

JupyLabBook_example

November 4, 2024

1 JupyLabBook @ SIRIUS

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

JupyterLab version: v3.2.3
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

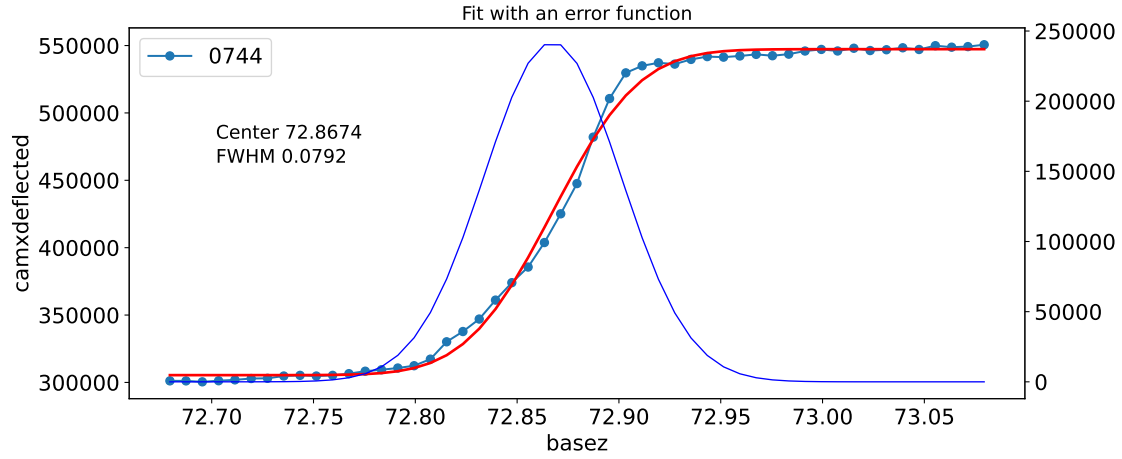
Fit with erf function.

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

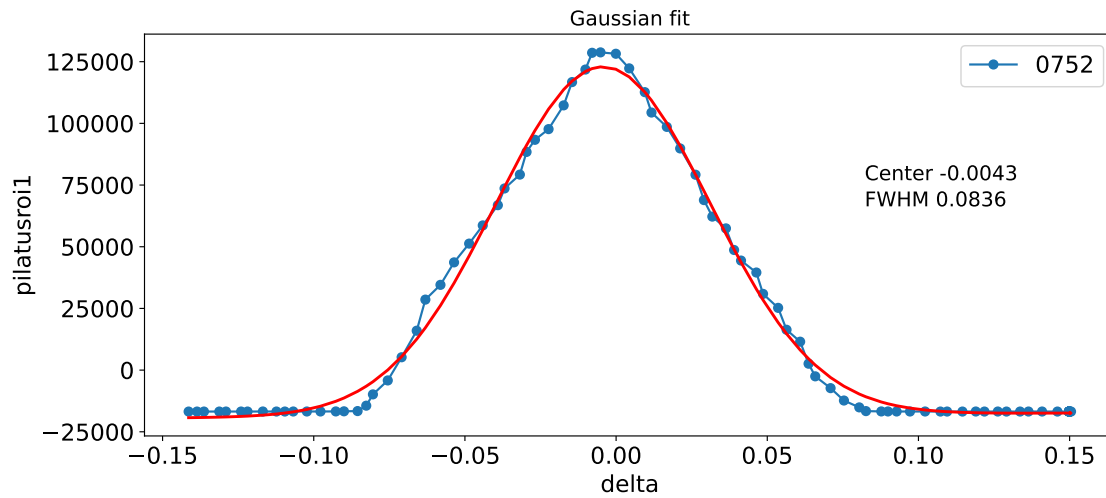


3.1.2 SIRIUS_2020_03_11_0752: continuous_ascan delta -.15 .15 100 1

Absorbers: Al 1000micron

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

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



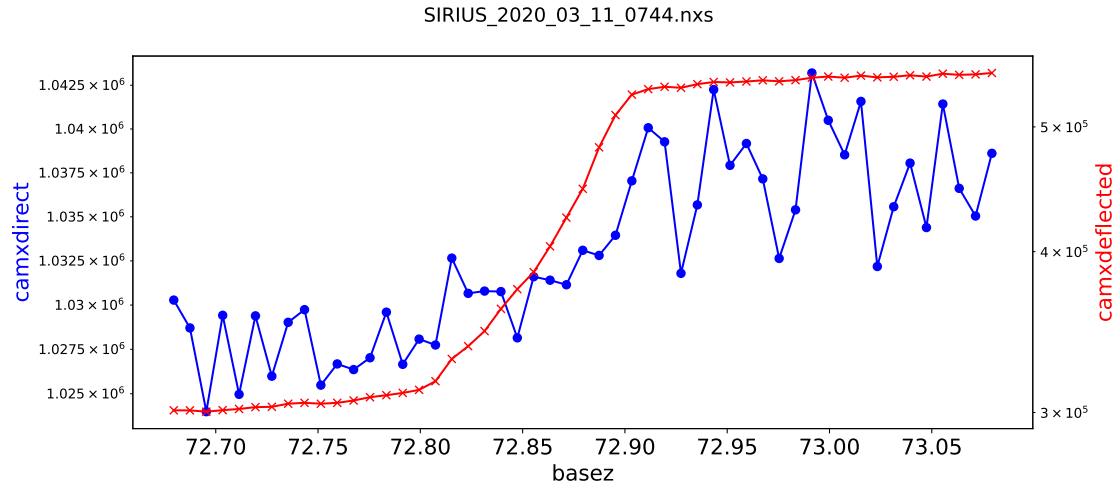
With two curves, in log.

3.1.3 SIRIUS_2020_03_11_0744: dscan basez -.2 .2 50 .1

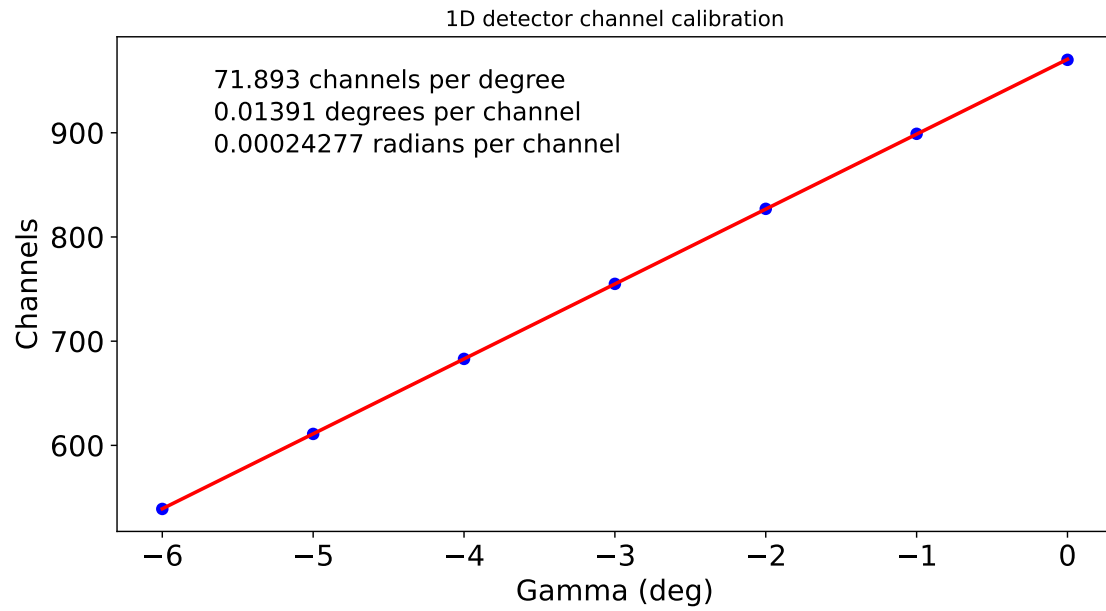
Absorbers: No Absorbers

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

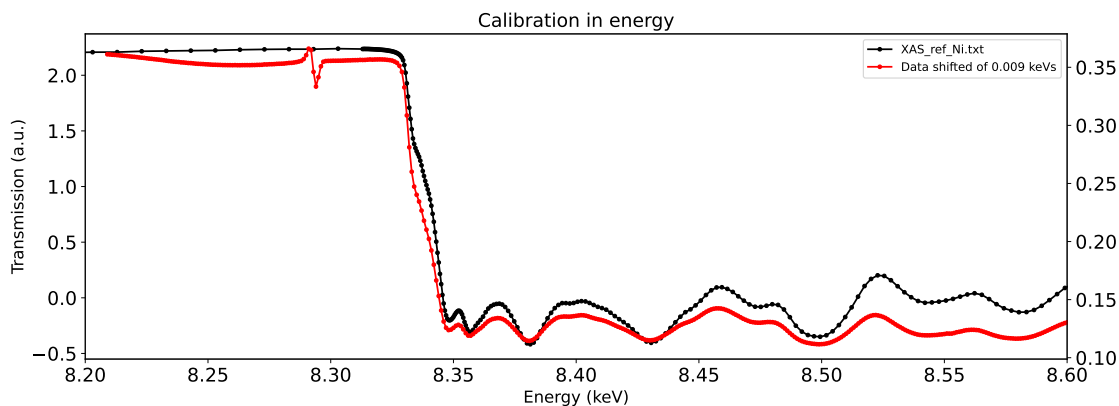
Ending time: 2020-03-11 16:53:42.791704



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 :

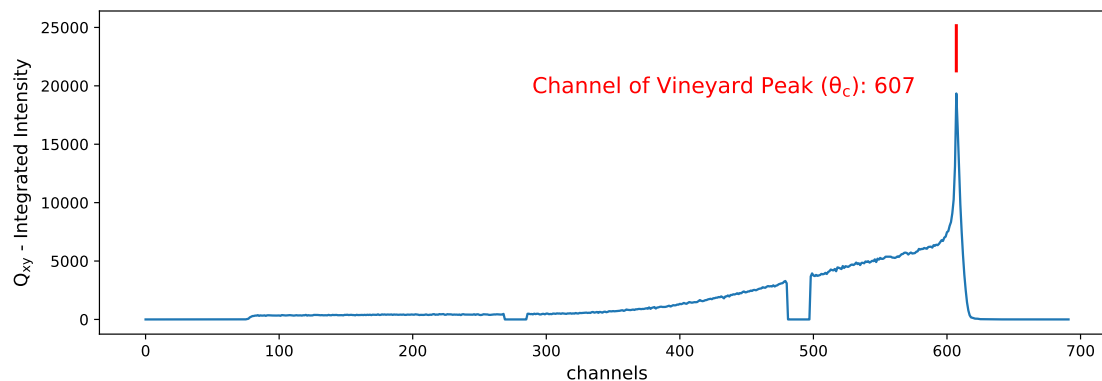
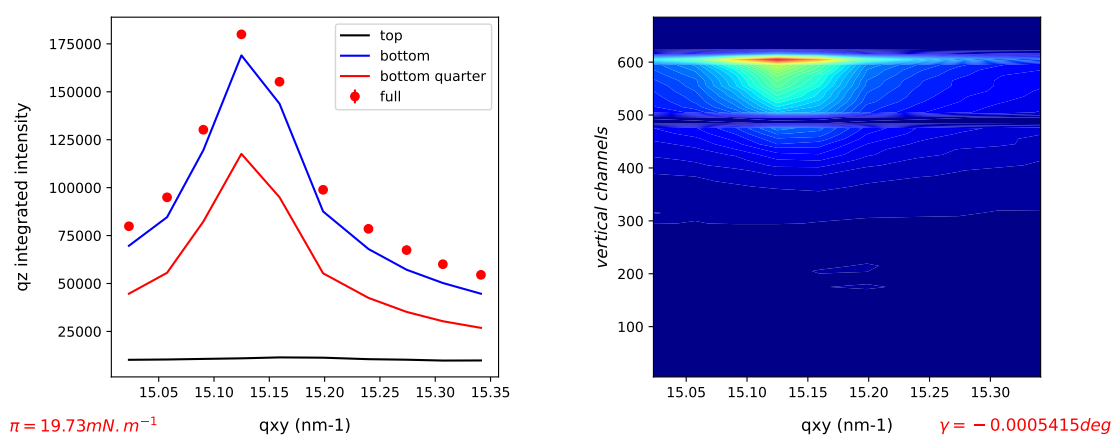
```
user/SIRIUS_2020_03_12_0756.nxs
. Number of data points: 10
. Available Counters:
0 -----> delta
1 -----> zs
2 -----> gamma
3 -----> hu36energy
4 -----> xs
5 -----> energydcm
6 -----> current
7 -----> mon2
8 -----> surfacepressure
9 -----> areapermolecule
10 -----> qxy
11 -----> pilatus
12 ----->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

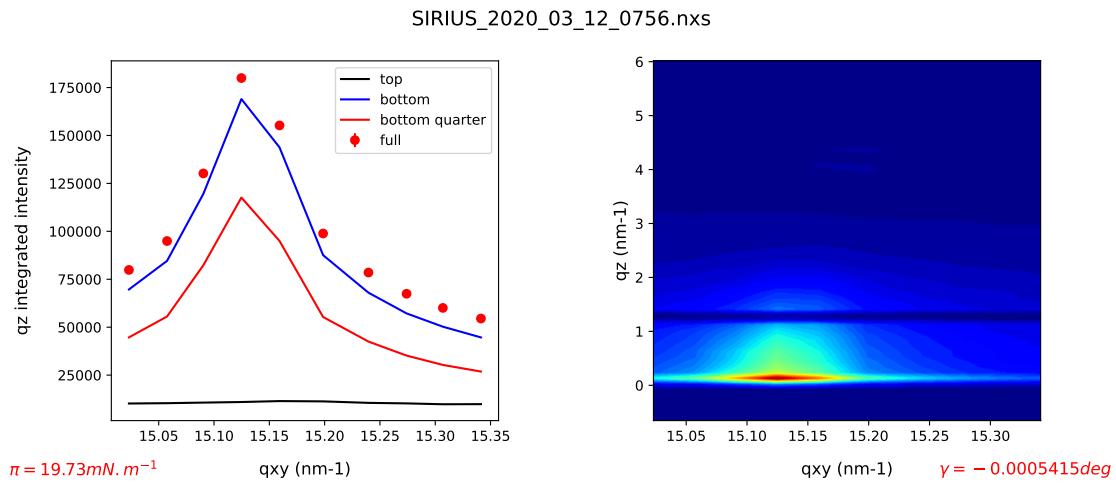
The variable `sensors` to add allows one to print the average value of a sensor on top of the figure.

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: No absorbers (wheel); No fast absorbers
Starting time: 2020-03-12 11:16:03.090248
Ending time: 2020-03-12 11:16:51.901126
mon2 = 9.338210916612297
```

zs = -40.431232115



```
. 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
```

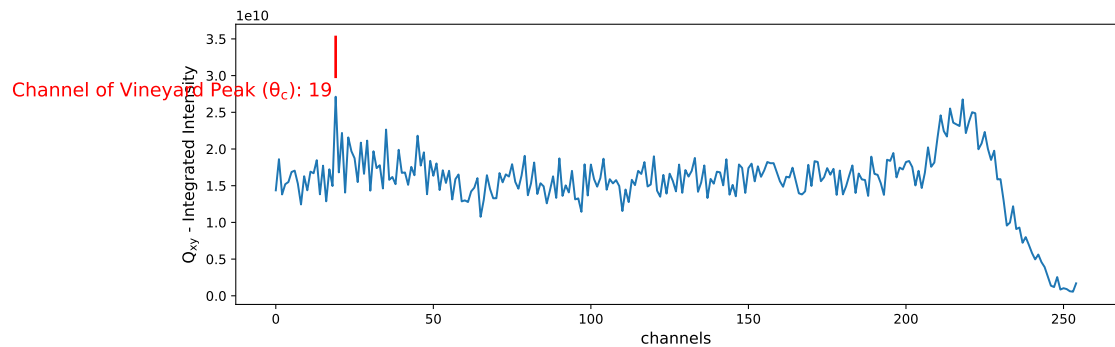
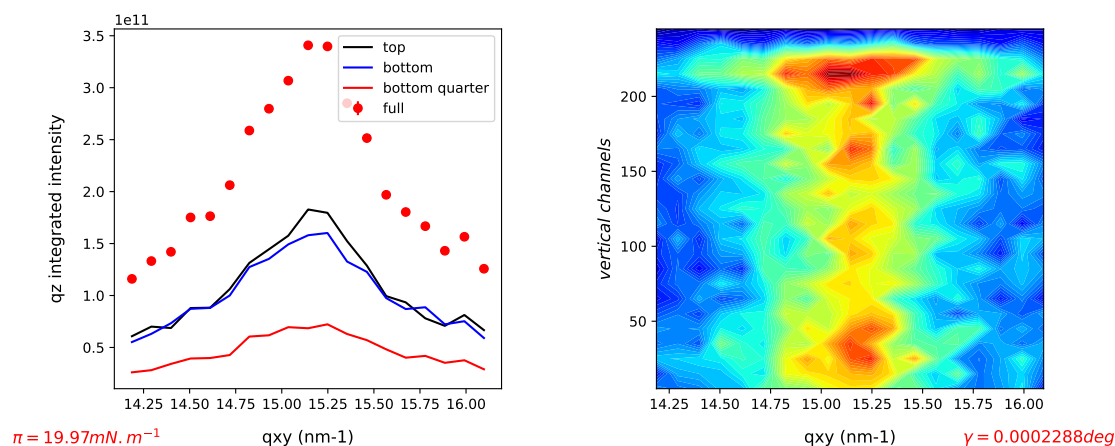
5 GIXD with UFXC

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

- Open Nexus Data File :

user/SIRIUS_2023_06_21_1770.nxs

. Number of data points: 19

. Available Counters:

```

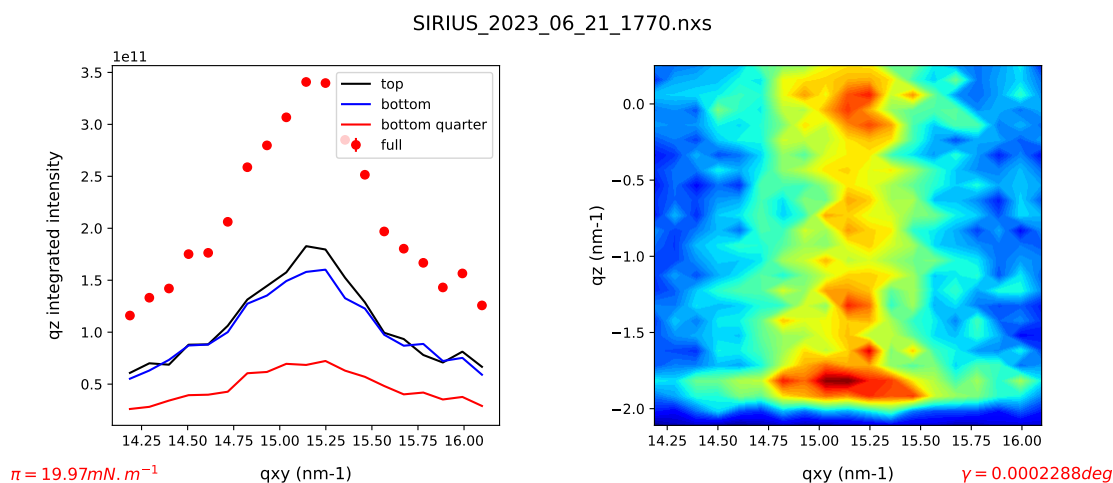
0 -----> delta
1 -----> zs
2 -----> baseztrait
3 -----> alphax
4 -----> gamma
5 -----> xs
6 -----> energydcm
7 -----> current

```

```

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  $19.97 \pm 0.003764$  mN/m
. Area per molecule data found, mean value  $0.1936 \pm 6.869e-05$  nm2 per
molecule
. Gamma motor data found, mean value 0.0002288 deg
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
mon2 = 13.13576863980607
zs = -40.190264414999994

```



```

. Original, non binned, matrix saved in:
data/SIRIUS_2023_06_21_1770_1D.mat
. Scalar data saved in:
data/SIRIUS_2023_06_21_1770_1D.dat
. qz values saved in:
data/SIRIUS_2023_06_21_1770_1D_qz.dat10
. Binned matrix saved in:

```

```

data/SIRIUS_2023_06_21_1770_1D.mat10
. XYZ data saved in:
data/SIRIUS_2023_06_21_1770_1D.moy10
. qz values saved in:
data/SIRIUS_2023_06_21_1770_1D_qz.dat20
. Binned matrix saved in:
data/SIRIUS_2023_06_21_1770_1D.mat20
. XYZ data saved in:
data/SIRIUS_2023_06_21_1770_1D.moy20
. qz values saved in:
data/SIRIUS_2023_06_21_1770_1D_qz.dat40
. Binned matrix saved in:
data/SIRIUS_2023_06_21_1770_1D.mat40
. XYZ data saved in:
data/SIRIUS_2023_06_21_1770_1D.moy40
. Figure saved in:
data/SIRIUS_2023_06_21_1770_1D.pdf

```

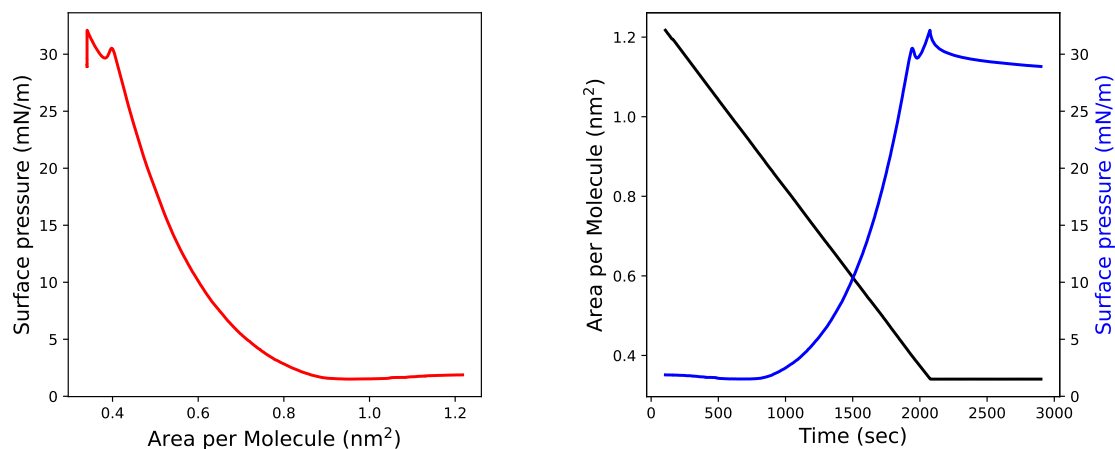
6 Isotherm

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

SIRIUS_Isotherm_2019_02_17_01544



7 1D plot

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

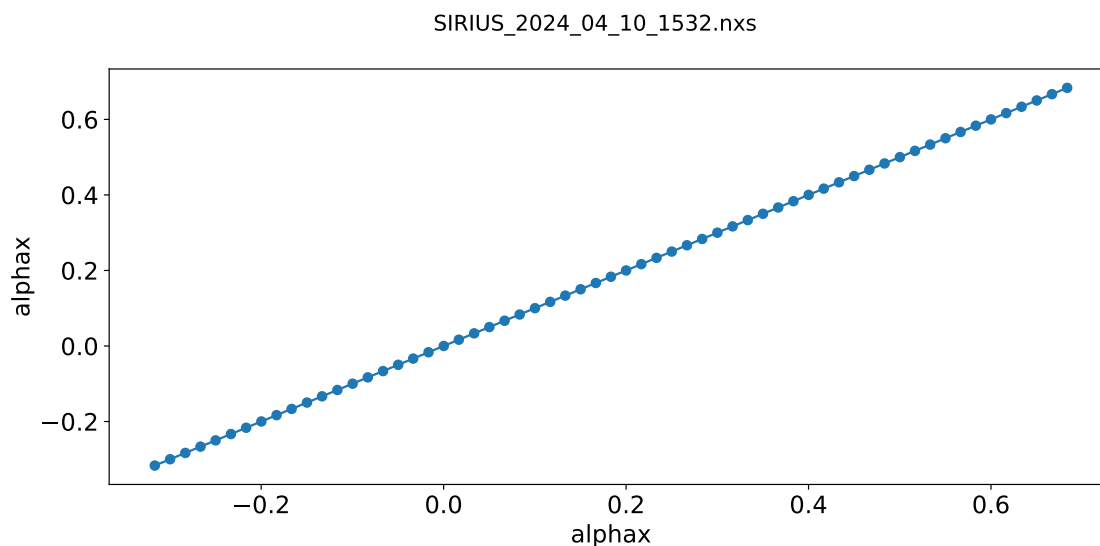
Generates SIRIUS_2024_04_10_1532.dat

7.0.1 SIRIUS_2024_04_10_1532: dscan alphax -0.5 0.5 60 .1

Absorbers: No absorbers (wheel); No fast absorbers

Starting time: 2024-04-10 15:23:55.466288

Ending time: 2024-04-10 15:24:40.793473



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

Absorbers: No absorbers (wheel); No fast absorbers

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

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

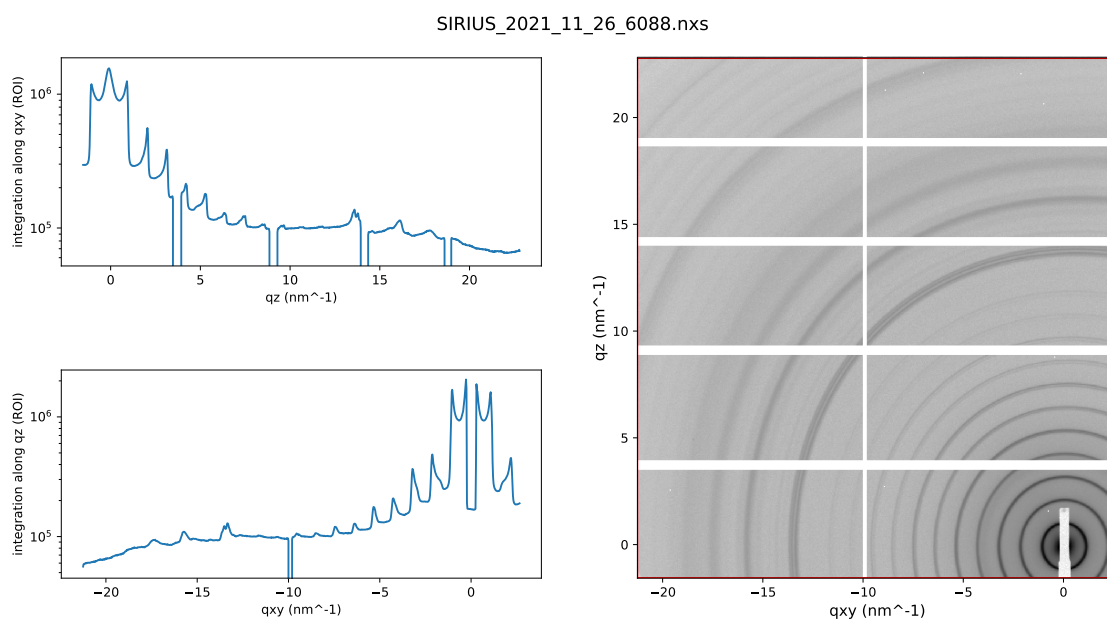
gamma found: gamma = -0.9997 deg

delta found: delta = -8.875 deg

thetai is forced to the value: thetai = 0 deg

mon2 = 0.4538712091743946

zs = -71.586768605



8.2 GIWAXS

8.2.1 SIRIUS_2021_11_26_6103: tscan 10 10

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

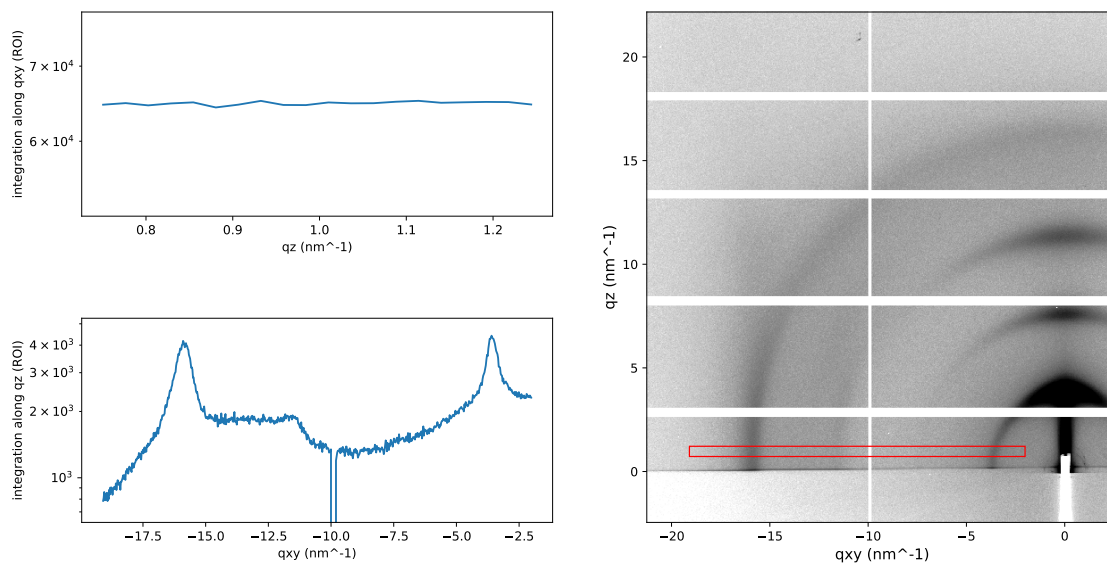
Ending time: 2021-11-26 12:40:16.870662

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

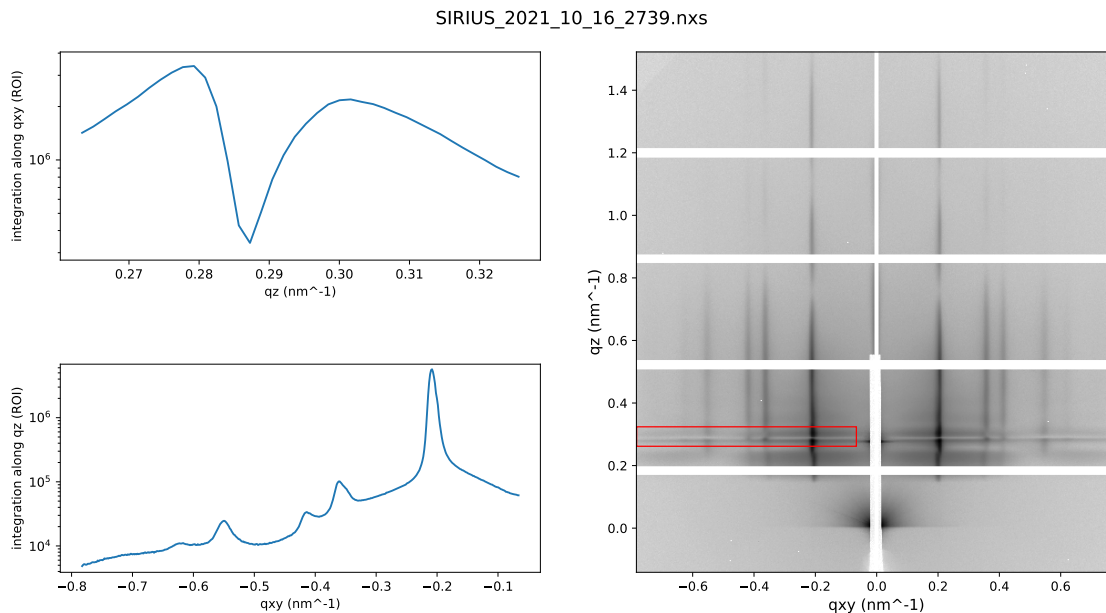
Starting time: 2021-10-16 18:47:21.180836

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

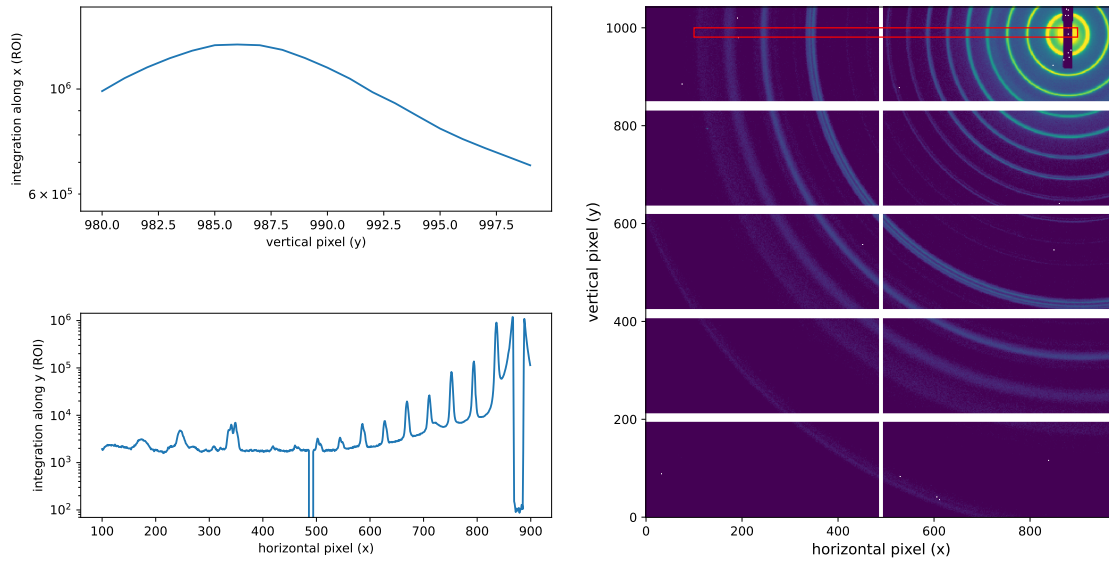
9.1.1 SIRIUS_2021_11_26_6088: tscan 5 5

Absorbers: No absorbers (wheel); No fast absorbers

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

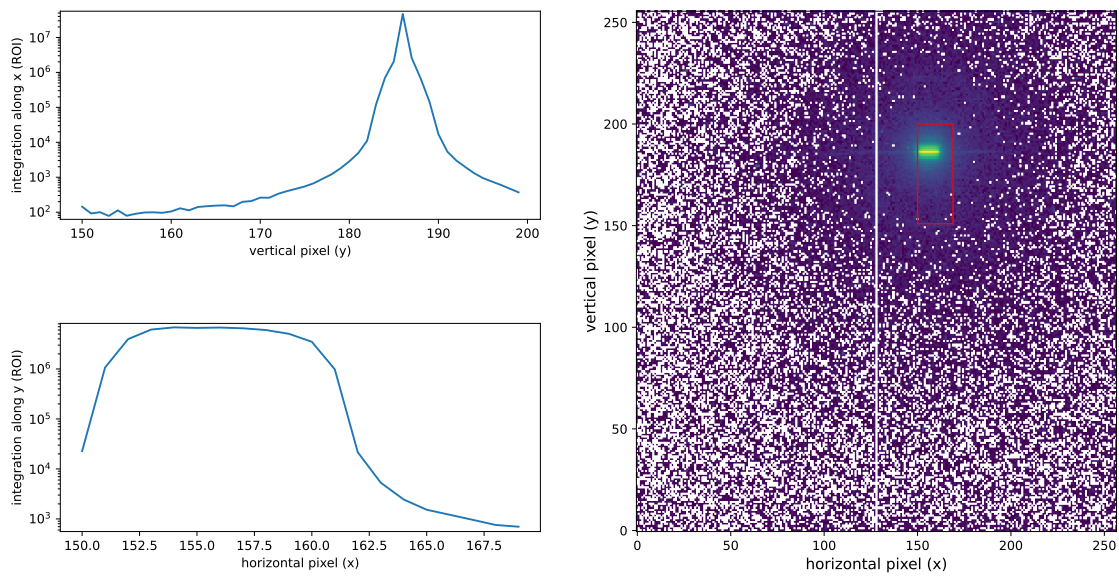
```

Absorbers: No absorbers (wheel); No fast absorbers

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

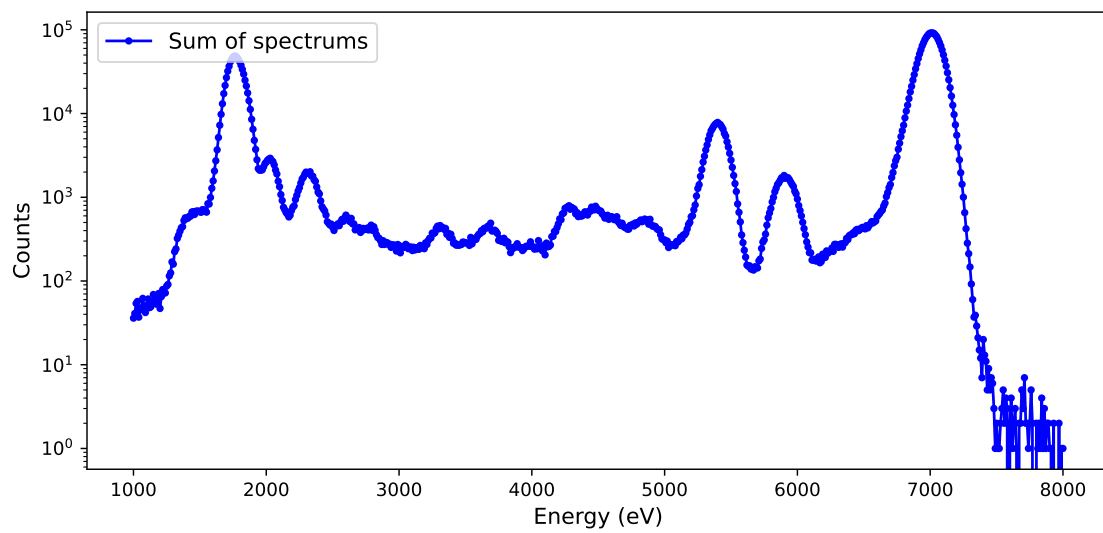
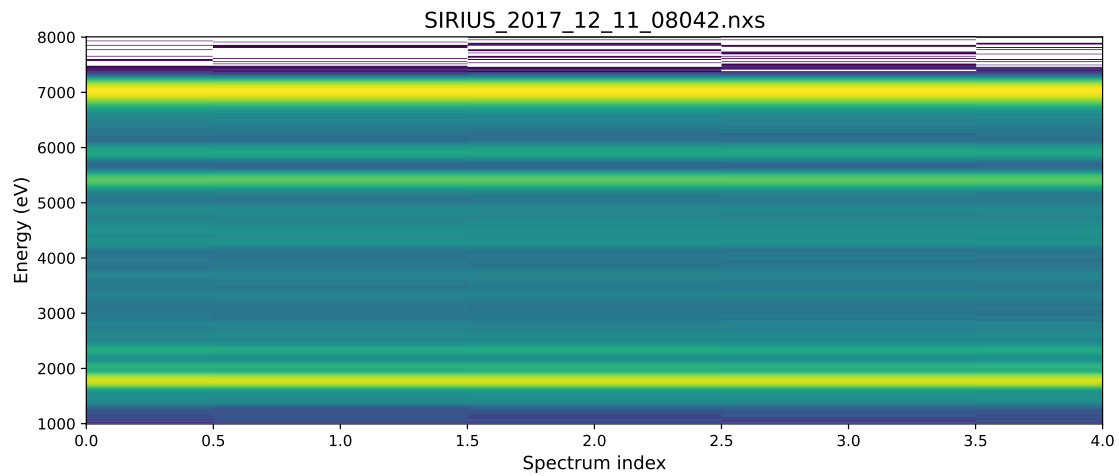
- Open Nexus Data File :

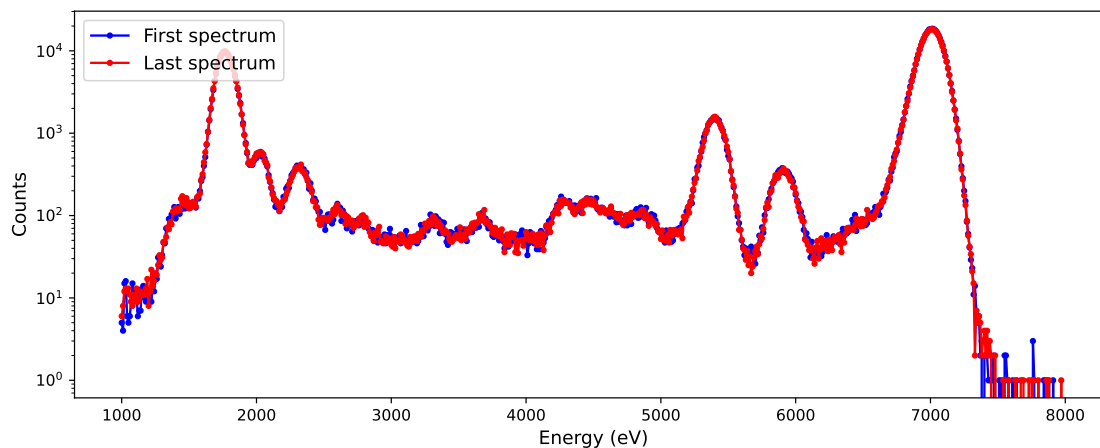
```
user/SIRIUS_2017_12_11_08042.nxs
. Number of data points: 5
. Available Counters:
    0 -----> alphax
    1 -----> gamma
    2 -----> delta
    3 -----> ys
    4 -----> ds1hg
    5 -----> os2hg
    6 -----> zs
    7 -----> alphax
    8 -----> gamma
    9 -----> hu36energy
   10 -----> xs
   11 -----> 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 -----> fluoocr01
   26 -----> fluoocr02
   27 -----> fluoocr03
   28 -----> fluospectrum00
   29 -----> fluospectrum01
   30 -----> fluospectrum02
   31 -----> fluospectrum03
   32 -----> fluoocr00
   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
. Valid data between points 0 and 4
```

Absorbers: No absorbers (wheel); No fast absorbers

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

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





```
. Dat file saved in:
data/SIRIUS_2017_12_11_08042.dat
. Spectrum(s) saved in:
data/SIRIUS_2017_12_11_08042_fluospectrum*.mat
. Figure spectrogram saved in:
data/SIRIUS_2017_12_11_08042_spectrogram.pdf
. Figure sum saved in:
data/SIRIUS_2017_12_11_08042_sum.pdf
. Figure first/last saved in:
data/SIRIUS_2017_12_11_08042_first_last.pdf
```

10.2 SDD 1-element

10.2.1 SIRIUS_Fluo_2020_07_03_0042: tscan 500 30

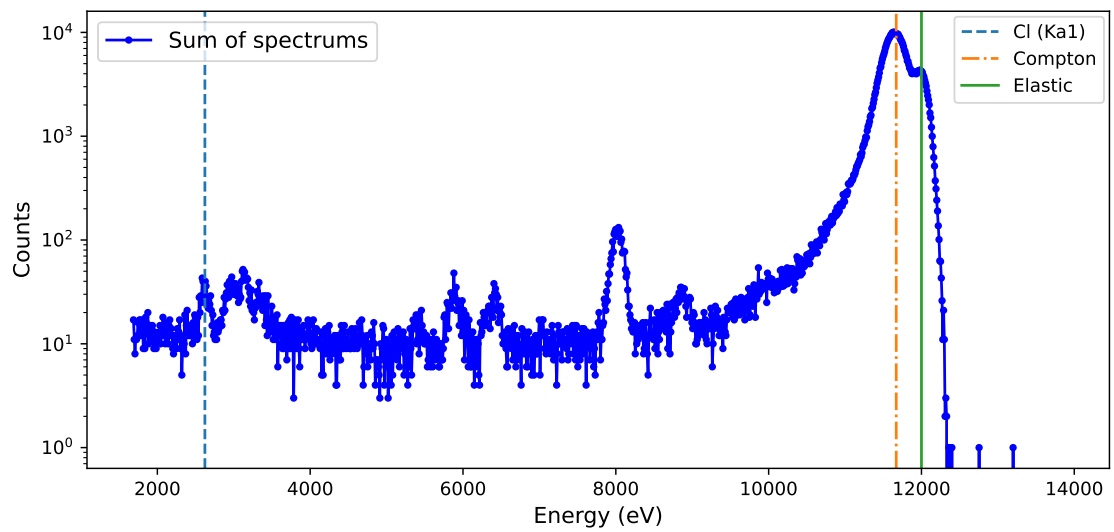
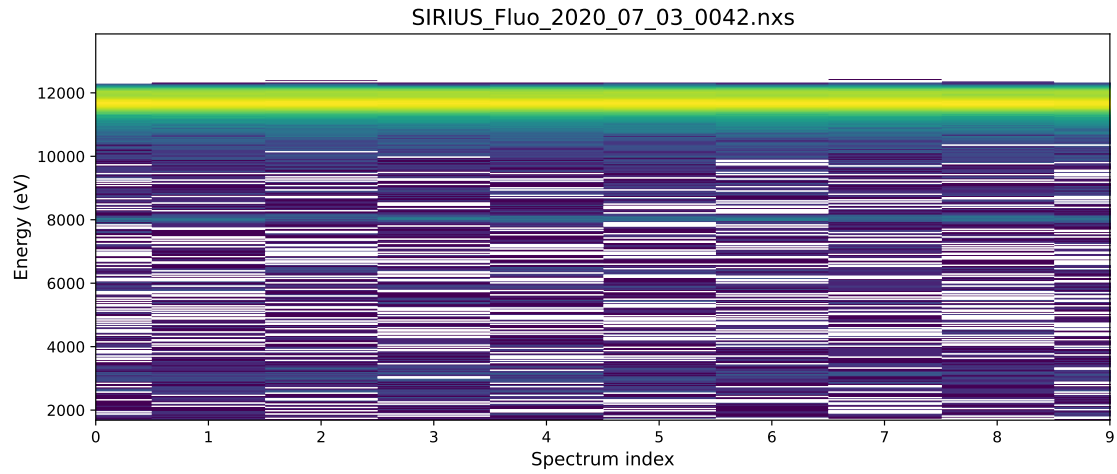
- Open Nexus Data File :

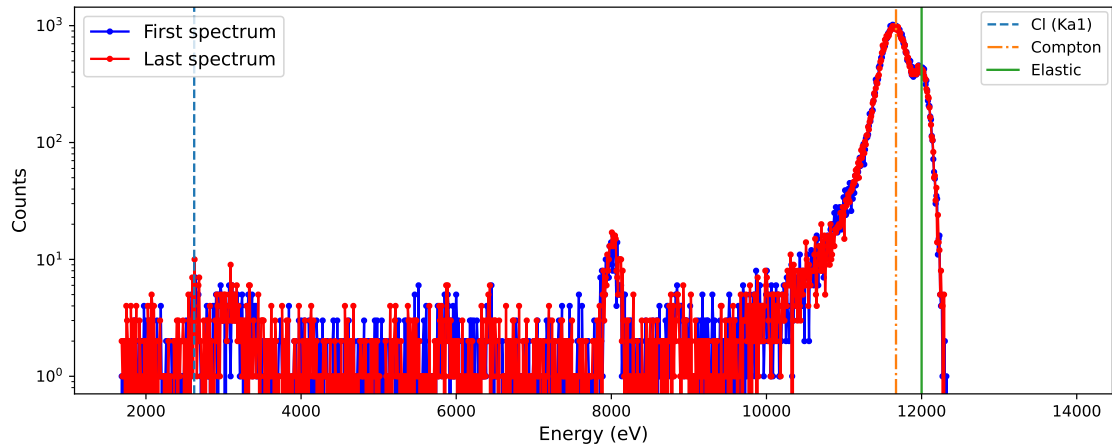
```
user/SIRIUS_Fluo_2020_07_03_0042.nxs
. Number of data points: 10
. Available Counters:
0 -----> ys
1 -----> zs
2 -----> xs
3 -----> surfacepressure
4 -----> areapermolecule
5 -----> fluo01
6 -----> fluo02
7 -----> fluo03
8 -----> fluo04
9 -----> fluoicr04
10 -----> fluoocr04
11 -----> fluospectrum04
```

```

12 -----> qxy
13 -----> integration_time
14 -----> sensorsRelTimestamps
15 -----> sensorsTimestamps
. Valid data between points 0 and 9
Starting time: 2020-07-03 11:01:00.235891
Ending time: 2020-07-03 11:05:34.198804
zs = -40.8671648075

```

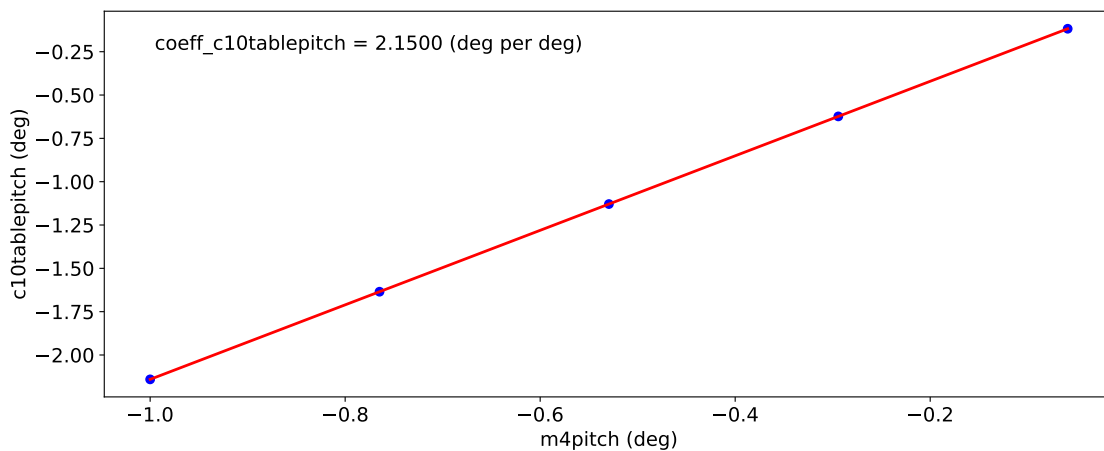


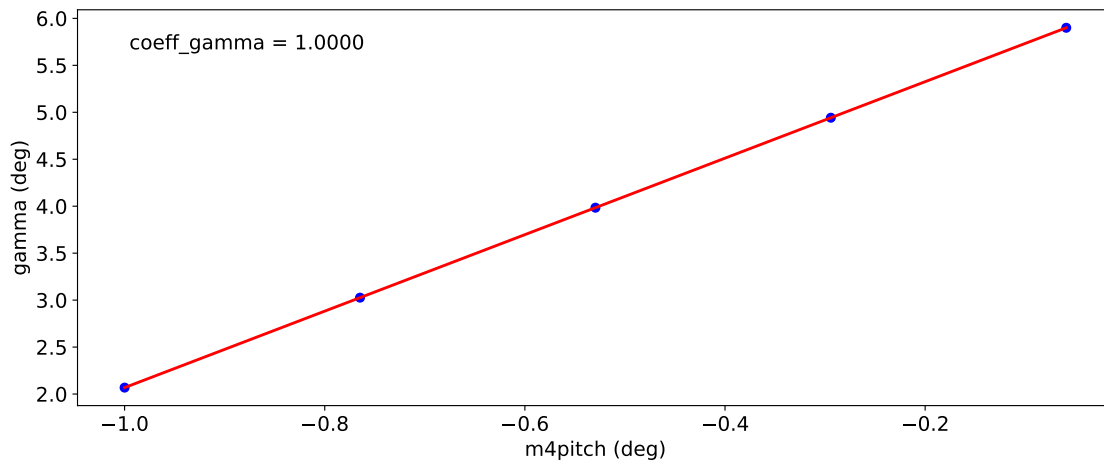
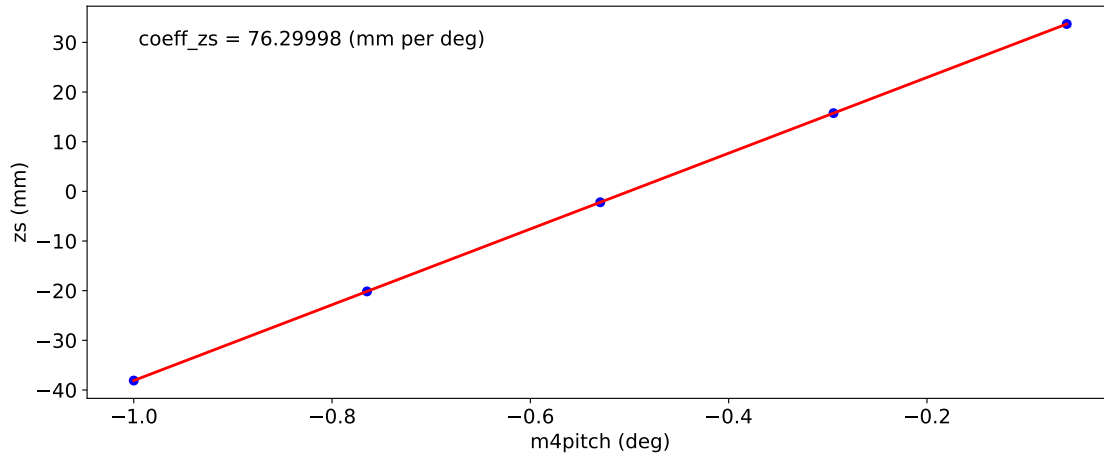


```
. Dat file saved in:
data/SIRIUS_Fluo_2020_07_03_0042.dat
. Spectrum(s) saved in:
data/SIRIUS_Fluo_2020_07_03_0042_fluospectrum*.mat
. Figure spectrogram saved in:
data/SIRIUS_Fluo_2020_07_03_0042_spectrogram.pdf
. Figure sum saved in:
data/SIRIUS_Fluo_2020_07_03_0042_sum.pdf
. Figure first/last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

11 XRR

11.1 Calibration XRR (liquid)



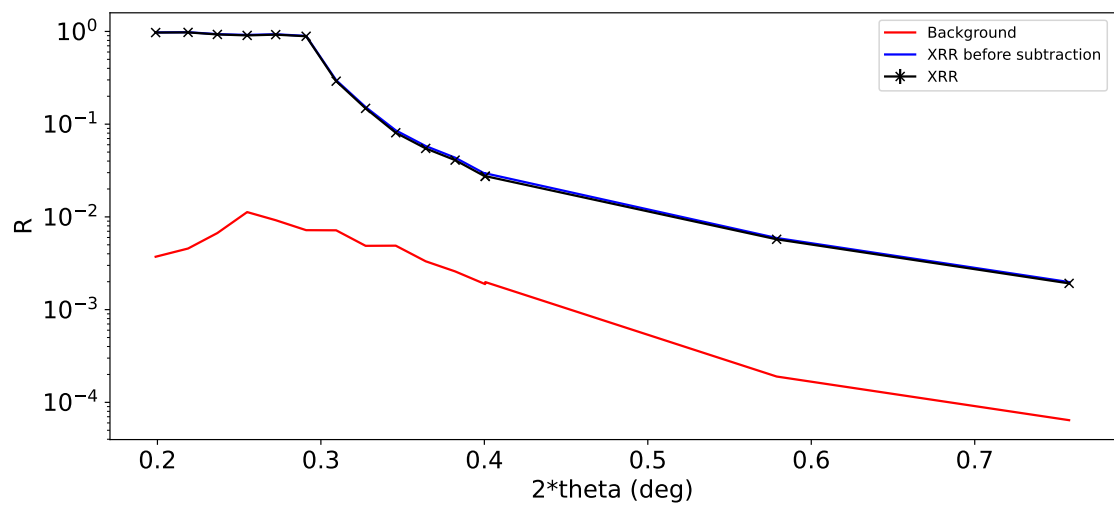
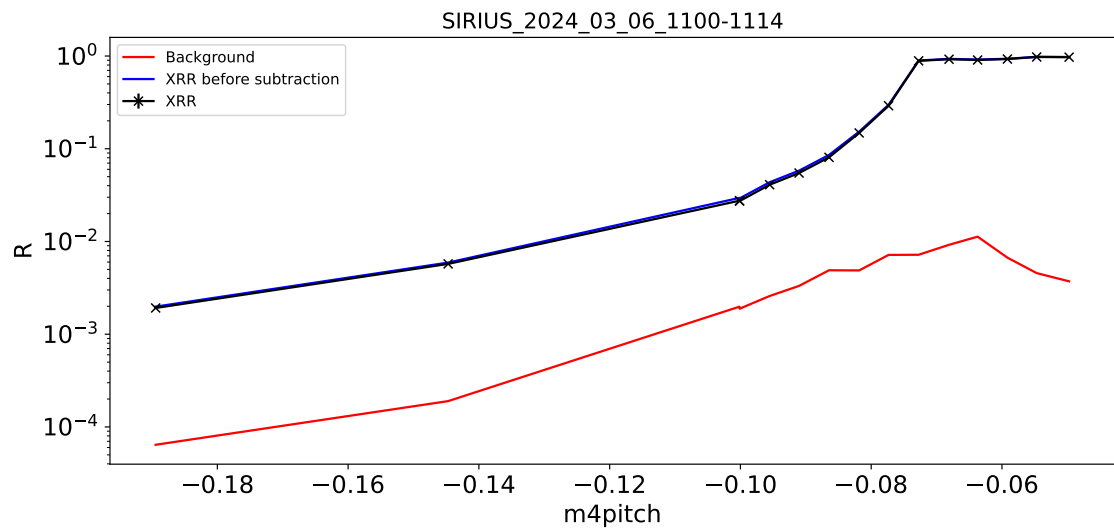


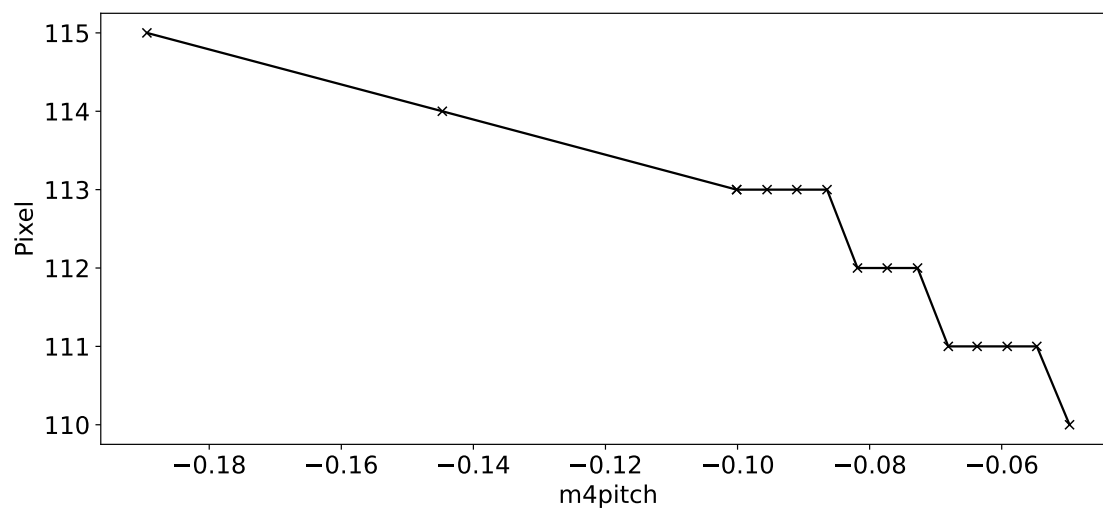
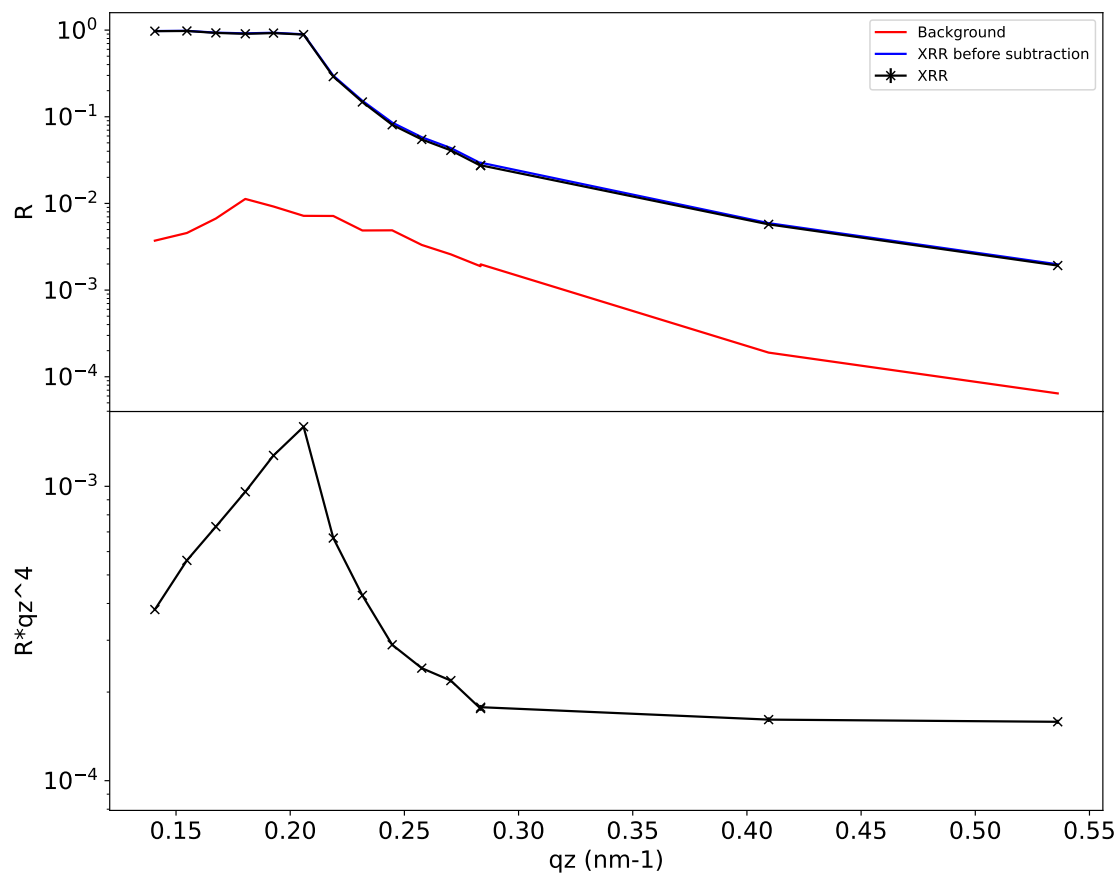
11.2 Scan XRR (liquid)

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!

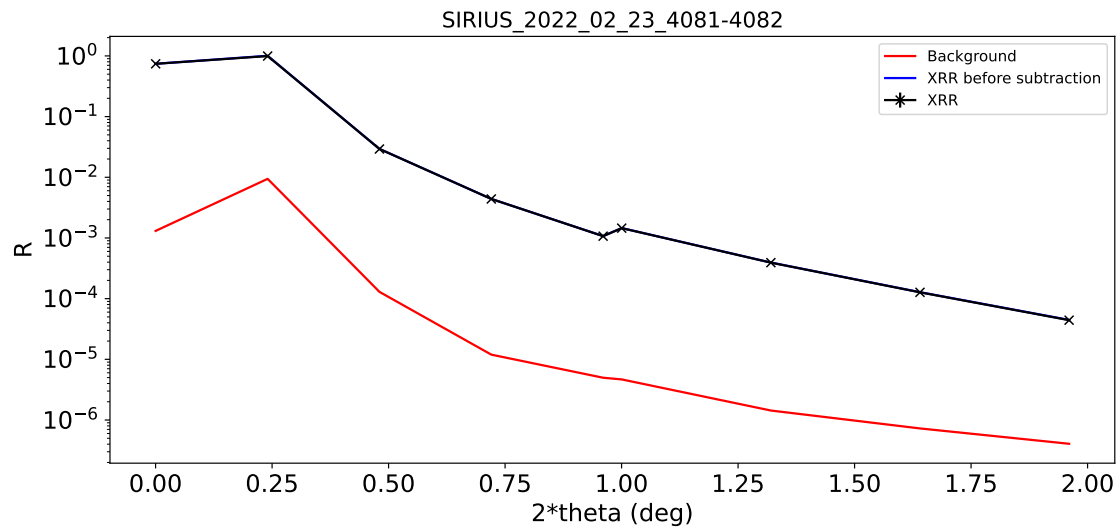
11.3 Scan XRR (solid)

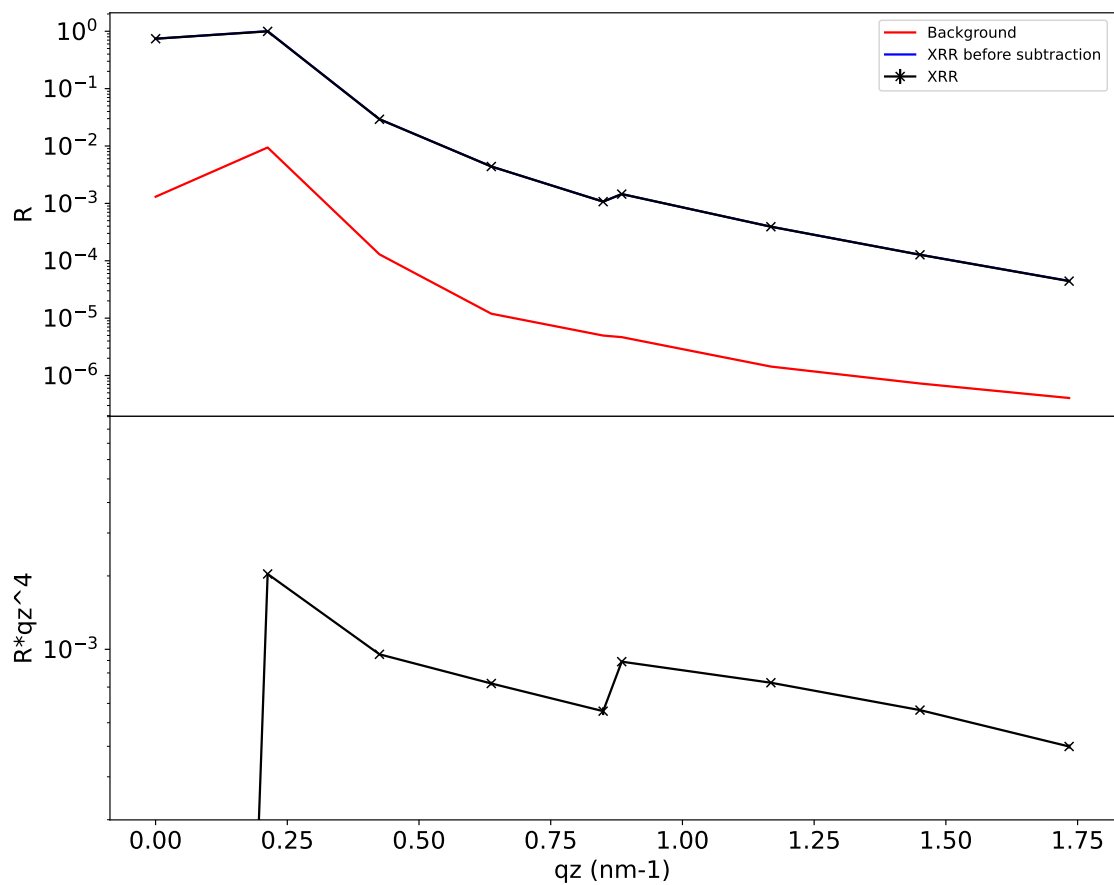
Select all the scans of the XRR series and click on Plot XRR (solid). Here we show only a few points for the example.

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!

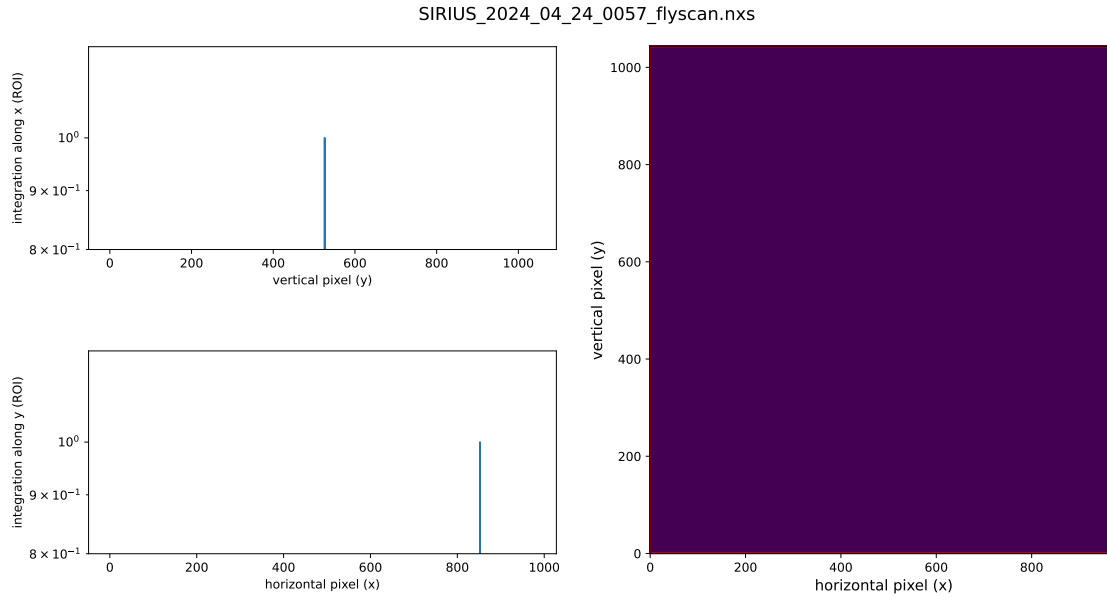
12 Flyscan

Extract a scan obtained using SOLEIL's flyscan.

12.0.1 SIRIUS_2024_04_24_0057_flyscan

mon2 = 0.10676705278456211

zs = -42.293922177499994



13 Insert script

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

13.0.1 script_with_loop.ipy

```
%shopen
%amove delta -40
%run reset_motors.ipy
%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.ipy
    %run cont_regh_abs.ipy #127 #129 #131 #133

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

    #%run cont_regh_abs.ipy
    %run cont_regh_abs.ipy #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

```

14 Insert positions

14.0.1 wm alphax gamma

alphax	gamma
0.0266	0.0002

14.0.2 wm gamma

gamma
19.9999

15 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

```

16 Save/load params

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

17 Export

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

This is a big remark.

And here is a small remark.