Selective Detection and Classification of Compounds by GCxGC-TOFMS

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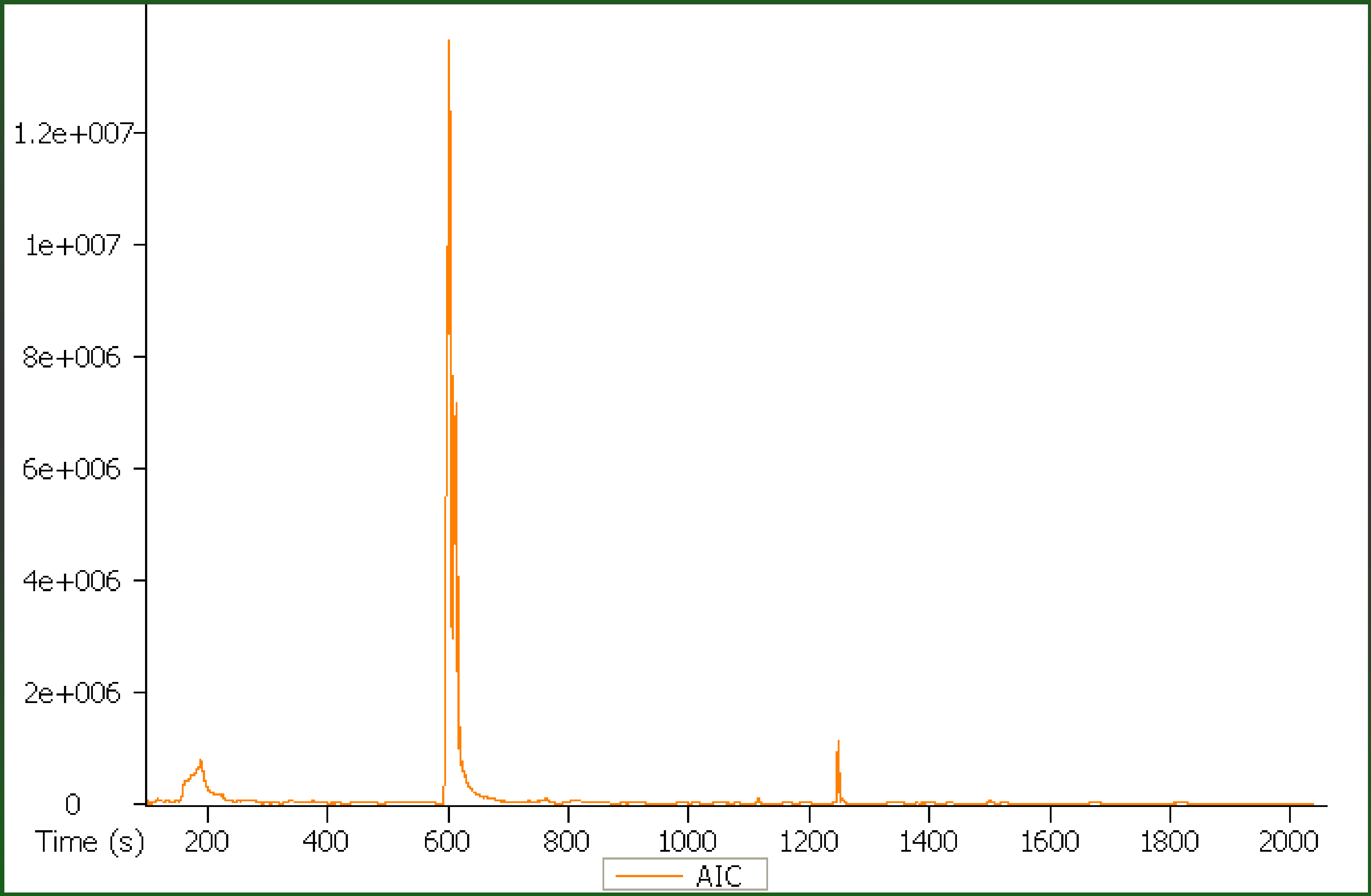
Life Science and Chemical Analysis Solution

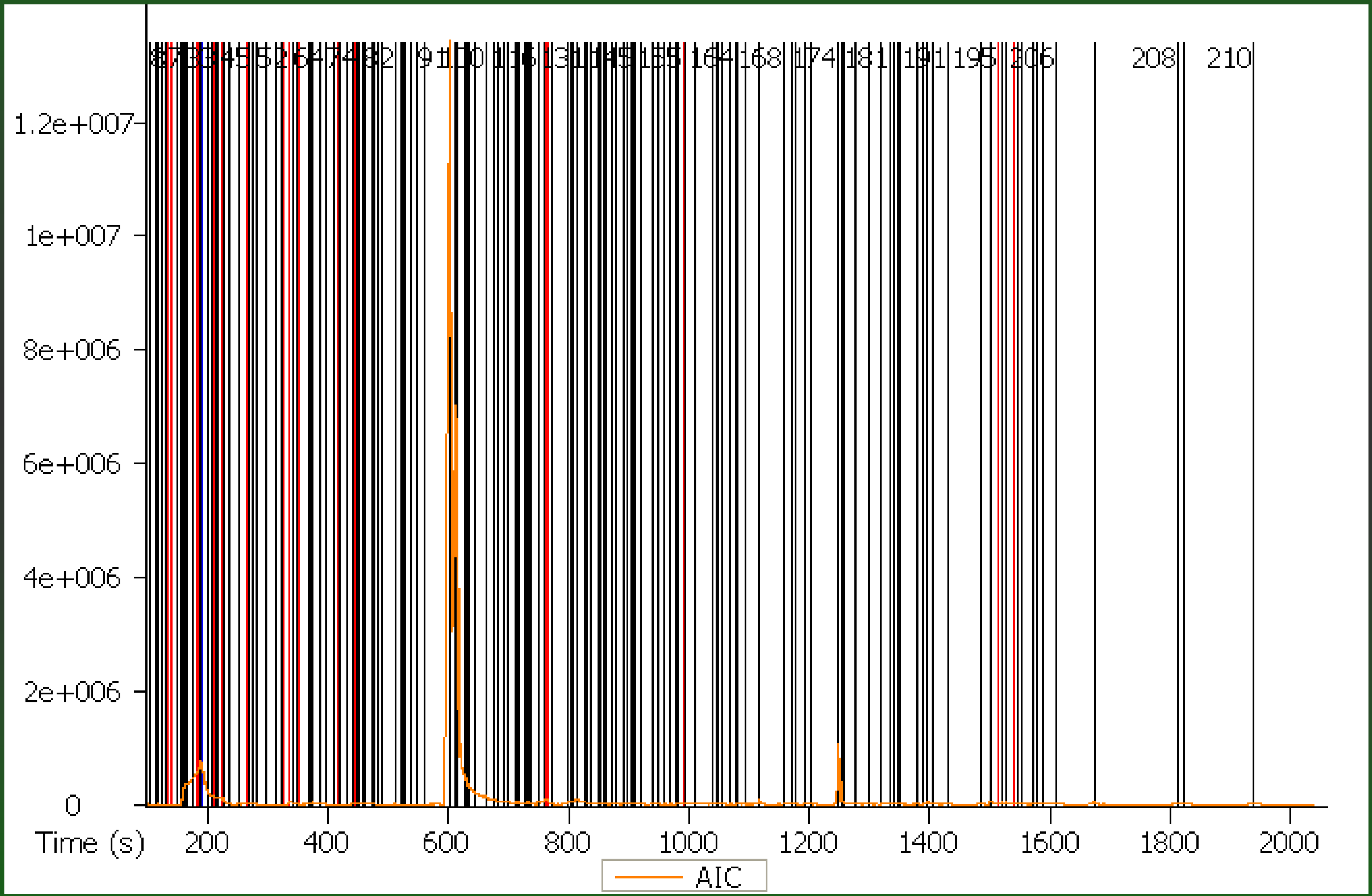
Overview

- GCxGC -MS provides significantly more information about a sample
- Automated selection of peaks based on mass spectral features can quickly identify compounds of interest
- Using such identification complex mixtures can be compared based on individual compounds and/or summaries of classes of compounds identified

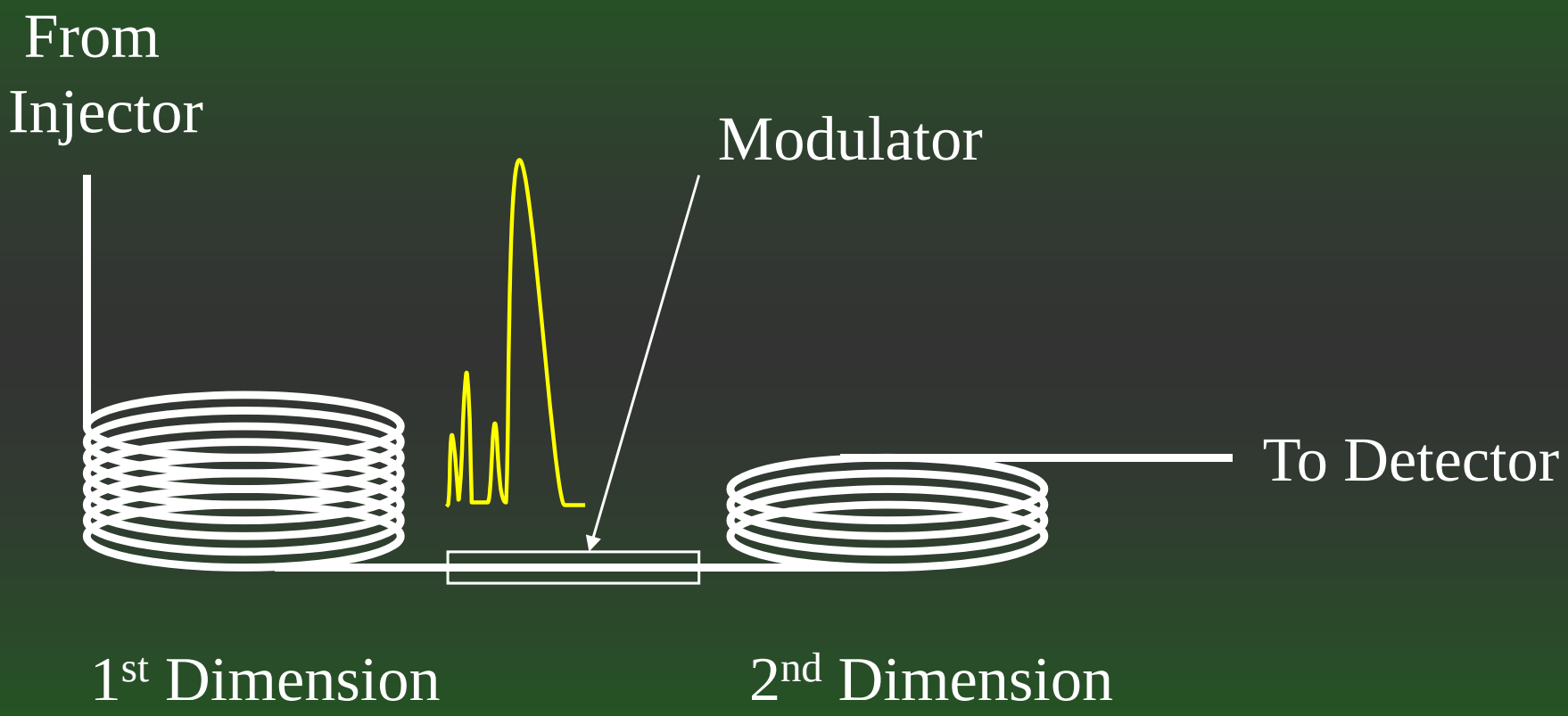
We can find a lot in smoke…



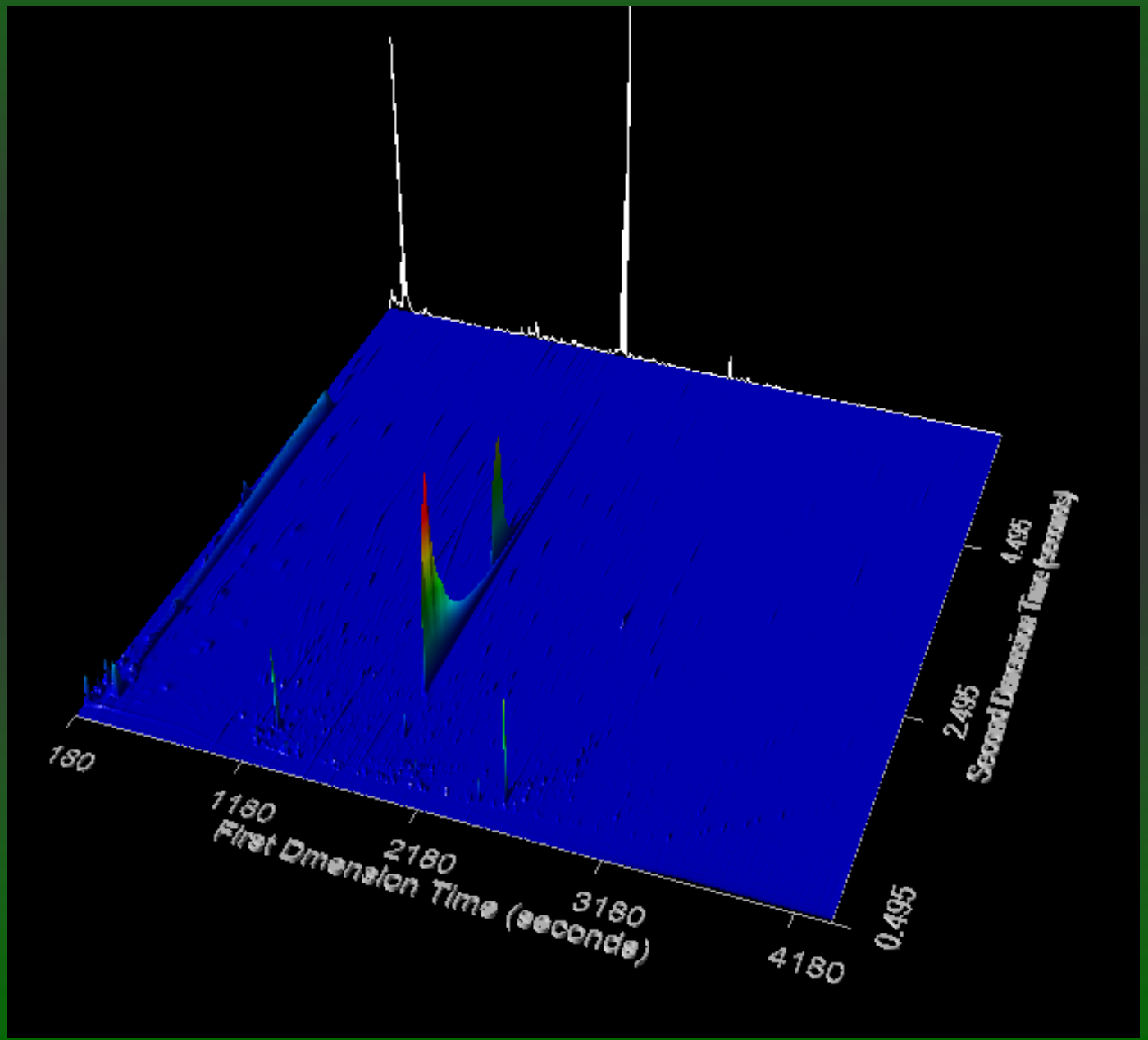
We can find a lot in smoke…



Adding Another Dimension to GC



And, with GCxGC we find it…



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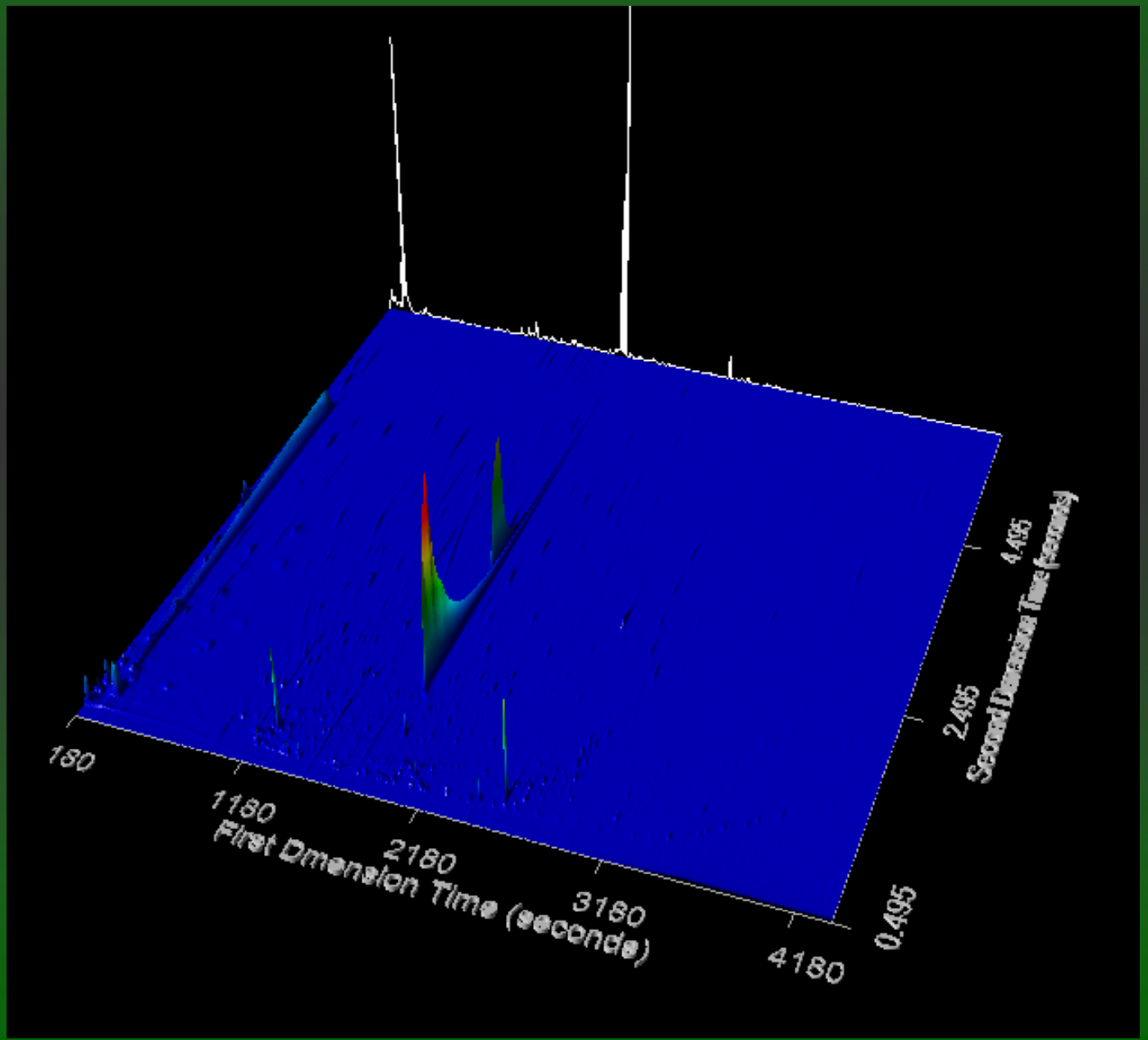

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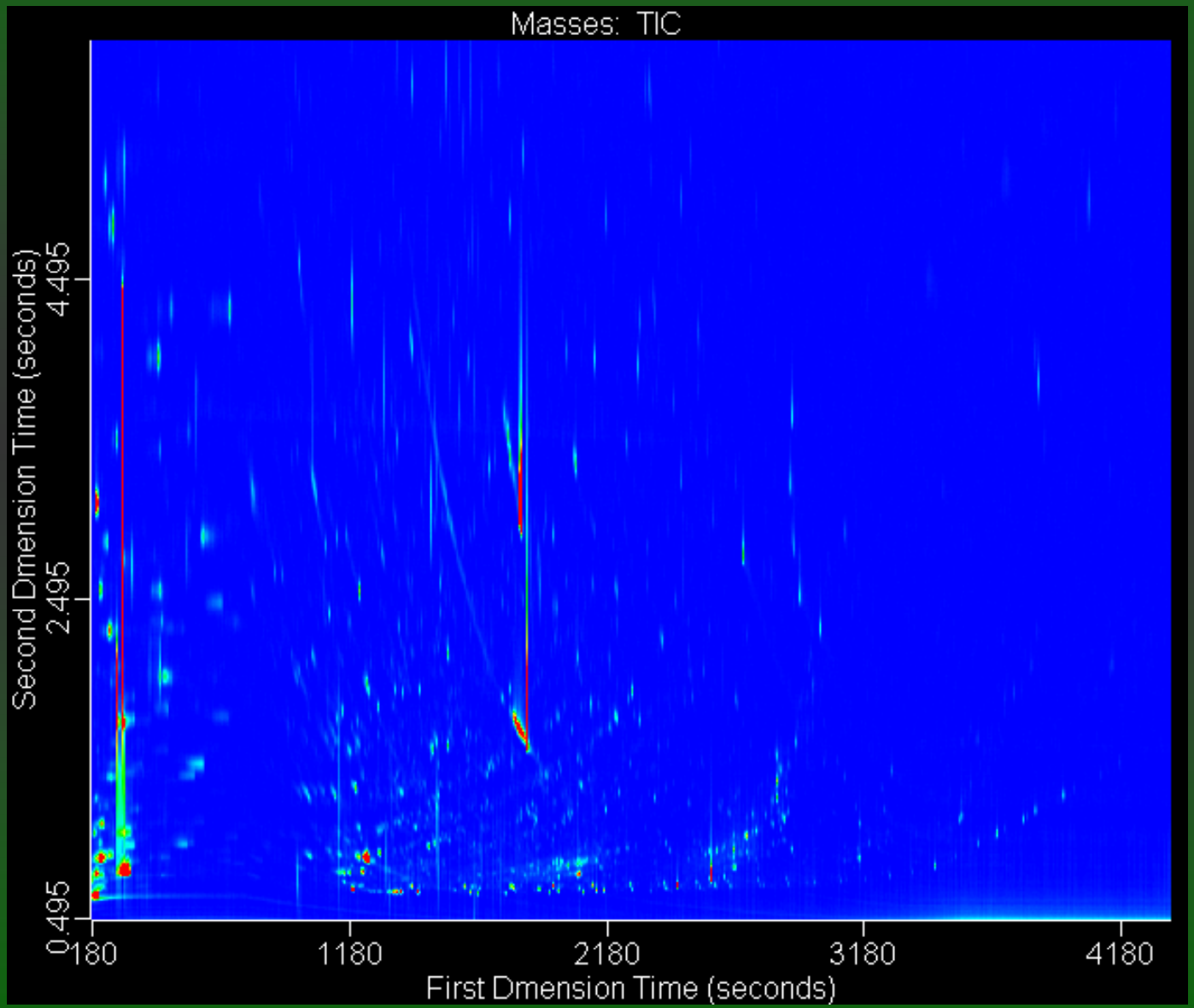

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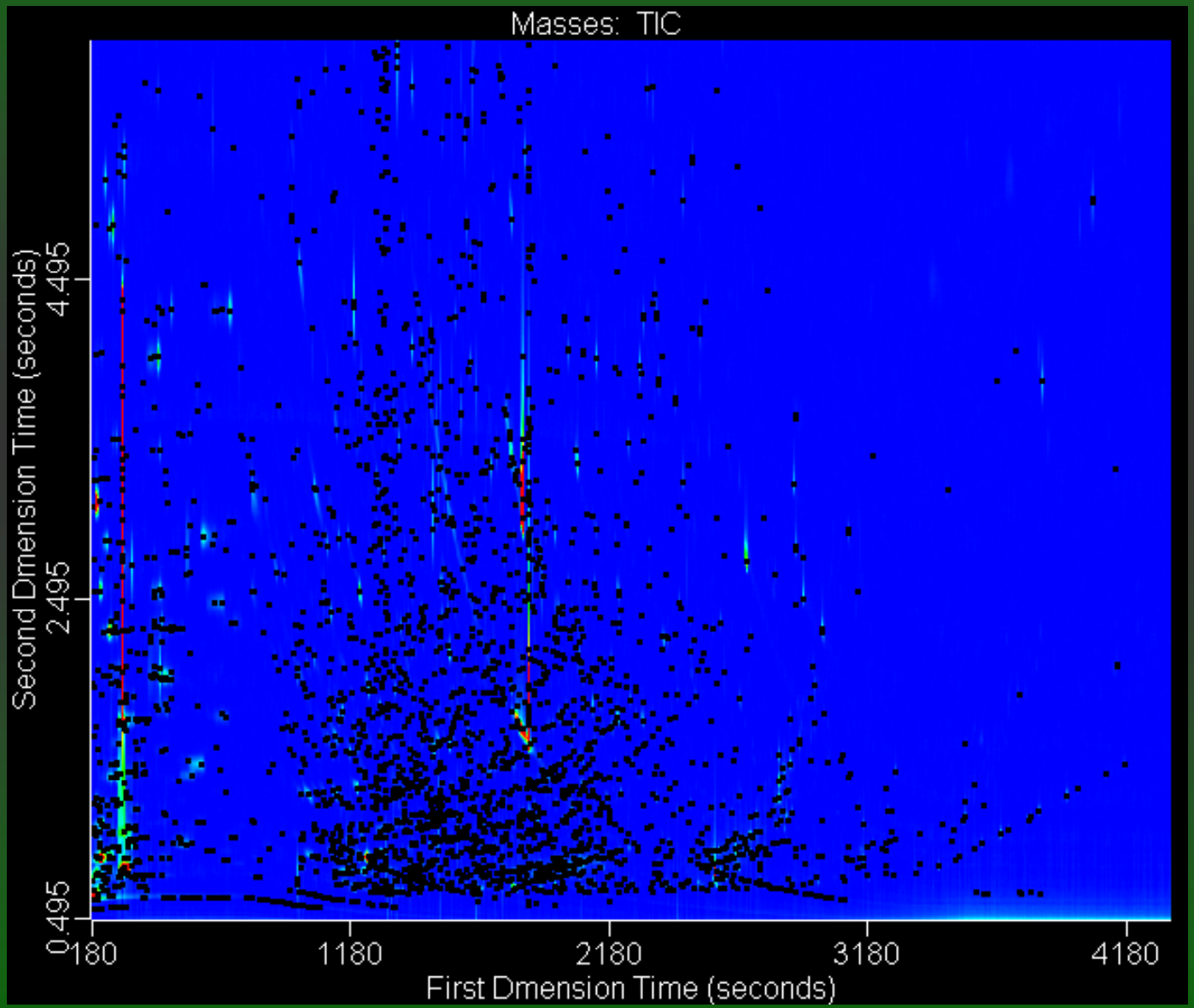
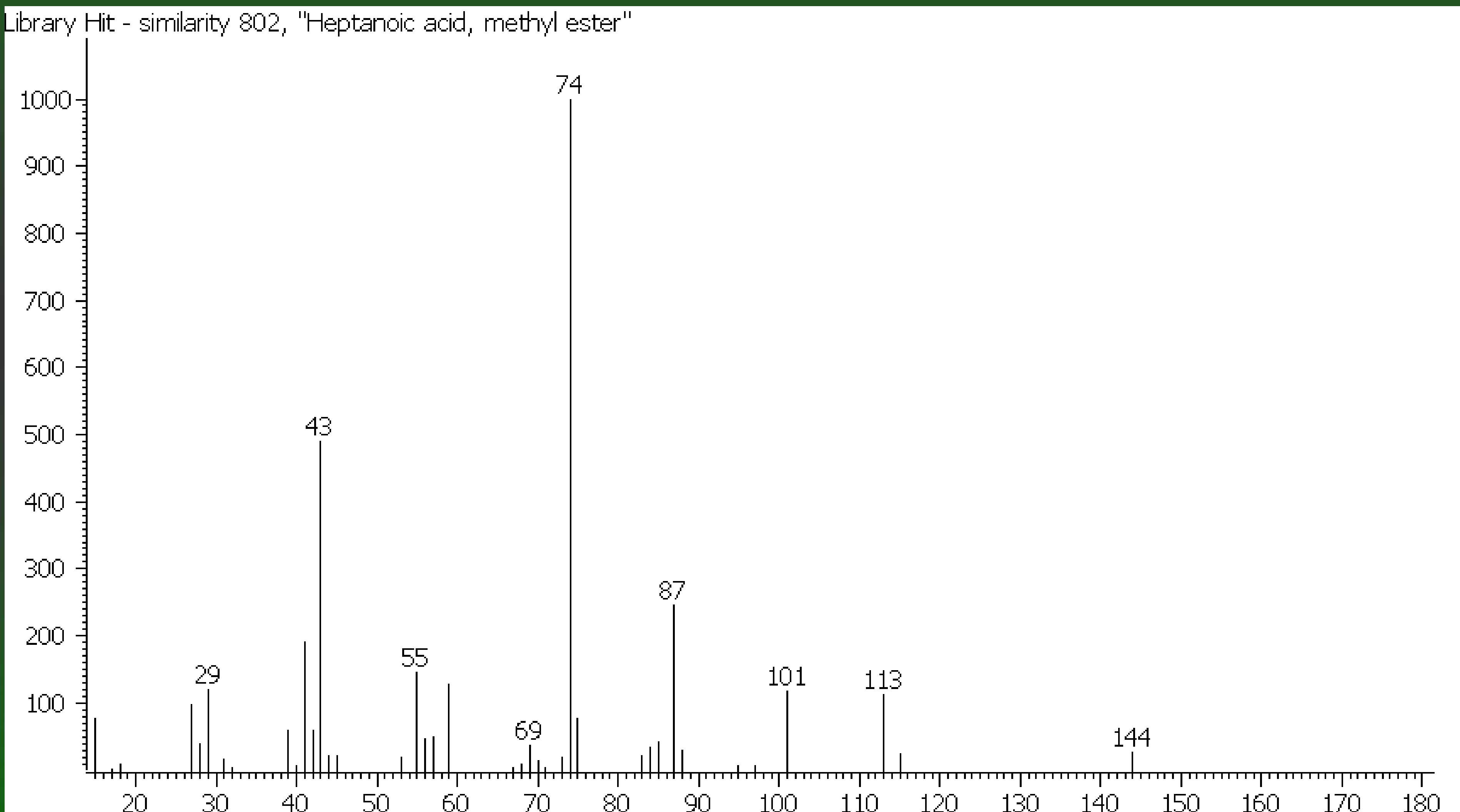


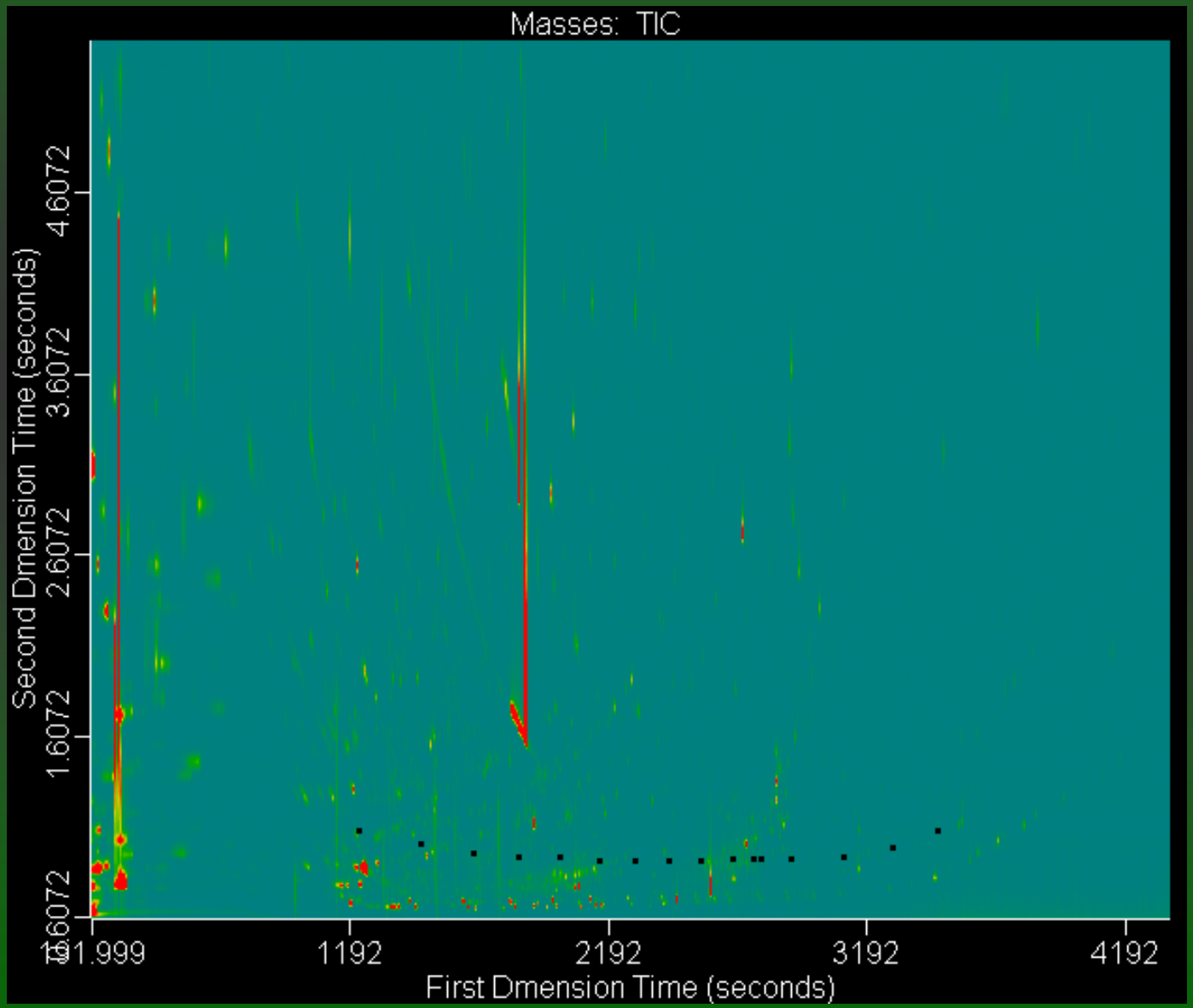
Typical Spectra of Fatty Acid Methyl Esters



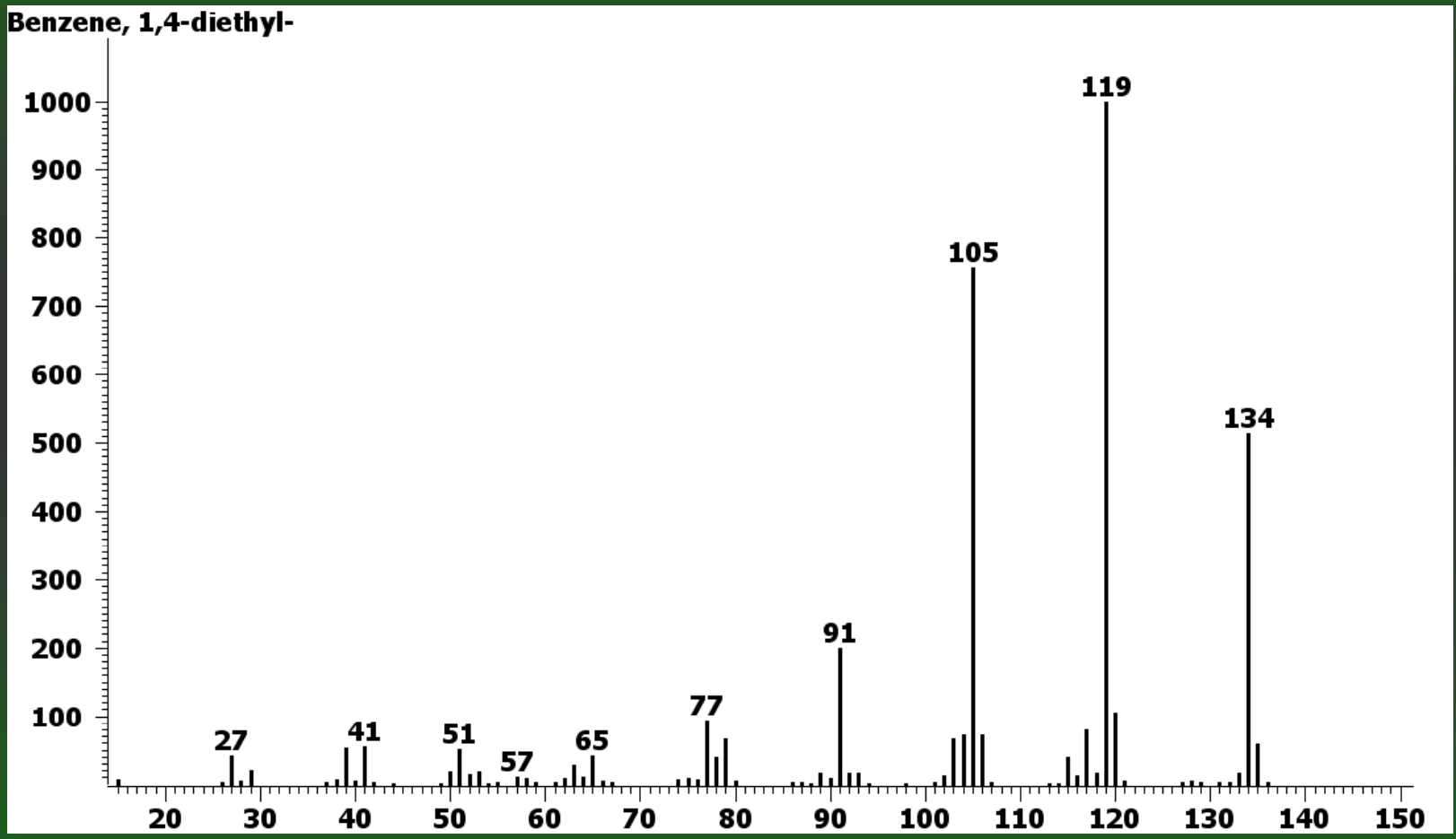
Filter for FAMES

```
Function fame()
   fame =  _
  ((Abundance(55) > 300 Or Abundance(43) > 300) _
 And Abundance(87) > 300  _
 And Abundance(74) > 300) _
 Or _
 (rank(1) = 74 And rank(2) = 87  _
  And  _ Abundance(rank(3)) < 300)
End Function
```

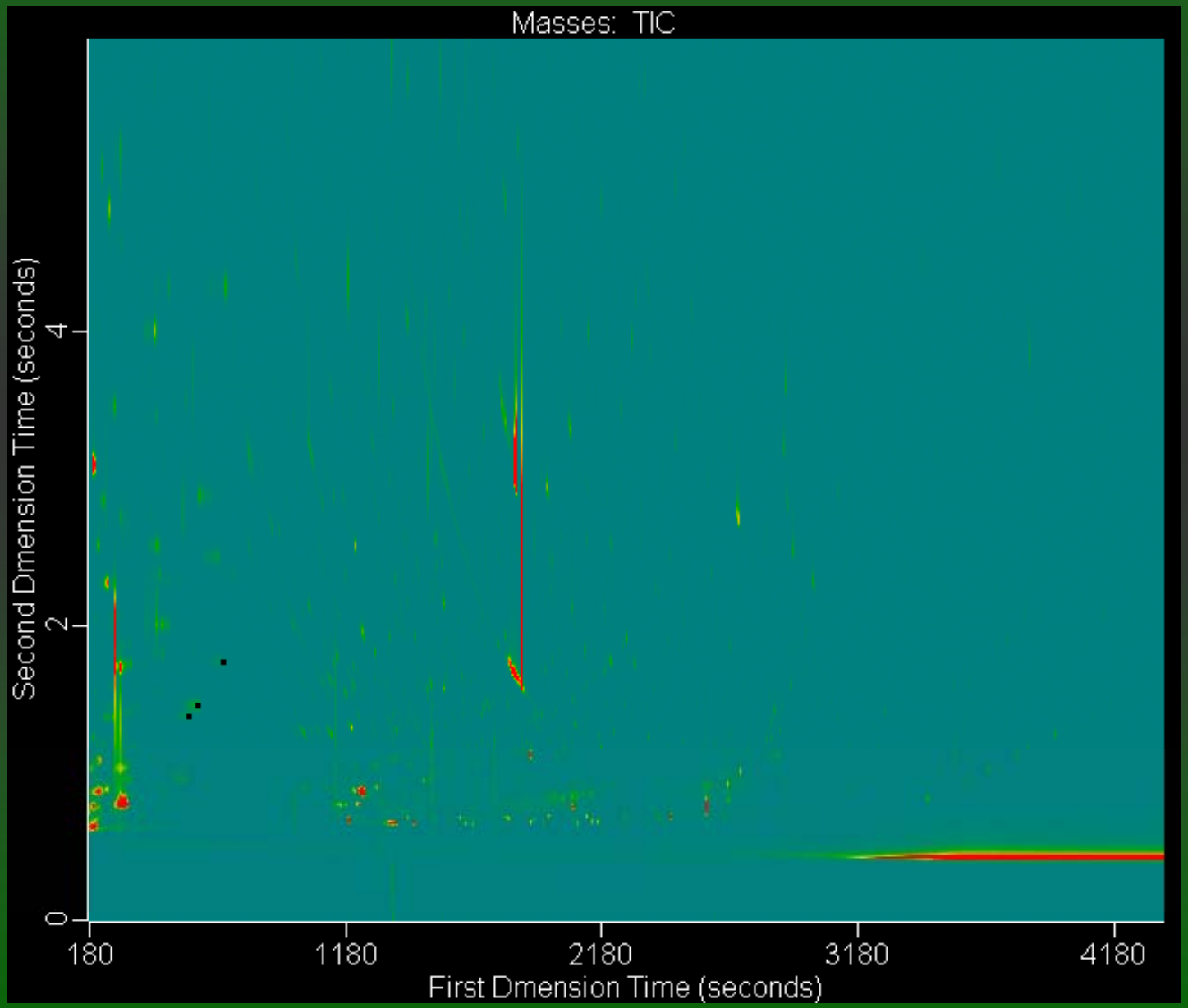
FAMES Automatically Identified



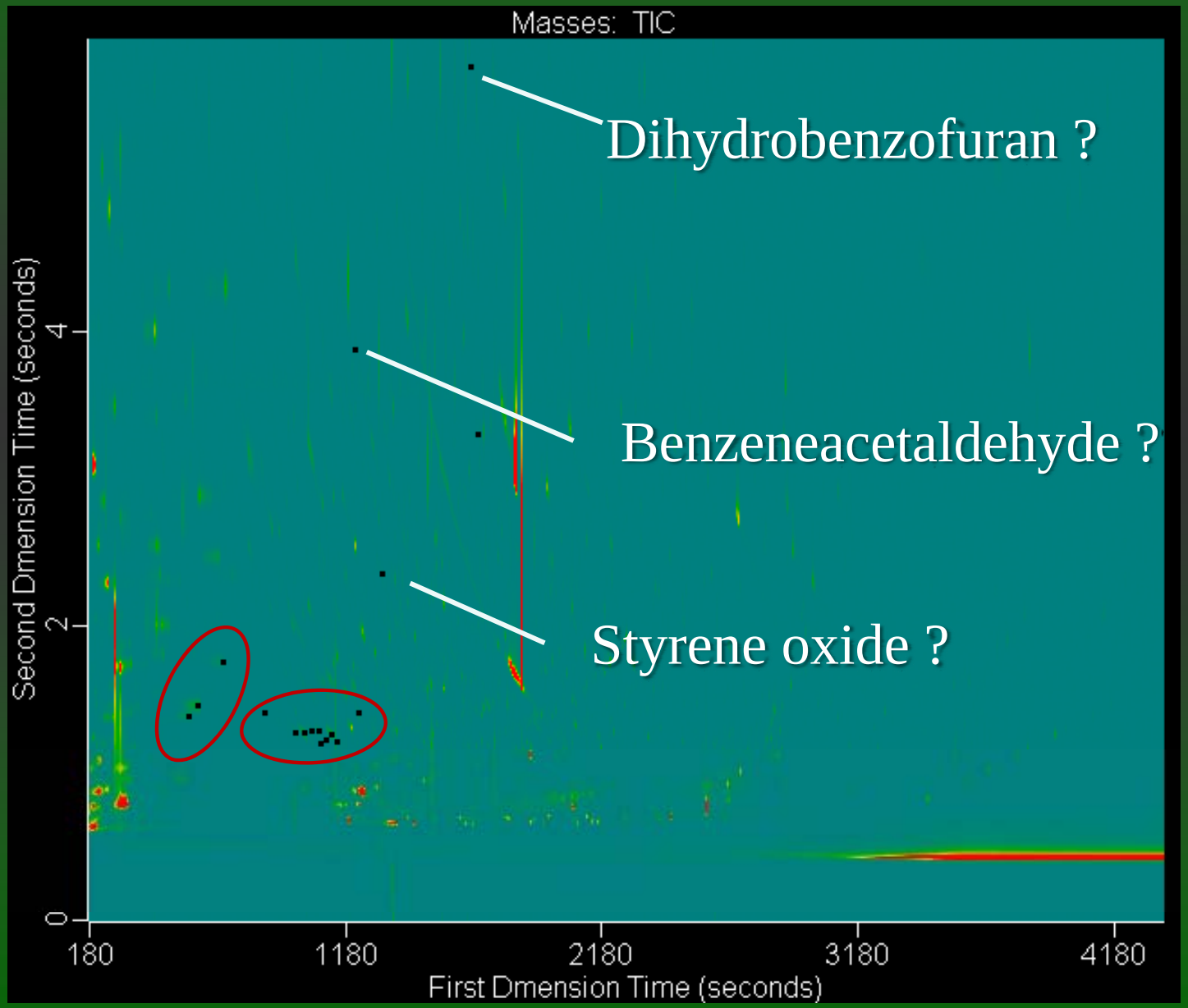
Alkyl Benzenes



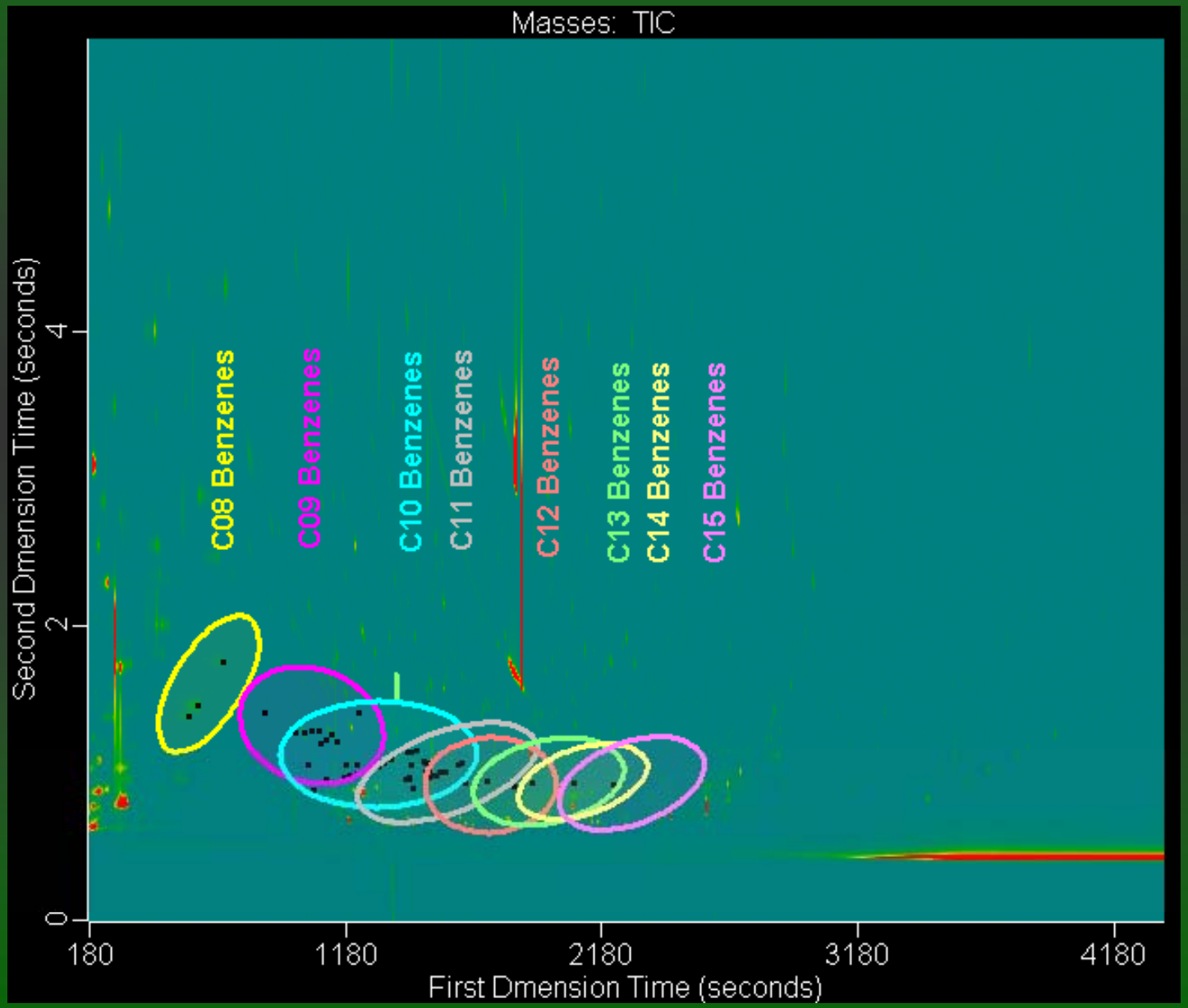
C2 Substituted Benzenes



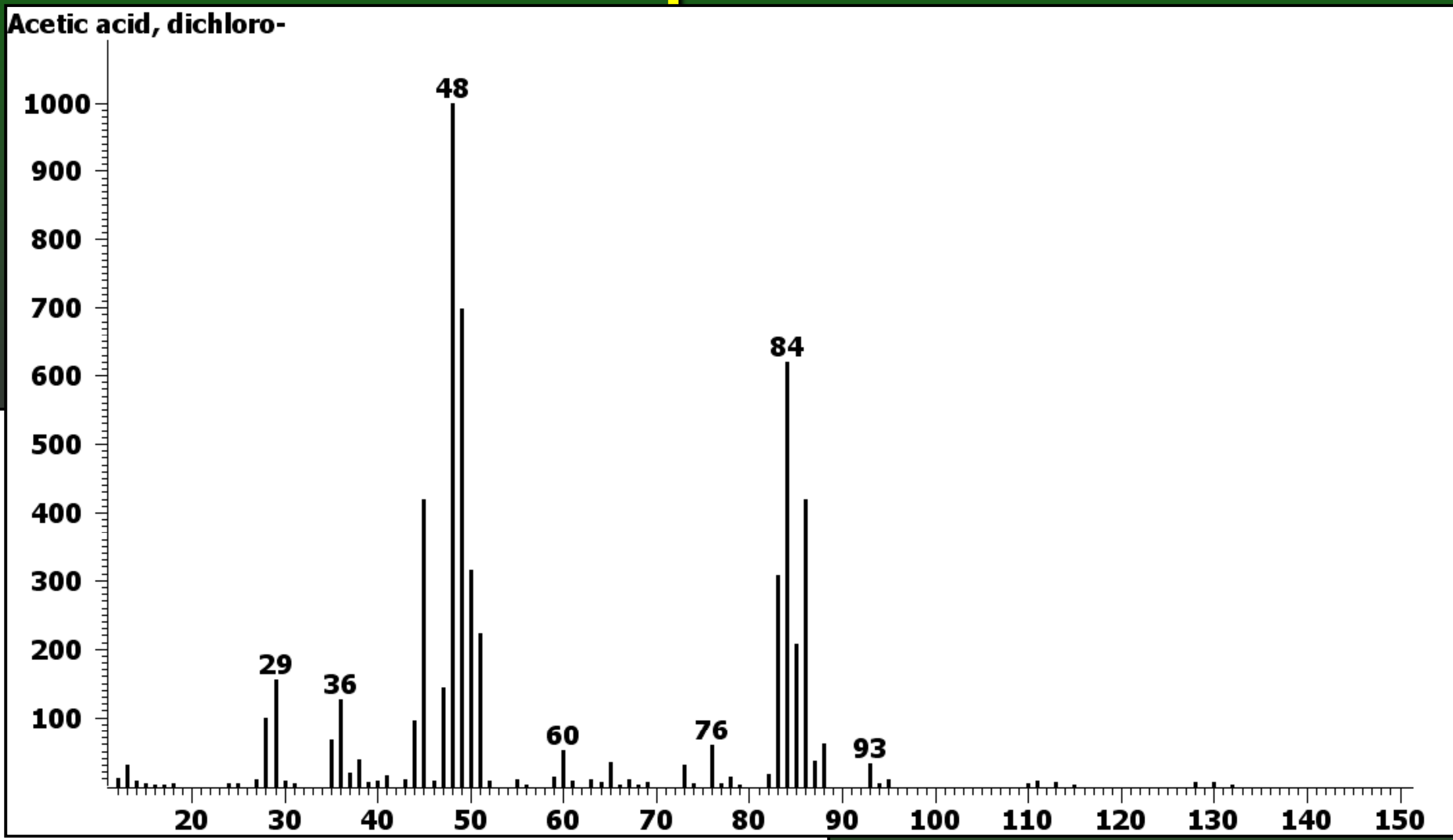
C2 and C3 Substituted Benzenes

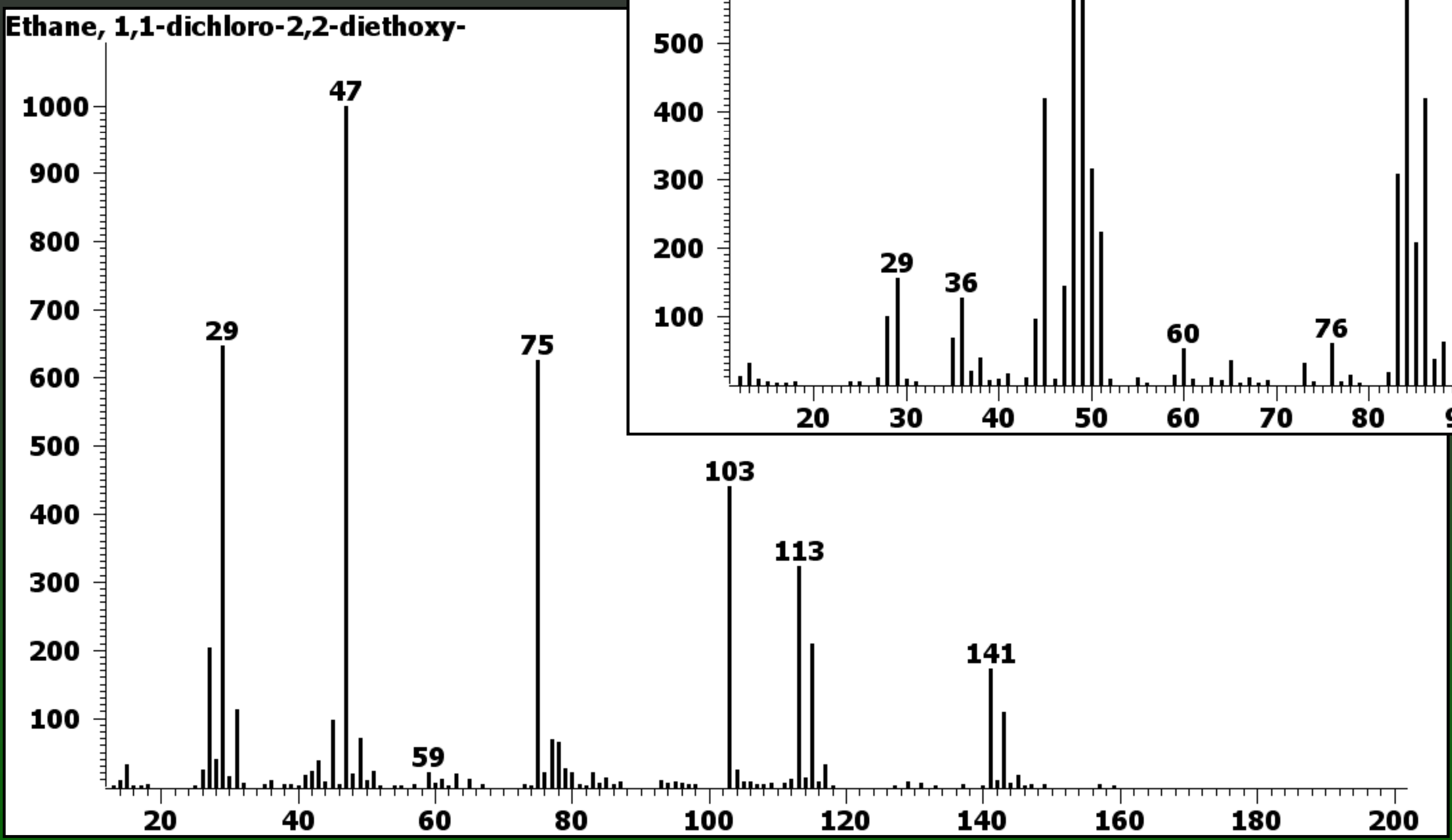


Substituted Benzenes

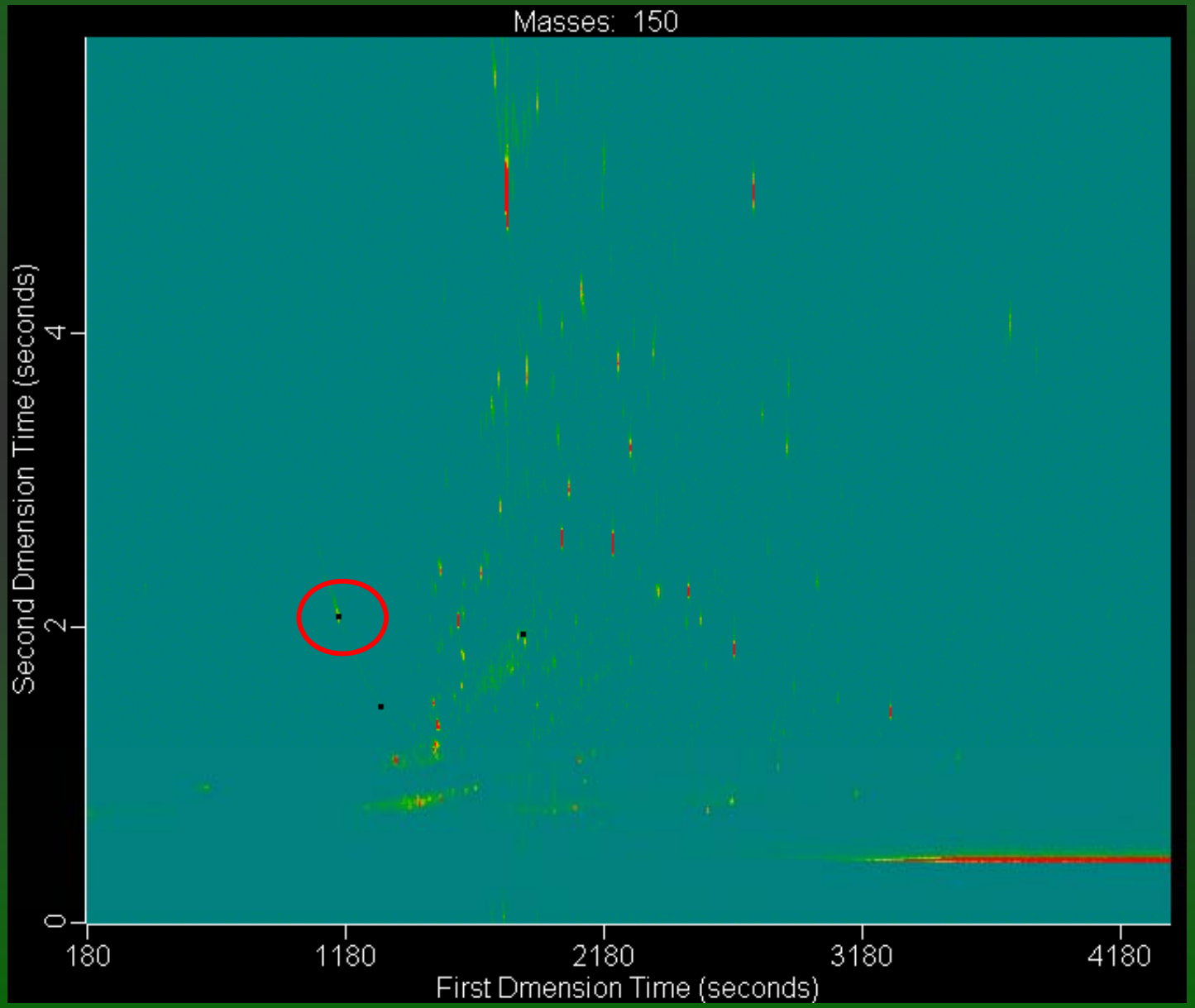


Chlorinated Compounds

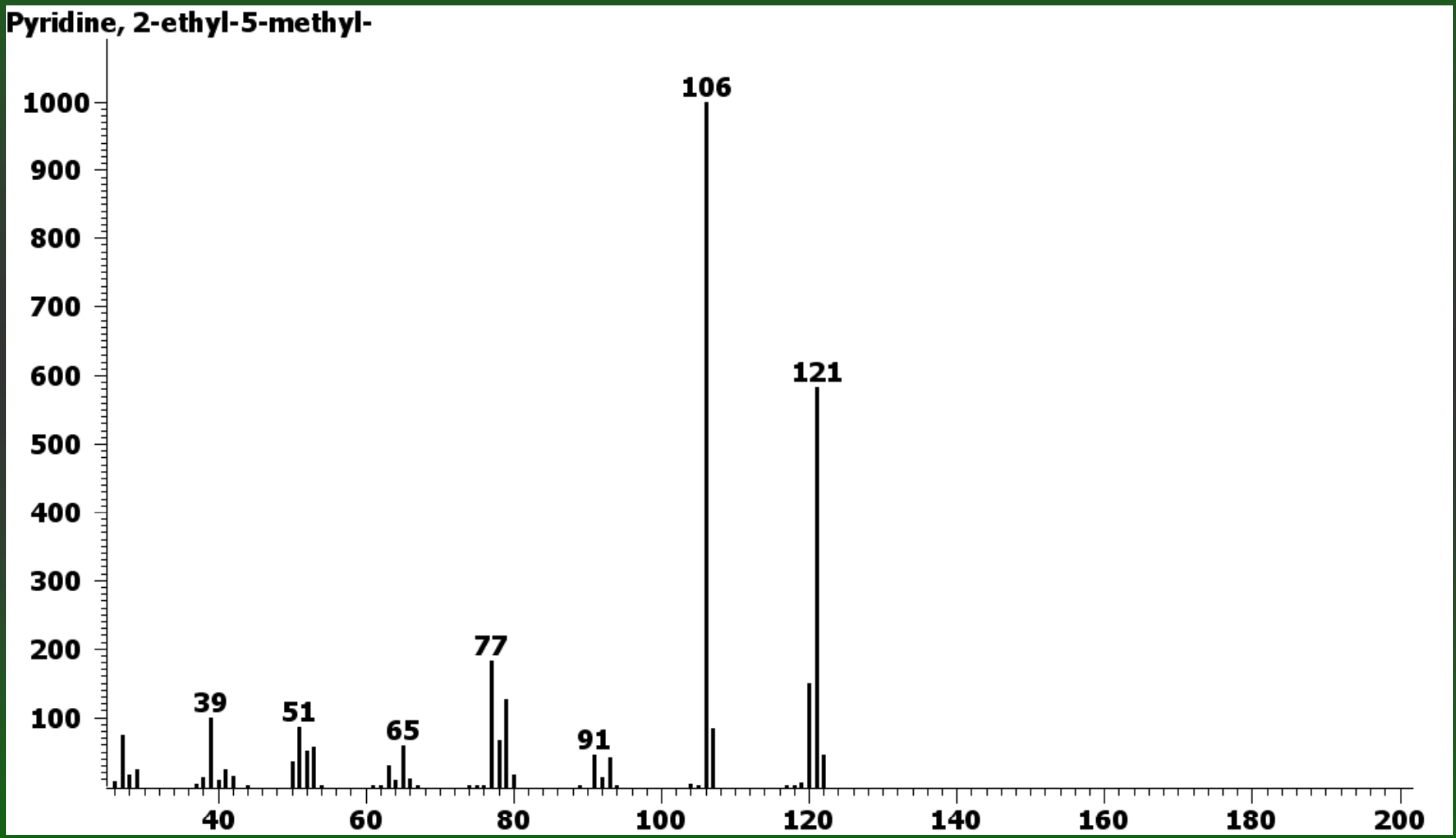




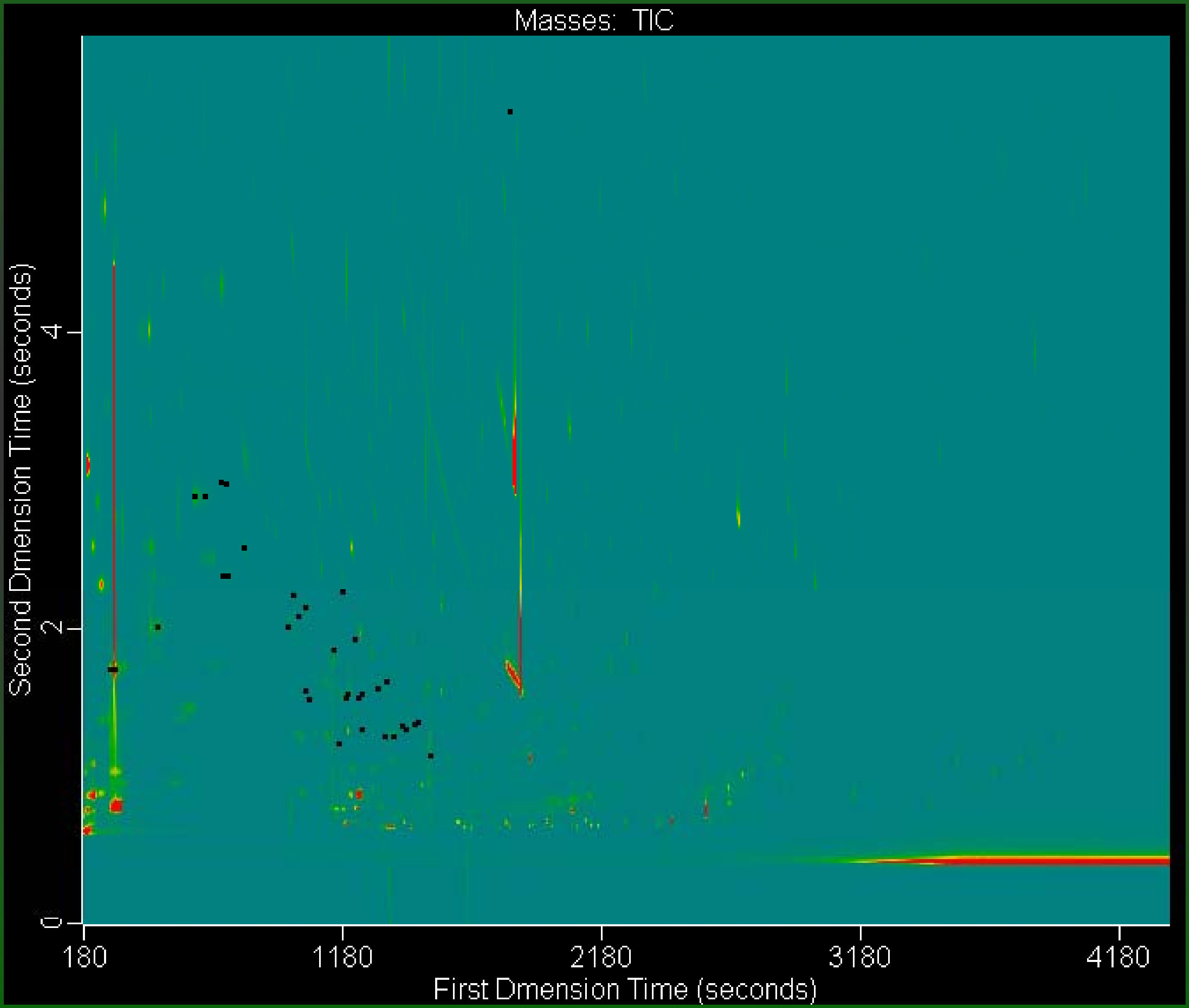
In smoke – six match, 3 are noise



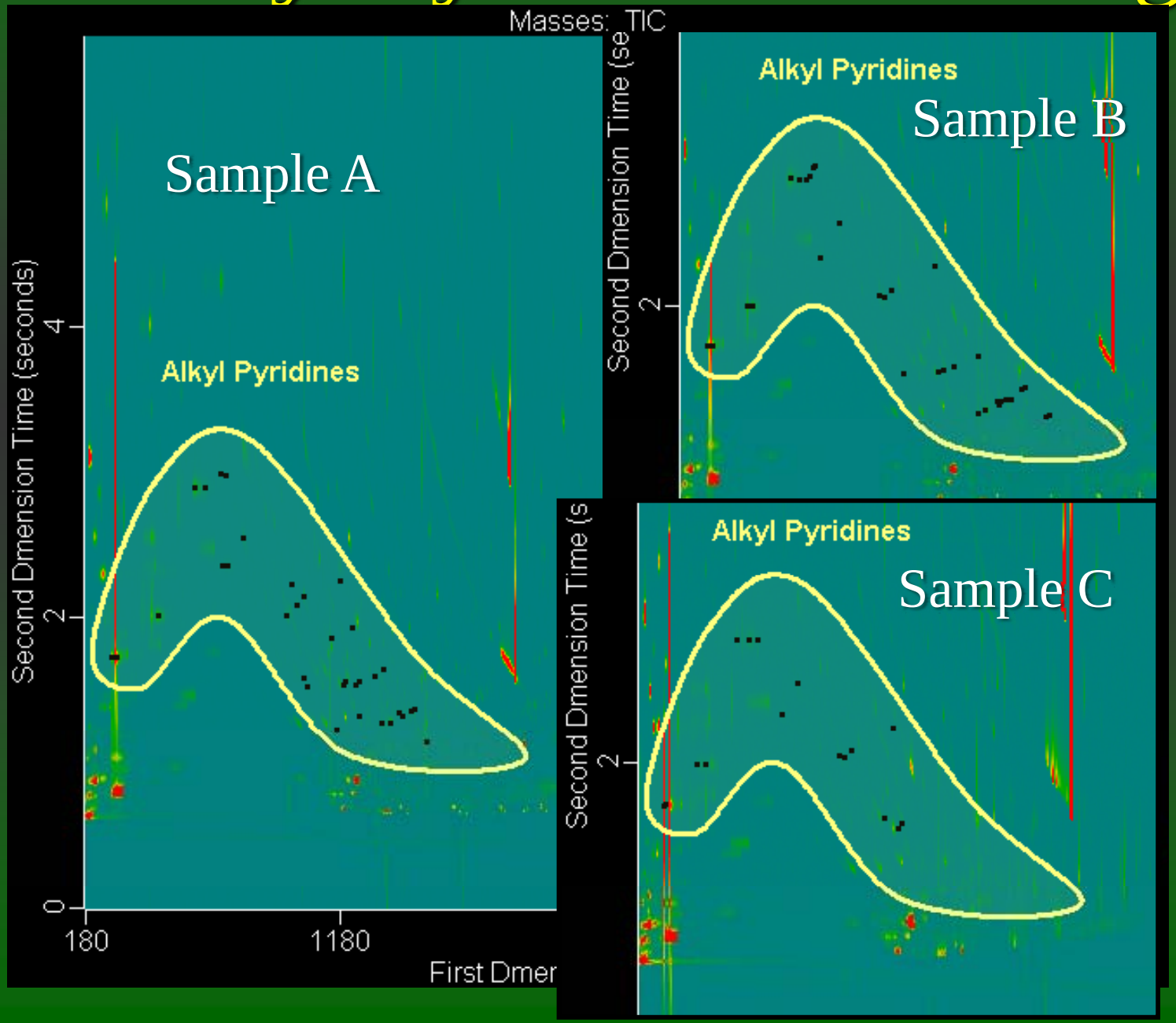
A Typical Alkyl Pyridine



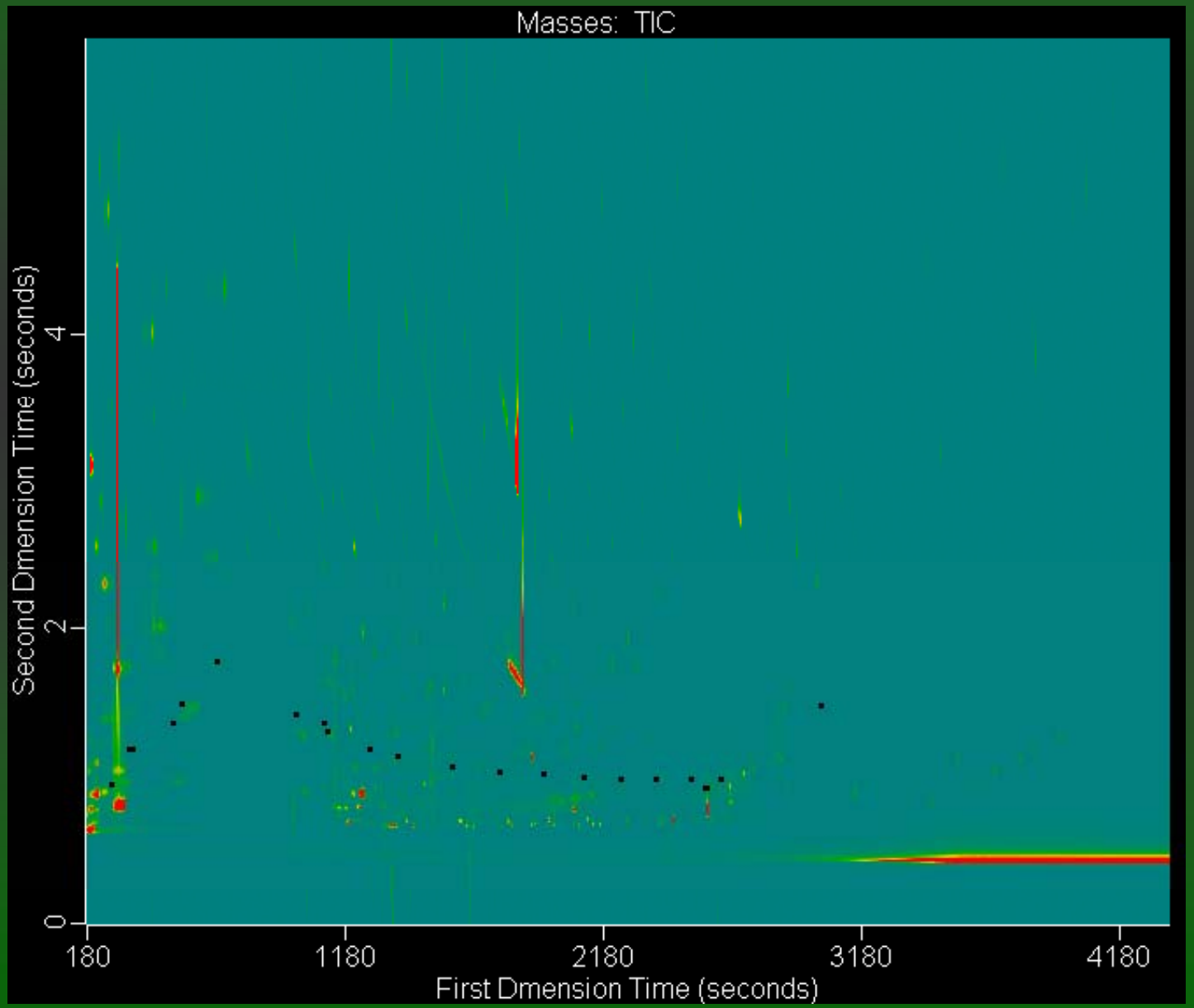
Alkyl Pyridines



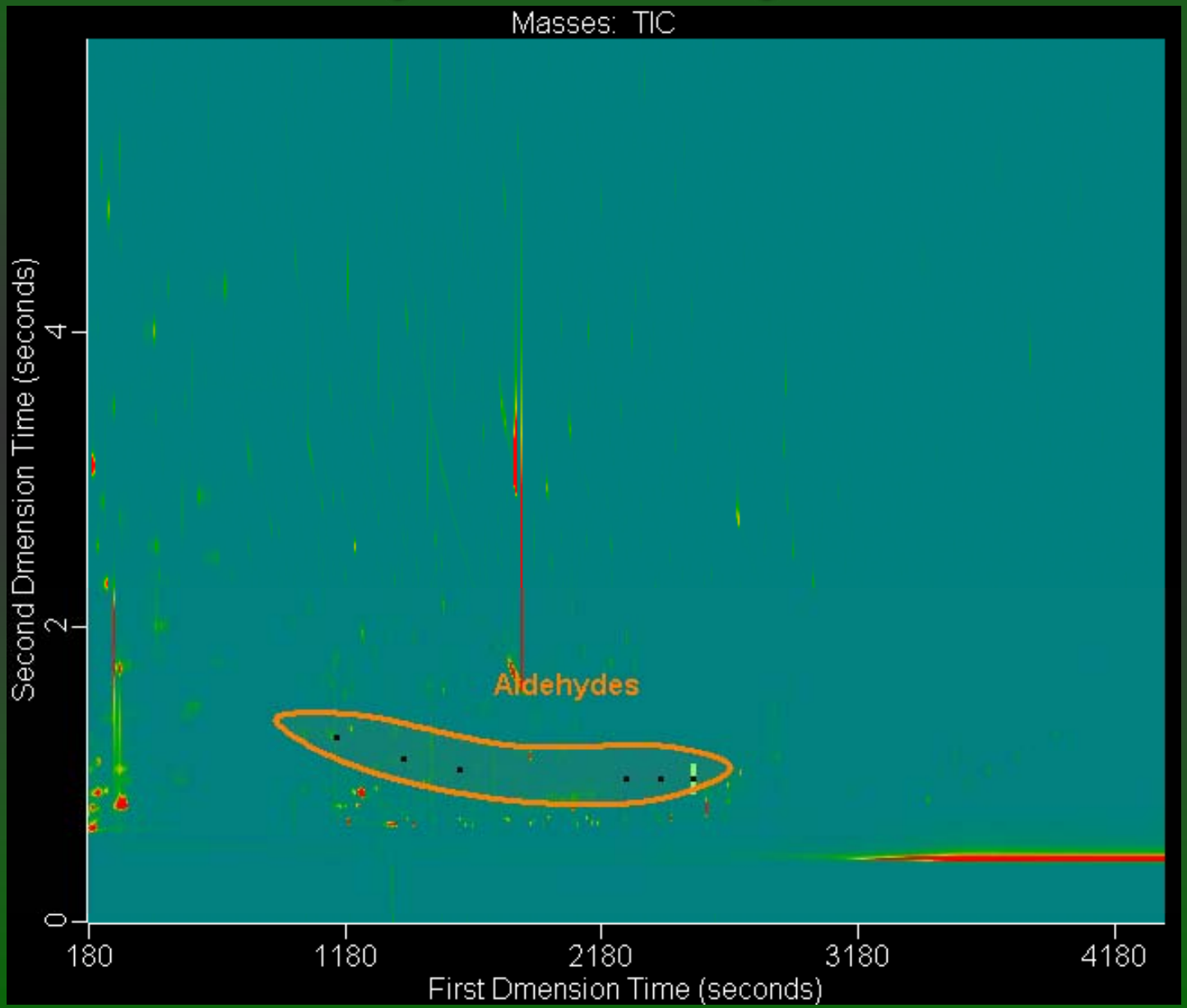
Alkyl Pyridines – two Cigarettes



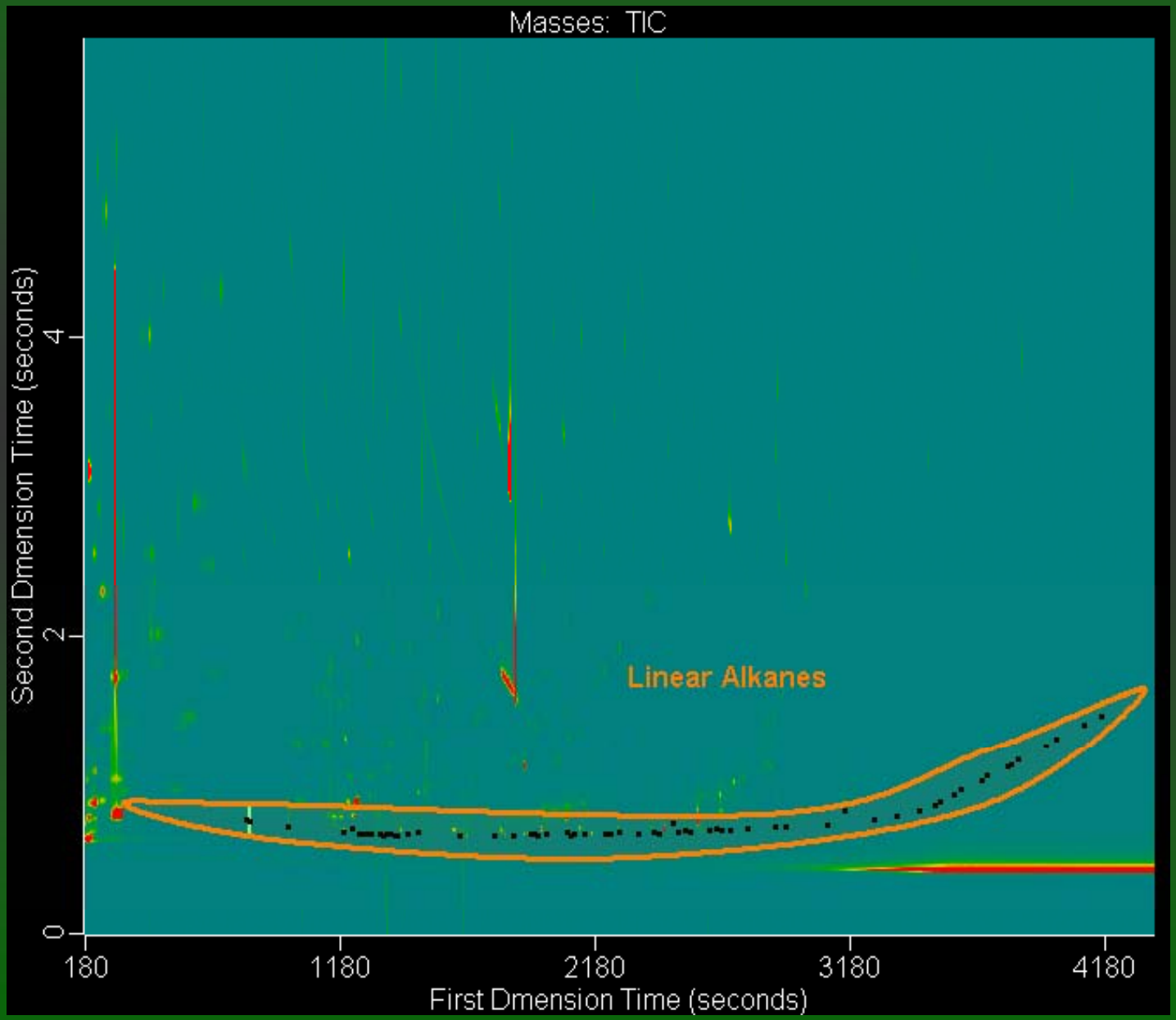
Methyl Alkyl Ketones



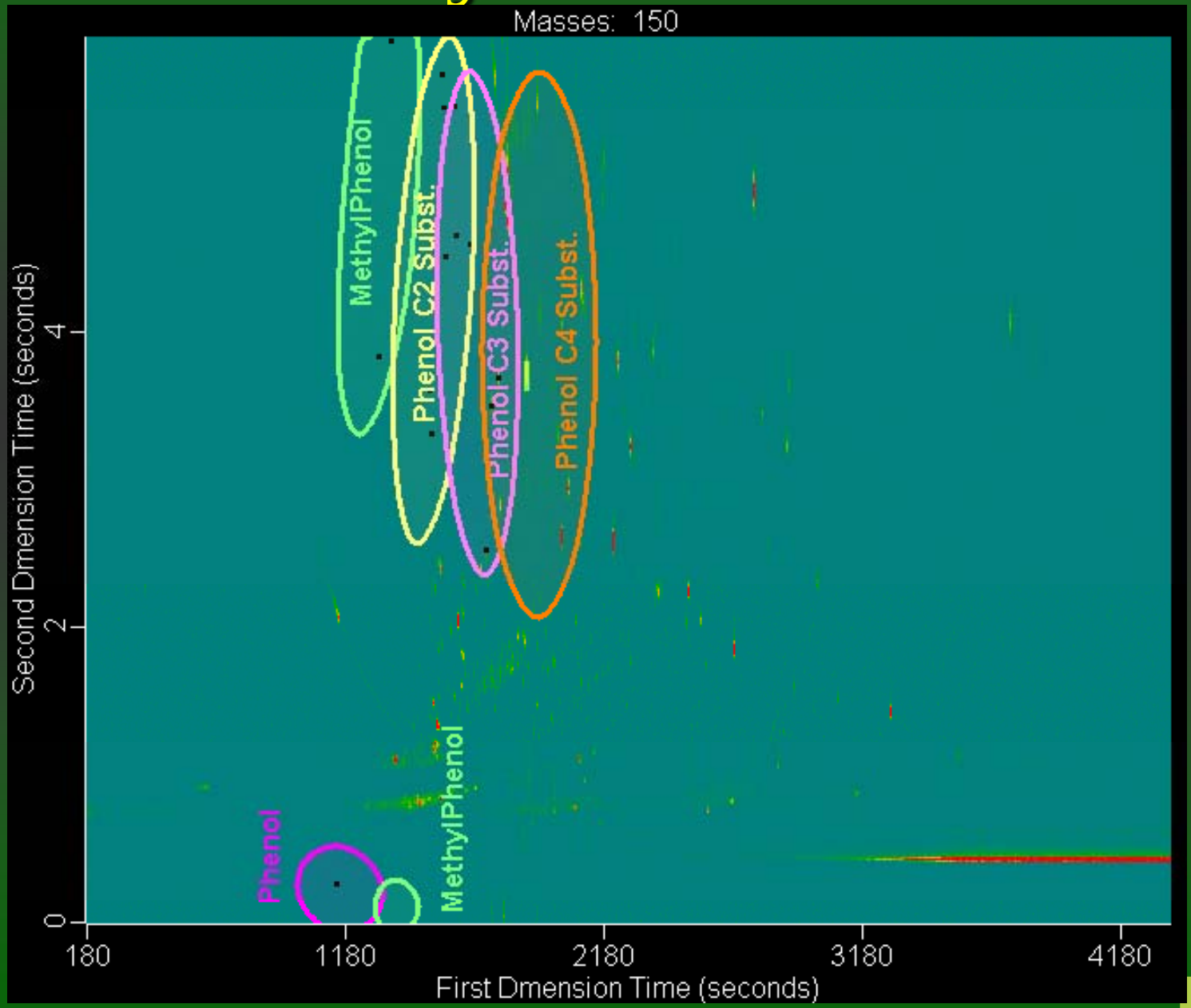
Alkyl Aldehydes



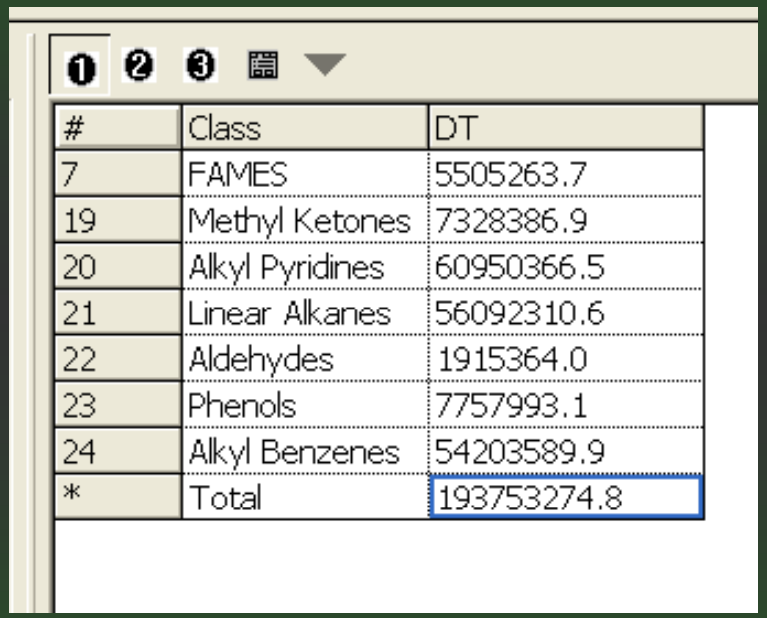
Linear Alkanes



Alkyl Phenols

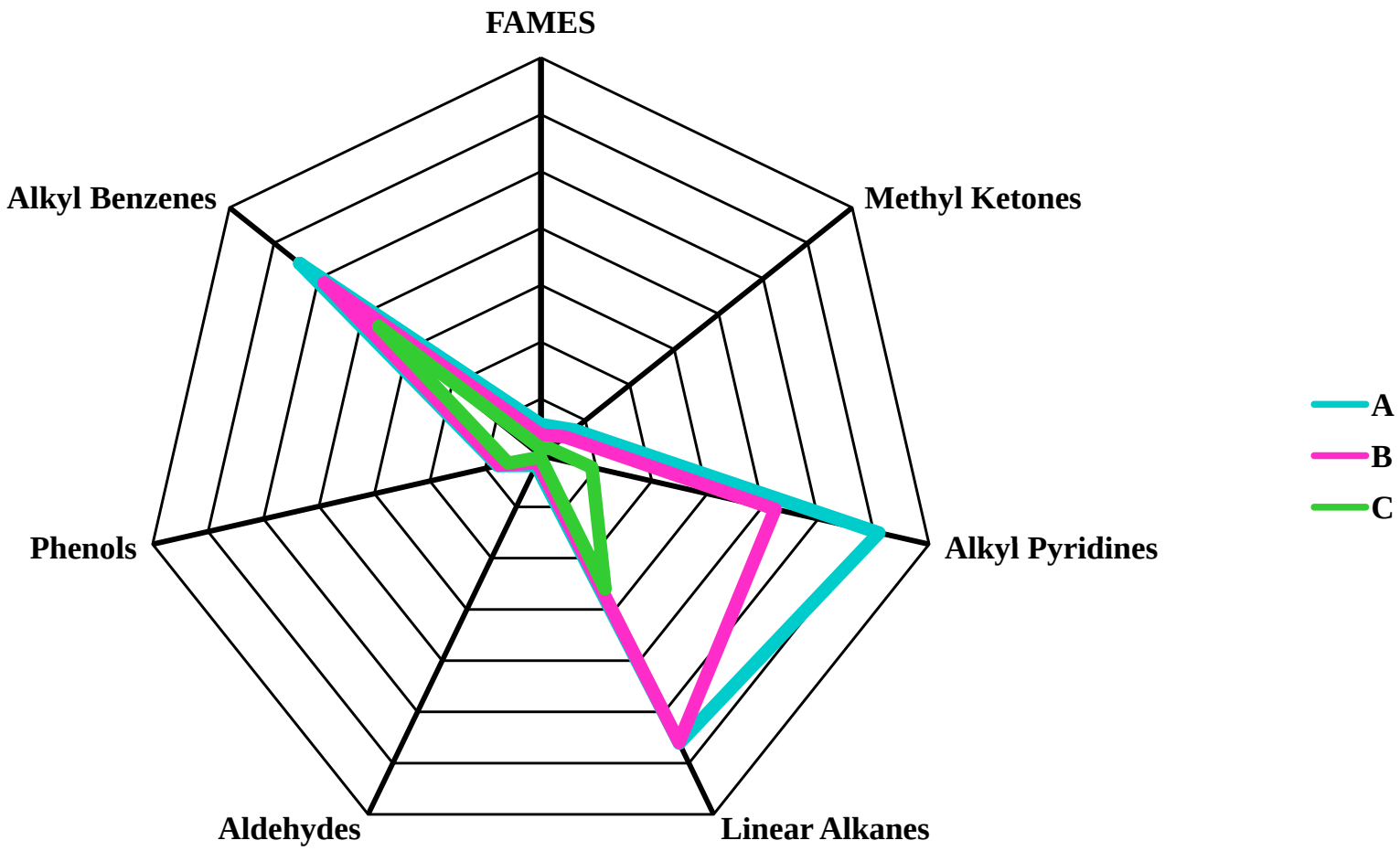


For Comparisons – Area Summaries



#	Class	DT
7	FAMES	5505263.7
19	Methyl Ketones	7328386.9
20	Alkyl Pyridines	60950366.5
21	Linear Alkanes	56092310.6
22	Aldehydes	1915364.0
23	Phenols	7757993.1
24	Alkyl Benzenes	54203589.9
*	Total	193753274.8

Side by Side…



Conclusions

- Automatic filtering can be used to identify compounds belonging to classes of interest.
- Summary information for classes can be used to highlight differences.
- Chromatographic information (peaks, spectra, areas) remain available for further investigation.

Acknowledgements

- Serban Moldoveanu (of R.J. Reynolds)
- LECO Corporation