

APP013 – DXR App Note on Software Features

Auto Exposure

Auto exposure adjusts the exposure conditions to produce a final spectrum with a specified signal-to-noise ratio (S/N). This feature is Patent Pending.

The Auto exposure option is enabled only when the Background Handling option 'Use smart background' is selected.

Experiment Setup - C:\My Documents\OMNIC\WRParam\Default.exp

Collect | Bench | Quality | Advanced | CCD Array | Alignment | Mapping | Series

Estimated time for this collection: 00:00:04

Collect exposure time (sec): 1.0

Preview exposure time (sec): 0.5

Sample exposures: 2

Background exposures: 16

Final format: Shifted spectrum (cm-1)

Correction: Fluorescence

Cosmic ray threshold: Medium

☐ Photobleach time (min): 0.0

☒ Preview data collection

☒ Auto exposure Desired S/N: 100

Maximum collect time (min): 5

File Handling

☒ Save automatically Base name: C:\My Documents\Omnica\autosave\0001.spa

Background Handling

☐ Collect background before each sample

☐ Maximum age for background: 1000 minutes

☒ Use smart background

Experiment title: Almega

Experiment description: Almega default experiment file

Help Open Save Save As OK Cancel

When you select Auto exposure, the controls for Collect exposure time (sec) and Sample exposures are disabled. The controls for Desired S/N and Maximum collect time (min) become enabled. This occurs because Auto exposure automatically sets these parameters in order to achieve the SNR you request in the Desired S/N control.

Desired S/N – This value controls the total collect time (exposure and number of scans). Higher S/N values require longer collect times.

Maximum collect time (min) – The maximum number of minutes allowed for the complete Collect Sample operation to reach the desired S/N.

OMNIC takes a preliminary scan (2x1-sec exposures) from which it measures signal and noise. From these results, it estimates the exposure time and number of

scans required to achieve the desired S/R. Exposure time is preferentially increased before the number of exposures because this gives better results. At least 2 exposures are always collected so that cosmic rays can be rejected. For strong signals, the exposure time may be limited by CCD overflow. In this case, the number of exposures is increased.

The preliminary scan signal measurement is the maximum signal in the spectral range. When Final format = Shifted spectrum, the spectrum below 150 cm⁻¹ is ignored to eliminate any residual laser bleed. An [AutoBaseline O4 L20] operation is performed on the preliminary scan before measuring the maximum signal. We have found this effectively removes baseline offset in most cases giving a more accurate signal measurement.

The preliminary scan noise measurement is the OMNIC peak-to-peak noise calculation over a 150 cm⁻¹ wide region. This region is moved across the spectrum and the minimum noise result is retained as the noise measurement.

Summary

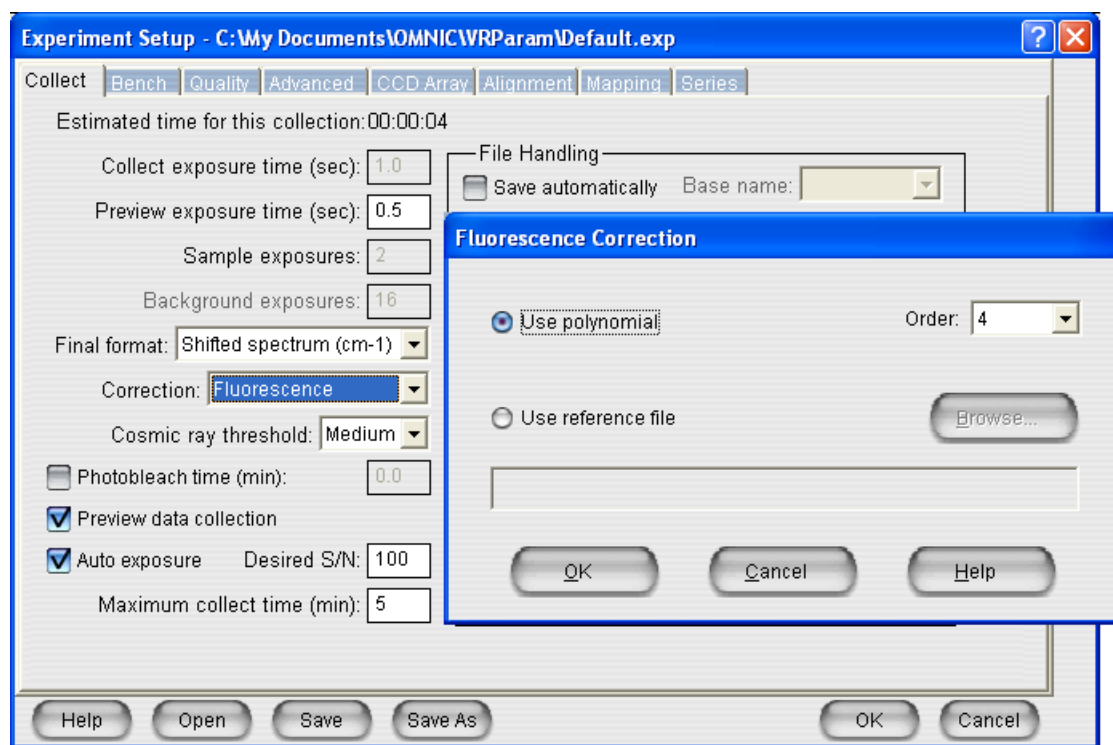
If the Auto exposure option is disabled, the Background Handling option 'Use smart background' has not been selected. Select this option to enable Auto exposure.

If the Use smart background option is disabled, OMNIC has not yet completed the initial smart background data collection. This takes approximately 3 days (weekend) when the system is idle. See the information in Smart Background for details.

Fluorescence correction

Fluorescence correction attempts to remove the effects of fluorescence as part of the sample collection process. The correction is applied after the sample spectrum is collected and before it is displayed.

This same operation can be run after a sample is collected using the command: Process > Other Corrections > Fluorescence. I recommend using this approach first to determine which type of correction works best. Then, assuming you will be collecting the same type of samples, you can apply this correction to the collection pipeline as described here.



Select Fluorescence from the Corrections drop-down list. The Fluorescence Correction dialog is displayed.

There are two methods for fluorescence correction: polynomial fit and reference file subtraction. Select one of these options.

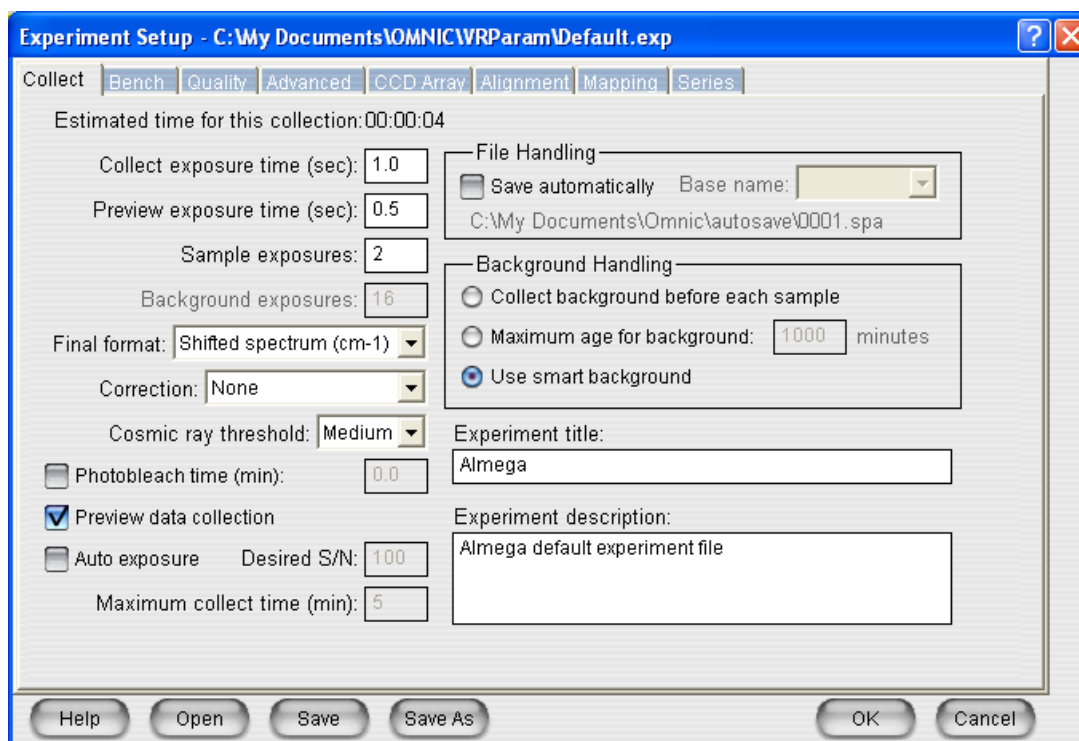
Use Polynomial attempts to fit a polynomial to the spectral baseline then subtracts the polynomial. You must specify a polynomial order from 1 to 6. Order = 4 is a good starting point. This option is best when the fluorescence shows as a very

gentle sloping baseline. It does not work well when fluorescence exhibits a definite peak such as glass fluorescence with the 780 nm laser.

Use reference file auto-subtracts a file which you specify from the collected spectrum. You will need to generate your own reference file for this option. I do this by collecting a sample exhibiting the fluorescence. Then use the Process > Straight line command to remove all sample peaks leaving just the fluorescence background. Then use the Process > Smooth > 25 command one (or more) times to smooth the baseline removing noise. Save this as your reference then select this file using the Browse button in the Fluorescence Correction dialog.

Smart Background

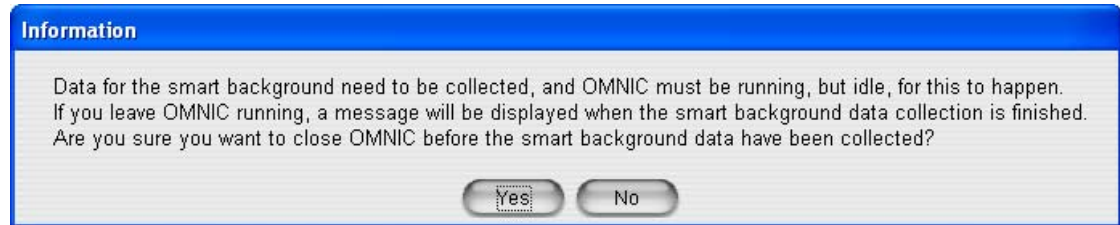
A new Background Handling option is Use smart background. A smart background is a fake background generated from a model of the CCD's response to exposure time. When this option is selected, the Background exposures control is disabled and you never have to wait for another background collection. This feature is Patent Applied For.



This option is disabled when a OMNIC is first installed because no background model exists yet. It takes about 3 days of OMNIC idle time to collect all the data for the smart background model. OMNIC idle time is defined as the OMNIC application open with no activity such as data collection (including scheduled calibrations) and data analysis (menu commands and macros).

The OMNIC idle time does not need to be consecutive; we recognize that people need to continue to use their system. When the system is idle for more than 5 minutes, it will begin collecting data for the smart background model. This activity is not noticeable other than the Experiment control in the OMNIC toolbar having a gray background. As soon as you do some OMNIC activity, the smart background collection is suspended and intermediate results are saved. The next time OMNIC is idle, it picks up where it left off.

If you close OMNIC before the smart background model is complete, a message is displayed as shown above. We recommend clicking the No button and leave OMNIC running.



When all data for the smart background model is complete, a message to this effect is displayed. The Use smart background option is now enabled in the Background Handling section of the Collect tab in Experiment Setup. (A file named bdata006250.vrb is written to the VRMCal folder containing the smart background model.)

The smart background feature uses the full CCD bin range from rows 6 through 250 for both the background model and subsequent Collect Sample operations. The bin range specified on the CCD Array tab of Experiment Setup is ignored as is the state of the 'Select rows automatically' option on the Advanced tab.