UNIVERSITÉ
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Ecole de Pharmacie
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Conversion of mass spectrometry files:
open format & open source tools for MS

LC-MS et substances naturelles
06-05-2015

Pierre-Marie Allard
Université de Genève

Why convert ?

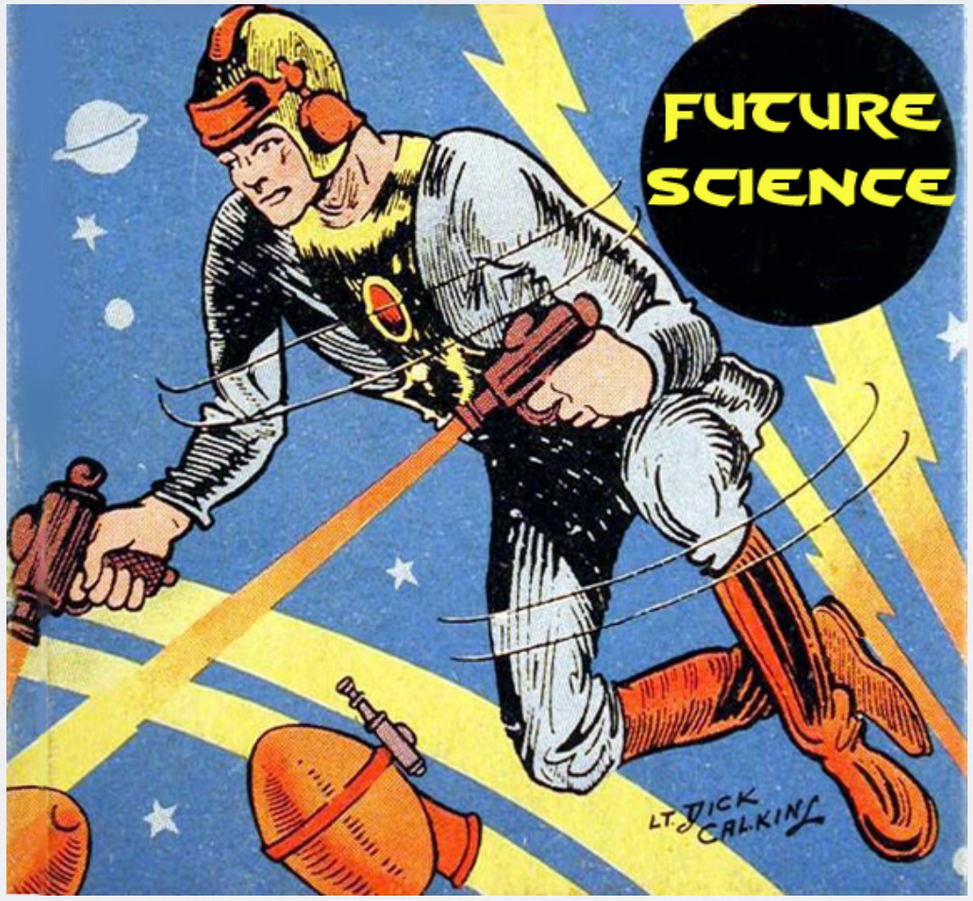
Why open-format ?

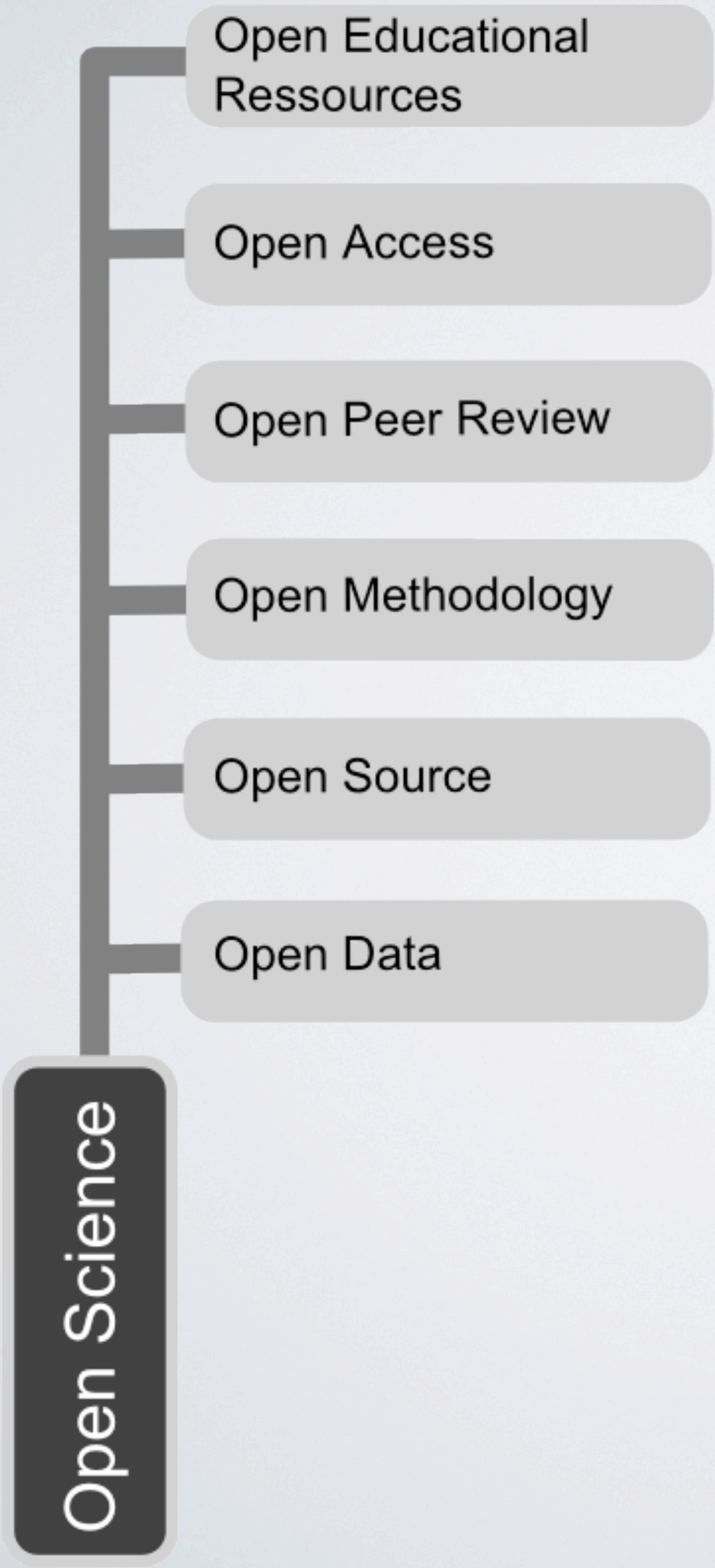
Why open-source ?

Why open-data ?

Because :

OPEN-SCIENCE
is the
FUTURE




Open Educational Ressources
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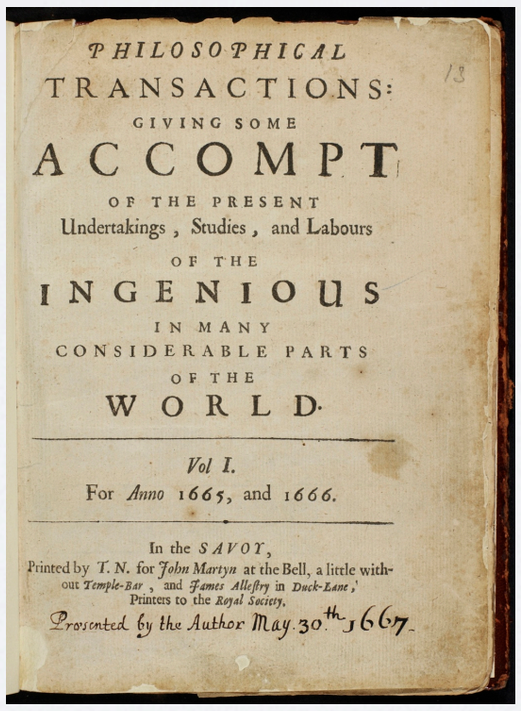
1665 1991 - 2001 - ...

Galileo, Isaac Newton
Kepler

Secret science


PHILOSOPHICAL
TRANSACTIONS:
GIVING SOME
ACCOMPT
OF THE PRESENT
Undertakings, Studies, and Labours
OF THE
INGENIOUS
IN MANY
CONSIDERABLE PARTS
OF THE
WORLD.
Vol I.
For Anno 1665, and 1666.
In the SAVOY,
Printed by T. N. for John Martyn at the Bell, a little without Temple-Bar, and James Allestry in Duck-Lane;
Printers to the Royal Society.
Presented by the Author May. 30th 1667.

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Living articles

RESEARCH ARTICLE

REVISED Sub-strains of *Drosophila* Canton-S differ markedly in their locomotor behavior [v2; ref status: indexed, http://f1000r.es/57i]

Julien Colomb[1], Björn Brembs[2]

Author affiliations

[1] Institute of Biology – Neurobiology, Freie Universität, Berlin, Germany
[2] Institute of Zoology – Neurogenetics, Universität Regensburg, Regensburg, Germany

Grant information: The author(s) declared that no grants were involved in supporting this work.

Abstract

We collected five sub-strains of the standard laboratory wild-type *Drosophila melanogaster* Canton Special (CS) and analyzed their walking behavior in Buridan's paradigm using the CeTrAn software. According to twelve different aspects of their behavior, the sub-strains fit into three groups. The group separation appeared not to be correlated with the origin of the stocks. We conclude that founder effects but not laboratory selection likely influenced the gene pool of the sub-strains. The flies' stripe fixation was the parameter that varied most. Our results suggest that differences in the genome of laboratory stocks can render comparisons between nominally identical wild-type stocks meaningless. A single source for control strains may settle this problem.

Corresponding author: Björn Brembs

How to cite: Colomb J and Brembs B. Sub-strains of *Drosophila* Canton-S differ markedly in their locomotor behavior [v2; ref status: indexed, http://f1000r.es/57i] *F1000Research* 2015, **3**:176 (doi: 10.12688/f1000research.4263.2)

Open Peer Review

Referee Status: ✓ ✓ ✓

	Invited Referees 1	2	3
REVISED version 2 published 21 avr. 2015			
version 1 published 30 juil. 2014	✓ report	✓ report	✓ report

1 **Gregg Roman**, University of Houston, USA
2 **Josh Dubnau**, Cold Spring Harbor Laboratory, USA
3 **Hiromu Tanimoto**, Tohoku University, Japan
Vladimiros Thoma, Tohoku University, Japan

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J. Colomb and B. Brembs F1000Research 3, 176; 2014

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Version 1

Referee Report 02 sept. 2014

Hiromu Tanimoto, Graduate School of Life Sciences, Tohoku University, Japan
Vladimiros Thoma, Graduate School of Life Sciences, Tohoku University, Japan

Views 59 Cite

✓ **Approved**

Colomb and Brembs reported an important piece of information that highlights large differences in the walking trajectory of six substrains of a wild-type *Drosophila* strain (Canton S) in the so-called Bridan paradigm. Drawing conclusions from behavioral comparisons of strains could ... *Continue reading*

Respond or Comment

Referee Report 15 août 2014

Josh Dubnau, Cold Spring Harbor Laboratory, USA

Views 76 Cite

✓ **Approved**

This is an interesting manuscript that I hope will be read widely. In this field, we give a lot of lip service to controlling genetic background because we all know it is important. But often, "wild type" lines such as ... *Continue reading*

Respond or Comment

J. Colomb and B. Brembs F1000Research 3, 176; 2014

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Current Referee Status: ✓ ✓ ✓

Version 1

Referee Report 02 sept. 2014

Hiromu Tanimoto, Graduate School of Life Sciences, Tohoku University, Japan
Vladimiros Thoma, Graduate School of Life Sciences, Tohoku University, Japan

✓ **Approved**

Colomb and Brembs reported an important piece of information that highlights large differences in the walking trajectory of six substrains of a wild-type *Drosophila* strain (Canton S) in the so-called Bridan paradigm. Drawing conclusions from behavioral comparisons of strains could therefore be moot, if the tested strains do not share the same genetic background (at least for the Buridan paradigm).

This report is presented in a clear and succinct way. In addition, the authors invite submission of data by other labs, and the addition of these new data will be plotted in Fig. 4. This is an interesting endeavor which nicely uses the function of this journal. One has yet to keep in mind that fly behavior can be dramatically affected by 'unwritten' lab conditions (e.g. fly food, rearing conditions), and therefore the new data from other labs might not be comparable to the current dataset. One suggestion for the contributing labs to circumvent this caveat is to use one (or more) of the strains analyzed in this study and to check the reproducibility.

In addition, I have a few minor comments that may be addressed:

1. The authors argue that the basis of the behavioral variability is differences in the genetic background, but other reasons (e.g. epigenetic differences) can conceivably contribute to the variability as well.

2. The authors state that there was a significant effect of the replicate on Principal Component 2 (page 3, left column, third line from bottom), but later state that "(…) sub-strain differences were comparable in the two replicates conducted one year apart" (page 5, left column, line 5 from top). Either of the statements should be amended.

3. "A" in "PCA" stands for analysis. Use "PCA" instead of "PCA analysis". My understanding of PCA is "Principal Component Analysis" rather than "Principle Component Analysis" the authors use in the paper. Use PC1, PC2, PC3 in the axes of Fig.2 and Fig. 4.

We have read this submission. We believe that we have an appropriate level of expertise to confirm that it is of an acceptable scientific standard.

Competing Interests: No competing interests were disclosed. *Close*

J. Colomb and B. Brembs F1000Research 3, 176; 2014

Living figures

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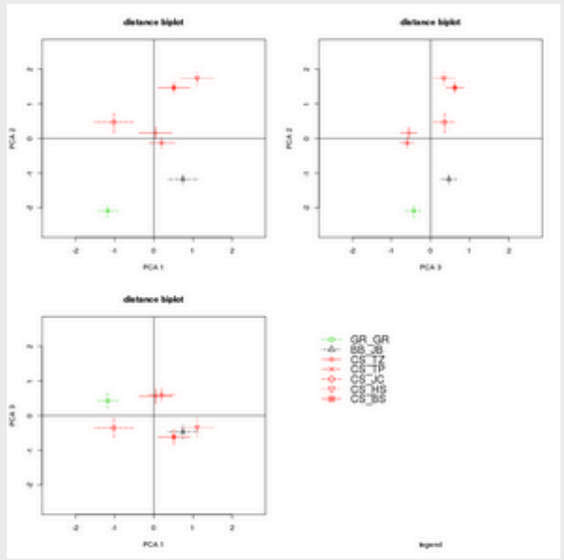

Figure 4. Updating principal component analysis of Canton S strains.

Results from the PCA obtained using the same analysis as for Figure 2, but with data uploaded from different laboratories. The version of this figure on the *F1000Research* site is 'living'; it will automatically re-plot as and when new data for other Canton S strains are submitted, and users can visualize previous versions of this figure. The conclusions of this article only relate to the data available at the time of publication. The prefixes in the key are the initials of the data contributor (except CS_ strains, which were tested by Julien Colomb); full names and affiliations can be found in the figure legend of the article on the *F1000Research* site. The suffixes denote the initials of the principal investigators from where each sub-strain was sourced. The BB_JB (Jose Botella) strain was ordered from the Bloomington stock center (stock #1) approx. seven years ago. BB_JB falls within the range of variability seen so

...

GR_GR: Added on 22 avr. 2015 by Gregg Roman, Stefani Garcia and Miguel de la Flor at Department of Biology and Biochemistry, University of Houston, TX, USA. DOI: 10.5256/f1000research.4263.d46290 | Download data | Cite data
BB_JB: Added on 21 avr. 2015 by Björn Brembs at Institute of Zoology – Neurogenetics, Universität Regensburg, Germany. DOI: 10.5256/f1000research.4263.d46234 | Download data | Cite data
CS_TZ: Added on 30 juil. 2014 by Julien Colomb at Institute of Biology – Neurobiology, Freie Universität, Berlin, Germany. DOI: 10.5256/f1000research.4263.d46232 | Download data | Cite data
CS_TP: Added on 30 juil. 2014 by Julien Colomb at Institute of Biology – Neurobiology, Freie Universität, Berlin, Germany. DOI: 10.5256/f1000research.4263.d46231 | Download data | Cite data
CS_JC: Added on 30 juil. 2014 by Julien Colomb at Institute of Biology – Neurobiology, Freie Universität, Berlin, Germany. DOI: 10.5256/f1000research.4263.d46230 | Download data | Cite data
CS_HS: Added on 30 juil. 2014 by Julien Colomb at Institute of Biology – Neurobiology, Freie Universität, Berlin, Germany. DOI: 10.5256/f1000research.4263.d46229 | Download data | Cite data

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J. Colomb and B. Brembs F1000Research 3, 176; 2014

Open projects

Nature **431**, 931-945 (21 October 2004) | doi:10.1038/nature03001; Received 29 July 2004; Accepted 7 September 2004

Finishing the euchromatic sequence of the human genome

International Human Genome Sequencing Consortium

1. A list of authors and their affiliations appears in the Supplementary Information

Correspondence to: Correspondence and requests for materials should be addressed to F .S. Collins (Email: fc23a@nih.gov), E. S. Lander (Email: lander@broad.mit.edu), J. Rogers (Email: jrh@sanger.ac.uk) or R. H. Waterston (Email: waterston@gs.washington.edu).
The sequence described here has been deposited in public databases, with the 24 human chromosomes having accession numbers NC000001 to NC000024.

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The vision of OSDD: Open Source Drug Discovery aims to provide affordable healthcare for neglected diseases.
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The motto of OSDD is "affordable health care for all".

OPEN SOURCE MALARIA

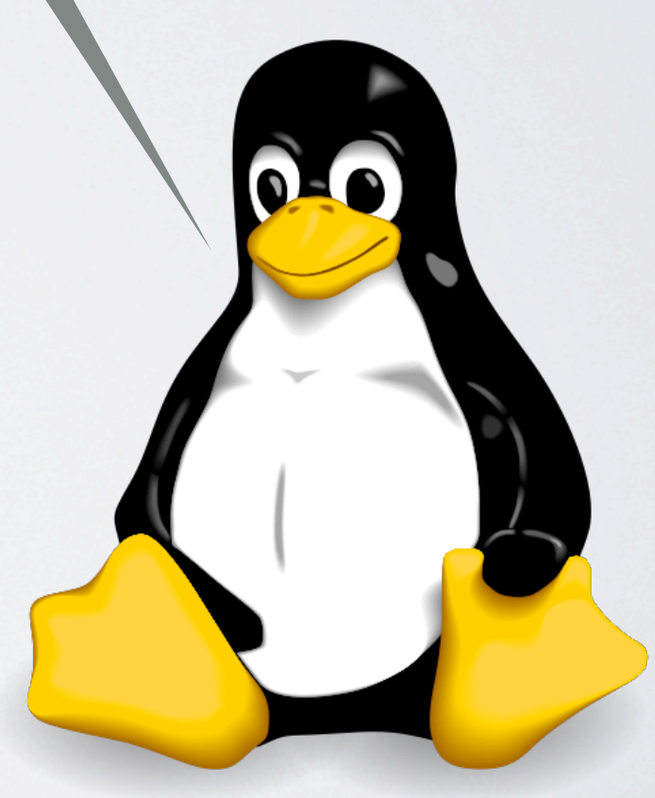
Looking for New Medicines

2011, Todd's lab, University of Sydney

«Thus the iterative cycle of analog synthesis in response to biological data that is normally guided by luck and medchem intuition is now guided by the intuition of the collective.»

Linus's law

« Given enough eyeballs, all bugs are shallow. »



OPEN SOURCE MALARIA

Looking for New Medicines

Join The Team

Open research is where anyone can take part at any level of the project, that all data and ideas are shared and there are no patents. **You are welcome, whatever your expertise.**

At the moment the main focus is on finding a new medicine by improving some molecules originally discovered by Big Pharma and put into the public domain, something called open source drug discovery. Much of what we need is based in science (chemistry and biology), but there are important things you can do if you're outside those fields.

You just have to adhere to the Six Laws:

First Law: All data are open and all ideas are shared
Second Law: Anyone can take part at any level of the project
Third Law: There will be no patents
Fourth Law: Suggestions are the best form of criticism
Fifth Law: Public discussion is much more valuable than private email
Sixth Law: The project is bigger than, and is not owned by, any given lab.

The default licence for everything in the OSM project is CC-BY, meaning you can use whatever you want for any reason (including to make money) provided you cite the project.

How to get involved:

If you like the sound of open research and curing malaria, then join in! Here's how:

- Check out the current To Do List for details of what's needed right now - help resolve an issue, comment on things that you think need to be done, or post any of your suggestions/ideas.
- Follow the G+, Twitter and Facebook pages.
- Read up on where we are and what we've published on the Wiki and sign up if you want to make changes.
- Check out the fresh chemical and biological data in the Lab Notebooks.
- Watch the regular Online Meetings and maybe come along to the next one.
- If you're a chemist, make a molecule that the project needs so that it can be screened for activity.

OPEN SOURCE MALARIA

Looking for New Medicines

First Law: All data are open and all ideas are shared
Second Law: Anyone can take part at any level of the project
Third Law: There will be no patents
Fourth Law: Suggestions are the best form of criticism
Fifth Law: Public discussion is much more valuable than private email
Sixth Law: The project is bigger than, and is not owned by, any given lab.

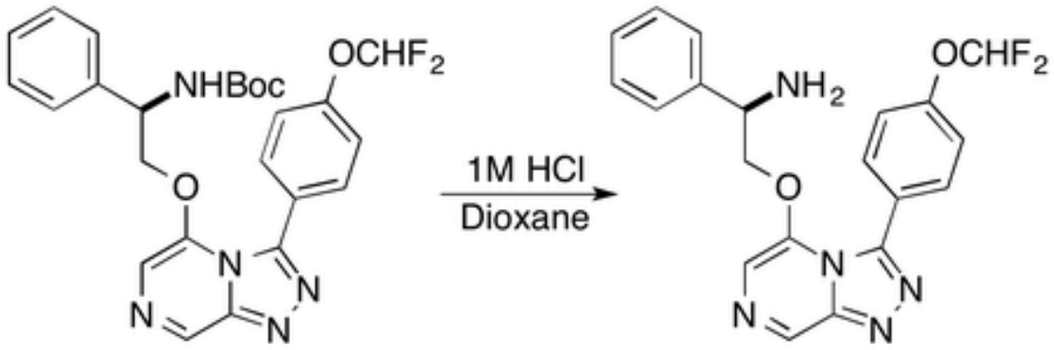
Triazolopyrazine Series

Synthesis of the triazolopyrazine series

Older Entries >>

Synthesis of (R)-2-((3-(4-(difluoromethoxy)phenyl)-[1,2,4]triazolo[4,3-a]pyrazin-5-yl)oxy)-1-phenylethan-1-amine (AEW 231-1)

30th April 2015 @ 04:49



Procedure:

Crude AEW 229-1 (~0.34 mmol) was dissolved in dioxane (1 mL) and then HCl (1 mL, 1 M aqueous solution) was added and the reaction mixture stirred at room temperature for

Strings:

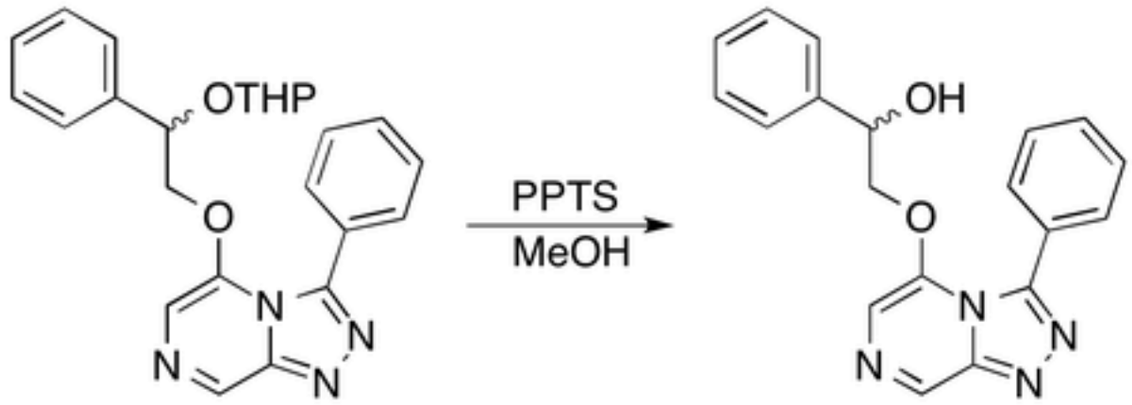
InChI=1S/C25H25F2N5O4
/c1-25(2,3)36-24(33)29-19(16-7-5-4-6-8-16)15-34-21-14-28-13-20-30-31-22(32(20)21)17-
/h4-14,19,23H,15H2,1-3H3,(H,29,33)

to

Synthesis of 1-phenyl-2-((3-phenyl-[1,2,4]triazolo[4,3-a]pyrazin-5-yl)oxy)ethan-1-ol (AEW 230-1)

30th April 2015 @ 04:23

Started 9.30 am posted 13.25 due to lack of internet connectivity.



Procedure:

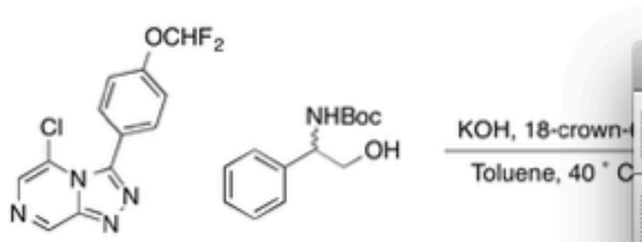
Crude AEW 128-1 (~0.43 mmol, 1 equiv.) was dissolved in MeOH (1.5 mL) and PPTS (11 mg, 0.043 mmol, 0.1 equiv.) was added and the reaction mixture stirred at room temperature for ten minutes.

Disaster: clamp broke and the flask fell into oil bath.

Rescue: Tried to extract into DCM (20 mL), didn't work so shook with HCl (1 M, 10 mL) for ten minutes in separating funnel then washed organic layer with water (10 mL), brine (5 mL) and dried ($MgSO_4$), filtered and evaporated to give a brown oily product surrounded with silca oil. Carefully pipetted of majority of oil and then resubmitted to the same reaction conditions and stirred for 2 hours.

Synthesis of 3-(4-(difluoromethoxy)phenyl)-5-(2-phenyl-2-((tetrahydro-2H-pyran-2-yl)oxy)ethoxy)-[1,2,4]triazolo[4,3-a]pyrazine (AEW 229-1)

29th April 2015 @ 09:34



Procedure:

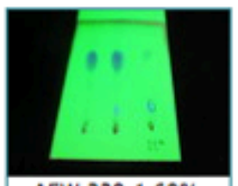
SM (100 mg, 0.34 mmol, 1 equiv) was added to toluene (2 r
mmol, 1 equiv), potassium hydroxide (67 mg, 1.18 mmol,
mmol, 0.07 equiv). The reaction was stirred at room temp
mixture) and then heated to 40°C (bath temperature) fo
minutes still SM - stirred for a further 30 minutes. Reaction

The sample was cooled to room temperature and diluted
extracted with EtOAc (3 x 10 mL). Fluorescent yellow solu
washed with water (1 x 4 mL) until the aqueous layer becar
dried over Na_2SO_4. The orange/yellow fluoro solution v
pressure and in vacuo to yield a black/green oil that was dri

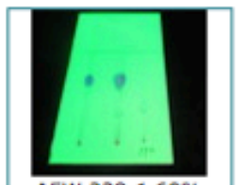
Crude NMR looks promising. Subjected crude directly to dep

Data:

TLC 60% EtOAc in Hex, 30 then 60 mins



AEW 229-1 60% EtOAc in Hex 30 mins.JPG

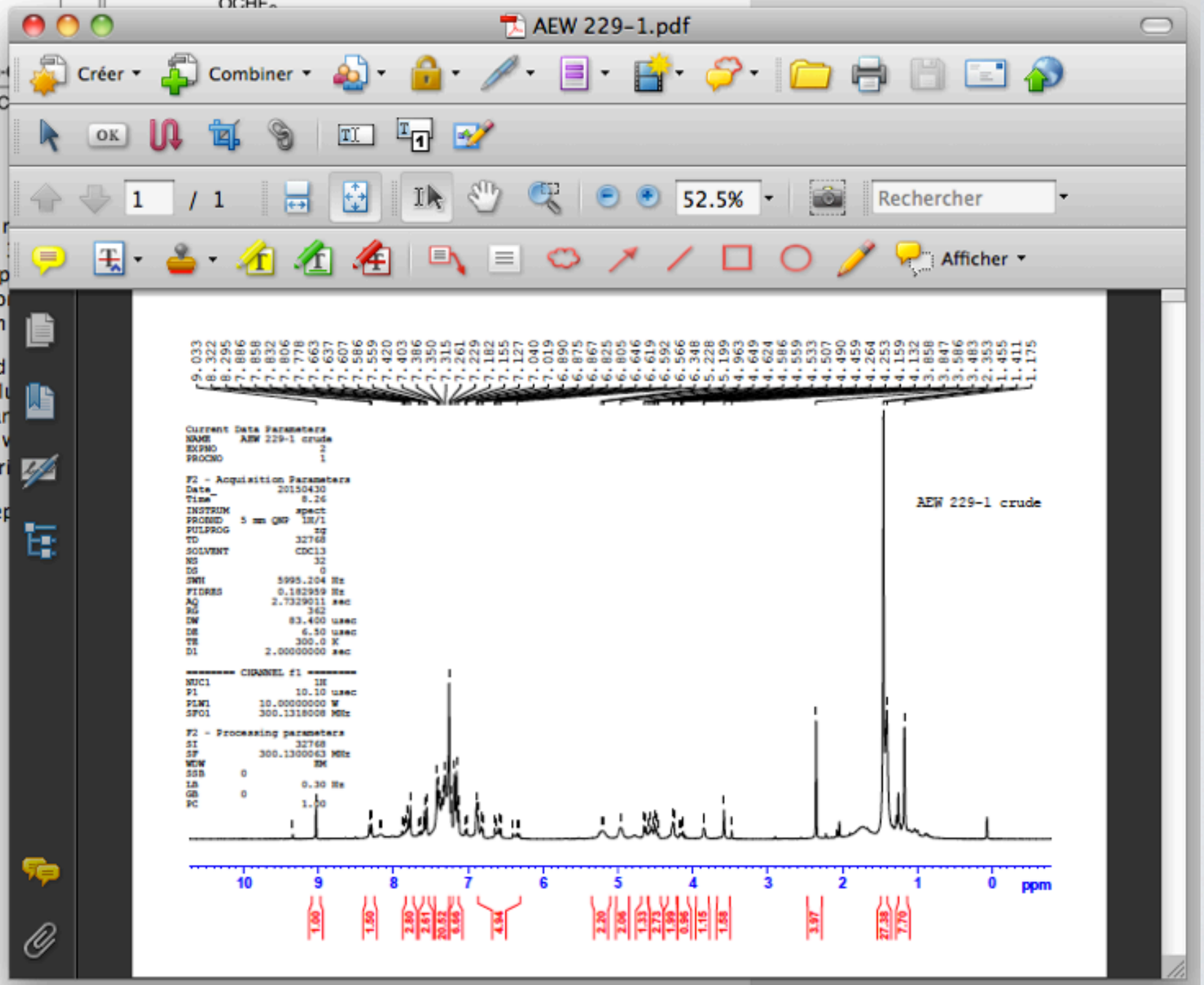


AEW 229-1 60% EtOAc in Hex 1 h.JPG

Crude NMR 300 MHz

AEW 229-1.pdf

AEW 229-1 crude.zip



Evaluation of Latest Series 4 Analogs in Ether and Amide Series

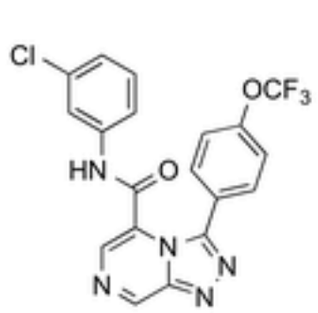
17th November 2014 @ 17:48

A set of 12 compounds were sent to Syngene for evaluation against blood stage asexual NF54 strain of Plasmodium falciparum.

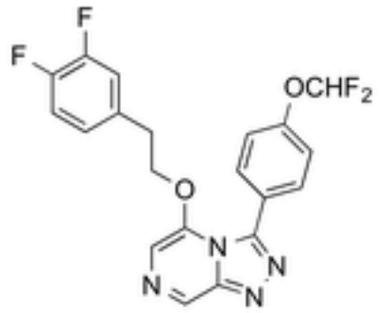
Samples sent for in vitro efficacy evaluation against Plasmodium falciparum asexual blood stage

Data were received (via the ScienceCloud portal at MMV) on October 10th. Data for one compound was missing, and subsequently received on Oct 23rd. Data:

Potency *vs.* Pfal NF54 (μM)



0.234
OSM-S-271
MMV675963
CLogP: 5.15



0.281
OSM-S-260
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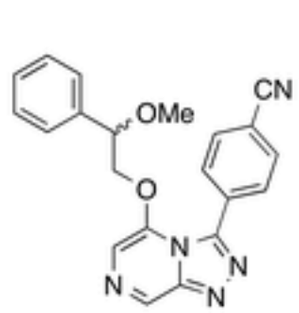
CLogP: 4.87



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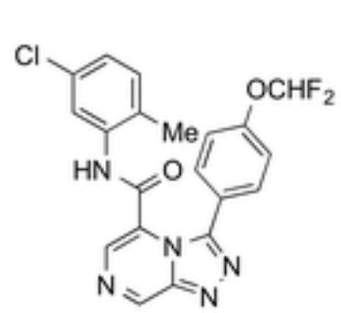
CLogP: 3.04



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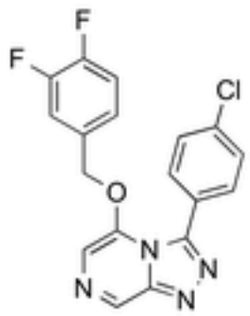
CLogP: 4.33



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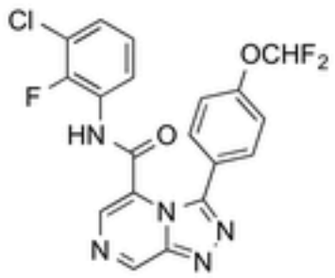
CLogP: 4.76



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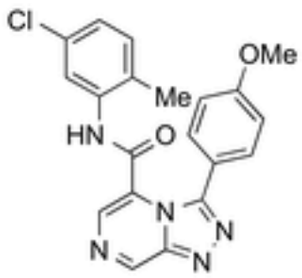

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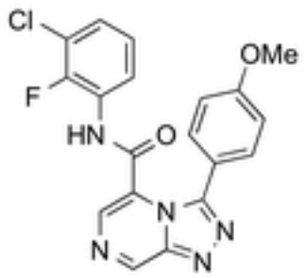

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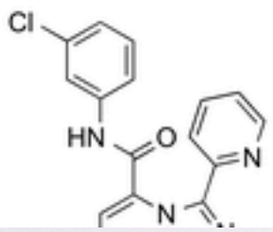
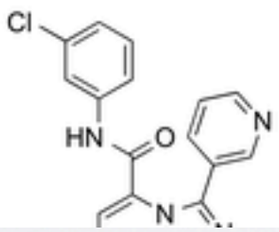
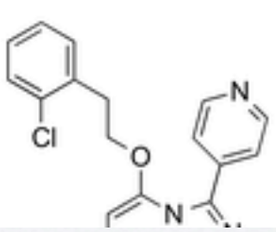
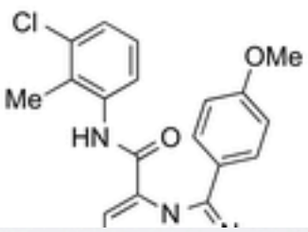
CLogP: 3.58









OSDDMalaria

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Toutes les activités

OSDDMalaria a mis en ligne une vidéo. il y a 1 mois

Open Source Malaria Intro Video
de OSDDMalaria
il y a 1 mois • 31 vues
Background to the Open Source Malaria consortium, featuring several of the contributors. If you like the idea, please vote for us in the Thinkable Open Innovation competition! …

OSDDMalaria a mis en ligne une ou plusieurs vidéos • a publié un bulletin • a ajouté une vidéo à Is Open Source Drug Discovery Practical?
il y a 9 mois

Is Open Source Drug Discovery Practical? (4/4)

Is Open Source Drug Discovery Practical? (4/4)
de OSDDMalaria
il y a 9 mois • 33 vues
"Is Open Source Drug Discovery Practical?"
WHO/TDR HQ, Geneva, September 19th, 2013 …

OSDDMalaria a mis en ligne une ou plusieurs vidéos • a publié un bulletin • a ajouté une vidéo à Is Open Source Drug Discovery Practical?

OpenSourceMalaria / OSM_To_Do_List

Watch 32 | Star 11 | Fork 4

Issues | Pull requests | Labels | Milestones

is:issue is:open

New issue

109 Open ✓ 186 Closed

Author | Labels | Milestones | Assignee | Sort

ELN Housekeeping for synthesis of J11-1 1
#295 opened 2 days ago by ConorGraham

Sydney Grammar Page for SGS 4-1 1
#294 opened 2 days ago by ConorGraham

Diagram Describing Open Science/OSM Workflow Collaboration Request Non-Science PR 2
#293 opened 11 days ago by mattodd

Should we buy a molecule from a CRO? question Search/Data Needed Series 4 Synthetic Chemistry Needed 4
#292 opened 16 days ago by mattodd

Consider Topliss Decision Tree for Series 4 Christmas Top 10 Compound List question Series 4 0
#291 opened 17 days ago by mattodd

Series 4 Wiki Strings Initial Housekeeping Administration Series 4 27
#290 opened on 1 Apr by mattodd

Primary Google indexing of OSM structures via InChIKey 4
#289 opened on 27 Mar by cdsouthan

Collection of Previous Work Towards Series 4 Pharmacophore Model --> ELN Search/Data Needed Series 4 4
#287 opened on 25 Mar by mattodd

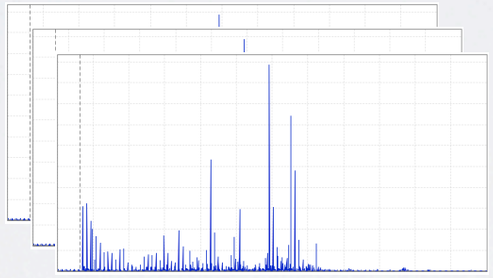
How do we search, store, index, annotate molecules? Administration High Priority question 68
#285 opened on 23 Mar by drc007

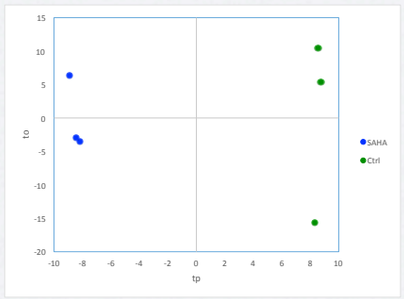
Votes Needed for Thinkable Open Innovation Competition Collaboration Request Non-Science PR 0
#284 opened on 3 Mar by mattodd

(S)-3-(4-(difluoromethoxy)phenyl)-5-(2-methoxy-2-phenylethoxy)-[1,2,4]triazolo[4,3-a]pyrazine 2
Being Synthesised Now Series 4 Synthetic Chemistry Needed
#278 opened on 15 Jan by alintheopen


KEEP
CALM
AND
USE
OPEN SOURCE

Open-source in MS





Open-source in MS

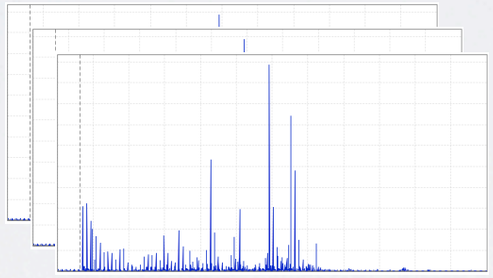
Thermo SCIENTIFIC

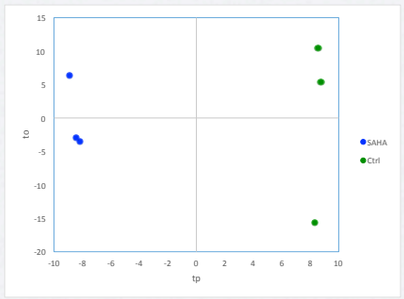
BRUKER

AB SCIEX

Agilent Technologies

? ? ?





Open-source in MS

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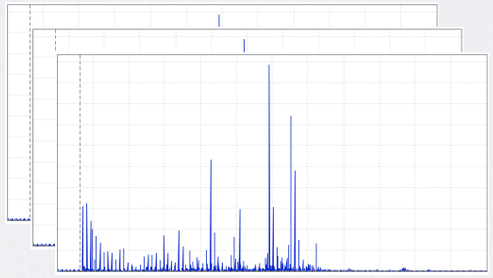
? ? ?

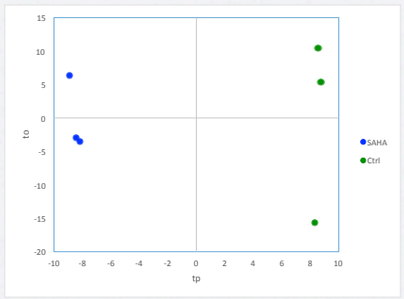
binary, vendor-controlled

.wiff .d .RAW .raw

text or XML based

.mgf .mzXML .netCDF





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? ? ?

binary, vendor-controlled

.wiff .d .RAW .raw

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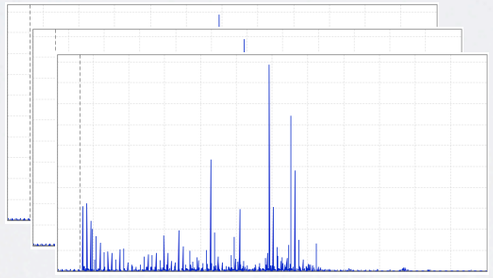
.mgf .mzXML .netCDF

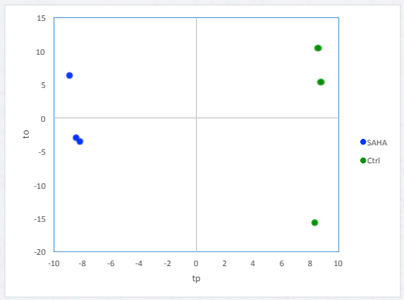


Analyst®

Xcalibur™

Masslynx™

MassHunter®



XCMS

OpenMS

MzMine

Open-source in MS

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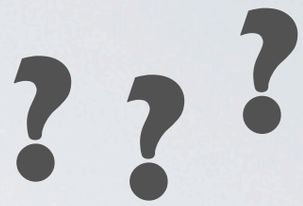

.wiff .d .RAW .raw

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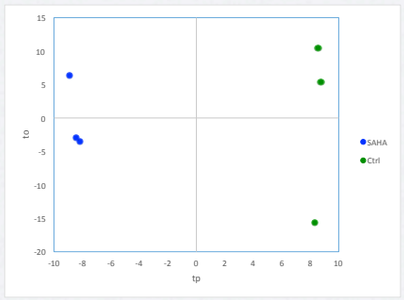
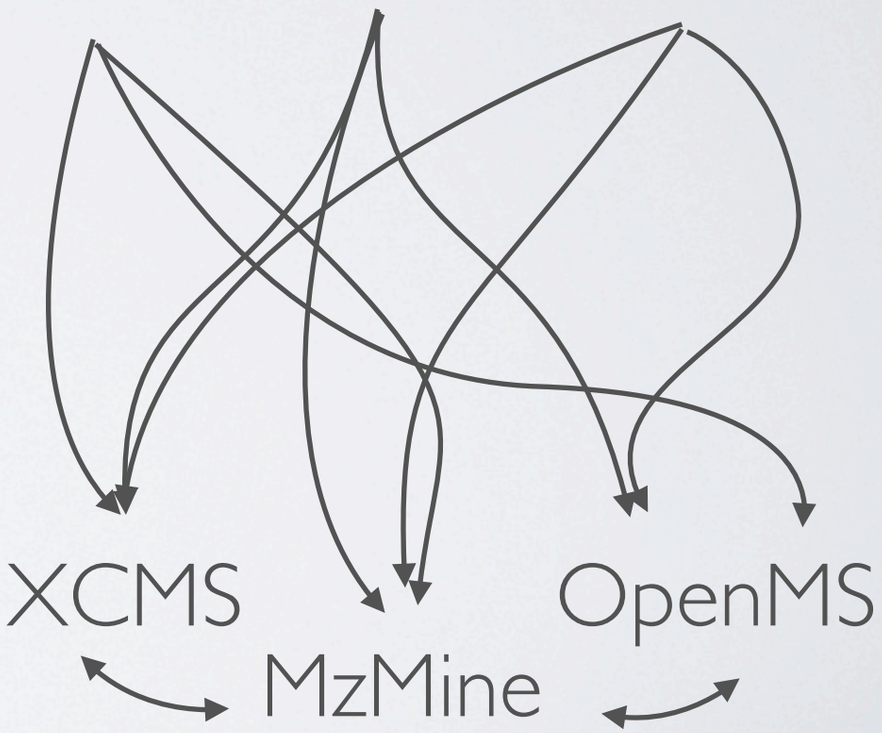


.mgf .mzXML .netCDF



XCMS MzMine OpenMS

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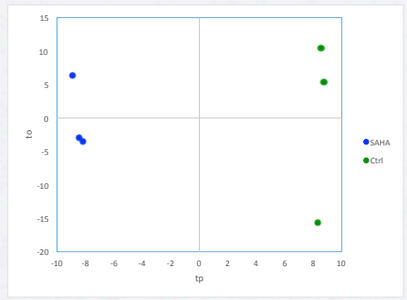

.mgf .mzXML .netCDF

XCMS

MzMine

OpenMS

Open-source in MS

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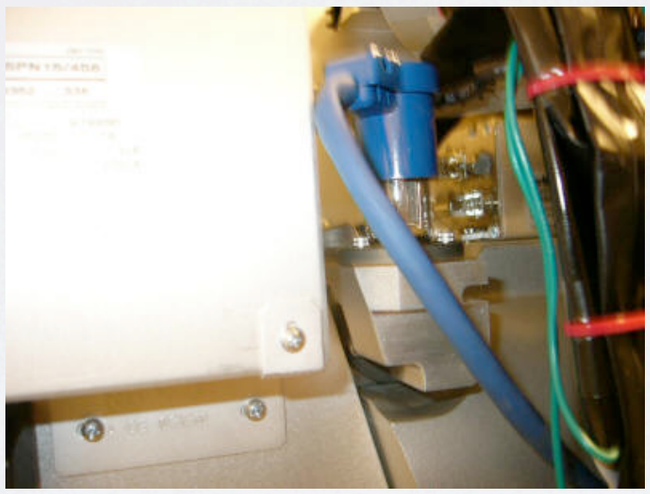
? ? ?

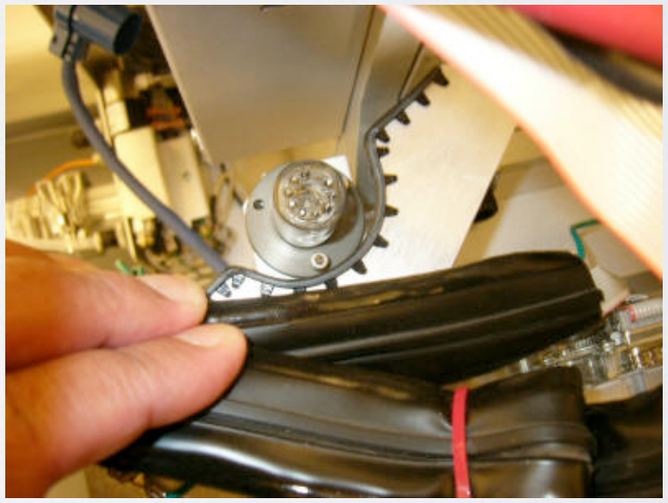
"How I Fixed That" at IonSource

return to DIY index | return to IonSource

Changing the Ion Gauge on a Quantum Triple Quadrupole Mass Spectrometer

Thermo-Scientific ion-gauge part# 00105-01525 cost approximately $500.00.
Necessary equipment: 4mm hex-wrench





http://www.ionsource.com/howifixedthat/

Open-source in MS

.wiff .d .RAW .raw

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MassHunter®

Xcalibur™

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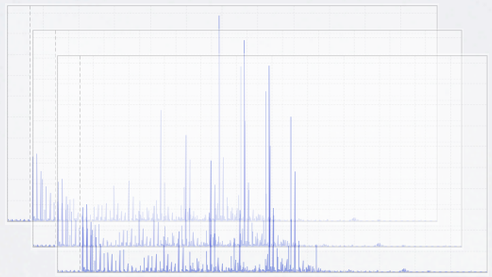
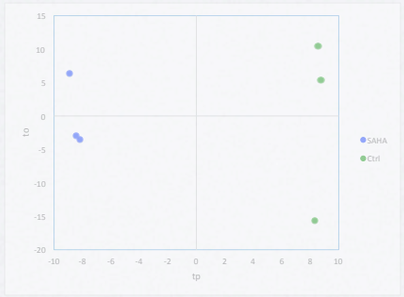




.mgf .mzXML .netCDF

XCMS

MzMine

OpenMS

Tool of the trade

http://proteowizard.sourceforge.net/

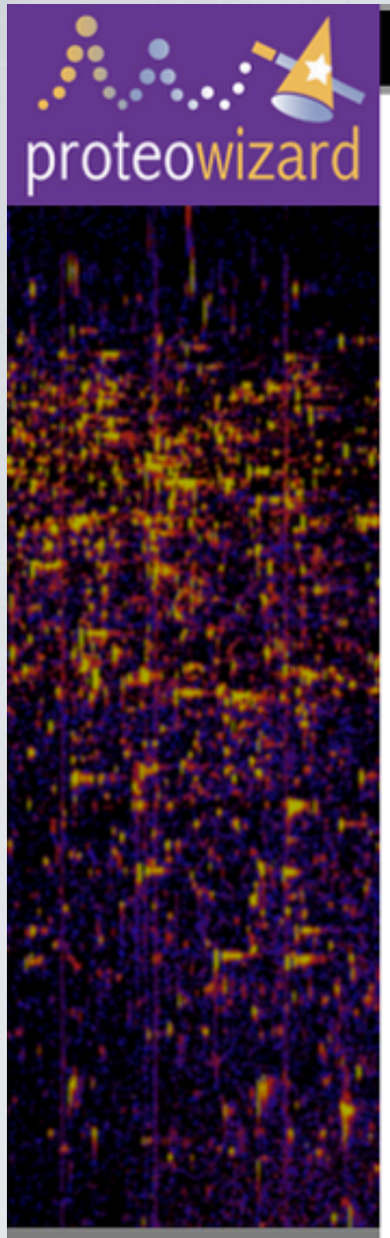
msconvert
- command line tool
-GUI

A cross-platform toolkit for mass spectrometry and proteomics

Matthew C Chambers, Brendan Maclean, Robert Burke, Dario Amodei, Daniel L Ruderman, Steffen Neumann, Laurent Gatto, Bernd Fischer, Brian Pratt, Jarrett Egertson, Katherine Hoff, Darren Kessner, Natalie Tasman, Nicholas Shulman, Barbara Frewen, Tahmina A Baker, Mi-Youn Brusniak, Christopher Paulse, David Creasy, Lisa Flashner, Kian Kani, Chris Moulding, Sean L Seymour, Lydia M Nuwaysir, Brent Lefebvre + ***et al.***

Affiliations | **Corresponding author**

Nature Biotechnology **30**, 918–920 (2012) | doi:10.1038/nbt.2377
Published online 10 October 2012



proteowizard

info download user docs dev docs contact

ProteoWizard Downloads

Get ProteoWizard (3 steps)

Step 1, Choose Download Type:

Please note that reading and conversion of vendor formatted files only works on Windows (or Windows Emulation). All other functionality of ProteoWizard is fully platform independent.

Windows 64-bit installer(able to convert vendor files except T2D)

Step 2, Read License Agreements

Pwiz Core | AB Sciex WiffReader | Agilent MHDAC | Bruker CompassXtract | Shimadzu SFCS | Thermo msFileReader | Waters WRDAC

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Agilent Mass Hunter Data Access Component Library
Bruker CompassXtract
Shimadzu SFCS
Thermo-Scientific MSFileReader Library
Waters Raw Data Access Component Library

Step 3, Click below to agree to Licenses and get ProteoWizard

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Notes:

Please cite us in your publications:

A cross-platform toolkit for mass spectrometry and proteomics. Chambers, M.C., MacLean, B., ... Mallick, P. Nature Biotechnology 30, 918-920 (2012). [article]

Step 2, Read License Agreements

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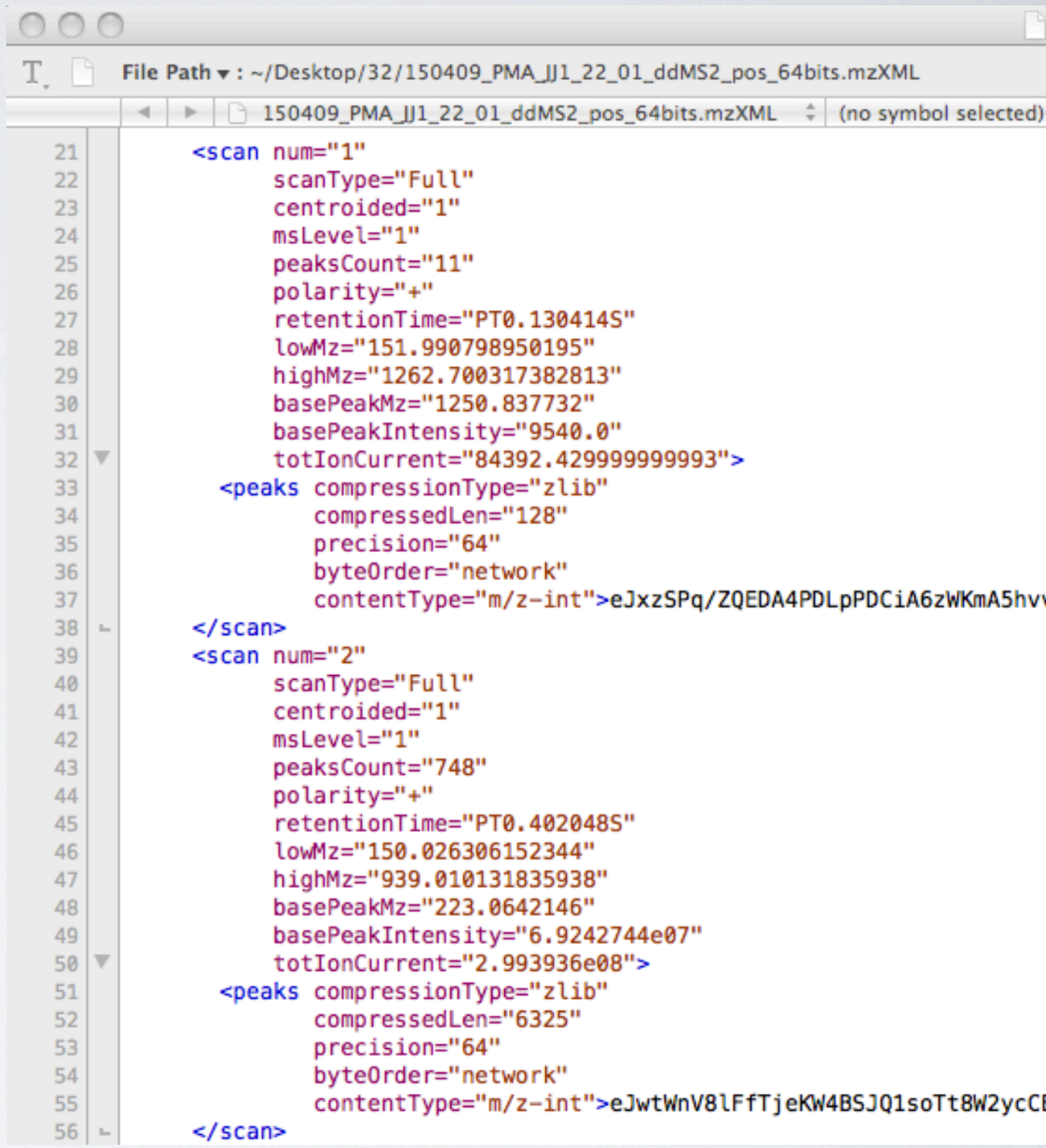
binary


File Path : /Volumes/PMA_Data/RAW_PMA/Epigen_Mod_201...S1_YS2/neg/raw/150203_PMA_JJ1_4_01_neg.raw
150203_PMA_JJ1_4_01_neg.raw

XML


File Path : ~/Desktop/32/150409_PMA_JJ1_22_01_ddMS2_pos_64bits.mzXML
150409_PMA_JJ1_22_01_ddMS2_pos_64bits.mzXML
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ProteoWizard Downloads

Get ProteoWizard (3 steps)

Step 1, Choose Download Type:

Please note that reading and conversion of vendor formatted files only works on Windows (or Windows Emulation). All other functionality of ProteoWizard is fully platform independent.

Windows 64-bit installer(able to convert vendor files except T2D)

For End Users

Step

- Windows 64-bit installer(able to convert vendor files except T2D)
- Windows installer (able to convert vendor files)
- Macintosh (NOT able to convert vendor files)
- Linux 64 bit (NOT able to convert vendor files)
- Windows tar.bz2 (able to convert vendor files)
- Windows 64-bit tar.bz2 (able to convert vendor files except T2D)

For Developers

- Source, bjam build (includes vendor reader support)
- Source, bjam build (NO 3rd party reader support (e.g. vendors, mz5))
- Source, MSVC build (NO 3rd party reader support (e.g. vendors, mz5))
- Source, GNU Autotools build (NO 3rd party reader support (e.g. vendors, mz5))

icense listed
does, however,
d redistribution.

By accepting the license terms for this software, you agree to comply with the restrictions imposed on you by the license agreements of the software libraries on which it depends:

AB Sciex WIFF Reader Library
Agilent Mass Hunter Data Access Component Library
Bruker CompassXtract
Shimadzu SFCS
Thermo-Scientific MSFileReader Library
Waters Raw Data Access Component Library

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MSConvert

List of Files File of file names

File: Browse

About MSConvert

Add Remove

F:\RAW_PMA\Epigen_Mod_2013_2015\15_03_EM_1
F:\RAW_PMA\Epigen_Mod_2013_2015\15_03_EM_1
F:\RAW_PMA\Epigen_Mod_2013_2015\15_03_EM_1
F:\RAW_PMA\Epigen_Mod_2013_2015\15_03_EM_1

Filters

MS Level

Levels: 1 – 1

Add Remove

Filter	Parameters

Output Directory:

F:\RAW_PMA\Epigen_Mod_2013_2015\1 Browse

Options

Output format: mzXML Extension:

Binary encoding precision: 64-bit 32-bit

Write index: Use zlib compression:

TPP compatibility: Package in gzip:

Use numpress linear compression:

Use numpress short logged float compression:

Use numpress short positive integer compression:

Use these settings next time I start MSConvert

Start

Peak list: 150409_PMA_JJ1_22_01_ddMS2_pos_64bits.mzXML chromatogramsGM2 deisotoped

ID	Average m/z	Average RT	Identity	Comment	Peak shape	150409_PI Status
99	250.143882751464840000	2.26762		1037 : MZ=250....		
98	249.159790039062500000	1.96917		1035 : MZ=249....		
231	357.300445556640600000	4.38692		1250 : MZ=357....		
453	529.302307128906200000	1.87652		1567 : MZ=529....		
225	355.284439086914060000	4.13402		1242 : MZ=355....		
123	266.158142089843750000	1.87652		1071 : MZ=266....		
465	538.236083984375000000	4.25200		1582 : MZ=538....		
201	335.196594238281250000	2.10933		1213 : MZ=335....		
337	434.232498168945300000	3.94613		1409 : MZ=434....		
313	409.312149047851560000	4.60632		1367 : MZ=409....		
33	194.081283569335940000	1.46233		901 : MZ=194.0...		
338	434.290649414062500000	4.30065		1410 : MZ=434....		
100	250.143814086914060000	2.35360		1038 : MZ=250....		
254	376.283966064453100000	3.93832		1283 : MZ=376....		
407	499.280273437500000000	2.26762		1502 : MZ=499....		
363	463.188430786132800000	3.70110		1445 : MZ=463....		
6	157.085983276367200000	1.58622		864 : MZ=157.0...		
76	232.133117675781250000	1.87652		1007 : MZ=232....		
494	571.280639648437500000	3.34333		1623 : MZ=571....		
43	204.101959228515620000	1.85360		912 : MZ=204.1...		
504	582.300964355468800000	4.66017		1637 : MZ=582....		
378	480.231262207031250000	4.40992		1464 : MZ=480....		
13	169.049575805664060000	1.43923		874 : MZ=169.0...		
81	233.136642456054700000	2.26762		1013 : MZ=233....		
265	388.254150390625000000	1.47757		1302 : MZ=388....		
239	363.227844238281250000	2.61662		1263 : MZ=363....		

Peak list: 150409_PMA_JJ1_22_01_ddMS2_pos_32bits.mzXML chromatogramsGM2 deisotoped

ID	Average m/z	Average RT	Identity	Comment	Peak shape	150409_PM Status
99	250.143882751464840000	2.26762		182 : MZ=250.1...		
98	249.159790039062500000	1.96917		180 : MZ=249.1...		
231	357.300445556640600000	4.38692		395 : MZ=357.3...		
453	529.302307128906200000	1.87652		712 : MZ=529.3...		
225	355.284439086914060000	4.13402		387 : MZ=355.2...		
123	266.158142089843750000	1.87652		216 : MZ=266.1...		
465	538.236083984375000000	4.25200		727 : MZ=538.2...		
201	335.196594238281250000	2.10933		358 : MZ=335.1...		
337	434.232498168945300000	3.94613		554 : MZ=434.2...		
313	409.312149047851560000	4.60632		512 : MZ=409.3...		
33	194.081283569335940000	1.46233		46 : MZ=194.08...		
338	434.290649414062500000	4.30065		555 : MZ=434.2...		
100	250.143814086914060000	2.35360		183 : MZ=250.1...		
254	376.283966064453100000	3.93832		428 : MZ=376.2...		
407	499.280273437500000000	2.26762		647 : MZ=499.2...		
363	463.188430786132800000	3.70110		590 : MZ=463.1...		
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494	571.280639648437500000	3.34333		768 : MZ=571.2...		
43	204.101959228515620000	1.85360		57 : MZ=204.10...		
504	582.300964355468800000	4.66017		782 : MZ=582.3...		
378	480.231262207031250000	4.40992		609 : MZ=480.2...		
13	169.049575805664060000	1.43923		19 : MZ=169.04...		
81	233.136642456054700000	2.26762		158 : MZ=233.1...		
265	388.254150390625000000	1.47757		447 : MZ=388.2...		
239	363.227844238281250000	2.61662		408 : MZ=363.2...		

64bits precision
10.6 Mo

32bits precision
9.4 Mo

conversion of Waters .RAW files
is not made correctly with Proteowizzard

Same Waters .RAW file converted with Databridge

Proteowizzard

Peak list: 131001_SC_PMA_1_3_1_POS01.CDF chromatogramsGM2

ID	Average m/z	Average RT	Identity	Comment	Peak shape	13100 Status
1	107.0507	0.58		1 : MZ=107.050...		
2	123.0450	0.32		2 : MZ=123.045,...		
3	127.0405	0.59		4 : MZ=127.040...		
4	127.0410	1.59		6 : MZ=127.041,...		
5	130.5327	5.29		7 : MZ=130.533...		
6	131.5330	5.30		9 : MZ=131.533,...		
7	137.0247	1.12		10 : MZ=137.02...		
8	137.0246	1.60		11 : MZ=137.02...		
9	139.9885	5.28		12 : MZ=139.98...		
10	143.0599	5.32		14 : MZ=143.06...		
11	149.0222	0.59		16 : MZ=149.02...		
12	151.0452	5.36		17 : MZ=151.04...		
13	152.0457	5.30		27 : MZ=152.04...		
14	152.5470	5.29		55 : MZ=152.54...		
15	153.0441	5.30		56 : MZ=153.04...		
16	154.9912	0.09		61 : MZ=154.99...		
17	155.0336	0.43		70 : MZ=155.03...		
18	155.0346	0.66		71 : MZ=155.03...		
19	155.0354	1.12		73 : MZ=155.03...		
20	155.0354	1.59		74 : MZ=155.03...		
21	159.0650	0.52		76 : MZ=159.06...		
22	159.9705	0.10		77 : MZ=159.97...		
23	160.0760	0.36		78 : MZ=160.07...		
24	168.0996	0.41		80 : MZ=168.09...		
25	172.0414	0.25		94 : MZ=172.04...		
26	176.9713	5.85		95 : MZ=176.97...		
27	177.0562	0.82		99 : MZ=177.05...		

Peak list: 131001_SC_PMA_1_3_1_POS.mzXML chromatogramsGM2

ID	Average m/z	Average RT	Identity	Comment	Peak shape	13100 Status
1	107.0014	0.58		661 : MZ=107.0...		
2	122.9934	0.32		662 : MZ=122.9...		
3	126.9884	0.59		664 : MZ=126.9...		
4	126.9889	1.59		666 : MZ=126.9...		
5	130.4802	5.29		667 : MZ=130.4...		
6	131.4804	5.30		669 : MZ=131.4...		
7	136.9715	1.12		670 : MZ=136.9...		
8	136.9714	1.60		671 : MZ=136.9...		
9	139.9350	5.28		672 : MZ=139.9...		
10	143.0061	5.32		674 : MZ=143.0...		
11	148.9678	0.59		688 : MZ=148.9...		
12	149.0212	0.70		689 : MZ=149.0...		
13	150.9906	5.36		696 : MZ=150.9...		
14	151.0463	5.20		706 : MZ=151.0...		
15	151.9911	5.30		708 : MZ=151.9...		
16	152.4924	5.29		736 : MZ=152.4...		
17	152.9894	5.30		737 : MZ=152.9...		
18	154.9353	5.39		738 : MZ=154.9...		
19	154.9363	0.09		742 : MZ=154.9...		
20	154.9787	0.43		751 : MZ=154.9...		
21	154.9797	0.66		752 : MZ=154.9...		
22	154.9805	1.12		754 : MZ=154.9...		
23	154.9805	1.59		755 : MZ=154.9...		
24	159.0098	0.52		757 : MZ=159.0...		
25	159.9152	0.10		758 : MZ=159.9...		
26	160.0208	0.36		759 : MZ=160.0...		
27	168.0438	0.41		761 : MZ=168.0...		

> 0.1 Da difference

Microsoft Excel 2010

Command Prompt

MassLynx V4.1

MSConvert

ChemBioFinder Ultra 13.0

Xcalibur

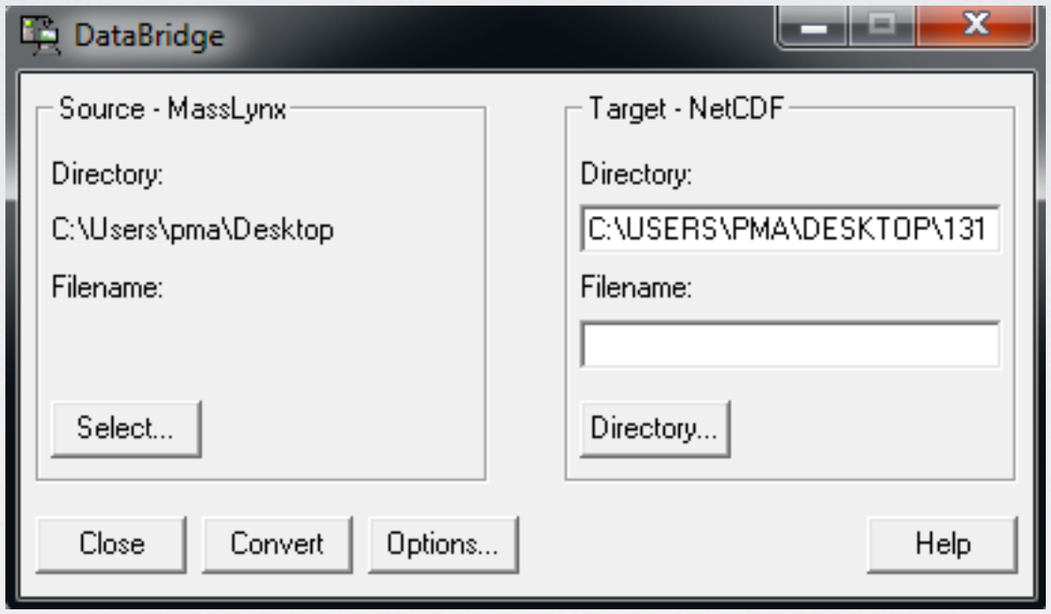
Microsoft Access 2010

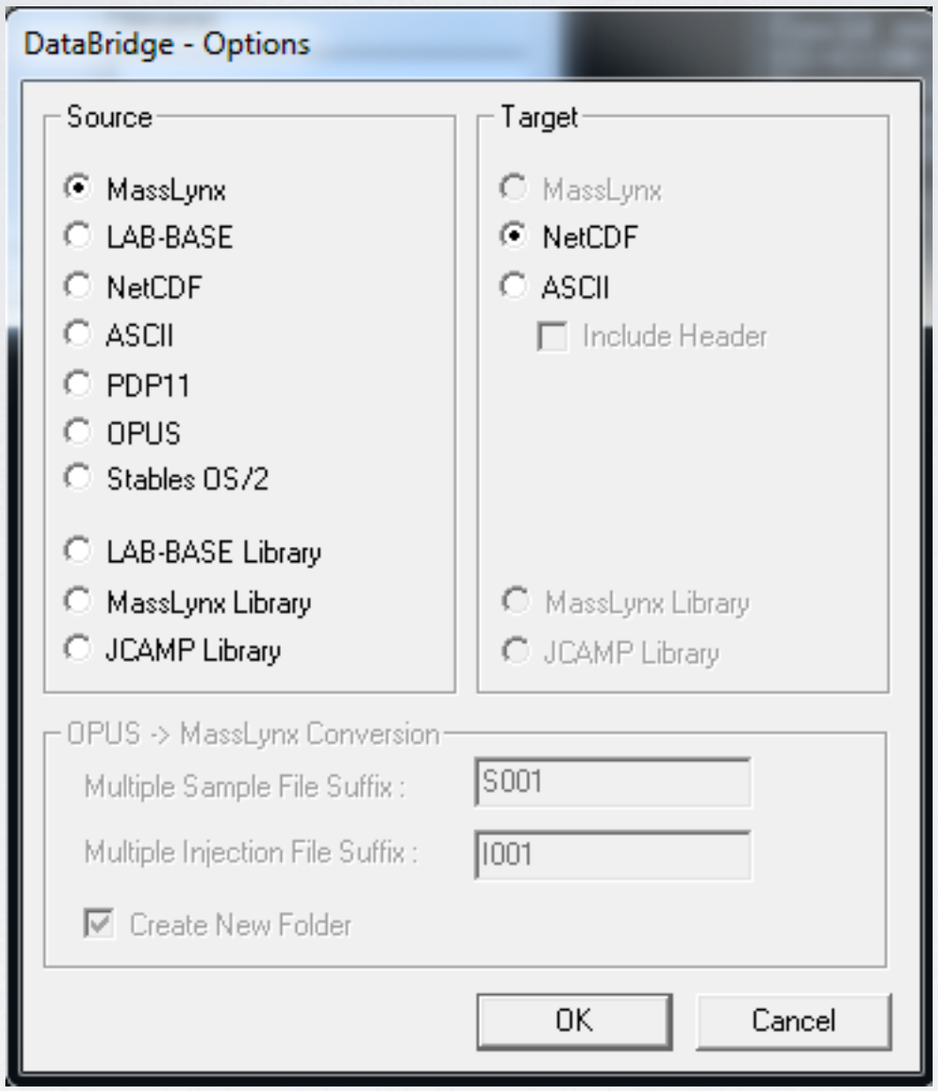
Getting Started

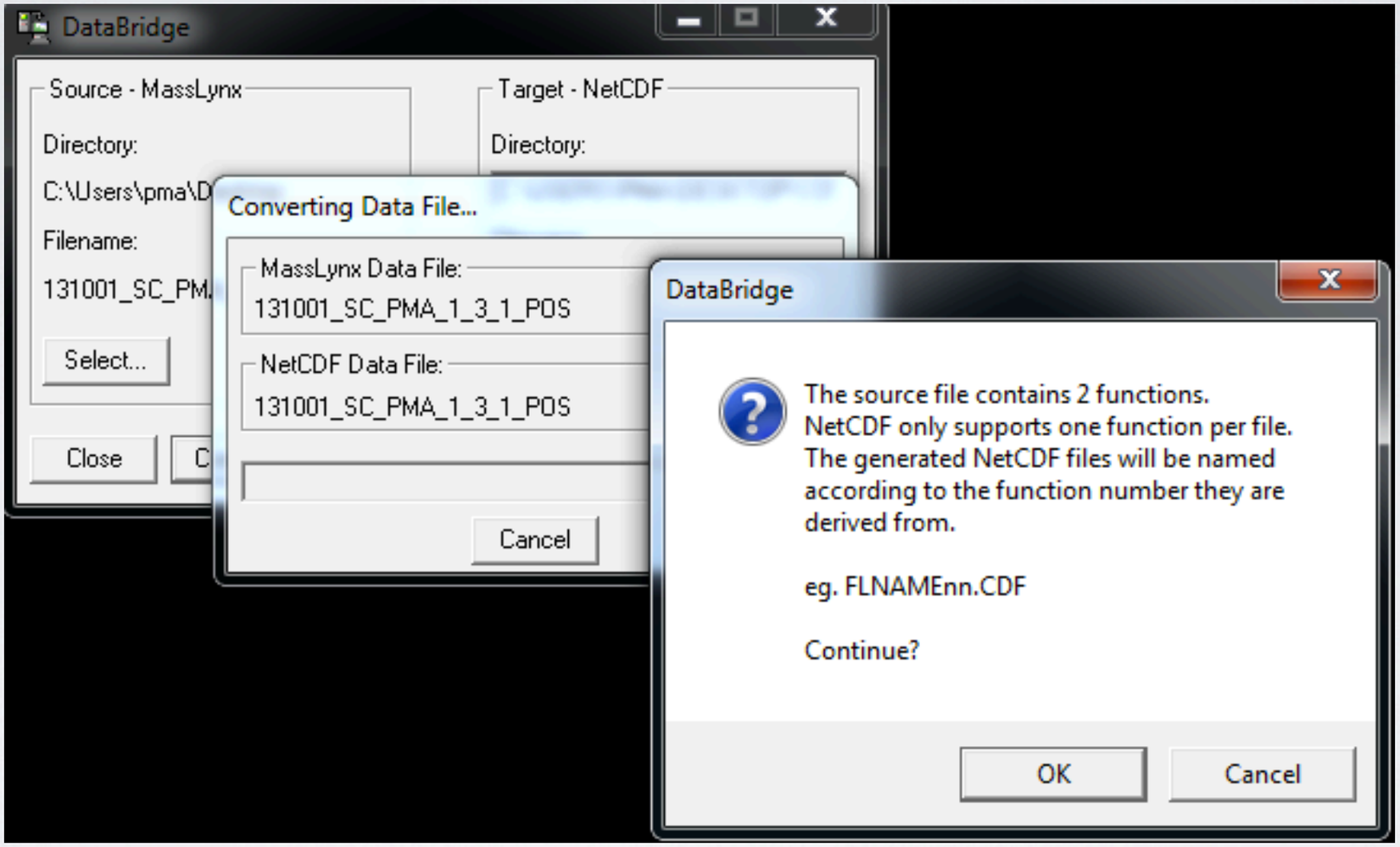
Databridge

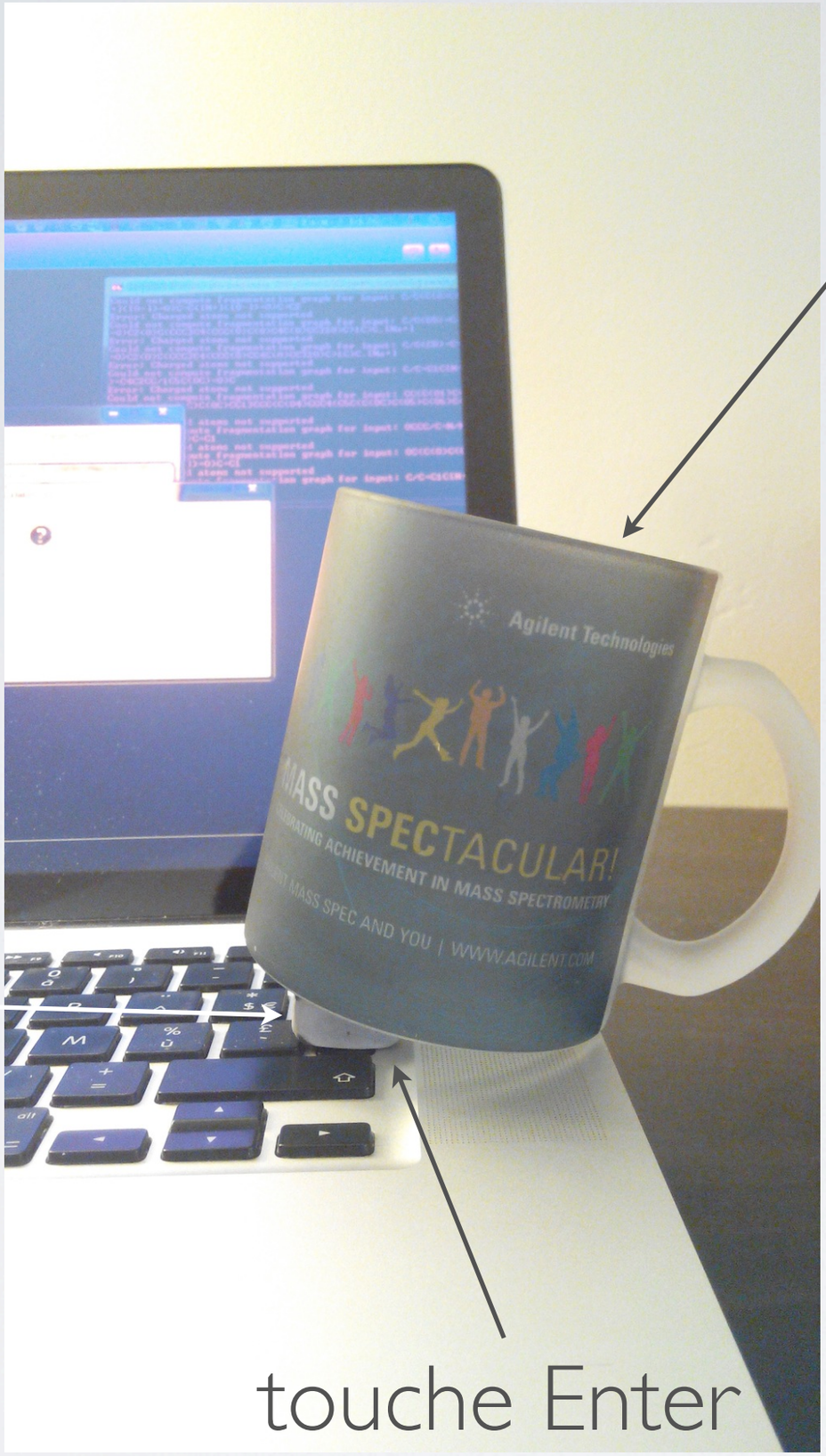
Windows Media Center

All Programs


DataBridge
Source - MassLynx
Directory:
C:\Users\pma\Desktop
Filename:
Select...
Target - NetCDF
Directory:
C:\USERS\PMA\DESKTOP\131
Filename:
Directory...
Close
Convert
Options...
Help


DataBridge - Options
Source
MassLynx
LAB-BASE
NetCDF
ASCII
PDP11
OPUS
Stables OS/2
LAB-BASE Library
MassLynx Library
JCAMP Library
Target
MassLynx
NetCDF
ASCII
Include Header
MassLynx Library
JCAMP Library
OPUS -> MassLynx Conversion
Multiple Sample File Suffix :
S001
Multiple Injection File Suffix :
I001
Create New Folder
OK
Cancel


DataBridge
Source - MassLynx
Directory:
C:\Users\pma\D
Filename:
131001_SC_PM
Select...
Close
Target - NetCDF
Directory:
Converting Data File...
MassLynx Data File:
131001_SC_PMA_1_3_1_POS
NetCDF Data File:
131001_SC_PMA_1_3_1_POS
Cancel
DataBridge
The source file contains 2 functions.
NetCDF only supports one function per file.
The generated NetCDF files will be named according to the function number they are derived from.
eg. FLNAMEnn.CDF
Continue?
OK
Cancel



Guillaume Marti & Samuel Bertrand (unpublished work)

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stanstrup / chemhelper Watch 1

R functions helpful in working with chemical data

117 commits 1 branch 0 releases 1 contributor

branch: master chemhelper / +

Updated README with latest functions.

stanstrup authored on 24 Mar latest commit a240c44118

R	Added letter notation functions.	3 months ago
inst/extdata	fixed orbiwarp fix example	6 months ago
man	grammar	2 months ago
DESCRIPTION	Updated README with latest functions.	a month ago
NAMESPACE	Added letter notation functions.	3 months ago
README.md	Updated README with latest functions.	a month ago

README.md

chemhelper

https://github.com/stanstrup/chemhelper

chemhelper

R functions helpful in working with chemical data. A number of functions to help analyze metabolomics data processed with xcms/CAMERA.

Data conversion and fixes

- `convert.waters` : Converts files from Waters .raw format to mzData. MassLynx need to be installed and masswolf need to be in path. (this works around the problem of properly converting Waters data described in the supplementary of dx.doi.org/10.1007/s00216-013-6954-6).

https://github.com/stanstrup/chemhelper

Open-format in MS

using open-format allows:

-acces to a range of data treatment solutions
-treat files from different vendors on same plateform (collaboration)
-share your data with the community, reproducibility of data treatment
-support of old file format (no data rot)

main open format in metabolomics:

-many of them but .mzXML is the standard (opinions ?)

to convert to mzXML:

-msconvert in Proteowizzard (be careful with Waters .RAW files)

Proteomics Standards Initiative

HUPO Proteomics Standards Initiative

Specifications

mzML 1.1.0 Specification

From 2005–2008 there has existed two separate XML formats for encoding raw spectrometer output: mzData developed by the PSI and mzXML developed at the Seattle Proteome Center at the Institute for Systems Biology. It was recognized that the existence of two separate formats for essentially the same thing generated confusion and required extra programming effort. Therefore the PSI, with full participation by ISB, has developed a new format by taking the best aspects of each of the precursor formats to form a single one. It is intended to replace the previous two formats. This new format was originally given a working name of dataXML. The final name is mzML.

On 2008-06-01, mzML 1.0.0 was released.

In early 2009, several implementation efforts have identified a few minor shortcomings in mzML 1.0.0. Since no vendors have yet released software supporting mzML 1.0, but have identified a few minor problems with it, the working group has decided to release an update in June 2009. It is expected that all software will support mzML 1.1 as the long-term-stable format instead of 1.0. Below are the available documents and initial implementations. We encourage the community to begin implementing mzML 1.1.0, to phase out use of mzData and mzXML, and to send feedback to psidev-ms-dev@lists.sourceforge.net.

On 2009-06-01, mzML 1.1.0 was released. There are no planned further changes as of early 2013.

Open-format in MS

more on MS formats :

Mol Cell Proteomics. 2012 Dec; 11(12): 1612–1621.
PMCID: PMC3518119
Published online 2012 Sep 6. doi: 10.1074/mcp.R112.019695

File Formats Commonly Used in Mass Spectrometry Proteomics[*]

Eric W. Deutsch[‡§]

From the ‡Institute for Systems Biology, Seattle, WA 98109

§ To whom correspondence should be addressed: Eric W. Deutsch, Institute for Systems Biology, 401 Terry Ave. North, Seattle, WA 98109,, Tel.: Phone: 206-732-1397, E-mail: eric.deutsch@systemsbiology.org.

Open-format in MS

Some open-format are designed to organize MS study results AFTER the analysis

.mzTAB

Technological Innovation and Resources

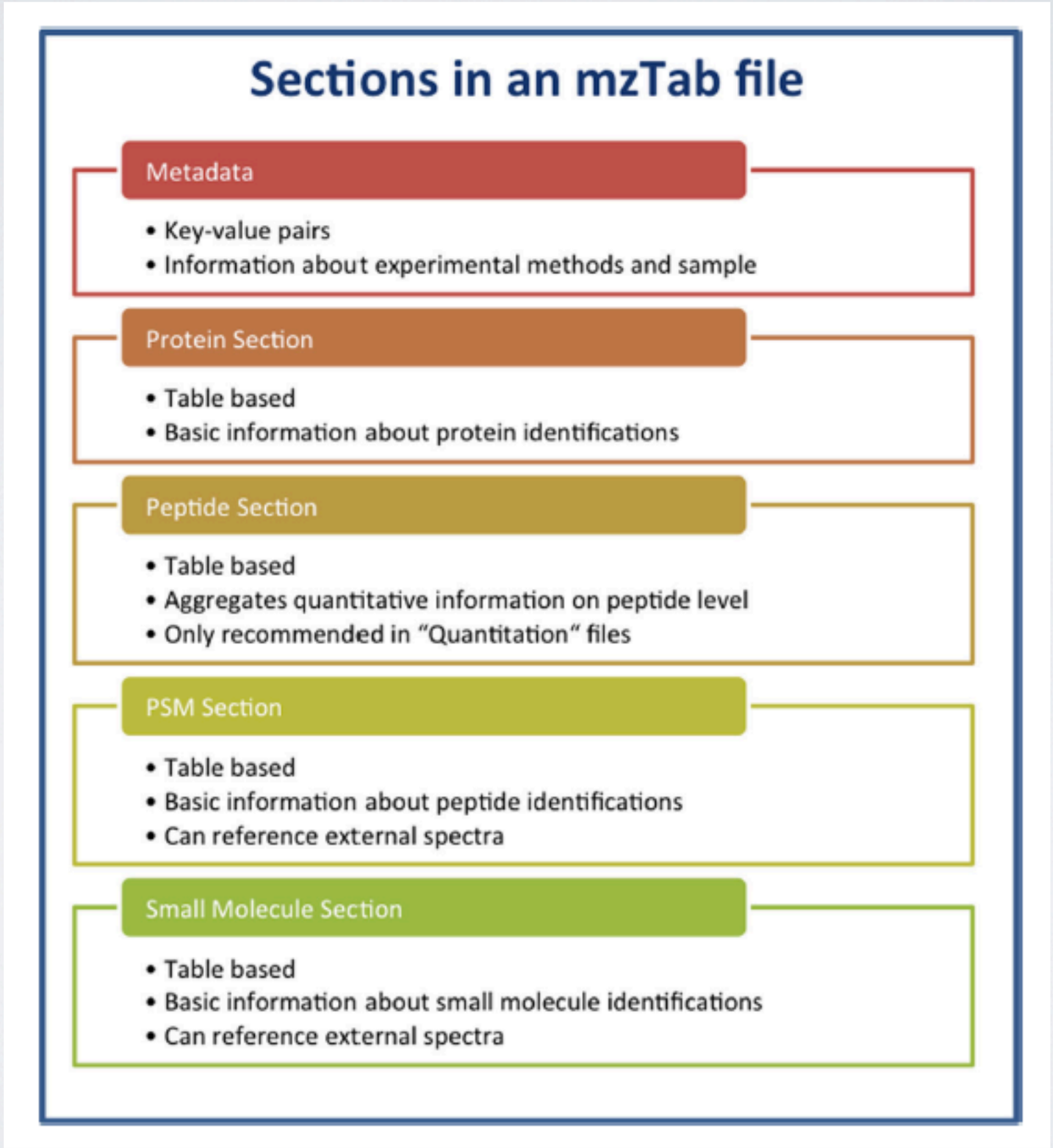
✂ *Author's Choice*

The mzTab Data Exchange Format: Communicating Mass-spectrometry-based Proteomics and Metabolomics Experimental Results to a Wider Audience*[S]

Johannes Griss‡§¶, Andrew R. Jones¶‖, Timo Sachsenberg**, Mathias Walzer**, Laurent Gatto‡‡, Jürgen Hartler§§¶¶, Gerhard G. Thallinger§§¶¶, Reza M. Salek‡, Christoph Steinbeck‡, Nadin Neuhauser‖‖, Jürgen Cox‖‖, Steffen Neumann[a], Jun Fan[b], Florian Reisinger‡, Qing-Wei Xu‡[c], Noemi del Toro‡, Yasset Pérez-Riverol‡, Fawaz Ghali‖, Nuno Bandeira[d], Ioannis Xenarios[efg], Oliver Kohlbacher**[h], Juan Antonio Vizcaíno‡[i], and Henning Hermjakob‡

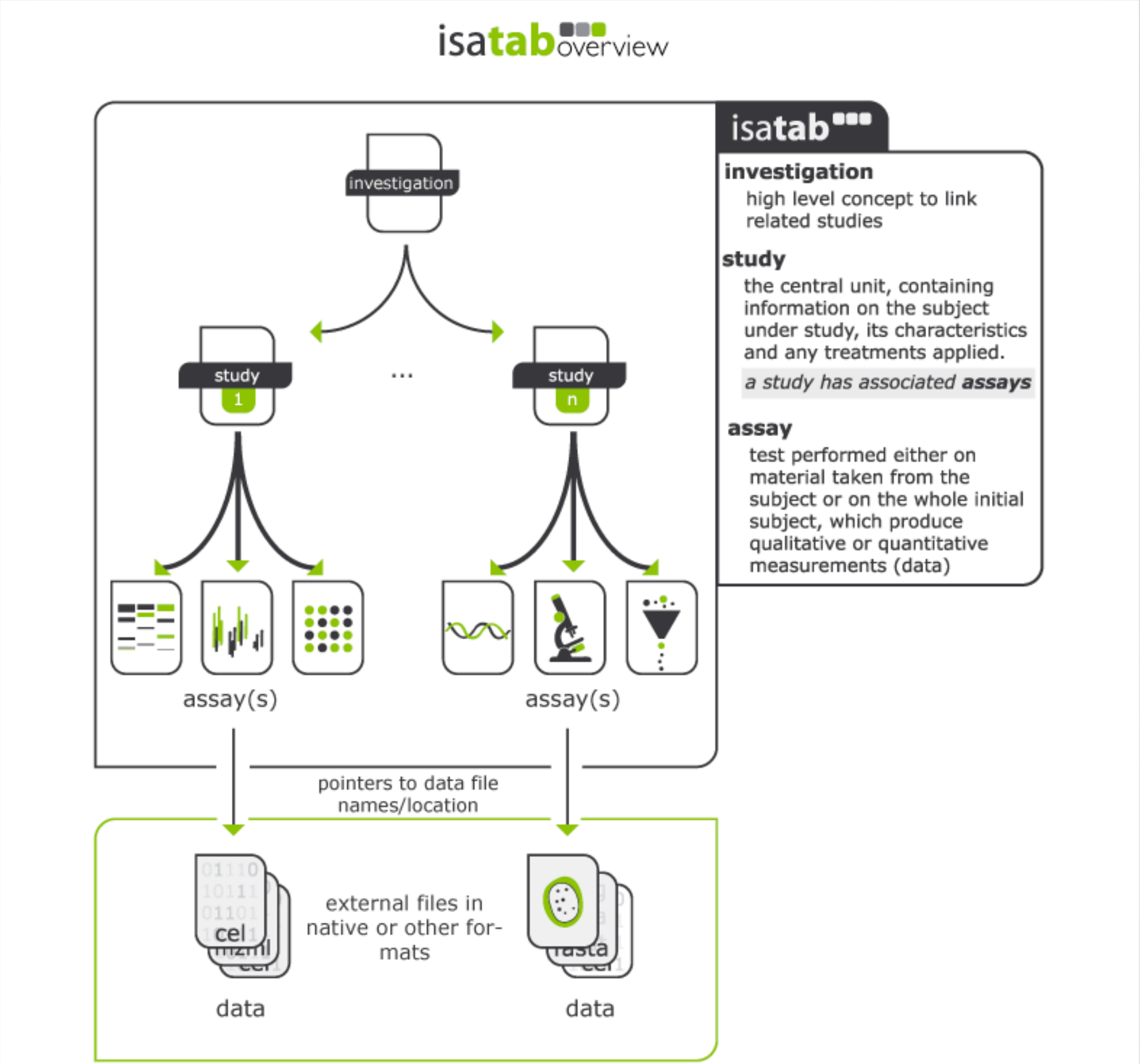
Open-format in MS

.mzTAB



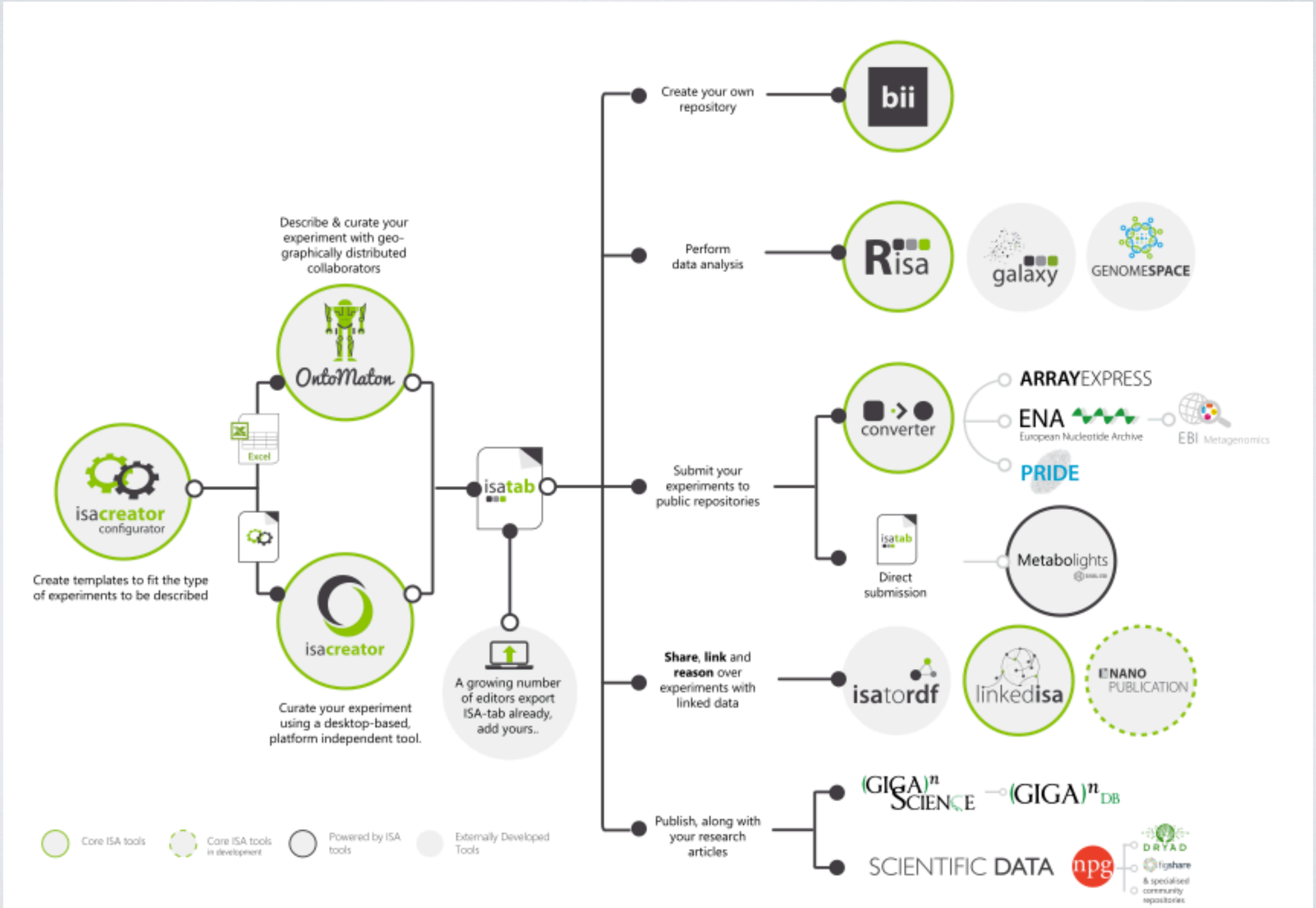
Open-format in MS

.isaTAB



Open-format in MS

.isaTAB



Open-format in MS

.isaTAB direct submission of study to Metabolights

Nucleic Acids Research Advance Access published October 29, 2012

Nucleic Acids Research, 2012, 1–6
doi:10.1093/nar/gks1004

MetaboLights—an open-access general-purpose repository for metabolomics studies and associated meta-data

Kenneth Haug[1], Reza M. Salek[1,2,3], Pablo Conesa[1], Janna Hastings[1], Paula de Matos[1], Mark Rijnbeek[1], Tejasvi Mahendraker[1], Mark Williams[1], Steffen Neumann[4], Philippe Rocca-Serra[5], Eamonn Maguire[5], Alejandra González-Beltrán[5], Susanna-Assunta Sansone[5], Julian L. Griffin[2,3] and Christoph Steinbeck[1,*]

[1]European Bioinformatics Institute, Wellcome Trust Genome Campus, Hinxton, Cambridgeshire CB10 1SD, [2]MRC HNR, Elsie Widdowson Laboratory, Fulbourn Road, Cambridge CB1 9NL, [3]Department of Biochemistry and Cambridge Systems Biology Centre, University of Cambridge, Cambridge CB2 1GA, UK, [4]Department of Stress- and Developmental Biology, Leibniz Institute of Plant Biochemistry, Weinberg 3, 06120 Halle, Germany and [5]Oxford e-Research Centre, University of Oxford, 7 Keble Road, Oxford OX1 3QG, UK

Open-format in MS

.isaTAB direct submission of study to Metabolights

MTBLS170: Solvent fractions of an aqueous extract of yerba mate (Ilex paraguariensis)

Share Study | View all files

Submitted: **24-Feb-2015** ,Release date: **19-Mar-2015**

Caroline Rempe

Other identifiers: yerba_mate_GCMS_profiles

The aqueous extract of yerba mate, a South American tea beverage made from Ilex paraguariensis leaves, has demonstrated bactericidal and inhibitory activity against bacterial pathogens, including methicillin-resistant Staphylococcus aureus (MRSA). The gas chromatography-mass spectrometry (GC-MS) analysis of two unique fractions of yerba mate aqueous extract revealed 8 identifiable small molecules in those fractions with antimicrobial activity. For a more comprehensive analysis, a data analysis pipeline was assembled to prioritize compounds for antimicrobial testing against both MRSA and methicillin-sensitive S. aureus using forty-two unique fractions of the tea extract that were generated in duplicate, assayed for activity, and analyzed with GC-MS. As validation of our automated analysis, we checked our predicted active compounds for activity in literature references and with used authentic standards to test for antimicrobial activity. 3,4-dihydroxybenzaldehyde showed the most antibacterial activity against MRSA at low concentrations in our bioassays. In addition, quinic acid and quercetin were identified using random forests analysis and 5-hydroxy pipecolic acid was identified using linear discriminant analysis. We additionally also generated a ranked list of unidentified compounds that may contribute to the antimicrobial activity of yerba mate against MRSA. Here we utilized GC-MS data to implement an automated analysis that resulted in a ranked list of compounds that likely contribute to the antimicrobial activity of aqueous yerba mate extract against MRSA.

Study Design Description | Protocols | Samples | Assay | Study Files

Protocol	Description
Sample collection	Dried leaves of a single commercial brand of yerba mate tea (Taragui; Argentina; 100% leaves; I. paraguariensis) were purchased from a local international supermarket and finely ground to a particle size < 300 µm using a commercial food blender (Oster, Boca Raton, Fla., USA). Sterile deionized water was added to ground leaves at a ratio of 3.6 ml to 1 g ground tissue, was allowed to stand for 2 h at 4°C with occasional mixing to maximize extraction and was subsequently centrifuged at 5000 × g for 30 min. Aqueous extracts were then subjected to dialysis at 4°C against deionized water for 36 h using a 3500 MWCO SnakeSkin® pleated dialysis tubing (ThermoFisher Scientific, Rockford, Ill., USA). Dialyzed extracts were then centrifuged at 5000 × g for 30 min to remove large insoluble particles and frozen at -80°C. Frozen extracts were lyophilized using Labconco FreeZone 12 L Freeze Dry System (Labconco, Kansas City, Missouri, USA) to concentrate them. Lyophilized extracts were stored at room temperature in a sealed container until testing.
Extraction	Lyophilized aqueous yerba mate extract was further extracted with 10%, 20%, 30%, 40%, 50%, 60%, 70%, 80%, and 90% solvent (methanol or acetonitrile) and centrifuged at 13,000 × g for 30 min to separate them into two fractions: the pellet (not soluble in solvent concentration) and the supernatant (soluble in solvent concentration). Fractions were subsequently dried using a SpeedVac Concentrator (Savant Industries, Inc., Farmingdale, N.Y., USA). Lyophilized solvent-extracts were weighed, resuspended in sterile water to a concentration of 40 mg/ml and stored at -20 °C until bio-assays or derivitization for GC-MS.

Open-format in MS

.isaTAB direct submission of study to Metabolights

MTBLS170: Solvent fractions of an aqueous extract of yerba mate (Ilex paraguariensis)

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Study Design Description | Protocols | Samples | Assay | Study Files

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List of study files

Type part of a filename and press enter to select. Prefix with ! to deselect.

Select	File
☐	120613B-13.CDF
☐	050214B-06.CDF
☐	013014B_14.CDF

Where to find open ressource & tools for MS ?

http://www.ms-utils.org

ms-utils.org

ms-utils.org
- About
- Software List
- Editing Policies
- FAQ
- ChangeLog

related sites
- ExPASy tools
- NBIC BioAssist
- PNNL Tools
- SPC Proteomic Tools

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Software List

platforms, pipelines and libraries

CPAS	LIMS and analysis tools for proteomics data (includes msInspect)		
CPFP	Central Proteomics Facilities Pipeline [1] (demo here)		
GenePattern	platform for integrative genomics and proteomics (includes PEPPeR [2] and other tools for proteomics)	Java	
InSilicoSpectro	open source proteomics library (of Perl functions) [3]	Perl	
libfbi	a fast implementation of box intersection for correspondence estimation in peak picking, alignment, etc.	C++	
Mass-up	utility with full GUI for proteomics data analysis, particularly MALDI-TOF	Java	
MASSyPup	a lightweight Linux live distribution prepackaged with a wide range of tools for MS and MS/MS data analysis		
mspire	MS data processing in Ruby, including mzML reader/writer, *in-silico* digestion, isotopic pattern calculation etc. [4]	Ruby	
OpenMS	library for the analysis, reduction and visualization of LC-MS(/MS) data	C++	
PAPPSO	Plateforme d'Analyse Protéomique de Paris Sud-Ouest	Java	
PatternLab	suite of pattern recognition software for interpretation of quantiative proteomics data [5]	.NET	
pFind Studio	computational platform for mass spectrometry-based proteomics, including pFind [6], pNovo [7] and pQuant [8]	Java	
PeptideShaker	platform for interpretation of proteomics identification results from multiple search engines [9]	Java	
PRIDE Toolsuite	a selection of tools and libraries for interacting with data in PRIDE	Java	
Proteios	pipeline/LIMS for proteomics experiments and analysis	Java	
Proteomatic	platform for creating MS/MS data analysis workflows using scripts [10]	C++	
ProteoWizard	open source library for proteomics tools development (supports mzML) [11]	C++	
pymzML	Python module to parse mzML data based on cElementTree [12]	Python	
Pyteomics	framework for proteomics data analysis, supporting mzML, MGF, pepXML and more [13]	Python	
QuPE	integrated environment for storage, analysis and integration of proteomics data (requires login) [14]	Java	web
Rproteomics	set of routines for analyzing proteomics data, an XML database to store the results and a user interface	R	
TPP	Institute for Systems Biology "Trans-Proteomic Pipeline"		
XCMS	software package (in R) for metabolite profiling from LC-MS data	R	

data visualization and analysis

cdfread	a simple reader of mass spectra in netCDF	C
COMSPARI	compares two datasets in netCDF or ASCII format	C

https://github.com/

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Search mass spectrometry Search

Repositories 120
Code 43,443
Issues 82
Users 5

We've found 120 repository results Sort: **Best match**

dbaileychess/CSMSL C# ★ 8 ⑂ 4
C# **Mass** **Spectrometry** Library
Updated on 13 Oct 2014

Languages

R 25
Python 17
Ruby 13
C# 10
Matlab 7
C++ 7
Java 5
JavaScript 4
HTML 3
C 2

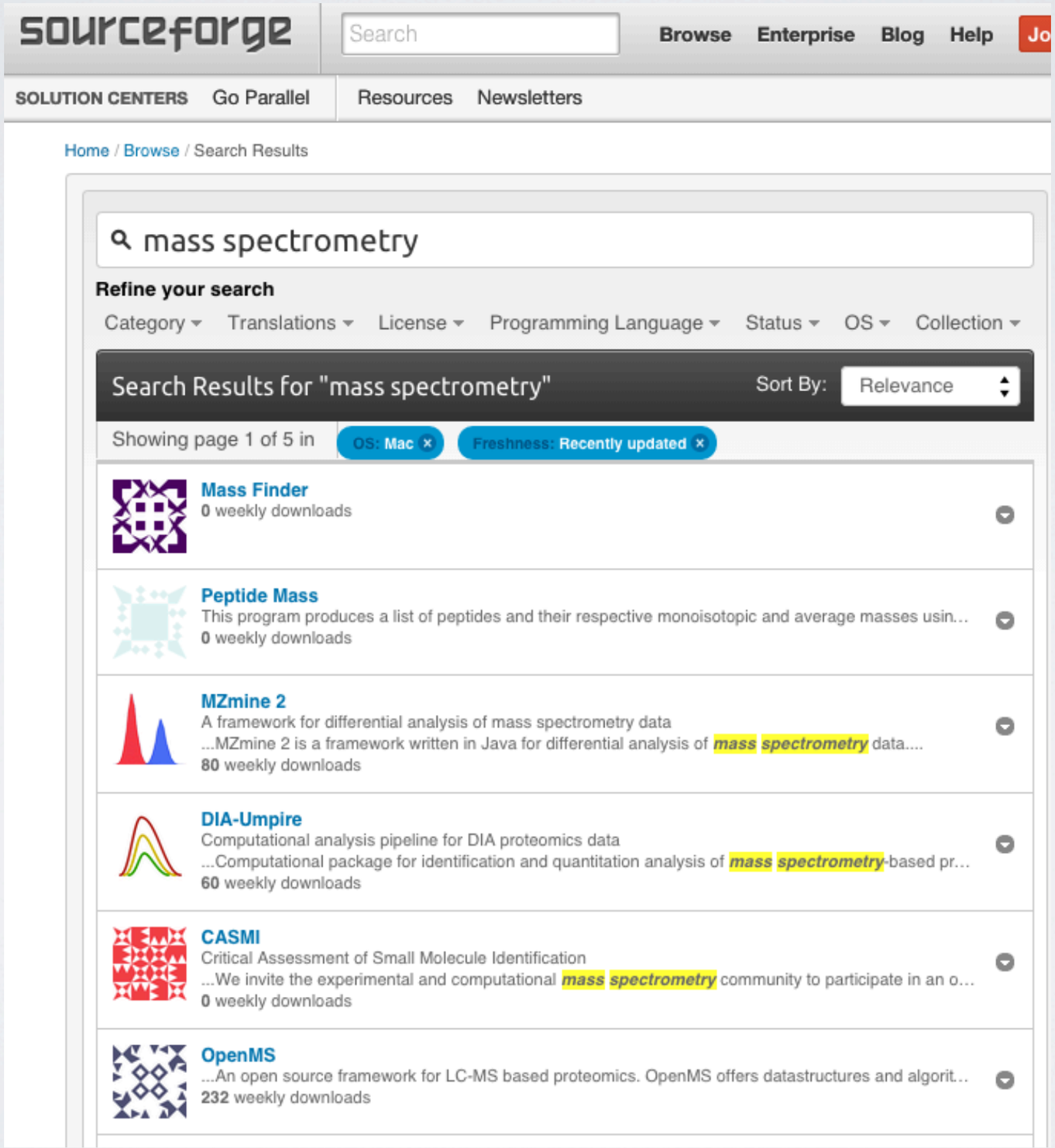
pymzml/pymzML Python ★ 17 ⑂ 16
pymzML - an interface between Python and mzML **Mass** **spectrometry** Files
Updated on 17 Dec 2014

princelab/mspire Ruby ★ 12 ⑂ 3
mass **spectrometry** proteomics in ruby
Updated on 3 Aug 2014

Advanced search Cheat sheet

dbaileychess/Compass C# ★ 8 ⑂ 5
Coon OMSSA (Open **Mass** **Spectrometry** Search Algorithm) Proteomic Analysis Software Suite.
Updated on 29 Oct 2014

http://sourceforge.net/



A nice solution ...

Research article

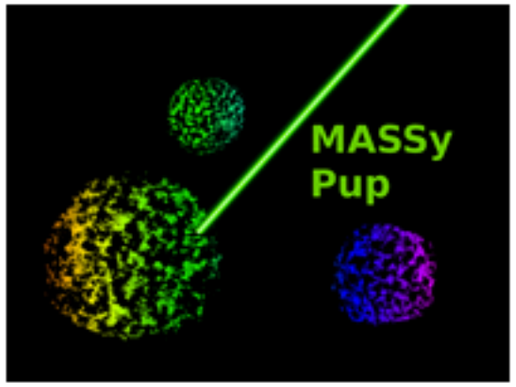
Journal of MASS SPECTROMETRY

Received: 12 September 2013 Revised: 5 November 2013 Accepted: 18 November 2013 Published online in Wiley Online Library

(wileyonlinelibrary.com) DOI 10.1002/jms.3314

MASSyPup — an 'Out of the Box' solution for the analysis of mass spectrometry data

Robert Winkler*



MASSyPup is a Puppy Linux based Live distribution with is focused on the analysis of mass spectrometry data.

The system runs from DVD, USB and hard drive (with or without installation). The software is collected from free sources and may distributed with/ without data. It runs completely from RAM (if there is sufficient memory available) and therefore it is extremely fast.

The distribution contains many programs for mass spectrometry data conversion, data processing, mass spectrometry imaging (MSI), metabolomics and proteomics, such as: ESIprot, imzML Converter, mmass, MZmine, OpenMZxy, OpenChrom, PepNovo, PeptideShaker, ProteoWizard tools (mscovert), R with XCMS and rJava, SearchGUI, SpiderMass, UniNovo, X!Tandem, X!Tandem Parser/ Viewer (see ms-util.org).

Further, various programming languages and libraries are installed, such as: Java, Phython, Perl, g++, which facilitates the development and installation/ compilation of custom programs.

Questions ?
Discussion ?
Merci !

A demain !