

Example

May 27, 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

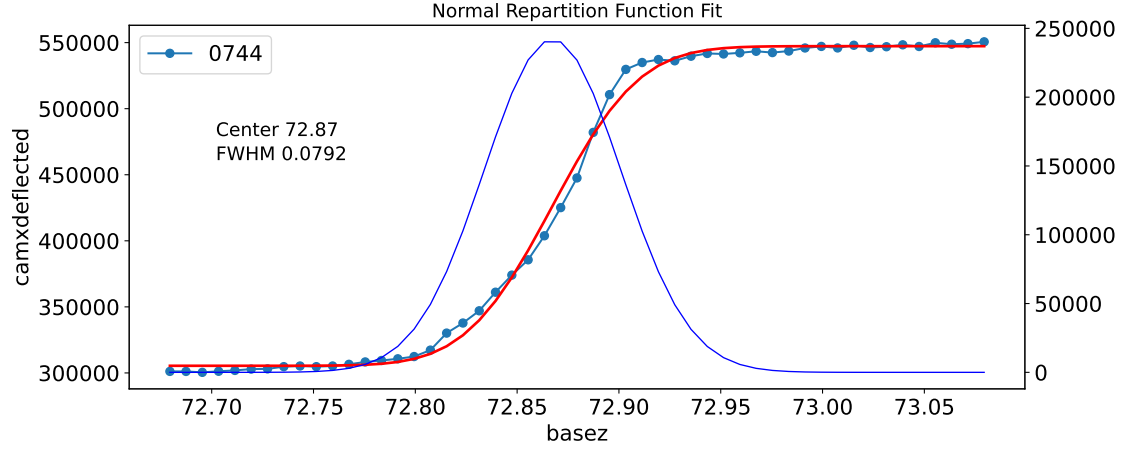
Here we show functions used during beamline alignment.

LaTeX formula can be used in the text:

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

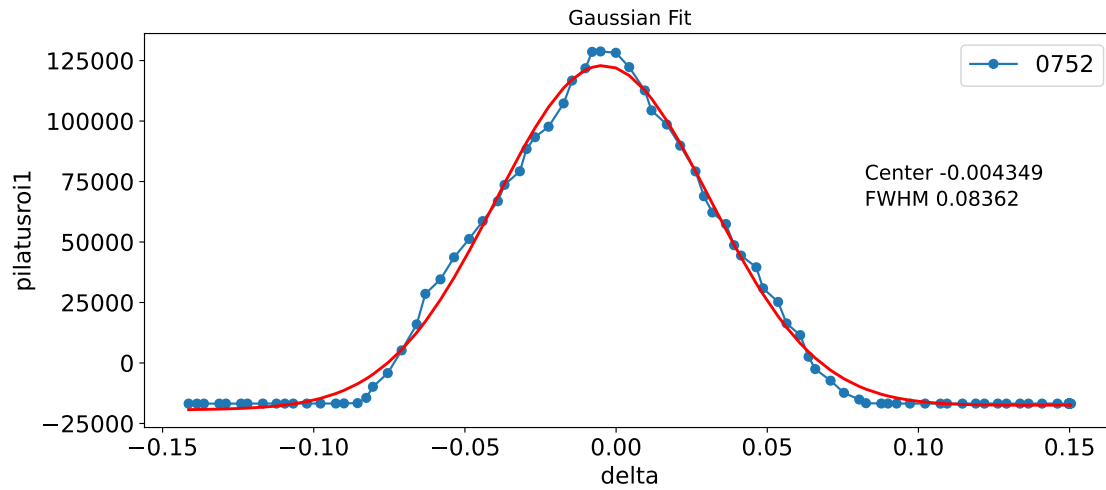
2.1 Subsection

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



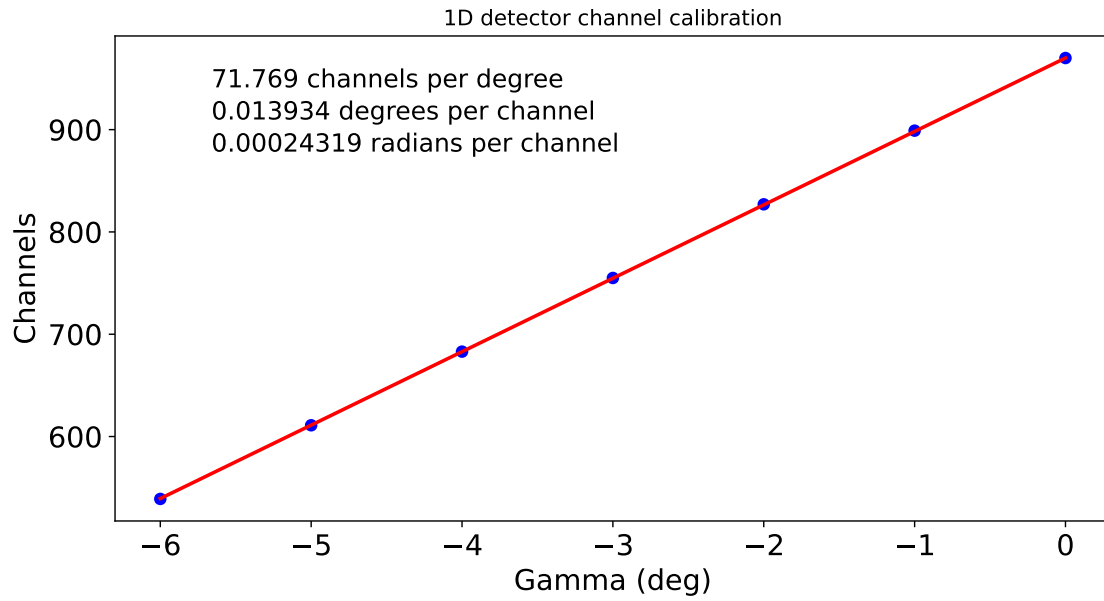
Fit with erf function.

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



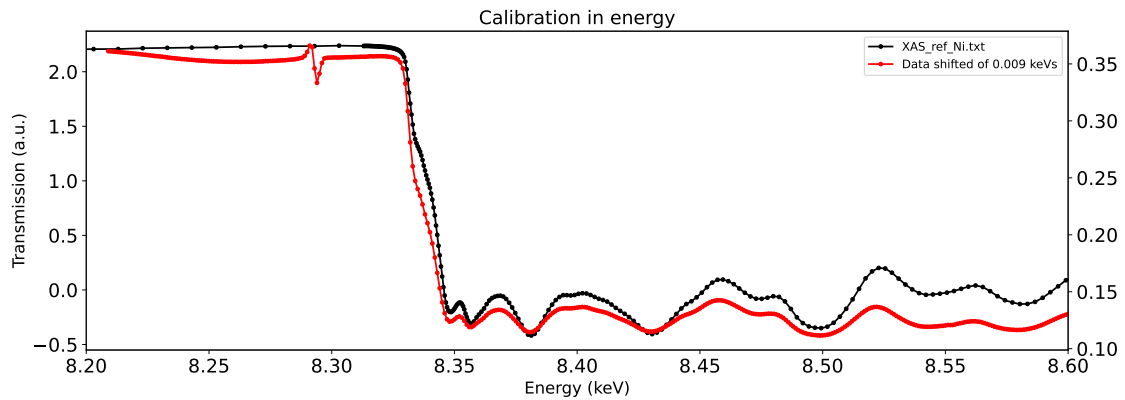
Fit with Gaussian function.

2.2 Calibration thetaz



2.3 Calibration energy

2.3.1 SIRIUS_2022_03_29_0374: ascan energydcm 8.2 8.6 400 .1



Current value of braggdcm = 13.7745

Current value of energydcm = 8.333

Do at the current energy: setposition braggdcm 13.7593

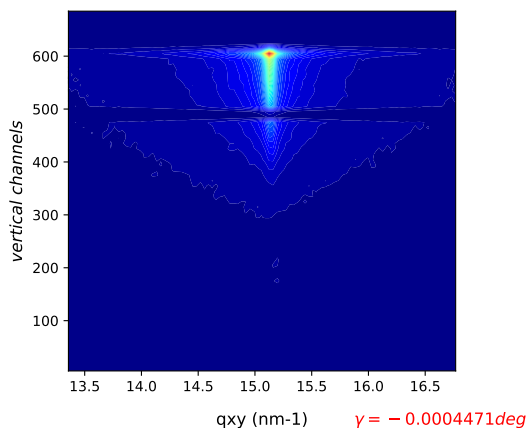
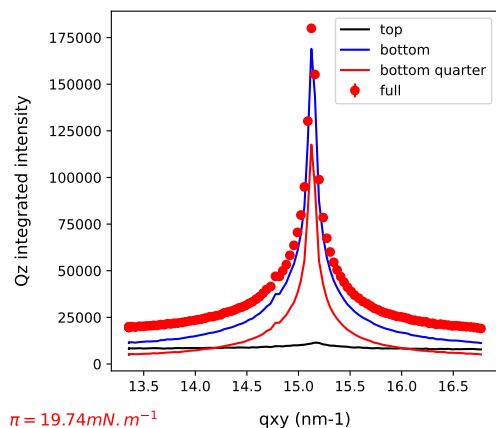
3 GIXD

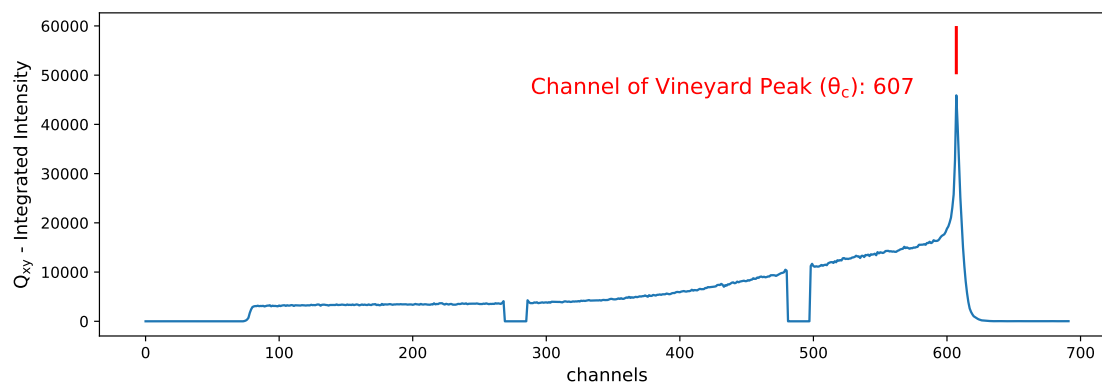
3.0.1 SIRIUS_2020_03_12_0756: continuous_ascan delta -24 -19 100 5

- 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





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

Channel0: 607

Extraction of the Yoneda-Vineyard peak.

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

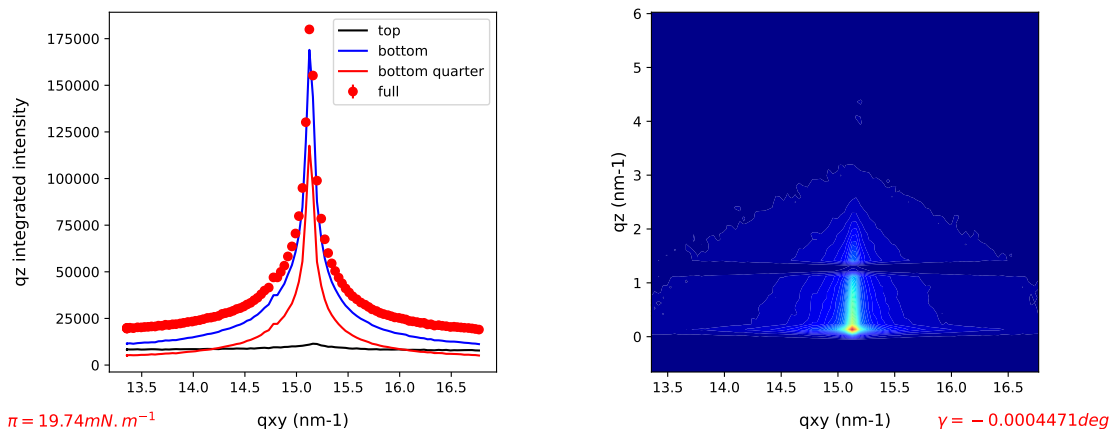
. Surface pressure data found, mean value 19.74 ± 0.006119 mN/m

. 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
Starting time: 2020-03-12 11:12:23.131901
Ending time: 2020-03-12 11:21:30.975287

SIRIUS_2020_03_12_0756.nxs



. 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

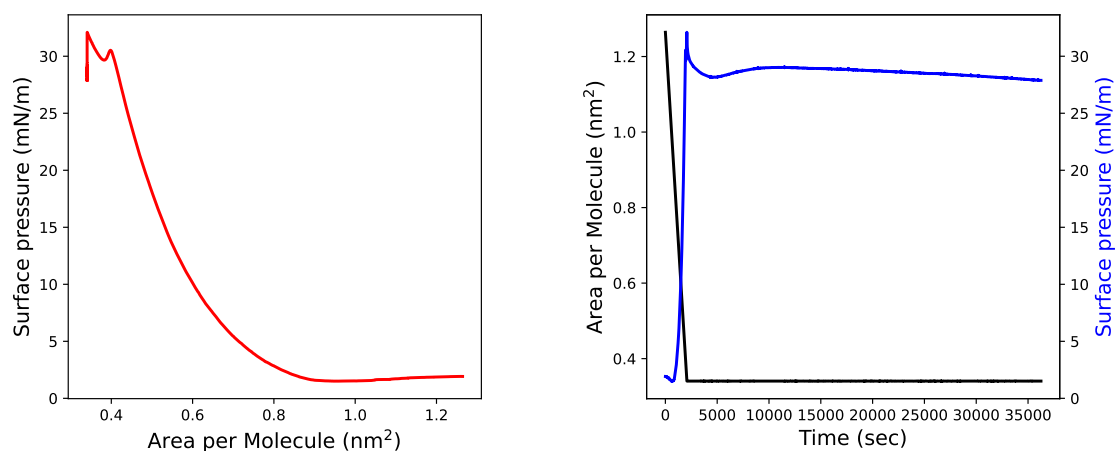
4 Isotherm

4.0.1 SIRIUS_Isotherm_2019_02_17_01544: isotherm 1.97 46 35000 1

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

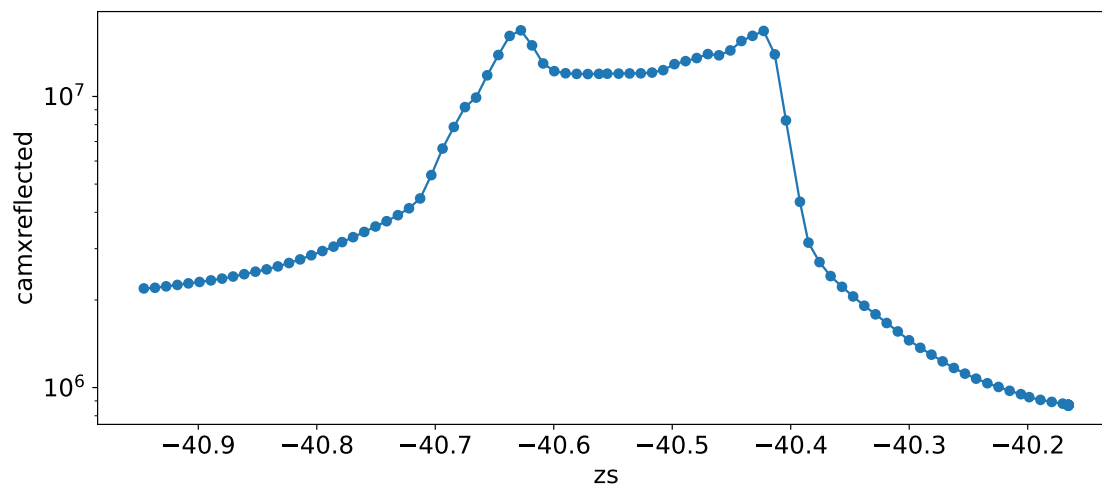
Ending time: 2019-02-18 02:56:07.101908

SIRIUS_Isotherm_2019_02_17_01544



5 1D plot

5.0.1 SIRIUS_2020_03_12_0760: run cont_regh.ipynb



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

6 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

6.0.1 SIRIUS_2021_11_26_6088: tscan 5 5

Absorbers: 29 - Vide

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

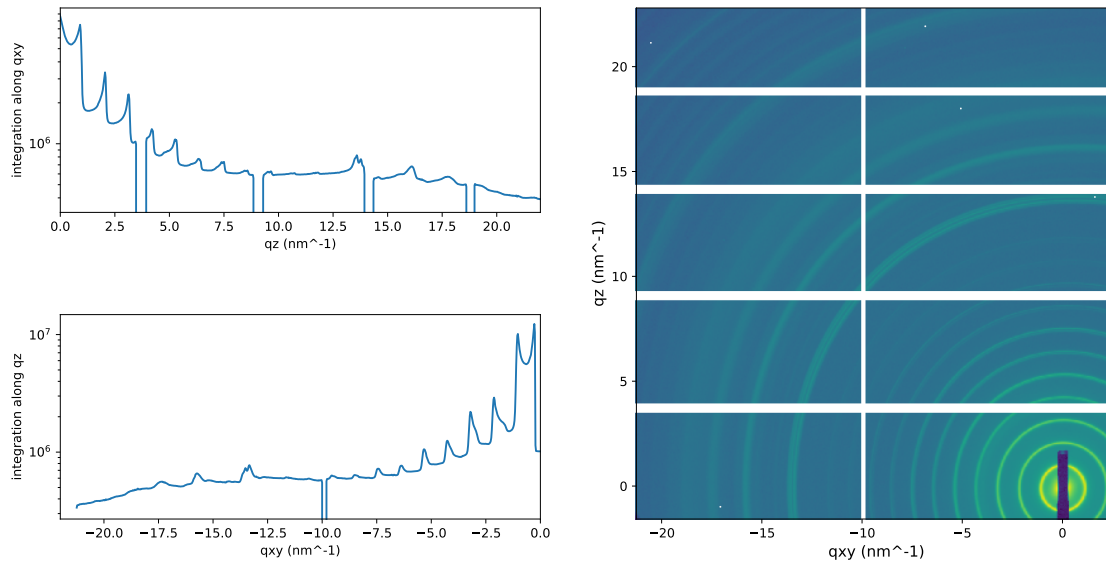
Ending time: 2021-11-26 10:35:36.820896

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



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

6.0.2 SIRIUS_2021_11_26_6103: tscan 10 10

Absorbers: 29 - Vide

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

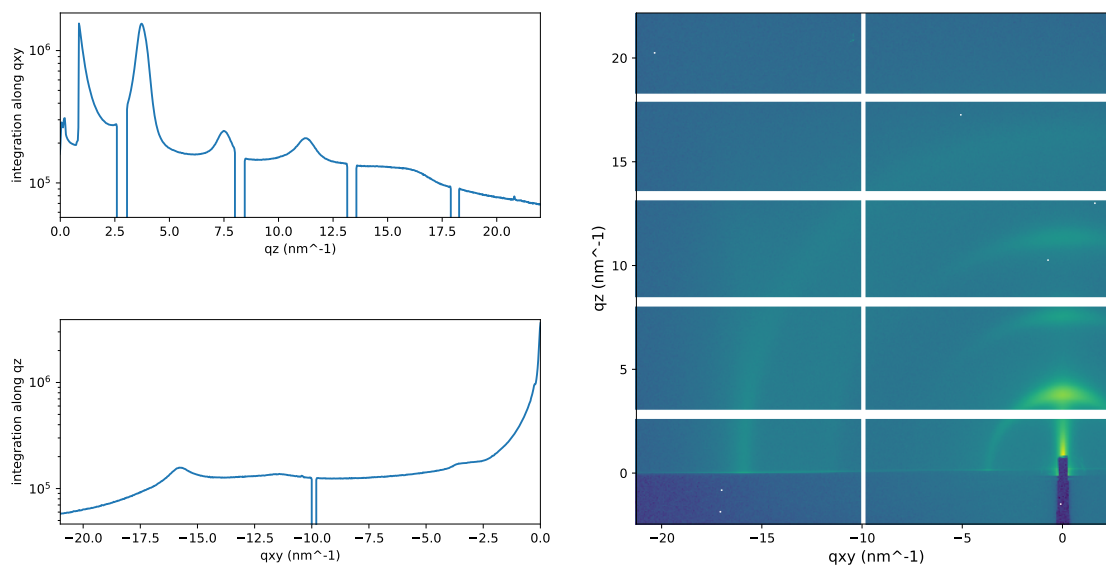
Ending time: 2021-11-26 12:40:27.880773

gamma found: gamma = -2 deg

delta found: delta = -8.875 deg

thetai (alphax) found: thetai = 0.1 deg

SIRIUS_2021_11_26_6103.nxs



GIWAXS on a P3HT film.

6.0.3 SIRIUS_2021_10_16_2739: run scan_0_18.ipy

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

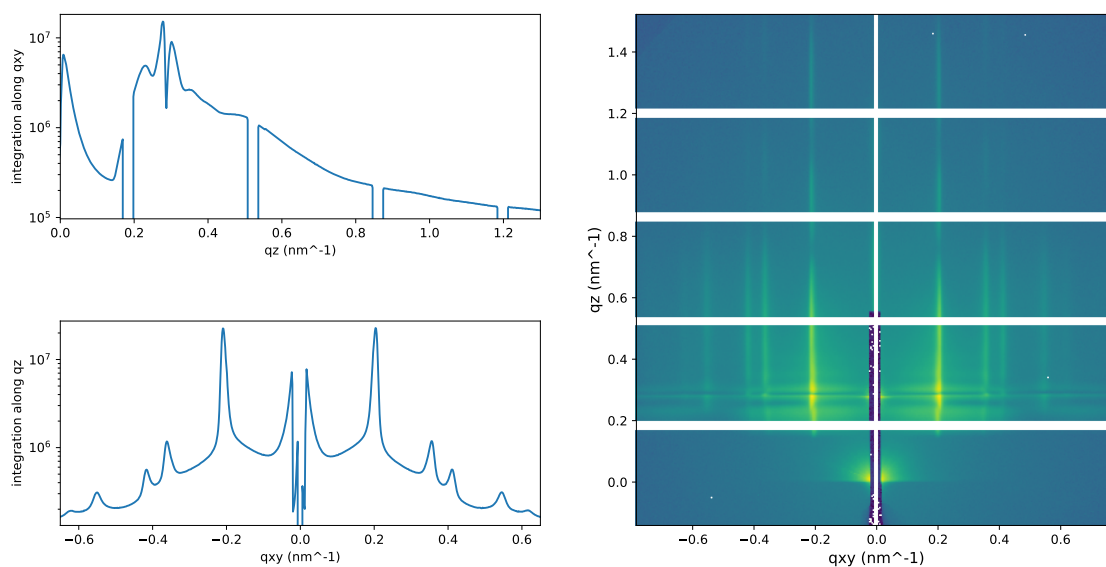
Ending time: 2021-10-16 18:47:31.474466

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

SIRIUS_2021_10_16_2739.nxs



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

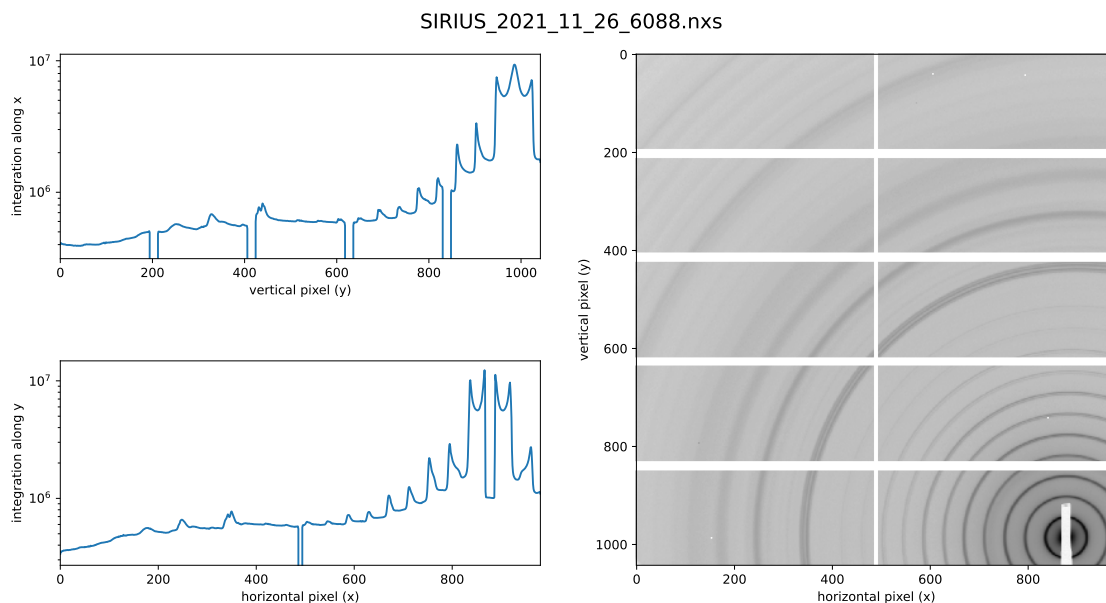
7 Plot 2D detector

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

7.0.1 SIRIUS_2021_11_26_6088: tscan 5 5

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

Ending time: 2021-11-26 10:35:36.820896



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

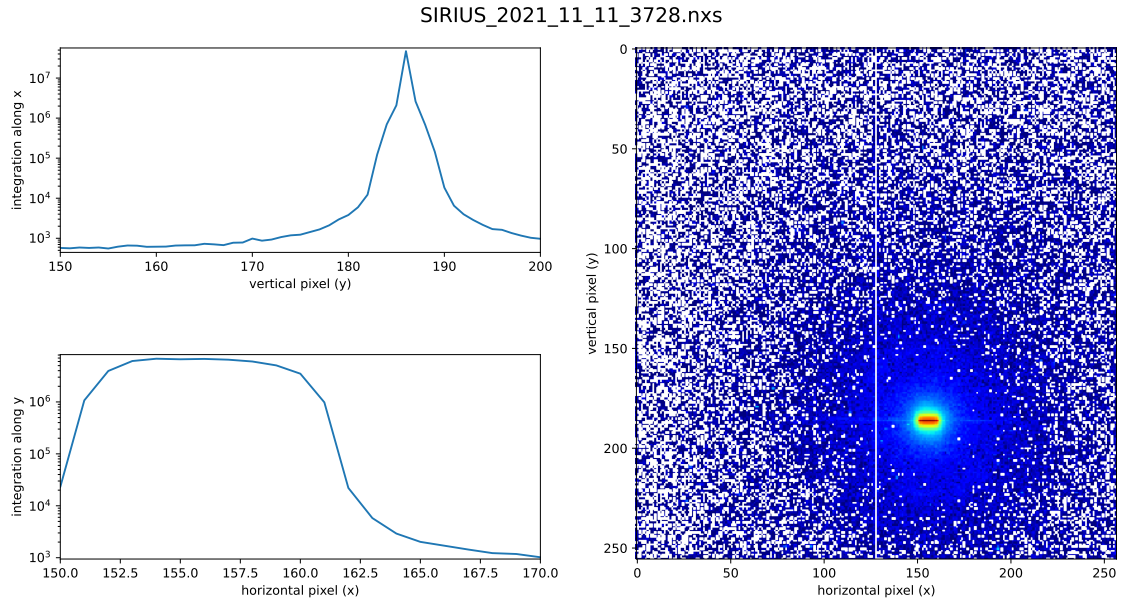
7.0.2 SIRIUS_2021_11_11_3728: tscan 2 9

. 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 -----> fluocr00
21 -----> fluocr01
22 -----> fluocr02
23 -----> fluocr03
24 -----> commandfemtoionchamber
25 -----> ufx
26 -----> ufxroi2
27 -----> integration_time
28 -----> sensorsRelTimestamps
29 -----> sensorsTimestamps
```

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

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



Works also with the detector UFXC.

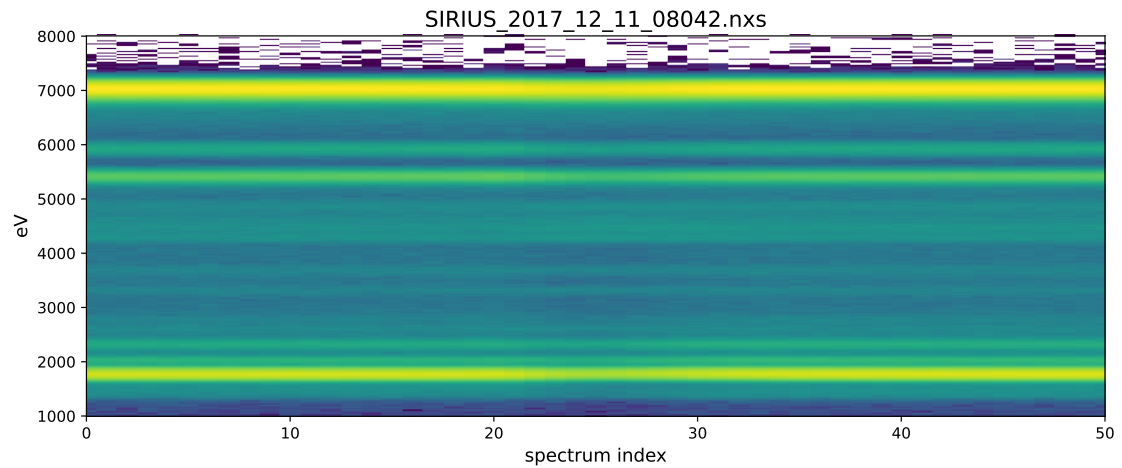
8 XRF

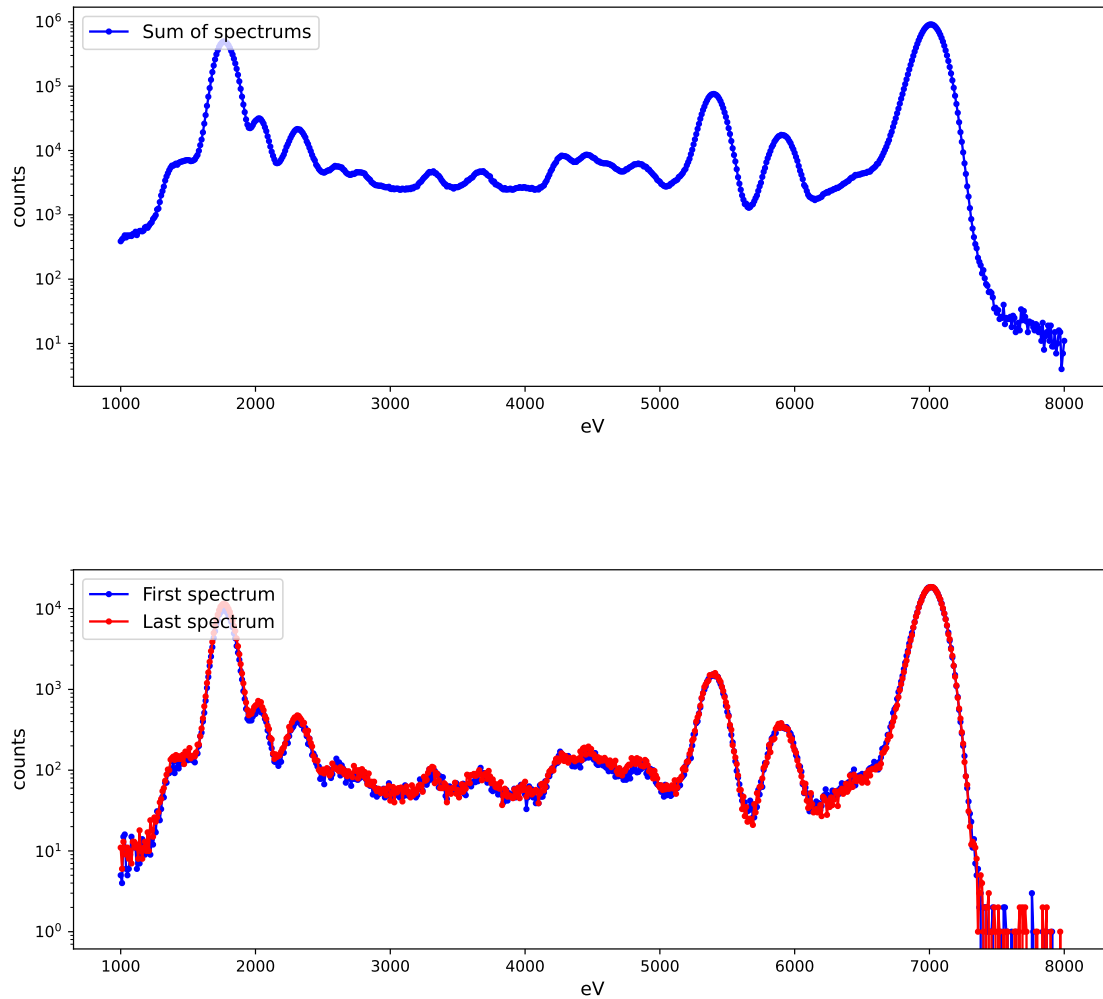
8.0.1 SIRIUS_2017_12_11_08042: run xsw7.ipy

Absorbers: Al 200micron

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

Ending time: 2017-12-11 06:43:25.042858





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

8.0.2 SIRIUS_Fluo_2020_07_03_0042: tscan 500 30

- Open Nexus Data File :

```

recording/SIRIUS_Fluo_2020_07_03_0042.nxs
. Number of data points: 501
. Available Counters:
    0 -----> ys
    1 -----> zs
    2 -----> xs
    3 -----> surfacepressure
    4 -----> areapermolecule

```



```

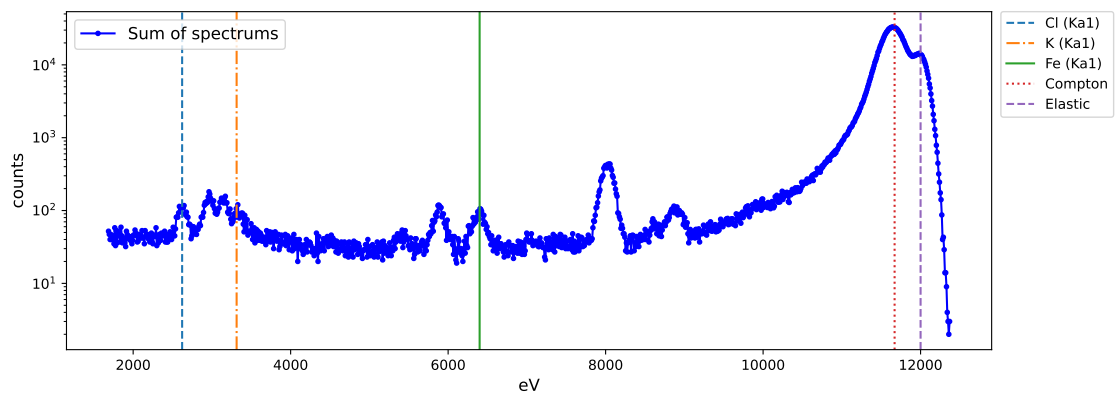
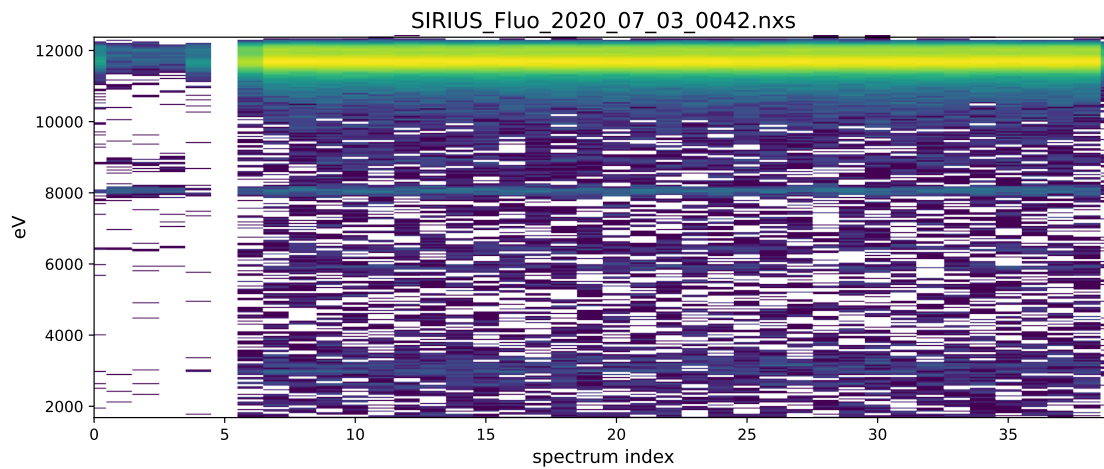
5 -----> fluo01
6 -----> fluo02
7 -----> fluo03
8 -----> fluo04
9 -----> fluoicr04
10 -----> fluocr04
11 -----> fluospectrum04
12 -----> qxy
13 -----> integration_time
14 -----> sensorsRelTimestamps
15 -----> sensorsTimestamps

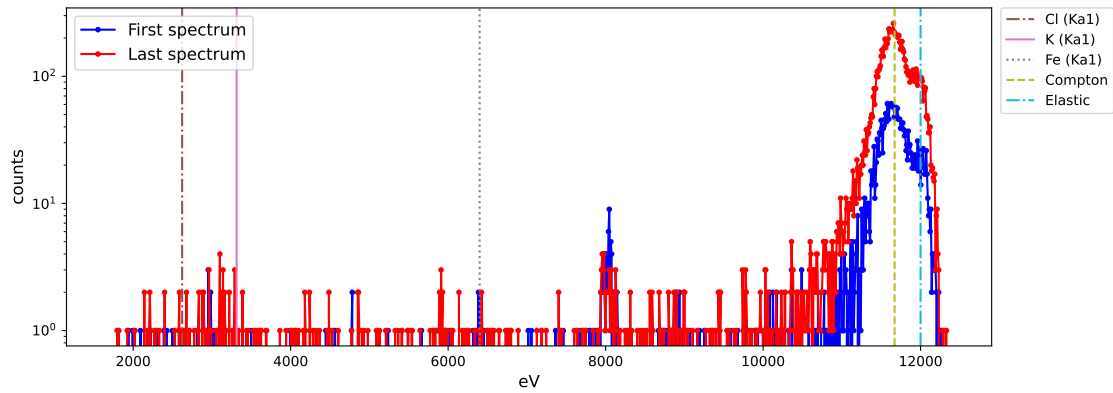
```

Absorbers: Al 800micron

Starting time: 2020-07-03 10:50:51.344430

Ending time: 2020-07-03 11:14:11.671638





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

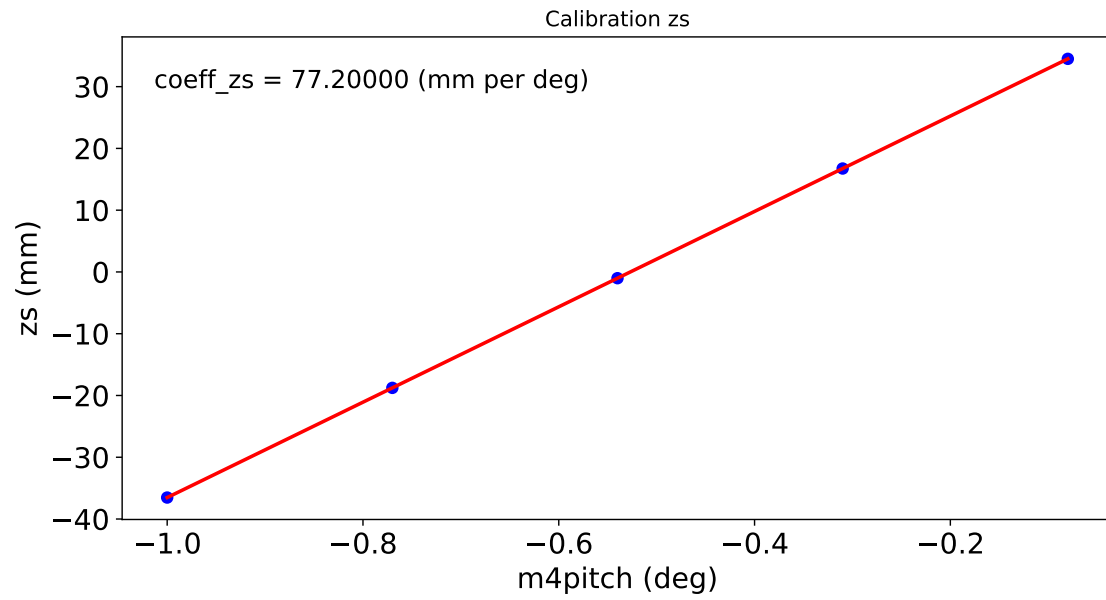
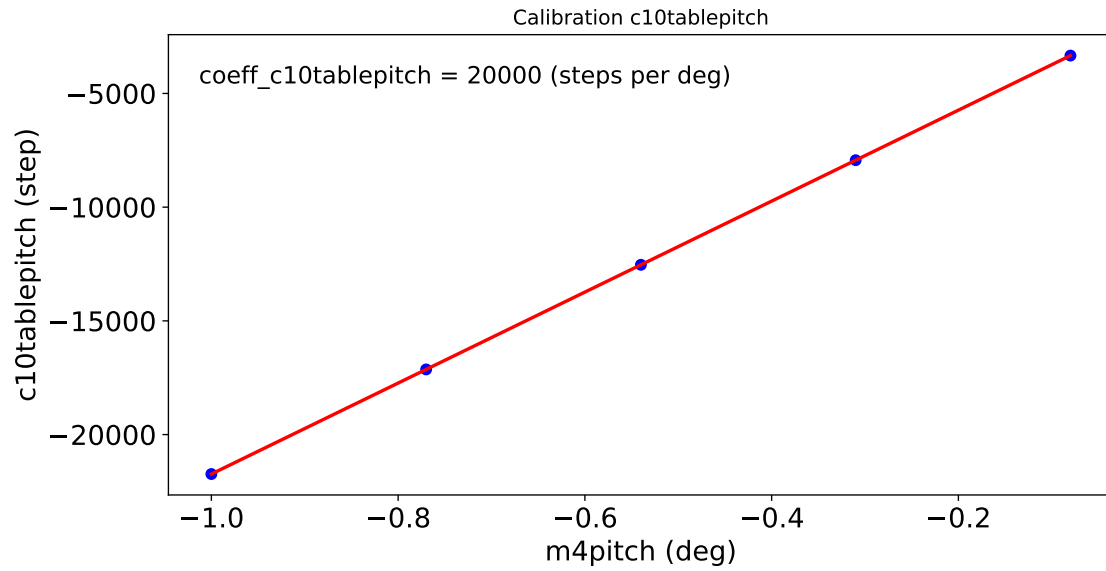
Plot XRF from the 1-element detector, in eVs and with peak identification.

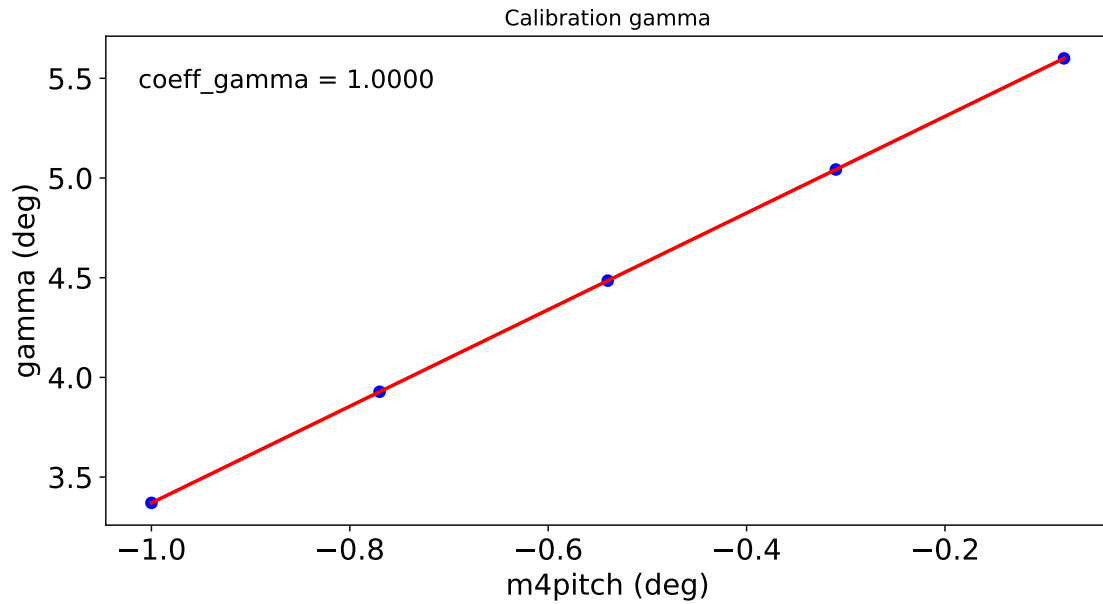
Generates:

- SIRIUS_Fluo_2020_07_03_0042_fluospectrum04.mat
- SIRIUS_Fluo_2020_07_03_0042.dat

9 XRR

9.1 Calibration XRR (liquid)





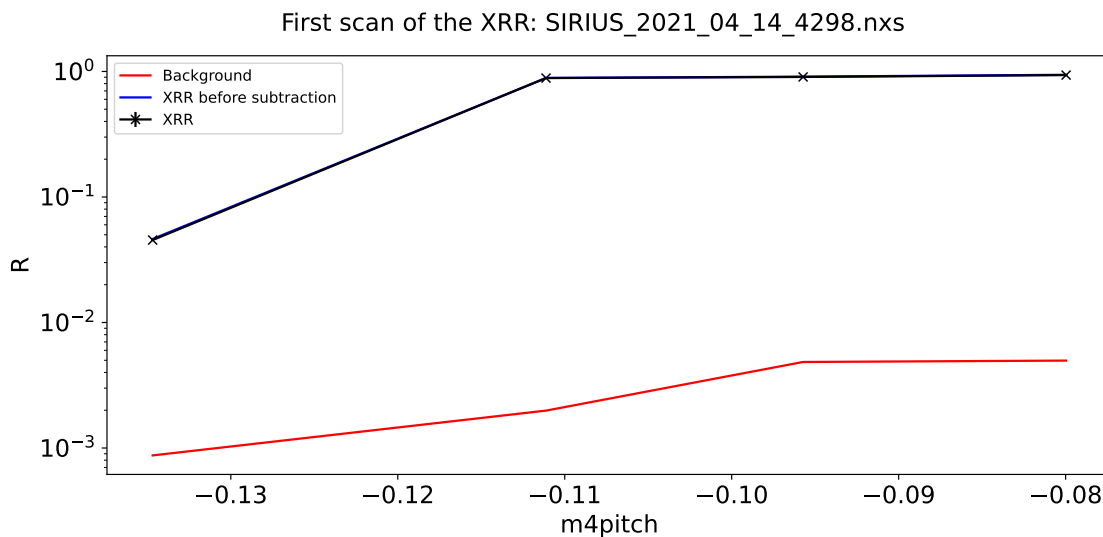
To start the calibration click on Calib. XRR (liquid).

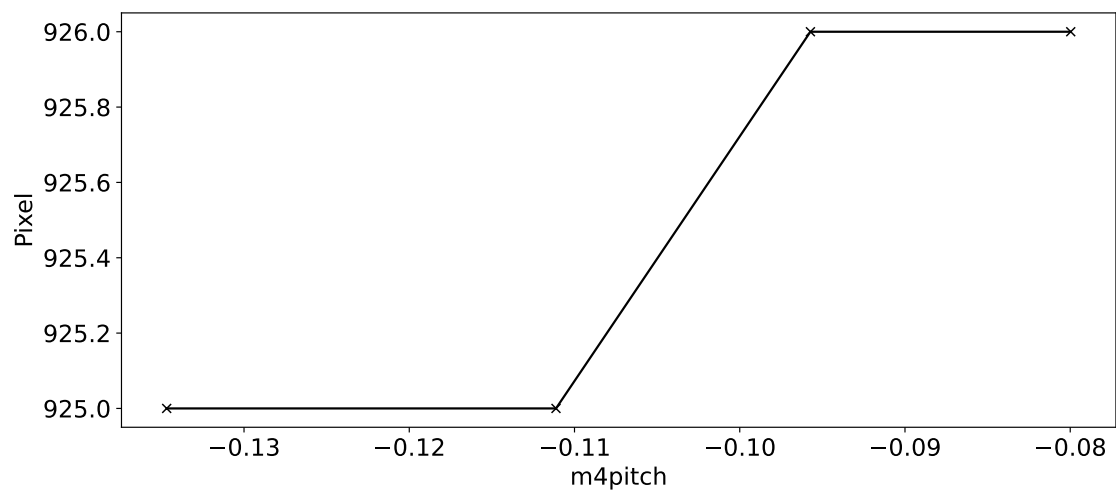
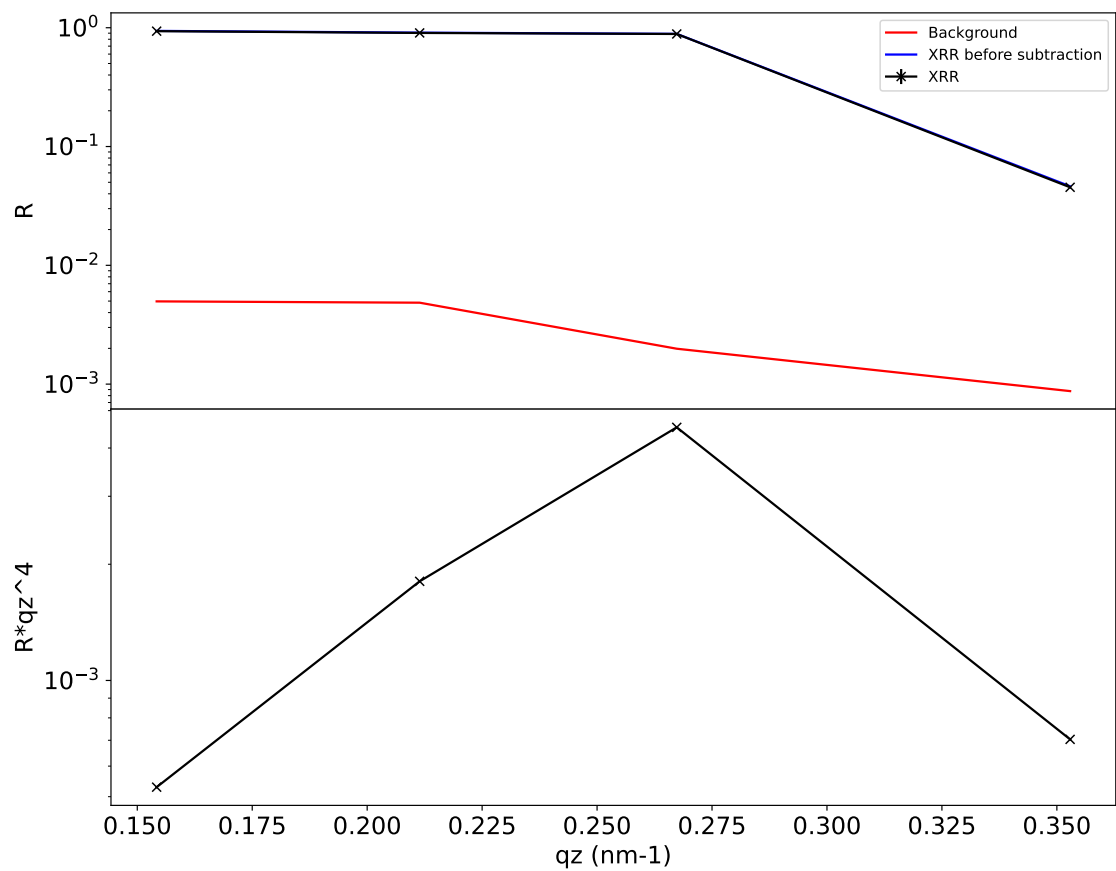
9.2 Scan XRR (liquid)

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

9.2.1 SIRIUS_2021_04_14_4298: No command found

Direct extracted from SIRIUS_2021_04_14_4297.nxs: direct=2.44385e+12





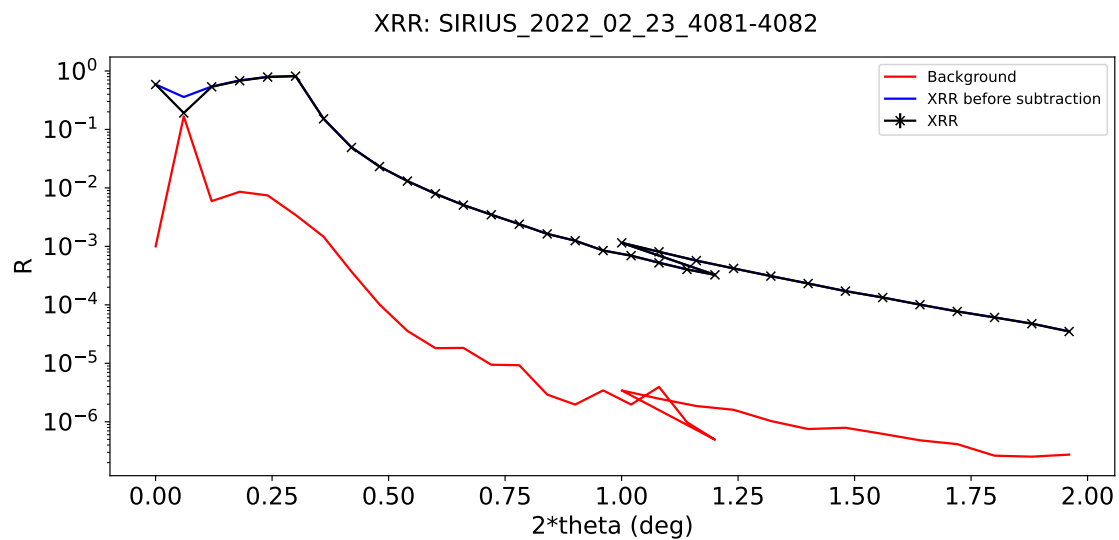
9.3 Scan XRR (solid)

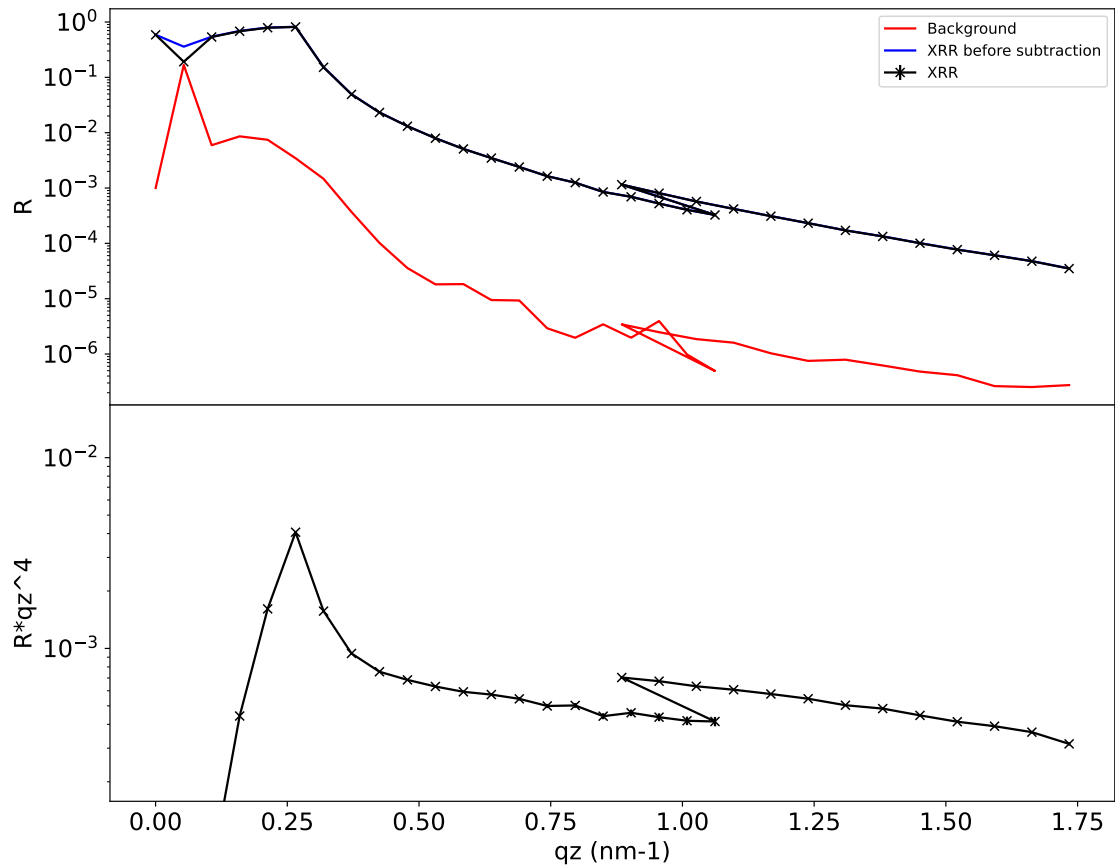
Select all the scans of the XRR series and click on Plot XRR (solid). Here we show only a few points for the example.

9.3.1 SIRIUS_2022_02_23_4081: run scan_XRR.ipy

Background taken: up down

Direct extracted from SIRIUS_2022_02_23_4080.nxs: direct=4.17113e+13





10 Insert script

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

10.0.1 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.ipynb
    %run cont_regh_abs.ipynb #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

```

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
	1.00196	-89.57961	90.42039	-0.00580	-0.08252
Degrees	deg	deg	deg		

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

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`.

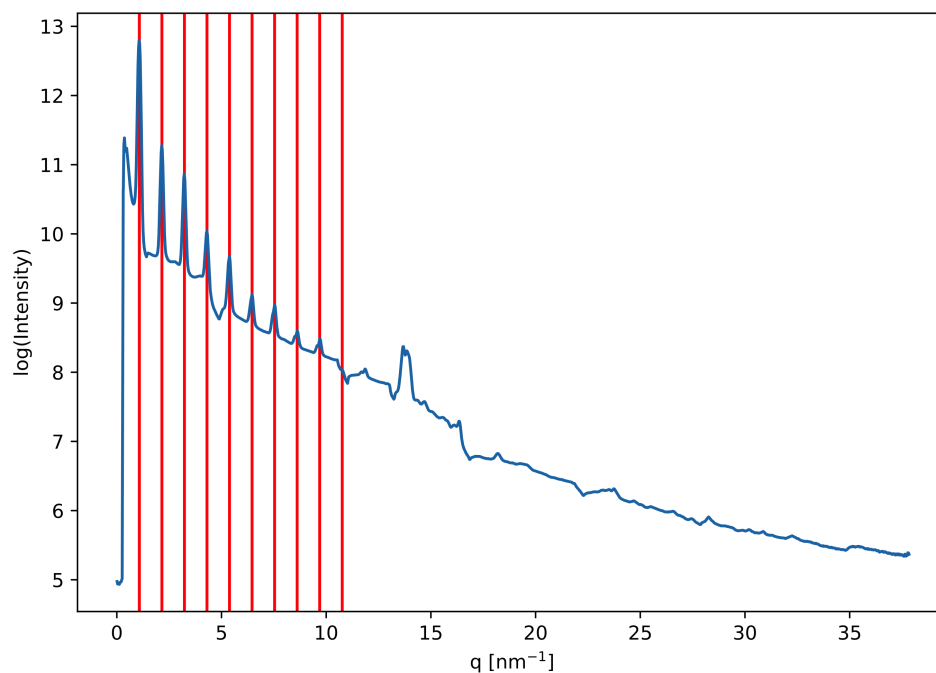
```
Fri, 26 Nov 2021 14:13:34 ct 1 pilatus
Fri, 26 Nov 2021 14:13:56 tscan 10 10 #6109
Fri, 26 Nov 2021 14:17:29 shclose
Fri, 26 Nov 2021 14:26:40 run config_alignment.ipyn
Fri, 26 Nov 2021 10:34:48 ct 1 pilatus
```

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**.