## **COMPREHENSIVE SCREENING OF AN ENVIRONMENTAL** WATER SAMPLE WITH HRMS COUPLED WITH IMS AND AN INTEGRATED SCIENTIFIC INFORMATION SYSTEM

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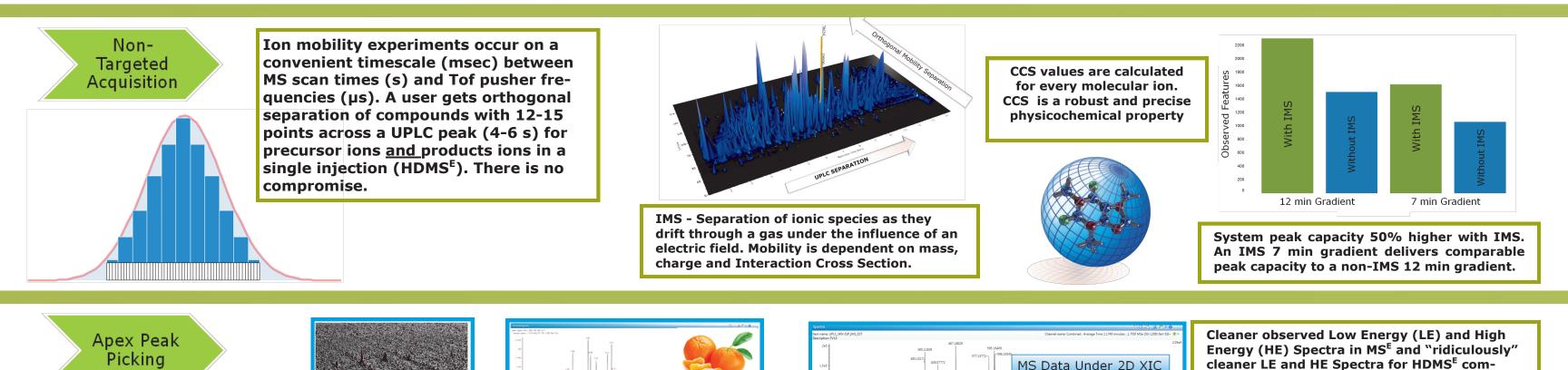
### **INTRODUCTION**

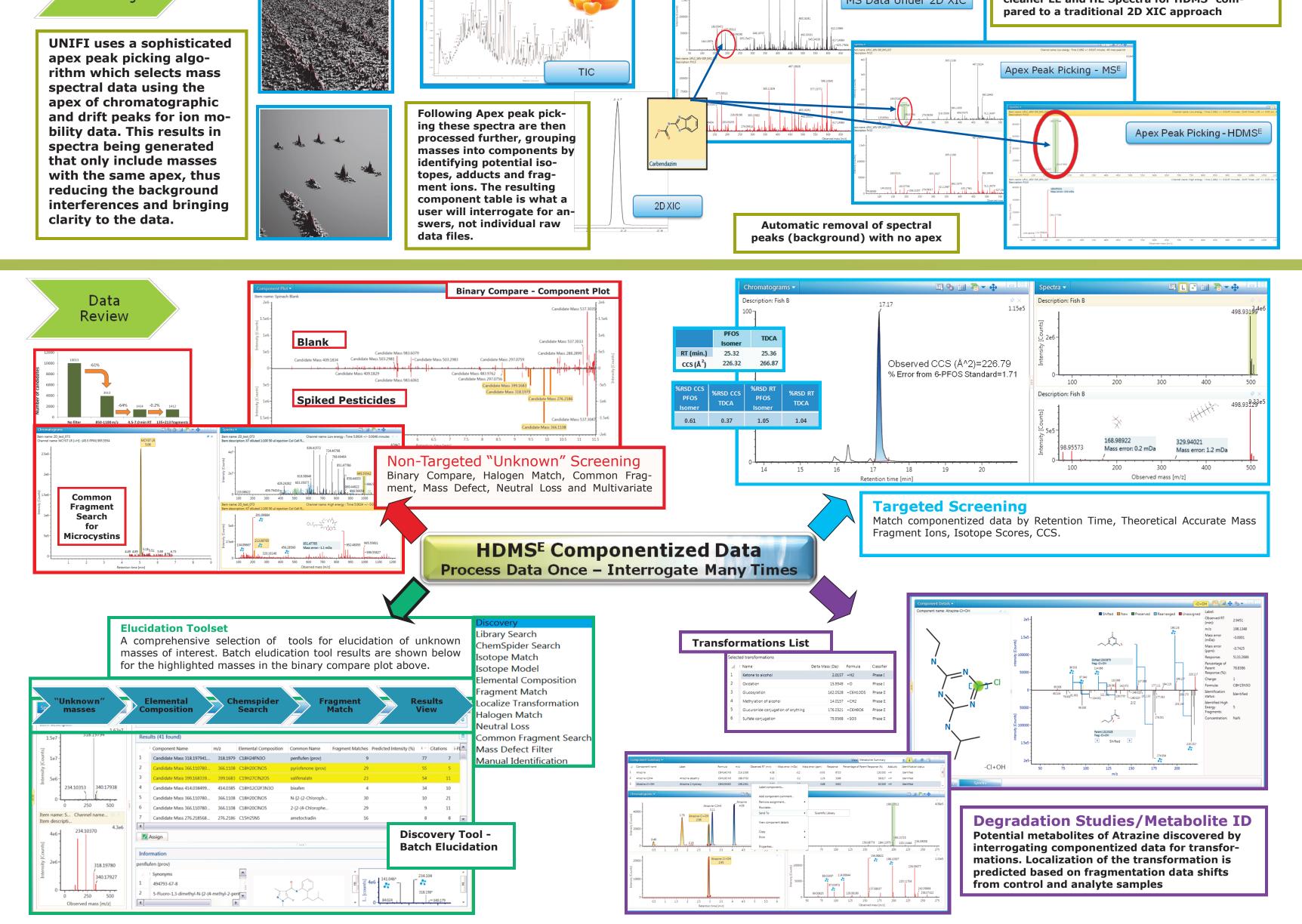
Companies and environmental regulatory authorities are looking toward High Resolution Mass Spectrometry (HRMS) to expand the scope of their screening methods. Improvements in mass spectrometer sensitivity and highly selective acquisition techniques allow users to find more compounds in a single injection than ever before, whether by a targeted analysis or via elucidation of unknown, or non-targeted masses of interest. Advancements in the Informatics used to process, interact and review non-targeted HRMS datasets have also increased markedly. Here we demonstrate how the use of modern informatics (UNIFI) can be used to comprehensively screen environmental samples for a range of contaminants in a given target list, as well as look for non-targeted or unknown compounds of interest. A typical experiment workflow is shown in the diagram below. We focus on the steps highlighted in green, typically the rate determining steps in getting from injection to report. Coupling ion mobility with HRMS, the use of Apex peak

substantially increases peak capacity but conventional 2D Extracted Ion interrogate comprehensive datasets This ensures a user can reduce the from vial to file.



picking and componentization<sup>1</sup> not only enables a user to process data beyond the Chromatogram (XIC) approach and  $(HDMS^E)^2$  without the need to reprocess data. injection to result bottleneck and quickly get





#### CONCLUSIONS

- The collection of a non-targeted comprehensive dataset incorporating UPLC and ion mobility separations (HDMS<sup>E</sup>) in combination with a sophisticated apex peak algorithm
  maximizes peak capacity for a given injection.
- Componentization of data following Apex peak picking enables a user to process data and interrogate it in many ways, without the need for reprocessing.
- Interrogation of data for targeted, non-targeted and unknown masses of interest is possible within a single integrated scientific information system (UNIFI).

#### REFERENCES

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

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