

timsCompare: Effortlessly compare and extract data from Bruker MS methods

Tobias Kroniger¹

¹Bruker Daltonik GmbH, Fahrenheitstraße 4, 28359 Bremen, Germany

Introduction

The increasing complexity of acquisition modes in trapped ion mobility spectrometry and quadrupole time-of-flight instruments has made method development and troubleshooting a challenging task. Comparing mass spectrometer method files manually is tedious. Further, method reporting in scientific publications is frequently incomplete or ambiguous, hindering reproducibility. To address this, I present timsCompare, a standalone, desktop application designed to enable the offline parsing, visualization, and comparison of instrument methods. This allows researchers to download raw data directly from online repositories and reverse-engineer the ground-truth acquisition parameters, eliminating the dependency on potentially inadequate text descriptions in manuscripts. By bridging the gap between acquisition and reporting, it fosters better reproducibility and transparent method sharing within the mass spectrometry community.

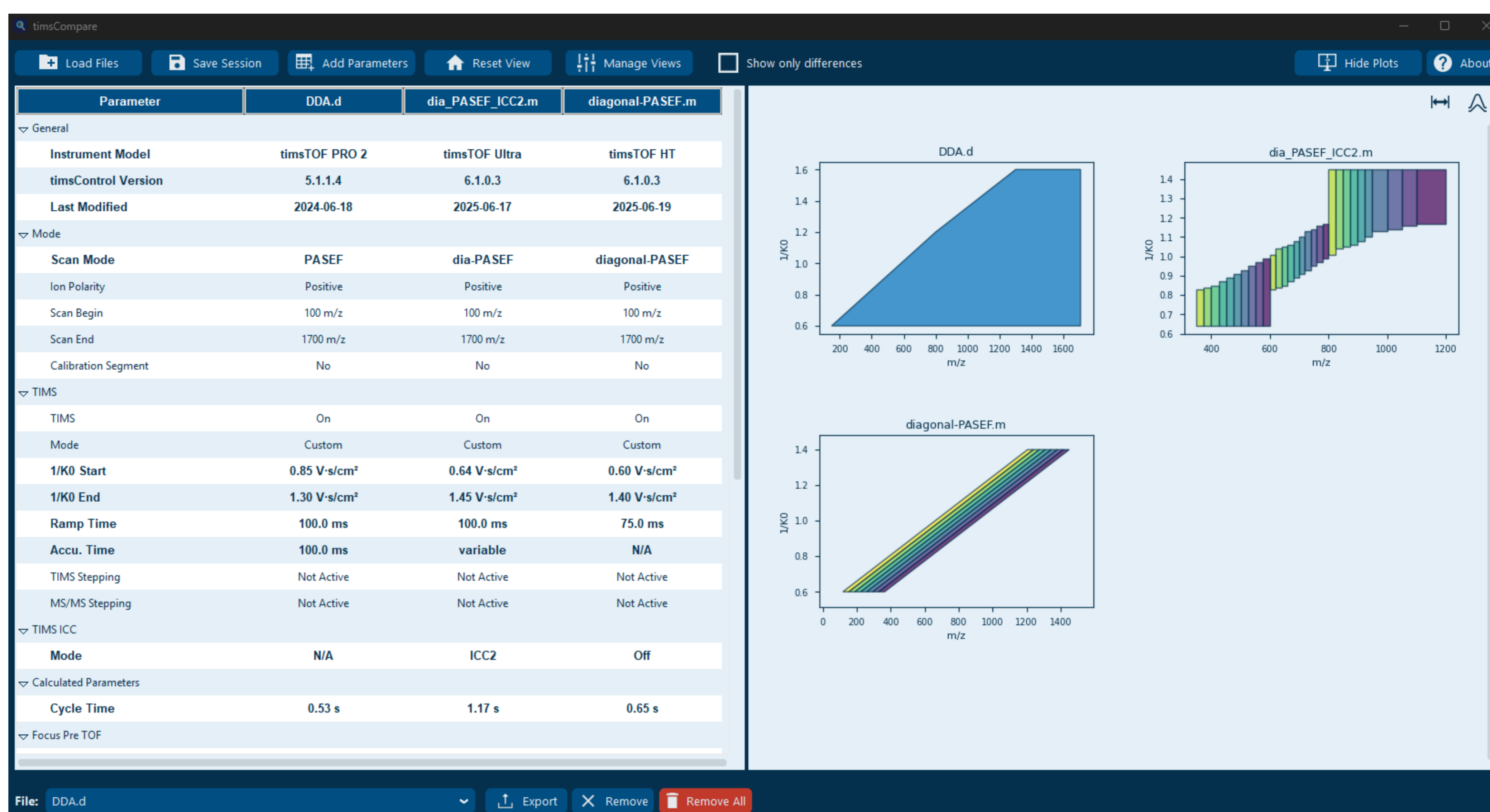


Fig. 1 Main window interface

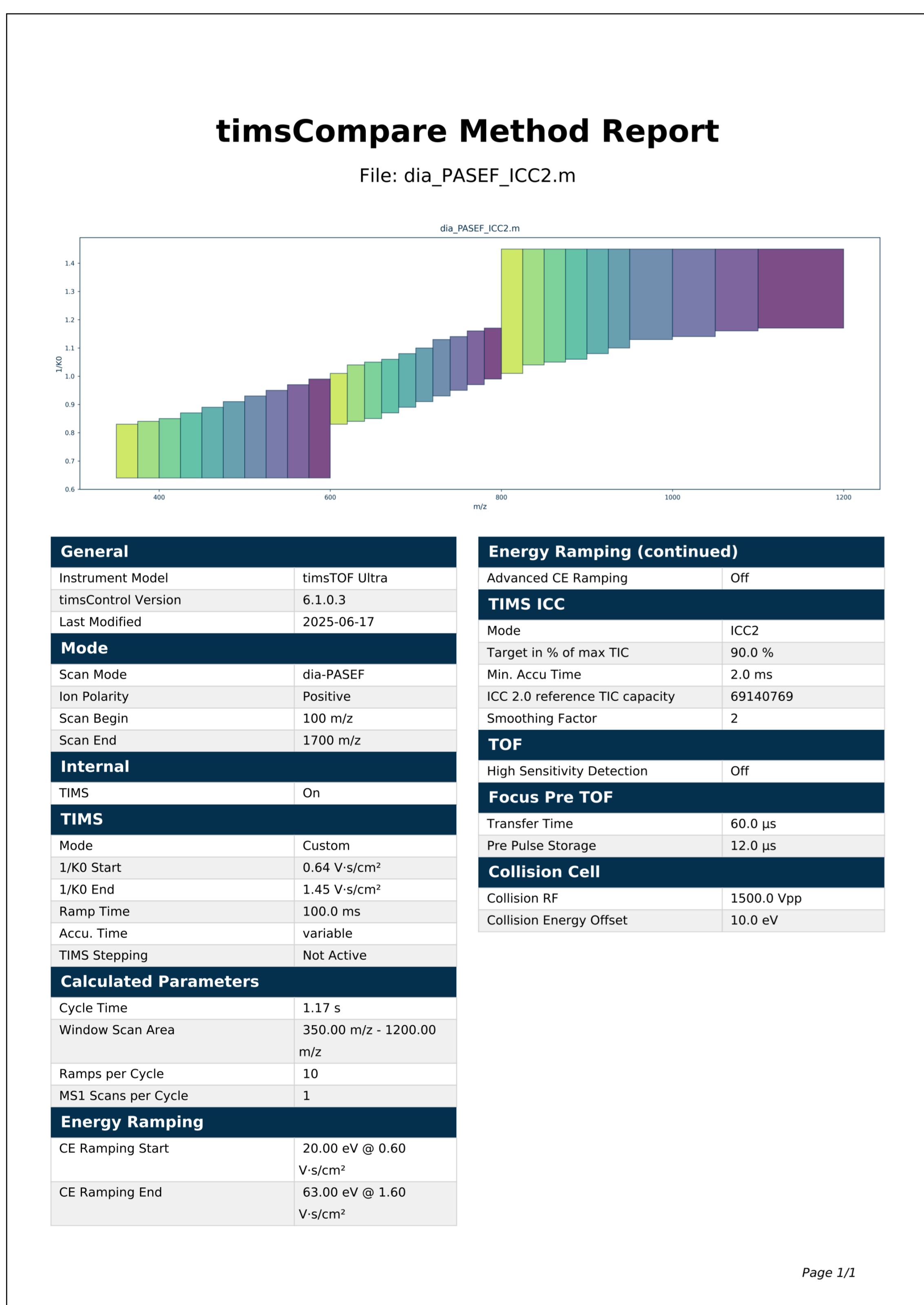


Fig. 2 Method report layout

Summary

timsCompare significantly reduces the barrier to compare and optimize Bruker acquisition methods. By providing an offline, instrument-independent platform for detailed inspection, it empowers researchers to quickly troubleshoot experiments, share methods, and compare their parameters against those from online repositories or previous acquisitions. Ultimately, the tool transforms method files into transparent, shareable assets, enabling the community to validate published data and deploy new applications more effectively.

Disclaimer: timsCompare is an independent, third-party tool and is not an official Bruker product, nor is it affiliated with or supported by Bruker.

Results

timsCompare provides an immediate side-by-side tabular view of loaded methods, automatically highlighting parameter differences in bold. It natively supports one-segment and multi-segment acquisitions, enabling users to compare specific time segments within a single file or across multiple datasets. To facilitate collaboration, the application introduces a proprietary compressed session format (.tcs). This allows researchers to encapsulate parsed metadata and visualizations into lightweight files (<1MB), which can be shared via email and opened without access to the original raw data.

Beyond textual parameters, timsCompare visualizes isolation schemes—including PASEF polygons, dia-PASEF windows, and diagonal-PASEF slices. These definitions can be exported directly to timsControl-compatible text files, streamlining method transfer from raw data to new methods. For documentation, the integrated Report Wizard generates comprehensive PDF or CSV method reports for laboratory notebooks or publications featuring smart column batching to handle large-scale comparisons across multiple pages.

How to get timsCompare

The windows installer for timsCompare is freely available at <https://github.com/kronigert/timsCompare>. Feel free to use the QR-code to get to the GitHub repository:

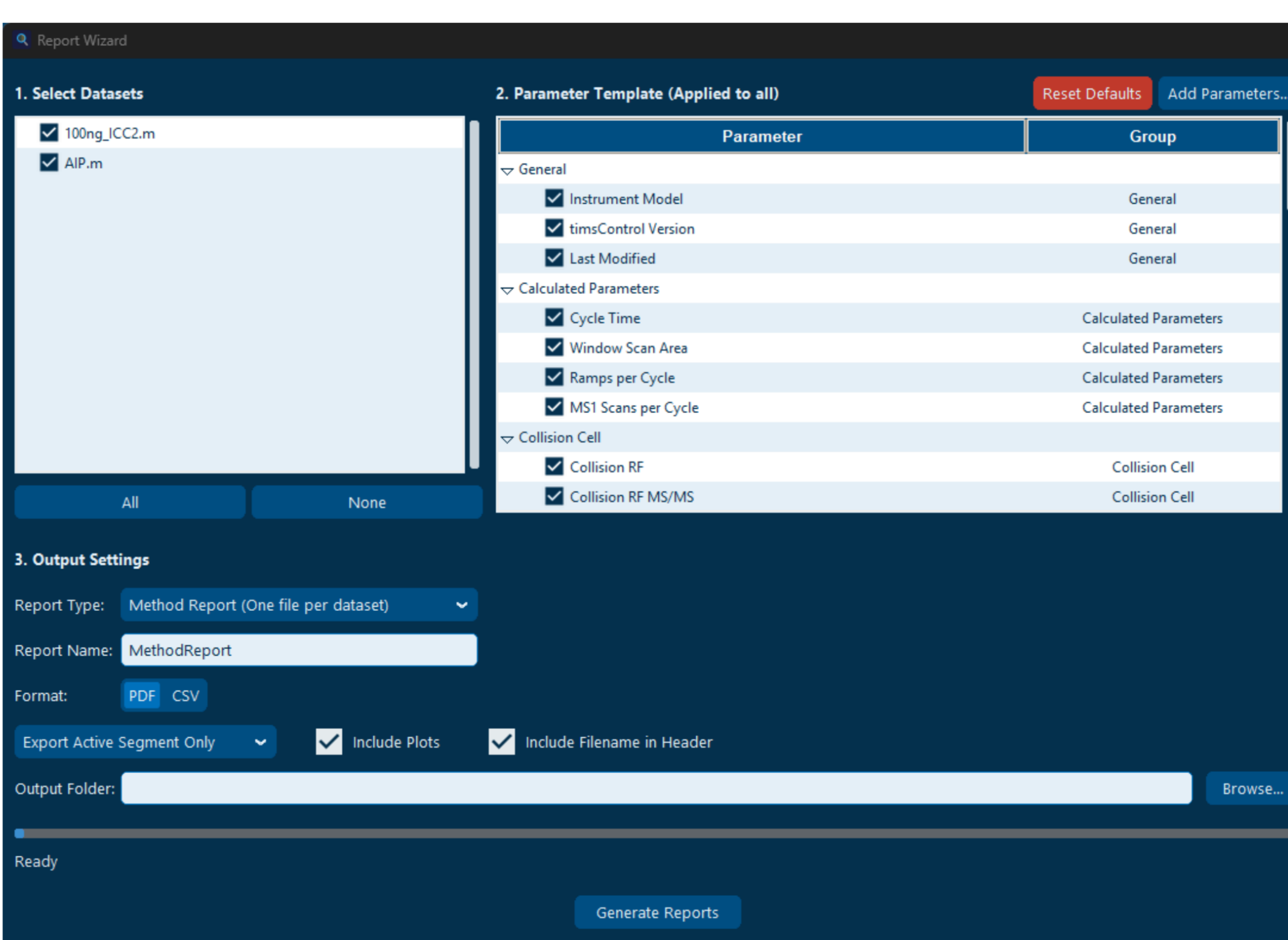


Fig. 3 Report wizard interface

Conclusion

- Accelerates Method Development and Troubleshooting: Replaces manual inspection with automated, side-by-side comparison and visualization.
- Ensures Reproducibility: Extracts ground-truth parameters directly from raw files, eliminating reporting ambiguity.

Software Tools