



ÚOCHB ^{AV}
IOCB PRAGUE

Proteomický ELIXIR

proteomická komunita v rámci ELIXIR CZ

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Neformální proteomické setkání 1.12.2017

ELIXIR - European infrastructure for biological information

Data infrastructure for Europe life-science research:



Data



Interoperability



Tools



Compute



Training



- 21 Members
- 1 Observer

www.elixir-europe.org

- ELIXIR Nodes build local bioinformatics capacity throughout Europe
- Over 140 institutes involved in ELIXIR Nodes

ELIXIR-CZ

RNDr. Jiří Vondrášek, Ph.D.
Head of the ELIXIR CZ Node



prof. RNDr. Jaroslav Koča, DrSc.
Chair of the ELIXIR CZ Board



Ing. Hana Pergl Šustková
Project Manager ELIXIR CZ



ELIXIR CZ Consortium

- Institute of Organic Chemistry and Biochemistry of the CAS – coordinating Institute
- CESNET, z.s.p.o.
- Masaryk University
- Charles University
- Palacky University
- Institute of Microbiology of the CAS
- Institute of Molecular Genetics of the CAS
- Institute of Biotechnology of the CAS
- Biology Centre of the CAS
- University Hospital of St. Anna in Brno
- University of Chemistry and Technology Prague
- University of South Bohemia
- University of West Bohemia
- Czech Technical University in Prague

The future of proteomics in ELIXIR

Strategic workshop

Tübingen, **1.-2. března 2017**

Oliver Kohlbacher, Juan Vizcaino – organizátoři

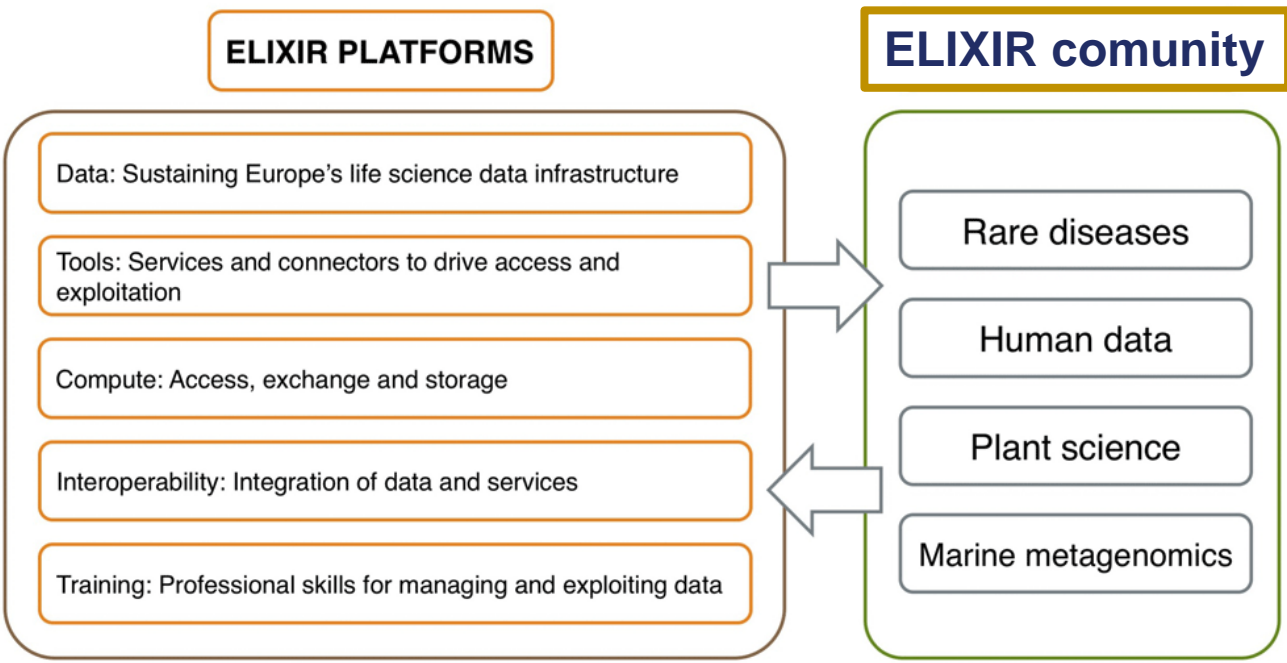
+ zástupci 11 EU států - české zastoupení – Jiří Vondrášek, Petr Novák, Martin Hubálek

Vysledek: white paper

A community proposal to integrate proteomics activities in ELIXIR

Vizcaíno JA, Walzer M, Jiménez RC et al. [A community proposal to integrate proteomics activities in ELIXIR](#) [version 1]. F1000Research 2017, 6:875

Stávající struktura



3 nové „Use cases“

Od září 2017

- Proteomics
- Metabolomics
- Galaxy

Proteomics

The Proteomics Use Case aims to align ELIXIR activities with the needs of scientists researching the expression and interactions of proteins. Merging sustainable proteomics resources into existing ELIXIR Platforms and Use Cases would help integrate proteomics data with multi-omics data, improve data processing and analysis pipelines and create guidelines for proteomics data management and annotation.

Možnosti využití ELIXIR CZ pro proteomickou práci

- výpočetní a archivační kapacita + nástroje

Instalované proteomické nástroje

- MASCOT
- GALAXY

- <https://galaxy-dev.metacentrum.cz/galaxy/>

OpenMS (cca 140 skriptů), OMSSA, Peptideshaker, etc.


možnost instalace dalších nástrojů nejlépe z


<https://toolshed.g2.bx.psu.edu>

Účet v MetaCentru může získat každý zaměstnanec či student akademické instituce v ČR

<https://metavo.metacentrum.cz/cs/application/index.html>

Galaxy – Analyze data

Tools 

search tools 

Statistics

Graph/Display Data

SAM

Utilities

OpenMS

[FuzzyDiff](#) Compares two files, tolerating numeric differences.

[MRMapper](#) MRMapper maps measured chromatograms (mzML) and the transitions used (TraML)

[ConsensusMapNormalizer](#) Normalizes maps of one consensusXML file

[OpenSwathChromatogramExtract](#) Extract chromatograms (XIC) from a MS2 map file.

[FileFilter](#) Extracts or manipulates portions of data from peak, feature or consensus-feature files.


[RTPredict](#) Predicts retention times for peptides using a model trained by RTModel.

[IDExtractor](#) Extracts 'n' peptides randomly or best 'n' from idXML files.





[IDScoreSwitcher](#) Switches between different scores of peptide or protein hits in identification data

[SpectraFilterBernNorm](#) Applies thresholdfilter to peak spectra.

[IDRipper](#) Split protein/peptide identification file into several files according to annotated file origin.

BaselineFilter Removes the baseline from profile spectra using a top-hat filter. (Galaxy Version 2.2.0) 

input raw data file

   4: 171111_Bgal1.mzml 

(-in)

Length of the structuring element (should be wider than maximal peak width - see documentation)

3.0

(--struc_elem_length)


Unit of 'struc_elem_length' paramete

Thomson

DataPoints


(--struc_elem_unit)

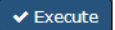
The name of the morphological filter to be applied

tophat 

(-method) If you are unsure, use the default


Advanced Options

Hide Advanced Options 



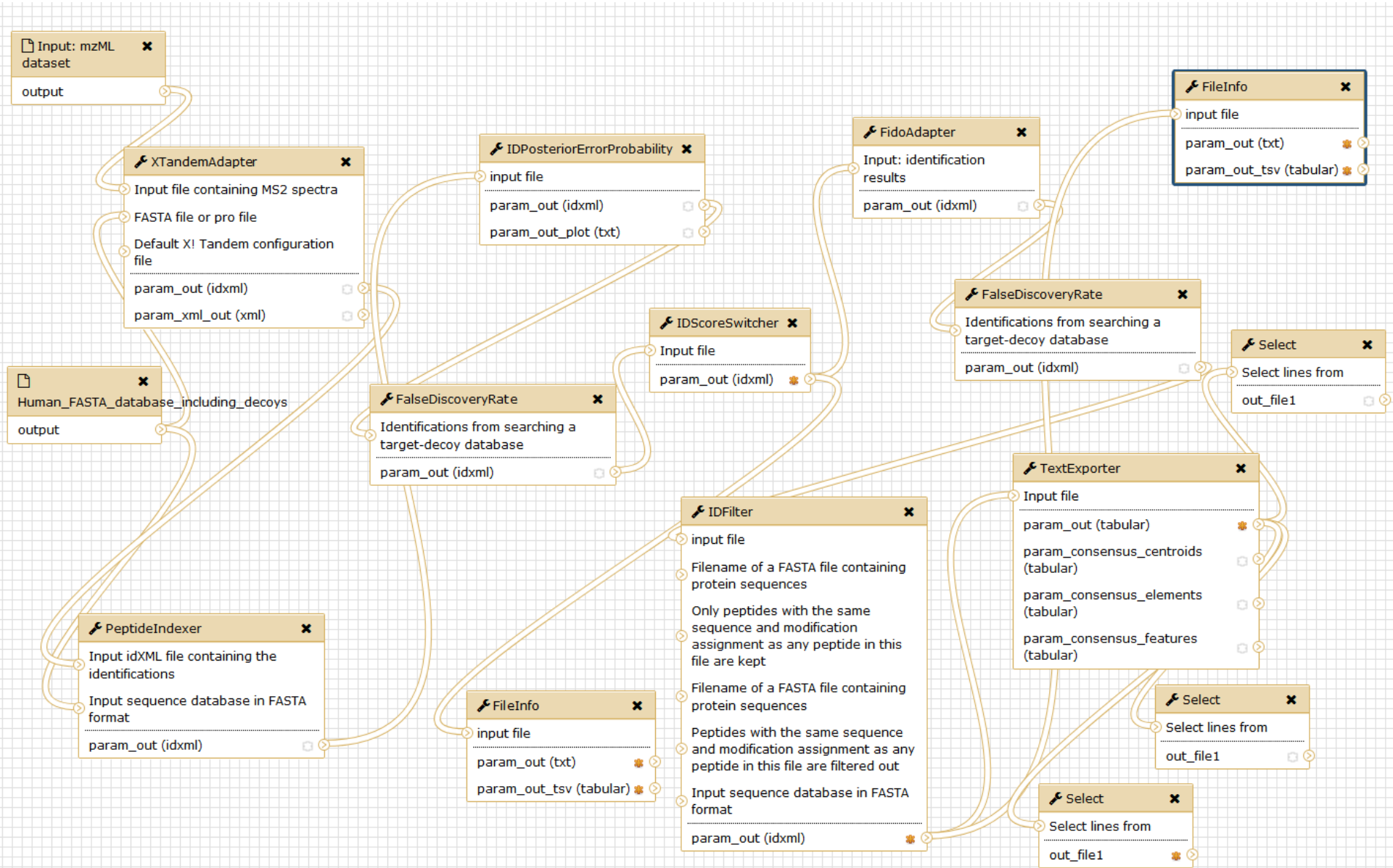
Removes the baseline from profile spectra using a top-hat filter.

For more information, visit http://ftp.mi.fu-berlin.de/OpenMS/release-documentation/html/TOPP_BaselineFilter.html

Citations 

Sturm, Marc and Bertsch, Andreas and Gröpl, Clemens and Hildebrandt, Andreas and Hussong, Rene and Lange, Eva and Pfeifer, Nico and Schu
OpenMS – An open-source software framework for mass spectrometry. In *BMC Bioinformatics*, 9 (1), pp. 163. [doi:10.1186/1471-2105-9-163][Li

Galaxy – workflow



Links

- <https://galaxyproject.github.io/training-material/topics/introduction/>
- <http://galaxyproject.github.io/training-material/topics/proteomics/>
- <https://github.com/galaxyproject/training-material>
- <https://toolshed.g2.bx.psu.edu/>
- <https://www.openms.de/>
- <http://ftp.mi.fu-berlin.de/pub/OpenMS/release-documentation/html/index.html>
- <https://compomics.com/>
- <https://compomics.github.io/>
- <https://compomics.com/bioinformatics-for-proteomics/>
- <https://bio.tools/?page=4&q=proteomics&sort=score>