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## Introduction

- Reliable instrument performance (Reproducibility of retention time, accurate mass, isotope patterns, CCS, MS/MS spectra) is the foundation of trustworthy data
  - Regular investigation of instrument performance by system suitability testing (SST) is essential
  - Long term tracking of instrument performance as key QA/QC tool
- QC Data should cover both immediate status und track long term trends
- Further requirements: minimal operator error, affordability in time and personnel resources
  - Necessity of semi-automated and software-driven procedures
  - Evaluation of QSee™ Performance Test Software (Bruker Daltonics, Germany) over a 6-month period as a fully integrated System Suitability Testing Suite

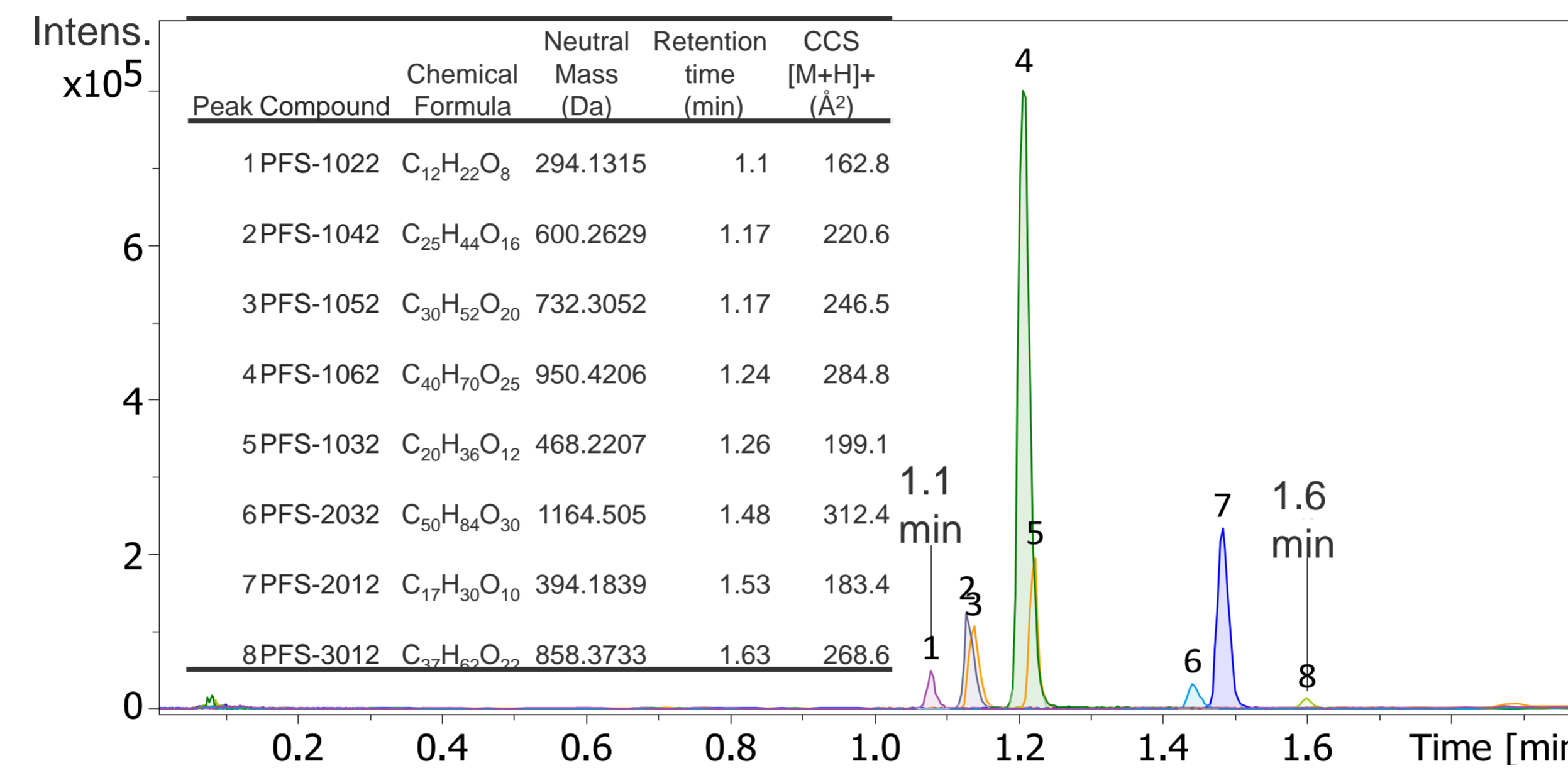


Figure 2: Extracted Ion Chromatogram of QSee-8 reference mixture in positive mode, Table shows QSee-8 Mixture compounds

## Methods

- QC data were acquired on multiple LC-timsTOF Systems (Elute + timsTOF Pro 2 (Tübingen), Agilent 1290 + timsTOF HT, Agilent 1290 + timsMetabo (Bremen)) using the QSee Performance Test Software
- Short gradient of 5 min total using water and acetonitrile (0.1% FA each) with RP columns (C8/C18), 95% to 1%A in 2.6 min
- QSee-8 standard mixture consisting of eight synthetic compounds with 290 to 1200 Da (Polymer Factory, Sweden), target concentration 10 µg/ml
- Triplicate injections of QC mixture and blanks at beginning, middle and end
- Tracked parameters: m/z (error), peak area, mSigma, RT (error), peak width, CCS (error)
- Automatic generation of result reports with clear pass / fail criteria
- Transfer of results data into TwinScope for longitudinal monitoring

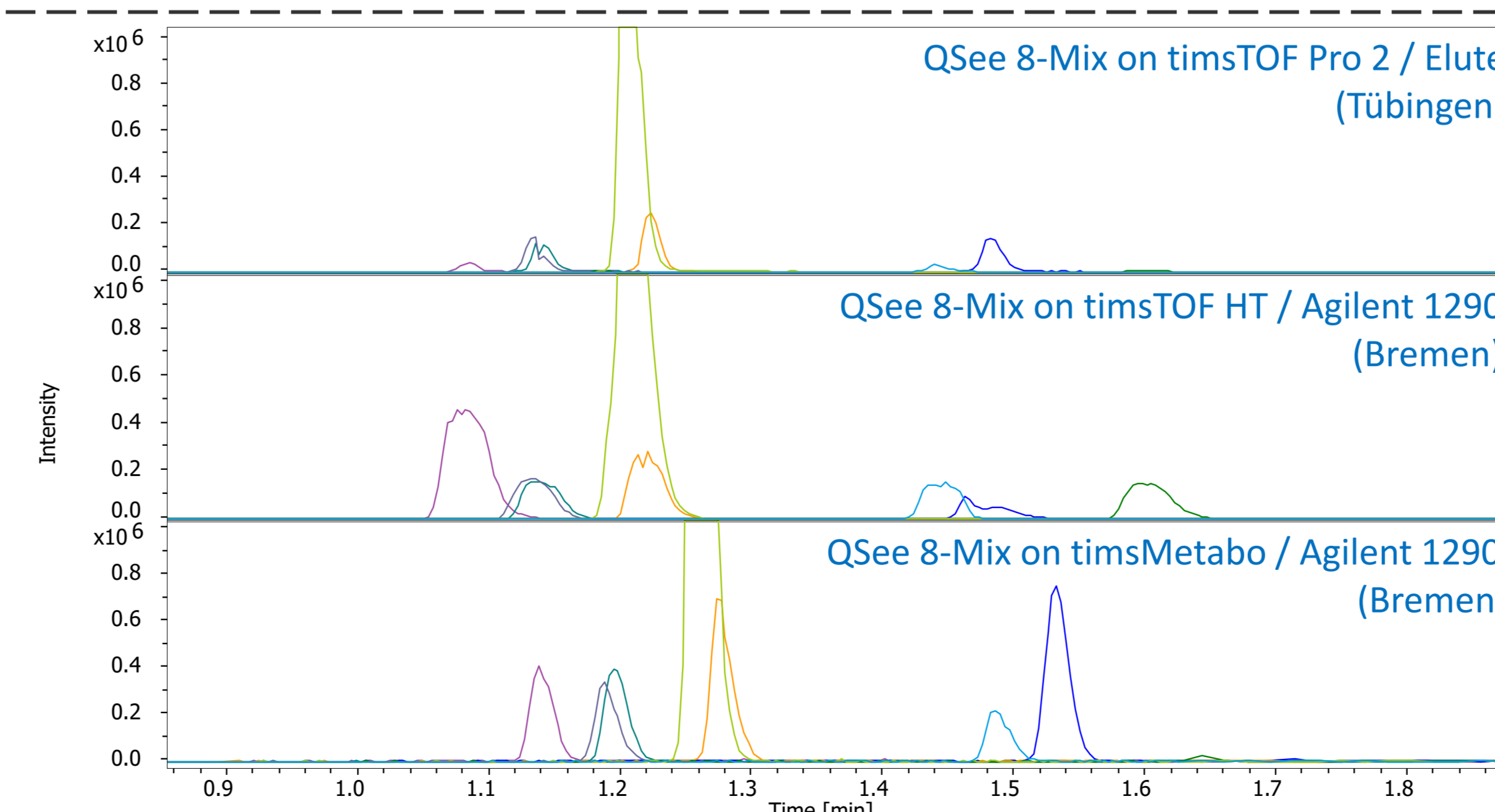


Figure 2: EIC of QSee-8 mixture of three tested LC-timsTOF system configurations

## Results

- Deviations in QSee indicated system issues which could subsequently be identified and mitigated:
  - Reduced peak area (sprayer contamination) -> Front-End cleaning
  - Shifted retention times (pump leak in B) -> pump repair

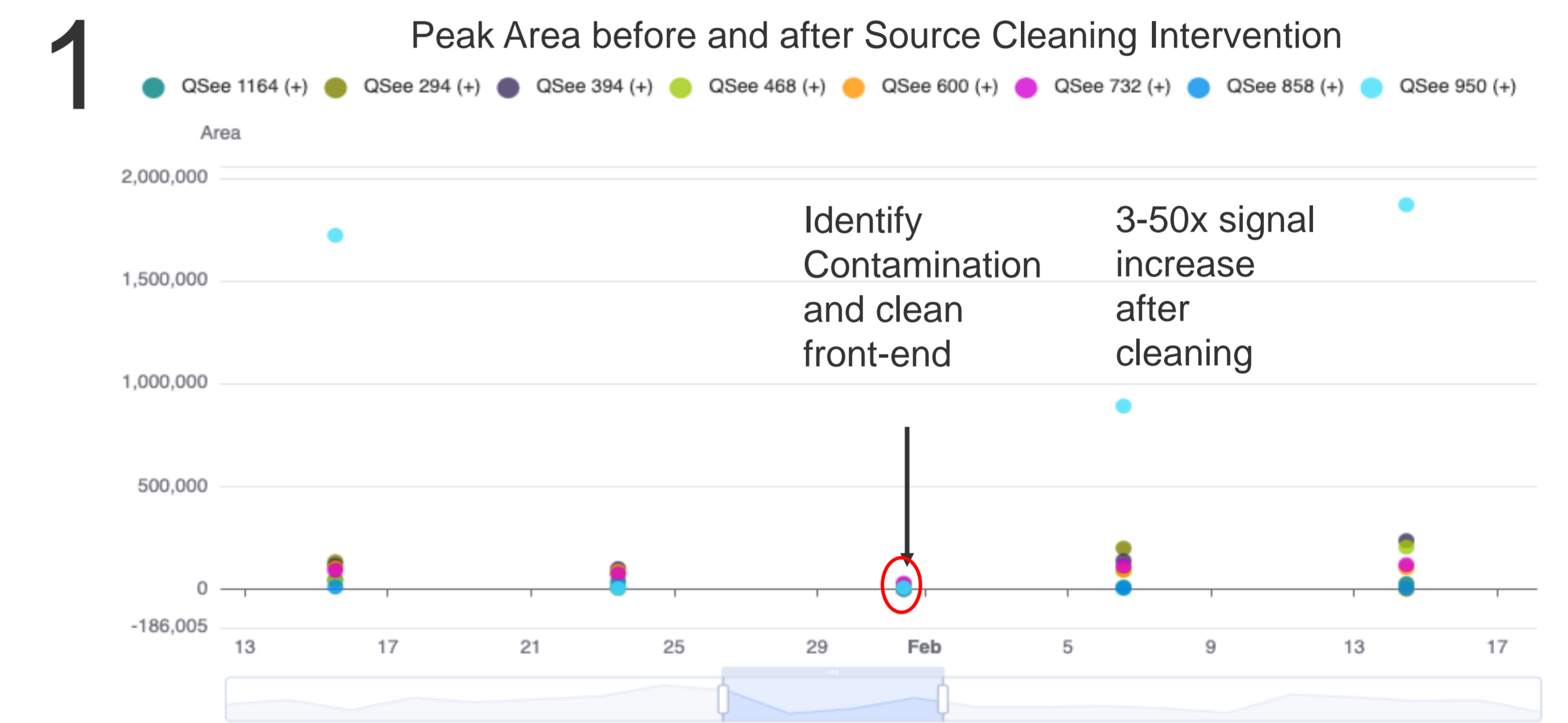


Figure 4: 1) Reduction in peak area due to Front-End contamination, areas restored after cleaning 2) Retention time deviation in a singular QSee run allowed for identification of a minor leak in pump B, RT is restored to baseline after cleaning of check valve

## Summary

- QSee provides straightforward System Suitability Testing with minimal operator effort (30 min setup + 90 min runtime)
- Automated data integration provides valuable longitudinal system overview
- Standardized workflows for long term reproducibility

**Conflict of interest statements:** SM and MRL are employees of Bruker Daltonics GmbH & Co. KG. Bruker Daltonics manufactures LC-MS instrumentation, consumables, and timsTOF instruments. CT reports a research grant by Bruker Switzerland AG.

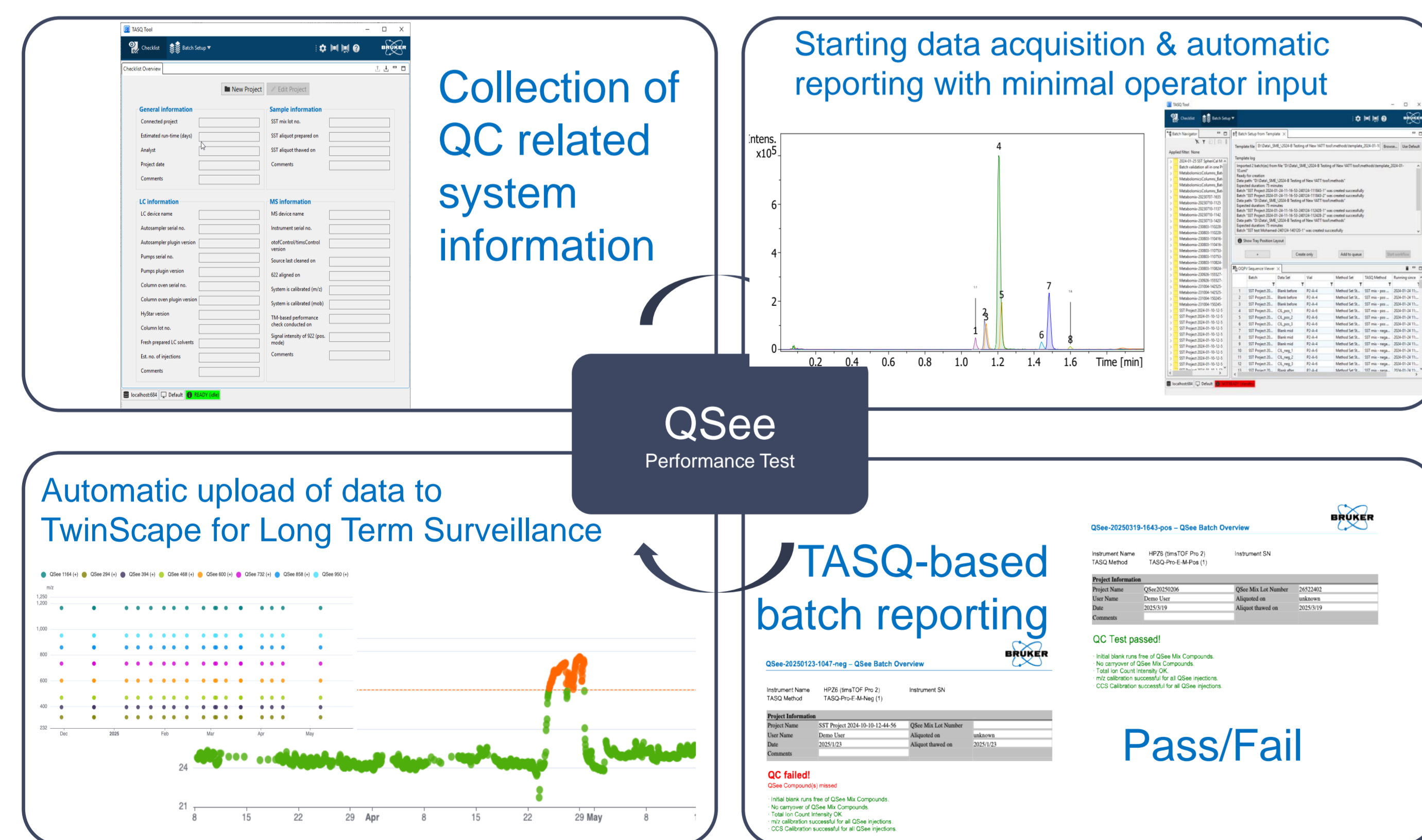


Figure 1: Process Diagram of the QSee Performance Test

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