Ivium application note: Peak finding and baseline correction

In addition to the automatic peakfind function, the IviumSoft contains a more advanced "peak finding/ base line subtraction" tool. It is also accessible from the Analysis options above the graph. The advanced option will allow the operator to manipulate the automatic peak-search parameters, or manually add/remove peaks, subtract a baseline and process the results.

Activating **Peakfind advanced,** will open a window that contains:
- Automatic peak find tool, and its editable parameters.
- Manual peak addition tool.
- Peak results list, and peak removal functions.
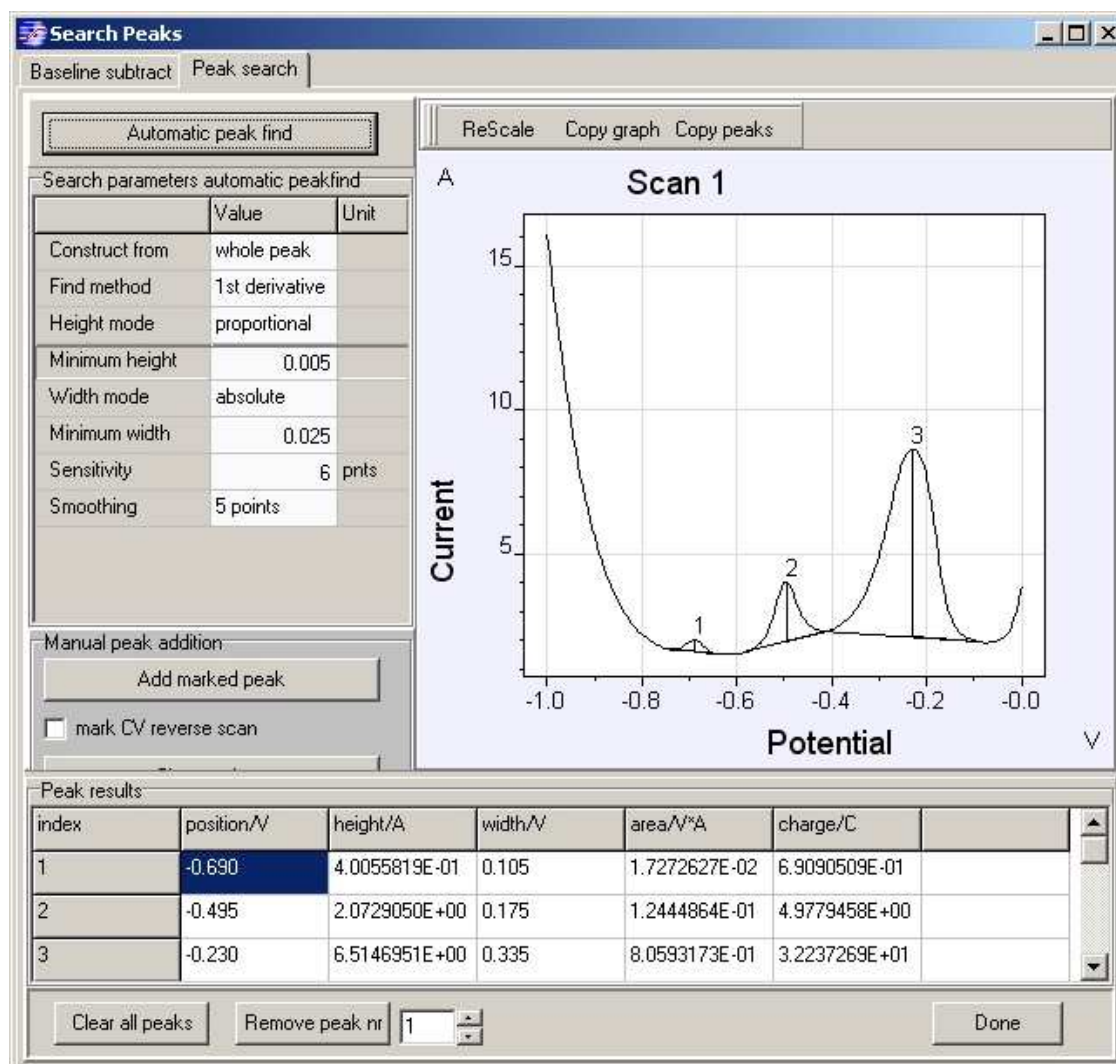- Graphical presentation of the data with found/added peaks drawn in.

Figure 1: Automatic peakfind example with whole peak and 1ˢᵗ derivative selected

The **automatic peak find tool** is located on the top left panel. It has an execute search button, and below a list of parameters that will be applied during automatic search actions:

Construct from: whole peak / front flank / rear flank

Selecting whole peak will construct a full peak, while front flank will only use the rising part of the peak, and rear flank only the descending flank. Whole peak is best suited for peaks with clearly defined flanks and horizontal baselines. Front peak is appropriate when the tail of the peak is "smeared out", or has a steep baseline, or is close to the scan boundaries, as is often the case in Cyclic Voltammetry.

Find Method: 1st derivative / 2nd derivative

Selects the control variable for the method that is used by the algorithm that determines where peaks start and end. The 1st derivative method is more sensitive to small peaks, but only works well when the baseline is (nearly) horizontal. The 2nd derivative technique can cope with sloped baselines, as is often the case for fast scan techniques, as Linear Sweep or Cyclic Voltammetry.

Height mode: proportional / absolute

Refers to the minimum height.

Minimum height: in absolute height mode it defines the absolute minimum height for a peak, while in proportional mode, it defines the minimum fraction from the maximum value in the whole scan.

Width mode: proportional / absolute

Refers to the minimum width.

Minimum width: in absolute width mode it defines the absolute minimum width for a peak, while in proportional mode, it defines the minimum fraction from the range of the scan.

Sensitivity: number of consecutive points that must fulfill the begin & end criteria for a peak to be accepted. A higher number usually expands the peak

Smoothing: Apply smoothing on the data from which the peaks are to be determined. Use higher levels (more points) on noisy data. Note that the underlying data will not be changed.
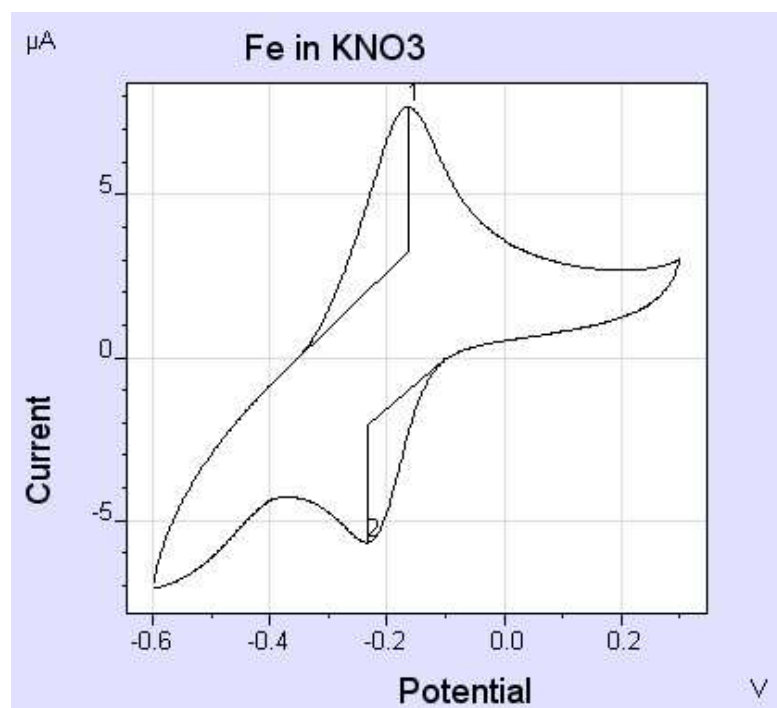

Figure 2: automatic peakfind example with front-flank and 2nd derivative selected

Manual peak addition tool : peaks can be added manually by first marking (left-mouse-click) the desired locations in the graph, and thereafter pressing the Add marked peak button. Peaks can be added either from 2 marks or from 3 marks. When 3 markers are set, these are taken as the beginpoint, toppoint, and the endpoint of the peak. When 2 markers are set, these are taken as the beginpoint and the endpoint of the peak, while the top is determined automatically.

When Cyclic Voltammograms are edited, the checkbox must be checked before markers on the reverse scan can be set.

Note that manual addition works independent of the peak search parameters, and always whole peaks are added.
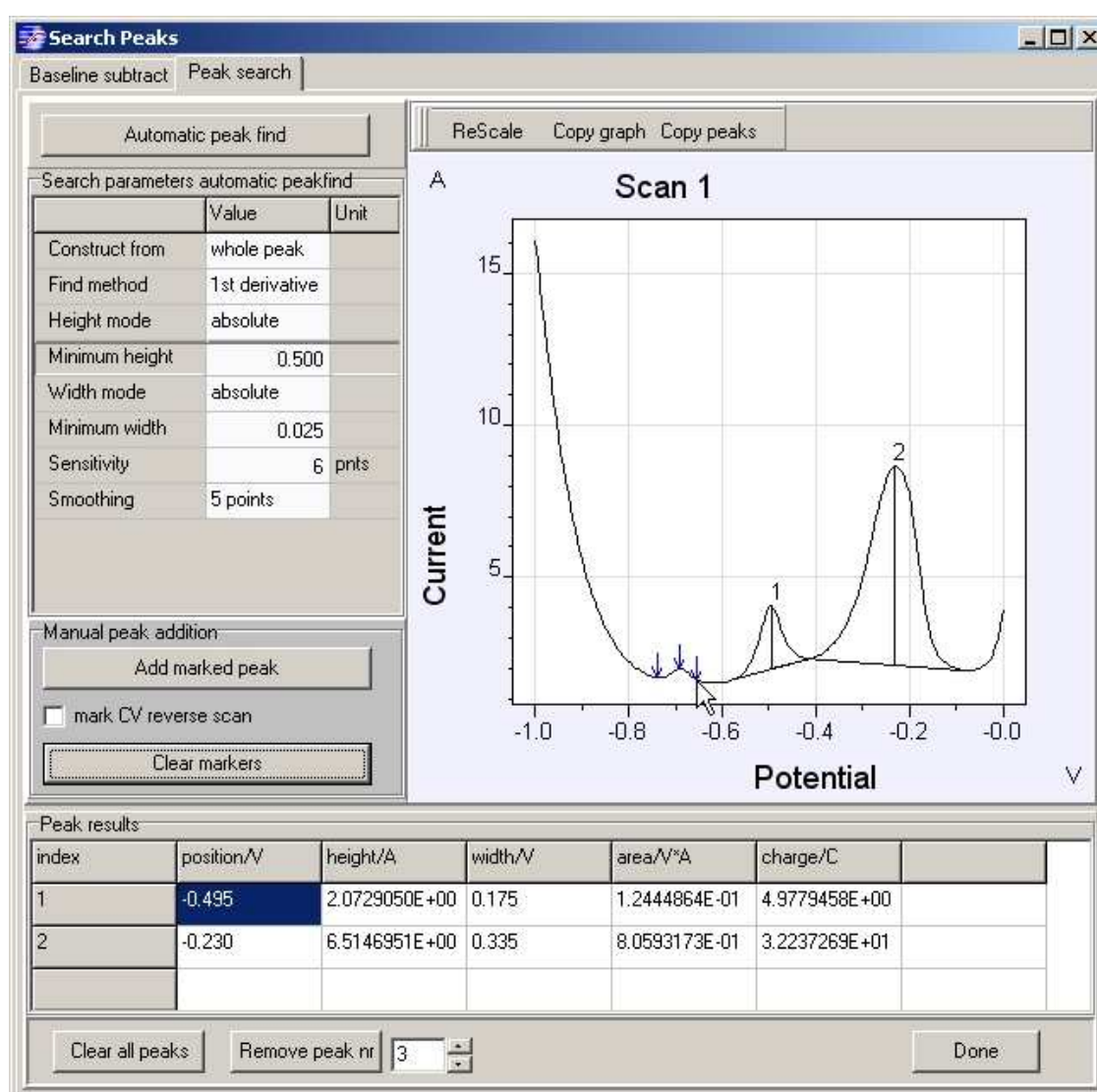

Figure 3:adding peaks manually - beginpoint, toppoint and the endpoint of the peak

Baseline subtraction: sometimes it is convenient to remove the baseline before the peak-analysis is executed. To activate the baseline subtraction tool, select the "Baseline subtract" tabsheet.
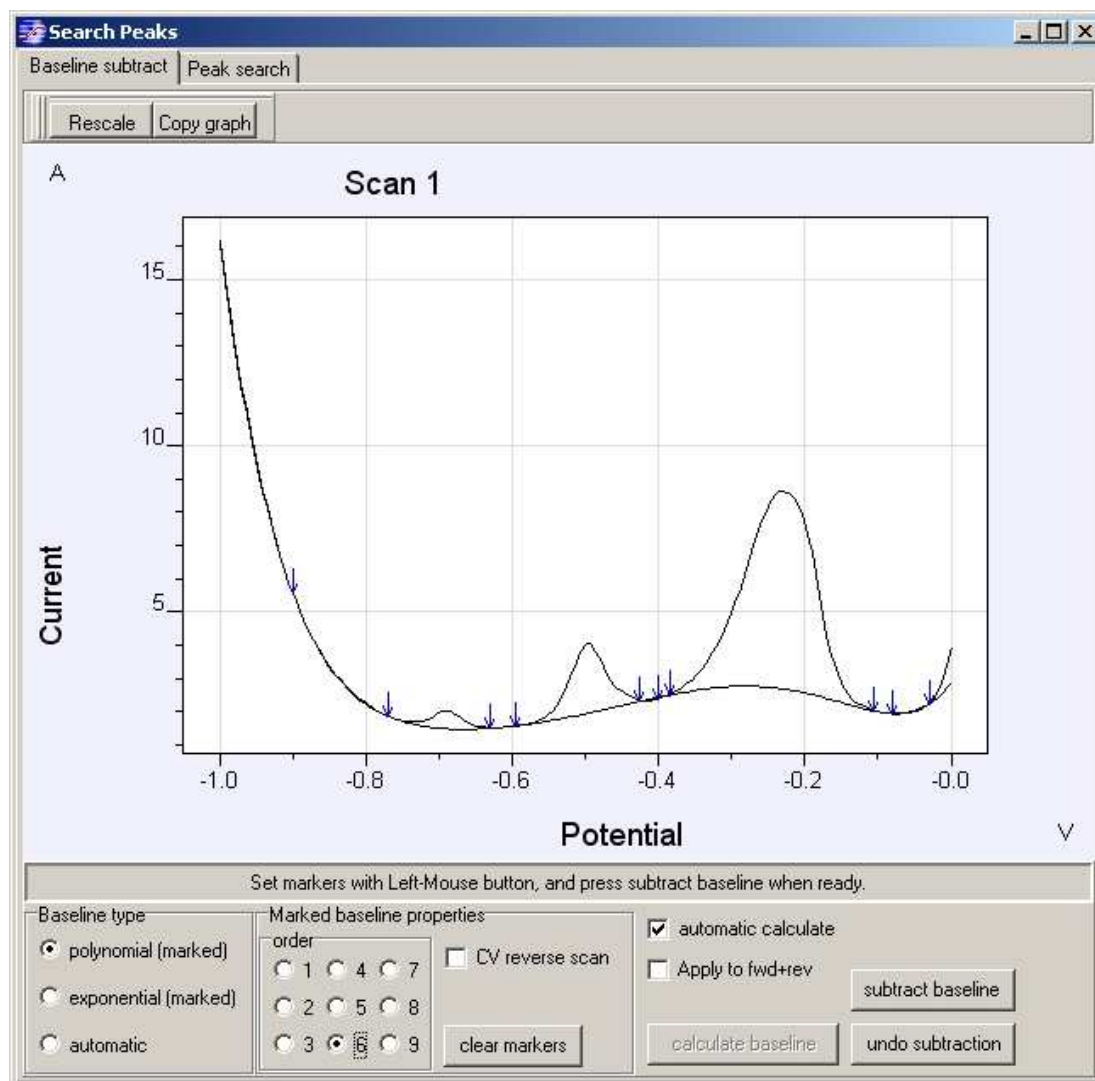

Figure 4: example of baseline subtraction with a 6th order polynomial

The operator should use left-mouse clicks to set anchor-points (markers) to which the baseline is fitted. The software will recalculate the baseline automatically after the addition of each anchor-point, unless this is disabled with the indicated checkbox. There is no limit to the number of anchor-points. When the projected baseline is satisfactory, press <subtract baseline>, and the data correction will be applied. **Please note that this procedure will change the underlying data**, **and prior calculated peakdata will be cleared.**

Three baseline types are available:
- Polynomial: 1st order corresponds to linear, 2nd to parabolic, etc.
- Exponential: the sum of exponents of increasing order, up to the indicated value.
- Automatic: automatically constructed baseline using the "moving average" method.

The baseline order can be set from 1 to 9. However the order will always be lower than the number of data points, for example on 3 anchor-points the baseline order is limited to 2.
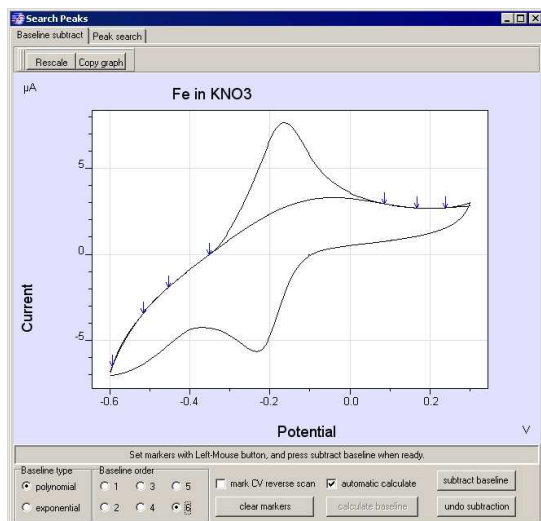

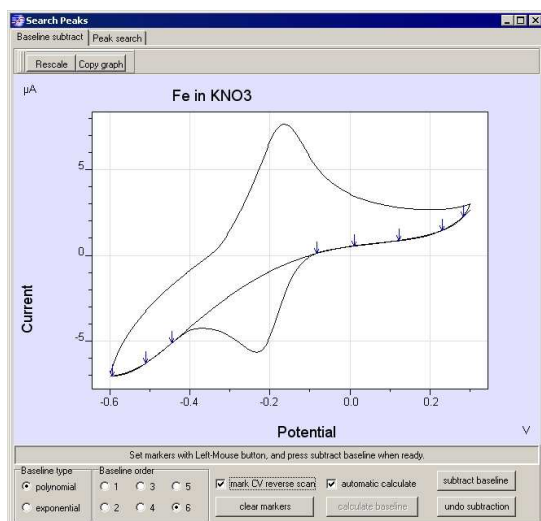*Figure 5a: baseline determination of CV forward scan*

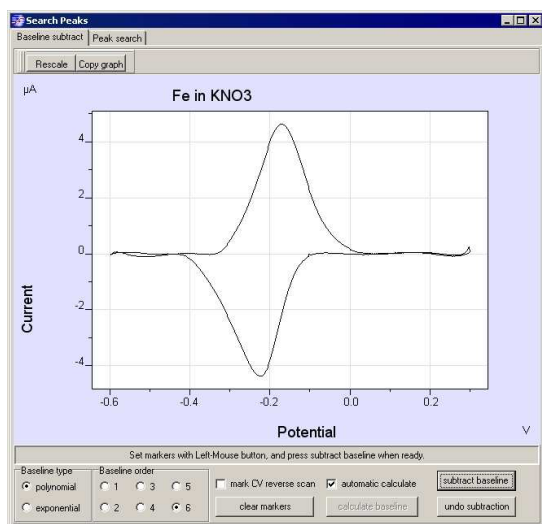*Figure 5b: baseline determination of CV reverse scan*

Figure 5c: CV after baseline subtraction

Note that for Cyclic Voltammograms, forward and reverse scan baselines have to be subtracted separately. Use the "mark CV reverse scan" checkbox to select each branch.