Basic Scripting in DTSA-II

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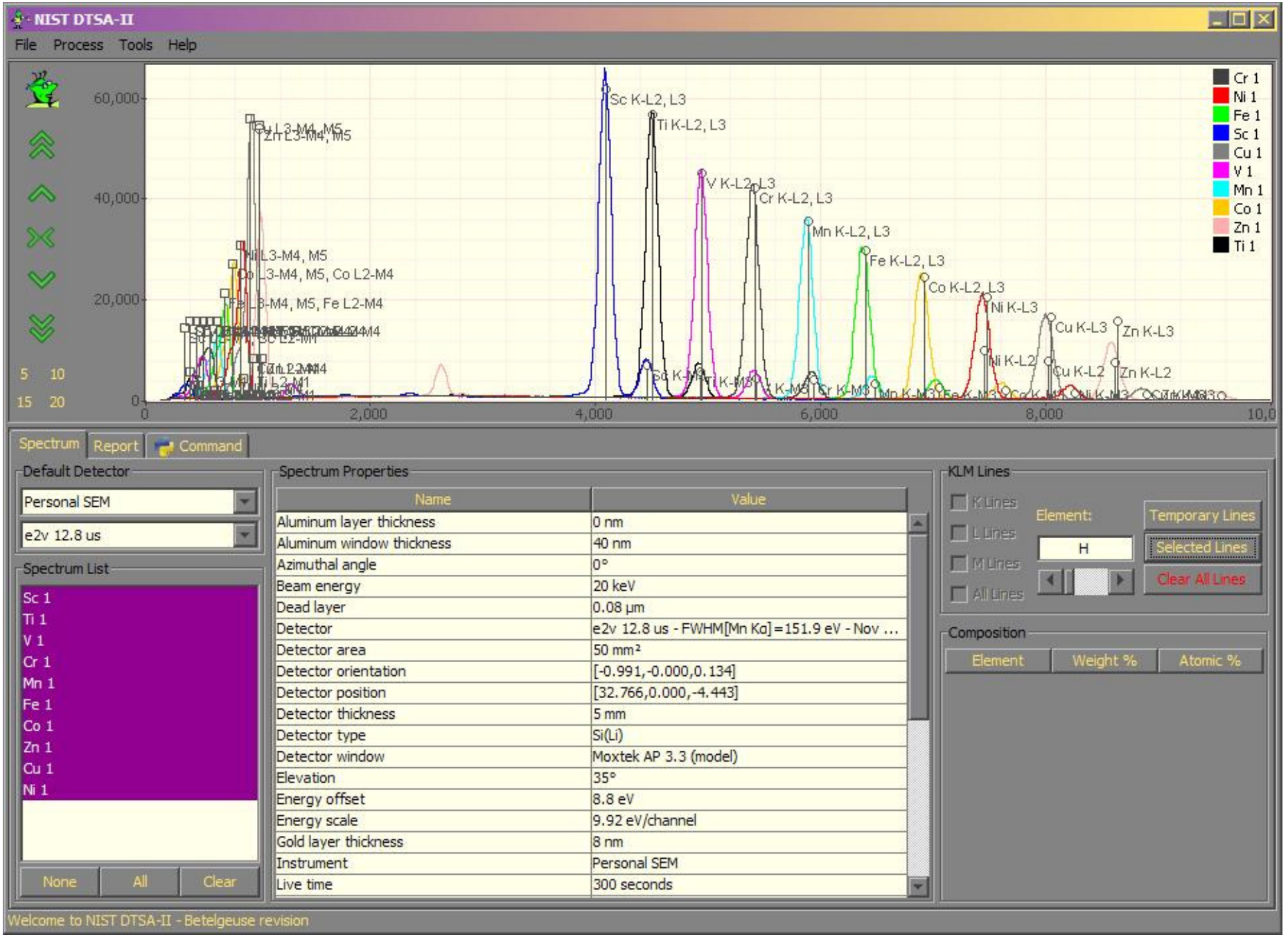
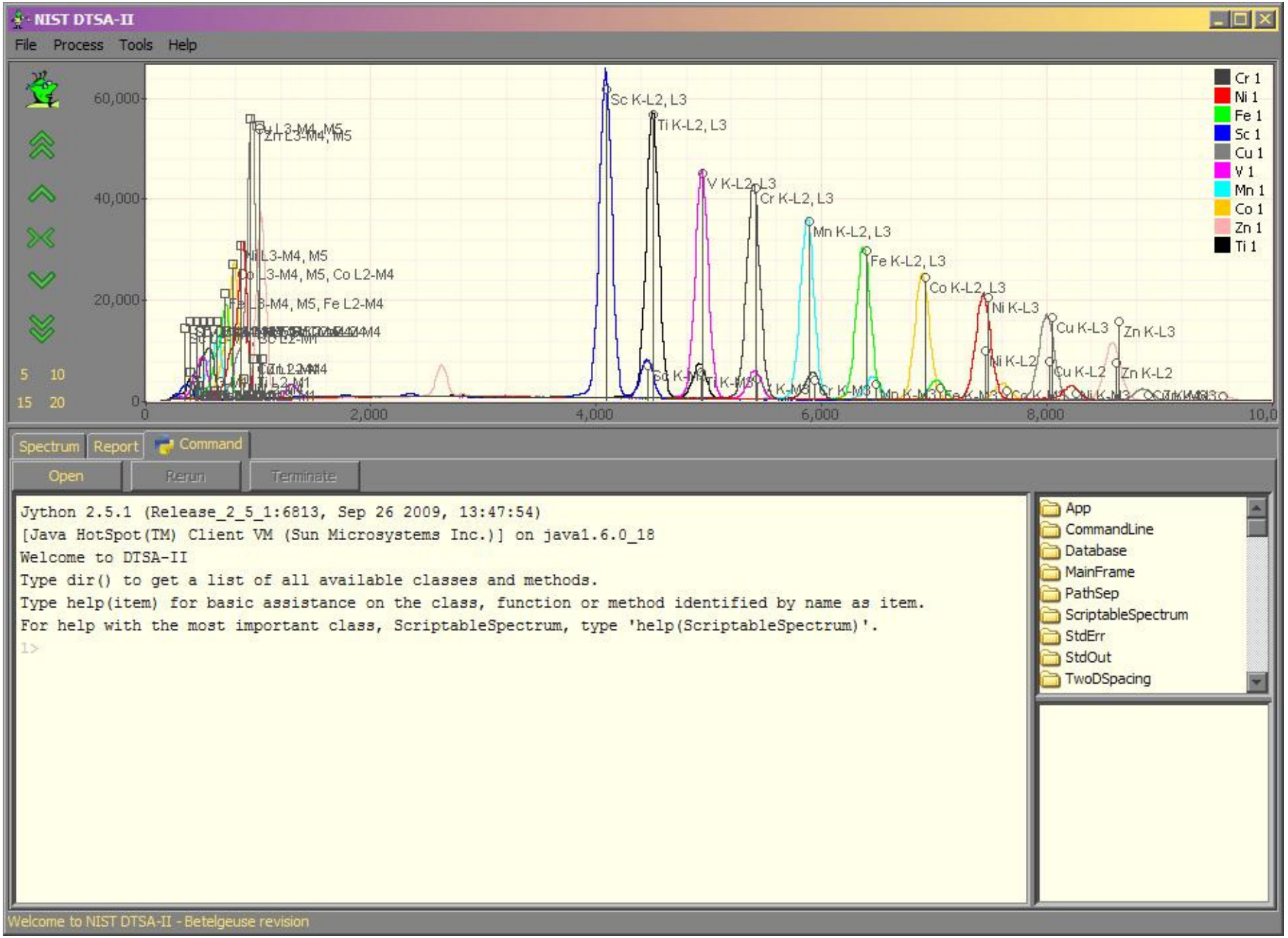
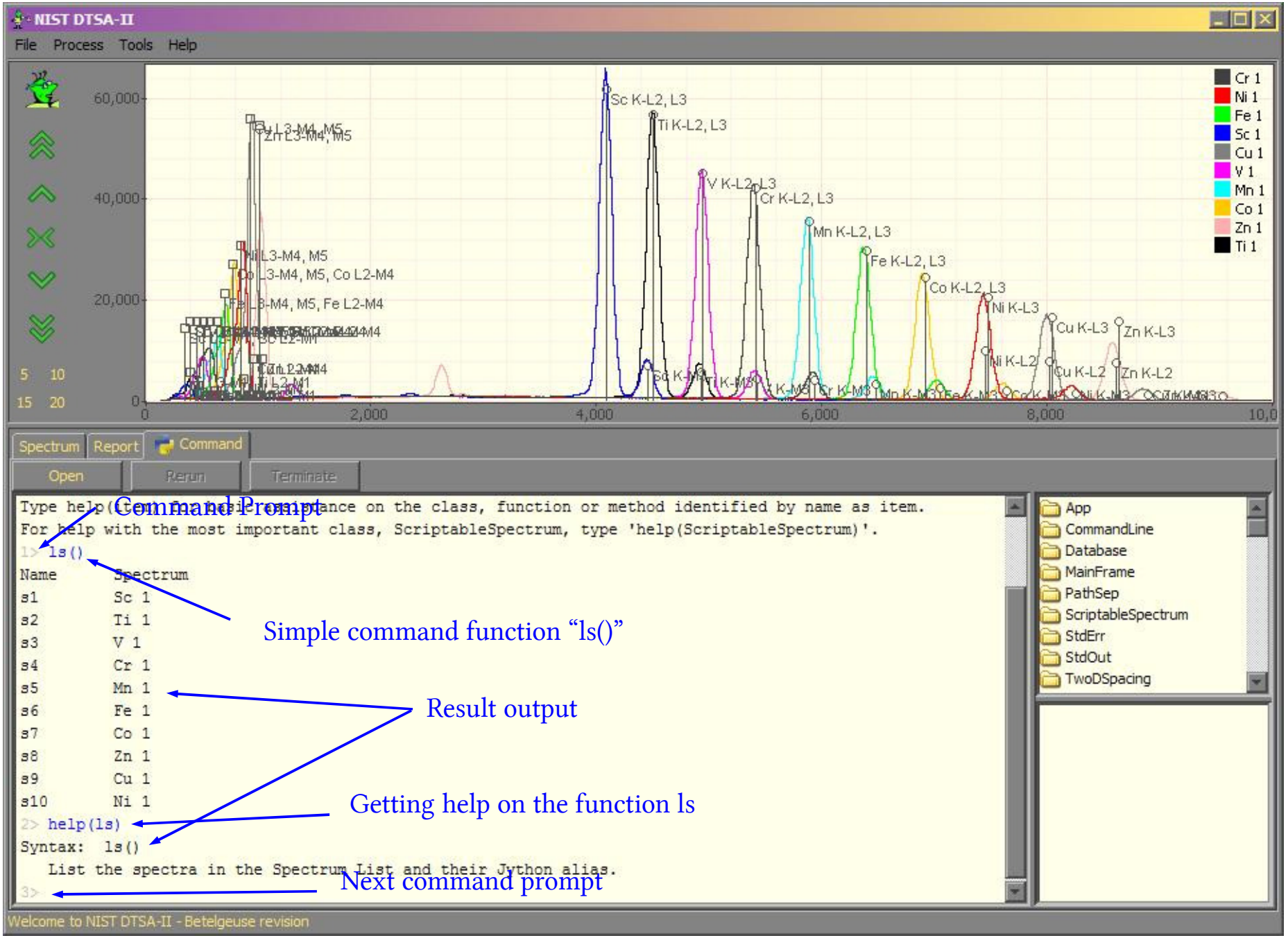

NIST DTSA-II
File Process Tools Help
Sc K-L2, L3
Ti K-L2, L3
V K-L2, L3
Cr K-L2, L3
Mn K-L2, L3
Fe K-L2, L3
Co K-L2, L3
Ni K-L3
Cu K-L3
Zn K-L3
Ni K-L2
Cu K-L2
Zn K-L2
Cr 1
Ni 1
Fe 1
Sc 1
Cu 1
V 1
Mn 1
Co 1
Zn 1
Ti 1
60,000
40,000
20,000
0
2,000
4,000
6,000
8,000
Spectrum
Report
Command
Default Detector
Personal SEM
e2v 12.8 us
Spectrum List
Sc 1
Ti 1
V 1
Cr 1
Mn 1
Fe 1
Co 1
Zn 1
Cu 1
Ni 1
None
All
Clear
Spectrum Properties
Name
Value
Aluminum layer thickness 0 nm
Aluminum window thickness 40 nm
Azimuthal angle 0°
Beam energy 20 keV
Dead layer 0.08 µm
Detector e2v 12.8 us - FWHM[Mn Kα]=151.9 eV - Nov ...
Detector area 50 mm²
Detector orientation [-0.991,-0.000,0.134]
Detector position [32.766,0.000,-4.443]
Detector thickness 5 mm
Detector type Si(Li)
Detector window Moxtek AP 3.3 (model)
Elevation 35°
Energy offset 8.8 eV
Energy scale 9.92 eV/channel
Gold layer thickness 8 nm
Instrument Personal SEM
Live time 300 seconds
KLM Lines
K Lines
L Lines
M Lines
All Lines
Element:
H
Temporary Lines
Selected Lines
Clear All Lines
Composition
Element
Weight %
Atomic %
Welcome to NIST DTSA-II - Betelgeuse revision


NIST DTSA-II
File Process Tools Help
60,000
40,000
20,000
0
0
2,000
4,000
6,000
8,000
Sc K-L2, L3
Ti K-L2, L3
V K-L2, L3
Cr K-L2, L3
Mn K-L2, L3
Fe K-L2, L3
Co K-L2, L3
Ni K-L3
Cu K-L3
Zn K-L3
Ni K-L2
Cu K-L2
Zn K-L2
Cr 1
Ni 1
Fe 1
Sc 1
Cu 1
V 1
Mn 1
Co 1
Zn 1
Ti 1
Spectrum
Report
Command
Open
Rerun
Terminate
Jython 2.5.1 (Release_2_5_1:6813, Sep 26 2009, 13:47:54)
[Java HotSpot(TM) Client VM (Sun Microsystems Inc.)] on java1.6.0_18
Welcome to DTSA-II
Type dir() to get a list of all available classes and methods.
Type help(item) for basic assistance on the class, function or method identified by name as item.
For help with the most important class, ScriptableSpectrum, type 'help(ScriptableSpectrum)'.
1>
App
CommandLine
Database
MainFrame
PathSep
ScriptableSpectrum
StdErr
StdOut
TwoDSpacing
Welcome to NIST DTSA-II - Betelgeuse revision

Overview

- Python 2.5 Syntax Scripting
  - General purpose, object oriented programming language
- Libraries
  - Access to all Java libraries
  - Access to all DTSA-II quantitative algorithms
  - Access to other algorithms not available through the DTSA-II GUI


NIST DTSA-II
File Process Tools Help
Sc K-L2, L3
Ti K-L2, L3
V K-L2, L3
Cr K-L2, L3
Mn K-L2, L3
Fe K-L2, L3
Co K-L2, L3
Ni K-L3
Cu K-L3
Zn K-L3
Ni K-L2
Cu K-L2
Zn K-L2
Cr 1
Ni 1
Fe 1
Sc 1
Cu 1
V 1
Mn 1
Co 1
Zn 1
Ti 1
Spectrum
Report
Command
Open
Rerun
Terminate
Type help(item) to obtain assistance on the class, function or method identified by name as item.
For help with the most important class, ScriptableSpectrum, type 'help(ScriptableSpectrum)'.
1> ls()
Name Spectrum
s1 Sc 1
s2 Ti 1
s3 V 1
s4 Cr 1
s5 Mn 1
s6 Fe 1
s7 Co 1
s8 Zn 1
s9 Cu 1
s10 Ni 1
2> help(ls)
Syntax: ls()
List the spectra in the Spectrum List and their Jython alias.
3>
App
CommandLine
Database
MainFrame
PathSep
ScriptableSpectrum
StdErr
StdOut
TwoDSpacing
Welcome to NIST DTSA-II - Betelgeuse revision
Command Prompt
Simple command function "ls()"
Result output
Getting help on the function ls
Next command prompt

Useful Utility Commands

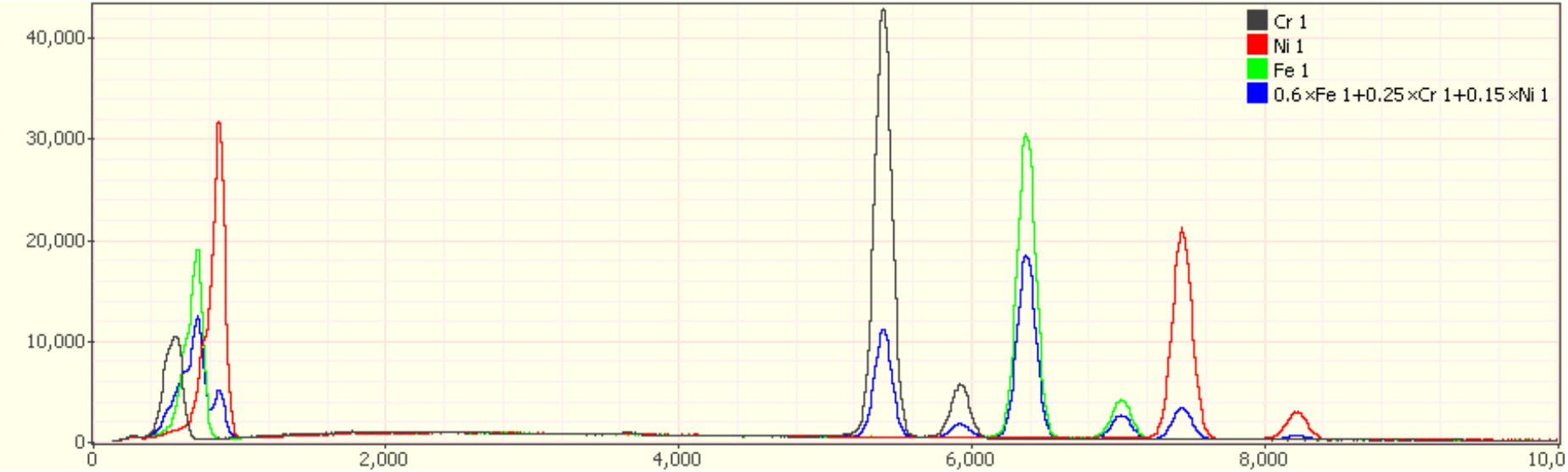
Generic Python Utility Methods

dir()	Displays a list of global functions, classes and variables
dir(obj)	Displays a list of methods and properties of the object *obj*
help()	Displays global help
help(obj)	Displays help on the object obj

DTSA-II Specific Utility Methods

ls()	Displays a list of all spectra in the Spectrum List with aliases ('s?' where ? is an integer)
spectra()	Returns a list object containing the spectra in the Spectrum List. spectra(True) returns only the selected spectra.
listDetectors()	Displays a list of all available detectors with aliases ('d?' where ? is an integer)
getElement()	GUI to select a single element
getElements()	GUI to select multiple elements
createMaterial()	GUI to select or create a new Composition or Material

Spectrum Math



Assign the result to the variable "*res*"

Construct a spectrum that is 0.6·Fe 1 + 0.25·Cr 1 + 0.15·Ni 1

```
3> res=(0.6*s6+0.25*s4+0.15*s10)
4> res.display()
```

Show the spectrum in the DTSA-II spectrum display

Operations: +, -, *, abs()

- You don't need to declare variables.
- Variable type is defined by what it contains.

Command “dir(res)” returns a list of the names of the “methods” available for use with the contents of the variable “res”

Calling convention is:
var.method()

```
3> res=(0.6*s6+0.25*s4+0.15*s10)
4> res.display()
5> dir(res)
['NullSpectrum', '__add__', '__class__', '__delattr__', '__dict__', '__doc__', '__eq__' '__ge__', '__getat-
tribute__', '__getitem__', '__getslice__', '__gt__', '__hash__', '__initProxy__', '__init__', '__le__',
'__len__', '__lt__', '__module__', '__mul__', '__ne__', '__new__', '__reduce__', '__reduce_ex__', '__re-
pr__', '__rmul__', '__setattr__', '__str__', '__sub__', '__supernames__', '__weakref__', '_getPyInstance',
'_getPySystemState', '_setPyInstance', '_setPySystemState', 'abs', 'applyLLT', 'autoOffset', 'back-
groundCorrect', 'beamEnergy', 'channel', 'channelCount', 'channelWidth', 'class', 'classDictInit',
'clone', 'compareTo', 'composition', 'display', 'duaneHunt', 'energies', 'energy', 'equals', 'finalize',
'firstNonZeroChannel', 'fromXML', 'getChannelCount', 'getChannelWidth', 'getClass', 'getCounts',
'getFWHMatMnKa', 'getProperties', 'getWrapped', 'getZeroOffset', 'hashCode', 'initializeSpectru-
mIndex', 'lastNonZeroChannel', 'liveTime', 'maxChannel', 'notify', 'notifyAll', 'offset', 'partition', 'peak-
Integral', 'positiveDefinite', 'probeCurrent', 'properties', 'property', 'remap', 'rename', 'save', 'scale',
'setAsStandard', 'setEnergyScale', 'setFWHMatMnKa', 'setLiveTime', 'setProbeCurrent', 'smooth',
'subSample', 'super__toString', 'super__toXML', 'takeOffAngle', 'toDouble', 'toString', 'toXML',
'totalCounts', 'wait', 'wrapped', 'zeroOffset']
6> res.getChannelWidth()
9.924458080007994
7> help(res.smooth)
Syntax:  s.smooth()
   Performs a fifth-order Savitzky-Golay filter on the spectrum s.
```

Getting help on a method

Get the string representation of “res”
and call it “oldName”

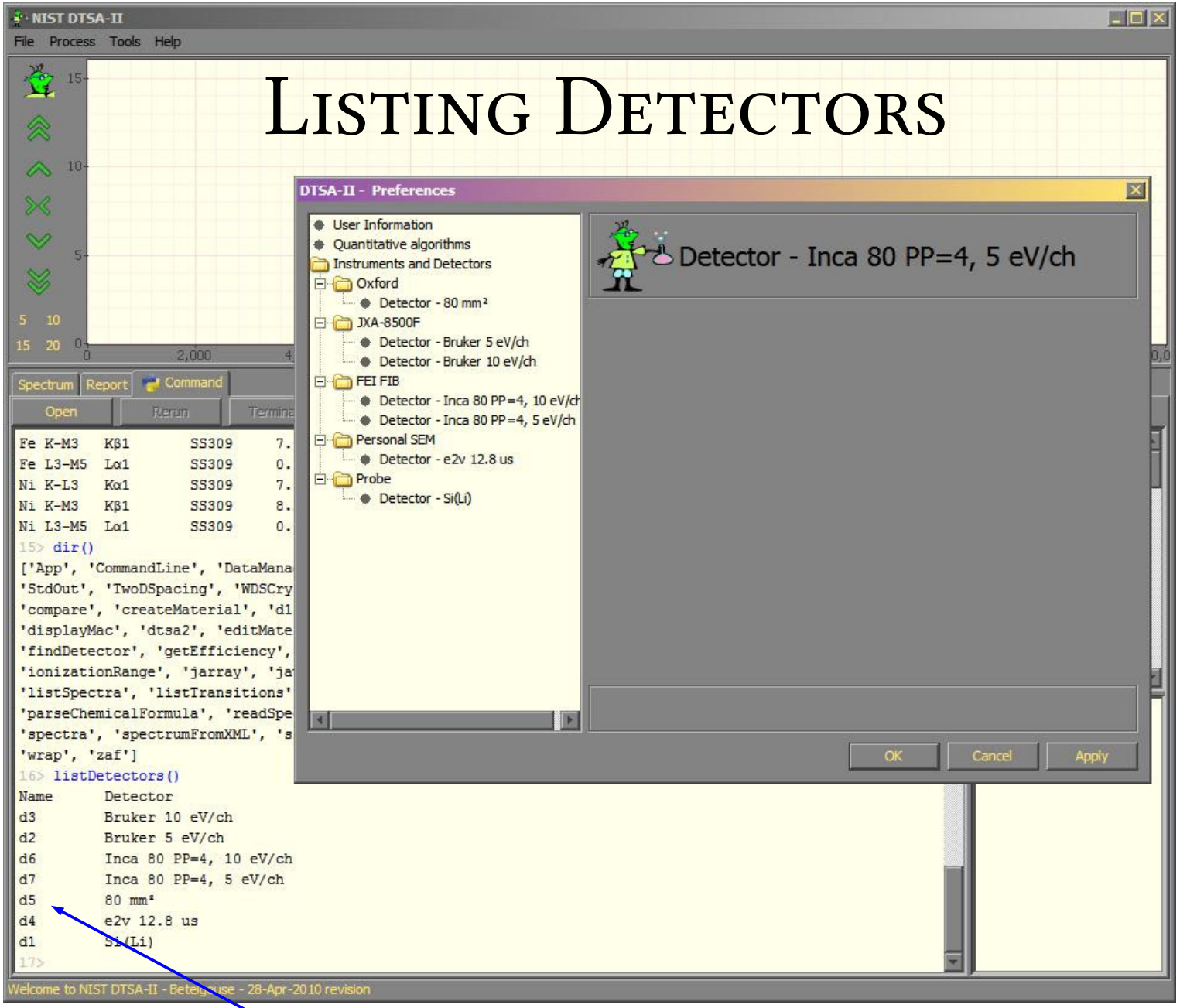
```
12> oldName=str(res)
13> oldName
'Sum[0.6\xd7Fe 1+0.25\xd7Cr 1+0.15\xd7Ni 1]'
14> res.rename("Bogus")
15> res.rename(oldName)
```

Give the spectrum the name “Bogus”

Set it back to the original name.

The method “rename” takes a single argument.

Listing Detectors



Detector alias (for referring to the detector within scripts)

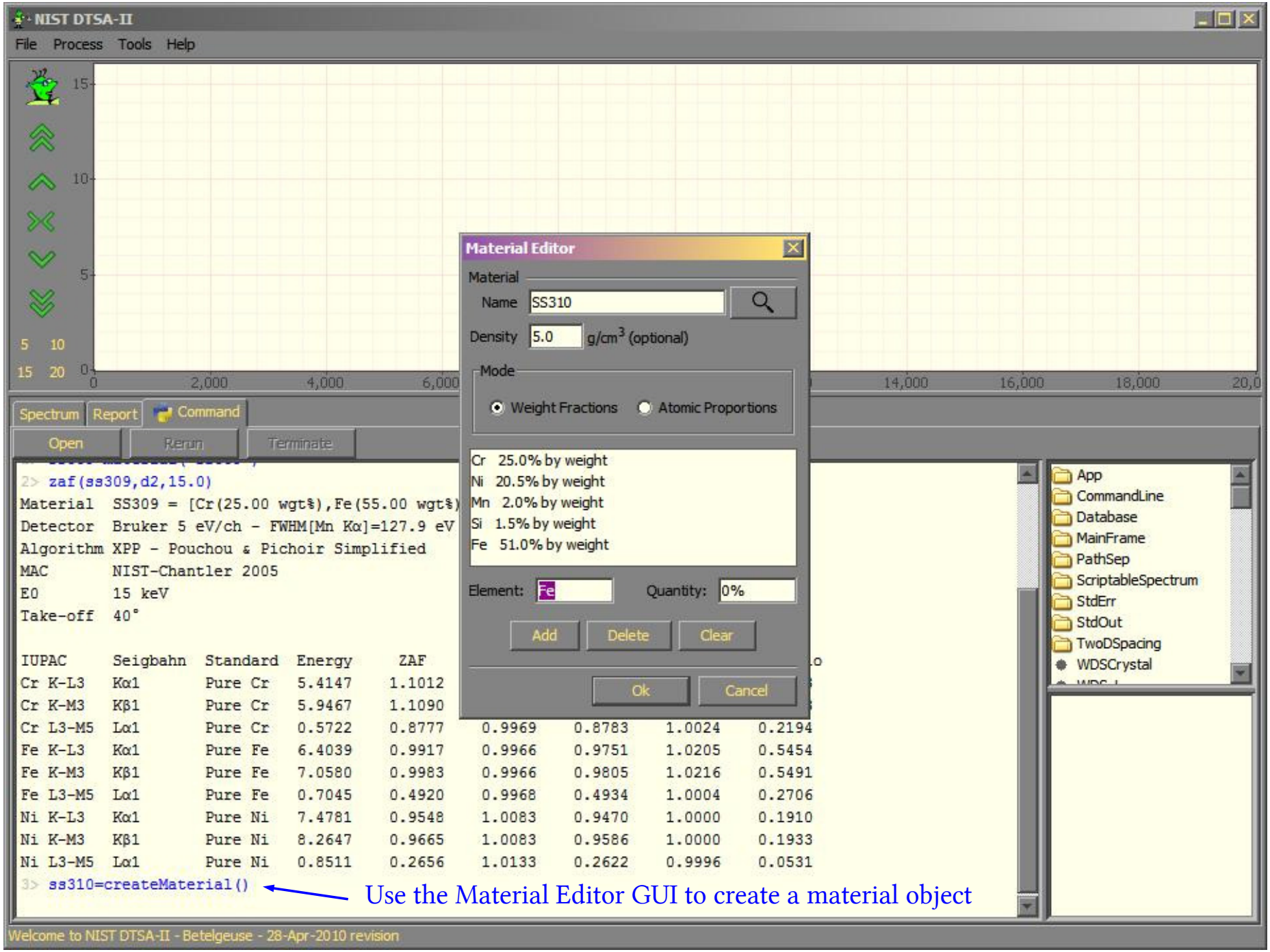
Basic ZAF calculations

Create a material object

Calculate the ZAF correction for the material "ss309" for the detector "d2" at "15.0" keV.

```
1> ss309=material("SS309")
2> zaf(ss309,d2,15.0)
Material  SS309 = [Cr(25.00 wgt%),Fe(55.00 wgt%),Ni(20.00 wgt%),Σ=100.00,5 g/cc]
Detector  Bruker 5 eV/ch - FWHM[Mn Kα]=127.9 eV - Sep 1, 2009 12:00:01 AM
Algorithm XPP - Pouchou & Pichoir Simplified
MAC       NIST-Chantler 2005
E0        15 keV
Take-off  40°

IUPAC     Seigbahn  Standard  Energy     ZAF        Z          A          F       k-ratio
Cr K-L3   Kα1       Pure Cr   5.4147    1.1012    0.9997     0.9939     1.1084    0.2753
Cr K-M3   Kβ1       Pure Cr   5.9467    1.1090    0.9997     0.9952     1.1147    0.2773
Cr L3-M5  Lα1       Pure Cr   0.5722    0.8777    0.9969     0.8783     1.0024    0.2194
Fe K-L3   Kα1       Pure Fe   6.4039    0.9917    0.9966     0.9751     1.0205    0.5454
Fe K-M3   Kβ1       Pure Fe   7.0580    0.9983    0.9966     0.9805     1.0216    0.5491
Fe L3-M5  Lα1       Pure Fe   0.7045    0.4920    0.9968     0.4934     1.0004    0.2706
Ni K-L3   Kα1       Pure Ni   7.4781    0.9548    1.0083     0.9470     1.0000    0.1910
Ni K-M3   Kβ1       Pure Ni   8.2647    0.9665    1.0083     0.9586     1.0000    0.1933
Ni L3-M5  Lα1       Pure Ni   0.8511    0.2656    1.0133     0.2622     0.9996    0.0531
3>
```



Use the Material Editor GUI to create a material object

ZAF against specific standards

```
13> ss310=createMaterial()
14> zaf(ss310,d2,15.0,stds={"Fe":"SS309","Cr":"SS309","Ni":"SS309"})
Material  SS310 = [Si(1.50 wgt%),Cr(25.00 wgt%),Mn(2.00 wgt%),Fe(51.00 wgt%),Ni(20.50 wgt%),Σ=100.00,5
g/cc]
Detector  Bruker 5 eV/ch - FWHM[Mn Kα]=127.9 eV - Sep 1, 2009 12:00:01 AM
Algorithm XPP - Pouchou & Pichoir Simplified
MAC       NIST-Chantler 2005
E0        15 keV
Take-off  40°

IUPAC     Seigbahn  Standard  Energy     ZAF      Z        A        F       k-ratio
Si K-L3   Kα1       Pure Si   1.7397     0.7178   1.1516   0.6228   1.0008   0.0108
Si K-M3   Kβ1       Pure Si   1.8290     0.7532   1.1516   0.6535   1.0009   0.0113
Cr K-L3   Kα1       SS309     5.4147     0.9913   0.9977   0.9997   0.9939   0.9913
Cr K-M3   Kβ1       SS309     5.9467     0.9911   0.9977   0.9998   0.9936   0.9911
Cr L3-M5  Lα1       SS309     0.5722     0.9890   0.9980   0.9912   0.9999   0.9890
Mn K-L3   Kα1       Pure Mn   5.8987     1.0043   0.9776   0.9973   1.0302   0.0201
Mn K-M3   Kβ1       Pure Mn   6.4904     0.9762   0.9776   0.9734   1.0259   0.0195
Mn L3-M5  Lα1       Pure Mn   0.6332     0.4405   0.9764   0.4502   1.0021   0.0088
Fe K-L3   Kα1       SS309     6.4039     0.9983   0.9976   0.9999   1.0008   0.9257
Fe K-M3   Kβ1       SS309     7.0580     0.9965   0.9976   0.9982   1.0007   0.9240
Fe L3-M5  Lα1       SS309     0.7045     0.9527   0.9980   0.9546   1.0000   0.8834
Ni K-L3   Kα1       SS309     7.4781     0.9991   0.9975   1.0016   1.0000   1.0241
Ni K-M3   Kβ1       SS309     8.2647     0.9987   0.9975   1.0013   1.0000   1.0237
Ni L3-M5  Lα1       SS309     0.8511     1.0242   0.9980   1.0262   1.0000   1.0498
15>
```

Defaults to pure elements.

Use the specified standard

Note: When quantified using a similar standard,
the Z, A and F terms are all close to 1.
This is likely to produce accurate quantifications!!!

Tabulating Elemental Data

listEdges("Pb")

```
17> listEdges("Pb")
IUPAC     Siegbahn  Energy (keV)
Pb K      Pb K      88.0045
Pb L1     Pb LI     15.8608
Pb L2     Pb LII    15.2
Pb L3     Pb LIII   13.0352
Pb M1     Pb MI     3.8507
Pb M2     Pb MII    3.5542
Pb M3     Pb MIII   3.0664
Pb M4     Pb MIV    2.5856
Pb M5     Pb MV     2.484
Pb N1     Pb NI     0.8936
Pb N2     Pb NII    0.7639
Pb N3     Pb NIII   0.6445
Pb N4     Pb NIV    0.4352
Pb N5     Pb NV     0.4129
Pb N6     Pb NVI    0.1429
Pb N7     Pb NVII   0.1381
Pb O1     Pb OI     0.1473
Pb O2     Pb OII    0.1048
Pb O3     Pb OIII   0.086
Pb O4     Pb OIV    0.0218
Pb O5     Pb OV     0.0192
18>
```

listTransitions("Fe")

```
18> listTransitions("Fe")
IUPAC     Siegbahn  Weight    Energy    Wavelength
                              (keV)       (Å)
Fe K-L3   Kα1       1         6.4039    1.93607
Fe K-L2   Kα2       0.5118    6.3909    1.94001
Fe K-M3   Kβ1       0.11895   7.058     1.75665
Fe K-M2   Kβ3       0.0684    7.058     1.75665
Fe K-M5   Kβ5       0.0001    7.1084    1.74419
Fe L3-M5  Lα1       1         0.7045    17.5989
Fe L3-M4  Lα2       0.1144    0.7045    17.5989
Fe L3-M1  Lℓ        0.10529   0.6152    20.1535
Fe L2-M4  Lβ1       0.16704   0.7175    17.28
Fe L2-M3  Lβ17      0.0001    0.6671    18.5855
Fe L2-N1  Lγ5       0.0045    0.718     17.268
Fe L2-M1  Lη        0.0511    0.6282    19.7364
Fe L1-M3  Lβ3       0.0479    0.7921    15.6526
Fe L1-M2  Lβ4       0.02569   0.7921    15.6526
19>
```

listData("Si")

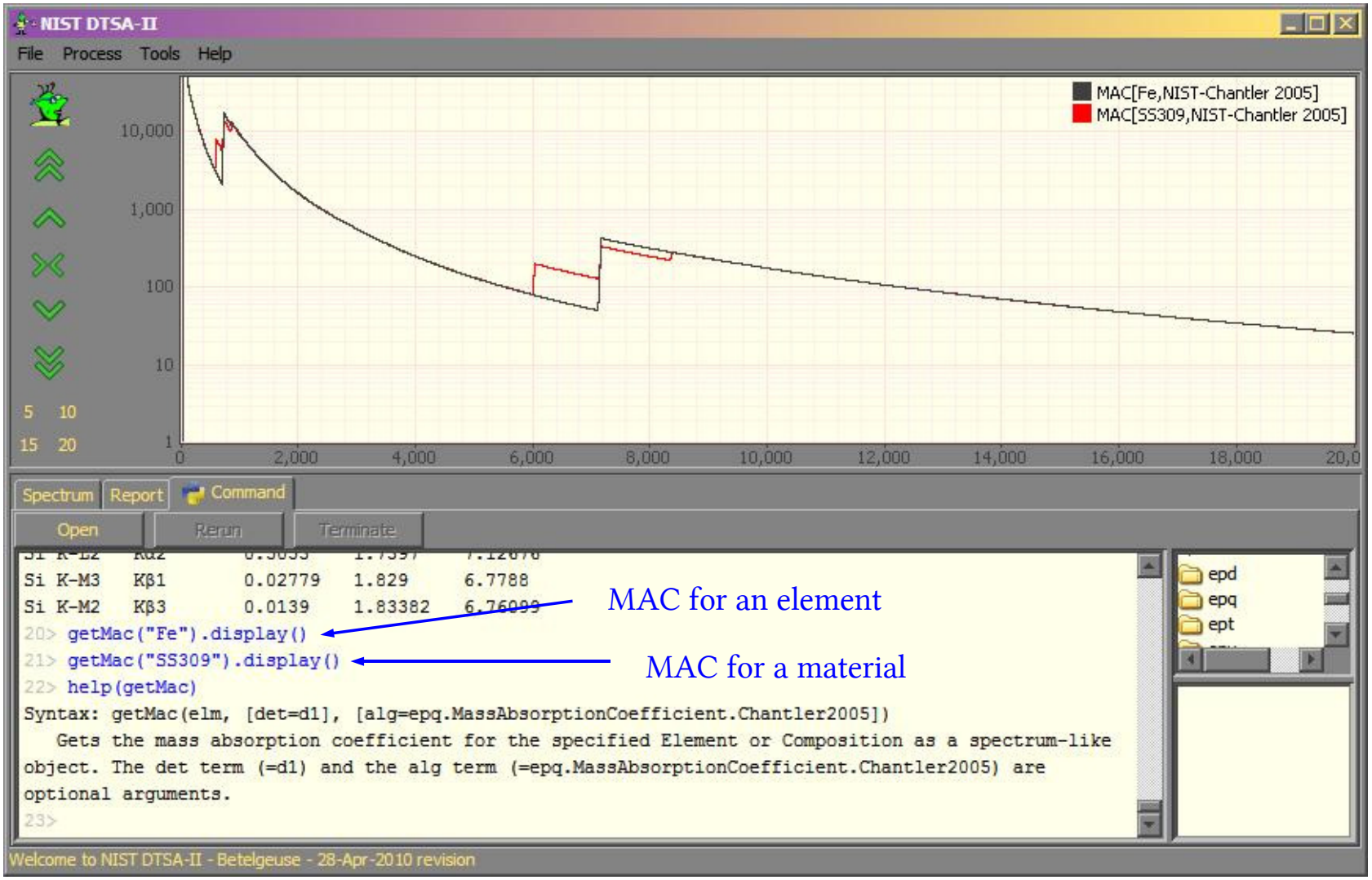
```
19> listData("Si")
Abbrev    Name      Z         A
Si        Silicon   14        28.0855

IUPAC     Siegbahn  Energy (keV)
Si K      Si K      1.8389
Si L1     Si LI     0.1487
Si L2     Si LII    0.0992
Si L3     Si LIII   0.0992
Si M1     Si MI     0.0113572
Si M2     Si MII    0.00508305

IUPAC     Siegbahn  Weight    Energy    Wavelength
                              (keV)       (Å)
Si K-L3   Kα1       1         1.7397    7.12676
Si K-L2   Kα2       0.5053    1.7397    7.12676
Si K-M3   Kβ1       0.02779   1.829     6.7788
Si K-M2   Kβ3       0.0139    1.83382   6.76099
20>
```

listData(..) = listEdges(...) + listTransitions(...) + extra

Displaying MAC data



MAC for an element

MAC for a material

getMac(...) actually creates a spectrum-like object. Hence the call to the method "display()" plots the MAC on the spectrum window (which I've scaled to log10.)

Calculating MAC data

```
23> help(mac)
Syntax: mac(mat, xx, [alg=epq.MassAbsorptionCoefficient.Chantler2005])
   where mat is a material or element (by name, Material or Element object), xx is an element,
atomic shell or x-ray transition and alg is the tabulation to use (by default Chantler2005).
Displays the mass absorption coefficient for the specified element or x-ray transition in the
specified material.
24> mac("SS309","Fe")
XRT        MAC
           (cm^2/g)
Fe K-L2    163.494
Fe K-L3    162.578
Fe K-M2    125.719
Fe K-M3    125.719
Fe K-M5    128.58
Fe L1-M2   10924.9
Fe L1-M3   10924.9
Fe L2-M1   6774.49
Fe L2-M3   5878.88
Fe L2-M4   11044.9
Fe L2-N1   11026.4
Fe L3-M1   7117.92
Fe L3-M4   5661.85
Fe L3-M5   5661.85
25>
```

For all transitions associated with an element.

For a specific transition in IUPAC notation.

```
27> mac("SS309",transition("Fe L3-M5"))
XRT        MAC
           (cm^2/g)
Fe L3-M5   5661.85
```

Useful Objects

Creating various types of useful objects:

element:	creates epq.Element objects
atomicShell:	creates epq.AtomicShell objects
material:	creates either epq.Composition or epq.Material objects.

```
29> elm=element("Fe")
30> shell=atomicShell("Fe L3")
31> xrt=transition("Fe L3-M5")
32> comp=material("Fe2O3")
33> mat=material("Fe2O3",5.24)
```

Many of the objects manipulated from the command line are actually Java objects. Many are from one of the libraries within *epq.jar*

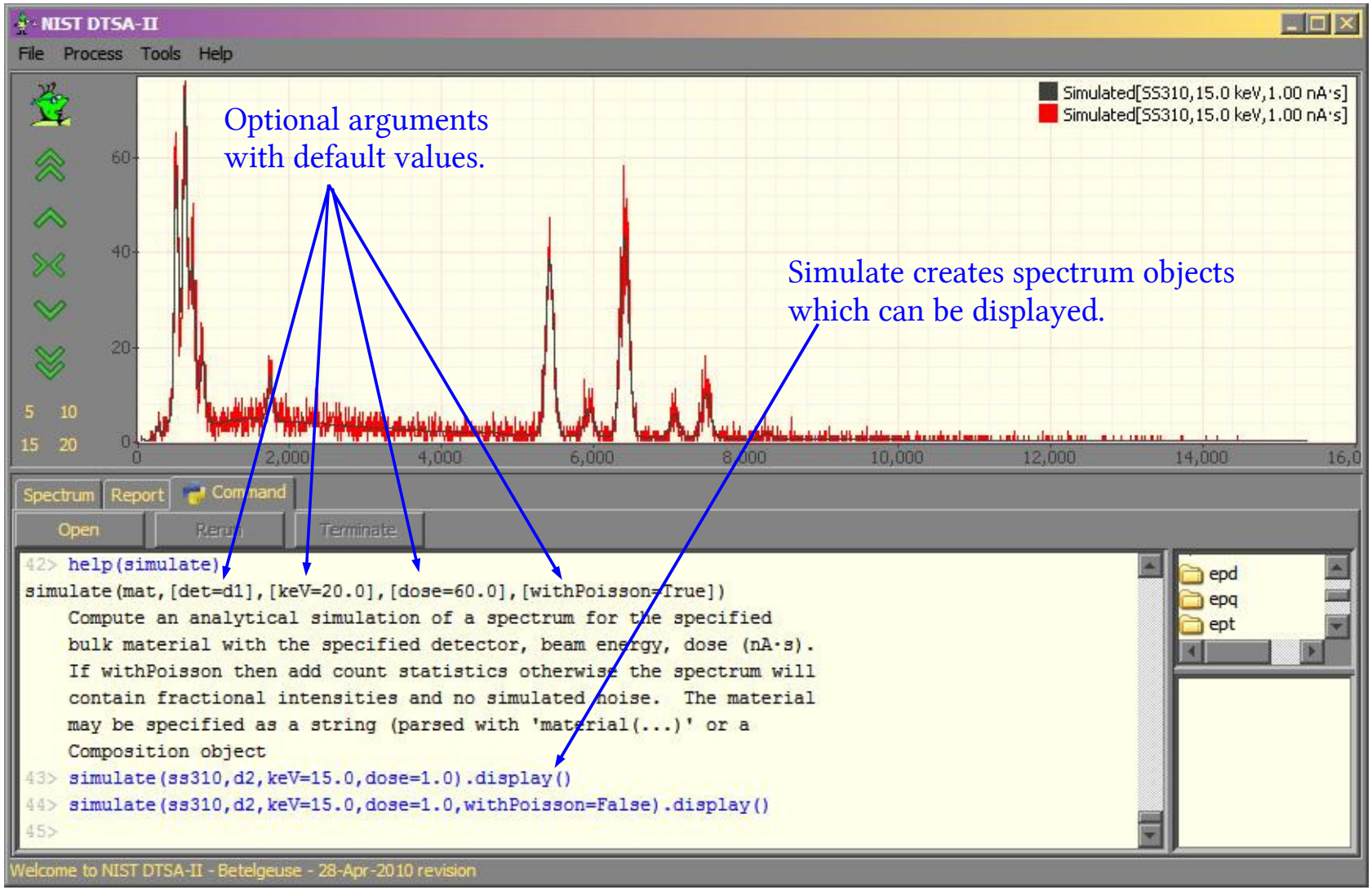
The fully qualified name of the Element object is:
gov.nist.microanalysis.EPQLibrary.Element
This is a little verbose so within the scripting the alias:
epq.Element
is equivalent.

Common aliases:

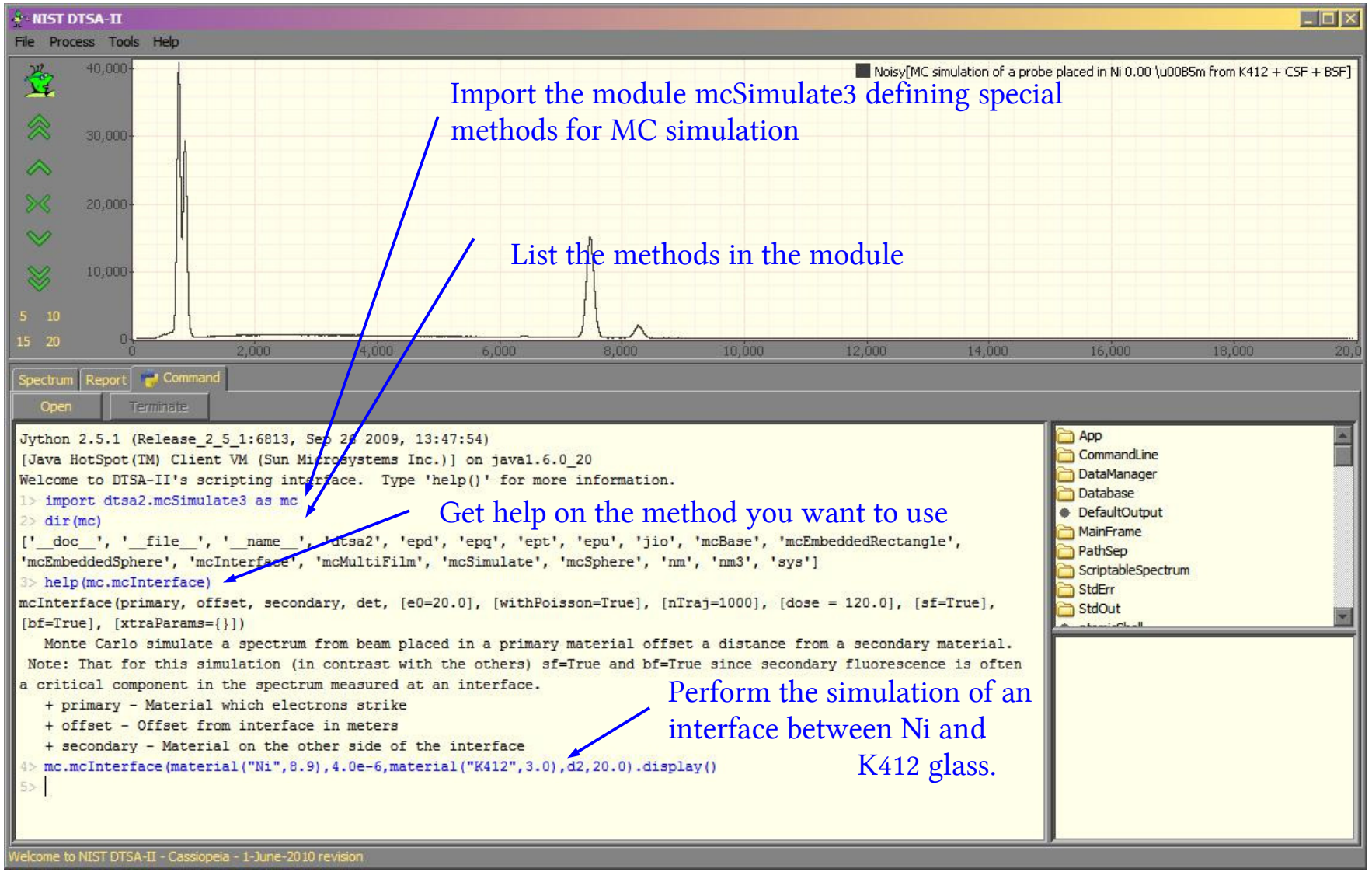
epq	*gov.nist.microanalysis.EPQLibrary*
epu	*gov.nist.microanalysis.Utility*
ept	*gov.nist.microanalysis.EPQTools*
epd	*gov.nist.microanalysis.EPQLibrary.Detector*

Library documentation:
http://www.cstl.nist.gov/div837/837.02/epq/dtsa2/JavaDoc/index.html

Quick Simulation

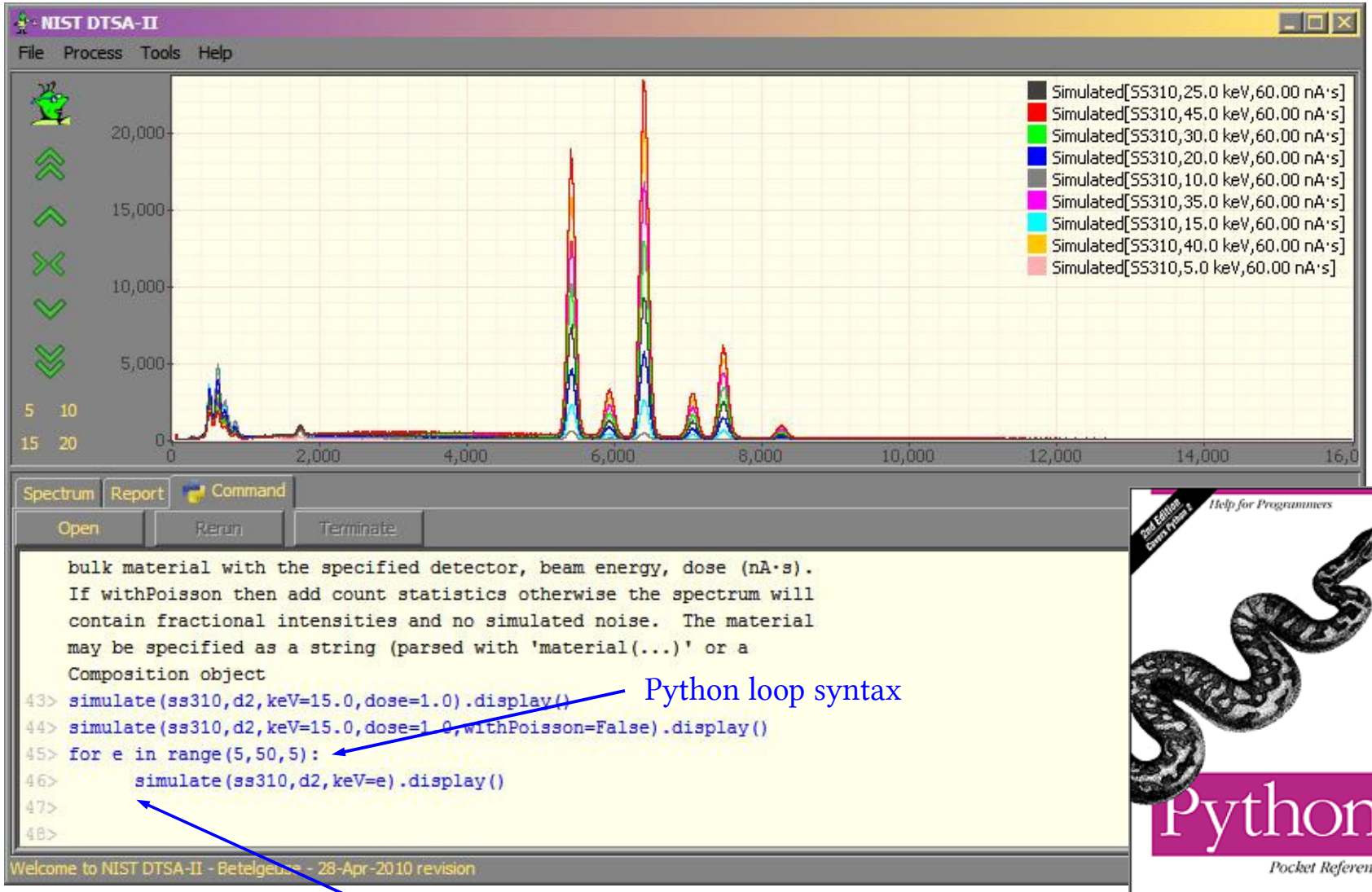


Monte Carlo Simulation



'help(mc)' provides help on the module aliased 'mc'

Loops



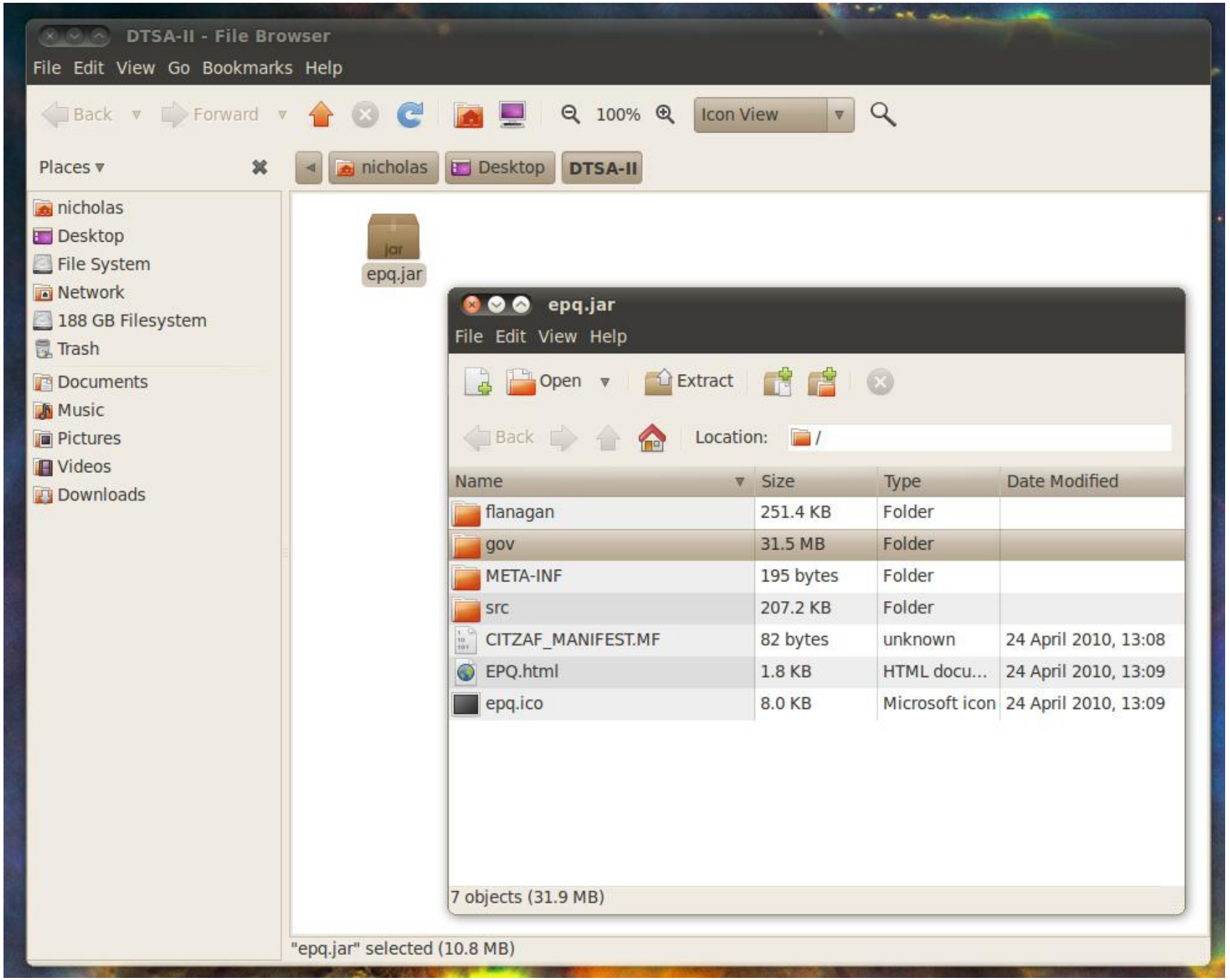
Python loop syntax

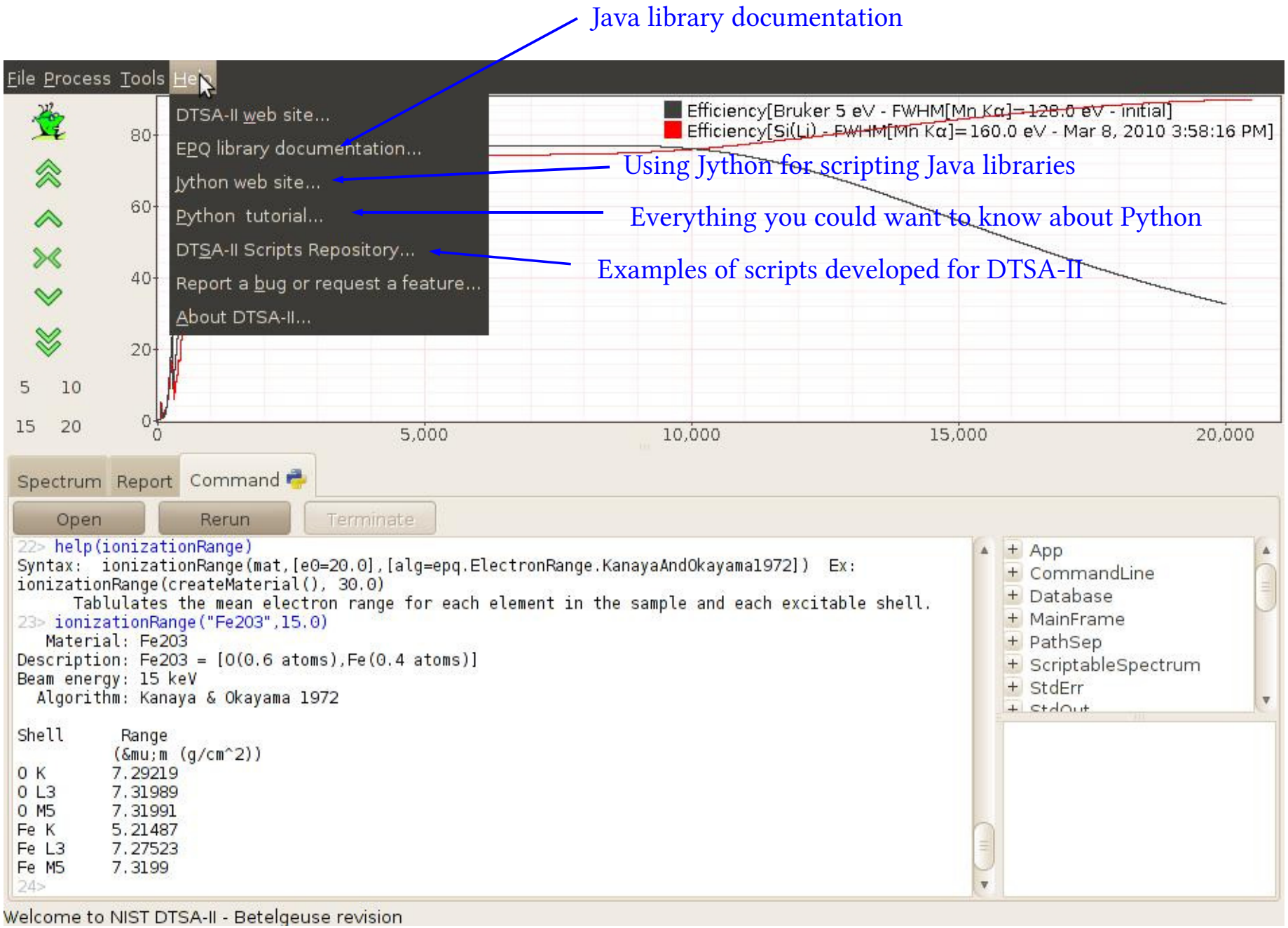
Indention dictates structure

```
22> help(ionizationRange)
Syntax:  ionizationRange(mat,[e0=20.0],[alg=epq.ElectronRange.KanayaAndOkayama1972])  Ex:
ionizationRange(createMaterial(), 30.0)
      Tablulates the mean electron range for each element in the sample and each excitable shell.
23> ionizationRange("Fe2O3",15.0)
   Material: Fe2O3
Description: Fe2O3 = [O(0.6 atoms),Fe(0.4 atoms)]
Beam energy: 15 keV
  Algorithm: Kanaya & Okayama 1972

Shell      Range
          (&mu;m (g/cm^2))
O K       7.29219
O L3      7.31989
O M5      7.31991
Fe K      5.21487
Fe L3     7.27523
Fe M5     7.3199
24>
```

If you hand ionizationRange a Material (Composition + density) the output is in μm otherwise for Compositions it is in μm (g/cm^3).


DTSA-II - File Browser
File Edit View Go Bookmarks Help
Back
Forward
100%
Icon View
Places
nicholas
Desktop
DTSA-II
nicholas
Desktop
File System
Network
188 GB Filesystem
Trash
Documents
Music
Pictures
Videos
Downloads
jar
epq.jar
epq.jar
File Edit View Help
Open
Extract
Back
Location:
/
Name
Size
Type
Date Modified
flanagan
251.4 KB
Folder
gov
31.5 MB
Folder
META-INF
195 bytes
Folder
src
207.2 KB
Folder
CITZAF_MANIFEST.MF
82 bytes
unknown
24 April 2010, 13:08
EPQ.html
1.8 KB
HTML docu...
24 April 2010, 13:09
epq.ico
8.0 KB
Microsoft icon
24 April 2010, 13:09
7 objects (31.9 MB)
"epq.jar" selected (10.8 MB)


Java library documentation
File Process Tools Help
DTSA-II web site...
EPQ library documentation...
Jython web site...
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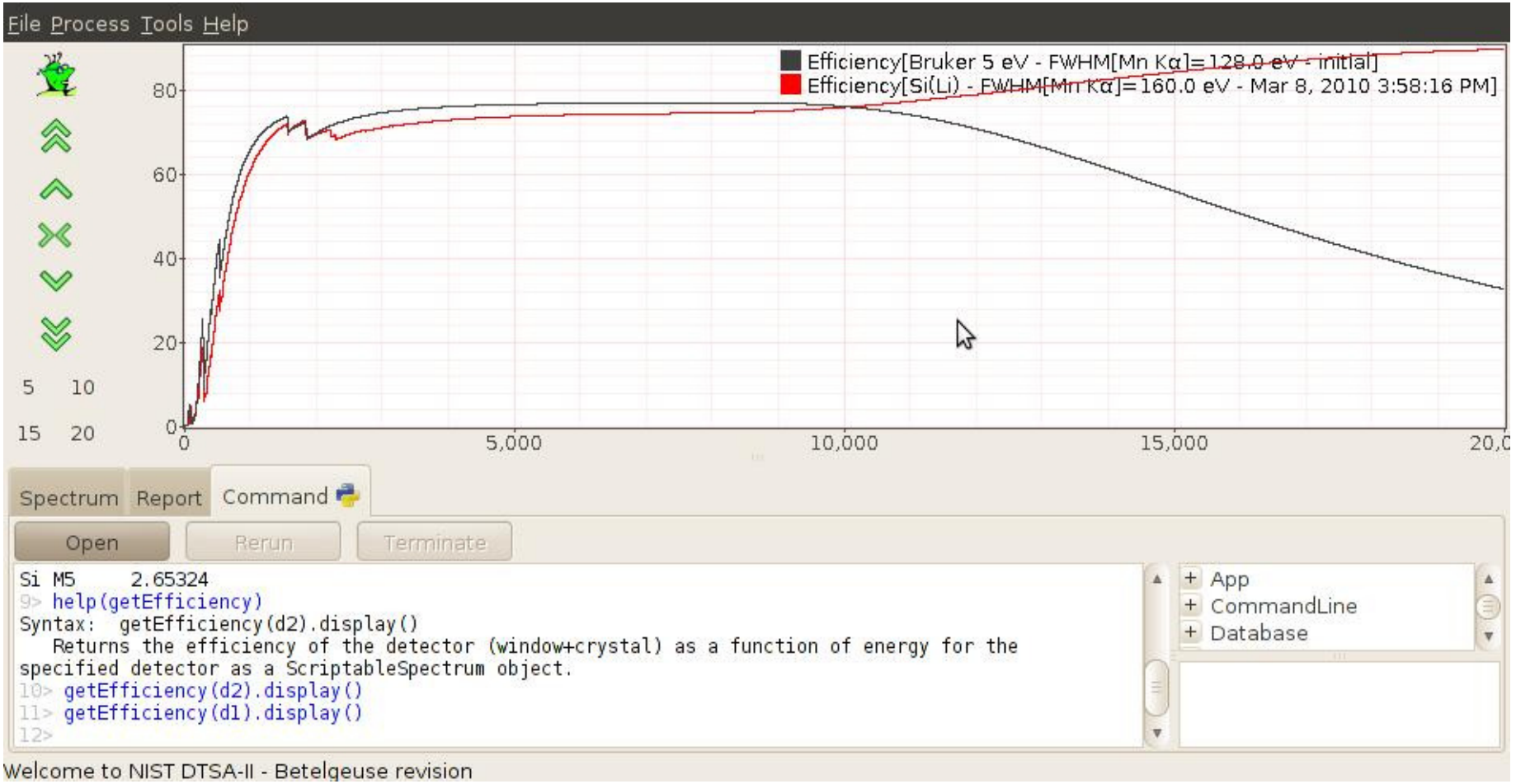
About DTSA-II...
Using Jython for scripting Java libraries
Everything you could want to know about Python
Examples of scripts developed for DTSA-II
Efficiency[Bruker 5 eV - FWHM[Mn Kα]=128.0 eV - Initial]
Efficiency[Si(Li) - FWHM[Mn Kα]=160.0 eV - Mar 8, 2010 3:58:16 PM]
Spectrum
Report
Command
Open
Rerun
Terminate
22> help(ionizationRange)
Syntax: ionizationRange(mat,[e0=20.0],[alg=epq.ElectronRange.KanayaAndOkayama1972]) Ex:
ionizationRange(createMaterial(), 30.0)
Tablulates the mean electron range for each element in the sample and each excitable shell.
23> ionizationRange("Fe2O3",15.0)
Material: Fe2O3
Description: Fe2O3 = [O(0.6 atoms),Fe(0.4 atoms)]
Beam energy: 15 keV
Algorithm: Kanaya & Okayama 1972
Shell Range
(μm (g/cm^2))
O K 7.29219
O L3 7.31989
O M5 7.31991
Fe K 5.21487
Fe L3 7.27523
Fe M5 7.3199
24>
App
CommandLine
Database
MainFrame
PathSep
ScriptableSpectrum
StdErr
Welcome to NIST DTSA-II - Betelgeuse revision



getEfficiency(d2) gets the effective quantum efficiency of the detector – includes window, support, dead layers, coatings, crystal geometry – as a spectrum-line object.

Notice how the SDD looses efficiency at high energies. This is due to the relative thinness of the detector (0.5 mm vs 3 mm for a conventional Si(Li). Also observe how the

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tc.py

```
for z in range(6,85):
    mat = material(epq.Element.byAtomicNumber(z).toAbbrev())
    tmp = "%d" % z
    for e0 in range(10,50,10):
        tc=epq.SpectrumUtils.totalCounts(simulate(mat,d2,e0))
        tmp = "%s\t%g" % ( tmp, tc)
    print tmp
```

Python Tab Width: 3 Ln 6, Col 34 INS