Triggered Acquisition support in Skyline-Daily 20.1.1.69

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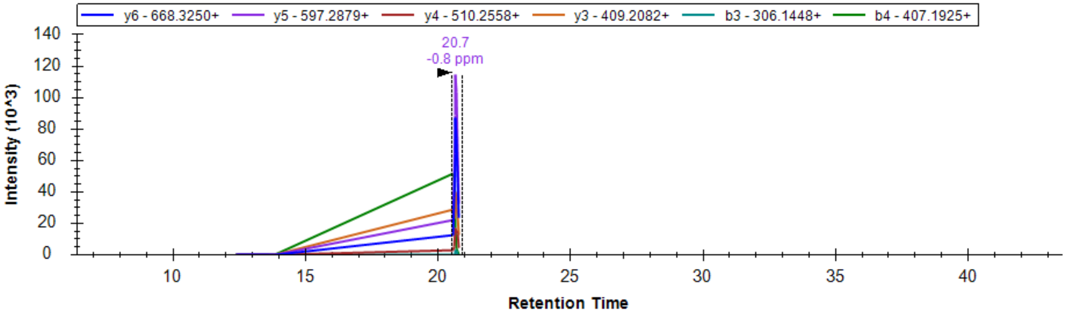
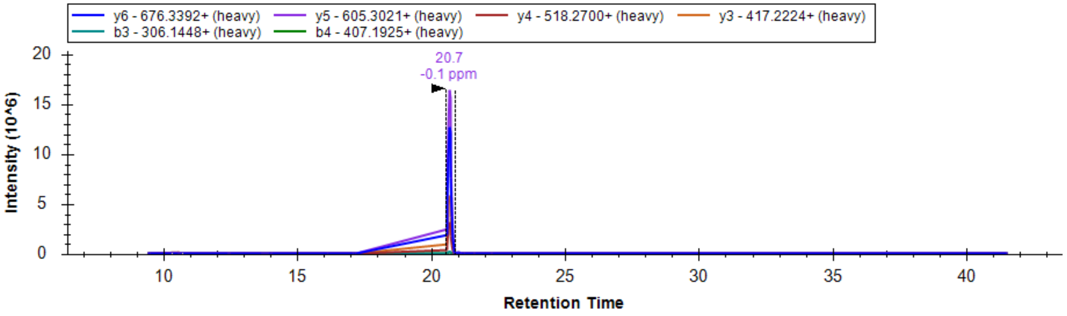
Introduction: Triggered acquisition methods

- In a triggered acquisition method, the mass spectrometer collects MS2 scans for a heavy peptide.
- When certain transitions are observed in the heavy spectra, the mass spectrometer begins collecting spectra for the light peptide.

The problem: triggered acquisition results in strange chromatograms

If there are gaps in the times at which matching MS2 scans were collected, they are drawn on the chromatogram as long straight lines.

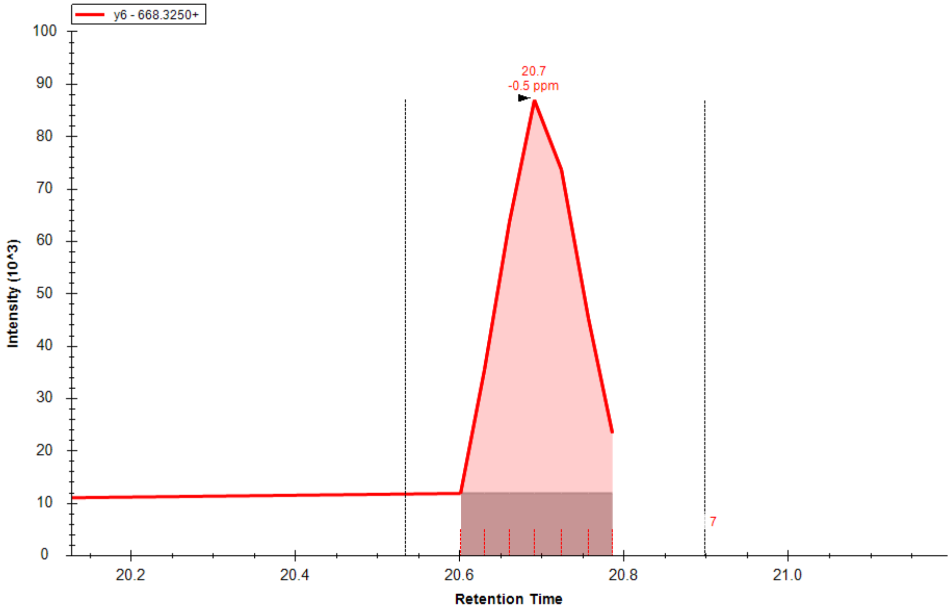




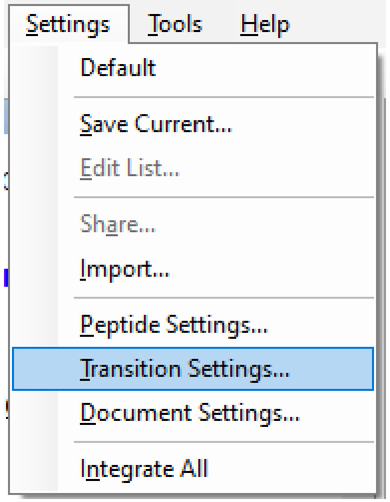
Peptide: FASTFDK

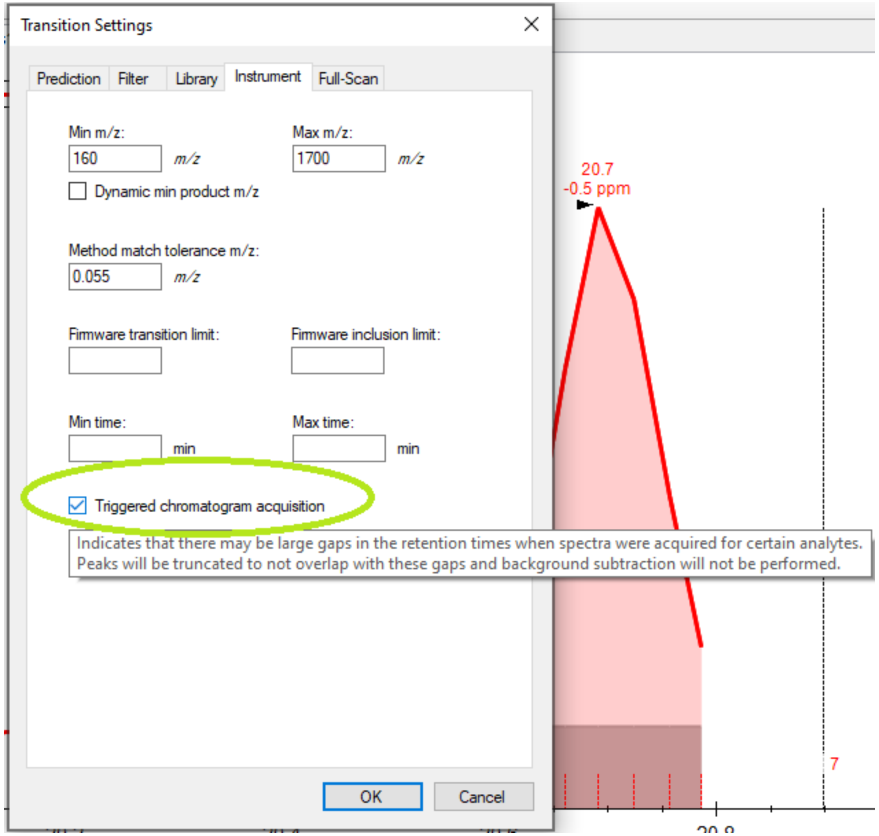
Gaps in collection time result in poor background estimation

- Skyline estimates the background level to be the lower of either the intensity at the start of the peak or at the end of the peak.
- This does not work well if the entire peak was not acquired.



New feature: Triggered Acquisition Setting





Min m/z: 160 m/z

Max m/z: 1700 m/z

☐ Dynamic min product m/z

Method match tolerance m/z: 0.055 m/z

Firmware transition limit:

Firmware inclusion limit:

Min time: min

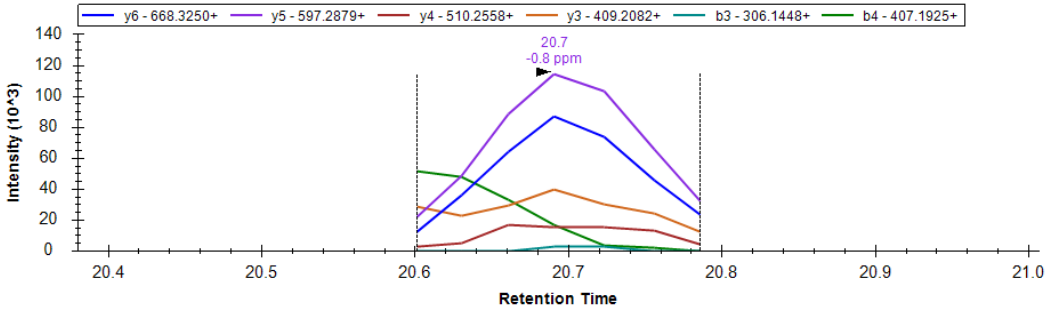
Max time: min

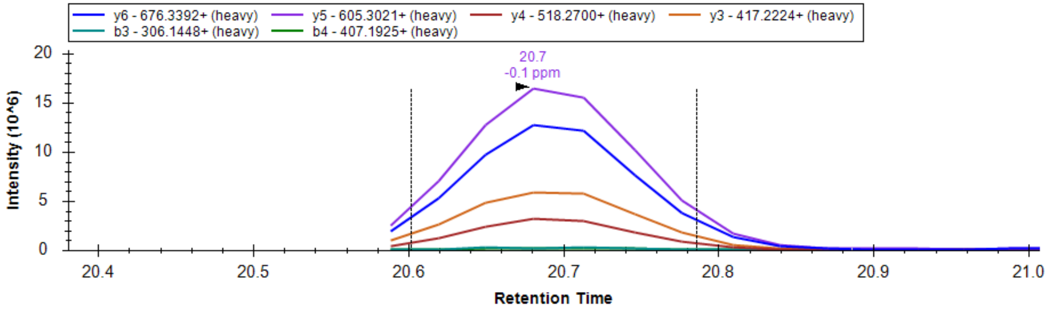
☑ Triggered chromatogram acquisition

Indicates that there may be large gaps in the retention times when spectra were acquired for certain analytes. Peaks will be truncated to not overlap with these gaps and background subtraction will not be performed.

With Triggered Acquisition turned on, Skyline recognizes the gaps in MS2 scan collection

Peak boundaries are constrained to range over which scans were collected for all of the precursors





Background subtraction does not happen if Triggered Acquisition is turned on