Example

December 7, 2020

1 Experimental setup

SIRIUS Beamline : Experiment 123456789

This is an example of JupyLabBook

- Type: Proposal
- Safety: Yellow
- Date: 12/03/2020-17/03/2020

- Main proposer: Doe
- Local contact: AH
- Users (on site): John Doe, Jane Doe
- Recording directory: /Users/arnaudhemmerle/Documents/Recherche/Analysis/JupyLabBook/recording/

- 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: 19
    - Polarisation: LH
    - Phase (deg): 0
    - Horizontal focalisation: False
    - Vertical focalisation: True
    - Horizontal beamsize (mm): 2
    - Vertical beamsize (mm): ~0.150

- Monitors and XBPM:
    - mon1:

- mon2: thick diamond
- mon3:
- mon4:
- Detectors: Pilatus on Delta-Gamma

- Remarks: This is an example.

2 Beamline alignment
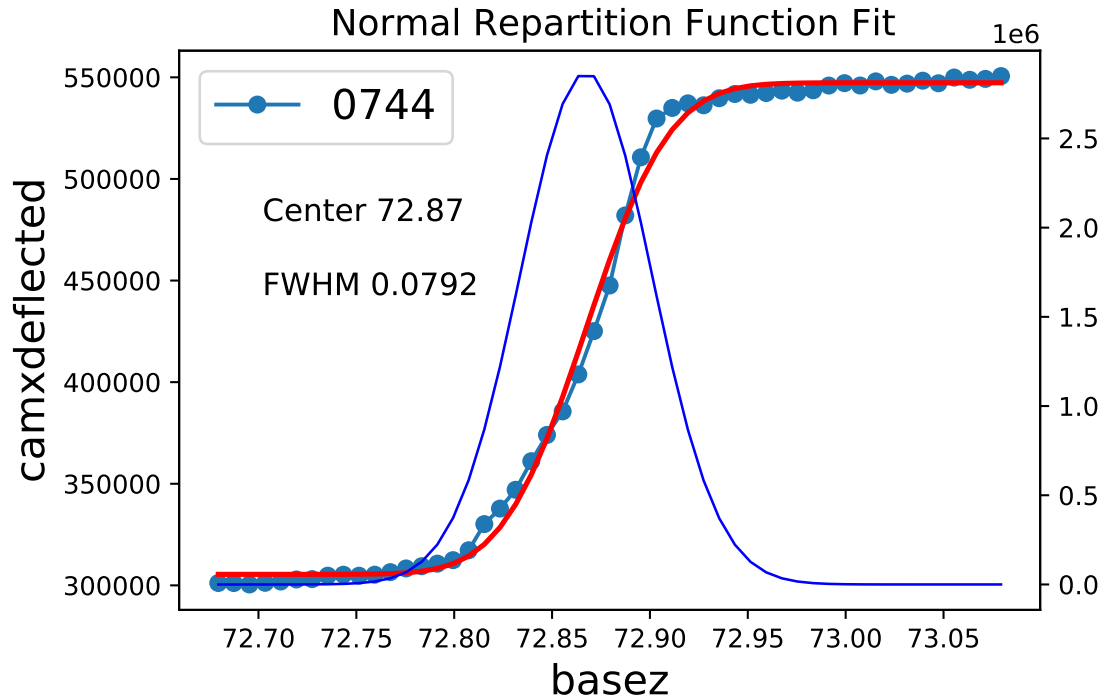
Here we show functions used during beamline aligment.

LaTeX formula can be used:
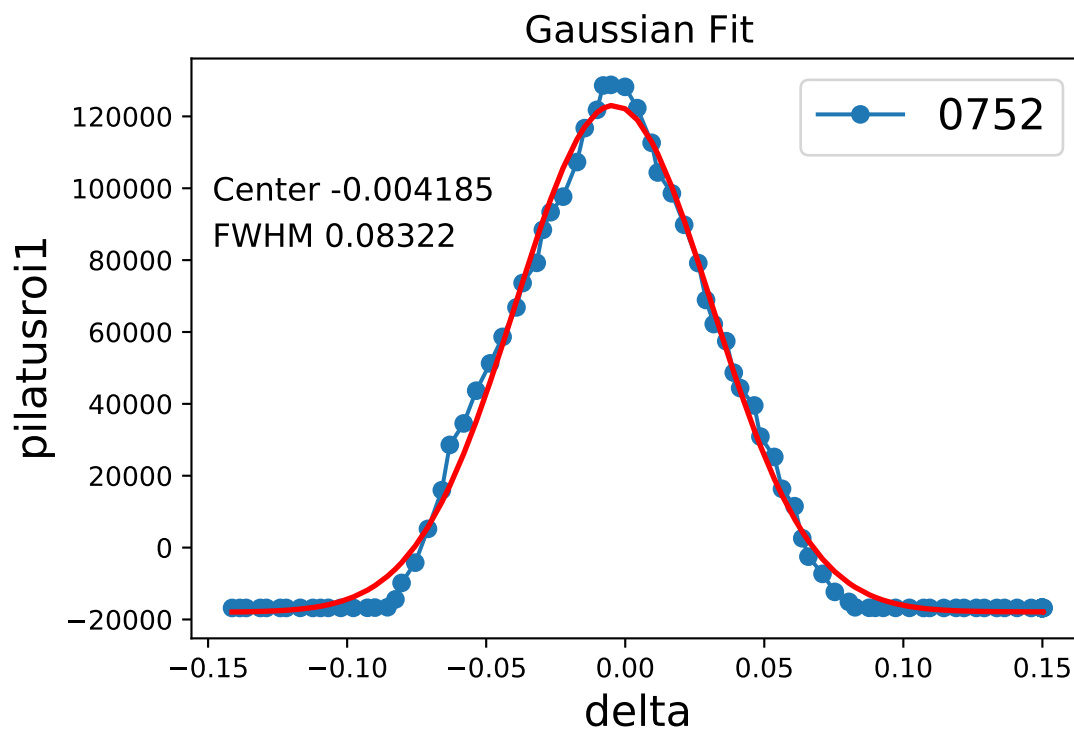$$\frac{786 - 558}{2 \times 2069} \times 0.0355 = 1.9 mrad$$

2.1 Subsection

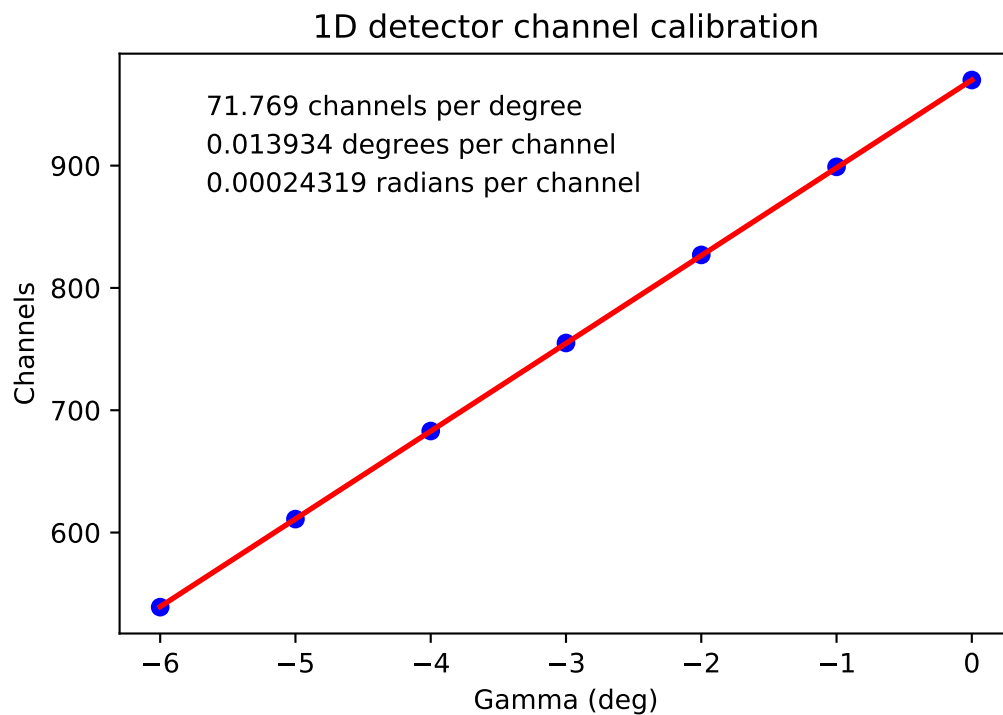### 2.1.1 SIRIUS_2020_03_11_0744: dscan basez -.2 .2 50 .1

Fit with erf function.

2.1.2 SIRIUS_2020_03_11_0752: One can edit the scan info here as well

Fit with a gaussian.

2.2   Calibration thetaz

1D detector channel calibration

71.769 channels per degree
0.013934 degrees per channel
0.00024319 radians per channel

Channels (y-axis), *Gamma (deg)* (x-axis)

3   GIXD

3.0.1   SIRIUS__2020__03__12__0756: continuous__ascan delta -24 -19 100 5

Extraction of the Vineyard.

```
- 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)

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

. Area per molecule data found, mean value 0.3557 ± 3.944e-05 nm2 per molecule

. Gamma motor data found, mean value -0.0004471 deg

SIRIUS_2020_03_12_0756.nxs

$\pi = 19.74 mN.m^{-1}$ qxy (nm-1)   qxy (nm-1) $\gamma = -0.0004471 deg$

Channel of Vineyard Peak (θ_c): 607
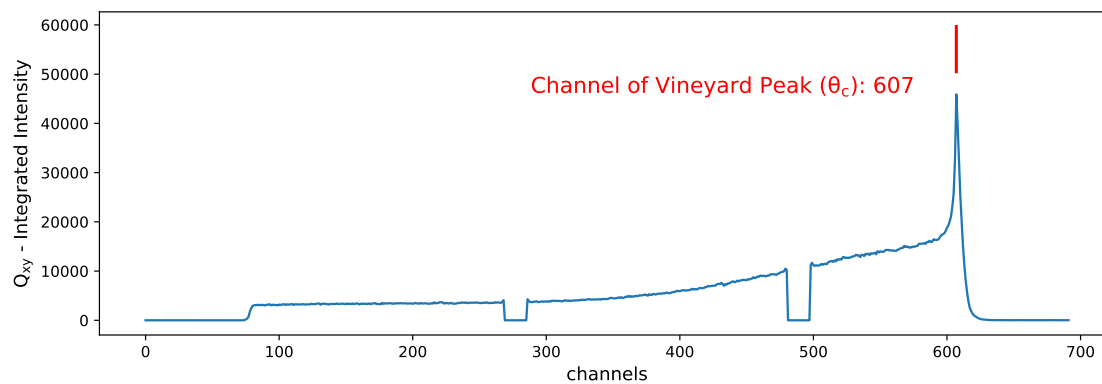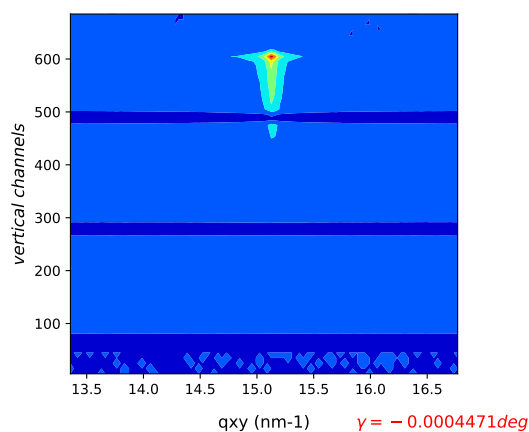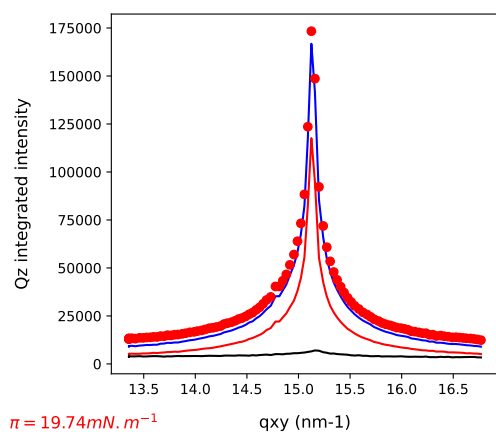
Data not saved. To save data, run a GIXD on the scan.
Channel0: 607

5

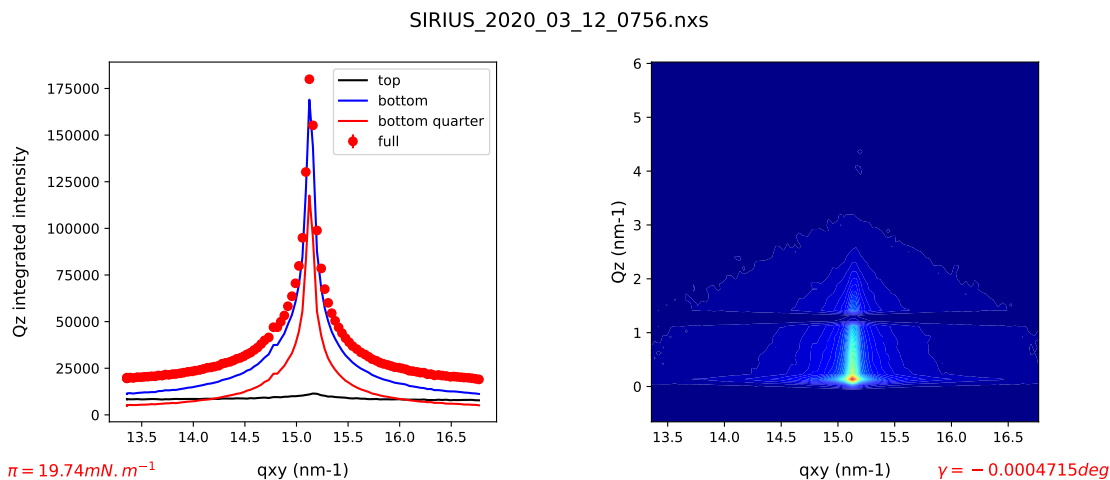### 3.0.2 SIRIUS_2020_03_12_0756: continuous_ascan delta -24 -19 100 5

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

```
. Absorbers: 29 - Vide
```

SIRIUS_2020_03_12_0756.nxs

3.0.3 SIRIUS_2020_03_12_0756: continuous_ascan delta -24 -19 100 5

It is possible to print all info on the scan and the counters.

```
- 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
```

. Absorbers: 29 - Vide
. 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 ± 0.006163 mN/m
. Area per molecule data found, mean value 0.3557 ± 3.866e-05 nm2 per molecule
. Gamma motor data found, mean value -0.0004715 deg
. 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

SIRIUS_2020_03_12_0756.nxs
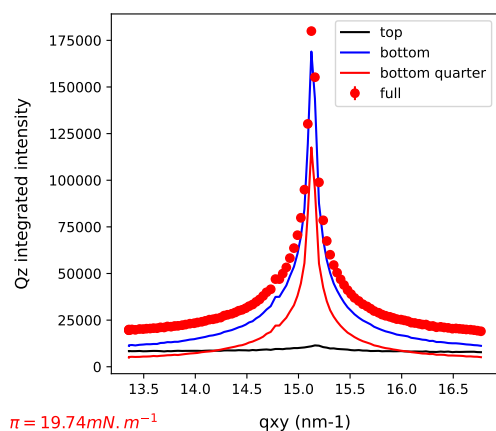
$\pi = 19.74 mN.m^{-1}$
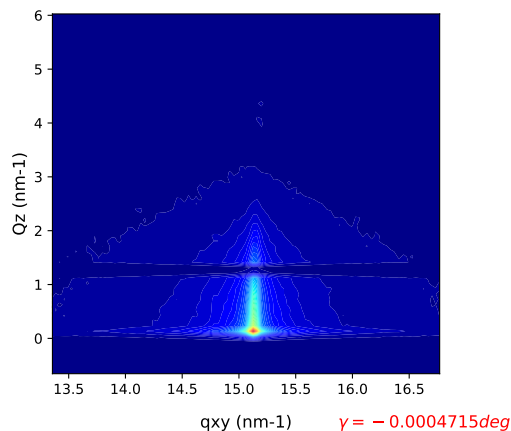
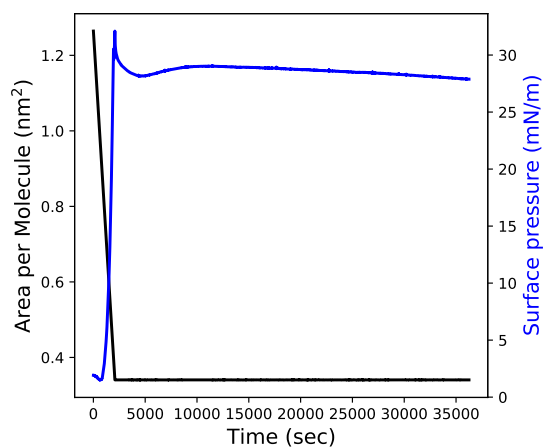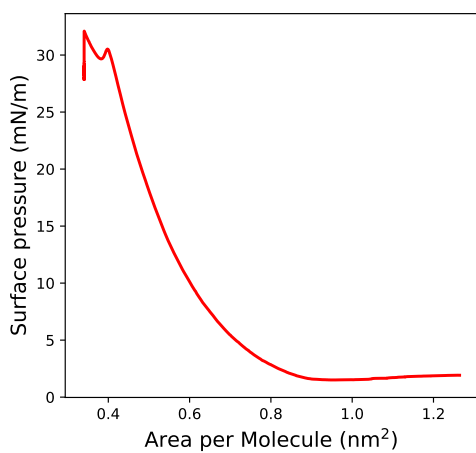$\gamma = -0.0004715 deg$

4 Isotherm

4.0.1 SIRIUS_Isotherm_2019_02_17_01544: isotherm 1.97 46 35000 1

Plot the isotherm. Generates SIRIUS_Isotherm_2019_02_17_01544.dat
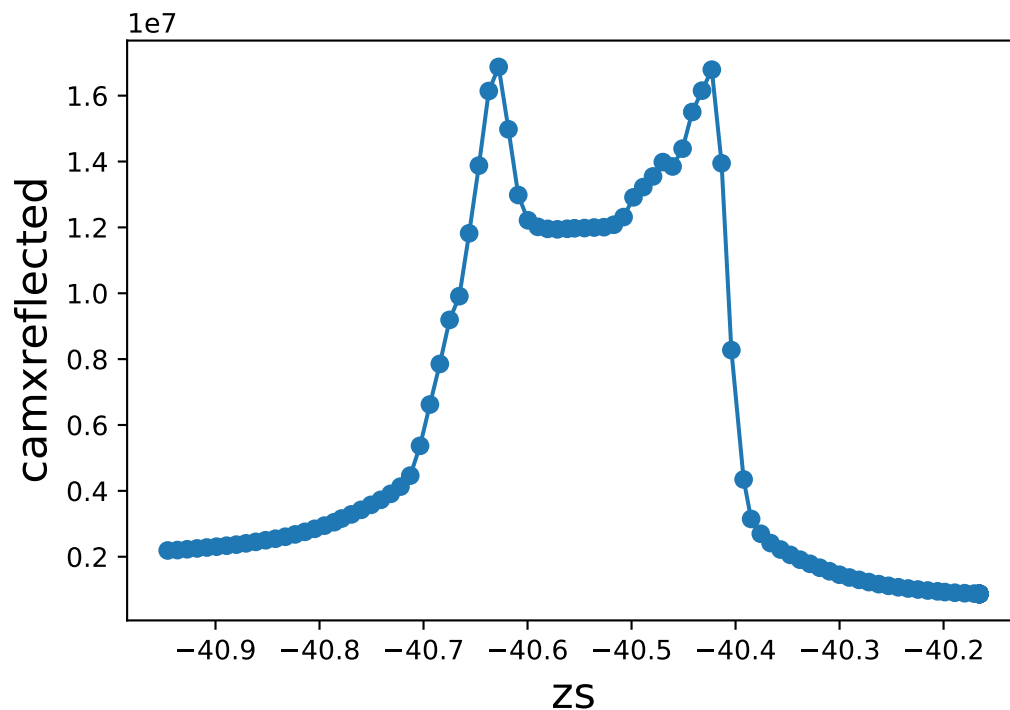
SIRIUS_Isotherm_2019_02_17_01544

5 1D plot

5.0.1 SIRIUS_2020_03_12_0760: run cont_regh.ipy

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

6 GIXS

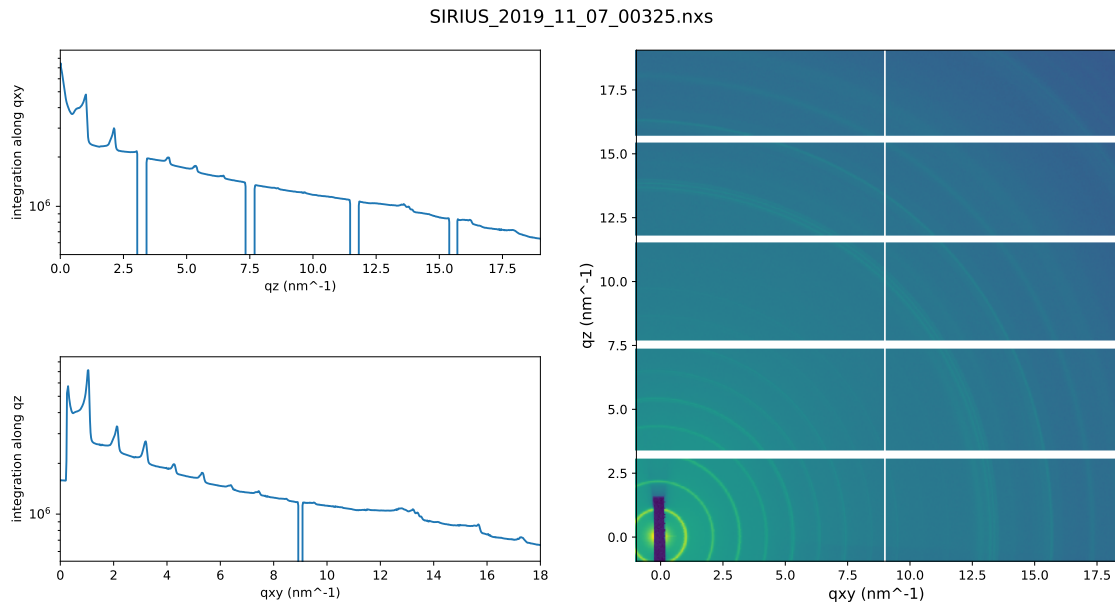### 6.0.1 SIRIUS_2019_11_07_00325: tscan 10 10

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_2019_11_07_00325_pilatus_sum.tiff
- SIRIUS_2019_11_07_00325_pilatus_sum.mat
- SIRIUS_2019_11_07_00325_integrated_qz.dat
- SIRIUS_2019_11_07_00325_integrated_qxy.dat

6.0.2 SIRIUS_2019_11_07_00325: tscan 10 10

```
. Absorbers: 29 - Vide

. No gamma found! gamma = 0
. No delta found! delta = 11.578
```
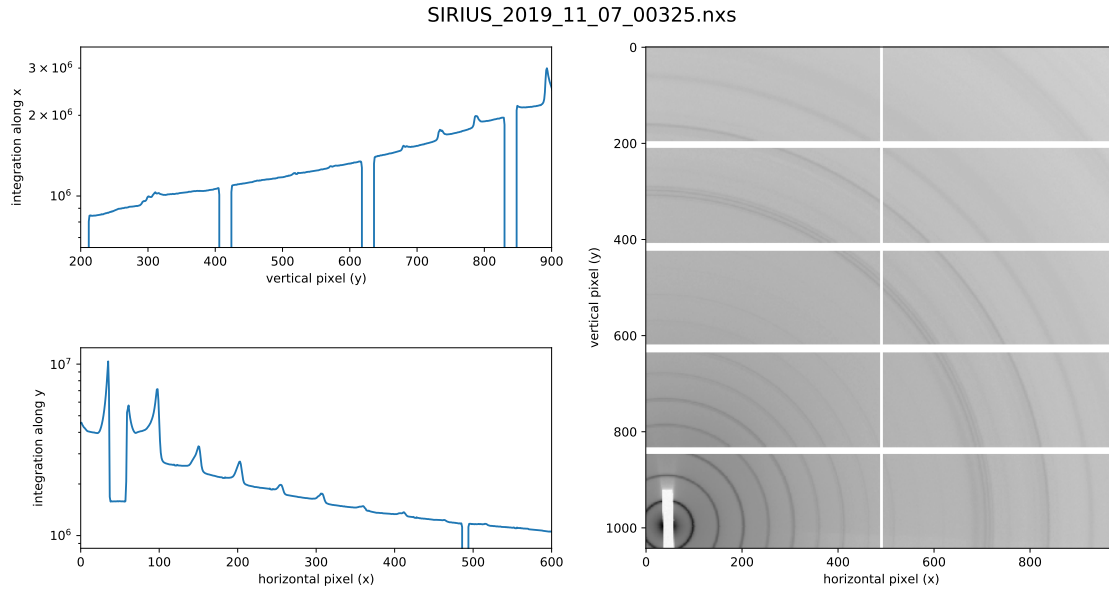
SIRIUS_2019_11_07_00325.nxs

7 Plot pilatus

7.0.1 SIRIUS_2019_11_07_00325: tscan 10 10

Plot the sum of the images from the Pilatus (time integration).
Generates:
- SIRIUS_2019_11_07_00325_pilatus_sum.tiff
- SIRIUS_2019_11_07_00325_pilatus_sum.mat
- SIRIUS_2019_11_07_00325_integrated_x.dat
- SIRIUS_2019_11_07_00325_integrated_y.dat

```
. Absorbers: 29 - Vide
```
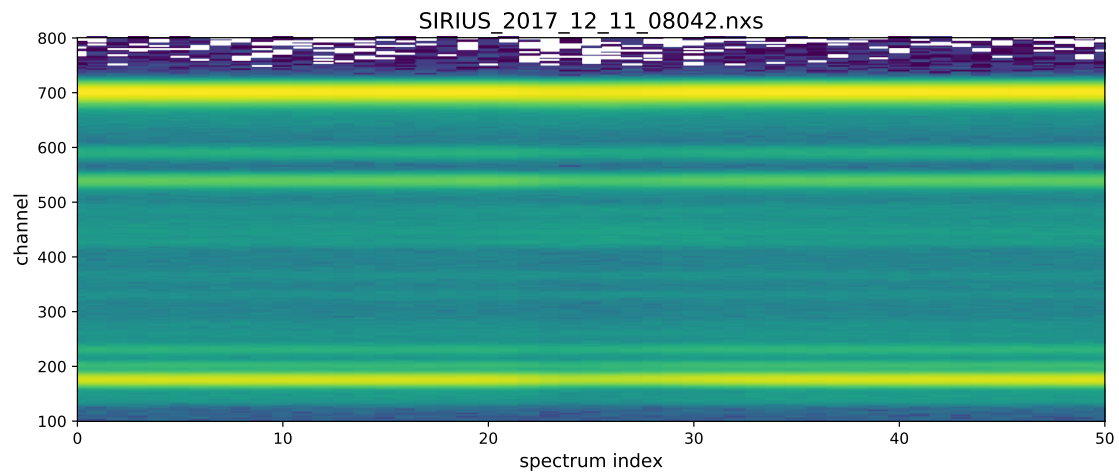
SIRIUS_2019_11_07_00325.nxs
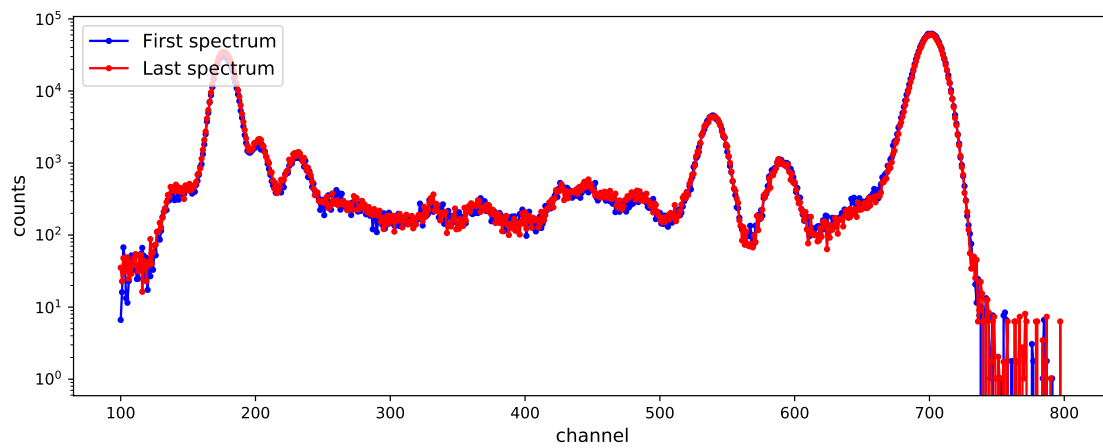
8 XRF

8.0.1 SIRIUS_2017_12_11_08042: run xsw7.ipy

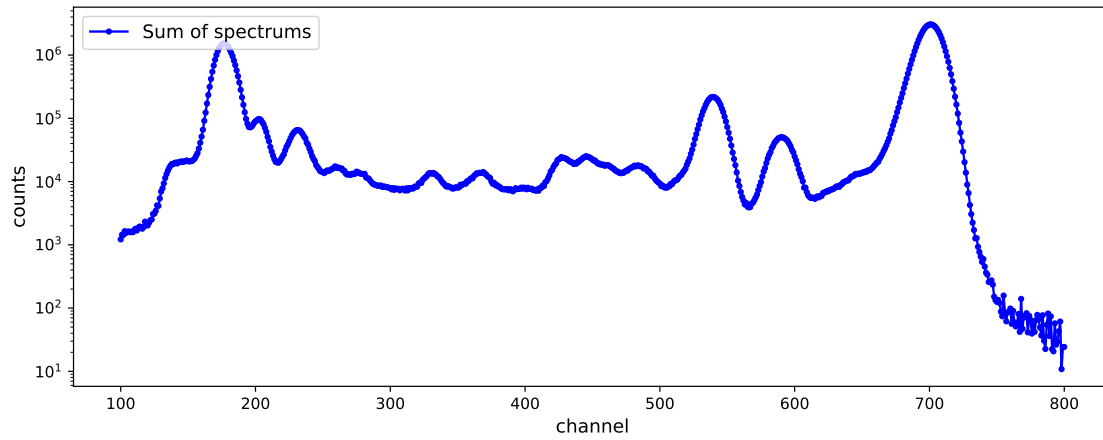Plot XRF from the 4-elements detector, in channels and without peak identification.
Generates:
- SIRIUS_2017_12_11_08042_fluospectrum.mat for each element
- SIRIUS_2017_12_11_08042.dat

    `. Absorbers: Al 200micron`

SIRIUS_2017_12_11_08042.nxs
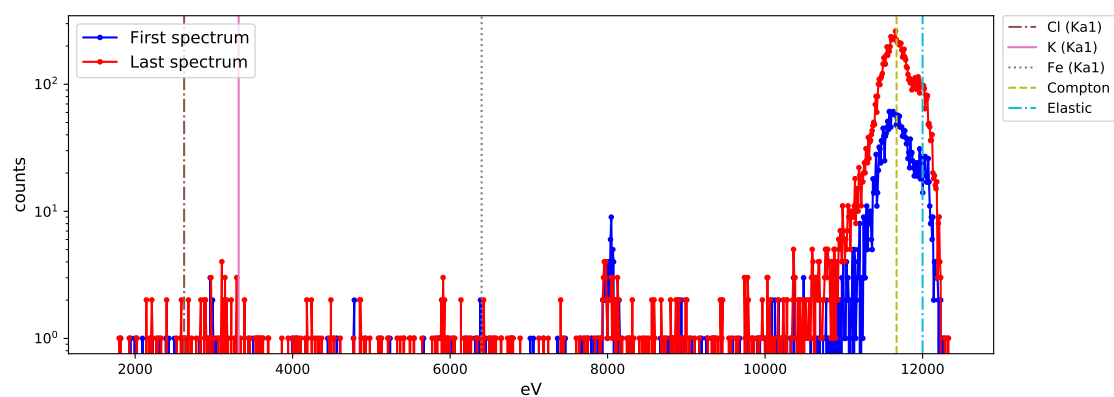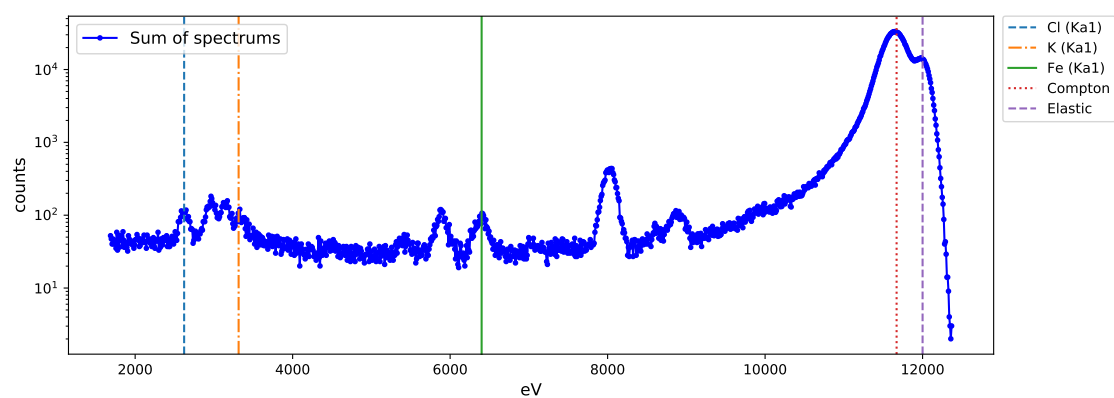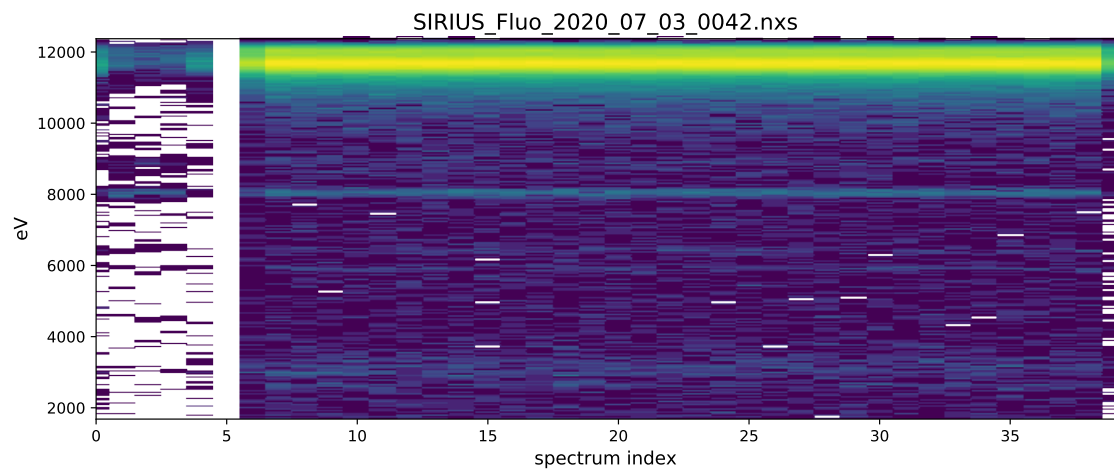
8.0.2 SIRIUS_Fluo_2020_07_03_0042: tscan 500 30

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

    . Absorbers: Al 800micron

9 Insert script

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

9.0.1 script_with_loop.ipy

```
%shopen
%amove delta -40
%run reset_motors.ipy
%amove delta -35
%continuous_ascan delta -35 -25 250 5 #123
%run reset_motors.ipy
for i in range(4):
    %amove delta -20
    %continuous_ascan delta -10 -3 175 5 #124 #126 #128 #130
    %run reset_motors.ipy
    %run cont_regh_abs.ipy #125 #127 #129 #131
for i in range(3):
    %amove delta -20
    %continuous_ascan delta -10 -3 175 5 #132 #135 #138
    %run reset_motors.ipy
    %run cont_regh_abs.ipy #133 #136 #139
    %run cont_regh_abs.ipy #134 #137 #140
for i in range(2):
    %amove delta -20
    %tscan 10 100 #141 #142

%continuous_ascan delta -35 -25 250 5 #143
%amove delta -40
%shclose
```

10 Insert positions

Positions extracted from the logs, using "'Insert positions"'.

10.0.1 wm zs

zs
-40.9178

10.0.2 wm diffracto

14

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	0.000	-15.727
			mrad	mrad	mm

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

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

11 Insert commands

Commands extracted from the logs, using "'Insert commands"'.

```
Wed, 11 Mar 2020 13:59:25 dmove m4tz 1
Wed, 11 Mar 2020 13:59:29 ct 1
Wed, 11 Mar 2020 13:59:37 amove m4pitch -.02
Wed, 11 Mar 2020 13:59:39 ct 1
```

```
Wed, 11 Mar 2020 13:59:50 dmove m4tz -.5
Wed, 11 Mar 2020 13:59:53 ct 1
Wed, 11 Mar 2020 13:59:56 dmove m4tz -.5
Wed, 11 Mar 2020 14:00:00 ct 1
Wed, 11 Mar 2020 14:00:12 dscan m4tz -.5 1.5 50 .1 #679
Wed, 11 Mar 2020 14:01:47 sigmoid_dscan m4tz -.4 .4 50 .1 #680
Wed, 11 Mar 2020 14:03:41 amove m4tz PEAK
Wed, 11 Mar 2020 14:03:50 dscan m4pitch -.5 .5 50 .1 #681
Wed, 11 Mar 2020 14:05:04 sigmoid_dscan m4tz -.4 .4 50 .1 #682
```
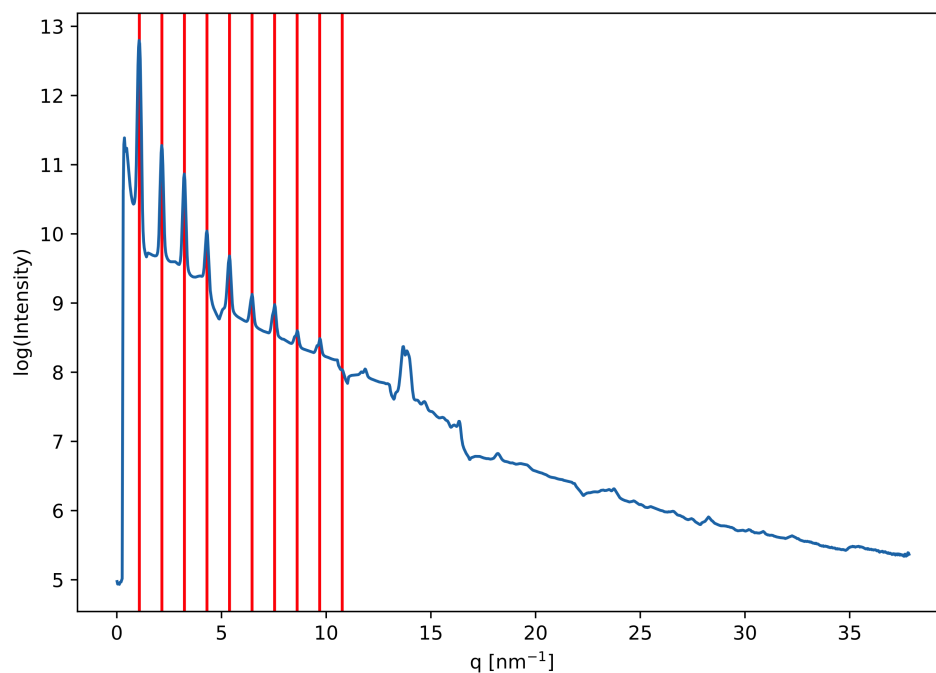
12   Convert logs

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

13   Insert an image

Using the command "Insert image".

14 Export to pdf

PDF generated by clicking on "'Export to pdf"'.