PRIDE Inspector: a tool to visualize and validate MS proteomics data

Rui Wang
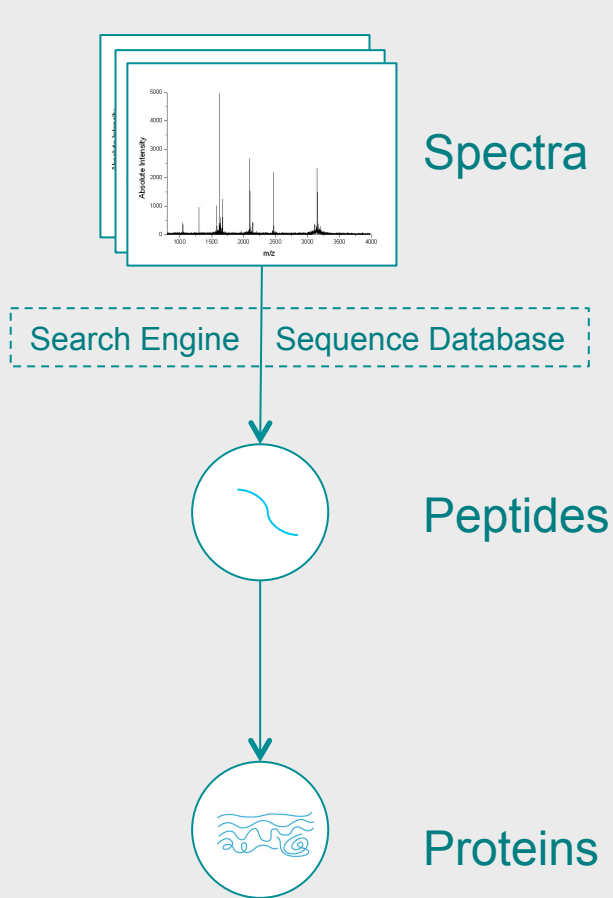
PRIDE Team, Proteomics Services Group
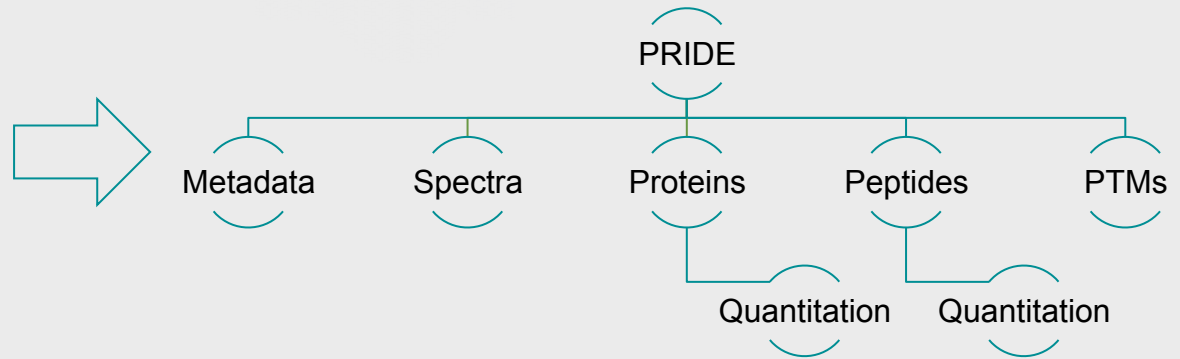
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Agenda

- PRIDE Repository

- Challenges

- PRIDE Inspector

- Future Plans

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PRoteomics IDEntifications Database (PRIDE)

Spectra

Public mass spec repository

Search Engine | Sequence Database

Peptides

PRIDE

Metadata   Spectra   Proteins   Peptides   PTMs

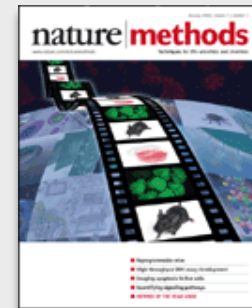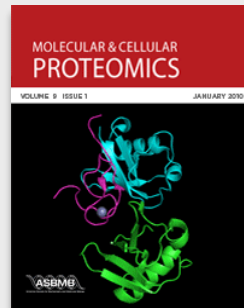Quantitation   Quantitation

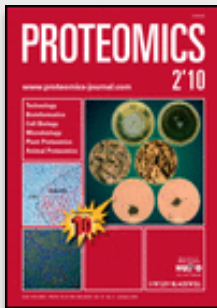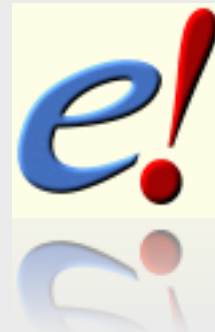Proteins

http://www.ebi.ac.uk/pride

- 151+ M Spectra
- 28+ M Peptides
- 5.8+ M Proteins

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PRoteomics IDEntifications Database (PRIDE)
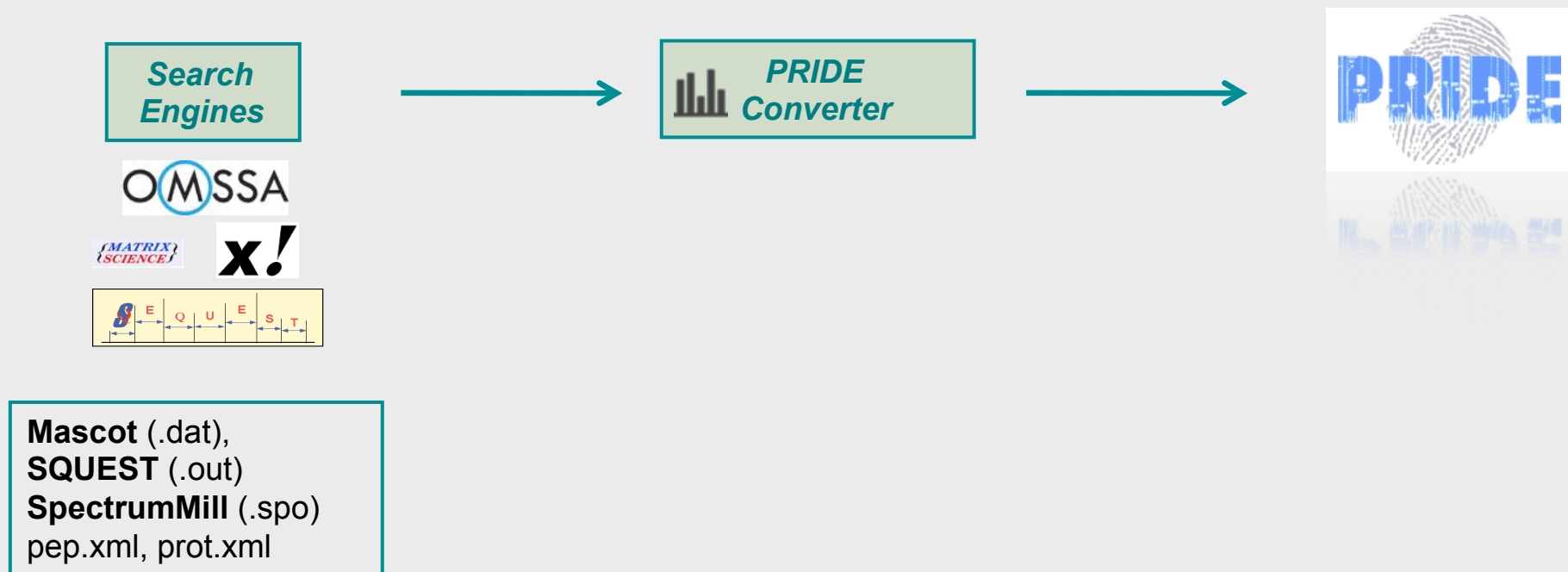
- Support for publications

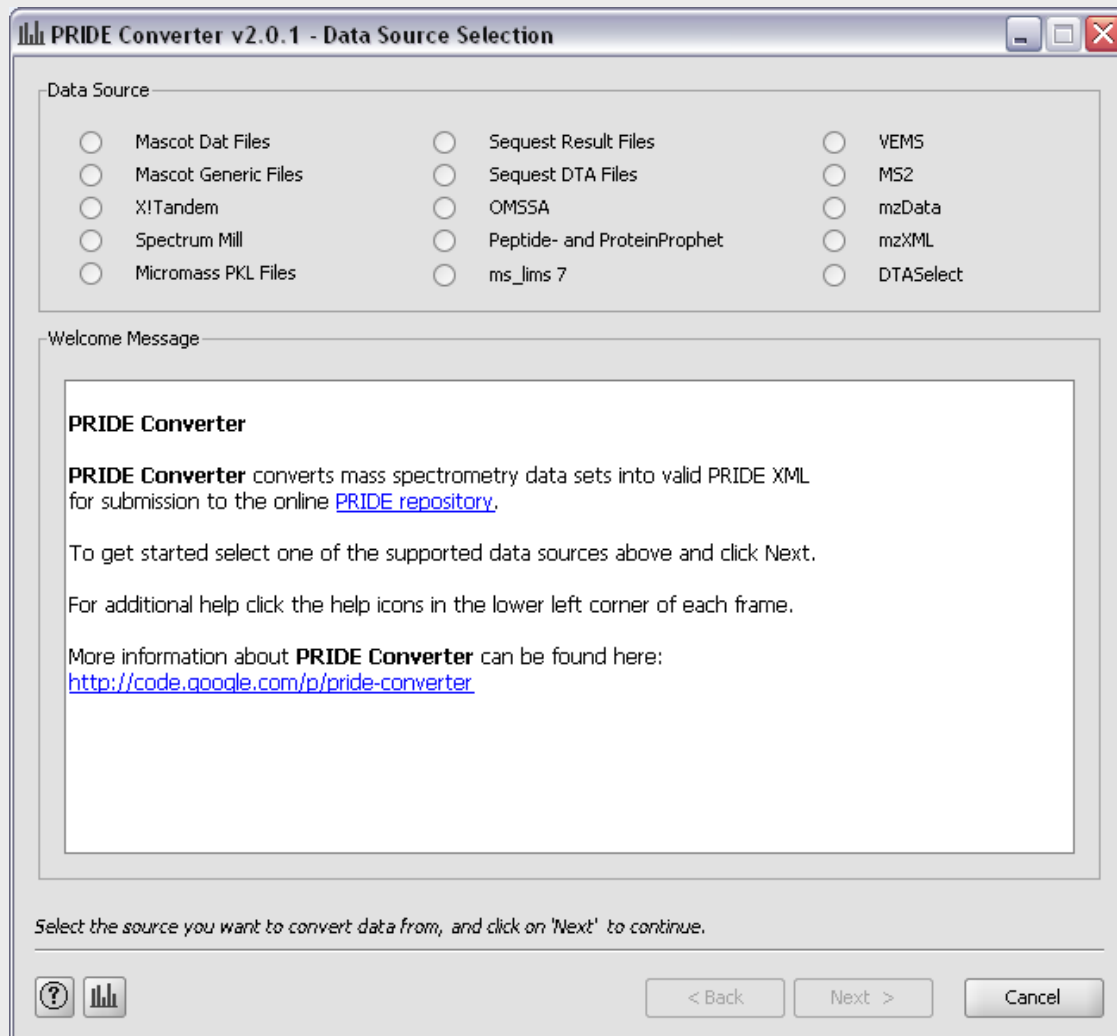- Reliable source of MS proteomics data for other resources

PRIDE Submission Workflow

Search Engines

PRIDE Converter

Mascot (.dat),
SQUEST (.out)
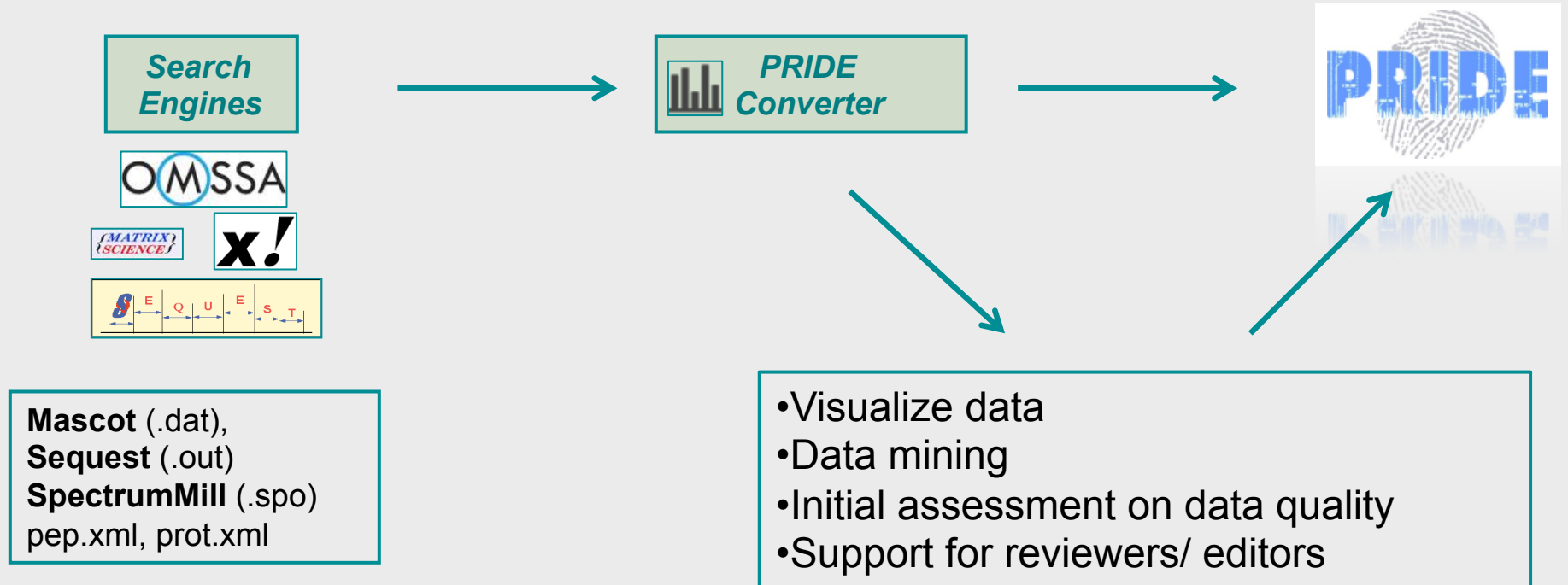**SpectrumMill** (.spo)
pep.xml, prot.xml

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PRIDE Converter

- Stand-alone tool for creating PRIDE XML files

- A variety of popular proteomics data formats

- Metadata using CVs/ Ontologies.

- GUI based tool, easy to use

- New version in development

http://code.google.com/p/pride-converter

PRIDE Repository: http://www.ebi.ac.uk

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The need for new tool

Search Engines

OMSSA

{MATRIX SCIENCE}   x!

SEQUEST

PRIDE Converter

PRIDE

Mascot (.dat),
Sequest (.out)
SpectrumMill (.spo)
pep.xml, prot.xml

- Visualize data
- Data mining
- Initial assessment on data quality
- Support for reviewers/ editors

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PRIDE Inspector

- Standard-alone tool
- 100% Java
- Open Source and Free

http://code.google.com/p/pride-toolsuite/

Java Web Start

Design

GUI Module

| Spectrum | Protein | Peptide | Charts |

Data Model Module

Service Module

Access Module

PRIDE XML | mzML | PRIDE DB

App Management

Task Management

Caching

Messaging

Property Management

Data Access Controller

Error Handling

PRIDE Inspector: http://code.google.com/p/pride-toolsuite

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Core Features

Fast loading of large *mzML* and *PRIDE XML* files.

Direct access to all PRIDE public database experiments.

Private experiment download facility.

PRIDE Inspector: http://code.google.com/p/pride-toolsuite

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Experiment Metadata View

27/09/2011   PRIDE Inspector: http://code.google.com/p/pride-toolsuite

Protein Centric View

PRIDE Inspector: http://code.google.com/p/pride-toolsuite

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Peptide Centric View

PRIDE Inspector: http://code.google.com/p/pride-toolsuite

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Spectrum Centric View

Summary Chart View

PRIDE Inspector: http://code.google.com/p/pride-toolsuite

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PRIDE Toolsuite

- PRIDE-Chart: Generating statistical chart

- PRIDE-mzGraph-Browser: Visualizing spectra or chromatogram

- PRIDE-JAXB: Reading PRIDE XML

- jmzML: Reading mzML

- XXIndex: Indexing large XML

PRIDE Inspector: http://code.google.com/p/pride-toolsuite

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Future Plan

- Better support for submitters and reviewers
  - Integration with PRIDE Converter
  - Quantitative data
  - Semantic validation
  - Summary report

- Better support for MS community
  - Additional formats: mzIdentML, MGF
  - Search PRIDE Database

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Search PRIDE

Additional Features

Acknowledgements

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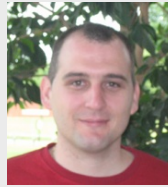
Florian Reisinger
Joe Foster
David Ovelleiro
Johannes Griss
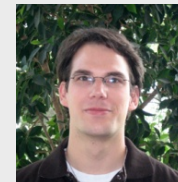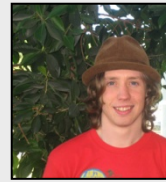
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Funding Sources
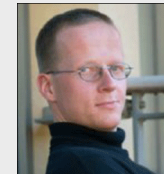
Funding

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Questions & Feedbacks

Contact us:

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