

ShinyCDS

An open-source R shiny-based software for the reproducible processing of chromatograms

Edouard Salingros – Gembloux Agro-Bio Tech, University of Liège, 5030 Gembloux, Belgium

The elephant in the room

Proprietary chromatography data software (CDS) and **proprietary data file formats** are obstacles to data integrity, reproducibility in sciences and regulatory compliance:

- **Blackbox:** algorithms are rarely disclosed in details
- **Costly licenses:** small labs and universities cannot afford...
- **Limited interoperability:** not all CDS can read all proprietary file formats
- **Planned obsolescence:** CDS usually become unusable at some point after a major update of the operating system (OS)
- **No universal open file format:** even the ANDI (.cdf) format proposed by the ASTM (the closest attempt to a universal format) is imperfect, as metadata are lost
- **Cognitive load:** CDS interfaces are often complex, with many features/options left unused or at their default settings. Switching between multiple CDS with different interfaces on a regular basis can be a burden

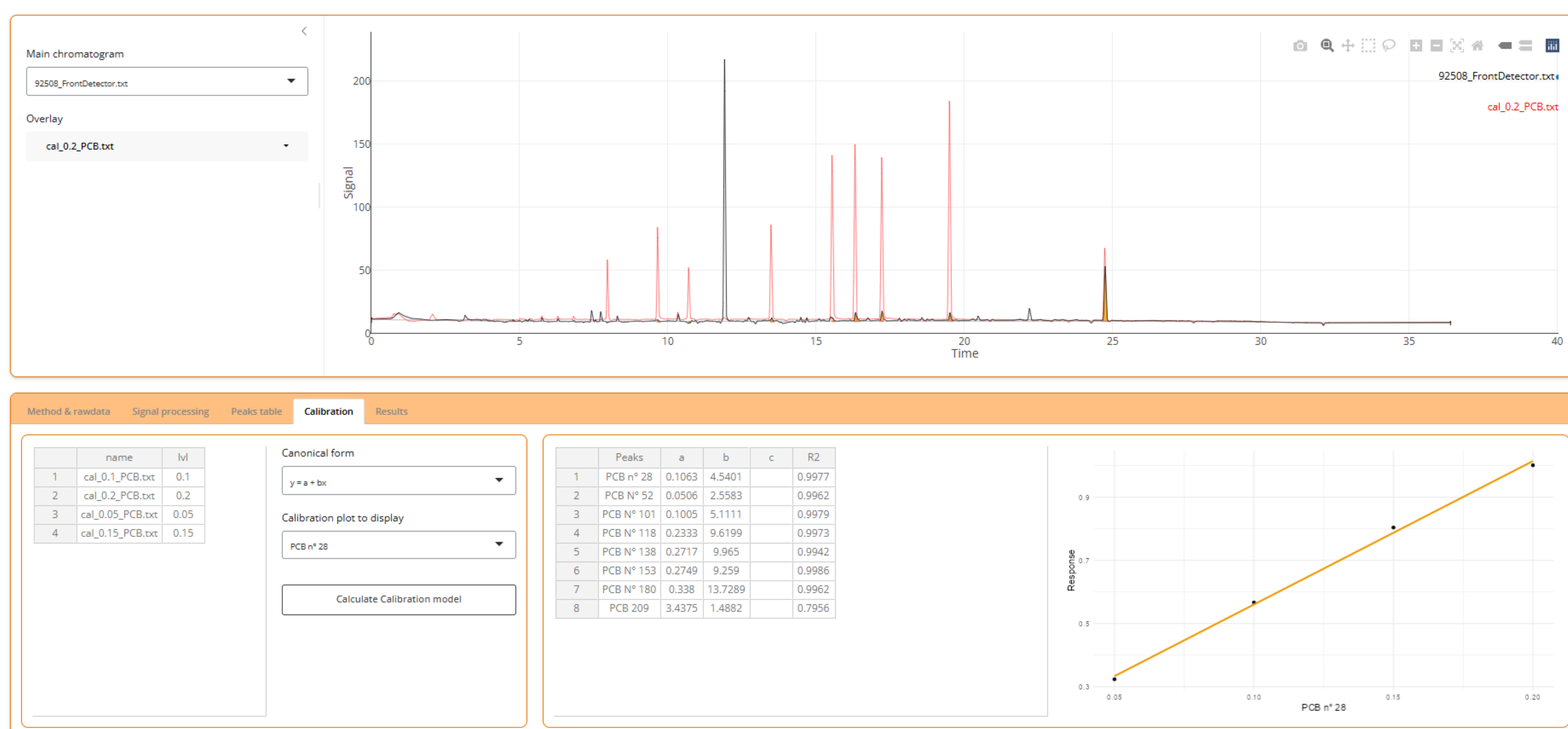
Custom open-source CDS

There is currently no fully open-source, generalist and free CDS available. OpenChrom [1], a well known alternative to mainstream proprietary CDS, only offers a limited version for free. Several alternatives to proprietary file formats have been discussed [2] but none arisen as universally accepted.

Although daunting at first glance, development of **custom CDS** has never been easier, using ever-improving open source languages and packages supported by active communities.

For example, in the R language [3], one of the most popular open languages for data analysis, various packages [4,5] make the development of applications truly accessible. Other packages allow parsing common proprietary file formats [6] and offer functions to achieve common operations on chromatographic data [7].

This work presents **ShinyCDS**, a fully functional CDS implemented as an R shiny app and leveraging existing resources.



Features & advantages of ShinyCDS

- ✓ Supports reading **raw data from various manufacturers for any separation method** (LC, GC, SFC, IMS, CE...), replacing the simultaneous use of multiple proprietary CDS
- ✓ Signal smoothing using **Savitsky-Golay**
- ✓ **Multiple baseline estimation methods**, including asymmetric least squares regression [8]
- ✓ **Automatic peak detection** and selection based on time windows
- ✓ Support for **internal standards** (relative retention time and relative area as signal)
- ✓ Support for **integration of fixed time ranges**
- ✓ **Methods can be saved** for easy reuse
- ✓ **Interactive user interface** allows direct visualisation of modifications by the user
- ✓ **Interactive chromatograms** with various zoom options, display of x-y coordinates on hovering and overlay of multiple injections
- ✓ Support for **high resolution png export** of chromatograms
- ✓ Reports available in **.xlsx, .docx and .pdf**
- ✓ Support for **export to database/LIMS**
- ✓ Can be **run locally** on a workstation using any OS, **or remotely** from a server (which can be on-site or off-site)
- ✓ The code can be **inspected and customised as needed** to implement new features or remove unused ones

Key R packages



References

- [1] Wenig, P. and Odermatt, J. (2020). BMC Bioinformatics,
- [2] Rauh, D. et al. (2022). Appl Chem, 94.
- [3] Ihaka, R. and Gentleman, R. (1996). J. Comput. Graph. Stat., 5.
- [4] Sievert, C. (2020). *Interactive Web-Based Data Visualization with R, plotly, and shiny*. Chapman and Hall/CRC.
- [5] Wickham et al. (2019). J. Open Source Softw., 4
- [6] Bass, E. (2026). chromConverter: Chromatographic File ConverterToolset.
- [7] Bass, E. (2026). chromatographR: Chromatographic Data Analysis

