The Use of GC/MS Methods for Chemically Characterizing Biomass-Burning Aerosols

Adrienne Lambert, Cade Christensen, Jason Surratt

Abstract

Africa has been overlooked when it comes to researching Biomass-Burning Emissions (1). The chemical characterization of African-specific fuels is important to understanding the possible chemical reactions that can form compounds dangerous to human health (3 & 4). The following experiment took extracted filter solutions from burned African-sourced fuels and used Gas Chromatography-Mass Spectrometry to discover the compounds associated with each fuel. The compounds found were compared. Many of the compounds identified were present in all of the fuels, other compounds were unique to fuels such as Olive, Mopane, Mosethla, and Acacia.

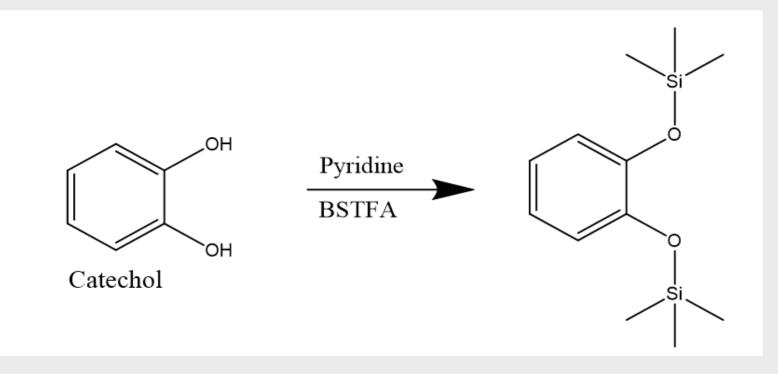
Methods

Preparing Samples For GCMS

- The filters collected from the burning chamber were extracted
- After the particles from the filters were extracted, a solution that isn't ready to be used on the GCMS is obtained
- To prepare the samples for GCMS analysis the extracted solution was dried completely, then the solutions was reconstituted with pyridine.
- Next, the reconstituted solution was derivatized using BSTFA
- The final solution was heated for 1 hour and then the samples were ready for GCMS analysis

Why we Derivatize the Solutions

- Many of the compounds used in this experiment are nonvolatile and by themselves wouldn't be picked up by the GCMS
- When derivatizing the hydrogen of the hydroxyl group is substituted with a trimethylsilyl group (TMS) (2)
- The TMS group makes the compound more volatile by lowering the boiling point
- This allows for the GCMS to heat the compound enough for it to vaporize and then be analyzed by the instrument

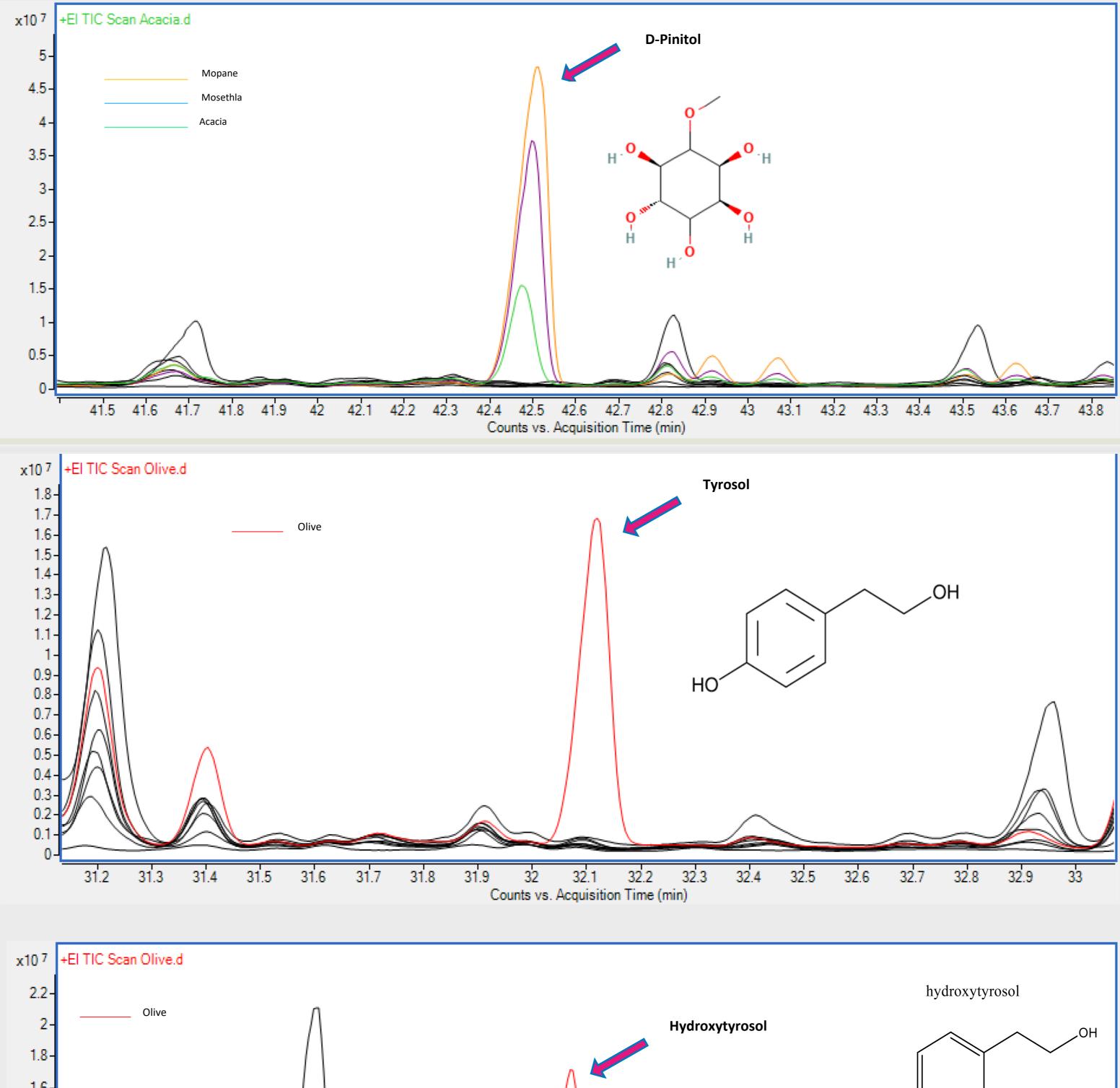


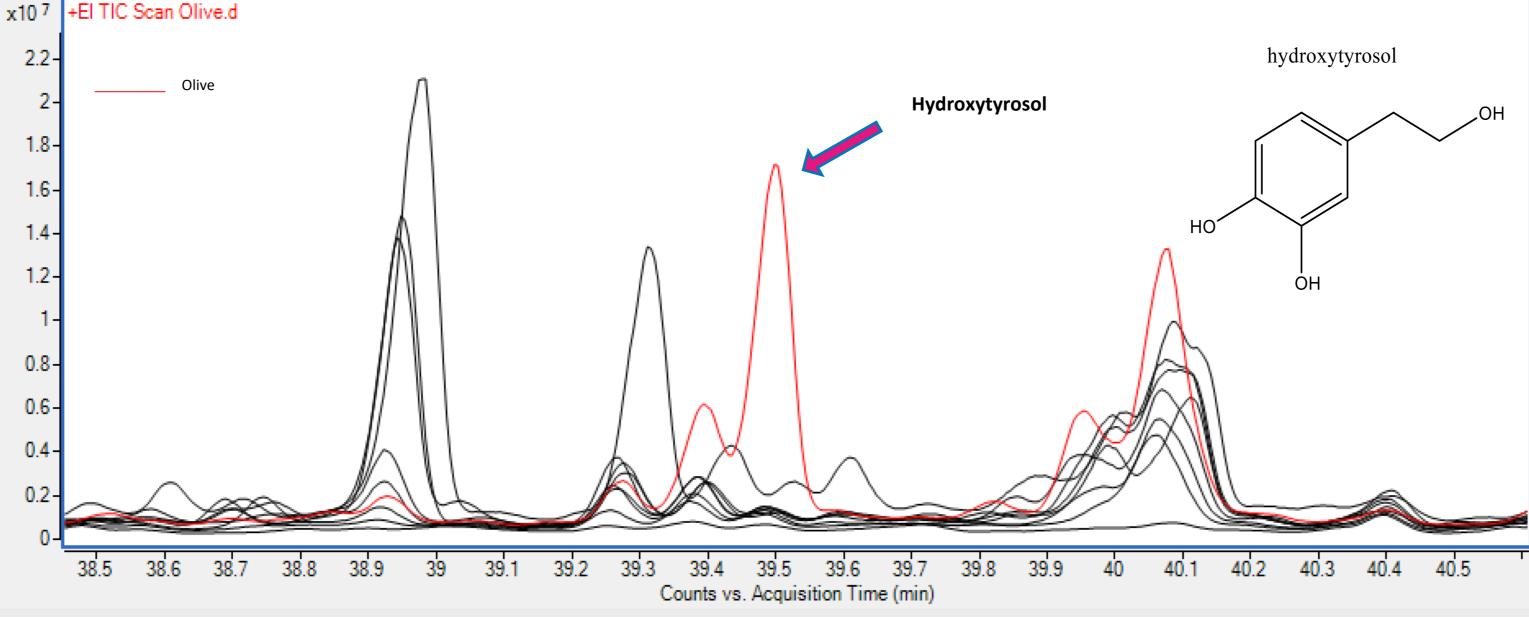
University of North Carolina at Chapel Hill – Department of Environmental Sciences and Engineering – Surratt Lab

Results

Table 1. The Different Compounds Detected in Each Fuel Along with Their Retention Times

		Detected in Fuel								
Compound	Retention Time (min) Estimate	Acacia	Dung	Grass	Mokala	Mopane	Mosethla	Mukusi	Olive	Wanza
Mannosan	38.1-38.2 (rough est.)	х		x	x	x	X	x	x	x
Galactosan	36.7-36.8 (rough est.)	х		х	X	x	X	X	х	x
Levoglucosan	37.6-37.8	х	X	x	X	X	X	x	X	x
Catechol	21.7-21.8	х	X	x	X	x	X	x	X	x
Resorcinol	24.5-24.6	х	X	x	X	x	X	x	X	x
Hydroquinone	25.3-25.4	х	X	x	X	X	X	x	X	x
Palmitic Acid	48.2-48.3	х	X	x	X	x	X	x	X	x
Glycerol	204-20.5	х	X	x	X	X	X	x	X	x
Coniferyl Alcohol	45.0-45.2	х		x	X	x	X	x	X	x
Sinapyl Alcohol	49.8-50.0	х			х	x	X	x	X	x
Lactic Acid	11.5	х	X	x	X	x	X	x	X	x
Glycolic Acid	12.1	х	X	x	X	x	X	x	X	x
Tyrosol	32								X	
2-(3,4-dihydroxyphenyl)-ethanol (hydroxytyroso	39.4								X	
Scopoletin	47.7								X	
D-Pinitol	42.3	х				x	X			
4-methylcatechol	24.8	х	x		x	x	X	x	x	x
pyrogallol	31.1	х		x	x	x	X	x	x	x
stearic acid	52.3	х	x	x	X	x	x	x	x	x





Compound Comparison Results

- The fuels analyzed were Acacia, Dung, Grass, Mokala, Mopane, Mosethla, Mukusi, Olive, and Wanza
- Dung had a different compound makeup than the rest of the fuels
- Unique compounds were found in Olive, Acacia, Mopane, and Mosethla

Chromatogram Results

- When looking at each fuel's chromatogram overlayed on top of one another there is a unique peak of D-Pinitol in the fuels Mopane, Mosethla, and Acacia.
- The D-Pinitol peak for Mopane is almost as high as the levoglucosan peak.
- Olive had three unique compounds that weren't found in any other fuel
- The unique compounds in Olive were Tyrosol, Hydroxytyrosol, and Scopoletin
- When analyzing all of the fuel's chromatograms overlayed the three unique compounds found in olive are significant





THE UNIVERSITY of NORTH CAROLINA at CHAPEL HILL

Objectives

- Understand how derivatizing can make an extracted filter solution detectable by the GCMS
- Be able to produce and analyze accurate chromatograms
- Investigate the chemical makeup of different Africansourced fuels
- Compare the chemical compounds found in each fuel
- Find unique compounds and compounds that overlap between fuels that can be investigated further
- Understand the future implications for atmospheric chemistry and public health

Conclusions

- Of the fuels that were tested, there were many compounds that were present in all the fuels There were also some compounds that were unique
- Dung and Olive had some unique compounds that will be further explored
- The data suggests that when different fuels are burned different compounds are produced and released
- This has implications for possible chemical reactions with sunlight and atmospheric gases along with the effects that these compounds can have on human health

References

- (1) Barker, P. A.; Allen, G.; Bannan, T.; Mehra, A.; Bower, K. N.; Pitt, J. R.; Bauguitte, S. J.-B.; Pasternak, D.; Fisher, R. E.; Lee, J. D.; Coe, H.; Gallagher, M.; Percival, C. J.; Nisbet, E. G. Airborne Measurements of Fire Emission Factors for African Biomass Burning Sampled during the MOYA Campaign, 2020. https://doi.org/10.5194/acp-2020-558.
- (2) Moldoveanu, S. C., & David, V. (2018). Derivatization Methods in GC and GC/MS. In (Ed.), Gas Chromatography - Derivatization, Sample Preparation, Application. IntechOpen. https://doi.org/10.5772/intechopen.81954
- (3) Akimoto, H., Global Air Quality and Pollution. Science, 2003. 302(5651).
- (4) Jolly, W.M., et al., Climate-induced variations in global wildfire danger from 1979 to 2013. Nature Communications, 2015. 6(1): p. 7537.