Direct sample analysis combined with a thermal gradient approach for routine testing of materials

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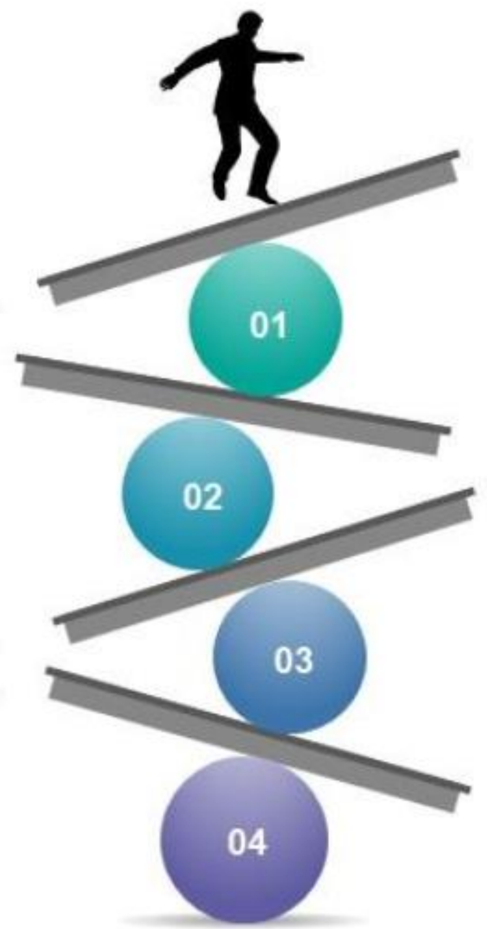
Waters Scientific Operations

Analytical challenges in Materials Testing Laboratories



1. Cost-efficient, fast analysis time from ‘sample to knowledge’
2. Robust, reliable analytical measurement
3. Quick result (pass/fail) from batch to batch
4. Minimal or no sample preparation (liquid or solids); reduce or eliminate the use of hazardous solvents

What is RADIAN ASAP?

Rapid Direct Analysis – Atmospheric pressure Solids Analysis Probe

- A novel, dedicated direct mass analysis system, engineered using proven and robust technologies
- Specifically designed for rapid, easy and low cost per sample analysis of solids and liquids.
- State of the art informatics tools to enable easy, real time results

Key features of RADIAN ASAP

- **Suitable for a wide range of samples**
  - High to low polarity analytes
  - Volatile and semi-volatile solids, liquids, and solutions
- **Simple analysis workflow**
  - Minimal to no sample preparation
  - Minimal training required
  - Open to use by non-expert personnel
- **Real time results for Raw Material & Formulation analysis**
  - LiveID & IonLynx software for real-time sample identification library matching compositional analysis
- **Fast**
  - Minimal time from sampling to result
- **Small footprint**
  - Make the most of available lab space
    W:34.4 cm/13.5”, H 27.1 cm/10.7”, D:73.0 cm/28.7”

How does RADIAN ASAP work?

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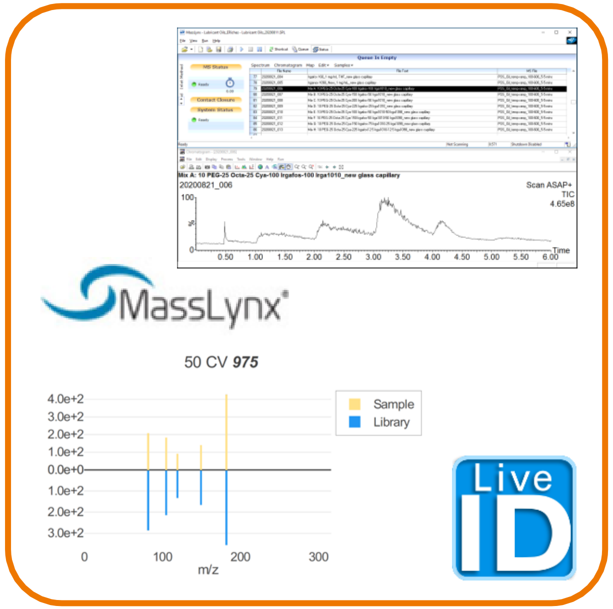
Analysis in four easy steps

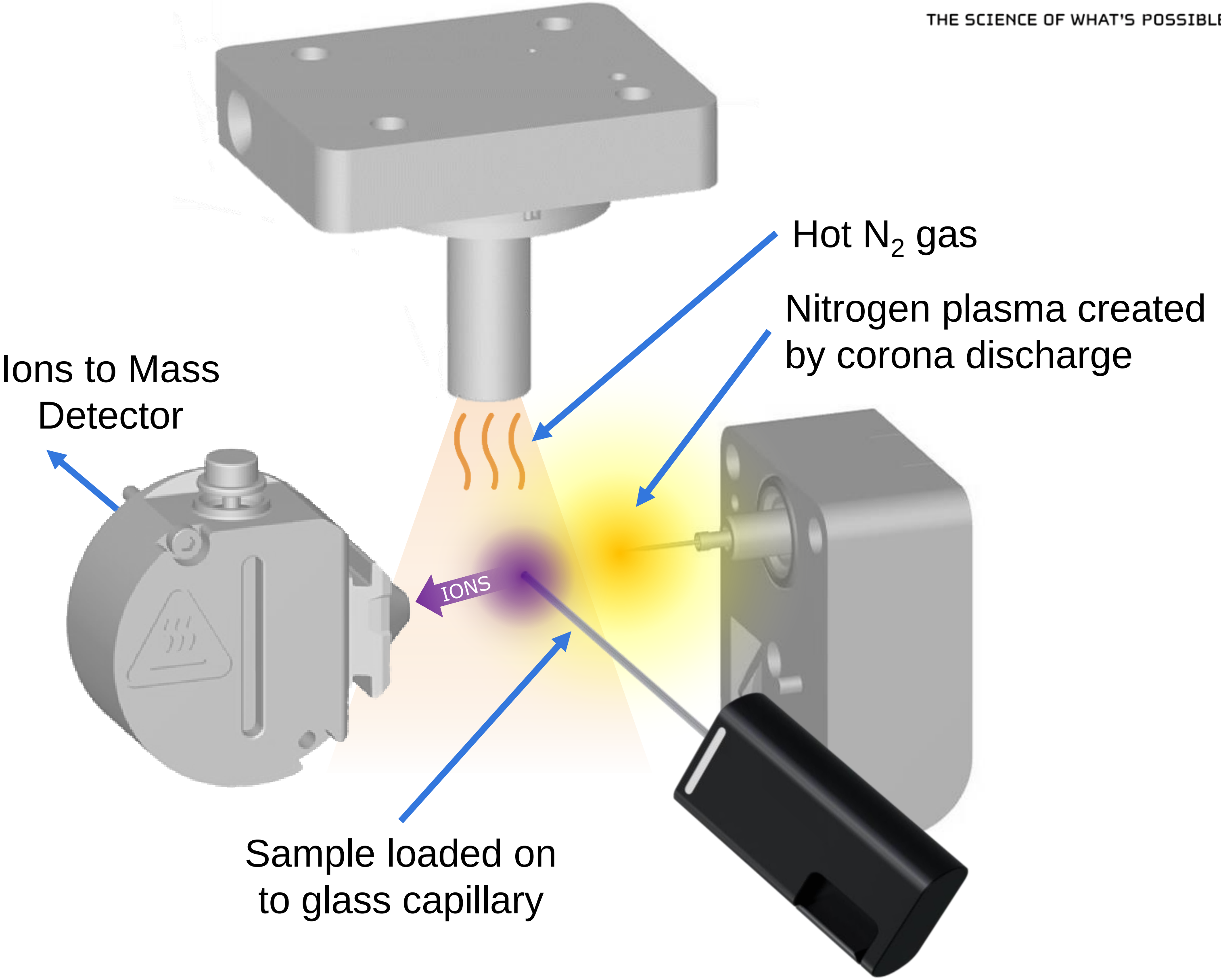


1. Clean the capillary
2. Load sample on capillary
3. Insert capillary to start acquisition
4. Real-time data visualization

How does RADIAN ASAP work?

The ASAP ionization process

- Sample is introduced into the corona discharge region on a glass rod
- Volatilised by stream of heated N_2
- Gaseous analyte molecules are ionised by N_2 plasma
- Gaseous ions are guided into the instrument and analysed by the single quadrupole analyser

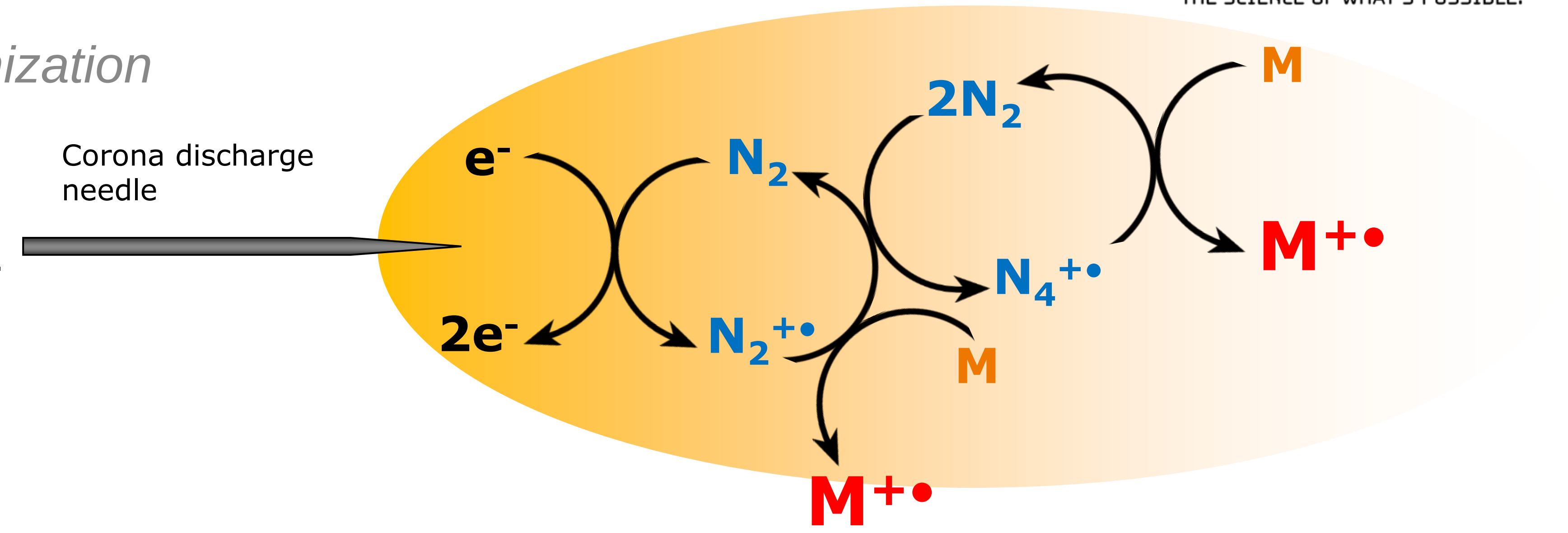


How does RADIAN ASAP work?

ASAP – The mechanism of ionization

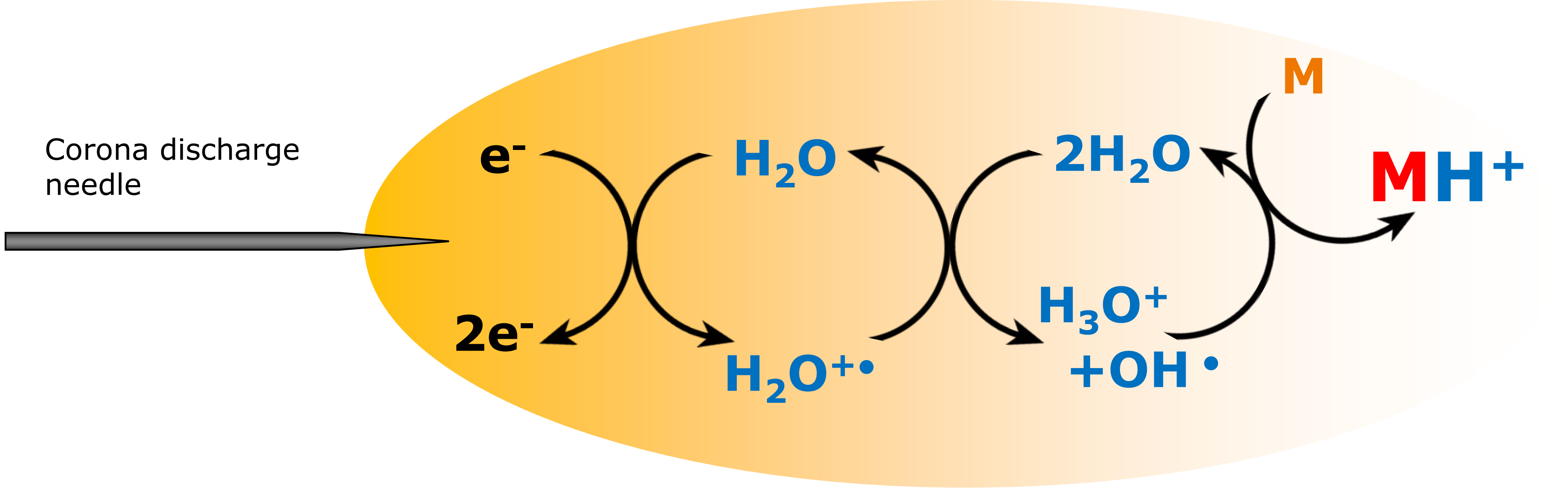
Charge Transfer

- Favoured by relatively non-polar compounds



Proton Transfer

- With presence of protic solvents such as H_2O or MeOH
- Favoured by relatively polar compounds



Horning, Anal. Chem, 1973, 45, 936-943

Example applications: Raw Materials Authenticity

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Raw Material Authenticity

- Chemical Industry:
  - Incoming raw materials need to be verified
  - Out of specification or contaminated substances need to be investigated
  - The quality of formulated products needs to be confirmed

- Decreasing the time to generate data on which decisions are made is key

- Reduction in analysis time allows laboratories to increase productivity and deliver results efficiently

Chemical Manufacturing Workflow

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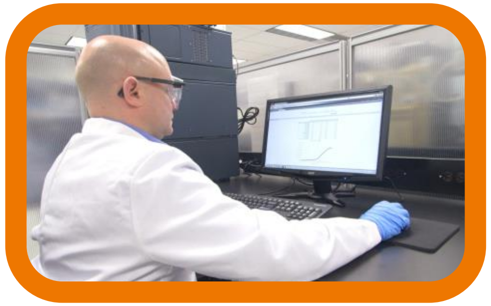
Receive Raw Materials	Verify Raw Materials	Formulate	Verify Formulation Batch QC testing
Quality Control Laboratories are responsible for ensuring all received raw materials conform to specification	QC Scientists utilize a range of analytical techniques to confirm the ID and purity of raw materials prior to formulation	Formulation Scientists design, prepare and test the formulations in iterative processes to develop new and improved products	Finished products are passed back to QC Scientists to perform batch release tests before release to market



Chemical Manufacturing Workflow – Current Analytical Technologies

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Receive Raw Materials → Verify Raw Materials → Formulate → Verify Formulation Batch QC testing

Identity & Purity Tests

In Process Monitoring
Prototype performance testing

Batch Release Testing

FTIR / UV Spec: time consuming sample prep, ambiguous results, no mass info

consuming, operator variability

LC / GC-MS: expensive, long analysis time, long queue

PAT: expensive to implement, requires expert operators

require expensive bespoke equipment

FTIR / UV Spec: time consuming sample prep, ambiguous results, no mass info

Requires specialist operators

LC / GC-MS: expensive, long analysis time, long queue

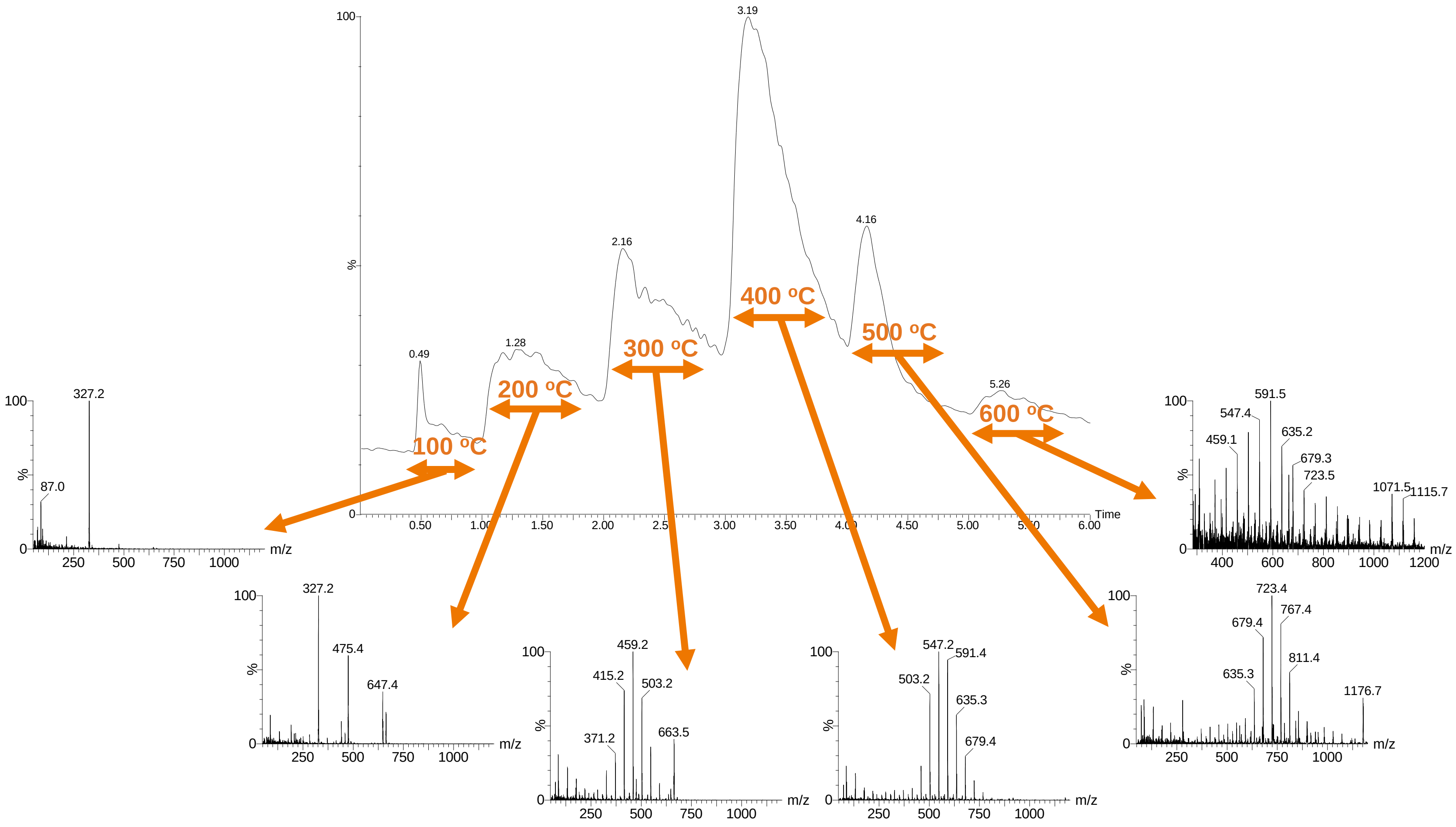
RADIAN ASAP: fast, rich mass spectral data for rapid decision making

Chemicals and Materials – Raw Material Authenticity

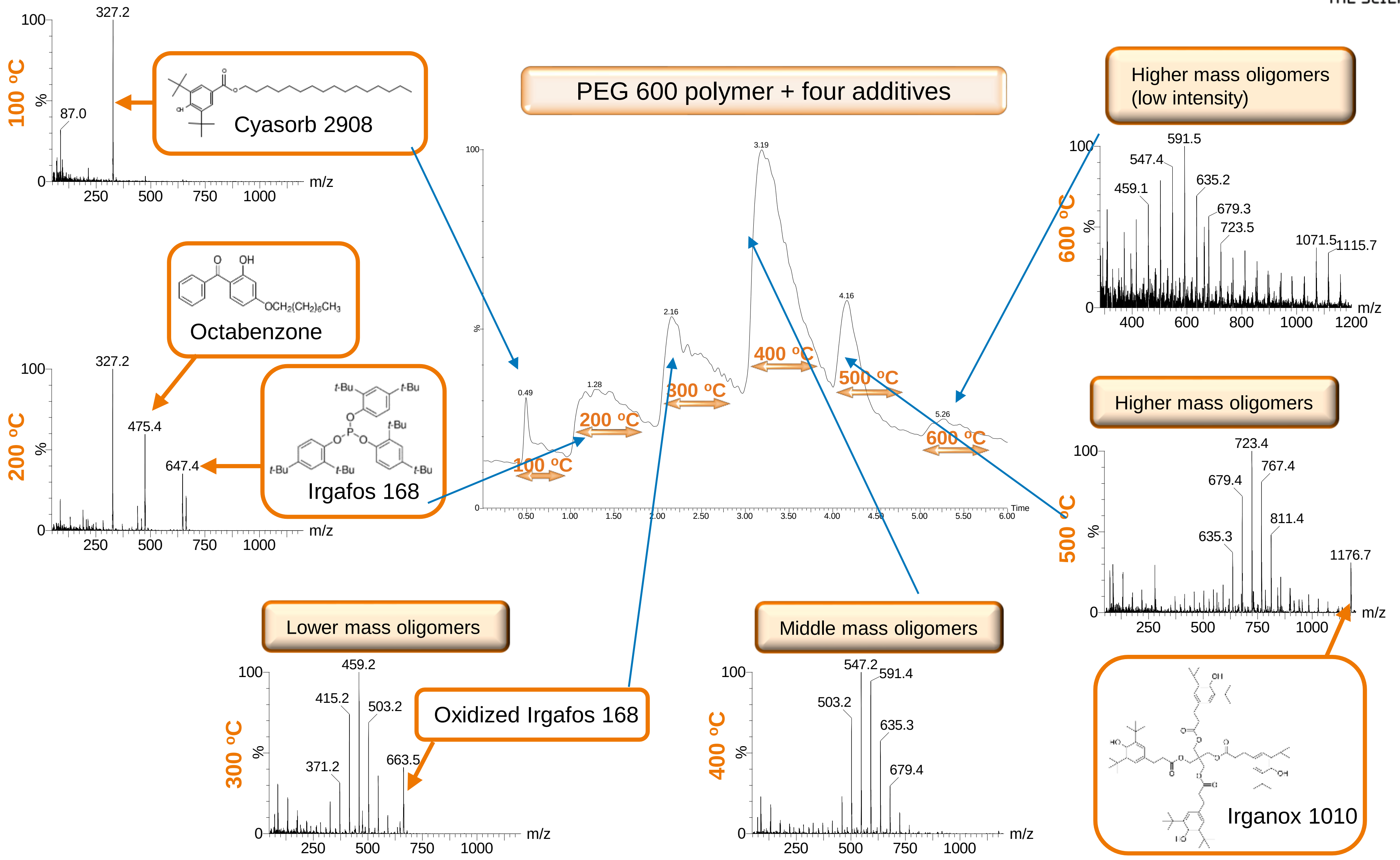
Temperature ramping as a tool for separation

- Temperature ramp separates compounds based upon boiling point
- Different spectra at different temperatures
- Basic deconvolution of complex samples

PEG 600 polymer + four additives



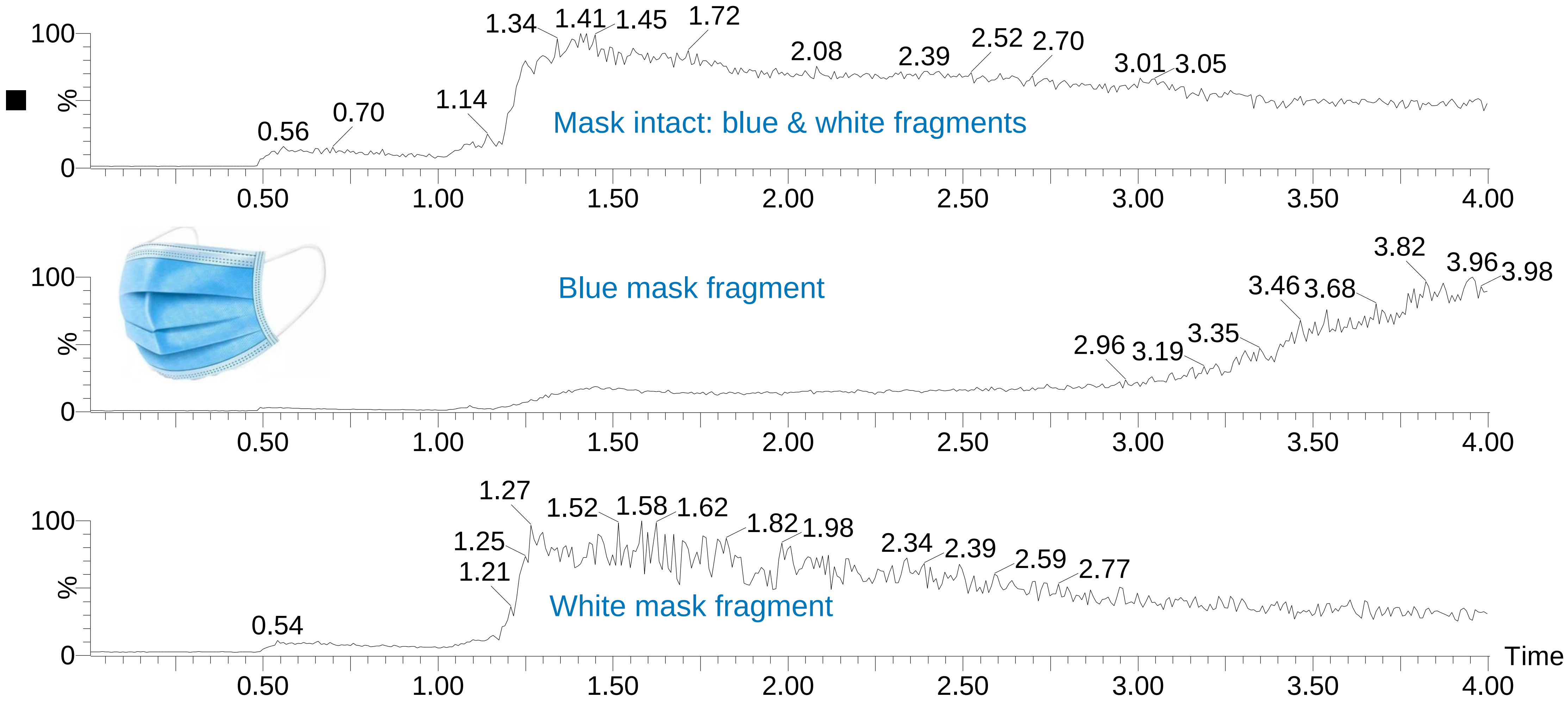
Rapid Analysis of Raw Polymeric Materials



Example applications: Face masks analysis

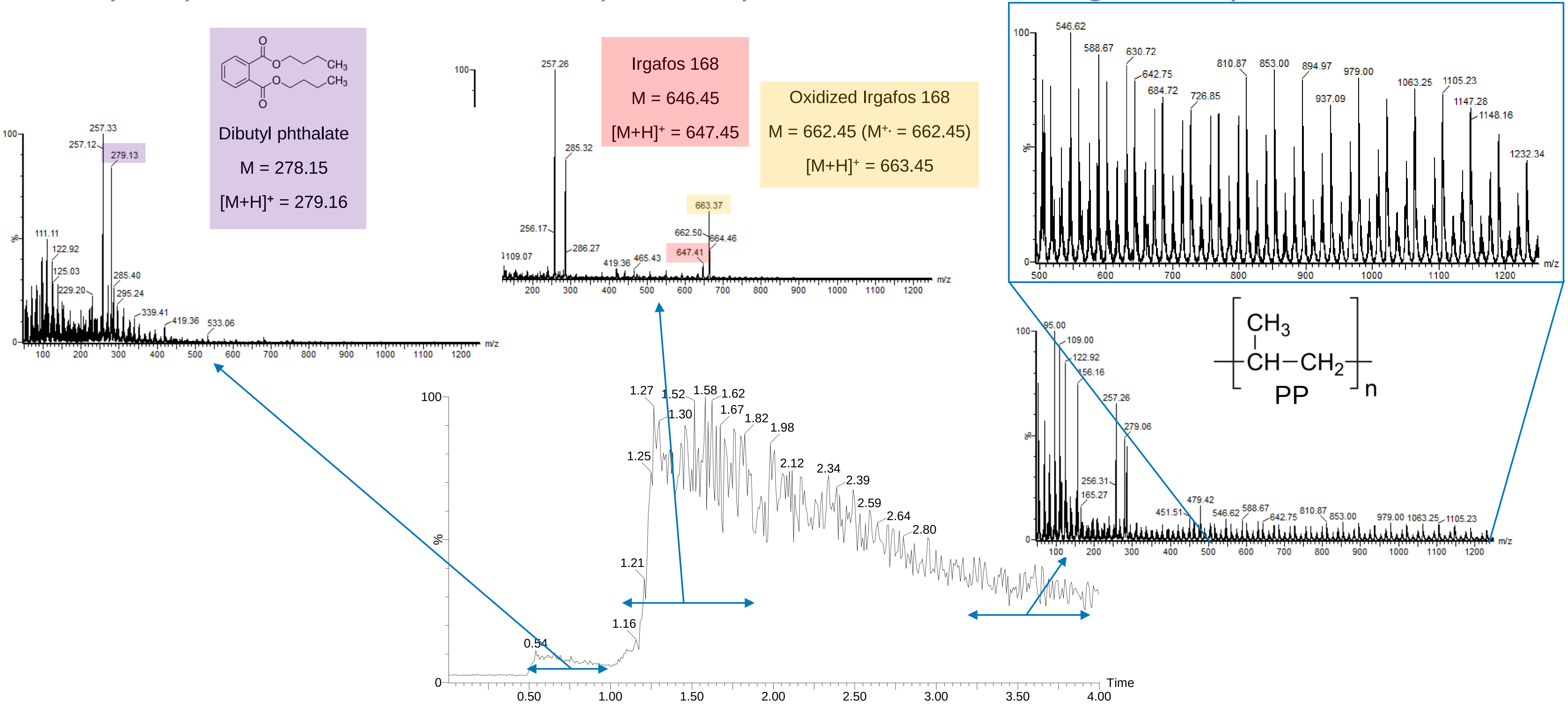
Manufactured Mask Sample

TIC for the white part, the blue part, and both parts together in positive ion mode



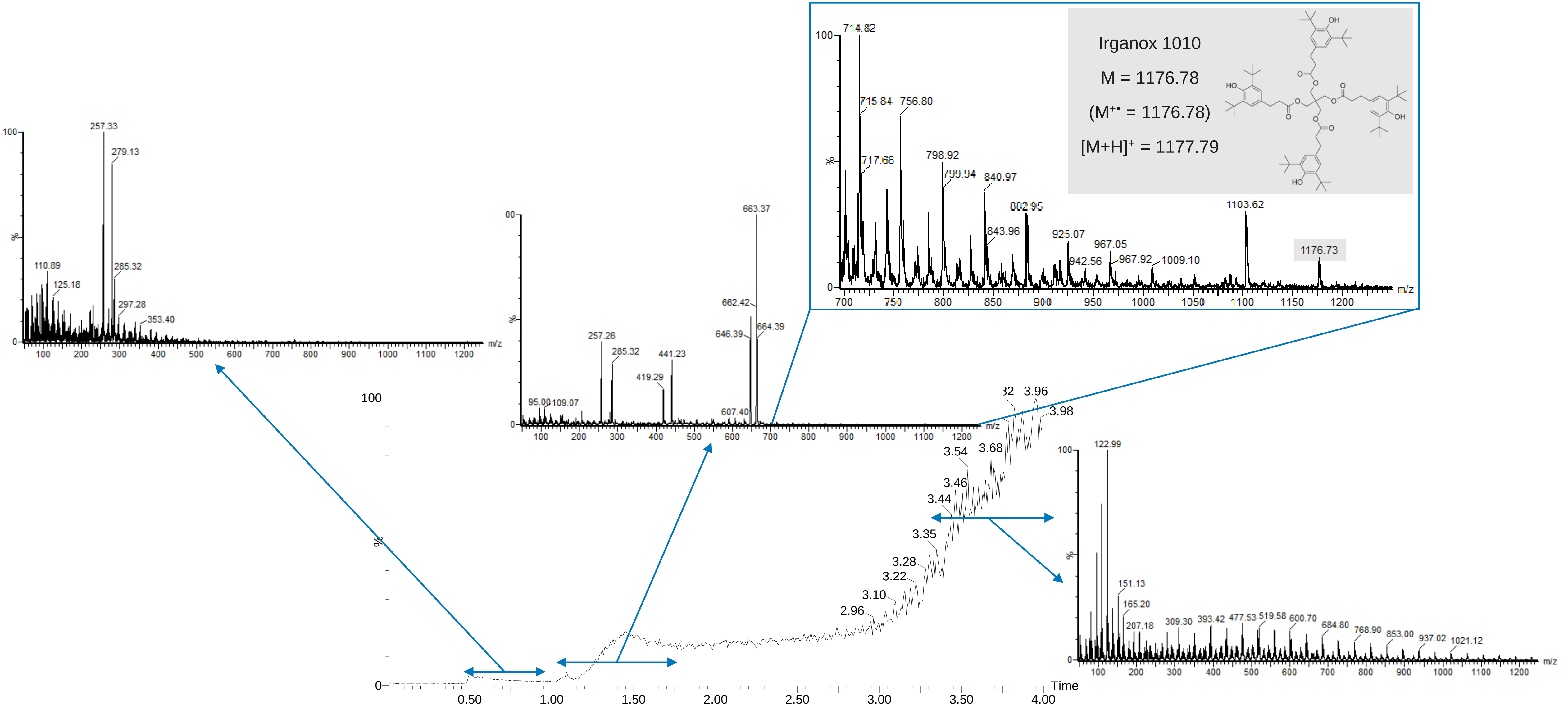
Results & Discussion: Manufactured Mask Sample

Example spectra at different time/temperature points for the white fragment in positive ion mode



Results & Discussion: Manufactured Mask Sample

Example spectra at different time/temperature points for the blue fragment in positive ion mode



Summary

- Compact, easy to use direct sampling mass detector
- Minimal need for training and system preparation, suitable for non-MS experts
- Rich mass spectral data obtained in as little as 30 seconds enables rapid decision making and increased workflow efficiency