

Broad Spectrum Analysis of a Complex Hydrocarbon Mixture by Mass Spectrometry

By Bhagya Gunatilleke

Project Funded by

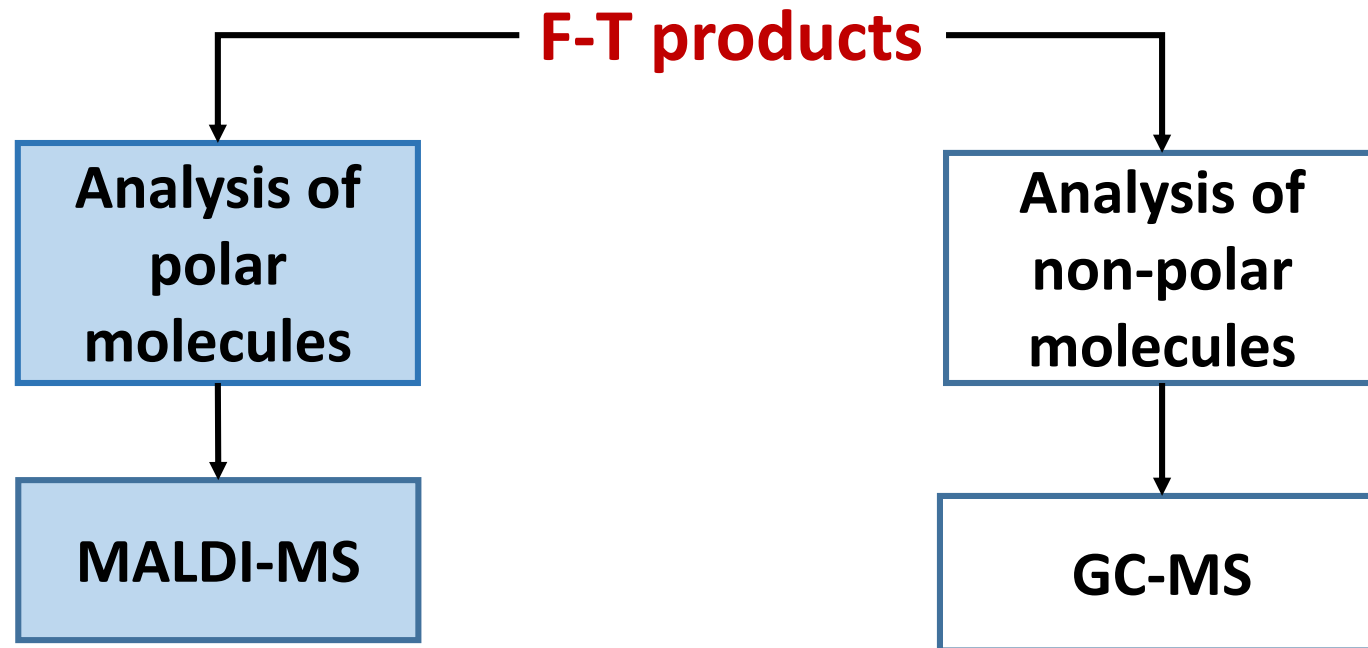
Anadarko Undergraduate Fellowships for Excellence in Energy Research

Fischer Tropsch Reaction

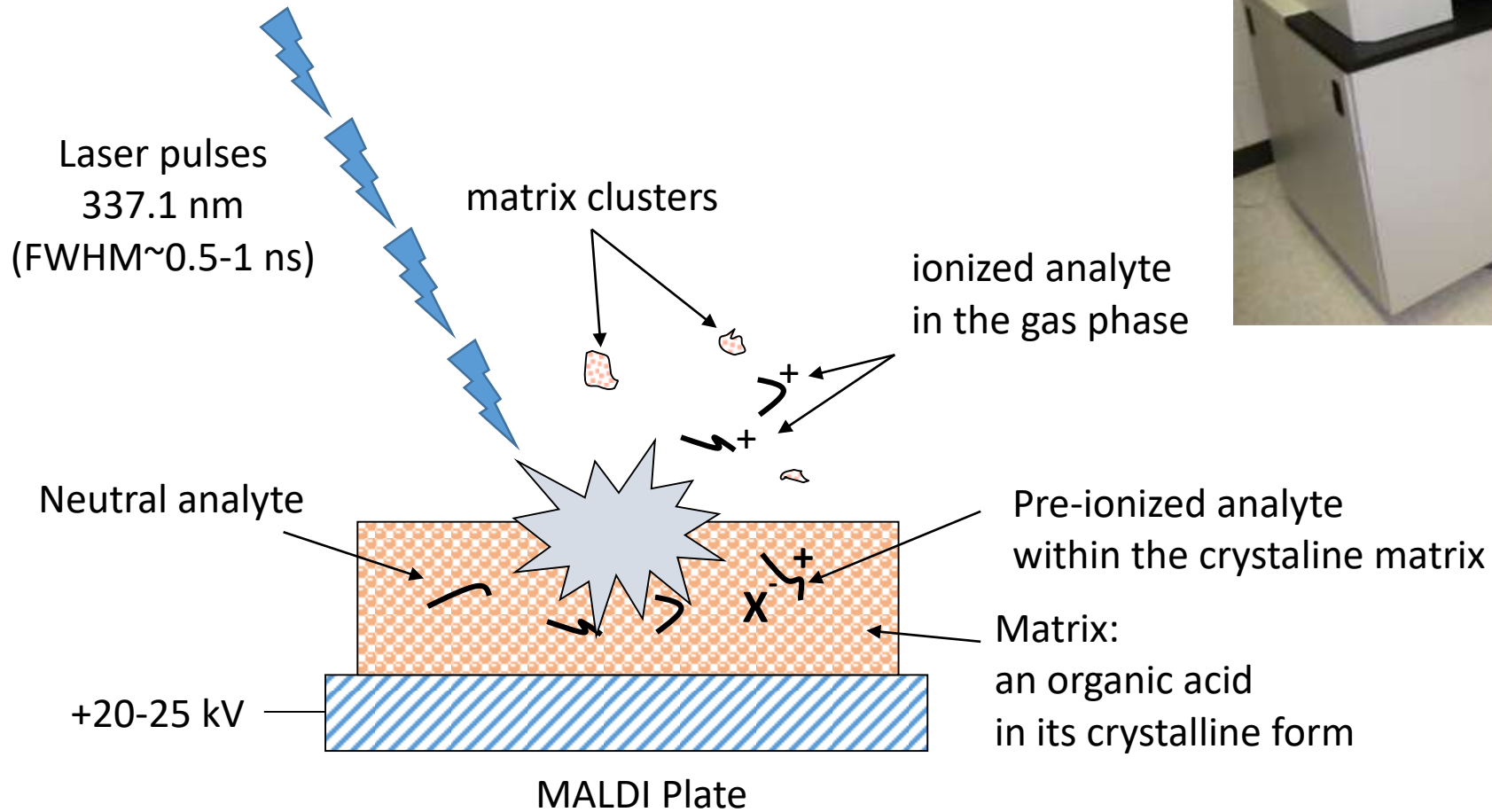
- Gas to liquids reaction
- $n \text{ CO} + (n+1) \text{ H}_2 \longrightarrow \text{C}_n \text{ H}_{(2n+2)} + n \text{ H}_2\text{O}$
- Reaction conditions : 300° C for 24 hr
- Catalyst – Co (Nano-particles)
- PVP(polyvinylpyrrolidone) as a surfactant



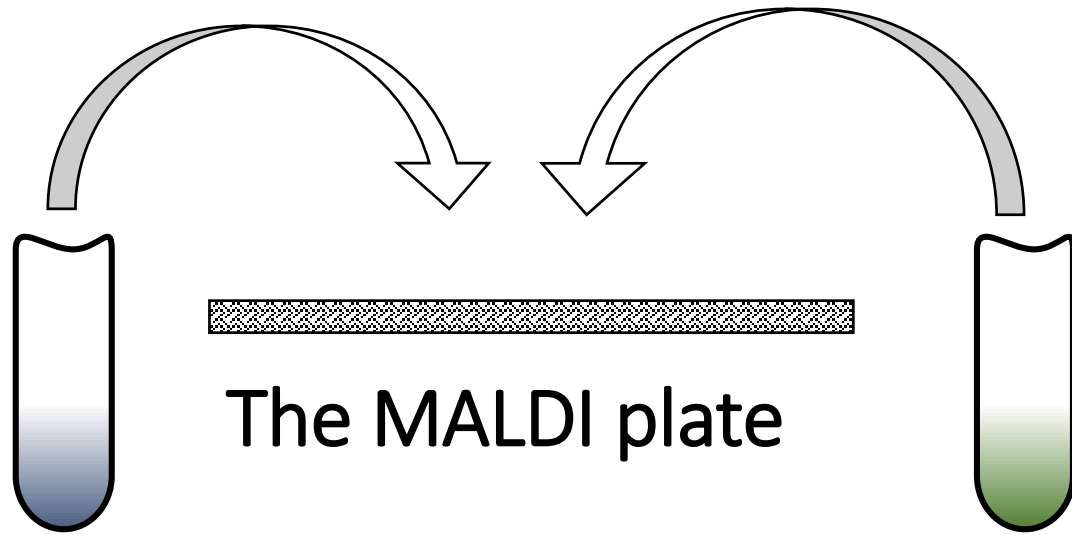
Strategy for complex sample analysis



Matrix-Assisted Laser Desorption/Ionization Mass Spectrometry (MALDI-MS)



Preparation for MALDI/MS analysis



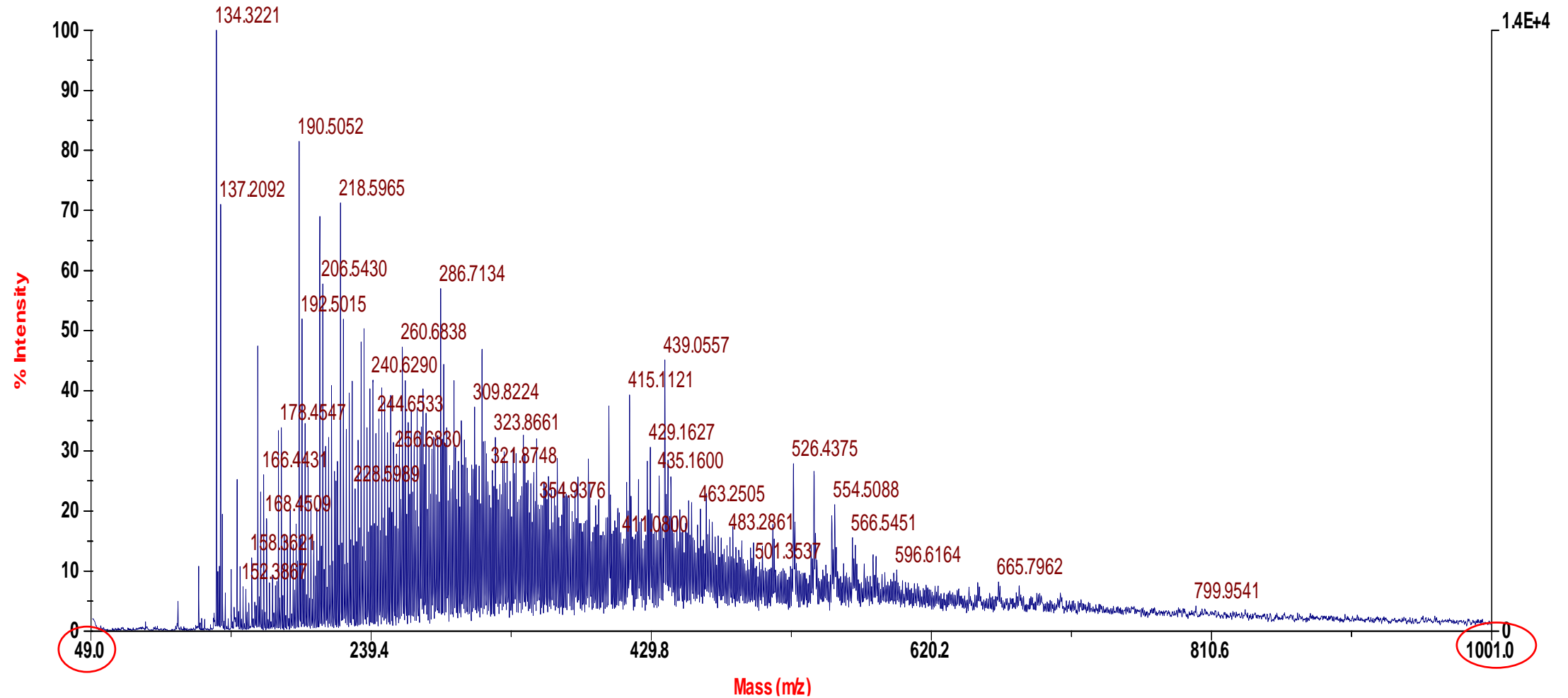
The sample

The matrix



• MALDI-MS analysis of F-T sample

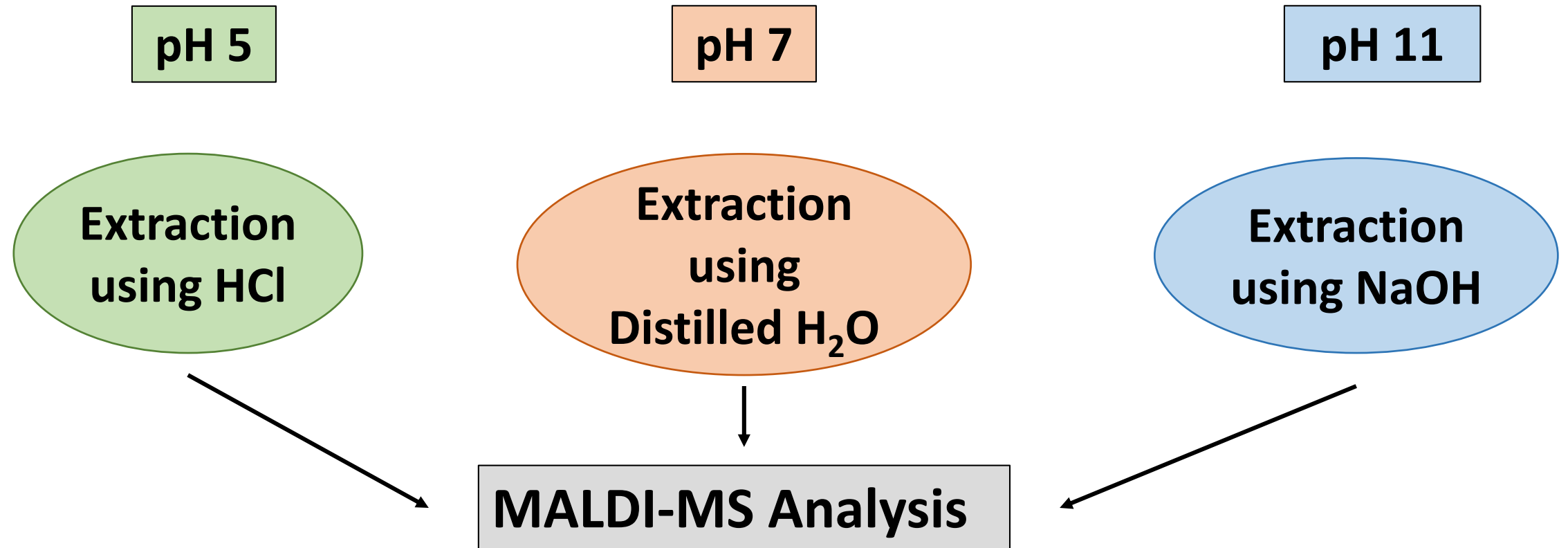
Voyager Spec #1[BP = 134.3, 13514]

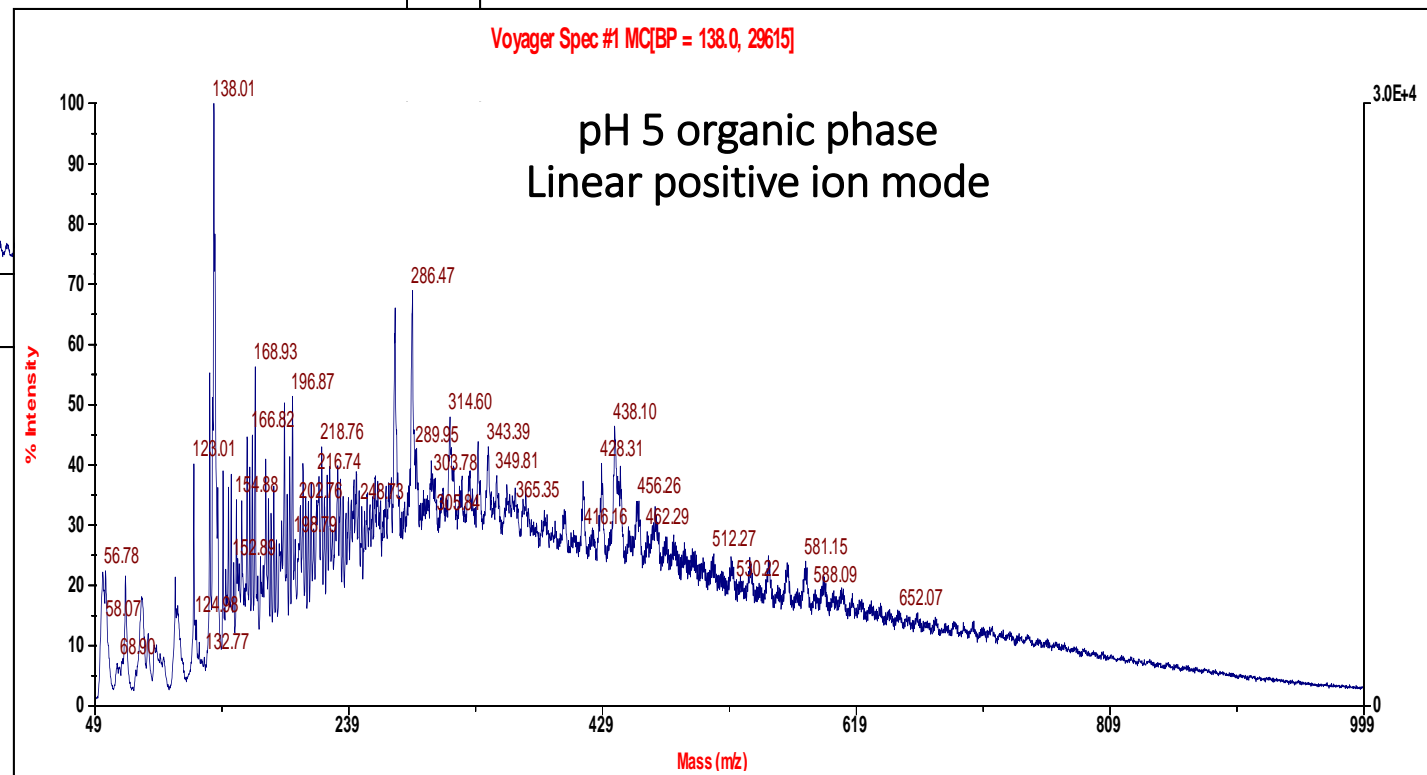
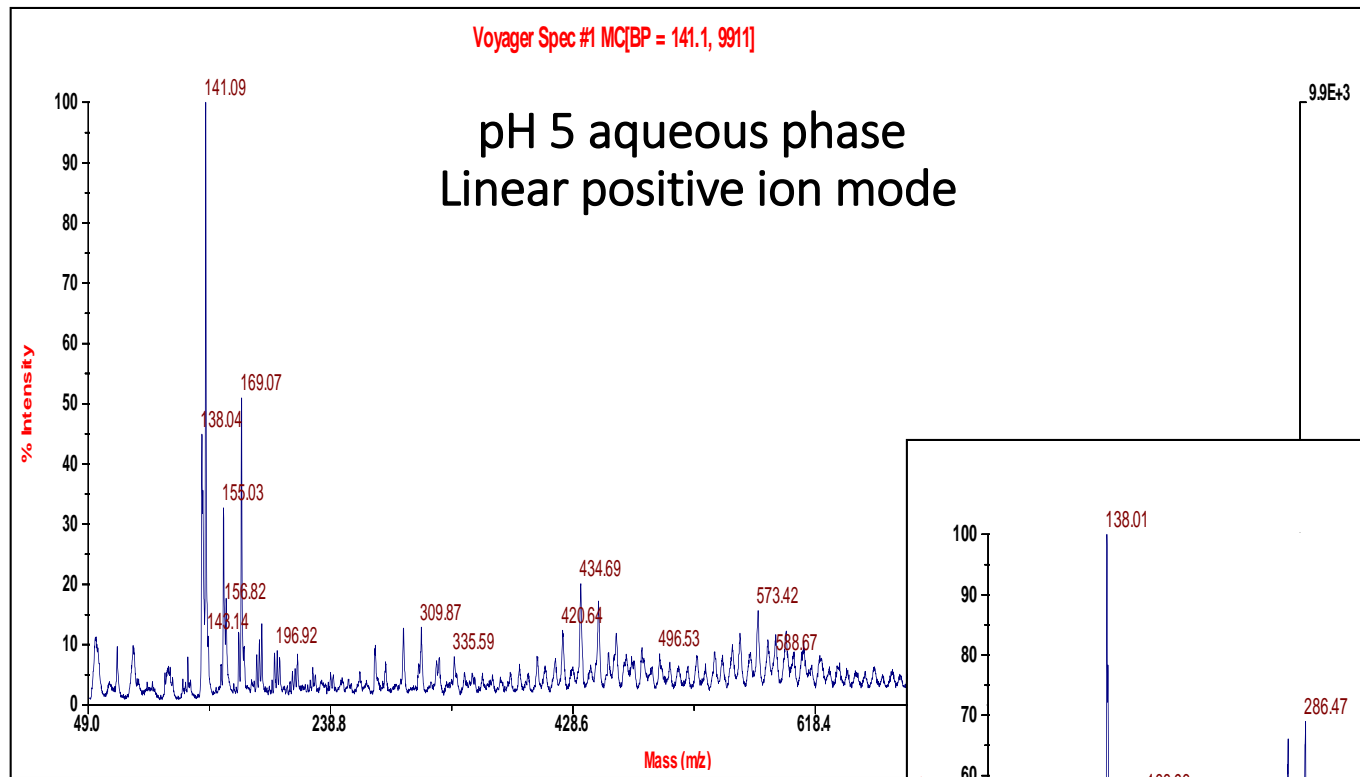


Conclusions from initial MALDI-MS analysis....

- Indicates highly complex mixture of low MW polar compounds
- These polar compounds may have acid/base behavior

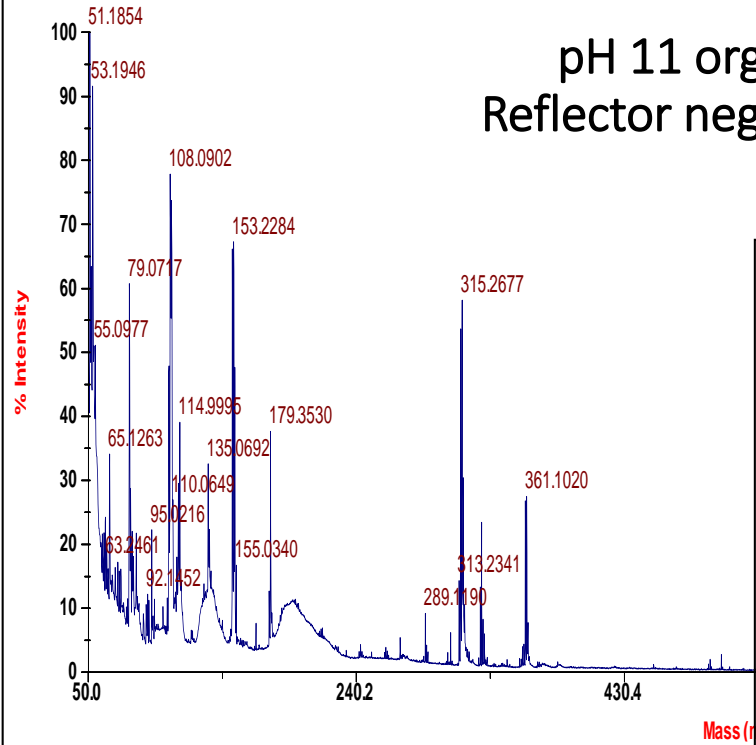
Analysis of acidic and basic compounds in the F-T mixture: Extraction using HCl & NaOH





Voyager Spec #1 MC[BP = 51.1, 49420]

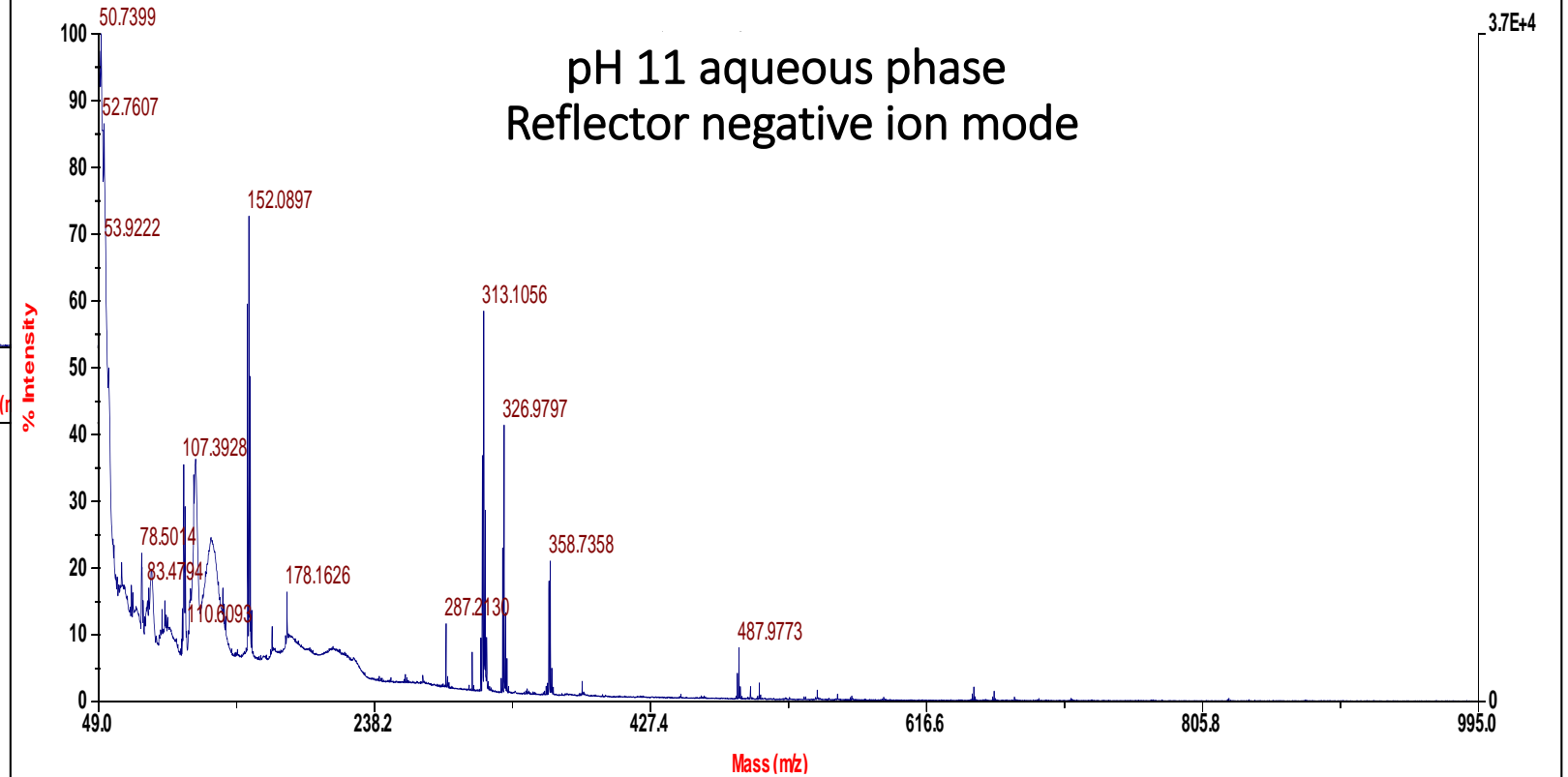
pH 11 organic phase Reflector negative ion mode



4.9E+4

Voyager Spec #1 MC[BP = 50.7, 37320]

pH 11 aqueous phase Reflector negative ion mode

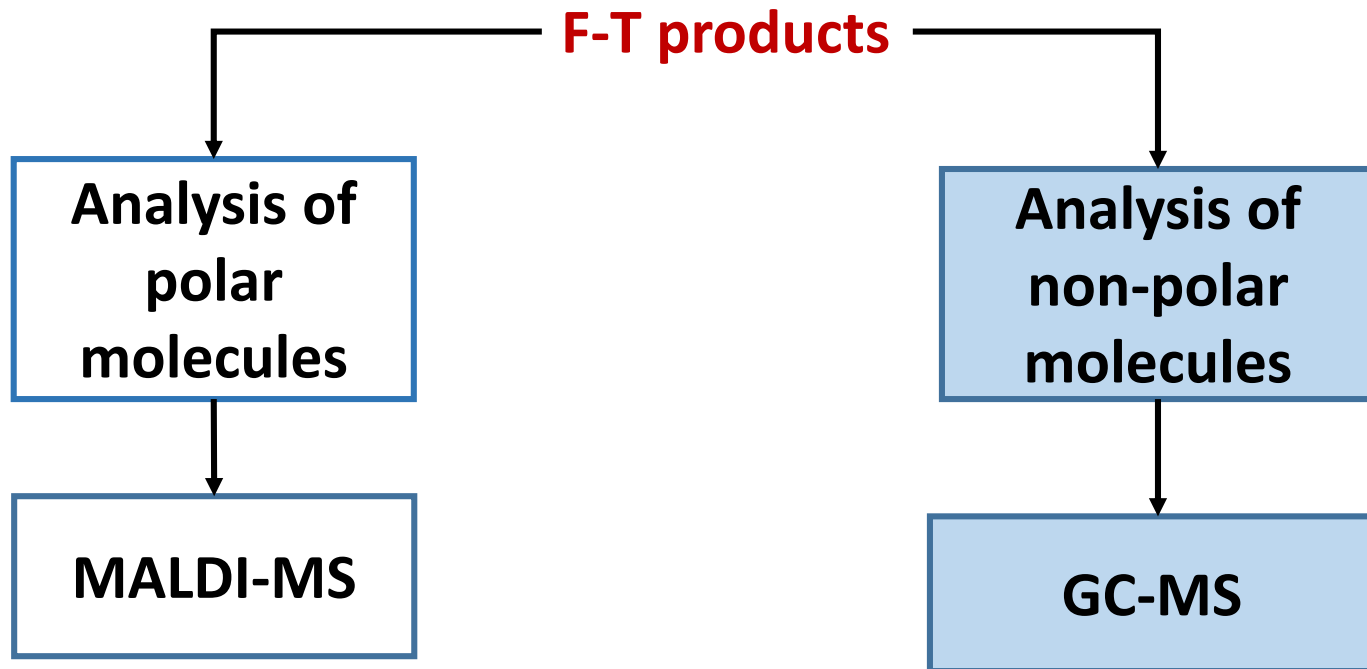


3.7E+4

Conclusions of the MALDI-MS measurements....

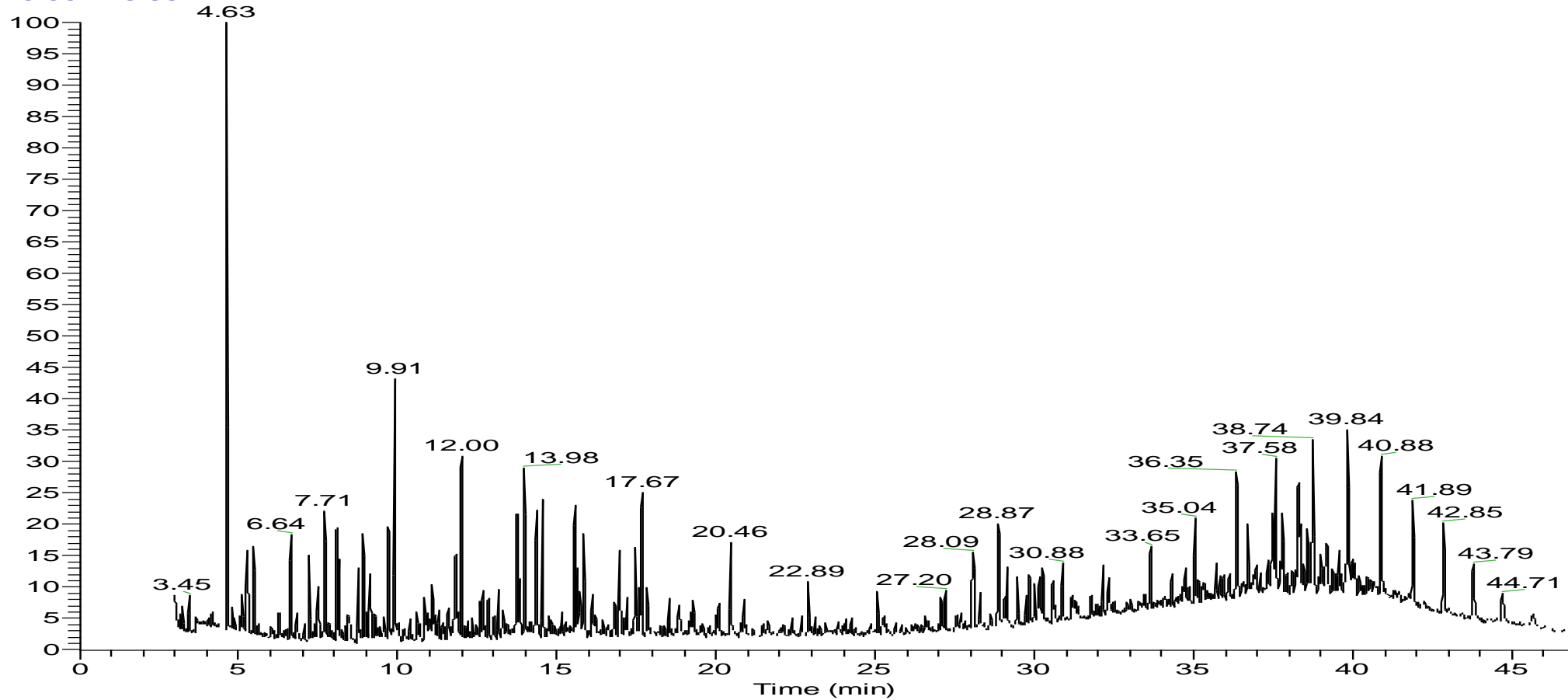
- Confirmation of the existence of acidic and basic compounds

Strategy for complex sample analysis



GC/MS analysis of the sample

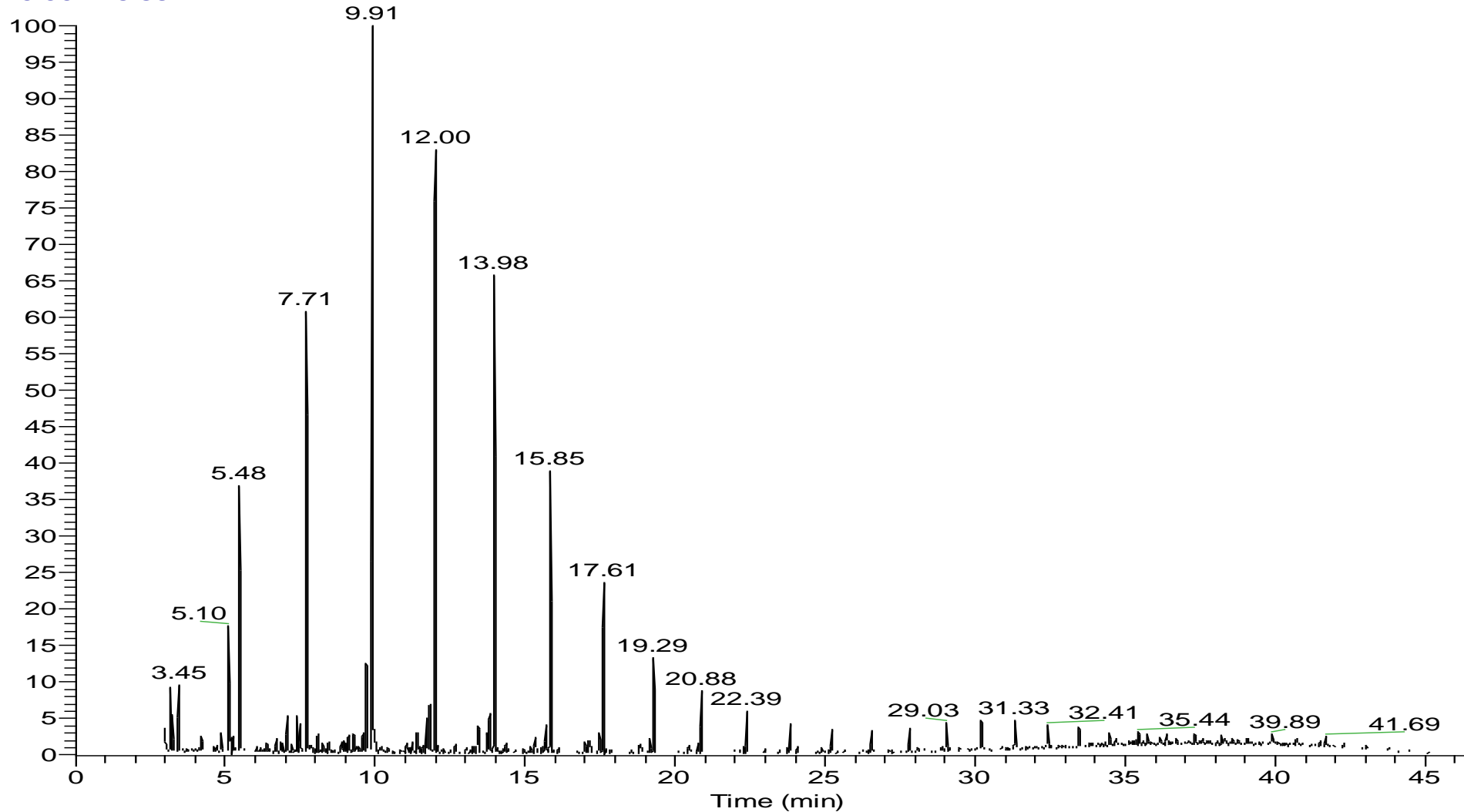
RT: 0.00 - 46.85



NL:
8.70E8
TIC MS
data16

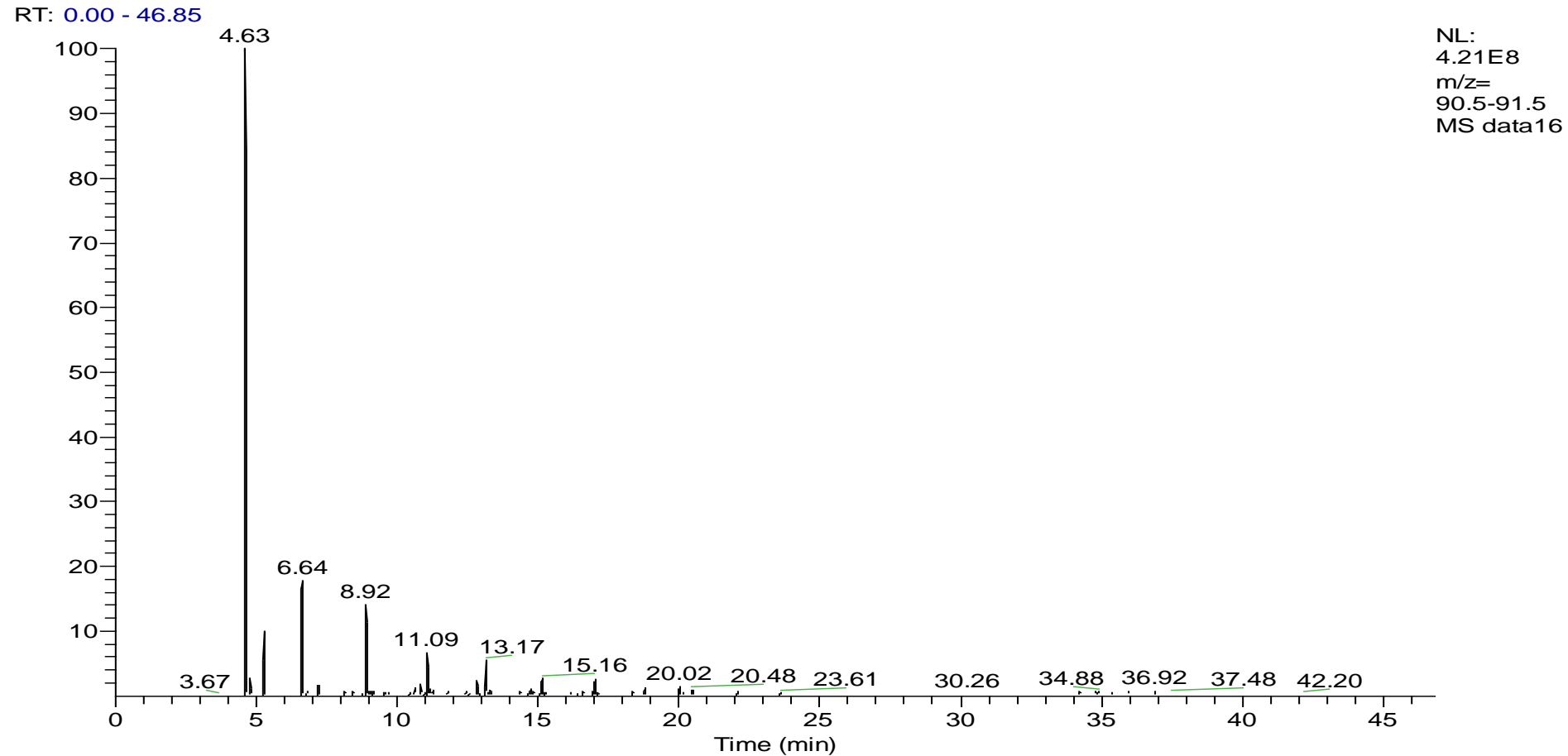
- Extracted Ion Chromatogram (XIC) for $m/z = 57$ (Alkanes)

RT: 0.00 - 46.85



NL:
1.01E8
 $m/z=$
56.5-57.5
MS data16

- Extracted Ion Chromatogram (XIC) for $m/z = 91, 105$ (methylbenzenes)



Conclusions of the GC-MS measurements....

- A complex mixture of non-polar compounds
- Confirmed existence of
 - Alkanes
 - Methyl benzenes
- Needs further analysis of spectra

Acknowledgements

- Research project partner - Cody Cervenka, Department of Chemistry
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