

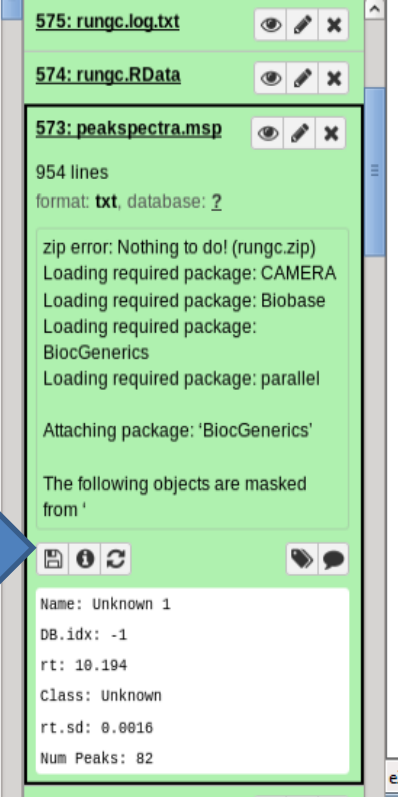
 	<h2>SOAP for peakspectra.msp file search with NIST MSSEARCH</h2>	<p>Redaction: GUITTON Yann Version: 20150408 Page 1 of 3</p> 
---	--	--

After the Galaxy workflow4metabolomics process for GCMS data you can download a peakspectra.msp file that can be searched against NIST MSSEARCH program on your GCMS computer.

To do so, follow this SOAP.

- 1- Download your **peakspectra.msp** file from galaxy website

Click on the floppy to start download



- 2- On your computer search for the program called nistms.exe (generally located on c:/NISTxx/MSSEARCH/ folder on the GCMS computer) and start it



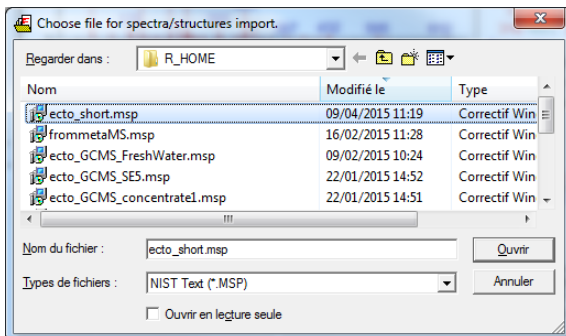


SOAP for peakspectra.msp file search with NIST MSSEARCH

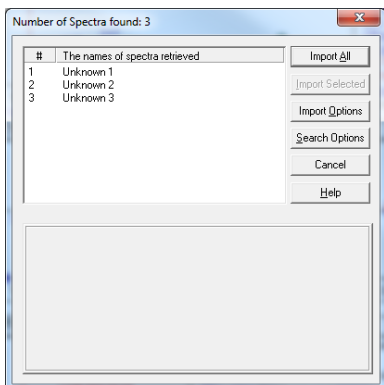
Redaction: GUITTON Yann
Version: 20150408
Page 2 of 3



3- On the menu: File→Open... and select the **peakspectra.msp**



4- Then Open and import all



5- The database search start automatically (or click on overwrite button)

6- Results

NIST MS Search 2.0 - [Quick, Penalize, Presearch Default - InLib = -194, 68 spectra]

File Search View Tools Options Window Help

1. Unknown 2

#	Src	Name
1	A	Unknown 1
2	A	Unknown 2
3	A	Unknown 3

Names / Structures / Spec List

gmd_20111121_md35_alk; replib; libr_gp; nist_n; 46636 total spectra

Mass Spectrum (Unknown 2):

- Major peaks at m/z 73, 116, 147, 190, 218, 233.
- Formula: C9H23NO2Si2
- MW: 233, CAS#: 27844-07-1, NIST#: 153056, ID#: 15453, DB: replib
- Contributor: Chemical Concepts
- 10 largest peaks: 116, 999, 73, 999, 147, 531, 147, 387, 190, 193, 75, 147, 59, 141, 118, 129, 74, 126, 100, 110
- Synonyms: no synonyms.

Mass Spectrum (I-Alanine, N-(trimethylsilyl)-, trimethylsilyl ester):

- Major peaks at m/z 73, 116, 147, 190, 218, 233.
- Formula: C9H23NO2Si2
- MW: 233, CAS#: 27844-07-1, NIST#: 153056, ID#: 15453, DB: replib
- Contributor: Chemical Concepts
- 10 largest peaks: 116, 999, 73, 494, 147, 137, 117, 116, 45, 63, 74, 43, 118, 40, 75, 39, 59, 35, 190, 34
- Synonyms: (replib) I-Alanine, N-(trimethylsilyl)-, trimethylsilyl ester

Names / Structures / InLib = -194, Hit List

Lib. Search Other Search Names Compare Librarian MSMS

Quick Quick Penalize

 	<p>SOAP for peakspectra.msp file search with NIST MSSEARCH</p>	<p>Redaction: GUITTON Yann Version: 20150408 Page 3 of 3</p> 
--	---	--

IF search do not start automatically please go to Options ->library search option and select Automatic Search On

