Building a Brand

Mass Spectrometry Service and Software Around LabKey Server

Brendan MacLean
Overview

- Me and LabKey
- Skyline
- Panorama
- Lessons Learned
Me

- LabKey Software Founder
- Worked on LabKey Server (originally CPAS) 5 years
- Left in 2008 for MacCoss Lab UW Genome Sciences
- No financial stake in LabKey
Early LabKey Decisions

- The Team
- Open Source
- Extendable
- Software platform with easy installation
- Supporting a **Hosted Service** ("in the cloud")
- Support scientists creating their own brands

“I don’t like Frameworks.”
– Alex MacLean (2013 – age 12)
Chromatography-based Quantification

- SRM – Selected ion chromatograms
- PRM – Extracted ion chromatograms
- DIA/SWATH – Extracted ion chromatograms
- DDA – Extracted ion chromatograms from MS1-only

<table>
<thead>
<tr>
<th>Acquisition</th>
<th>Targeted</th>
<th>Survey</th>
</tr>
</thead>
<tbody>
<tr>
<td>More Selective</td>
<td>PRM</td>
<td>DIA</td>
</tr>
<tr>
<td>Less Selective</td>
<td>SRM</td>
<td>DDA</td>
</tr>
</tbody>
</table>
Skyline Project Overview

- 10th years of development
- 9 developers
- over 500,000 lines of code – open source
- 60,000 lines of code for testing
- over 10,000 registered users
  - 2000 registered for Skyline-daily
- over 8000 instances started each week
- over 1700 citations
- funded by NIH and 6 instrument vendors

How can we help?
Skyline Web Site Visits (6 months)
Ion Mobility Support (unfiltered)
Ion Mobility Support (3D spectrum)
Calibrated Quantification

- **Henderson, Clinical Chemistry 2017**
  Skyline Performs as Well as Vendor Software in the Quantitative Analysis…

**Fig. 1.** Comparison of Skyline vs TargetLynx analysis of 25(OH)D concentrations from 154 serum samples and VDBG concentrations from 164 serum samples.

The Deming regression equation is shown (solid line), along with the line of unity (dashed line), and the Pearson correlation coefficient ($R^2$).
Small Molecule Support

Webinar 16: Small Molecule Research with Skyline (https://skyline.ms/webinar16.url)
Aggregating and Publishing

- Publish fully annotated Skyline documents
  - 85 public data sets (29 more in review)  
    Abbatilermo, et al. MCP Guidelines, 2017  
    Sharma, et al. MCP 2018

- Aggregate lab QC data
- Assay development
- Quantitative, PK/PD views

- Free hosted version (http://panoramaweb.org)
  - >310 separate projects so far (CPTAC, LINCS & ABRF sPRG)
  - >3900 data sets uploaded (>8000 QC documents)
  - User controlled security

- Locally installable server application
  - Roche, Genentech, J&J, Amgen, NCI and Merck…

- Free and open source (Apache 2.0)

Sharma, et al. J. Proteome Res. 2014
Early LabKey Decisions Revisited

- Publish fully annotated Skyline documents
  - 85 public data sets (29 more in review)
  
- Aggregate lab QC data
- Assay development
- Quantitative, PK/PD views

- Free hosted version ([http://panoramaweb.org](http://panoramaweb.org))
  - >310 separate projects so far (CPTAC, LINCS & ABRF sPRG)
  - >3900 data sets uploaded (>8000 QC documents)
  - User controlled security

- Locally installable server application
  - Roche, Genentech, J&J, Amgen, NCI and Merck…

- Free and open source (Apache 2.0)
Early LabKey Decisions Revisited

- Publish fully annotated Skyline documents
  - 85 public data sets (29 more in review)

- Aggregate lab QC data

- Assay development

- Quantitative, PK/PD views

- Free hosted version ([http://panoramaweb.org](http://panoramaweb.org))
  - >310 separate projects so far (CPTAC, LINCS & ABRF sPRG)
  - >3900 data sets uploaded (>8000 QC documents)
  - User controlled security

- Locally installable server application
  - Roche, Genentech, J&J, Amgen, NCI and Merck…

- Free and **open source** (Apache 2.0)

Sharma, et al. *J. Proteome Res.* 2014
Early LabKey Decisions Revisited

- Publish fully annotated Skyline documents
  - 85 public data sets (29 more in review)

- Aggregate lab QC data
- Assay development
- Quantitative, PK/PD views

- Free hosted version ([http://panoramaweb.org](http://panoramaweb.org))
  - >310 separate projects so far (CPTAC, LINCS & ABRF sPRG)
  - >3900 data sets uploaded (>8000 QC documents)
  - User controlled security

- Locally installable server application
  - Roche, Genentech, J&J, Amgen, NCI and Merck…

- Free and open source (Apache 2.0)

Sharma, et al. MCP 2018
Sharma, et al. MCP 2018
Abattiello, et al. MCP Guidelines, 2017
Early LabKey Decisions Revisited

- Publish fully annotated Skyline documents
  - 85 public data sets (29 more in review)

- Aggregate lab QC data
- Assay development
- Quantitative, PK/PD views

- Free hosted version ([http://panoramaweb.org](http://panoramaweb.org))
  - >310 separate projects so far (CPTAC, LINCS & ABRF sPRG)
  - >3900 data sets uploaded (>8000 QC documents)
- User controlled security

- Locally **installable** server application
  - Roche, Genentech, J&J, Amgen, NCI and Merck…

- Free and open source (Apache 2.0)

Sharma, et al. *J. Proteome Res.* 2014
Early LabKey Decisions Revisited

- Publish fully annotated Skyline documents
  - 85 public data sets (29 more in review)
    - Abbatiliso, et al. MCP Guidelines, 2017
    - Sharma, et al. MCP 2018

- Aggregate lab QC data
- Assay development
- Quantitative, PK/PD views

- Free hosted version (http://panoramaweb.org)
  - >310 separate projects so far (CPTAC, LINCS & ABRF sPRG)
  - >3900 data sets uploaded (>8000 QC documents)
  - User controlled security

- Locally installable server application
  - Roche, Genentech, J&J, Amgen, NCI and Merck…
- Free and open source (Apache 2.0)

Sharma, et al. J. Proteome Res. 2014
Early LabKey Decisions Revisited

- Publish fully annotated Skyline documents
  - 85 public data sets (29 more in review)
  - Aggregate lab QC data
  - Assay development
  - Quantitative, PK/PD views

- Free hosted version ([http://panoramaweb.org](http://panoramaweb.org))
  - >310 separate projects so far (CPTAC, LINCS & ABRF sPRG)
  - >3900 data sets uploaded (>8000 QC documents)
  - User controlled security

- Locally installable server application
  - Roche, Genentech, J&J, Amgen, NCI and Merck…

- Free and open source (Apache 2.0)

Sharma, et al. *J. Proteome Res. 2014*

Abbatiello, et al. MCP Guidelines, 2017
Sharma, et al. *MCP 2018*
Skyline/Panorama Workflow

1. **Build Method**
2. **Acquire Data**
3. **Evaluate Results**
4. **Refine**

Skyline

Publish to Panorama

Panorama

Store in a relational database

Explore results in a web-browser

Search Analyze Export

Download Skyline documents and chromatogram libraries

User Interface
Longitudinal System Suitability Tracking

Levey-Jennings
All Series

Peptides
ATEEQLK
DIP...
ELA...
ELG...
GIL...
GIS...
GLI...
HVL...
IGD...
LSS...
LTI...
LVN...
NGF...
SAA...
SFA...
SSA...
TAS...

Peak Area

Time

Lindsay Pino
Longitudinal System Suitability Tracking

Retention Time

Time

Levey-Jennings
All Series

Peptides
- ATEEQLK
- DIP...
- ELA...
- ELG...
- GIL...
- GIS...
- GLI...
- HVL...
- IGD...
- LSS...
- LTI...
- LVN...
- NGF...
- SAA...
- SFA...
- SSA...
- TAS...

Lindsay Pino
Longitudinal System Suitability Tracking

Levey-Jennings
All Series

Mass Error

Time

Lindsay Pino
Lessons Learned

- Extend – don’t build from scratch
- Make LabKey your team
  - Contracting what you can’t get done yourself
  - Helping your developers to be more successful
- Provide hosted services to
  - Collaborators
  - Customers
- Encourage them to install their own when necessary
- Build a reputation (brand)
Skyline Team

- Brendan MacLean
- Nick Shulman
- Brian Pratt
- Tobi Rohde
- Vagisha Sharma
- Nat Brace
- Kaipo Tamura
- Yuval Boss
Thank you Mike MacCoss!