

## I. The plot only option

```
perl cleaned_upgrade.plx B30_rl.log B30_mh.log B30_ml.log 1.txt
```

or

```
perl cleaned_upgrade.plx B30_rl.log B30_mh.log B30_ml.log plotonly
```

To generate data for plotting spectrum for each subcalculation (without extrapolation): simply replace the original output file name with “plotonly”). Main peak information will be printed out on to the screen and to the “outbands.txt” file.

## II. The advance shoulder detection option

```
extn,3
sigma,0.4
sdtrl,0.2
sdtrh,0.2
sdtml,0.2
|
sdtrllleft,0.2,0.2,0.2,0.2,#
sdtrllright,0.2,0.2,0.2,0.2,#
sdtrhlleft,#
sdtrhlright,#
sdtmlleft,#
sdtmlright,#
```

Basic shoulder detection parameters

Advance shoulder detection parameters

**Basic shoulder detection parameters:** set one sdt for each spectrum.

**Advance shoulder detection parameters:**

- set sdt parameters for each main peak on the spectrum.
- This option can be turned off by removing the section or placing “#” at the end, the program will go through basic shoulder detection as usual.
- The advance shoulder detection option can be turned off for one spectrum and turned on for another
- The number of sdtrllleft and sdtrllright values have to be the same as the number of main peaks on the spectrum. Ie. 4 main peaks on the rl spectrum, you need to give 4 numbers for sdtrllleft and sdtrllright.
- Place “NA” to replace a number: shoulder detection off for this side of this peak
- Place “df” to replace a number: use the same sdt value as in basic shoulder detection (the first one does the same thing as the second one)

```
extn,3
sigma,0.4
sdtrl,0.1
sdtrh,NA
sdtml,0.1

sdtrllleft,NA,df
sdtrllright,NA,0.08
sdtrhlleft,#
sdtrhlright,#
sdtmlleft,NA,df
sdtmlright,NA,df
```

```
extn,3
sigma,0.4
sdtrl,0.1
sdtrh,NA
sdtml,0.1

sdtrllleft,NA,0.1
sdtrllright,NA,0.08
sdtrhlleft,#
sdtrhlright,#
sdtmlleft,NA,0.1
sdtmlright,NA,0.1
```

Parameters

sdtrllleft: shoulder detection threshold for left side of the main peaks on rl spectrum

sdtrllright: shoulder detection threshold for right side of the main peaks on rl spectrum

...other parameters follow the same pattern