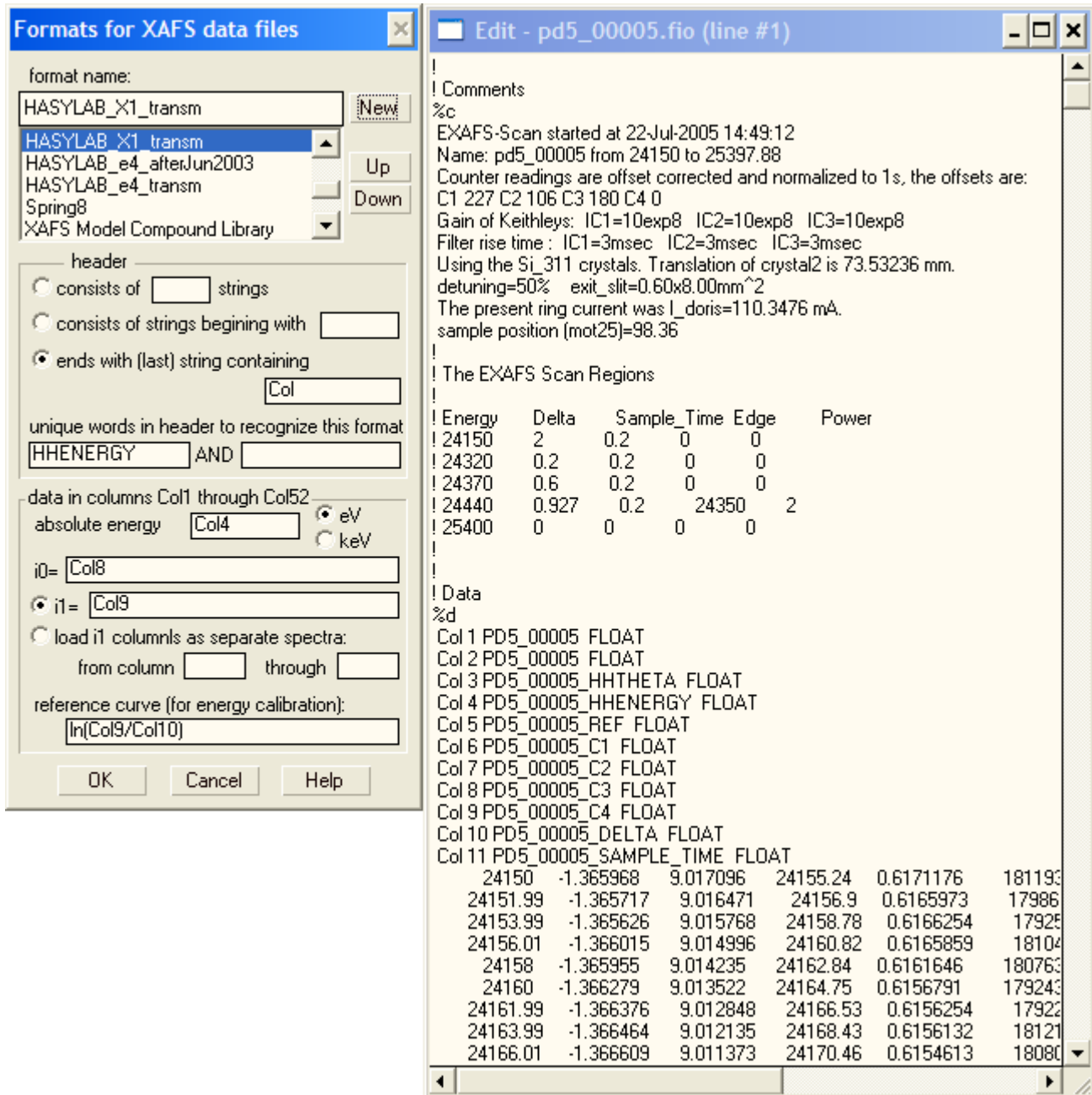


## VIPER (Visual Processing in EXAFS Researches)

- 'Formats...' dialog box



The image shows two windows from the VIPER software. The left window is the 'Formats for XAFS data files' dialog box, and the right window is an 'Edit' window showing the contents of a file named 'pd5\_00005.fio'.

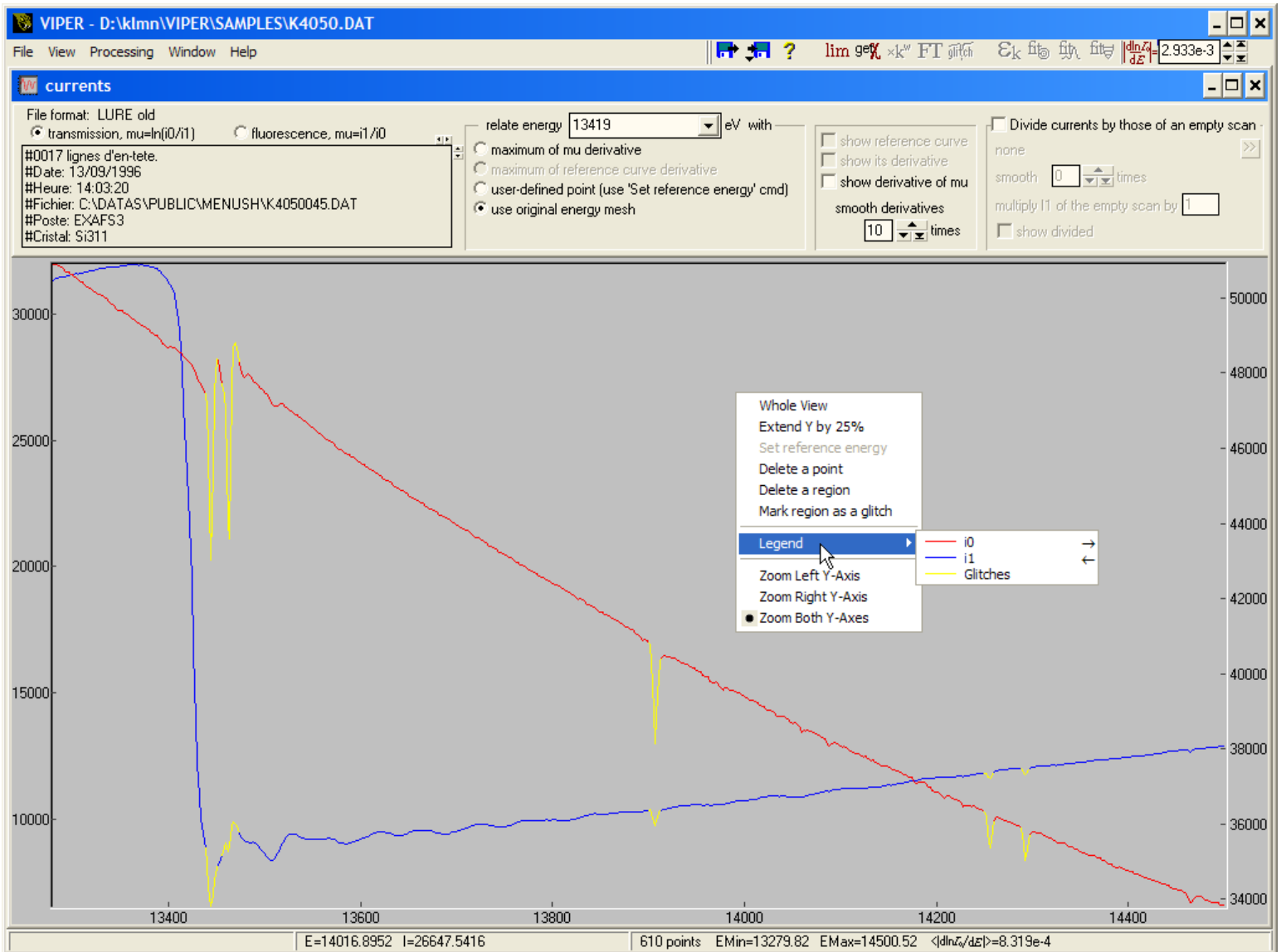
**Formats for XAFS data files dialog box:**

- format name: HASYLAB\_X1\_transm
- Header options:
  - consists of [ ] strings
  - consists of strings beginning with [ ]
  - ends with (last) string containing [ Col ]
- unique words in header to recognize this format: HHENERGY AND [ ]
- data in columns Col1 through Col52:
  - absolute energy: [ Col4 ]  eV  keV
  - i0 = [ Col8 ]
  - i1 = [ Col9 ]
  - load i1 columns as separate spectra: from column [ ] through [ ]
  - reference curve (for energy calibration): ln[Col9/Col10]

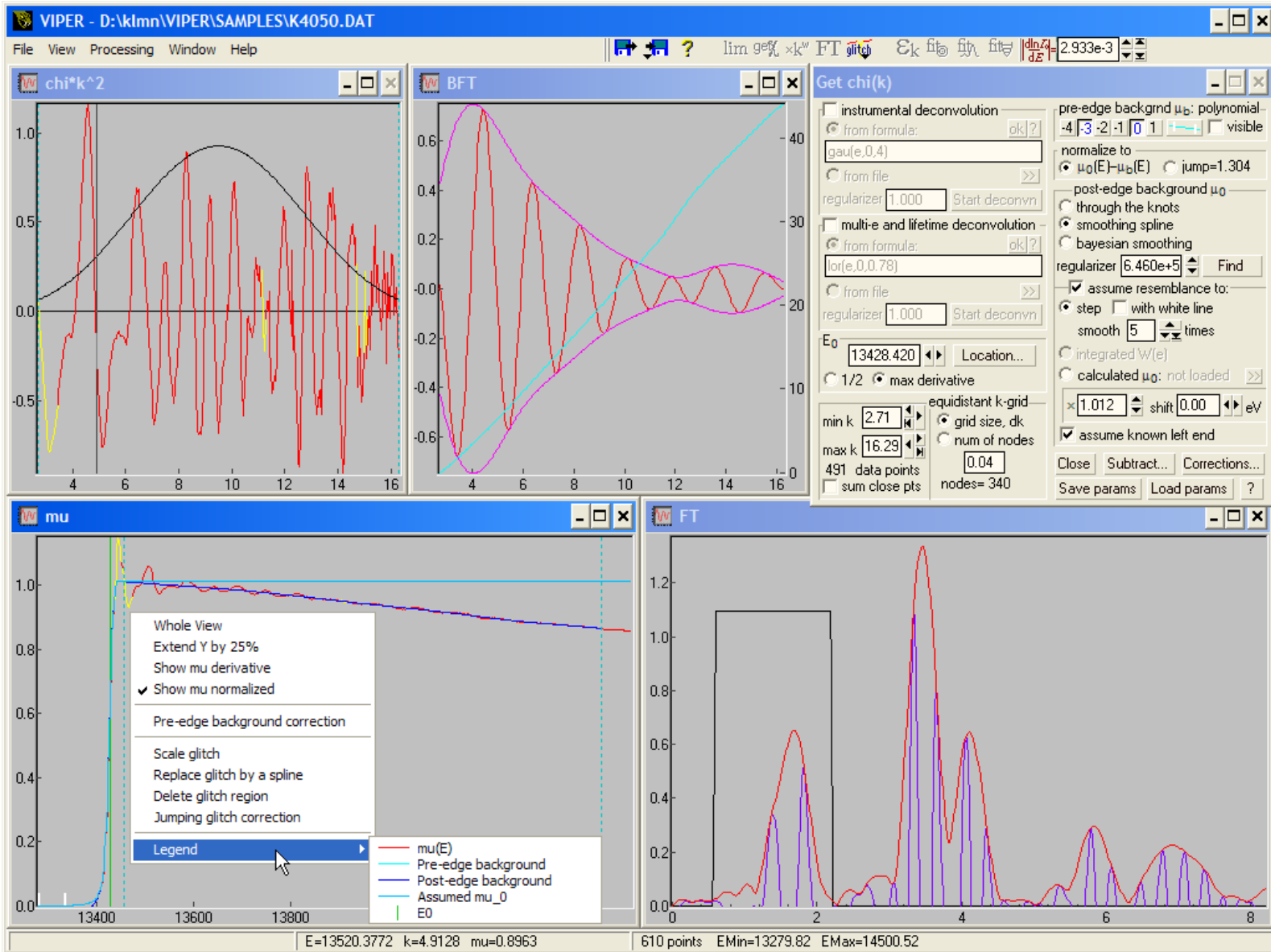
**Edit - pd5\_00005.fio (line #1):**

```
!
! Comments
%c
EXAFS-Scan started at 22-Jul-2005 14:49:12
Name: pd5_00005 from 24150 to 25397.88
Counter readings are offset corrected and normalized to 1s, the offsets are:
C1 227 C2 106 C3 180 C4 0
Gain of Keithleys: IC1=10exp8 IC2=10exp8 IC3=10exp8
Filter rise time : IC1=3msec IC2=3msec IC3=3msec
Using the Si_311 crystals. Translation of crystal2 is 73.53236 mm.
detuning=50% exit_slit=0.60x8.00mm^2
The present ring current was I_doris=110.3476 mA.
sample position (mot25)=98.36
!
! The EXAFS Scan Regions
! Energy   Delta   Sample_Time Edge   Power
! 24150    2      0.2      0     0
! 24320    0.2    0.2      0     0
! 24370    0.6    0.2      0     0
! 24440    0.927  0.2      24350 2
! 25400    0      0        0     0
!
! Data
%d
Col 1 PD5_00005 FLOAT
Col 2 PD5_00005 FLOAT
Col 3 PD5_00005_HHTHETA FLOAT
Col 4 PD5_00005_HHENERGY FLOAT
Col 5 PD5_00005_REF FLOAT
Col 6 PD5_00005_C1 FLOAT
Col 7 PD5_00005_C2 FLOAT
Col 8 PD5_00005_C3 FLOAT
Col 9 PD5_00005_C4 FLOAT
Col 10 PD5_00005_DELTA FLOAT
Col 11 PD5_00005_SAMPLE_TIME FLOAT
24150 -1.365968 9.017096 24155.24 0.6171176 181193
24151.99 -1.365717 9.016471 24156.9 0.6165973 17986
24153.99 -1.365626 9.015768 24158.78 0.6166254 17925
24156.01 -1.366015 9.014996 24160.82 0.6165859 18104
24158 -1.365955 9.014235 24162.84 0.6161646 180763
24160 -1.366279 9.013522 24164.75 0.6156791 179243
24161.99 -1.366376 9.012848 24166.53 0.6156254 17922
24163.99 -1.366464 9.012135 24168.43 0.6156132 18121
24166.01 -1.366609 9.011373 24170.46 0.6154613 18080
```

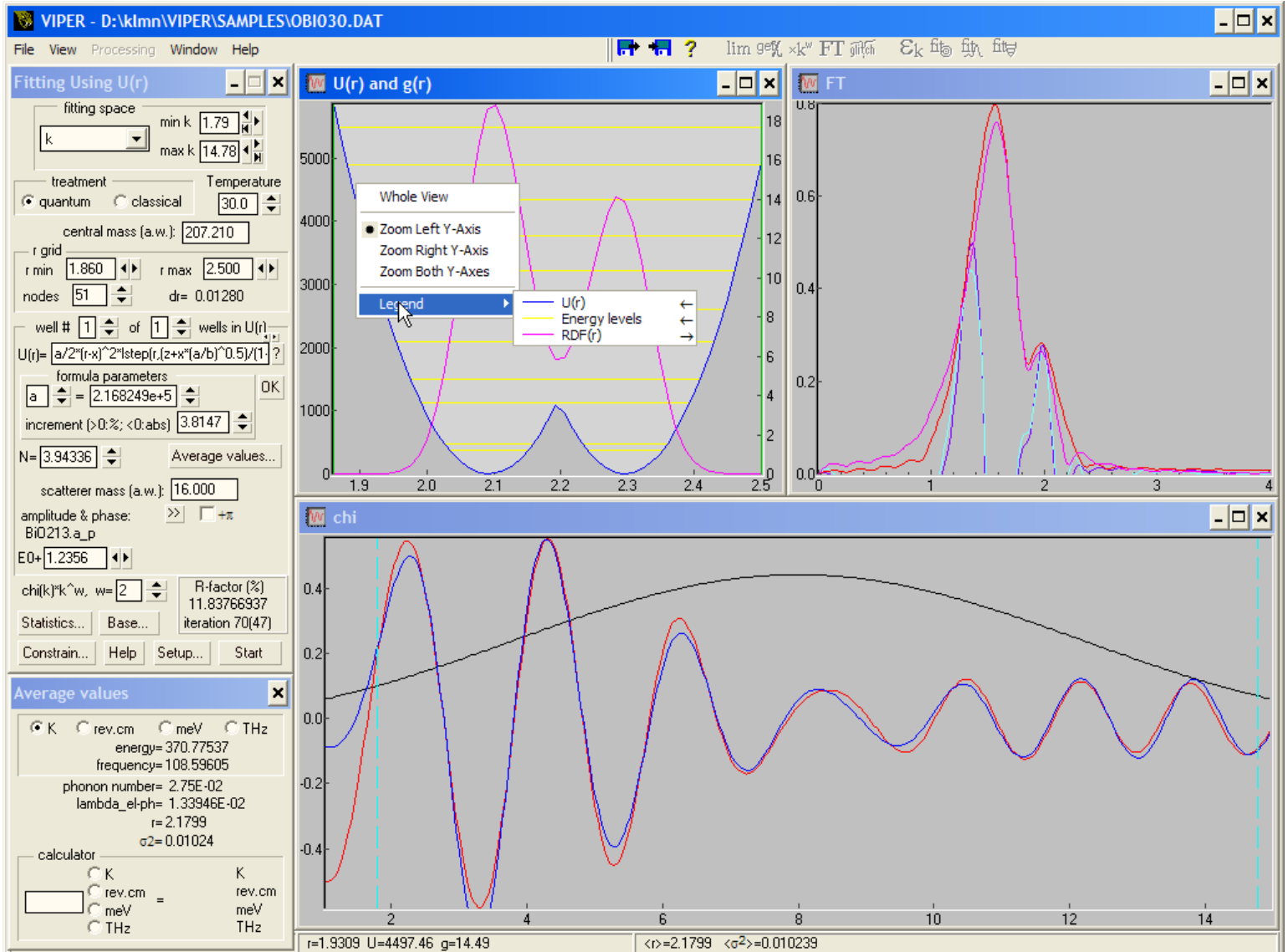
after opening an experimental file (containing currents of ionization chamber)



after pressing 'get  $\chi$ ' button



a filtered  $\chi(k)$  is loaded and the command 'fitting using U(r)' is performed



'Statistics' dialog box (after pressing 'Statistics...' button) with mapping and statistical tests

**Statistical evaluations (to redraw, press 'Statistics...')**

$\Delta R = 1.40 \rightarrow N = 2\Delta k \Delta R / \pi + 2 = 13.58$   
 $P = 6 \quad v = N \cdot P = 8$   
 colors  numbers  
 $x1\_b1 = 6.632e-1$

individual errors of data points  
 are proportional to  $k^m$ ,  $m = 1.5$   
 proportionality coefficient is unknown  
 known  
 from file  
 set equal, for all points =

$\chi^2$ -test: 8.00000000  $\chi^2$  and F-test

$\delta p_k$   
 independent  
 supreme projection  
 integrated  
 a priori space sizes:  
 reg-r = 0.00000  
 most probable  
 $\langle \chi^2 \rangle_{post} = 6.0000$

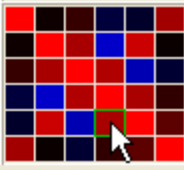
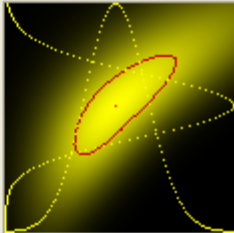
	min	max	pixels
X: $b1$	$2.2e+5$	$2.8e+5$	115
Y: $x1$	2.07	2.11	115

ellipticity param = 0.5138  
 $\chi^2$   exact  decomposed  
 correlation coefficient =  $7.404e-1$   
 confidence level  $0.393$

Start Save map

click right mouse

N1	e1	a1	b1	x1	z1
$\delta N1 = 2.169e-1$	$\delta e1 = 8.187e-1$	$\delta a1 = 1.408e+4$	$\delta b1 = 1.498e+4$	$\delta x1 = 1.855e-2$	$\delta z1 = 2.793e-2$

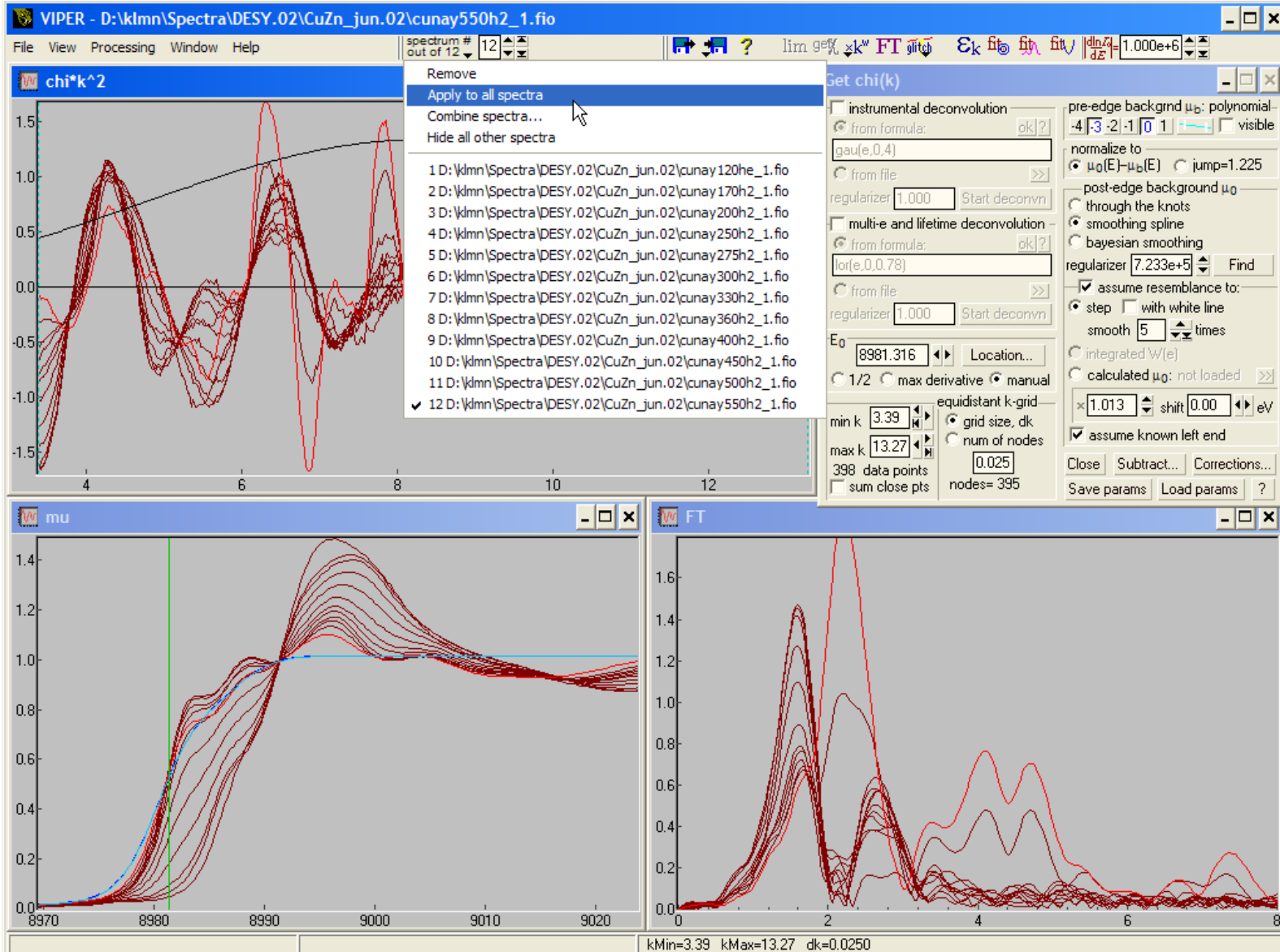
**F-test**

$\chi^2$  critical value  
 $v = 8 \quad c = 0.632 \quad \chi_8^{0.632} = 8.7026$

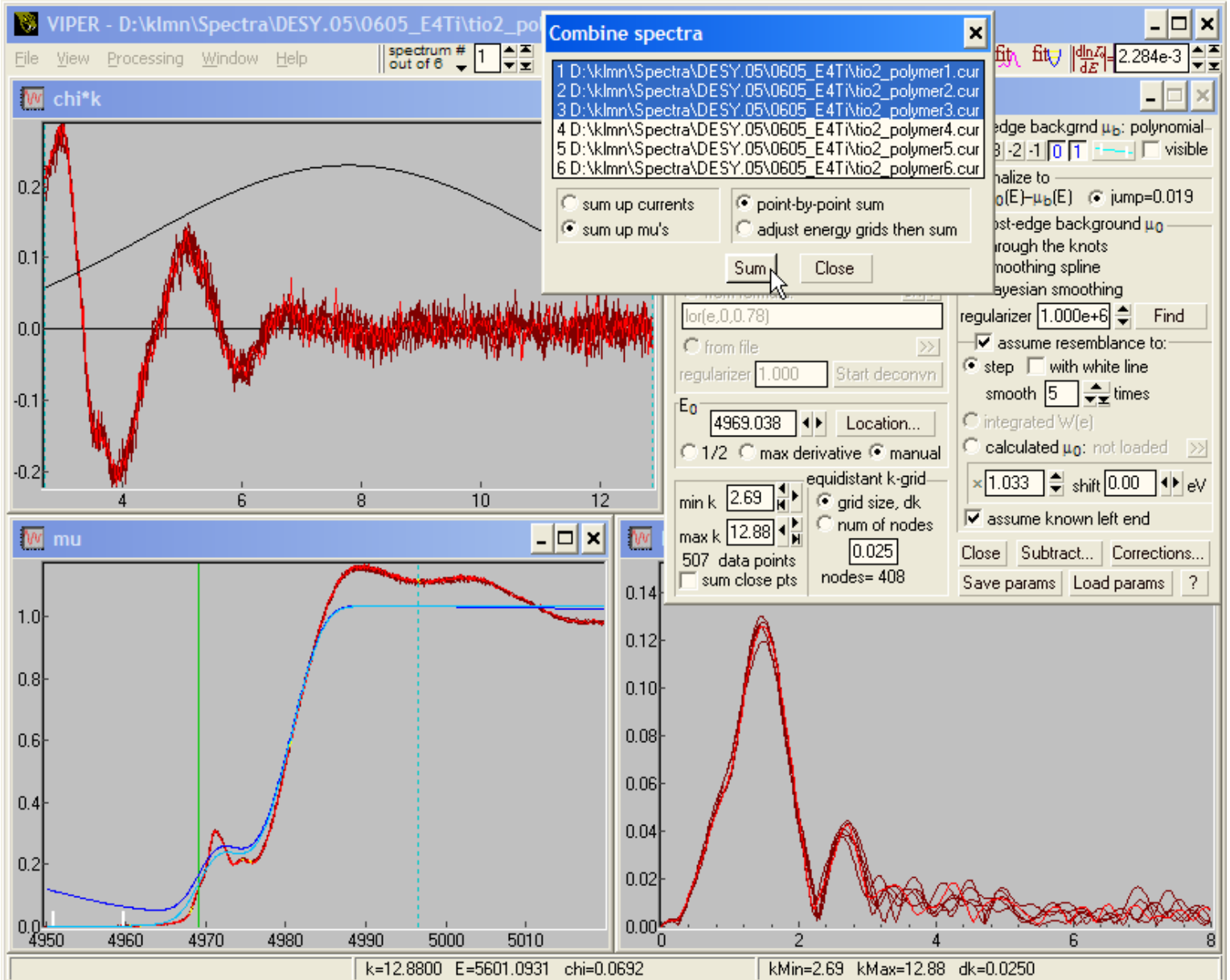
F-test  
 $v_1 = 8 \quad v_2 = 7 \quad \chi_1^2 = 8.00000000$   
 $\chi_2^2 = 7.05619989 \quad F_{1,7}^{0.632} = 0.936$   
 $c = 0.632$

Close Help

you can open as many files as you want (this is a series of CuZn-based catalysts under reduction treatment)



you can easily combine several spectra. Here are 6 fluorescence spectra ...





... combined into 2

