

## Ivium application note: Peak finding and baseline correction, revision 2

In addition to the automatic peakfind also present in the pocketpc software, the PalmSensPC program contains a more advanced “peak finding/ base line subtraction” tool. It is accessible from the Peaks menu, via the advanced operations option. The advanced option will allow the operator to manipulate the automatic peak-search parameters, or manually add/remove peaks, subtract baselines and process the results.

Activating **advanced operations**, will open an extra 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.

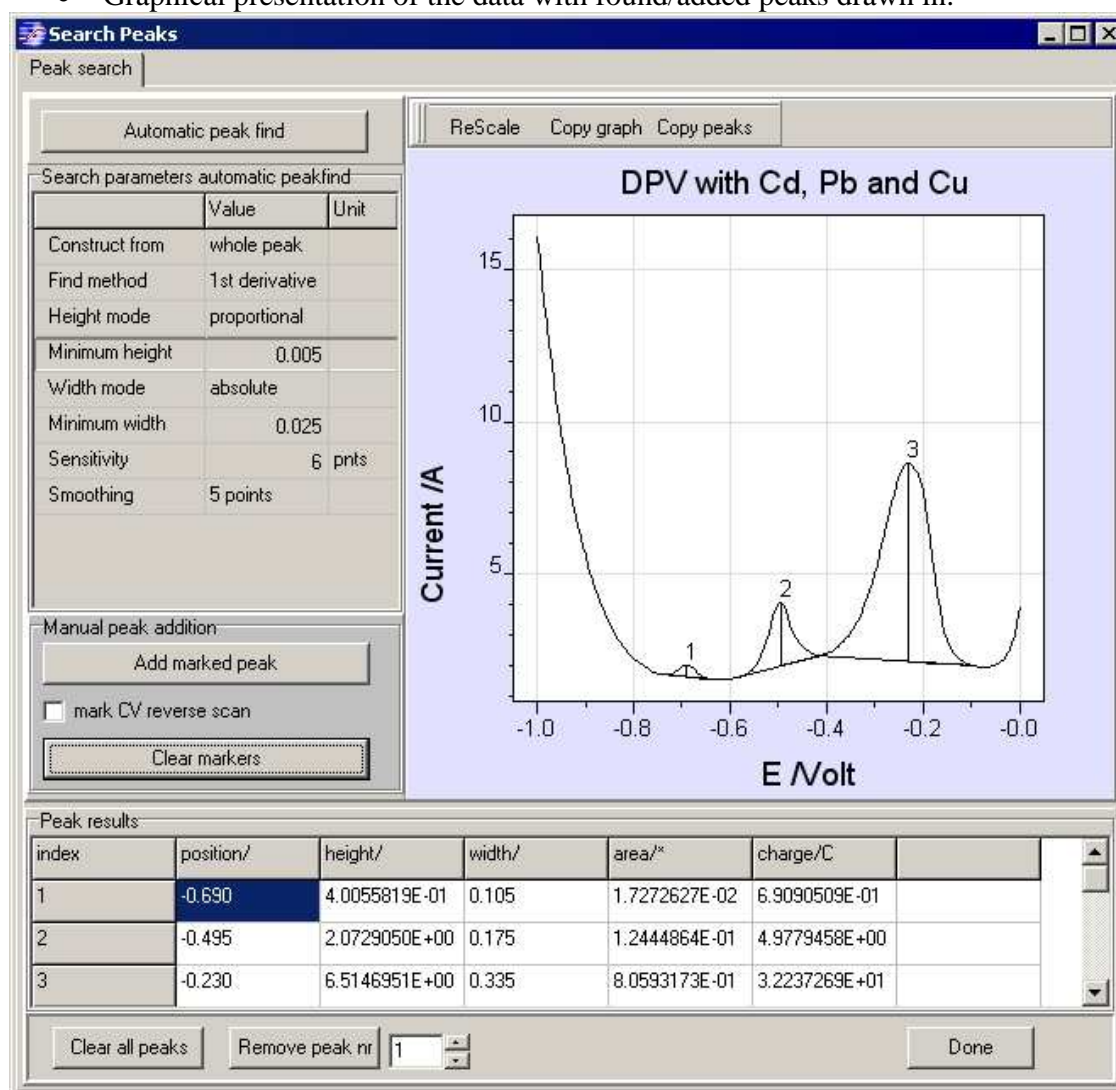


Figure 1: Automatic peakfind example with whole peak and 1<sup>st</sup> derivative selected

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** : 1<sup>st</sup> derivative / 2<sup>nd</sup> derivative

Selects the control variable for the method that is used by the algorithm that determines where peaks start and end. The 1<sup>st</sup> derivative method is more sensitive to small peaks, but only works well when the baseline is (nearly) horizontal. The 2<sup>nd</sup> 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.

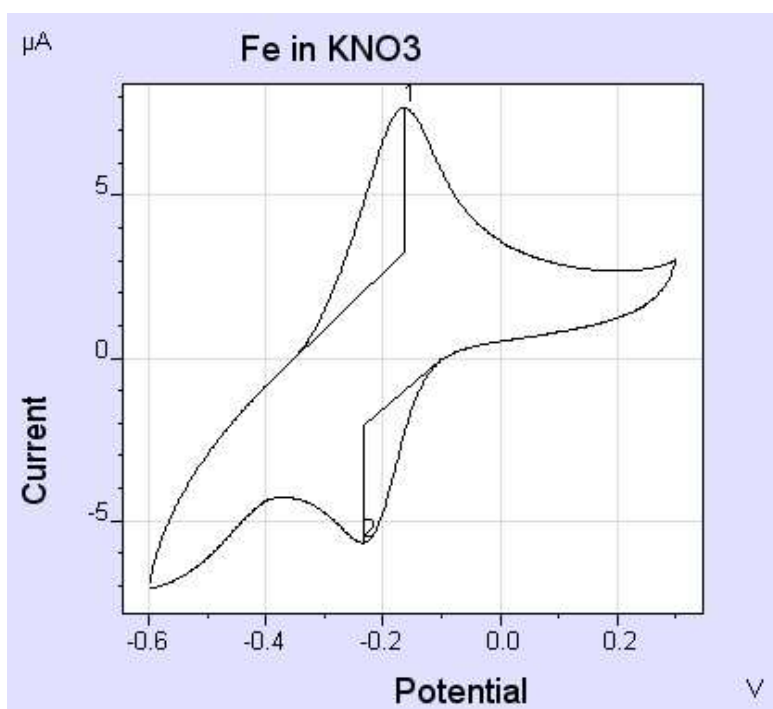


Figure 2: automatic peakfind example with front-flank and 2<sup>nd</sup> derivative selected

**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, top point, 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.

**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.

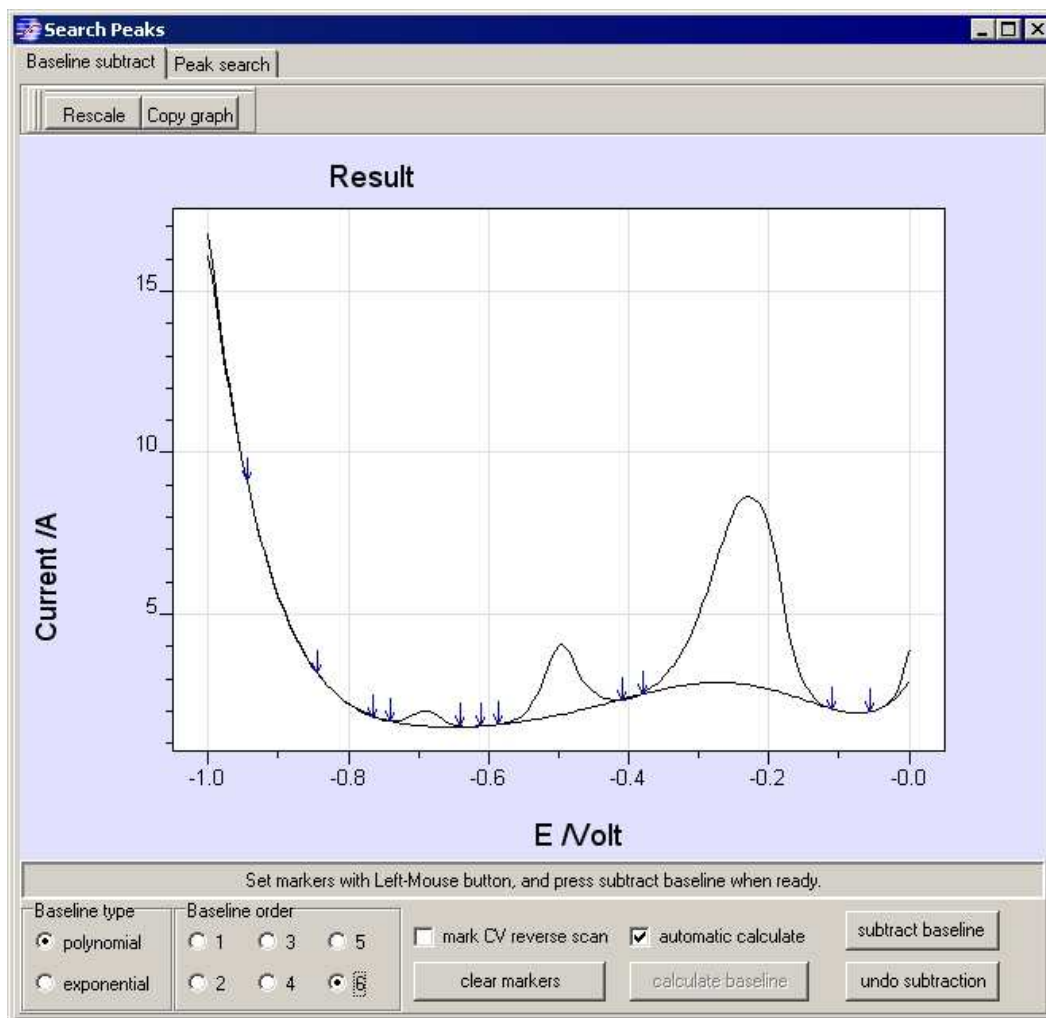


Figure 3: example of baseline subtraction with a 6<sup>th</sup> order polynomial

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.**

2 baseline types are available:

- Polynomial : 1<sup>st</sup> order corresponds to linear, 2<sup>nd</sup> to parabolic, etc.
- Exponential : the sum of exponents of increasing order, up to the indicated value.

The baseline order can be set from 1 to 6. 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.

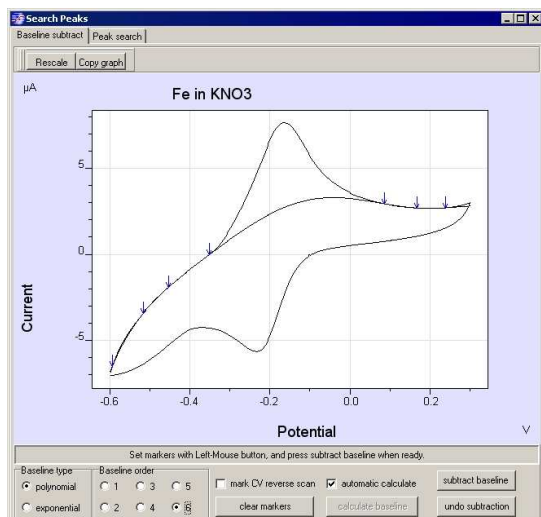


Figure 4a: baseline determination of CV forward scan

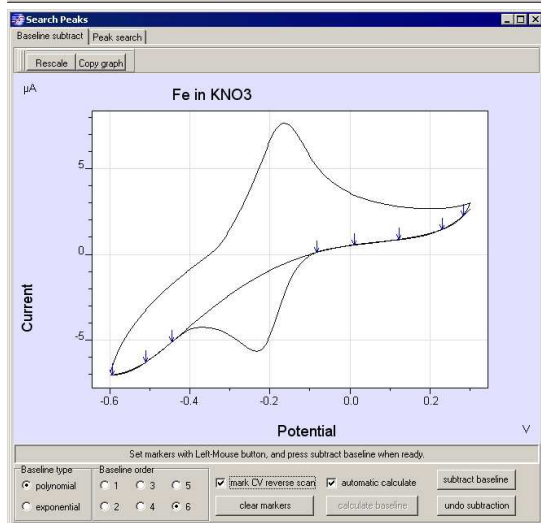


Figure 4b: baseline determination of CV reverse scan

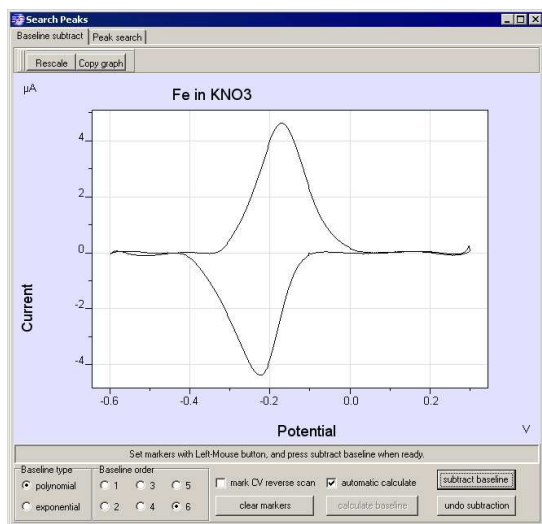


Figure 4c: CV after baseline subtraction

For Cyclic Voltammograms, forward and reverse scan baselines have to be subtracted separately. Use the “mark CV reverse scan” checkbox to select each branch.