

Quant Initialization

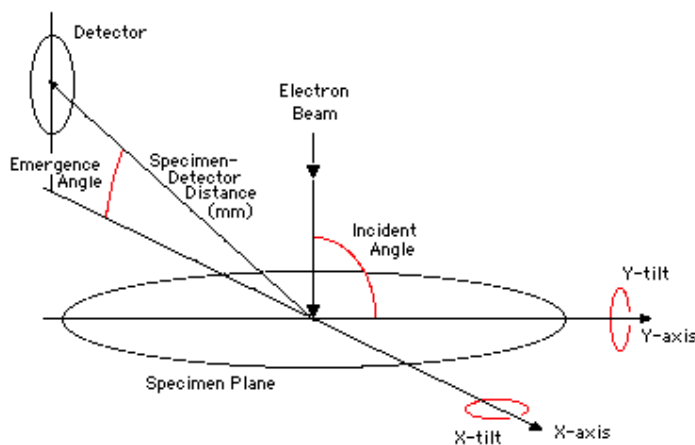
Before any quantitative results can be obtained, the **detector parameters** and the **analysis parameters** must be set. **Important Note: the system must be calibrated before meaningful quant results can be obtained!**

Quant Initialization - Detector Parameters

Detector Parameters are accessed via the menu command
Analysis → Setup Detector:

The user is allowed to select from a variety of **Window** types. Depending on the window type, the user can select from the list of **Crystal** types, if applicable. Depending on both the window and crystal types, the user can adjust the following **thickness** parameters: window, aluminum layer, crystal, front contact, dead layer, and ice layer. Not all thickness parameters are applicable, depending on the choice of window and crystal. The default **Physics** values used by Revolution for **electronic noise** and **Fano factor** are shown but cannot be changed by the user. The **linewidth** (at Manganese) is editable but it is highly recommended that the user allow the program to determine this value.

The four **Geometry** parameters are also available, defined in this diagram (**angles shown in red**):



When all **Setup Detector** settings are correct, hit **OK** to enter them into the program preferences.

Important operating note: A single well-defined emergence angle rarely reflects the actual measurement situation. Sample

surface properties cause this value to be ill-defined unless care has been taken to clean and polish the sample flat. In addition, the beam is being scanned across the sample from a point source, causing a slightly different emergence angle to apply for each pixel being probed. Therefore, the emergence angle value is at best an integrated effective value for the sample, and within limits can and should be treated as a freely adjustable parameter to maximize accuracy of quant results (see discussion of background subtraction below).

Quant Initialization - Analysis Parameters

Analysis Parameters are accessed via the menu command
Analysis → Setup Analysis:

Analysis Options

Methods → Determines whether Peak ID functionality is handled automatically by the program or allows manual intervention. Also used to select Bulk (ZAF) or Thin-Film (modified ZAF) analysis.

Peak Sensitivity → A measure of the peak-to-background ratio that must be exceeded before a peak is included for identification. Default value is 3.5.

Element Threshold (%) → A measure of the certainty required to label a peak as belonging to a particular element. If the membership function as determined by the fuzzy logic engine is less than the threshold value, then the peak does not belong to the element being tested. Within the internal database of elements, each element has its own measure of probability which is directly compared to the threshold value. These values are updated over time as the program becomes "smarter." Default value is 40.00.

Operating note: There is no straightforward interpretation of the threshold value except in the context of Fuzzy Logic, which is beyond the scope of this manual. Likewise, there is no straightforward procedure for adjusting the Peak Sensitivity and Element Threshold values to improve PeakID or Quant results. As a general rule, the primary strategy is to gradually reduce

Sensitivity; a secondary strategy is to lower the Threshold.

- Show ROIs** → When selected, highlights a spectrum with ROIs calculated by the program. **Note: these ROIs are not the ROIs associated with x-ray mapping or simple EDS acquisition!** These ROIs are not accessible to the user.
- Show Qual. Results** → Toggles display of the Qualitative report, which appears below a spectrum.
- Show Bkg Subtracted** → Toggles display of the background subtracted spectrum. The quality of a background-subtracted spectrum is crucial to the accuracy of any Quant results! (The background-subtracted spectra are most easily viewed in log scale).
- Use Standards** → Quantify with Standards. Required for accuracies better than about 5%. See [Making A Standard](#) further down this page for more information.
- Normalize** → Forces percentage calculations to add up to 100. If **off** while using standards, non-normalized results will be calculated for any elements that lack a standard or are specifically excluded.
- Treat as Oxides** → Attempts to classify elements as common oxides in conventional formulas (e.g., carbon dioxide, CO₂), according to the **Edit Oxides** table. Normalization is forced (calculated oxide percents will total 100). **Treat as Oxides** should be turned **off** for hydrocarbon (polymer) analysis. The treat-as-oxides check box will toggle the Normalize, Oxide Percent, and Cation checkboxes (see below).
- Edit Oxides** → Define which oxides to use for oxide analysis. The table consists of all commonly encountered oxides in EDS work. Entries can be manipulated with certain limitations. For example, CO₂ can be changed to CO, but N₂O₅ cannot be changed to an oxide without Nitrogen. Note: *changes to the Oxide table are not saved until both the Oxide table dialog and the Setup Analysis dialog are dismissed using the OK button!*
- Element by Difference** →
- Element by Stoichiometry** →

Result Options

- Display by** → Set Quant results to display by Chemical Symbol, Element Name, or Atomic Number. Default is **Chemical Symbol**.
- Sort Results by** → Set Quant results to sort by Chemical Symbol, Element Name, Atomic Number, Weight Percent, Atomic Percent, Oxide Percent, or Peak Energy. Default is **Atomic Number**.
- Weight Percent** → Toggle display of Weight Percent.
- Standard Deviation** → Toggle display of Standard Deviation. Only applies to calculation of Weight Percent.
- Atomic Percent** → Toggle display of Atomic Percent.
- Min. Detectability Limit** → Toggle display of Minimum Detectability Limit. Only applies to calculation of Weight Percent.
- Oxide Percent** → Toggle display of Oxide Percent. Only available if **Treat as Oxides** is on (see above).
- k-Ratios** → Toggle display of k-ratios. See discussion of [ZAF](#) and [Cliff-Lorimer](#) analysis methods.
- Intensities** → Toggle display of line Intensities. The intensities are the integrated counts for each ROI that is calculated by the program.
- Probability** → Toggle display of Probability. Probability is a confidence level that the results are correct. For Quant results, the probability values are a conglomerate of several of the results for each element.
- FWHM** → Toggle display of representative full-width at half-maximum for an element. *Note: the only meaningful measure of resolution is the FWHM at the Manganese line.*
- Use Line Labels** →
- ROI Counts** →
- Cations** →

Quant Initialization - ZAF and Cliff-Lorimer Corrections

Revolution 1.5.6 uses a standard ZAF correction for bulk analysis and a modified ZAF for thin-film analysis; the use of standards is **highly recommended** for accurate results.

The basic form for the ZAF correction is:

$$\frac{C}{C_{sd}} = \frac{I}{I_{sd}} \frac{F}{F_{sd}} \quad (1)$$

where **C** is concentration, **I** is x-ray line intensity, and **F** is the ZAF matrix correction. The subscript **SD** refers to the same quantities for the standard element in use for the analysis. If standardless analysis is being used, a mathematical model of

the standard is substituted.

The quantity **F** can be further broken down into multiple corrections:

$$F = F_z F_a F_f \quad (2)$$

which comprise effects due to atomic number (Z), which includes the effects of backscattering and stopping power, x-ray absorption (A), and x-ray fluorescence (F).

For any particular element, the ratio of intensities (sample/standard) is the k-ratio (a **measured** quantity):

$$k\text{-ratio} = \frac{I}{I_{sd}} \quad (3)$$

The ZAF correction generally applies to bulk specimens, defined as one that is thick enough that the x-ray generation volume for each element is contained within the sample. If bulk effects can be neglected (in thin-foil samples for example), the complex ZAF correction can be replaced by the Cliff-Lorimer simplification, in which a "k-factor" characterizes the relationship between elements.

For any 2 elements **A** and **B** this ratio is defined as the k-factor (an **entered** quantity):

$$k\text{-factor}_{AB} = \frac{C_A I_B}{C_B I_A} \quad (4)$$

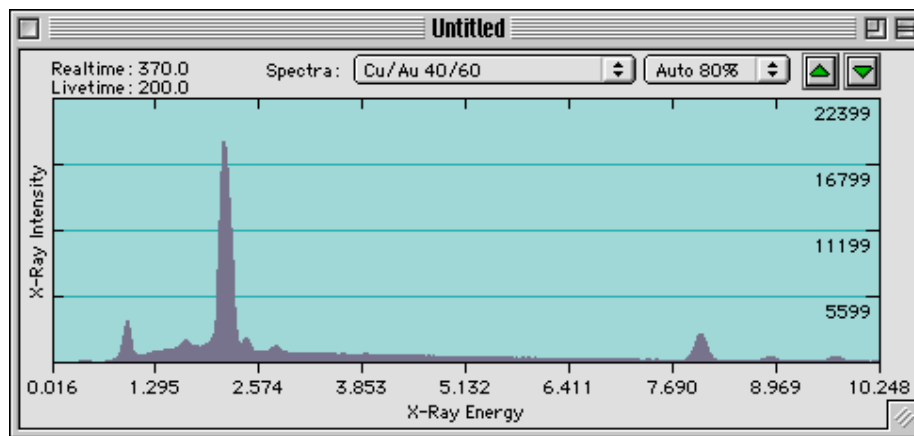
The Cliff-Lorimer approach can be extended to multielement systems by determining k-factors relative to a single element (often Si). Experimental determination of the k-factors accurately reflects both x-ray absorption effects in the sample and x-ray detector efficiency. Note the mathematical similarity between the k-factor and the ZAF correction (F) in Equation 1.

Strictly speaking, the ZAF correction requires a **standard** for each element that is being quantitatively analyzed. The Cliff-Lorimer correction requires a **k-factor** for every element that is being quantitatively analyzed, but a standard is only required for the initial characterization of the detector. Since it is ZAF only, Revolution cannot use, nor does it require, k-factors. The ZAF k-ratios reported in quantitative results are not related to the Cliff-Lorimer k-factors.

Peak Identification

Revolution's Peak ID feature allows the user to make quick and accurate identifications of elements in a spectrum. Clicking on the **id** button in the upper left of the EDX Spectra Mode Toolbar (see below) automatically analyzes the spectrum and presents an identification report. Peak Identification can be performed in either **automatic** or **manual** mode (below).

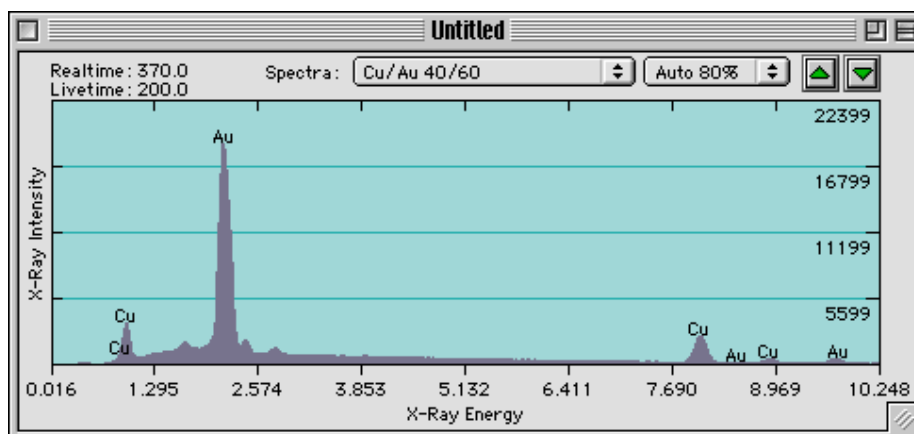
A sample spectrum in a catalog is shown below, before identification:



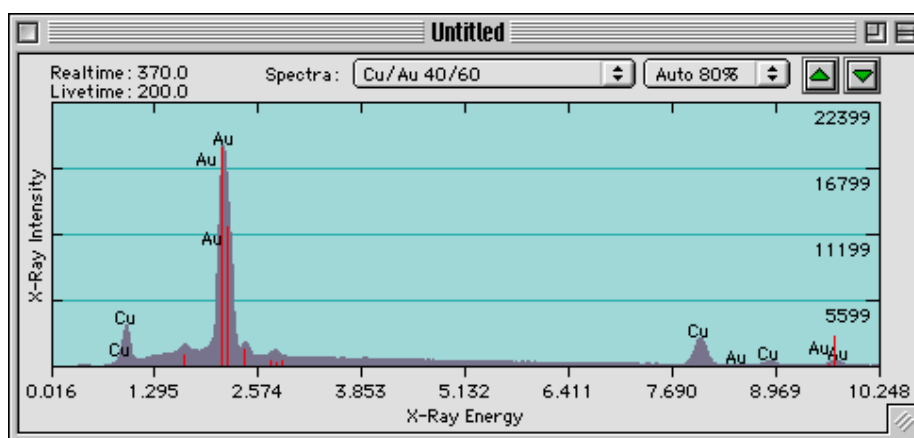
When a catalog is open and a spectrum is being acquired or has been acquired, the user may hit the **id** button (or select the **Analyze → Identify** menu item) at any time to perform a peak identification. During an acquisition, the peak identifications may "lock" (appear) and "unlock" (disappear) until sufficient statistics are obtained.



The element labels are displayed in proximity to each peak (here, Gold and Copper):



[KLM markers](#) can be independently overlaid at any time by right-clicking and selecting **Open KLMs** (Gold shown):

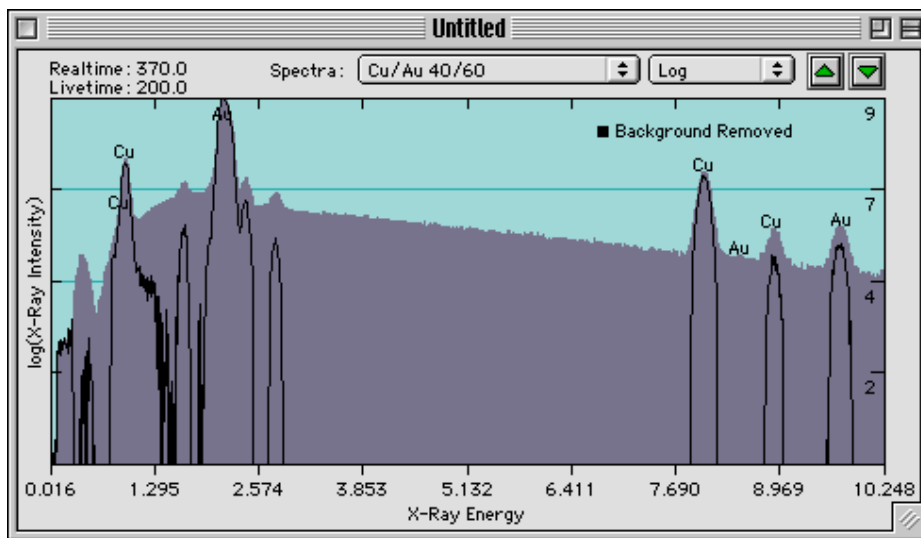


There are three additional options available with the qualitative PeakID capability, all accessed through the [Setup Analysis](#) dialog box (choose **Setup Analysis** from the **Analysis** menu): **Show ROIs**, **Show Qual. Results**, and **Show Bkg Subtracted**.

When **Show ROIs** is turned on, the Peak ID routines will automatically calculate a FWHM value for each identified peak and overlay the spectrum. Note that these ROIs are internally calculated and not accessible to the user. If the [manual ROI marker](#) for an element happens to be turned on, the **Show ROIs** function will override the manual ROI definition and overlay the true FWHM value for the element.

Show Bkg Subtracted

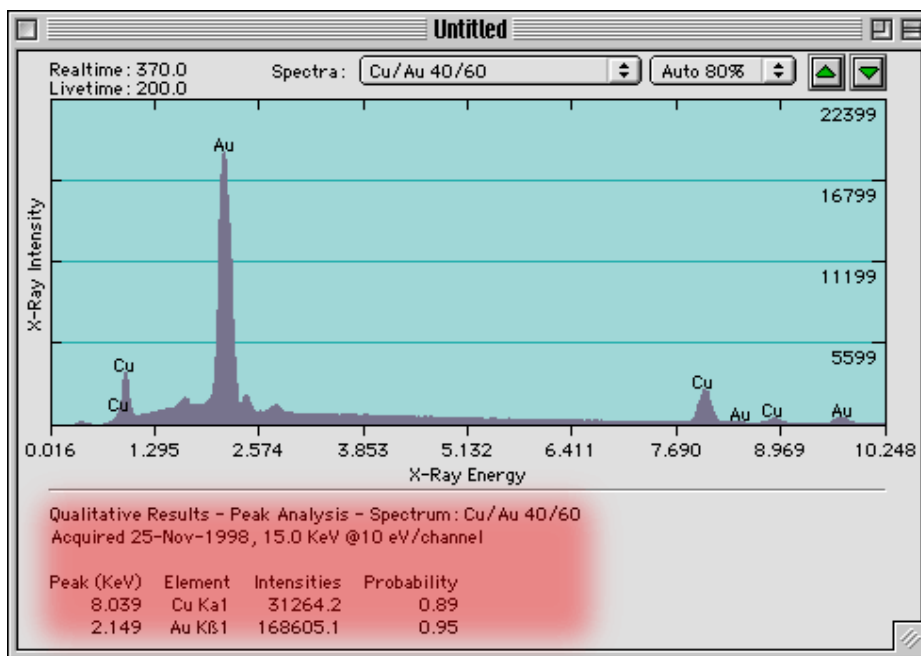
The **Show Bkg Subtracted** checkbox performs a background subtraction on the spectrum (shown in log scale for clarity):



Show Qual. Results

The **Show Qual. Results** checkbox performs a qualitative analysis on the spectrum and presents the results in a small report (highlighted).

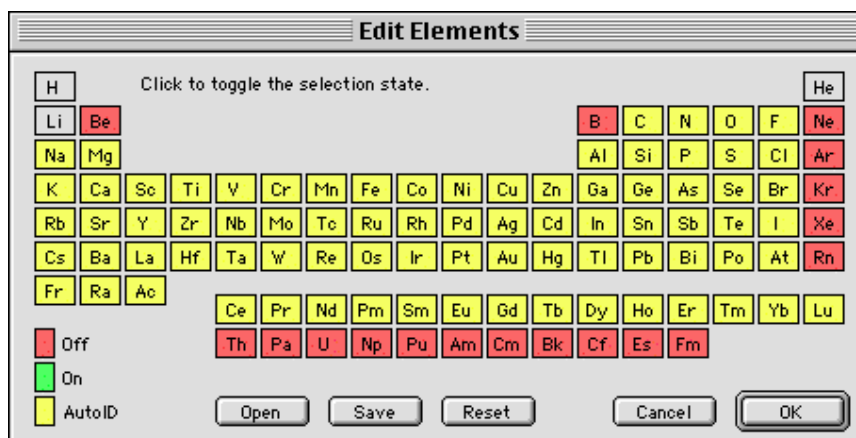
What appears in the report is determined by selections in the [Setup Analysis](#) dialog box.



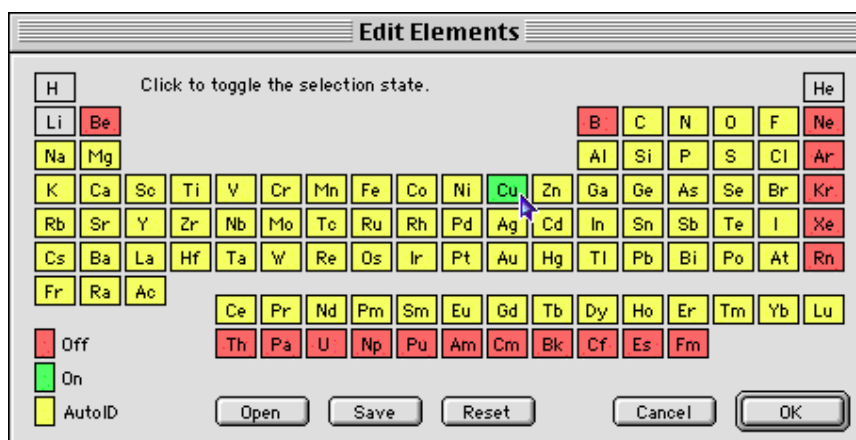
The report is able to identify primary peaks in the spectrum, assign elemental IDs, list relative intensities, and a probability (see [Setup Analysis](#) for definitions of these report items). The intensities are integrated counts in the element ROIs. The probability can be strongly affected by even a small miscalibration. Again, it is critical that a precise [calibration](#) be performed for accurate PeakID results.

There may be times when the Auto Peak ID returns questionable results. This may occur if an element's entry in the Fuzzy database is skewed, either because of poor calibration or a previous lack of identification. If a user knows what elements are present, the automatic capability can be manually overridden to force the Peak ID routines to analyze only selected possibilities. The ability to include or exclude elements from analysis has been incorporated into a master element periodic table.

Access this table by right-clicking in a spectrum window and selecting **Edit Elements** from the contextual menu:



By default, all elements are set to **AutoID** (except for a small group of elements that are turned off because they are rarely analyzed). By clicking any element, it will toggle on, off, and back to AutoID, with the requisite color change for easy determination.:



The three states are defined as:

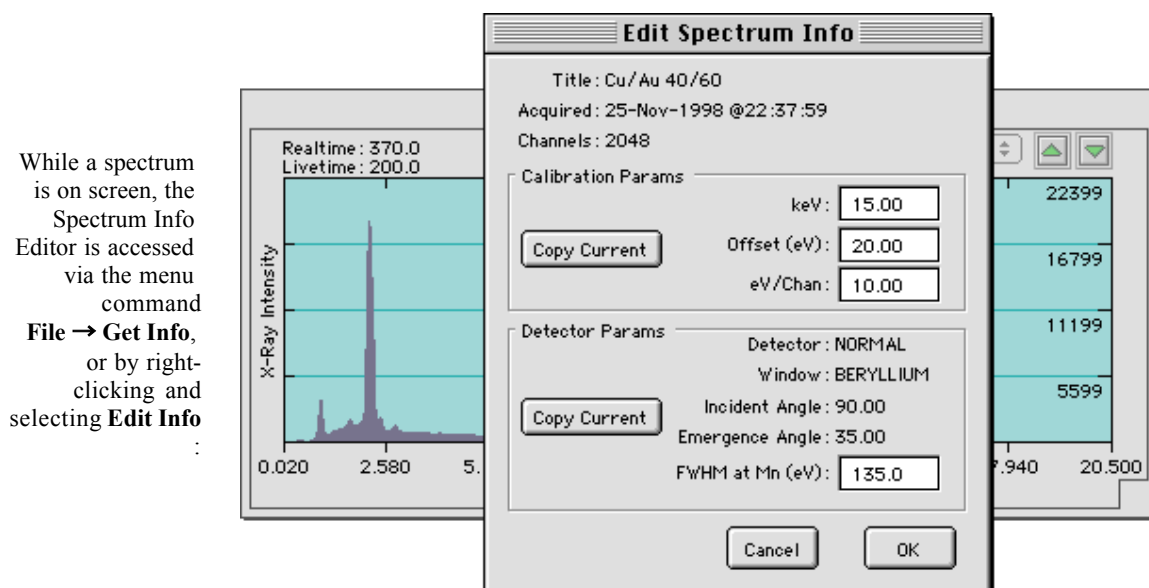
- **AutoID**: Revolution makes all decisions about whether to include an element as a possibility in the quant routines. This is the default state, recommended for most work.
- **On**: The user forces Revolution to **include** an element in the list of possible identifications. Revolution will try to continue including the element, even if it would normally be discarded from the ID list. This is useful if the element is at such a low concentration that its statistics are poor, or when the element has lines very close to other elements, causing the program difficulty making an automatic identification.
- **Off**: The user forces Revolution to **exclude** an element in the list of possible identifications. Revolution will try to continue excluding the element, even if it would normally be added to the ID list. This is useful if the element has lines very close to other elements, causing the program difficulty making an automatic identification.

The last configuration set by the user is remembered going forward; however, the user can **Save** a configuration and then **Open** it later for convenience. The **Reset** button places the entire table into its original default state. A **right-click** on any element allows one to set it to either AutoID, On, or Off, and has the added ability to turn the entire table off.

Peak Identification Operating Notes

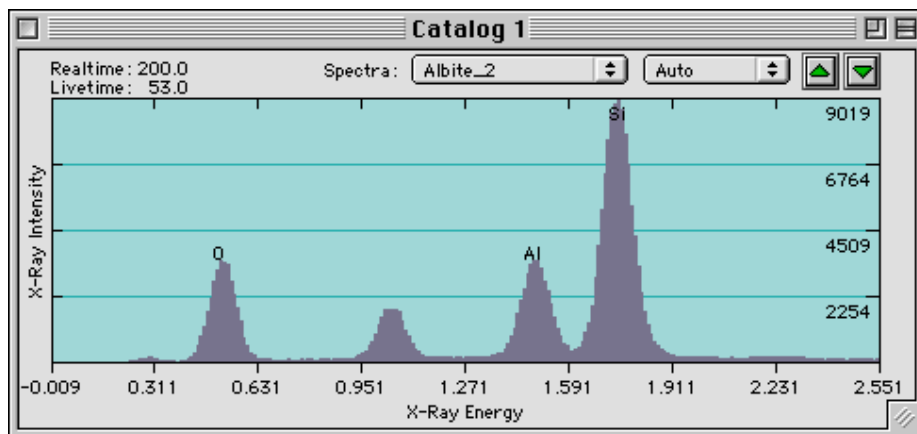
- When the Manual Identify Setup periodic table first appears, certain elements may be autoselected. The elements that are autoselected are picked first from current KLM markers (if any), then from the previous Quant results (if present), and then from the previous Manual ID elements (if previously selected). If none of these criteria match, the table will be blank and no Manual ID is possible until at least one element is selected.

- The X-ray energy axis (x-axis) will sometimes start with a non-zero number. This is because the spectrum, once autocalibrated, is adjusted by a software gain and offset so that peaks line up precisely according to accepted reference values. X-axis labels change accordingly, starting at the computed offset, even if that is a negative offset. So to some degree, aesthetics is traded for accuracy. A future feature will allow custom axis settings for reports.
- Sometimes Peak ID element labels are written on top of one another. The automatic label placement routine can't always keep each label in the clear if there are too many in one place. Either turn off the labels for some elements, or resize and zoom the spectrum window to make more space. Future updates will handle this presentation aspect better.
- When the spectrum is magnified for clarity, sometimes there appear more KLM markers for an element than there are Peak ID labels, or vice versa, instead of the expected one-to-one correspondence between the identifications and the markers. To avoid clutter, this is because Peak ID identifies whole peaks, and not all the energy lines that may contribute to each peak. This is done to avoid clutter, and helps avoid the problem noted in the previous bullet.
- In the Peak ID results for a spectrum, sometimes the probabilities are quite a bit less than 100%. This does not mean the ID is wrong. EDX calculations, especially the default ZAF standardless method, is not a science of 100% certainty. If probabilities for the elements of interest seem too low, there may be problems with the spectrum such as: (especially) miscalibration, insufficient acquisition time, inaccurate detector parameters, or contamination.
- An older spectrum may yield identifications that are not correct because it was acquired under a different calibration. However, all spectra have their own calibration data saved with them, and can be modified to bring the spectrum back into calibration.



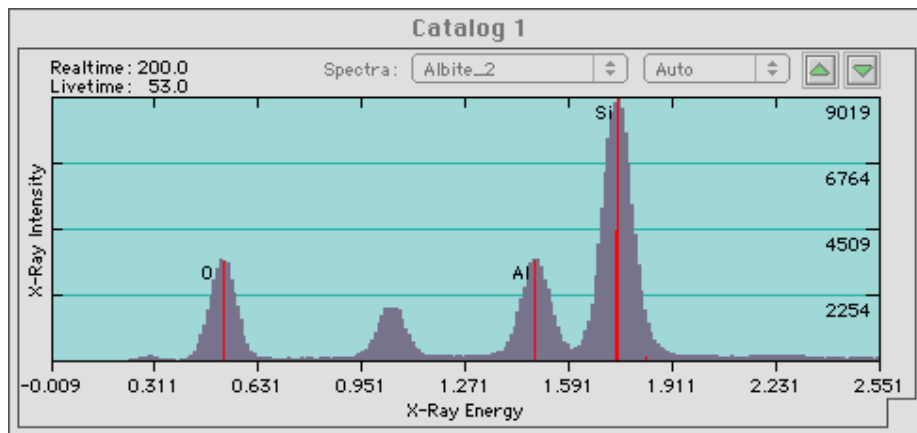
- In the default configuration of Revolution, some elements in the database have a relatively low probability assignment. It is possible that these peaks are visible in the spectrum but are not identified by the PeakID routines. The following procedure can be used to modify the Fuzzy database and create a correct identification. **Note:** *outside of calibration errors, the most likely cause of non-identification is poor statistics; before resorting to a modification of the database, make sure the problem cannot be fixed by acquiring for a longer time.*

Example spectrum after PeakID is performed which shows a single unidentified peak:



Select **Analyze** → **Learn Peaks** from the toolbar menu. The **Learn Peaks** dialog is displayed, listing **only** the elements that Revolution knows about for the spectrum in question (it can be moved so as to not obscure the spectrum window):

KLM markers for the known elements are automatically displayed



Learn Peaks

H																	He
Li	Be											B	C	N	O	F	Ne
Na	Mg											Al	Si	P	S	Cl	Ar
K	Ca	Sc	Ti	V	Cr	Mn	Fe	Co	Ni	Cu	Zn	Ga	Ge	As	Se	Br	Kr
Rb	Sr	Y	Zr	Nb	Mo	Tc	Ru	Rh	Pd	Ag	Cd	In	Sn	Sb	Te	I	Xe
Cs	Ba	La	Hf	Ta	W	Re	Os	Ir	Pt	Au	Hg	Tl	Pb	Bi	Po	At	Rn
Fr	Ra	Ac															
		Ce	Pr	Nd	Pm	Sm	Eu	Gd	Tb	Dy	Ho	Er	Tm	Yb	Lu		
		Th	Pa	U	Np	Pu	Am	Cm	Bk	Cf	Es	Fm	Ka1	Ka2	Ka3		
		Ka3	Ka3	La1	La2												

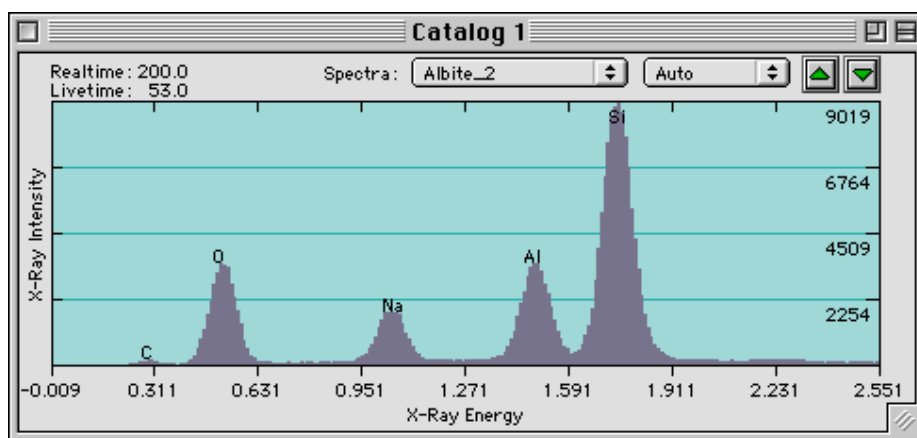
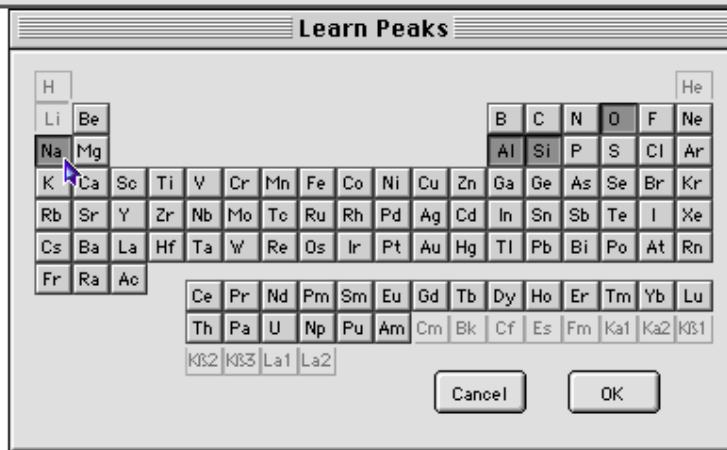
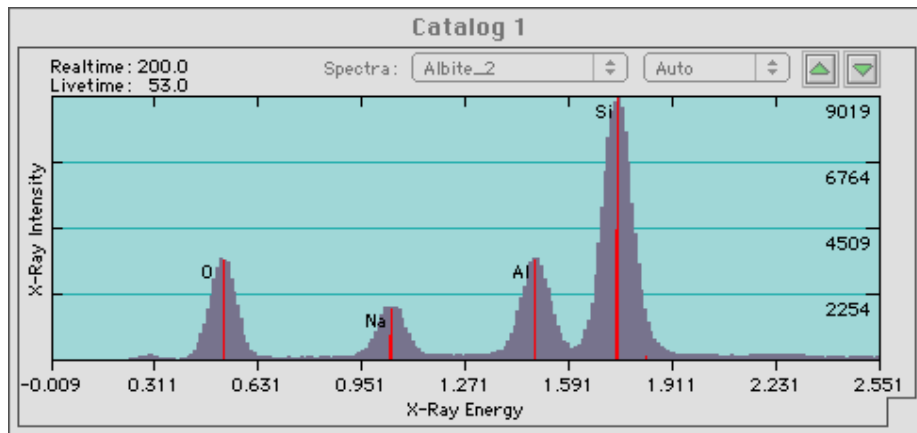
Cancel OK

Clicking on any element in the Learn Peaks dialog will automatically overlay the KLM marker for that element.

With 20-20 hindsight, the result for Sodium is shown:

The user can select as many element markers as necessary in an attempt to manually identify the unknown element(s). When the manual identification has been made, click OK in the Learn Peaks window.

Click yes in response to the dialog box that follows to update the element database



In most situations, the previously unidentified element will be identified, and the element will successfully be identified in subsequent measurements:

There are rare or unusual situations in which the Learn Peaks procedure still does not successfully identify peaks. Assuming that the calibration has been performed correctly, it is likely that one or both of the two parameters which control the PeakID calculation, **Sensitivity** and **Threshold**, are not adjusted appropriately for the sample in question (see [Setup Analysis](#) for more information).

In contrast to the above discussion, peaks that are consistently identified but which the user is certain do **not** exist in

the spectrum can be **unlearned**. The procedure is roughly the reverse: in the Learn Peaks dialog (above), Revolution will display all elements it thinks it knows about. An element can be clicked **off** and should **disappear** from the identification; however, this procedure is significantly more dependent on the values selected for Sensitivity and Threshold, and may not work as anticipated. A circumstance where an element must be "unlearned" is significantly less likely if the sample has good statistics associated with it to begin with.

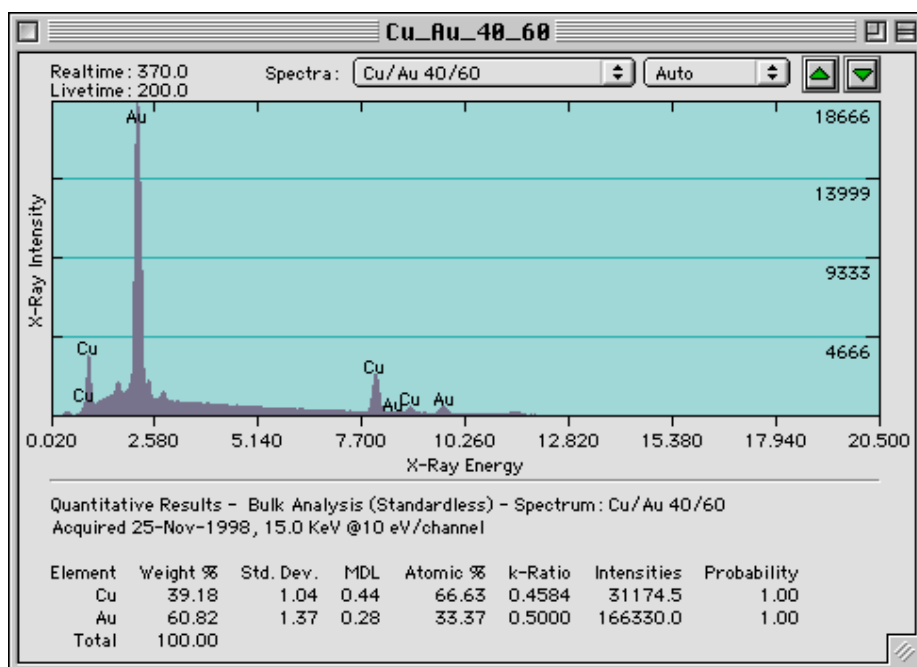
Analyzing all possible strategies for modifying the values of Sensitivity and Threshold, especially for unlearning peaks, is outside the current scope of this manual. Any user with problems in this area is encouraged to contact [4pi support](#).

Quant Analysis

With a catalog open and showing an acquired spectrum, click the Quant button on the EDX toolbar to activate quantitative analysis and display the quantitative results report:

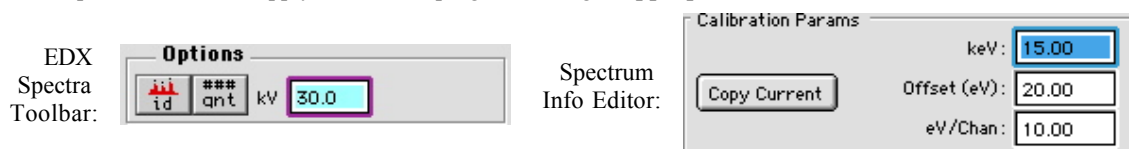


Note: on slower machines, leaving the **qnt** button selected during acquisition can cause undesirable system slowdowns as Revolution continuously tries to analyze the changing spectrum.

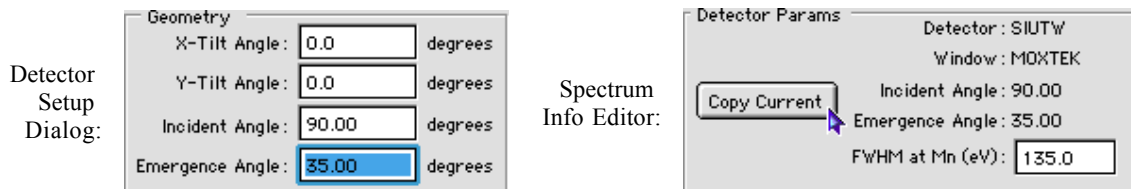


Quant Operating Notes

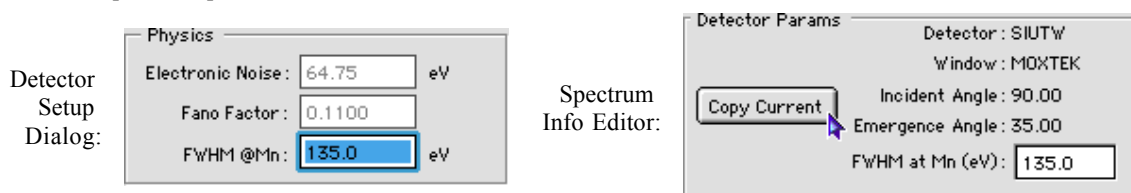
- For meaningful quant results, it is **critical** that all detector settings are correct, that the system has been autocalibrated, and that the correct parameters are entered in the EDX toolbar. If not, the quant results are likely to be wrong. Also review the reported eV/channel. A exact even-integer value such as the 10eV/channel default is unlikely if an autocalibration has been done.
- If the **Show ROIs** checkbox (above) is turned on while performing quant, new ROIs overlays calculated by the quant routines will override the [manually defined ROI](#) overlays.
- Be sure that the beam energy (the kV field in the EDX toolbar) is set correctly. If analyzing an existing spectrum, check the Spectrum Info and apply the current program setting **if appropriate**.



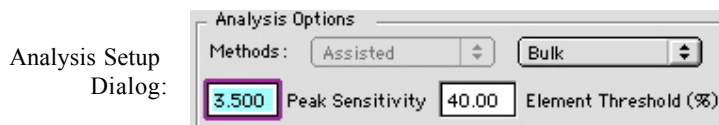
- Be sure the Emergence Angle is set correctly. As with beam energy, this number is critical for accurate analysis. If analyzing an existing spectrum, check the Spectrum Info Editor and apply the current program setting **if appropriate**.



- Check that the full-width at half-maximum resolution (FWHM) is correct. FWHM, normalized to Manganese, is less critical to accuracy but can cause incorrect identification of elements. If analyzing an imported spectrum that was not tagged with detector resolution information, the program will default to your detector's setting. Check the Spectrum Info and apply the current program setting **if appropriate**. Alternately, edit the resolution in the FWHM field. If you then save or export the spectrum from within Revolution, the FWHM will be saved with it.

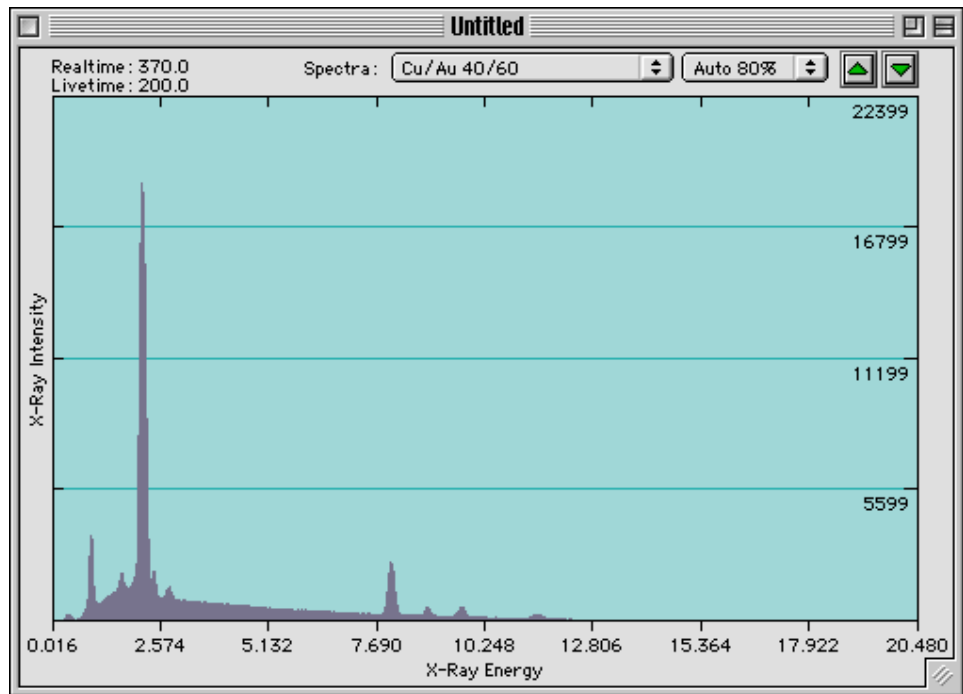


- If an element that is not in the sample continues to be identified by Revolution, try using **Analyze** → **Learn Peaks** to un-learn the errant peaks by deselecting the offending elements on the **Learn Peaks** periodic table (see above, this page).
- If a peak can't be removed by unlearning, try adjusting the **Sensitivity** in the [Setup Analysis](#) dialog box.

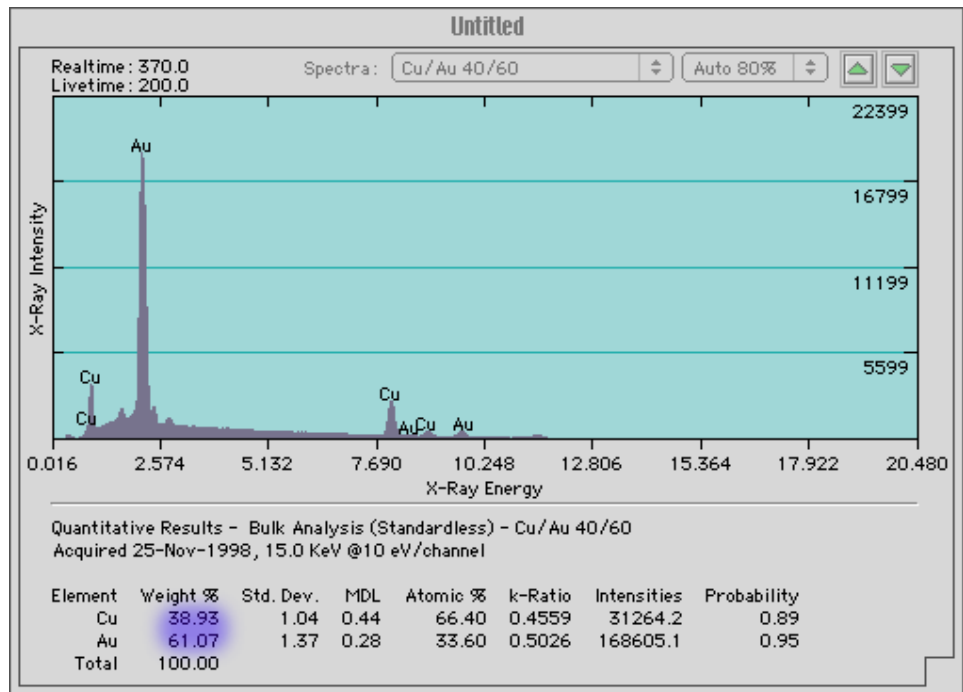


Making a Standard

Before a standard can be made, a spectrum must be acquired (in this example, a Copper and Gold sample, independently known to be a 40/60 mix):



A quant analysis performed on the spectrum should be close to the correct analysis (blue):



To create any standard, **make sure the spectrum to be used is displayed in the catalog**, select **Analyze → Make Standard**, and fill out the dialog box according to the known composition:

Enter values for up to 12 elements in the current spectrum in terms of: Weight Fraction, Weight Percent, Atomic Percent, Oxide Percent, or Number of Atoms. The values must sum close to 1.0 or 100% in order for the OK button to be enabled. **Clicking OK makes the current spectrum a standard.**

*Elements may be individually excluded. See examples under **Using a Standard** (below) for more information.*

The number of standards may be extended beyond the available edit fields in the dialog box.

*See discussion of **Import and Export** below.*

Setup Standard

Choose the concentration method and enter element symbols with associated concentration values. Changing methods will convert current values to the new method. Use the "Sum" to catch possible conversion or entry errors.

Method: Weight Fraction

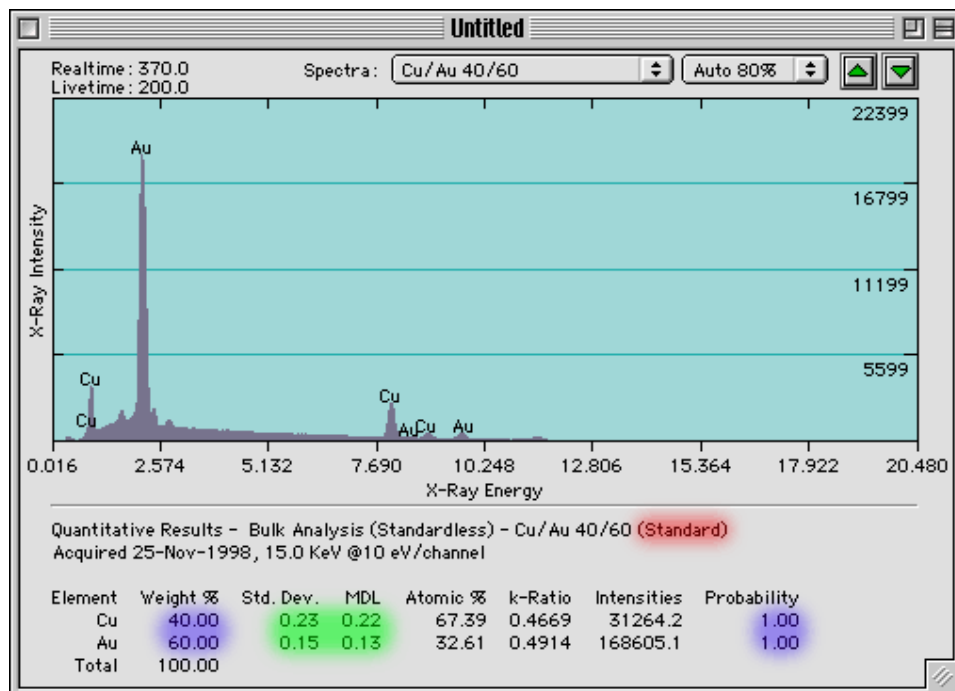
Element	Concentration	Exclude
Al	0.6	<input type="checkbox"/>
Cu	0.4	<input type="checkbox"/>
		<input type="checkbox"/>
		<input type="checkbox"/>
		<input type="checkbox"/>
		<input type="checkbox"/>
		<input type="checkbox"/>
		<input type="checkbox"/>
		<input type="checkbox"/>
		<input type="checkbox"/>
		<input type="checkbox"/>
		<input type="checkbox"/>
		<input type="checkbox"/>
		<input type="checkbox"/>

Sum = 1.000000

Import
Clear All
Export

Discard
Cancel
OK

Making the spectrum a standard necessarily changes the analysis. The Weight Percent and probability match the definition of the standard (blue). The spectrum is listed as a standard for reference (red). The [Standard Deviation and MDL](#) are generally reduced because the statistics exclude alternate analyses (green):



Operating note 1: For correct Quant analysis on any particular spectrum, all standard spectra as well as the target spectrum must have been acquired with a common ev/channel setting and the same accelerating voltage.

Operating note 2: The full Revolution Quant module must be active for either standardless quant (also known as "semi-quant") or quant with standards.

*Operating note 3: To remove a standard from consideration temporarily, close the catalog that contains it. Alternately, select the spectrum being used as a standard, select **Analyze** → **Edit Standard**, and exclude any or all elements from consideration. To eliminate the spectrum as a standard, click on **Discard** in the **Setup Standard** window. See the examples below for more clarification.*

Using a Standard

Revolution **checks all open catalogs** for standards when doing standards-based analysis. The following examples describe the way Revolution interacts with standards:

Example 1. Given a single Cu-Au sample, create 2 catalogs and acquire spectra into each. A spectrum from Catalog 1 is used to make a Gold standard. A spectrum from Catalog 2 is used to make a Copper standard. Neither element has been excluded. Analysis of any subsequent spectrum in any catalog will use the Gold standard from Catalog 1 and the Copper standard from Catalog 2 to perform quant.

Extended Example 1. If Catalog 2 is closed, no subsequent spectrum can be analyzed with the Copper standard until Catalog 2 is reopened. Such analysis will be mixed (and so noted in the report): Gold will be analyzed with the standard and all other elements (including Copper) will be analyzed using standardless quant. Note that for this single-element-standard example, the same thing can be achieved by excluding Copper rather than closing the catalog.

Example 2. Given a single Cu-Au-Mn sample, create a single catalog with 2 spectra. Spectrum 1 is used to make a Gold and Copper standard. Spectrum 2 is used to make a Gold and Manganese standard. No elements from either standard are excluded. Revolution will use as the Gold standard that spectrum which has the highest intensity Gold peak, under the assumption that the higher intensity peak has "better statistics." The same applies even if the 2 spectra are in different catalogs.

Extended Example 2. It is desired to use the **low-intensity** Gold standard instead of the default high-intensity standard. This is accomplished by selecting the Exclude checkbox in the Setup Standard dialog box for the spectrum with the higher Gold intensity.

Example 3. Given 3 Cu-Al-Mn samples, but with different percentages of Cu-Al-Mn in each sample. Acquire a spectrum from each sample into one or more catalogs. Create a standard for each spectrum. Analysis of any subsequent spectrum will use the highest intensity peaks found in any of the 3 spectra for each element, under the assumption that a higher intensity peak has "better statistics."

Extended Example 3. To modify the usage of the highest intensity peaks from multiple standards, edit each standard to Exclude any element to get the desired dependence.

Example 4. Spectrum 1 is used to make a standard per the method of Weight Fraction. Spectrum 2 is used to make a standard per the method of Atomic Percent. Revolution will perform an internal conversion so that both standards can be used.

Importing and Exporting a Standard

Data in a standard can be exported to disk for safekeeping. Simply choose the **Export** button in the Setup Standards window. If the standard is ever lost or corrupted, it can be imported again by using the **Import** button in the Setup Standards window.

An exported standards file can be opened with a text editor, edited, resaved, and imported again. This technique can be used to extend the number of elements in the standard to beyond the twelve that are displayed in the **Setup Standards** window.

The file is formatted in the following way:

```
[Global Factors]
Order=Descending
Number of Elements=2

[Type of Concentration]
Weight Fraction=1
Weight Percent=0
Atomic Percent=0
Oxide Percent=0
Number of Atoms=0

[Concentrations]
Element_1=Al
Concentration_1=0.600000
Ignore_1=0
Element_2=Cu
Concentration_2=0.400000
Ignore_2=0
```

The format of the file should be more or less self-explanatory. The **order** determines whether elements with the lowest concentrations or highest concentrations appear first when displayed in the **Setup Standards** window (**Ascending** or **Descending**). The **number of elements** *must* be set correctly. Only one **concentration type** should be set to true. For each element, the **two-letter designation** must be specified, followed by the **concentration** (a value between 0 and 1.0), followed by the **ignore** setting, which determines whether an element is excluded from the standard or not.

The file will not be imported if an illegal 2-letter element designation is used, or if there is a formatting error in the text file. If the concentrations do not add up to 1.0 (or 100%, as needed), the file will be imported, but the OK button will only be activated if the sum is close enough to the 100% point.