table1	Table	Normal	18.02.21 11:55	

A vertical sidebar on the right side of the image contains several icons, each enclosed in a red rounded rectangle. From top to bottom, the icons are:

- DAN SANS
- FIT (highlighted with a green rounded rectangle)
- FIT (with a scatter plot)
- SVD (with a color bar)
- JNSE
- ASCII 1D SANS

Red arrows point from the 'FIT' icon in the sidebar to the 'FIT' button in the COMPILER window, and from the 'DAN SANS' icon to the 'DAN SANS' button in the COMPILER window.

# Main Elements

## 1. Button Group

## 2. Function Explorer

2.1 Category List

2.2 Function List (in Active Category)

2.3 Active Category Line

2.4 Active Function Line

## 3. Browser of Parameters

3.1 Dependent Variable

3.2 Independent Variable

3.3 Number-of-Parameter Spin-Box

3.4 Table-of-Parameters

## 4. Tab of Tools

4.1 „Code“: C++ Function Editor (Main Function)

4.2 „+Include“: C++ Function Editor (Included Functions)

4.3 „+Fortran“: Fortran Function Editor (Included Functions)

4.4 „Info“: Information Editor (Current Function)

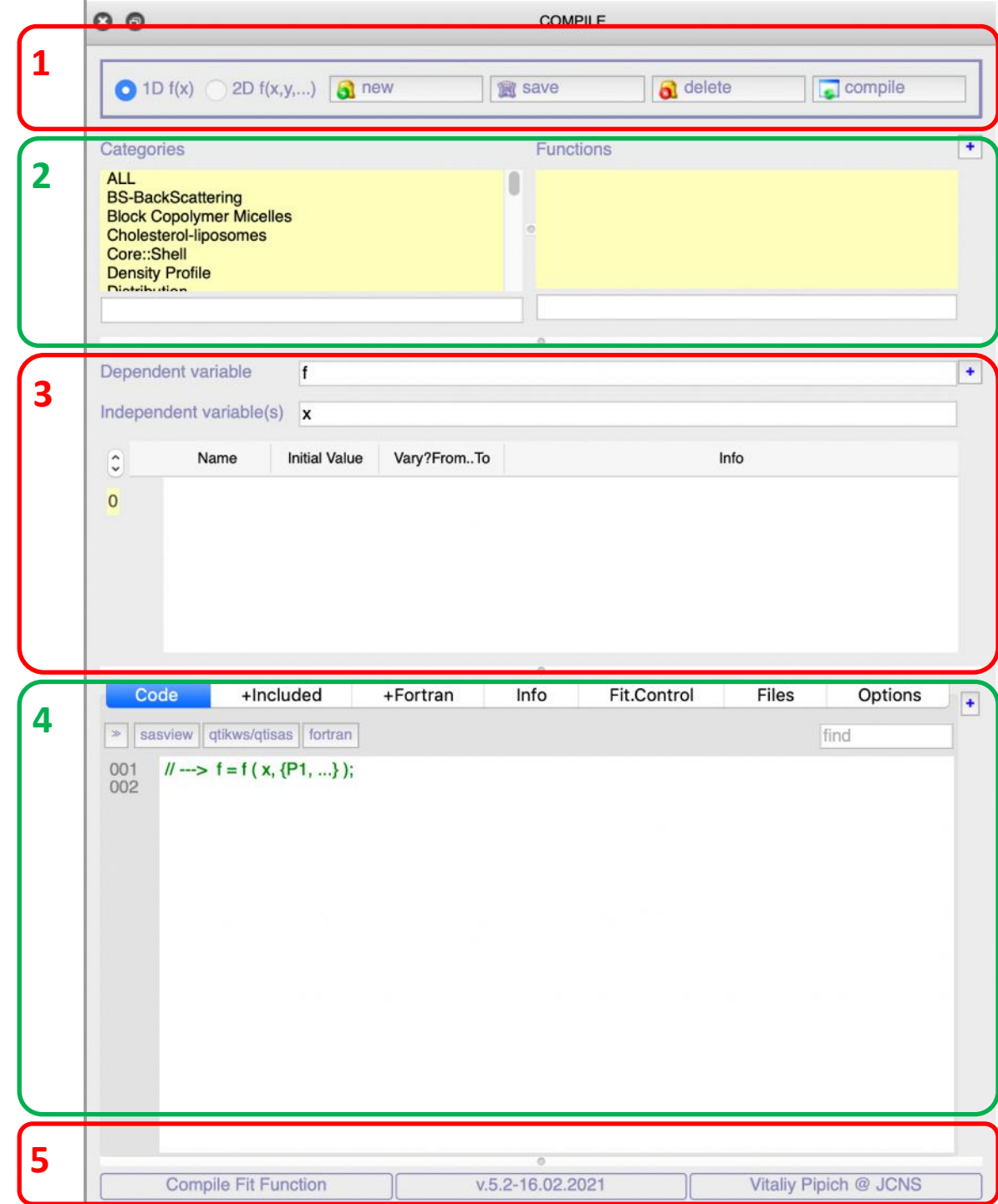
4.5 “Fit.Control”: Fitting Options (Current Function)

4.6 “Files”: Generated Files Viewer (Current Function)

4.7 “Options”: Fit-Compile Interface Options

## 5. Info Panel:

Name – Version – Author



## 2. Function Explorer: Open & Compile an Existing Function

1. Category Selection

The screenshot shows the 'COMPILE' window with the 'Categories' list on the left. The 'Form Factors' category is highlighted in yellow. A green arrow points to this category. The 'Functions' list on the right shows 'Cylinder-eFit' selected. Below the lists, the 'Dependent variable' is 'f' and the 'Independent variable(s)' is 'x'. At the bottom, there is a table with columns 'Name', 'Initial Value', 'Vary?From..To', and 'Info'. The table is currently empty.

2. Function Selection

The screenshot shows the 'COMPILE' window with the 'Categories' list on the left. The 'Form Factors' category is highlighted in yellow. A green arrow points to this category. The 'Functions' list on the right shows 'Cylinder-eFit' selected. Below the lists, the 'Dependent variable' is 'I' and the 'Independent variable(s)' is 'Q'. At the bottom, there is a table with columns 'Name', 'Initial Value', 'Vary?From..To', and 'Info'. The table contains the following data:

	Name	Initial Value	Vary?	From..To	Info
1 ^	L	500	<input checked="" type="checkbox"/>	1..10000	Length of Cylinder [A]
2 ^	R	20	<input checked="" type="checkbox"/>	1..1000	Radius of Cylinder [A]
3 ^	I0	1	<input type="checkbox"/>	0..1E6	Forward Scattering calculated [1/cm]
4 ^	bgd	0	<input type="checkbox"/>	0..10	Background [1/cm]
5 ^	sldCylinder	3e+10	<input type="checkbox"/>	..	SLD [1/cm/cm]
6 ^	sldSolvent	-5.6e+09	<input type="checkbox"/>	..	SLD [1/cm/cm]
7 ^	phi	0.01	<input checked="" type="checkbox"/>	0.001..1	volume fraction [0..1]

3. Compile Current Function

4. Results Log :  
check compilation status

The screenshot shows the 'Results Log' window with the following text:

```
<< compile >>  
<< compile status >> OK: function 'Cylinder-eFit' is ready
```

5. Check Options

The screenshot shows the 'COMPILE' window with the 'Code' tab selected. The code editor contains the following code:

```
260 double VolumeCylinder=M_PI*R*R*L; // volume in A^3  
261  
262 I0=phi*VolumeCylinder*1.0E-24*(sldCylinder-sldSolvent)*(sldCylinder-sldSolvent);  
263  
264 I=I0 * cylinder_form_factor(Q, R, L)+bgd;  
265  
266 beforeFiting(ParaM); //+++ eFit  
267
```

### 3. Parameters Browser: Example : Cylinder Form Factor

Expanding of the Parameter Browser Button

The screenshot shows the COMPILER interface with the parameter browser expanded. The 'Dependent variable' field is empty, and the 'Independent variable(s)' field contains 'Q'. A table of parameters is displayed below, with a spin box for the number of parameters set to 7. The code editor at the bottom shows the definition of the cylinder form factor.

Name	Initial Value	Vary?From..To	Info
1 ^ L	500	<input checked="" type="checkbox"/> 1..10000	Length of Cylinder [A]
2 ^ R	20	<input checked="" type="checkbox"/> 1..1000	Radius of Cylinder [A]
3 ^ I0	1	<input type="checkbox"/> 0..1E6	Forward Scattering calculated [1/cm]
4 ^ bgd	0	<input type="checkbox"/> 0..10	Background [1/cm]
5 ^ sldCylinder	3e+10	<input type="checkbox"/> ..	SLD [1/cm/cm]
6 ^ sldSolvent	-5.6e+09	<input type="checkbox"/> ..	SLD [1/cm/cm]
7 ^ phi	0.01	<input checked="" type="checkbox"/> 0.001..1	volume fraction [0..1]

```

260 double VolumeCylinder=M_PI*R*R*L; // volume in A^3
261 I0=phi*VolumeCylinder*1.0E-24*(sldCylinder-sldSolvent)*(sldCylinder-sldSolvent);
262
263 I=I0 * cylinder_form_factor(Q, R, L)+bgd;
264
265
266
267 beforeFiting(ParaM); //+++ eFit
    
```

The annotated screenshot highlights four key elements in the COMPILER interface:

- 3.1** Dependent Variable: The 'Dependent variable' field.
- 3.2** Independent Variable: The 'Independent variable(s)' field containing 'Q'.
- 3.3** Number-of-Parameters Spin-Box: The spin box showing the value '7'.
- 3.4** Table-of-Parameters: The table listing parameters L, R, I0, bgd, sldCylinder, sldSolvent, and phi with their initial values and ranges.

- 3.1 Dependent Variable
- 3.2 Independent Variable
- 3.3 Number-of-Parameters Spin-Box
- 3.4 Table-of-Parameters

## 3.4 Table-of-Parameters

	Name	Initial Value	Vary?	From..To	Info
3.4.1 1 ^	L	500	<input checked="" type="checkbox"/>	1..10000	Length of Cylinder [A]
2 ^	R	20	<input checked="" type="checkbox"/>	1..1000	Radius of Cylinder [A]
3 ^	I0	1	<input type="checkbox"/>	0..1E6	Forward Scattering calculated [1/cm]
4 ^	bgd	0	<input type="checkbox"/>	0..10	Background [1/cm]
5 ^	sldCylinder	3e+10	<input type="checkbox"/>	..	SLD [1/cm/cm]
6 ^	sldSolvent	-5.6e+09	<input type="checkbox"/>	..	SLD [1/cm/cm]
7 ^	phi	0.01	<input checked="" type="checkbox"/>	0.001..1	volume fraction [0..1]

3.4.1 Number of the current Parameter; pushing of the “^” symbol will shift pushed row up.

3.4.2 Names of parameters: defined in c++ code.

3.4.3 Initial Values of Parameters.

3.4.4 Check-box of initial adjustability of the parameters

3.4.5 Range of Parameters: if empty (“.”), range is [-inf . .+inf]

3.4.6 Info-Column: Description of Parameters

- **L, R, phi** : initially **fittable** parameters (adjustability could be changed in the fitting interface later)
- **bgd, sldCylinder, sldSolvent**: initially **fixed** parameters (adjustability could be changed in the fitting interface later)
- **I0**: parameter **calculated** inside of the function -> `I0=phi*VolumeCylinder*1.0E-24*(sldCylinder-sldSolvent)*(sldCylinder-sldSolvent);`
- **VolumeCylinder**:: Internal Variable (volume): `double VolumeCylinder=M_PI*R*R*L; // volume in A^3`

Dependent variable: I

Independent variable(s): Q

	Name	Initial Value	Vary?	From..To	Info
1 ^	L	500	<input checked="" type="checkbox"/>	1..10000	Length of Cylinder [A]
2 ^	R	20	<input checked="" type="checkbox"/>	1..1000	Radius of Cylinder [A]
3 ^	I0	1	<input type="checkbox"/>	0..1E6	Forward Scattering calculated [1/cm]
4 ^	bgd	0	<input type="checkbox"/>	0..10	Background [1/cm]
5 ^	sldCylinder	3e+10	<input type="checkbox"/>	..	SLD [1/cm/cm]
6 ^	sldSolvent	-5.6e+09	<input type="checkbox"/>	..	SLD [1/cm/cm]
7 ^	phi	0.01	<input checked="" type="checkbox"/>	0.001..1	volume fraction [0..1]

Code

```

260 double VolumeCylinder=M_PI*R*R*L; // volume in A^3
261
262 I0=phi*VolumeCylinder*1.0E-24*(sldCylinder-sldSolvent)*(sldCylinder-sldSolvent);
263
264 I=I0 * cylinder_form_factor(Q, R, L)+bgd;
265
266 beforeFiting(ParaM); //+++ eFit
267

```

## Functions

- *cylinder\_form\_factor(Q, R, L)*
- *beforeFiting(ParaM)*

Defined in **4.2 „+Include“: C++ Function Editor**

## 4.1 „Code“: C++ Function Editor

Inside of the “Code” we defined next function:

**I = I( Q, L, R, I0, bgd, sldCylinder, sldSolvent, phi )**

## 4.1 „Code“: C++ Function Editor

4.1.1 Useful (non-critical) tools [will be explained later]

4.1.2 Line Number in the generated C++ file (important during compilation/debugging)

4.1.3 C++ code editor I=I(Q, parameters)

4.1.4 Find text in the code editor (type text + “enter”)

4.1.5 Tab of Tools: expansion/shrinking button

The screenshot shows the C++ Function Editor interface. At the top, there are tabs: Code (selected), +Included, +Fortran, Info, Fit.Control, Files, and Options. A red box labeled 4.1.5 highlights a '+' button to the right of the Options tab. Below the tabs is a toolbar with buttons for '<<', 'para', 'flags', 'data', 'math', 'multi-function', 'sasview', 'qtikws/qtisas', and 'fortran'. A red box labeled 4.1.1 highlights this toolbar. To the right of the toolbar is a search box labeled 'find' with a green box labeled 4.1.4 around it. The main editor area shows C++ code with line numbers 260-268 on the left. A red box labeled 4.1.3 highlights the code area. A green box labeled 4.1.2 highlights the line numbers. The code is as follows:

```
260 double VolumeCylinder=M_PI*R*R*L; // volume in A^3
261
262 I0=phi*VolumeCylinder*1.0E-24*(sldCylinder-sldSolvent)*(sldCylinder-sldSolvent);
263
264 I=I0 * cylinder_form_factor(Q, R, L)+bgd;
265
266
267 beforeFiting(ParaM); //+++ eFit
268
```

## 4.2 „+Included“: C++ Editor of Functions

1. Change Active Tab to +Included

2. Push: Expanding of Tools Tab Button

Categories: End-cap-Thomas, Flo, Form Factors, Form Structure, General, Form Factors

Functions: Cylinder, Cylinder-OZ, Cylinder-eFit, Cylinder-eFit-I0, Cylinder-eFit

Dependent variable: I

Independent variable(s): Q

Name	Initial Value	Vary?From..To	Info
1 ^ L	500	<input checked="" type="checkbox"/> 1..10000	Length of Cylinder [A]
2 ^ R	20	<input checked="" type="checkbox"/> 1..1000	Radius of Cylinder [A]
3 ^ I0	1	<input type="checkbox"/> 0..1E6	Forward Scattering calculated [1/cm]
4 ^ bgd	0	<input type="checkbox"/> 0..10	Background [1/cm]
5 ^ sldCylinder	3e+10	<input type="checkbox"/> ..	SLD [1/cm/cm]
6 ^ sldSolvent	-5.6e+09	<input type="checkbox"/> ..	SLD [1/cm/cm]
7 ^ phi	0.01	<input checked="" type="checkbox"/> 0.001..1	volume fraction [0..1]

Code +Included +Fortran Info Fit.Control Files Options

```

260 double VolumeCylinder=M_PI*R*R*L; // volume in A^3
261
262 I0=phi*VolumeCylinder*1.0E-24*(sldCylinder-sldSolvent)*(sldCylinder-sldSolvent);
263
264 I=I0 * cylinder_form_factor(Q, R, L)+bgd;
265
266 beforeFitting(ParaM); //+++ eFit
267
268
  
```

Categories: End-cap-Thomas, Flo, Form Factors, Form Structure, General, Form Factors

Functions: Cylinder, Cylinder-OZ, Cylinder-eFit, Cylinder-eFit-I0, Cylinder-eFit

Dependent variable: I

Independent variable(s): Q

Name	Initial Value	Vary?From..To	Info
1 ^ L	500	<input checked="" type="checkbox"/> 1..10000	Length of Cylinder [A]
2 ^ R	20	<input checked="" type="checkbox"/> 1..1000	Radius of Cylinder [A]
3 ^ I0	1	<input type="checkbox"/> 0..1E6	Forward Scattering calculated [1/cm]
4 ^ bgd	0	<input type="checkbox"/> 0..10	Background [1/cm]
5 ^ sldCylinder	3e+10	<input type="checkbox"/> ..	SLD [1/cm/cm]
6 ^ sldSolvent	-5.6e+09	<input type="checkbox"/> ..	SLD [1/cm/cm]
7 ^ phi	0.01	<input checked="" type="checkbox"/> 0.001..1	volume fraction [0..1]

Code +Included +Fortran Info Fit.Control Files Options

```

018 #include <gsl/gsl_sf_bessel.h>
019 #include <gsl/gsl_integration.h>
020
021
022
  
```

```

179 struct data {double QL; double QR;};
180 //---
181 double cylinder_under_integral(double alfa, void * data)
182 {
183   double QL = ((struct data *)data)->QL;
184   double QR = ((struct data *)data)->QR;
185   double result;
186   //---
187   result= 2*gsl_sf_bessel_J1(QR*sin(alfa))/(QR*sin(alfa));
188   result*=sin(QL*cos(alfa)/2)/(QL*cos(alfa)/2);
189   result=result*result*sin(alfa);
190   //---
191   return result;
192 };
193 double cylinder_form_factor(double Q, double R, double L)
194 {
195   if (Q==0) return 1.0;
196   if (R*L==0) return 0.0;
197   //+++ integral control parameters
198   double IntegralAbs=0;
199   double IntegralRel=0.001;
200   int maxNumber=1000;
201   //---
202   double QL=Q*L;
203   double QR=Q*R;
204
205   gsl_integration_workspace * w = gsl_integration_workspace_alloc (maxNumber);
206   double result, error;
207   data data=(QL, QR);
208   gsl_function F;
209   F.function = &cylinder_under_integral;
210   F.params = &data;
211   gsl_integration_qags (&F, 0.0001, M_PI/2, IntegralAbs, IntegralRel, maxNumber, w, &result,
212   &error);
213   gsl_integration_workspace_free(w);
214   return result;
215 }
216
217 void beforeFitting(void * ParaM)
218 {
219
220   if ((beforeFit) return;
221
222   int minPoint=currentFirstPoint;
  
```

Code +Included +Fortran Info Fit.Control Files Options

```

#included Headers
018 #include <gsl/gsl_sf_bessel.h>
019 #include <gsl/gsl_integration.h>
020
021
022
  
```

Select Included Headers: ABC.h, cyl-coreshell-dens-profile.h, data-Management.h, Distributions.h, execute.h

```

179 struct data {double QL; double QR;};
180 //---
181 double cylinder_under_integral(double alfa, void * data)
182 {
183   double QL = ((struct data *)data)->QL;
184   double QR = ((struct data *)data)->QR;
185   double result;
186   //---
187   result= 2*gsl_sf_bessel_J1(QR*sin(alfa))/(QR*sin(alfa));
188   result*=sin(QL*cos(alfa)/2)/(QL*cos(alfa)/2);
189   result=result*result*sin(alfa);
190   //---
191   return result;
192 };
193 double cylinder_form_factor(double Q, double R, double L)
194 {
195   if (Q==0) return 1.0;
196   if (R*L==0) return 0.0;
197   //+++ integral control parameters
198   double IntegralAbs=0;
199   double IntegralRel=0.001;
200   int maxNumber=1000;
201   //---
202   double QL=Q*L;
203   double QR=Q*R;
204
205   gsl_integration_workspace * w = gsl_integration_workspace_alloc (maxNumber);
206   double result, error;
207   data data=(QL, QR);
208   gsl_function F;
209   F.function = &cylinder_under_integral;
210   F.params = &data;
211   gsl_integration_qags (&F, 0.0001, M_PI/2, IntegralAbs, IntegralRel, maxNumber, w, &result,
212   &error);
213   gsl_integration_workspace_free(w);
214   return result;
215 }
216
217 void beforeFitting(void * ParaM)
218 {
219
220   if ((beforeFit) return;
221
222   int minPoint=currentFirstPoint;
  
```

Cylinder-eFit

## 4.2 „+Included“: C++ Editor of Functions

4.2.1

```
#included Headers
018 #include <gsl/gsl_sf_bessel.h>
019 #include <gsl/gsl_integration.h>
020
021
022
```

4.1.4

```
Select Included Headers
ABC.h
cyl-coreshell-dens-profile.h
data-Management.h
Distributions.h
execute.h
#-aligned-Model.h
```

4.2.2

4.2.3

```
Included Functions
179 struct data {double QL; double QR;};
180 /*--
181 double cylinder_under_integral(double alfa, void * data)
182 {
183     double QL = ((struct data *)data)->QL;
184     double QR = ((struct data *)data)->QR;
185     double result;
186     /*--
187     result= 2*gsl_sf_bessel_J1(QR*sin(alfa))/(QR*sin(alfa));
188     result*=sin(QL*cos(alfa)/2)/(QL*cos(alfa)/2);
189     result=result*result*sin(alfa);
190     /*--
191     return result;
192 };
193 double cylinder_form_factor(double Q, double R, double L)
194 {
195     if (Q==0) return 1.0;
196     if (R*L==0) return 0.0;
197     /*+++ integral control parameters
198     double IntegralAbs=0;
199     double IntegralRel=0.001;
200     int maxNumber=1000;
201     /*--
202     double QL=Q*L;
203     double QR=Q*R;
204
205     gsl_integration_workspace * w = gsl_integration_workspace_alloc (maxNumber);
206     double result, error;
207     data data={QL, QR};
208     gsl_function F;
209     F.function = &cylinder_under_integral;
210     F.params = &data;
211     gsl_integration_qags (&F, 0.0001, M_PI/2, IntegralAbs, IntegralRel, maxNumber, w, &result,
212     &error);
213     gsl_integration_workspace_free(w);
214     return result;
215 }
216
217 void beforeFiting(void * ParaM)
218 {
219
220     if (!beforeFit) return;
221
222     int minPoint=currentFirstPoint;
```

4.2.1 Place for declaration of needed c++ headers

4.2.2 Line Number in the generated C++

4.2.3 C++ Function editor

[functions defined here could be called in the 4.1 function editor]

4.2.4 Headers Browser of header files

[ headers path: `./qtiSAS/FitFunctions/ IncludedFunctions/` ]

[ not used in this example ]

[ will be explained somewhere else ]

# GSL - GNU Scientific Library

# !!! integrated in Fit-Compile v 1.15

The GNU Scientific Library (GSL) is a numerical library for C and C++ programmers. It is free software under the GNU General Public License.

The library provides a wide range of mathematical routines such as random number generators, special functions and least-squares fitting. There are over 1000 functions in total with an extensive test suite.

Unlike the licenses of proprietary numerical libraries the license of GSL does not restrict scientific cooperation. It allows you to share your programs freely with others.

<https://www.gnu.org/software/gsl/>

#included Headers

```
018 #include <gsl/gsl_sf_bessel.h>
019 #include <gsl/gsl_integration.h>
020
021
022
```

In the Example we use 2 modules from GSL library

- Bessel Functions module ( we use  $J_1(x)$  function)
  - `gsl/gsl_sf_bessel.h`
  - <https://www.gnu.org/software/gsl/doc/html/specfunc.html?highlight=bessel>
- Numerical integral module
  - `gsl/gsl_integration.h`
  - <https://www.gnu.org/software/gsl/doc/html/integration.html>

```

1018 #include <gsl_sf_bessel.h>
1019 #include <gsl_integration.h>
1020
1021
1022
1023
1024
1025
1026
1027
1028
1029
1030
1031
1032
1033
1034
1035
1036
1037
1038
1039
1040
1041
1042
1043
1044
1045
1046
1047
1048
1049
1050
1051
1052
1053
1054
1055
1056
1057
1058
1059
1060
1061
1062
1063
1064
1065
1066
1067
1068
1069
1070
1071
1072
1073
1074
1075
1076
1077
1078
1079
1080
1081
1082
1083
1084
1085
1086
1087
1088
1089
1090
1091
1092
1093
1094
1095
1096
1097
1098
1099
1100
1101
1102
1103
1104
1105
1106
1107
1108
1109
1110
1111
1112
1113
1114
1115
1116
1117
1118
1119
1120
1121
1122
1123
1124
1125
1126
1127
1128
1129
1130
1131
1132
1133
1134
1135
1136
1137
1138
1139
1140
1141
1142
1143
1144
1145
1146
1147
1148
1149
1150
1151
1152
1153
1154
1155
1156
1157
1158
1159
1160
1161
1162
1163
1164
1165
1166
1167
1168
1169
1170
1171
1172
1173
1174
1175
1176
1177
1178
1179
1180
1181
1182
1183
1184
1185
1186
1187
1188
1189
1190
1191
1192
1193
1194
1195
1196
1197
1198
1199
1200
1201
1202
1203
1204
1205
1206
1207
1208
1209
1210
1211
1212
1213
1214
1215
1216
1217
1218
1219
1220
1221
1222
1223
1224
1225
1226
1227
1228
1229
1230
1231
1232
1233
1234
1235
1236
1237
1238
1239
1240
1241
1242
1243
1244
1245
1246
1247
1248
1249
1250
1251
1252
1253
1254
1255
1256
1257
1258
1259
1260
1261
1262
1263
1264
1265
1266
1267
1268
1269
1270
1271
1272
1273
1274
1275
1276
1277
1278
1279
1280
1281
1282
1283
1284
1285
1286
1287
1288
1289
1290
1291
1292
1293
1294
1295
1296
1297
1298
1299
1300
1301
1302
1303
1304
1305
1306
1307
1308
1309
1310
1311
1312
1313
1314
1315
1316
1317
1318
1319
1320
1321
1322
1323
1324
1325
1326
1327
1328
1329
1330
1331
1332
1333
1334
1335
1336
1337
1338
1339
1340
1341
1342
1343
1344
1345
1346
1347
1348
1349
1350
1351
1352
1353
1354
1355
1356
1357
1358
1359
1360
1361
1362
1363
1364
1365
1366
1367
1368
1369
1370
1371
1372
1373
1374
1375
1376
1377
1378
1379
1380
1381
1382
1383
1384
1385
1386
1387
1388
1389
1390
1391
1392
1393
1394
1395
1396
1397
1398
1399
1400
1401
1402
1403
1404
1405
1406
1407
1408
1409
1410
1411
1412
1413
1414
1415
1416
1417
1418
1419
1420
1421
1422
1423
1424
1425
1426
1427
1428
1429
1430
1431
1432
1433
1434
1435
1436
1437
1438
1439
1440
1441
1442
1443
1444
1445
1446
1447
1448
1449
1450
1451
1452
1453
1454
1455
1456
1457
1458
1459
1460
1461
1462
1463
1464
1465
1466
1467
1468
1469
1470
1471
1472
1473
1474
1475
1476
1477
1478
1479
1480
1481
1482
1483
1484
1485
1486
1487
1488
1489
1490
1491
1492
1493
1494
1495
1496
1497
1498
1499
1500
1501
1502
1503
1504
1505
1506
1507
1508
1509
1510
1511
1512
1513
1514
1515
1516
1517
1518
1519
1520
1521
1522
1523
1524
1525
1526
1527
1528
1529
1530
1531
1532
1533
1534
1535
1536
1537
1538
1539
1540
1541
1542
1543
1544
1545
1546
1547
1548
1549
1550
1551
1552
1553
1554
1555
1556
1557
1558
1559
1560
1561
1562
1563
1564
1565
1566
1567
1568
1569
1570
1571
1572
1573
1574
1575
1576
1577
1578
1579
1580
1581
1582
1583
1584
1585
1586
1587
1588
1589
1590
1591
1592
1593
1594
1595
1596
1597
1598
1599
1600
1601
1602
1603
1604
1605
1606
1607
1608
1609
1610
1611
1612
1613
1614
1615
1616
1617
1618
1619
1620
1621
1622
1623
1624
1625
1626
1627
1628
1629
1630
1631
1632
1633
1634
1635
1636
1637
1638
1639
1640
1641
1642
1643
1644
1645
1646
1647
1648
1649
1650
1651
1652
1653
1654
1655
1656
1657
1658
1659
1660
1661
1662
1663
1664
1665
1666
1667
1668
1669
1670
1671
1672
1673
1674
1675
1676
1677
1678
1679
1680
1681
1682
1683
1684
1685
1686
1687
1688
1689
1690
1691
1692
1693
1694
1695
1696
1697
1698
1699
1700
1701
1702
1703
1704
1705
1706
1707
1708
1709
1710
1711
1712
1713
1714
1715
1716
1717
1718
1719
1720
1721
1722
1723
1724
1725
1726
1727
1728
1729
1730
1731
1732
1733
1734
1735
1736
1737
1738
1739
1740
1741
1742
1743
1744
1745
1746
1747
1748
1749
1750
1751
1752
1753
1754
1755
1756
1757
1758
1759
1760
1761
1762
1763
1764
1765
1766
1767
1768
1769
1770
1771
1772
1773
1774
1775
1776
1777
1778
1779
1780
1781
1782
1783
1784
1785
1786
1787
1788
1789
1790
1791
1792
1793
1794
1795
1796
1797
1798
1799
1800
1801
1802
1803
1804
1805
1806
1807
1808
1809
1810
1811
1812
1813
1814
1815
1816
1817
1818
1819
1820
1821
1822
1823
1824
1825
1826
1827
1828
1829
1830
1831
1832
1833
1834
1835
1836
1837
1838
1839
1840
1841
1842
1843
1844
1845
1846
1847
1848
1849
1850
1851
1852
1853
1854
1855
1856
1857
1858
1859
1860
1861
1862
1863
1864
1865
1866
1867
1868
1869
1870
1871
1872
1873
1874
1875
1876
1877
1878
1879
1880
1881
1882
1883
1884
1885
1886
1887
1888
1889
1890
1891
1892
1893
1894
1895
1896
1897
1898
1899
1900
1901
1902
1903
1904
1905
1906
1907
1908
1909
1910
1911
1912
1913
1914
1915
1916
1917
1918
1919
1920
1921
1922
1923
1924
1925
1926
1927
1928
1929
1930
1931
1932
1933
1934
1935
1936
1937
1938
1939
1940
1941
1942
1943
1944
1945
1946
1947
1948
1949
1950
1951
1952
1953
1954
1955
1956
1957
1958
1959
1960
1961
1962
1963
1964
1965
1966
1967
1968
1969
1970
1971
1972
1973
1974
1975
1976
1977
1978
1979
1980
1981
1982
1983
1984
1985
1986
1987
1988
1989
1990
1991
1992
1993
1994
1995
1996
1997
1998
1999
2000
2001
2002
2003
2004
2005
2006
2007
2008
2009
2010
2011
2012
2013
2014
2015
2016
2017
2018
2019
2020
2021
2022
2023
2024
2025
2026
2027
2028
2029
2030
2031
2032
2033
2034
2035
2036
2037
2038
2039
2040
2041
2042
2043
2044
2045
2046
2047
2048
2049
2050
2051
2052
2053
2054
2055
2056
2057
2058
2059
2060
2061
2062
2063
2064
2065
2066
2067
2068
2069
2070
2071
2072
2073
2074
2075
2076
2077
2078
2079
2080
2081
2082
2083
2084
2085
2086
2087
2088
2089
2090
2091
2092
2093
2094
2095
2096
2097
2098
2099
2100
2101
2102
2103
2104
2105
2106
2107
2108
2109
2110
2111
2112
2113
2114
2115
2116
2117
2118
2119
2120
2121
2122
2123
2124
2125
2126
2127
2128
2129
2130
2131
2132
2133
2134
2135
2136
2137
2138
2139
2140
2141
2142
2143
2144
2145
2146
2147
2148
2149
2150
2151
2152
2153
2154
2155
2156
2157
2158
2159
2160
2161
2162
2163
2164
2165
2166
2167
2168
2169
2170
2171
2172
2173
2174
2175
2176
2177
2178
2179
2180
2181
2182
2183
2184
2185
2186
2187
2188
2189
2190
2191
2192
2193
2194
2195
2196
2197
2198
2199
2200
2201
2202
2203
2204
2205
2206
2207
2208
2209
2210
2211
2212
2213
2214
2215
2216
2217
2218
2219
2220
2221
2222
2223
2224
2225
2226
2227
2228
2229
2230
2231
2232
2233
2234
2235
2236
2237
2238
2239
2240
2241
2242
2243
2244
2245
2246
2247
2248
2249
2250
2251
2252
2253
2254
2255
2256
2257
2258
2259
2260
2261
2262
2263
2264
2265
2266
2267
2268
2269
2270
2271
2272
2273
2274
2275
2276
2277
2278
2279
2280
2281
2282
2283
2284
2285
2286
2287
2288
2289
2290
2291
2292
2293
2294
2295
2296
2297
2298
2299
2300
2301
2302
2303
2304
2305
2306
2307
2308
2309
2310
2311
2312
2313
2314
2315
2316
2317
2318
2319
2320
2321
2322
2323
2324
2325
2326
2327
2328
2329
2330
2331
2332
2333
2334
2335
2336
2337
2338
2339
2340
2341
2342
2343
2344
2345
2346
2347
2348
2349
2350
2351
2352
2353
2354
2355
2356
2357
2358
2359
2360
2361
2362
2363
2364
2365
2366
2367
2368
2369
2370
2371
2372
2373
2374
2375
2376
2377
2378
2379
2380
2381
2382
2383
2384
2385
2386
2387
2388
2389
2390
2391
2392
2393
2394
2395
2396
2397
2398
2399
2400
2401
2402
2403
2404
2405
2406
2407
2408
2409
2410
2411
2412
2413
2414
2415
2416
2417
2418
2419
2420
2421
2422
2423
2424
2425
2426
2427
2428
2429
2430
2431
2432
2433
2434
2435
2436
2437
2438
2439
2440
2441
2442
2443
2444
2445
2446
2447
2448
2449
2450
2451
2452
2453
2454
2455
2456
2457
2458
2459
2460
2461
2462
2463
2464
2465
2466
2467
2468
2469
2470
2471
2472
2473
2474
2475
2476
2477
2478
2479
2480
2481
2482
2483
2484
2485
2486
2487
2488
2489
2490
2491
2492
2493
2494
2495
2496
2497
2498
2499
2500
2501
2502
2503
2504
2505
2506
2507
2508
2509
2510
2511
2512
2513
2514
2515
2516
2517
2518
2519
2520
2521
2522
2523
2524
2525
2526
2527
2528
2529
2530
2531
2532
2533
2534
2535
2536
2537
2538
2539
2540
2541
2542
2543
2544
2545
2546
2547
2548
2549
2550
2551
2552
2553
2554
2555
2556
2557
2558
2559
2560
2561
2562
2563
2564
2565
2566
2567
2568
2569
2570
2571
2572
2573
2574
2575
2576
2577
2578
2579
2580
2581
2582
2583
2584
2585
2586
2587
2588
2589
2590
2591
2592
2593
2594
2595
2596
2597
2598
2599
2600
2601
2602
2603
2604
2605
2606
2607
2608
2609
2610
2611
2612
2613
2614
2615
2616
2617
2618
2619
2620
2621
2622
2623
2624
2625
2626
2627
2628
2629
2630
2631
2632
2633
2634
2635
2636
2637
2638
2639
2640
2641
2642
2643
2644
2645
2646
2647
2648
2649
2650
2651
2652
2653
2654
2655
2656
2657
2658
2659
2660
2661
2662
2663
2664
2665
2666
2667
2668
2669
2670
2671
2672
2673
2674
2675
2676
2677
2678
2679
2680
2681
2682
2683
2684
2685
2686
2687
2688
2689
2690
2691
2692
2693
2694
2695
2696
2697
2698
2699
2700
2701
2702
2703
2704
2705
2706
2707
2708
2709
2710
2711
2712
2713
2714
2715
2716
2717
2718
2719
2720
2721
2722
2723
2724
2725
2726
2727
2728
2729
2730
2731
2732
2733
2734
2735
2736
2737
2738
2739
2740
2741
2742
2743
2744
2745
2746
2747
2748
2749
2750
2751
2752
2753
2754
2755
2756
2757
2758
2759
2760
2761
2762
2763
2764
2765
2766
2767
2768
2769
2770
2771
2772
2773
2774
2775
2776
2777
2778
2779
2780
2781
2782
2783
2784
2785
2786
2787
2788
2789
2790
2791
2792
2793
2794
2795
2796
2797
2798
2799
2800
2801
2802
2803
2804
2805
2806
2807
2808
2809
2810
2811
2812
2813
2814
2815
2816
2817
2818
2819
2820
2821
2822
2823
2824
2825
2826
2827
2828
2829
2830
2831
2832
2833
2834
2835
2836
2837
2838
2839
2840
2841
2842
2843
2844
2845
2846
2847
2848
2849
2850
2851
2852
2853
2854
2855
2856
2857
2858
2859
2860
2861
2862
2863
2864
2865
2866
2867
2868
2869
2870
2871
2872
2873
2874
2875
2876
2877
2878
2879
2880
2881
2882
2883
2884
2885
2886
2887
2888
2889
2890
2891
2892
2893
2894
2895
2896
2897
2898
2899
2900
2901
2902
2903
2904
2905
2906
2907
2908
2909
2910
2911
2912
2913
2914
2915
2916
2917
2918
2919
2920
2921
2922
2923
2924
2925
2926
2927
2928
2929
2930
2931
2932
2933
2934
2935
2936
2937
2938
2939
2940
2941
2942
2943
2944
2945
2946
2947
2948
2949
2950
2951
2952
2953
2954
2955
2956
2957
2958
2959
2960
2961
2962
2963
2964
2965
2966
2967
2968
2969
2970
2971
2972
2973
2974
2975
2976
2977
2978
2979
2980
2981
2982
2983
2984
2985
2986
2987
2988
2989
2990
2991
2992
2993
2994
2995
2996
2997
2998
2999
3000

```

$$cylinder\_form\_factor(Q, R, L) = \int_0^\pi F^2(Q, L, R, \alpha) \sin(\alpha) d\alpha$$

```

double cylinder_form_factor(double Q, double R, double L)
{
    if (Q==0) return 1.0;
    if (R*L==0) return 0.0;
    //+++ integral control parameters
    double IntegralAbs=0;
    double IntegralRel=0.001;
    int maxNumber=1000;
    //---
    double QL=Q*L;
    double QR=Q*R;

    gsl_integration_workspace * w = gsl_integration_workspace_alloc (maxNumber);
    double result, error;
    data data={QL, QR};
    gsl_function F;
    F.function = &cylinder_under_integral;
    F.params = &data;
    gsl_integration_qags (&F, 0.0001, M_PI/2, IntegralAbs, IntegralRel, maxNumber, w, &result, &error);
    gsl_integration_workspace_free(w);
    return result;
}

```

$$F(Q, L, R, \alpha) = cylinder\_under\_integral(\alpha, data) = 2 \times \frac{J_1[QR \sin(\alpha)]}{QR \sin(\alpha)} \times \frac{\sin[QL \cos(\alpha)/2]}{QL \cos(\alpha)/2}$$

```

double cylinder_under_integral(double alfa, void * data)
{
    double QL = ((struct data *)data)->QL;
    double QR = ((struct data *)data)->QR;
    double result;
    //---
    result= 2*gsl_sf_bessel_J1(QR*sin(alfa))/(QR*sin(alfa));
    result*=sin(QL*cos(alfa)/2)/(QL*cos(alfa)/2);
    result=result*result*sin(alfa);
    //---
    return result;
};

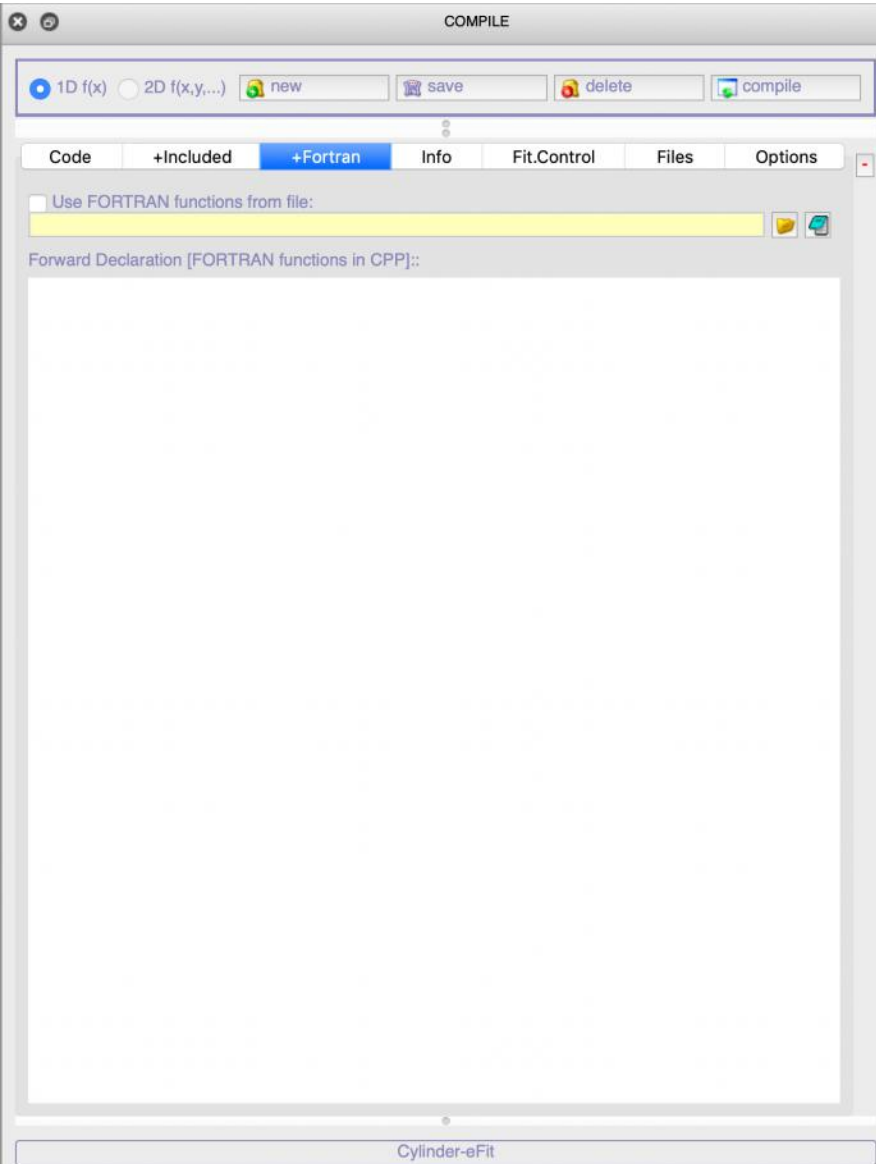
```

- Bessel Functions module ( we use J1(x) function)
  - <https://www.gnu.org/software/gsl/doc/html/specfunc.html?highlight=bessel>
- Numerical integral module
  - <https://www.gnu.org/software/gsl/doc/html/integration.html>

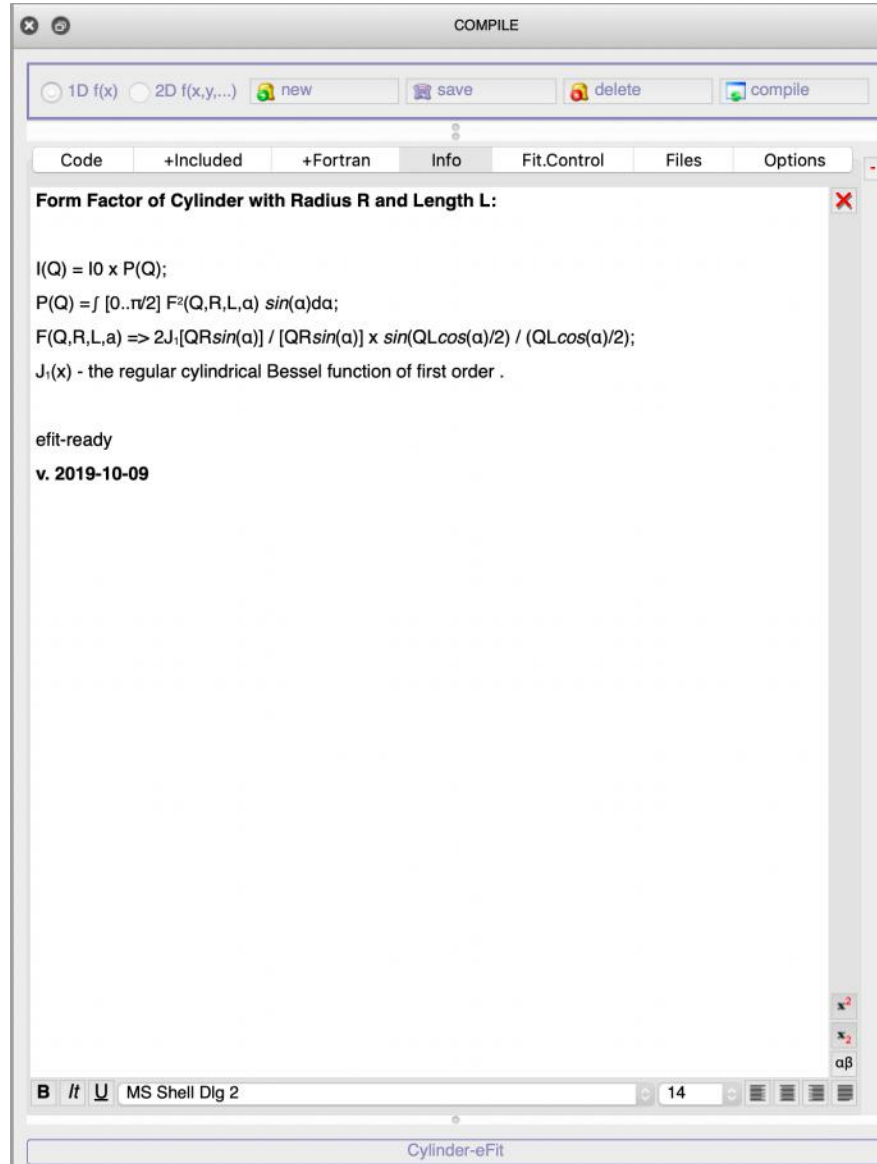
## 4.3 „+Fortran“: Fortran Function Editor

In current example we do not use any Fortran function.

<https://www.qtisas.com/compile/fortran>

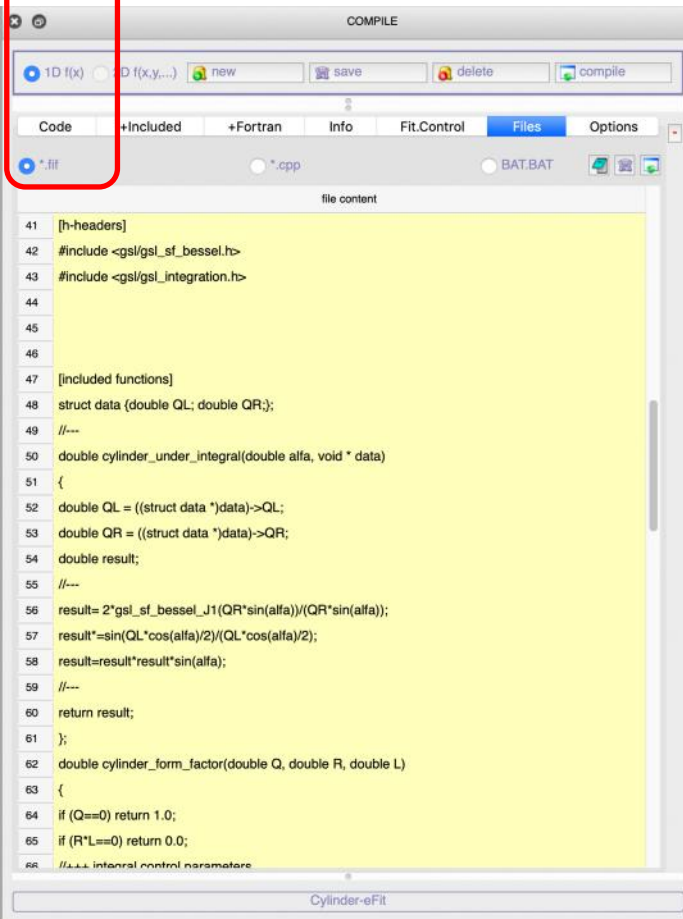


## 4.4 „Info“: Information Editor



## 4.6 “Files”: Generated Files Viewer

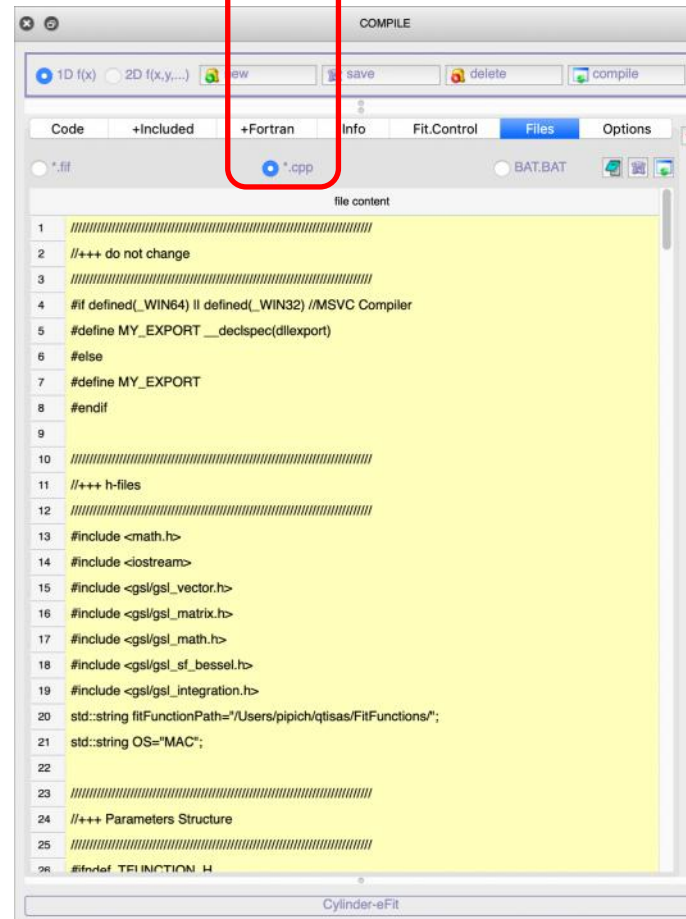
4.6.1



The screenshot shows the 'COMPILE' application window with the 'Files' tab selected. The file list at the bottom shows '\*.fif' as the active file. The main text area displays the content of the \*.fif file, which includes C++ code for header files and function definitions.

```
41 [h-headers]
42 #include <gsl/gsl_sf_bessel.h>
43 #include <gsl/gsl_integration.h>
44
45
46
47 [included functions]
48 struct data {double QL; double QR;};
49 //---
50 double cylinder_under_integral(double alfa, void * data)
51 {
52 double QL = ((struct data *)data)->QL;
53 double QR = ((struct data *)data)->QR;
54 double result;
55 //---
56 result= 2*gsl_sf_bessel_J1(QR*sin(alfa))/(QR*sin(alfa));
57 result*=sin(QL*cos(alfa)/2)/(QL*cos(alfa)/2);
58 result=result*result*sin(alfa);
59 //---
60 return result;
61 };
62 double cylinder_form_factor(double Q, double R, double L)
63 {
64 if (Q==0) return 1.0;
65 if (R*L==0) return 0.0;
66 //+++ integral control parameters
```

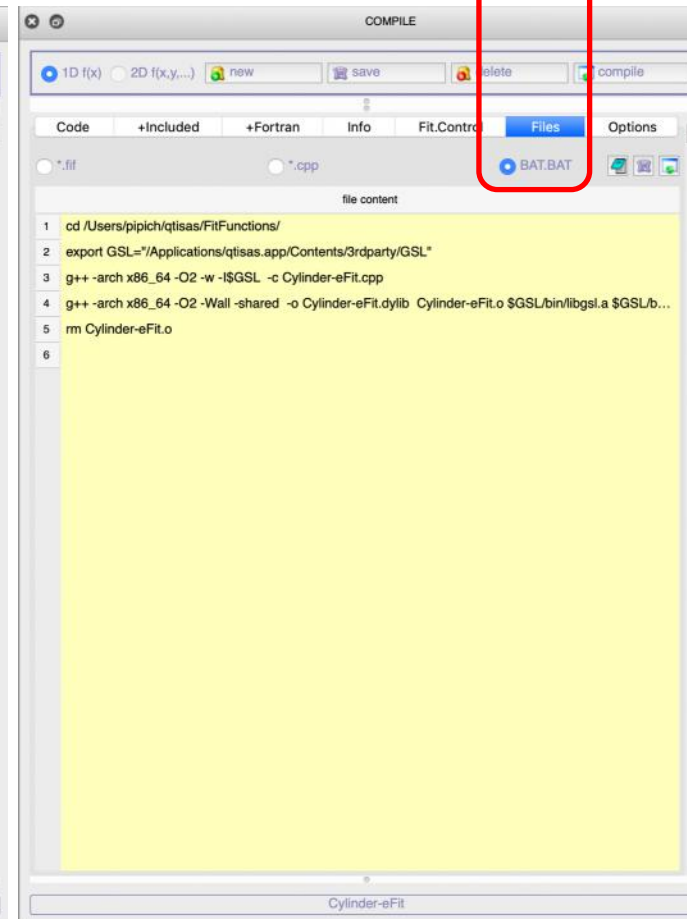
4.6.2



The screenshot shows the 'COMPILE' application window with the 'Files' tab selected. The file list at the bottom shows '\*.cpp' as the active file. The main text area displays the content of the \*.cpp file, which is a C++ source file generated from the \*.fif file.

```
1 //-----
2 //+++ do not change
3 //-----
4 #if defined(_WIN64) || defined(_WIN32) //MSVC Compiler
5 #define MY_EXPORT __declspec(dllexport)
6 #else
7 #define MY_EXPORT
8 #endif
9
10 //-----
11 //+++ h-files
12 //-----
13 #include <math.h>
14 #include <iostream>
15 #include <gsl/gsl_vector.h>
16 #include <gsl/gsl_matrix.h>
17 #include <gsl/gsl_math.h>
18 #include <gsl/gsl_sf_bessel.h>
19 #include <gsl/gsl_integration.h>
20 std::string fitFunctionPath="/Users/pipich/qtisas/FitFunctions/";
21 std::string OS="MAC";
22
23 //-----
24 //+++ Parameters Structure
25 //-----
26 #ifdef DEFINITION_H
```

4.6.3



The screenshot shows the 'COMPILE' application window with the 'Files' tab selected. The file list at the bottom shows 'BAT.BAT' as the active file. The main text area displays the content of the BAT.BAT script file, which contains compilation commands for the \*.cpp file.

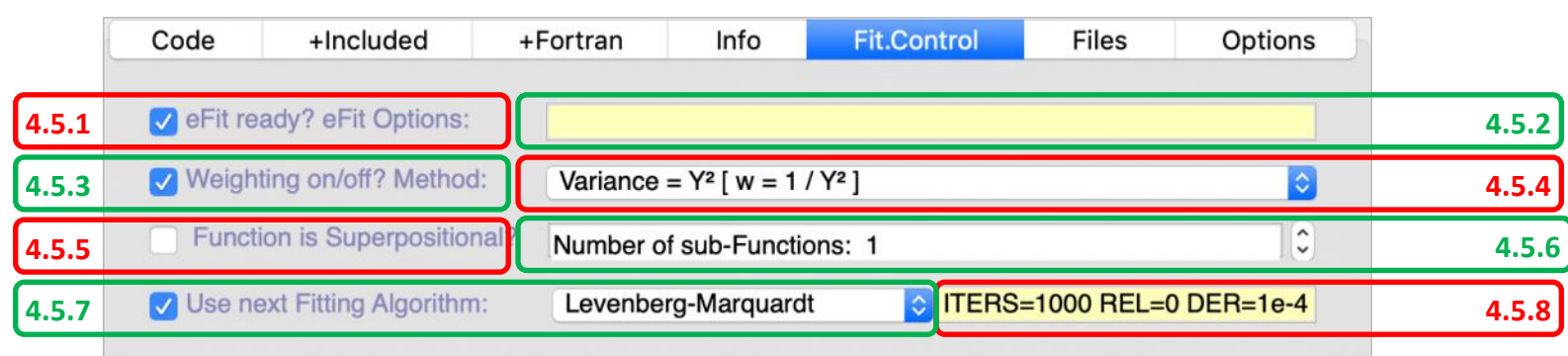
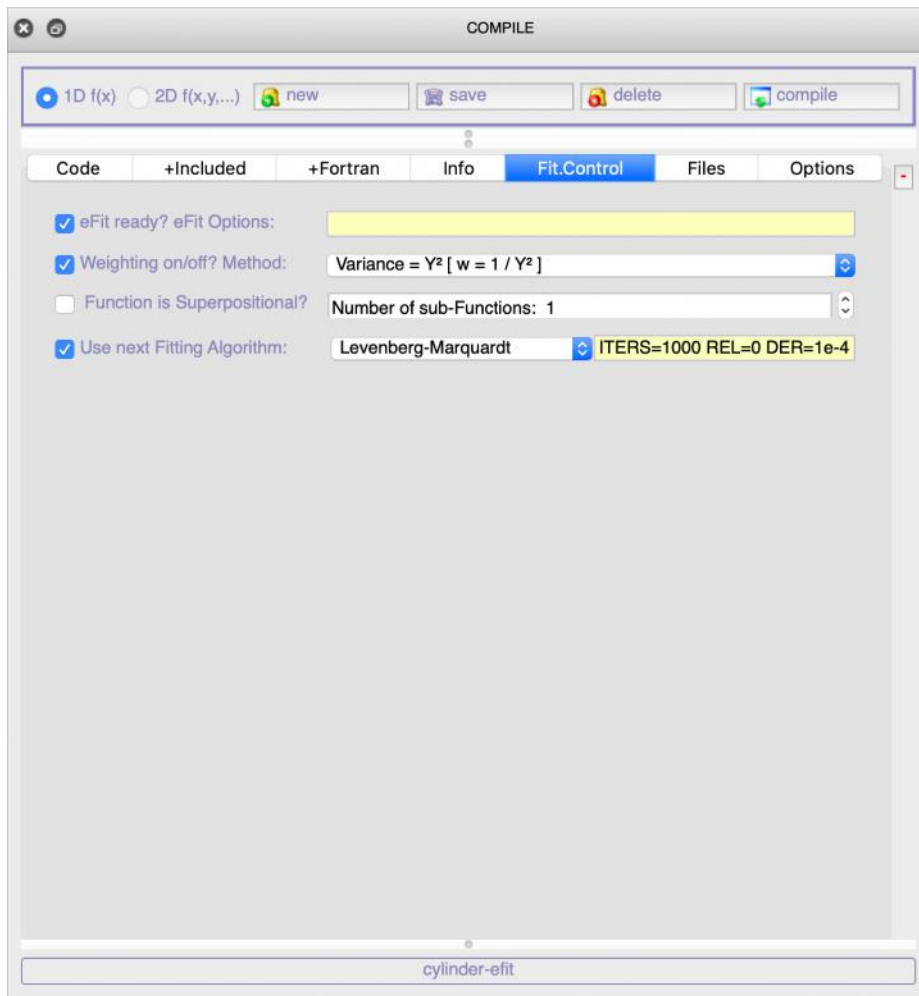
```
1 cd /Users/pipich/qtisas/FitFunctions/
2 export GSL="/Applications/qtisas.app/Contents/3rdparty/GSL"
3 g++ -arch x86_64 -O2 -w -I$GSL -c Cylinder-eFit.cpp
4 g++ -arch x86_64 -O2 -Wall -shared -o Cylinder-eFit.dylib Cylinder-eFit.o $GSL/bin/libgsl.a $GSL/b...
5 rm Cylinder-eFit.o
6
```

4.6.1 Information from the interface is saved in \*.fif file

4.6.2 FIF-file is converted to c++ file: \*.cpp

4.6.3 c++ file is compiled by **BAT.BAT** script file

## 4.5 “Fit.Control”: Fitting Options



Fit-control for the active function.

4.5.1 Check-Box: eFit-ready

4.5.2 Line-Edit: eFit-Options [see next page]

4.5.3 Check-Box: By default use **Weighting** for the active function if checked

4.5.4 Combo-box: default **Weighting** Method for the active function

4.5.5 Check-Box: super positional Function: if checked function has several sub-functions. Info will be here: <https://www.qtisas.com/fitting/superpositional-fit>

4.5.6 Number of sub-functions

4.5.7 Check-Box: default **Fitting** algorithm for the active function

4.5.8 Options for active fitting algorithm

## 4.5.1 "Fit.Control": Check-Box: eFit-Option

e-FIT



Weighting

e-Fit+++

Method:

Variance =  $Y^2$

default eFit procedure:

Function is Superpositional?

Number of sub

[1]

Script :: Before Fit

Fitting Algorithm:

Levenberg-M

"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:

"no-reslog": to skip it

"yes-res-in-plot": to show results in graph

## 4.5.8 "Fit.Control": Options for active fitting algorithm

MODE=3 ITERS=1000 REL=0 DER=1e-4

### simplex:

SD=... MODE=... ITERS=... REL=... CONVRATE=...

### levenberg:

SD=... MODE=... ITERS=... REL=... ABS=... DER=...DSSV=

### genetic:

SD=...GENCOUNT=...GENSIZE=...ITERS=...SELRATE=...MUTRATE=...SEED=...MODE=...

Algorithm [GenMin]

Significant Digits 9 SD=

**Genetic Algorithm Options [GenMin]**

Genome count 100 GENCOUNT=

Genome size 5 GENSIZE=

Max. # of Generations 500 ITERS=

Selection Rate 0.05 SELRATE=

Mutation Rate 0.03 MUTRATE=

Random Seed 1 SEED=

Local Search [levenberg] MODE=

Algorithm Nelder-Mead Simplex

Significant Digits 9 SD=

**Simplex Options**

Simplex Mode [nmsimplex2] MODE=

Convergence Rate 1.0: normal convergence CONVRATE=

**Stopping Criteria:**

Maximal # Iterations 1000 ITERS=

Relative Tolerance 0 REL=

Algorithm Levenberg-Marquardt

Significant Digits 9 SD=

**Levenberg-Marquardt Options**

Levenberg Mode [delta, scaled] MODE=

Derivative Step Size 1e-4 DER=

**Stopping Criteria:**

Maximal # Iterations 1000 ITERS=

Absolute Tolerance 0 ABS=

Relative Tolerance 0 REL=

Reaching Constant  $\chi^2$   Derivative Step Size Variation DSSV=

# 4.7 "Options": Fit-Compile Interface Options

