MUNI | RECETOX

E5020 – Analysis of nontarget MS data

0 - Organization

What are we going to do?

Lectures – **theoretical** understanding of the **concepts**, methods and algorithms

Practical – **applying** tools implementing those **methods** to process data using Galaxy

Course Objectives

At the end of this course, you will:

- know different approaches to separation and detection of molecules with a focus on liquid and gas chromatography
- know the principles of mass spectrometry (MS) instrumentation
- know basic MS data formats and related terminology
- know which steps are involved in processing untargeted MS data
- based on data type, methodology used and molecule type, select and apply methods for data processing
- be able to work with software for MS data analysis using Galaxy

Agenda

Date	Topic	Class	Teacher
20.02.	**Organization and Introduction**	Lecture	Helge Hecht
27.02.	**Instrumental Analysis – Chromatography, Mass Spectrometry & Acquisition methods**	Lecture	Thomas Contini
05.03.	**Introduction to -omics**	Lecture	Elliott Price
12.03.	**Introduction to untargeted mass spectrometry data & pre-processing**	Lecture	Helge Hecht
19.03.	**Getting started with Galaxy, exploring the data and pre-processing Feature detection from instrumental data**	Practical Lecture	Helge Hecht
26.03. & 02.04.	**No classes**		
09.04.	**Feature detection from instrumental data**	Practical	Thomas Contini
16.04.	**From features to spectra (deconvolution)**	Lecture	Helge Hecht
23.04.	**From features to spectra (deconvolution)**	Practical	Helge Hecht
30.04.	**Annotation – from spectra to compounds**	Lecture	Helge Hecht
07.05.	**Annotation – from spectra to compounds**	Practical	Helge Hecht
14.05. & 21.05.	**TBA**	TBA	TBA

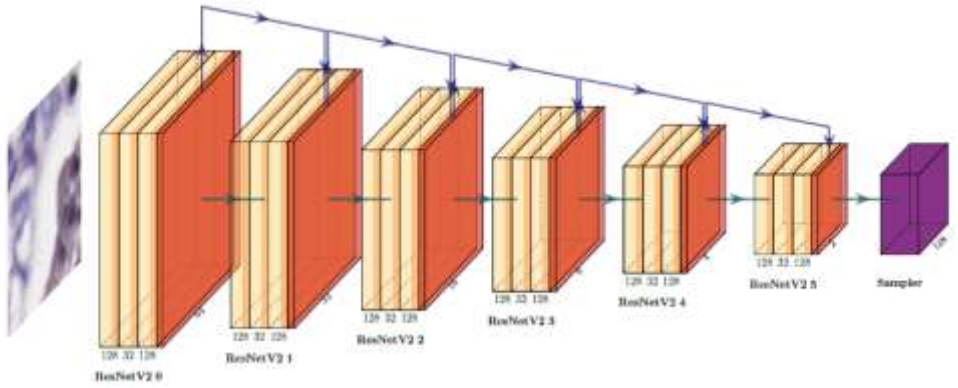
General Information

- Contact the course coordinator: eva.budinska@recetox.muni.cz
- Contact me: helge.hecht@recetox.muni.cz
- Course information & (interactive) syllabus available in IS
- Interactive syllabus contains
  - a summary of each session
  - accompanying slides after each lesson
  - link to anonymous feedback form
- Attendance is not compulsory (but highly encouraged!)
- Assessment via written exam based the slides (100%)
- Additional information and examples are linked in the slides

A little about myself

Helge Hecht – Spectrometric Data Processing & Analysis Research Infrastructure (SpecDatRI)

- BSc in **Informatik: Games Engineering**
- MSc in **Computer Science (TUM)**
- **Research assistant** working with Building Information Modeling (BIM)
- **Software engineer** in Thermo Scientific
- **PhD student** at RECETOX with Jana Klánová & Elliott James Price
- Developing tools for **mass spectrometry data processing** in the RECETOX RI



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Discussion

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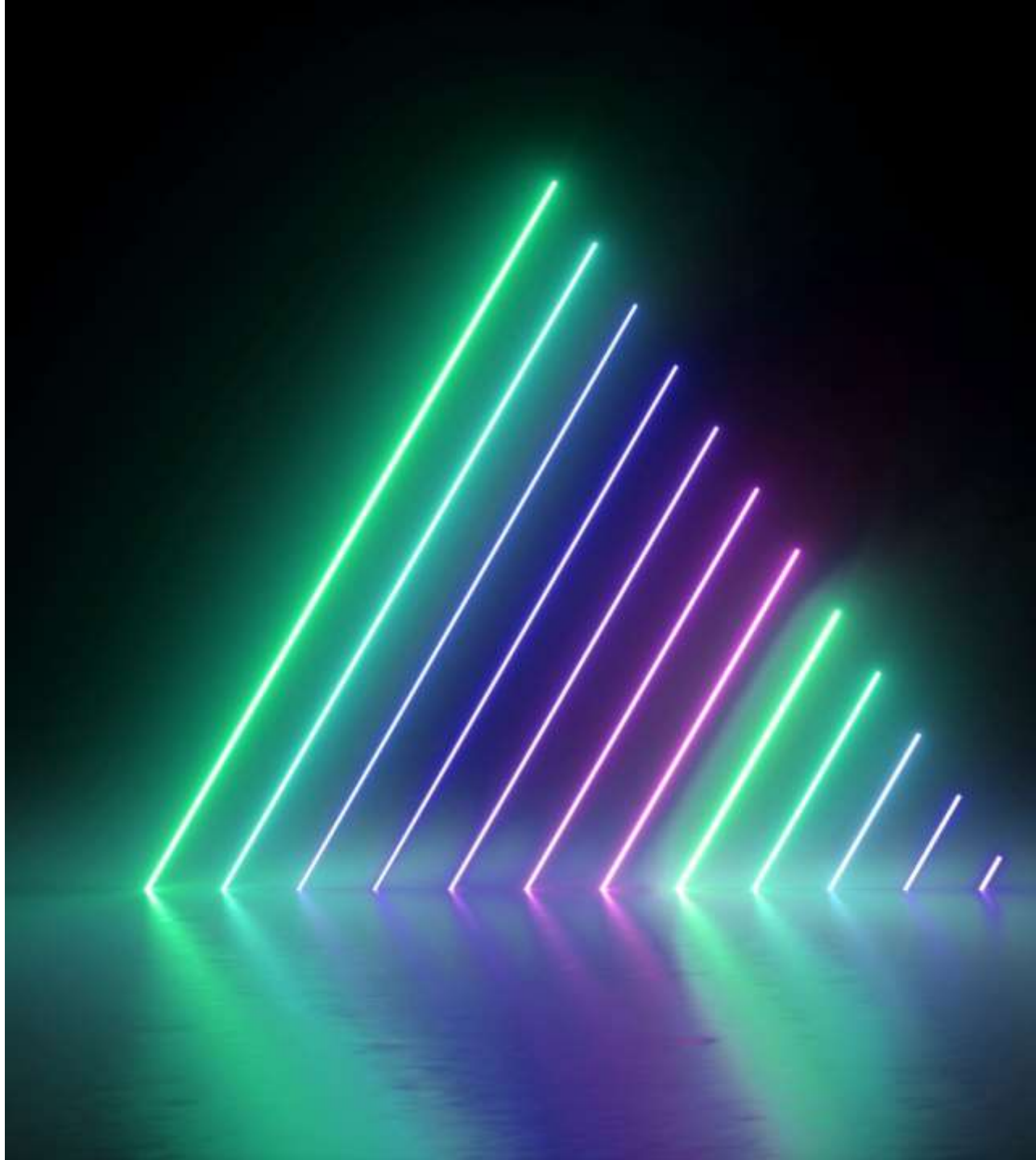
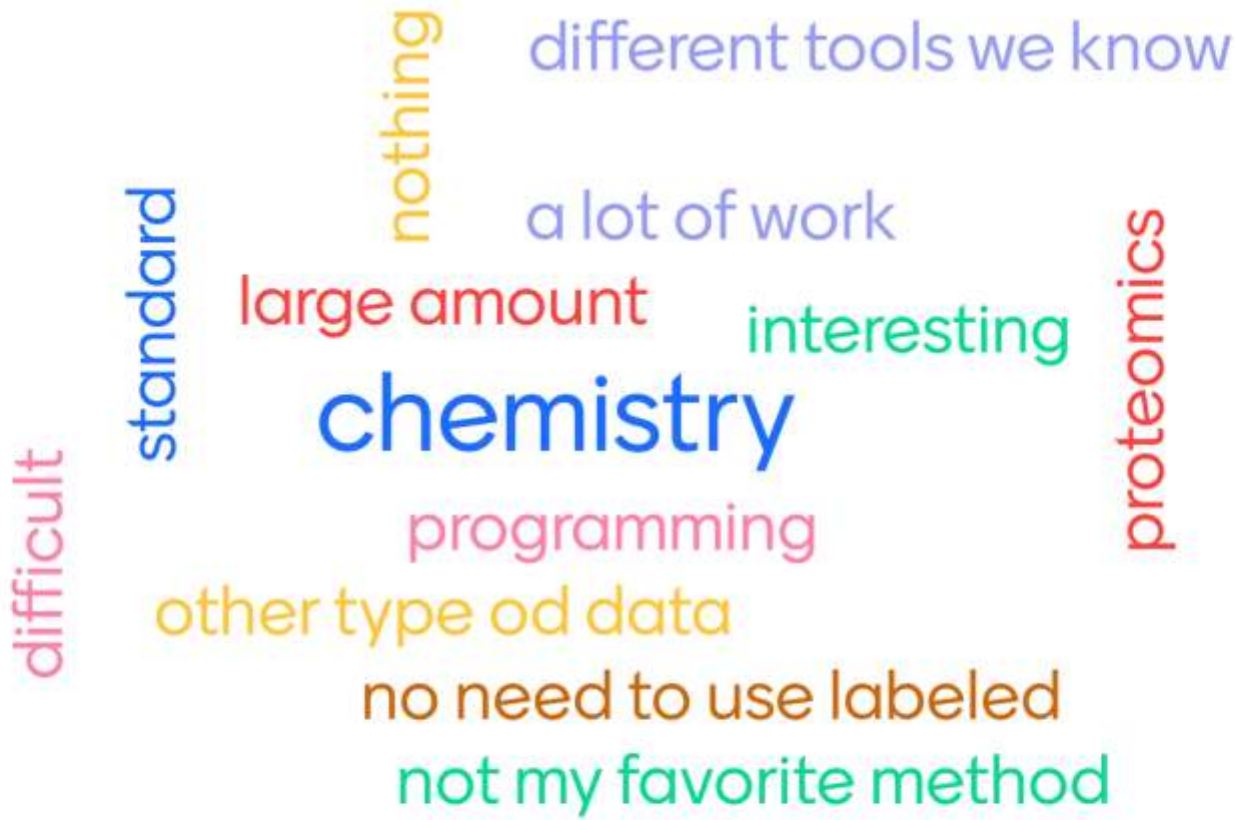


What do you think of when you hear "Analysis of non-targeted mass spectrometry data"?

14 responses



How do you usually process data?

Statistics and visualization in R

Clean, normalize, visualize

Genome data analysis using Python, specifically Numpy

Control, edit, perform analysis

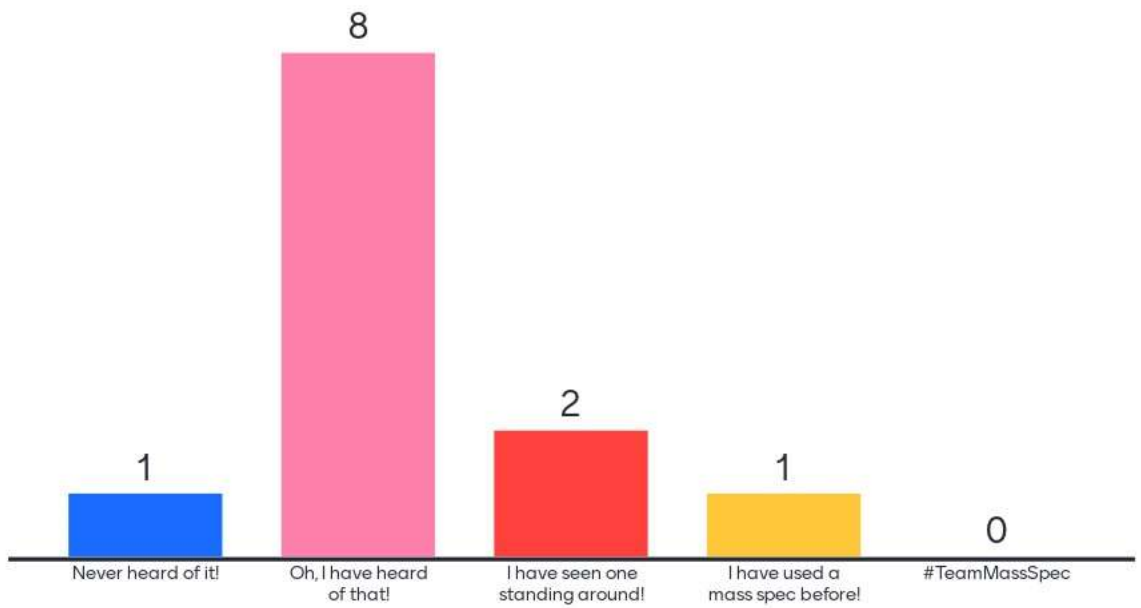
I look at them, try to understand them and then based on my goal I use coresponding tools to process the data

In R software or Python - gene or genome analysis

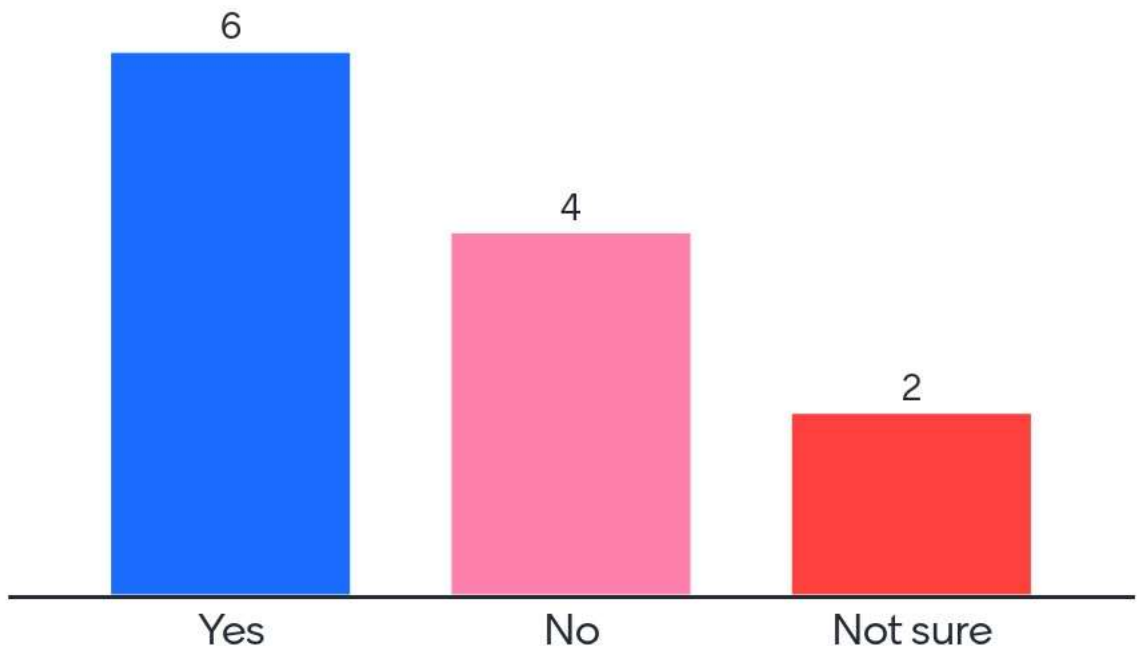
By my scripts or validated tools

Obtaine (measurements) - clean up - visualise

How familiar are you with mass spectrometry?



Have you heard of the Galaxyproject before?



Introduction - Lectures

Lectures – theoretical understanding of the concepts, methods and algorithms

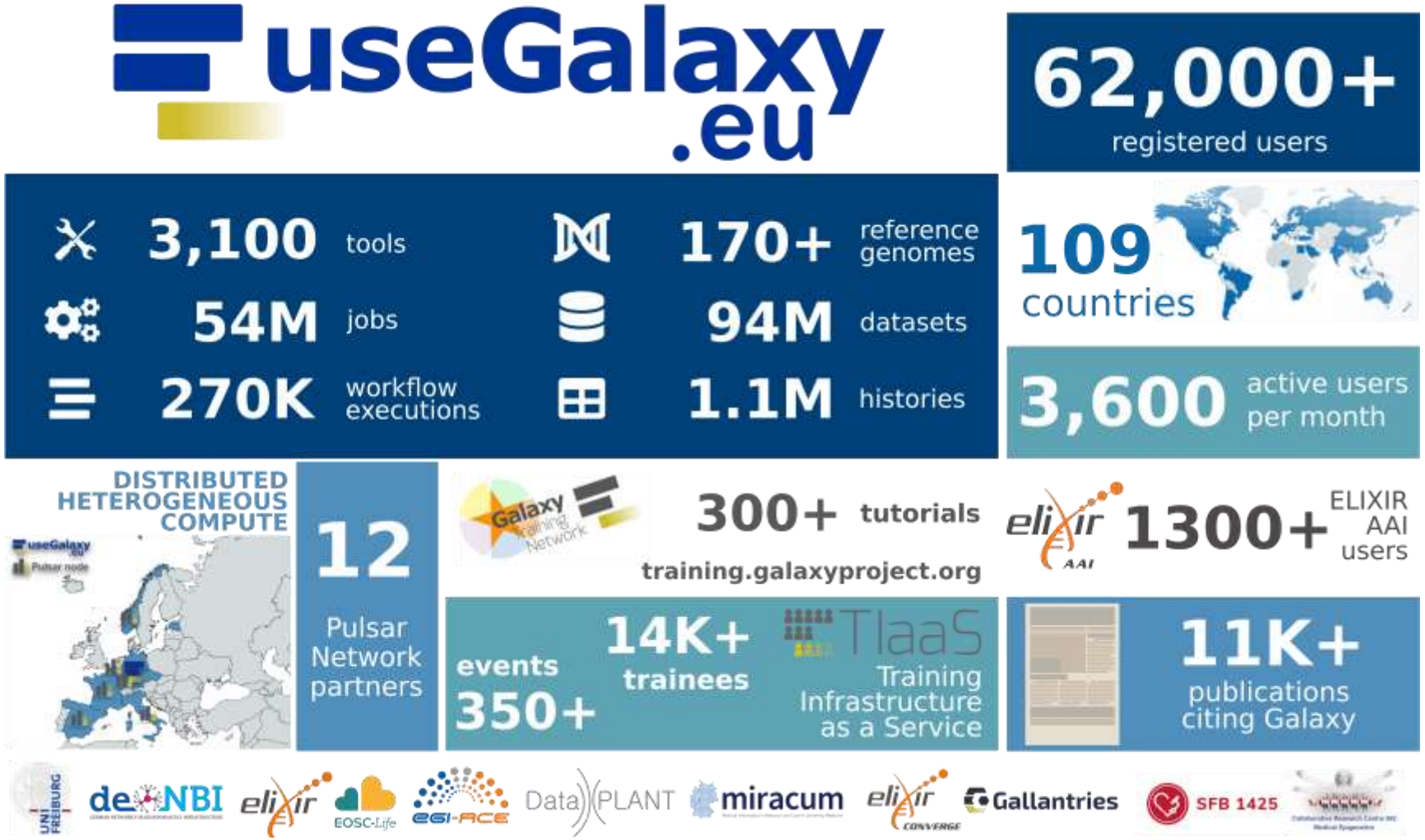
- Learning the instrumental analytical platforms
- Experiment design and research questions – introduction to (mass spectrometry based) –omics
- Understanding of the data and related terminology
- Algorithms and methods behind data processing software

Introduction - Practical

applying tools implementing those methods to process data using Galaxy

- Getting familiar with the Galaxy platform
- Learn about existing tools implementing the concepts discussed in the lectures
- Use those tools to process example data
- Each practical is based on a Galaxy Training Network Tutorial which can be studied also independently at home

Introduction – Practical – Galaxy Servers



… and many more!

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Introduction – Practical - TIaaS

Training **I**nfrastructure **a**s **a** **S**ervice

- dedicated environment for teaching
- registration link for each practical in the interactive syllabus in IS
- no own device or software setup required
- all data and steps are recorded and accessible from any device with a web browser

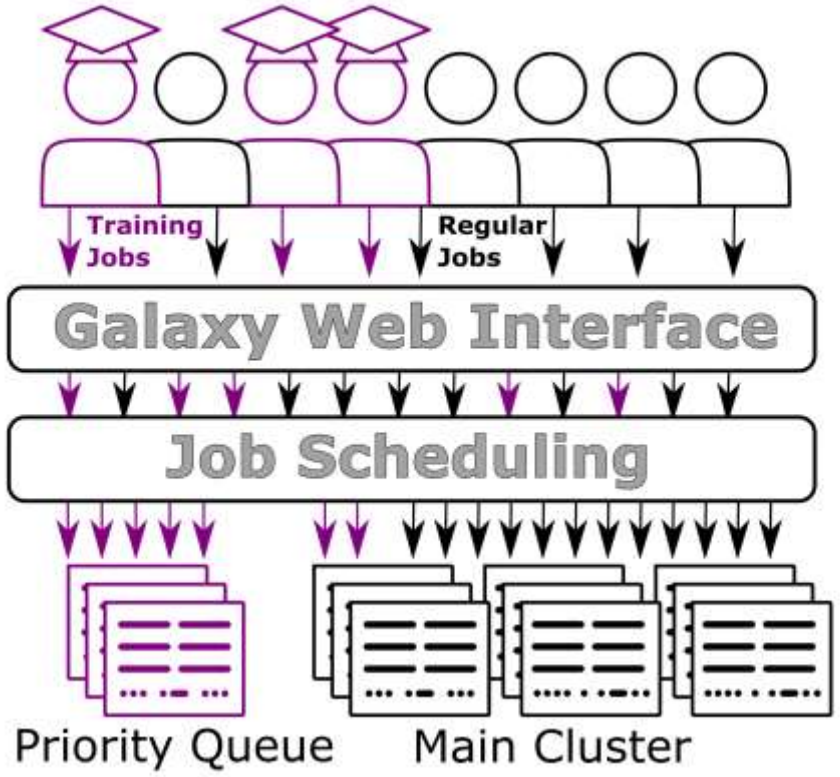

Figure taken from 10.1093/gigascience/giad048

Next time…

We are talking about

1. Chromatography
2. Mass Spectrometry
3. Data Acquisition Methods

with Thomas Contini.