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ISQ EC AND ISQ EM

TIPS AND TRICKS: ISSUE 6

The effects of the chromatography filter

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Keywords

Single quadrupole mass spectrometer, ISQ EC, ISQ EM, Chrom Filter

Goal

Better understanding of the Chromatographic Filter and its effects

Introduction

The Thermo Scientific™ ISQ™ EC and EM single quadrupole mass spectrometers were developed with chromatographers in mind. As a result, some data settings are predefined to assure straightforward, hassle-free data acquisition. One of these settings is the Chromatography Filter.

Guideline

The Chromatography Filter has a fixed setting in Component Mode and Basic Mode. In Scan mode it can be adjusted by the operator. By default, it is set to 3.000 s (seconds) peak width at half maximum (Figure 1).

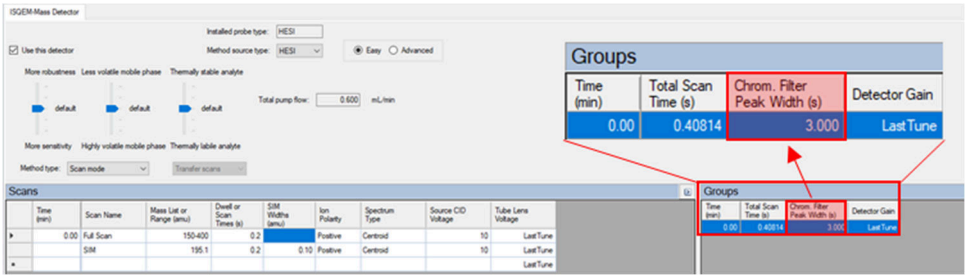

Figure 1. ISQ EC/EM Pane of the Method Editor. In Scan Mode the Chromatography Filter Setting is located on the right (marked in red). By default, the value is set to 3.000 s.

Applying the Chromatography Filter results in a light smoothing of the data and noise reduction. The peak area is not affected.

Smoothing

The filter applies a gaussian smoothing over the detected peaks in order to reduce artificial signal variation introduced by electronic or detector noise. Peak detection is done based on the peak width setting. Ideally, the selected value should approximate the full-width half-maximum value of the analyte peaks. In fact, the algorithm works well even if the peak width is under or a bit overestimated. If the actual peak width is wider than the set value the smoothing will not be as efficient, If the actual peak is narrower than the set value the smoothing will result in slightly increased peak width. In any case the area of the peak is conserved. These effects are highlighted in Figure 2.

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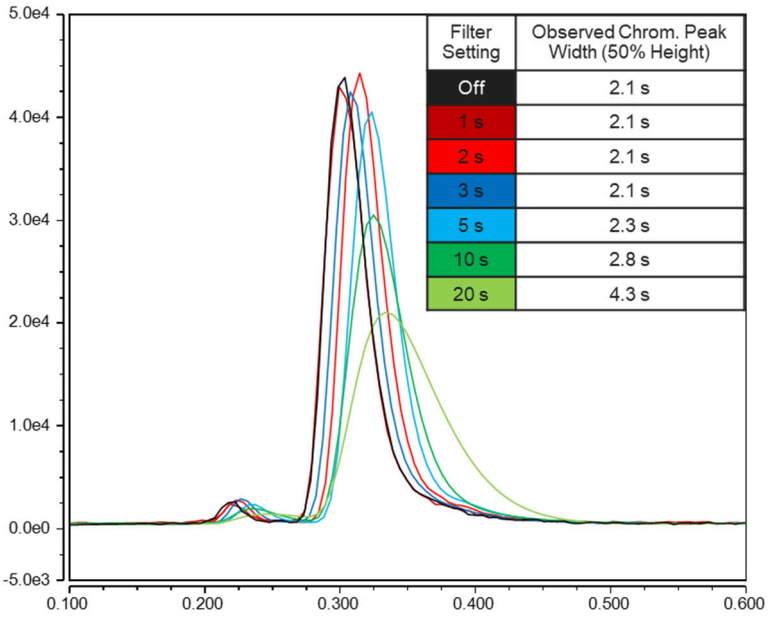

Figure 2. Reserpine acquisition with different Chromatography Filter settings. The coloring of the cells matches the colors or the respective chromatograms. Increasing the value of the Chromatography Filter from Off to 3 seconds did not change the observed chromatographic peak width. Setting the filter to 5 seconds slightly increased the observed peak width. At higher values (10 and 20 seconds) the filtering resulting in significant peak broadening. The observed peak area was not affected by the smoothing algorithm.

Noise reduction

The Chromatography Filter has a second component, particularly important for low intensity ions and background signals. It squelches the baseline if the signal is below a certain threshold. Then, it removes all signals below a level which is considered to only be electronic or detector noise. Once the signal exceeds this threshold the squelching is turned off and the complete signal is recorded. This effect becomes frequently noticeable with SIM scans that have a very low noise baseline away from the chromatographic peak. The observed baseline before and/or after the actual analyte signal can then be zero because the signal intensity is below the filter threshold, therefore, has been determined to be electronic noise, and is cut-off. Once the signal exceeds the electronic noise limit, the filter is switched off and the entire signal is recorded (Figure 3).

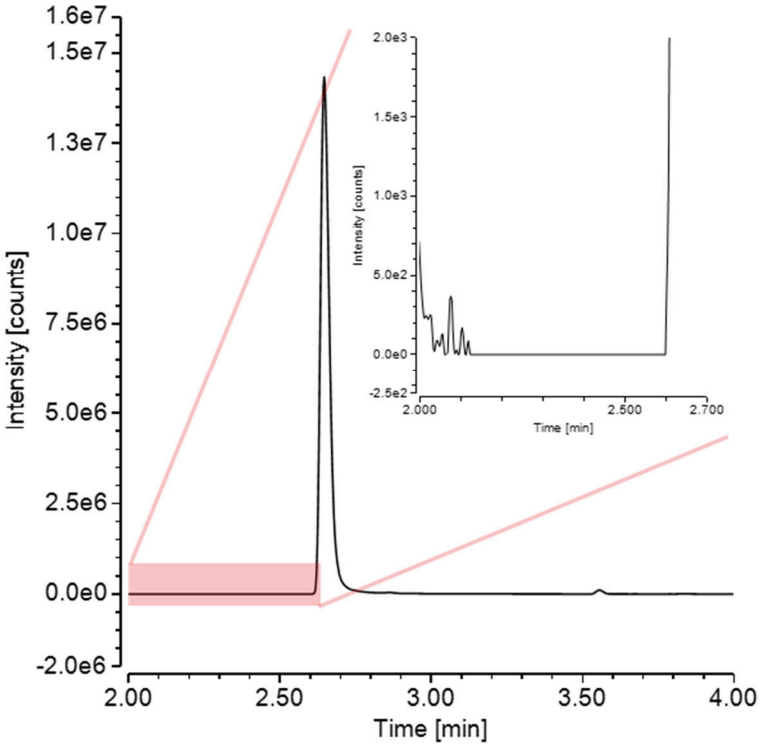

Figure 3. SIM acquisition showing baseline squelching effect away from the chromatographic peak. The baseline where the signal is cut off because the signal is below the filter limit is highlighted and enlarged (top right). The signal is recorded once the actual peak is detected because the filter threshold is surpassed.

Please note, the applied threshold value is independent of the peak width setting. It is automatically determined by the system based upon a variety of parameters and instrument settings. However, it is switched off if the Chromatographic filter is switched off.

Conclusion

The Chromatography Filter results in improved data because of smoothing and noise reduction. If this is not desired it can be switched off in Scan Mode by setting the peak width value to Off.

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