ABSTRACT

Ideally, a generic screening method will work for any compound. Targeted methods are useful, but they are non-optimal for new compounds that may elute at the same time. Acquisitonal mass spectrometry (MS/MS) is a highly effective way to ID/quantify unknowns. The use of high-resolution MS/MS acquisition in an ion trap MS1 is a close relative that acquires MS/MS that represent every precursor mass of interest at every point. However, there are some challenges. The deconvolution of MS/MS for intensity searching and calculation of ion ratios from fragments, requires that fragments from different compounds have a different chromatographic profile and elution time. Intensity searching with different fragmentation post-accumulation (or the use of precursor signal) is time consuming. Scanning SWATH acquisition enables measurement of both precursor mass and fragmentation for all compounds and elution times.

INTRODUCTION

Acquiring precursor ion information at the low collision energy. Thus, resulting in a cleaner spectrum than a simple MS1 scan. Additionally, this quadrupole dimension from scanning SWATH acquisition was used to distinguish precursor matching compound fragmentation signal. The information used to identify the fragmentation signal originating from internal standard and separate it from the background.

MATERIALS AND METHODS

Scanning SWATH acquisition technique continuously scans the quadrupole along the mass range, but events are recorded using each TOF (time of flight) pulse over a period on Q1 in a ramp. This way, every ion on a characteristic of the independent computer, mass, LC time, and GI. Quadrupole dimension in providing information used to identify the fragmentation signal originating from internal standard and separate it from the matching compound fragmentation acquisition. The quadrupole dimension is not available for the matching compound fragmentation acquisition.

Additionally, the isolation window for the precursor mass of interest. Acquisition is performed in steps: acquiring data from individual pulses enables a more sophisticated analysis. An extraction of a unique fragment ion interference makes it difficult to determine the correct retention time, unless it is known ahead of time. Processing scanning SWATH acquisition data for MS1 is almost identical to processing the standard SWATH format. Analysis is performed in different IS and separate it from the background.

CONCLUSIONS

• Scanning SWATH acquisition and processing can determine the correct signal intensity for shared fragments, even if they perfectly co-elute.

• The correct ion ratio for a diclobutrazol and penconazole almost perfectly co-elute. The correct ion ratio for diclobutrazol.

REFERENCES


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