

Example

June 11, 2021

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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
- Recording directory: Z:\com-sirius\users\2021\week15\
- 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.

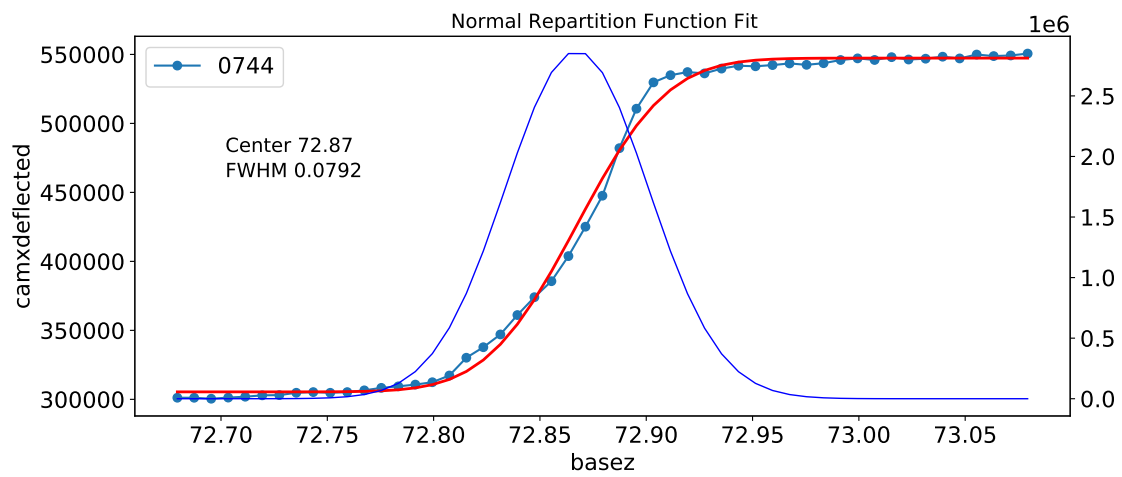
LaTeX formula can be used:

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

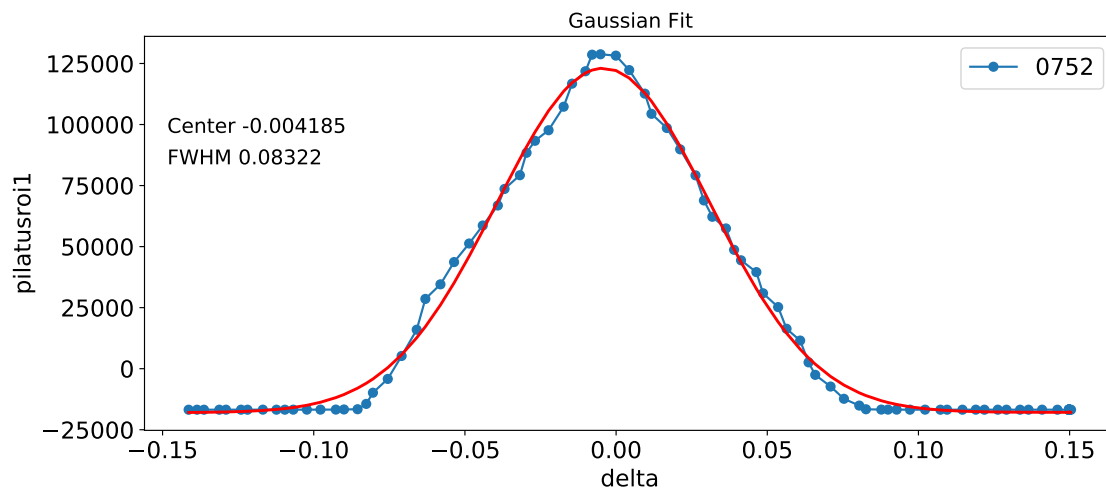
2.1 Subsection

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

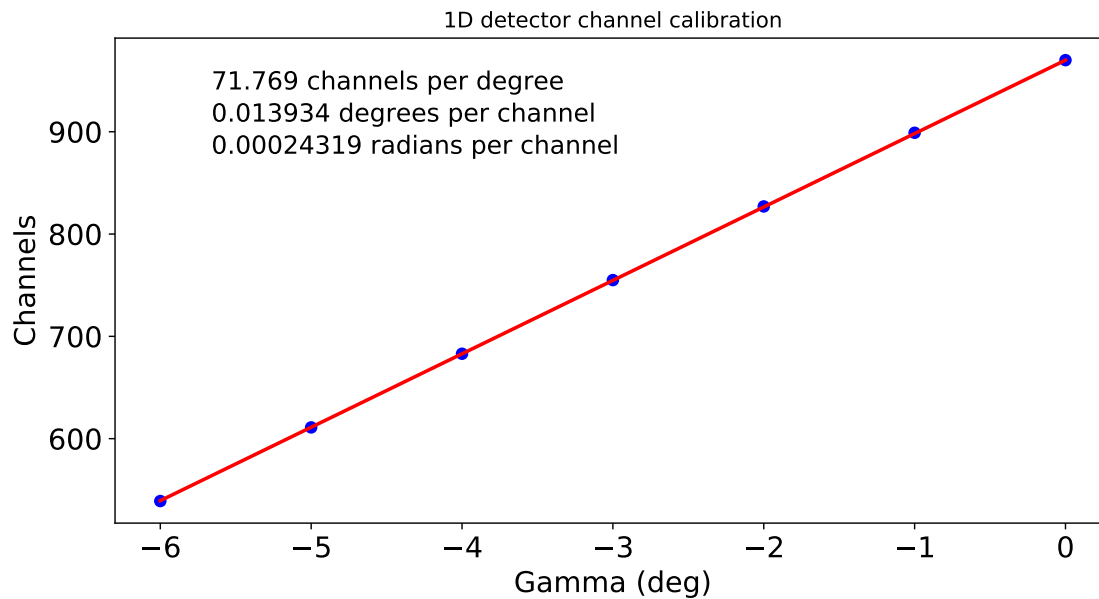
Fit with erf function.



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



2.2 Calibration thetaz



3 GIXD

3.0.1 SIRIUS_2020_03_12_0756: continuous_ascan delta -24 -19 100 5

Extraction of the Vineyard.

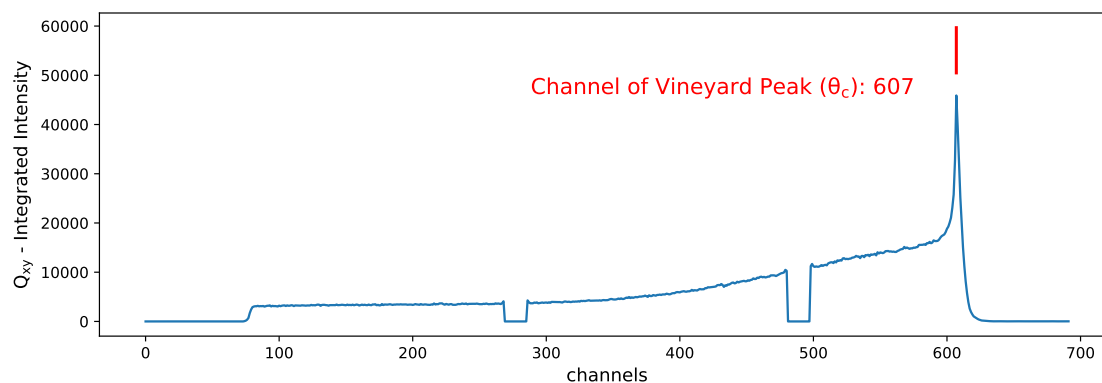
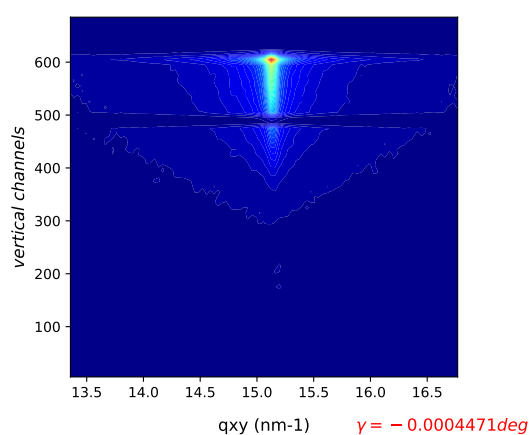
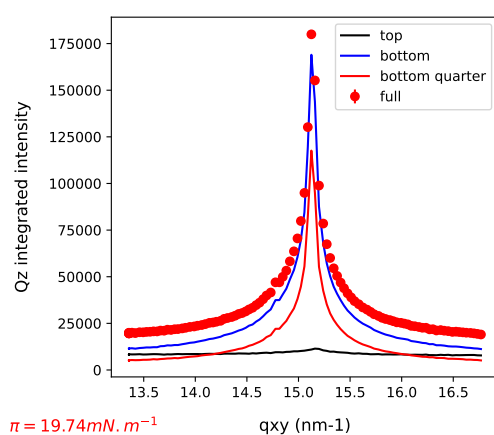
```
- Open Nexus Data File :
recording/SIRIUS_2020_03_12_0756.nxs
. Number of data points: 101
. Available Counters:
  0 -----> delta
  1 -----> zs
  2 -----> gamma
  3 -----> hu36energy
  4 -----> xs
  5 -----> energydcm
  6 -----> current
  7 -----> mon2
  8 -----> surfacepressure
  9 -----> areapermolecule
 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)
. 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

3.0.2 SIRIUS_2020_03_12_0756: continuous_ascan delta -24 -19 100 5

Classic GIXD with:

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

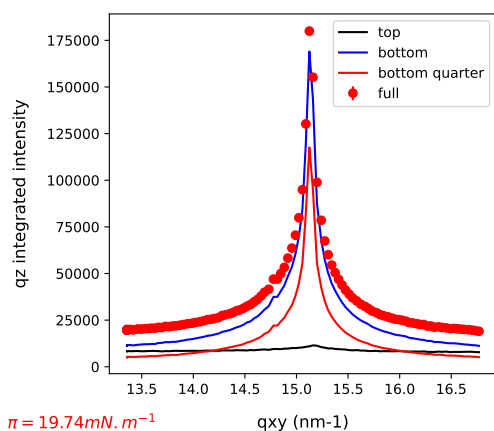
Generates:

- 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

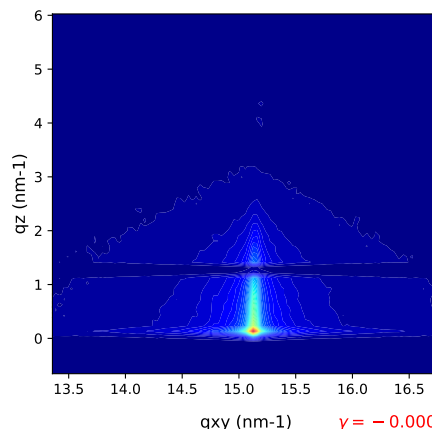
- Open Nexus Data File :

```
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 ± 3.944e-05 nm2 per
molecule
. Gamma motor data found, mean value -0.0004471 deg
Absorbers: 29 - Vide
```

SIRIUS_2020_03_12_0756.nxs



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



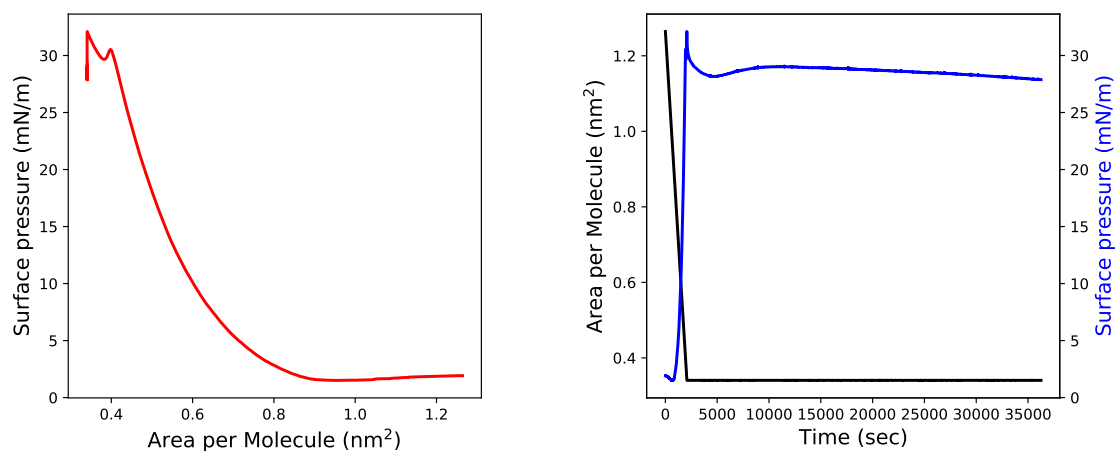
$\gamma = -0.0004471 \text{ deg}$

```
. 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
```


4 Isotherm

4.0.1 SIRIUS_Isotherm_2019_02_17_01544: isotherm 1.97 46 35000 1

SIRIUS_Isotherm_2019_02_17_01544

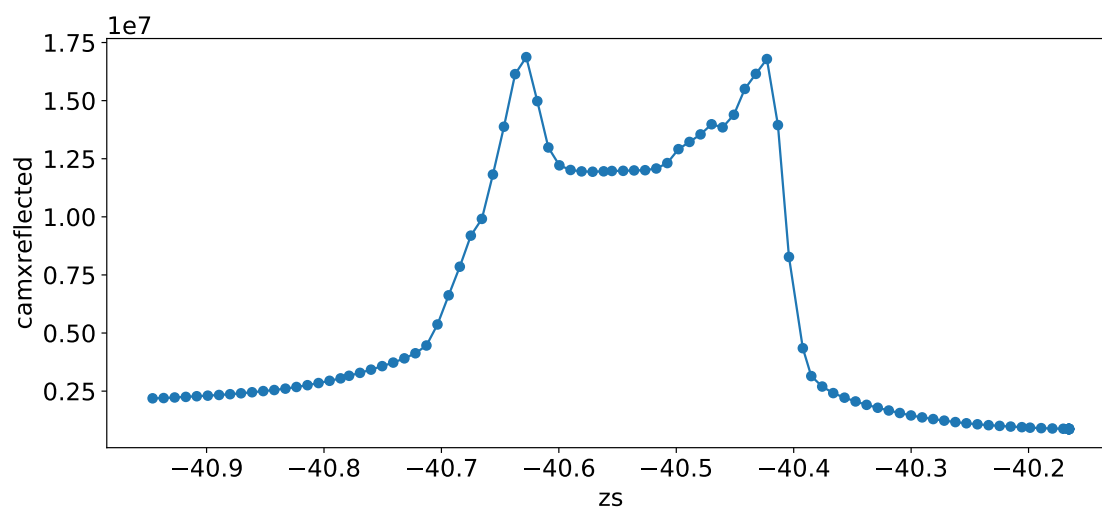


5 1D plot

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:

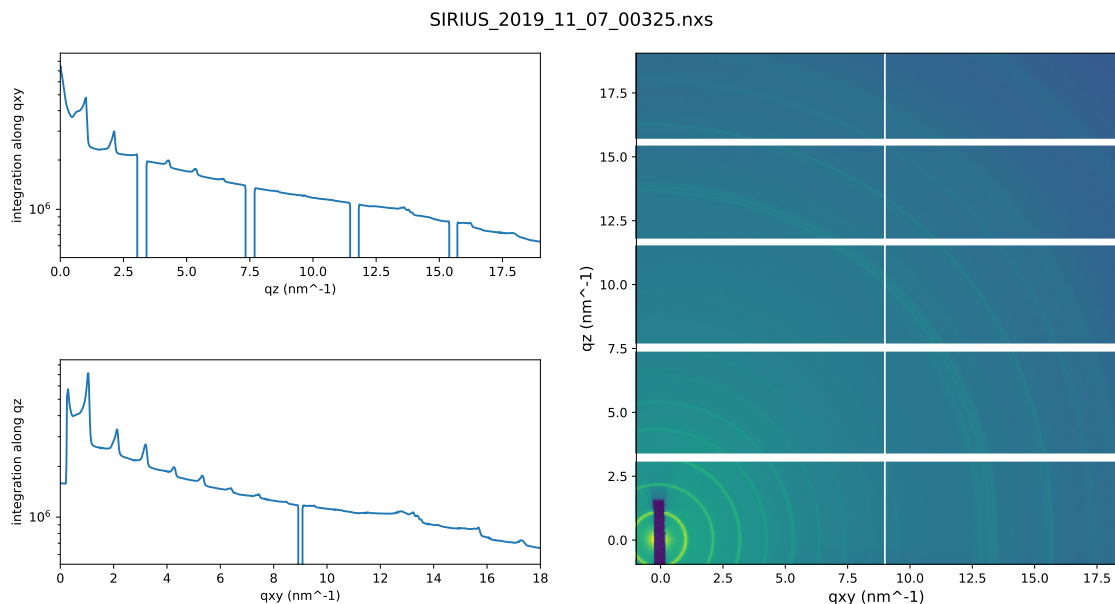
- SIRIUS_2019_11_07_00325_pilatus_sum.tiff
- SIRIUS_2019_11_07_00325_pilatus_sum.mat
- SIRIUS_2019_11_07_00325_integrated_qz.dat
- SIRIUS_2019_11_07_00325_integrated_qxy.dat

Absorbers: 29 - Vide

gamma is forced to the value: gamma = 0 deg

delta is forced to the value: delta = 11.58 deg

thetai is forced to the value: thetai = 0 deg



7 Plot Pilatus

7.0.1 SIRIUS_2019_11_07_00325: tscan 10 10

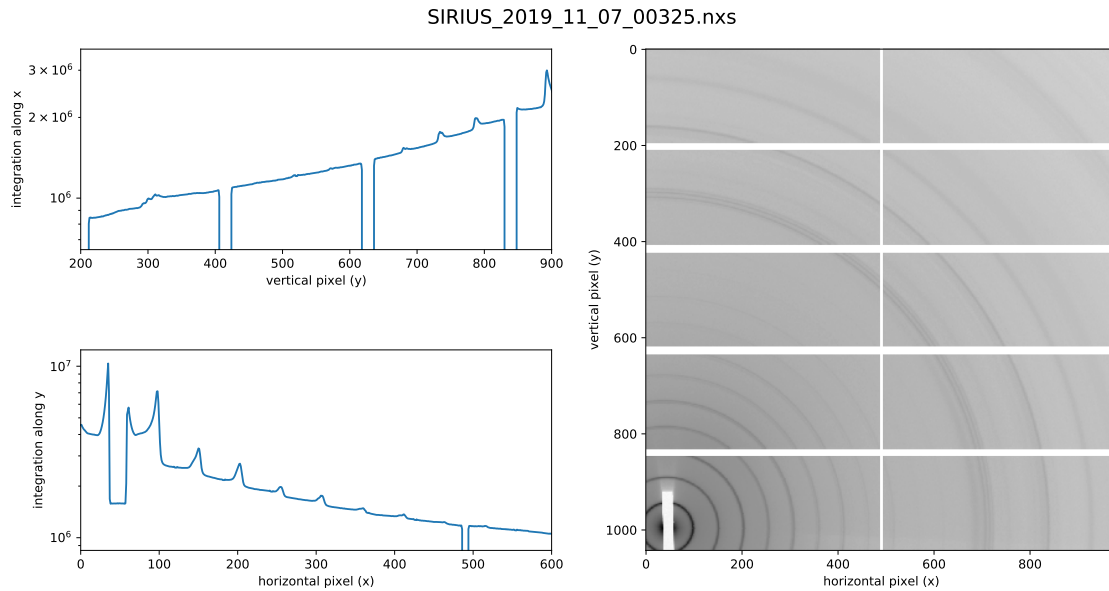
Plot the sum of the images from the Pilatus (time integration).

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



8 XRF

8.0.1 SIRIUS_2017_12_11_08042: run xsw7.ipynb

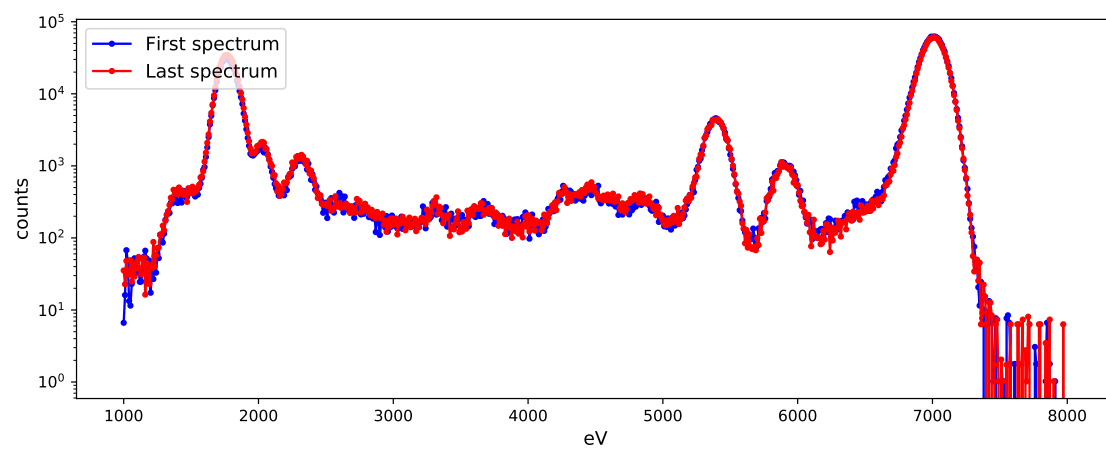
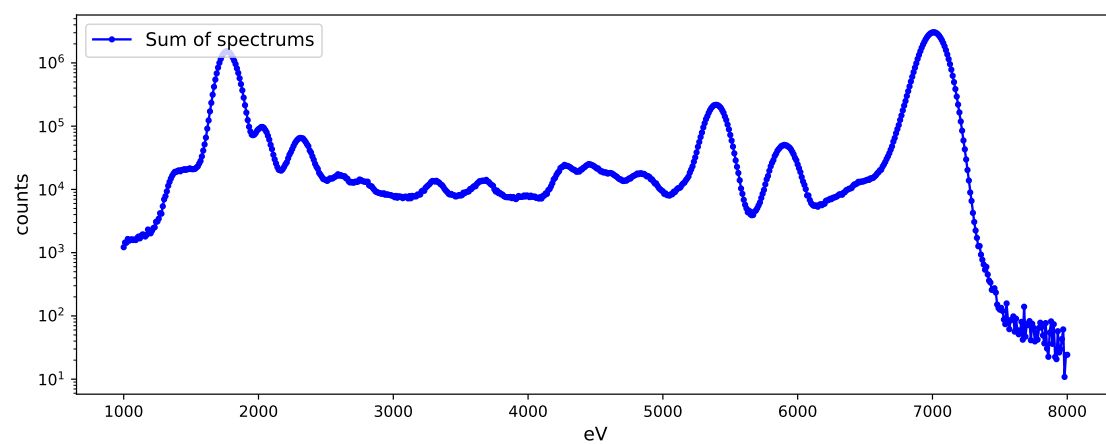
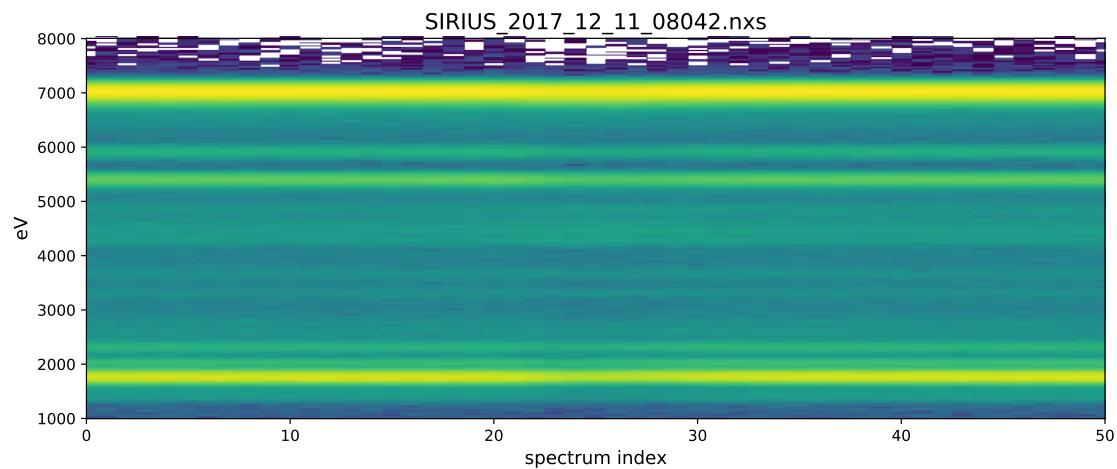
Plot XRF from the 4-elements detector, in channels and without peak identification.

Generates:

- SIRIUS_2017_12_11_08042_fluospectrum.mat for each element
- SIRIUS_2017_12_11_08042.dat

8.0.2 SIRIUS_2017_12_11_08042: run xsw7.ipynb

Absorbers: Al 200micron



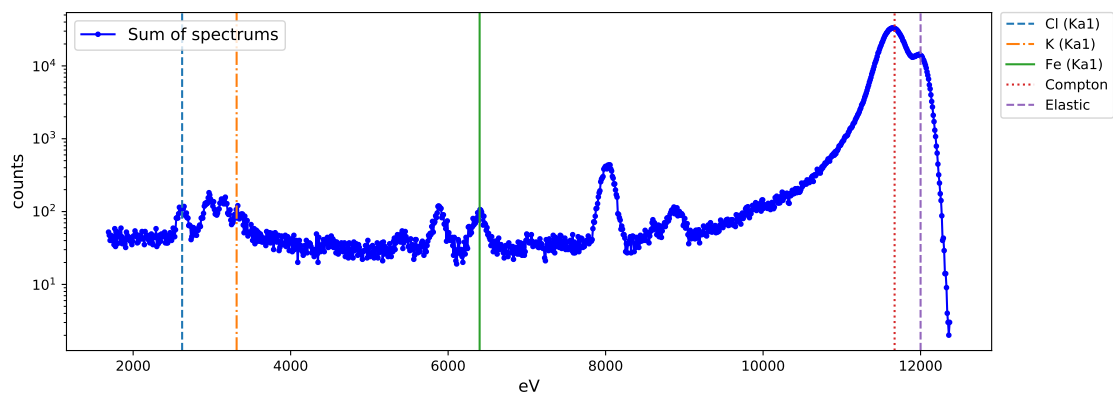
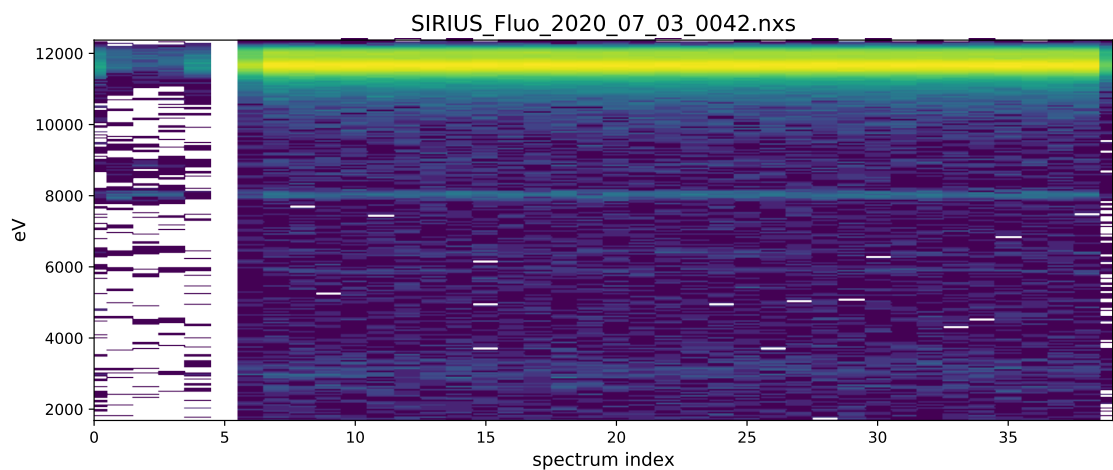
8.0.3 SIRIUS_Fluo_2020_07_03_0042: tscan 500 30

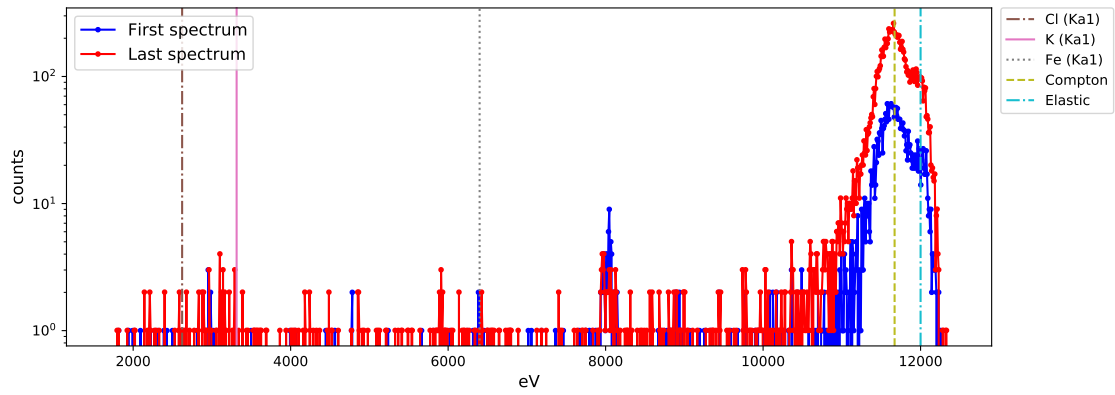
Plot XRF from the 1-element detector, in eVs and with peak identification.

Generates:

- SIRIUS_Fluo_2020_07_03_0042_fluospectrum04.mat
- SIRIUS_Fluo_2020_07_03_0042.dat

Absorbers: Al 800micron

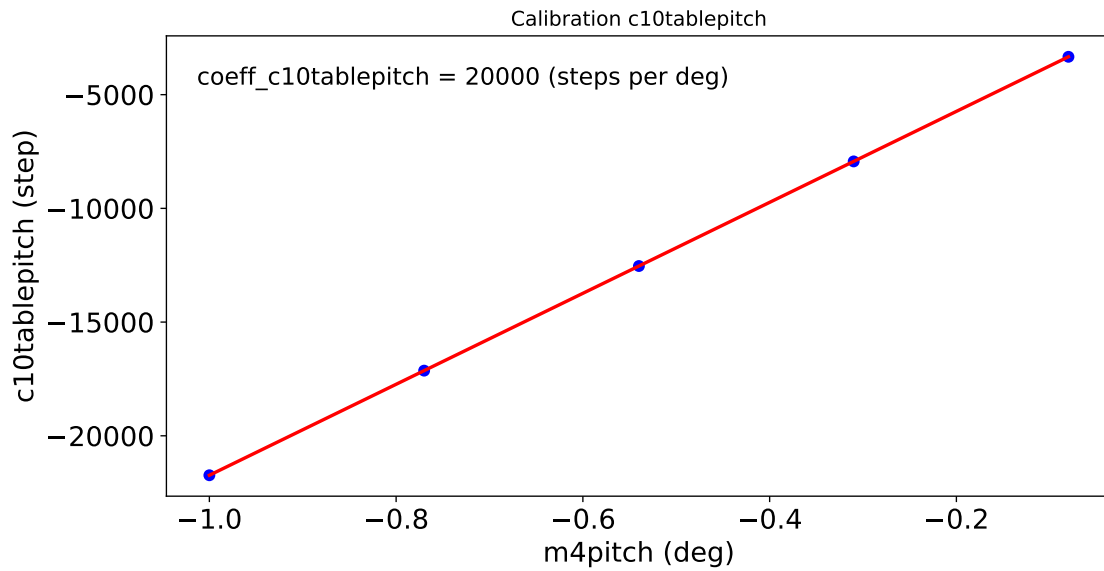


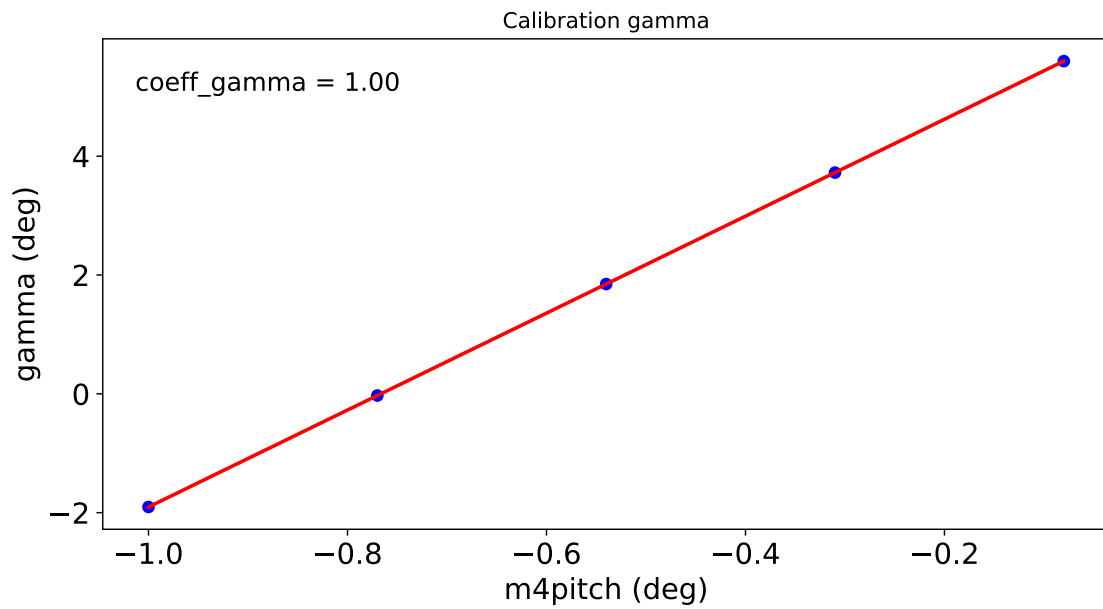
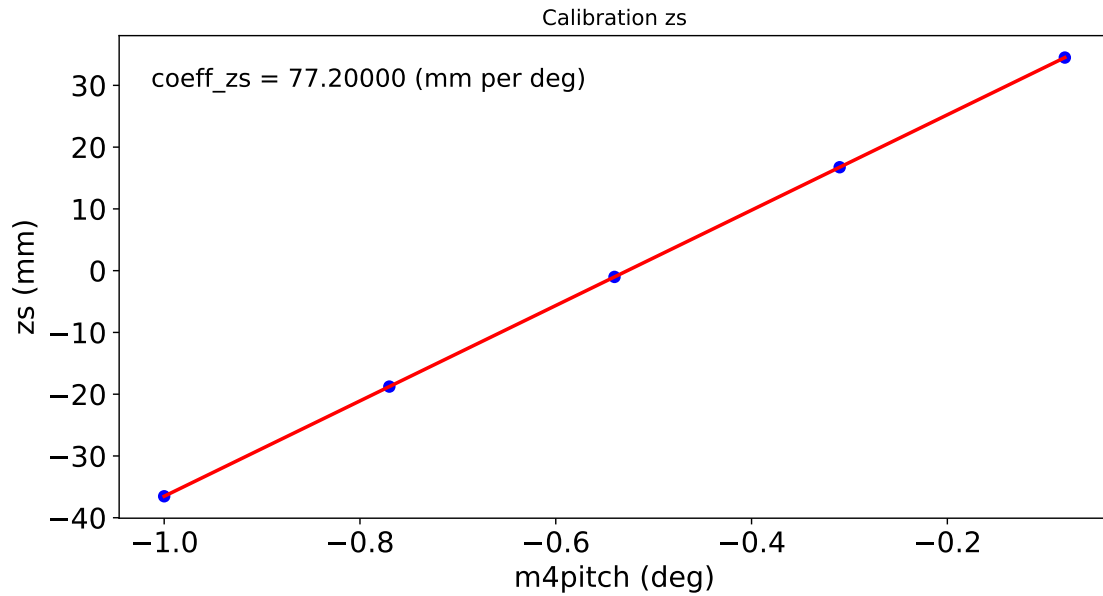


9 XRR

9.1 Calibration XRR

To start the calibration click on ''Calib. XRR''.



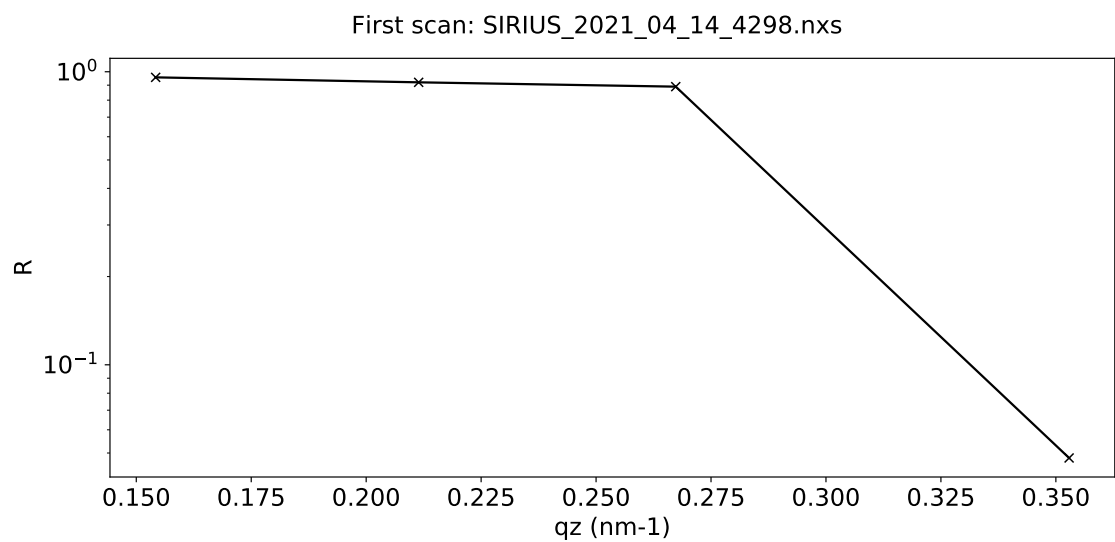
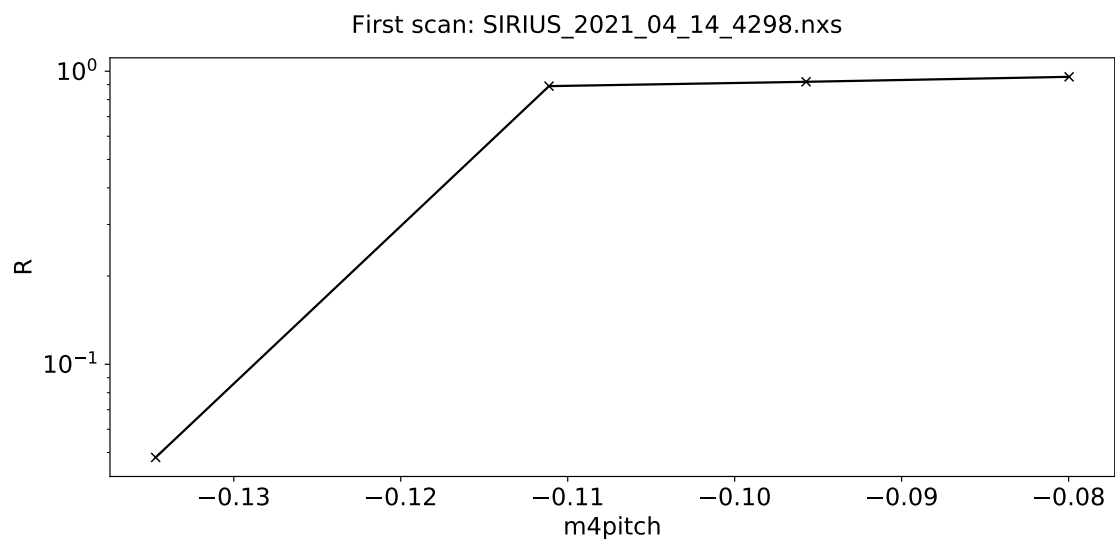


9.2 Scan XRR

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: run XRR.ipy

Direct extracted from SIRIUS_2021_04_14_4297.nxs: direct=2.45544e+12



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
%amove delta -35
%continuous_ascan delta -35 -25 250 5 #123
%run reset_motors.ipynb

for i in range(4):
    %amove delta -20
    %continuous_ascan delta -10 -3 175 5 #124 #126 #128 #130
    %run reset_motors.ipynb
    %run cont_regh_abs.ipynb #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.ipynb

    %run cont_regh_abs.ipynb #133 #136 #139
    %run cont_regh_abs.ipynb #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
```

11 Insert positions

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

11.0.1 wm m4

m4roll	m4pitch	m4tracks_mot	m4tz
2.10	-0.0802	1.001	2.42
deg	deg	mm	mm

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	0.000	-15.727
			mrاد	mrاد	mm

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

12 Insert commands

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

```

Wed, 11 Mar 2020 16:44:04 amove basez -67
Wed, 11 Mar 2020 16:44:11 amove basez 67
Wed, 11 Mar 2020 16:44:58 amove basez 75
Wed, 11 Mar 2020 16:46:26 shopen

```

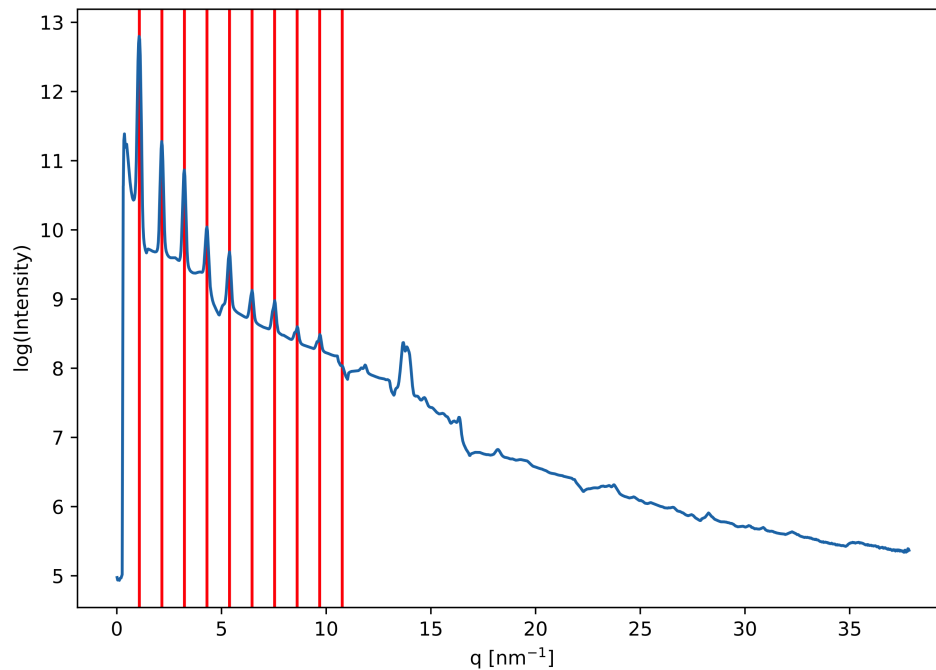
Wed, 11 Mar 2020 16:46:34 ct 1
Wed, 11 Mar 2020 16:46:47 ct 1
Wed, 11 Mar 2020 16:46:56 dmove basez 1

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 Export to pdf

PDF generated by clicking on “Export to pdf”.