Example

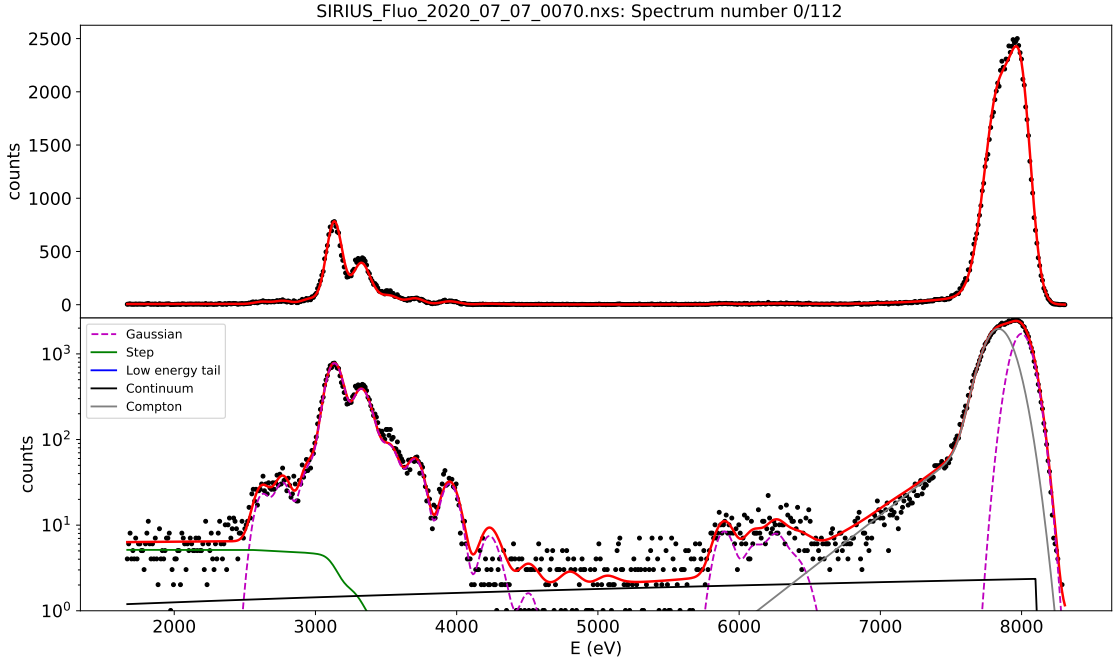
June 2, 2021

Contents

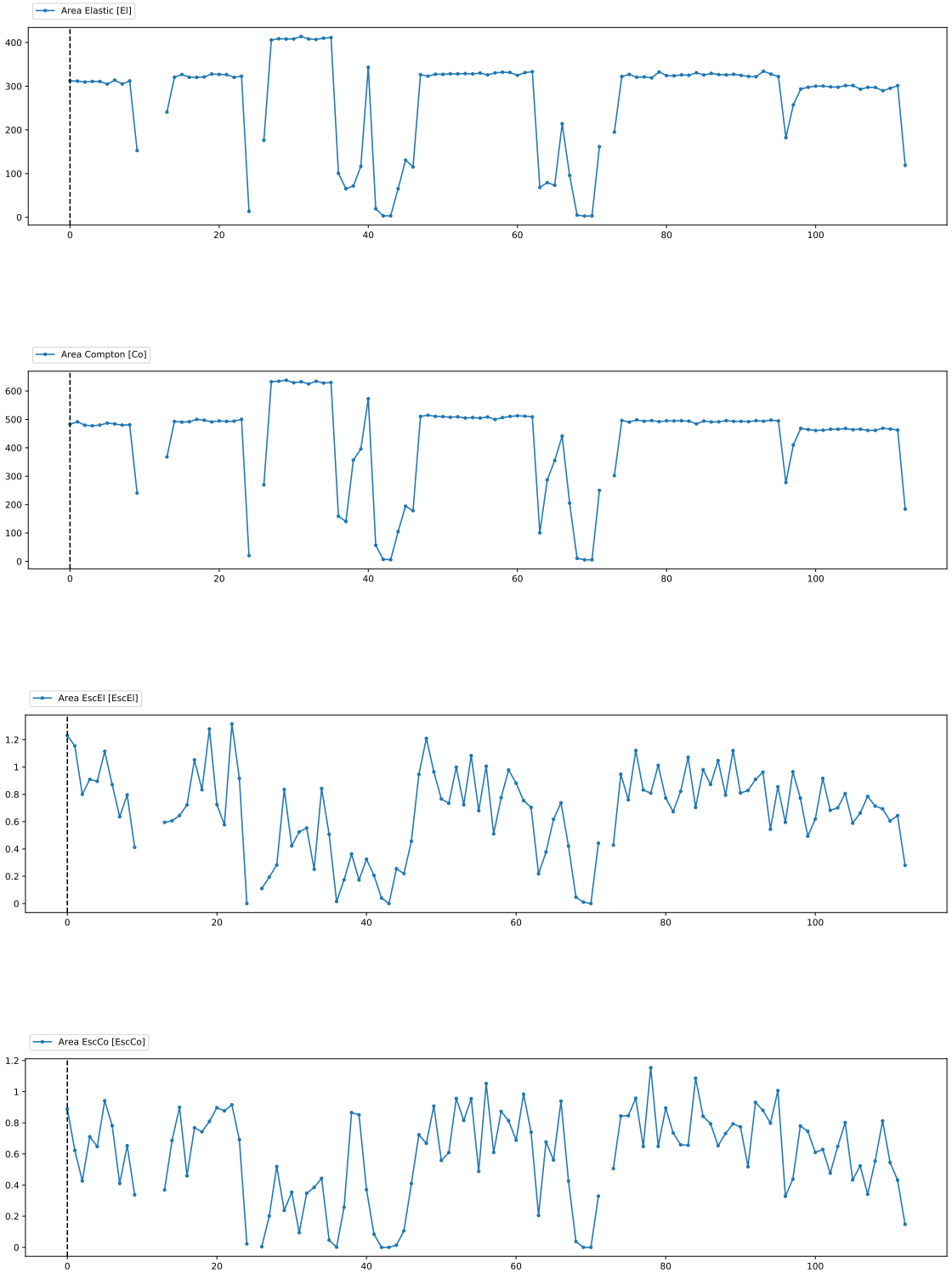
0.0.1 SIRIUS_Fluo_2020_07_07_0070

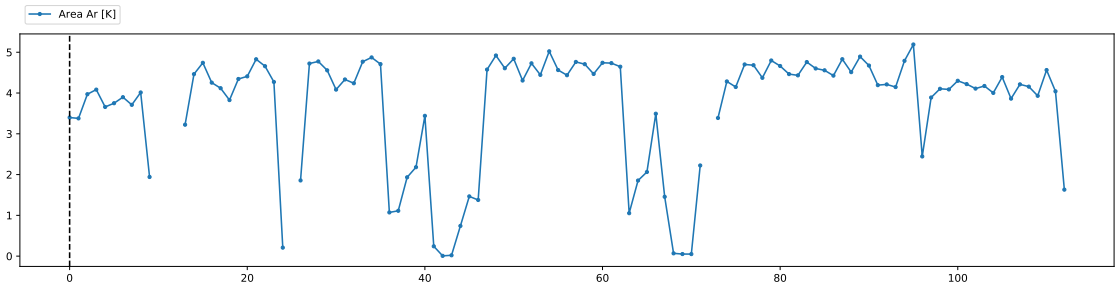
Spectrums with Cadmium and traces of Manganese and Iodine. We can see well the evolution of Cadmium with time.
The compton peak is quite large, but can be well modeled with a foot at low energy (gammaA=4.7, fA=0.1).

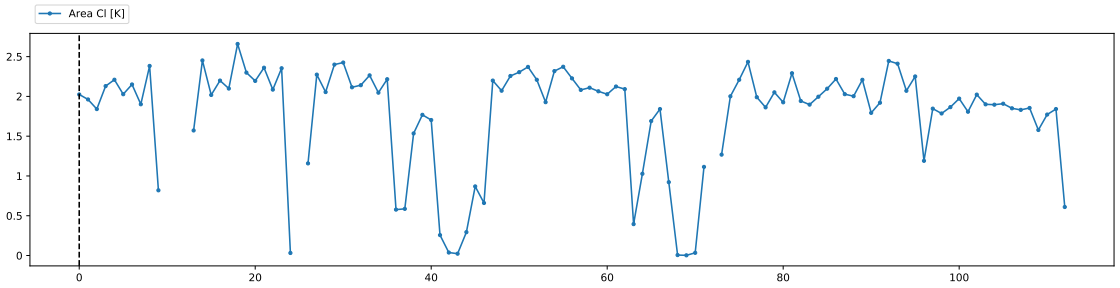
```
Fit results for SIRIUS_Fluo_2020_07_07_0070.nxs
Spectrum interval = [0,112]
Channel interval = [170,840]
List of chosen elements:  ['Element 4']
List of fitted parameters: ['sl', 'ct']

Initial fit parameters:
beam energy = 8000
gain = 9.9086; eV0 = -16.84
epsilon = 0.0036; fano = 0.115; noise = 0.10317
sl = 0; ct = 2
sfa0 = 0.89986; tfb0 = 0; twc0 = 0.1
fG = 1.41047; fA = 0.107121; fB = 0; gammaA = 4.71378; gammaB = 0
```

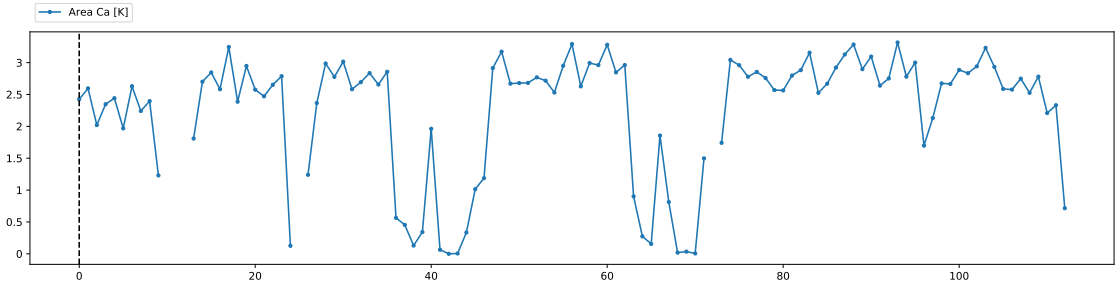


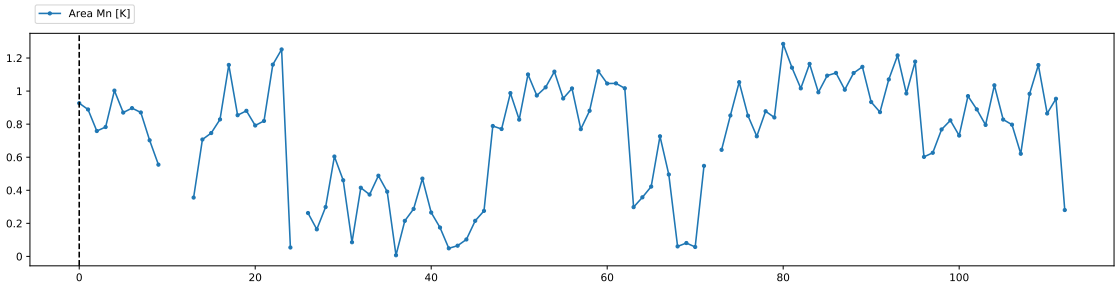
AREAS

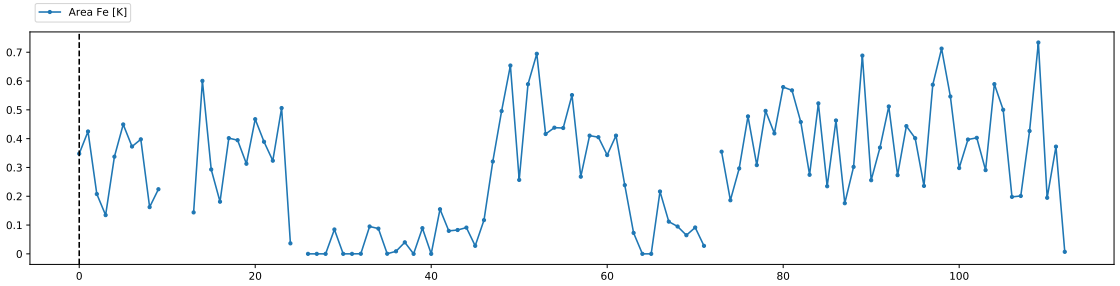

Area Elastic [El]
Area Compton [Co]
Area EscEl [EscEl]
Area EscCo [EscCo]

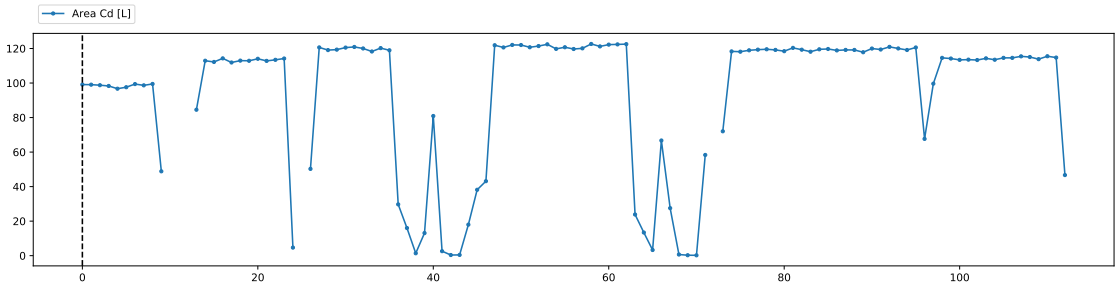

Area Ar [K]
0
1
2
3
4
5
0
20
40
60
80
100

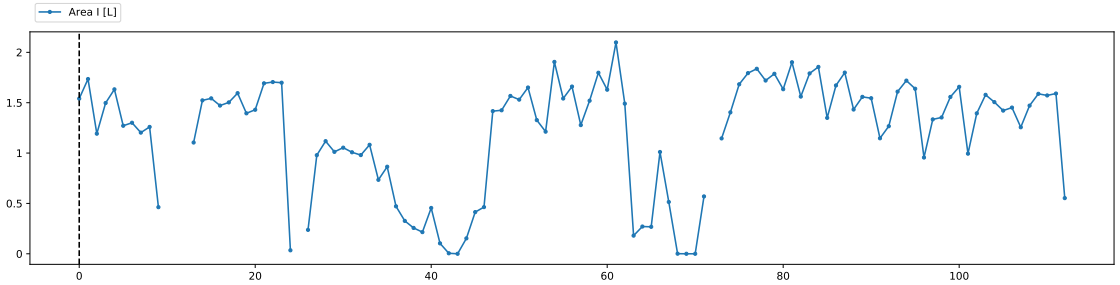

Area Cl [K]
0
0.5
1
1.5
2
2.5
0
20
40
60
80
100


Area Ca [K]
0
0.5
1
1.5
2
2.5
3
0
20
40
60
80
100

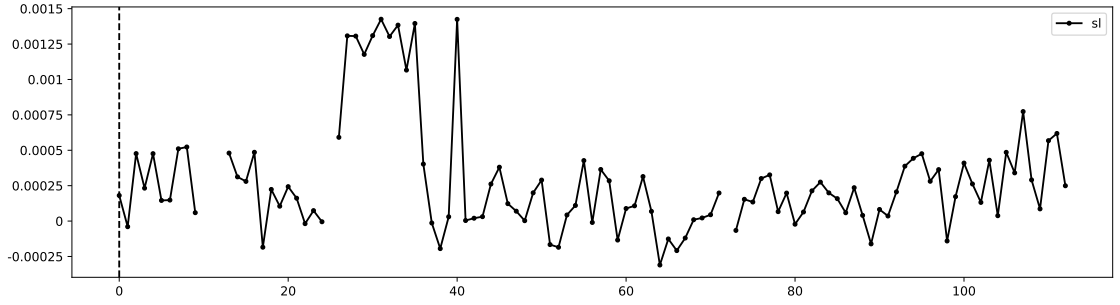

Area Mn [K]
0
0.2
0.4
0.6
0.8
1
1.2
0
20
40
60
80
100

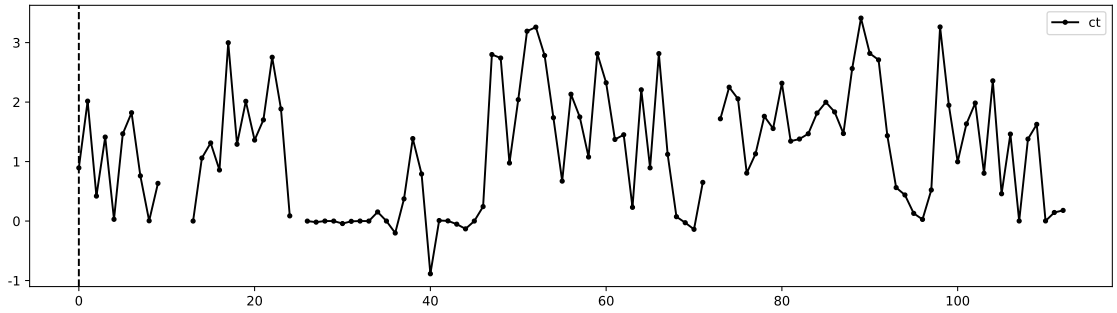






OTHER PARAMETERS

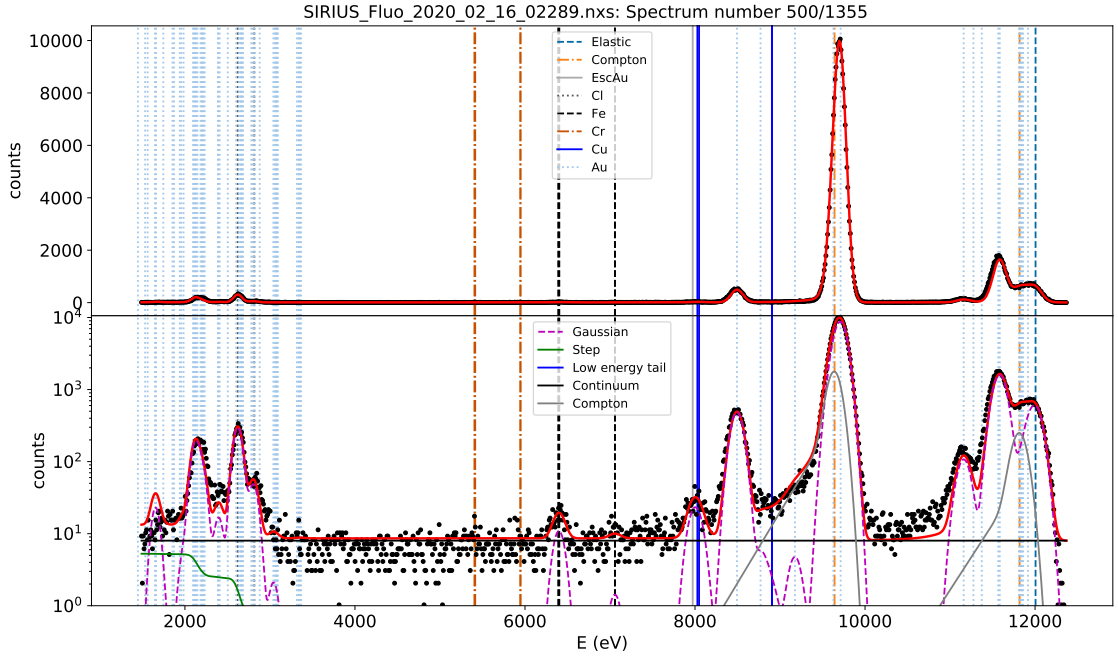




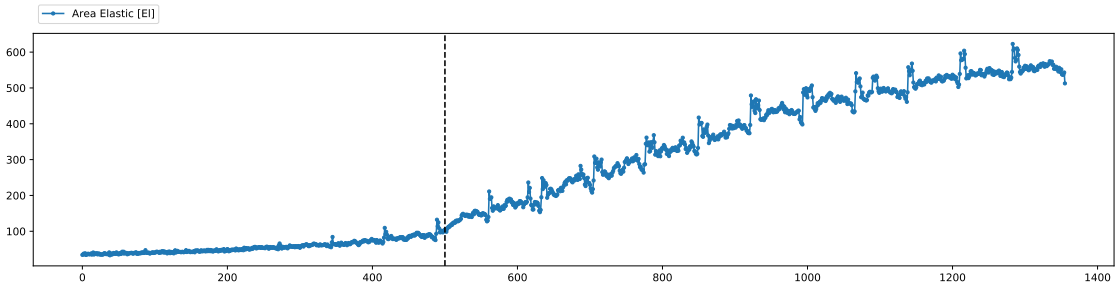
0.0.2 SIRIUS_Fluo_2020_02_16_02289

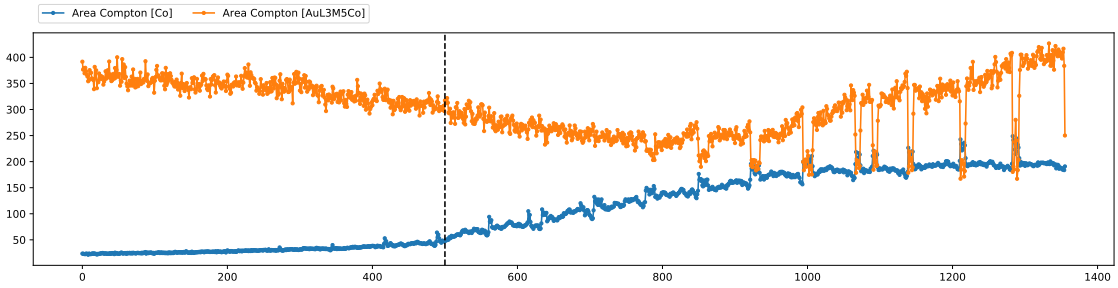
A series of spectrums which is a bit more difficult to fit, due to the many different lines of gold and their high intensities.
It is required to add a Compton peak for the Au La1 line. Do not forget to name it “Compton” as well.
We also add an escape peak for this Au La1 line. Do not name it ‘Au’! Here we name it ‘EscAuLa1’.
Another difficulty is the strong change of the nature of the interface, with an associated rise of the Compton scattering. All in all the fits are quite good even without any fitting parameters.

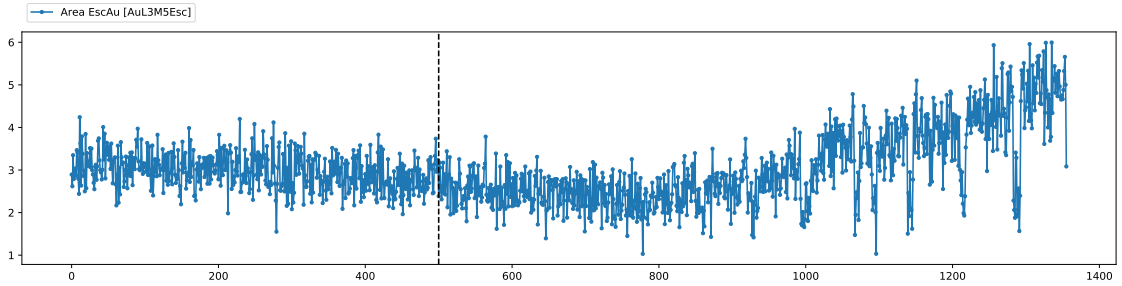
```
Fit results for SIRIUS_Fluo_2020_02_16_02289.nxs
Spectrum interval = [50,1405]
Channel interval = [150,1250]
List of chosen elements:  ['Element 4']
List of fitted parameters: []

Initial fit parameters:
beam energy = 12000
gain = 9.89; eV0 = 6
epsilon = 0.0036; fano = 0.115; noise = 0.08915
sl = 0; ct = 8
sfa0 = 0.8; tfb0 = 0; twc0 = 0.1
fG = 1.04571; fA = 0.238138; fB = 0; gammaA = 3; gammaB = 0
```

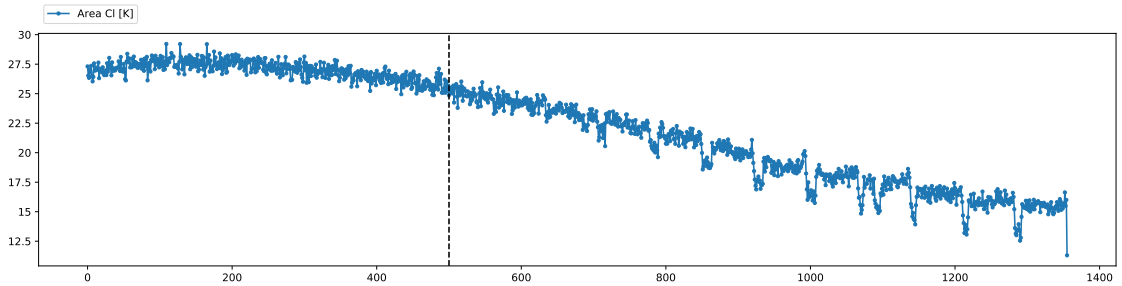

SIRIUS_Fluo_2020_02_16_02289.nxs: Spectrum number 500/1355
Elastic
Compton
EscAu
Cl
Fe
Cr
Cu
Au
Gaussian
Step
Low energy tail
Continuum
Compton
counts
E (eV)

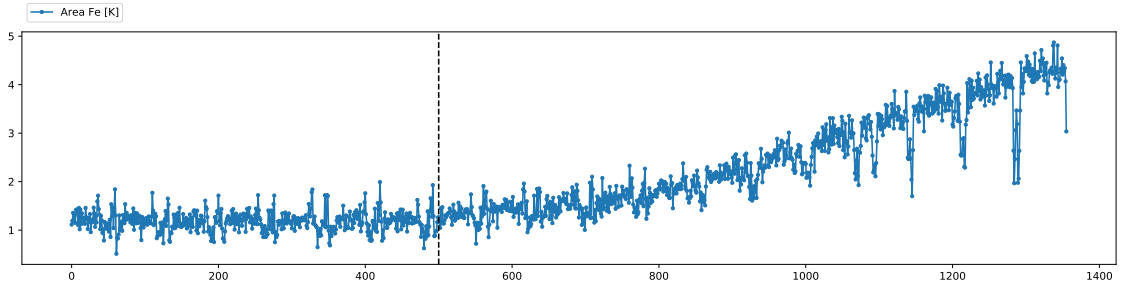
AREAS

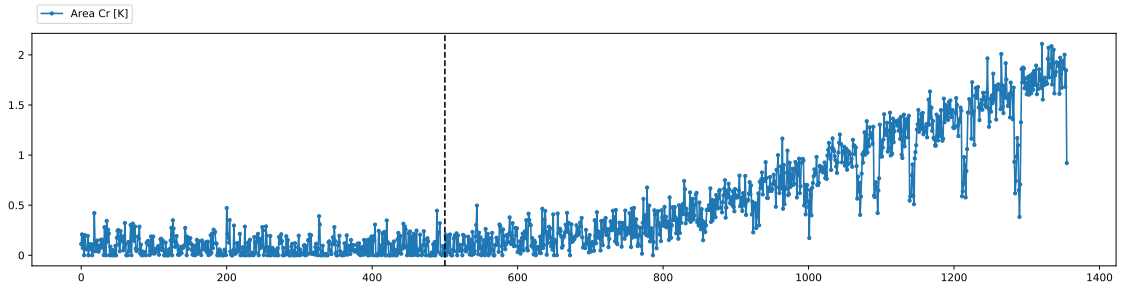

Area Elastic [El]

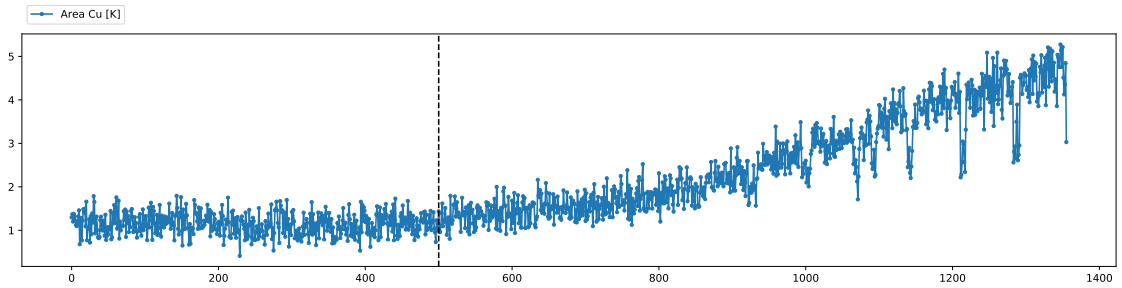

Area Compton [Co]
Area Compton [AuL3M5Co]

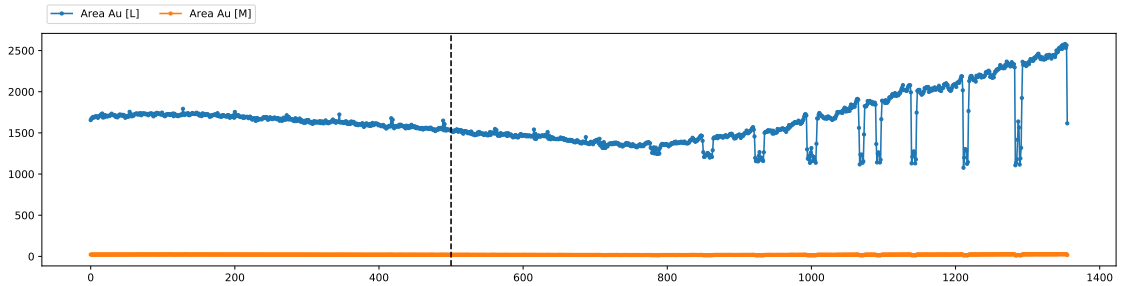

Area EscAu [AuL3M5Esc]
6
5
4
3
2
1
0
200
400
600
800
1000
1200
1400


Area Cl [K]
30
27.5
25
22.5
20
17.5
15
12.5
0
200
400
600
800
1000
1200
1400

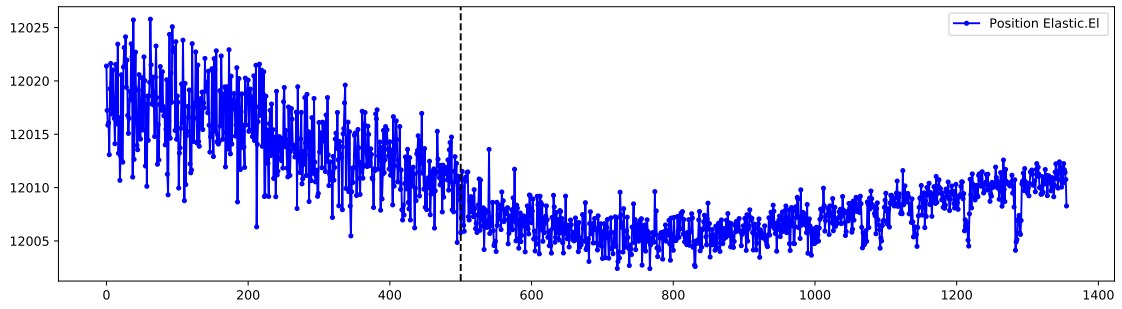

Area Fe [K]
5
4
3
2
1
0
200
400
600
800
1000
1200
1400

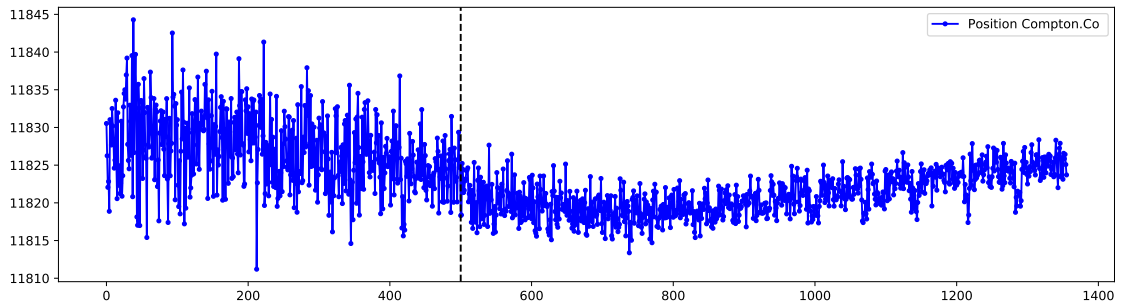

Area Cr [K]
2
1.5
1
0.5
0
200
400
600
800
1000
1200
1400

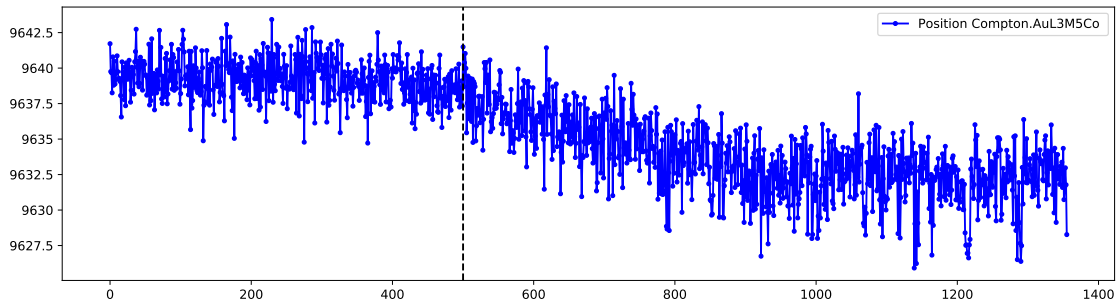

Area Cu [K]
5
4
3
2
1
0
200
400
600
800
1000
1200
1400


Area Au [L]
Area Au [M]
2500
2000
1500
1000
500
0
0
200
400
600
800
1000
1200
1400

POSITIONS


Position Elastic.El
12025
12020
12015
12010
12005
0
200
400
600
800
1000
1200
1400

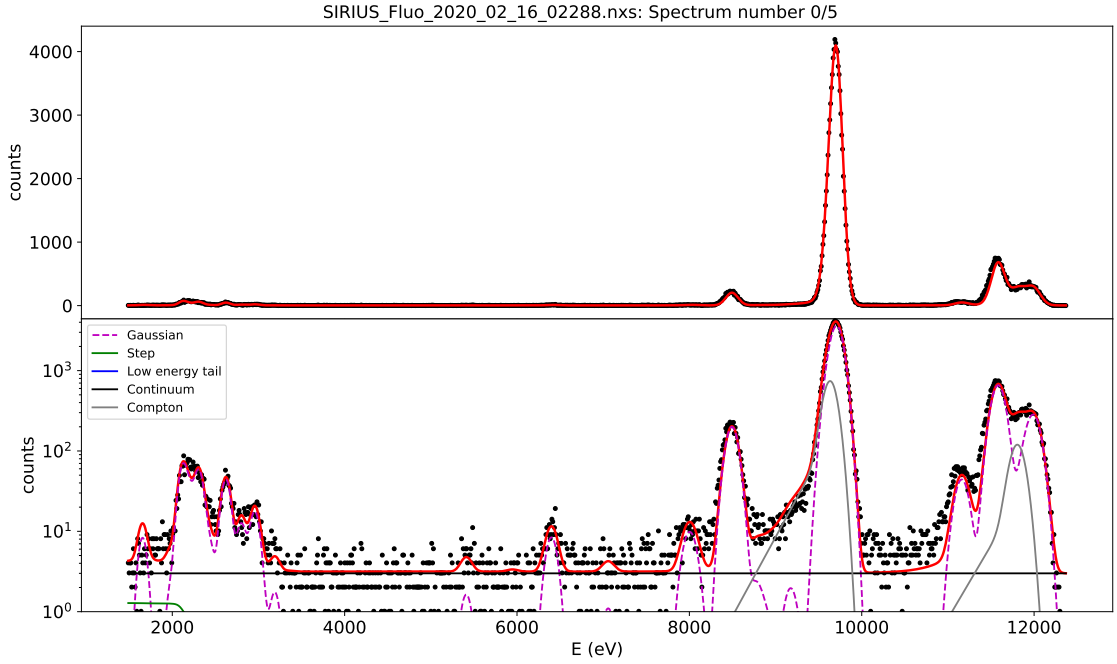

Position Compton.Co
11845
11840
11835
11830
11825
11820
11815
11810
0
200
400
600
800
1000
1200
1400



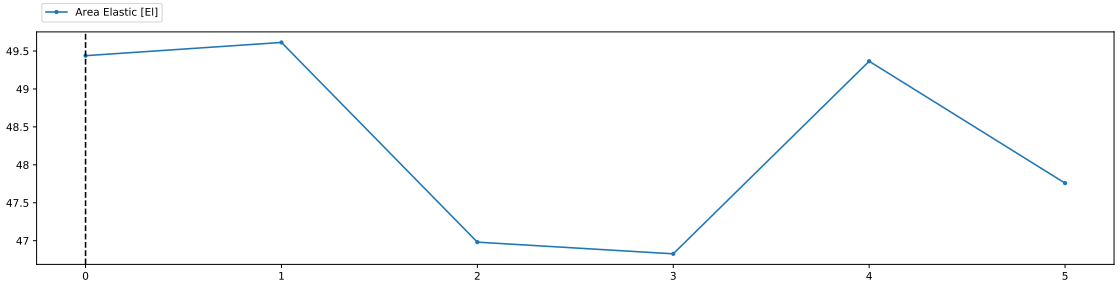
0.0.3 SIRIUS_Fluo_2020_02_16_02288

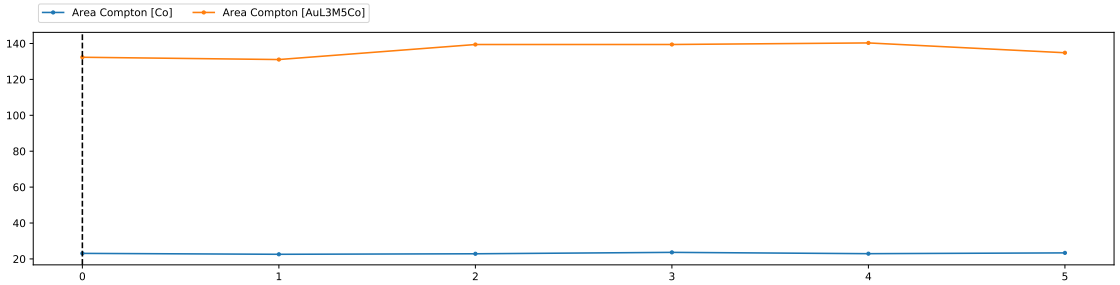
Spectrums from the same series as SIRIUS_Fluo_2020_02_16_02289.
Here to show that we can fit the curve with the same parameters as the previous one (only with a small adjustement of the noise via ct, and of the low energy step via sfa0).
Fitting all the time series may require a bit more work, with a noise continuously increasing (may be by fitting via sl and ct).
Here, the quantitative fitting allows one to show an increase of the Argon contribution as compared to the previous scan, and the potential contamination with Sulfur.

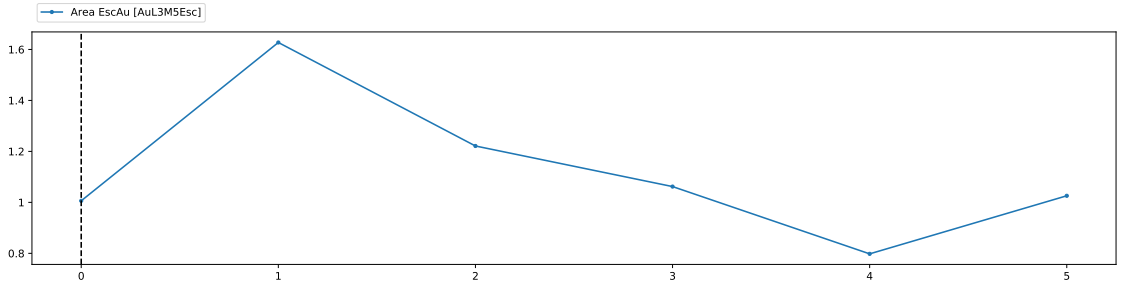
```
Fit results for SIRIUS_Fluo_2020_02_16_02288.nxs
Spectrum interval = [50,55]
Channel interval = [150,1250]
List of chosen elements:  ['Element 4']
List of fitted parameters: ['sfa0']

Initial fit parameters:
beam energy = 12000
gain = 9.89; eV0 = 6
epsilon = 0.0036; fano = 0.115; noise = 0.08915
sl = 0; ct = 3
sfa0 = 0.404519; tfb0 = 0; twc0 = 0.1
fG = 1.04571; fA = 0.238138; fB = 0; gammaA = 3; gammaB = 0
```

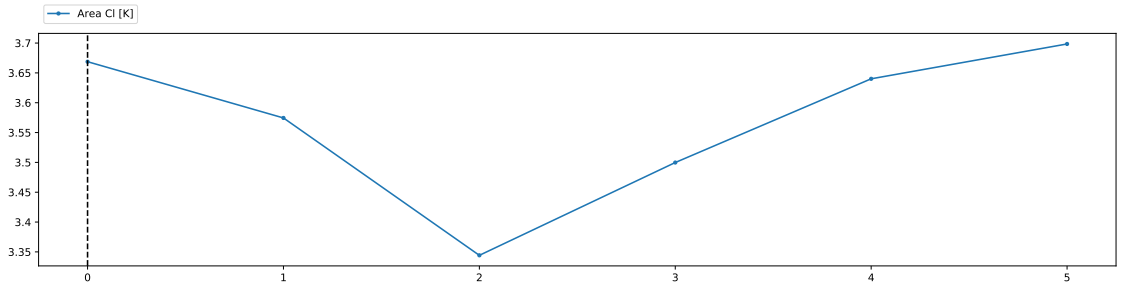

SIRIUS_Fluo_2020_02_16_02288.nxs: Spectrum number 0/5
counts
Gaussian
Step
Low energy tail
Continuum
Compton
E (eV)

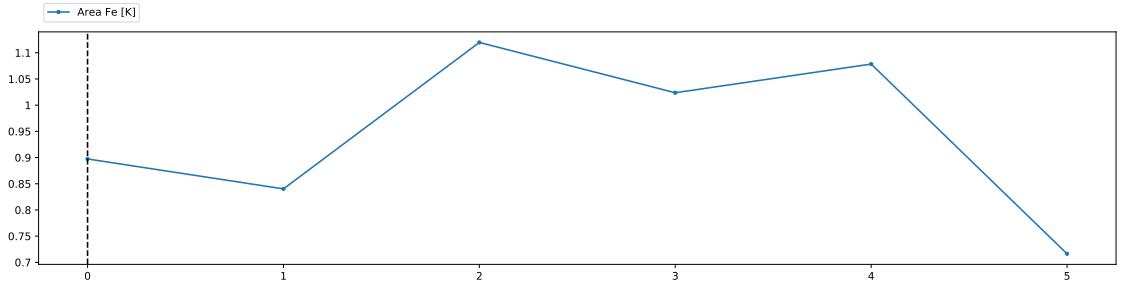
AREAS

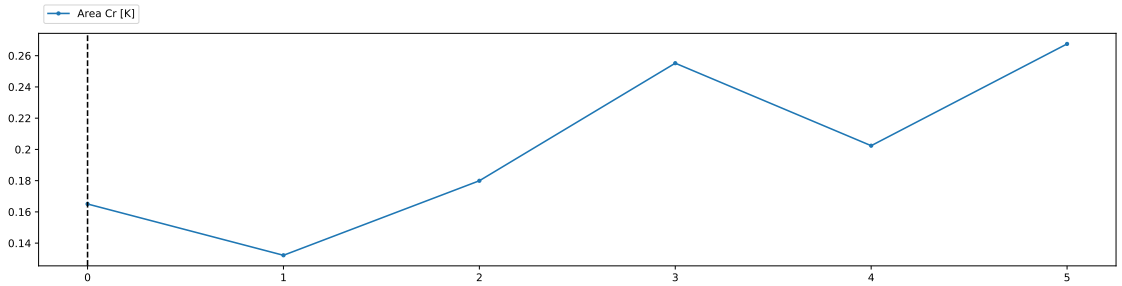

Area Elastic [El]

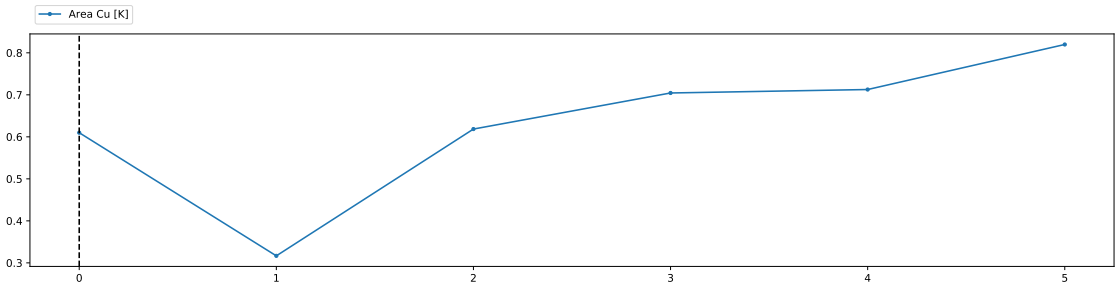

Area Compton [Co]
Area Compton [AuL3M5Co]

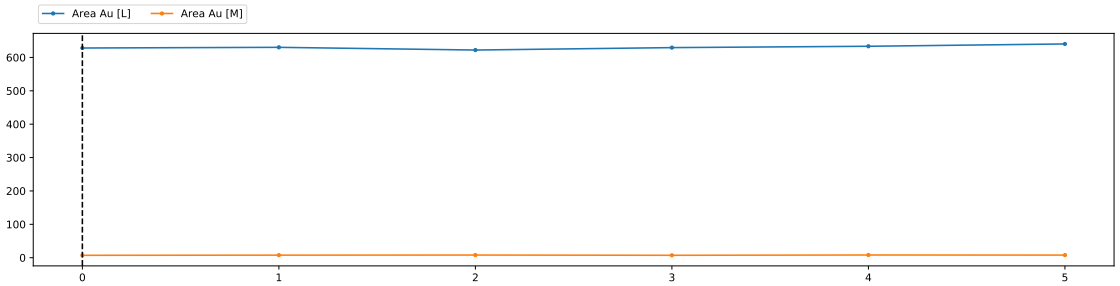

Area EscAu [AuL3M5Esc]
1.6
1.4
1.2
1
0.8
0
1
2
3
4
5

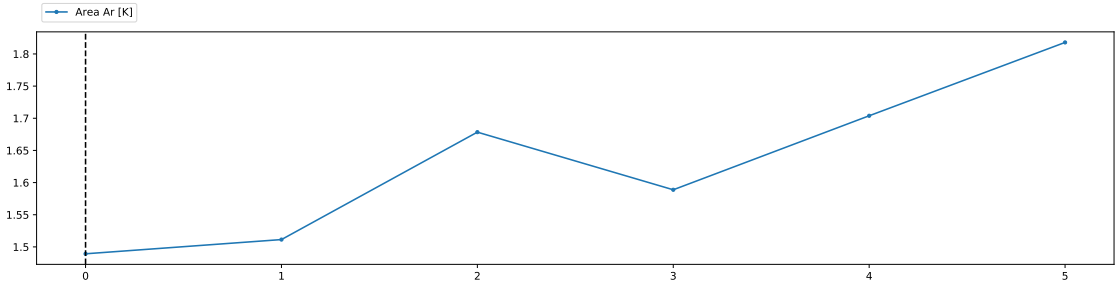

Area Cl [K]
3.7
3.65
3.6
3.55
3.5
3.45
3.4
3.35
0
1
2
3
4
5

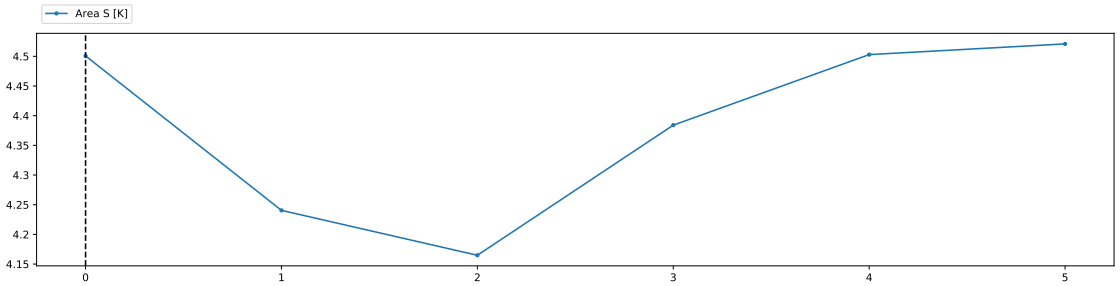

Area Fe [K]
1.1
1.05
1
0.95
0.9
0.85
0.8
0.75
0.7
0
1
2
3
4
5

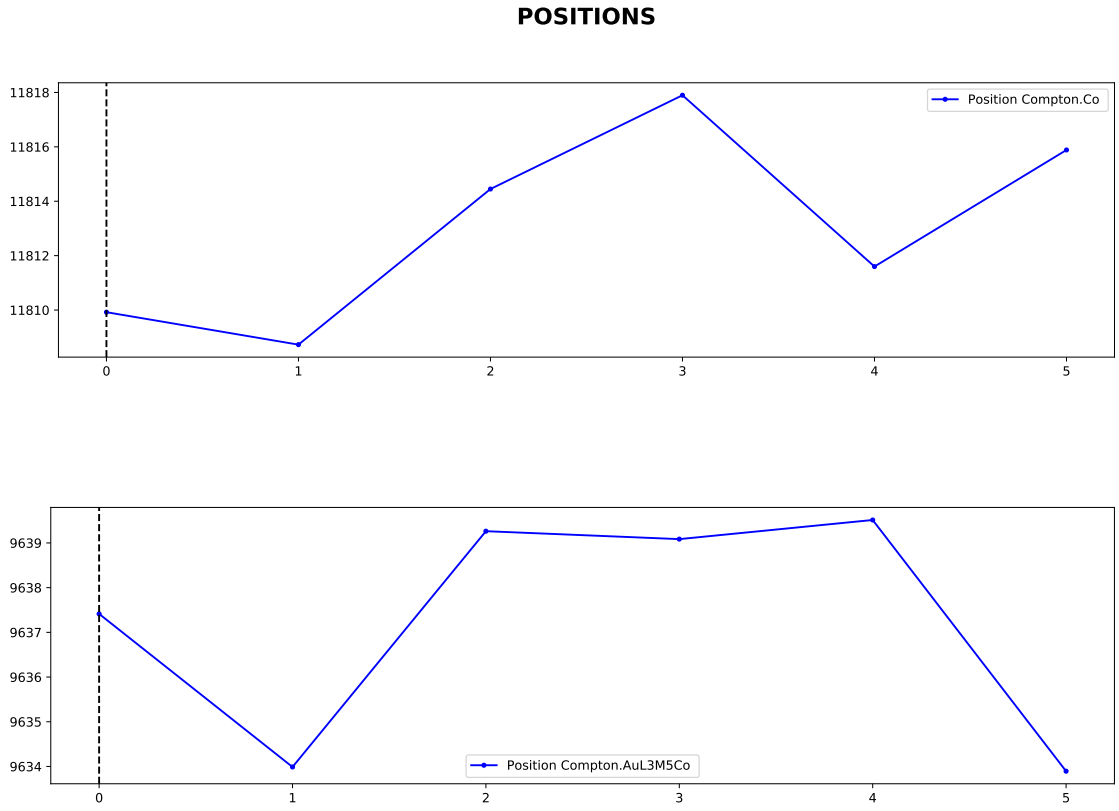

Area Cr [K]
0.26
0.24
0.22
0.2
0.18
0.16
0.14
0
1
2
3
4
5


Area Cu [K]
0.8
0.7
0.6
0.5
0.4
0.3
0
1
2
3
4
5


Area Au [L]
Area Au [M]
600
500
400
300
200
100
0
0
1
2
3
4
5


Area Ar [K]
1.8
1.75
1.7
1.65
1.6
1.55
1.5
0
1
2
3
4
5

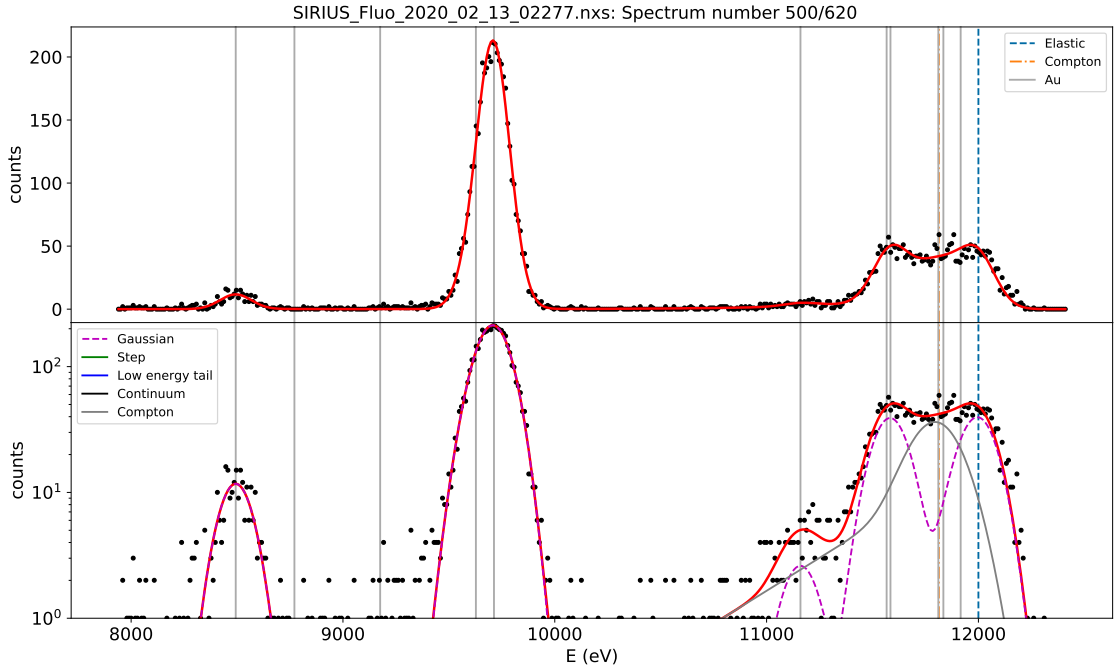

Area S [K]
4.5
4.45
4.4
4.35
4.3
4.25
4.2
4.15
0
1
2
3
4
5

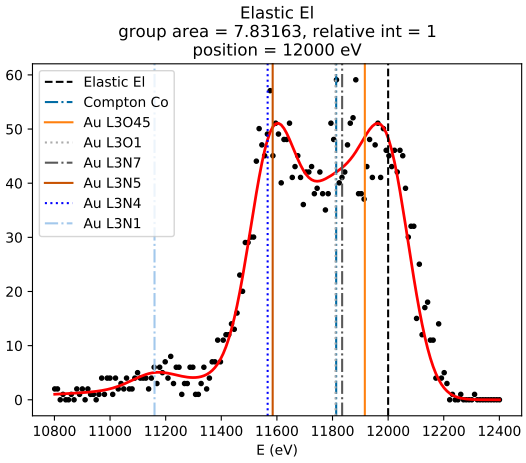


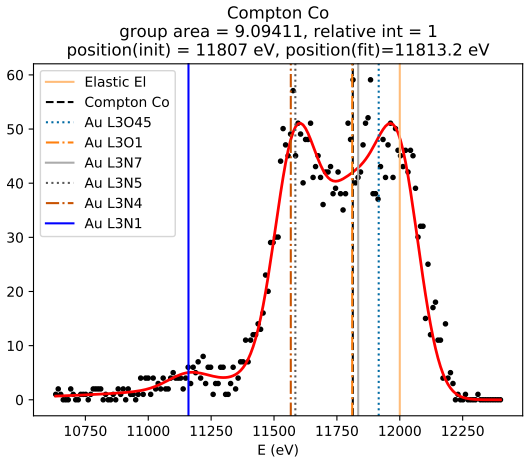
0.0.4 SIRIUS_Fluo_2020_02_13_02277

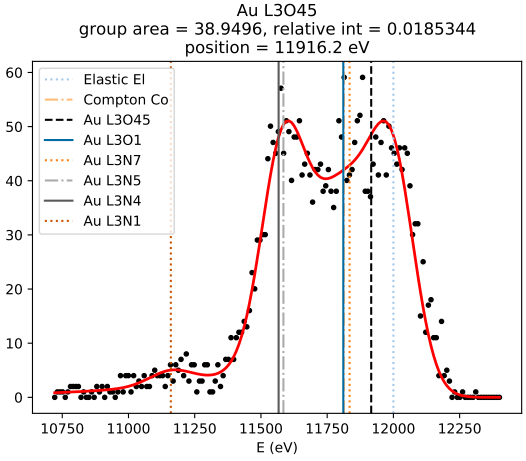
An example of fits with a limited number of peaks (only one line of Au, Compton and Rayleigh). The fit is therefore very fast, and quite good considering the low couting time per point. Conclusion: a quick and good analysis can be done by pointing only the most intense peaks.

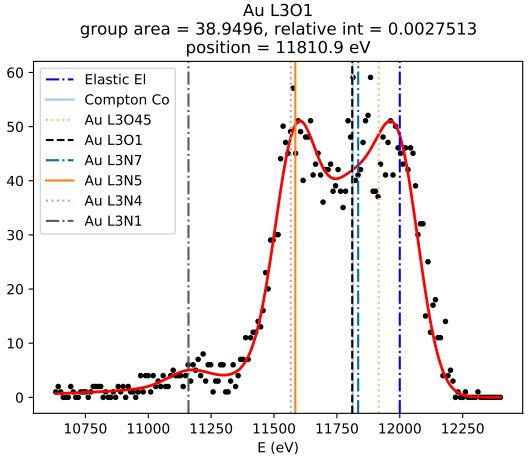
```
Fit results for SIRIUS_Fluo_2020_02_13_02277.nxs
Spectrum interval = [1,621]
Channel interval = [800,1250]
List of chosen elements:  ['Element 4']
List of fitted parameters: []

Initial fit parameters:
beam energy = 12000
gain = 9.9329; eV0 = -5.98
epsilon = 0.0036; fano = 0.115; noise = 0.10535
sl = 0; ct = 0
sfa0 = 0; tfb0 = 0; twc0 = 0.1
fG = 1.41047; fA = 0.52325; fB = 0; gammaA = 5; gammaB = 0
```

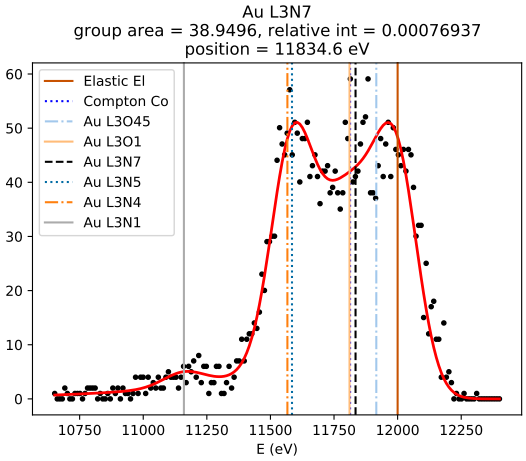


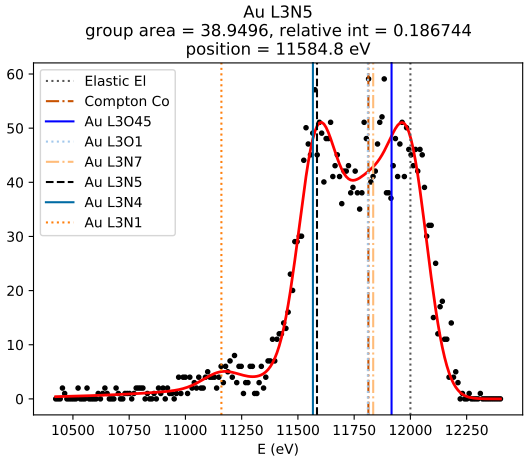

Elastic El
group area = 7.83163, relative int = 1
position = 12000 eV
Elastic El
Compton Co
Au L3O45
Au L3O1
Au L3N7
Au L3N5
Au L3N4
Au L3N1
E (eV)

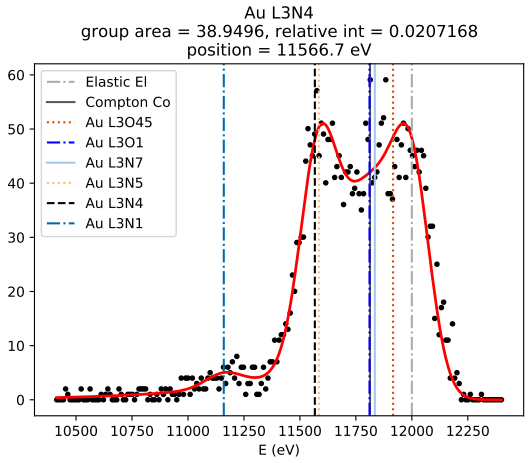

Compton Co
group area = 9.09411, relative int = 1
position(init) = 11807 eV, position(fit)=11813.2 eV
Elastic El
Compton Co
Au L3O45
Au L3O1
Au L3N7
Au L3N5
Au L3N4
Au L3N1
E (eV)

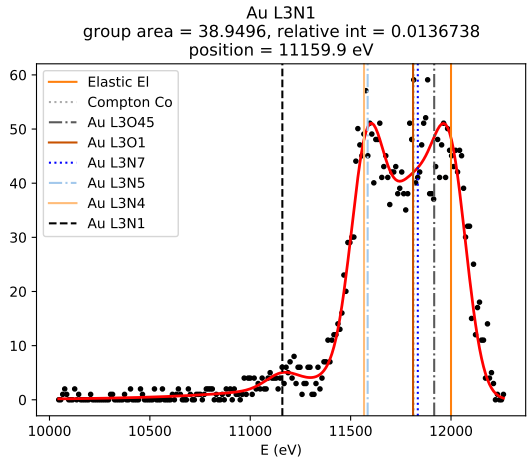

Au L3O45
group area = 38.9496, relative int = 0.0185344
position = 11916.2 eV
Elastic El
Compton Co
Au L3O45
Au L3O1
Au L3N7
Au L3N5
Au L3N4
Au L3N1
E (eV)

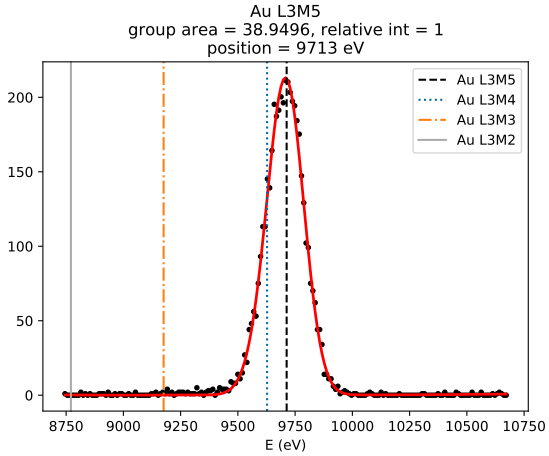

Au L3O1
group area = 38.9496, relative int = 0.0027513
position = 11810.9 eV
Elastic El
Compton Co
Au L3O45
Au L3O1
Au L3N7
Au L3N5
Au L3N4
Au L3N1
E (eV)

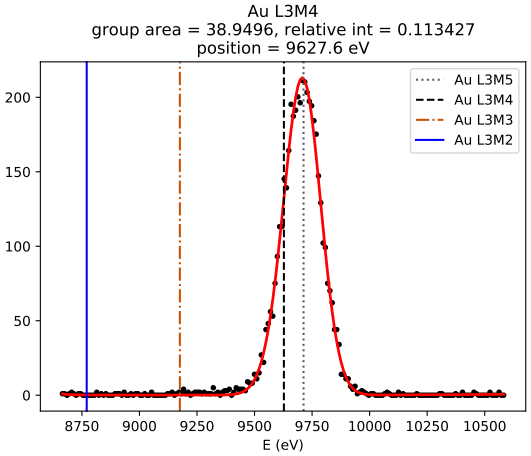

Au L3N7
group area = 38.9496, relative int = 0.00076937
position = 11834.6 eV
Elastic El
Compton Co
Au L3O45
Au L3O1
Au L3N7
Au L3N5
Au L3N4
Au L3N1
E (eV)

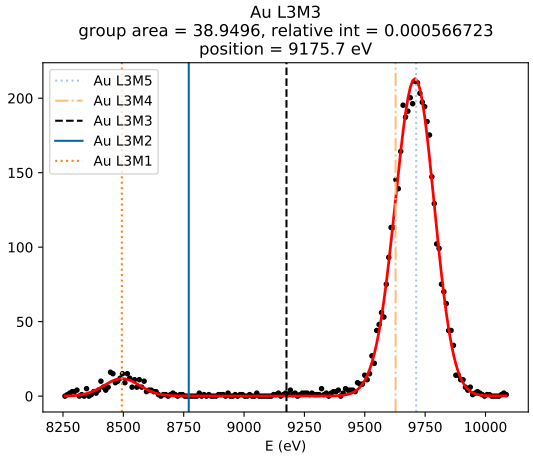

Au L3N5
group area = 38.9496, relative int = 0.186744
position = 11584.8 eV
Elastic El
Compton Co
Au L3O45
Au L3O1
Au L3N7
Au L3N5
Au L3N4
Au L3N1
E (eV)

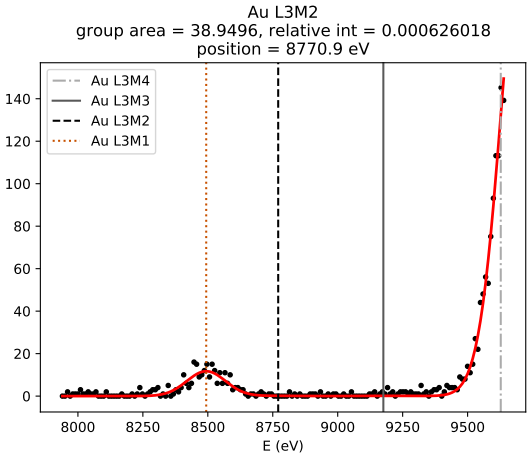

Au L3N4
group area = 38.9496, relative int = 0.0207168
position = 11566.7 eV
Elastic El
Compton Co
Au L3O45
Au L3O1
Au L3N7
Au L3N5
Au L3N4
Au L3N1
E (eV)

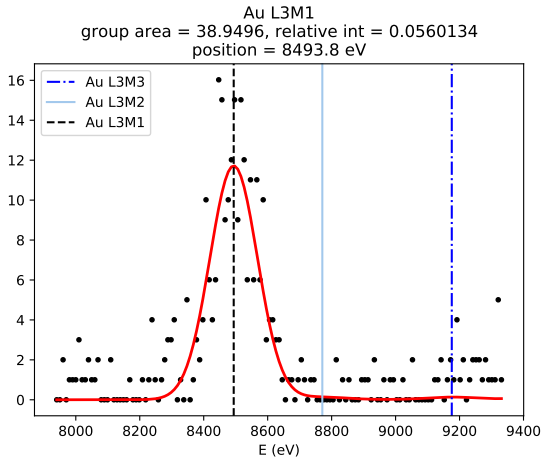

Au L3N1
group area = 38.9496, relative int = 0.0136738
position = 11159.9 eV
Elastic El
Compton Co
Au L3O45
Au L3O1
Au L3N7
Au L3N5
Au L3N4
Au L3N1
E (eV)


Au L3M5
group area = 38.9496, relative int = 1
position = 9713 eV
Au L3M5
Au L3M4
Au L3M3
Au L3M2
E (eV)

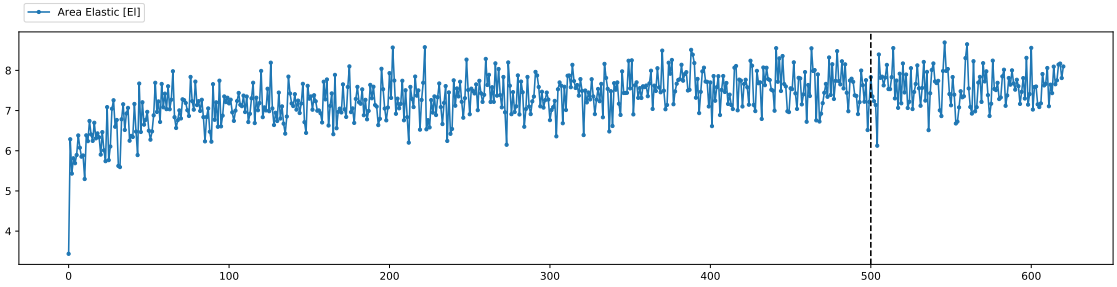

Au L3M4
group area = 38.9496, relative int = 0.113427
position = 9627.6 eV
Au L3M5
Au L3M4
Au L3M3
Au L3M2
E (eV)

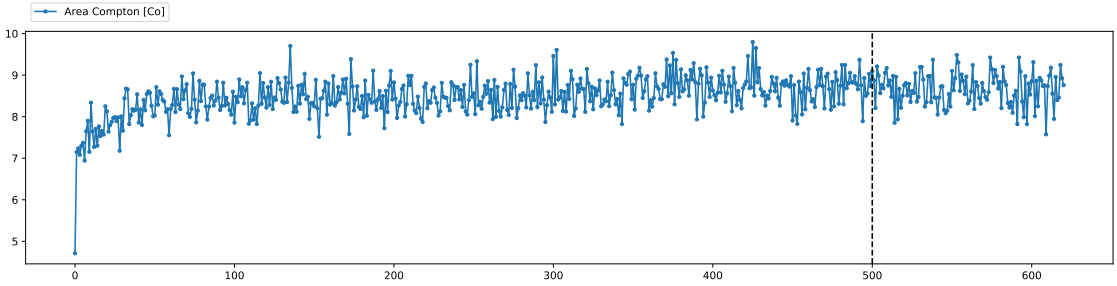

Au L3M3
group area = 38.9496, relative int = 0.000566723
position = 9175.7 eV
Au L3M5
Au L3M4
Au L3M3
Au L3M2
Au L3M1
E (eV)

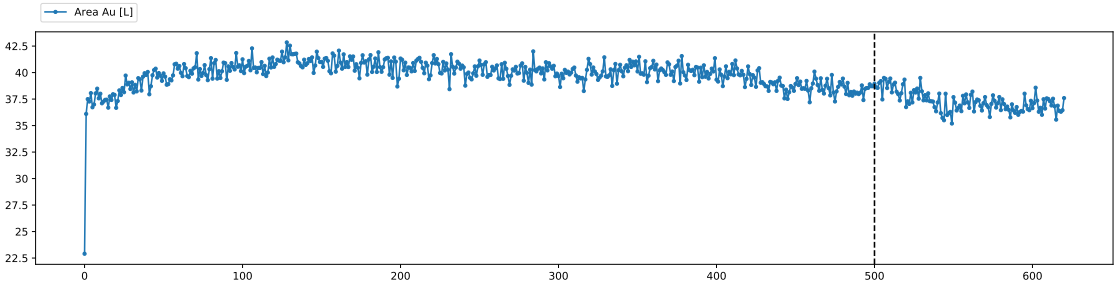

Au L3M2
group area = 38.9496, relative int = 0.000626018
position = 8770.9 eV
Au L3M4
Au L3M3
Au L3M2
Au L3M1
E (eV)

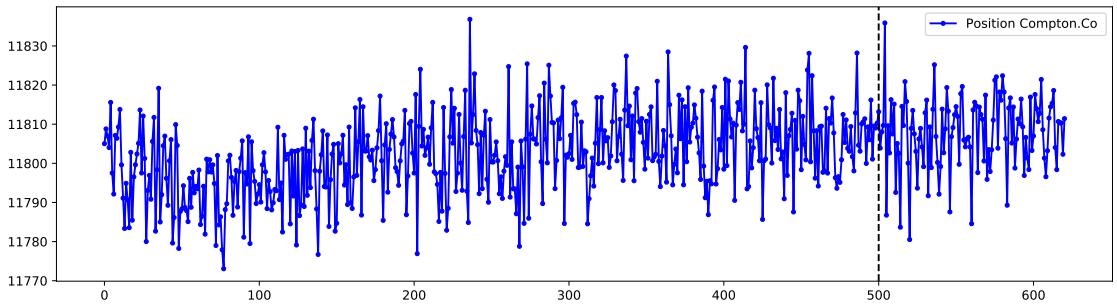

Au L3M1
group area = 38.9496, relative int = 0.0560134
position = 8493.8 eV
Au L3M3
Au L3M2
Au L3M1
E (eV)

AREAS


Area Elastic [El]


Area Compton [Co]

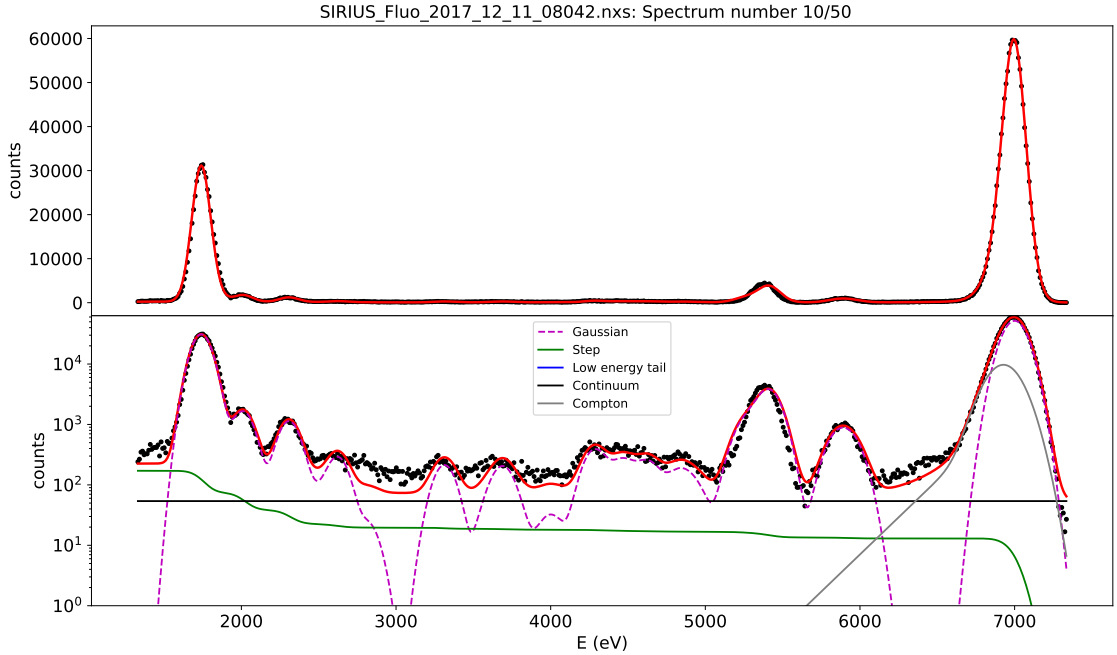

Area Au [L]



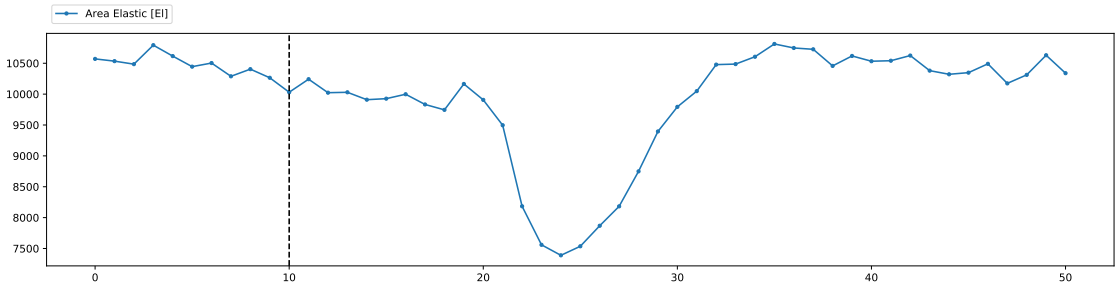
0.0.5 SIRIUS_Fluo_2017_12_11_08042

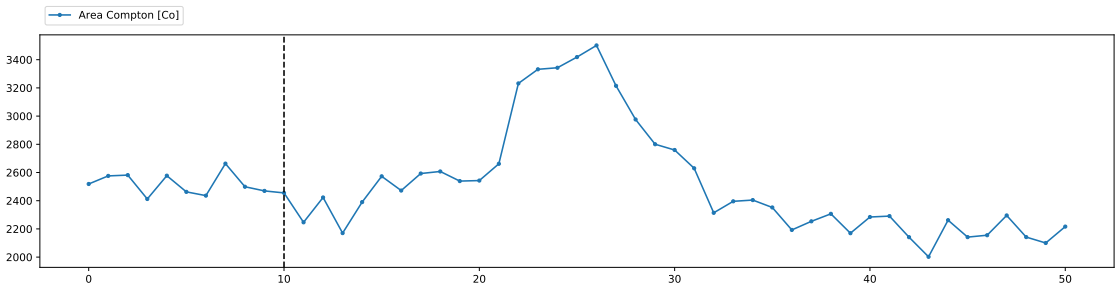
An example of an X-ray standing wave (XSW) experiment, fitted before subtraction with 55 peaks (8 atoms).
Here using a 4-elements detector.

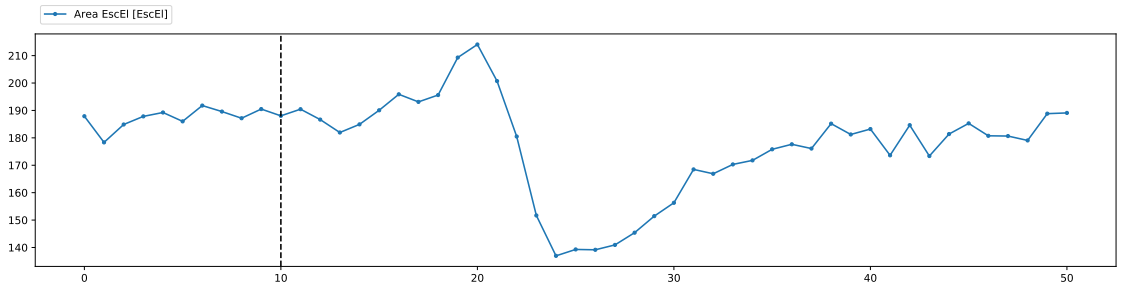
```
Fit results for SIRIUS_Fluo_2017_12_11_08042.nxs
Spectrum interval = [0,51]
Channel interval = [135,735]
List of chosen elements:  ['Element 0', 'Element 1', 'Element 2']
List of fitted parameters: ['ct']

Initial fit parameters:
beam energy = 7000
gain = 10.0065; eV0 = -20
epsilon = 0.0036; fano = 0.115; noise = 0.12973
sl = 0; ct = 92.61
sfa0 = 1; tfb0 = 0; twc0 = 0.1
fG = 1.377; fA = 0.09; fB = 0; gammaA = 2.3; gammaB = 0
```

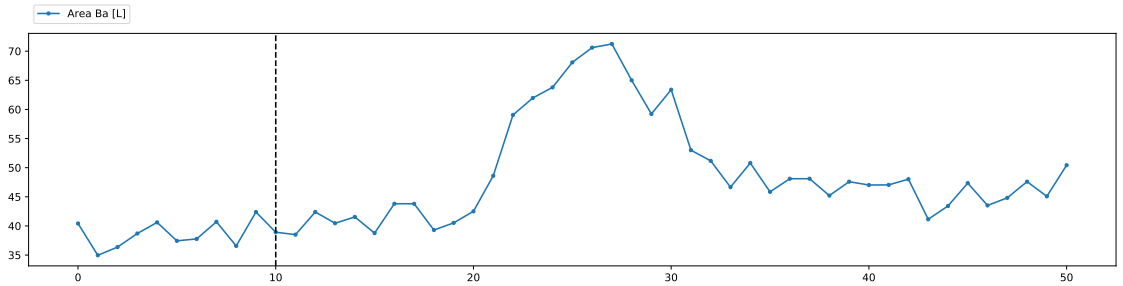

SIRIUS_Fluo_2017_12_11_08042.nxs: Spectrum number 10/50
counts
Gaussian
Step
Low energy tail
Continuum
Compton
E (eV)

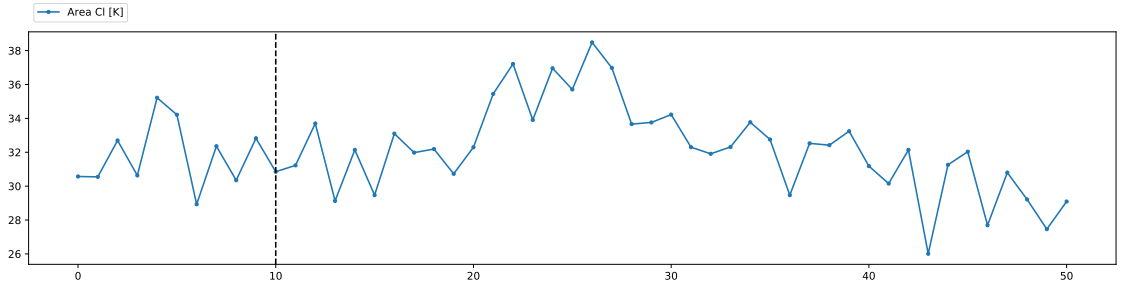
AREAS

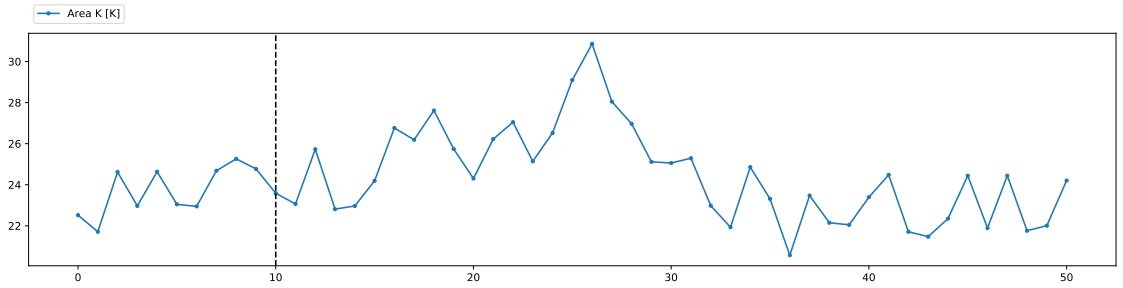

Area Elastic [El]

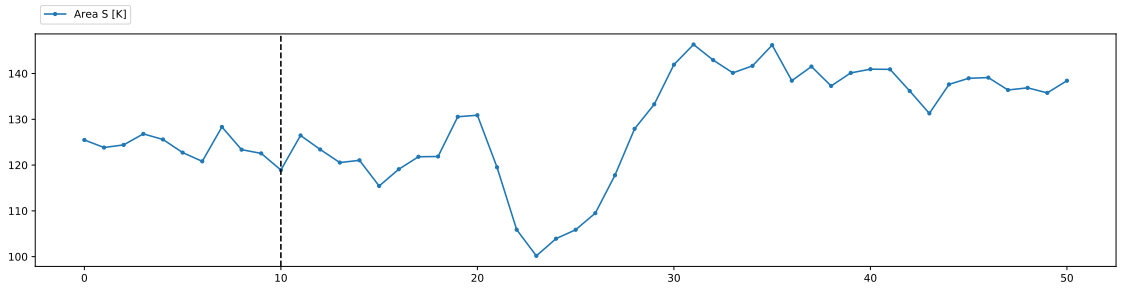

Area Compton [Co]

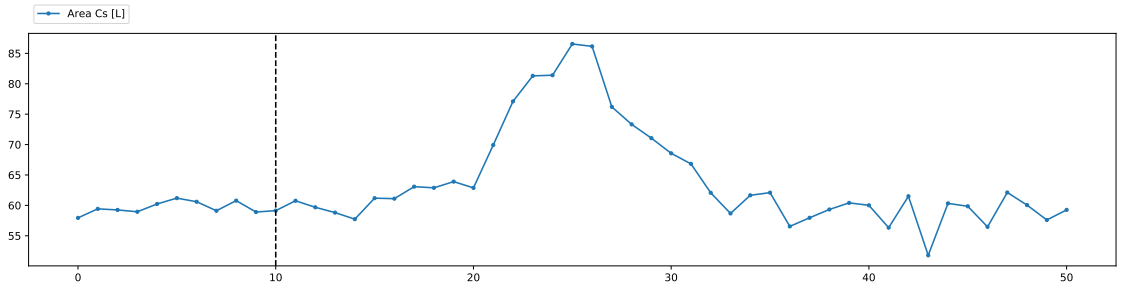

Area EscEl [EscEl]
210
200
190
180
170
160
150
140
0
10
20
30
40
50

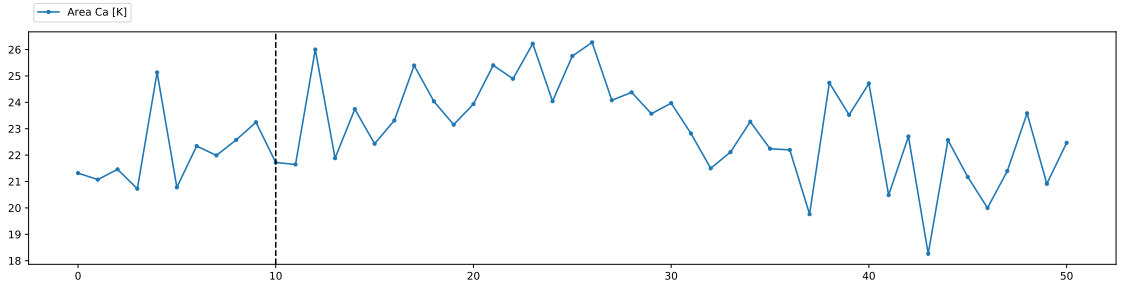

Area Ba [L]
70
65
60
55
50
45
40
35
0
10
20
30
40
50

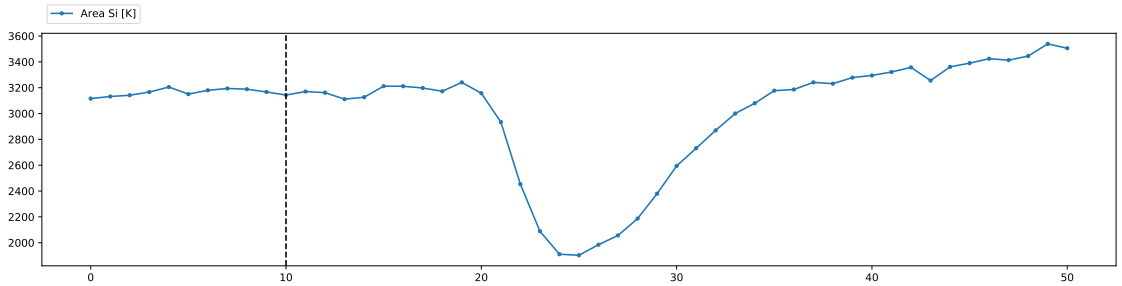

Area Cl [K]
38
36
34
32
30
28
26
0
10
20
30
40
50

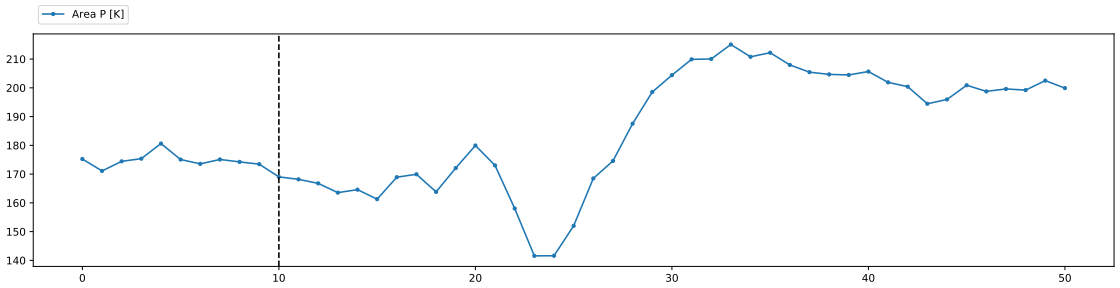

Area K [K]
30
28
26
24
22
0
10
20
30
40
50

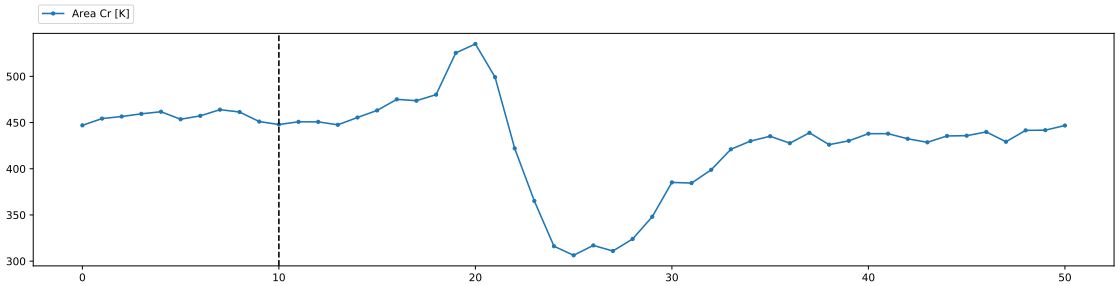

Area S [K]
140
130
120
110
100
0
10
20
30
40
50

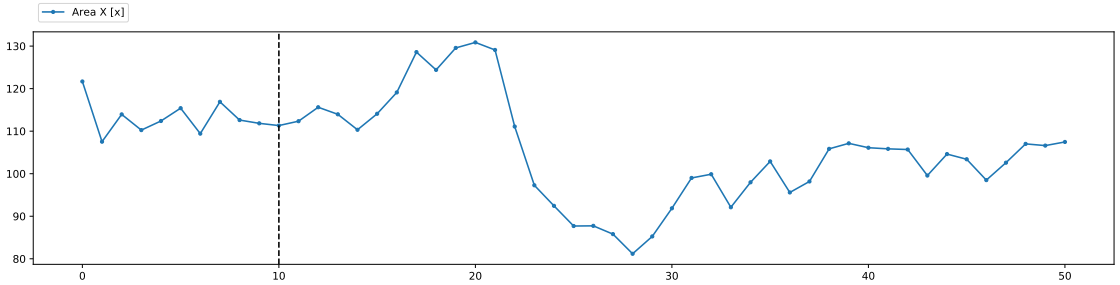

Area Cs [L]
85
80
75
70
65
60
55
0
10
20
30
40
50


Area Ca [K]
26
25
24
23
22
21
20
19
18
0
10
20
30
40
50

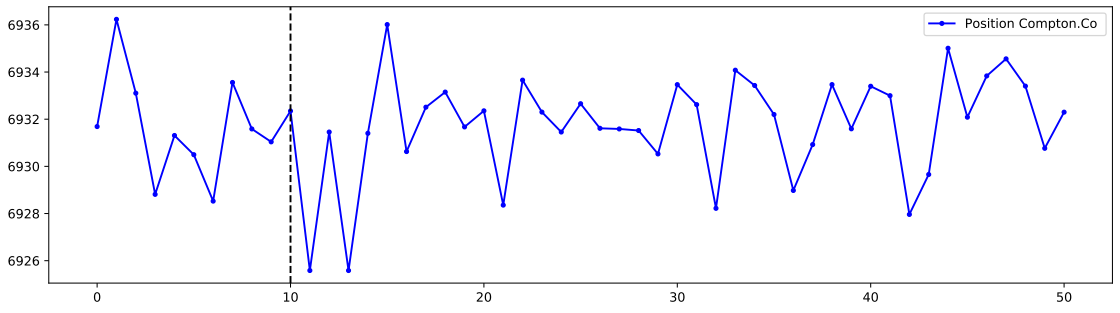

Area Si [K]
3600
3400
3200
3000
2800
2600
2400
2200
2000
0
10
20
30
40
50

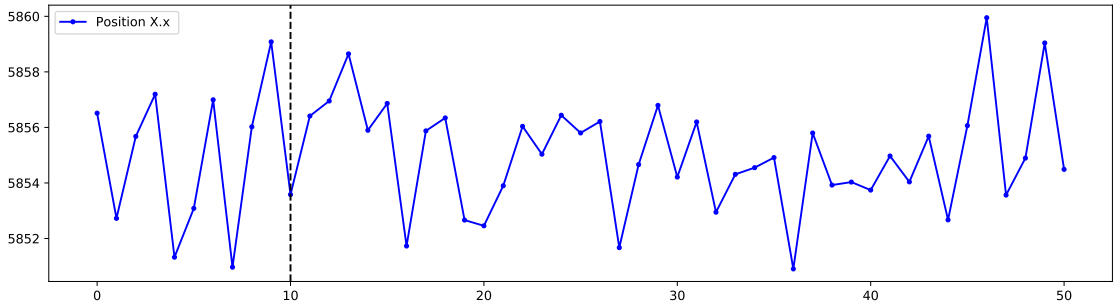

Area P [K]
210
200
190
180
170
160
150
140
0
10
20
30
40
50


Area Cr [K]
500
450
400
350
300
0
10
20
30
40
50


Area X [x]
130
120
110
100
90
80
0
10
20
30
40
50

POSITIONS


Position Compton.Co
6936
6934
6932
6930
6928
6926
0
10
20
30
40
50



OTHER PARAMETERS