

Observations on Spectra in MoNA Database

<https://onlinelibrary.wiley.com/doi/abs/10.1002/mas.21535>

Libraries That I will Evaluate: mona-lc-ms_spectra-142,886 MSMS spectra and mona-export-gc-ms_spectra-18,886 EI spectra

mona-lc-ms_spectra-142,886 spectra

-summed library merged from other libraries on MoNA

-mainly MSMS, both positive and negative, maybe contaminated with a small amount of EI

does contain:

mona-export-embl-mcf-1293 MSMS spectra
mona-export-fiehn_hilic-3060 MSMS spectra
mona-export-gnps-23801 MSMS spectra
mona-export-hmdb-7,415 MSMS spectra
mona-export-lc-ms-ms_negative_mode-42,468 MSMS spectra
mona-export-lc-ms-ms_positive_mode-91,806 MSMS spectra
mona-export-massbank-72.240 MSMS spectra
mona-export-vaniya-fiehn_natural_products_library-44,936, MSMS spectra
mona-export-metabobase-1,254 MSMS spectra
mona-export-riken_plasma-8,655 MSMS spectra

mona-export-experimental_spectra

-summed library merged of other libraries on MONA, probably not generally useful for creating a NIST database

-mixture of EI, and MSMS and even for some strange reason, some in-silico

-179,964 spectra of 180,047 ID range

-contains a lot of in-silico-spectra starting around 10-4300 ID number, searching some by EI simple not found in mona-export-in-silico spectra list of 490,087 spectra; also these in-silico have no structures

-does contain (*details of library origin shown at bottom of document*):

mona-export-fiehn_hilic 3060 spectra MSMS
mona-export-gnps 23801 MSMS
mona-export-hmdb 7415, MSMS
mona-export-lc-ms-ms_negative_mode 42468, MSMS
mona-export-lc-ms-ms_positive_mode 91,807, MSMS
mona-export-lc-ms_spectra 142,891, MSMS
mona-export-massbank 72,360 MSMS
mona-export-respect 6,374 MSMS
mona-export-vaniya-fiehn_natural_products_library, 44936
mona-export-embl-mcf, 1,293 MSMS
mona-export-gc-ms_EI spectra 18886

mona-export-rtx5_fiehnlib, 1,118 EI of derivatives not indicating actually TMS or oxime derivative, etc.
mona-export-volatile_fiehnlib-212 EI

-does not contain entries from:

mona-export-fahfa which is an in-silico library, 4390
mona-export-metabobase 1,254 MSMS spectra
mona-export-riken_plasma, 8,655 MSMS spectra

GNPS mona-export-gnps 23,801 spectra, Global Natural Products Social Molecular Networking, MSMS

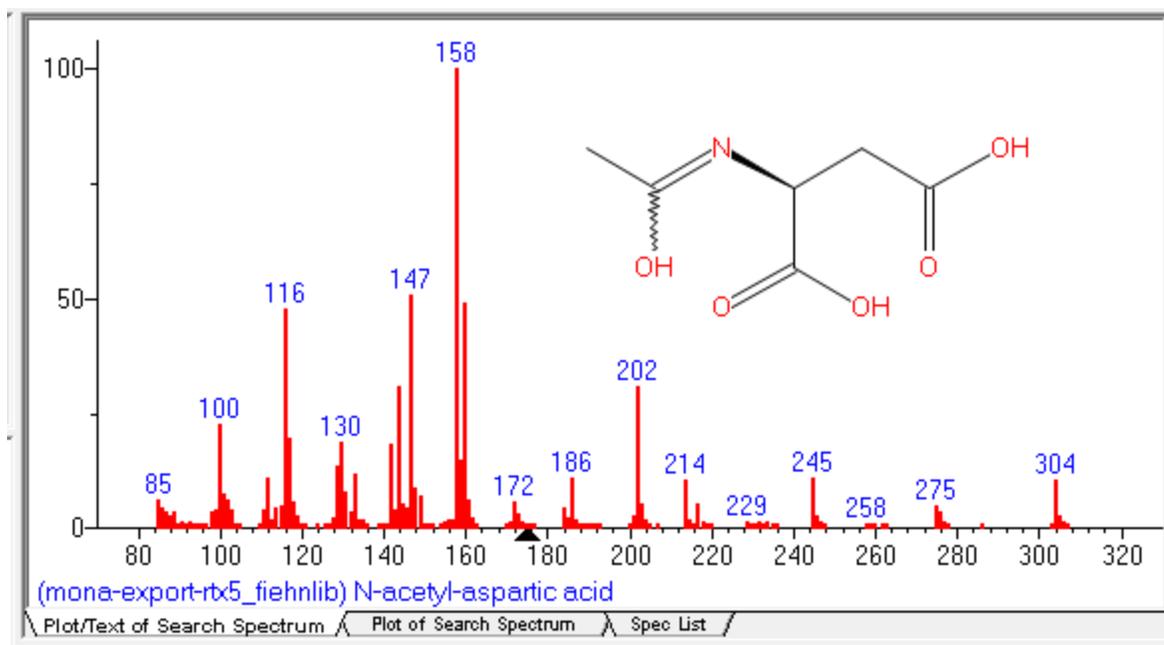
mona-export-hmdb-possibly Human Metabolome Database? Bruker?, 7413 spectra MSMS

mona-export-massbank-72360 spectra, probably the original collection?

https://www.researchgate.net/publication/45152587_MassBank_A_public_repository_for_sharing_mass_spectral_data_for_life_sciencesJ

mona-export-respect-6,374 spectra, Riken MSnspectral database for phytochemicals, MSMS;
<http://spectra.psc.riken.jp/>

mona-export-rtx5_fiehnlib-1,118 spectra, very strange spectra, says MS1 so assume EI, these spectra are actually derivatives as pointed out to me by Gary Mallard from NIST; unfortunately, they didn't point out which derivatives, e.g. TMS, oxime, etc. in the meta fields in the spectra; also didn't scan low enough to see m/z 73 for TMS derivatives; I searched and some are found in Wiley or NIST as the correct structure reflecting the derivatization



mona-export-fahfa-4,390, , in-silico; fatty acid esters of hydroxyl fatty acids, MSMS, see
<https://www.ncbi.nlm.nih.gov/pmc/articles/PMC4646931/> article

mona-export-fiehn_hilic 3060 spectra MSMS, does HILIC relate to type of chromatography used? see
<https://pubs.acs.org/doi/pdf/10.1021/acs.analchem.8b04698?rand=yhrhdgok>, Fiehn Laboratory UC Davis

mona-export-vaniya-fiehn_natural_products_library-44, 936 MSMS spectra, Fiehn Laboratory Natural Products, UC Davis

mona-export-volatile_fiehnlib-212 EI GCMS spectra, Fiehn Laboratory, UC Davis

mona-export-embl-mcf- Metabolomics Core Facility, 1,293 MS2 spectra, Pride Archive, Proteomics IDentifications Database? see <https://www.ebi.ac.uk/pride/archive/>; Wellcome Genome Campus, Hinxton, Carbridgeshire, UK; <https://www.embl.de/mcf/metabolomics-core-facility/>

mona-export-gc-ms_spectra-18,886 spectra, contains the EI library of mona-export-rtx5_fiehnlib, 1,118 EI spectra (original structure shown, actually TMS or oxime derivatives, no labeling in spectrum to reflect), and mona-export-volatile_fiehnlib-212, plus what?, maybe spectra from original MassBank collection?

mona-export-in-silico_spectra-490,087 in-silico spectra, not sure of origin, or classes of compounds, contains mona-export-lipidblast 485,796 spectra,

mona-export-lipidblast-LipidBlast in silico tandem mass spectrometry database for lipid identification <https://fiehnlab.ucdavis.edu/projects/lipidblast>, 485,796 MSMS and mona-export-fahfa-4,390

mona-export-metabobase-1254 MSMS spectra, possibly Bruker database, see <https://www.bruker.com/products/mass-spectrometry-and-separations/ms-software/metabolomics-spectral-libraries/overview.html>

mona-export-riken_plasma-8,655 MSMS spectra, possibly from <http://prime.psc.riken.jp/>

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