Tandem Quadrupole Purification

With single quadrupole directed purification, all ions generated in the source are passed through the quadrupole mass filter of the “Tandem” mode of operation. Only MS1 is static in this configuration. All ions generated in the source confer a specific neutral loss. Consequently, multiple fractions can be generated from a single m/z value. Additional analysis is then required to identify known fractions.

Example Data: Caffeine metabolites m/z 167 and 181

- For the peak present in the chromatogram, both the specific parent and specific daughter ions were collected. The chromatogram shows that only one fraction for each m/z was collected. In this example, only the 120 ng/g caffeine was used. Additional analysis is required to determine the neutral loss.

- Additional analysis is required to determine daughter ion.

Constant Neutral Loss Example Data

This example data shows the constant neutral loss of 57 acquisition and collection of the caffeine metabolites with m/z 167 and 181.

- 2 Fractions are collected. 1 for each m/z.
- Fractionation was performed using neutral loss and the specific neutral loss.

Applications for Fraction Collection from Constant Neutral Loss Acquisition

Mixed Trigger Collection

With constant neutral loss acquisition, the only products detected are the ones with the loss of the isobaric masses. Thus, in the case of caffeine the constant neutral loss of 57 was not detected. This leads to complete total ion chromatograms. Therefore, when targeting by a specific mass, the collected mass must contain the parent of interest and a specific neutral loss.

Collection Triggered with NC

When using the mode of collection and acquisition, all the peaks with a specific neutral loss are collected. This is valuable when the metabolites have a specific neutral loss that can easily be monitored. For the example collected at 100 ng/g in glucose (data not shown). The parent mass for each fraction is then neutralized and used as a criterion for the identification of the fraction.

In the constant neutral loss example shown, collection could also have been triggered from the 2,500 ng/g caffeine sample. Additional analysis of other neutral loss and constant neutral loss fractions would be required to find the desired fractions.

Preserver Ion Collection

Constant neutral loss fractionation can be used to collect a specific s/m/z combination. For example, if the specific daughter is detected, the method is triggered and the detector scans for the specific parent. This can be used as a background scan, where the target is known to have a specific mass and the neutral loss.

Collection of Neutral Loss Products

When using the mode of collection and fractionation, all the products with a specific neutral loss in the chromatogram are collected. This mode of fractionation is valuable when the metabolites are unknown, but there is a constant fragment or the compound that can be detected.

Additional Collection Options

- Mass spectrometric analysis exploits the fact that only ions with a neutral loss corresponding to that of interest are transmitted by the second quadrupole. This process allows for the metabolites to be detected without fragmentation. However, the second quadrupole may be used to selectively transmit only a subset of ions. The second quadrupole may be used to selectively transmit only a subset of ions.

- Mixed trigger fractionation allows for boolean logic strings to trigger collection from multiple different modes or at least beam fractionation and the analyzed fractions for both modes to detect different compounds.

- Weighted isotopic fractionation allows for the isotopic log of interest to trigger from multiple collection data streams. For example, each collection can occur only when there is a parent at a specific time or when a peak is present at a different time.

Conclusions

- Fraction collection with a tandem quadrupole mass spectrometer is now possible. It is a more specific s/m/z combination if different modes of data acquisition are used. Mixed, constant neutral loss and preserver Ion collection, allowing for improved sensitivity for fractionation collections.

- MS1 is a useful method by monitoring a specific parent and specific daughter. This more generally reduces the amount of ion fragments which requires previous knowledge of the parent / daughter transition.

- Constant neutral loss can be used as a method to collect a specific s/m/z combination. This method can be used as a background scan as long as the target is known to have a specific mass and the neutral loss.

- Collection with a constant neutral loss filter is valuable for the collection of neutral products. This mode of fractionation can be used to isolate the metabolites and collection of the neutral products. Additional analysis of different fractions can be performed.

- The different modes of collection have different applications based on the requirements of the study. It is true of all collection methods that the identification of the different samples is facilitated by targeted fragmentation.