Case Study I: Small Molecule Impurity ID

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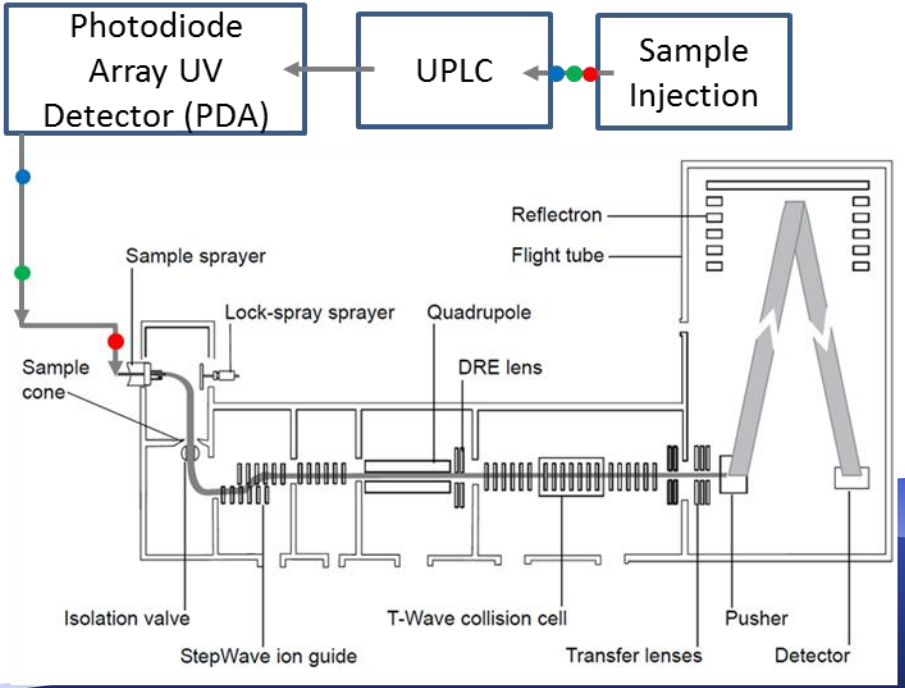
Determination of an Unknown E&L Impurity Based on **Accurate Mass** Detection, **Elemental Composition Matching**, Chemicals **Database Searching**, and MassFrontier **Theoretical Fragmentation**

CHALLENGE: Detection of Unknown E&L Impurity
SOLUTION: UPLC – UV – High Resolution Accurate Mass MS Analysis and MassFrontier Theoretical Fragment Library Searching Workflow

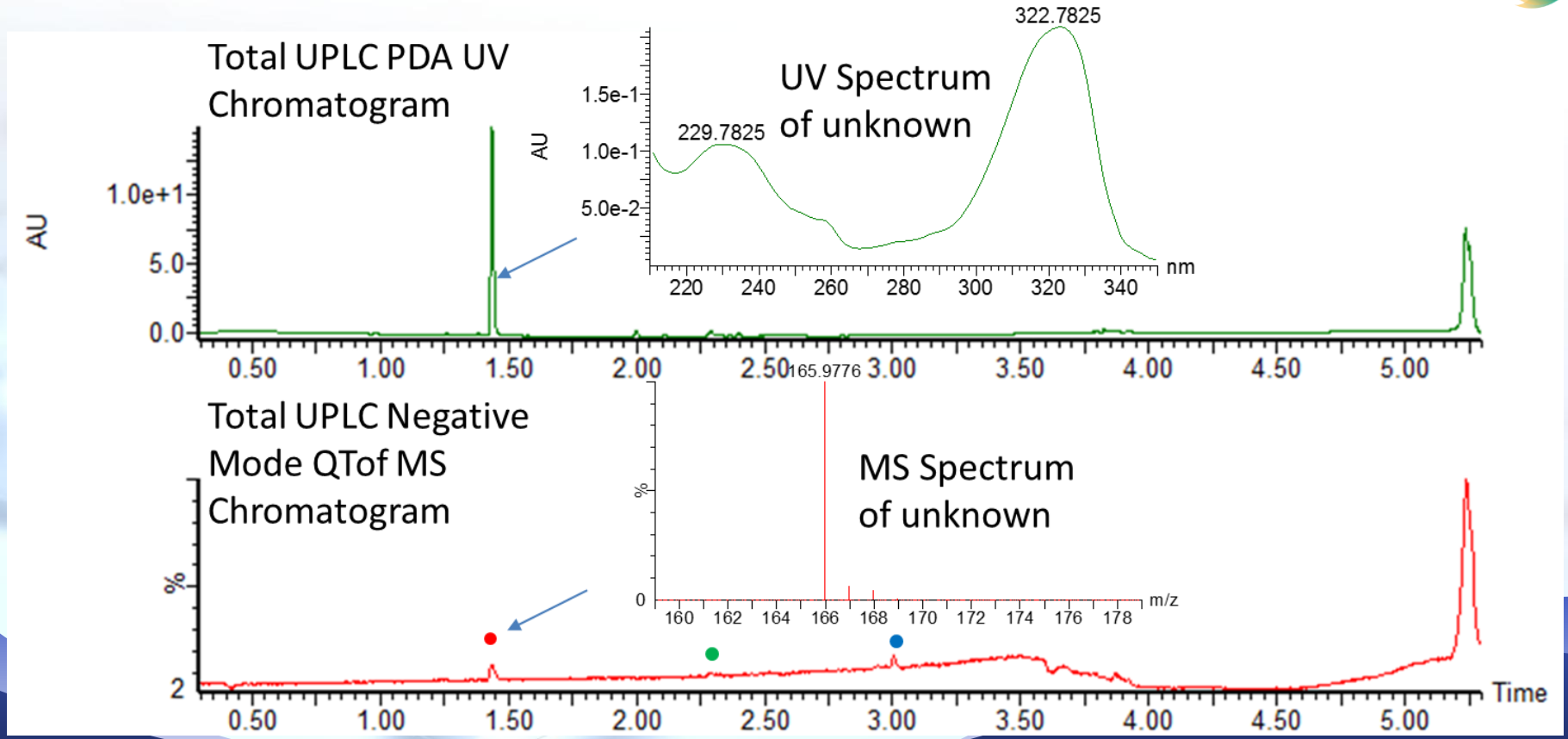
Step 1 - Accurate Mass UPLC-UV-QTof MS and MSMS Analysis

Acquity UPLC Coupled to G2-S (Waters) Q-Tof High Resolution Mass Spectrometer

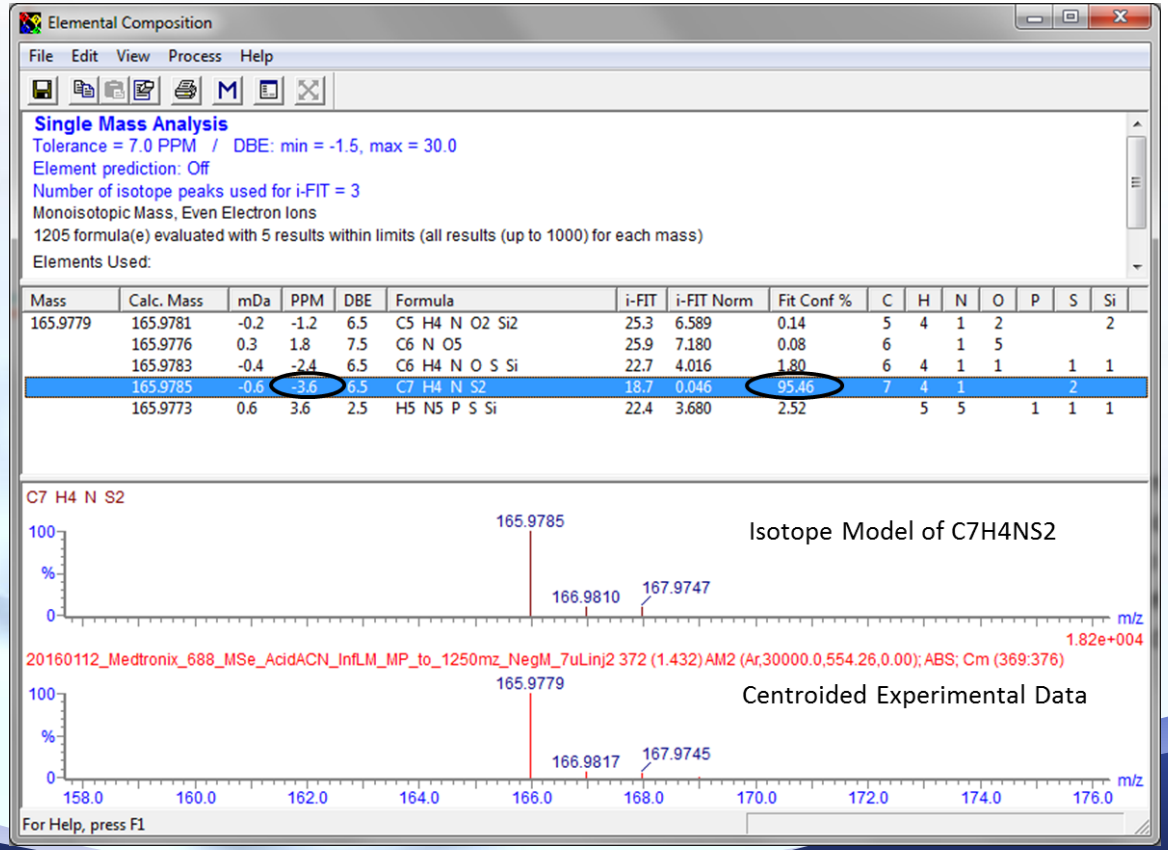
Chemical and Structural Identification of unknown component analytes comprising a complex mixture.



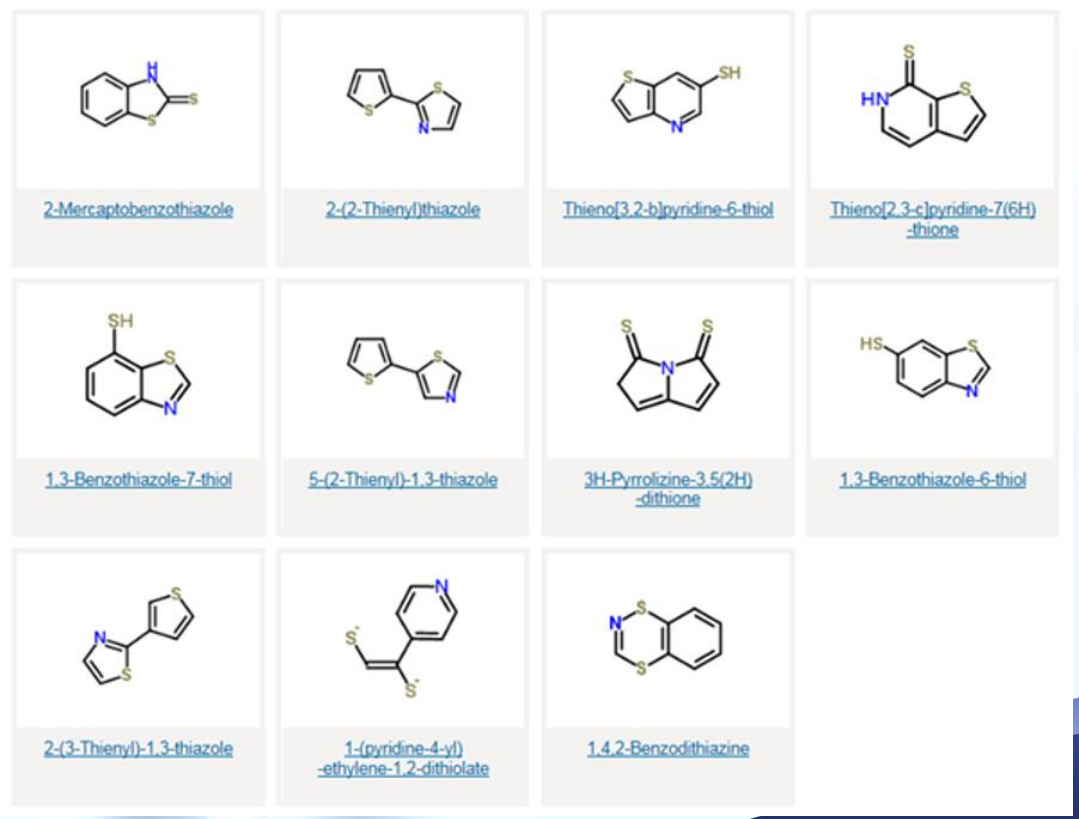
MS and UV Spectra of Unknown Impurity



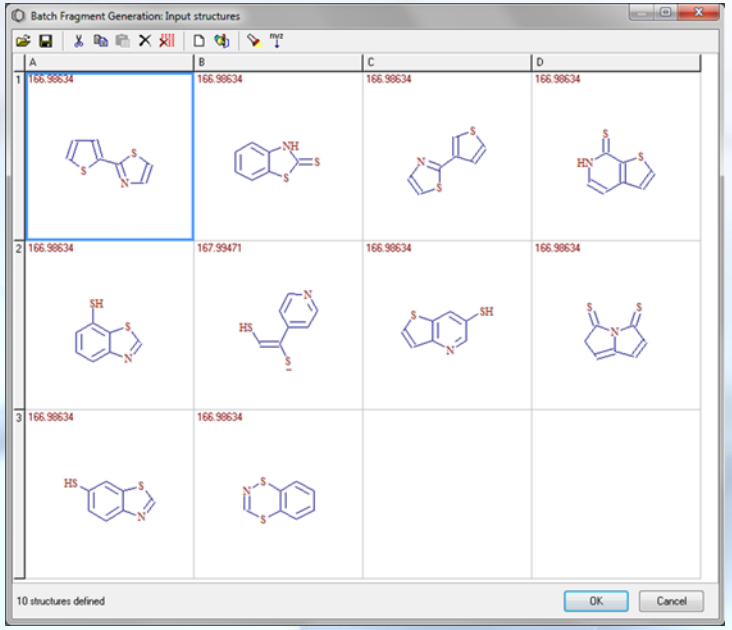
Step 2 – Elemental Composition Determination

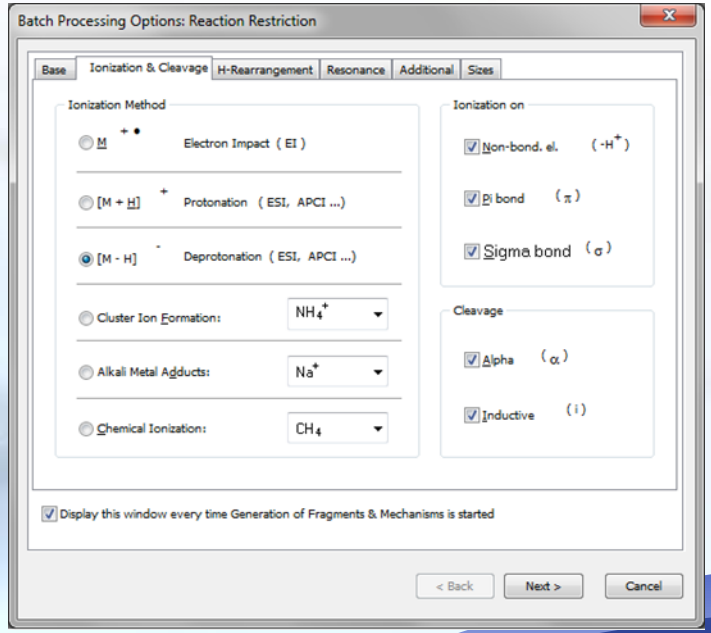


Step 3 – Elemental Composition Search of Online Databases



Step 4 – Mass Frontier Theoretical MSMS Spectra Calculation in Batch Fragmentation Mode

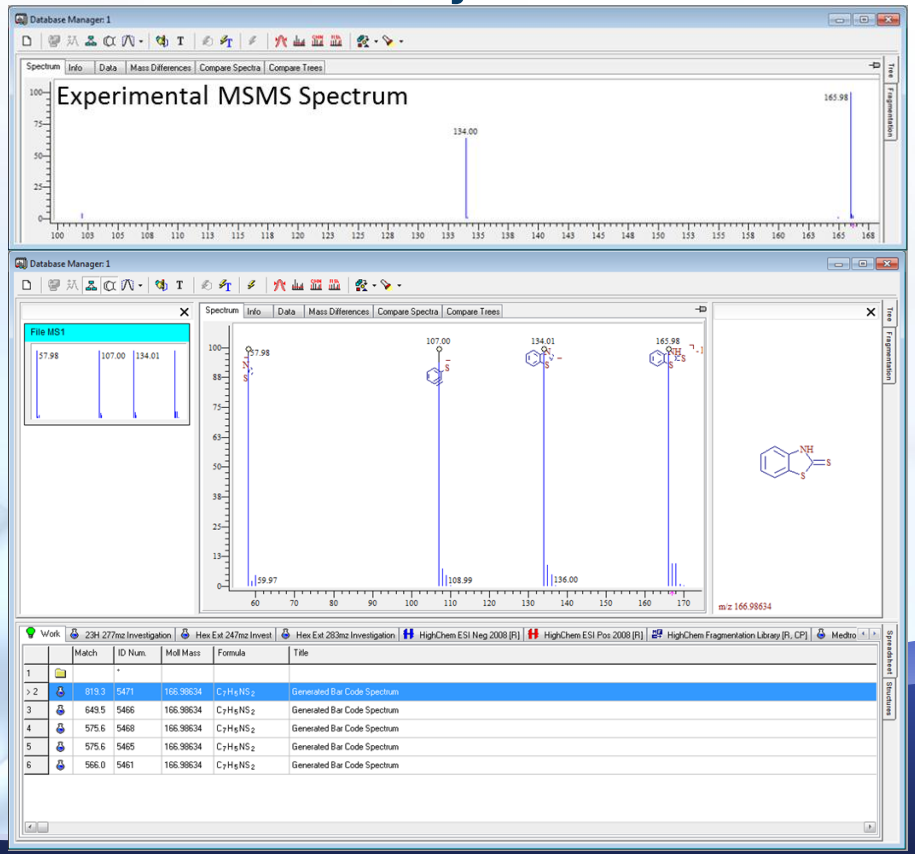




Step 5 – Search of Experimental MSMS Spectrum Against Calculated MassFrontier MSMS Library

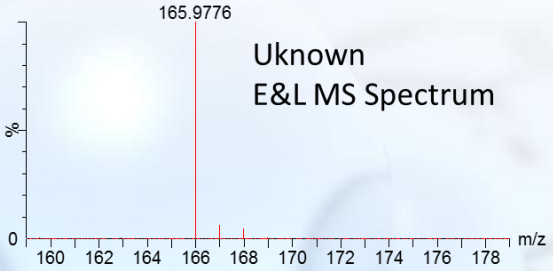
Top search match yielded a candidate for the unknown in the extractables and leachables study, namely

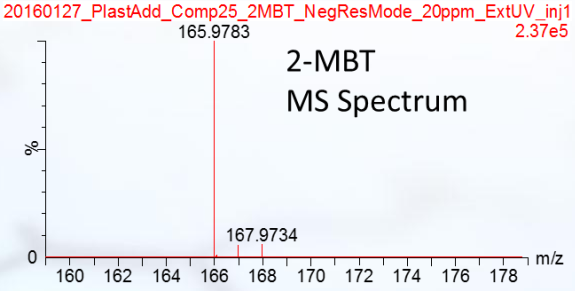
2-Mercaptobenzothiazole

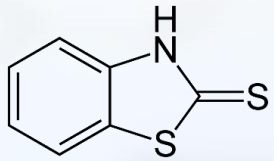


Step 6 – Confirmation of 2-mercaptobenzothiazole (2-MBT) as the correct identification of the extractables/leachables unknown

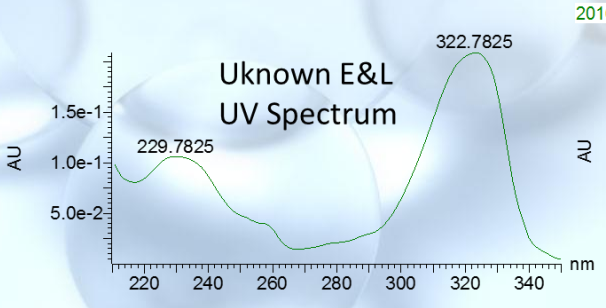
Experimental standard data confirmed the MassFrontier identification.

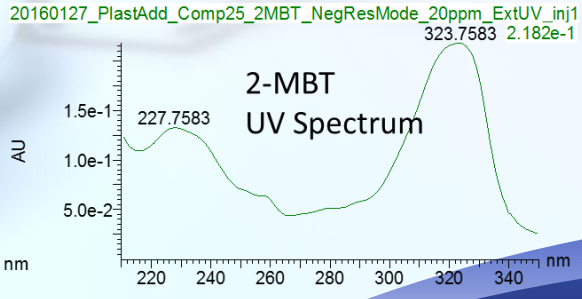






2-MBT





SUMMARY:

Mass Spec Lab's UPLC-UV-high resolution accurate mass workflow successfully identified a completely unknown E&L analyte present at trace levels (≅20 ppm) with no information other than that provided by the work flow.

We gratefully acknowledge technical assistance from HighChem (Bratislava, Slovakia, EU), the maker of MassFrontier, in assistance with the theoretical fragmentation spectral matching algorithms.

Questions?

More Information?

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