

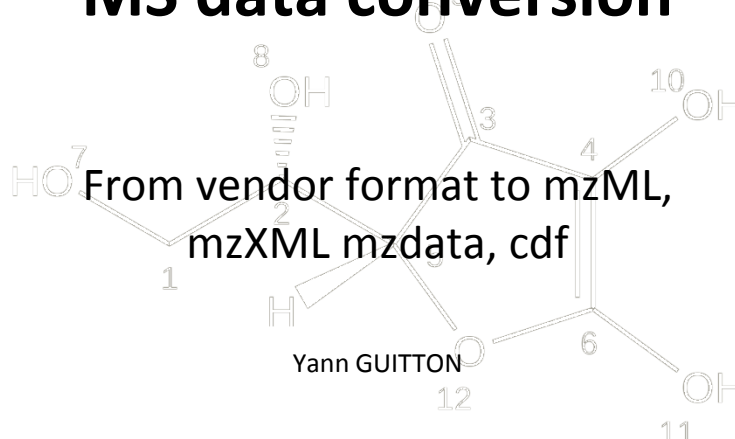


4 Wm

Workflow4metabolomics

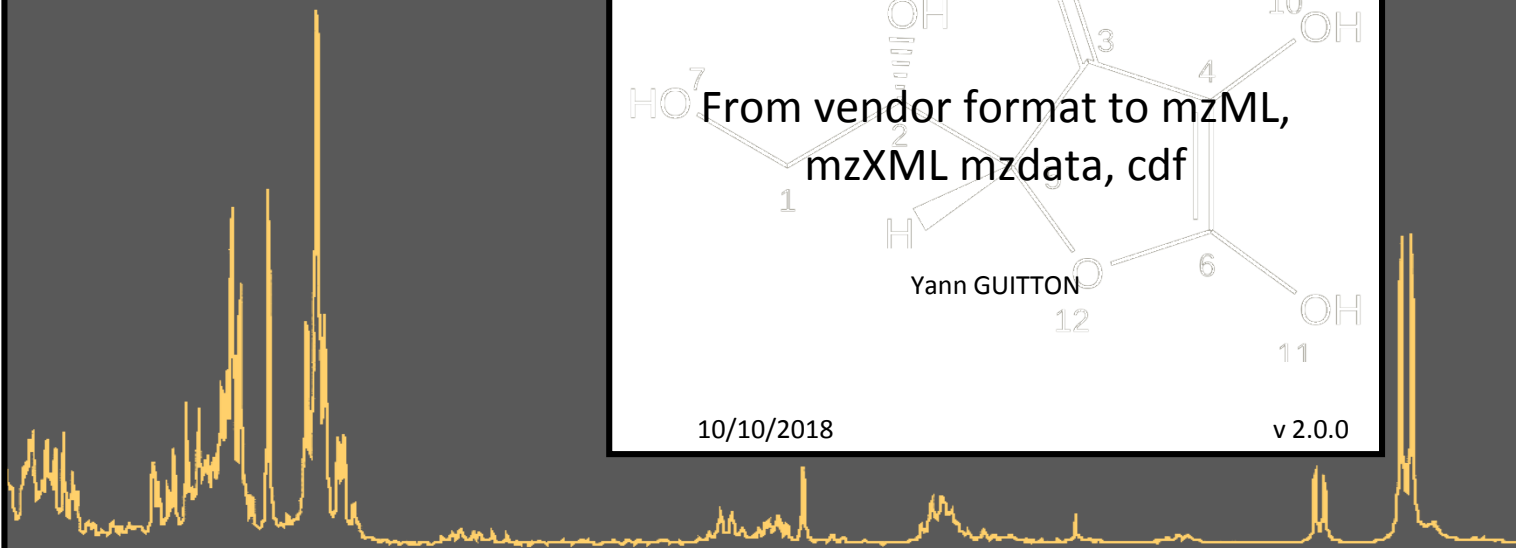


MS data conversion



10/10/2018

v 2.0.0



Msconvert a Magical tool

- <http://proteowizard.sourceforge.net/tools/msconvert.html>
- A Graphical User Interface
- Command lines for some advanced features (polarity switch data...)

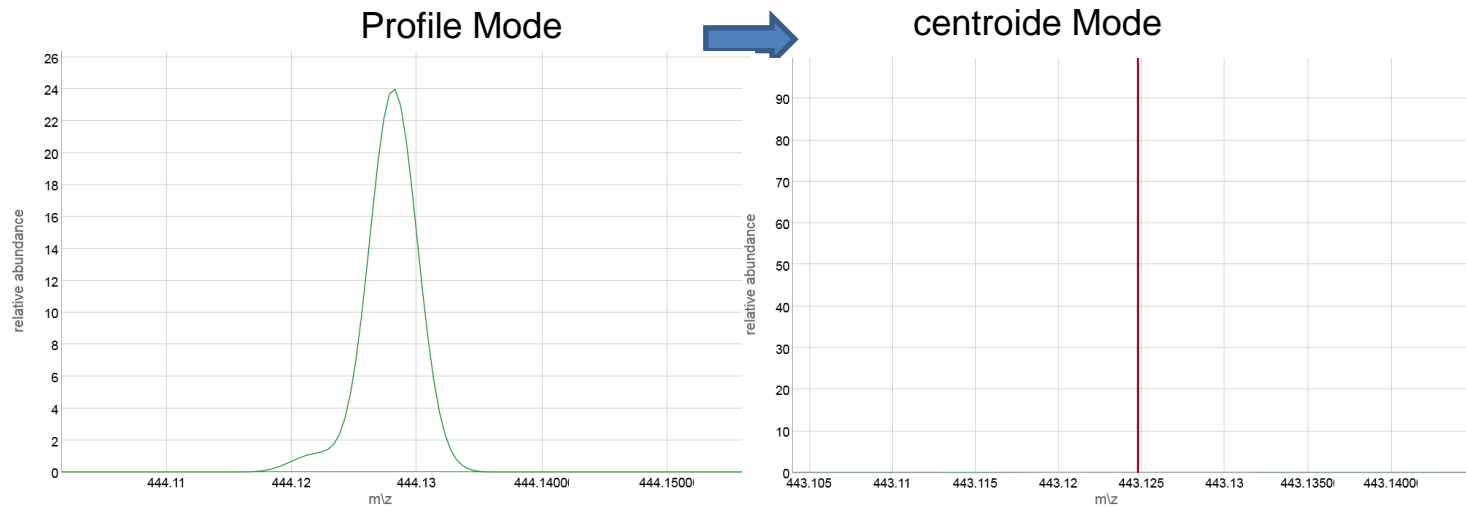
Vendor	Formats	Vendor Required Software	License
Agilent	MassHunter .d	distributed with ProteoWizard	MHDAC
Bruker	Compass .d, YEP, BAF, FID	distributed with ProteoWizard	
Thermo Fisher	RAW	distributed with ProteoWizard	MSFileReader
Waters	MassLynx .raw	distributed with ProteoWizard	WRDAC
Applied Biosystems	WIFF	distributed with ProteoWizard	Wiff Reader Library



Msconvert a Magical tool



XCMS centWave read ONLY centroided data

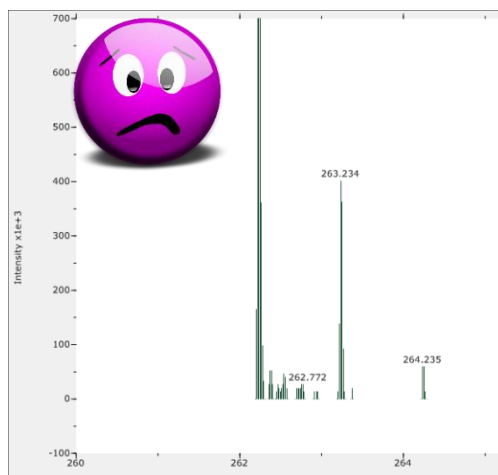


Msconvert a Magical tool

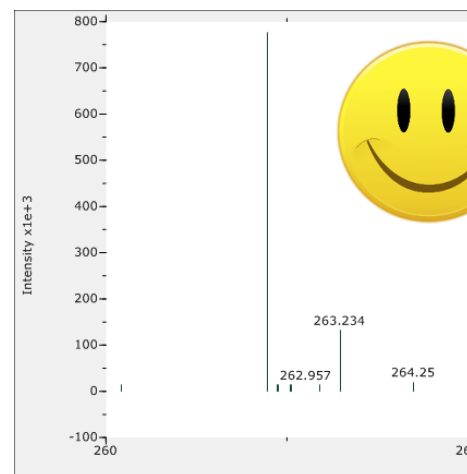


Bad conversion example

Msconvert
Profile Mode

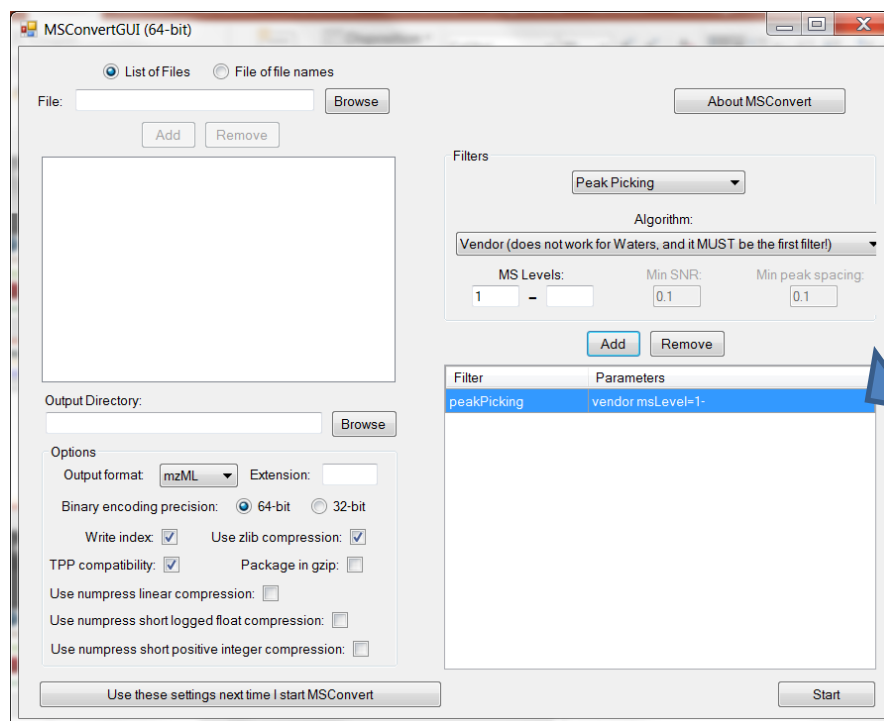


Msconvert
Centroided (peakpicking =TRUE)



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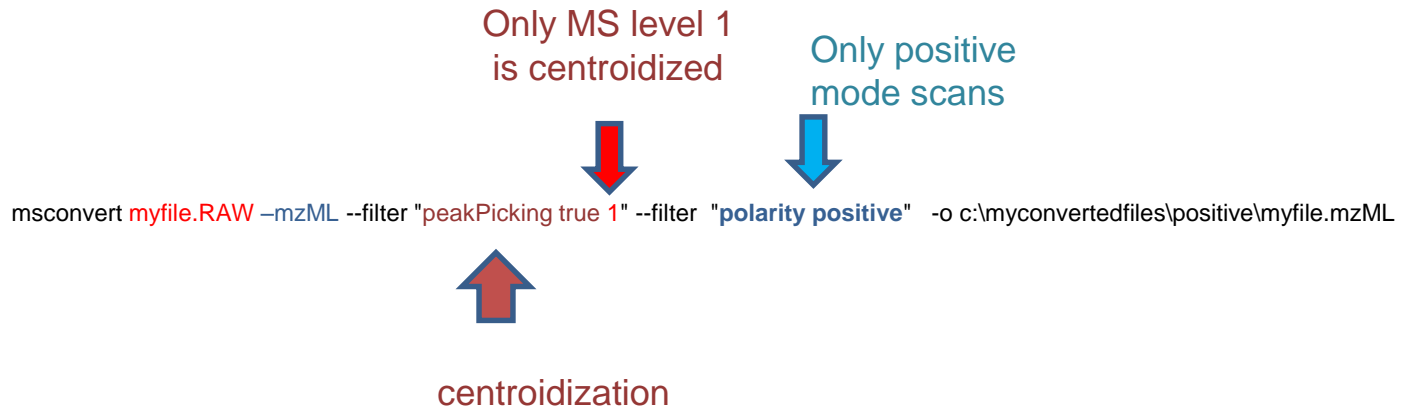


Mandatory if your data are in profile mode



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Hard cases: Waters QToF with LockMass,



Other conversion tools

- Vendor softwares (Waters databridge, Agilent MassHunter, Bruker compassXport)
- Open Source:

For Shimadzu, old vendor format (Agilent .d from Chemstation, Varian...)

openChrom

Agilent *.D (DATA.MS and MSD1.MS)
Agilent MassHunter (*.D)
Agilent ICP-MS (*.icp)
Bruker Flex MALDI-TOF MS (.fid)
Chromtech (*.dat)
Finnigan (*.RAW)
Finnigan ICIS (*.dat)
Finnigan ITDS (*.DAT)
Finnigan ITS40 (*.MS)
Finnigan MAT95 (*.dat)
MassLynx (*.RAW)
PerkinElmer (*.raw)
Shimadzu (*.qgd)
Varian SMS (*.SMS)
Varian XMS (*.XMS)
VG MassLab (*.DAT_001;1)
Waters (*.RAW)

 **OPEN**Chrom

<https://www.openchrom.net/>



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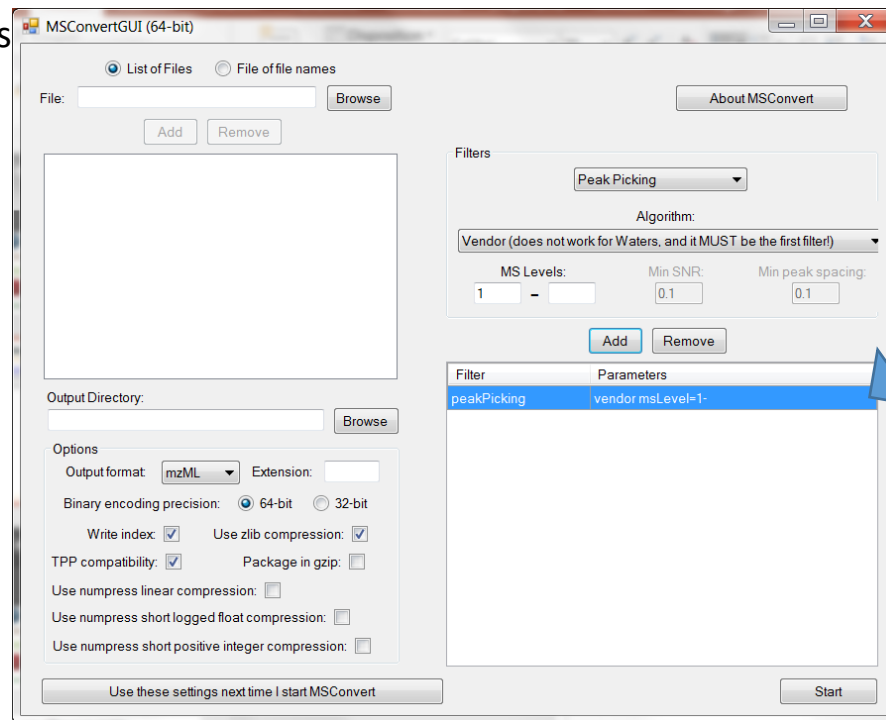
Mass++

<https://solutions.shimadzu.co.jp/form/msrl/license.html>



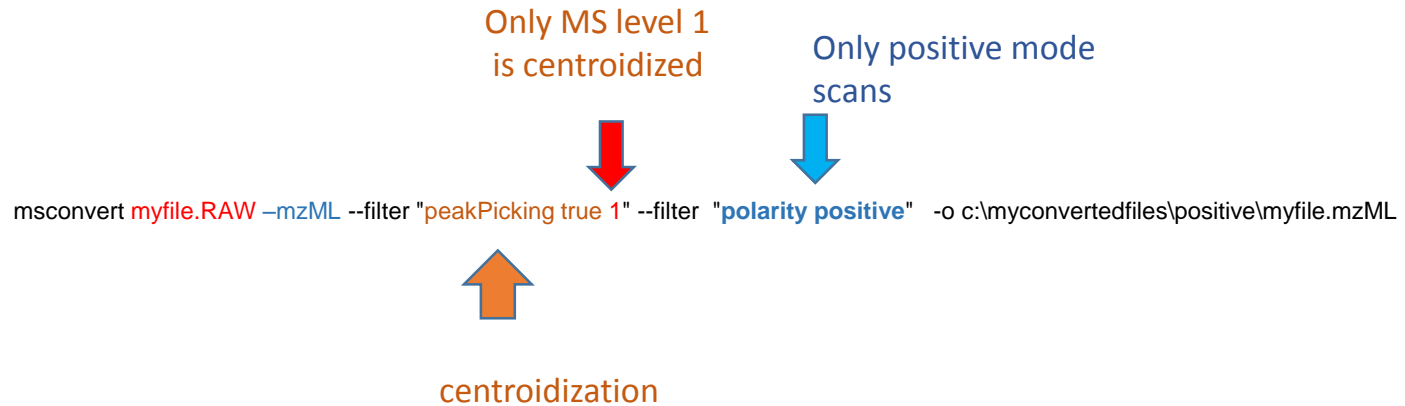
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- A Graphical User Interface
- Command lines



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<https://www.openchrom.net/>



<https://solutions.shimadzu.co.jp/form/msrl/license.html>