A NOVEL DATA-INDEPENDENT ACQUISITION STRATEGY FOR NON-TARGETED ACCURATE MASS CONTAMINANT SCREENING

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INTRODUCTION

Some people call them Non-Targeted acquisitions, some Data Independent Acquisitions (DIA). What does Non–Targeted screening mean to you?
Here, we discuss the use of a novel DIA method, SONAR, where precursor and product ion data are acquired with a sliding quadrupole window. We compare results of a SONAR acquisition, developed primarily for 'omic' experiments, to traditional DIA acquisition strategies such as full scan low and high collision energy acquisition (MS^E[1]), and its ion-mobility enhanced variant (HDMS^E) for use in contaminant screening.

METHODS

Well characterized samples from a collaborator

Reported Residues	Reprted (ng/g)	UPLC-TQS micro	APGC-TQS micro	UPLC-Vion	Xevo G2-XS Sonar
Azoxystrobin	21	✓	-	✓	✓
Bifenthrin*	161	-	✓	-	
Boscalid	131	✓	✓	✓	✓
Captan*	30	-	✓	-	
Cypermethrin*	34	-	✓	-	
Fenhexamid	116	✓	-	✓	✓
Imidacloprid	T	✓	-	✓	✓
Iprodione*	51	-	✓	-	
Pyraclostrobin	18	✓	-	✓	✓

* GC Amenable

Excellent results correlation for all samples (Blackberry shown) using 3 different systems, 5 acquisition types

Tandem Quad (TQ-S micro)
LC and APGC MSMS

Non-IMS Enabled Tof (Xevo G2-XS)
MS^E and SONAR

IMS Enabled Tof (VION)
HDMS^E

All accurate mass data was **Apex peak picked and componentized [2]** in UNIFI software. Utilizing informatics to align and display data across all channels results in cleaner spectra

Focus ! Azoxystrobin in Blackberry

Focus ! All MS data shown here is for 21 ng/g azoxystrobin in blackberries using MS^E, HDMS^E and SONAR acquisitions

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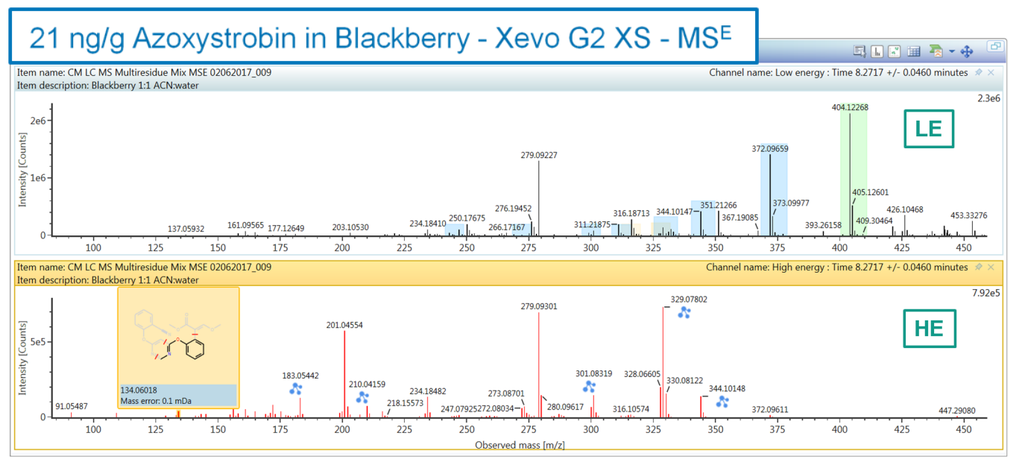
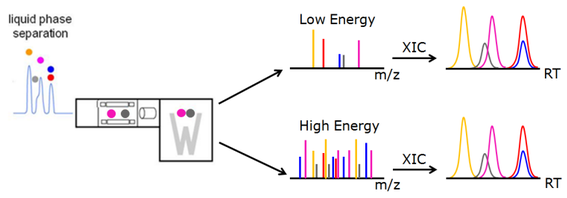


DIA



MS^E Summary

- Fast Acquisition: GC and UPLC compatible
- Accurate mass precursor and fragment ions
- Spectral Cleanup with Apex Peak picking
- Most sensitive Data Independent Acquisition

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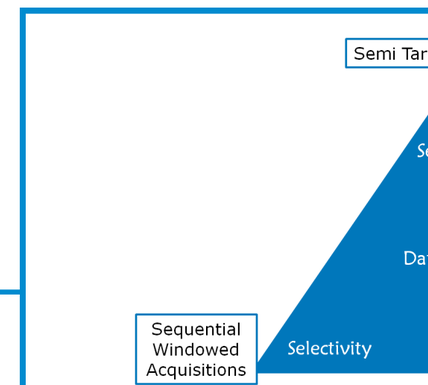
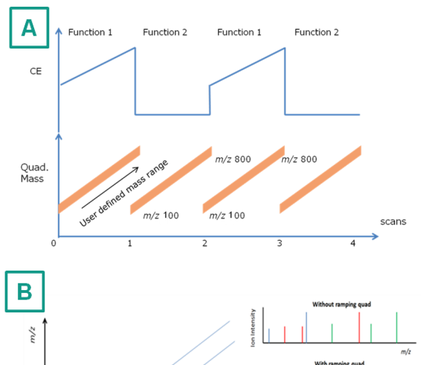
HDMS^E Summary

- Orthogonal separation of all parent ions using ion mobility – potential separation of isomeric species
- Fast Acquisition: GC and UPLC compatible
- Accurate mass precursor and fragment ions
- Spectral Cleanup with Apex Peak picking, RT alignment and Drift Time alignment
  - Library searchable spectra
  - Speedy target list screening data review
  - Aids in elucidation of unknowns



New DIA strategies like SONAR bridge the gap between selectivity (specificity), speed and sensitivity. Where do different or your acquisition methods fit?

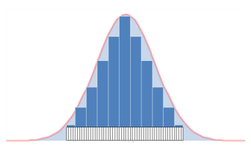


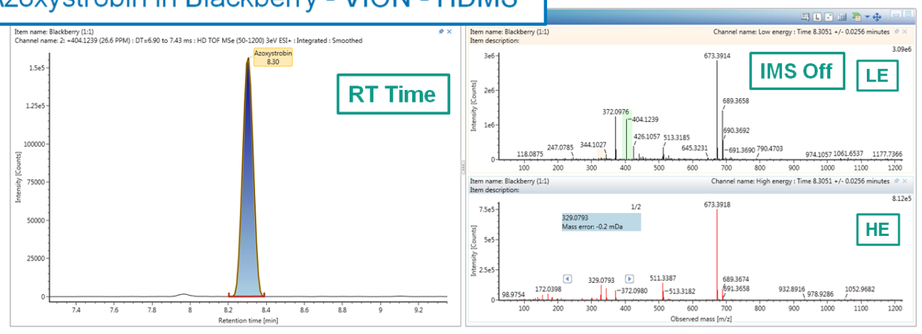
(A) SONAR acquisition schematic. Consists of 1 scan at a high collision energy (CE) followed by another at low CE. During each period the quadrupole is swept over a predetermined mass range, with a defined mass window.

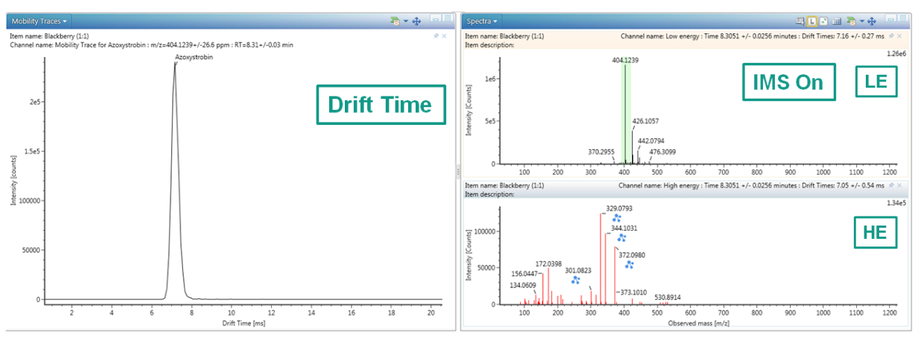
(B) Schematic of the scanning quadrupole and alignment of the precursor and fragment ions.

DIA with IMS

21 ng/g Azoxystrobin in Blackberry - VION - HDMS^E







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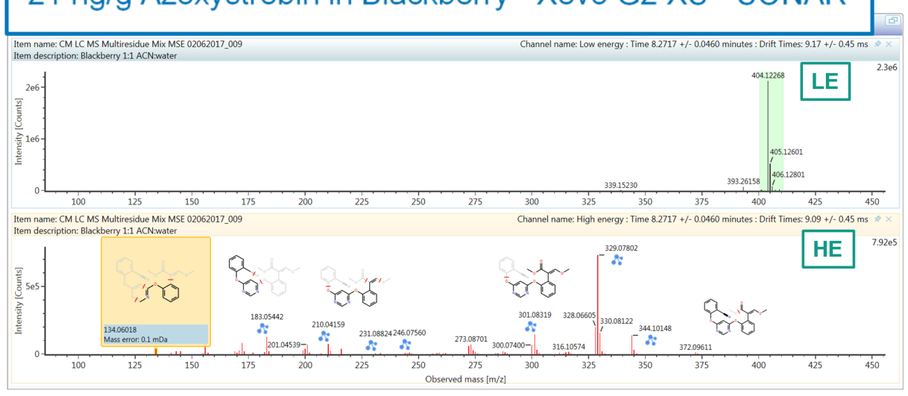
DIA Scanning Quad

SONAR Summary

- Fast Acquisition: GC and UPLC compatible
- Accurate mass precursor and fragment ions
- Spectral Cleanup with Apex Peak picking and quadrupole scanning windows
  - Library searchable spectra
  - Speedy target list screening data review
  - Aids in elucidation of unknowns

SONAR™

21 ng/g Azoxystrobin in Blackberry - Xevo G2 XS - SONAR



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CONCLUSIONS

- **Data independent acquisition strategies afford a robust, generic approach which generate rich, comprehensive datasets amenable to automated analysis such as contaminant screening.**
- **On ion mobility enabled instruments, HDMS^E experiments enable clean up of data in more complex matrices via drift time correlation of precursor and of product ions.**
- **On non-ion mobility instruments, as well as established strategies such as MS^E, swept scan approaches such as SONAR— while primarily targeted for 'omics experiments—do offer the scope for an intermediate level of specificity between MS^E and targeted MSMS. To this end, the next steps should be to perform a validation to establish SONAR as a fit for purpose method for contaminant screening.**

REFERENCES

1.MS^E White Paper: http://www.waters.com/webassets/cms/library/docs/720004036en.pdf
2.Componentization White Paper http://www.waters.com/webassets/cms/library/docs/720004597en.pdf

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