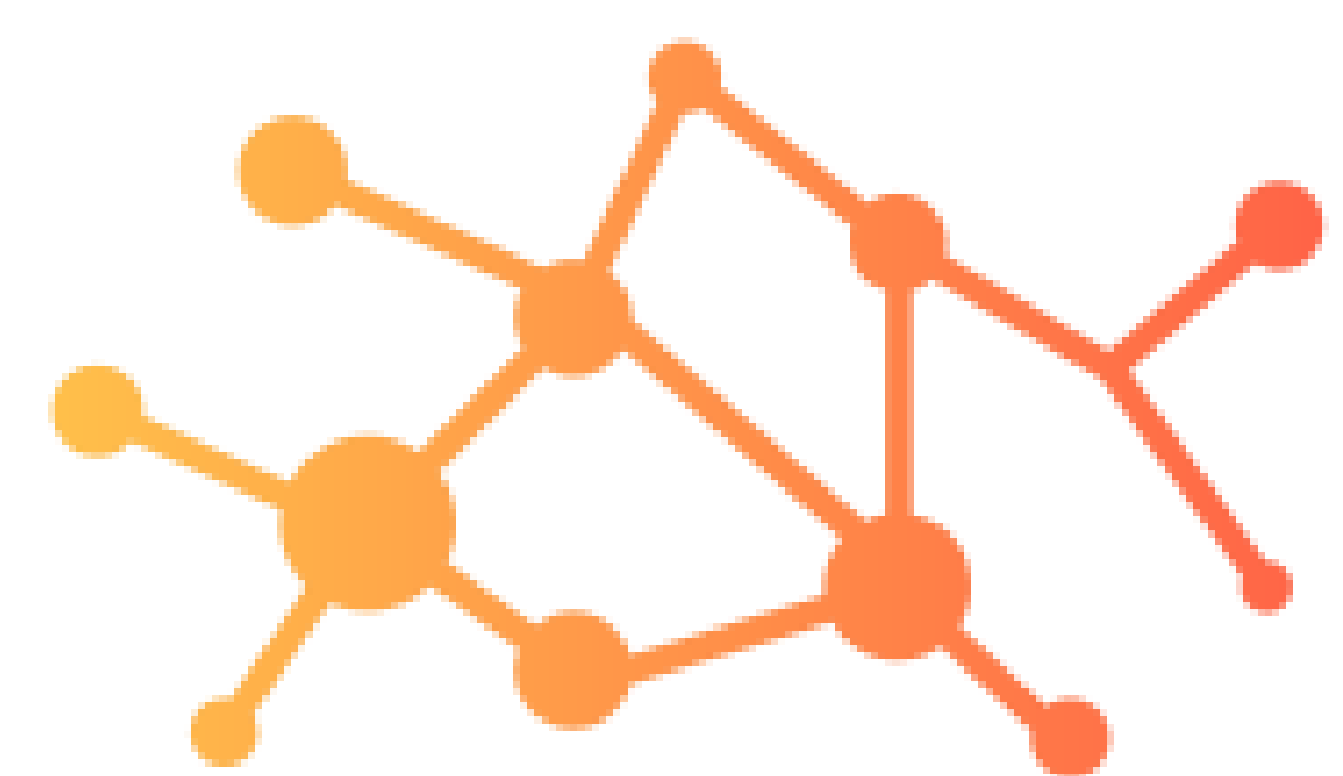


Abstract

We developed PASER (Parallel Database Search Engine in Real-Time), which performs database searching in parallel with data acquisition on a high-speed timsTOF Pro mass spectrometer. To perform a database search in real-time, PASER adopts a fast IP2GPU search engine. Using PASER, we demonstrate the simultaneous completion of database searching and MS spectra acquisition. The PASER search engine can keep up with the 120Hz MS/MS-acquisition speed of the timsTOF Pro instrument, saving significant time by elimination of separate data extraction and protein database search steps, thus enabling true high-throughput proteomics data analysis in an automated way. PASER is scalable and can perform searches on data from multiple timsTOF instruments without compromising the search speed on any of the data analyses.



PASER

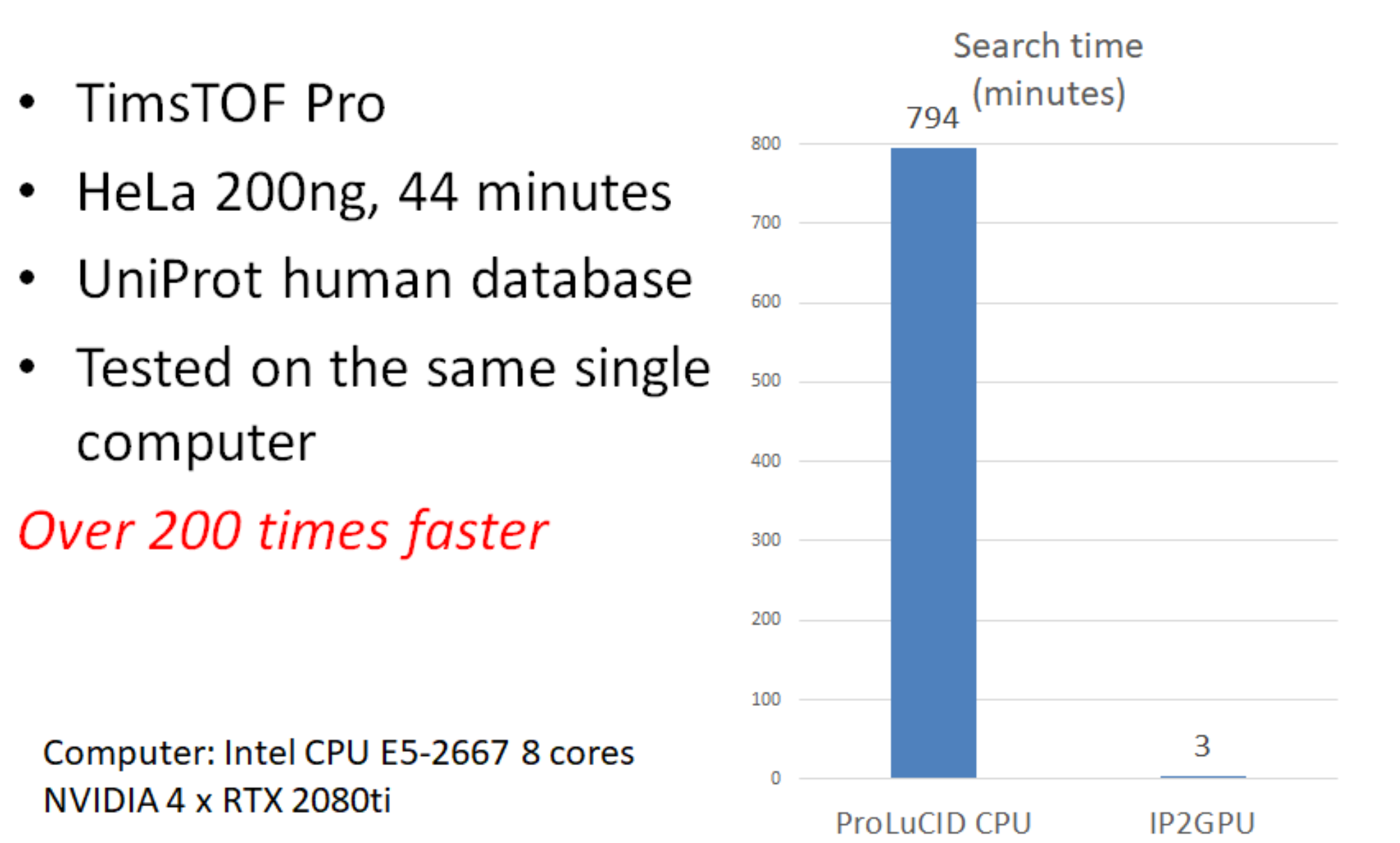
Deeper Faster Smarter

Extremely fast search engine

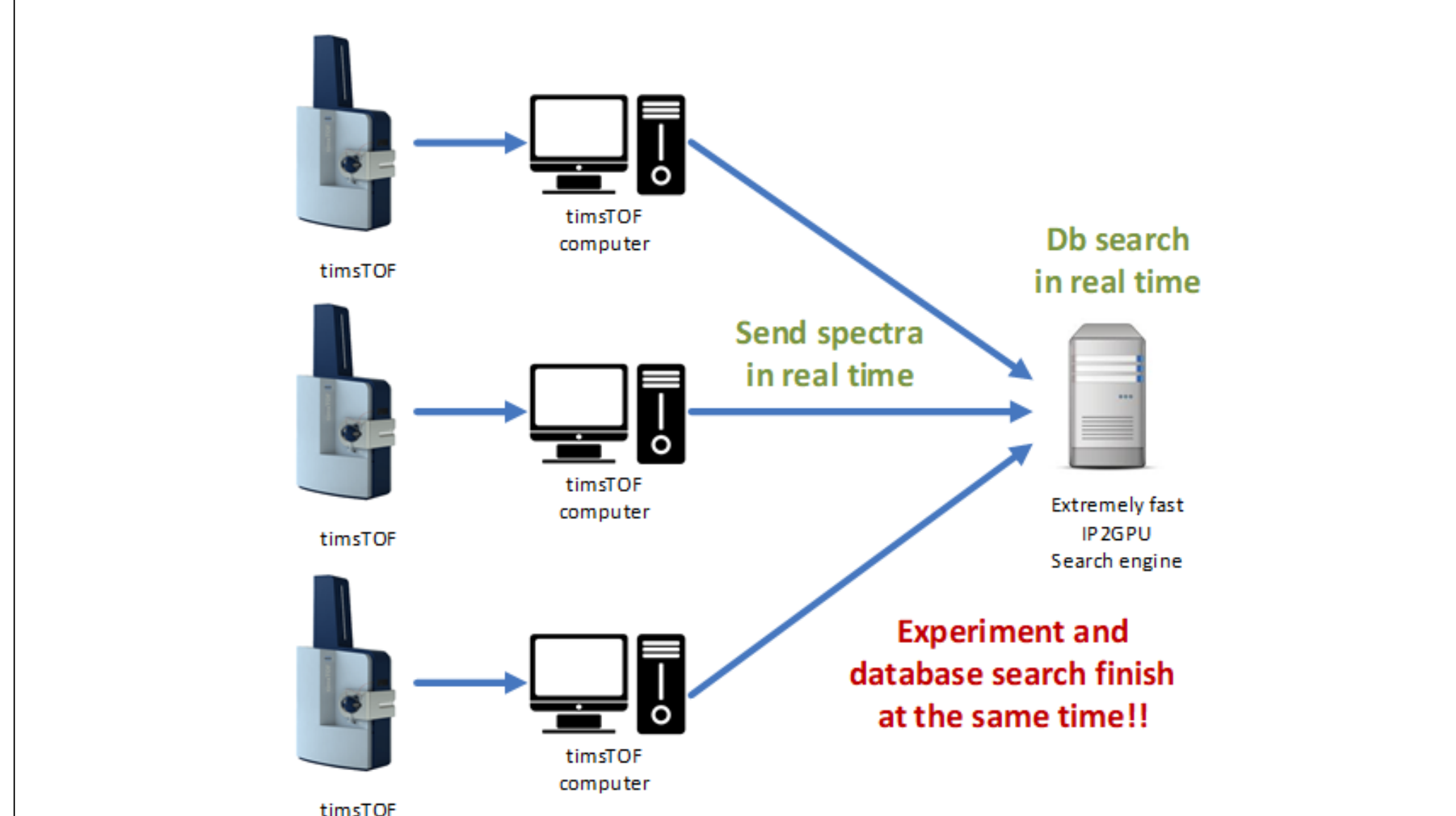
CPU vs IP2GPU Search Time

- TimsTOF Pro
- HeLa 200ng, 44 minutes
- UniProt human database
- Tested on the same single computer

Over 200 times faster



PASER Overview



Experimental design

Evaluation of PASER

- timsTOF Pro
- HeLa, 200ng
- 6 runs

Run 1	Run 2	Run 3	Run 4	Run 5	Run 6
R1	NR1	R2	NR2	R3	R4

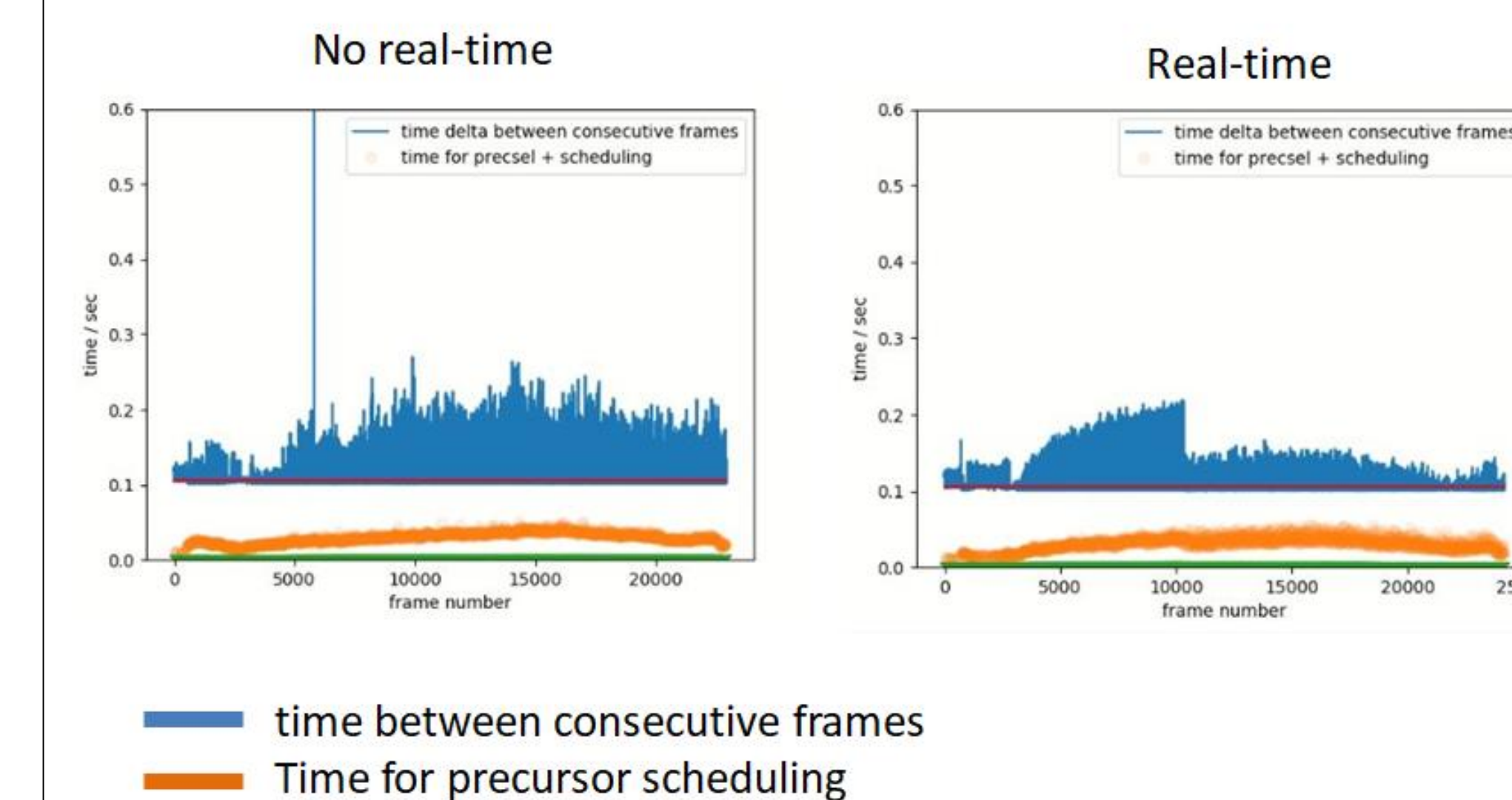
R: real-time

NR: no real-time

No slow down on scanning time

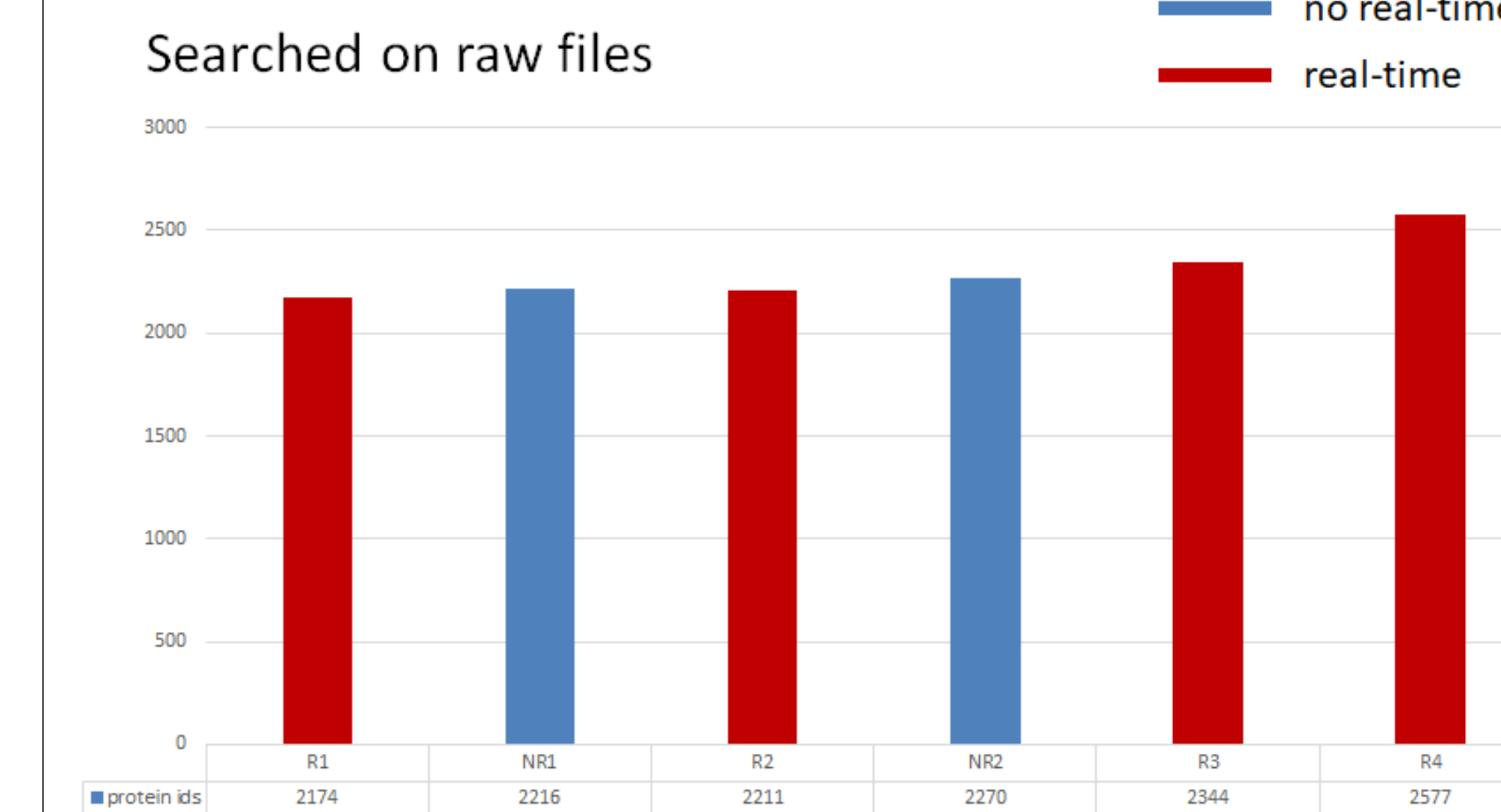
Instrument Scanning Time

RT does not affect instrument scanning speed



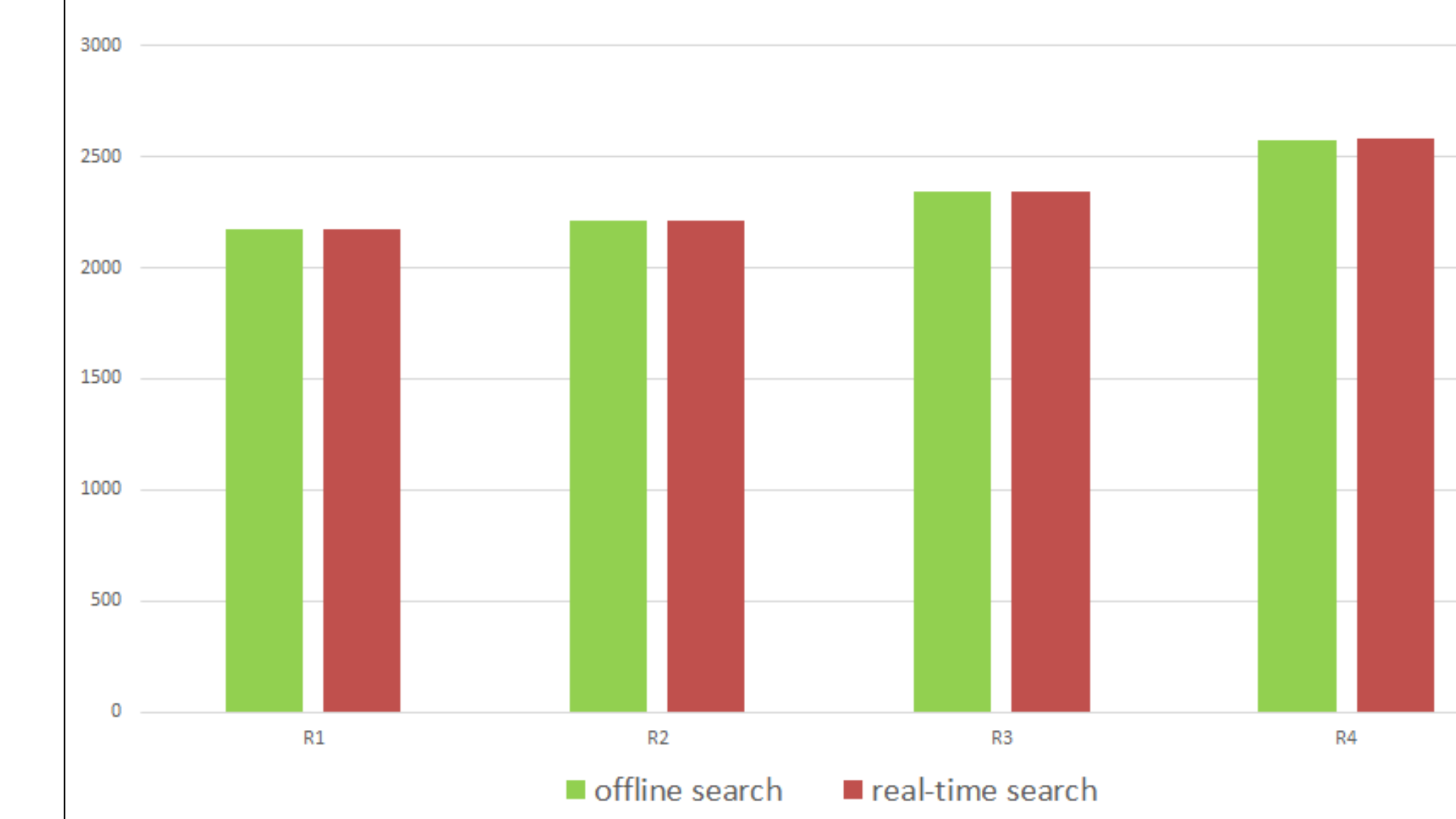
Realtime vs No Realtime generates consistent results

Number of Protein IDs



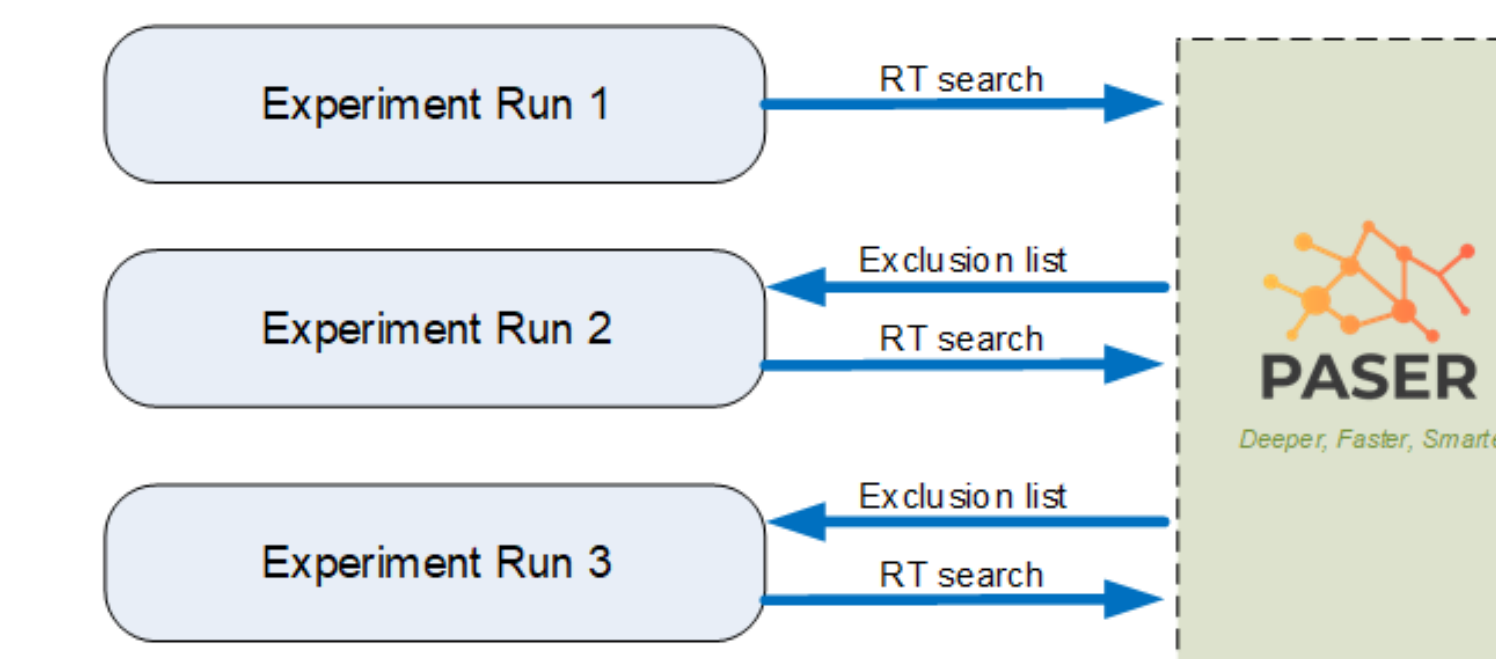
Realtime and Offline search generates identical results

RT vs Offline Search Protein IDs



Exhaustively pick low abundant peaks

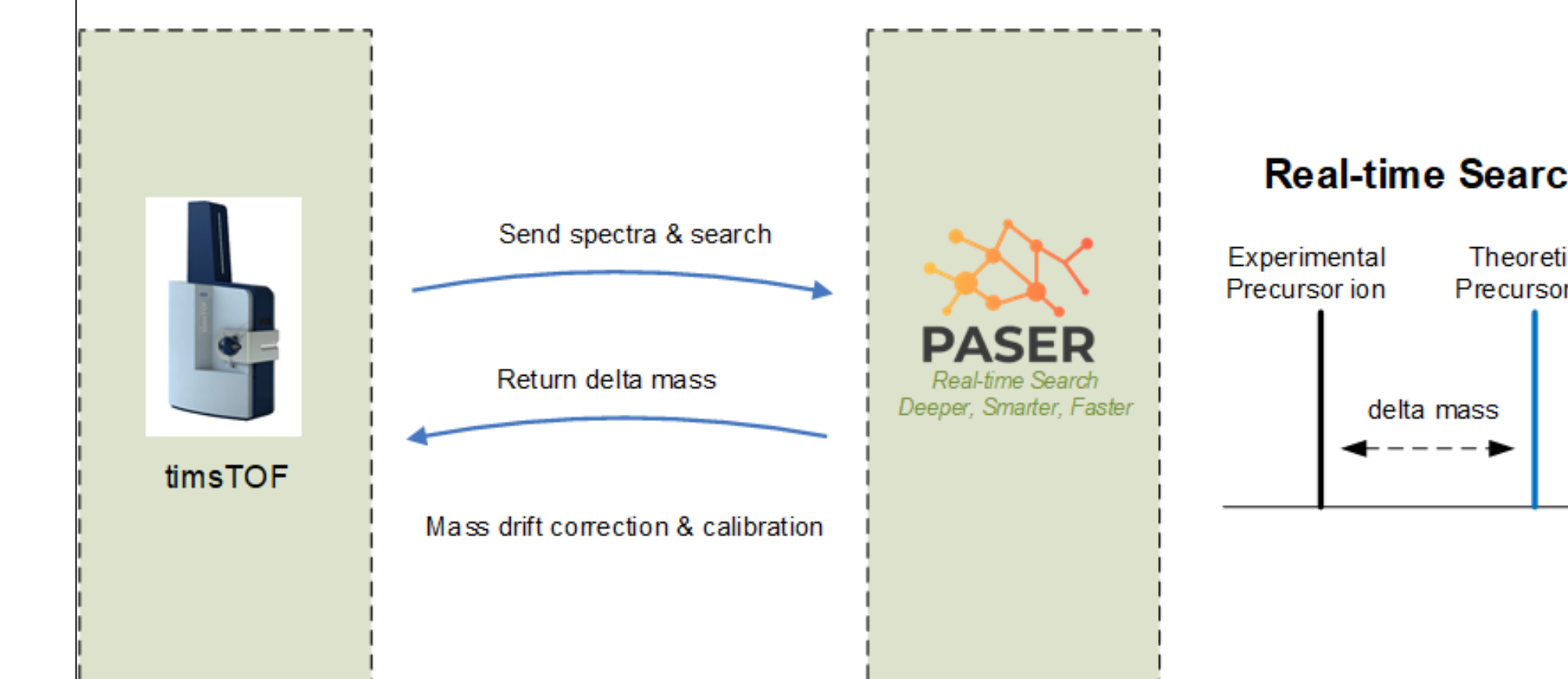
Dynamic Exclusion List



- Auto sampler
- Identify peptides in real-time
- Build exclusion list automatically
- Exclude previously identified peptides and pick ions deeper
- exhaustively search down precursor ions

Application on labeled samples

Dynamic Mass Drift Correction & Calibration



Conclusion

PASER provides extremely efficient protein database search strategies. The search can be completed simultaneously with timTOF data acquisition by dramatically reducing separate data extraction and search time.

References

1. T. Xu, S. K. Park, J. D. Venable, J.A. Wohlschlegel, J. K. Diedrich, D. Cociorva, B. Lu, L. Liao, J. Hewel, X. Han, CCL. Wong, B. Fonslow, C. Delahunty, Y. Gao, H. Shah, and J. R. Yates, 3rd, ProLuCID: an improved SEQUEST-like algorithm with enhanced sensitivity and specificity, J Proteomics, 2015
2. Integrated Proteomics Pipeline (IP2) – www.integratedproteomics.com