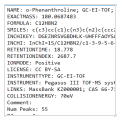

Oct 28, 2019

Steps for Building an Open Source EI-MS Mass Spectral Library for GC-MS -based Metabolomics

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1 *Works for me* dx.doi.org/10.17504/protocols.io.8txhwpn

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ABSTRACT

The objective of this protocol is to provide a set of instructions/ steps to guide ANY NEW USER to generate an open source EI-MS mass spectral library to aid in interpretation of GC-EI-MS spectral data for metabolomics research. Users need to appreciate and acknowledge the efforts of developers who have helped build and released their EI-MS spectral data and associated meta-data for free use and distribution from Mass Bank of North America (MoNA), RIKEN, GOLM Metabolome Database, Cayman, SWGDRUG, and NIST among others.

1 **From individual open source libraries download all the ".msp" or ".txt" files. Save them locally somewhere in a new folder. The names and links of the available open source spectral / retention time EI-MS libraries are:**

2 **MoNA- Mass bank of North America: https://mona.fiehnlab.ucdavis.edu/downloads**
RTX5 Fiehnlib (1,118 spectra)
GC-MS Spectra (15,114 spectra)
ReSpect (6,374 spectra)
HMDB (8,540 spectra)
MetaboBASE (1,254 spectra)

3 **RIKEN EI-MS Spectra**: http://prime.psc.riken.jp/Metabolomics_Software/MS-DIAL/index.html

Fiehn BinBase DB (Rtx5-Sil MS, predicted Kovats RI, 1021 records)
RIKEN DB (Rtx5-Sil MS, Kovats RI, 241 records)
Kazusa DB (Rtx5-Sil MS, Kovats RI, 273 records)
GL-Science DB (InertCap 5MS-NP, Kovats RI, 494 records)
Osaka Univ. DB (CPSil-8CB, Kovats RI, 430 records)
Fiehn BinBase DB (Rtx5-Sil MS, FAMEs RI, 1021 records)
RIKEN DB (Rtx5-Sil MS, predicted Fiehn RI, 241 records)
Kazusa DB (Rtx5-Sil MS, predicted Fiehn RI, 273 records)
GL-Science DB (InertCap 5MS-NP, predicted Fiehn RI, 494 records)
Osaka Univ. DB (CPSil-8CB, predicted Fiehn RI, 430 records)

4 **Cayman Spectral Library (**70eV EI mass spectral data of hundreds of Cayman Chemical's emerging forensic drug standards): https://www.caymanchem.com/forensics/publications/csl Needs registration and then one can download these spectra for free.

5 **GOLM Metabolome Database (**mass spectral reference library from biological specimens) : http://gmd.mpimp-golm.mpg.de/download/ (several options available depending on the column-type (VAR5/ MDN35) and RI marker used: FAME or Alkane mixes)

6 **SWGDRUG MS Library Version 3.6 (October 19, 2019):** http://www.swgdrug.org/ms.htm 3160 spectra

7

NIST, **USA** offers several EI-MS spectra for free as well: https://chemdata.nist.gov/dokuwiki/doku.php?id=chemdata:start NIST 17 GC Method / Retention Index MS Library- Extensive collection of GC retention indices with method information

8 **Now, open a notepad (.txt) file (do not save!) and drag one of these (any!) .msp library file onto this file and now save it as "YOUR NAME Library" (no file extension needed) just as it is (then it automatically is saved as .msp file format and you can scroll through to see the format/ style.**

9 **Now open, multiple .txt Notepad files and keep dragging the individual .msp files into these .txt files.**

10 **Copy these spectral information from the open .msp files one by one and copy out to "YOUR NAME Library" and let it keep growing. Just copy entire text files one after the other sequentially into a single .msp file.**

11 **That's it, "YOUR NAME GC-EI-MS" open source library is ready to go and be used for MS-DIAL spectral matching for spectra and/ RI or can be added to your AMDIS (NIST, USA) search as well.**