

Example

February 5, 2022

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1 Experimental setup

SIRIUS Beamline : Experiment 1234

Example

- Type: Proposal
- Safety: Yellow
- Date: 11/06/21-12/06/21
- Main proposer: Hemmerle
- Local contact: Arnaud
- Users (on site): Person 1, Person 2, Person 3, Person 4
- Machine:
 - Current: 450 mA
 - Mode: 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: 12
 - Polarisation: LH
 - Phase (deg): 0
 - Horizontal focalisation: False
 - Vertical focalisation: True
 - Horizontal beamsize (mm): 2
 - Vertical beamsize (mm): 0.5
- Monitors and XBPM:
 - mon1:
 - mon2:
 - mon3:
 - mon4: thick diamond
 - Detectors: None
- Remarks: This is an example.

2 Beamline alignment

Here we show functions used during beamline alignment.

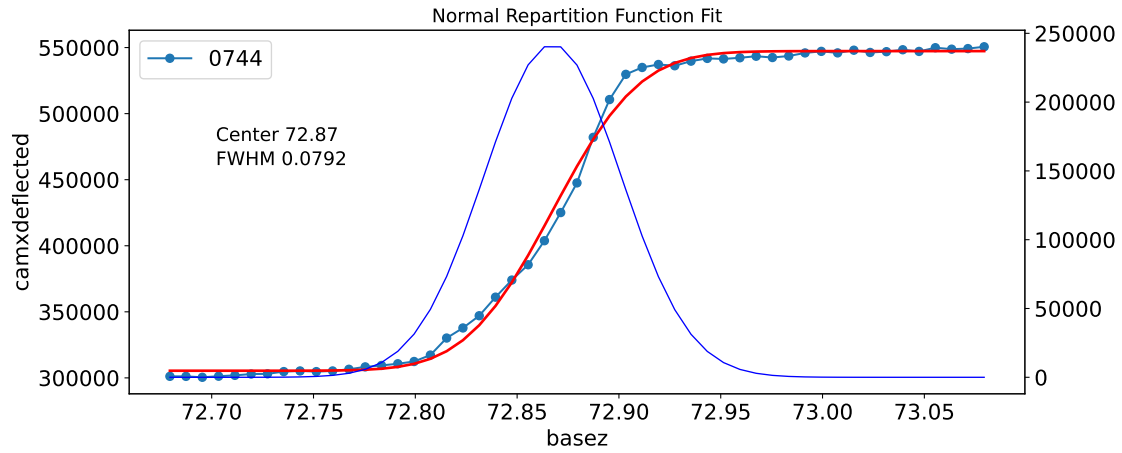
LaTeX formula can be used in the text:

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

2.1 Subsection

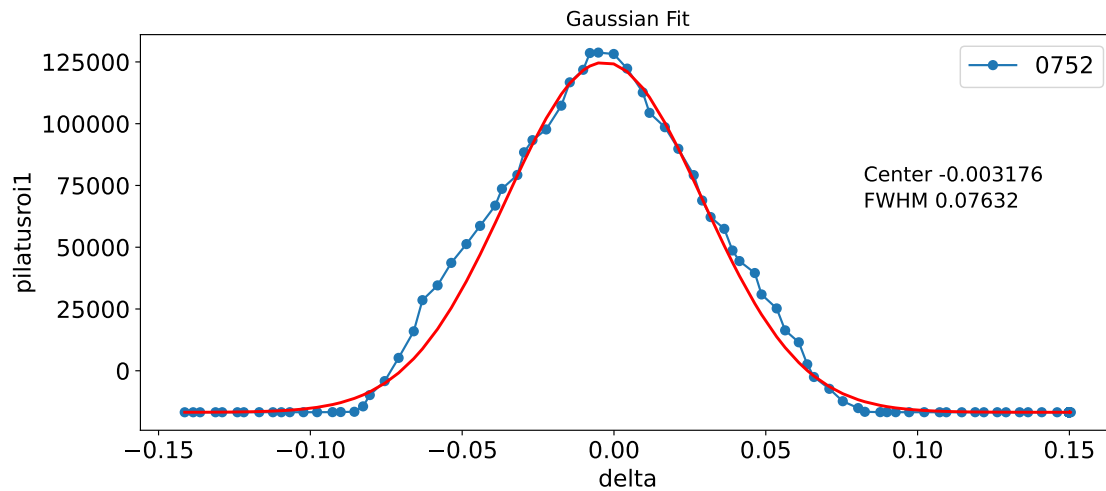
Fit with erf function.

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

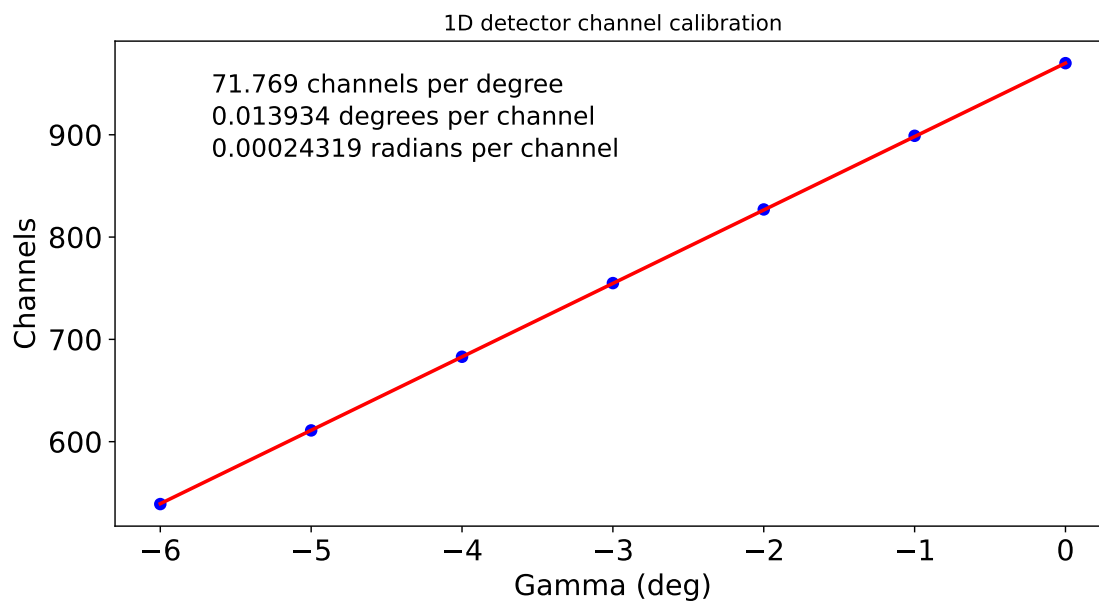


Fit with Gaussian function.

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



2.2 Calibration thetaz



3 GIXD

Extraction of the Yoneda-Vineyard peak.

3.0.1 SIRIUS_2020_03_12_0756: continuous_ascan delta -24 -19 100 5

- Open Nexus Data File :

recording/SIRIUS_2020_03_12_0756.nxs

. Number of data points: 101

. Available Counters:

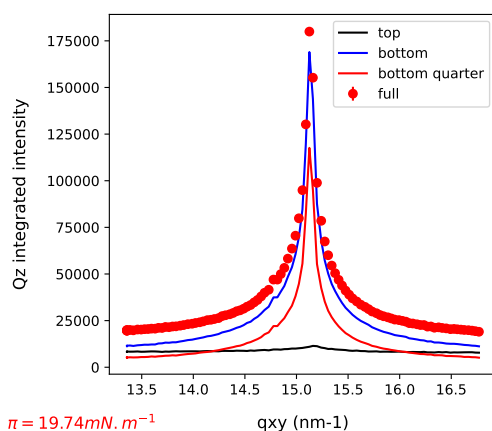
0	----->	delta
1	----->	zs
2	----->	gamma
3	----->	hu36energy
4	----->	xs
5	----->	energydcm
6	----->	current
7	----->	mon2
8	----->	surfacepressure

```

9 -----> areapermolecule
10 -----> qxy
11 -----> pilatus
12 -----> pilatusroi1
13 -----> integration_time
14 -----> sensorsRelTimestamps
15 -----> sensorsTimestamps
. Pilatus data found, (column 11, alias pilatus)
. qxy data found, (column 10, alias qxy)
. Valid data between points 0 and 100
. Surface pressure data found, mean value  $19.74 \pm 0.006119$  mN/m
. Area per molecule data found, mean value  $0.3557 \pm 3.944e-05$  nm2 per
molecule
. Gamma motor data found, mean value  $-0.0004471$  deg

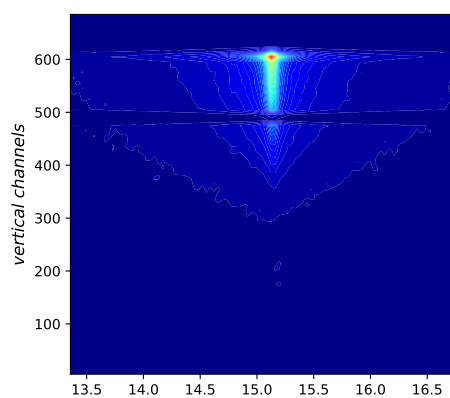
```

SIRIUS_2020_03_12_0756.nxs



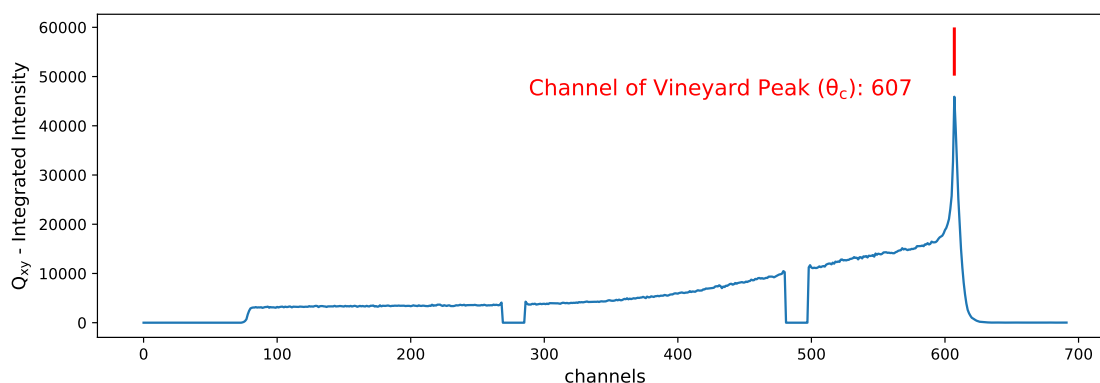
$\pi = 19.74 \text{ mN} \cdot \text{m}^{-1}$

qxy (nm-1)



qxy (nm-1)

$\gamma = -0.0004471 \text{ deg}$



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

Channel0: 607

3.0.2 SIRIUS_2020_03_12_0756: continuous_ascan delta -24 -19 100 5

- Open Nexus Data File :

recording/SIRIUS_2020_03_12_0756.nxs

. Number of data points: 101

. 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
```

. Pilatus data found, (column 11, alias pilatus)

. qxy data found, (column 10, alias qxy)

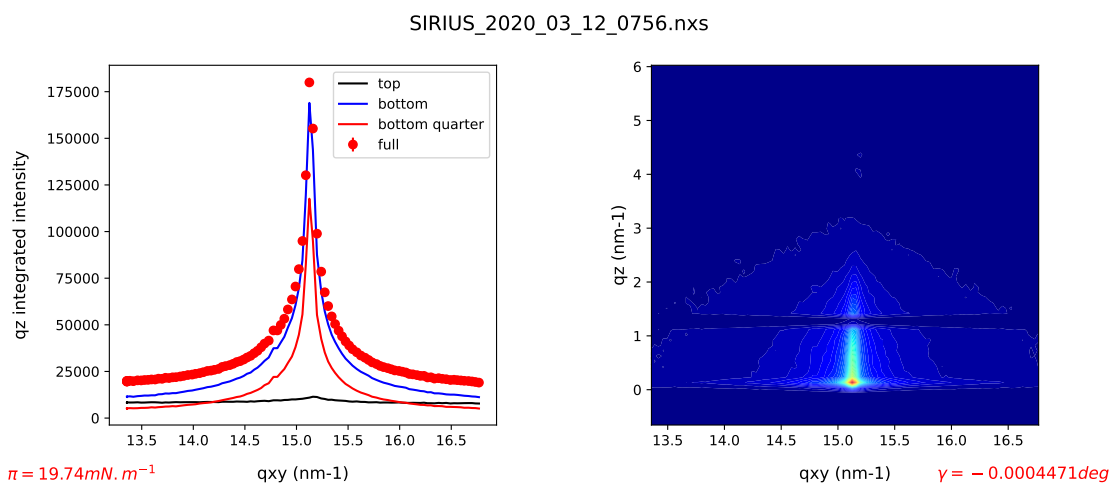
. Valid data between points 0 and 100

. Surface pressure data found, mean value 19.74 ± 0.006119 mN/m

. Area per molecule data found, mean value $0.3557 \pm 3.944e-05$ nm² per molecule

. Gamma motor data found, mean value -0.0004471 deg

Absorbers: 29 - Vide



```

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

```

Classic GIXD with:

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

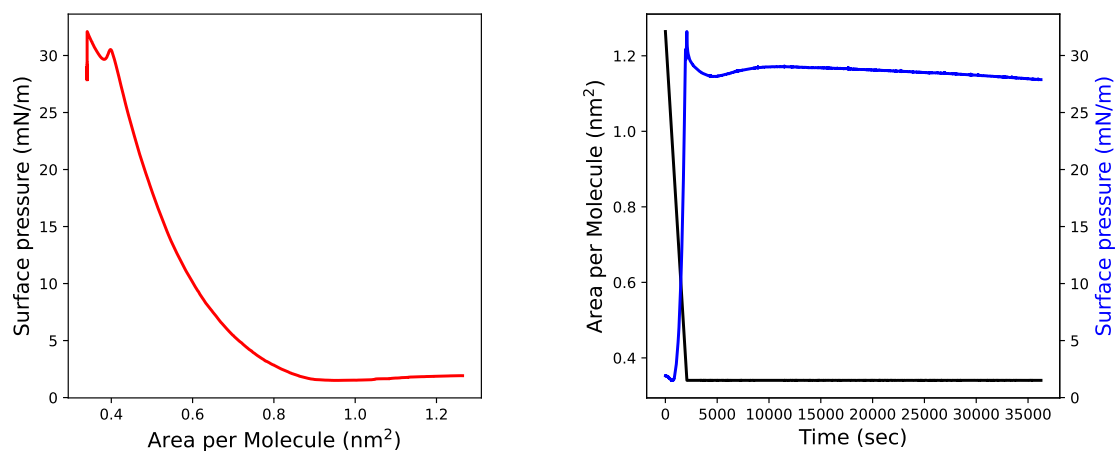
Generates:

- 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 Isotherm

4.0.1 SIRIUS_Isotherm_2019_02_17_01544: isotherm 1.97 46 35000 1

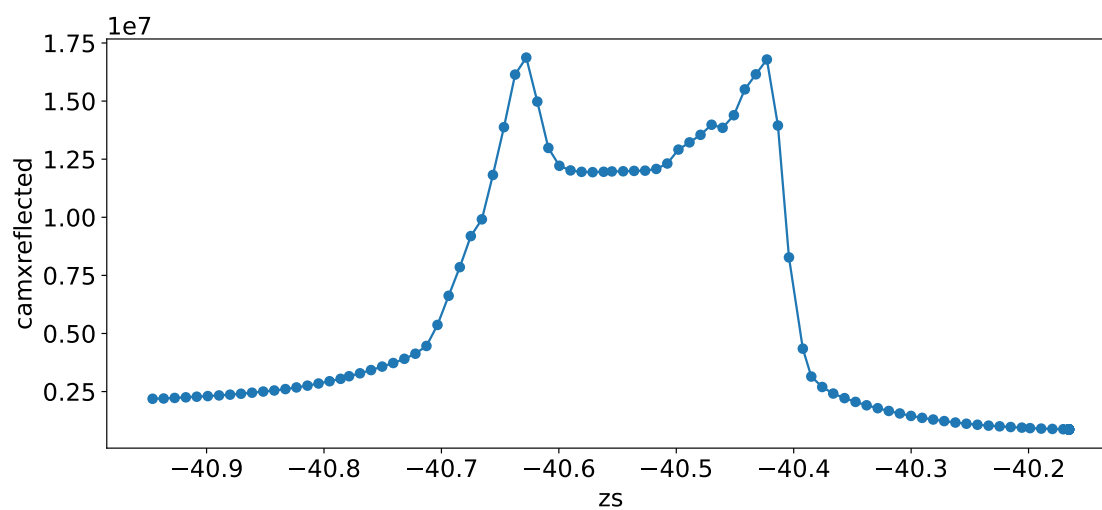
SIRIUS_Isotherm_2019_02_17_01544



5 1D plot

Add a 1D plot by clicking on Add plot to report. Generates SIRIUS_2020_03_12_0760.dat

5.0.1 SIRIUS_2020_03_12_0760: run cont_regh.ipy



6 GIXS

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

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

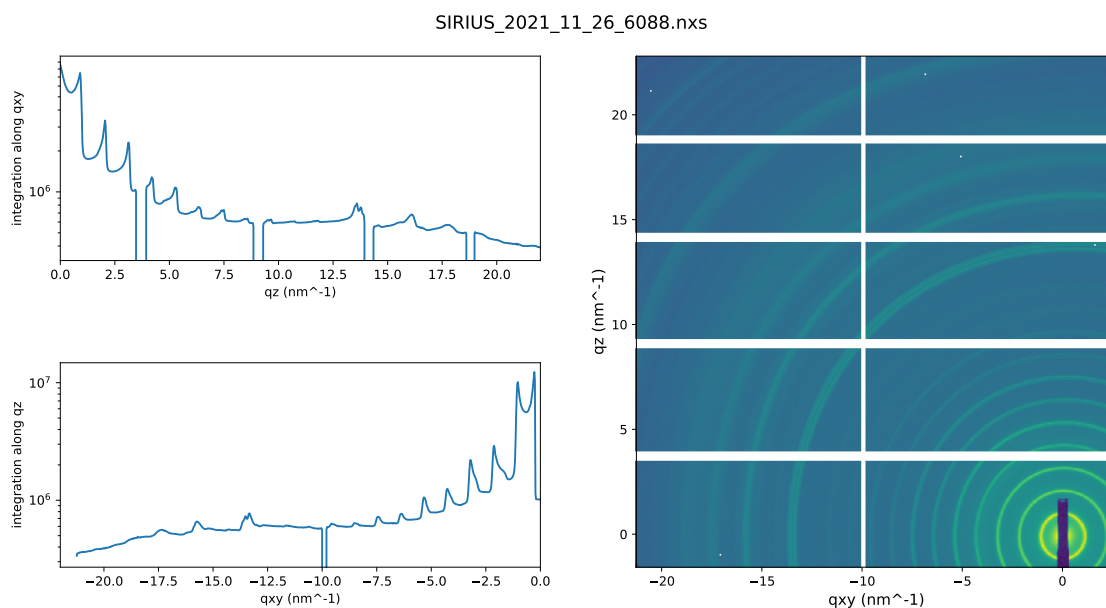
6.0.1 SIRIUS_2021_11_26_6088: tscan 5 5

Absorbers: 29 - Vide

gamma found: gamma = -0.9997 deg

delta found: delta = -8.875 deg

thetai is forced to the value: thetai = 0 deg



GIWAXS on a P3HT film.

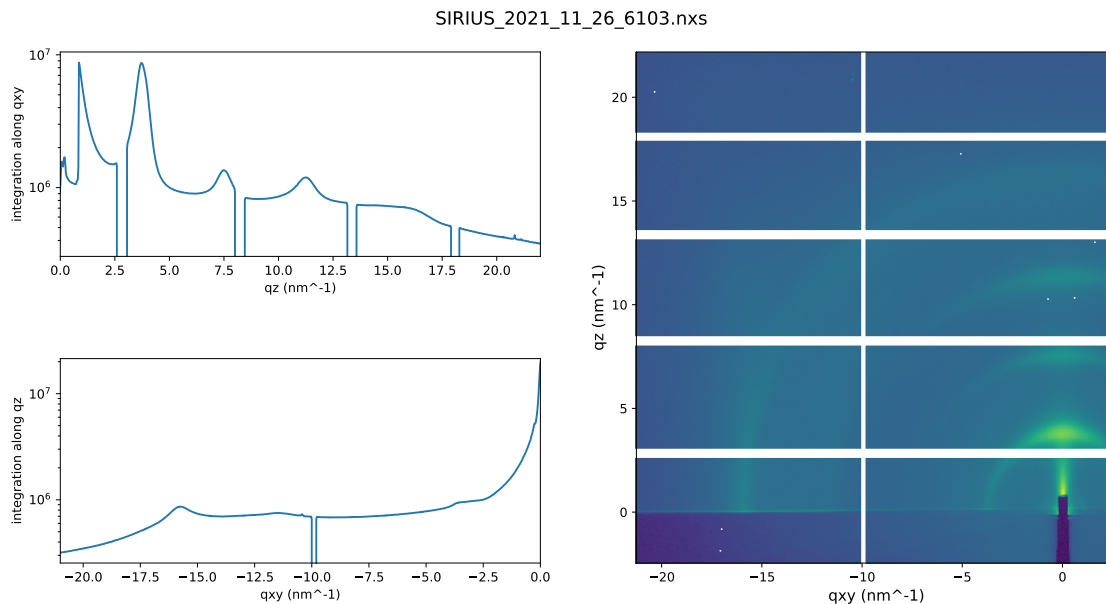
6.0.2 SIRIUS_2021_11_26_6103: tscan 10 10

Absorbers: 29 - Vide

gamma found: gamma = -2 deg

delta found: delta = -8.875 deg

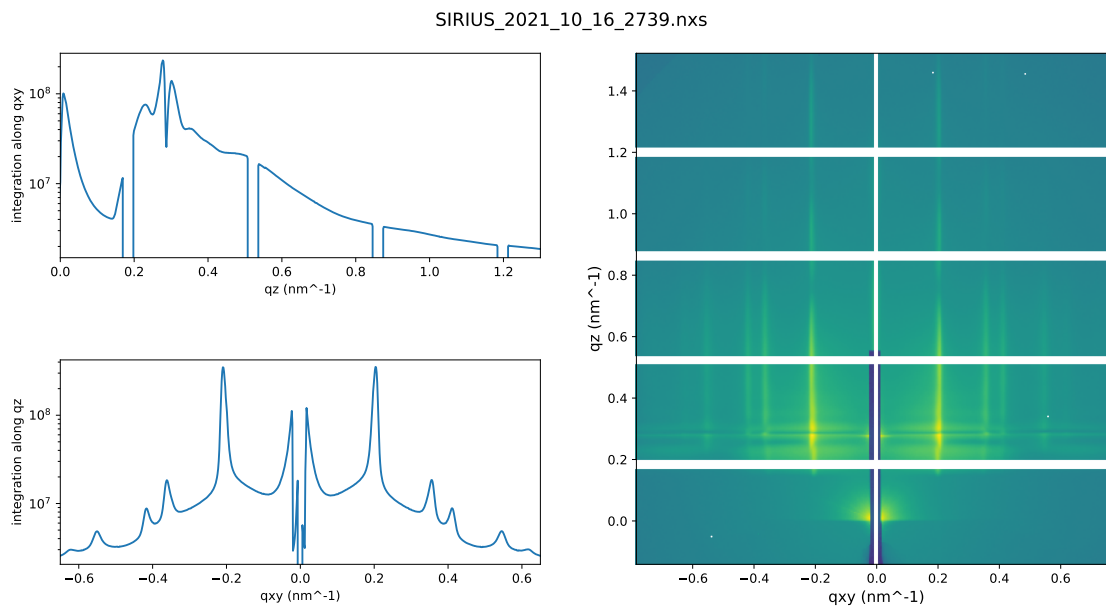
thetai (alphax) found: thetai = 0.1 deg



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

6.0.3 SIRIUS_2021_10_16_2739: run scan_0_18.ipy

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



7 Plot 2D detector

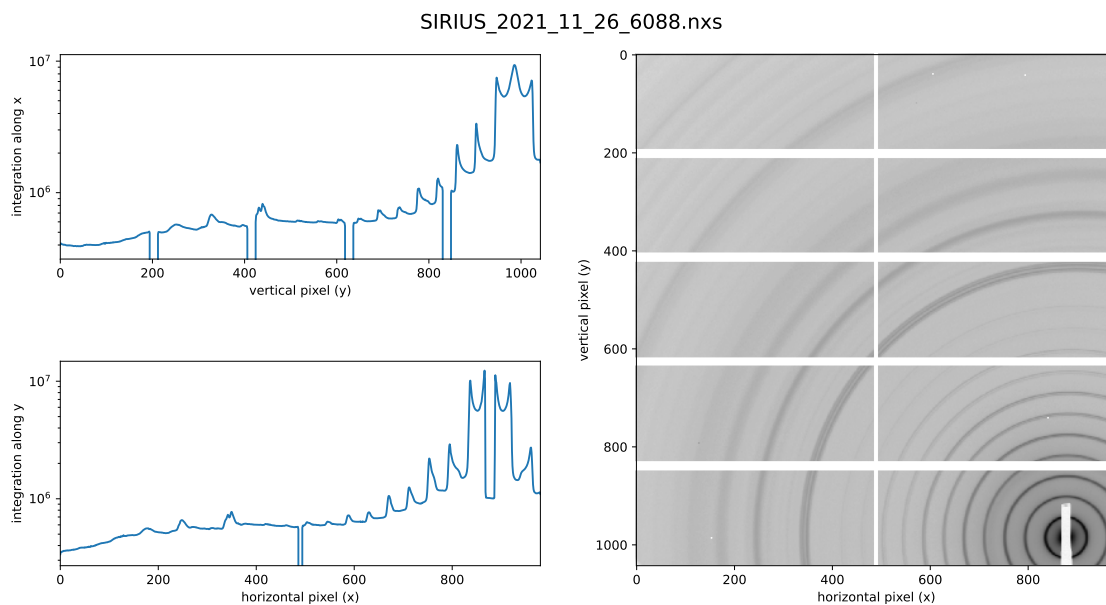
Plot the sum of the images from a 2D detector. Can also extract and save all the individual images if `save='all'`.

Here with the 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

7.0.1 SIRIUS_2021_11_26_6088: tscan 5 5



Works also with the detector UFXC.

7.0.2 SIRIUS_2021_11_11_3728: tscan 2 9

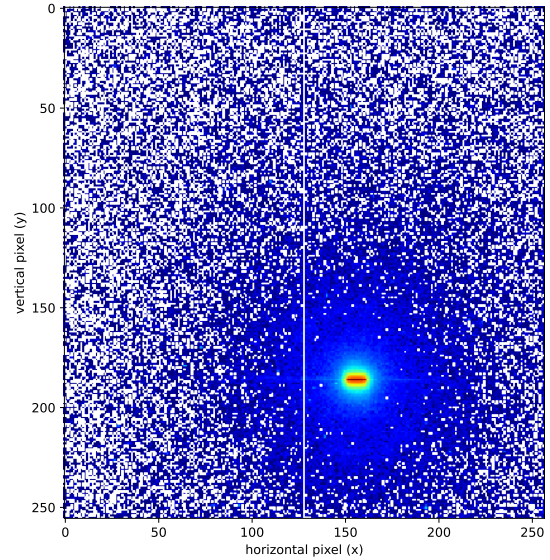
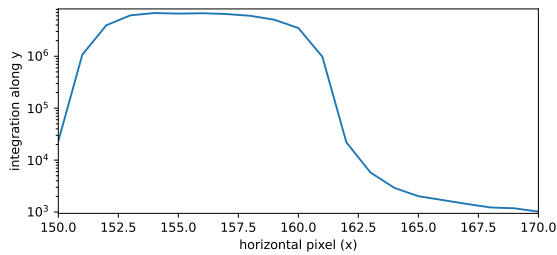
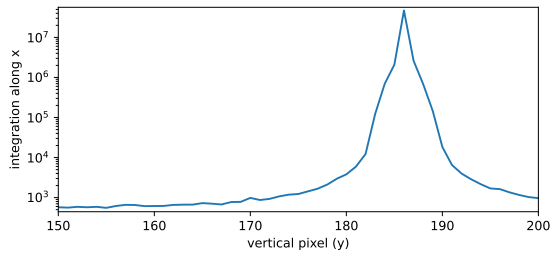
```
. Available Counters:  
0 -----> delta  
1 -----> shg
```

```

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

```

SIRIUS_2021_11_11_3728.nxs



8 XRF

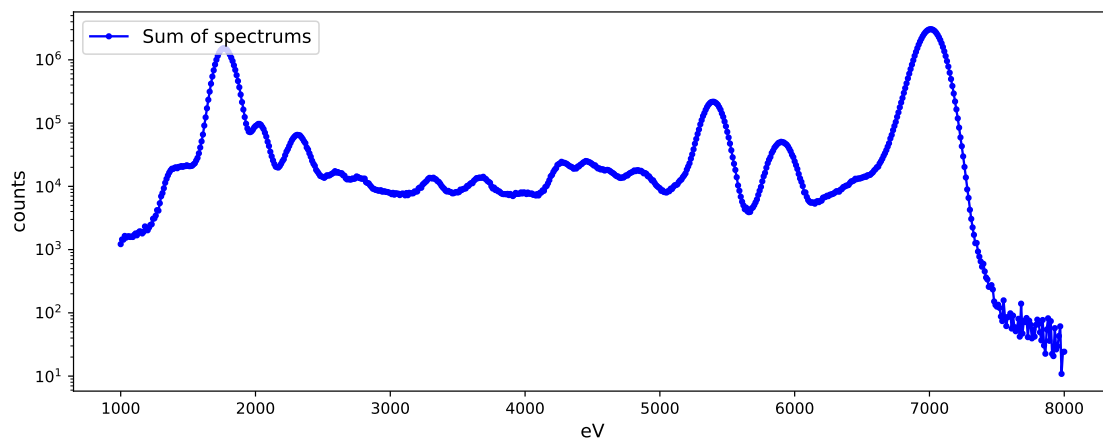
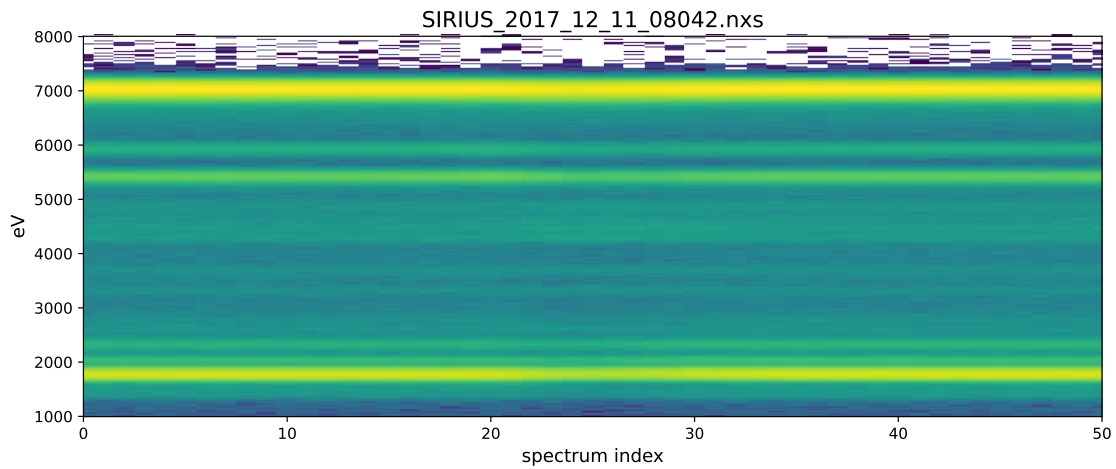
Plot XRF from the 4-elements detector, in channels and without peak identification.

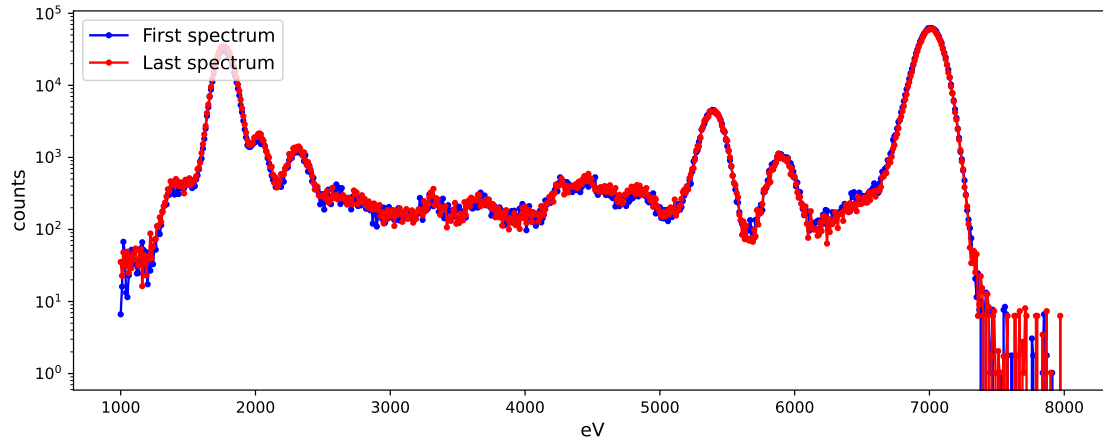
Generates:

- SIRIUS_2017_12_11_08042_fluospectrum.mat for each element
- SIRIUS_2017_12_11_08042.dat

8.0.1 SIRIUS_2017_12_11_08042: run xsw7.ipy

Absorbers: Al 200micron





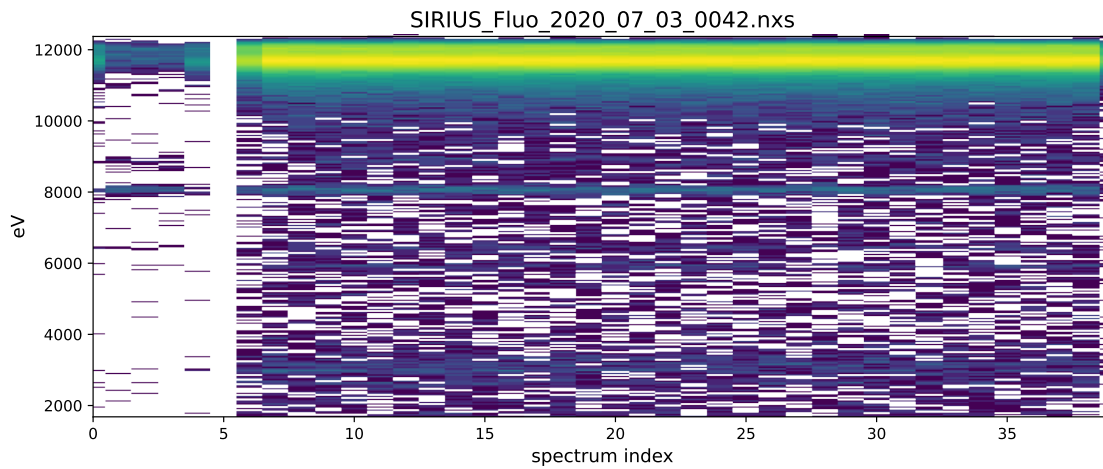
Plot XRF from the 1-element detector, in eVs and with peak identification.

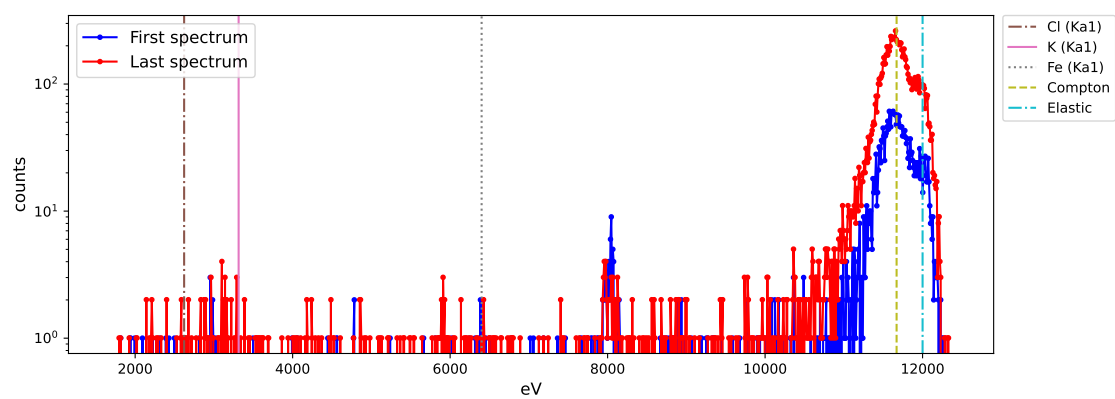
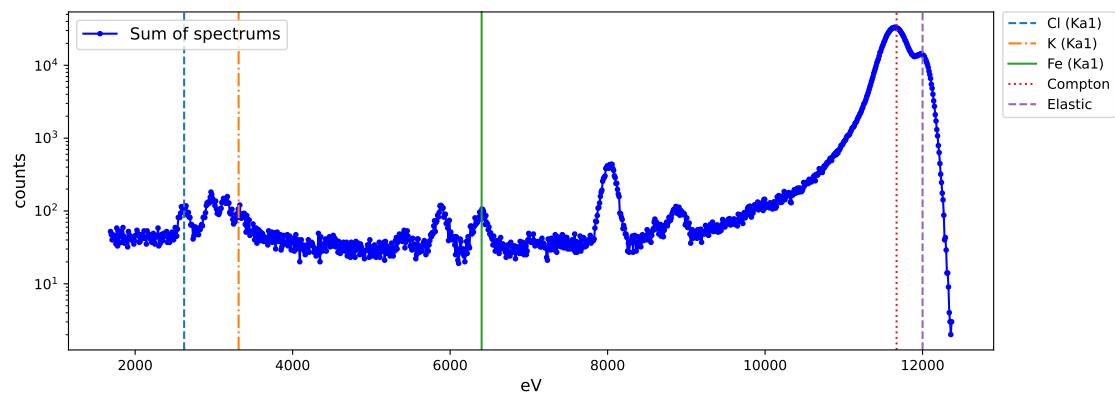
Generates:

- SIRIUS_Fluo_2020_07_03_0042_fluospectrum04.mat
- SIRIUS_Fluo_2020_07_03_0042.dat

8.0.2 SIRIUS_Fluo_2020_07_03_0042: tscan 500 30

Absorbers: Al 800micron

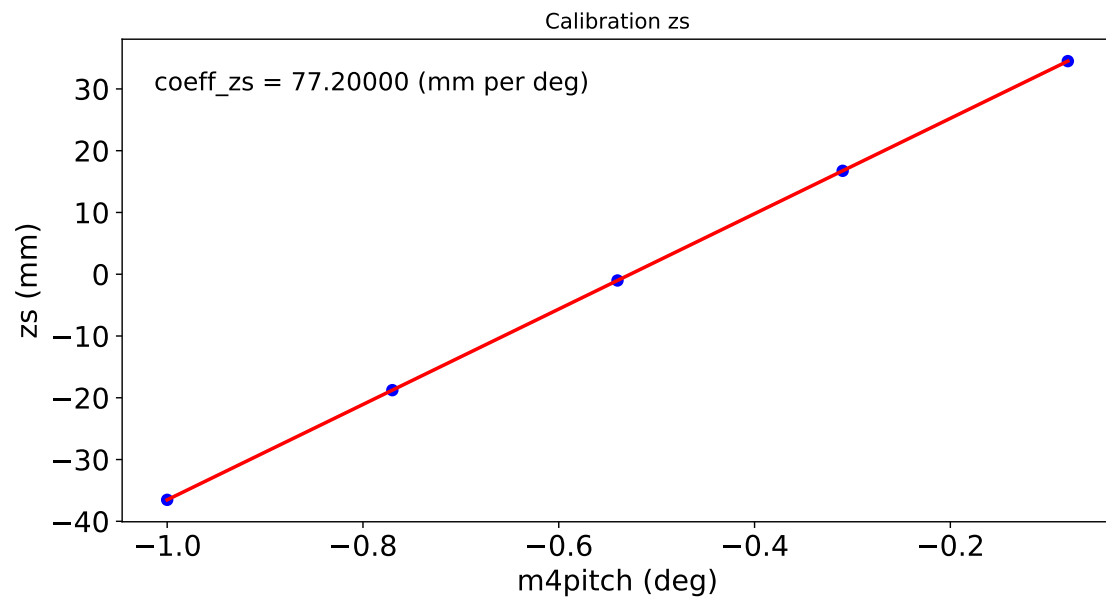
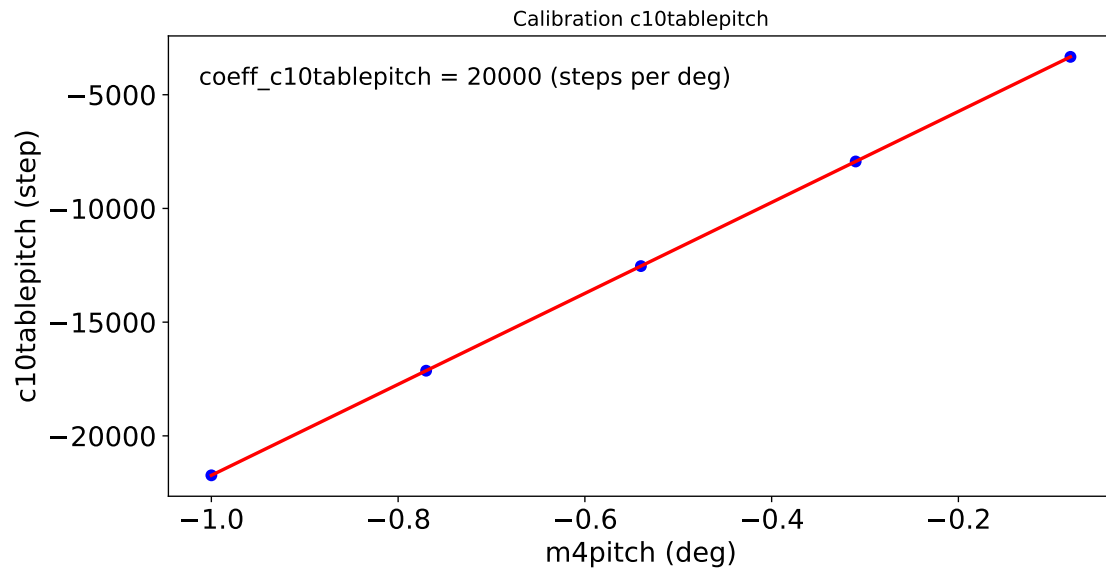


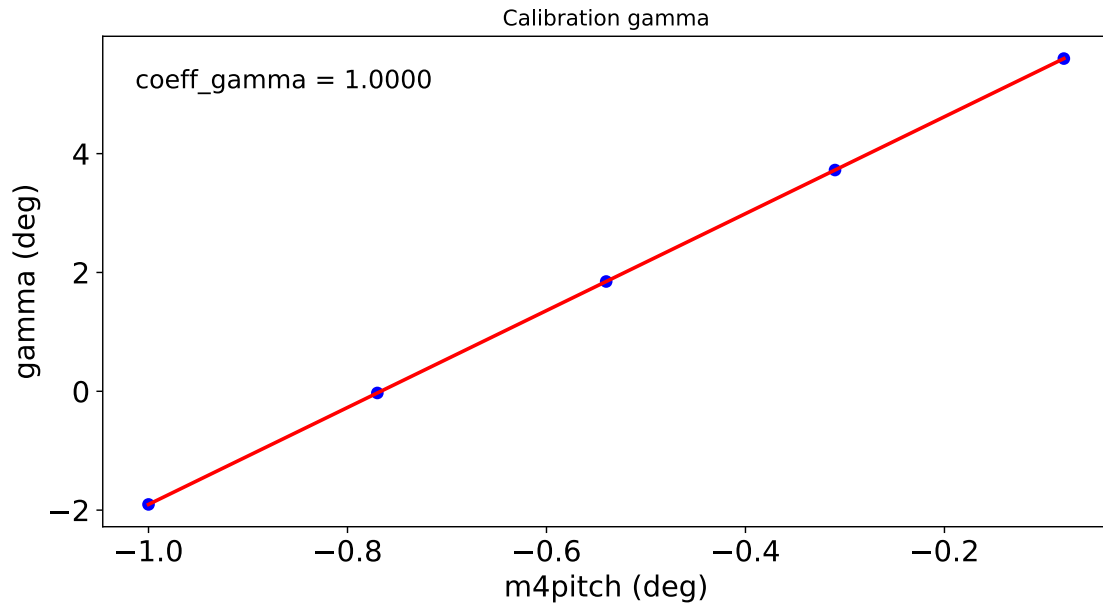


9 XRR

To start the calibration click on Calib. XRR.

9.1 Calibration XRR



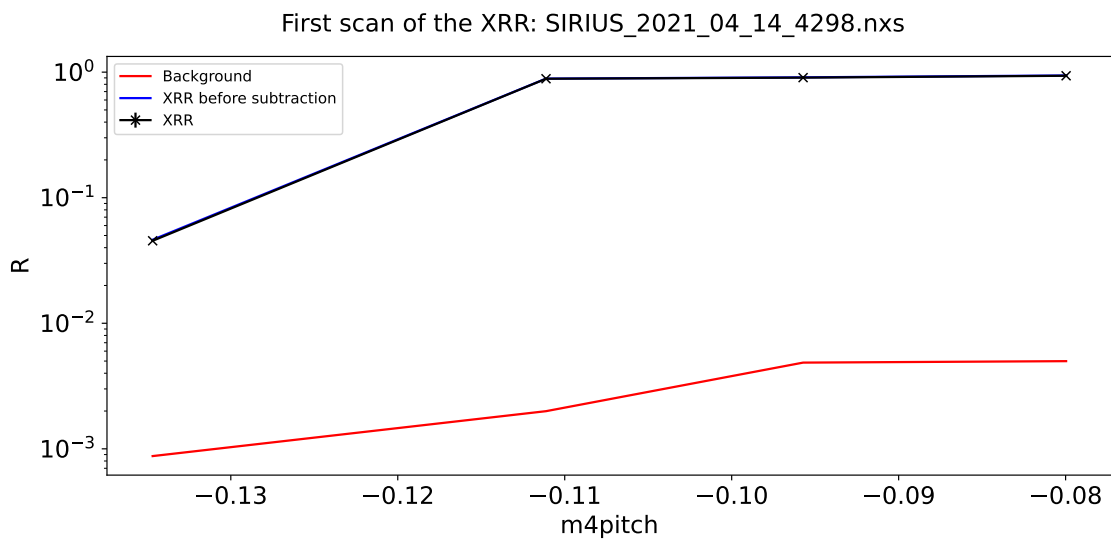


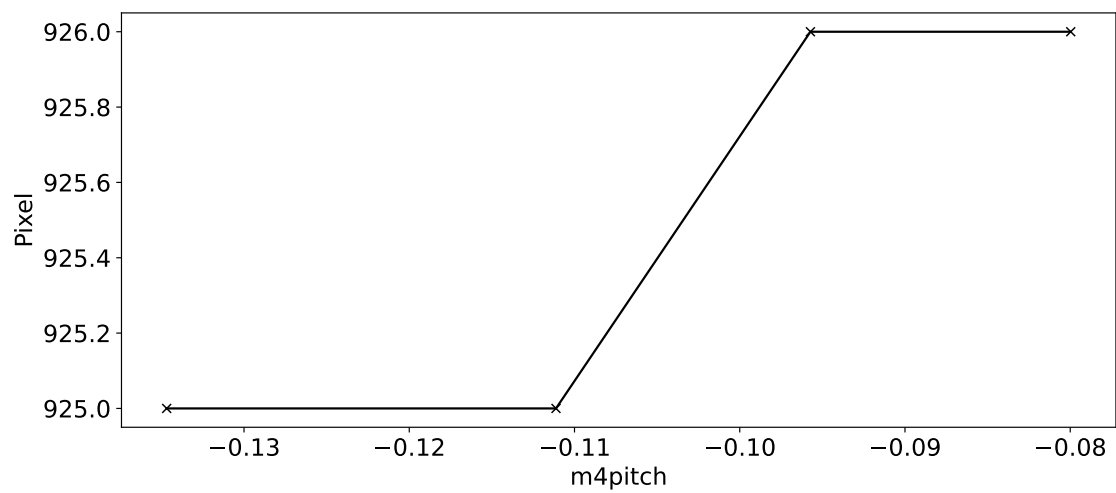
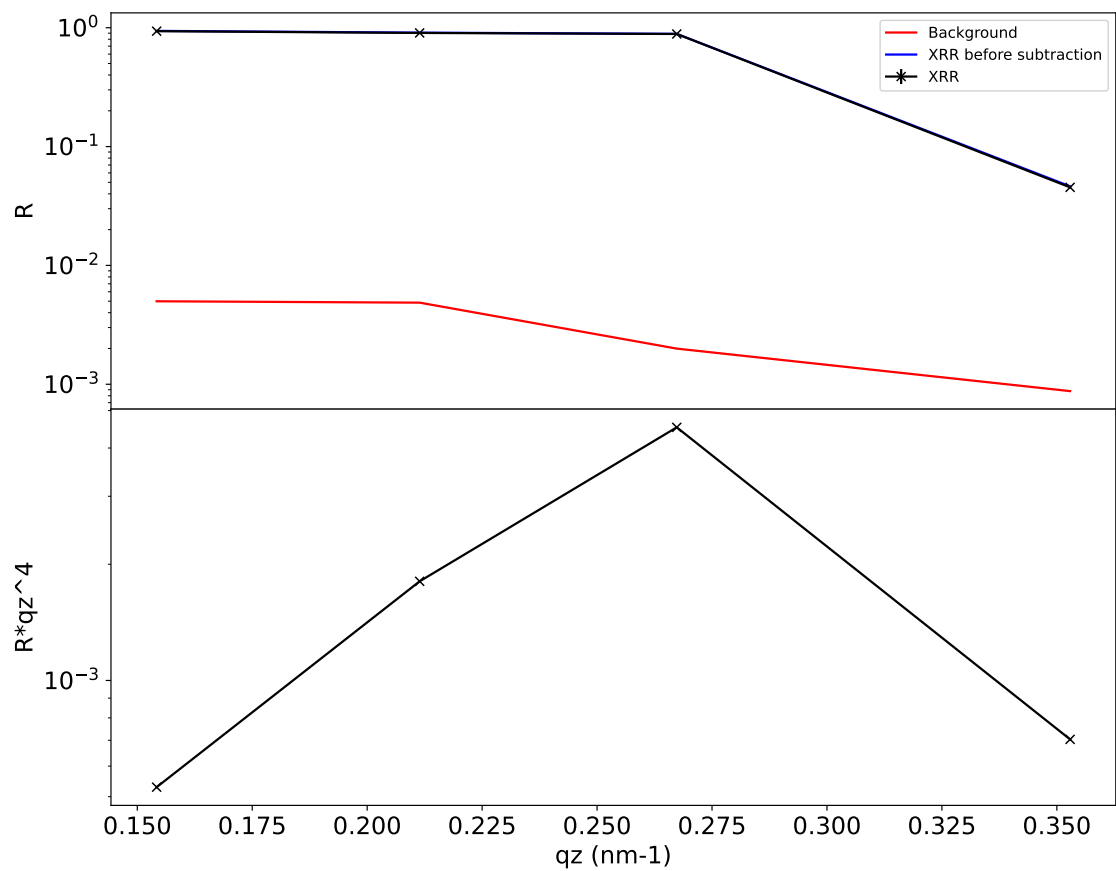
9.2 Scan XRR

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

9.2.1 SIRIUS_2021_04_14_4298: No command found

Direct extracted from SIRIUS_2021_04_14_4297.nxs: direct=2.44387e+12





10 Insert script

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

10.0.1 script_with_loop.ipy

```
%shopen
%amove delta -40
%run reset_motors.ipy
%continuous_ascan delta -35 -25 250 5 #123
%tscan 10 10 #124

for i in range(4):
    %amove delta -20
    %continuous_ascan delta -10 -3 175 5 #125 #127 #129 #131
    %run reset_motors.ipy
    %run cont_regh_abs.ipy #126 #128 #130 #132

for i in range(3):
    %amove delta -20
    %dscan delta -10 -3 175 5 #133 #135 #137
    %run reset_motors.ipy

    #%run cont_regh_abs.ipy
    %run cont_regh_abs.ipy #134 #136 #138

for i in range(2):
    %amove delta -20
    %tscan 10 100 #139 #140
    %slist scan add camxdirect

%continuous_ascan delta -35 -25 250 5 #141
# %tscan 10 10
%shclose
```

11 Insert positions

Positions extracted from the logs, using `Insert positions`.

11.0.1 wm alphax gamma

alphax	gamma
2.0679	4.1401

11.0.2 wm diffracto

deltacodeur	euchi	euth	euphi	kappa_h	kappa_k
Degrees	1.00196 deg	-89.57961 deg	90.42039 deg	-0.00580	-0.08252

kappa_l	qxy	qxy0	qz	basexPoint	basexTrait
-0.18486	2.0556 nm-1	23.82 nm-1	-0.92 nm-1	-15.7275	-15.7274

basezPlan	basezPoint	basezTrait	basepitch	baseroll	basex
71.1257	71.1257	71.1257	-0.0000 mrad	0.000 mrad	-15.727 mm

baseyaw	basez	alphax	alphay	delta	delta0
-0.000 mrad	71.126 mm	0.2998	0.2000	-2.9110	-34.2322

deltaa	etaa	gamma	kappav	mu	kphi
0.0000	0.0000	1.2997	1.3080	-179.9997	0.0000

thetaa	thetah	komega	xs	ky	ys
0.0000	0.0185	0.0000	0.0000	-0.1000	0.0000

kz	zs	kx
0.0000	-41.9999	-0.1000

12 Insert commands

Commands extracted from the logs, using `Insert commands`.

```
Fri, 26 Nov 2021 14:13:34 ct 1 pilatus
Fri, 26 Nov 2021 14:13:56 tscan 10 10 #6109
```

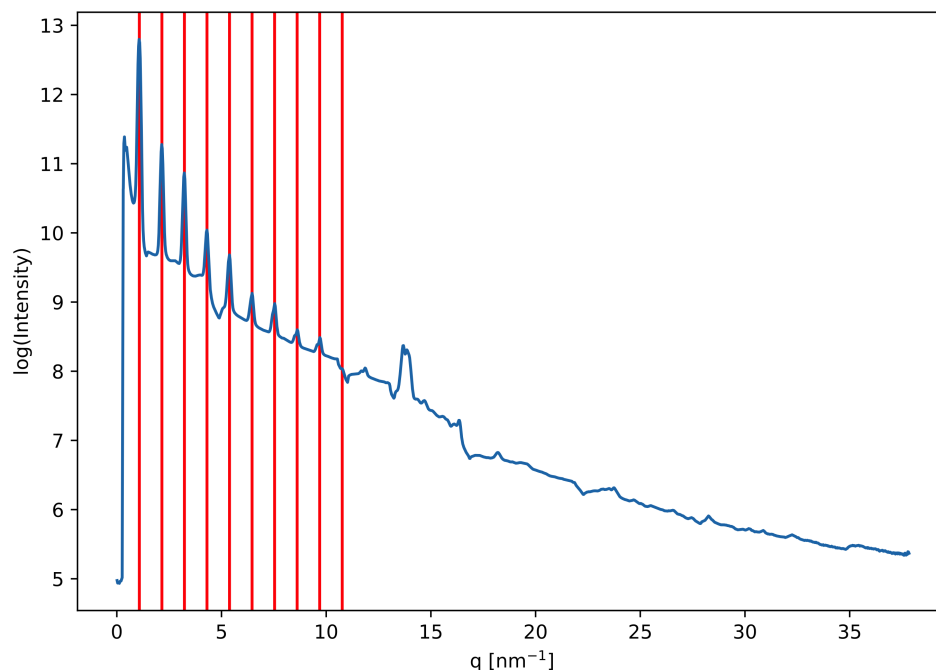
```
Fri, 26 Nov 2021 14:17:29 shclose  
Fri, 26 Nov 2021 14:26:40 run config_alignment.ipyn  
Fri, 26 Nov 2021 10:34:48 ct 1 pilatus
```

13 Convert logs

Human-readable logs generated in the folder `/working/readable_logs/` by clicking on **Convert logs**.

14 Insert an image

Using the command `Insert image`.



15 Save/load state

Save the current state of the notebook (the variable `expt`) by clicking on **Save state**.

Load the previous state of the notebook by clicking on **Load state**(for example after creating a new notebook).

16 Insert text

Use the button `Insert text` to insert text into the report.

17 Export to pdf

PDF generated by clicking on `Export to pdf`.