benefits of open science

lennart martens

lennart.martens@vib-ugent.be
computational omics and systems biology group
VIB / Ghent University, Ghent, Belgium

Open science creates very many opportunities but it does take some work to get it right

- Open science should not serve to police scientists, but to provide opportunities
- Creating an open data ecosystem is not trivial, but with a bit of work, it can certainly be done
- Scientists should not ask themselves whether there will be open science, but rather what they will be able to do thanks to open science

Why should we share our work?

Our biggest challenge is to make it work!

What can we do with open science?

Of sedimentation, opportunity, and (an absence of) dragons

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We usually think we need open science to prevent bad things from happening

- While open science helps prevent some cases of fraud or low quality work being published, it is certainly not a panacea (cfr. peer review)
- Simultaneously, fraud is regularly detected:
  - in the absence of the source data
  - from papers published in closed access journals
  - without any of the code or metadata available
- Why should we define the use of open science through an application with negative connotation?

Instead, we should rather focus on the good that comes from open science

- Open science makes the work accessible to anyone
- Open science allows people to build much more efficiently on previous work
- Open science helps maximize the usefulness of each individual research effort
- Data tend to have a (much!) longer shelf life than our (limited) interpretations
- Open science fosters creativity, and stimulates revolutionary research

Why should we really have open science?

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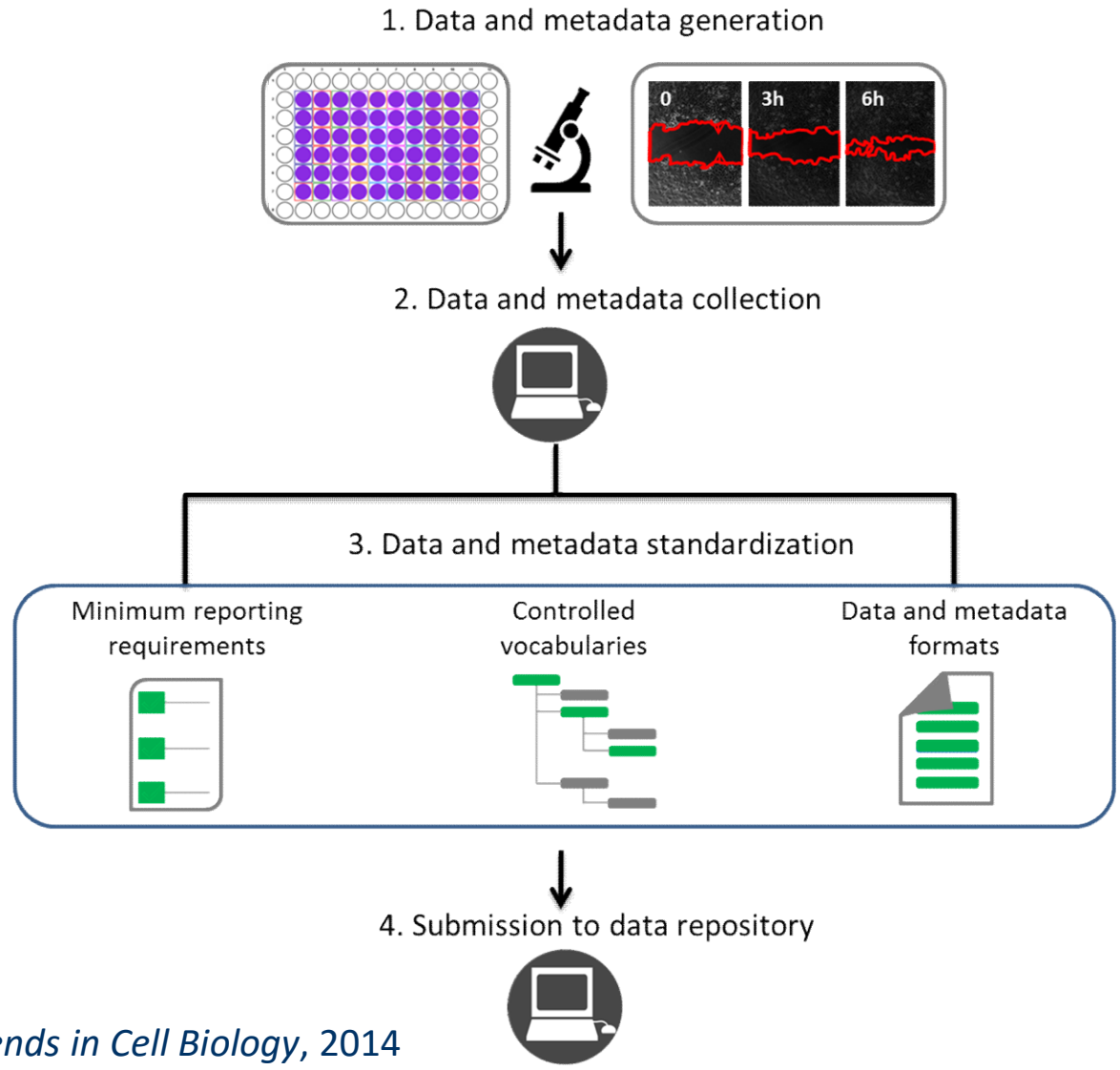
Making open science work requires a bit of effort from every scientist

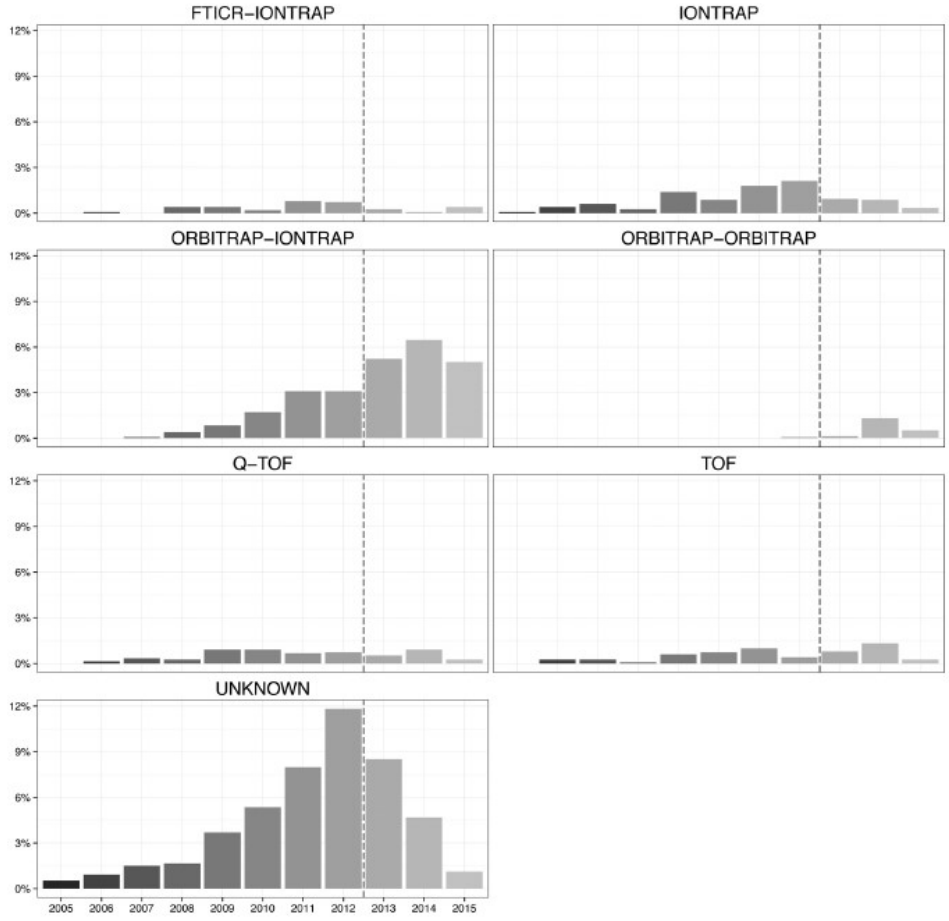
- The data that is obtained should be accompanied by the associated metadata
- The code that is written should be understandable, documented, and hosted at a reliable site
- The protocols should be provided clearly and in full
- The interpretations should be clearly linked to the data (*full provenance*)
- Everything should be licensed in a permissible way

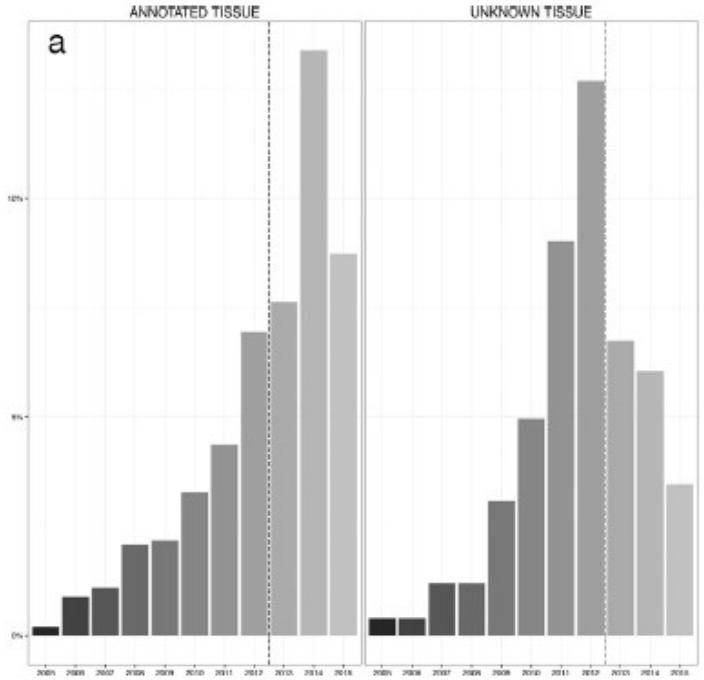
Any open data exchange ecosystem requires standardization



Masuzzo, *Trends in Cell Biology*, 2014

But scientists are human, and very fallible - especially when extra effort is required





Verheggen, *EuPA Open Proteomics*, 2015

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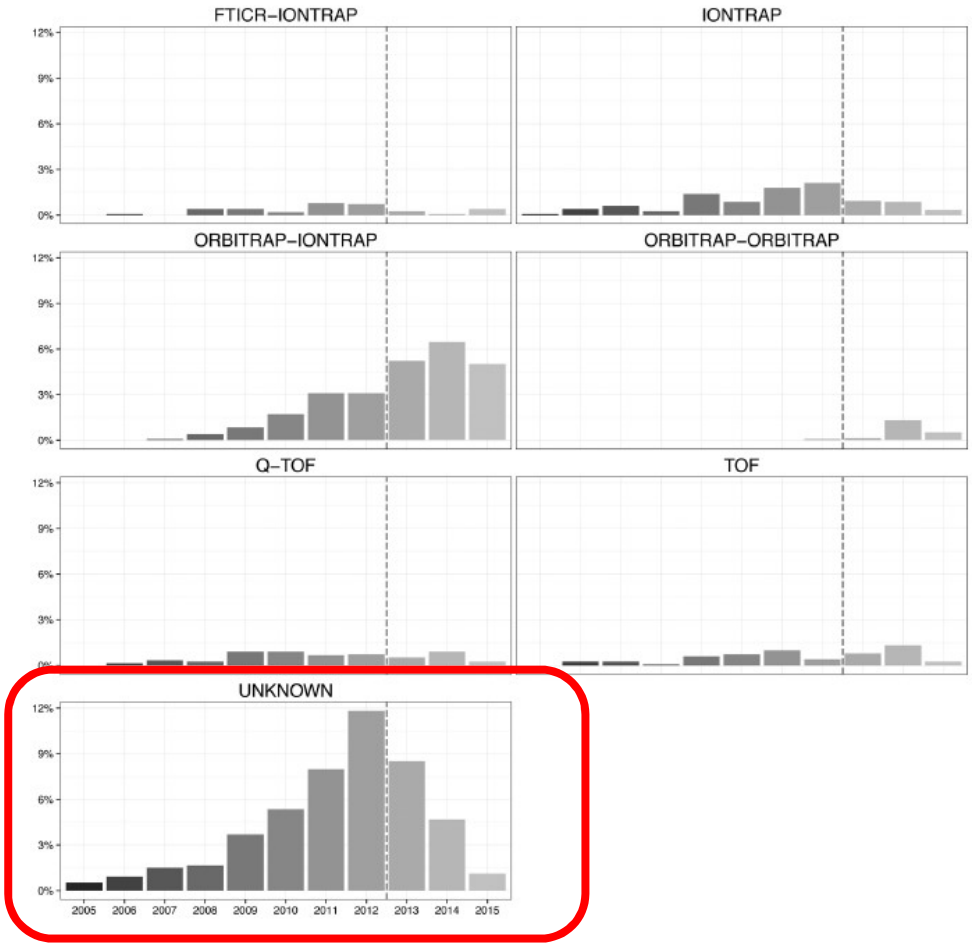
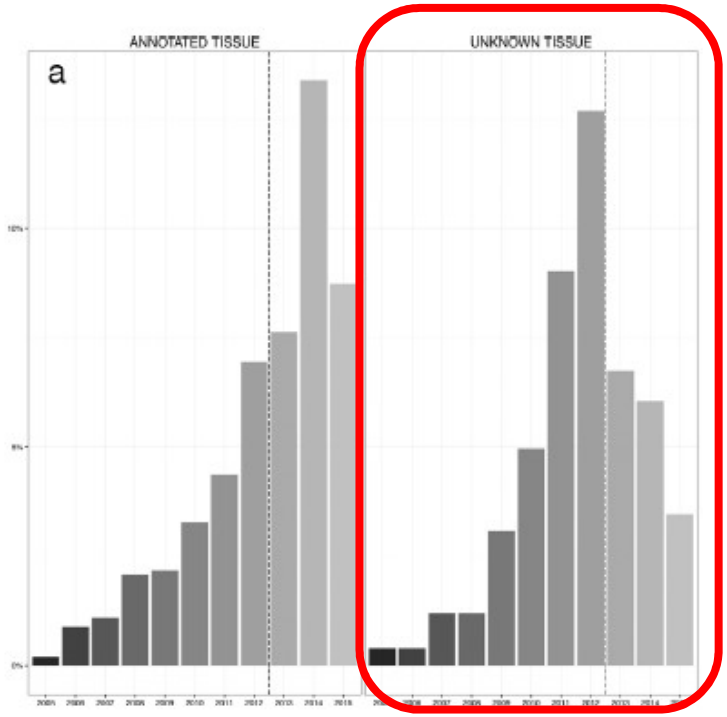
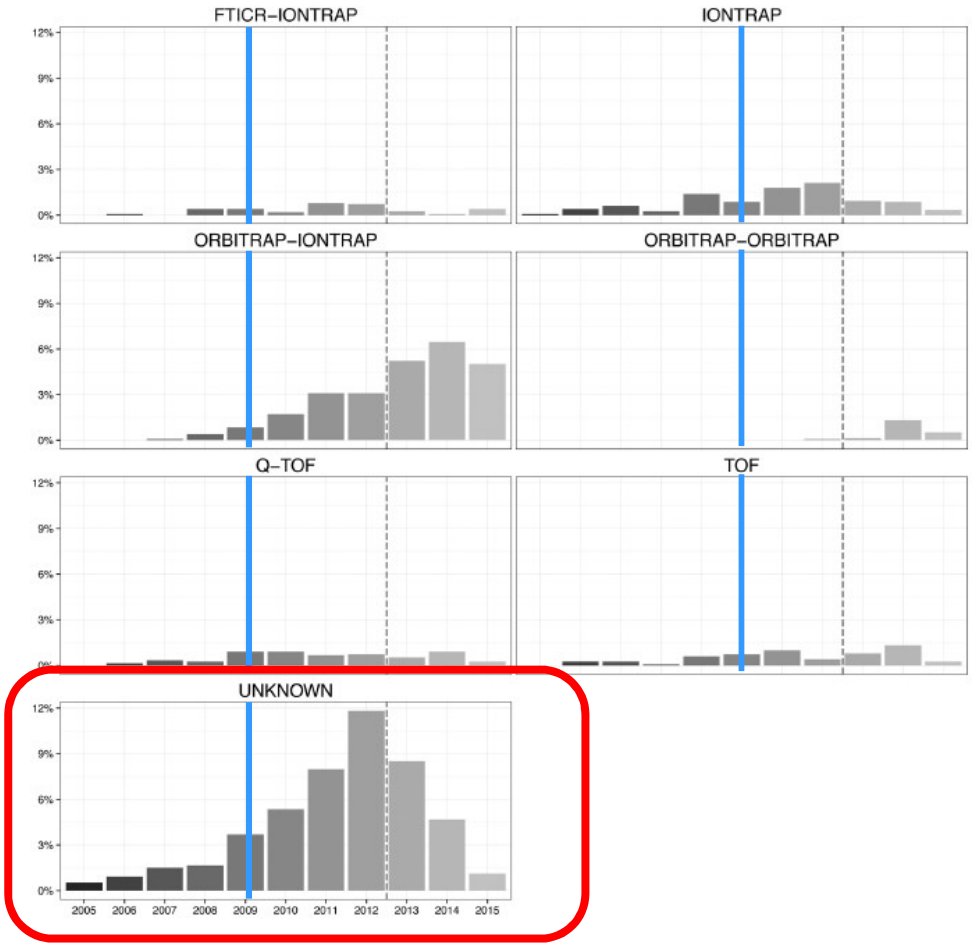
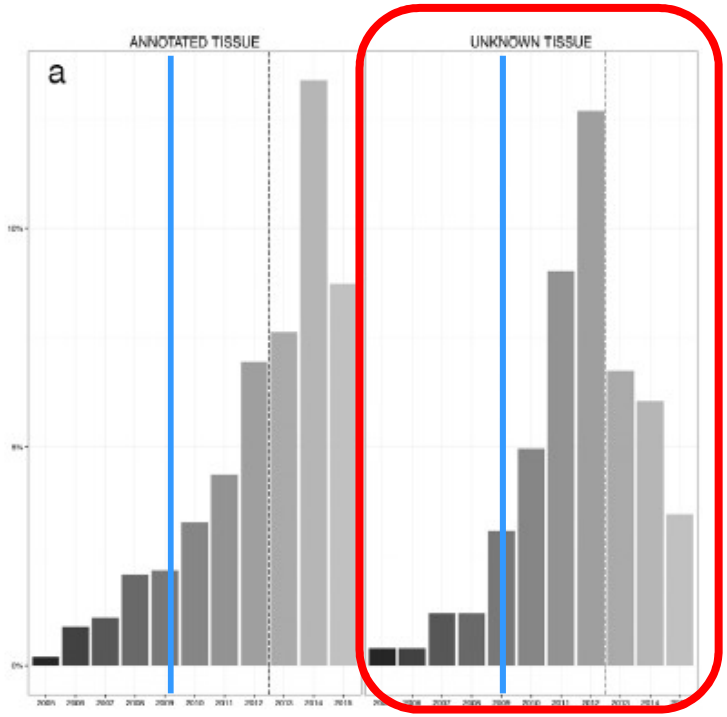




Verheggen, *EuPA Open Proteomics*, 2015

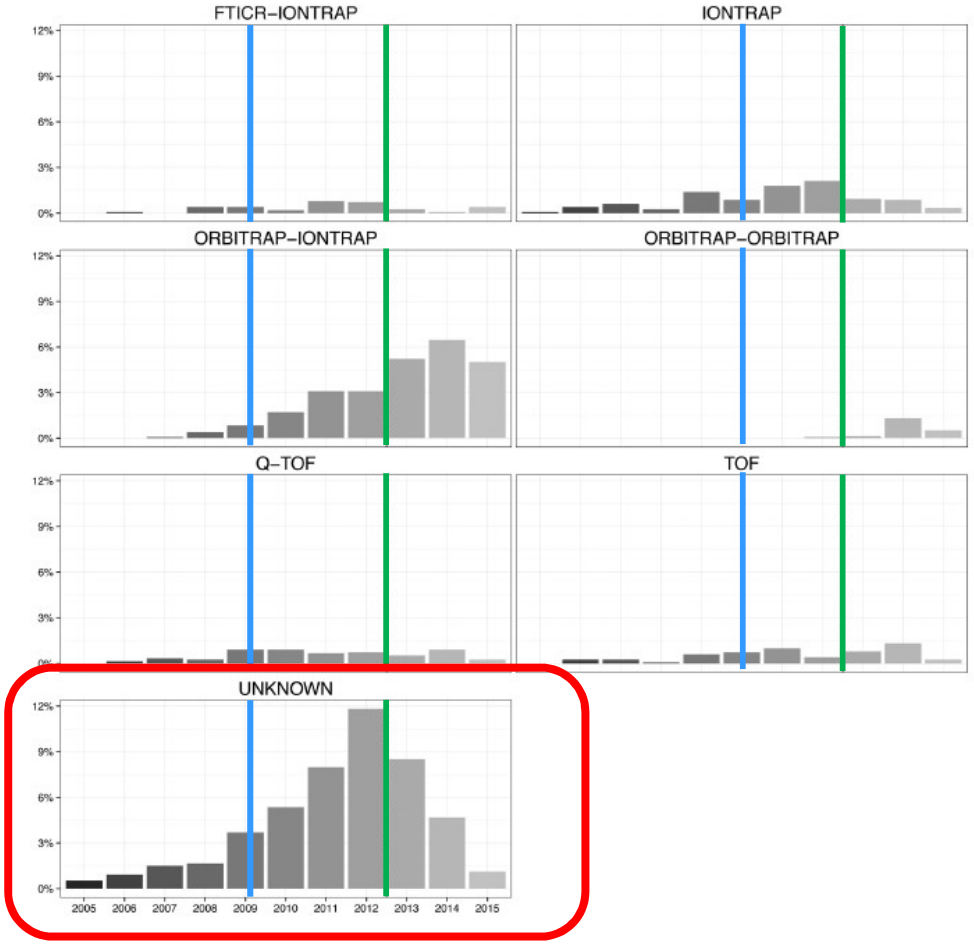
The arrival of user-friendly submission tools did not nothing to reverse reporting trends

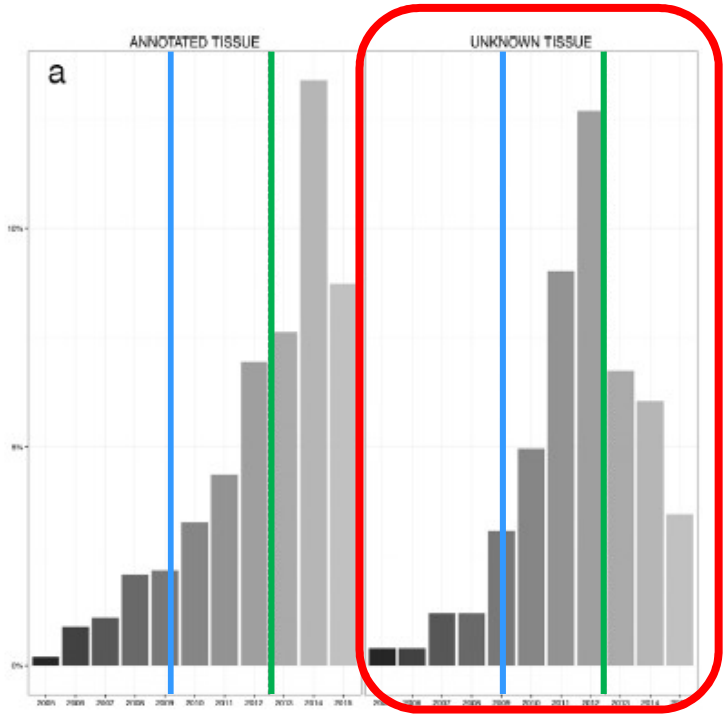




Verheggen, *EuPA Open Proteomics*, 2015

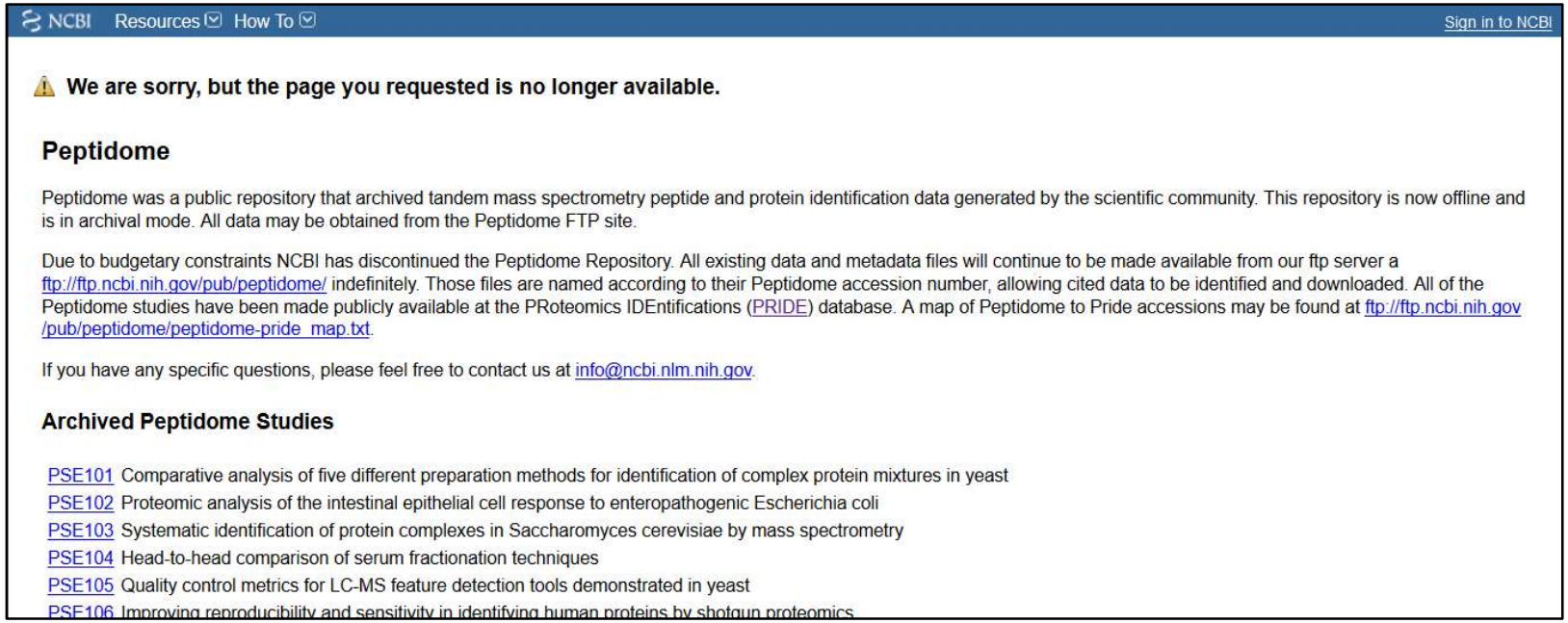
Manual curation of submissions, equivalent to restrictive policing, did help





Verheggen, *EuPA Open Proteomics*, 2015

Mid-to long-term storage of data is expensive and thus very difficult to fund and maintain



NCBI Resources How To Sign in to NCBI

We are sorry, but the page you requested is no longer available.

Peptidome

Peptidome was a public repository that archived tandem mass spectrometry peptide and protein identification data generated by the scientific community. This repository is now offline and is in archival mode. All data may be obtained from the Peptidome FTP site.

Due to budgetary constraints NCBI has discontinued the Peptidome Repository. All existing data and metadata files will continue to be made available from our ftp server a ftp://ftp.ncbi.nih.gov/pub/peptidome/ indefinitely. Those files are named according to their Peptidome accession number, allowing cited data to be identified and downloaded. All of the Peptidome studies have been made publicly available at the PRoteomics IDEntifications (PRIDE) database. A map of Peptidome to Pride accessions may be found at ftp://ftp.ncbi.nih.gov/pub/peptidome/peptidome-pride_map.txt.

If you have any specific questions, please feel free to contact us at info@ncbi.nlm.nih.gov.

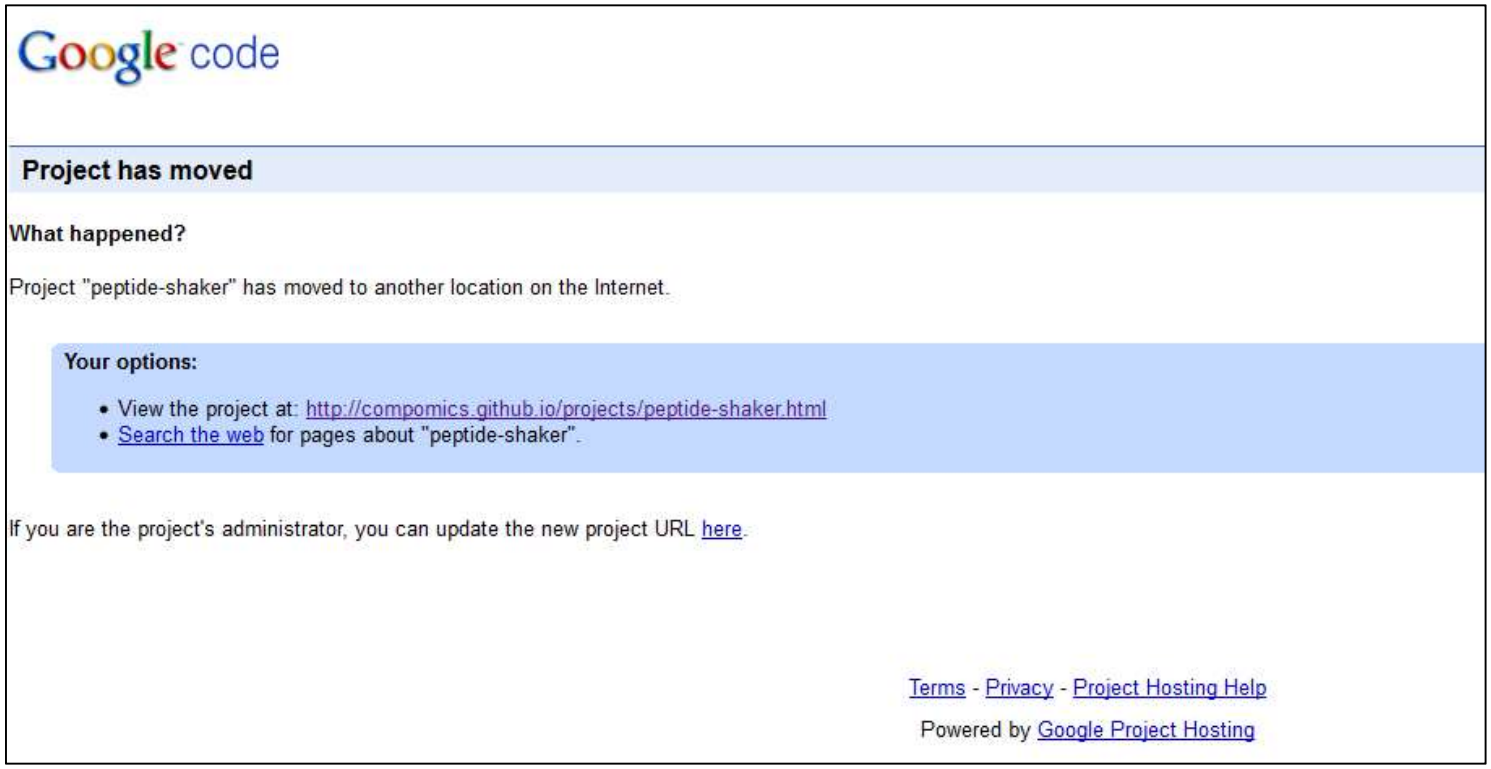
Archived Peptidome Studies

PSE101 Comparative analysis of five different preparation methods for identification of complex protein mixtures in yeast
PSE102 Proteomic analysis of the intestinal epithelial cell response to enteropathogenic Escherichia coli
PSE103 Systematic identification of protein complexes in Saccharomyces cerevisiae by mass spectrometry
PSE104 Head-to-head comparison of serum fractionation techniques
PSE105 Quality control metrics for LC-MS feature detection tools demonstrated in yeast
PSE106 Improving reproducibility and sensitivity in identifying human proteins by shotgun proteomics

http://www.ncbi.nlm.nih.gov/peptidome

Slotta, *Nature Biotechnology*, 2009; Csordas, *Proteomics*, 2013; Martens, *Proteomics*, 2013

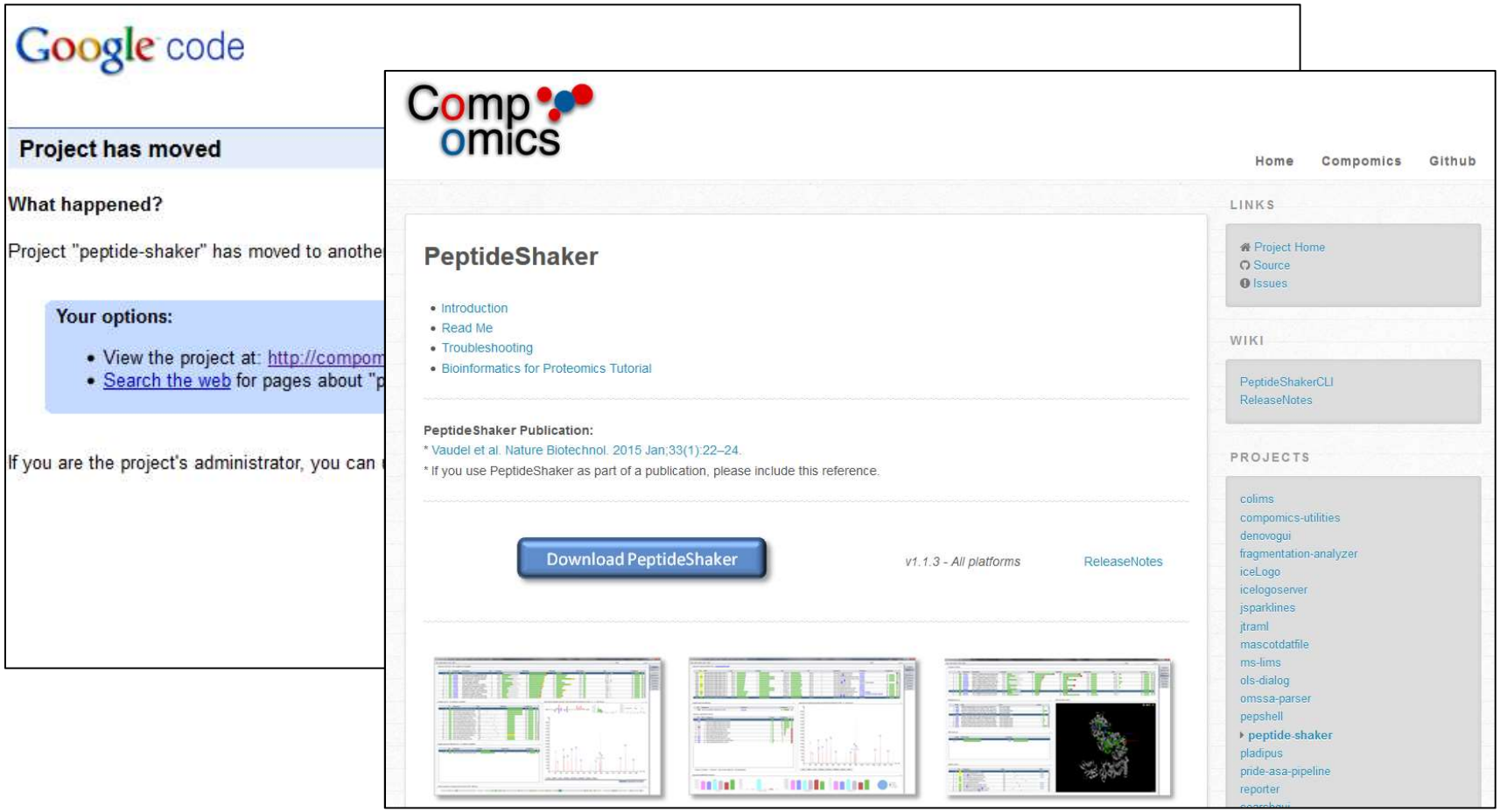
And as responsible caretaker of your stuff, you will sometimes need to take action too



http://peptide-shaker.googlecode.com

Vaudel, *Nature Biotechnology*, 2015

Maintaining what you do is not trivial, not cheap, and considered unwise by senior PIs



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Vaudel, *Nature Biotechnology*, 2015

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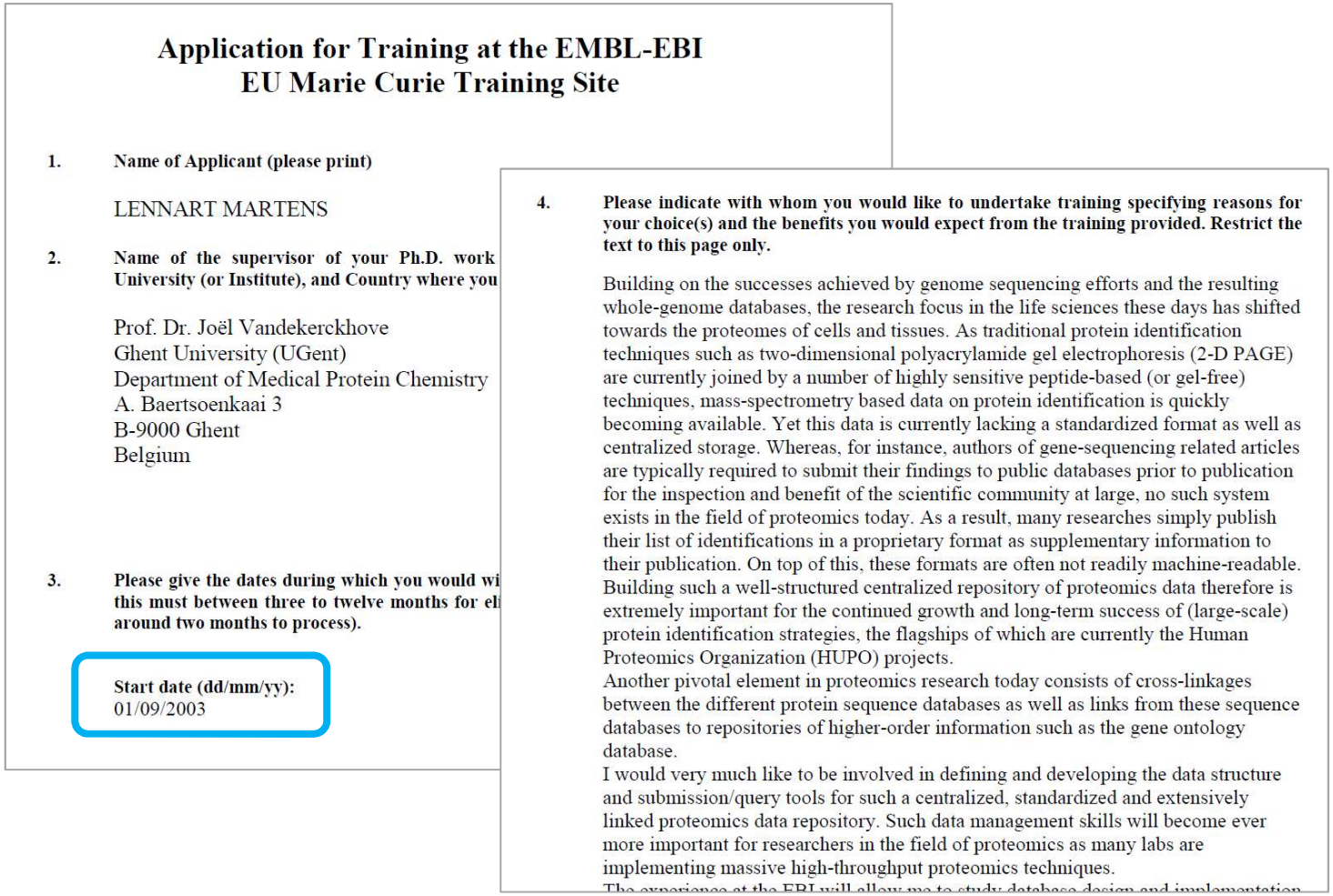
The PRIDE database was started to allow (orthogonal) re-analysis of proteomics data



Application for Training at the EMBL-EBI
EU Marie Curie Training Site

1. **Name of Applicant (please print)**

LENNART MARTENS

2. **Name of the supervisor of your Ph.D. work University (or Institute), and Country where you**

Prof. Dr. Joël Vandekerckhove
Ghent University (UGent)
Department of Medical Protein Chemistry
A. Baertsoenkaai 3
B-9000 Ghent
Belgium

3. **Please give the dates during which you would wi this must between three to twelve months for eli around two months to process).**

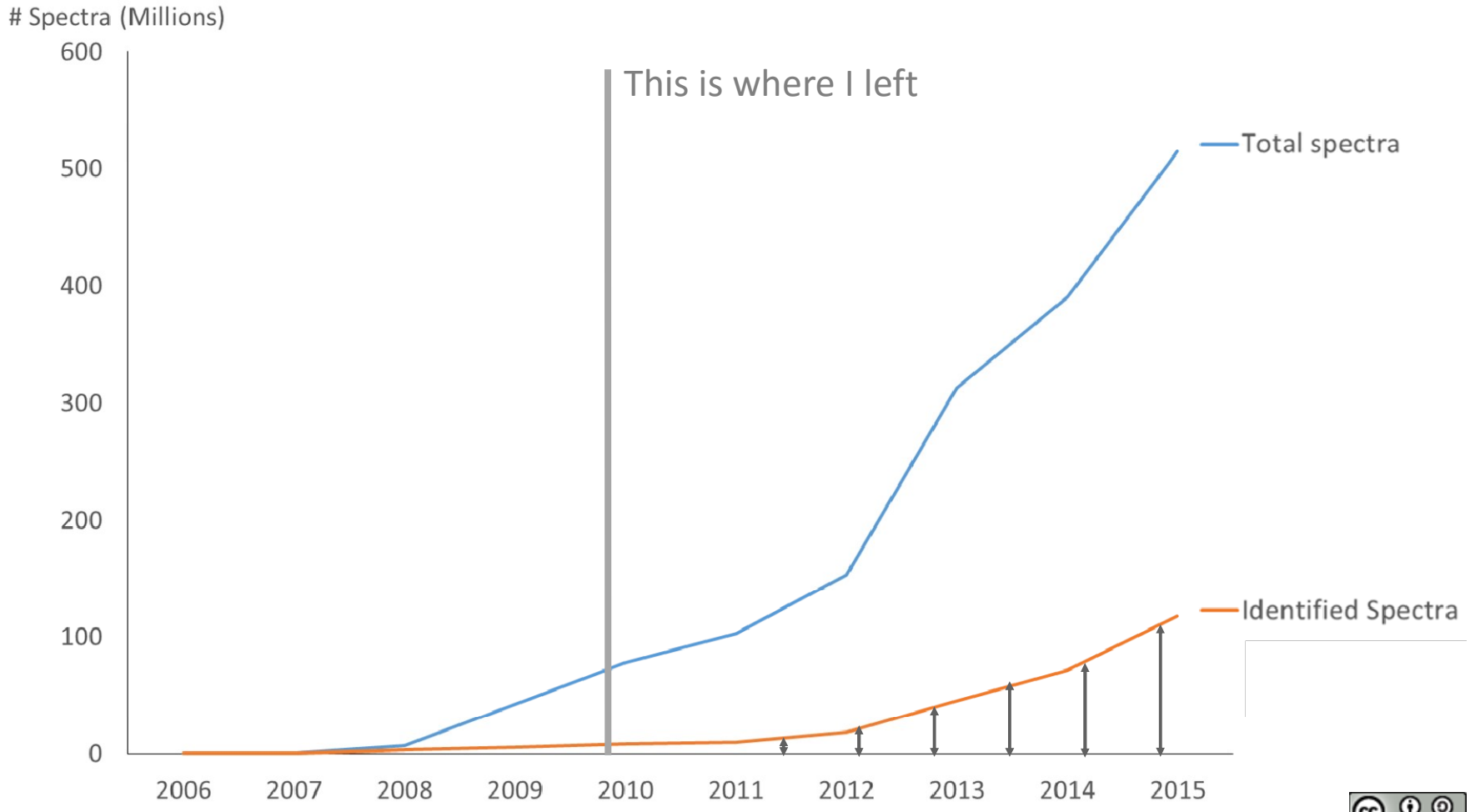
Start date (dd/mm/yy):
01/09/2003

4. **Please indicate with whom you would like to undertake training specifying reasons for your choice(s) and the benefits you would expect from the training provided. Restrict the text to this page only.**

Building on the successes achieved by genome sequencing efforts and the resulting whole-genome databases, the research focus in the life sciences these days has shifted towards the proteomes of cells and tissues. As traditional protein identification techniques such as two-dimensional polyacrylamide gel electrophoresis (2-D PAGE) are currently joined by a number of highly sensitive peptide-based (or gel-free) techniques, mass-spectrometry based data on protein identification is quickly becoming available. Yet this data is currently lacking a standardized format as well as centralized storage. Whereas, for instance, authors of gene-sequencing related articles are typically required to submit their findings to public databases prior to publication for the inspection and benefit of the scientific community at large, no such system exists in the field of proteomics today. As a result, many researches simply publish their list of identifications in a proprietary format as supplementary information to their publication. On top of this, these formats are often not readily machine-readable. Building such a well-structured centralized repository of proteomics data therefore is extremely important for the continued growth and long-term success of (large-scale) protein identification strategies, the flagships of which are currently the Human Proteomics Organization (HUPO) projects.
Another pivotal element in proteomics research today consists of cross-linkages between the different protein sequence databases as well as links from these sequence databases to repositories of higher-order information such as the gene ontology database.
I would very much like to be involved in defining and developing the data structure and submission/query tools for such a centralized, standardized and extensively linked proteomics data repository. Such data management skills will become ever more important for researchers in the field of proteomics as many labs are implementing massive high-throughput proteomics techniques.
The experience at the EBI will allow me to study database design and implementation

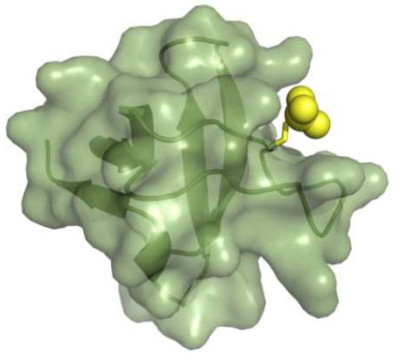
Martens, EuPA Open Proteomics, in press

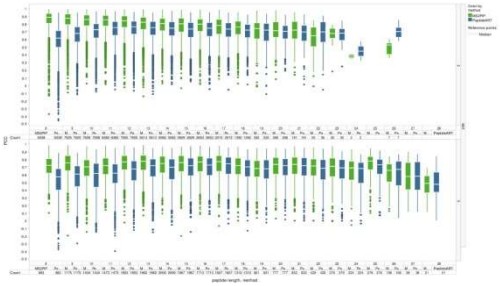
A large amount of post-consumer MS data is collected in public databases such as PRIDE

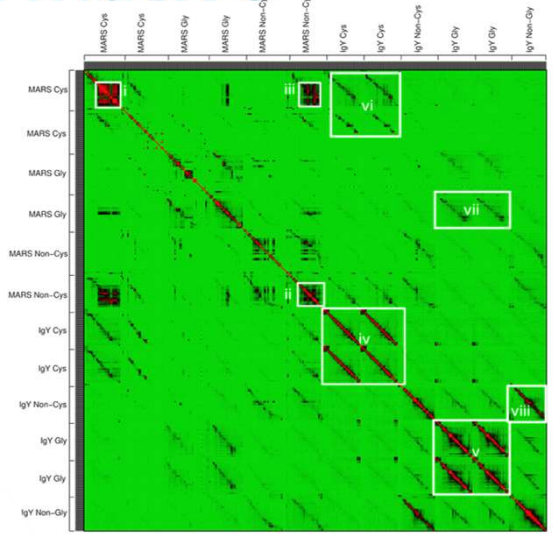


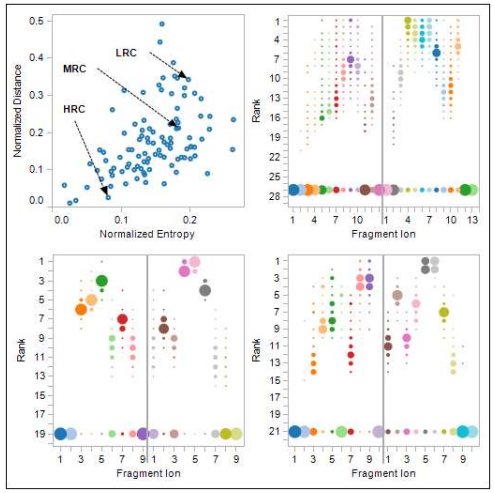
Martens, Proteomics, 2005

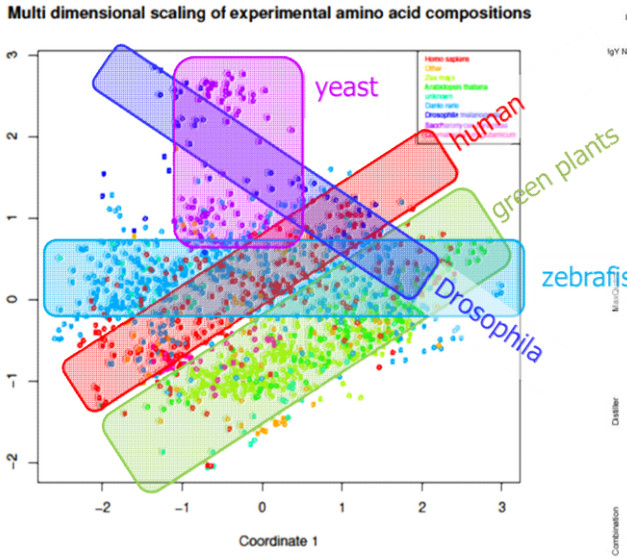
The identified peptides reported by the community proved highly informative

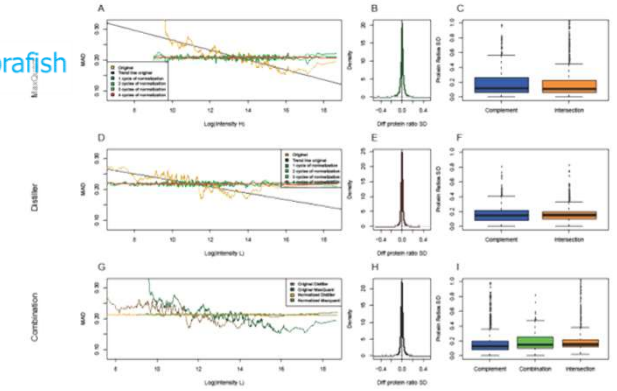






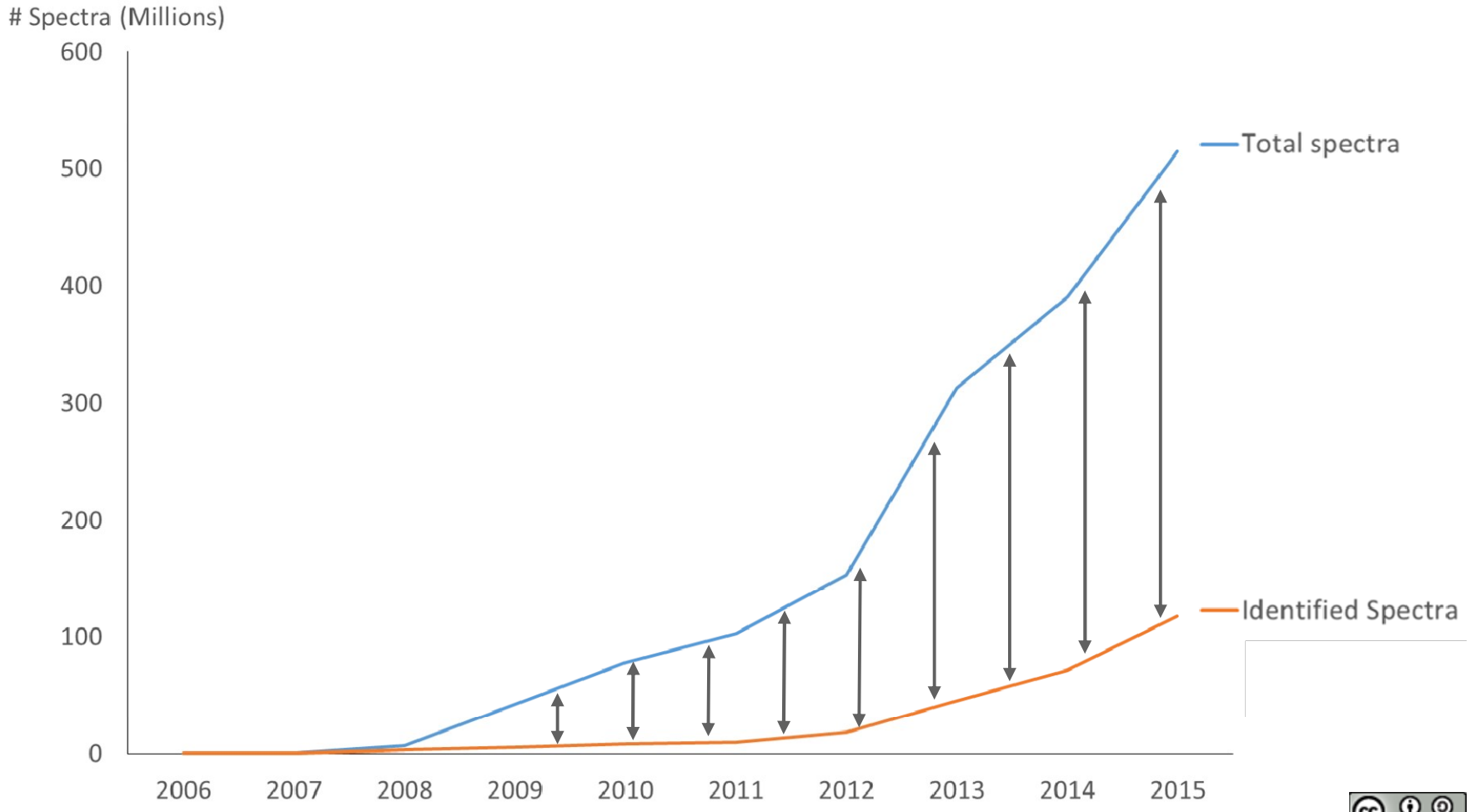




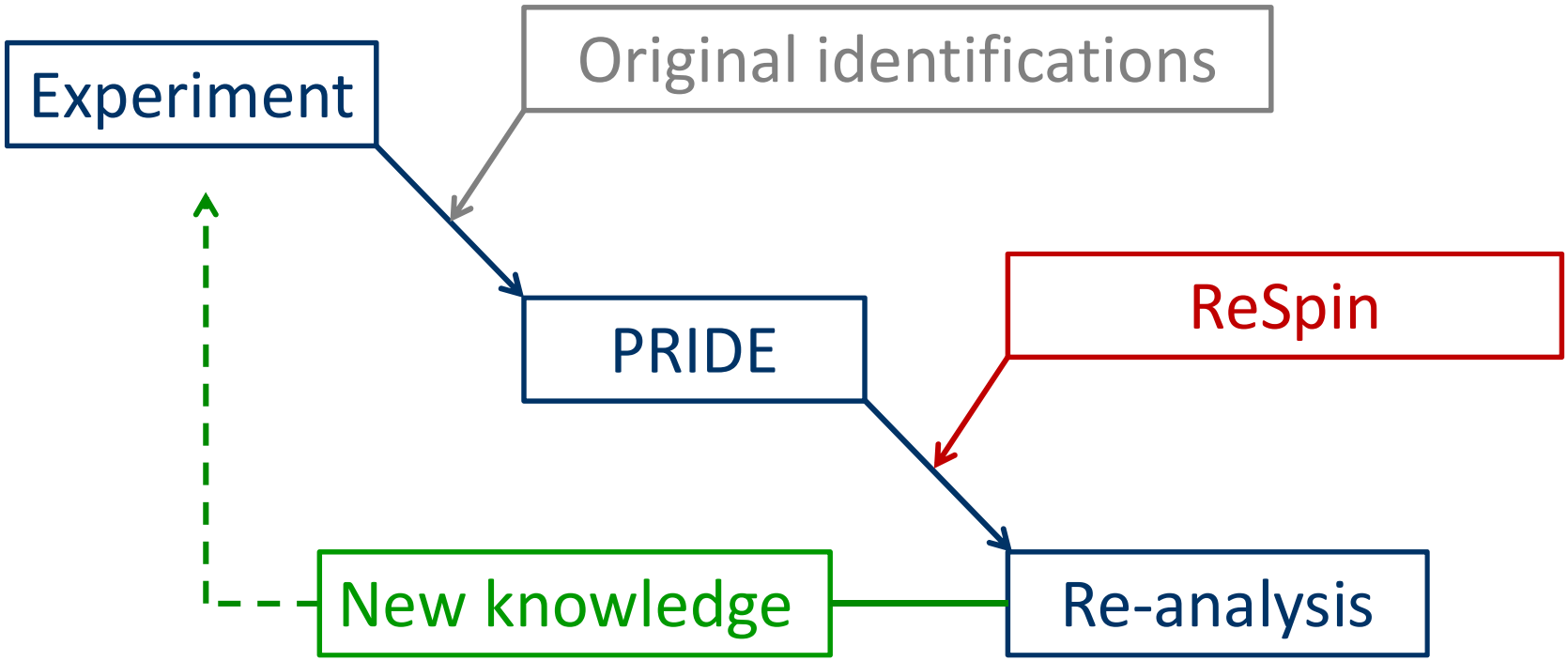


Foster, Proteomics, 2011; Colaert, Nature Methods, 2011; Barsnes, Proteomics 2011, Vandermarliere, Proteomics 2013; Degroeve, Bioinformatics 2013

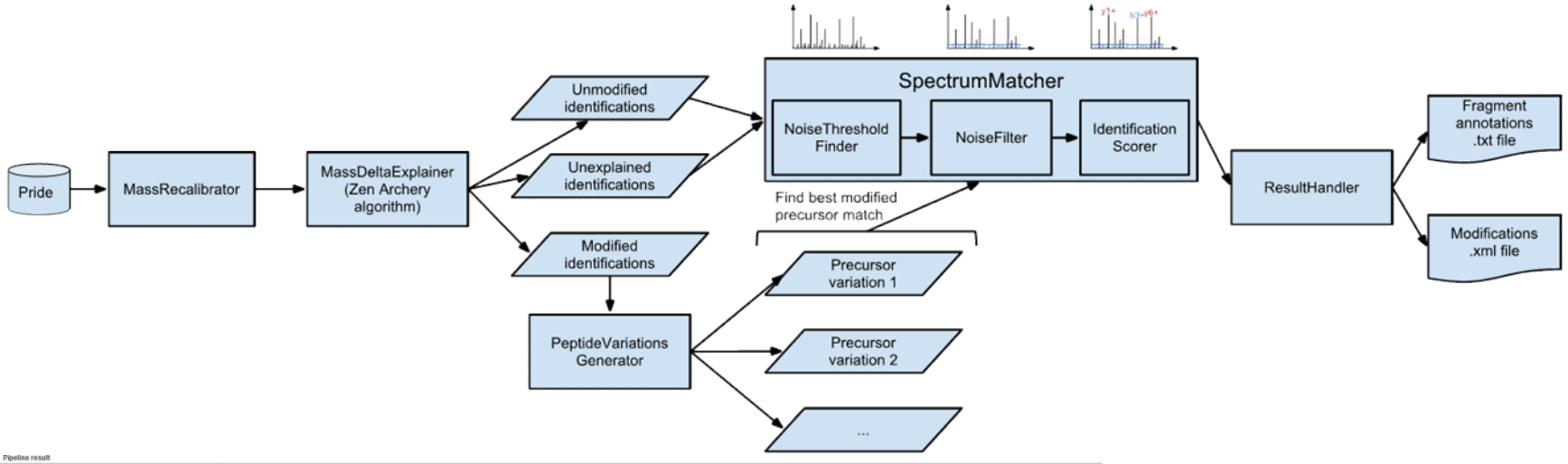
Meanwhile, we took an interest in the unidentified part of the data

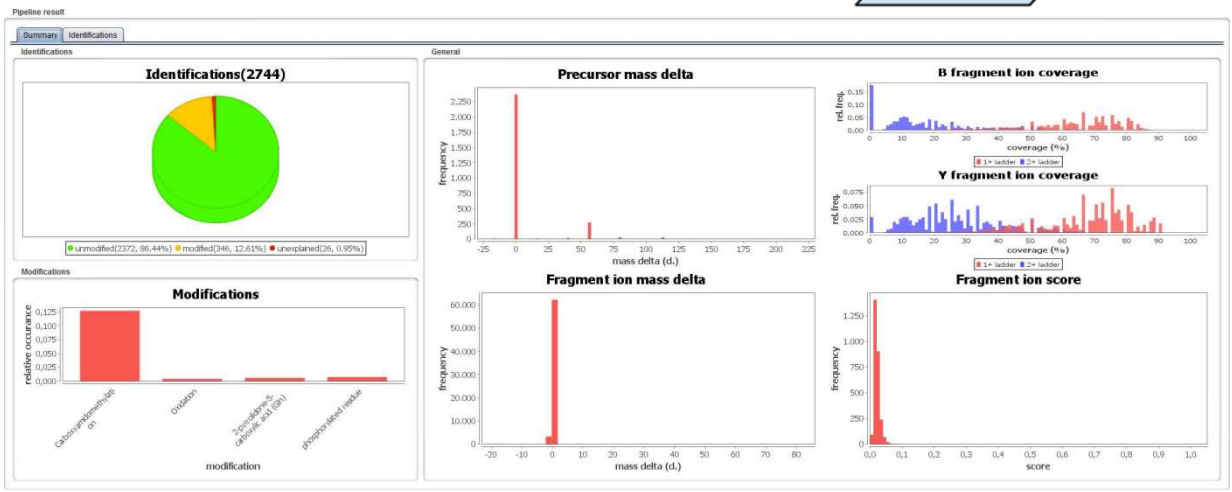


We built the ReSpin pipeline to enable fast re-processing of proteomics data in new ways



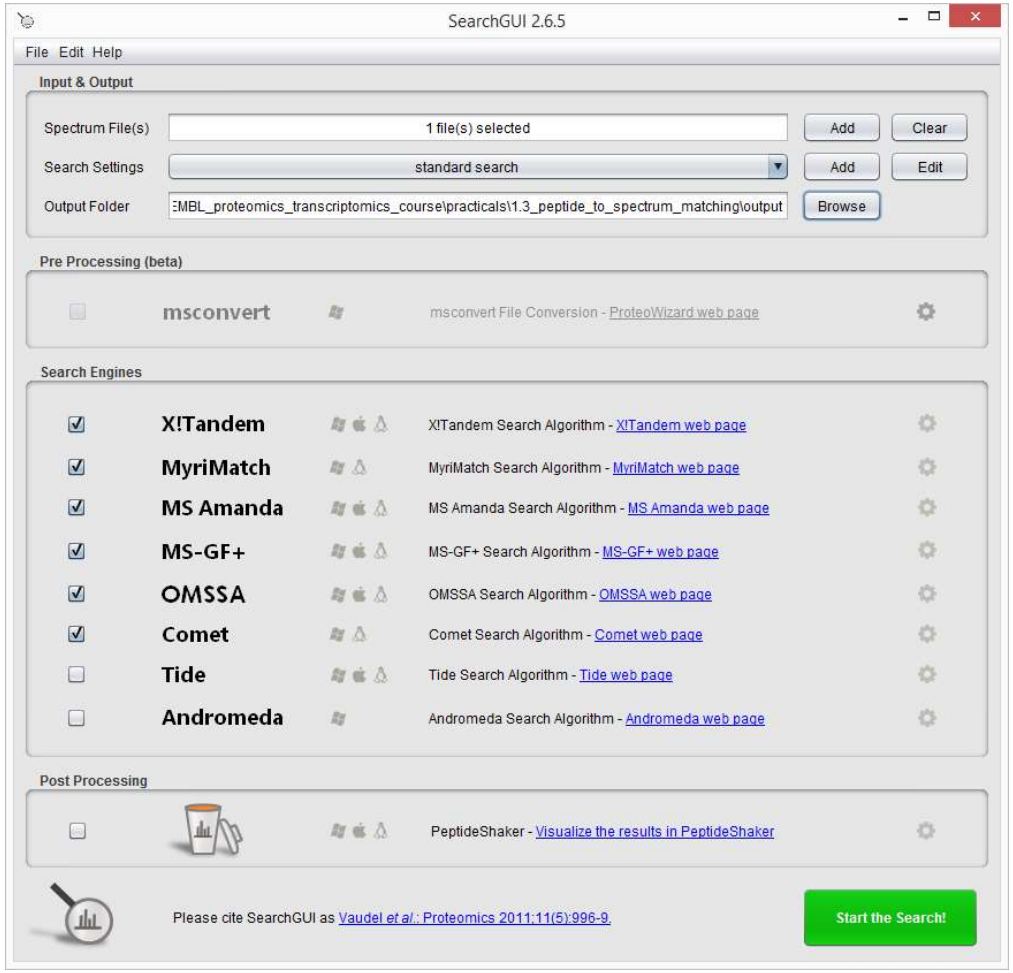
First of all, we had to understand the data to allow reliable re-interpretation





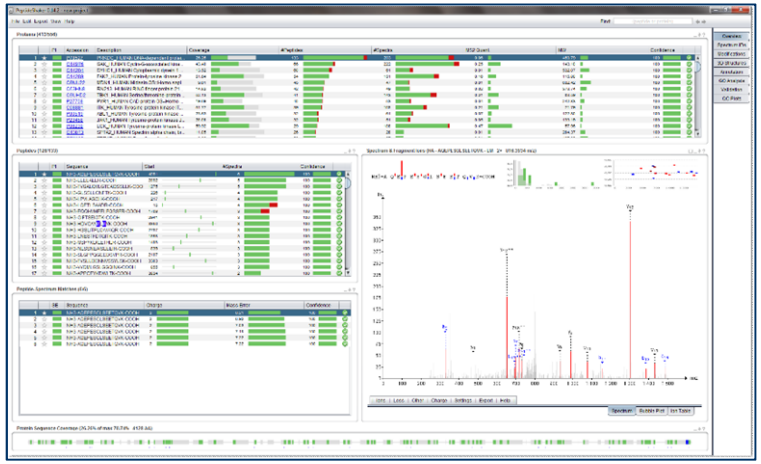
http://compomics.github.io/projects/pride-asa-pipeline.html
Hulstaert, Journal of Proteomics, 2013

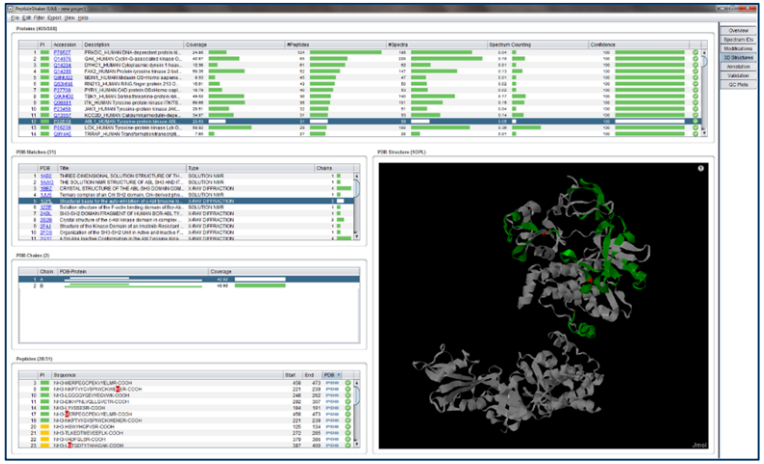
Then we had to make it easy to re-analyze these data with multiple search algorithms

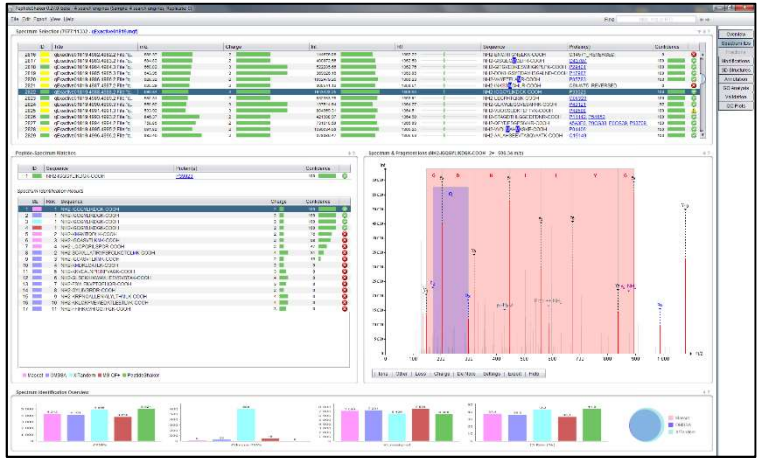


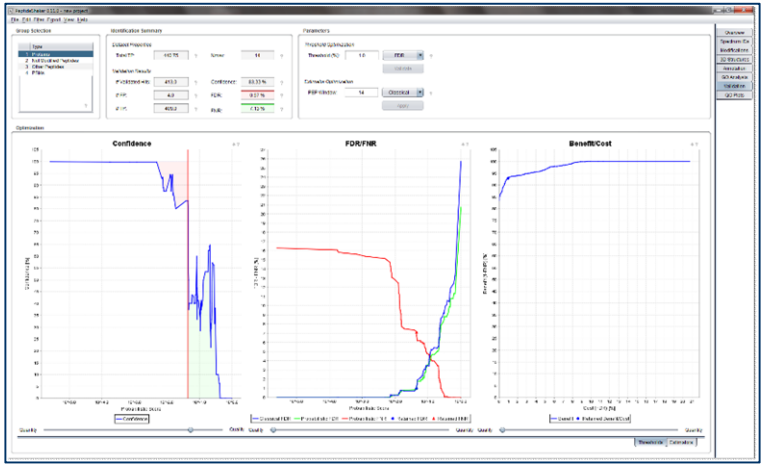
http://compomics.github.io/projects/searchgui.html
Vaudel, Proteomics, 2011

And finally, a means to collate, process and validate the results from our re-analyses



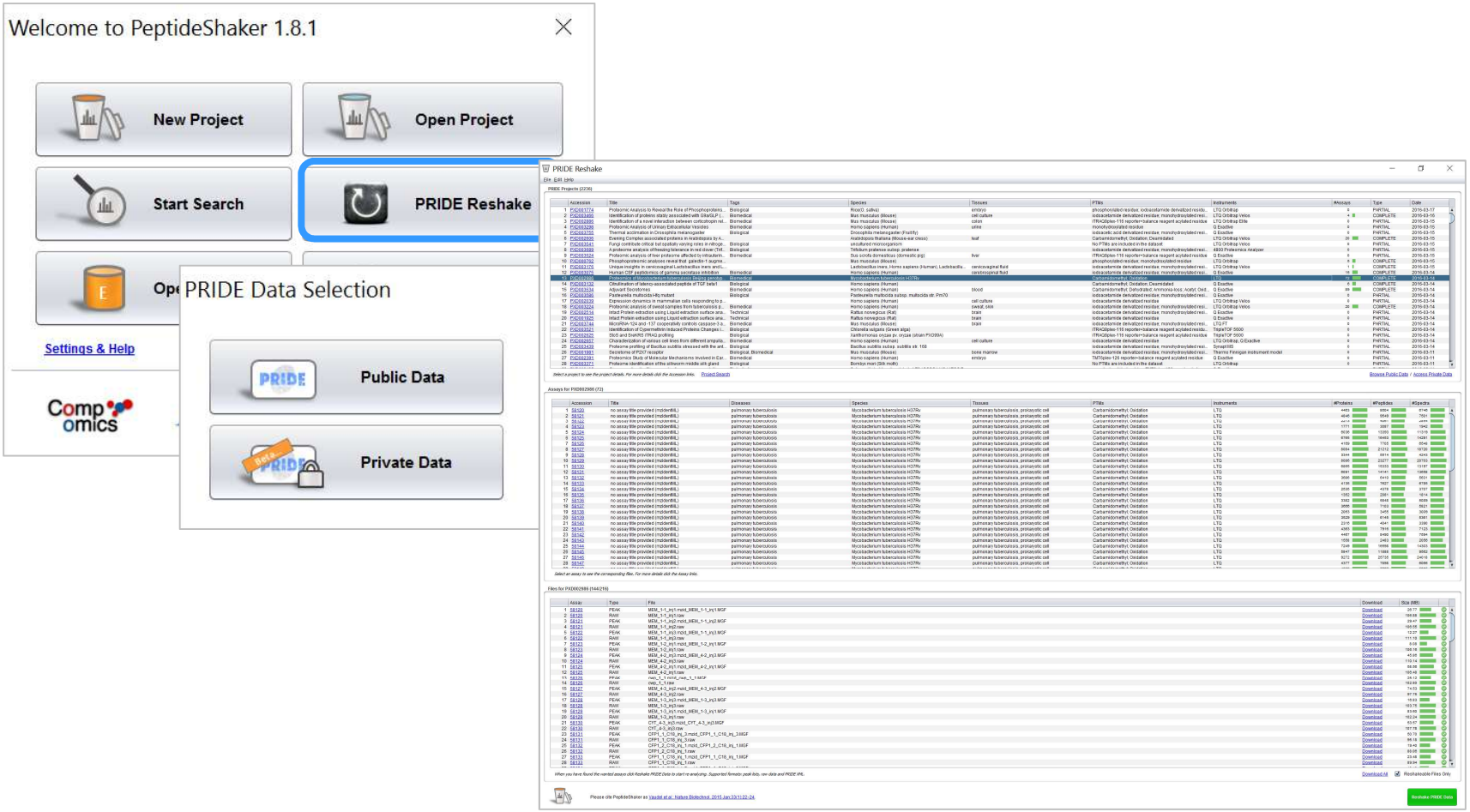






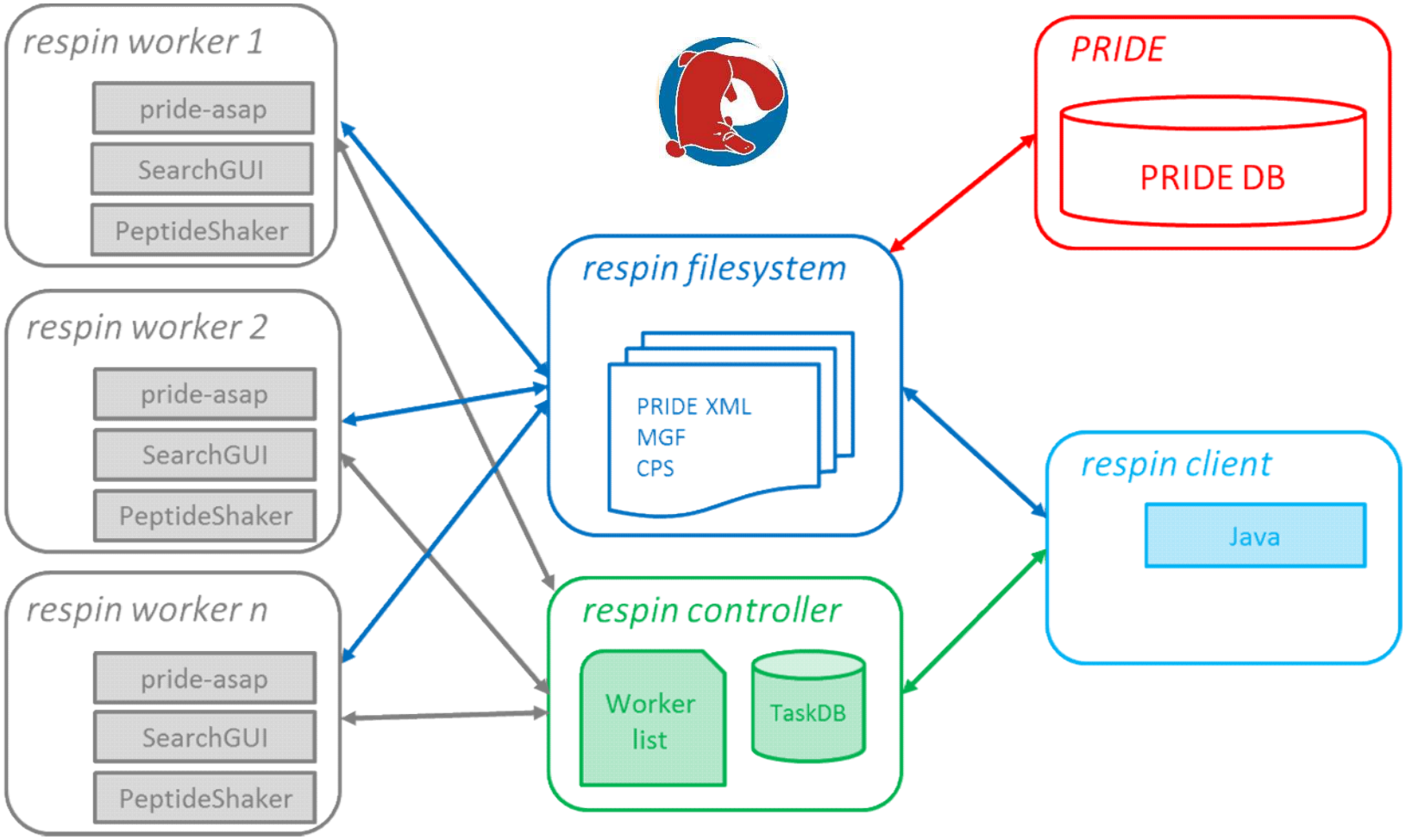
http://compomics.github.io/projects/peptide-shaker.html
Vaudel, Nature Biotechnology, 2015

Incidentally, anyone can reprocess public data with PeptideShaker and about ten mouseclicks



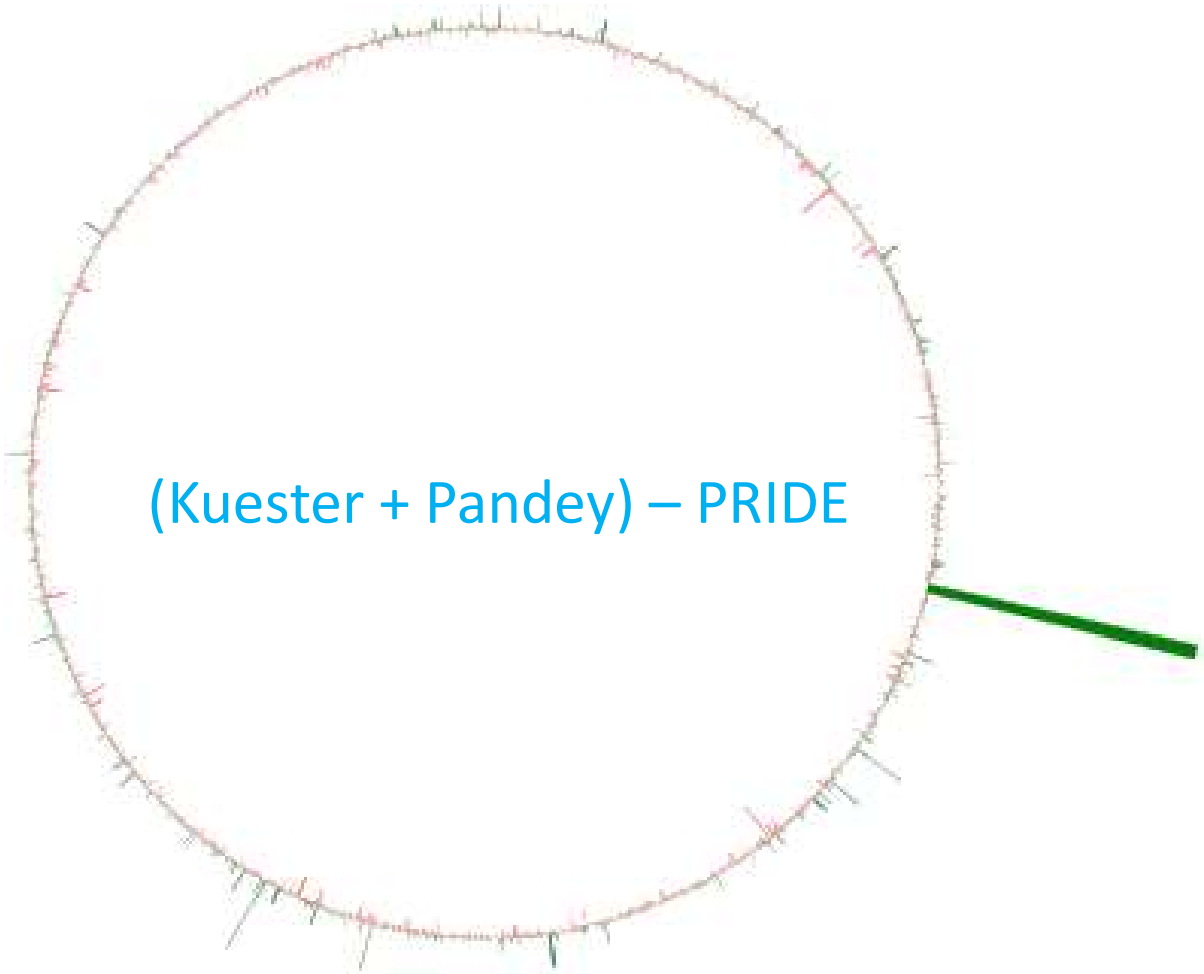
Vaudel, Nature Biotechnology, 2015

We then automated everything on our Pladipus custom grid engine



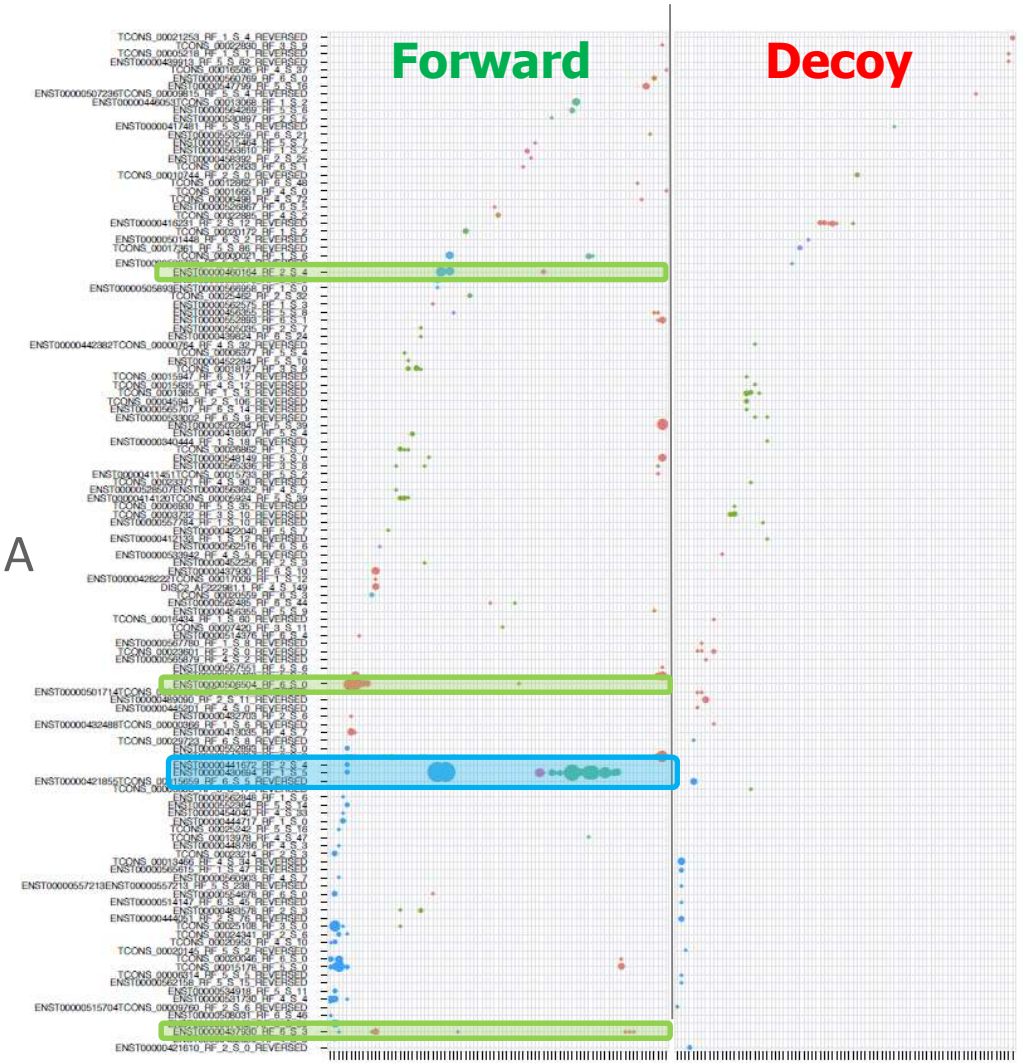
http://compomics.github.io/projects/pladipus.html
Verheggen, Journal of Proteome Research, 2016

Combining data sets brings clear benefits



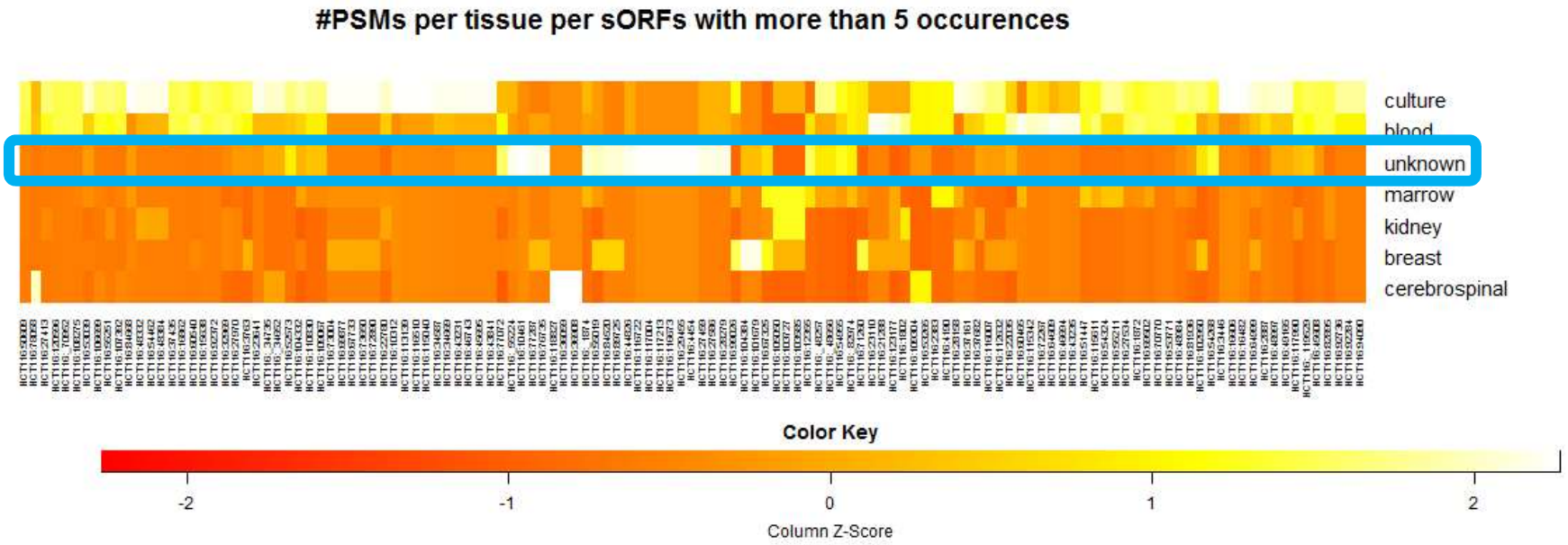
Vizcaíno, Nature Biotechnology, 2014; Wilhelm, Nature, 2014; Kim, Nature, 2014

We already went hunting for translated lncRNAs, but we found very few (< 1%)



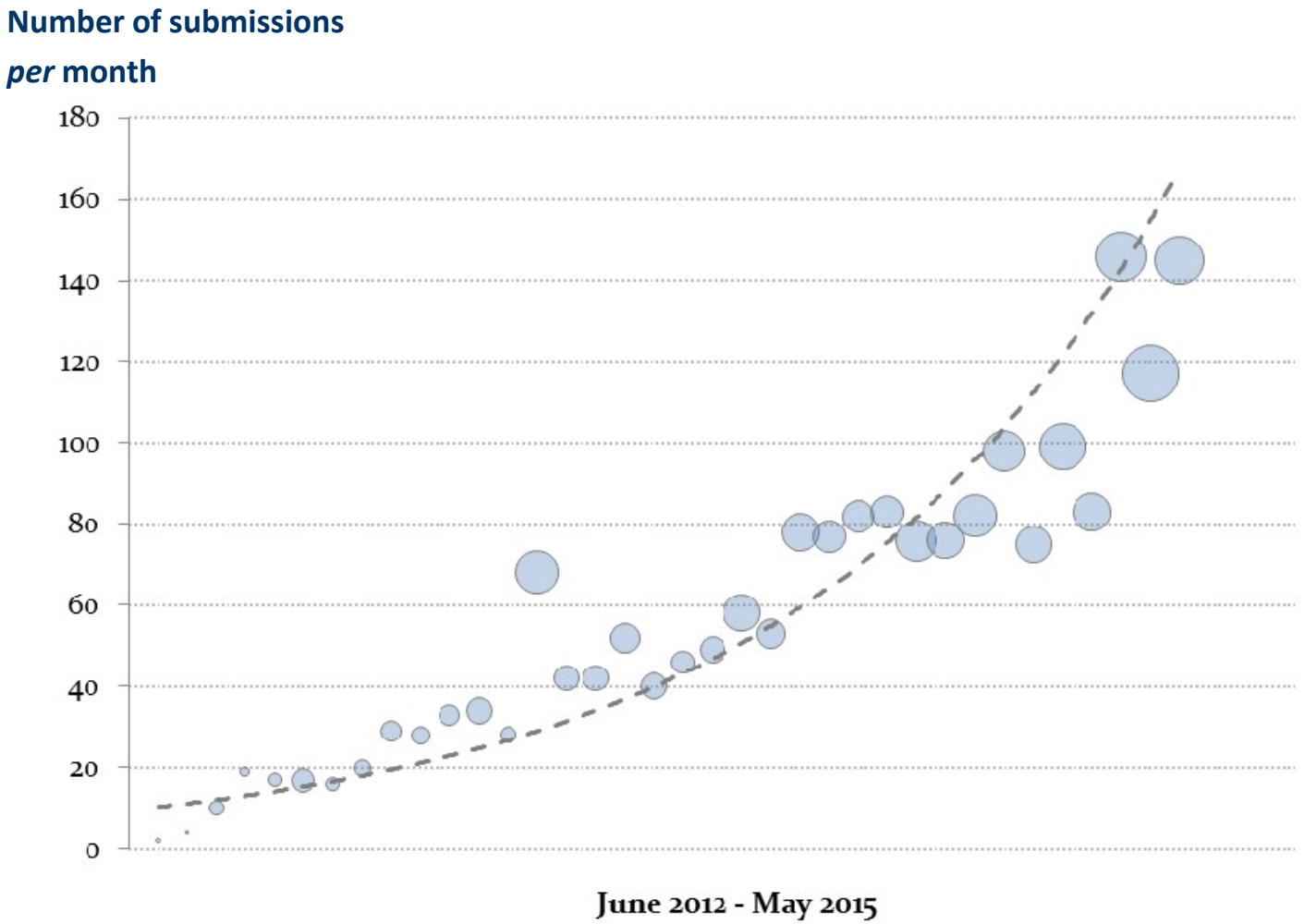
Volders, NAR, 2013; Volders, NAR, 2015

We were able to help confirm expression of small ORFs across human tissues



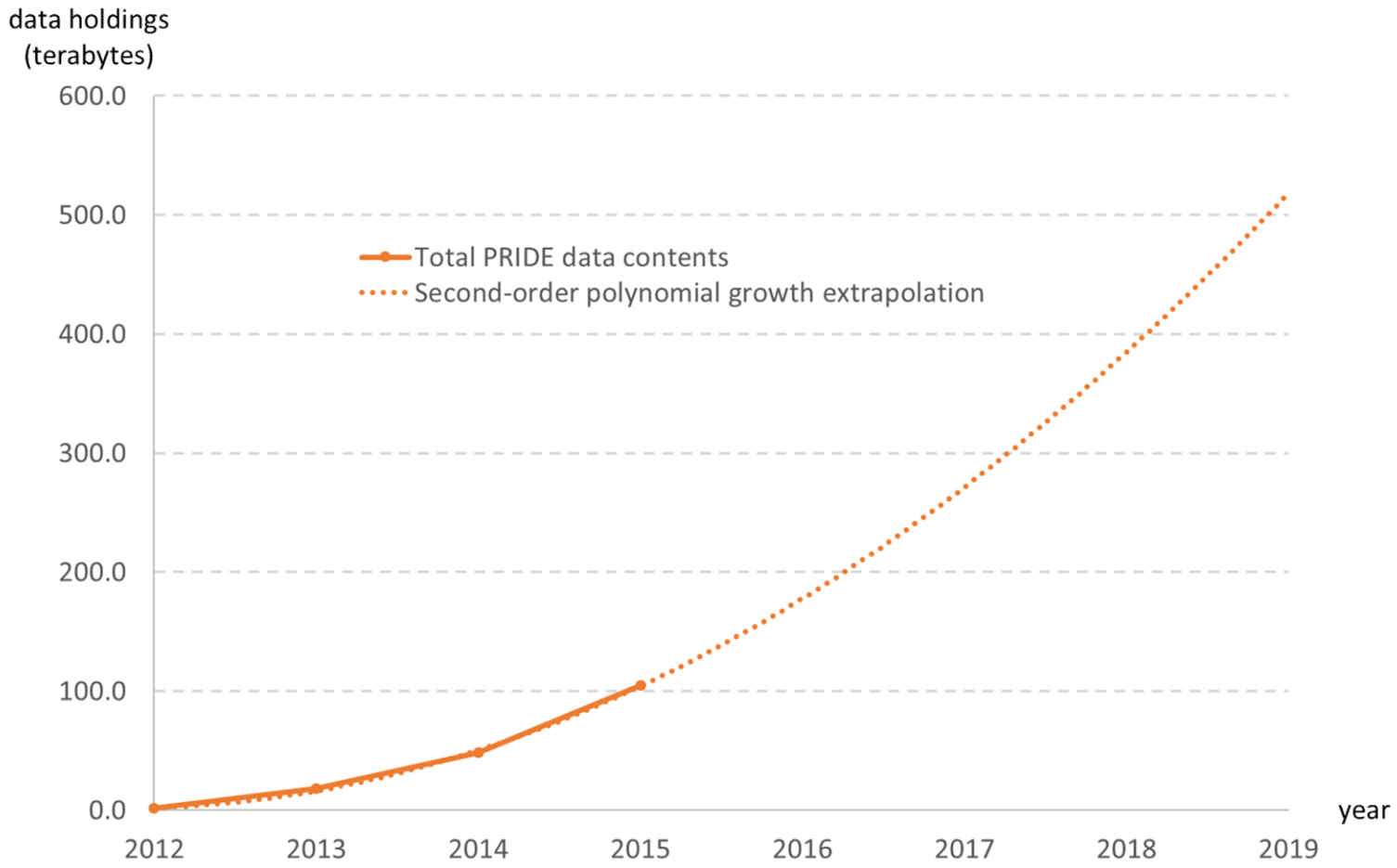
Olexiouk, NAR, 2016

Data growth is increasing in PRIDE; more, and ever bigger data sets are submitted daily



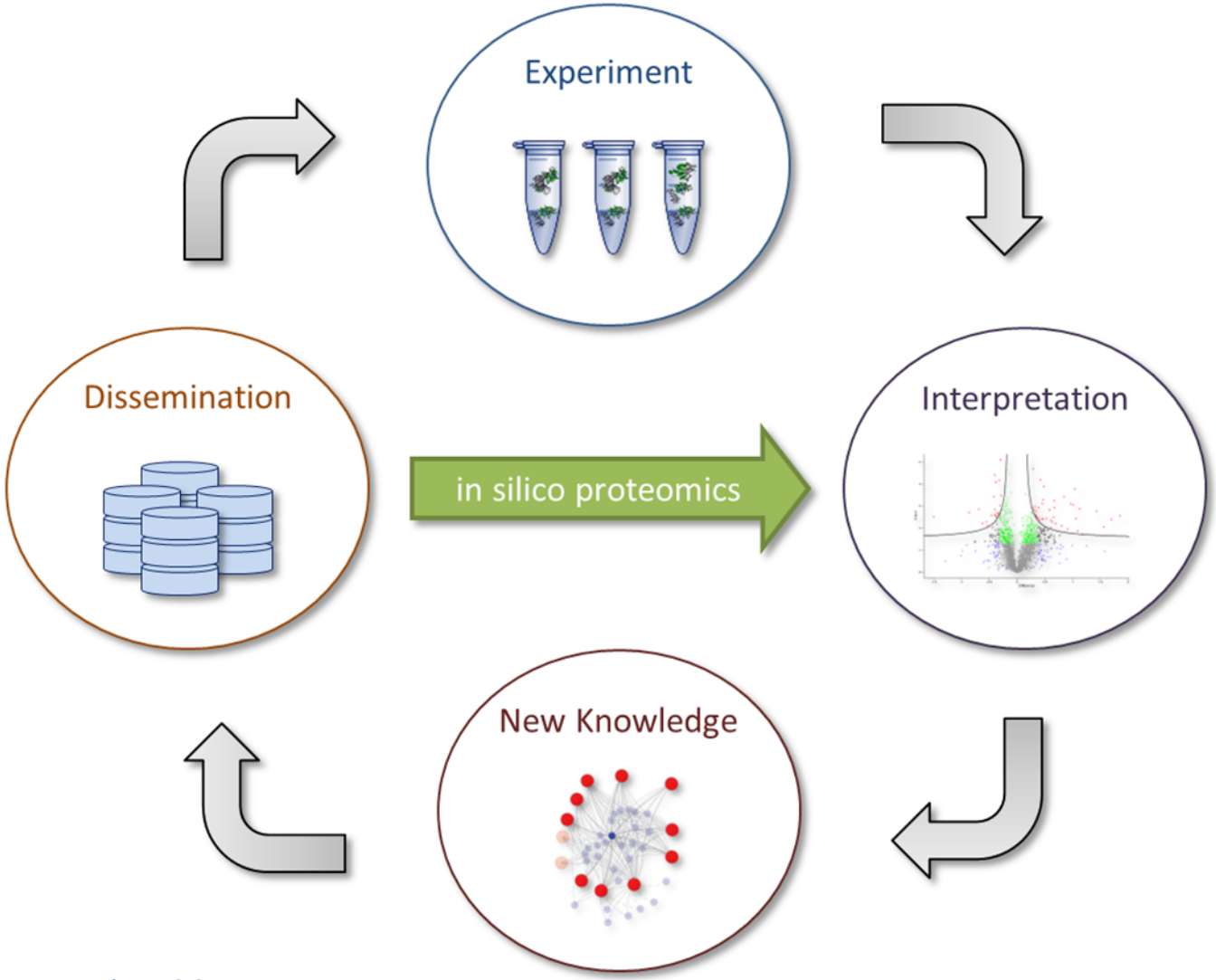
Vaudel, Proteomics, 2015

Projections for data growth in PRIDE are therefore quite impressive



Courtesy of Dr. Juan Antonio Vizcaíno, Proteomics Team Leader, EMBL-EBI

All of the available data simply bristle with opportunity



Vaudel, Proteomics, 2015

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A sociologist's take on our efforts towards (orthogonal) data reuse

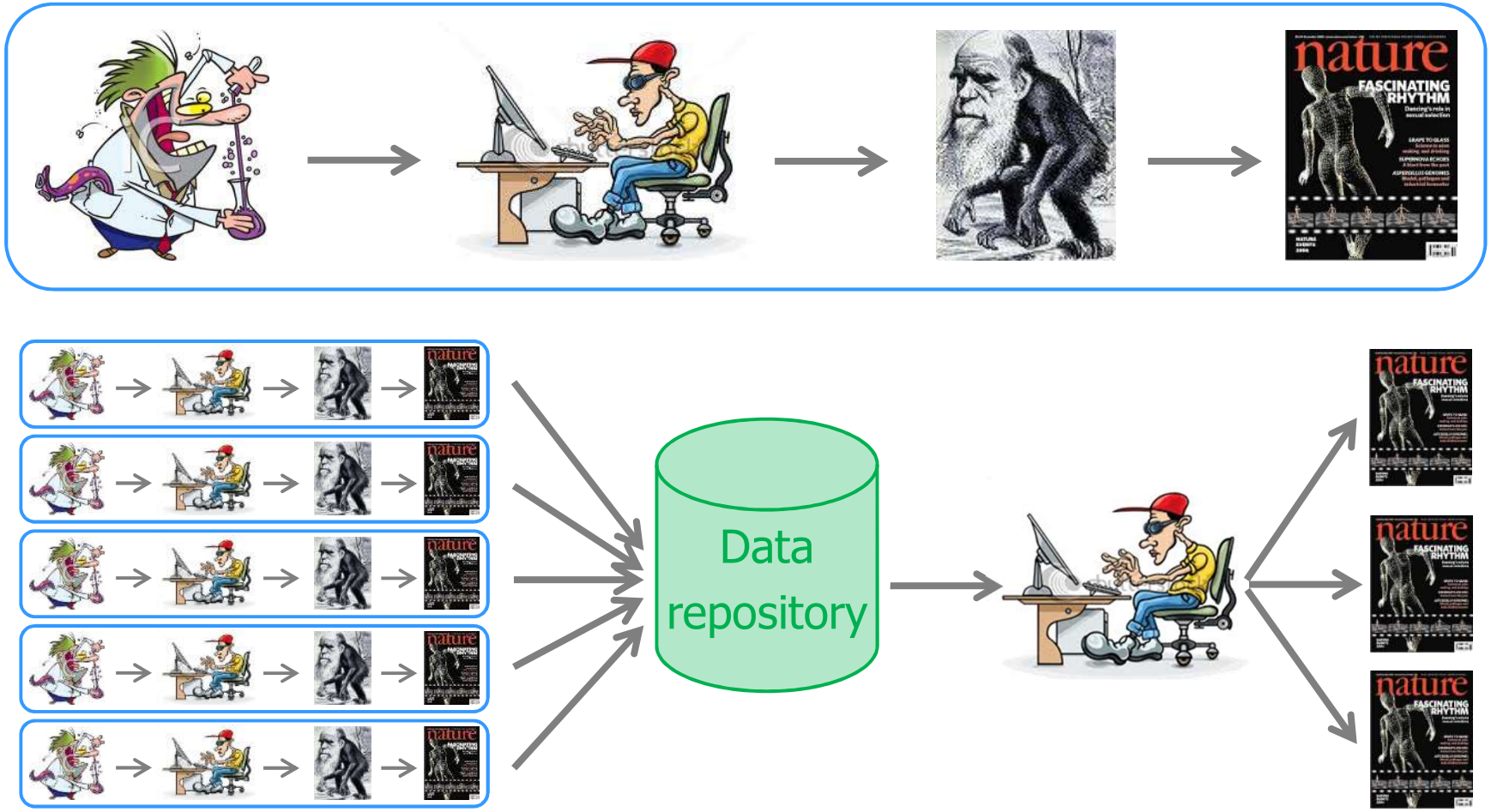
"This desire to reactivate data is widespread, and Klie et al. are not alone in wanting to show that 'far from being places where data goes to die' (Klie et al., 2007: 190), **such data collections can be mined for valuable information that could not be obtained in any other way**."

"In attempting to **reactivate sedimented data** in order to enable its re-use, their first step was ..."

"... they are experiments in seeing, in furnishing ways of seeing how data on proteins could become re-usable, could be reactivated as **collective property rather than the by-product of publication**."

Mackenzie and McNally, *Theory, Culture and Society*, 2013

One of the big ideas in science will be the (ortogonal-) re-use of (big) public data



And now think about open science, and imagine the opportunities

- What could you do with open science? What could you study? What could you learn?

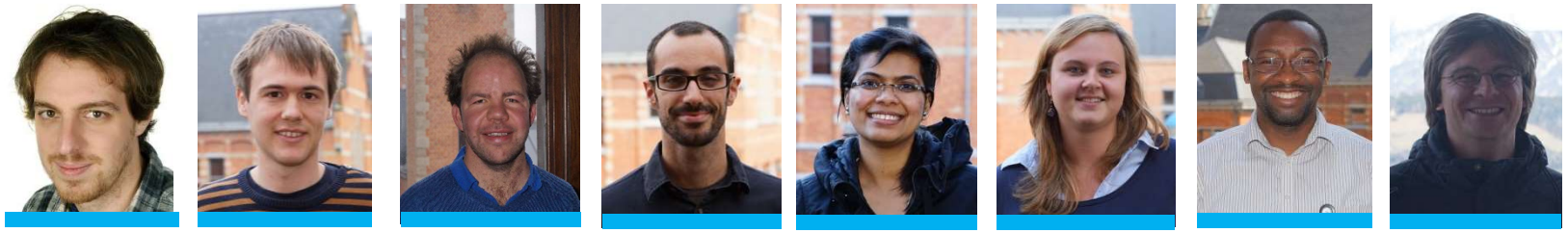
- What opportunities would present themselves, if…
  - All data (in your field) were available online
  - All algorithms (in your field) were available online
  - All publications (in your field) were open access

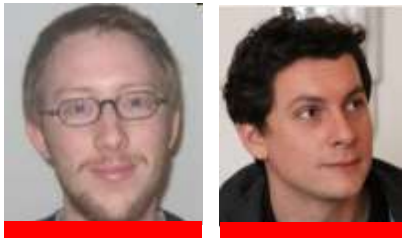
- Most of these opportunities are not little steps forward; instead they promise to be revolutionary!

J.R.R. Tolkien, *A Conversation with Smaug*

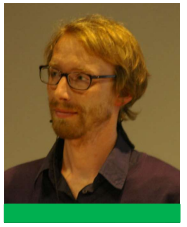
Here is treasure of unlimited size, with all dragons chased away – *now what will you do?*

https://www.flickr.com/photos/fantasy-art-and-portraits/2884954207
(CC BY-NC-SA 2.0)





Comp omics



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