

Resolving the Partially Resolved: GC-MS Data Processing Tools

Megan R. Pearl,¹ Jonell N. Smith,² Mark H. Van Benthem,¹ and James M. Hochrein²

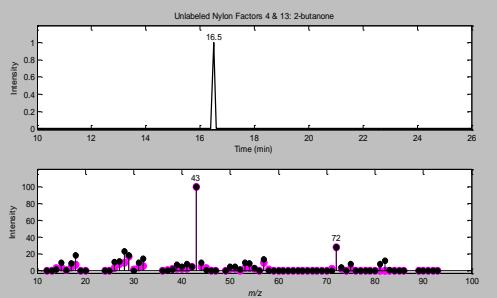
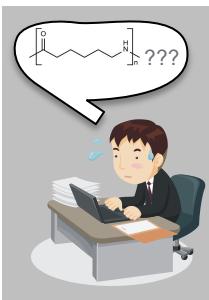
¹Materials Characterization Department, 1822

²Materials Reliability Department, 1825

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Analysis

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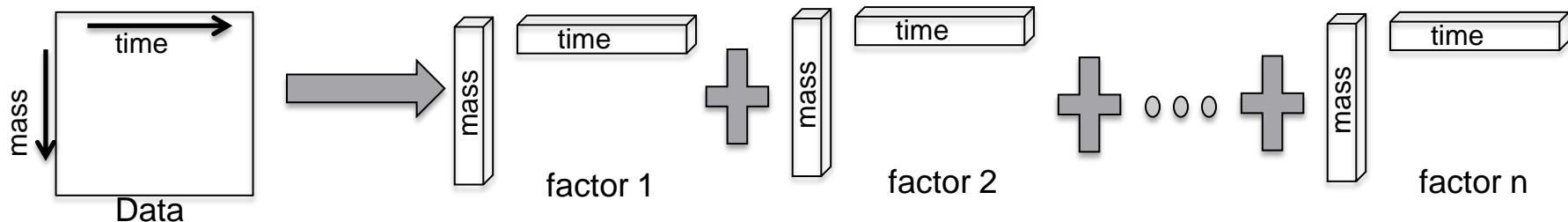


Factor Analysis

- Data reduction using PCA.
- Decompose the data into n factors.

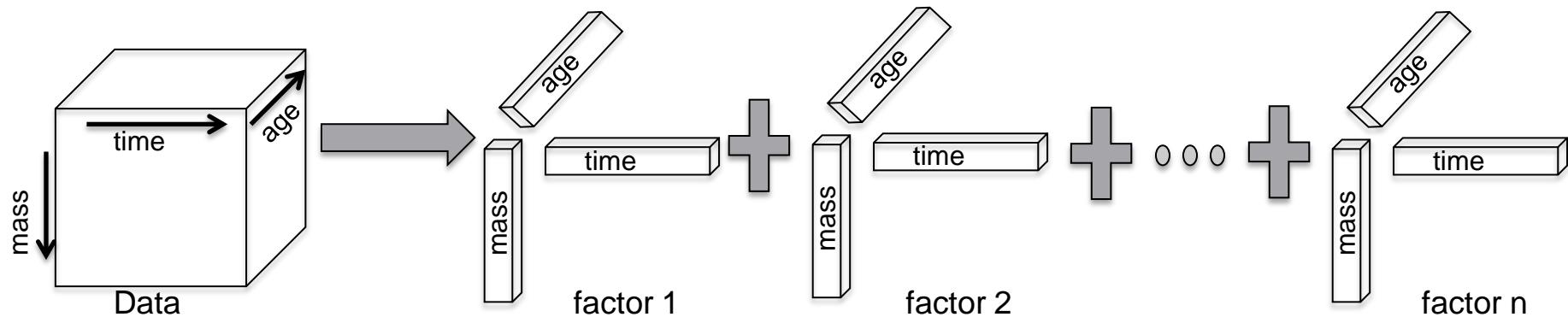
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 - Parallel Factor Analysis (PARAFAC2) → Changes in compounds with time

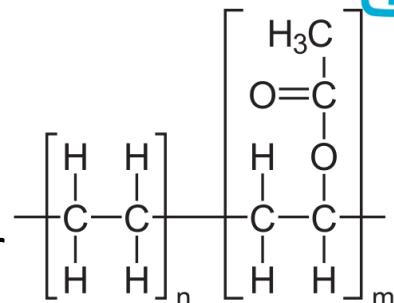


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 - Different polymers, different components
 - Labeled vs. unlabeled
 - Changes over time

Different Polymers

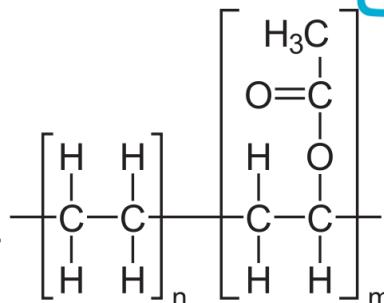
- Ethylene-vinyl acetate (EVA)
 - Hot glue sticks, ski boot padding, fishing rods, cigarette paper, plastic wrap clinginess enhancer



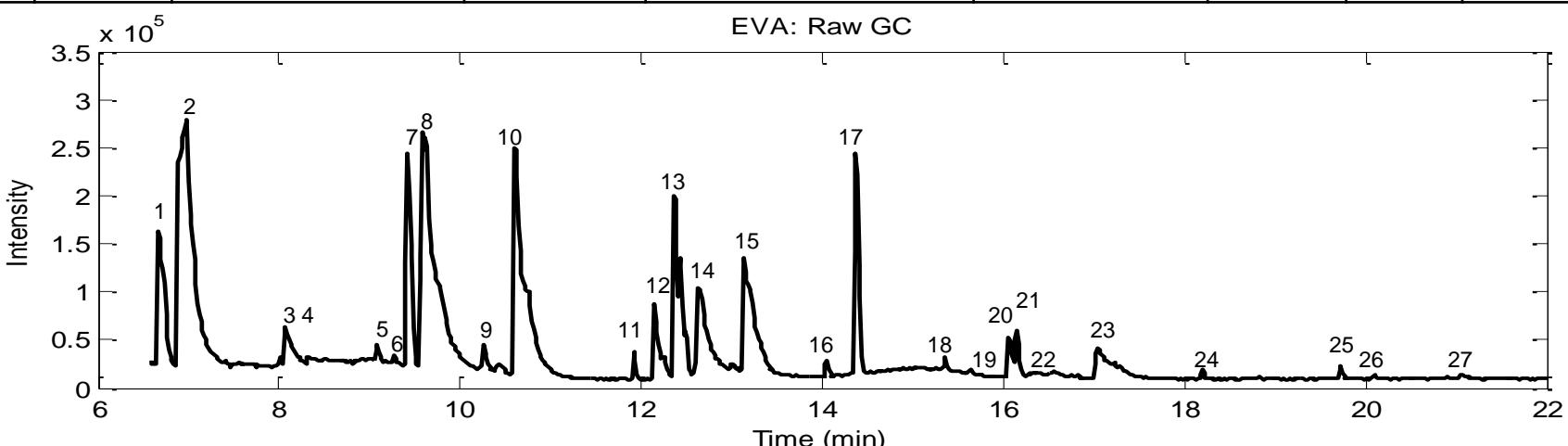
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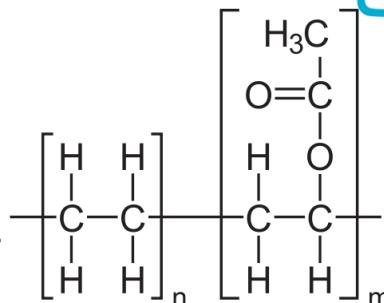
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1-propene, 2-methyl	acetaldehyde	ethyl chloride	methyl formate	1-pentene	pentane	furan	propanal	acetone
10	11	12	13	14	15	16	17	18
acetic acid methyl ester	1-hexene	acetic acid ethenyl ester	butanal	2-butanone	ethyl acetate	butane, 1-chloro	benzene	1-heptene
19	20	21	22	23	24	25	26	27
heptane	pentanal	2-hexene, 5,5-dimethyl	2-pentanone	2-pentene, 3,4,4-trimethyl	Pentane, 1-chloro	1-octene	octane	hexanal



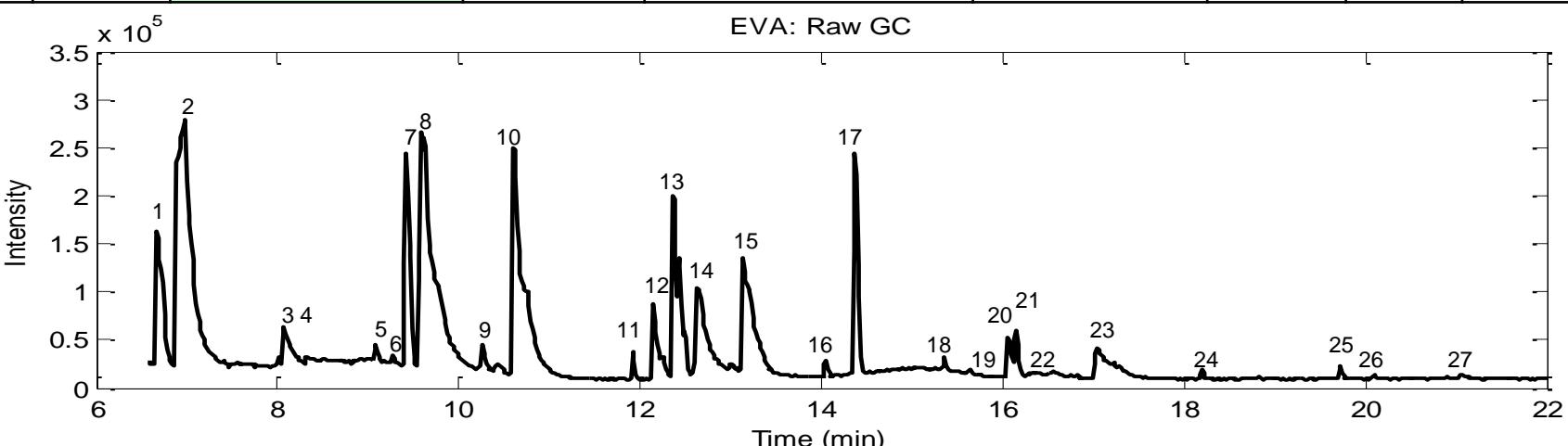
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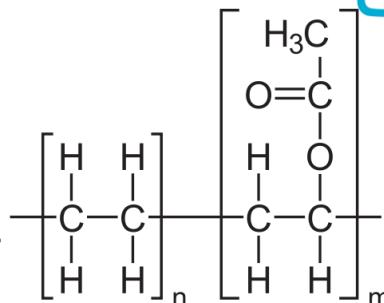
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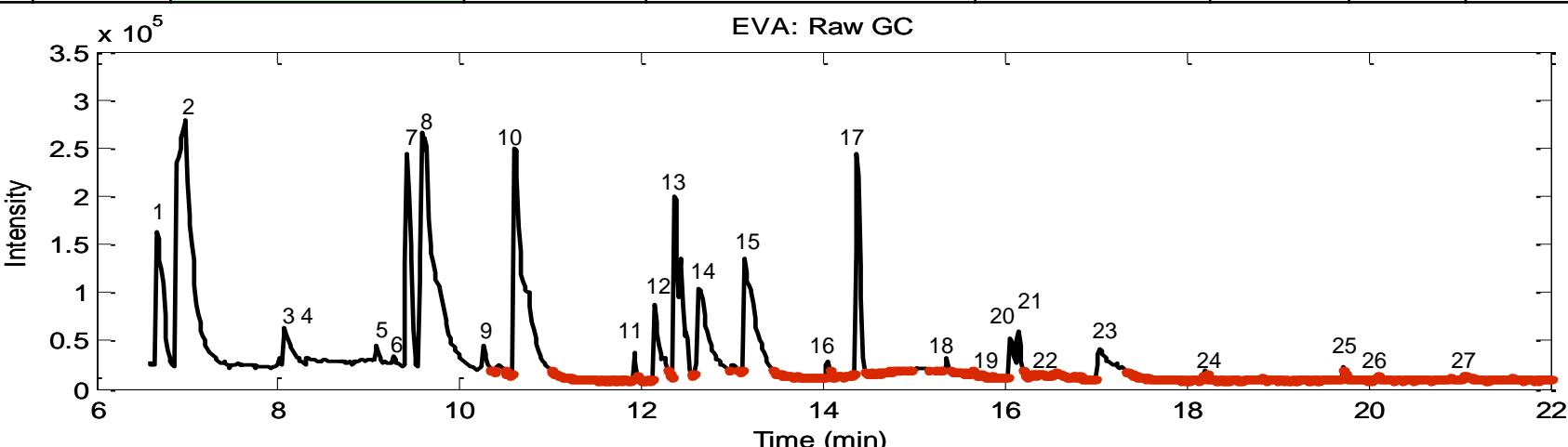
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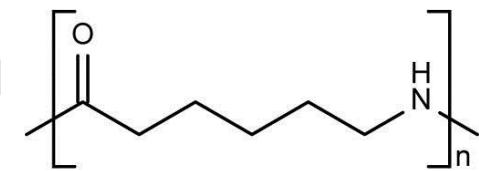


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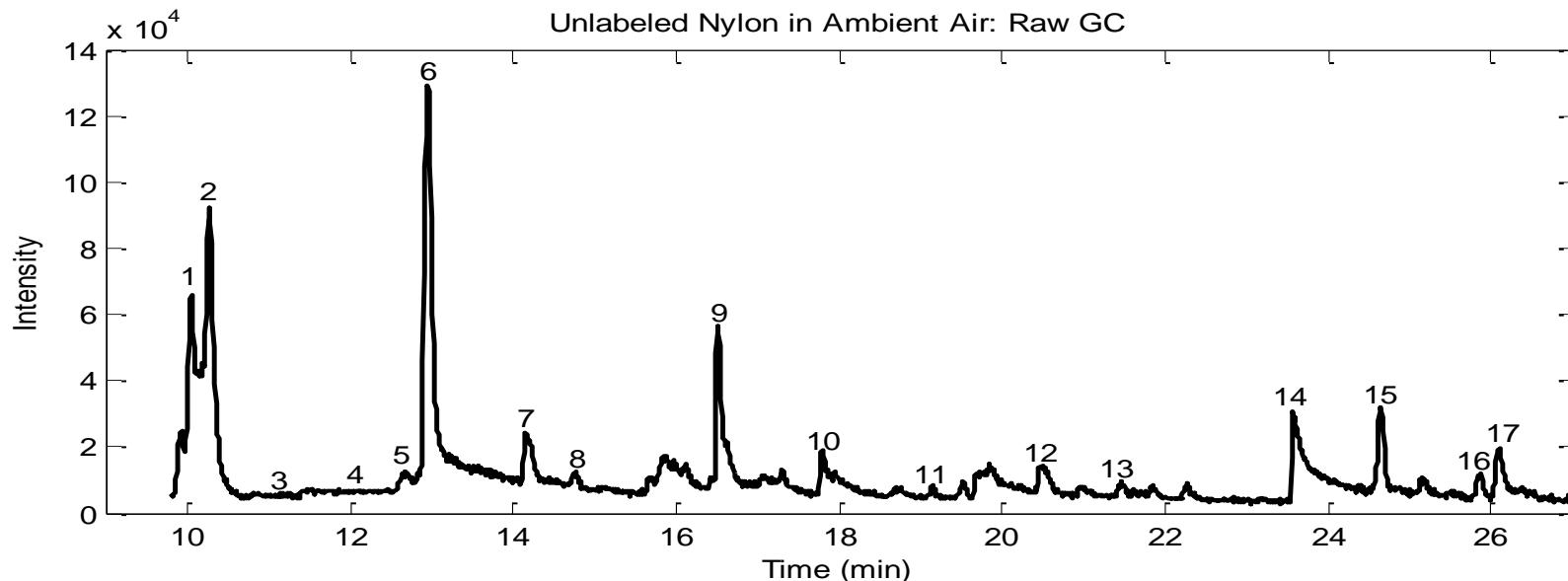


Different Polymers

- Nylon
 - Bridal veils, screws, vehicle tires, toothbrush, musical strings, fabrics...and many other commercial items



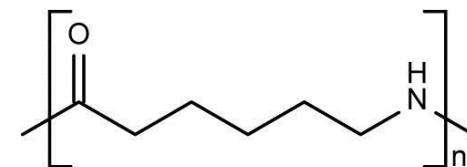
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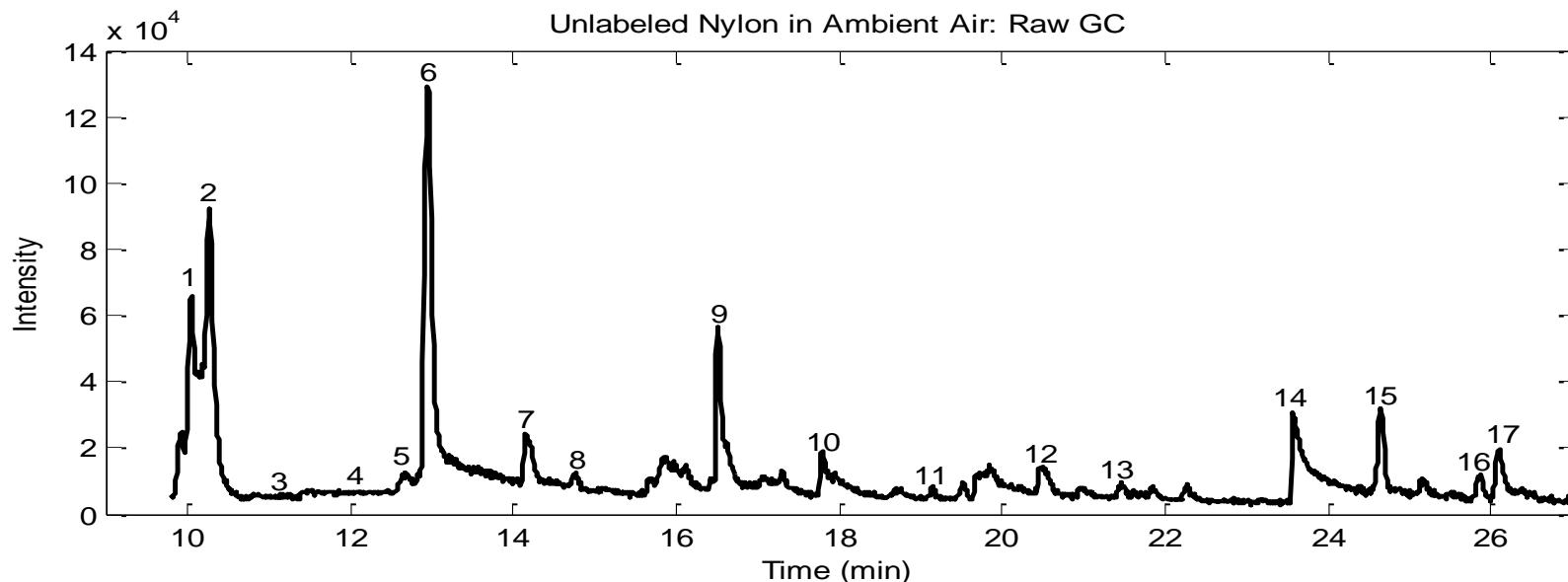
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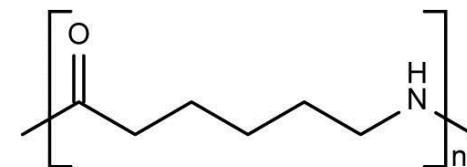
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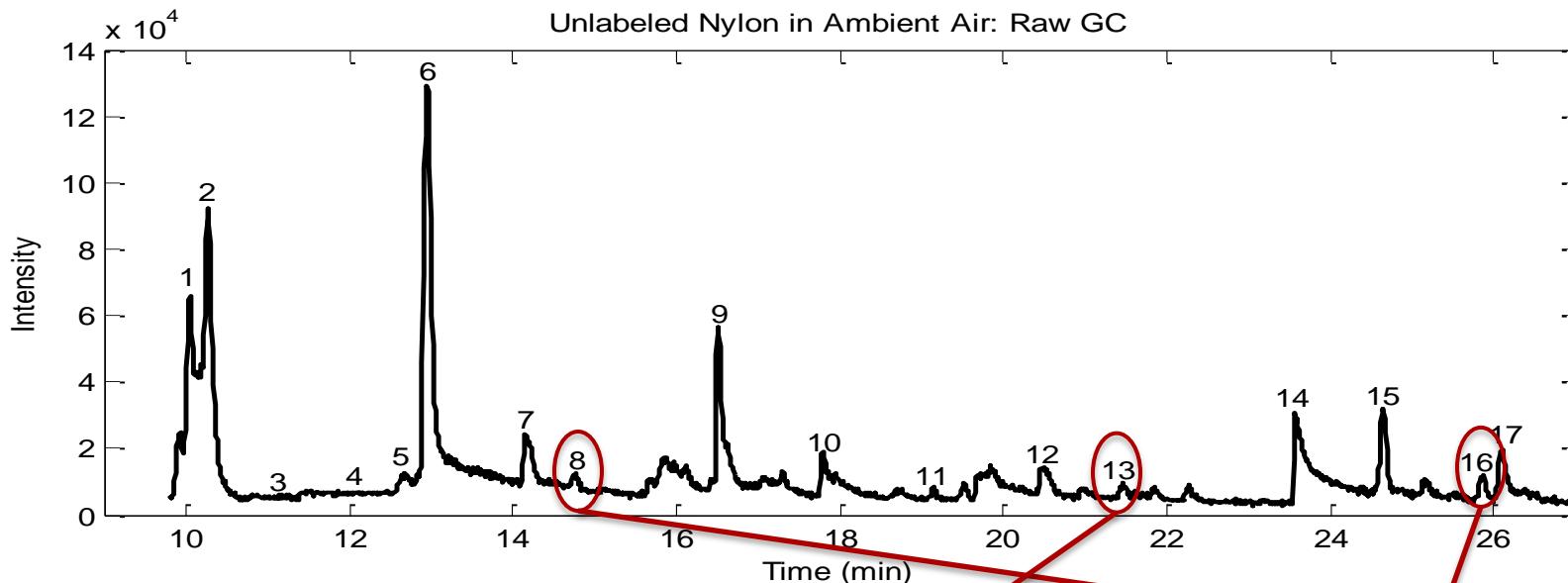
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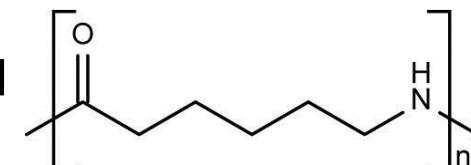
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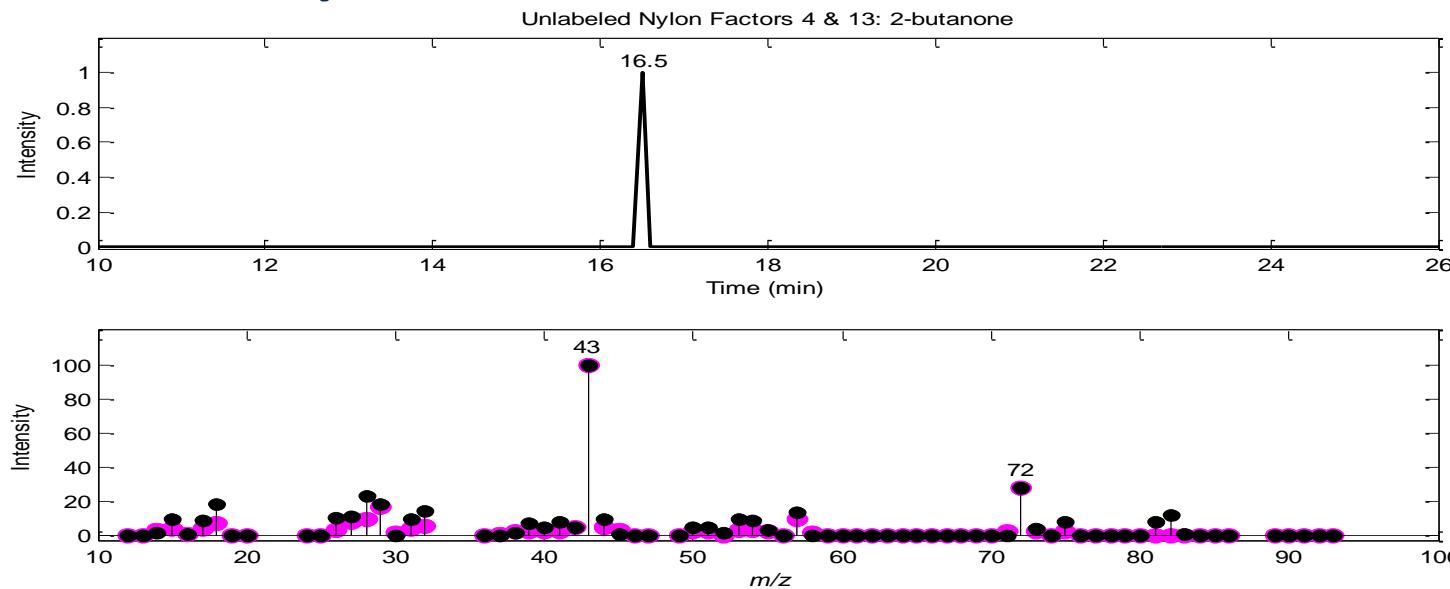
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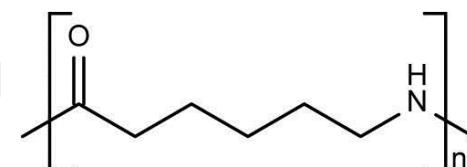
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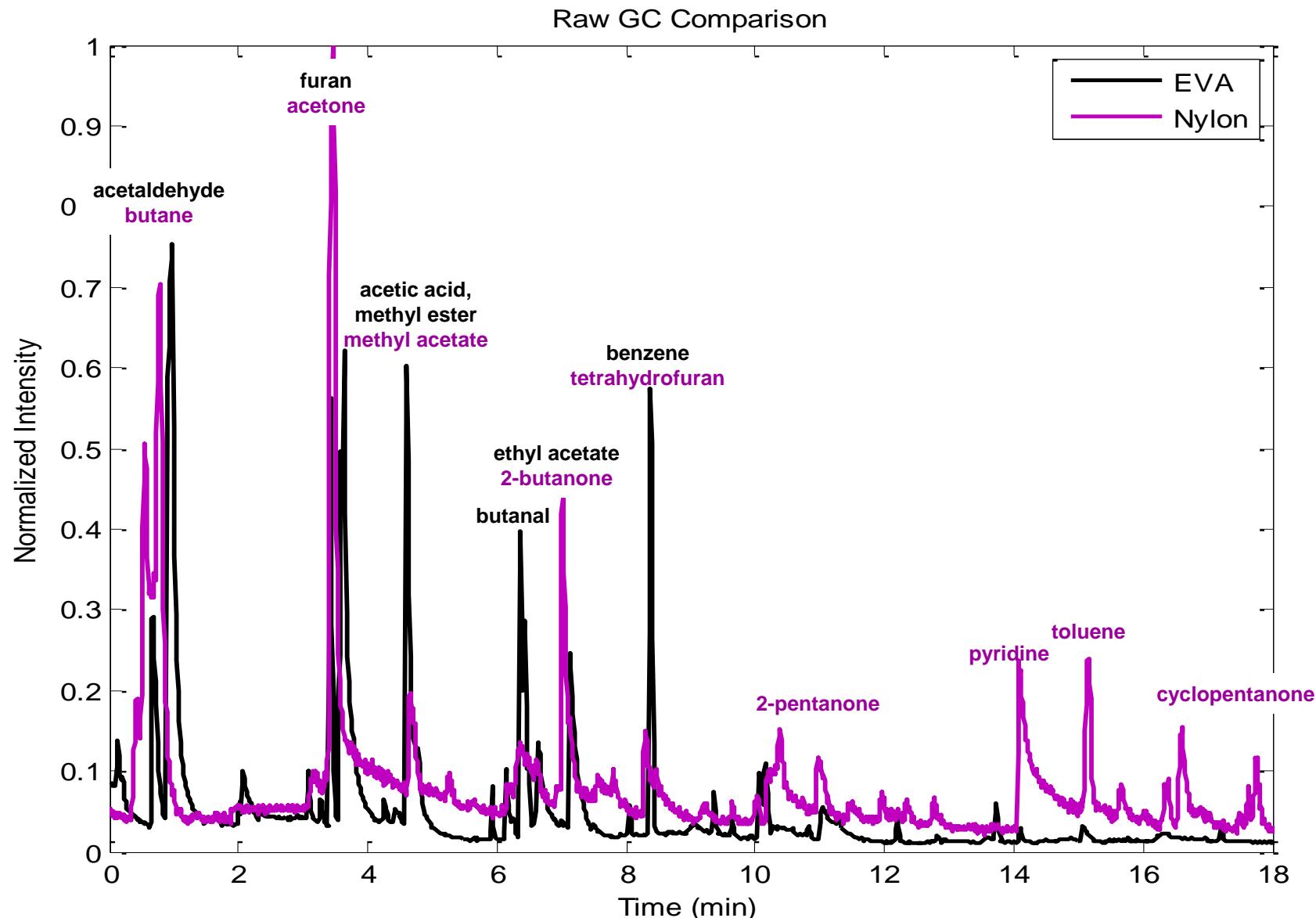
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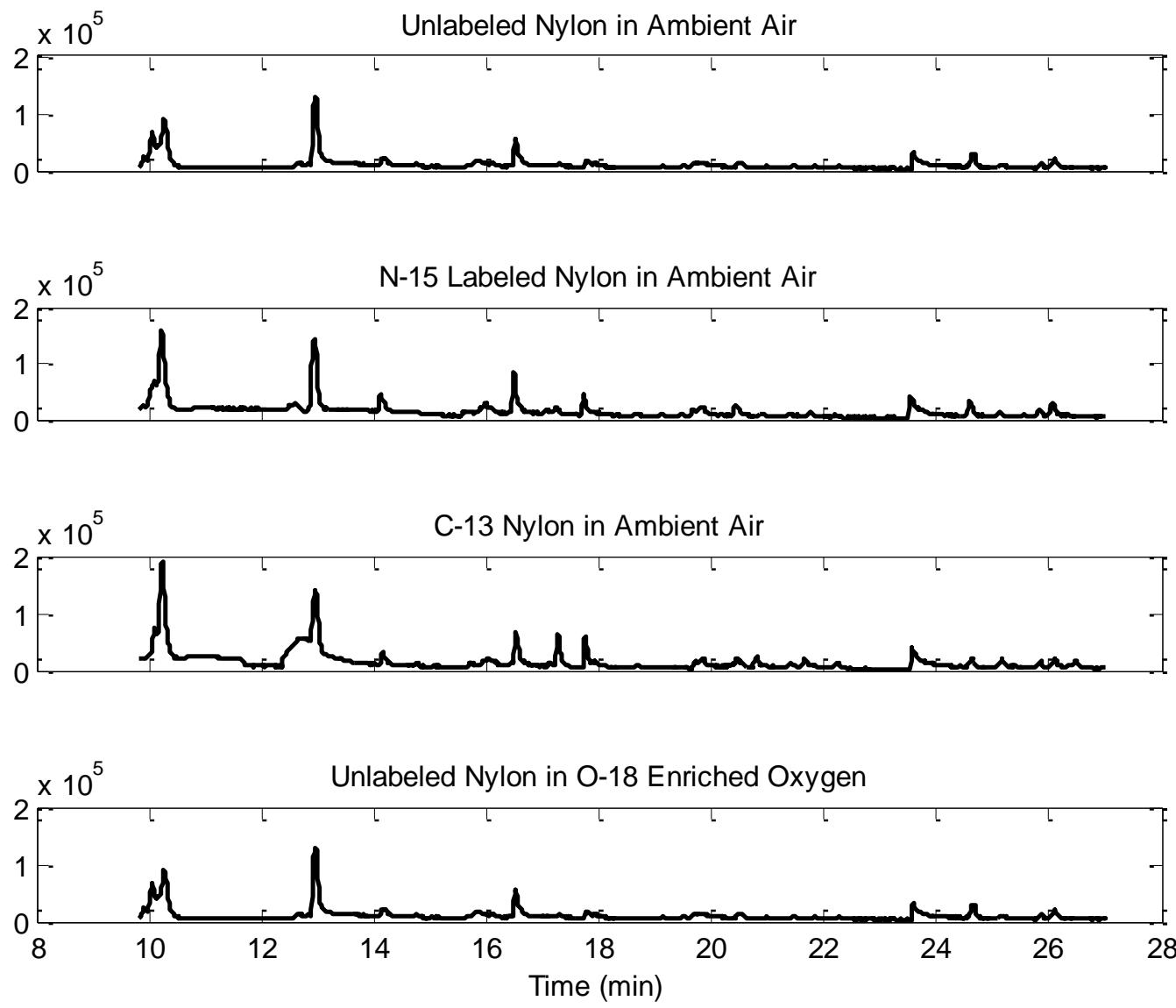
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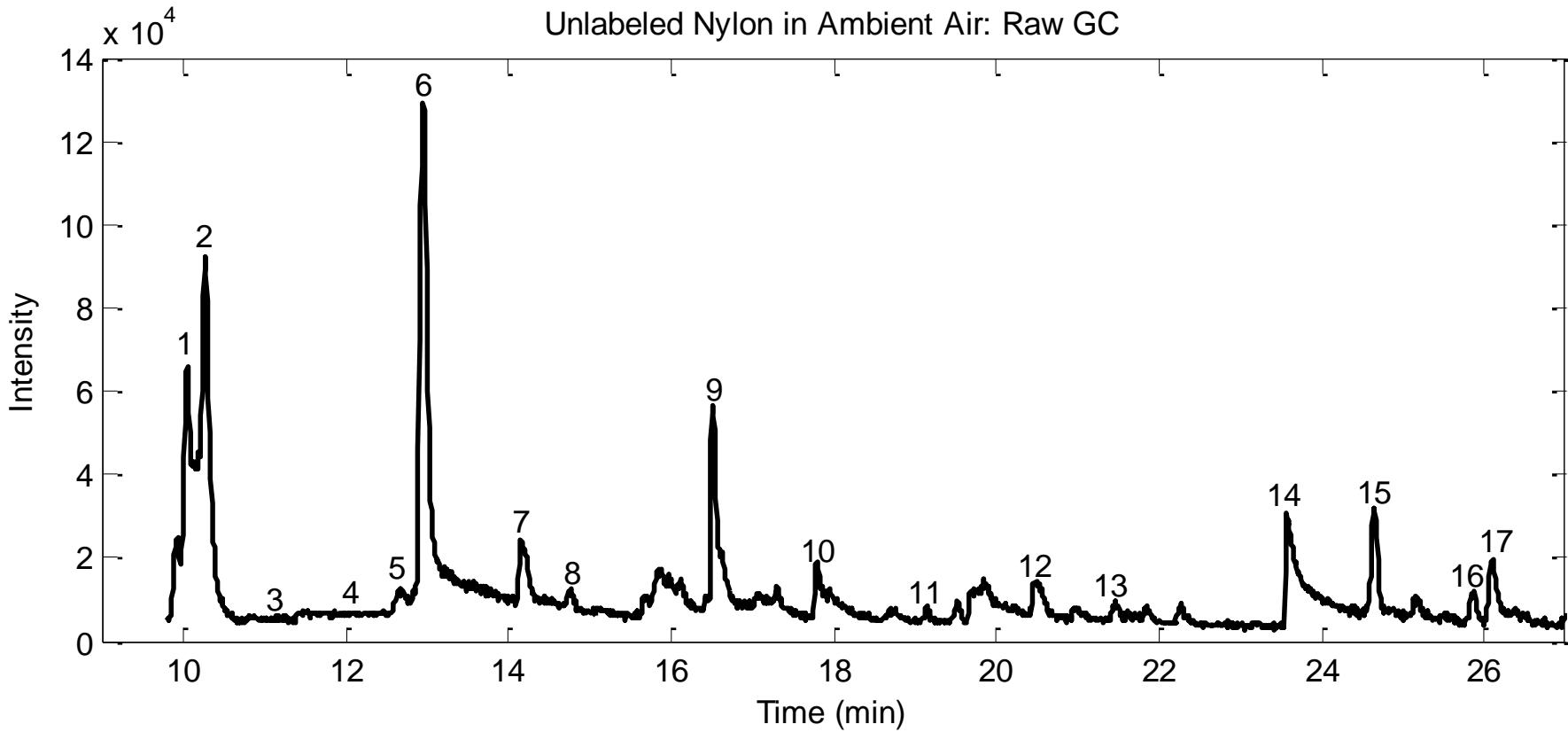
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Labeled vs. Unlabeled: GC



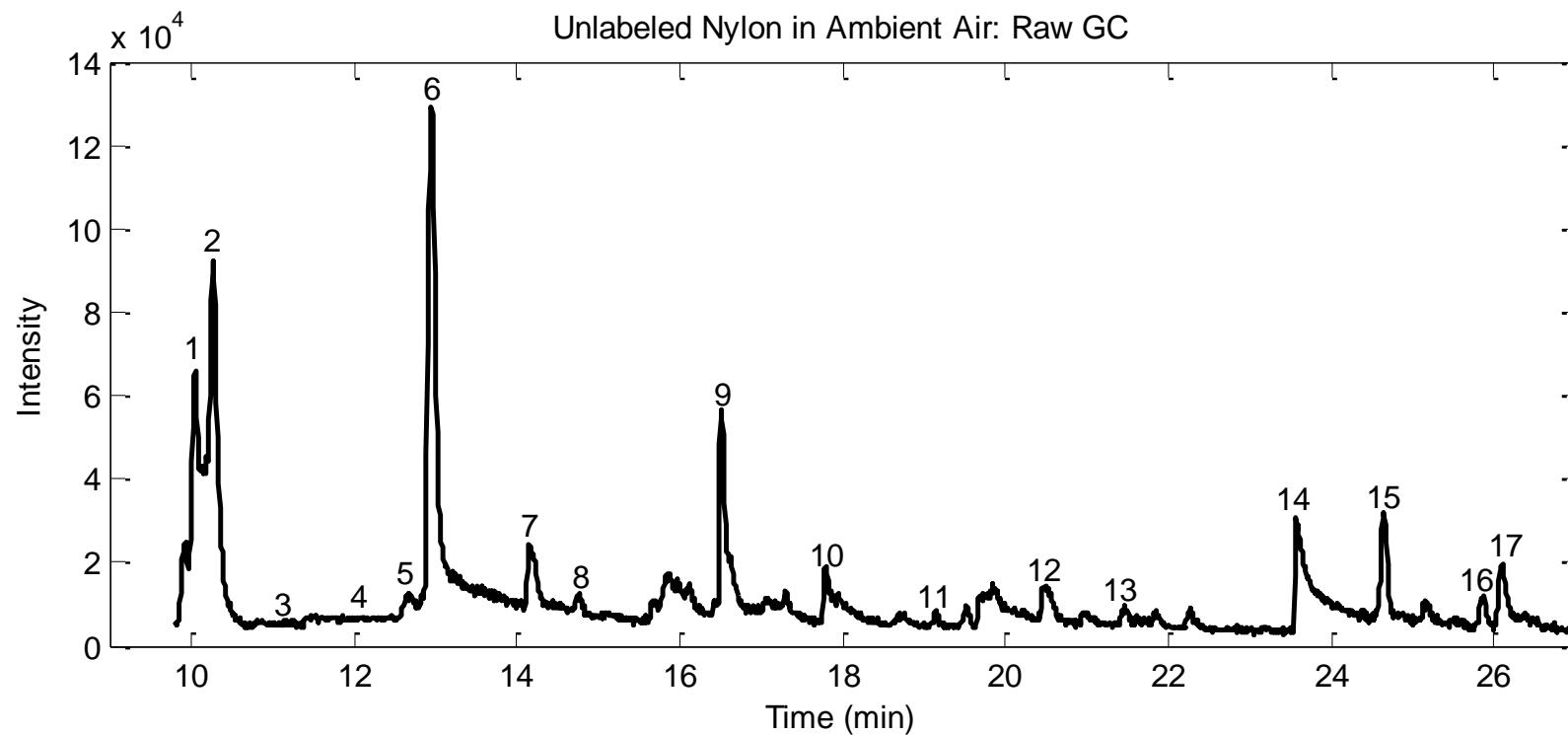
Labeled vs. Unlabeled: GC



Labeled vs. Unlabeled: MS

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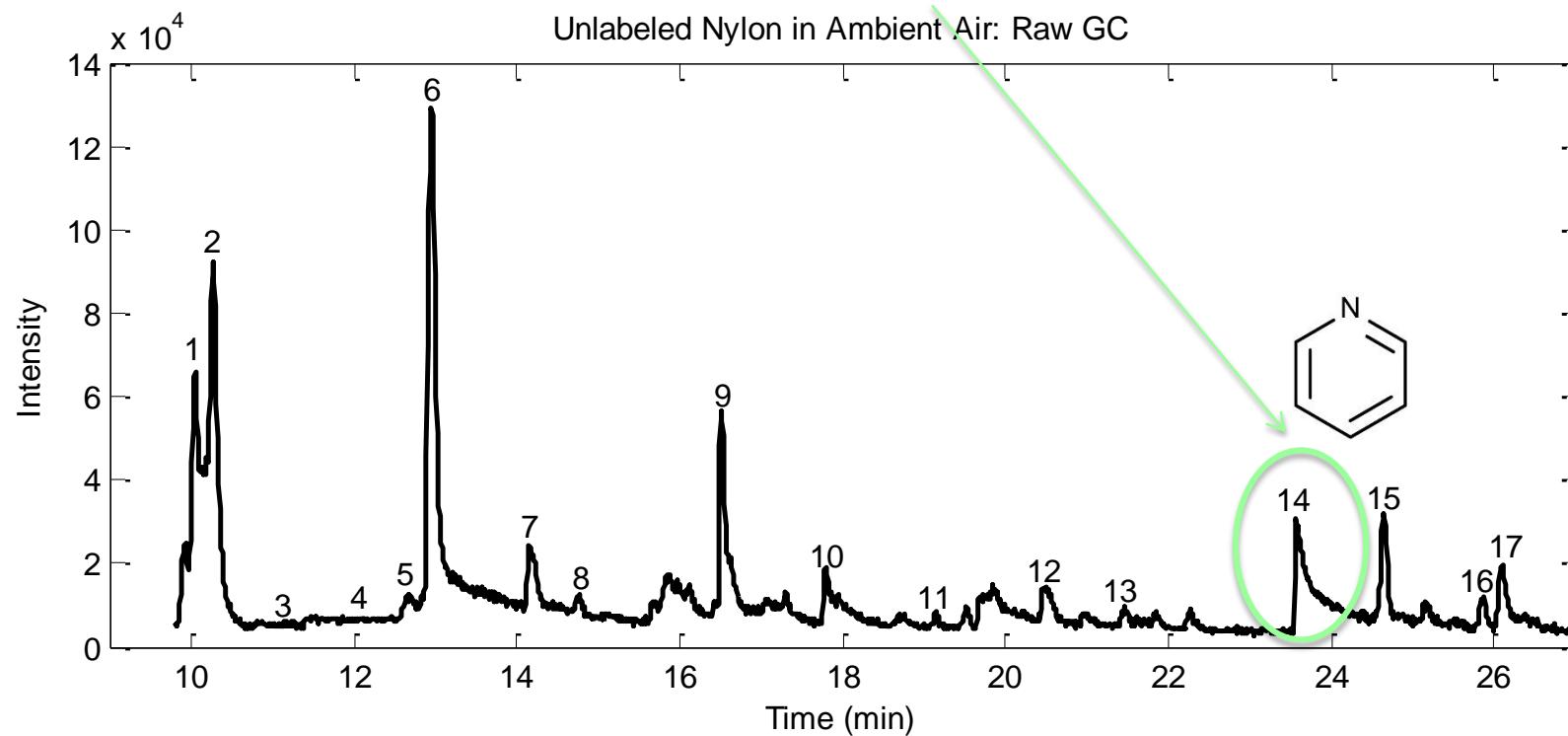
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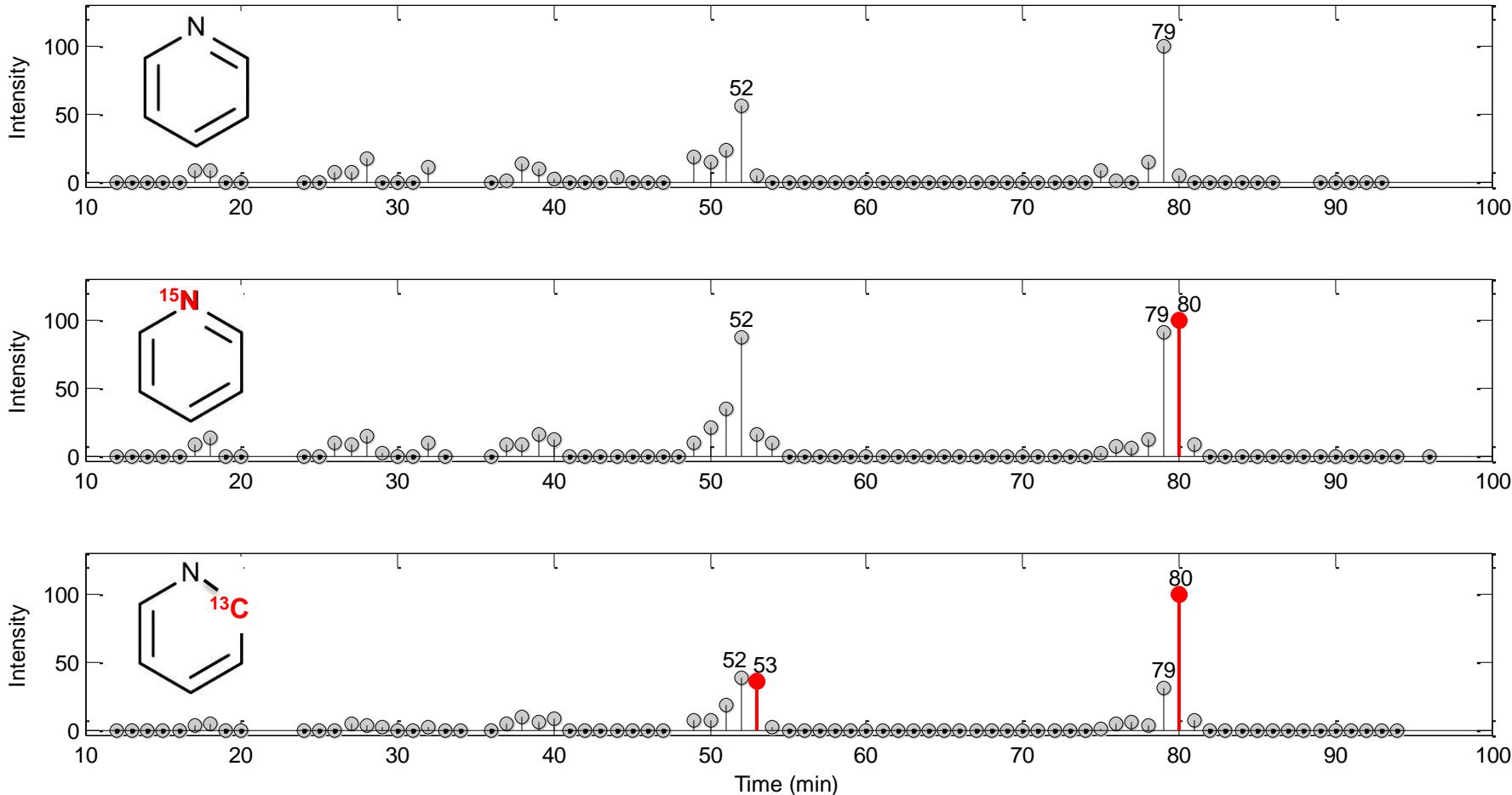
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Labeled vs. Unlabeled: MCR Factors



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Changes with Time

- PARAFAC2: multi-way parallel factor analysis
- Models data in the presence of retention time shifts or shape changes of profiles.
 - No aligning of peaks is necessary.
 - Reduces computational effort.
- Literature:
 - 2005: Classification of pectins with different ester distributions
 - Zachariassen *et al. Chemometrics & Intelligent Laboratory Systems, 83*
 - 2007: Classification of aged petroleum oils
 - Ebrahimi *et al. Journal of Chromatography A, 1166*

Conclusion

- MCR is excellent data exploration tool for first approximation.
- Reduce analysis time from days or weeks to possibly a single day.
- Requires no *a priori* sample knowledge.
- Work to be done:
 - Improve peak recognition for peaks close to baseline.
 - Multi-way analysis of aging studies on a single polymer.
 - Multi-way analysis of labeled vs. unlabeled.

Acknowledgements

- Jim Aubert, 1822
 - Manager
- Mark Van Benthem, 1822
 - Mentor
- James Hochrein, 1825
 - Mentor
- Funding
 - Enhanced Surveillance Campaign

Thank you for your time!