Tutorial Webinar #20

Using **Skyline Batch** for Large-Scale DIA

With

Brendan MacLean (Principal Developer)
Ali Marsh (Development Intern)
Nat Brace (Project Manager)

Agenda

- Welcome from the Skyline team!

- Introduction and overview with **Brendan MacLean**

- Introduction to Skyline Batch with **Ali Marsh**

- Tutorial on using Skyline Batch from **Ali Marsh**

- Tutorial on creating a template file with **Brendan MacLean**

- Audience Q&A – submit questions to Google Form:

  https://skyline.ms/QA4Skyline.url

Skyline Team

Nat Brace

Vagisha Sharma

Brian Connolly

Brendan MacLean

Rita Chupalov

Ali Marsh

Nick Shulman

Kaipo Tamura

Brian Pratt

Matt Chambers

Windows Batch Scripts for Running Skyline

- Created for Navarro, Nature Biotech. 2016
- First presented in Skyline Tutorial Webinar 14 – https://skyline.ms/webinar14.url
- Used again in Skyline Tutorial Webinar 15 – https://skyline.ms/webinar15.url
- Used to teach May Institute 2018-2020
- Used in Searle, Nature Comm. 2018
- Used in Vaca Jacome, Nature Methods, 2020
- Used in MacLean oral (Prosit) and poster (diaPASEF) at ASMS 2020

#14: Large Scale DIA
(Jan 2017)
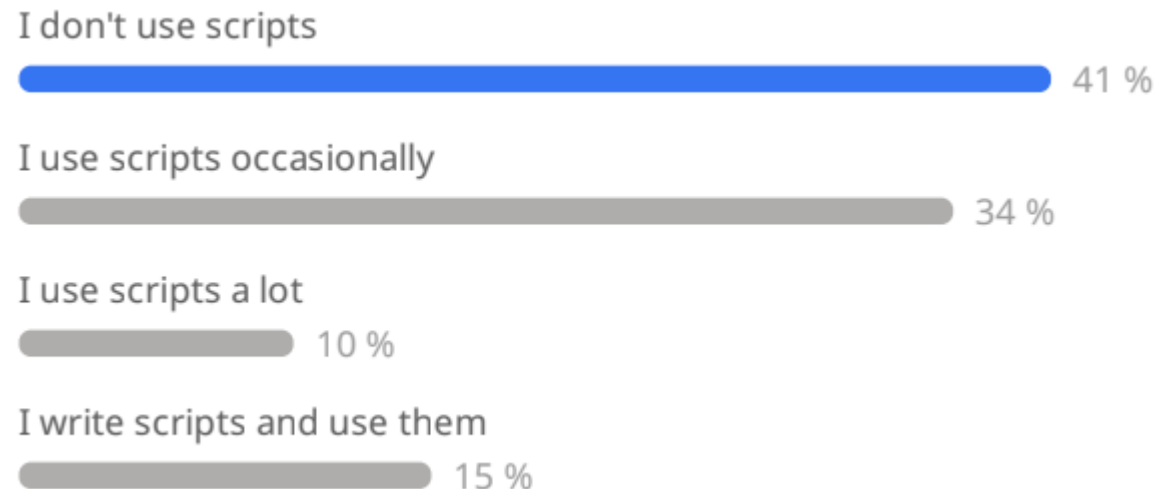
#15: Optimizing Large Scale DIA
(Apr 2017)

Q: Do Skyline users use these scripts?

- Require a user to slightly but expertly **edit the scripts**

- AutoQC Loader increasingly popular
  - Runs Skyline command-line based on GUI configuration
  - Nice UI for monitoring processing logs

Replacing Scripts with Skyline Batch GUI

- Intern Ali Marsh of MIT CS joined Skyline Team for 1 year

- Goal: Replace the scripts with a GUI

- Proof of concept 1: Replace the scripts in webinars 14 and 15

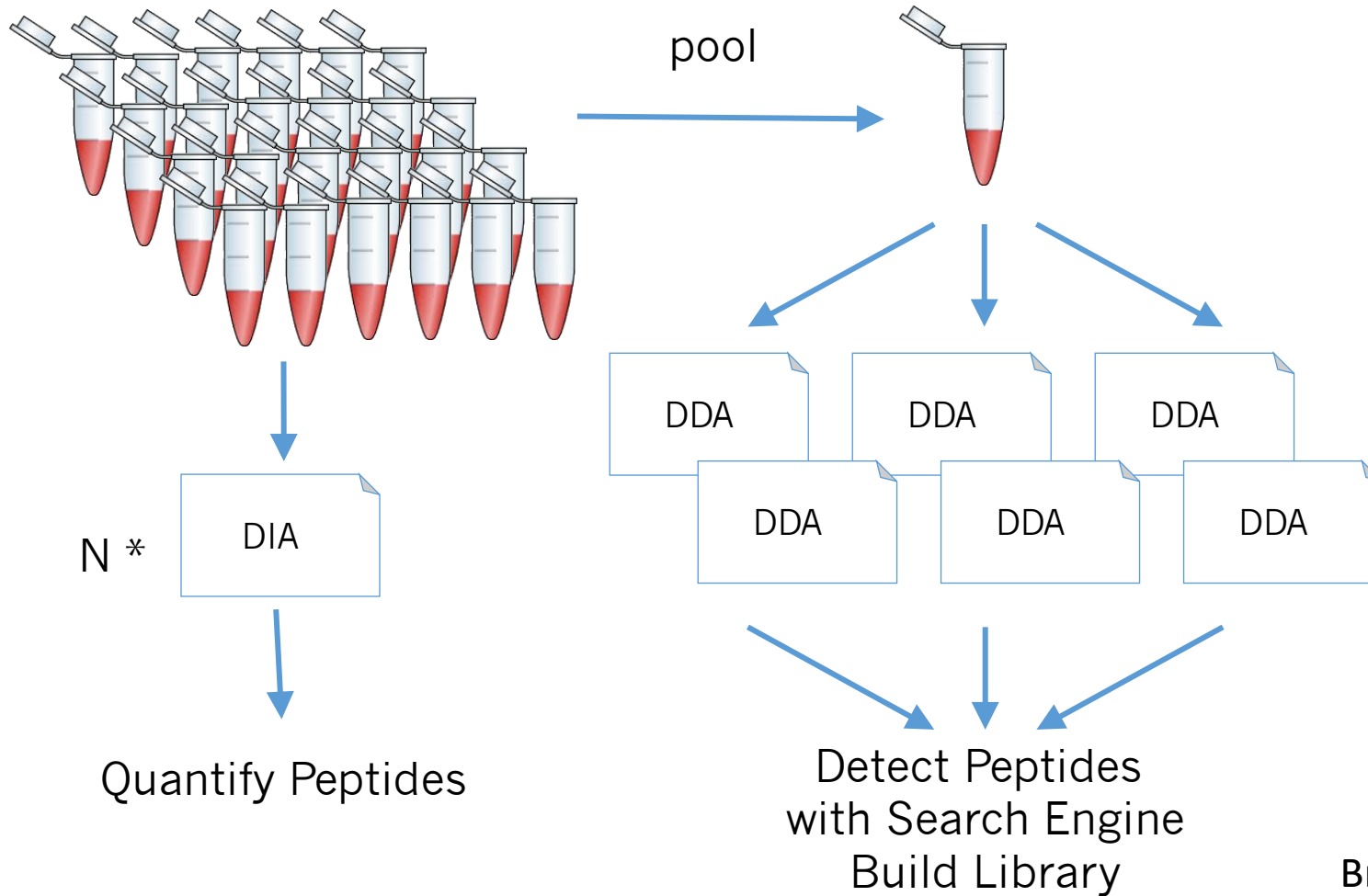- Proof of concept 2: Replace the scripts and teach in May Institute
  - https://computationalproteomics.khoury.northeastern.edu/
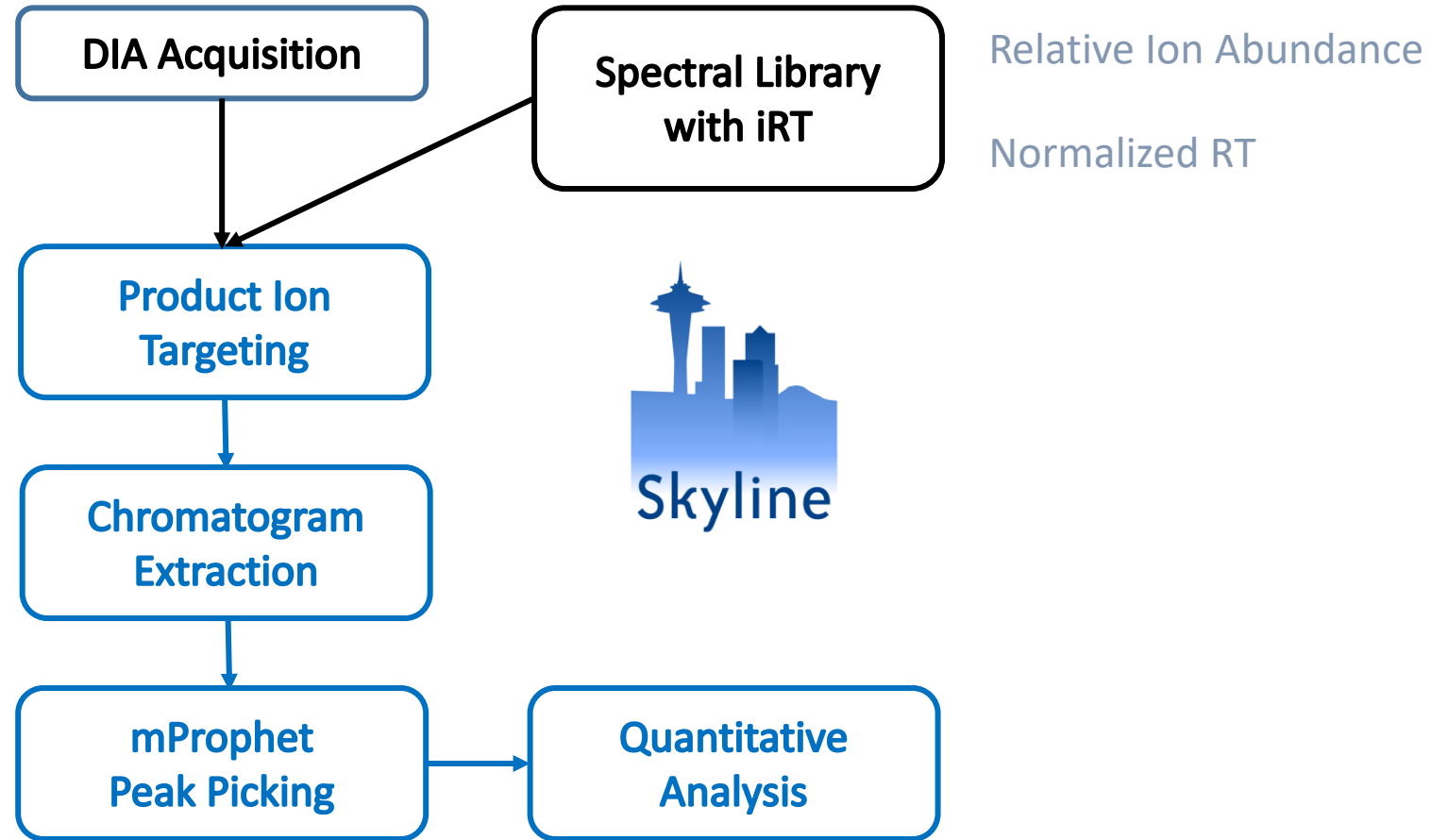 - What is your scripting expertise?

- https://skyline.ms/batch.url

I don't use scripts

41 %

I use scripts occasionally

34 %

I use scripts a lot

10 %

I write scripts and use them

15 %

Two Phase Experiment

N * Quantitative Samples

1 * Detection Samples

pool

DDA   DDA   DDA

DDA   DDA   DDA

N *   DIA

Quantify Peptides

Detect Peptides
with Search Engine
Build Library

Bruderer, et al. & Reiter, *MCP, 2015*

Prior Knowledge Workflow

DIA Acquisition

Spectral Library with iRT

Relative Ion Abundance

Normalized RT

Product Ion Targeting

Skyline

Chromatogram Extraction

mProphet Peak Picking

Quantitative Analysis

Reiter, Rinner, et al.
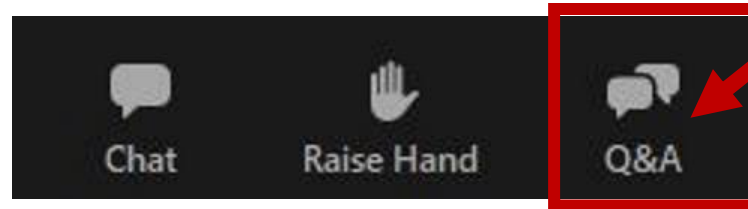*Nature Methods*, 2011

Learn More

- Webinar #21? Trapped Ion Mobility diaPASEF
  - With Ben Collins (data collected, tutorial drafted)
- Weeklong Courses 2022 ?
  - University of Washington – July
  - Buck Institute – April
  - Northeastern May Institute – May 9 – 22
  - PRBB, Barcelona – November
- Workshops and Conferences 2020 ?
  - **Skyline User Group Meeting "at ASMS" – October (webinar)**
  - Pre-ASMS course – October 30 & 31

Listings updated in **Join Us** section of Skyline homepage:

https://skyline.ms/Skyline.url

Questions?

- Ask any questions at the Q&A form in Zoom:

- Take the post-webinar survey:

https://skyline.ms/survey4webinar.url

Skyline Tutorial Webinar #20

This ends this Skyline Tutorial Webinar.

Please give us feedback on the webinar at the following survey:

https://skyline.ms/survey4webinar.url

A recording of today's meeting will be available shortly at the Skyline website.

We look forward to seeing you at a future Skyline Tutorial Webinar.