



Utility of Tier 1 Analysis in Hydrocarbon Forensics

EPA-NEMC 2024

Kesavalu M. Bagawandoss, Ph.D., J.D. | 08-06-2024

SAFER
GREENER
SMARTER

SGS



Agenda



- Introduction
- Why do we need Hydrocarbon Fingerprinting ?
- How do Hydrocarbons get into the Environment?
- What is necessary to perform Fingerprinting?
- Two Tracks of Data Collection
- Analytical Tiers
- Methods and Choices
- Matrices
- Sample Collection and Shipping
- Laboratory Information (Data Presentation)
- Summary



Whole Oil Analysis Forensics

Introduction

- Methods
- Most methods will require modifications
- ASTM methods are specific to the matrix
- Two tracks - regulatory requirements & forensic outcomes
- Need expertise for methods, analysis and interpretation
- Tiered Approach to Characterization
- Need a lot of information - Historical and Current



Why do we need Hydrocarbon Fingerprinting?

- Characterization of Product
 - Determination of Source
 - Multiple Sources?
- Range of Approximate Time of Release
 - Allocation of Liability



How do Hydrocarbons get into the Environment?



- Spills
- Leaks
- Explosions
- Natural Seeps
- Emissions

What is necessary to perform Fingerprinting?

- Samples from Site
- Source Product or Products
- Historical Background
- All other Information

MORE INFORMATION THE BETTER !!!





Two Tracks of Data Collection

- Regulatory Aspects
- Determination of Source/ Multiple Sources

Analytical Tiers

- Tier I – GC/FID*
- Tier II – GC/MS (SHC's, PAH/APAH's, BIOMARKERS, PIANO)
- Tier III – CSIA (Carbon Stable Isotope Analysis)
- *Products comparison
- Whole Oil Analysis (GC/FID)
- Other Parameters... additives, metals, wear metals, sulfur, organic Pbs, Mn etc..
- P (Paraffins), I (Isoparaffins), A (Aromatics), N (Naphthenes), O (Olefins)



Methods and Choices

ASTM Methods

- ASTM D7900 (Detailed Hydrocarbon Analysis (DHA))
- ASTM D6730 Mod. (DHA Analysis)
- ASTM D8003 HPLIS (n-C1 through n-C24)
- ASTM D2887
- ASTM D7169
- ASTM D3328 (whole Oil)
- Physical Parameters by ASTM methods
- ASTM D7363 (SPE method)
- ASTM D5739 (Extraction and Analysis)





Methods and Choices

EPA Methods

GC Methods

- SW846 8015 Mod. (whole Oil)
- Ethanol

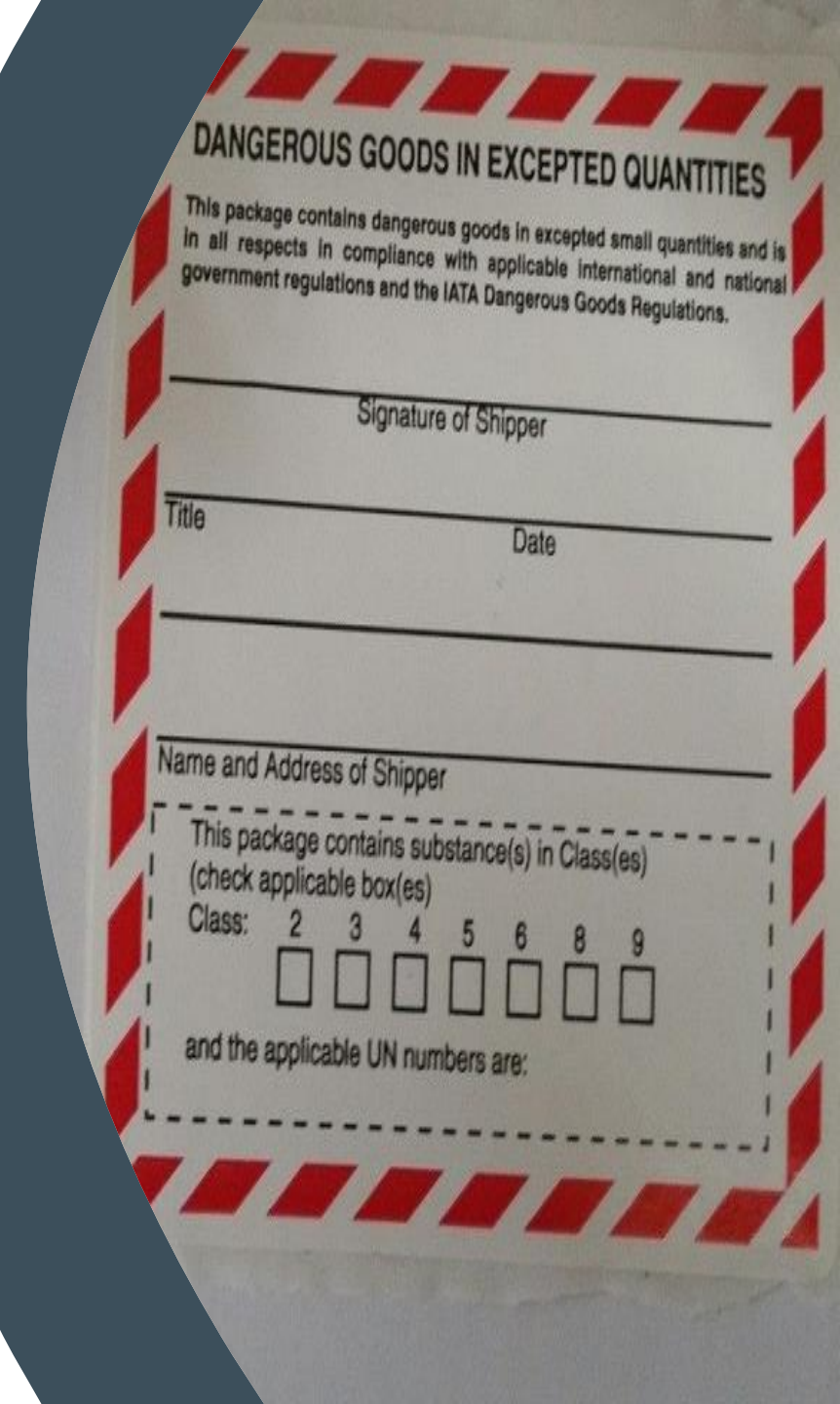
GC/MS Methods

- SW846 8260 Mod. (GC/MS)
- SW 46 8270D Mod. (GC/MS)
- SW846 8272 (Draft Method)(GC/MS)
- SW846 8270 Mod., for Organic Leads and Mn
- GC/GC methods
- SW846 6010D for metals (Pb, Cr, Ni, V etc...) including Sulfur



Sample Collection and Shipping

- Normal Sample Collection Protocols
- GW & Soils – Regular Protocols
- Product Samples - Special Handling
- DOT Shipping Rules
- Exempted Quantity Shipping
- 30 ml VOA Vials
- No more than 300 ml in a Shipment
- Requires Exempted Quantity Label on the outside of the Shipment





Laboratory Information

- GC/FID traces
- Total Ion Chromatograms
- Overlays based on Source Product or SGS Library
- Overlays comparison over time
- Overlays based on excavations at various intervals
- Data Interpretation Reports

Matrices

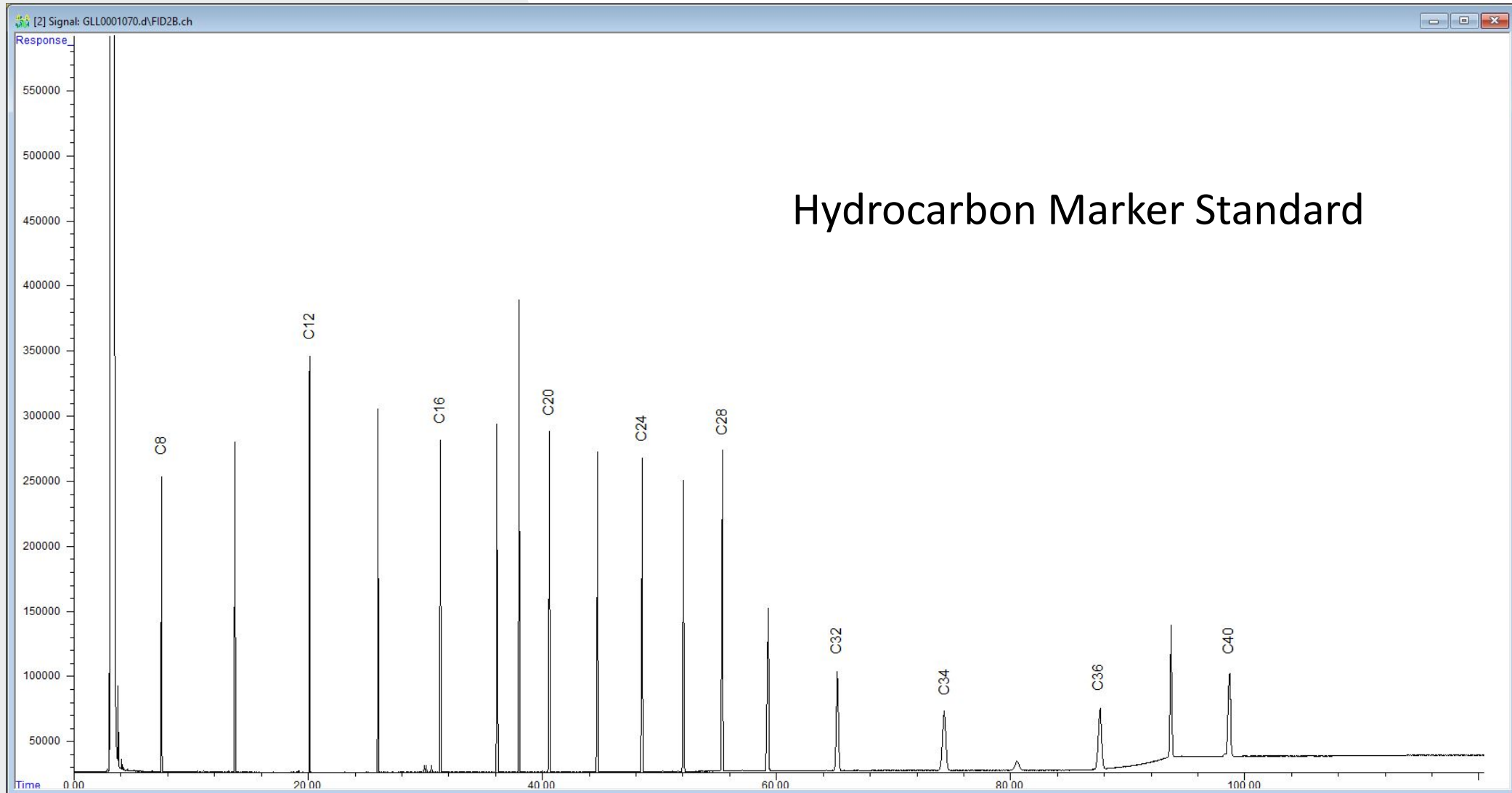
- Pure Product
- NAPL (Nonaqueous Phase Liquids) (Light and Dense)
- Soils & Sediments
- Water
- Matrix Combinations

Method Choice based on Matrix (ASTM or EPA)

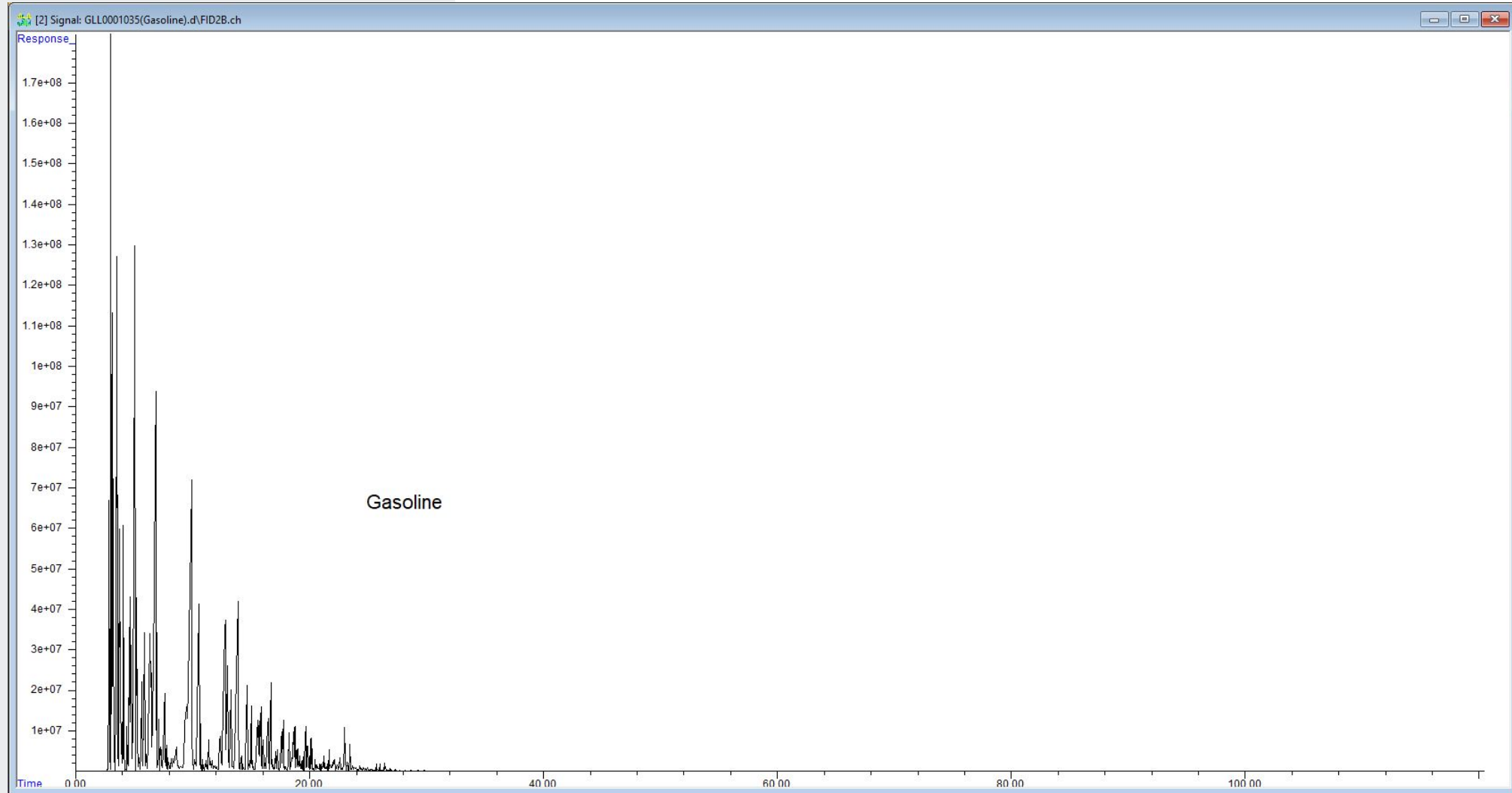


GC/FID Traces and Overlays

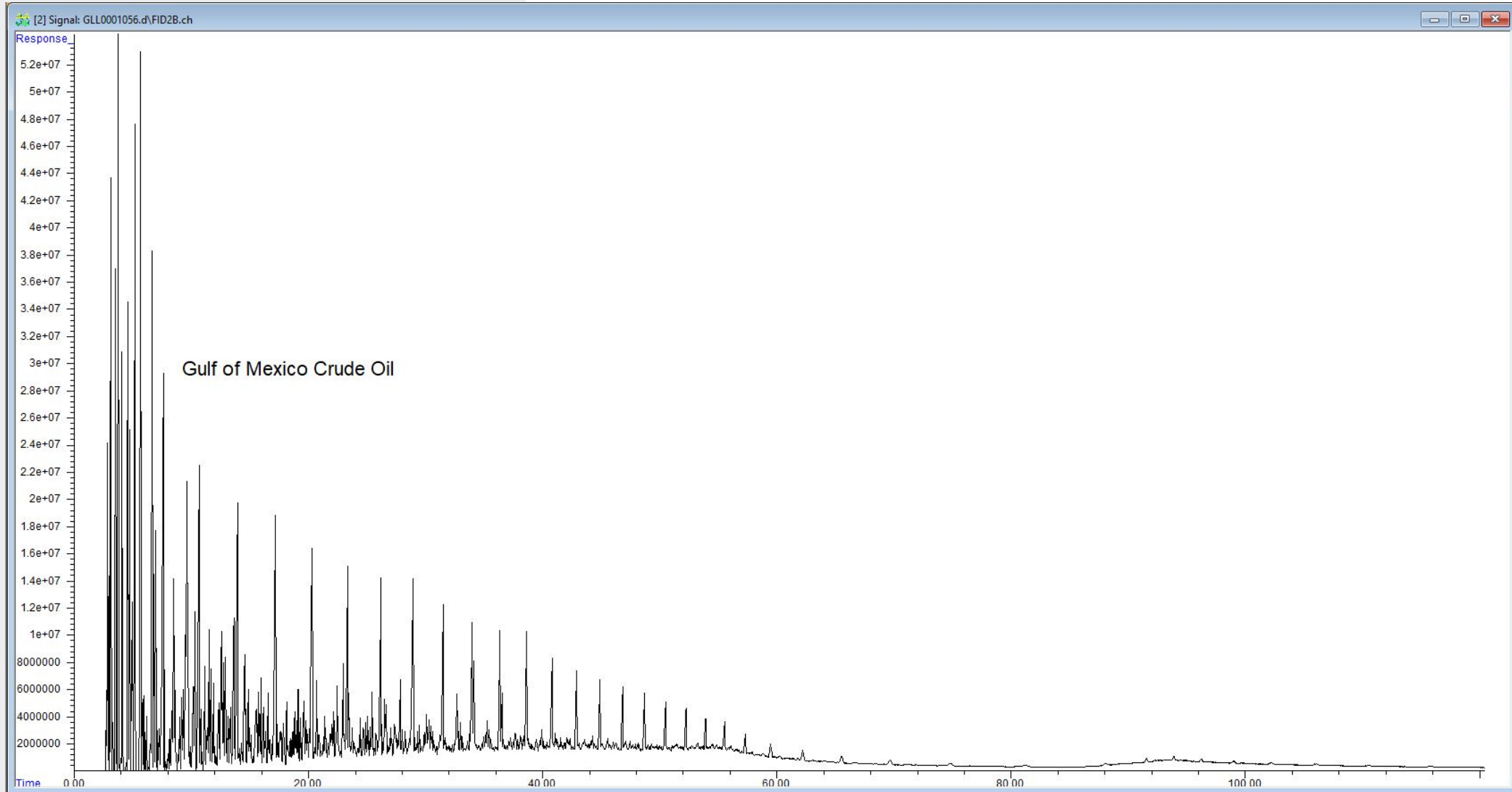
Laboratory Information



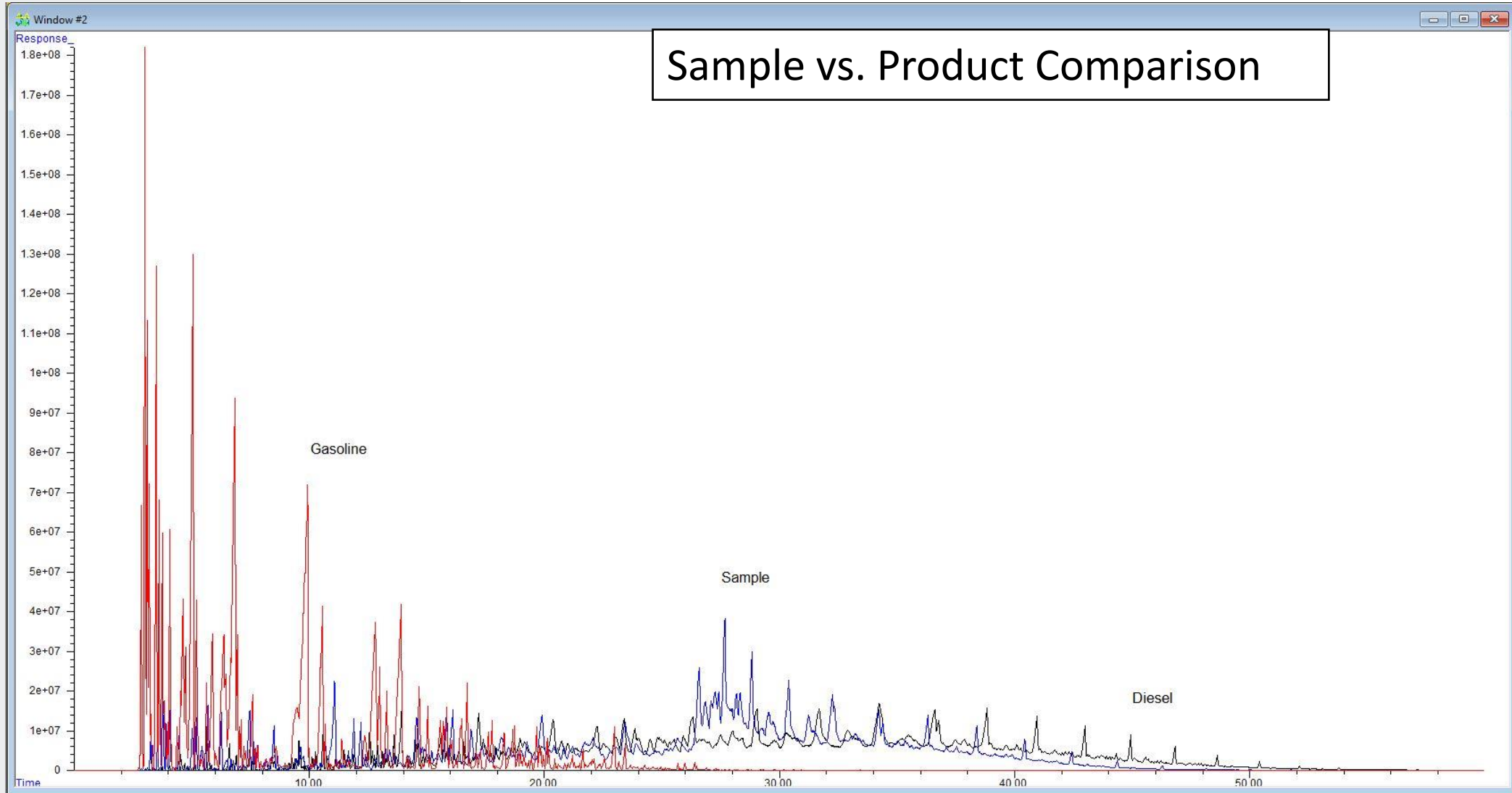
Laboratory Information



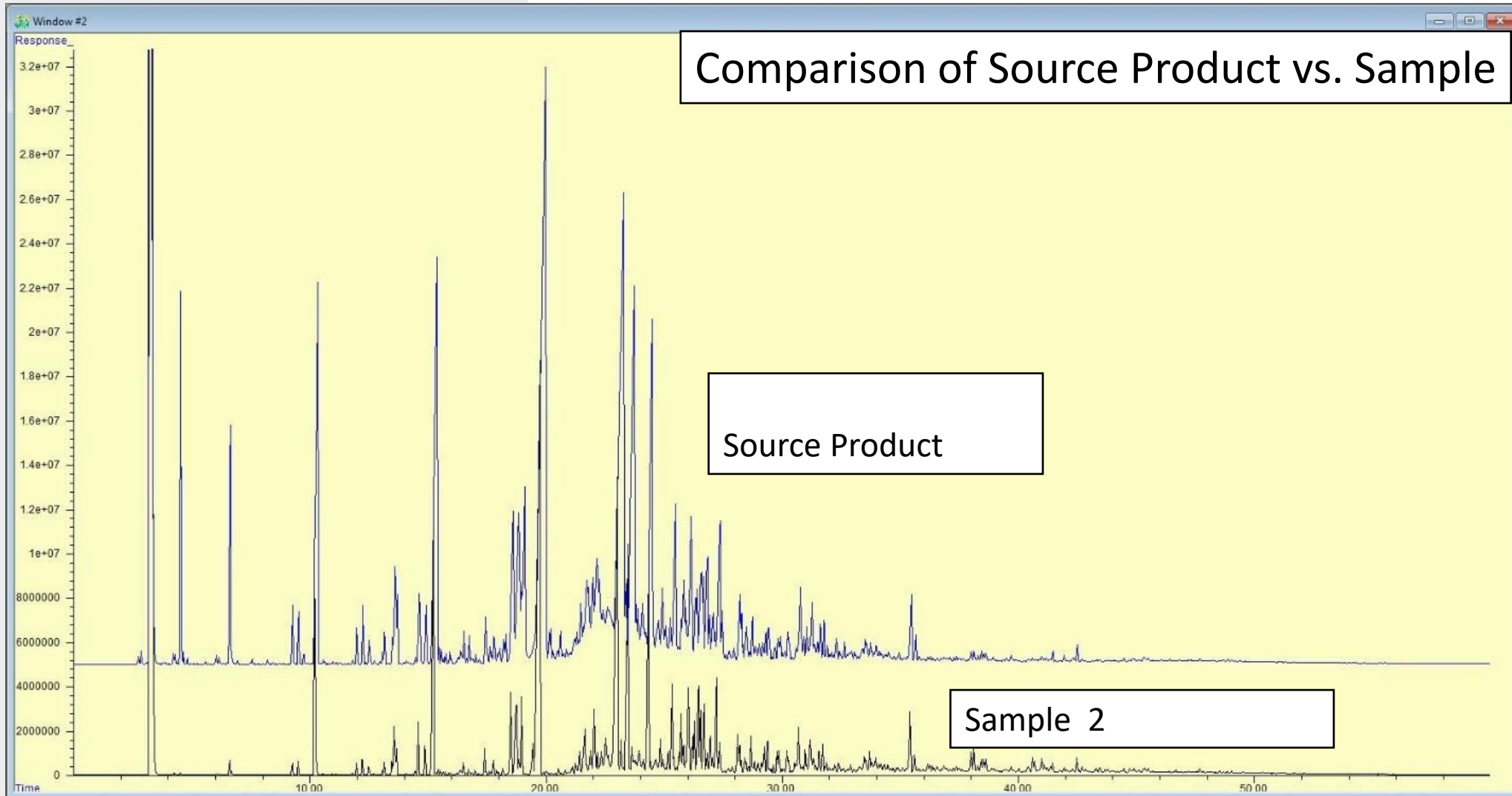
Laboratory Information



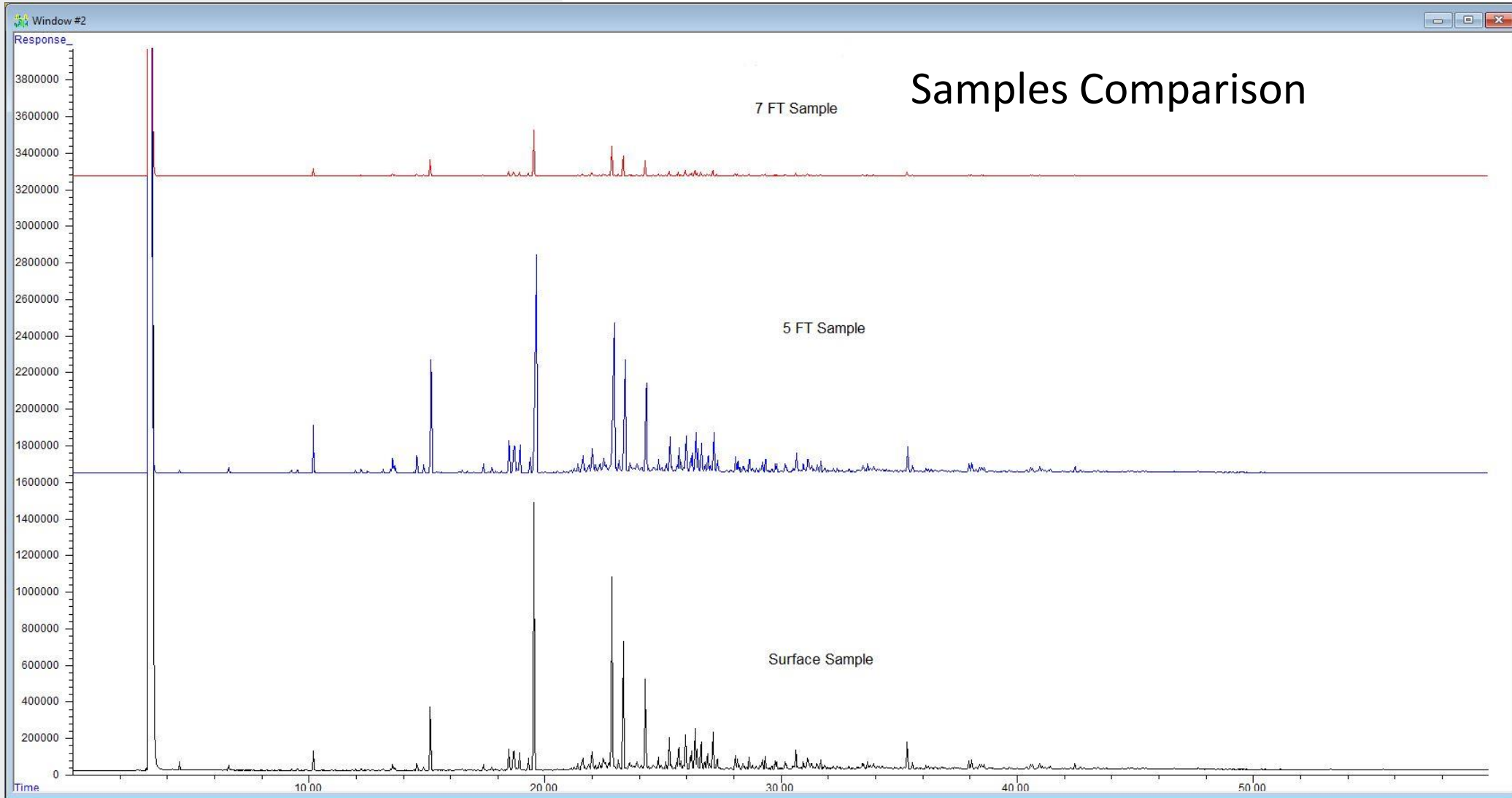
Laboratory Information



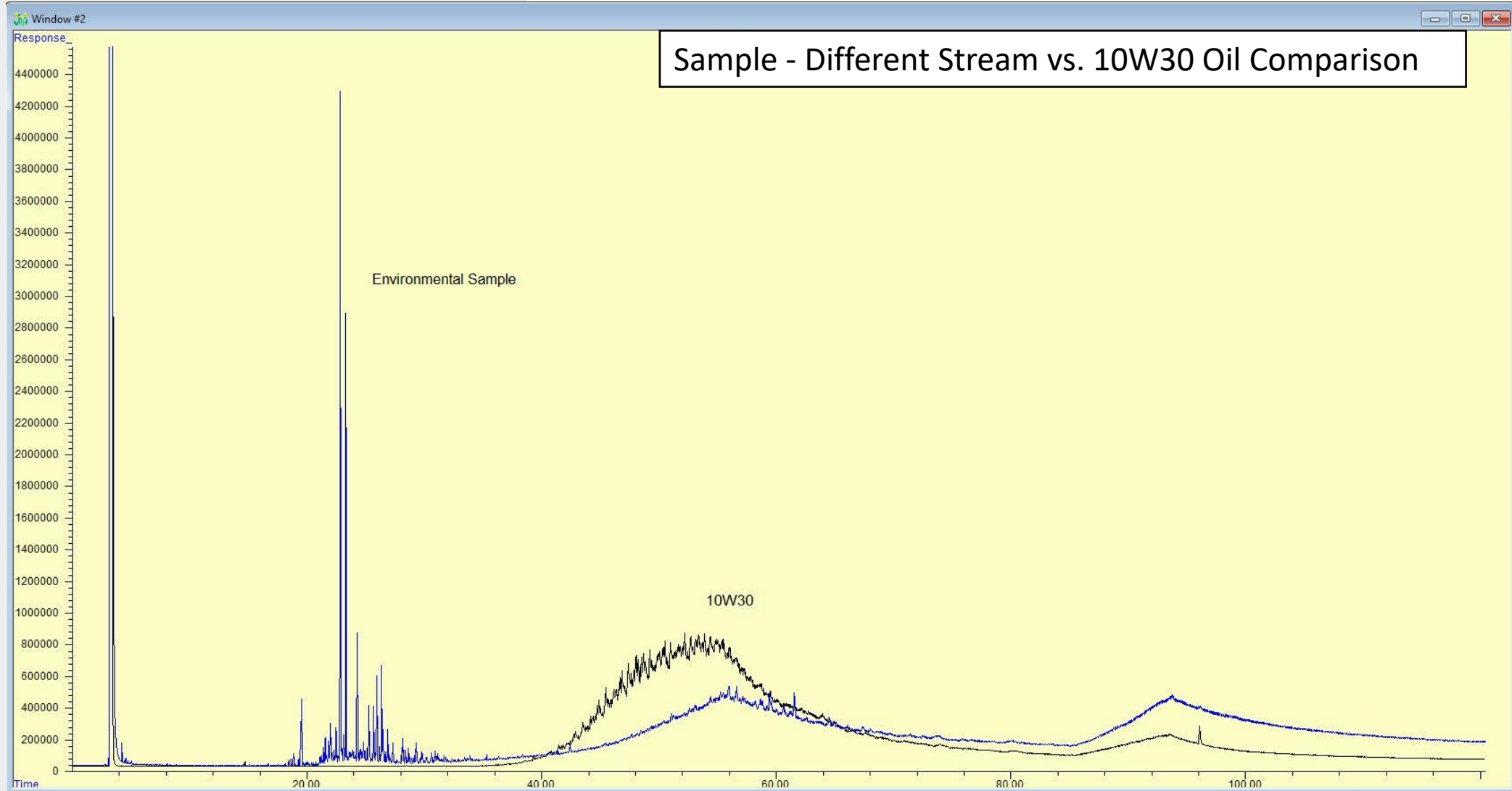
Laboratory Information



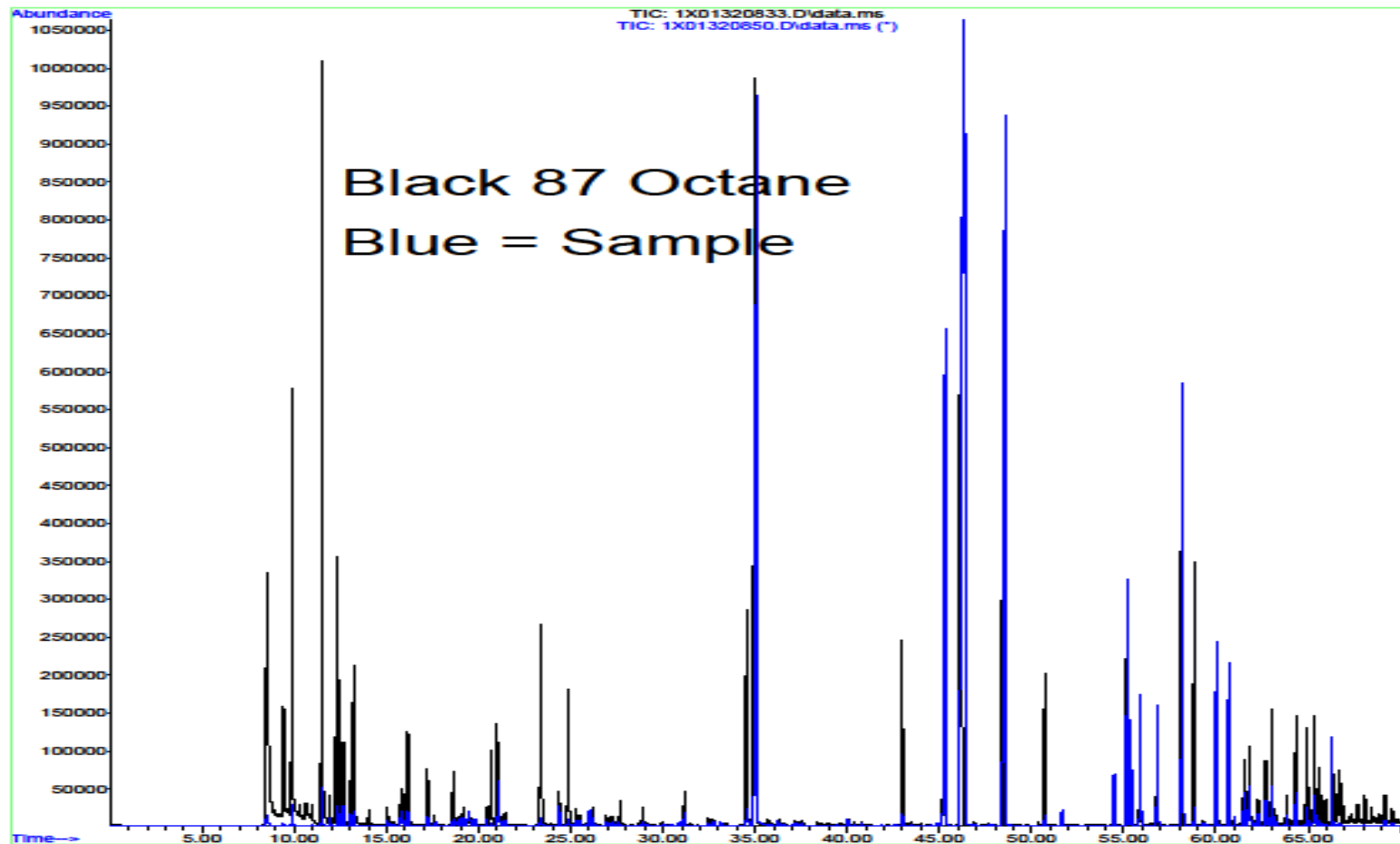
Laboratory Information



Laboratory Information



PIANO Analysis – Sample vs. Product Comparison



Summary

- Tier 1 Analysis is a powerful tool
- GC/FID traces of Samples
- Overlays to compare with product library
- Sites can be characterized or remediated by using Whole Oil Analysis with final regulatory required analysis
- Data Interpretation Reports
- Tier 2 analysis can be undertaken based on Whole Oil Analysis





Questions?
Thoughts?
Concerns?

Acknowledgements to my colleagues:
Benjamin Hentschel
Roger Johnson
Marketing team