Evaluation of Vapor Pressures of Ignitable Liquids, Water and Fire Debris Analysis, and the Effects on Extraction

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Abstract

Fire debris analysts examine evidence from fire scenes for ignitable liquids to assist fire investigators determine whether a fire was accidental or intentional. The primary goal of fire and emergency crews is to quickly extinguish the fire. Therefore, fire debris evidence often arrives in the laboratory wet having been sealed in airtight metal cans. Analysts typically extract samples by placing an activated charcoal strip (ACS) in the container, heating it, and desorbing the compounds with a solvent for GC-MS analysis. Previous studies investigated factors such as extraction time, activated charcoal strip (ACS) saturation, and adsorption efficiency. However, advances in ACS manufacturing and substantial improvements in gas chromatography-mass spectrometry (GC-MS) sensitivity present an opportunity to build upon these earlier findings. Furthermore, older studies often employed complex ignitable liquid mixtures like gasoline, which complicated interpretation and limited the ability to conduct semi-quantitative analyses. This study investigated ACS extraction using current ASTM E1412 guidelines while simplifying the analysis by focusing on ten representative compounds: ethanol, isooctane, n-heptane, toluene, 1-octene, 1,2,4-trimethylbenzene, n-decane, indane, naphthalene, and n-heptadecane. Extractions used varied starting volumes and extraction times. The objective was to compare predicted headspace concentrations with GC-MS responses and to evaluate the influence of water. Contrary to predictions, higher vapor pressure compounds were not consistently observed in greater abundance during shorter extractions. Instead, ACS affinity appeared to govern adsorption. Other experimental parameters were found to be significant; desorption solvent volume affected compound recovery and GC-MS detector saturation, while adsorption times showed little variation, suggesting that equilibrium is reached more quickly than previously reported. Water had a limited overall effect, but its presence did prevent the detection of ethanol in wet samples. This was likely due to ethanol's adsorption by the water.

Experimental

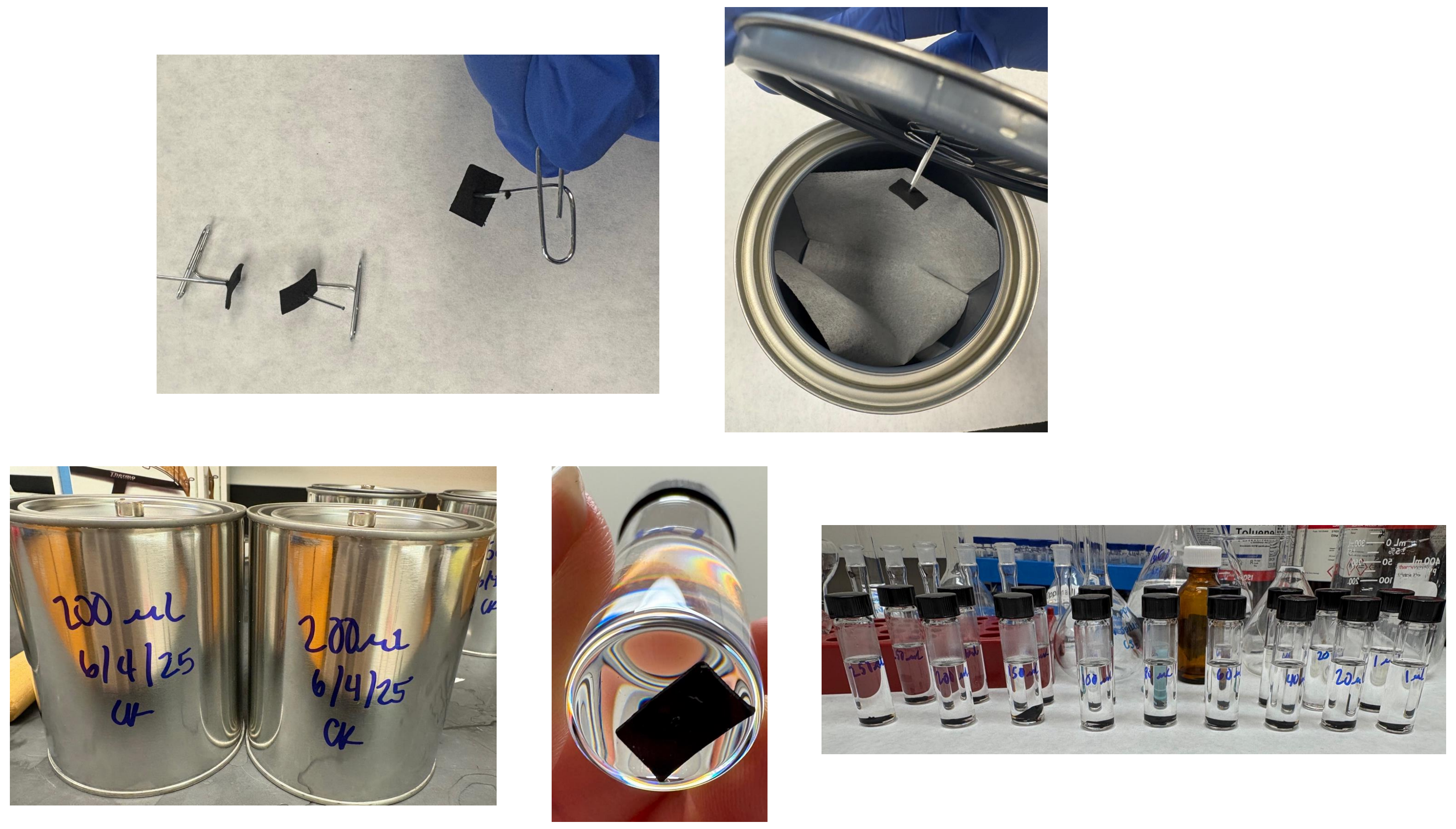
1.Prepare extraction following ASTM E1412 guidelines

2.Place a KimTech wipe inside quart-sized air-tight metal cans, and spike with various volumes of ten-compound mixture or gasoline, depending on the study being done

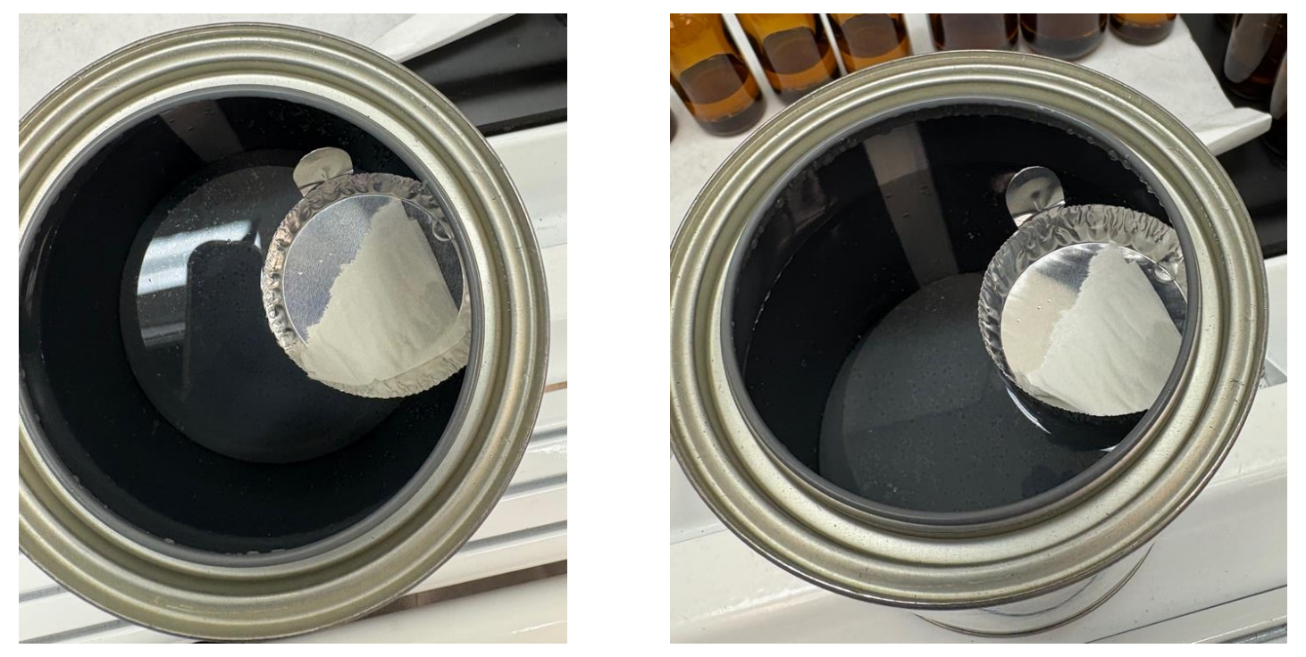
3. Heat samples in the oven at 65°C for 2 hours overnight (approx. 16 hours)

4. Extract ACSs with 10 mL of CS_2 spiked with 100 ppm of s-Tetrachloroethane (ISTD)

Preparation of the Air-tight Metal Cans and Extraction Vials



Preparation of the Air-tight Metal Cans for Water Study



Results

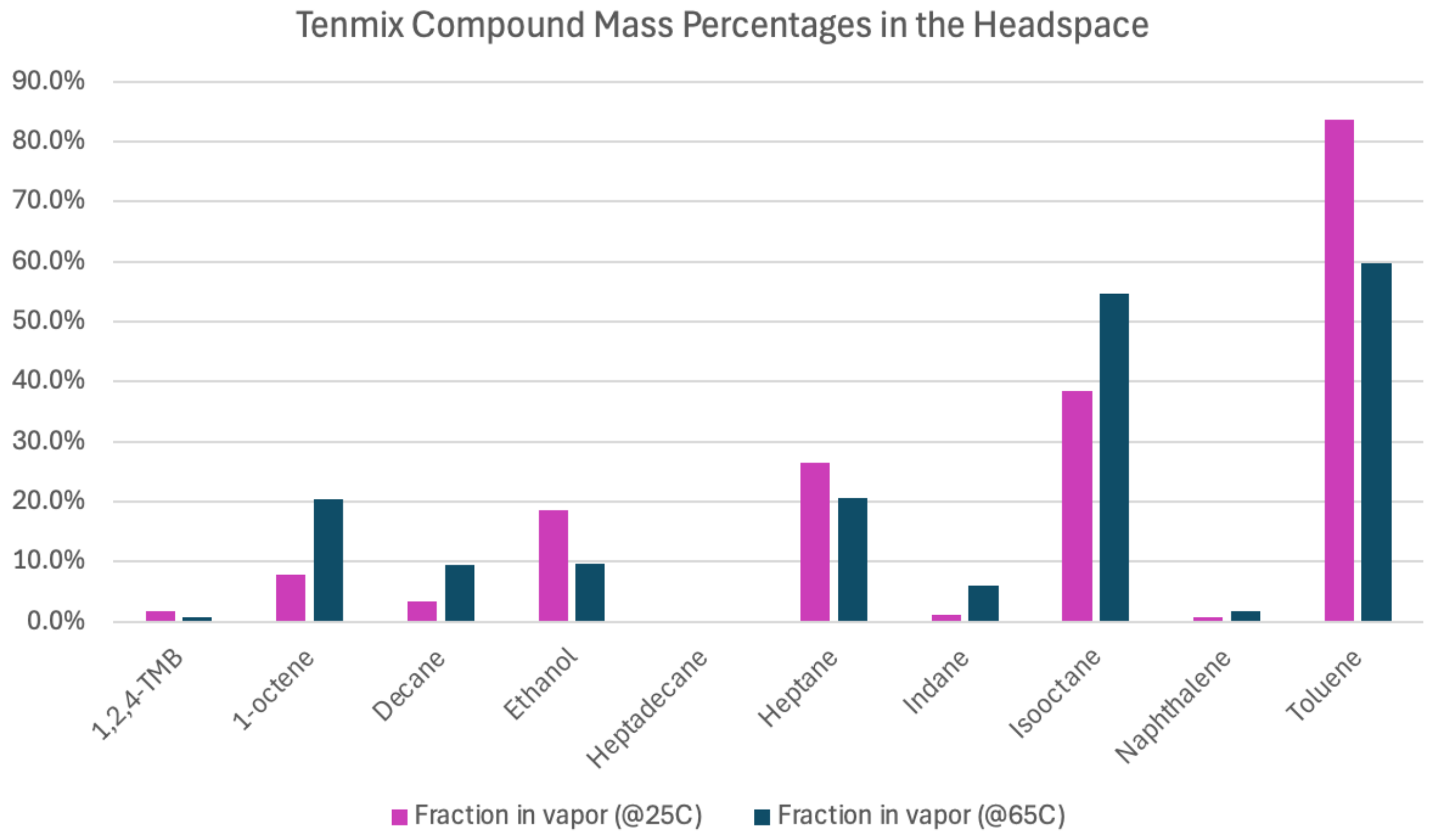


Figure 1: Calculated Mass Percentages of the Ten-compound Mixture in the Headspace

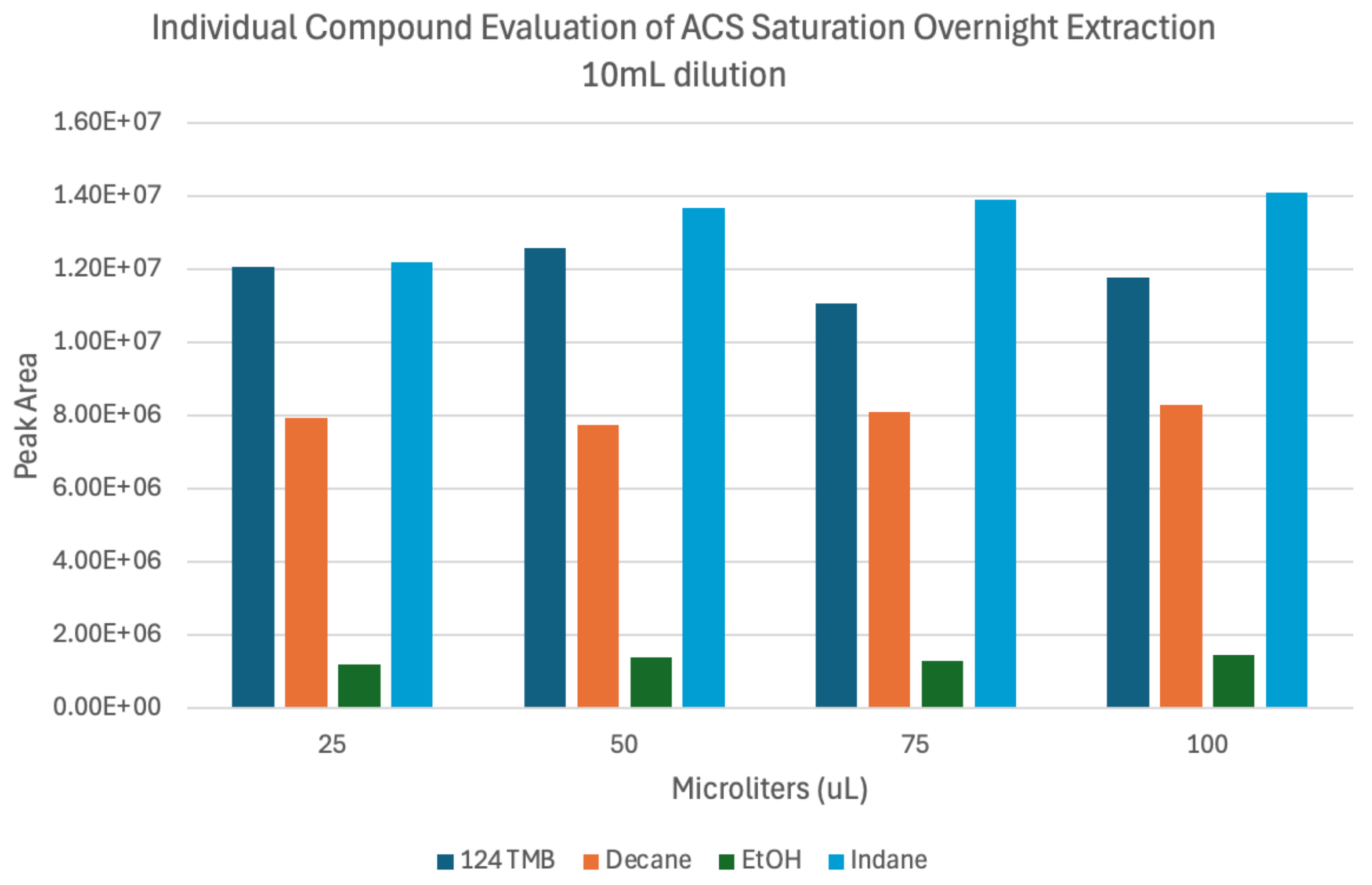


Figure 2: Individual Compound ACS Capacity as Measured by GC-MS Response

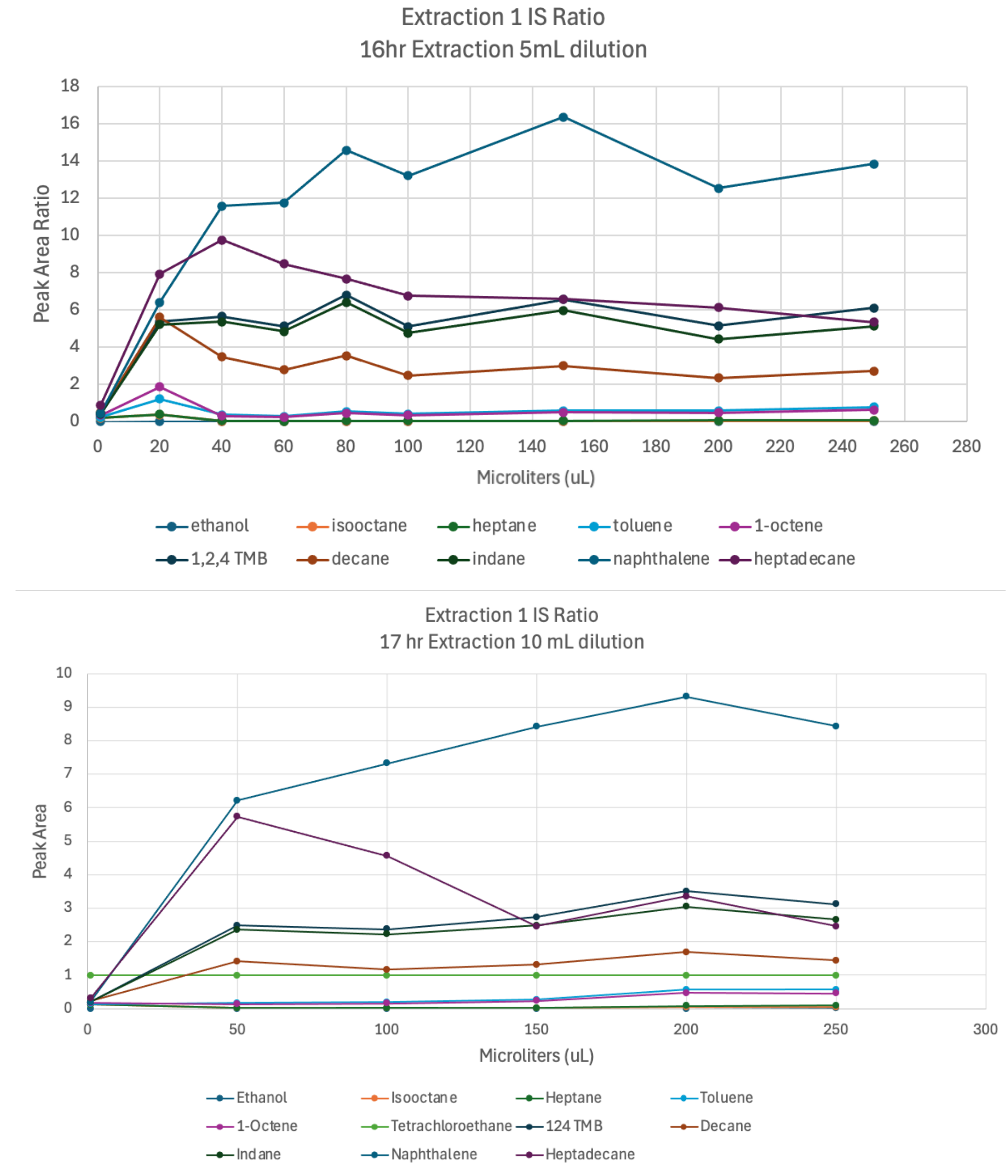
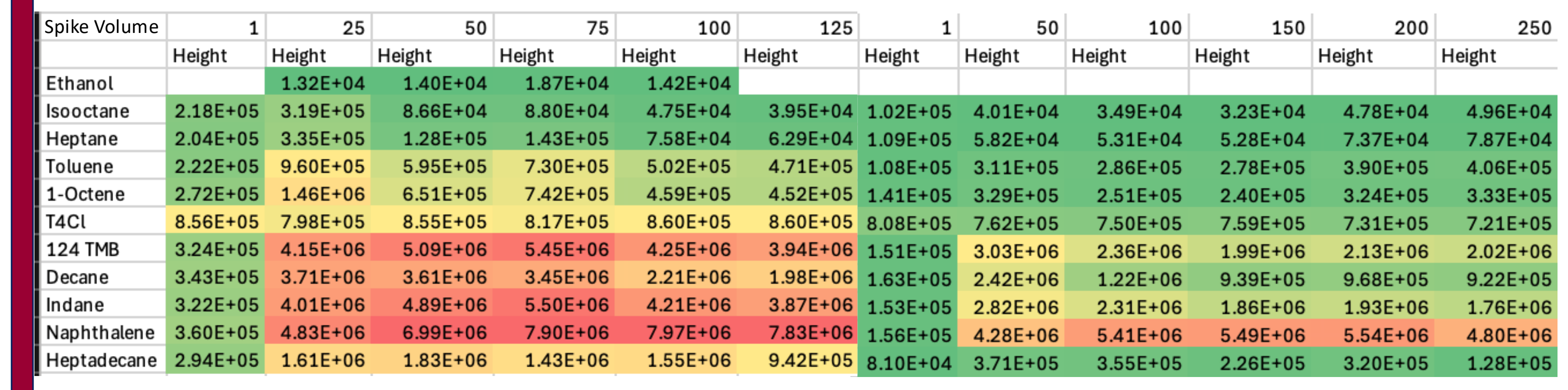


Figure 3&4: Differences in Relative Quantitation Curves Using 5 mL Versus 10 mL as the Solvent Extraction Volume

5mL Extraction Volume | 10mL Extraction Volume



Spike Volume	1	25	50	75	100	125	1	50	100	150	200	250
	Height	Height	Height	Height	Height	Height	Height	Height	Height	Height	Height	Height
Ethanol		1.32E+04	1.40E+04	1.87E+04	1.42E+04							
Isooctane	2.18E+05	3.19E+05	8.66E+04	8.80E+04	4.75E+04	3.95E+04	1.02E+05	4.01E+04	3.49E+04	3.23E+04	4.78E+04	4.96E+04
Heptane	2.04E+05	3.35E+05	1.28E+05	1.43E+05	7.58E+04	6.29E+04	1.09E+05	5.82E+04	5.31E+04	5.28E+04	7.37E+04	7.87E+04
Toluene	2.22E+05	9.60E+05	5.95E+05	7.30E+05	5.02E+05	4.71E+05	1.08E+05	3.11E+05	2.86E+05	2.78E+05	3.90E+05	4.06E+05
1-Octene	2.72E+05	1.46E+06	6.51E+05	7.42E+05	4.59E+05	4.52E+05	1.41E+05	3.29E+05	2.51E+05	2.40E+05	3.24E+05	3.33E+05
T4Cl	8.56E+05	7.98E+05	8.55E+05	8.17E+05	8.60E+05	8.60E+05	8.08E+05	7.62E+05	7.50E+05	7.59E+05	7.31E+05	7.21E+05
124 TMB	3.24E+05	4.15E+06	5.09E+06	5.45E+06	4.25E+06	3.94E+06	1.51E+05	3.03E+06	2.36E+06	1.99E+06	2.13E+06	2.02E+06
Decane	3.43E+05	3.71E+06	3.61E+06	3.45E+06	2.21E+06	1.98E+06	1.63E+05	2.42E+06	1.22E+06	9.39E+05	9.68E+05	9.22E+05
Indane	3.22E+05	4.01E+06	4.89E+06	5.50E+06	4.21E+06	3.87E+06	1.53E+05	2.82E+06	2.31E+06	1.86E+06	1.93E+06	1.76E+06
Naphthalene	3.60E+05	4.83E+06	6.99E+06	7.90E+06	7.97E+06	7.83E+06	1.56E+05	4.28E+06	5.41E+06	5.49E+06	5.54E+06	4.80E+06
Heptadecane	2.94E+05	1.61E+06	1.83E+06	1.43E+06	1.55E+06	9.42E+05	8.10E+04	3.71E+05	3.55E+05	2.26E+05	3.20E+05	1.28E+05

Figure 5&6: Reduction in Oversaturation of the GC-MS Detector by Increasing Solvent Extraction Volume (red denotes ULL has been reached)

*Note: over dilution (ethanol) also occurs

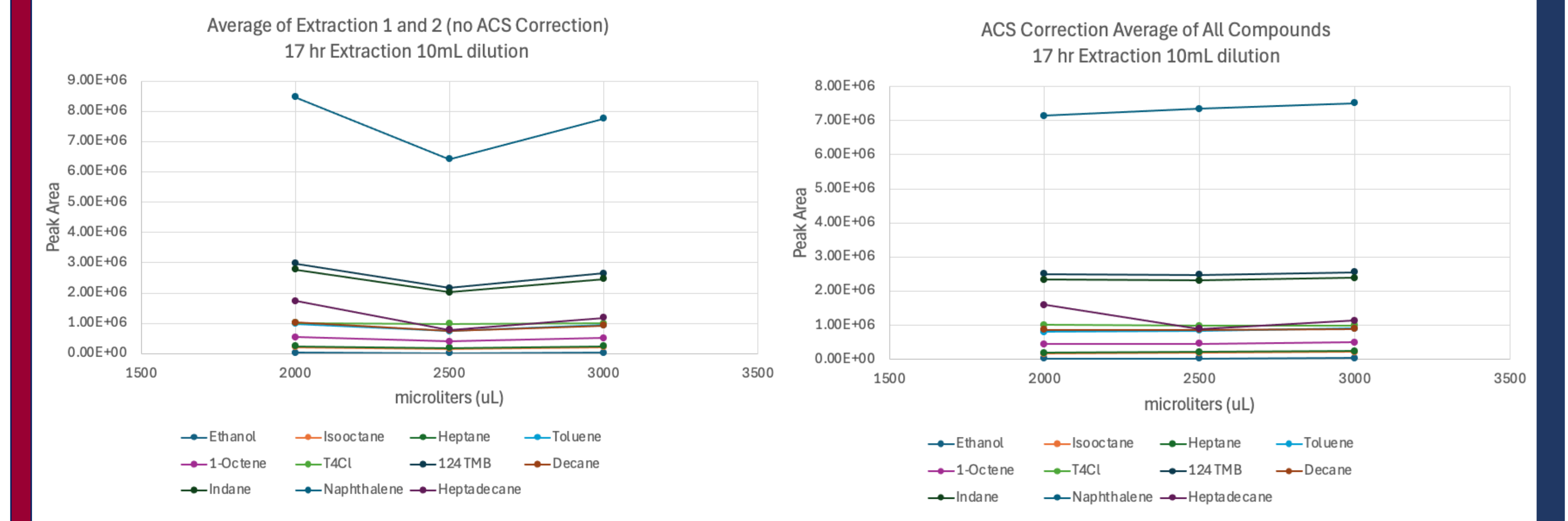


Figure 7&8:Comparing Adsorption Trends of Compounds with and without ACS Correction Factor

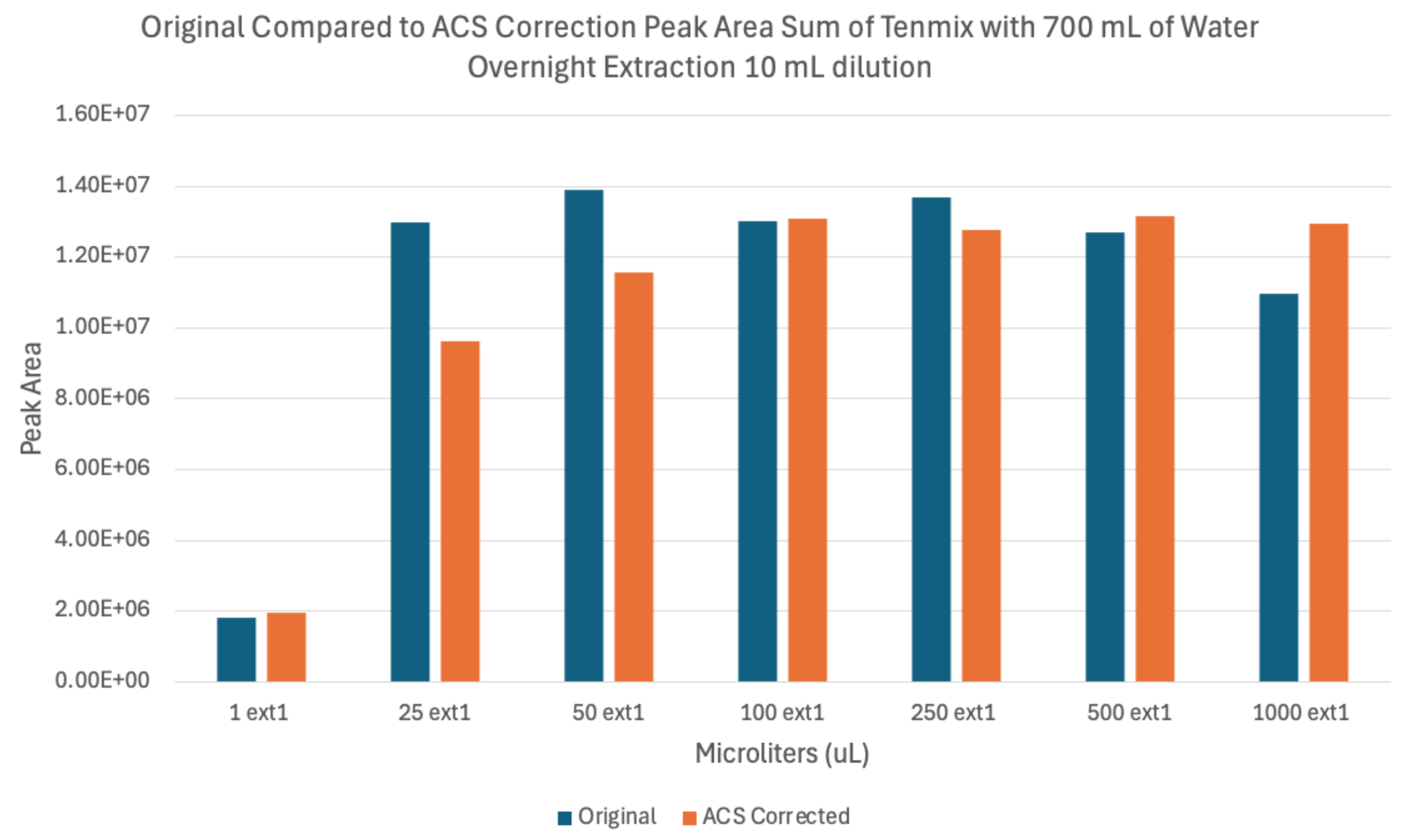


Figure 9: Comparing Peak Sum Areas with and without ACS Correction Factor

Conclusions

- One hypothesis being proposed is that the ACS capacity is reached in a manner similar to an organized closet (with affinity being the defining characteristic)
- Water does not appear to affect adsorption much other than on ethanol, in this instance, due to affinity (or hydrophilic nature)
- ACS size, volume, or weight have an impact on quantitation studies (this is a demonstrable result)
- 2-hour and 16-hour extractions appear to have similar results suggesting that equilibrium takes place faster than expected
- Increase in extraction volume improved semi-quantitation capabilities by reducing detector saturation effects
- Confirmation of other studies that suggest that affinity takes precedence over concentration, even when accounting for large differences in vapor pressure

Future Study

- Water study testing the effects of molecular sieves
- Conduct additional ambient extractions for comparison purposes
- Test additional methods for potential improvements to the fire debris analysis methods

References

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2. Evans, M; Games, C. Quantifying Ignitable Liquids in Fire Debris: Possible or Problematic? Fire and Arson Investigator 2012
3. Newman, R; Dietz, W.R; Lothridge, K, The Use of Activated Charcoal Strips for Fire Debris Extractions by Passive Diffusion. Part 1: The Effects of Time, Temperature, Strip Size, and Sample Concentration. *Journal of Forensic Sciences* **1996**, *41*(3), 361-370; DOI: 10.1520/JFS13922J
4. *Activated Charcoal Strips: Instruction Manual & Technical Guide For Forensic Laboratories*. https://arrowheadforensics.com/content/a-z/Activated%20Charcoal%20Strip%20Tech%20Guide.pdf (accessed 2025-06-03).

Acknowledgement

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