

MOBILion/Agilent Acorn Data Processing with Skyline

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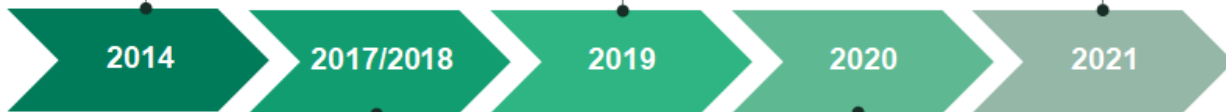
The ACORN Project | What is it?

Invented at Pacific Northwest National Laboratory in 2014

MOBILion has exclusive license to the SLIM technology

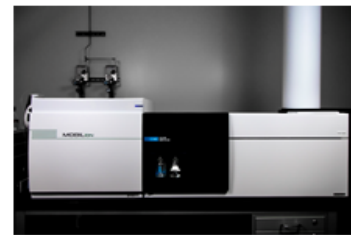


Dr. Richard D. Smith
Photo Courtesy of
Pacific Northwest
National Lab



MOBILion Planning for Commercialization Begins

Team and technology continue growing, key applications identified, and beta unit planned



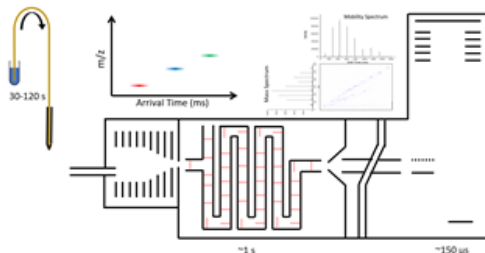
MOBILion Commercial Launch
ACORN SLIM-QTOF

MOBILion Begins its Journey

The first team members join and start to build out proof of concept

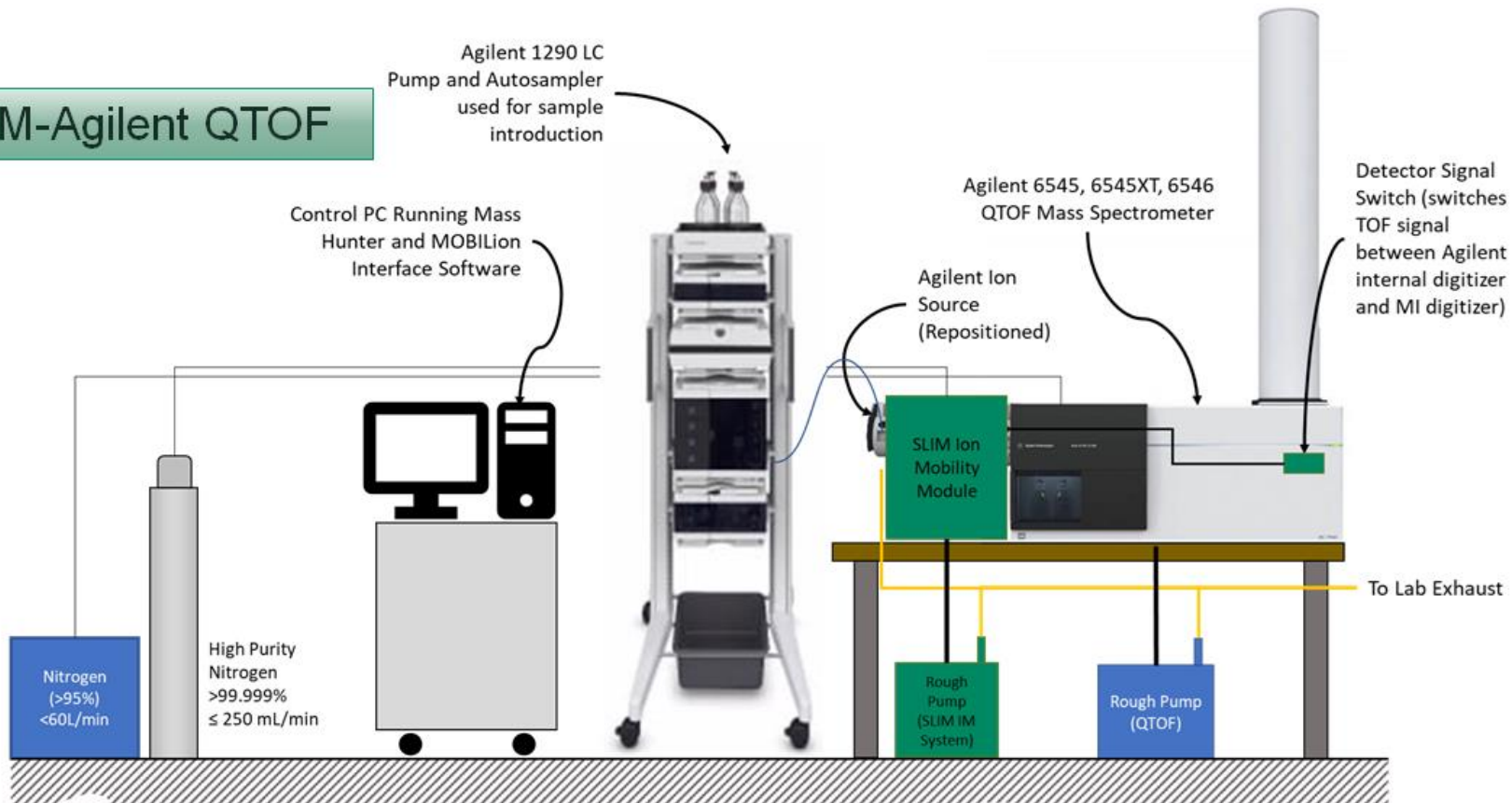
MOBILion Launches Beta Units in the Field

Vanderbilt, CCRC, BATL, UW, Agilent beta units deployed

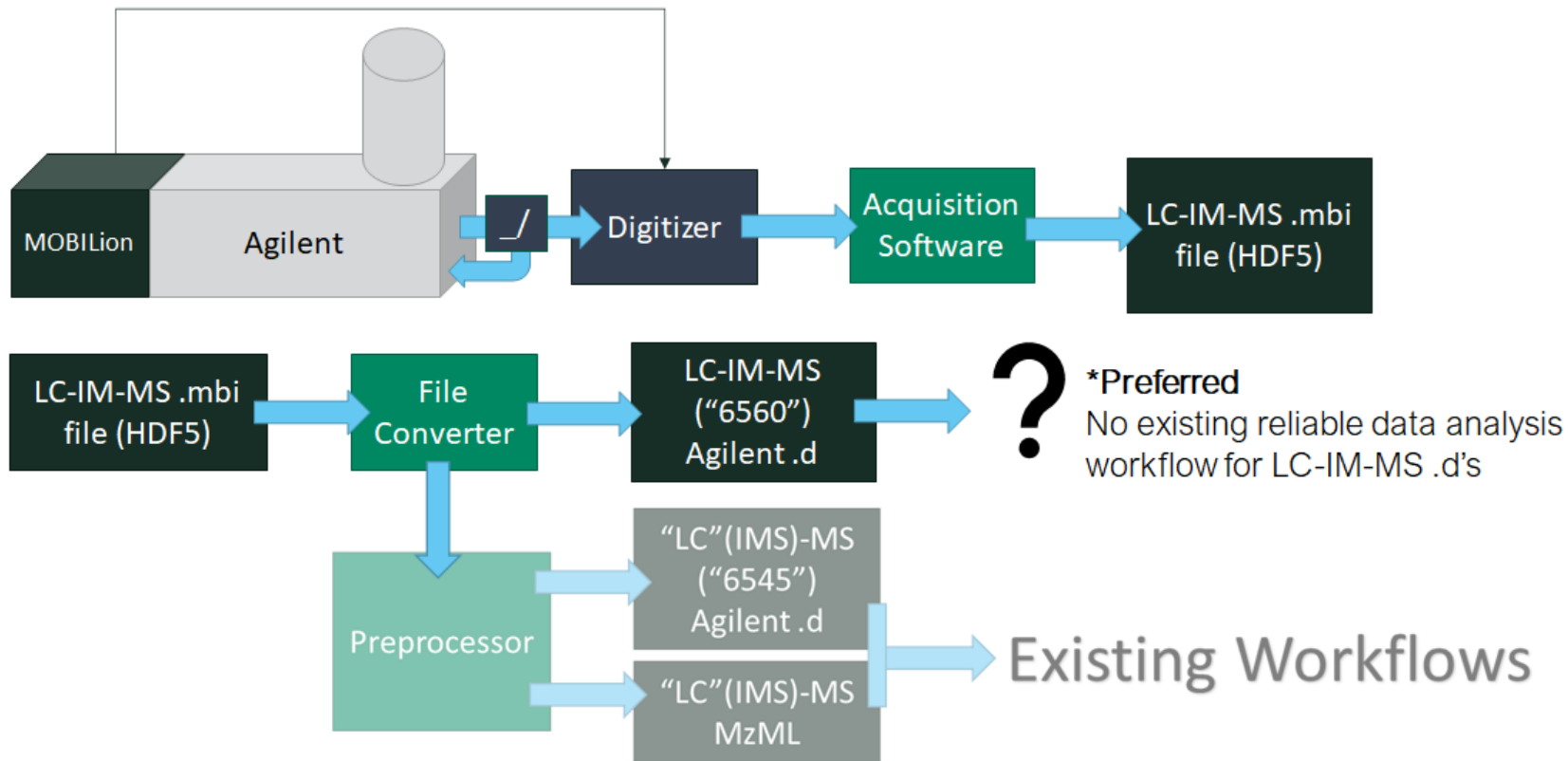


The ACORN Project | How We Will Integrate

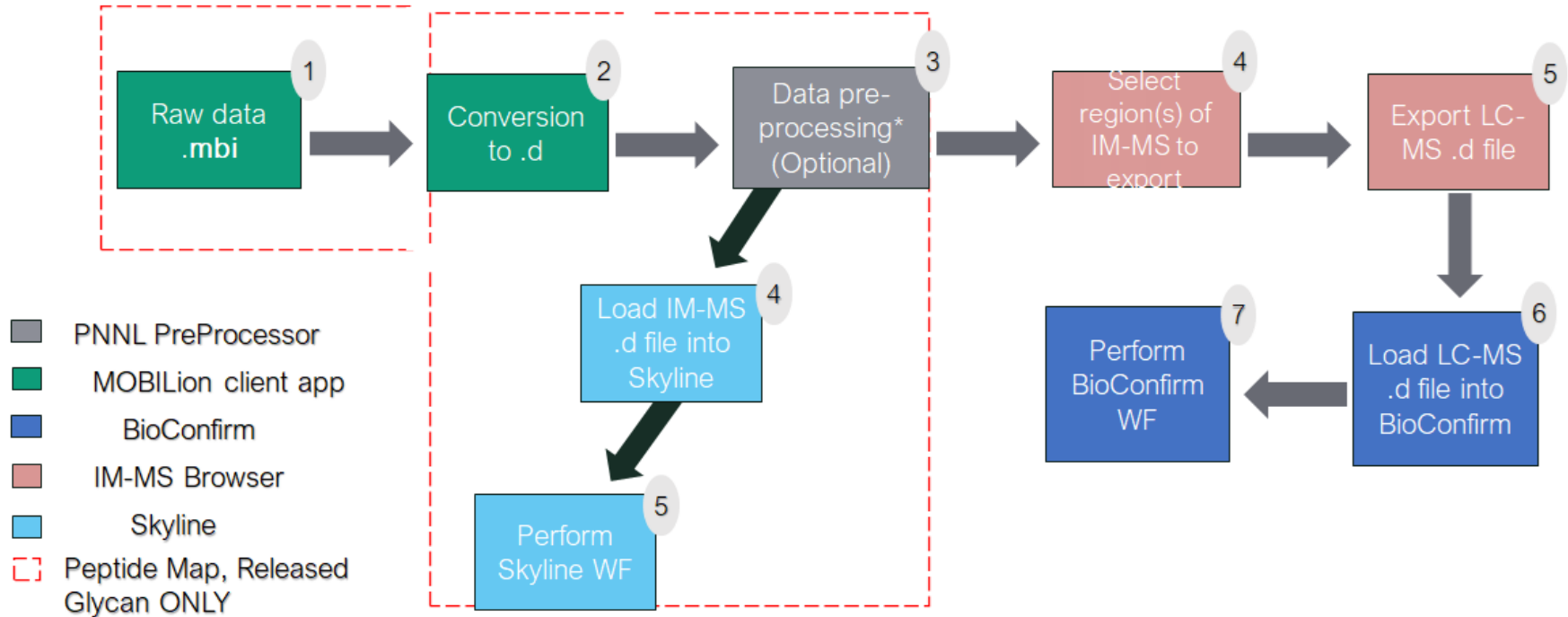
SLIM-Agilent QTOF



MOBILion Data Acquisition



Intact & Subunit Analysis, Targeted Released Glycan Analysis, Peptide Mapping



*pre-processing = binning / smoothing

Confidential/Proprietary

Ideas for Enhanced IM support in Skyline

Drift time predictor

Non-linear CCS calibration support

Ability to view drift spectrum

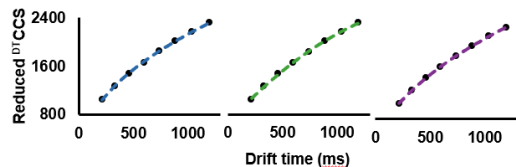
Annotation of chromatographic peaks with ccs/arrival time

Suggested improvement/toggle for heat map display

Non-linear CCS calibration

CCS Calibration of SLIM Drift Times

	Power	2 nd order polynomial	3 rd order polynomial
Eq. Form	$y = Ax^B$	$y = Ax^2+Bx+C$	$y = Ax^3+Bx^2+Cx+D$
Corr. (R ²)	0.9995	0.9997	0.9999
Avg. Error	0.48%	0.45%	0.12%



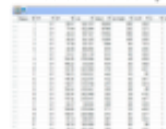
CCS Calibration with SLIM Data in IM-MS Browser

1 Find drift times

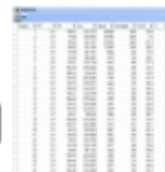
2 Save coefficients

```
<?xml version="1.0" encoding="utf-8"?>
<SLIMmsCalibration>
  <FileVersion>1</FileVersion>
  <Polynomial>
    <C0>109.62659248963419</C0>
    <C1>0.41002497602805255</C1>
    <C2>-0.00021572696963293082</C2>
    <C3>6.1430025380998662E-08</C3>
  </Polynomial>
</SLIMmsCalibration>
```

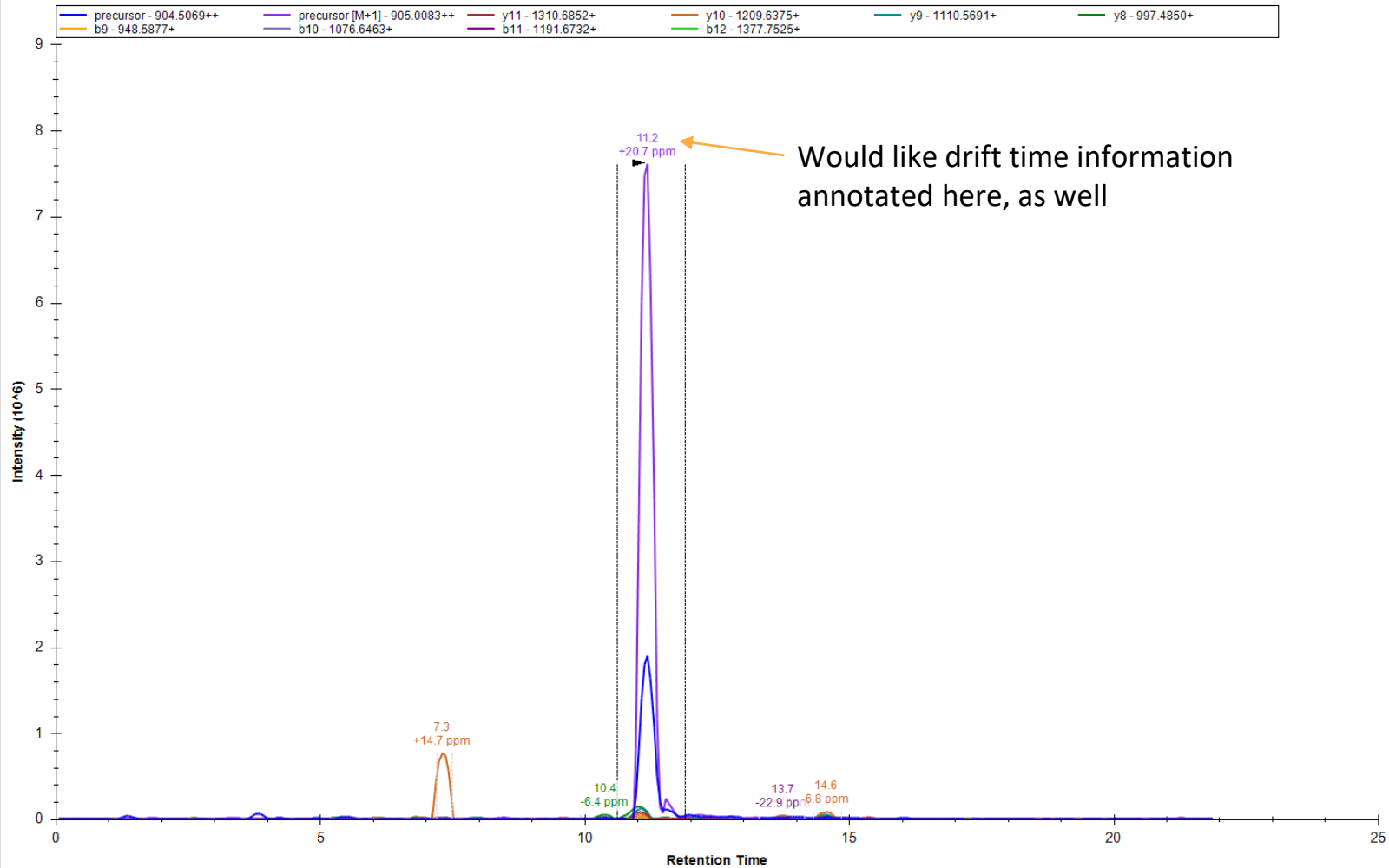
If SLIMmsCal.xml is present, it will be used to compute CCS



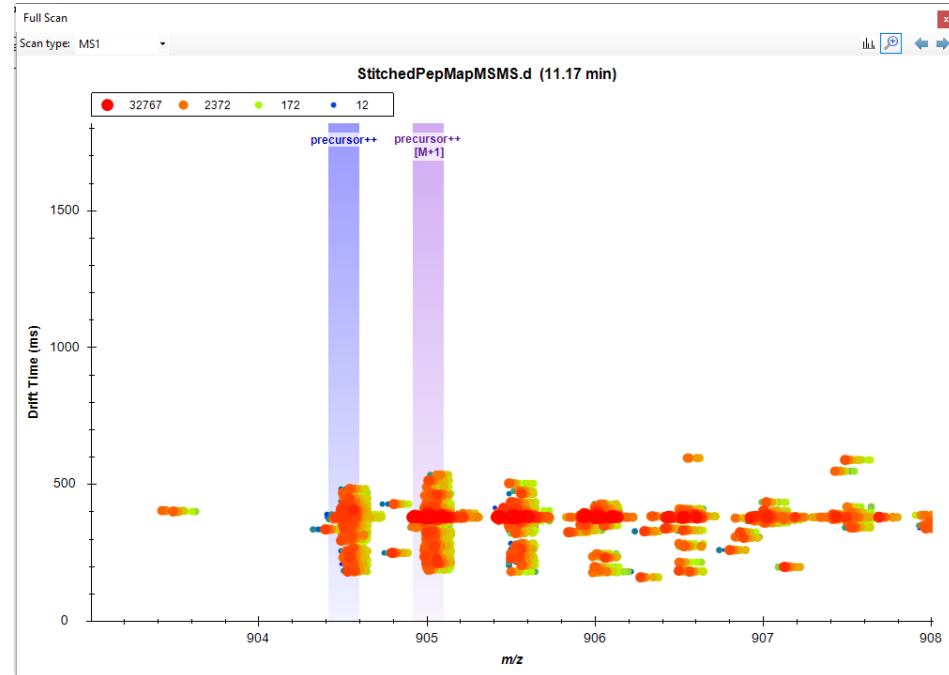
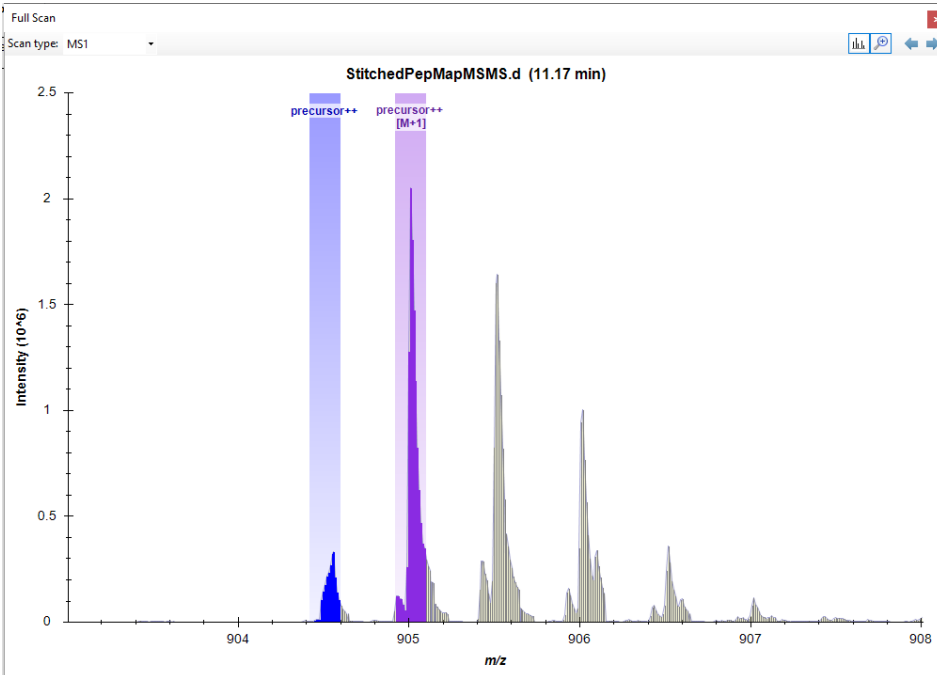
If not, it will use the preferred order: OverrideImmsCal.xml > DefaultImmsCal.xml (and perform a standard linear conversion)



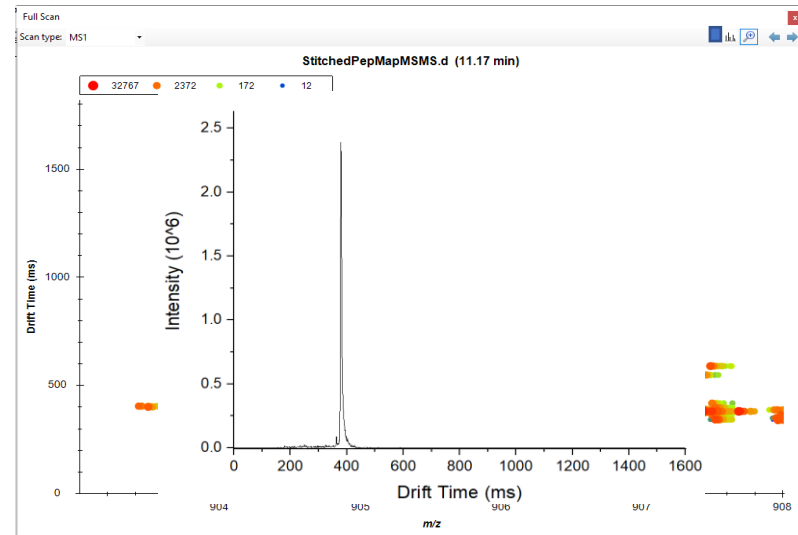
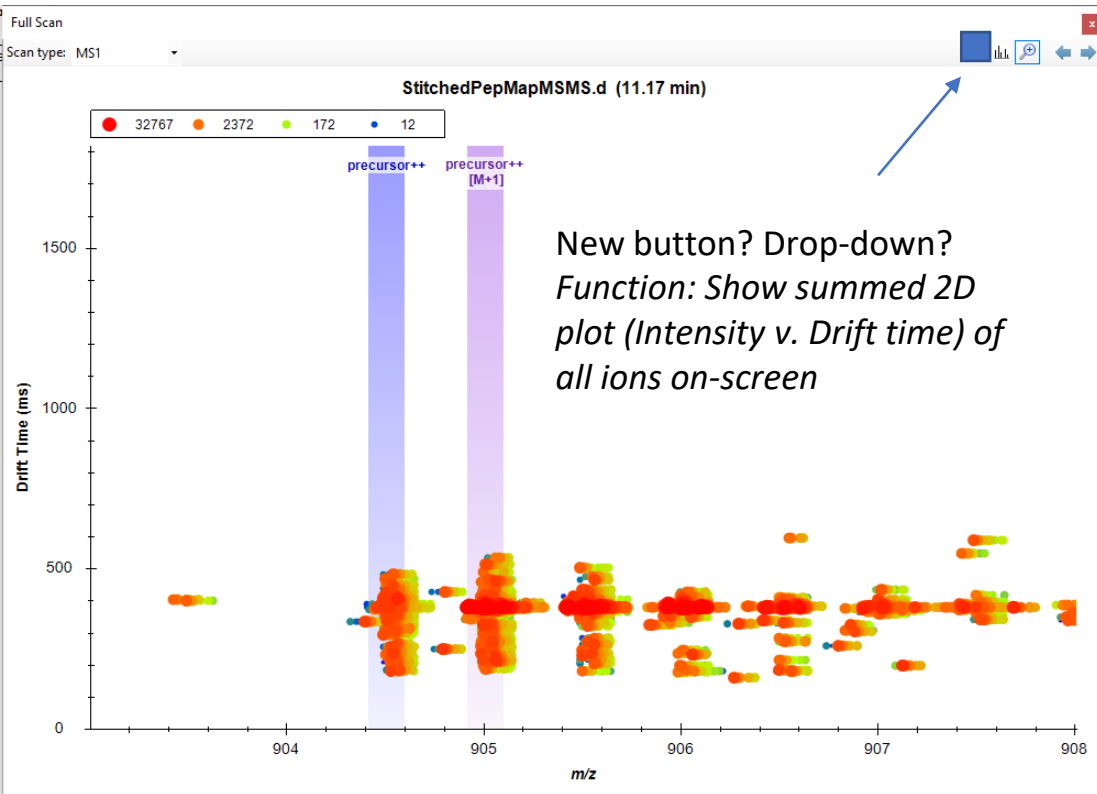
3 Feature finding



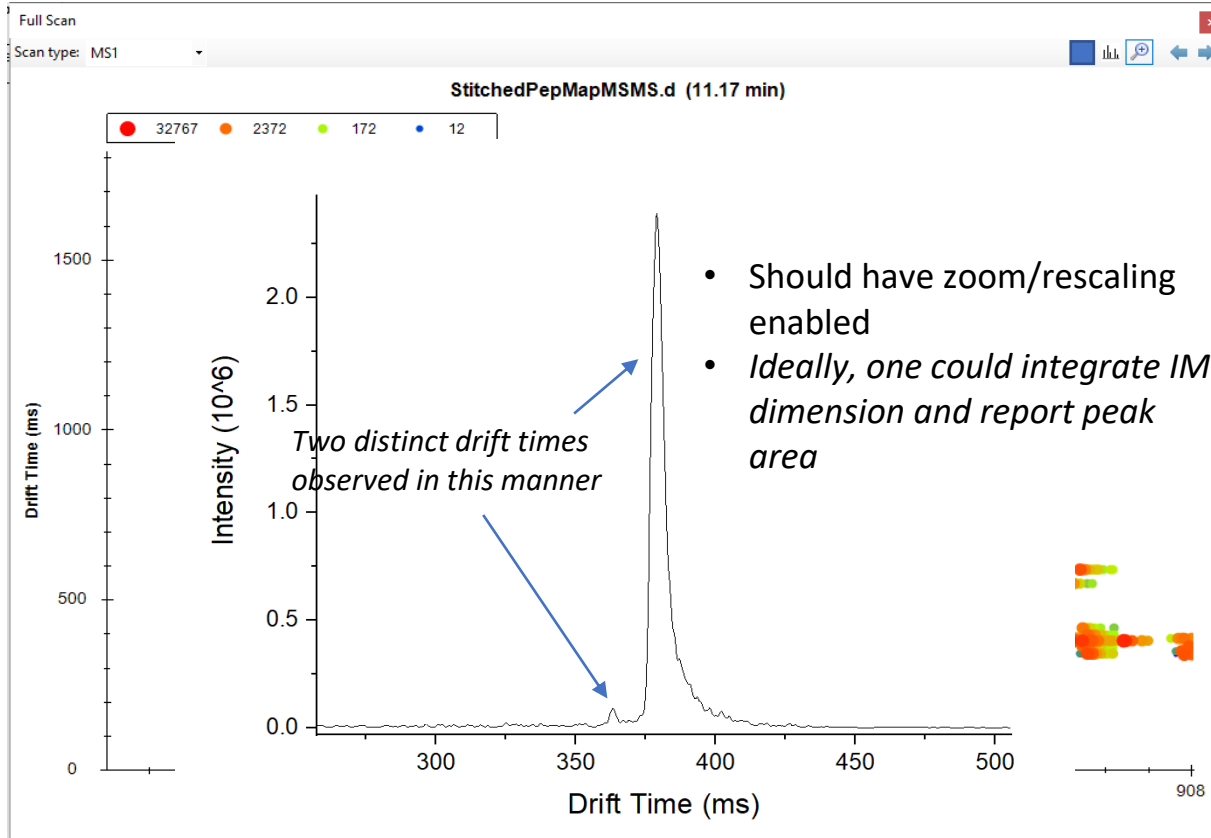
Current Data Visualization



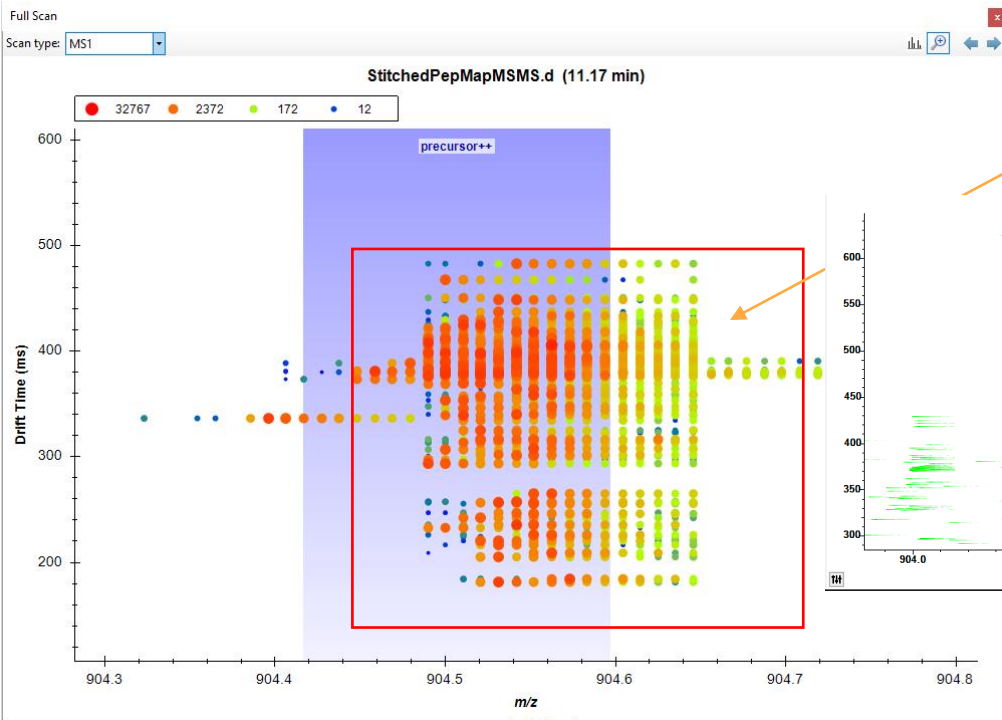
Proposed Data Visualization



Visualization of IM Dimension



Heat Map Data Visualization (Nice to have)



Would like this to be more continuous, rather than dots

