

General Workflow For Confident Identification of Unknown Compounds in Forensic, Petroleum, Food, Environmental, and Biological Materials: The GC-HRT Advantage

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Introduction

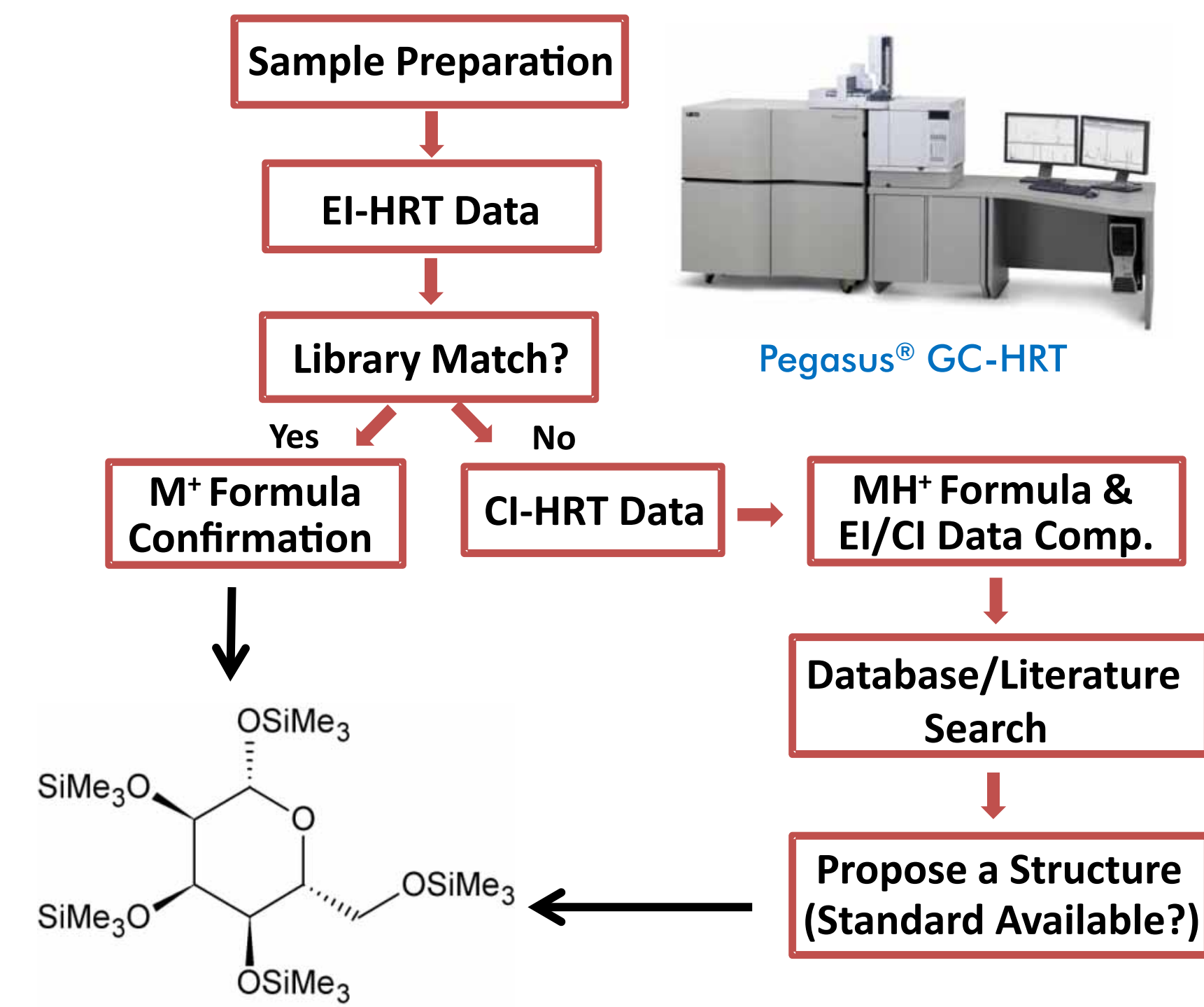
Pegasus GC-HRT is an ideal tool for the analysis of a wide variety of samples.

Advantages:

- Fast Acquisition Rates (up to 200 spectra/s)
- Chromatographic Resolution
- High Resolving Power (Up to $R = 50k$)
- High Resolution Deconvolution™ (HRD™)
- High Quality Spectral Data
- Superior Mass Accuracy (< 1 ppm)
 - Fragment Ions
 - Molecular Ions
 - Adducts

• **One Injection → Rich Data**

Workflow



Discussion

Complementary ionization methods and high resolution time of flight mass spectrometry facilitate compound identification:

EI-HRT

- Database searching (e.g., NIST, Wiley)
- Formulae determination—fragment and molecular ions
- Retention Indices

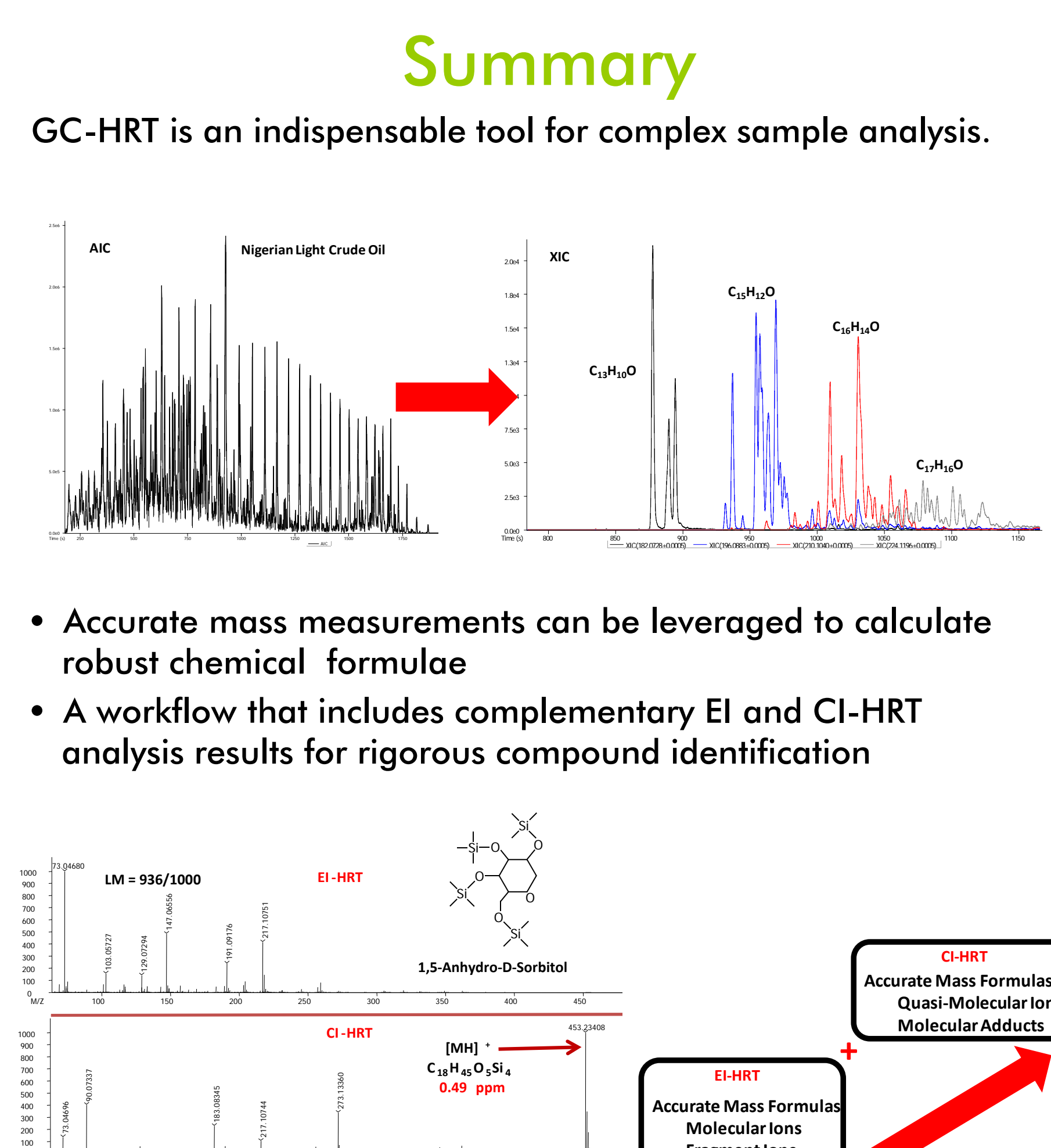
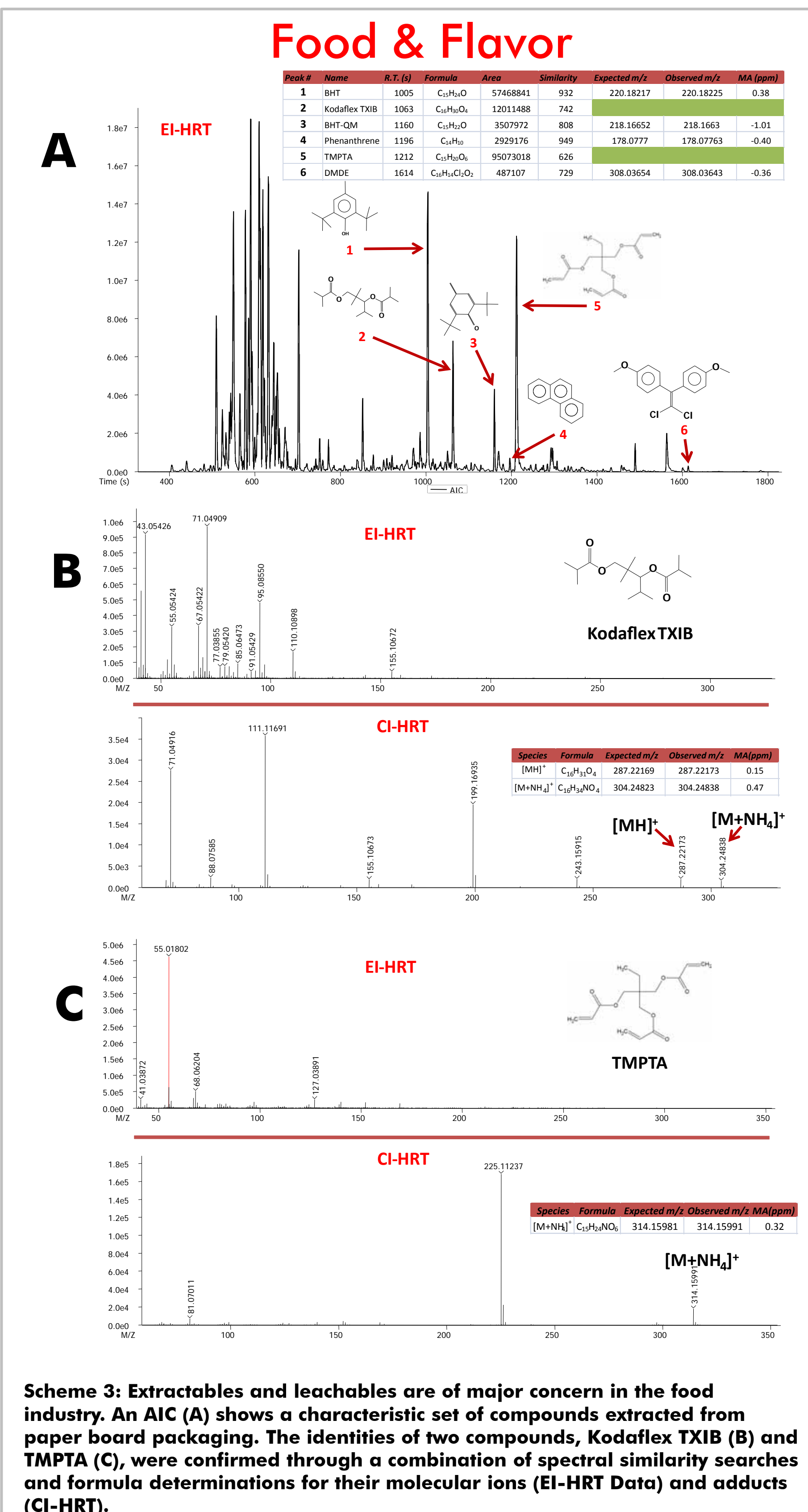
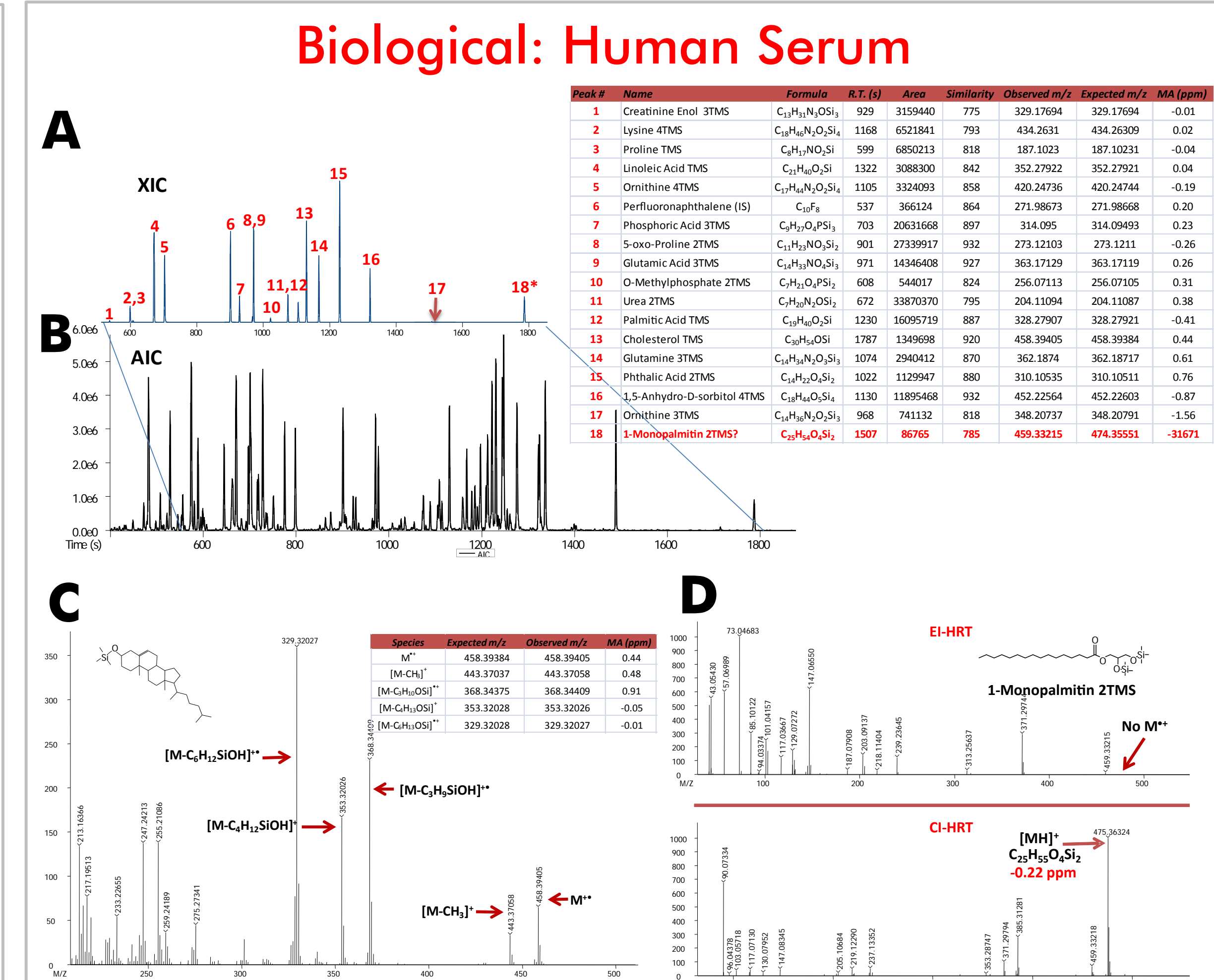
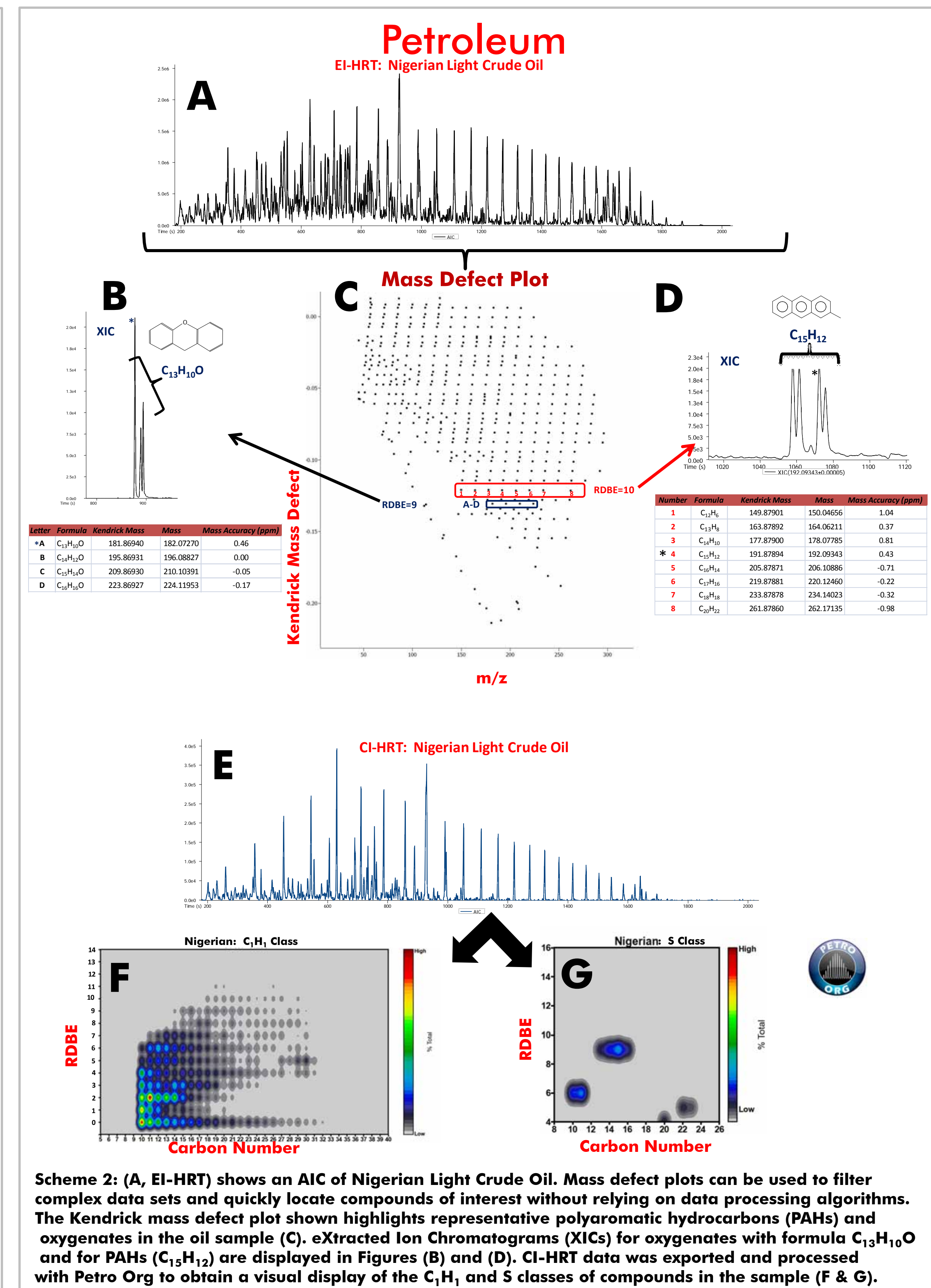
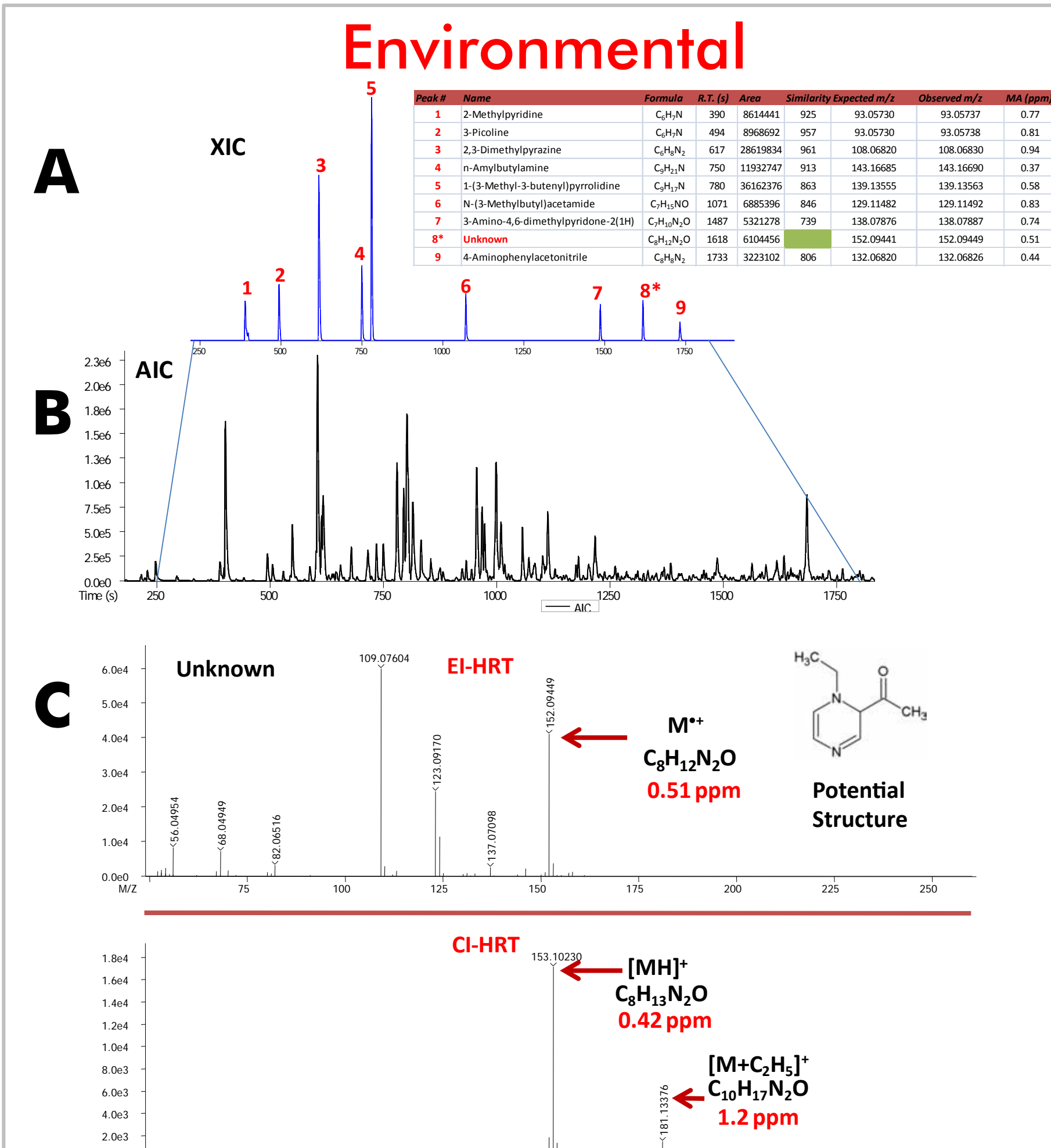
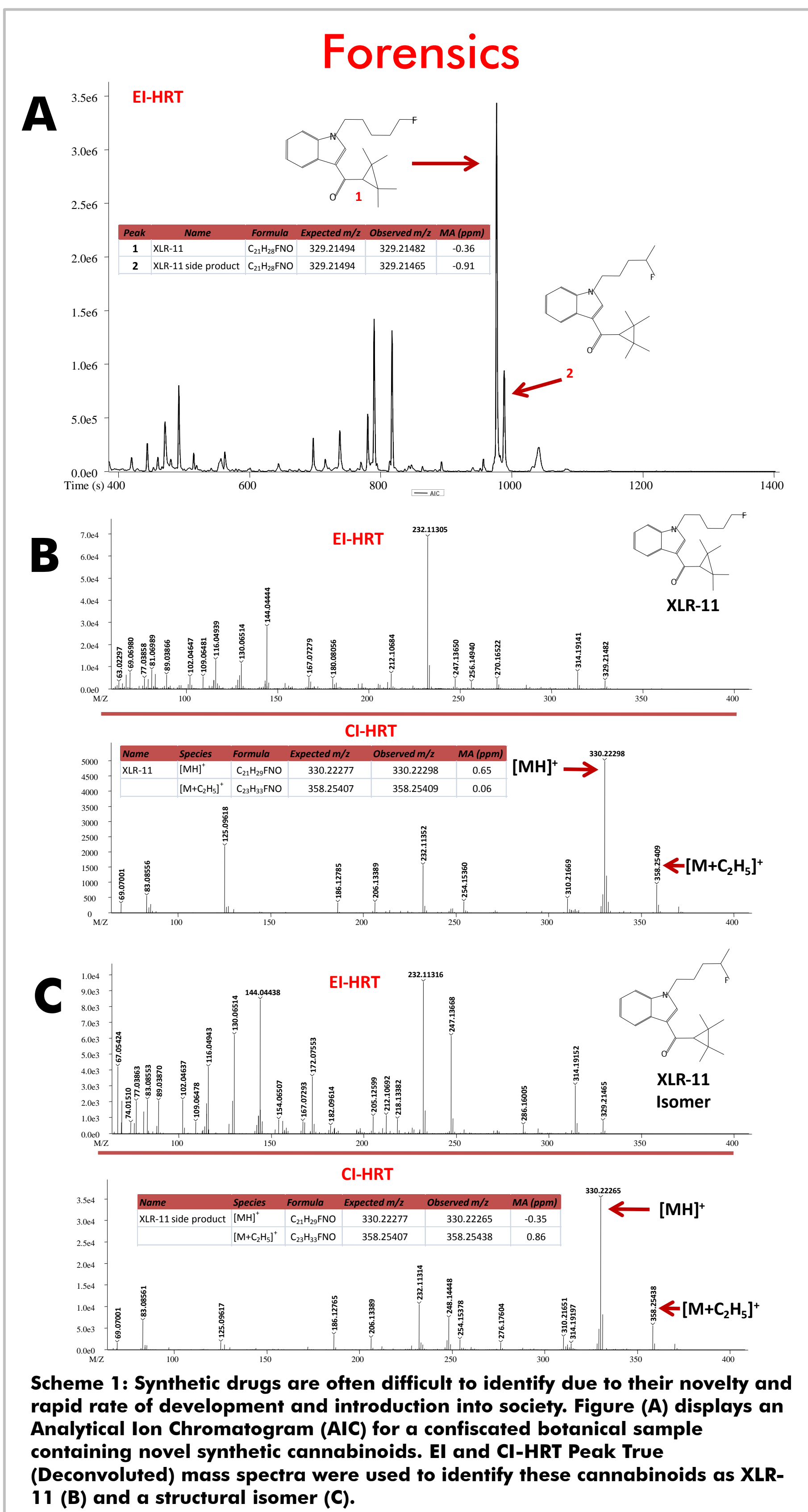
CI-HRT

- Formulae determination—molecular adducts

ChromaTOF-HRT® Software Tools

- Kendrick plots for quick analysis of complex samples
- Launch ChemSpider database searches

Data



Scheme 1: Synthetic drugs are often difficult to identify due to their novelty and rapid rate of development and introduction into society. Figure (A) displays an Analytical Ion Chromatogram (AIC) for a confiscated botanical sample containing novel synthetic cannabinoids. EI and CI-HRT Peak True (Deconvoluted) mass spectra were used to identify these cannabinoids as XLR-11 (B) and a structural isomer (C).

Scheme 2: (A) EI-HRT shows an AIC of Nigerian Light Crude Oil. Mass defect plots can be used to filter complex data sets and quickly locate compounds of interest without relying on data processing algorithms. The Kendrick mass defect plot shown highlights representative polyaromatic hydrocarbons (PAHs) and oxygenates in the oil sample (C). eXtracted Ion Chromatograms (XICs) for oxygenates with formula $C_{13}H_{10}O$ and for PAHs ($C_{13}H_{12}$) are displayed in Figures (B) and (D). CI-HRT data was exported and processed with Petro Org to obtain a visual display of the $C_{13}H_{10}$ and S classes of compounds in the sample (F & G).

Scheme 3: Extractables and leachables are of major concern in the food industry. An AIC (A) shows a characteristic set of compounds extracted from paper board packaging. The identities of two compounds, Kodaflex TXIB (B) and TMPTA (C), were confirmed through a combination of spectral similarity searches and formula determinations for their molecular ions (EI-HRT Data) and adducts (CI-HRT).

GC-HRT is an indispensable tool for complex sample analysis.

• Accurate mass measurements can be leveraged to calculate robust chemical formulae

• A workflow that includes complementary EI and CI-HRT analysis results for rigorous compound identification

• **More Confident I.D.s**