

Igor Technical Notes

WaveMetrics Technical Support

#020-B: Peak Areas

Written by:
Mar 1992

James Prouty

Modified:
Sep 1993

James Prouty

This revision addresses Igor Pro compatibility.

We started with the TN020 Peak Measurement experiment and created the Peak Areas experiment. This experiment is useful when you have data containing a large number of closely spaced periodic bipolar peaks, and you need “rough and ready” estimates of the peak parameters. Other peak shapes can be measured if they are identified manually (with cursors), or if the peak identification functions are re-written. This experiment does not fit a function to peaks; it just measures the amplitudes, widths, and areas.

Accompanying files:

‘Peak Areas’ -- Sample experiment.

Supporting files (from the ‘Sample XOPs Folder’ of the ‘Igor Extras Disk’):

‘Execute’ -- XOP containing the Execute operation. **The ‘Execute’ XOP is not needed and is not compatible with Igor Pro.**

Related files:

‘TN020 Peak Measurement’ -- Sample experiment (Fits Gaussian and Lorentzian peaks).

‘TN020-A Custom Peak Measurement’ -- Sample experiment (Fits Voigt and Template peaks).

The Peak Areas experiment is for measuring a large number of peaks, and for estimating and removing a piece-wise linear baseline.

The Peak Areas experiment features:

- Full support of equally-spaced or X-Y data representation.
- Baseline (background) estimation and removal.
 - Any built-in Igor function may be fit to the baseline at multiple areas indicated with the cursors.
- Peak Identification
 - Manual or automatic identification of peak start and end. Automatic peak identification is currently adequate for data similar to that shown in the graph on page 2.

- Baseline generation
Creates a piece-wise linear baseline from data minima or maxima. This baseline may then be removed from the data, or accounted for during the peak measurement process.
- Peak Measurement
Report of amplitudes, positions, widths (FWHMs), and areas of peaks excluding the baseline. The area calculation uses either rectangular integration, trapezoidal integration, or counts.

Peak Areas Requirements

The experiments require Igor 1.24 or later. At least 1 megabyte of memory should be allocated to Igor 1.2. If you use color, allocate at least 1.5 megabytes. A floating point coprocessor is highly recommended.

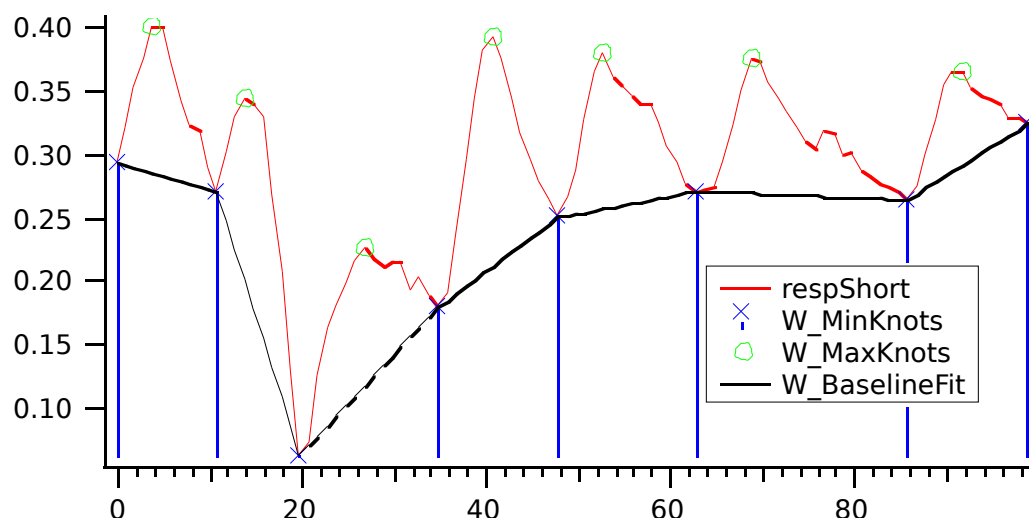
Installing the Supporting Files

Igor 1.2 users must copy the ‘Execute’ XOP into the folder containing the ‘Igor’ application.

Igor Pro has a built-in Execute, so the XOP is not required.

How To Use The Peak Areas Experiment

After installing any XOP(s), launch Igor, and open the ‘Peak Areas’ experiment. A graph with a sample series of peaks will appear.



You can use this data to become familiar with the experiment, or you can import your own using the standard techniques; see “loading” and “Browse Waves” in the manual’s index. If you import your own data, you should create a graph which displays it as equally-spaced or X-Y data.

Pull down the Macros menu to see what this experiment contains:

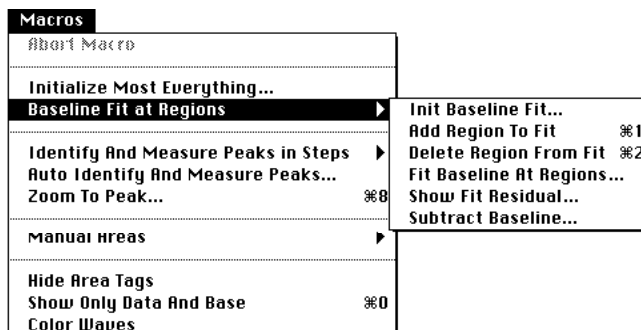


Initialize Most Everything...

This macro announces to the experiment which waves are your data and their representation (equally-spaced or X-Y). Use this macro to analyze new data, or start over with old data. The data is converted to double precision.

Baseline Fit at Regions

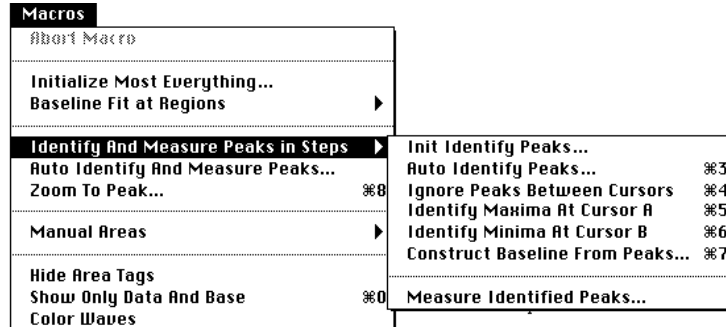
This hierarchical menu contains **almost** everything related to baseline estimation and removal, and is the same as the Baseline menu in the Peak Measurement experiment. See Technote #020:



One additional baseline-related item is found in the 'Identify And Measure Peaks in Steps' menu, described below.

Identify And Measure Peaks in Steps

This hierarchical menu contains the macros related to identifying and measuring peaks. You can employ the cursors to identify the **start** and **end** of peaks, or you can use the ‘Auto Identify Peaks...’ macro to identify peaks automatically. Once identified, the peaks can be measured.



The menu items are listed in approximate order of use.

Init Identify Peaks...

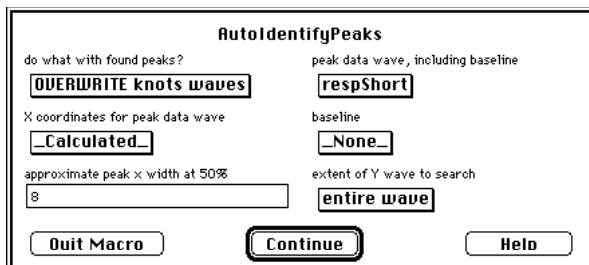
This macro initializes the process of “identifying” peaks — manually or automatically — to provide peak start and end locations to the ‘Measure Identified Peaks...’ macro.

The peaks are identified through two waves, “W_MinKnots” and “W_MaxKnots”. These waves are the same size as the data wave, which is “respShort” in our example here. The values in these waves are set to NaN (“Not a Number”) where there is no minima or maxima, and to the value of the data wave where there is a local minima or maxima.

The cursors are used to identify peaks or modify automatically identified peaks, so this macro makes sure the cursors are displayed in the graph.

Auto Identify Peaks...

The ‘Auto Identify Peaks’ macro scans the data wave looking for local minima and sets the value of the wave “W_MinKnots” to NaN where there is none, or to the value of the data wave where a local minima exists. Similar computations result in “W_MaxKnots” values identifying local maxima.



The ‘approximate peak x width at 50%’ value is used to specify the window over which local minima and maxima are computed. A data value is a local maxima if it is the highest value within the window

centered about itself. Ties are resolved in the favor of the left-most maxima or minima.

NOTE: The functions ‘IsBestMinMax’ and ‘IsLocalMinMax’ are used to automatically identify the minima and maxima. If you have a more useful identification method, try modifying these to suit your needs. **The current algorithm works best with bi-polar peaks that have a fairly regular frequency of occurrence, such as the data shown in this Technical Note.**

The ‘Auto Identify Peaks...’ macro allows you to add the identified minima and maxima to those already defined in the knots waves, or to overwrite the knots waves with the identified minima and maxima, which ignores previously identified peaks. “OVERWRITE...” is usually the correct choice.

‘baseline’ is often “_None_”, but could be the result of a baseline fit from the ‘Baseline Fit at Regions’ macros.

NOTE: ‘baseline’ gets set to “W_BaselineFit” by the ‘Construct Baseline From Peaks...’ and ‘Auto Identify And Measure Peaks...’ macros.

After identifying the peaks, the two “knots waves” are appended to the graph in a manner which identifies the maxima (circles) and minima (crosses). You can change the number and location of minima and maxima using the cursors and the three following macros.

Ignore Peaks Between Cursors

Place the cursors around or on any minima or maxima, then invoke this macro (using the menu, or the command-4 key equivalent). All minima and maxima under either cursor or between the cursors are removed from the knots waves.

Identify Maxima At Cursor A

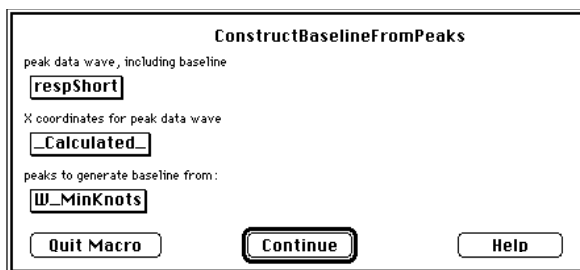
Place cursor A (the circle cursor) on the data value you wish to be considered a maxima, and then invoke this macro.

Identify Minima At Cursor B

Place cursor B (the square cursor) on the data value you wish to be considered a minima, and then invoke this macro.

Construct Baseline From Peaks...

This macro creates a piece-wise linear baseline from the identified minima or maxima:



The resulting baseline is wave “W_BaselineFit”, which is appended to the graph. It becomes the default baseline wave.

This baseline wave can then be subtracted from the data, but the ‘Measure Identified Peaks...’ macro does

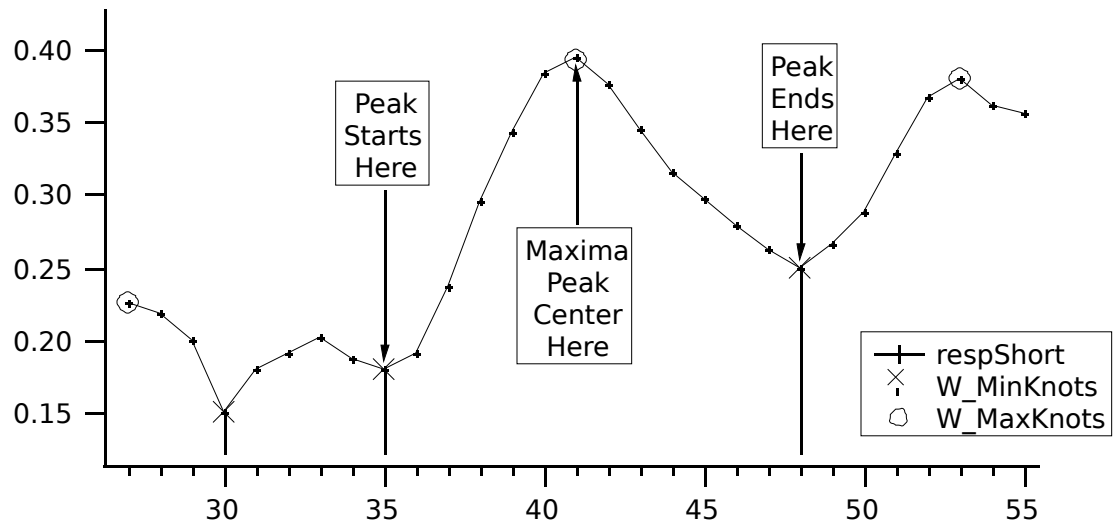
#020-B: Peak Areas
not require this to be done.

Measure Identified Peaks...

This macro uses peak locations described by the “knots waves” to create a table named “PeakReportTable” which contains the amplitude, width, center position, and area of each identified peak. It also contains the peak start in the wave named “W_PkX1”, the peak end in “W_PkX2”, and the starting x location of the FWHM in “W_PkXwL”. The area of all the peaks (taken together) is printed to the history window.

You choose whether the table of peak parameters is sorted by amplitude, center location, width (FWHM), or area. Area may be computed by rectangular integration, trapezoidal integration, or counts.

NOTE: This macro considers a positive peak to start from the minima that precedes the peak’s maxima. The peak ends at the minima that follows the peak’s maxima:



A Report layout is generated containing a graph of the data and the the table named “PeakReportTable”.

Auto Identify And Measure Peaks...

This menu item combines most of the steps in the ‘Identify And Measure Peaks in Steps’ hierarchical menu into a single dialog (which is the ‘InitIdentifyPeaks’ dialog):

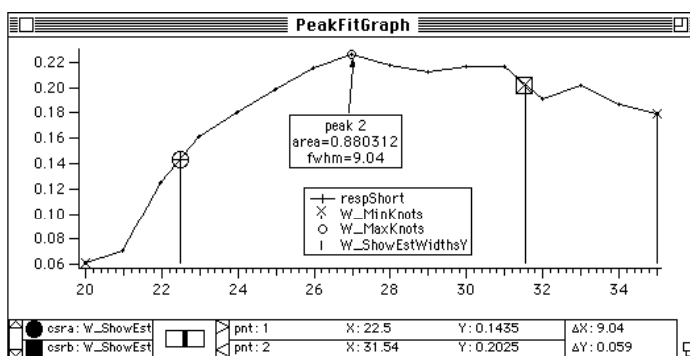
InitIdentifyPeaks

peak data wave, including baseline	X coordinates for peak data wave
<input type="text" value="respShort"/>	<input type="text" value="._Calculated._"/>
baseline	peak polarity
<input type="text" value="._None._"/>	<input type="text" value="positive"/>
approximate peak x width at 50%	default integration type
<input type="text" value="0.8"/>	<input type="text" value="integrate trapezoidal"/>

This is effective when the automatic peak detector correctly identifies peaks and baseline minima. See the description for ‘Auto Identify Peaks’ for the importance of the value labelled “approximate peak x width at 50%”.

Zoom To Peak

Give the row number (see the ‘Point’ column) in the PeakReportTable, and this macro will zoom the graph to display only the corresponding peak. If desired, a tag showing the measurements for the peak is displayed as well. The wave “W_ShowEstWidthsY” and the cursors indicate where the peak width starts and ends, and where the half amplitude levels were:



Manual Areas

Same as the “Areas’ menu hierarchy in TN020, “Peak Measurement and Fitting”. This hierarchical menu contains the macros related to computing areas over a single region of the peak data wave, and the baseline wave if there is one. The cursors are used to select the region of measurement.

Hide Area Tags

Removes area tags created by ‘ZoomToPeak’ or ‘AreaBetweenCursors’.

Show Only Data and Base

This macro removes all waves from the target window, except the current peak data and baseline waves. (It also keeps all waves whose names end in “X”, because it is impolite to remove x waves from underneath y waves.) The removed waves are not killed. This macro is invoked by typing command-0 (zero, not oh).

If you have another wave you want to keep on the graph, set the global string g_keep to the name of that wave before invoking the macro.

Color Waves

This macro (which also appears in the 'Graph Macros' menu) is used by the experiment to color the waves in each graph to aid in distinguishing one wave from another. It also applies other style preferences such as minor ticks, curve smoothing, and legends.

If you don't use color with Igor, or prefer a different graph presentation (such as turning off axis standoff), you should change this macro to make waves distinguishable from one another. The experiment calls this macro when it appends a wave, so you'll get your own presentation.

Waves and their Uses

respShort	Sample peak data, aka "the data wave".
W_BaseCoefs	Baseline coefficients from 'Fit Baseline at Regions', this is passed to the PolyMorph function. This is paired with W_BasePM. See the procedure window for a description of the format of the coefficients. Note that, for implementation reasons, W_BaseCoefs[0] is NaN.
W_BaselineFit	Output wave of 'Fit Baseline at Regions...' and 'Construct Baseline From Peaks', this is each macro's idea of the best fit of the baseline to the peak data wave. It has the same scaling and number of points as the peak data wave. After it is created, it becomes the default baseline wave.
W_BasePM	Baseline coefficients descriptor for PolyMorph ("PM") from 'Fit Baseline at Regions', this is copied to the global wave W_PM for access by the PolyMorph function. This is paired with W_BaseCoefs.
W_BaseRegion	Annotation and weighting wave used in identifying regions of the peak data wave as belonging to the baseline of the data. Used by most of the 'Baseline' macros.
W_PkAmps	Output of the 'MeasureIdentifiedPeaks' macro, it contains the baseline-corrected amplitudes of the identified peaks.
W_PkAreas	Output of the 'MeasureIdentifiedPeaks' macro, it contains the baseline-corrected areas of the identified peaks.
W_PkCenters	Output of the 'MeasureIdentifiedPeaks' macro, it contains the center locations in x coordinates of the identified peaks.
W_PkFWHMs	Output of the 'MeasureIdentifiedPeaks' macro, it contains the Full Width at Half Maximums of the identified peaks.
W_PkX1,W_PkX2	Output of the 'MeasureIdentifiedPeaks' macro, they contain the peak start and end x locations of the identified peaks.
W_PkXwL	Output of the 'MeasureIdentifiedPeaks' macro, it contains the

starting x location of the Full Width at Half Maximums of the identified peaks.

W_PM

Function coefficients **descriptor** used by PolyMorph (“PM”) from ‘Fit Peaks And Baseline...’, this is usually a copy of “W_BasePM”.

W_ResidBaseX

Annotation wave for ‘Show Fit Residual...’ when invoked from the ‘Baseline’ hierarchical menu, the x coordinates of the standard deviation lines.

W_ResidBaseY	Annotation wave for ‘Show Fit Residual...’ when invoked from the ‘Baseline’ hierarchical menu, the y coordinates of the standard deviation lines.
W_ShowEstWidthsX	Annotation wave shows the widths of identified peaks (x coordinates). See the ‘Zoom To Peak...’ macro.
W_ShowEstWidthsY	Annotation wave shows the widths of identified peaks (y coordinates). See the ‘Zoom To Peak...’ macro.
W_sigma	Curve fit output wave. See the Igor manual’s “Analysis” section.
W_tmp,W_tmp0	Temporary working waves.
W_tmp1,W_tmp2	Temporary working waves.

Revisions:

V1.3	Removed smooth, lhair, and minor ticks settings from the ColorWaves macro. (9/24/93)
------	--

References:

- [1] TN020: Peak Measurement and Fitting
- [2] TN020-A: Custom Peak Measurement and Fitting