

# JupyLabBook\_example

March 6, 2024

## 1 JupyLabBook @ SIRIUS

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```
<IPython.core.display.Javascript object>

JupyterLab version: v3.2.0
More info on: https://gitlab.synchrotron-soleil.fr/sirius-beamline/notebooks/JupyterLabBook

Data reduction will be saved in the folder:
    data/
The nexus files should be in the folder:
    user/
The logs should be in the folder:
    user/logs/
The params should be in the folder:
    ../../lib/params/
The scripts should be in the folder:
    user/scripts/
Notebook name:
    JupyterLabBook_example.ipynb
Default parameters loaded.

<IPython.core.display.Javascript object>
```

## 2 Experimental setup

### SIRIUS Beamline: Experiment 1234

**This notebook is an example showing all the different things that can be done**

- Type: Proposal
- Safety: Yellow
- Date: 11/06/21-12/06/21
- Main proposer: Hemmerle
- Local contact: Arnaud
- Users (on site): AH-DH-CDH
- Machine:
  - Current: 450 mA
  - Mode: Hybrid Top-up
- Optics:
  - DCM: Si111
  - MGM: Not used
  - M1: M1-A Pt Track
  - M2: M2 Pt Track
  - M3: No M3
  - M4: M4 Pt Track
- Beam:

- Fixed/Variable energy: Fixed
- Energy (keV): 8
- Wavelength (nm): 0.155
- Harmonic: 16
- Polarisation: LH
- Phase (deg): 0
- Horizontal focalisation: False
- Vertical focalisation: True
- Horizontal beamsize (mm): 2
- Vertical beamsize (mm): 0.1
- Monitors and XBPM:
  - mon1:
  - mon2: thick diamond
  - mon3:
  - mon4: thick diamond
  - Detectors: Pilatus on delta/gamma Fluo 1 elem on side
- Remarks: This is an example.

### 3 Beamline alignment

Here we show functions used during beamline alignment.

LaTeX formula can be used in the text:

$$\frac{786 - 558}{2 \times 2069} \times 0.0355 = 1.9 \text{ mrad}$$

#### 3.1 Subsection

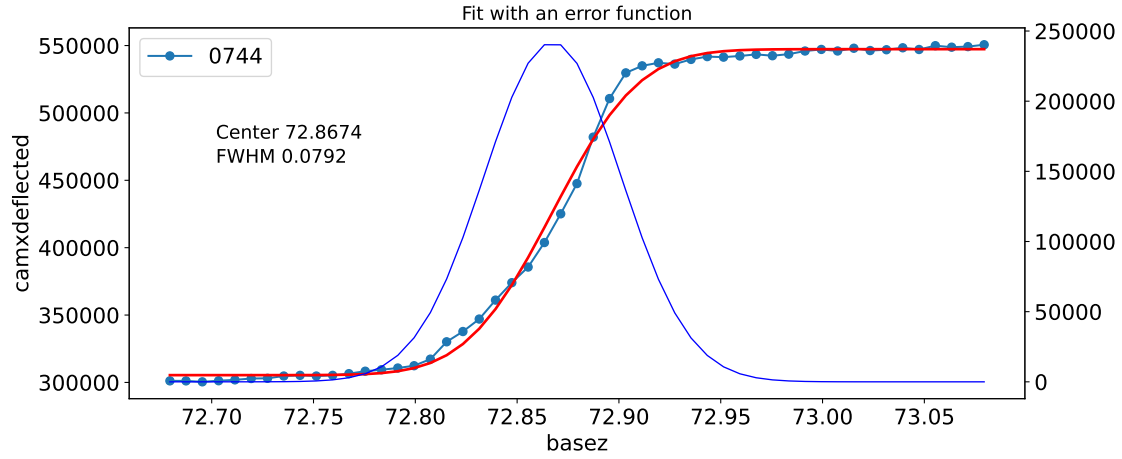
Fit with erf function.

##### 3.1.1 SIRIUS\_2020\_03\_11\_0744: dscan basez -.2 .2 50 .1

Absorbers: No Absorbers

Starting time: 2020-03-11 16:52:56.910030

Ending time: 2020-03-11 16:53:42.791704

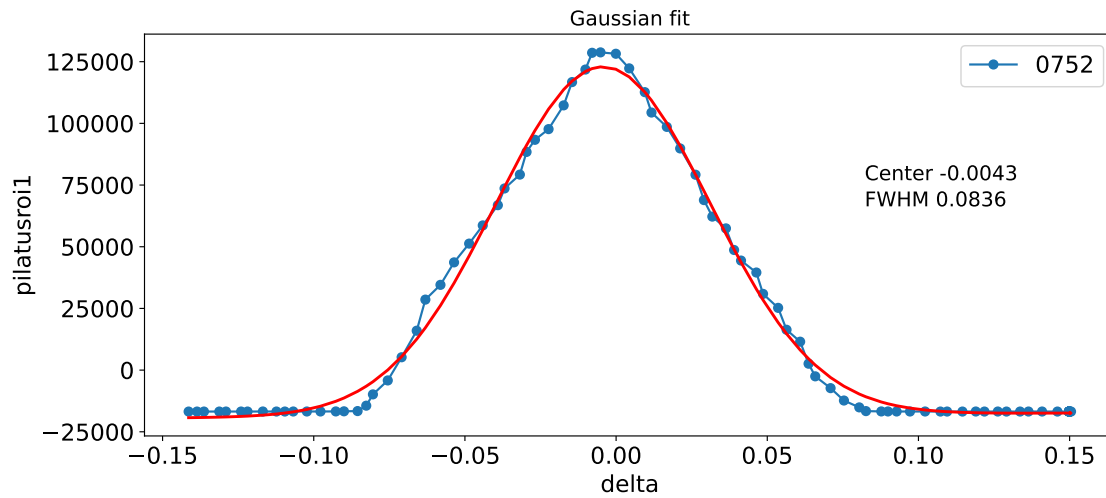


### 3.1.2 SIRIUS\_2020\_03\_11\_0752: continuous\_ascan delta -.15 .15 100 1

Absorbers: Al 1000micron

Starting time: 2020-03-11 18:41:13.266293

Ending time: 2020-03-11 18:44:06.972633



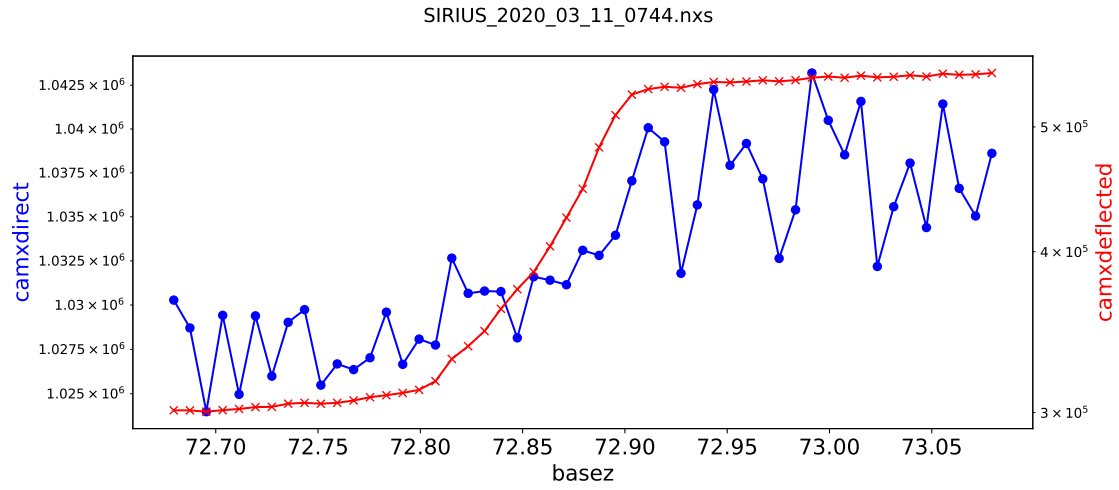
With two curves, in log.

### 3.1.3 SIRIUS\_2020\_03\_11\_0744: dscan basez -.2 .2 50 .1

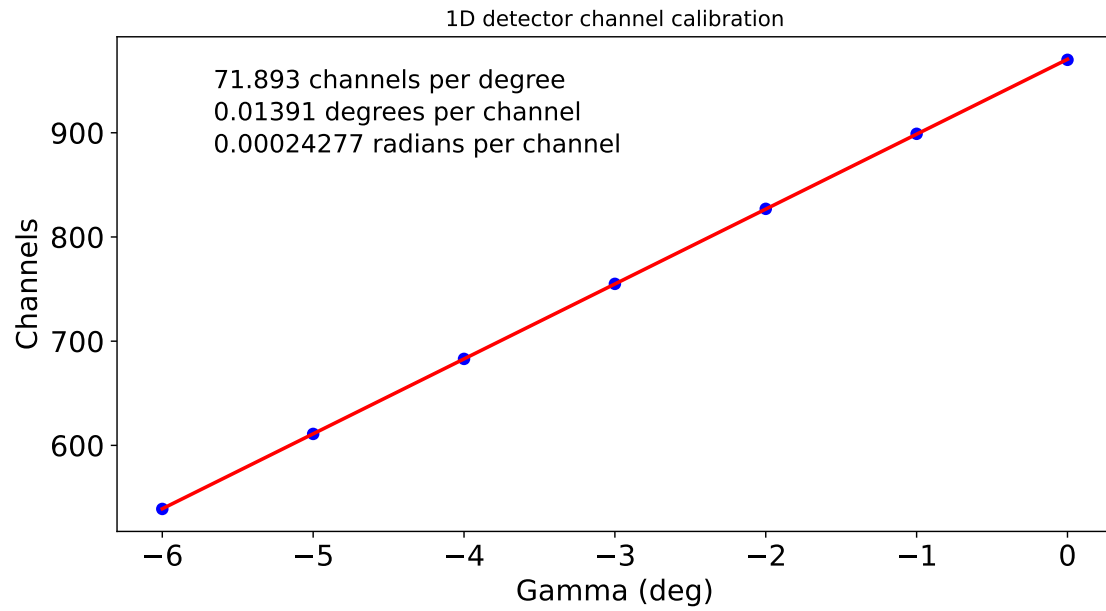
Absorbers: No Absorbers

Starting time: 2020-03-11 16:52:56.910030

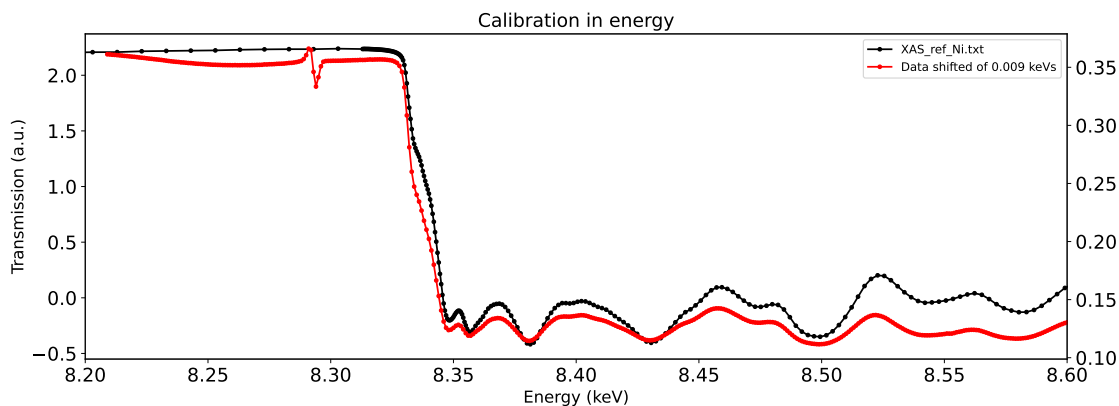
Ending time: 2020-03-11 16:53:42.791704



### 3.2 Calibration thetaz



### 3.3 Calibration energy



Current value of braggdcm = 13.7745

Current value of energydcm = 8.333

Do at the current energy: setposition braggdcm 13.7593

## 4 GIXD with Pilatus

### 4.1 Yoneda peak

Extraction of the Yoneda-Vineyard peak.

#### 4.1.1 SIRIUS\_2020\_03\_12\_0756: continuous\_ascan delta -24 -19 100 5

##### - Open Nexus Data File :

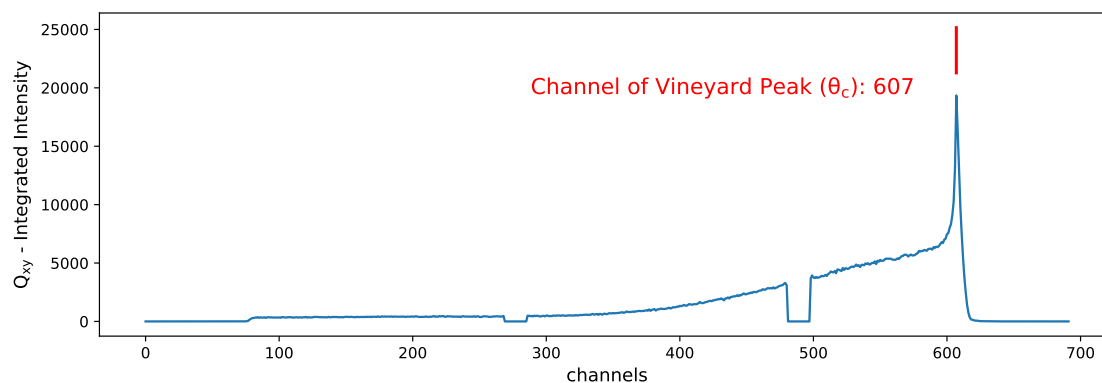
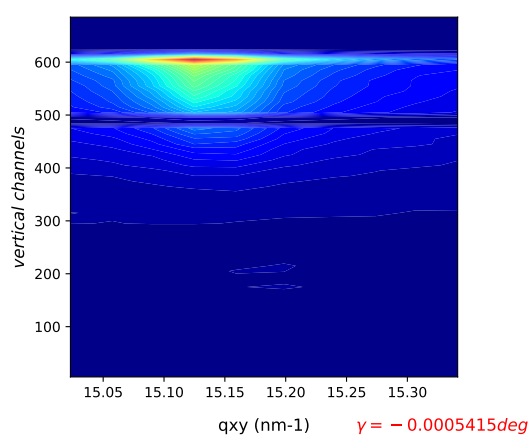
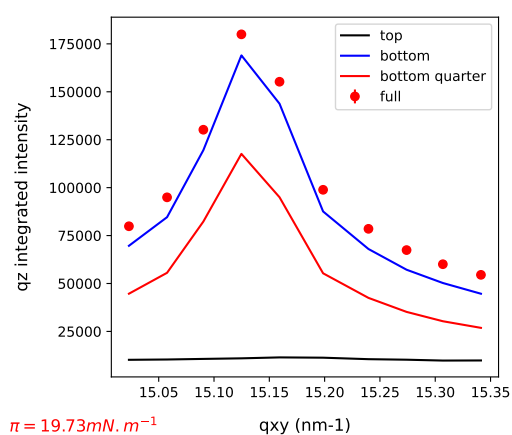
```
user/SIRIUS_2020_03_12_0756.nxs
. Number of data points: 10
. Available Counters:
  0 -----> delta
  1 -----> zs
  2 -----> gamma
  3 -----> hu36energy
  4 -----> xs
  5 -----> energydcm
  6 -----> current
  7 -----> mon2
  8 -----> surfacepressure
  9 -----> areapermolecule
 10 -----> qxy
 11 -----> pilatus
 12 -----> pilatusroi1
```

```

13 -----> integration_time
14 -----> sensorsRelTimestamps
15 -----> sensorsTimestamps
. 2D detector data found, (column 11, alias pilatus)
. qxy data found, (column 10, alias qxy)
. Valid data between points 0 and 9
. Surface pressure data found, mean value 19.73 ± 0.005632 mN/m
. Area per molecule data found, mean value 0.3558 ± 1.942e-05 nm2 per
molecule
. Gamma motor data found, mean value -0.0005415 deg
Starting time: 2020-03-12 11:16:03.090248
Ending time: 2020-03-12 11:16:51.901126

```

SIRIUS\_2020\_03\_12\_0756.nxs



Data not saved. To save data, run a GIXD on the scan.  
Channel0: 607



## 4.2 Process GIXD

Classic GIXD with:

$$q_{xy} = \frac{4\pi}{\lambda} \sin\left(\frac{2\theta}{2}\right)$$

Generates:

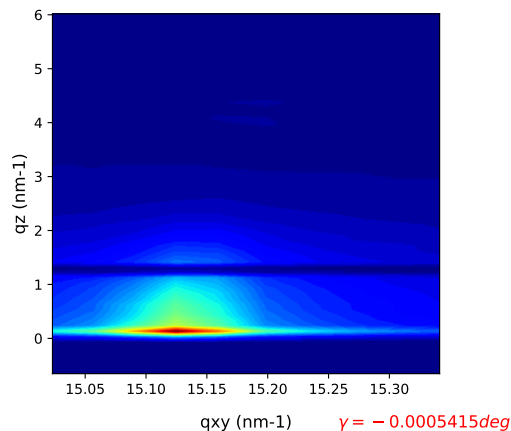
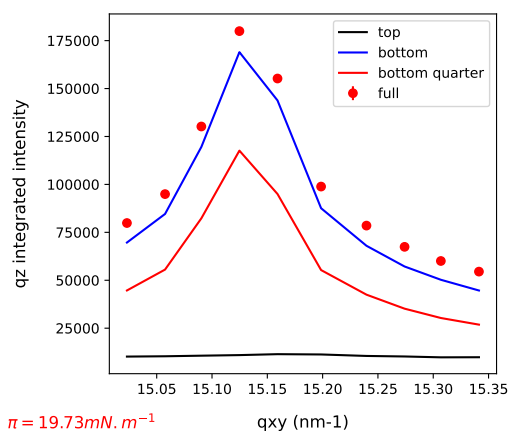
- SIRIUS\_2020\_03\_12\_0756\_1D\_qz.dat for each binning
- SIRIUS\_2020\_03\_12\_0756\_1D.dat
- SIRIUS\_2020\_03\_12\_0756\_1D.mat for each binning
- SIRIUS\_2020\_03\_12\_0756\_1D.moy for each binning

### 4.2.1 SIRIUS\_2020\_03\_12\_0756: continuous\_ascan delta -24 -19 100 5

#### - Open Nexus Data File :

```
user/SIRIUS_2020_03_12_0756.nxs
. Number of data points: 10
. Available Counters:
    0 -----> delta
    1 -----> zs
    2 -----> gamma
    3 -----> hu36energy
    4 -----> xs
    5 -----> energydcm
    6 -----> current
    7 -----> mon2
    8 -----> surfacepressure
    9 -----> areapermolecule
   10 -----> qxy
   11 -----> pilatus
   12 -----> pilatusroi1
   13 -----> integration_time
   14 -----> sensorsRelTimestamps
   15 -----> sensorsTimestamps
. 2D detector data found, (column 11, alias pilatus)
. qxy data found, (column 10, alias qxy)
. Valid data between points 0 and 9
. Surface pressure data found, mean value 19.73 ± 0.005632 mN/m
. Area per molecule data found, mean value 0.3558 ± 1.942e-05 nm2 per
molecule
. Gamma motor data found, mean value -0.0005415 deg
Absorbers: 29 - Vide
Starting time: 2020-03-12 11:16:03.090248
Ending time: 2020-03-12 11:16:51.901126
```

SIRIUS\_2020\_03\_12\_0756.nxs



```
. Original, non binned, matrix saved in:
data/SIRIUS_2020_03_12_0756_1D.mat
. Scalar data saved in:
data/SIRIUS_2020_03_12_0756_1D.dat
. qz values saved in:
data/SIRIUS_2020_03_12_0756_1D_qz.dat10
. Binned matrix saved in:
data/SIRIUS_2020_03_12_0756_1D.mat10
. XYZ data saved in:
data/SIRIUS_2020_03_12_0756_1D.moy10
. qz values saved in:
data/SIRIUS_2020_03_12_0756_1D_qz.dat20
. Binned matrix saved in:
data/SIRIUS_2020_03_12_0756_1D.mat20
. XYZ data saved in:
data/SIRIUS_2020_03_12_0756_1D.moy20
. qz values saved in:
data/SIRIUS_2020_03_12_0756_1D_qz.dat40
. Binned matrix saved in:
data/SIRIUS_2020_03_12_0756_1D.mat40
. XYZ data saved in:
data/SIRIUS_2020_03_12_0756_1D.moy40
. Figure saved in:
data/SIRIUS_2020_03_12_0756_1D.pdf
```

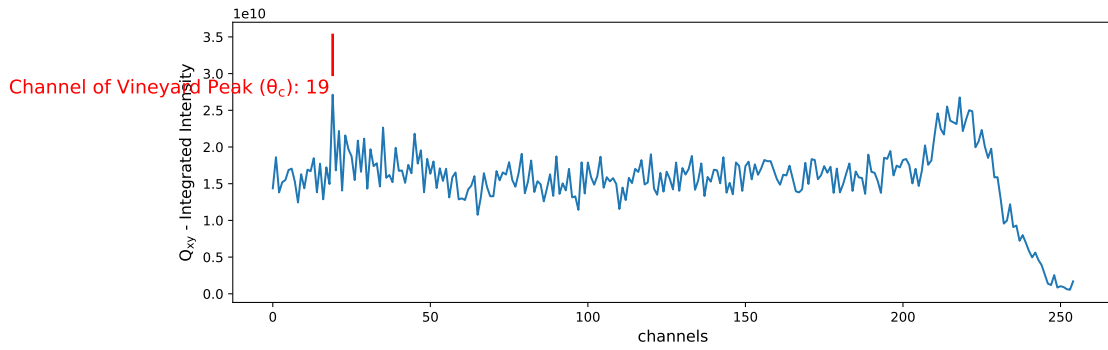
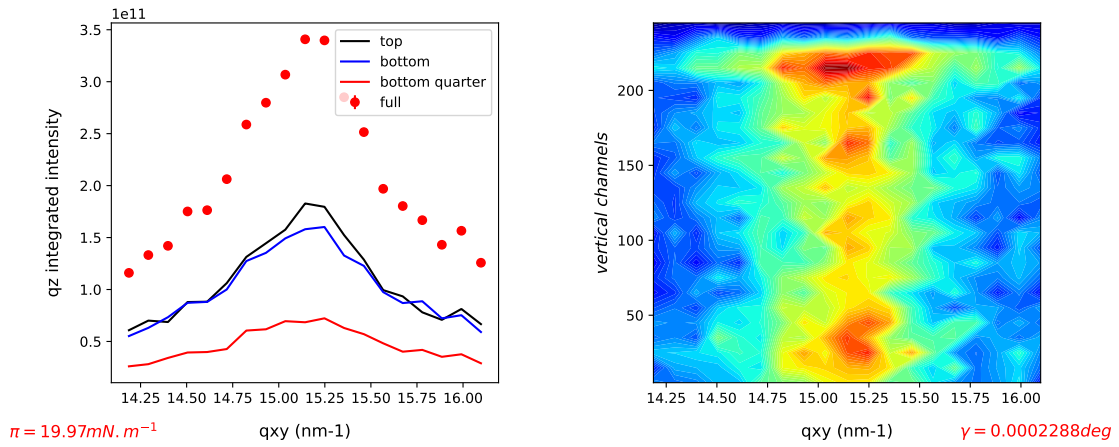
## 5 GIXD with UFXC

### 5.0.1 SIRIUS\_2023\_06\_21\_1770

#### - Open Nexus Data File :

```
user/SIRIUS_2023_06_21_1770.nxs
. Number of data points: 19
. Available Counters:
    0 -----> delta
    1 -----> zs
    2 -----> baseztrait
    3 -----> alphax
    4 -----> gamma
    5 -----> xs
    6 -----> energydcm
    7 -----> current
    8 -----> mon2
    9 -----> surfacepressure
   10 -----> areapermolecule
   11 -----> qxy
   12 -----> mon4
   13 -----> ufxc
   14 -----> ufxcroi1
   15 -----> integration_time
   16 -----> sensorsRelTimestamps
   17 -----> sensorsTimestamps
. 2D detector data found, (column 13, alias ufxc)
. qxy data found, (column 11, alias qxy)
. Valid data between points 0 and 18
. Surface pressure data found, mean value 19.97 ± 0.003764 mN/m
. Area per molecule data found, mean value 0.1936 ± 6.869e-05 nm2 per
molecule
. Gamma motor data found, mean value 0.0002288 deg
Starting time: 2023-06-21 17:07:12.139154
Ending time: 2023-06-21 17:13:19.507741
```

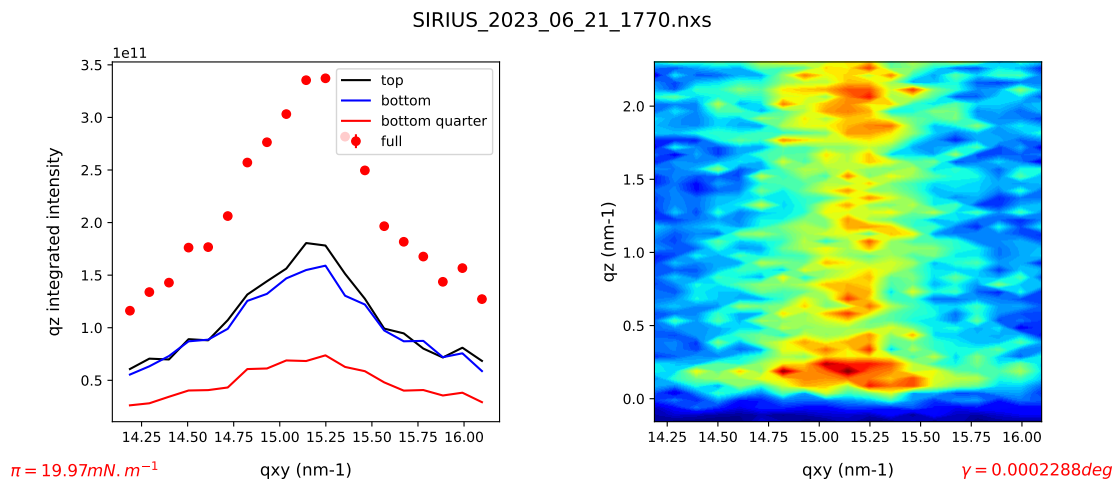
SIRIUS\_2023\_06\_21\_1770.nxs



Data not saved. To save data, run a GIXD on the scan.  
Channel0: 19

## 5.0.2 SIRIUS\_2023\_06\_21\_1770

Absorbers: No absorbers found in the log  
Starting time: 2023-06-21 17:07:12.139154  
Ending time: 2023-06-21 17:13:19.507741

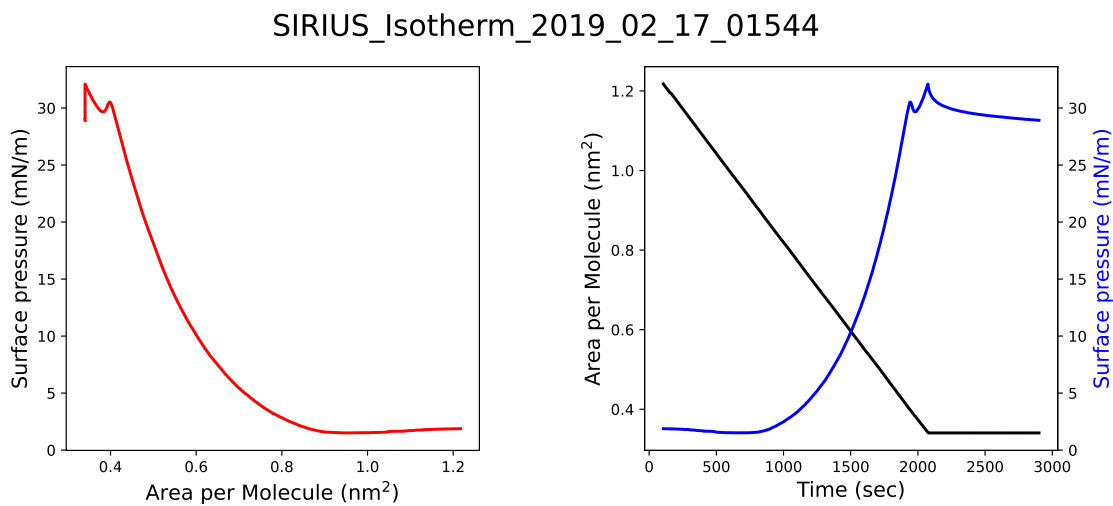


## 6 Isotherm

### 6.0.1 SIRIUS\_Isotherm\_2019\_02\_17\_01544: isotherm 1.97 46 35000 1

Starting time: 2019-02-17 16:52:00.519142

Ending time: 2019-02-17 17:43:46.021957



## 7 1D plot

Add a 1D plot by clicking on Add plot to report.

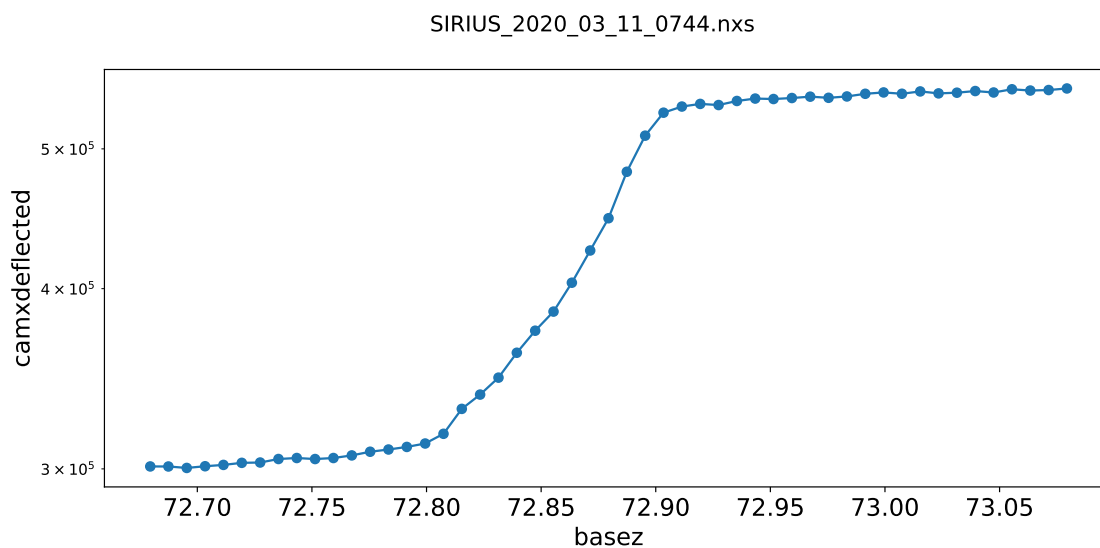
Generates SIRIUS\_2020\_03\_11\_0744.dat

### 7.0.1 SIRIUS\_2020\_03\_11\_0744: dscan basez -.2 .2 50 .1

Absorbers: No Absorbers

Starting time: 2020-03-11 16:52:56.910030

Ending time: 2020-03-11 16:53:42.791704



## 8 GIXS

GIXS:  $q_z$  vs  $q_{xy}$ .

Image and profiles with the approximation  $q_{xy} = \frac{4\pi}{\lambda} \sin\left(\frac{2\theta}{2}\right)$ .

Generates:

- SIRIUS\_2021\_11\_26\_6088\_pilatus\_sum.tiff
- SIRIUS\_2021\_11\_26\_6088\_pilatus\_sum.mat
- SIRIUS\_2021\_11\_26\_6088\_integrated\_qz.dat
- SIRIUS\_2021\_11\_26\_6088\_integrated\_qxy.dat

### 8.1 WAXS

WAXS on Ag Behenate for calibration. Use the GIXS command with thetai forced to 0.

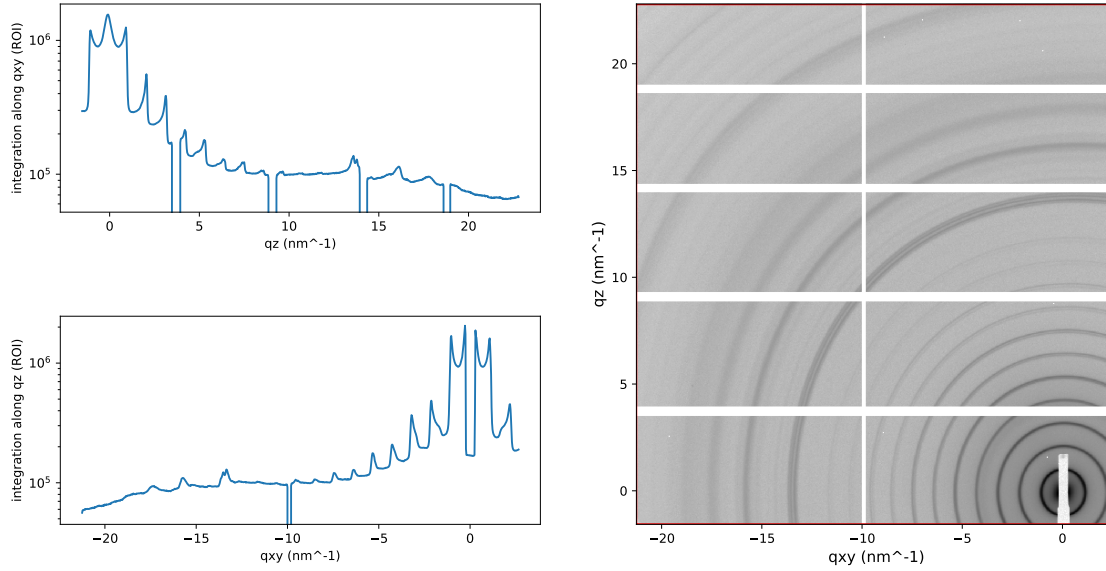
#### 8.1.1 SIRIUS\_2021\_11\_26\_6088: tscan 5 5

Starting time: 2021-11-26 10:35:05.759991

Ending time: 2021-11-26 10:35:05.759991

gamma found: gamma = -0.9997 deg  
delta found: delta = -8.875 deg  
thetai is forced to the value: thetai = 0 deg

SIRIUS\_2021\_11\_26\_6088.nxs



## 8.2 GIWAXS

### 8.2.1 SIRIUS\_2021\_11\_26\_6103: tscan 10 10

Starting time: 2021-11-26 12:40:16.870662

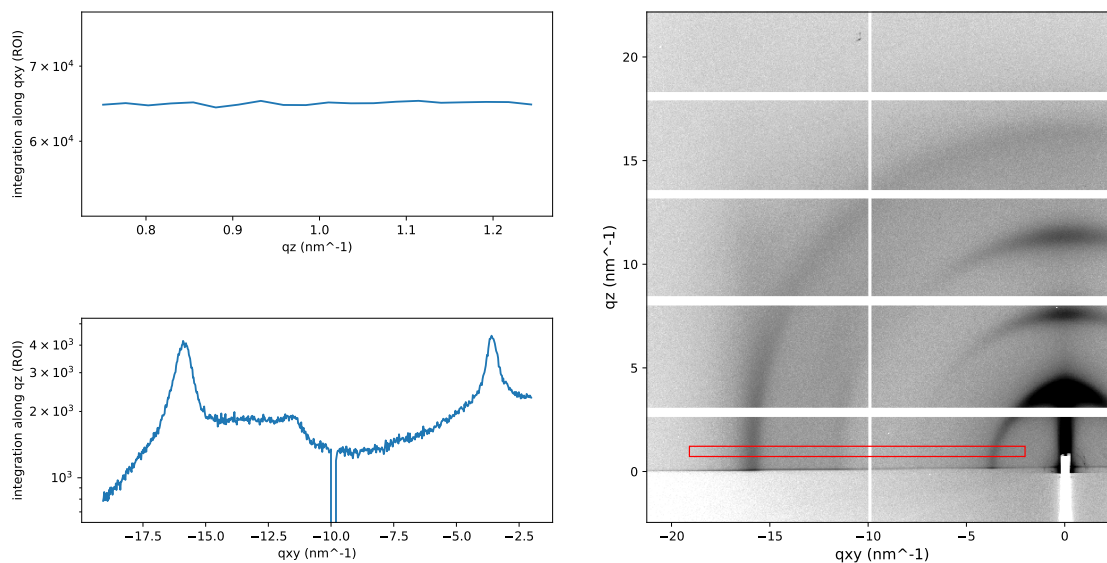
Ending time: 2021-11-26 12:40:16.870662

gamma found: gamma = -2 deg

delta found: delta = -8.875 deg

thetai (alphax) found: thetai = 0.1 deg

SIRIUS\_2021\_11\_26\_6103.nxs



### 8.3 GISAXS

GISAXS image. Delta and gamma have to be forced to zero (the detector is not on the diffractometer).

#### 8.3.1 SIRIUS\_2021\_10\_16\_2739: run scan\_0\_18.ipy

Absorbers: 29 - Vide

Starting time: 2021-10-16 18:47:21.180836

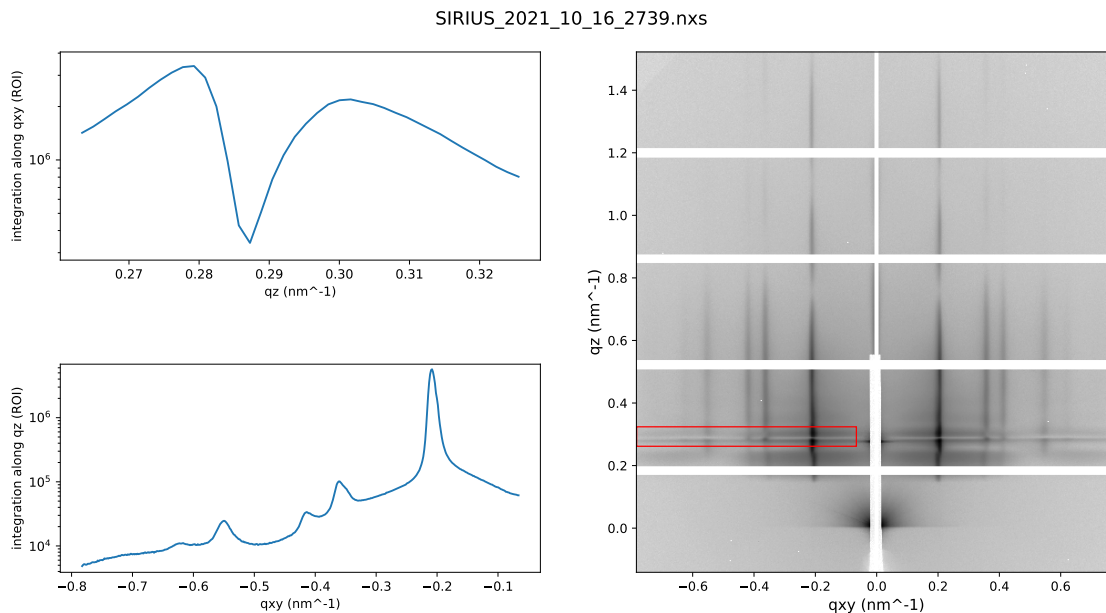
Ending time: 2021-10-16 18:47:21.180836

gamma is forced to the value: gamma = 0 deg

delta is forced to the value: delta = 0 deg

thetai (alphax) found: thetai = 0.18 deg





## 9 Plot area detector

Plot the sum of the images out of a 2D detector. Can also extract and save all the individual images if **Save each** is ticked.

### 9.1 Pilatus

Here with Pilatus.

Generates:

- SIRIUS\_2021\_11\_26\_6088\_pilatus\_sum.tiff
- SIRIUS\_2021\_11\_26\_6088\_pilatus\_sum.mat
- SIRIUS\_2021\_11\_26\_6088\_integrated\_x.dat
- SIRIUS\_2021\_11\_26\_6088\_integrated\_y.dat

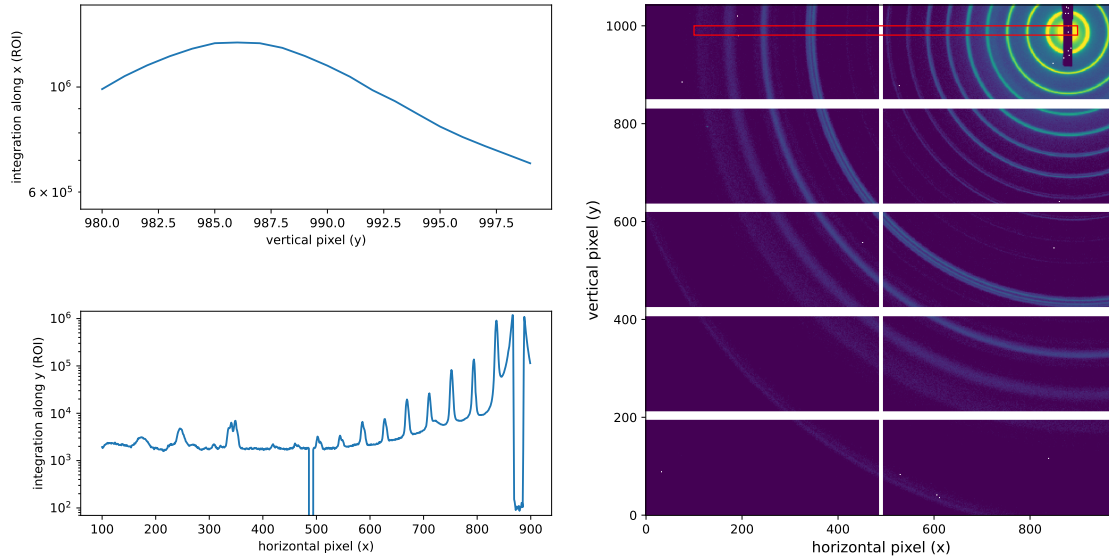
#### 9.1.1 SIRIUS\_2021\_11\_26\_6088: tscan 5 5

Absorbers: 29 - Vide

Starting time: 2021-11-26 10:35:05.759991

Ending time: 2021-11-26 10:35:05.759991

SIRIUS\_2021\_11\_26\_6088.nxs



## 9.2 UFXC

### 9.2.1 SIRIUS\_2021\_11\_11\_3728: tscan 2 9

```
. Available Counters:
0 -----> delta
1 -----> shg
2 -----> zs
3 -----> alphax
4 -----> gamma
5 -----> xs
6 -----> energydcm
7 -----> svg
8 -----> current
9 -----> mon2
10 -----> fluoicr00
11 -----> fluoicr01
12 -----> fluoicr02
13 -----> fluoicr03
14 -----> fluospectrum00
15 -----> fluospectrum01
16 -----> fluospectrum02
17 -----> fluospectrum03
18 -----> mon4
19 -----> ionchamber
20 -----> fluoocr00
```

```

21 -----> fluoocr01
22 -----> fluoocr02
23 -----> fluoocr03
24 -----> commandfemtoionchamber
25 -----> ufx
26 -----> ufxroi2
27 -----> integration_time
28 -----> sensorsRelTimestamps
29 -----> sensorsTimestamps

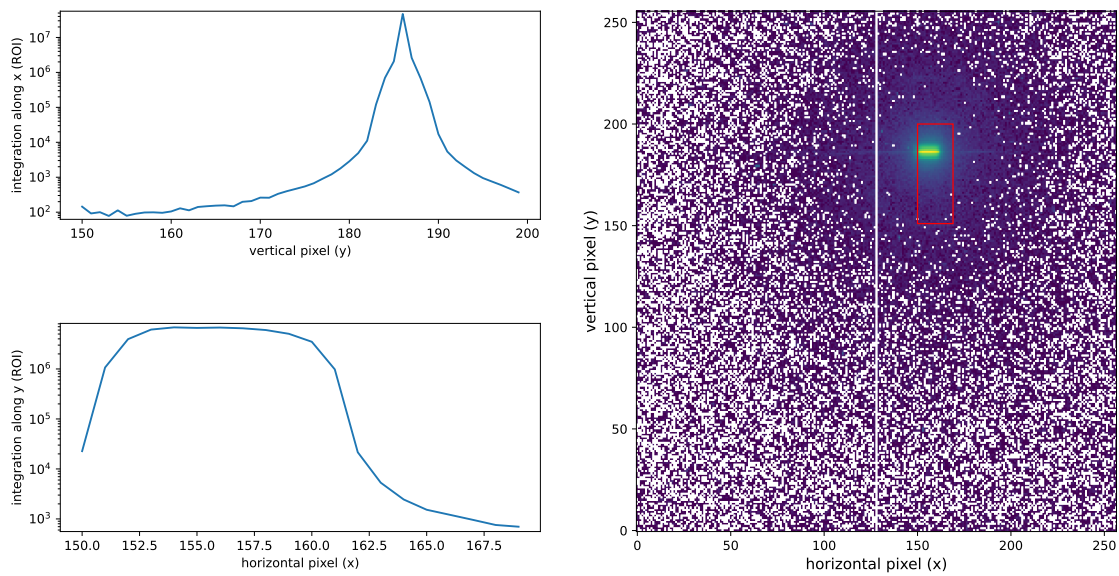
```

Absorbers: Al 100micron

Starting time: 2021-11-11 14:37:28.024263

Ending time: 2021-11-11 14:37:46.813598

SIRIUS\_2021\_11\_11\_3728.nxs



## 10 XRF

### 10.1 SDD 4-elements

Plot XRF from the 4-elements detector, in channels and without peak identification.

Generates:

- SIRIUS\_2017\_12\_11\_08042\_fluospectrum.mat for each SDD element
- SIRIUS\_2017\_12\_11\_08042.dat

### 10.1.1 SIRIUS\_2017\_12\_11\_08042: run xsw7.ipy

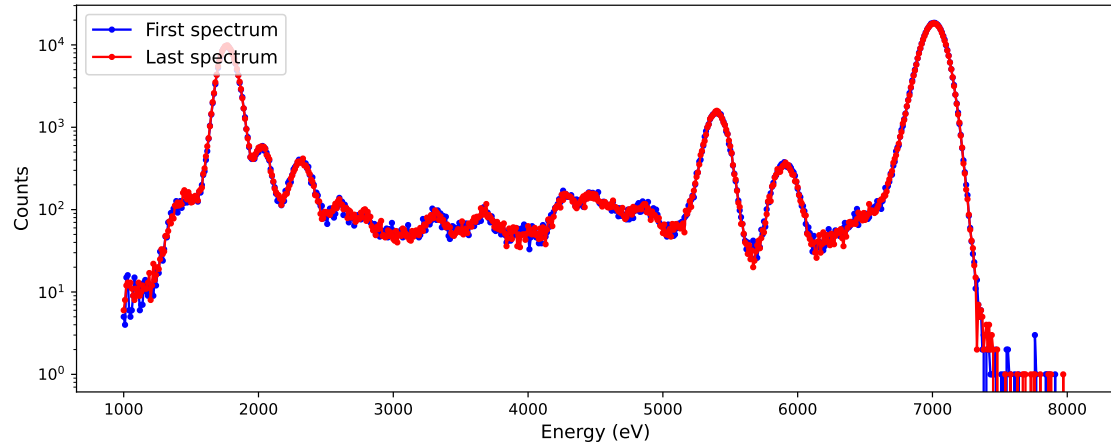
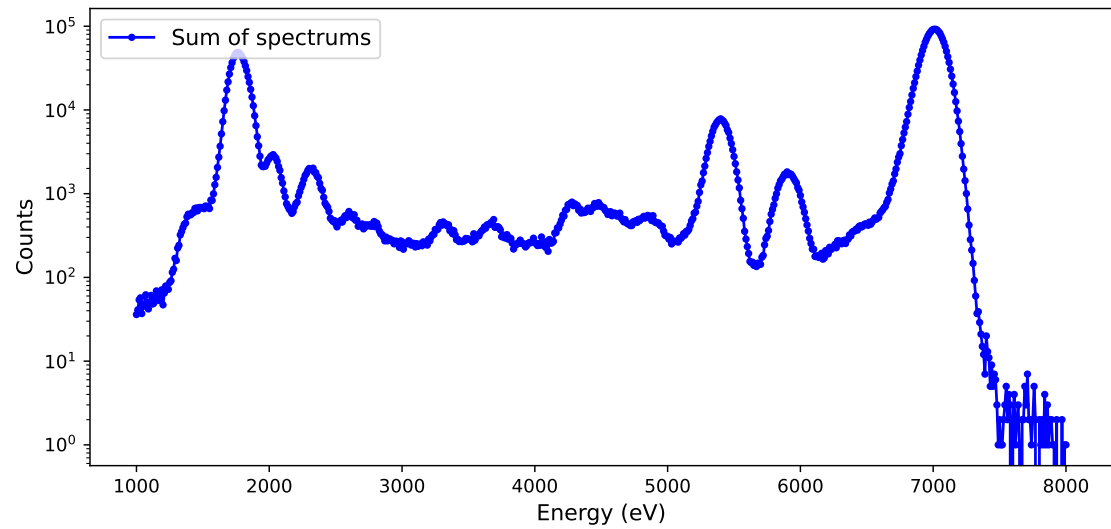
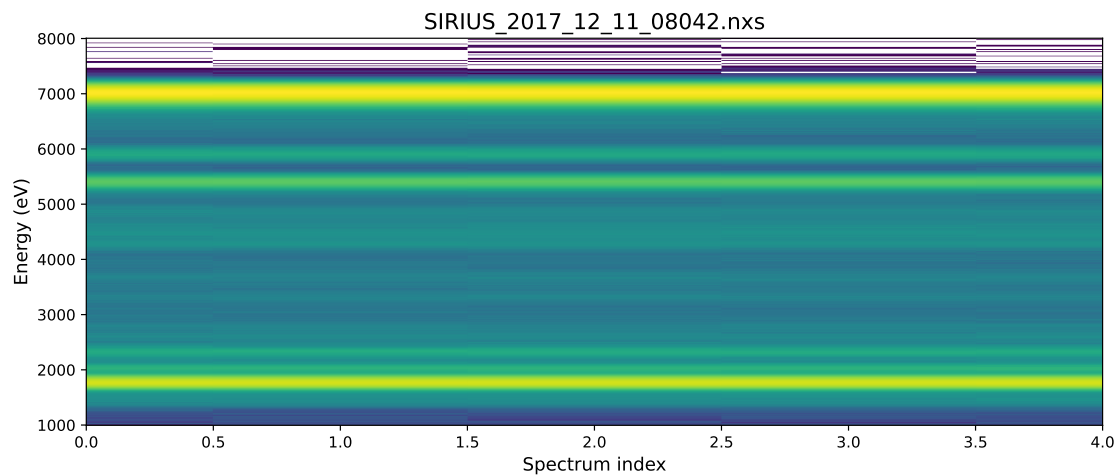
. Available Counters:

```
0 -----> alphax
1 -----> gamma
2 -----> delta
3 -----> ys
4 -----> ds1hg
5 -----> os2hg
6 -----> zs
7 -----> alphax
8 -----> gamma
9 -----> hu36energy
10 -----> xs
11 -----> thetah
12 -----> ds2hg
13 -----> ss1hg
14 -----> current
15 -----> mon2
16 -----> dioderefl
17 -----> fluo00
18 -----> fluo01
19 -----> fluo02
20 -----> fluo03
21 -----> fluoicr00
22 -----> fluoicr01
23 -----> fluoicr02
24 -----> fluoicr03
25 -----> fluocr01
26 -----> fluocr02
27 -----> fluocr03
28 -----> fluospectrum00
29 -----> fluospectrum01
30 -----> fluospectrum02
31 -----> fluospectrum03
32 -----> fluocr00
33 -----> mon4
34 -----> gainfemtodioderefl
35 -----> integration_time
36 -----> sensors_rel_timestamps
37 -----> sensorsTimestamps
38 -----> i15-c-cx1/ex/v2_grp_alphax.rot/rot
39 -----> i15-c-cx1/ex/v2_grp_gamma.rot/rot
```

Absorbers: Al 200micron

Starting time: 2017-12-11 06:24:58.182355

Ending time: 2017-12-11 06:26:26.813347

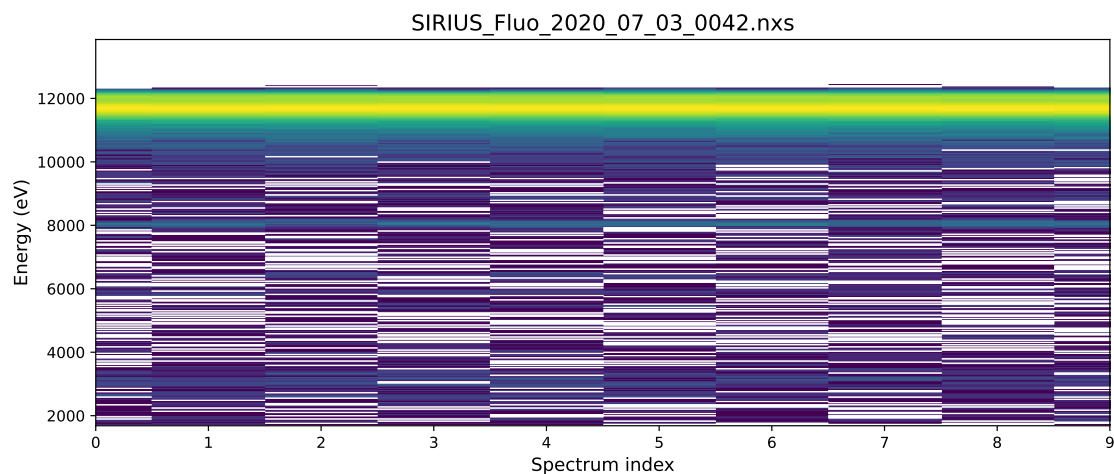


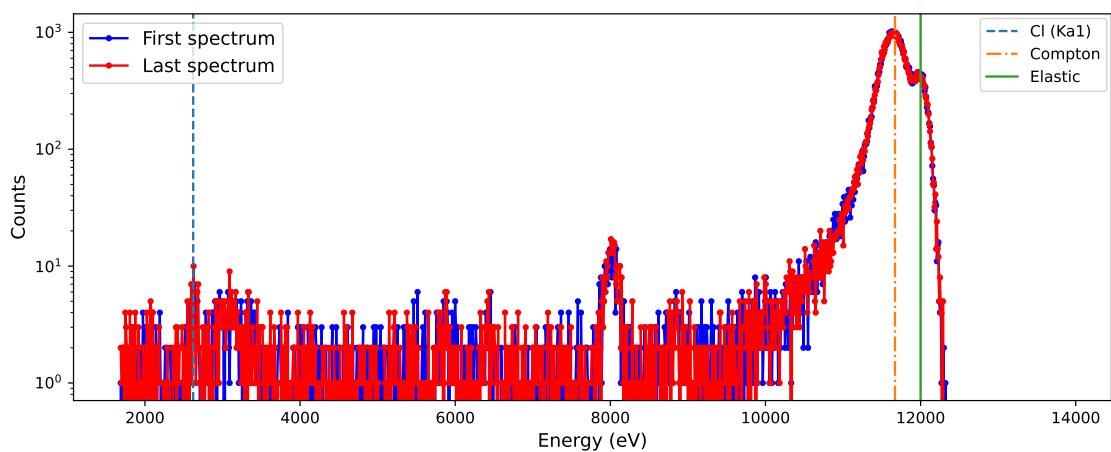
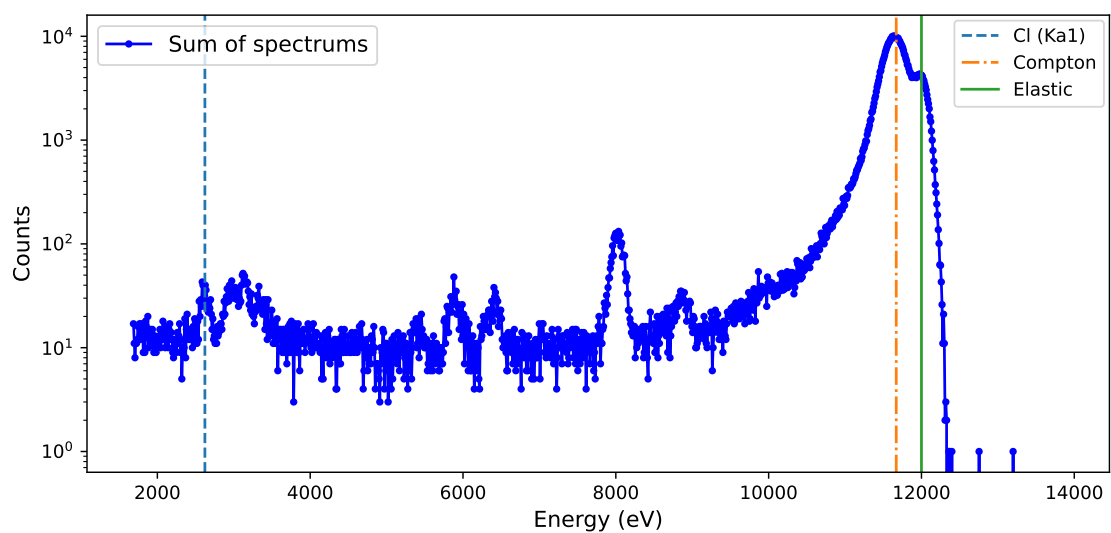
## 10.2 SDD 1-element

### 10.2.1 SIRIUS\_Fluo\_2020\_07\_03\_0042: tscan 500 30

#### - Open Nexus Data File :

```
user/SIRIUS_Fluo_2020_07_03_0042.nxs
. Number of data points: 10
. Available Counters:
    0 -----> ys
    1 -----> zs
    2 -----> xs
    3 -----> surfacepressure
    4 -----> areapermolecule
    5 -----> fluo01
    6 -----> fluo02
    7 -----> fluo03
    8 -----> fluo04
    9 -----> fluoicr04
   10 -----> fluoocr04
   11 -----> fluospectrum04
   12 -----> qxy
   13 -----> integration_time
   14 -----> sensorsRelTimestamps
   15 -----> sensorsTimestamps
. Valid data between points 0 and 9
Absorbers: Al 800micron
Starting time: 2020-07-03 11:01:00.235891
Ending time: 2020-07-03 11:05:34.198804
```

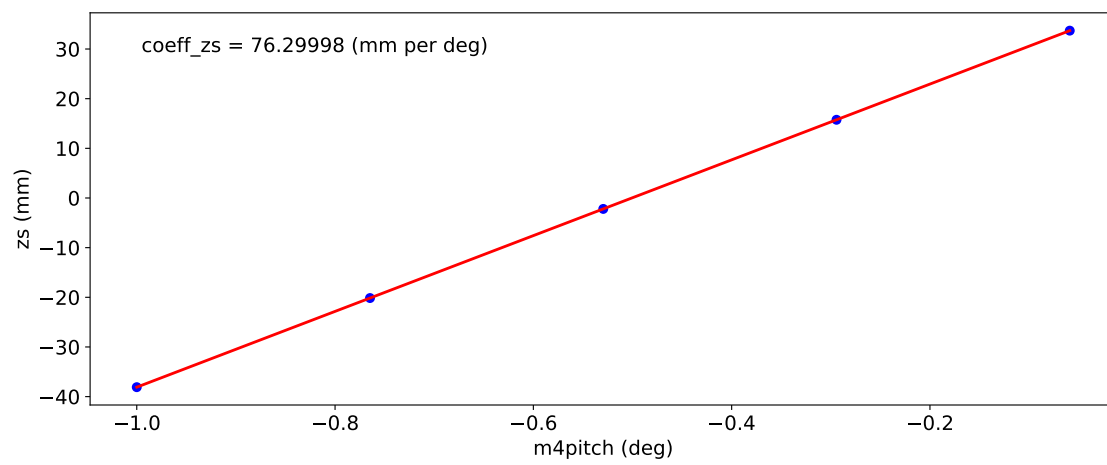
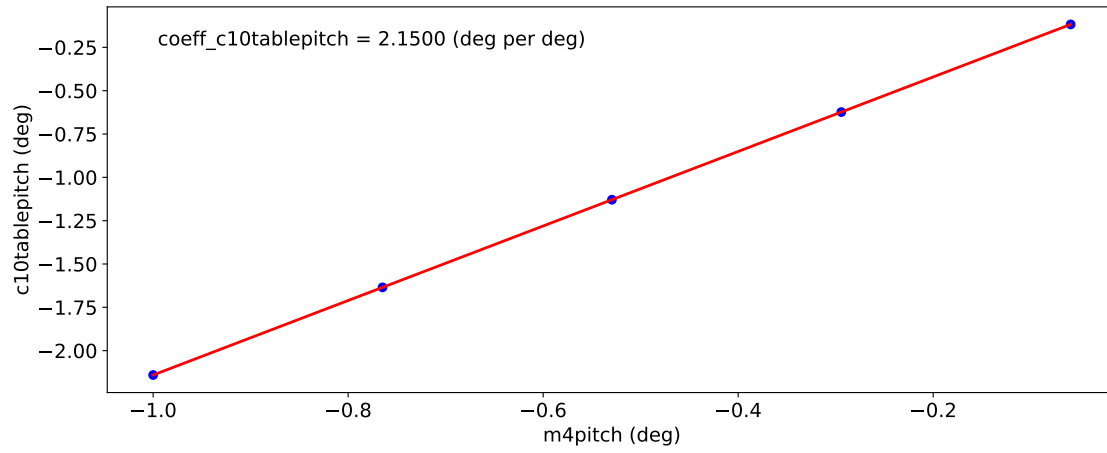




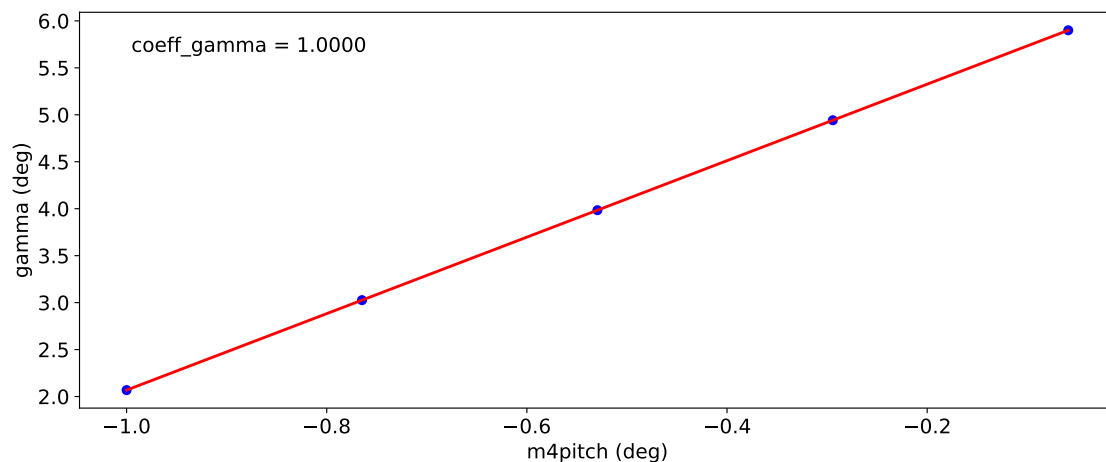
```
. Dat file saved in:
data/SIRIUS_Fluo_2020_07_03_0042.dat
. Spectrum(s) saved in:
data/SIRIUS_Fluo_2020_07_03_0042_fluospectrum*.mat
. Figure spectrogram saved in:
data/SIRIUS_Fluo_2020_07_03_0042_spectrogram.pdf
. Figure sum saved in:
data/SIRIUS_Fluo_2020_07_03_0042_sum.pdf
. Figure first/last saved in:
data/SIRIUS_Fluo_2020_07_03_0042_first_last.pdf
```

## 11 XRR

### 11.1 Calibration XRR (liquid)







## 11.2 Scan XRR (liquid)

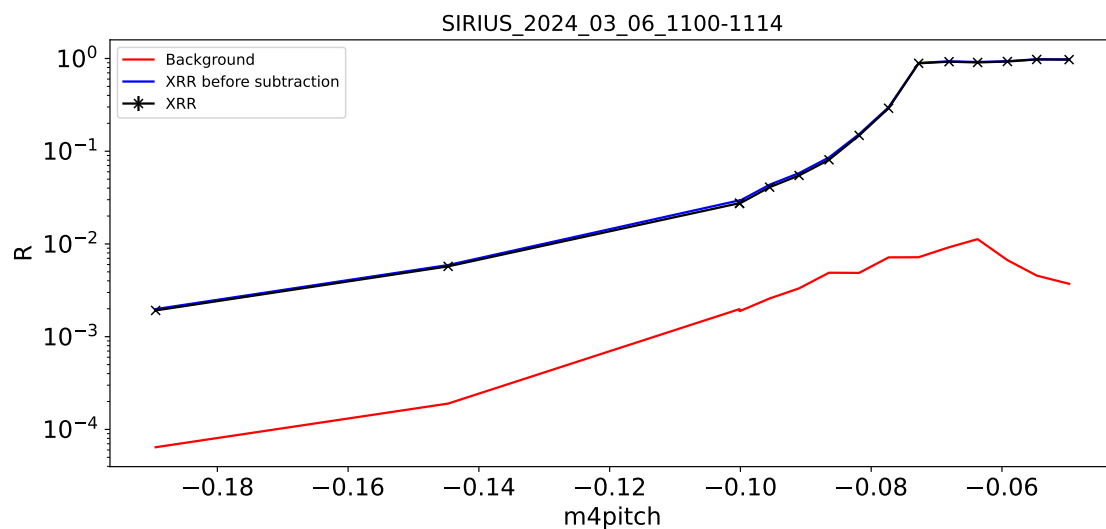
Select the first scan of the XRR series and click on Plot XRR (liquid). Here we show only a few points for the example.

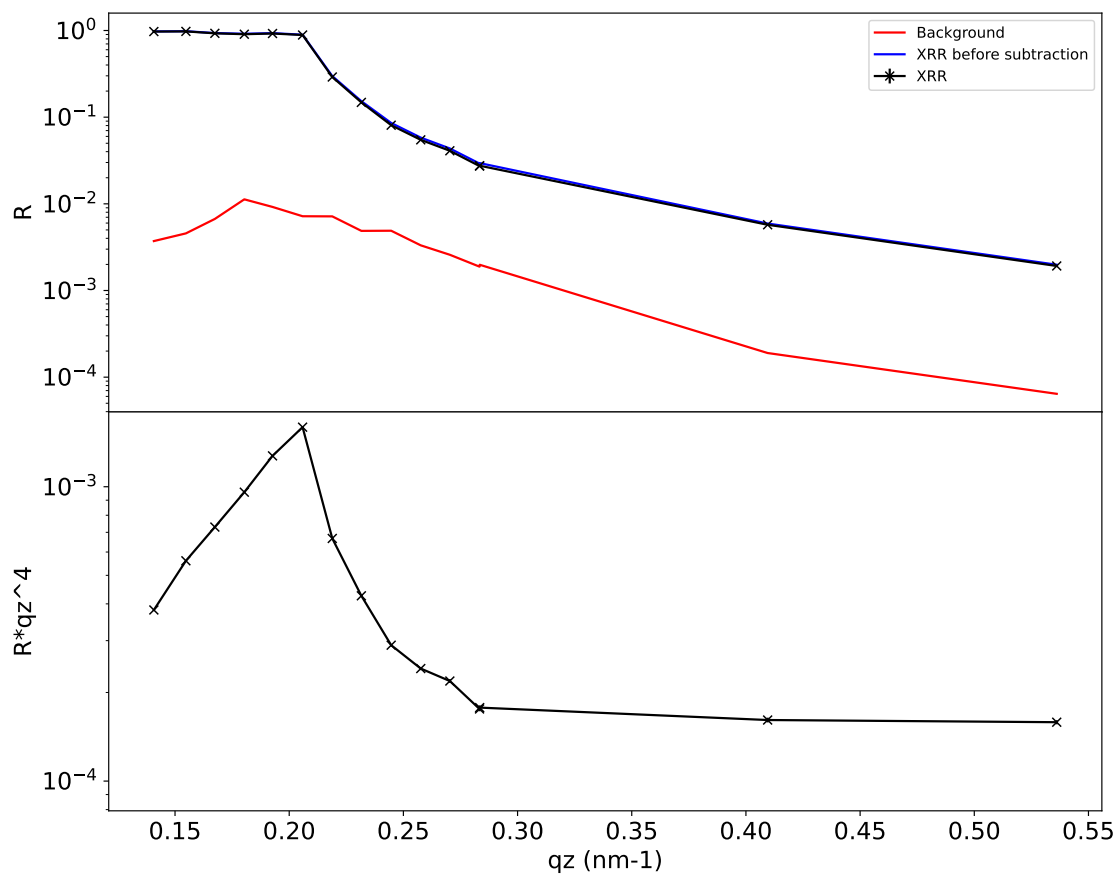
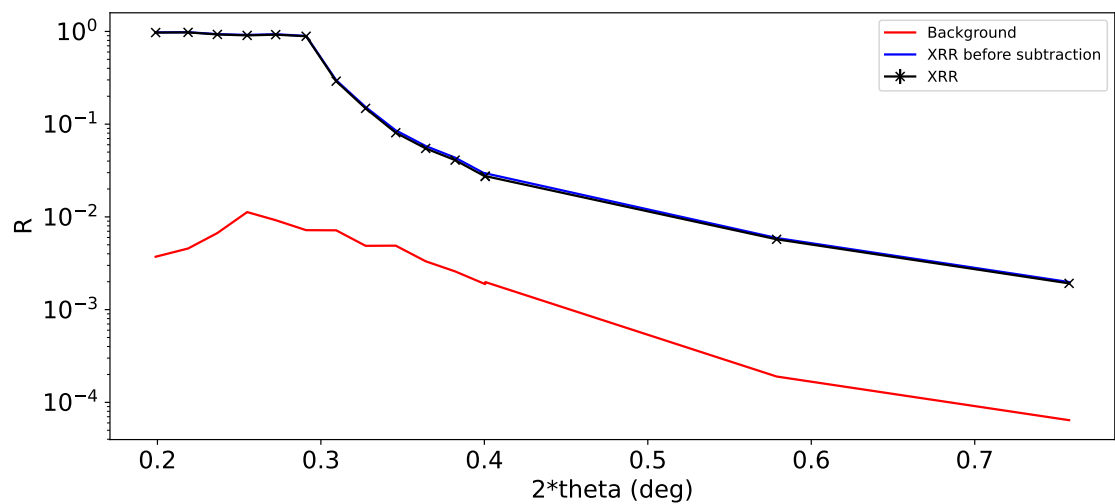
### 11.2.1 SIRIUS\_2024\_03\_06\_1100

Direct extracted from SIRIUS\_2024\_03\_06\_1099.nxs: direct=2.36655e+13

Starting time: 2024-03-06 17:26:18.892705

Ending time: 2024-03-06 17:30:02.152732





Save in progress...  
Save done!

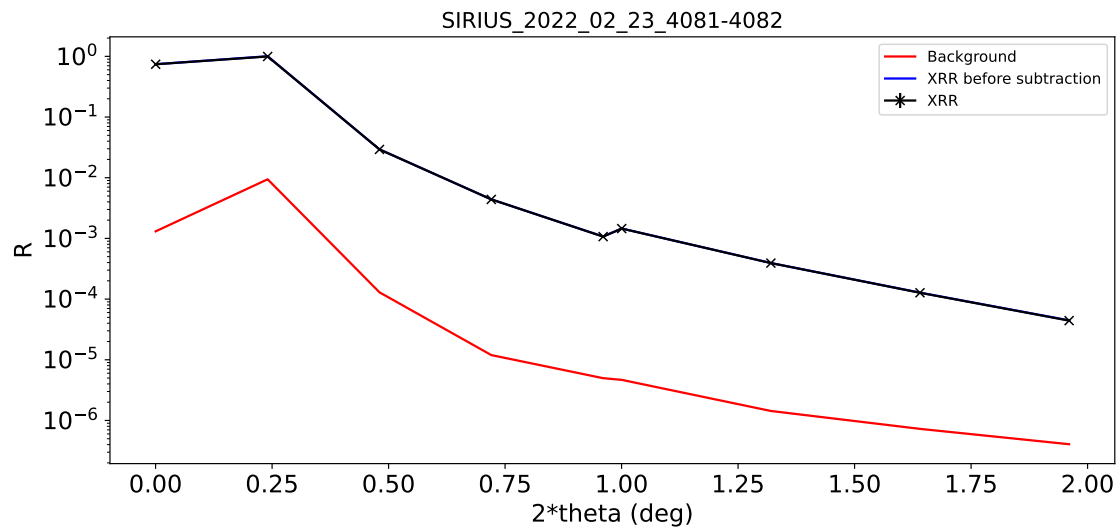
### 11.3 Scan XRR (solid)

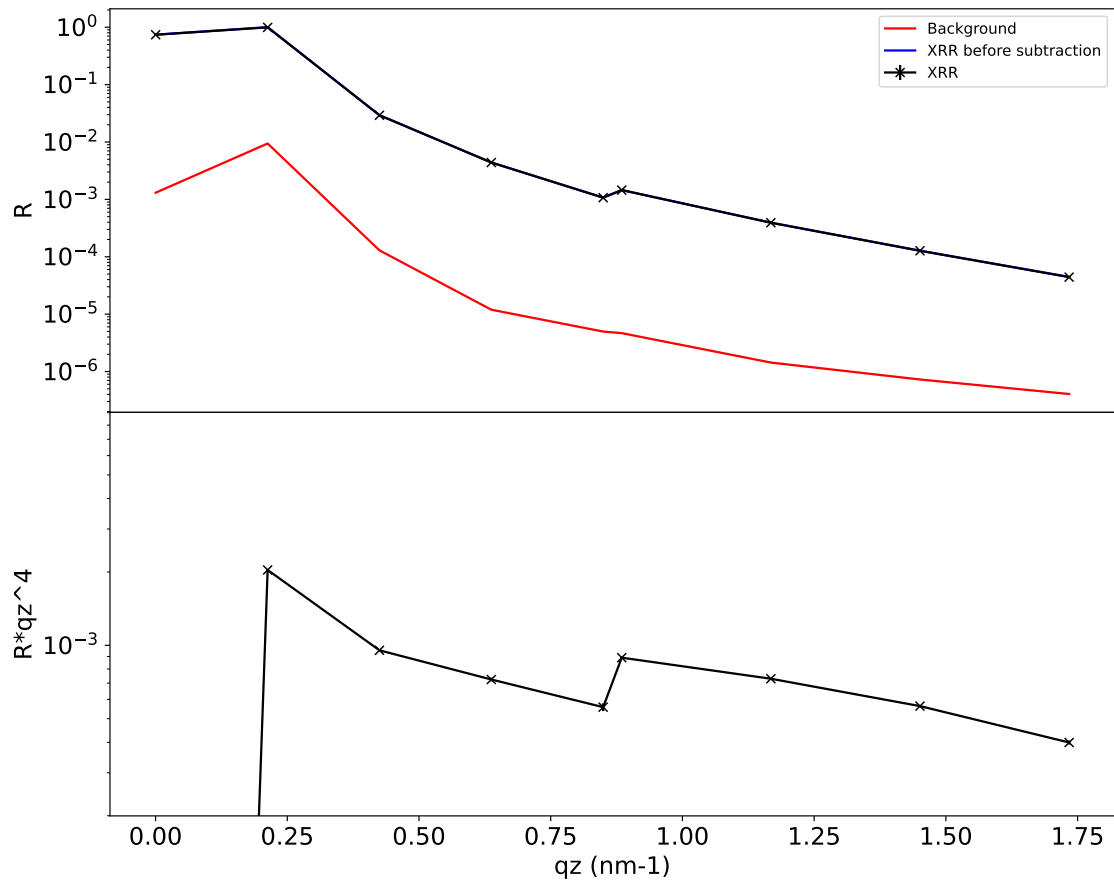
Select all the scans of the XRR series and click on Plot XRR (solid). Here we show only a few points for the example.

#### 11.3.1 SIRIUS\_2022\_02\_23\_4081: run scan\_XRR.ipynb

Starting time: 2022-02-23 14:29:48.620166

Ending time: 2022-02-23 14:38:23.898086





Save in progress...

Save done!

## 12 Insert script

Script inserted (with automatic scan numbering) using `Insert script`.

### 12.0.1 script\_with\_loop.ipynb

```
%shopen
%amove delta -40
%run reset_motors.ipynb
%continuous_ascan delta -35 -25 250 5 #124
%tscan 10 10 #125

for i in range(4):
    %amove delta -20
    %continuous_ascan delta -10 -3 175 5 #126 #128 #130 #132
```

```

%run reset_motors.ipyn
%run cont_regh_abs.ipyn #127 #129 #131 #133

for i in range(3):
    %amove delta -20
    %dscan delta -10 -3 175 5 #134 #136 #138
    %run reset_motors.ipyn

    #%run cont_regh_abs.ipyn
    %run cont_regh_abs.ipyn #135 #137 #139

for i in range(50):
    %amove delta -20
    %tscan 10 100 #140 #141 #142 #143 #144 #145 #146 #147 #148 #149 #150 #151
    #152 #153 #154 #155 #156 #157 #158 #159 #160 #161 #162 #163 #164
    #165 #166 #167 #168 #169 #170 #171 #172 #173 #174 #175 #176 #177
    #178 #179 #180 #181 #182 #183 #184 #185 #186 #187 #188 #189
    %slist scan add camxdirect

%continuous_ascan delta -35 -25 250 5 #190
# %tscan 10 10
%shclose

```

## 13 Insert positions

### 13.0.1 wm alphax gamma

alphax	gamma
0.0266	0.0002

### 13.0.2 wm gamma

gamma
19.9999

## 14 Insert commands

```

Mon, 11 Dec 2017 05:27:55 ct 10 fluoICR00 fluoICR01 fluoICR02
Mon, 11 Dec 2017 05:30:13 amove xs 0
Mon, 11 Dec 2017 06:03:15 amove xs 2

```

## 15 Save/load params

Save/load the current state of the notebook (the variable `jlb.expt`).

## 16 Export

Save the notebook, export it to PDF, and convert logs to a more convenient file format.

**Remarks can be inserted in bold red !**

**Like that.**