True Plug and Play Chromatography

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The Overarching Infometrix Goal

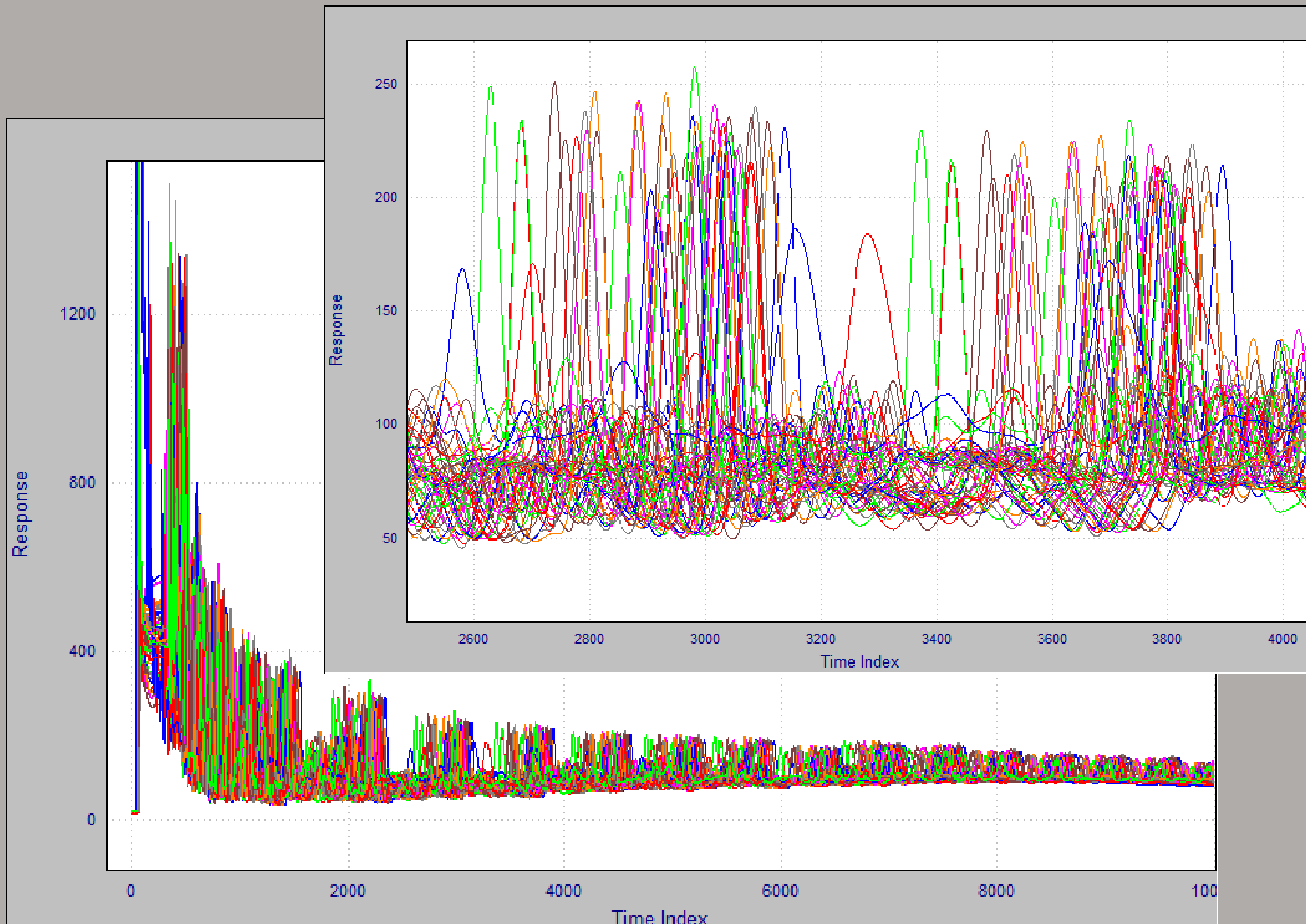
- The process world has a disconnect as we reduce staffing and add more analyzers to the monitoring and control mix.
- More data does not get us into a better position to achieve our quality objectives; we must extract the information content.
- As much as possible, we need to make the interpretation more automated, objective and do so in the highest quality manner.
- We also need to cut the lifecycle costs, which means lower costs of installation, maintenance and training of personnel.

Alaska North Slope crude oil

- Same container of oil analyzed over 2 ½ years
- 1% crude in CS_2
- The chromatography is challenging
  - Column changes every 3-6 weeks
  - Inlet liner every week
  - Work burden: need to recalibrate every 8-12 hours
  - Some band focusing due to inlet at +30°C and column at -20°C

The quintessential column drift problem

Chromatograms – RT drift

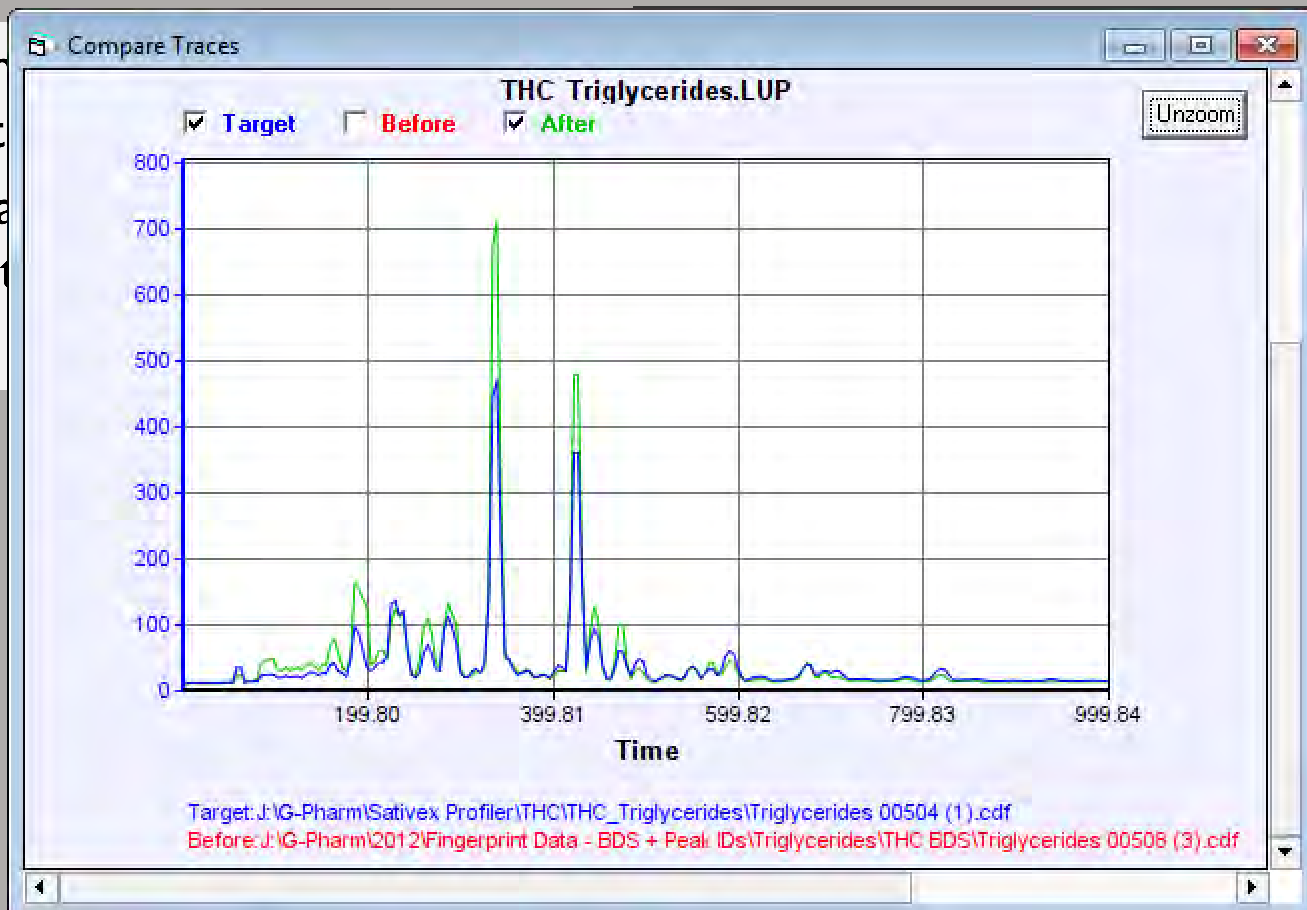


Correlation Optimized Warping (COW)

- Alignment is successful using a combination of algorithms based on chromatographic correlation
- Key is the COW algorithm initially developed by a research group in Denmark and similar to one used in voice recognition
- The advantage is that alignment can be done at any time; it does not require hardware adjustments that only correct future samples (as is the case with pressure modulation)

Alignment setup and processing

- For each
paramet
- Range ca
only that
interest



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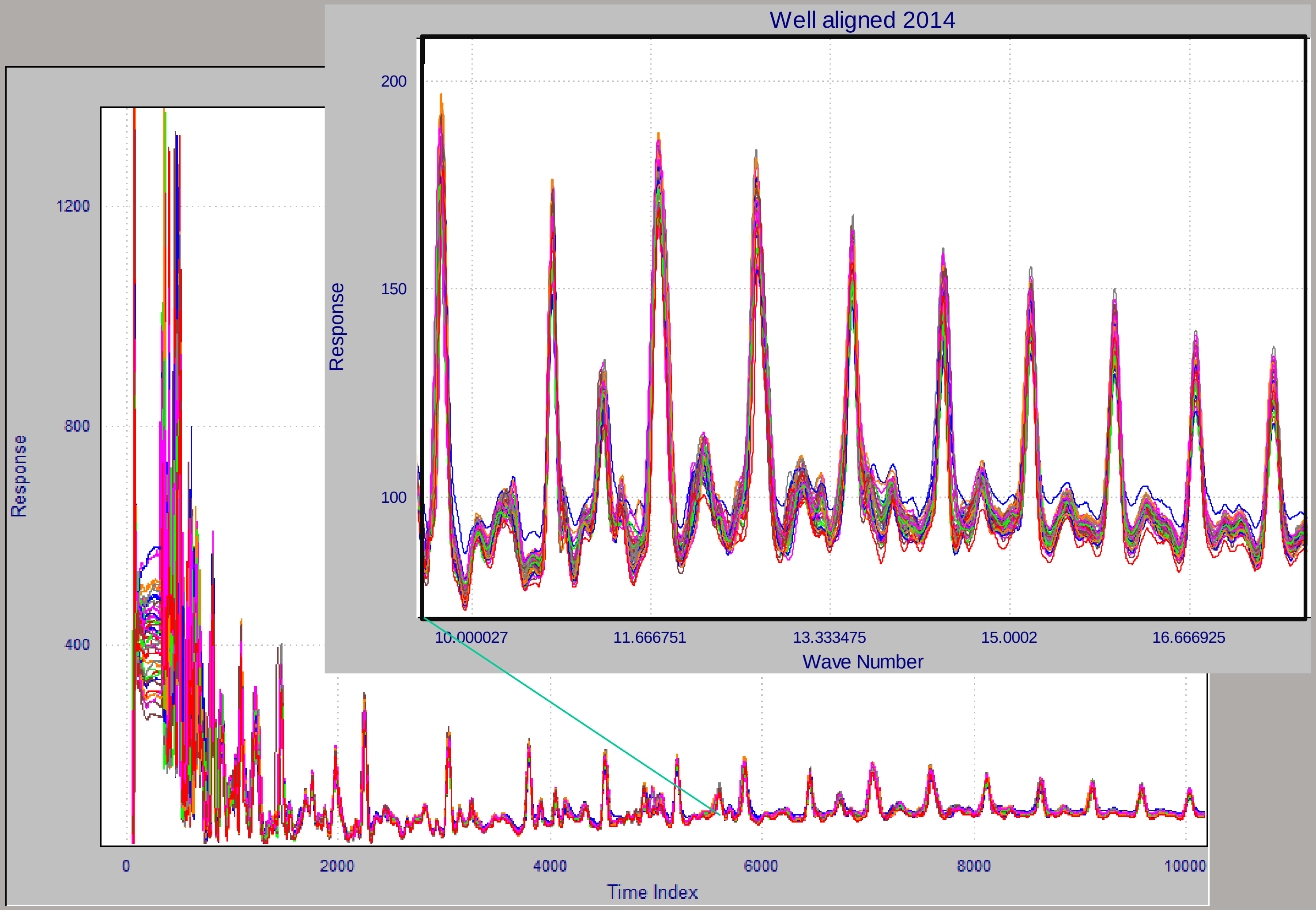
Aligned profiles – 2014



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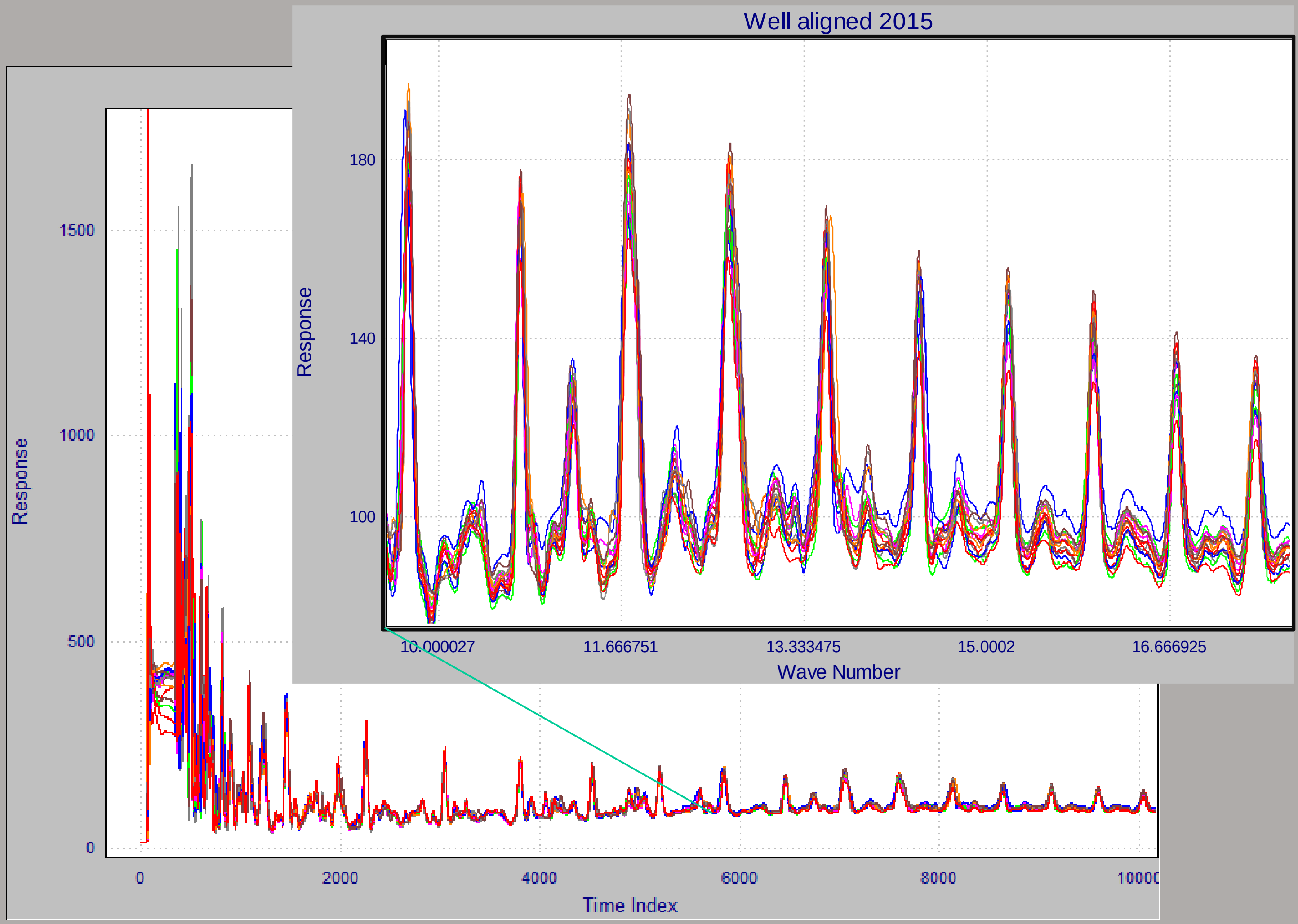
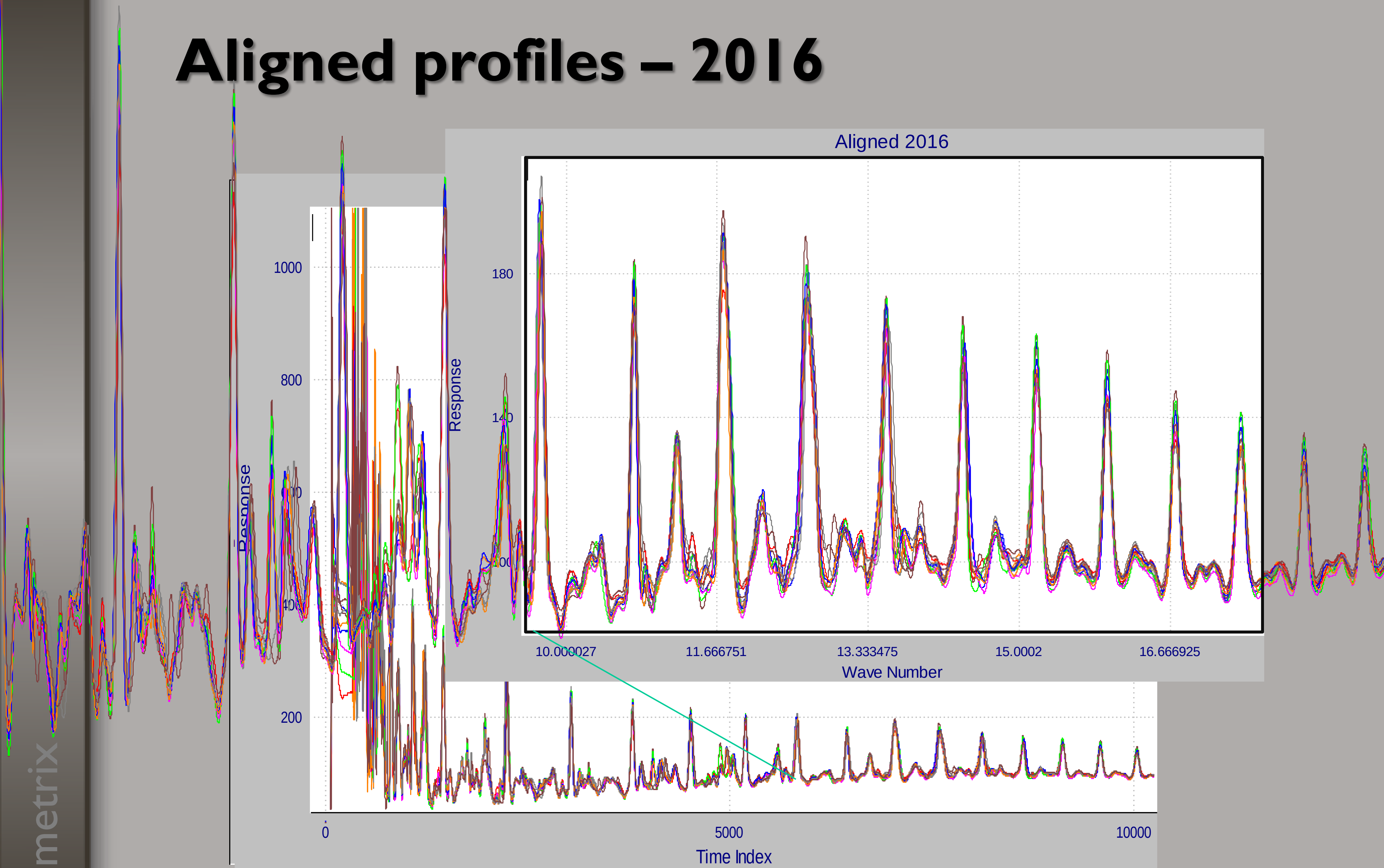
Aligned profiles – 2015



Aligned profiles – 2016



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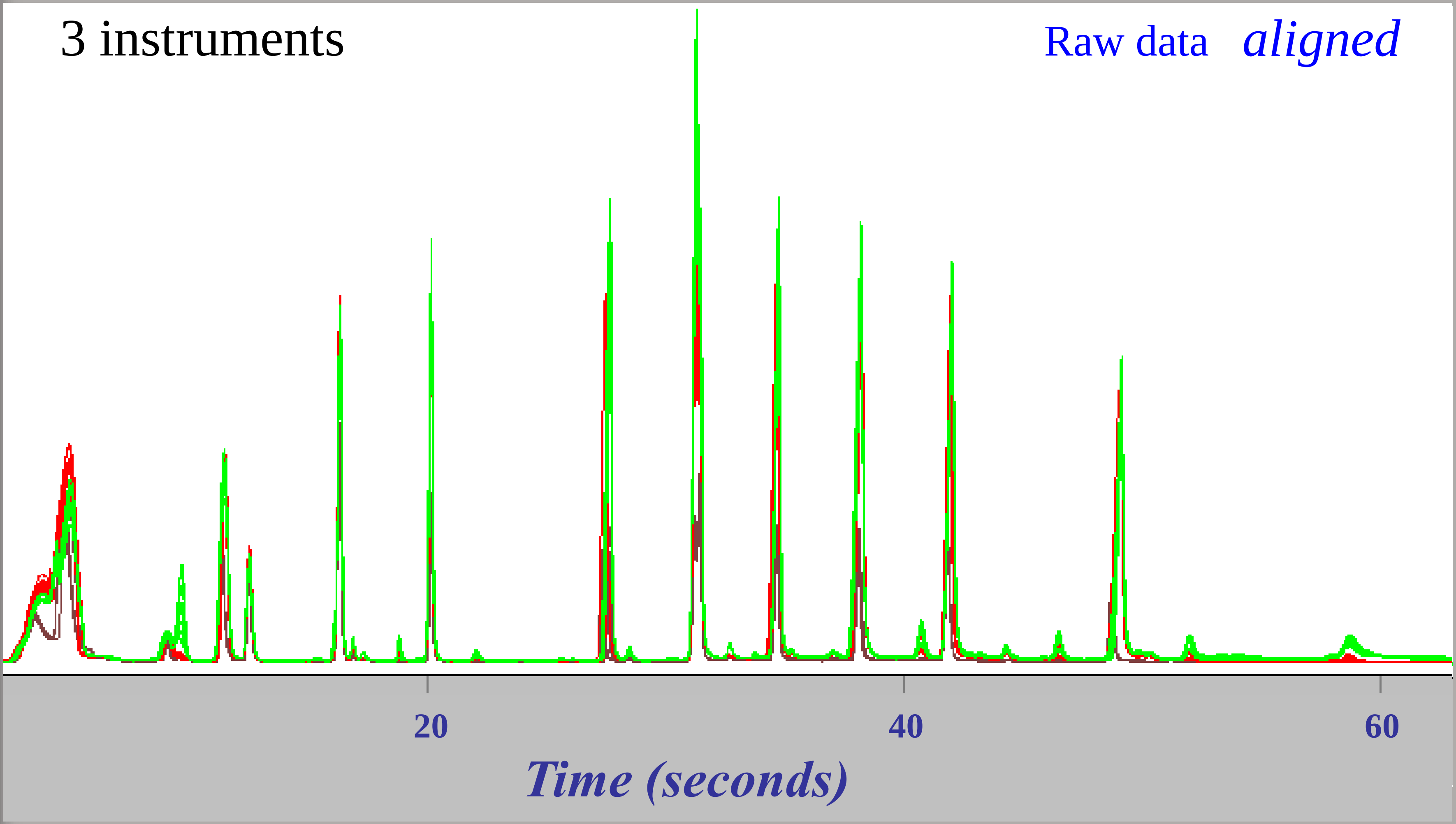
Automated alignment across instruments

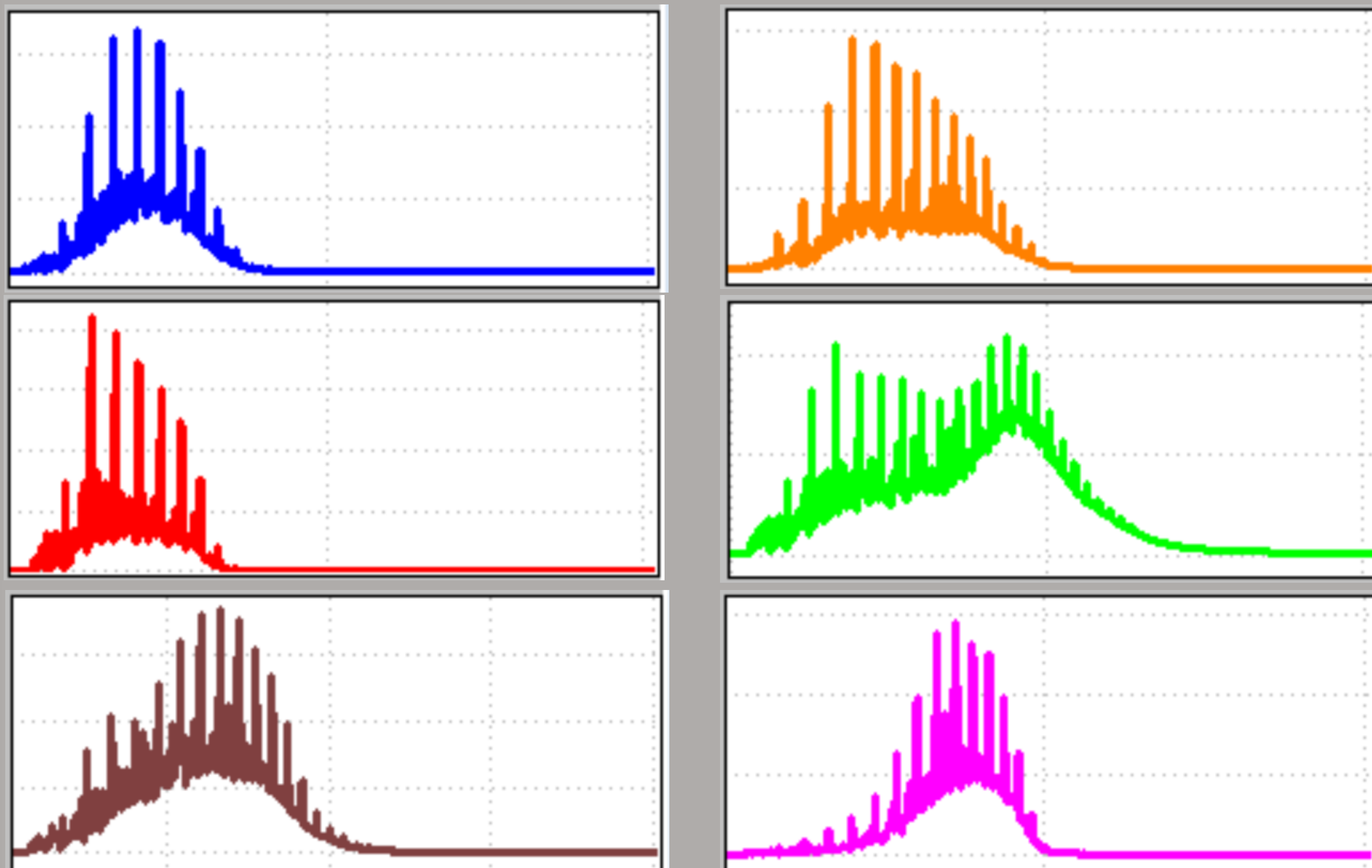


Taking this a step beyond

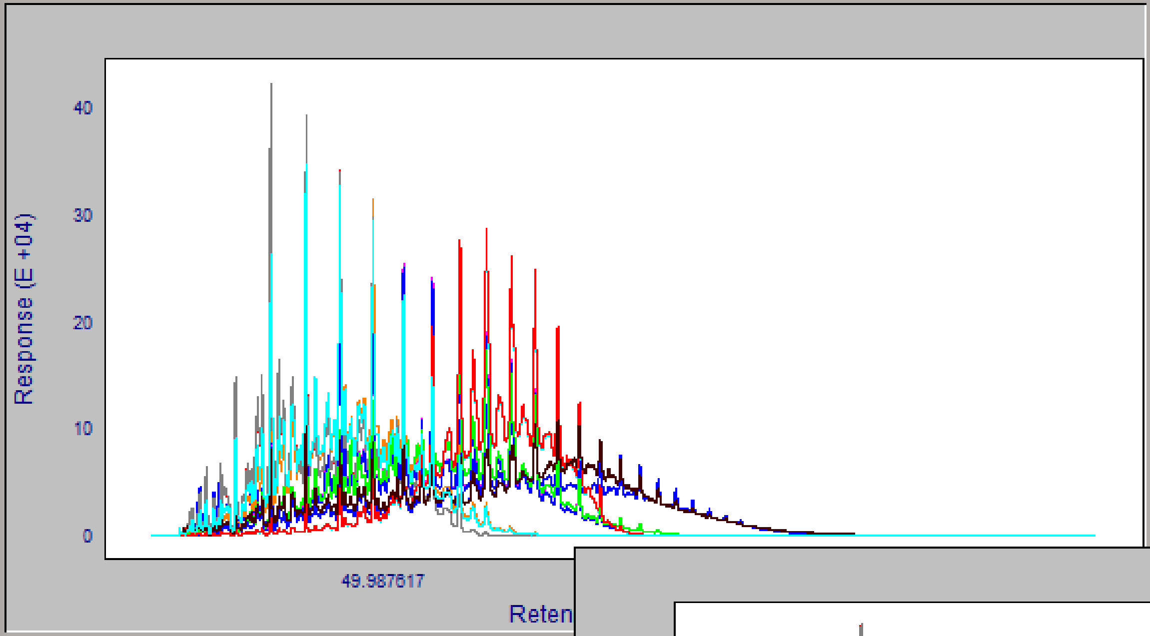
- Think about how alignment relates to simulated distillation…
  - We run an n-paraffin standard to correlate temperature to retention time.
  - We use this new axis to map the cumulative percent of total area as we progress along this set of temperatures.

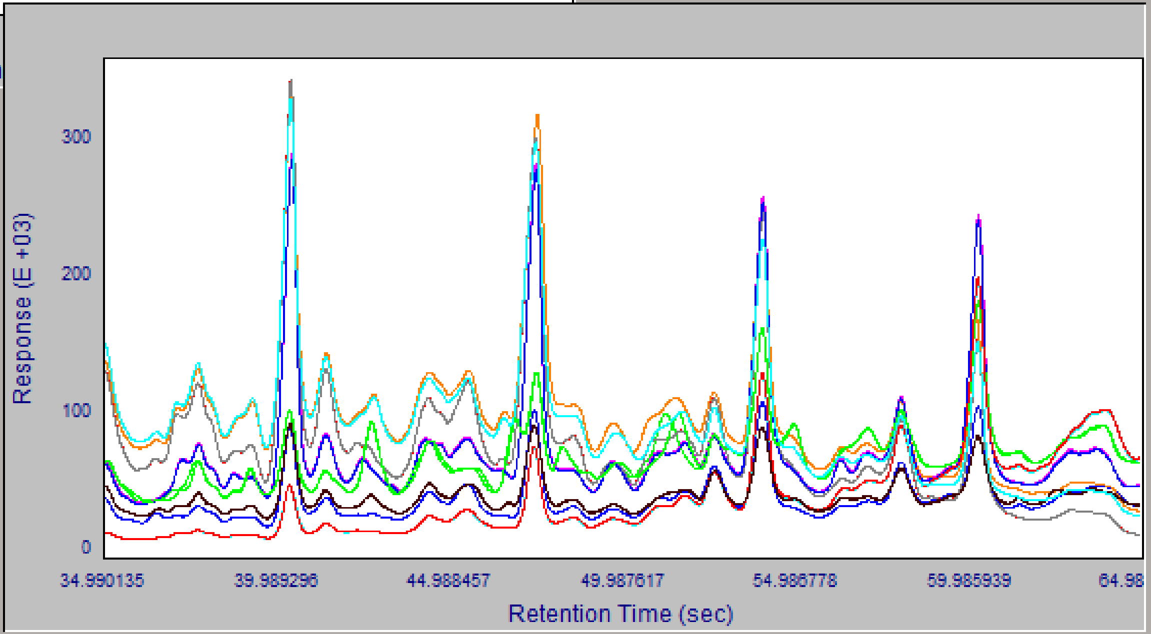
SimDist test samples

ASTM 7798 ILS

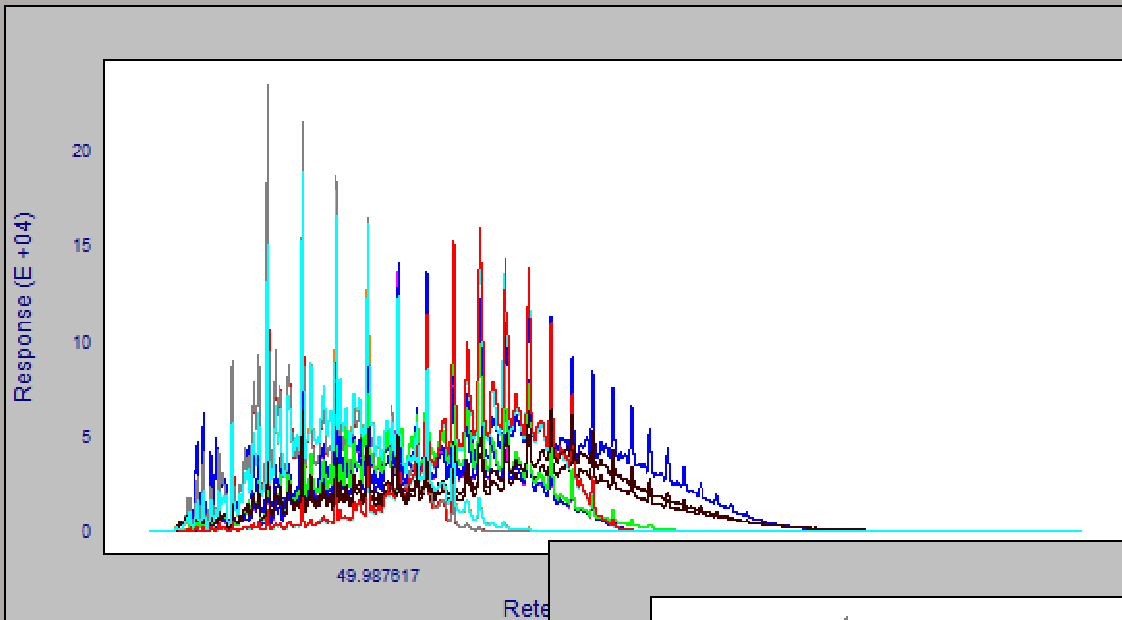


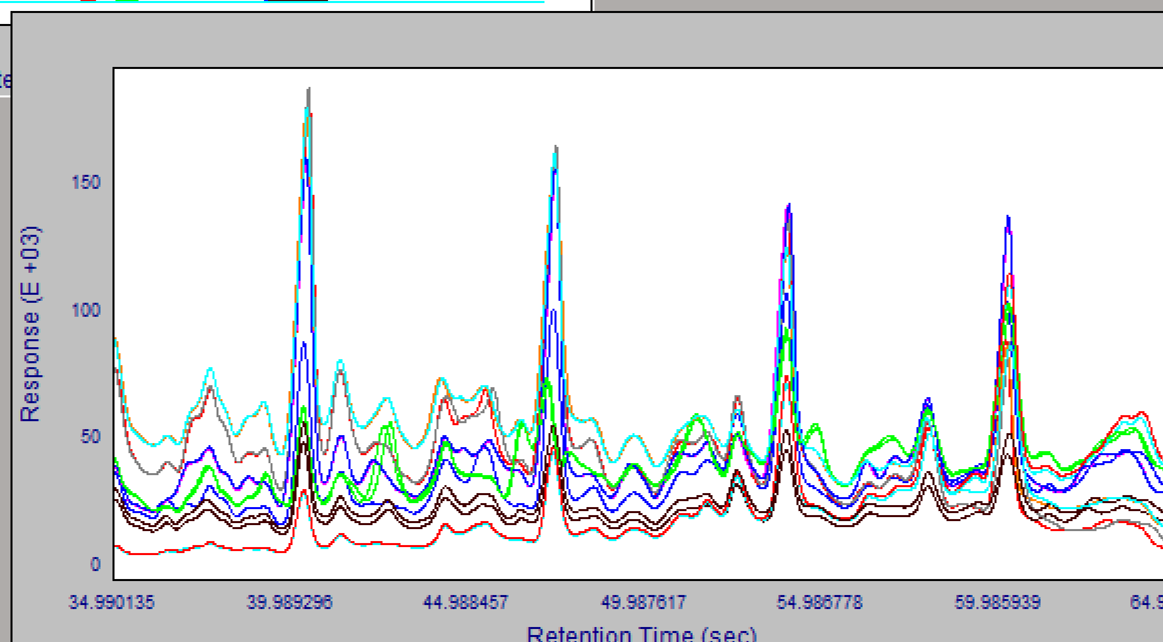
Location 1 – aligned to the Location 1 standard



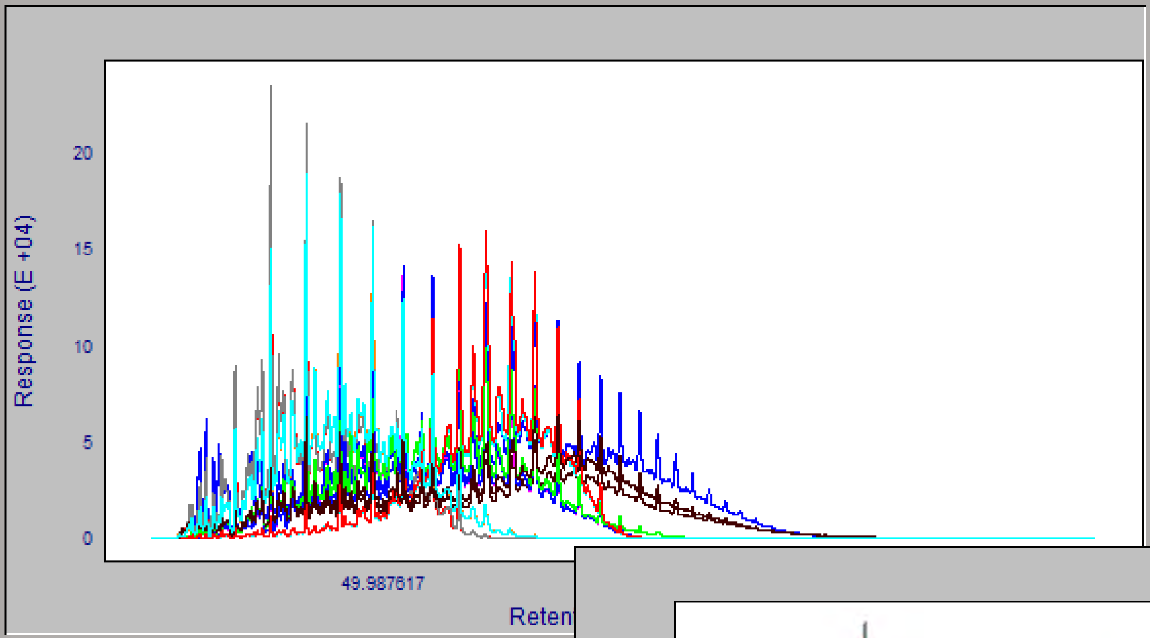


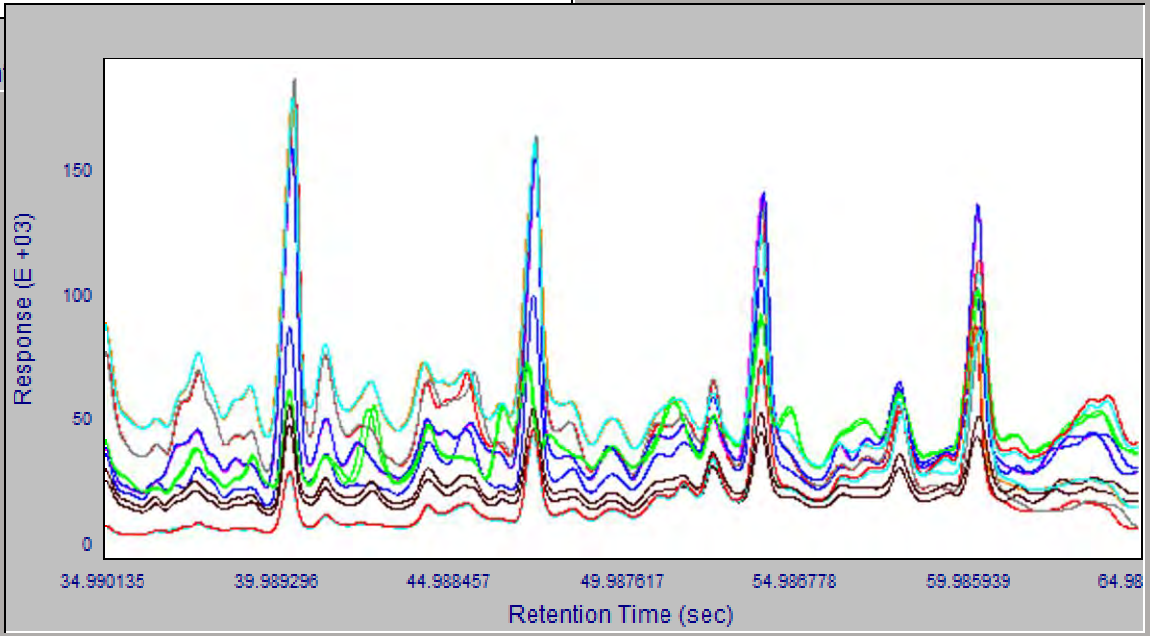
Location 2 – aligned to the Location 2 standard



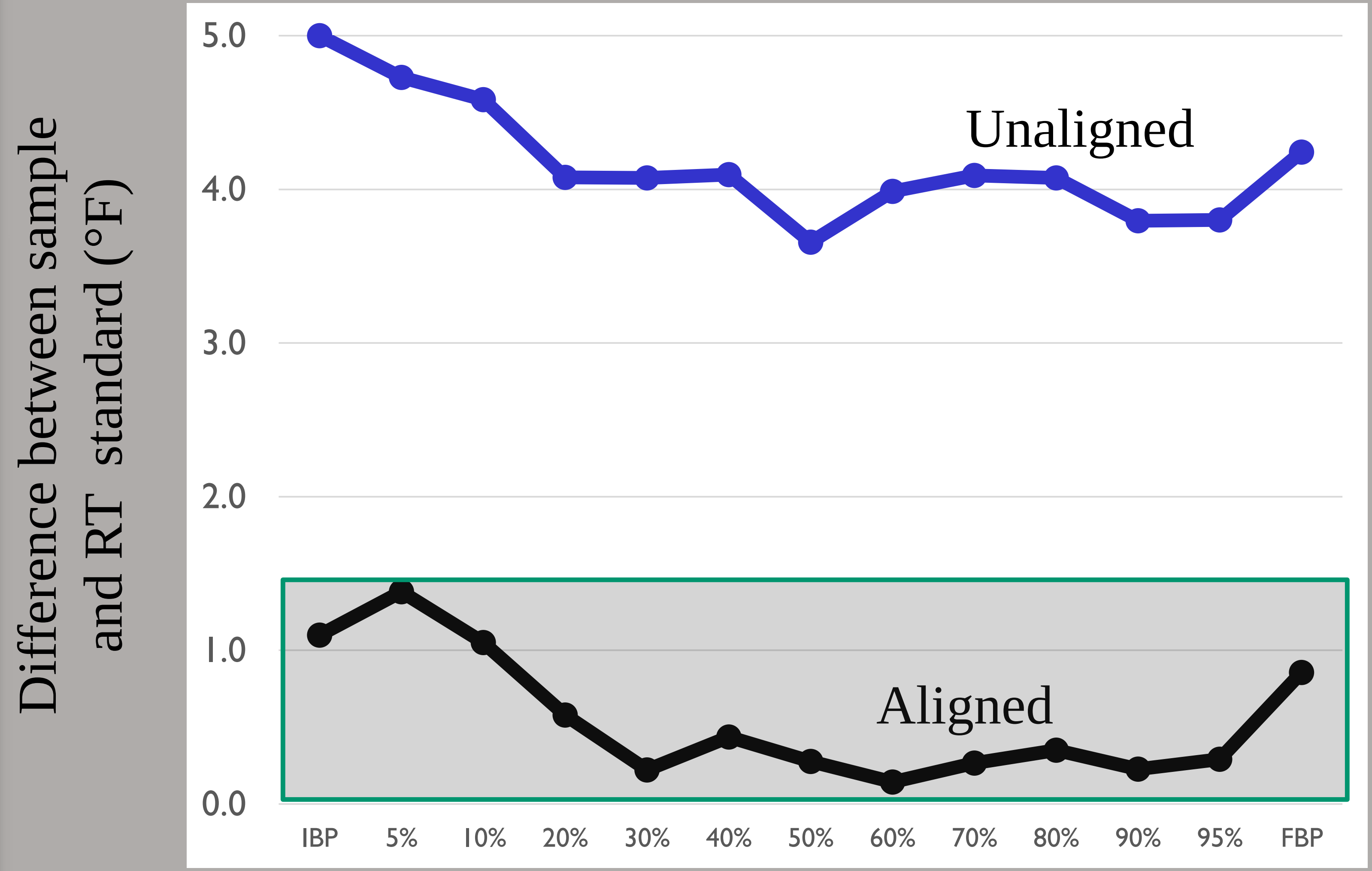


Location 2 – aligned to the <u>Location 1</u> standard





Impact of alignment



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Continuous data interpretation

We can correct retention times to match an application-specific relevant sample

You can use this to make all instruments performing a similar task to look identical (Plug and Play)

This raises the possibility of having a universal calibration

At the least, the frequency with which we really need to run calibration standards is significantly lower that what is currently being done.

PLUS validation of a multivariate instrument

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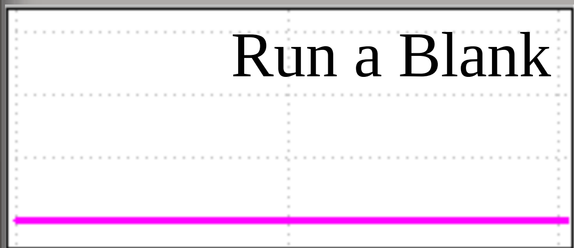
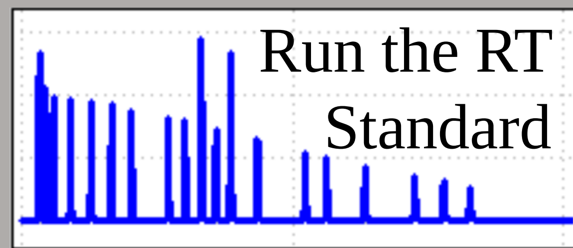
SimDist D7798: lab versus on-line

Laboratory



Pass



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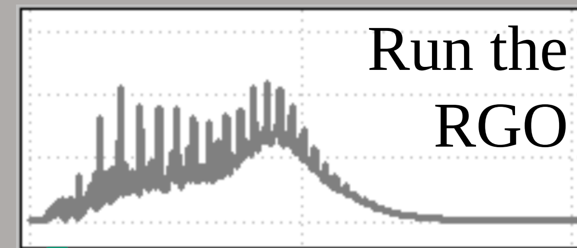

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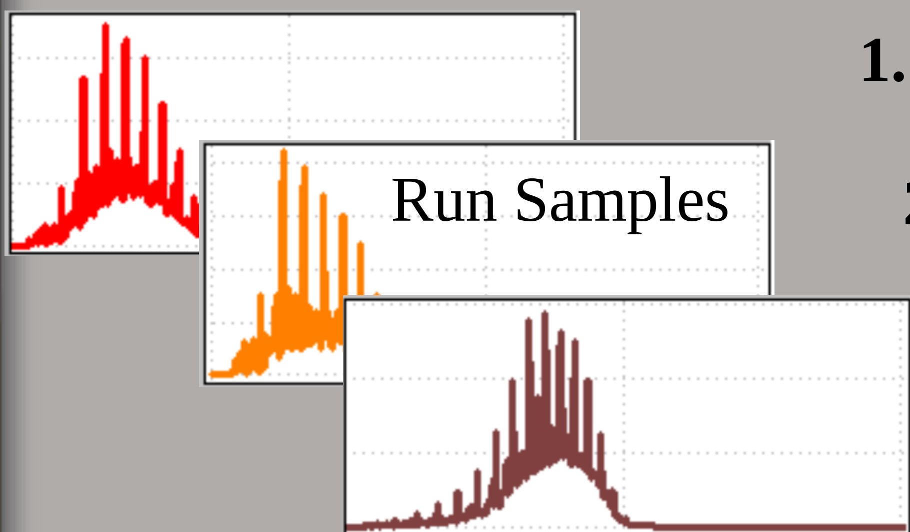

1. Run a Blank

to ensure a clean system

2. Run the n-Paraffin Standard

relates retention time to temperature

3. Run the Reference

to check results with a known

4. Run Samples

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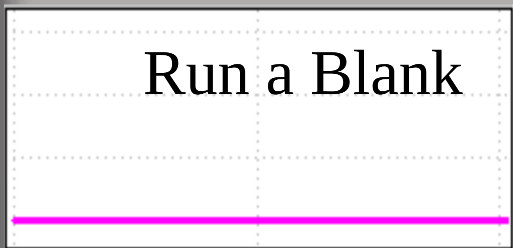
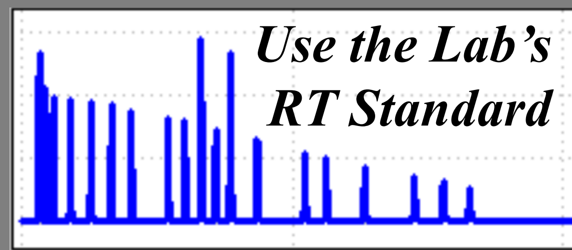
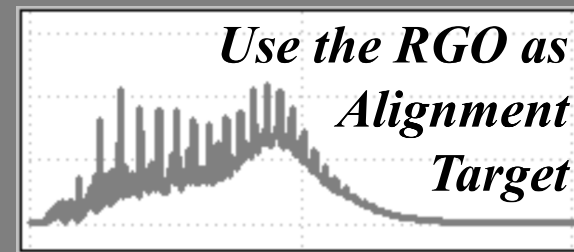
SimDist D7798: lab versus on-line

On-Line



Chromatographic files from the laboratory





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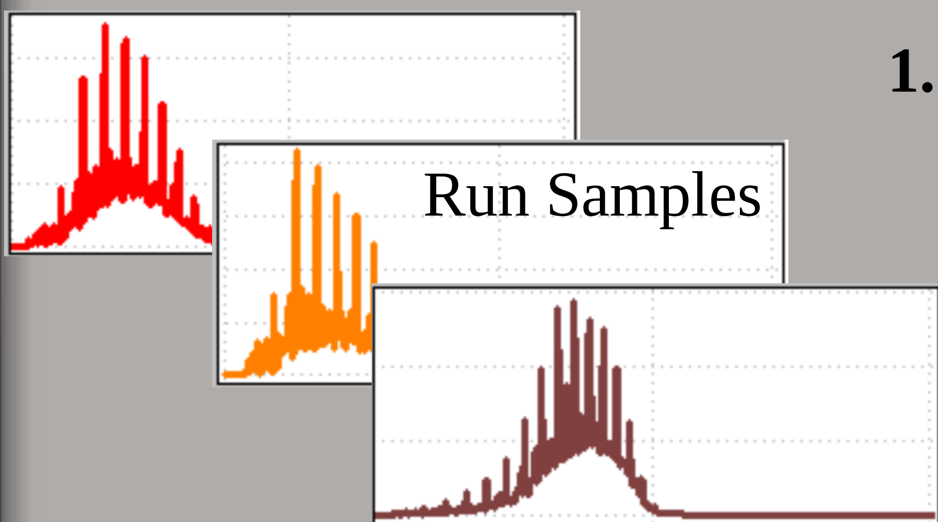

1. Run a Blank
to ensure a clean system

2. Use the *same* n-Paraffin Standard
from the run in the laboratory

3. Use the RGO or Process Sample
as an alignment target

4. Run Samples

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Delivering information

Just having the measurements does not translate into control

- Remember, there are not enough skilled technicians to handle even the current workload.
- Chemometrics aids the processing problem with 2 technologies:
  - Alignment enables us to sell instruments that have vastly-lower calibration requirements.
  - Interpretation algorithms automate the generation and the qualification of the information derived from the raw data.

And if we can make all of our instruments look as much alike as possible.

Interchangeability
Common interpretive base

Acknowledgements

- Robert Lorenz, Chevron
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