

RESEARCH WEEK 2020

A Tour of the Mass Spectrometry Facility



Dr. Stefana Egli

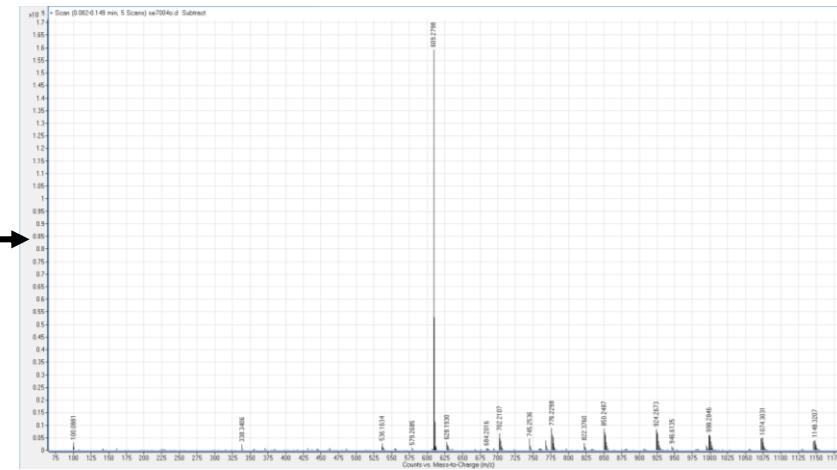
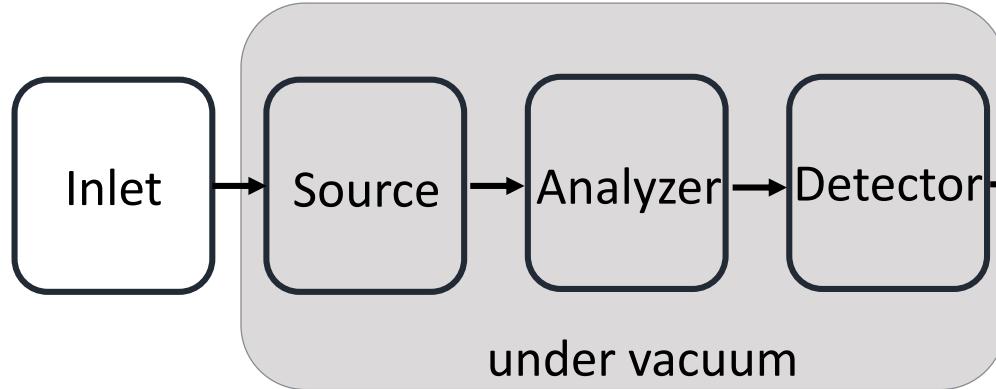
Research Laboratory Coordinator II, CCART, CREATI
Adjunct Professor in Chemistry



- Training (data acquisition and processing)
- Assistance with method optimization
- Support and collaboration in research projects
- Maintenance and troubleshooting of equipment
- Assistance with major equipment acquisition
- Service analysis

Mass Spectrometry

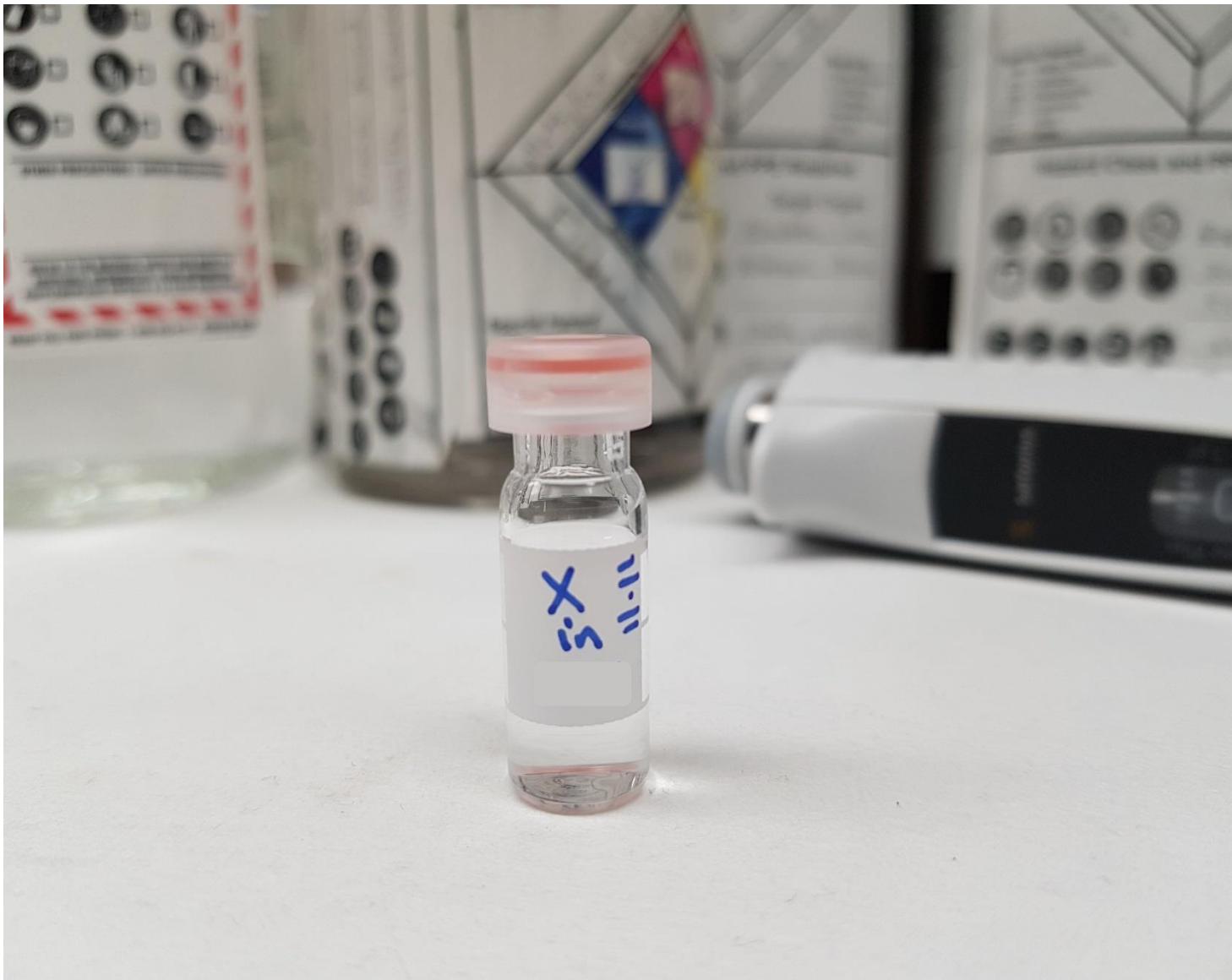
- Chemical compounds converted into gaseous ions (with or without fragmentation) are ordered based on their mass to charge ratios and relative abundance



- Quantification of known compounds
- Mass confirmation of (synthesis) compounds
- Structure elucidation
- Chemical properties determination (polymers!)



- Agilent 6890 GC - 5973 MS EI (quadrupole)
- Agilent 7890 GC - 5975 MSD EI/CI (quadrupole)
- Agilent 1260 HPLC - UV/DAD - 6230 MS (TOF)
- Agilent 1290 UHPLC-UV/DAD - Sciex 5600 TripleTOF (qTOF)
- Bruker ultrafleXtreme MALDI TOF TOF
- Agilent 7100 CE-UV



Analyze a group of compounds in a relatively unknown sample

Scenario 1

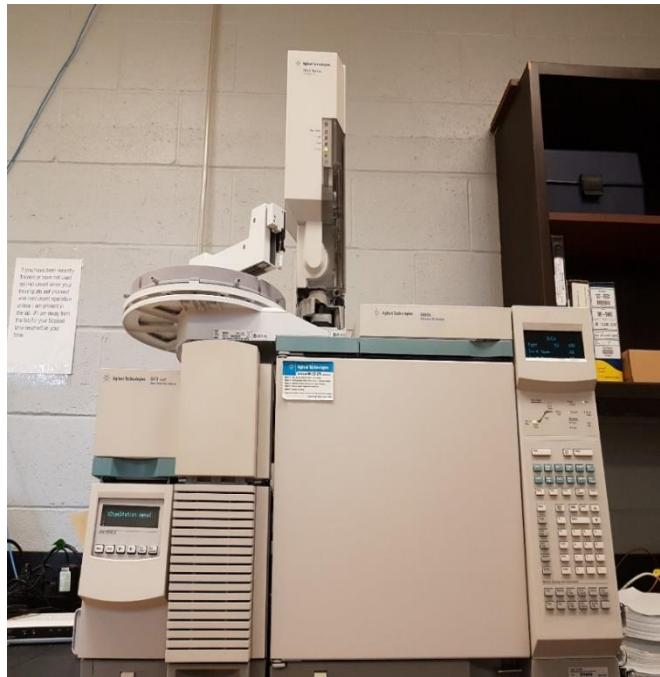
Volatile or semi-volatile compounds



C-CART Options:

Gas Chromatography - Mass Spectrometry

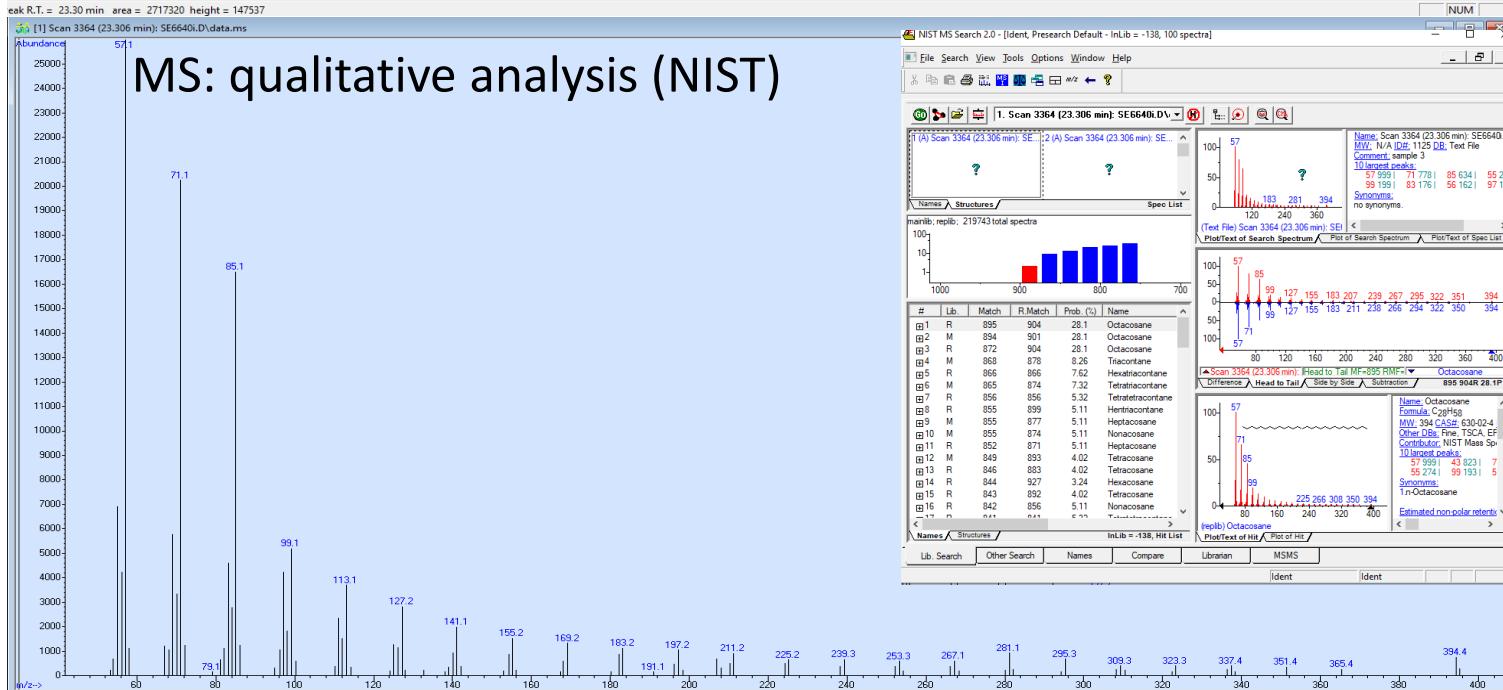
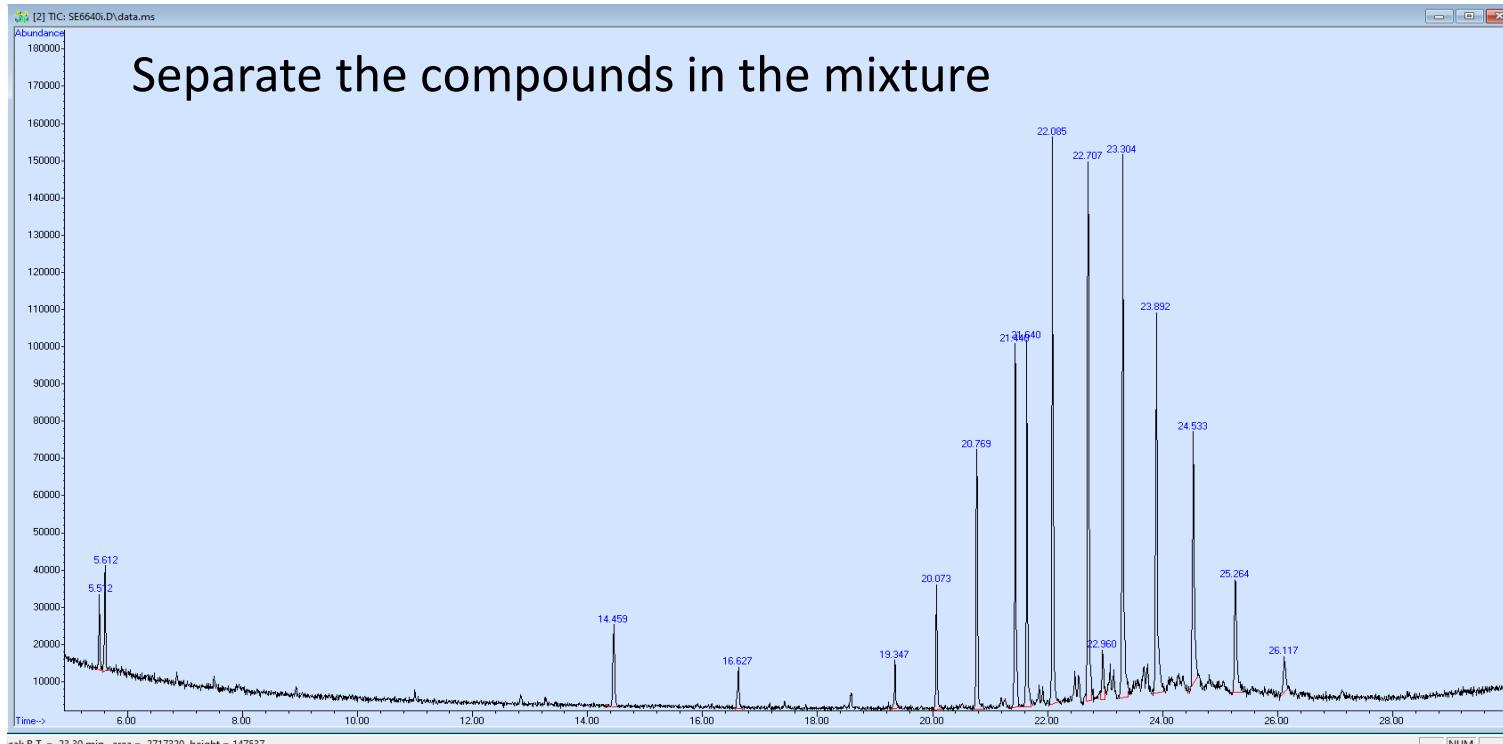
Agilent 6890 GC-MS EI



Agilent 7890 GC-MS EI/CI



- Split/splitless injector with auto sampler (100-vial tray)
- Separation (DB-5MS, ZB-5MS plus, ZB-WAX plus, VF 23-ms)
- MS analysis: 1.6 – 800/1050 Da
- EI and CI sources
- Qualitative analysis (access to NIST library) - SCAN
- Quantitative analysis - SIM



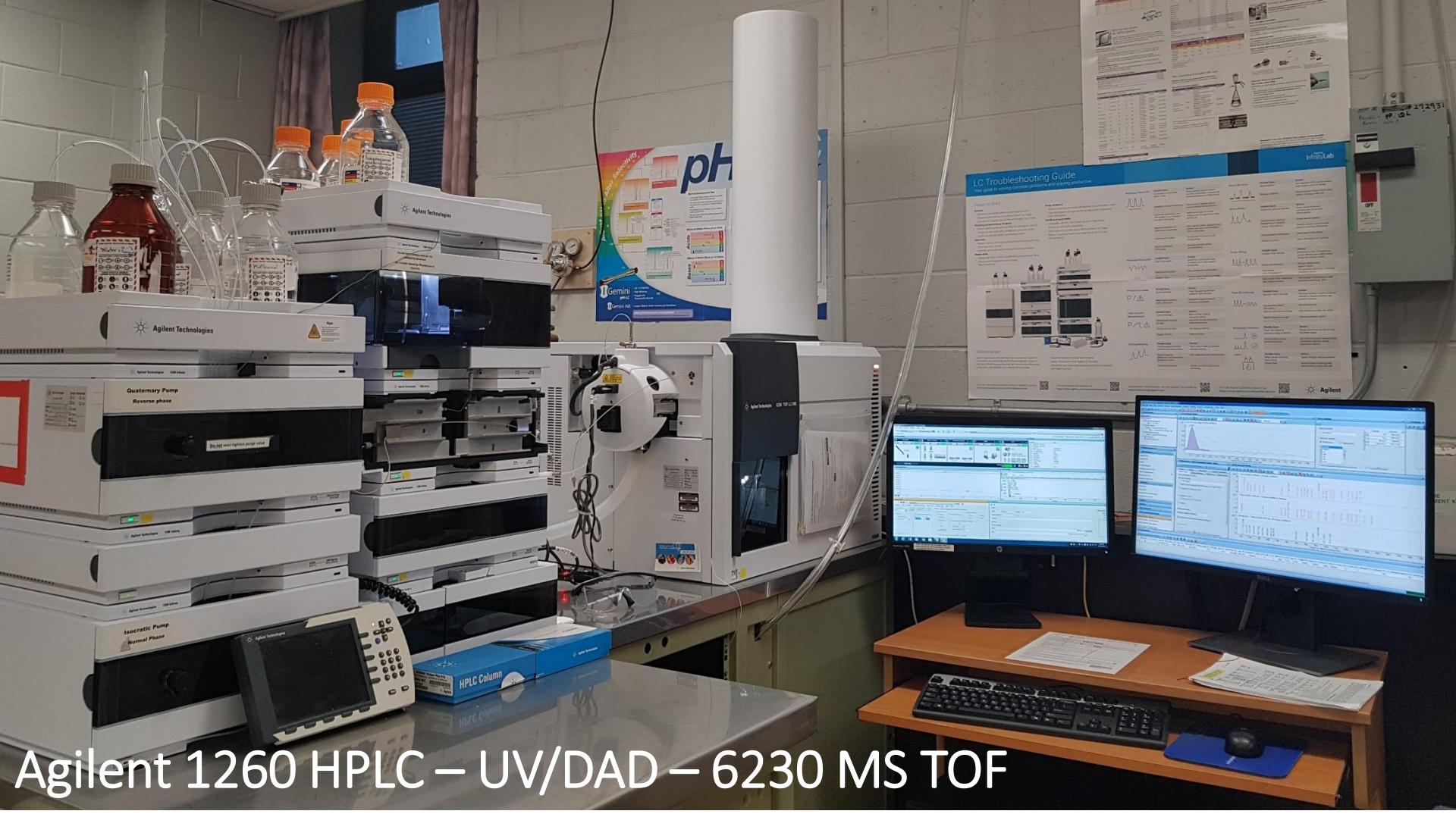
Scenario 2

Aqueous sample containing non-volatile compounds



C-CART Options:

LC-UV-MS (TOF) and LC-UV-MS/MS (qTOF)

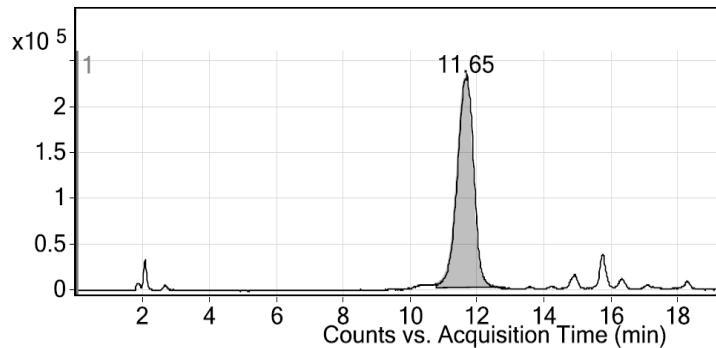


Agilent 1260 HPLC – UV/DAD – 6230 MS TOF

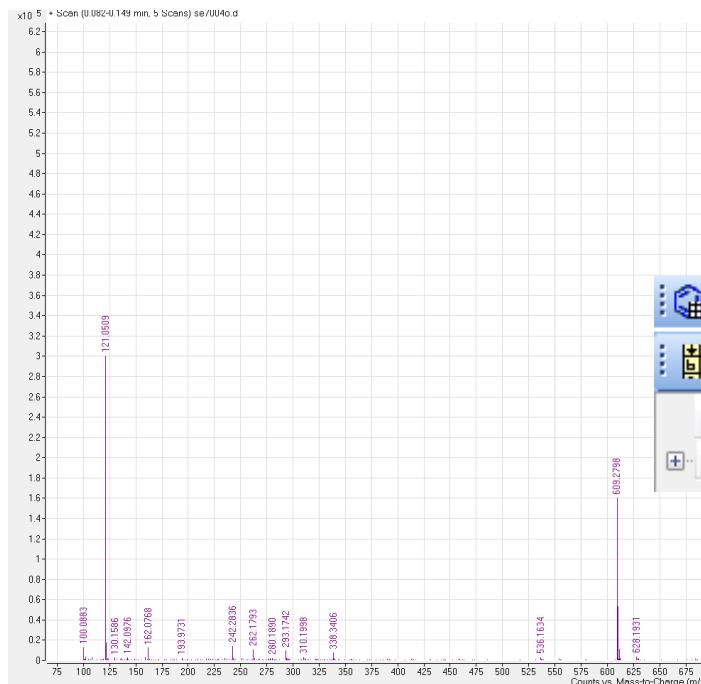
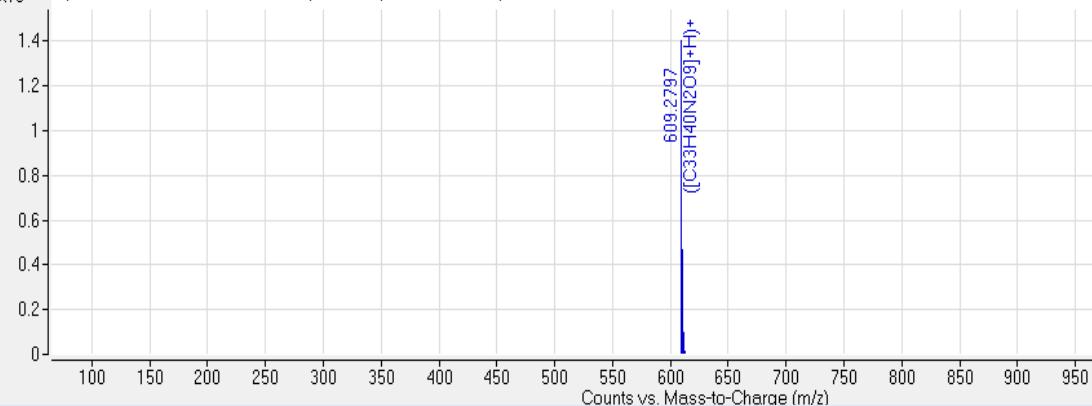
- Separation (a few columns available)
- UV-VIS diode array detector (wavelength range 190 – 600 nm)
- ESI and APPI ionization sources
- High resolution MS (up to 15,000)
- Mass range: 50 - 3200 m/z

User Chromatograms

Fragmentor Voltage 175 Collision Energy 0 Ionization Mode ESI



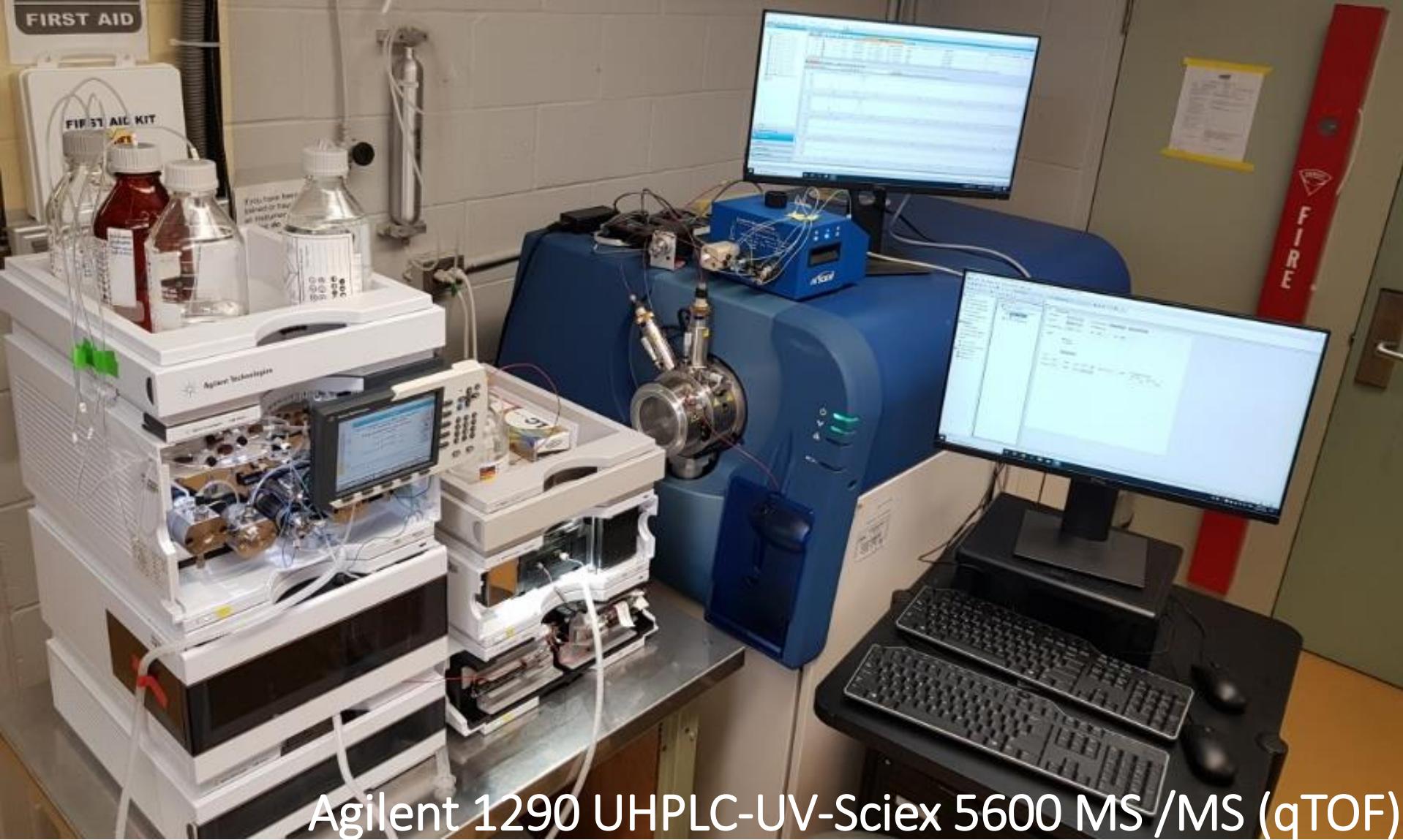
x10⁵ Cpd 1: C₃₃ H₄₀ N₂ O₉: + FBF Spectrum (0.082-0.165 min) se7004o.d Subtract



Compound List

Automatically Show Columns	Cpd	Formula	Score	Mass	Mass (Tgt)	Diff (Tgt. ppm)
<input checked="" type="checkbox"/>	1	C ₃₃ H ₄₀ N ₂ O ₉	95.89	608.27229	608.27338	-1.79

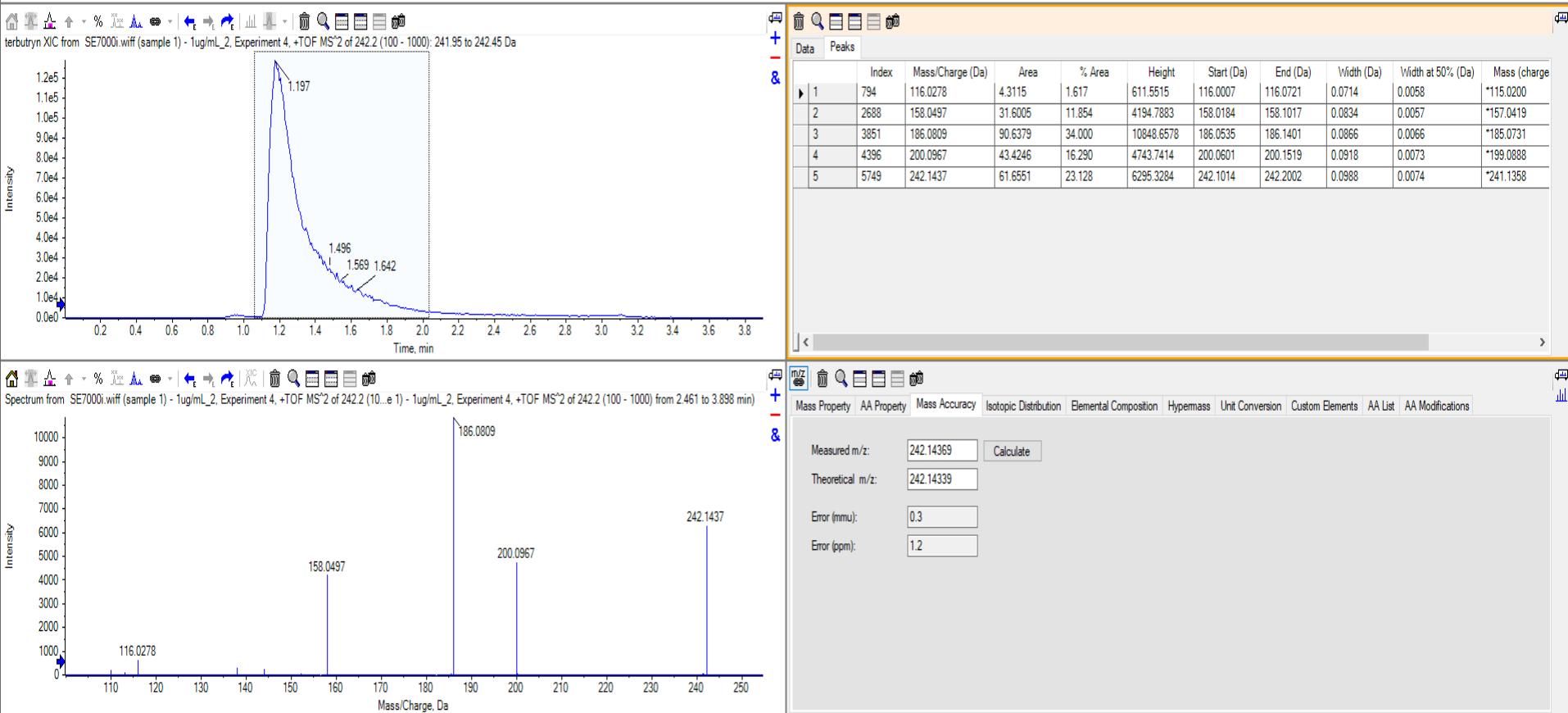
- Chromatographically separate the compounds in the mixture
- Confirm the mass of compounds
- Show fragmentation pattern



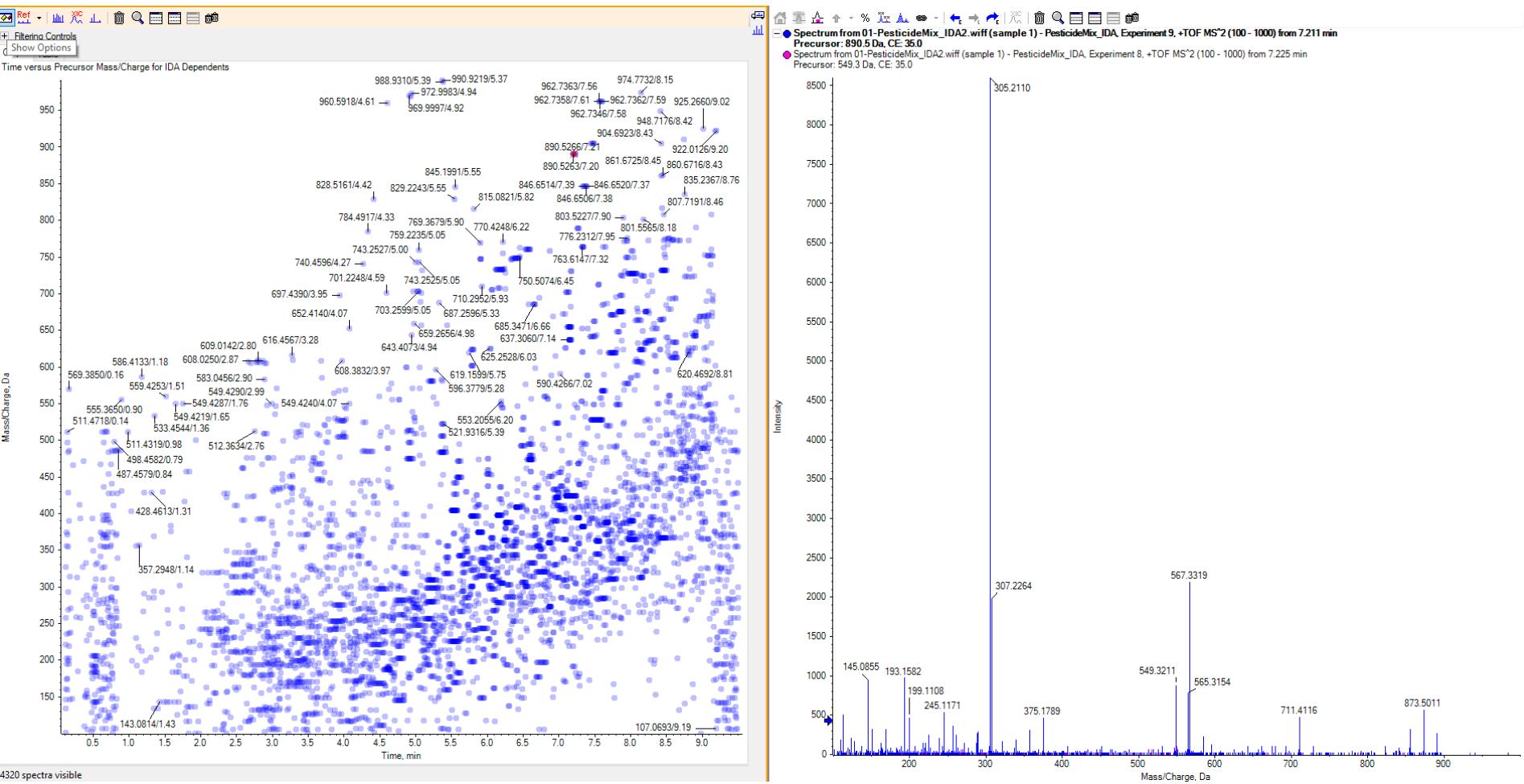
Agilent 1290 UHPLC-UV-Sciex 5600 MS /MS (qTOF)

- Superior mass range
- Targeted and untargeted mass analysis

- ESI and APCI ionization
- Data mass accuracy for compounds up to 40,000 Da
- High resolution (up to 35,000)
- MS and MS/MS (Product Ion) experiments

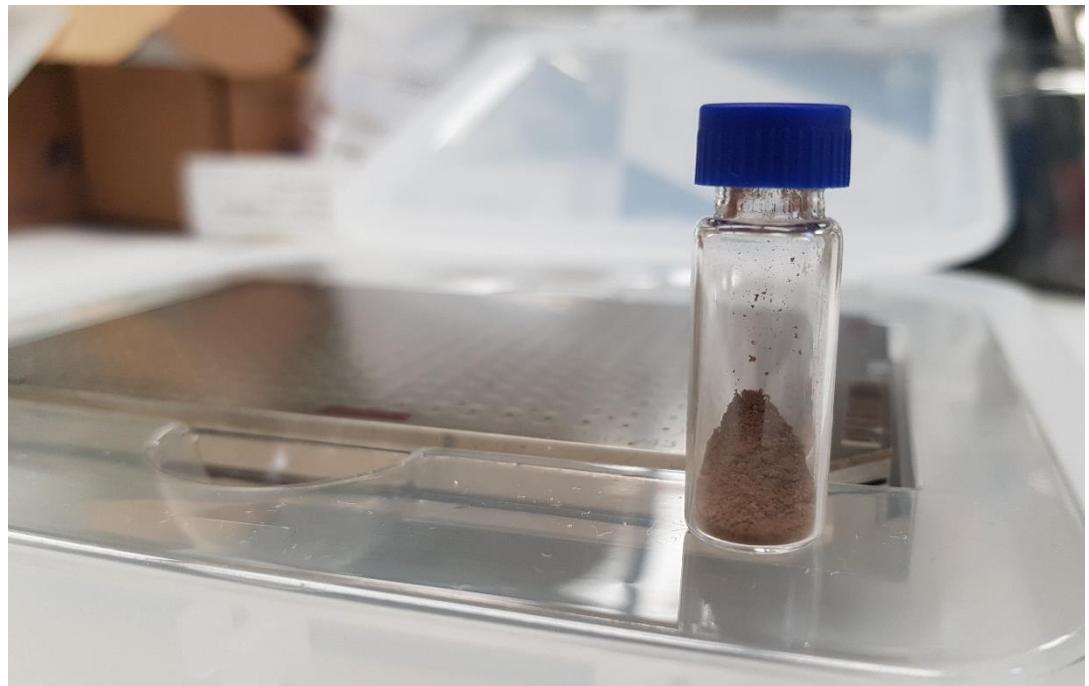


- A highly complex sample
- Information dependent acquisition (IDA)
- Sequential window acquisition of all theoretical fragment ion spectra (SWATH)



Scenario 3

High molecular mass compound



C-CART Option:

MALDI TOF-TOF

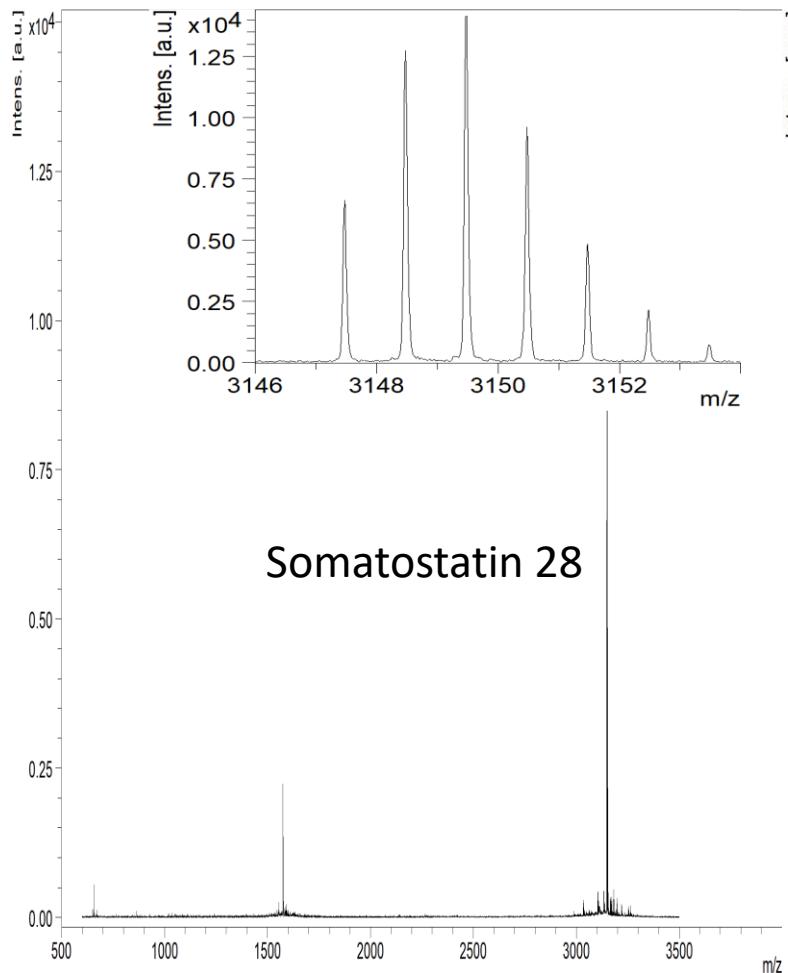
Bruker ultrafleXtreme MALDI TOF TOF



- Rapid top-down sequence confirmation of biopharmaceuticals
- Direct mass determination of very high molecular species
- Mass range up to 500 kDa

Reflector mode

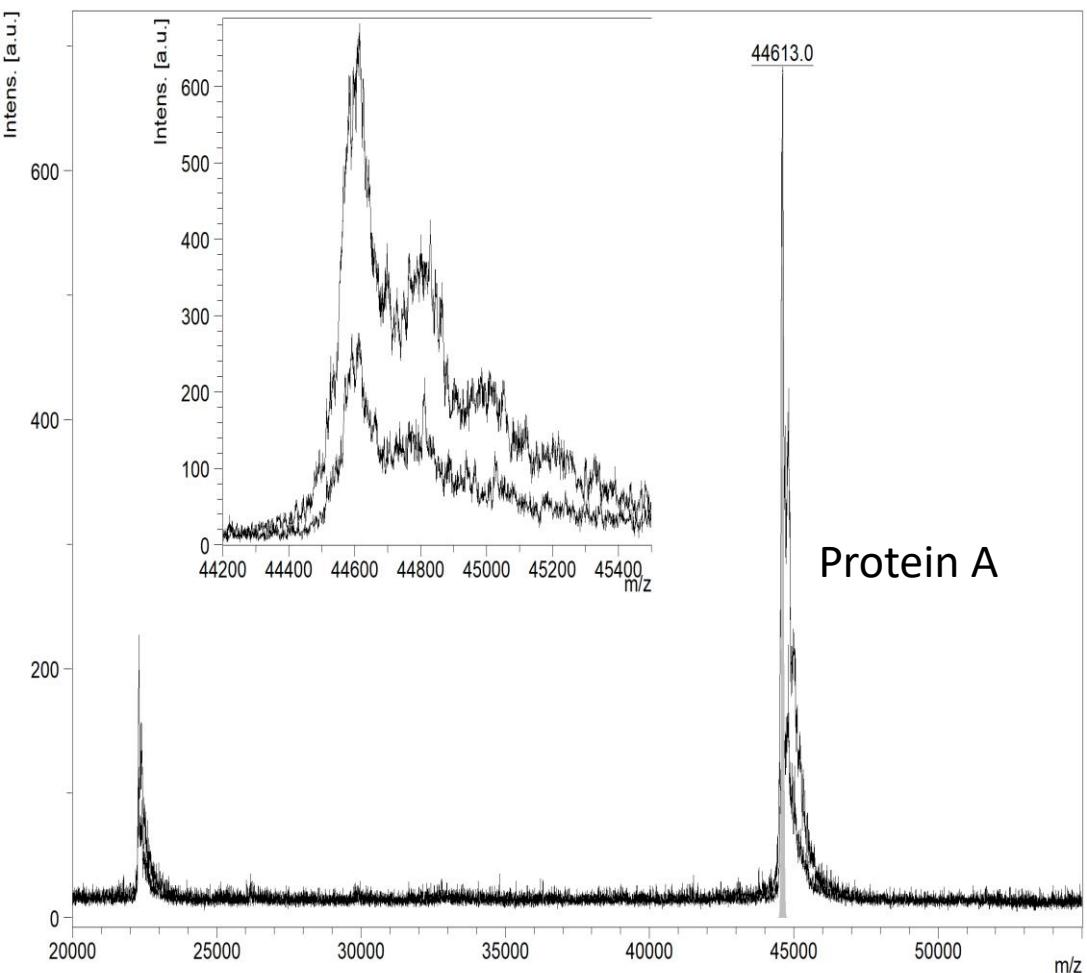
- Mass 3,147.474 Da
- Resolution: 45,000



Somatostatin 28

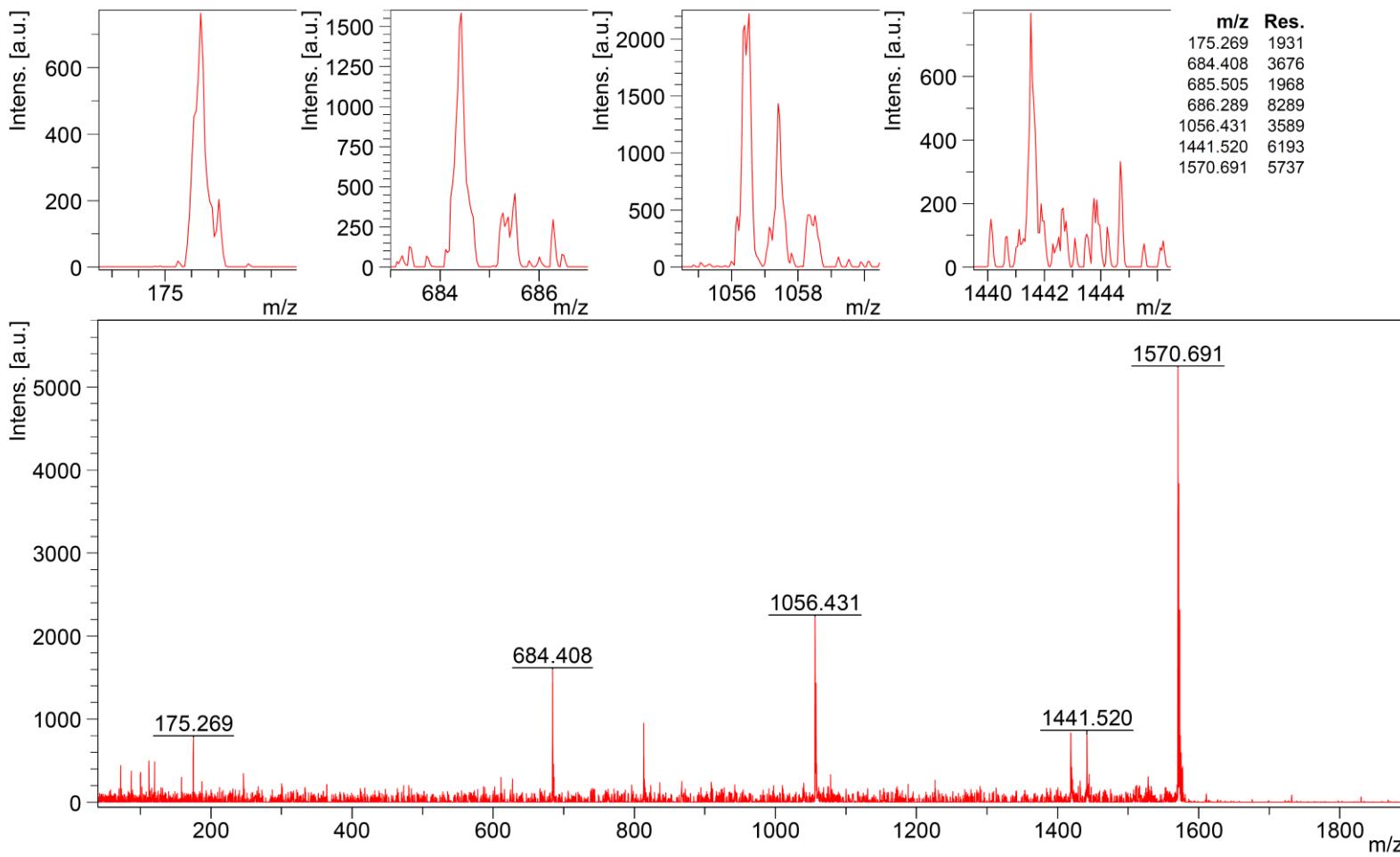
Linear mode

- Mass 44,613.0 Da
- Resolution: 516

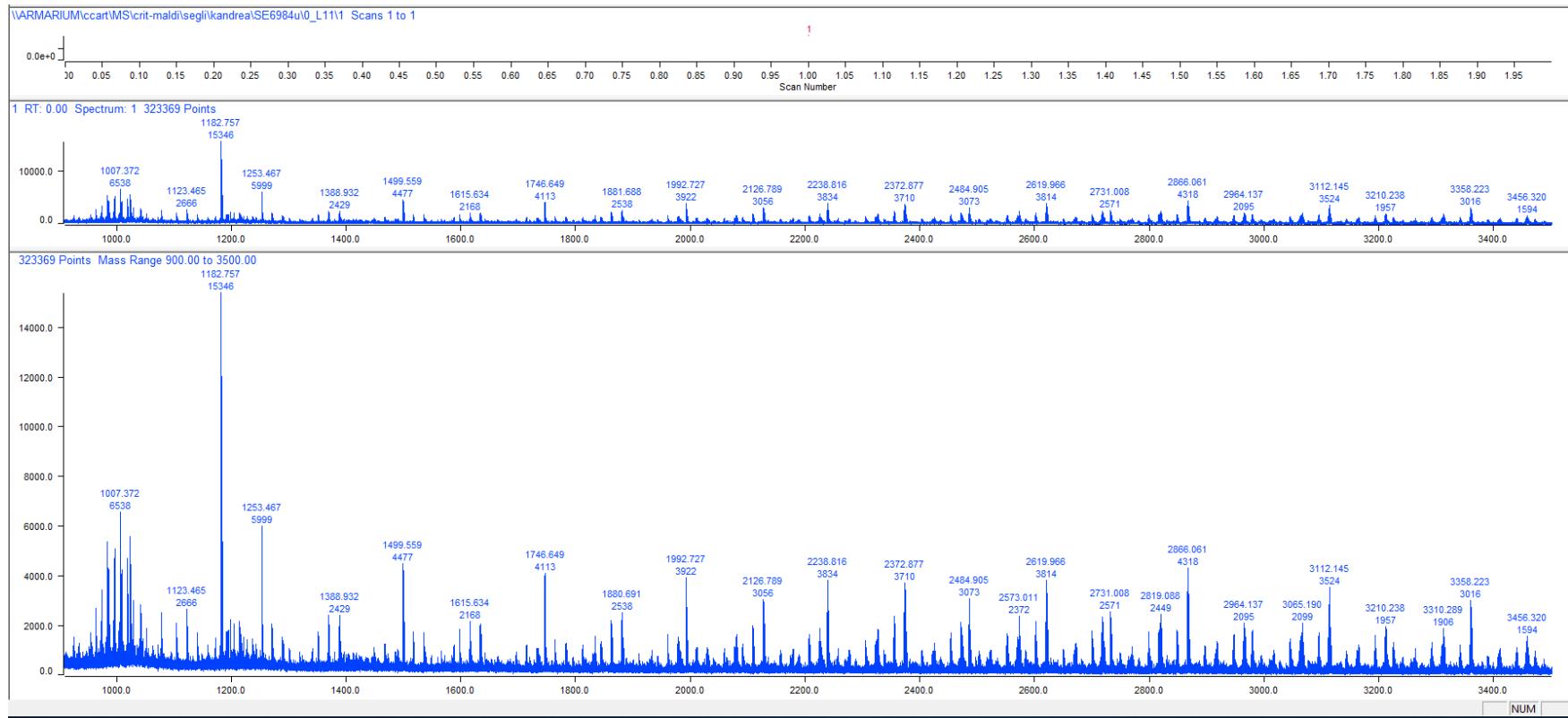


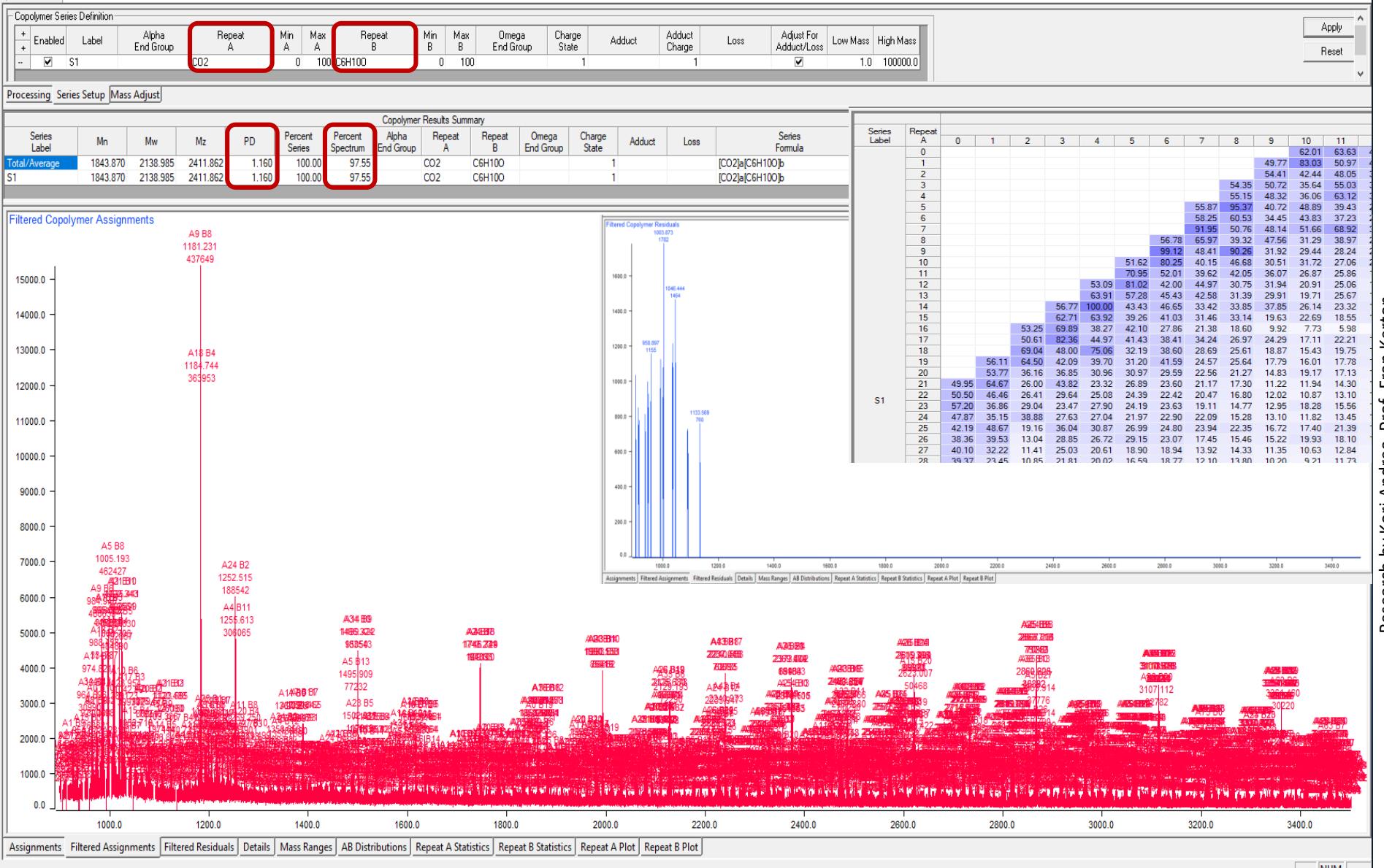
Protein A

- MS/MS (LIFT technique)
- Precursor 1570.691 Da
- Fragments 175.269 Da, 684.408 Da, 1056.431 Da and 1441.520 Da

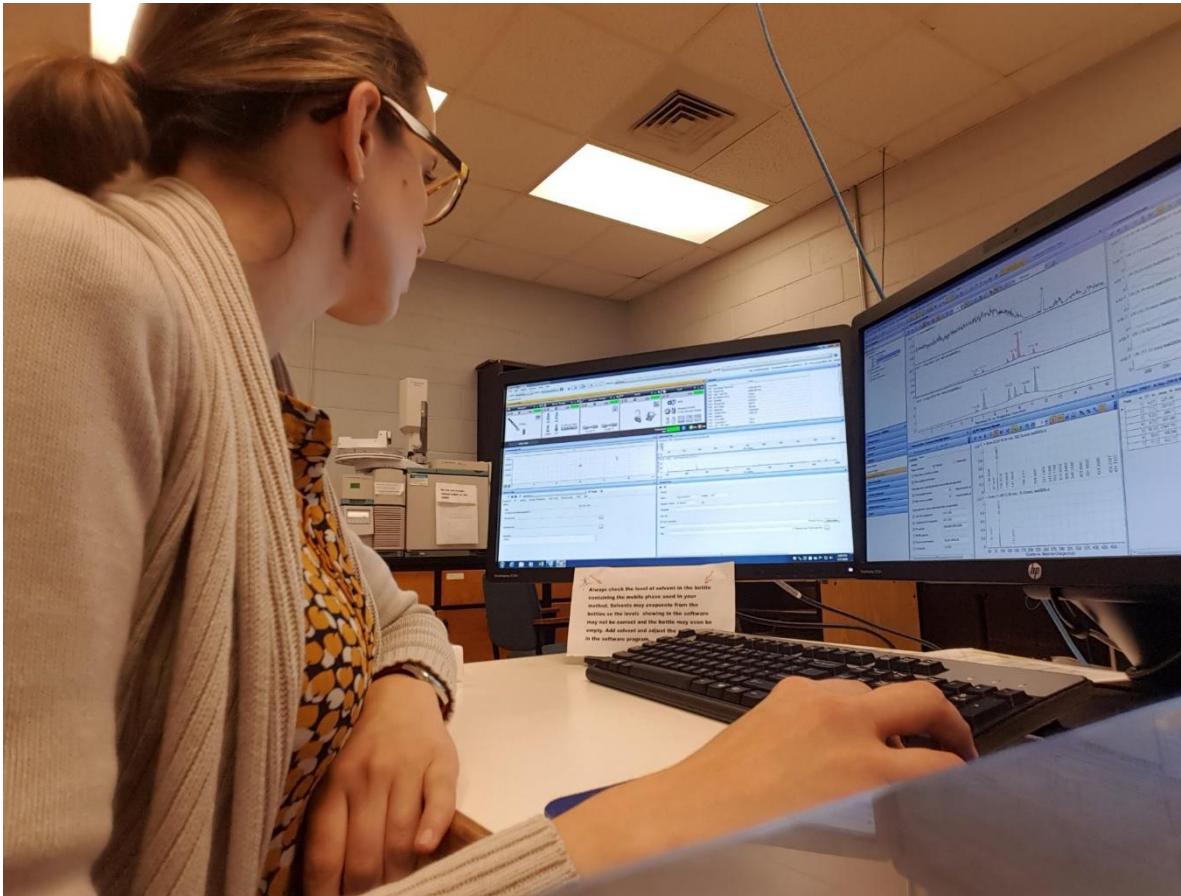


Characterization of a polymer (natural or synthetic)

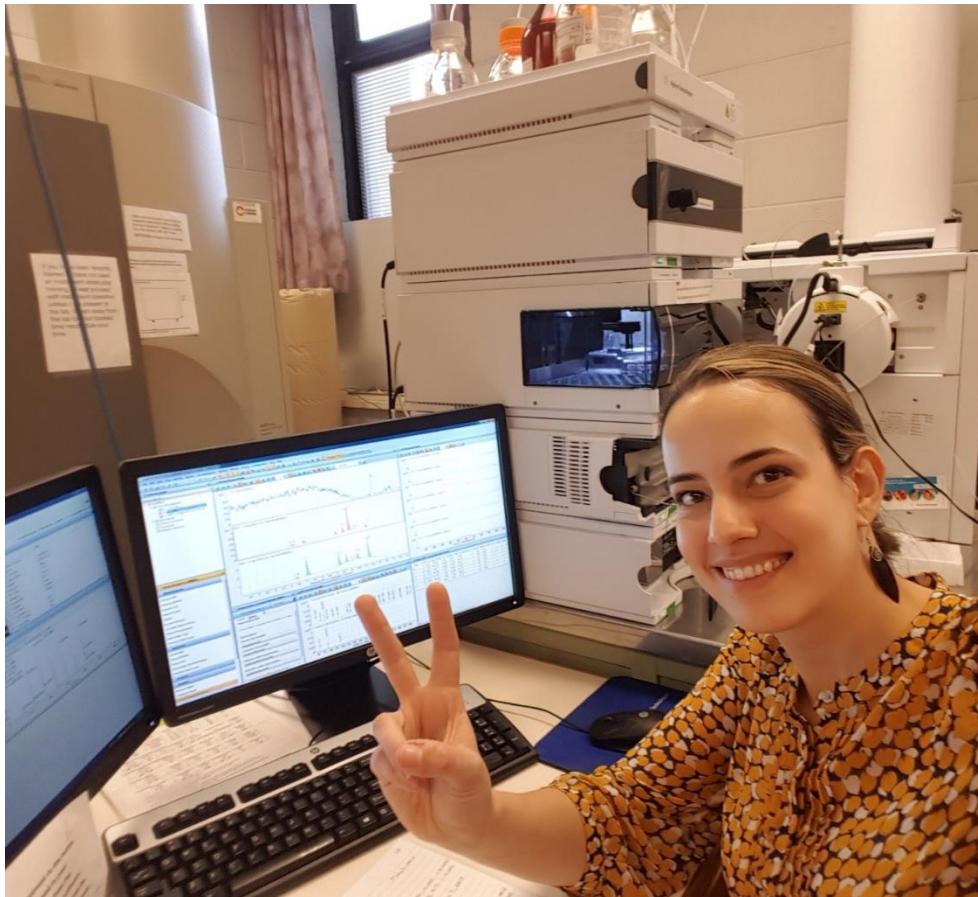




- Characterization/confirmation of copolymer subunit
- Assistance to determine the nature of the end unit
- Polydispersity determination for synthetic polymers



Access your processed data from
a shared lab computer or your own!



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