A LOW-CODE WEB APPLICATION FOR RELATIVE RETENTION TIME (RRT) ALIGNMENT ACROSS LC SYSTEMS

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INTRODUCTION

Retention time shifts in liquid chromatography (LC) are unavoidable. Absolute retention times are highly dependent on column and analysis conditions which can become an obstacle to comparing chromatographic data across LC systems.

Here we demonstrate the ability to align multiple complex chromatograms from different LC systems in an interactive web application using relatively few lines of code and utilizing the Empower™ Chromatography Data Software (CDS) Software Development Toolkit (SDK).

The Empower CDS SDK can be used to monitor one or more Empower databases and extract data into a cloud environment where data from multiple projects, systems &/ or Empower instances can be queried and accessed efficiently from a web application using cloud tools like Elasticsearch and Amazon S3. (Figure 1)

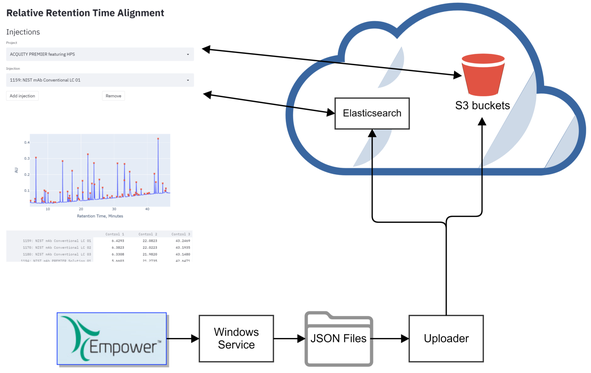

Figure 1. Application Architecture

RESULTS

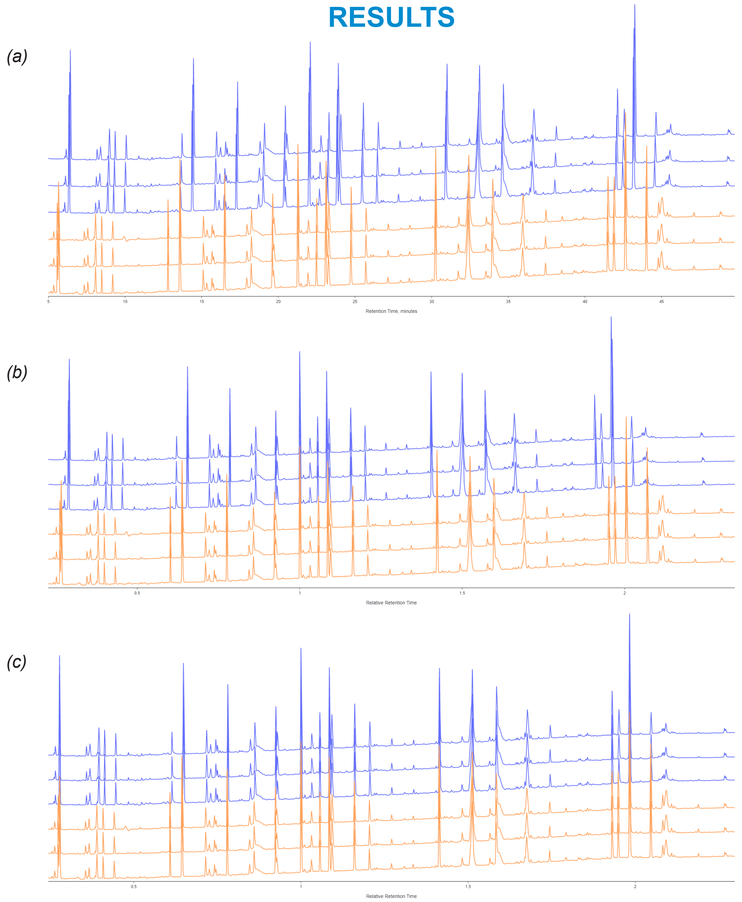

*Figure 2. NIST mAb Tryptic digest chromatography data. ACQUITY PREMIER CSH C18 1.7µm 2.1 x 100mm **(Orange)** ACQUITY CSH C18 1.7µm 2.1 x 100 mm **(Blue)***
(a) Unaligned; (b) conventional RRT alignment; (c) multi-point RRT alignment

METHODS

- Chromatographic data was extracted from the Empower CDS system using the Empower SDK and converted to a JSON format.
- Metadata was sent to an Elasticsearch engine where it is indexed for flexible and efficient text-based querying via a web API.
- Raw chromatographic data was stored in Amazon S3 buckets.
- The web application was developed in the Python™ programming language using Streamlit™ tools to build the UI.
- Alignment is performed using piecewise linear interpolation between common “anchor” peaks.

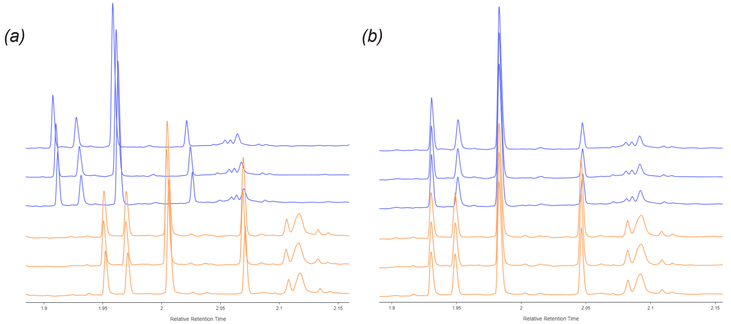

Figure 3. Zoomed area of data from Figure 1
(a) Conventional RRT alignment; (b) multi-point RRT alignment

CONCLUSION

- Alignment of complex chromatograms across different LC systems in a highly interactive web application using relatively few lines of code is possible.
- The conventional approach, whereby retention times are expressed relative to the measured retention time of a single standard peak, doesn’t produce good alignment across the entire time range in these complex data sets, see Figures 2(b) & 3(a).
- Using multiple common "anchor" peaks as RRT standard peaks provides much improved peak alignment between data from the different LC systems, see Figures 2(c) & 3(b).

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