

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

¹*Materials Characterization Department, 1822*

²*Materials Reliability Department, 1825*

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Analysis

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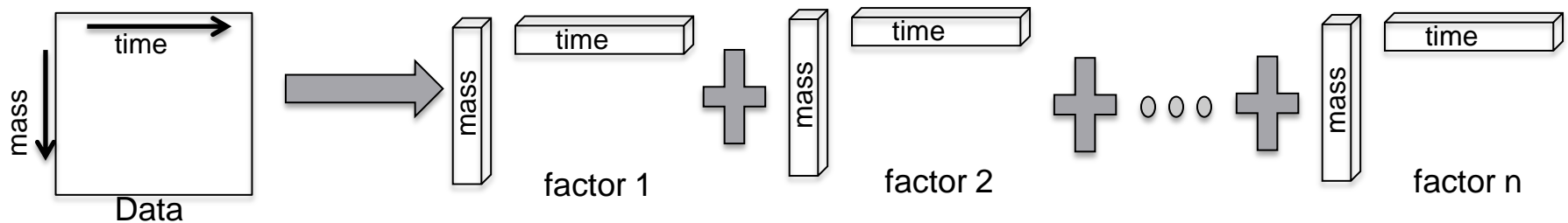


Factor Analysis

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

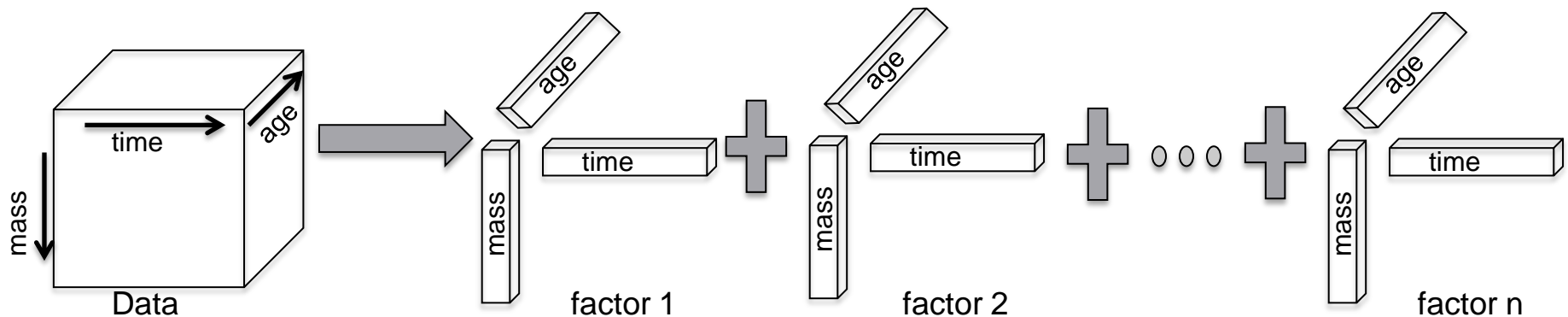
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 - Parallel Factor Analysis (PARAFAC2) → Changes in compounds with time



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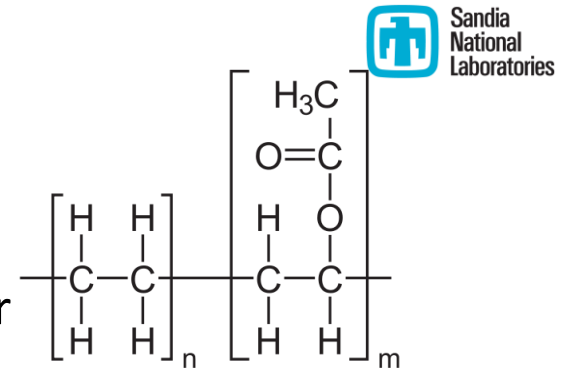
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- *Applications:*

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

Different Polymers

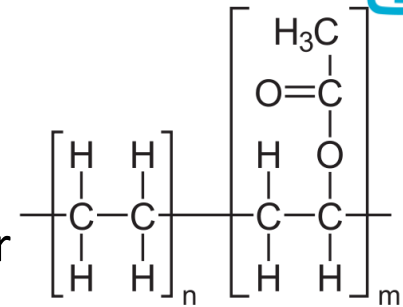
- Ethylene-vinyl acetate (EVA)
 - Hot glue sticks, ski boot padding, fishing rods, cigarette paper, plastic wrap clinginess enhancer



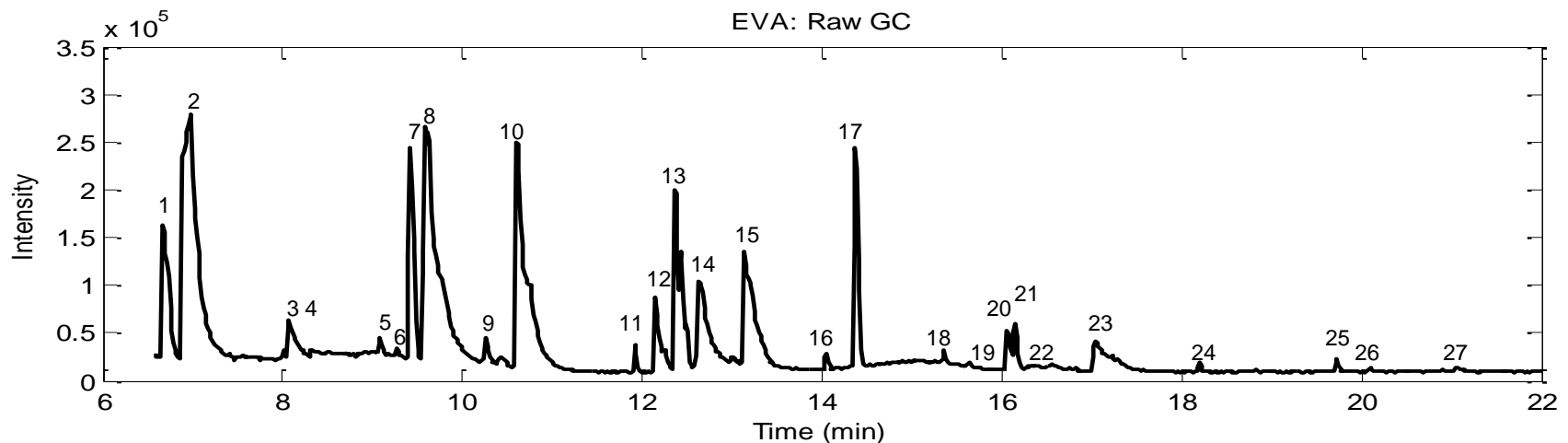
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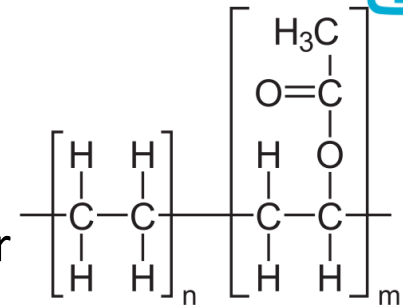
1			2		3		4		5		6		7		8		9	
1-propene, 2-methyl			acetaldehyde		ethyl chloride		methyl formate		1-pentene		pentane		furan		propanal		acetone	
10			11		12		13	14		15		16		17		18		
acetic acid methyl ester			1-hexene		acetic acid ethenyl ester		butanal	2-butanone		ethyl acetate		butane, 1-chloro		benzene		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		



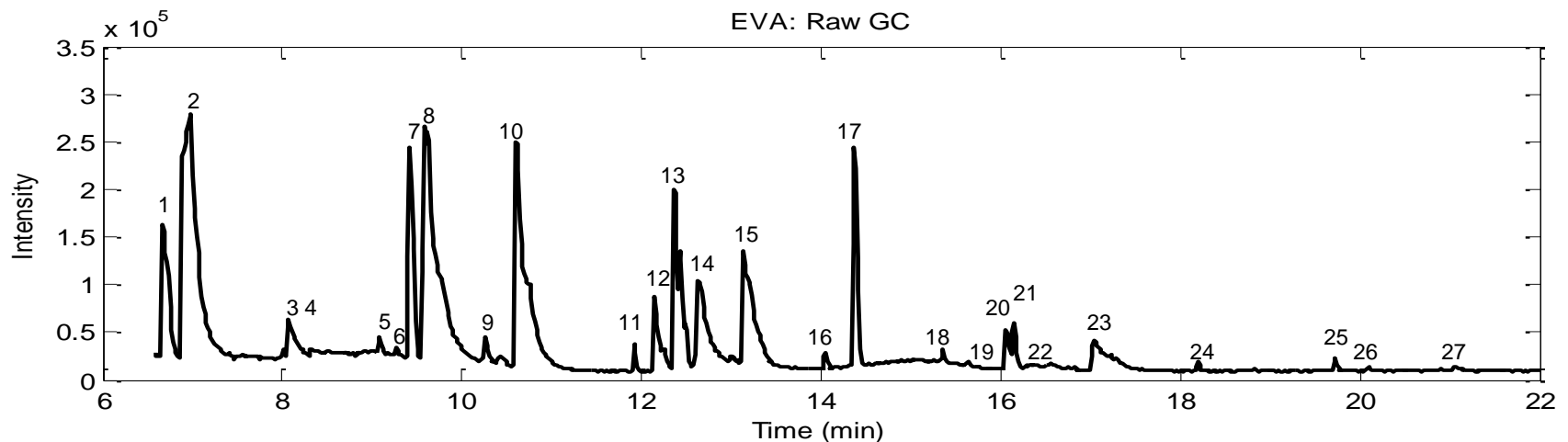
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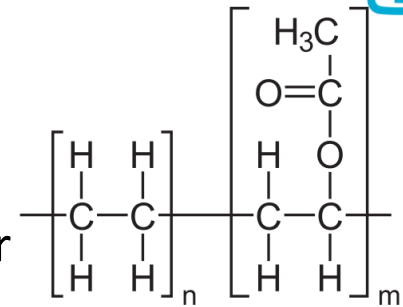
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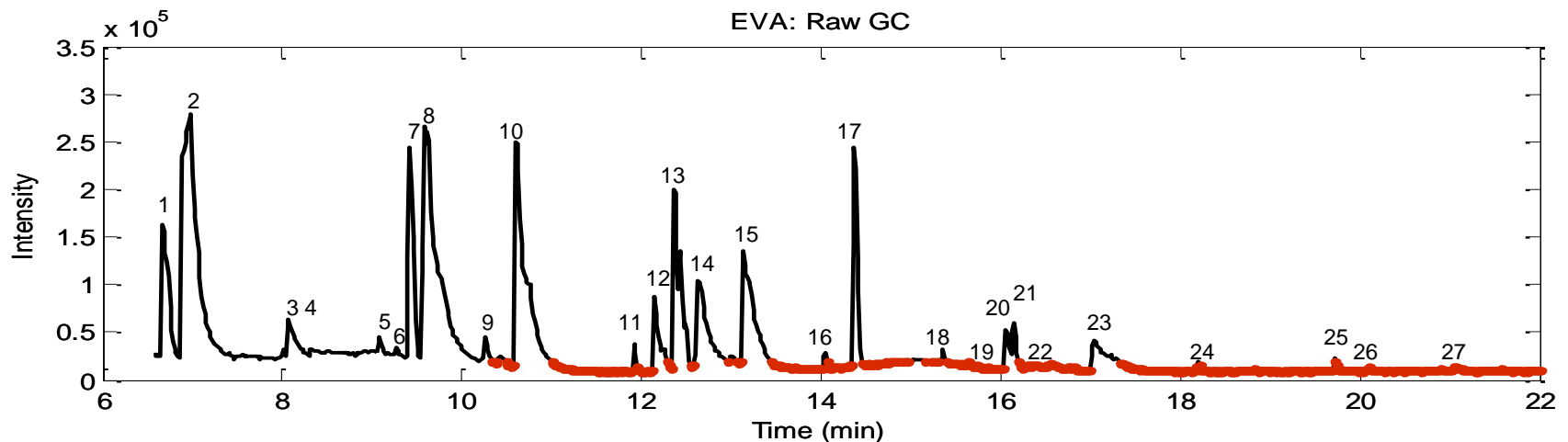
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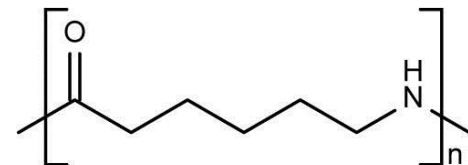
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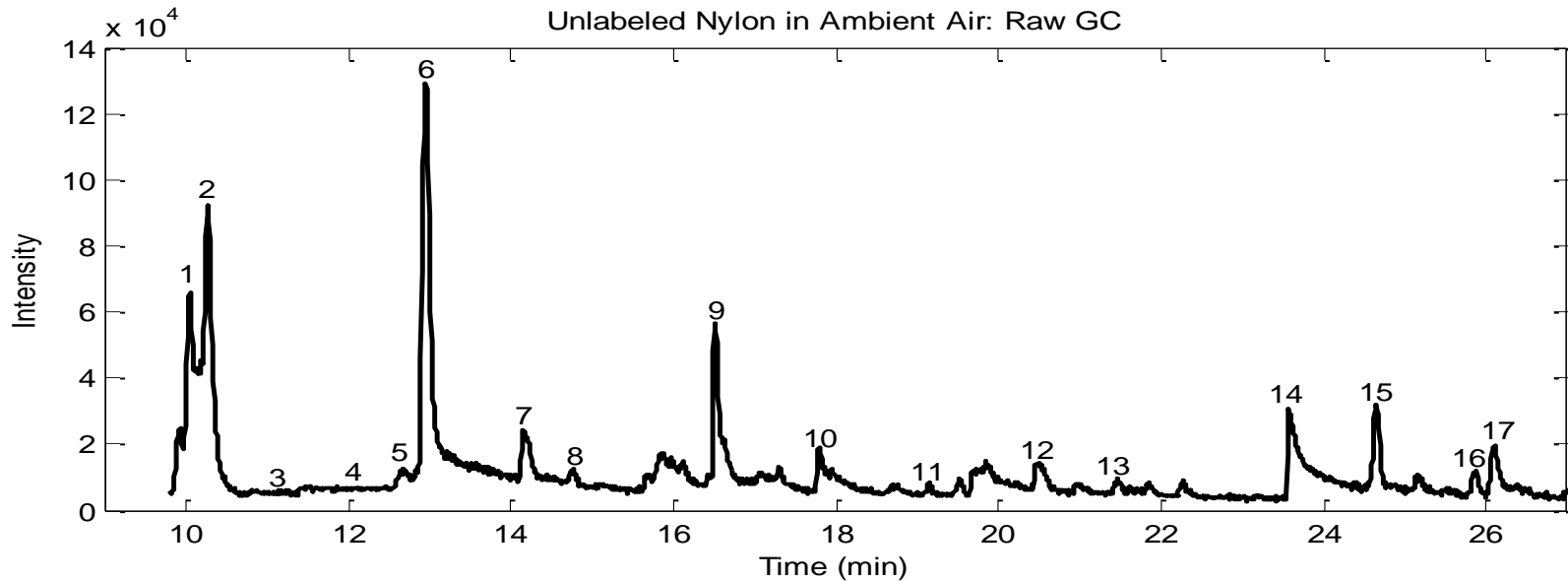
Different Polymers

- Nylon

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



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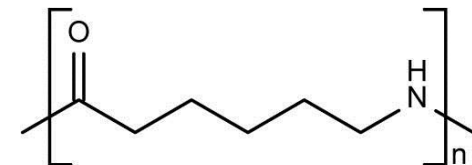


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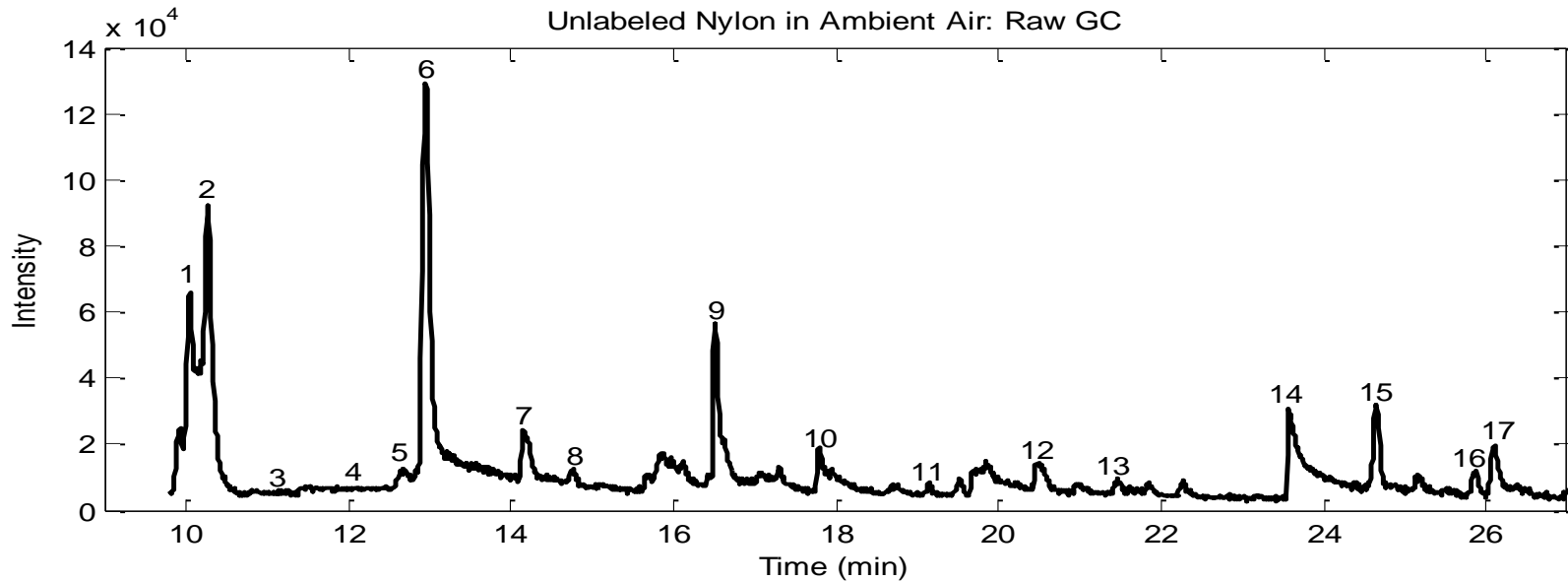
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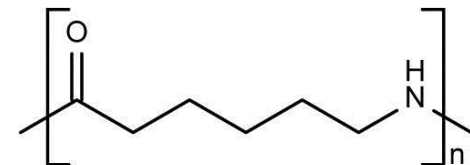
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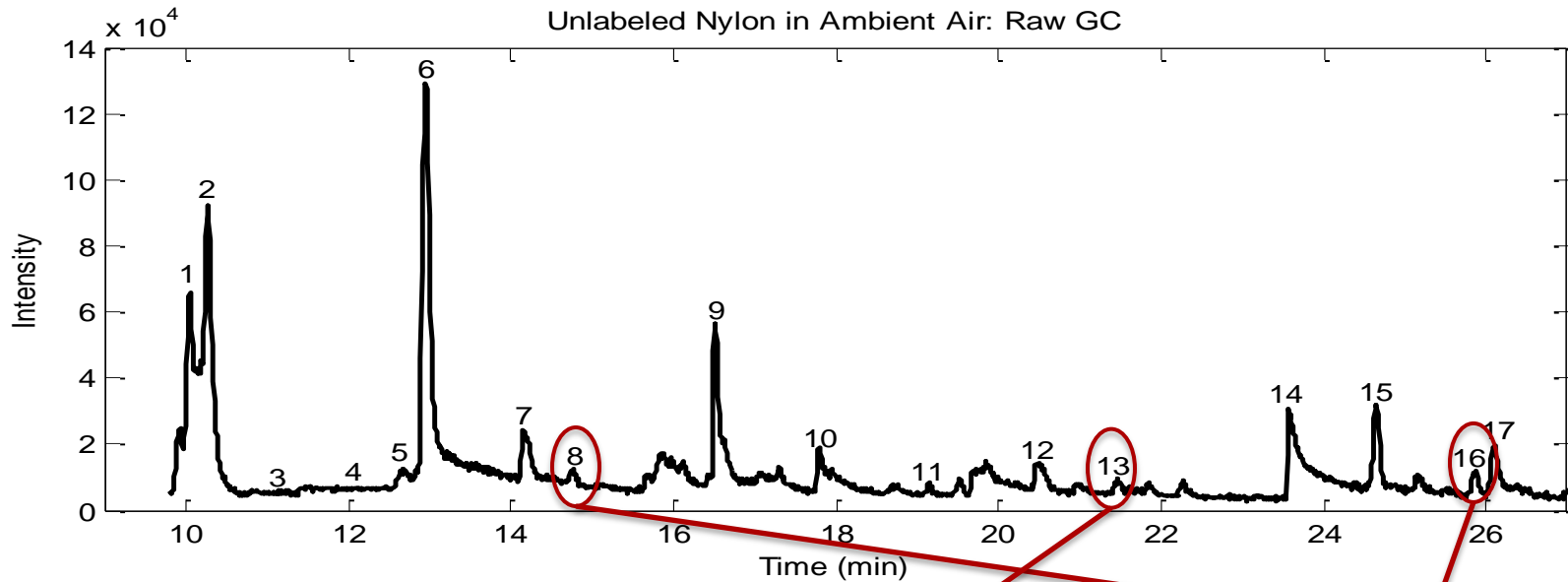
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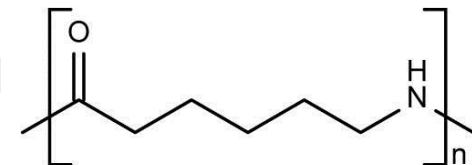
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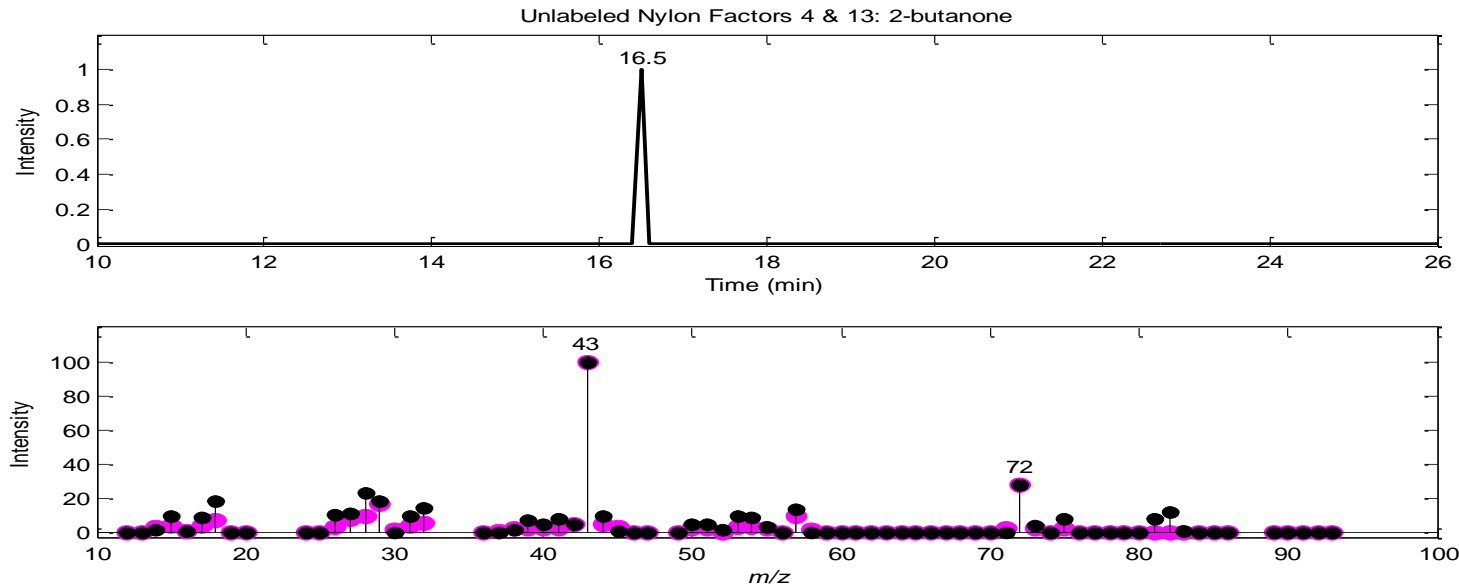
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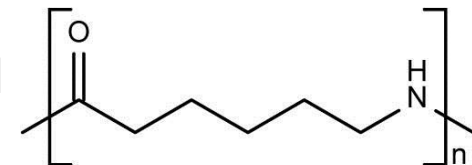
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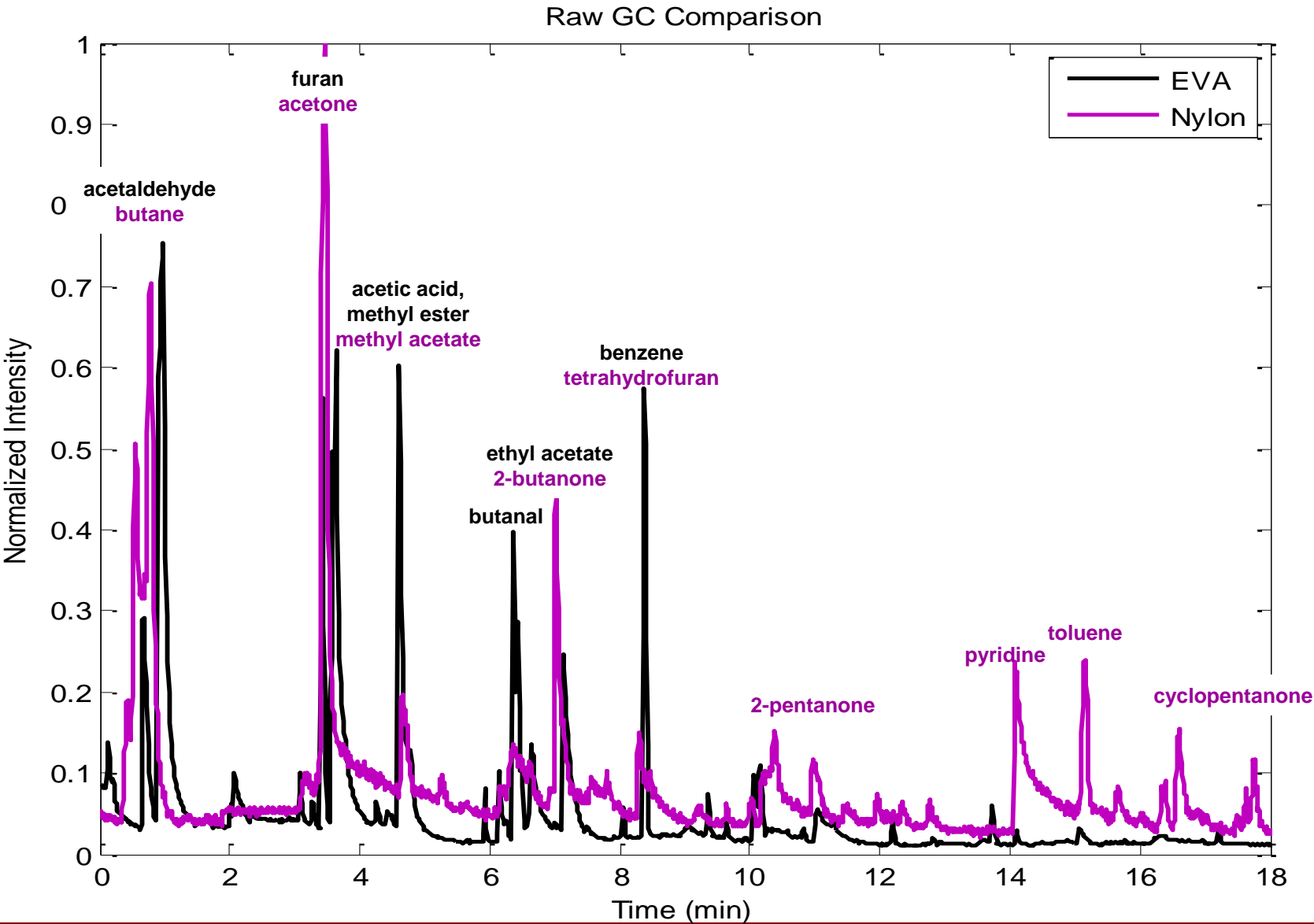
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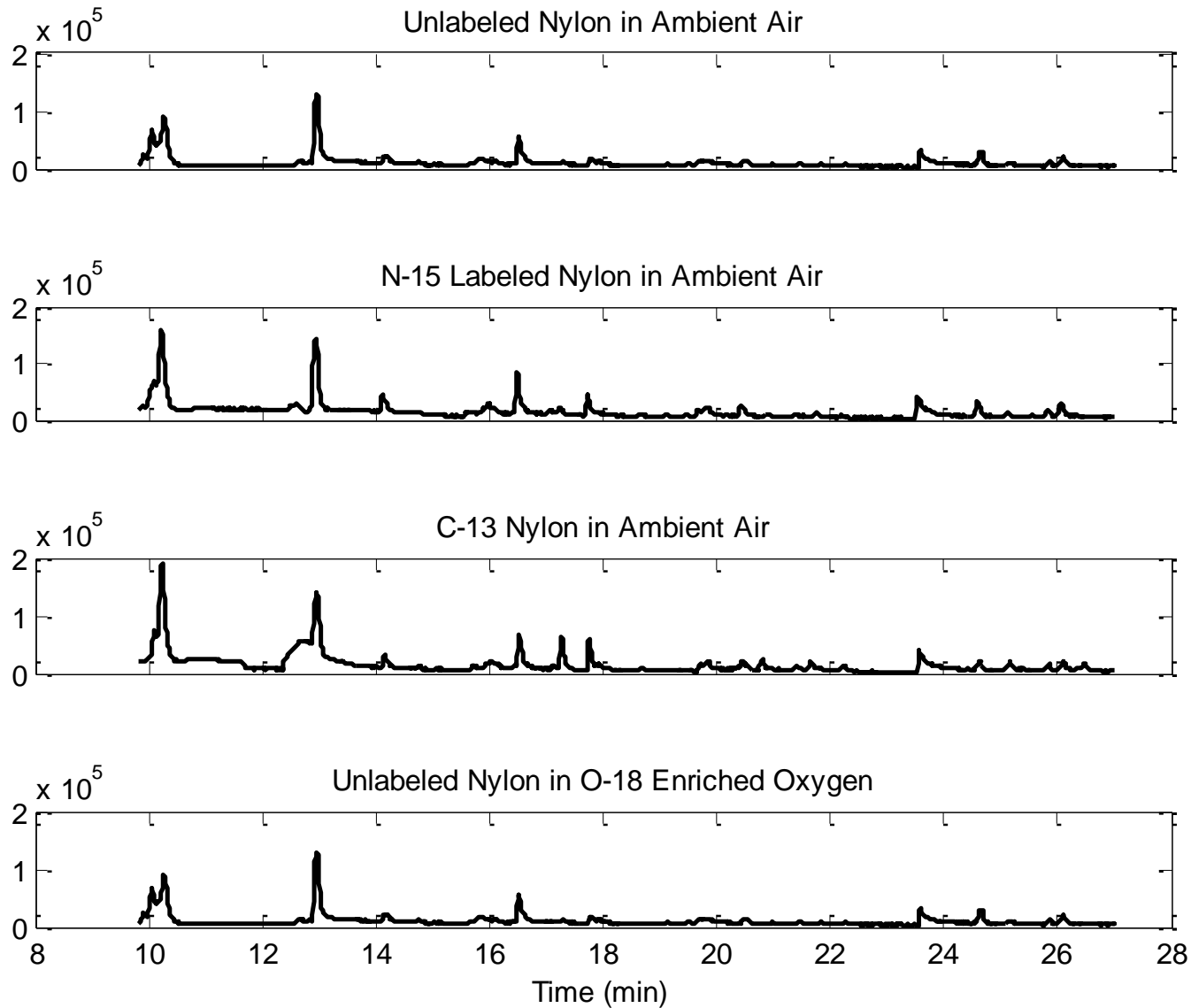
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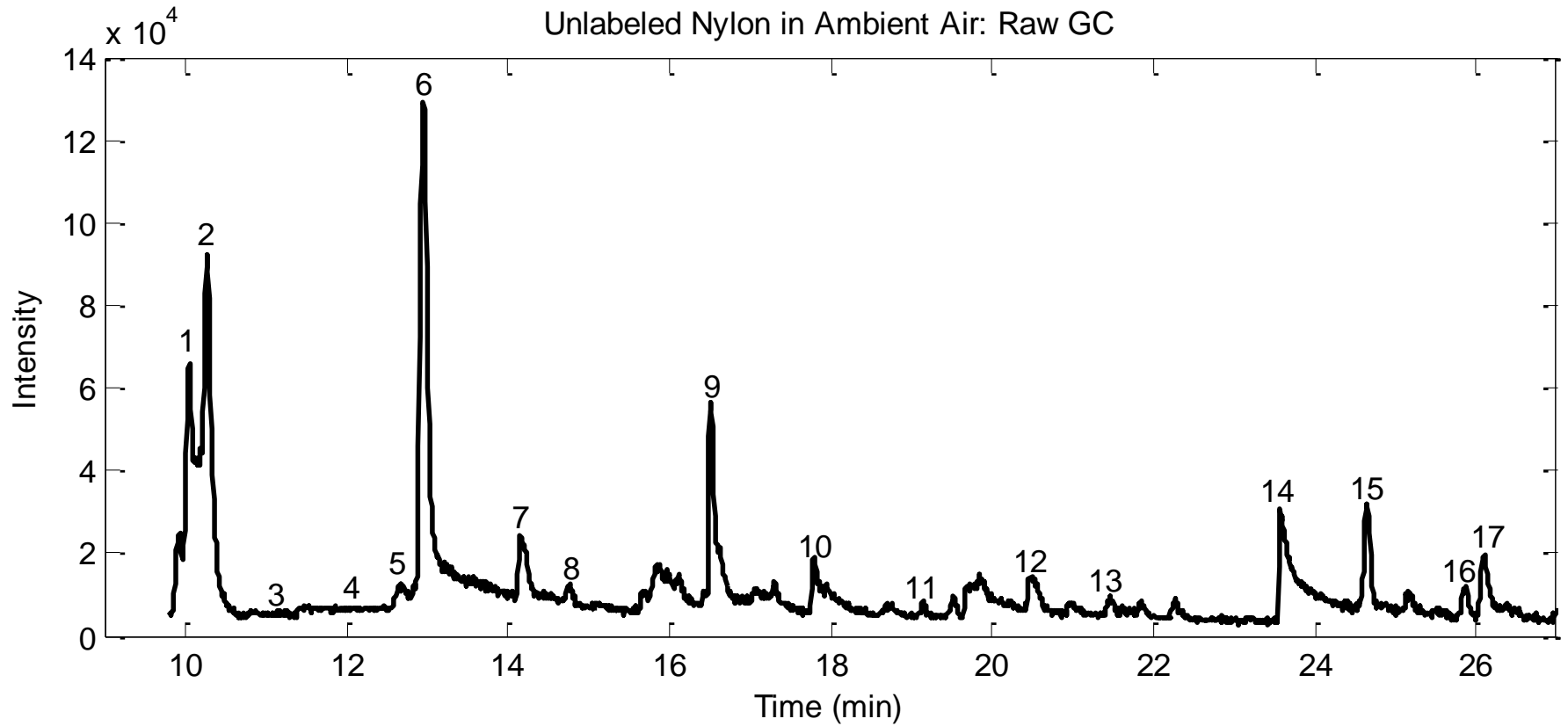
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Labeled vs. Unlabeled: GC



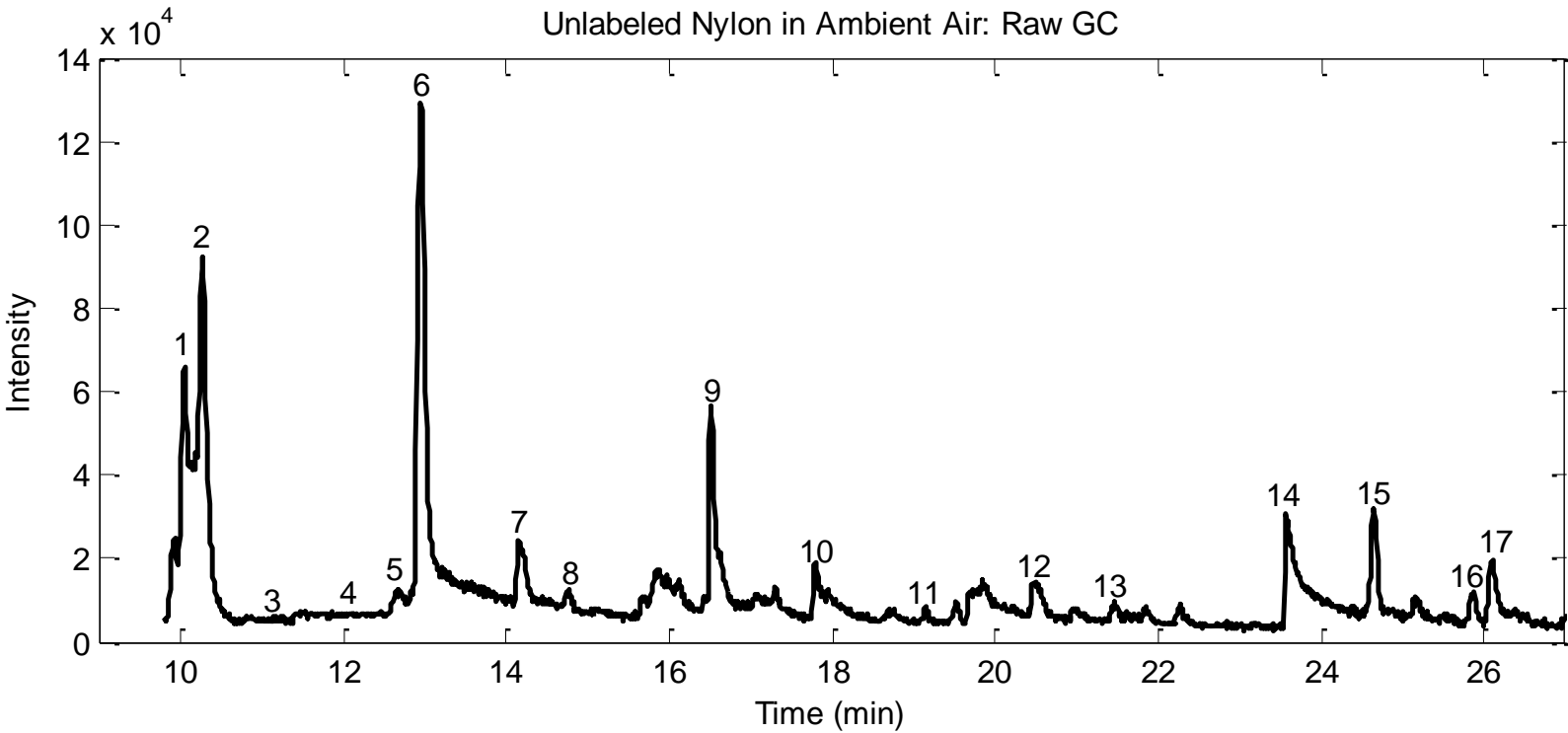
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Labeled vs. Unlabeled: MS

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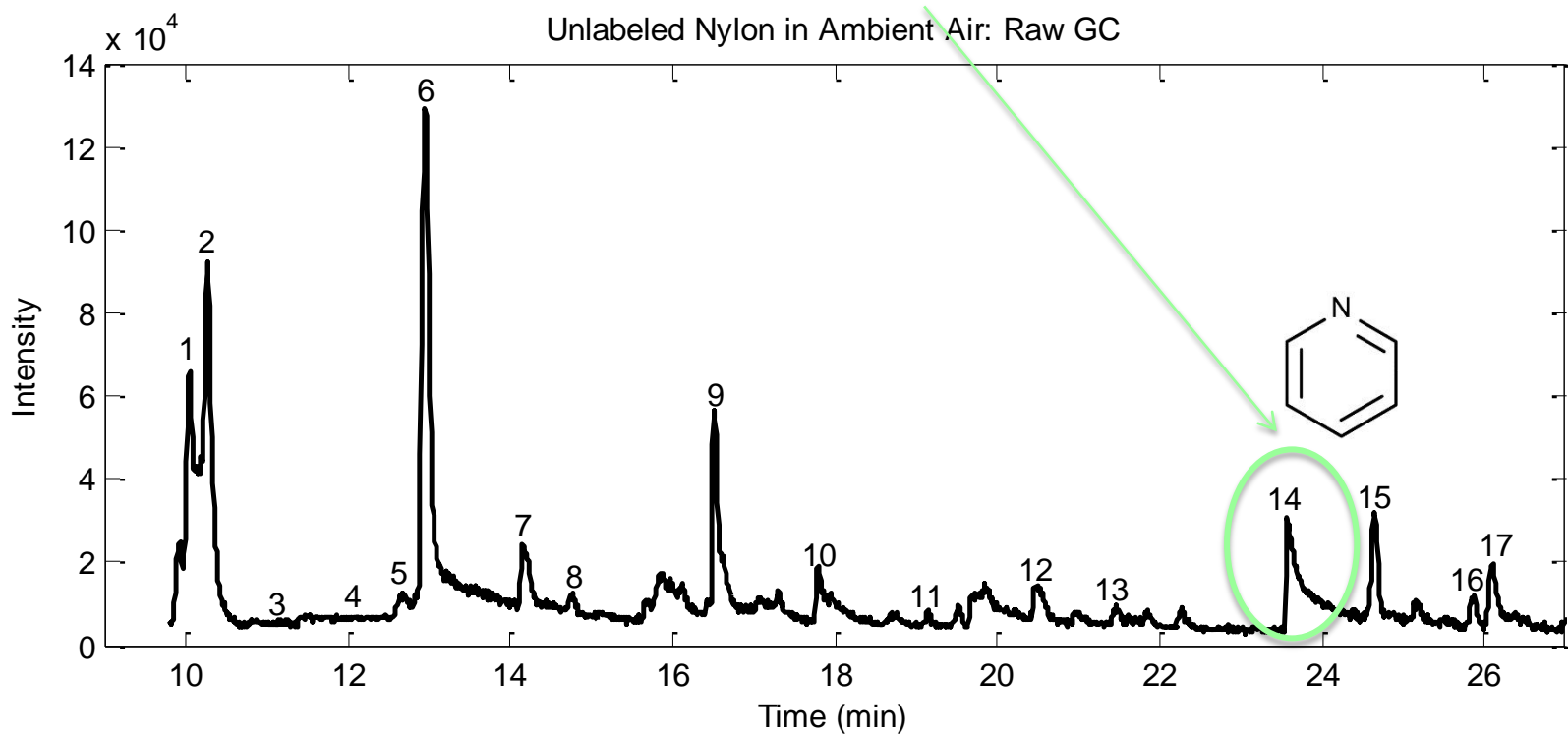
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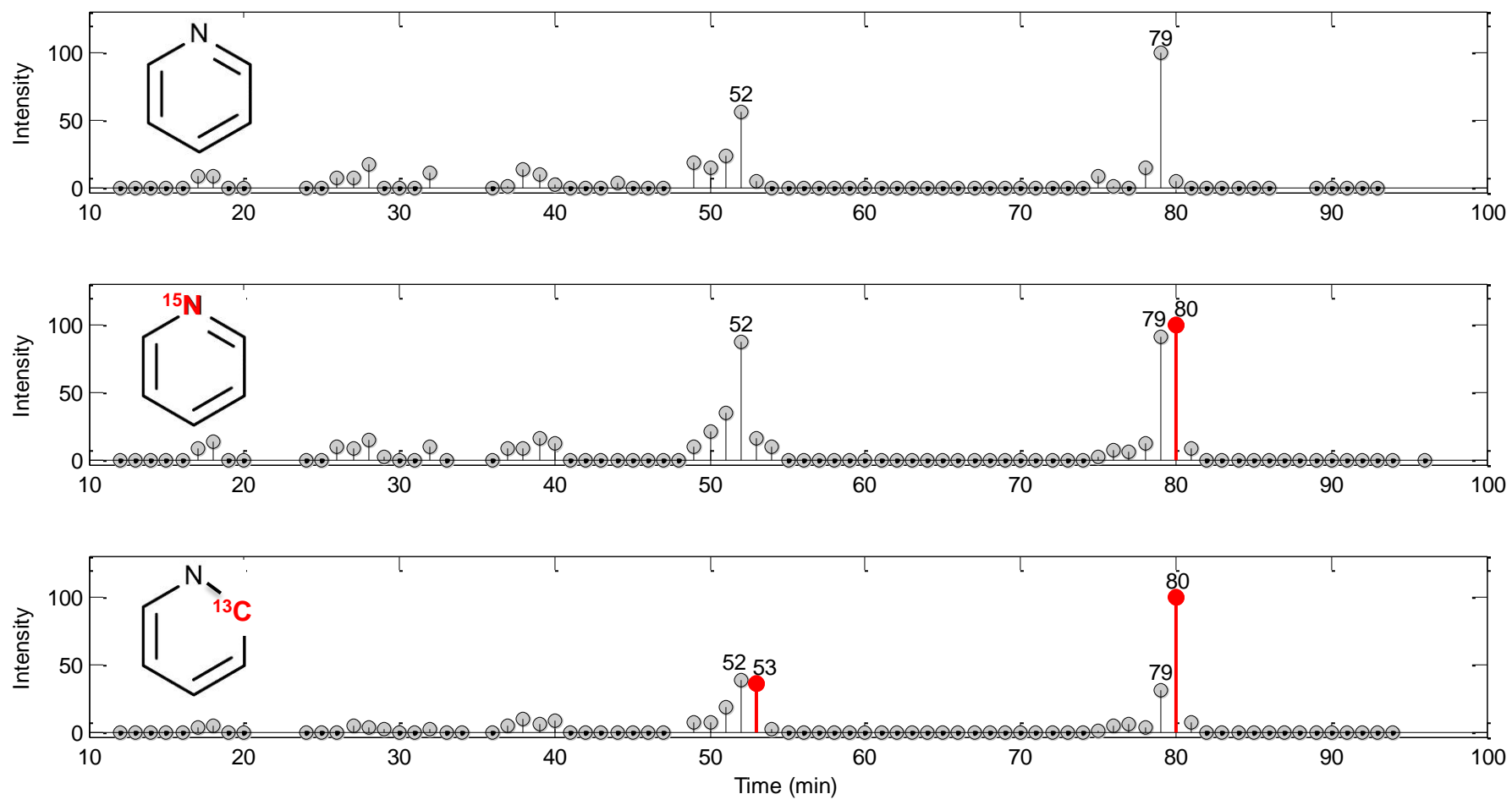
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Labeled vs. Unlabeled: MCR Factors



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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!