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SpectraWorks²: Advanced spectral analysis for liquid scintillation counters.

Author

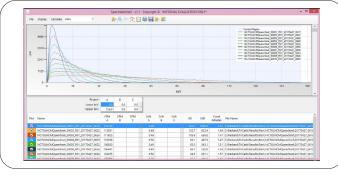
Dr. Ronald Edler Revvity

Introduction

In the past, Quantulus™ 1220 liquid scintillation counters were delivered with the EasyView and Low Level and Super Low-Level instruments of the Tri-Carb™ series with the SpectraWorks software. These programs allowed the user to load and analyze the recorded spectra. With the conversion to the Windows 10 interface, the SpectraWorks² software has now been delivered for all Tri-Carb and Quantulus liquid scintillation counters. This software can now load and edit all spectra of the Tri-Carb series of instruments and the Quantulus GCT 6220. In addition to the sample spectra, the guard spectra and the auxiliary spectra can also be opened in the software. This application is intended to give a brief introduction into the possibilities of the software. The software can be opened via the desktop icon or also from the QuantaSmart software under Replay with "Analyze Spectra". Opening with "Analyze Spectra" requires at least the QuantaSmart software version 5.2 or later versions.

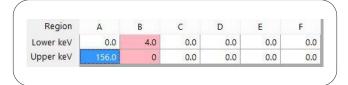
The main screen

Figure 1 displays the main screen of the SpectraWorks² software which appears when the software is opened.



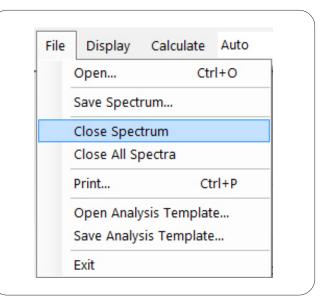
| Figure 1: The main screen of the SpectraWorks² software.

Spectra can be opened via the QuantaSmart software or within the SpectraWorks² software with the "File Open" command. The upper area of the main screen is designed for displaying the spectra, the lower area for the energy regions with the counts and file names in a kind of Excel table. The "File", "Display", "Calculate" and a drop-down menu are available in the main menu, in the latter the scaling of the X axis can be selected. Alternatively, you can enter a numerical value for the end of the energy range via the keyboard into the drop-down menu. If you do not want to display all spectra, you can do this by removing ticks in the plot box in the lower table. All spectra can also be displayed or removed from the display via the display menu. The current energy range is highlighted with a colored background. Optionally, as in this example, a legend can be displayed on the right side. The Y-axis of the spectra is automatically scaled but can also be scaled manually using the scroll bar on the right. The division between the upper part for the spectral view and the lower part with the table can be made via a separating bar. Up to 6 energy regions can be set up in SpectraWorks² on the main screen between the spectra and the table as shown in Figure 2:



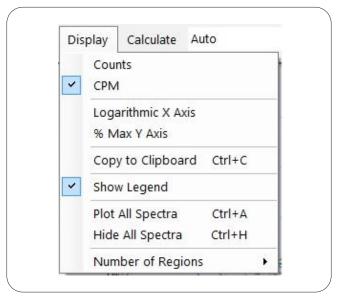
| Figure 2: Defining energy regions.

By clicking on the individual cells, they are activated, and energy values can be entered for the window. Invalid numbers are pinked. Active cells are highlighted in blue. When new valid numbers are entered, the table below is immediately updated. Using the File menu, you can not only open, close and save spectra, but also open and save analysis templates as shown in Figure 3.



| Figure 3: The file menu.

A template is a quick way to load settings in SpectraWorks². In this template the number of regions, the energy windows and the presentation in counts or CPM can be saved and reloaded for new evaluations.



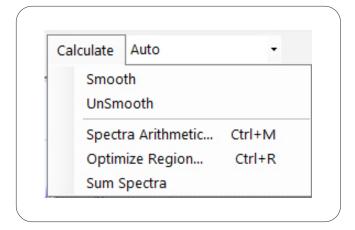
| Figure 4: The display menu.

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In addition to the number of regions, counts can also be scaled to CPM or to a logarithmic X-axis in the display menu.

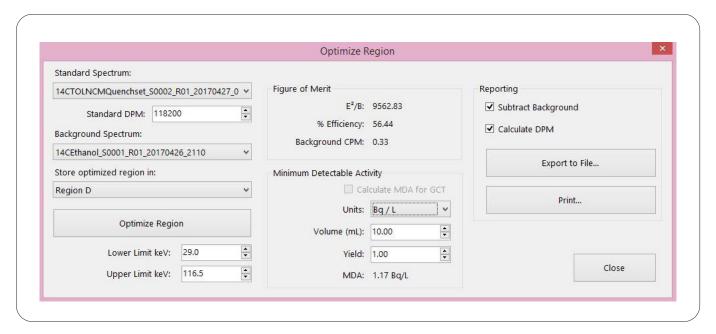
The table below the spectra shows the CPM or counts values and $\sigma\text{-values}$ for each valid energy window. In addition, the measurement time as well as the SIS and tSIE values are indicated, the latter only if an external standard was used for the measurement. The file name is also specified.

The "Calculate" menu allows arithmetic operations with the raw data without changing these raw data. All changes are only visible visually on the screen. However, the newly calculated data can be stored as spectra under a new name. Spectra can be smoothed, added and subtracted, or multiplied by constants. The latter can, for example, be used to convert the CPM values into DPM values by dividing them by the counting efficiency. With "Sum Spectra" there is the possibility to combine spectra from repeat counting and/or cycles in a single spectrum.



| Figure 5: The calculate menu.

Both the channel contents of the multi-channel analyzer and the measurement times are summed. A particularly interesting point in this menu is the point "Optimize Region ..." This menu item allows the very fast and easy optimization of the energy window for the measurement.



| Figure 6: The optimize region dialog window.

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A standard or sample spectrum and a background spectrum are required to calculate the optimized energy window, as shown in Fig 6. The calculated energy window, the figure of merit, the counting efficiency and the background are displayed. If the activity of the standard is known as in this example, the detection limit can also be calculated according to the formula of Curry as given below, in this case 1.17 Bq/L. A report for this calculation can be printed or saved as a file.

$$MDA = \frac{3.0 + \left(3.29 \cdot \sqrt{u(C_{BKG})} \cdot \left(\sqrt{C_{BKG}}\right)\right)}{StdEfficiency \cdot \left(\frac{Volume}{1000}\right) \cdot Yield \cdot CountingTime \ in \ Minutes}$$

Where $u(C_{BKG})$ is the uncertainty of the background count rate, and C_{BKG} is the background count rate. If the activity of the standard is known and "Calculate DPM" has been activated under "Reporting", the DPM value also appears in the report.

In addition to the menus discussed so far, some buttons for the most common menu items are available in the SpectraWorks² software in the main menu bar for quick access to these, as shown below:



In the order from left to right these points allow the spectra to be opened, spectral arithmetic, spectrum smoothing, copying to the clipboard, printing, saving, closing a spectrum or closing all spectra.

For the SpectraWorks² software, single licenses or multiple licenses are available on USB sticks. During the installation, one license is copied to the computer with the SpectraWorks² software. A second license can be used to evaluate data with the SpectraWorks² software in an office on a second computer. The USB stick should be kept carefully. When the SpectraWorks² software is uninstalled, the license is copied back from the computer to the USB stick and is then available for installations on other computers.



