

Lib2NIST v1.0.9.18(beta) command line options

Starting from version 1.0.0.6 (beta), the Lib2NIST library conversion utility can be run from a batch file. This possibility is reserved for advanced users and is not necessary for most conversions.

Important: In all input text files, lines must end with Carriage Return/Line Feed characters (CRLF, "\r\n")

General Lib2NIST command line options rules:

- Options are separated by spaces.
- Options are not case-sensitive.
- If an option must contain spaces, it should be enclosed in "double quotes". If a quoted option ends with a backslash, one more backslash must be added before the closing double quote, e.g. "c:\my libraries\\"
- Options containing characters equal sign "=" or colon ":" should not have spaces around them.
- Since the command line is read by Lib2NIST from left to right, meaning of an option may be affected by options located to the left from it.
- Variable parts of options described below are in ***Bold Italics***; fixed parts (necessary to recognize options) are in **Bold**.
- Lib2NIST differentiates between options according to the following characteristic features:
 - starting with a slash "/"
 - starting with a slash and containing an equal sign "=" or colon ":" inside
 - starting with an equal sign "=" (an output library or file name)
 - ending with a backslash "\" (an output path)
 - file (path)name with a predefined extension (.INI or .LOG)
- Lib2nist_dll.dll is not aware of Windows Registry and does not use .INI files.

COMMAND LINE OPTIONS

The following command line options are recognized. Whenever a file name without the path is used as a command line option, the current path or the default path from the Windows Registry or .INI file is used.

/LOGn (example: /LOG3). Write logfile, details level 3.

- Contents of all dialogs informing the user about errors and warnings are redirected to the logfile. All questions asked in the dialog (non-logged) mode are automatically answered Yes and logged. Lib2NIST automatically terminates upon completion.
- n=0..11 sets level of warnings; the greater the n, the more detailed information is written into the logfile.
- The default logfile name is Lib2NIST.LOG; it is located on the current path.
- Most of the warnings lines contained in the logfile start with the level number (for example, L3 for details level 3)
- Lines without indentation refer to the spectrum ID located below them.

Logfile.LOG Logfile (path)name, must have extension .LOG

- Set custom logfile name or pathname. If **/LOGn** option is not used, level n is 0.
- If neither **/LOGn** nor **Logfile.LOG** option is used then the logging is disabled.
- If containing Logfile folder does not exist, it will be created if possible.

/LOGINI Dump current Windows Registry settings

- Dump current Lib2NIST Windows Registry settings (as they are at the startup) into the file Lib2NistSaved.INI located on the current path.

Inifile.INI Custom initialization file; must have extension .INI

- Read settings from this file; missing settings are read from the Windows Registry. Changes in settings will be written to this file instead of the Registry. If this file does not exist, it is created and Windows Registry settings are saved in it. This option prevents Registry from changing.

/DeleteINI Delete initialization file.(Infile.INI) upon Lib2NIST exit (*not implemented*).

InputFile or InputLibrary One or more Input datafiles or library names with full pathnames.

- This option suppresses normally displayed on startup "Select Input Library or DataFile" dialog and starts conversion immediately.
- Datafiles must have extensions from the following list: .SDF, .MSP, .JDX, .DX, .HPJ, .JX, .JC, .JCM
- HP/Agilent MS library folders should have extension ".L"
- NIST MS User library is recognized according to the contents of the library directory.
- Full pathname overrides .INI and Windows Registry input path settings
- INI file setting of [Directory] Input= overrides Windows Registry settings
- /UCP option (see below) overrides .INI and Windows Registry input path settings unless full pathname is specified.

/InpList=pathname (no spaces around '=' allowed.) File *pathname* contains input file or library full pathnames, one per line. No quotes, leading or trailing spaces allowed.

/UCP or /UseCurrentPathForInputData Use current path for input datafile or library

- In case of missing path in the **InputFile** or **InputLibrary** this option forces Lib2NIST to use current path instead of INI file setting of [Directory] Input=.. It is also used in case of a relative **OutputPath**.

OutputPath Set destination path. Must end with a backslash, "\".

- Write conversion results to the specified path. This option overrides .INI file setting of [Directory] Output=. If no output path has been specified, current path is used. If **OutputPath** does not exist, it will be created if possible.

=OutputName Set single destination file or library name. No spaces after "=" allowed. .

- Write conversion results of all input files and/or libraries to the specified destination. This option creates one library or datafile out of several input libraries and/or files. The option turns off after the completion of the first successful conversion. If the name is invalid, then the option is ignored.

=OutputPath\OutputName Set single destination file or library. No spaces after "=" allowed. .

- Write conversion results of all input files and/or libraries to the specified destination. This option creates one library or datafile out of several input libraries and/or files. If **OutputPath** does not exist it will be created if possible. The option turns off after the completion of the first successful conversion; however, it overrides .INI file setting of [Directory] Output=. If the pathname is invalid, then the option is ignored.

/1stID=nnn Set the first output spectrum ID; create sequential IDs. No spaces allowed.

- Set the value of the ID of the first spectrum to be converted. All other spectra will have sequential ID values. This option temporarily overrides ini or Windows Registry [Output]KeepIDs=1 setting and forces the IDs to be written into the output file(s). This option does not apply to HP-JCAMP output.

Example: /1stID=1500

/NOEXTRA Ignore HP-JCAMP-specific extra data in comments

- Without this option Lib2NIST recognizes |BP:nnn|MP:nnn|RI:nnn| within the comments of the input spectra as boiling point, melting point and retention index values. When BP, MP, or RI is defined, this information in the same format is added to the comments in the output NIST MS User library spectra and in the output .MSP file. This option enforces old behavior of Lib2NIST when comments are not interpreted and are left unchanged.

/NoAlias Do not create a folder with file alias.msd in NIST MS Search folder.

- Normally, when Lib2NIST creates a library, it also creates a subfolder in NIST MS Search base folder that contains file ALIAS.MSD. The only line in this folder is the path pointing to the newly created library. After NIST MS Search has been restarted, this file provides to the MS Search a link to the new library. The ALIAS.MSD creation may be prevented in two ways: use /NoAlias option or line NIST=<None> in the Directory section of the ini file.

/Tab4QC Output TAB4QC lines for all spectra

/Norm9999 Special intensity normalization if max. intensity is 9999 or 10000

/ToV2000 Add V2000 and M END to older versions of molfiles; incompatible with /CopySdf2Sdf

/IsotopesInFormula Allow isotopes in format [13C]2H6 – incompatible with NIST MS Search.

/AllowNoPeaks Do not require mass spectral peaks. Useful for creating chemical structure library.

/Z Do not discard mass spectral peaks that have zero abundances; see also /Z:S below.

/KeepAbund Copy original peak abundances from the input to the output text file

/OldRI If output text format is HP JCAMP (.hpl), output RI in old format (no ##Library_RI=...)

/ShortRiLabel Produce 1-letter RI label in <RETENTION INDEX> (e.g. n=123 instead of StdNP=123)

/McSDF¹ or /MultilineCommentSdf – merge multiline Comment and Contributor in input SDF

/StdRounding Round m/z in imported EI spectra to the nearest integer.

/Rounding=Mpy,Add Mpy=multiplier, Add=subsequent shift. StdRounding sets Mpy=1, Add=0

/OutLib Output MS Library. Equivalent to Output Format = NIST MS Library)

/OutMSP² Output .MSP file. Equivalent to Output Format = Text File (.MSP)

/OutSDF Output SDfile. Equivalent to Output Format = SDFFile (.SDF)

/OutJCAMP Output JAMP file. Equivalent to Output Format = HP JCAMP File (.HPJ)

/com2tag Extract and remove tagged expressions³ from the comment. An example of tagged

¹ Also charge -- or ++ in PRECURSOR TYPE is replaced with 2- or 2+.

The following **input** <INSTRUMENT TYPE> strings are replaced:

| input | new <INSTRUMENT TYPE> | new <IONIZATION> | Separation= |
|--------------|--------------------------|------------------|-------------|
| EI-QTOF | Q-TOF | EI | |
| ESI-IT | IT/ion trap | ESI | |
| ESI-ITFT | IT-FT/ion trap with FTMS | ESI | |
| ESI-QTOF | Q-TOF | ESI | |
| GC-EI-TOF | Other | EI | GC |
| LC-APCI-QTOF | Q-TOF | APCI | LC |
| LC-ESI-IT | IT/ion trap | ESI | LC |
| LC-ESI-ITFT | IT-FT/ion trap with FTMS | ESI | LC |
| LC-ESI-QFT | HCD | ESI | LC |
| LC-ESI-QQ | QqQ | ESI | LC |
| LC-ESI-QQQ | QqQ | ESI | LC |
| LC-ESI-QTOF | Q-TOF | ESI | LC |

where tagged expression Separation=GC or Separation=LC is added to the <COMMENT>.

² To output MSP file with linked molfiles, instead of /OutMSP use /OutMSP_and_Mol_linked_by_NISTrn, /OutMSP_and_Mol_linked_by_ID, /OutMSP_and_Mol_linked_by_CASrn, or /OutMSP_and_Mol_linked_by_CASrn_ID.

³ In /com2tag mode, tagged expressions are expected to have format Tag=value or Tag="value" and are separated by spaces. Inside the tagged expression, spaces are allowed only in the quoted value. Letter case in the Tag is ignored. Accepted tags are AUX, Charge, Collision_energy or CollisionV, Collision_gas, Compound_type, Cone_voltage or In-source_voltage or ConeV, Instrument, Instrument_type, Ion_Formula, Ion_mode, Ion_MW, Ion_name, Ionization, Known_impurity, Mass_range, Maximum_intensity, Peptide_mods or Mods, Peptide_sequence, Precursor_m/z or Mz_exact, Precursor_type, Pressure, Related_CAS#, Salt, Salt/mix_CAS#, Sample_inlet, Special_fragmentation, Spectrum_type. MW with a decimal point and value ≥ 1 is interpreted as exact mass. If the same tag is already present in the spectrum then it is not extracted and left in the comment.

expression is `Ion_type=[M+H]+`. Technically, tagged expressions are moved into `$.nn-` type synonyms. Supported formats are NIST MS library, text files in MSP and SDF formats.

/MsmIncNames In case of MS/MS library output, create MS Search Names window content specific for NIST 14 MS/MS libraries. Precursor type or in-source spectrum type entries in the spectra are required. Incompatible with `/PepIncNames` option.

/PepIncNames In case of MS/MS library output, create MS Search Names window content specific for NIST Tandem Peptide Libraries. Incompatible with `/MsmIncNames` option.

/MSKEY=*ms_label* /SDFKEY=*sdf_label* Merge linked mass spectral file and SDfile into one output. No spaces around "=" allowed

- Convert mass spectral data from .MSP or JCAMP format and data (including structures) from the linked to it SDfile. *ms_label* and *sdf_label* in the command line should be substituted with corresponding labels located in the input files.
- The SDfile must have the same name as the mass spectral datafile and have extension .SDF; it should be located in the same directory as the mass spectral datafile.
- Mass spectra and SDfile data blocks are linked into pairs by character-to-character identical *ms-value* and *sdf-value* located within them:

ms_label: *ms-value* (in MSP-file) or
##*ms_label* = *ms-value* (in JCAMP-MS file)

and

> <*sdf_label*>
sdf-value
(blank line)

- Leading and trailing spaces in *ms-value* and *sdf-value* are ignored. Letter case is not ignored.
- Names of the labels *ms_label*, *sdf_label* should not contain white spaces, ?, /, +, -, <, >, (,), [,], |, *, or punctuation characters (, ; :).
- One SDfile block can be linked to several mass spectra.
- Example: Word NAME can serve as an example of both *ms_label* and *sdf_label* if names in the mass spectra and SDfile blocks can be used for linking, that is, are identical and unique. In this case, word HYDROGEN could be both *ms-value* and *sdf-value* to link hydrogen mass spectrum and structure together.
- Minimal set of command line options to add structures from str.SDF to inp.SDF and write results to out.SDF:
`/OutSdf /CopySdf2Sdf "inp.SDF" "=out.SDF" "/StructSource=str.SDF" /MSKEY=inp_label /SDFKEY=str_label`
where labels *inp_label* are in *inp.SDF*, *str_label* - in *str.SDF*. Double quotes are used to allow spaces inside. *inp.SDF*, *out.SDF*, *str.SDF* may be full pathnames to SDFfiles.
- Molfile name may be placed in the input spectrum. Use tags **molfilename:** and **<MOLFILE NAME>** in .MSP and SDFfile, respectively. The *ms-* or *sdfkey* value, if present, will be added to the end of it.

/msp2peplib Convert NIST peptide library MSP file (typically, *_consensus_final_true_lib.MSP) into a peptide MS/MS library. Implies options `/IncludeSynonyms:Y /KeepIDs:N /MwFromFormula:N /MsmOnly:Y /Msm2008-Compat:N /UseSubset:N /Z /NOEXTRA /StdRounding /OutLib`. It is not advisable to change these options. Option `/msp2peplib` sorts library spectra by precursor m/z values for faster searching, shortens protein names, truncates lists of homologues, encodes references and removes unused ones into an overflow file. It creates two peptide library-specific files, "references.txt" and "overflow.txt". Created in the library folder file "__log.txt" may be safely deleted.

/MspLinkedByNISTrn Add "Text File (.MSP) + MOLfiles linked by NIST#" option to Output Format drop

down list box, which creates molfiles named N<NIST r.n.>.MOL. When converting a filename.MSP file accompanied by filename.MOL folder containing molfiles, the molfiles are picked up according to (1) NIST r.n., (2) CAS r.n., (3) ID number.

- /PeakMzDecPlaces=*n*** Round peak m/z values to *n* decimal places. This may be overridden in the input MSP or SDF file⁴; *n* = **keep** means do not change m/z values by removing trailing zeroes
- /PrecurMzDecPlaces=*n*** Round precursor m/z values to *n* decimal places. *n* = **keep** means do not change m/z values by removing trailing zeroes
- /AccuratePeakMZ** In MS/MS Spectra Only mode (also set by **/MsmsOnly:S** option), accurate peak m/z and intensities in the range 0.01-999 are saved in a MS/MS library even though a spectrum does not have precursor m/z and *Spectrumtype* does not begin with *in-source* or *accurate*⁵. The integer m/z peaks used for EI search are saved as for an EI spectrum.

In options below, S is letter Y or N

- /IncludeSynonyms:S** Same as “Include Synonyms” check box in Options dialog.
- /KeepIDs:S**⁶ Same as “KeepIDs Unchanged” check box in Options dialog.
- /MakeInChIKeys:S** Calculate InChIKey from each input chemical structure, add it to the spectrum, and use it for indexing output library. Default: **Y** except JCAMP output. In case of **N**, InChIKey, if present in the input spectrum, is used for indexing. If no InChIKeys were found or created, file *inchikey.inu* contains strings “None” instead of missing InChIKeys..
- /MwFromFormula:S** Same as “MW from chem. formula” check box in Options dialog.
- /MsmsOnly:S** Same as “MS/MS spectra only” check box in Options dialog. Create MS/MS or in-source library, including Glycopeptide library
- /Msms2008-Compat:S** Same as “2008 MS Search compatible” check box in Options dialog.
- /KeepStruct:S** with **/OutLib** only: Do not save in a library only a single copy of multiple identical structures
- /Minset** Create only *user.dbu*, *user.inu*, *mztxt.dbu*, *mztxt.inu*, *precmz.inu*, *usrstruc.db* & *struct* index files.

⁴ For example, to set maximal number of peak m/z decimal places to 4 in a MSP file spectrum, include in the spectrum line

Max_m/z_decimal_places: 4

Include in SDfile the following 2 lines followed by a blank line in a SDfile spectrum:

```
> <MAX M/Z DECIMAL PLACES>
```

```
4
```

Note that this entry, as well as precursor m/z entry must precede mass spectral peaks.

⁵ In an MSP file, line *Spectrum_type*: *in-source* or *Spectrum_type*: *accurate* makes Lib2NIST save the accurate product peak m/z even though the spectrum does not have precursor m/z. In an SDfile, the following 3 lines

```
> <SPECTRUM TYPE>
```

```
in-source
```

(the 3rd line is blank) have the same effect. This line should be located before the peak list. In these cases, integer m/z peaks used for EI search are saved as if the spectrum were MS/MS.

⁶ **S=Y** is ignored, as well as “KeepIDs Unchanged” check box in Options dialog, when creating a read-only (e.g. MS/MS) library. To override, use **/KeepIDs=Yes**. However, note that in this case the conversion will fail if it encounters spectrum ID = 65,536×N, where N=1, 2, 3, ... or two equal IDs. If input spectra do not have IDs, not more than 65,535 spectra may be converted into a library. If **S=N**, the output spectra do not have ID = 64K and a multiple of 64K=65536.

/UseSubset:S Same as check box "Use subset".

/[F]Subset={ID|CASrn|NISTrn},{All|First},{Pathname|String} FSubset – from file, Subset – from string

/Z:S Y – the same as /Z. N – discard mass spectral peaks that have zero abundances even though the spectra are treated as MS/MS

/SdfRemAliases Remove alias lines from molfile

/SdfSetKnownValences, /SdfSetAllValences, /SdfClearKnownValences – molfile output options

/BL=nn Set average bond length in chemical structures

/SdfFormula=str Tag for chemical formula in input SDF file

/SdfMw=nn Tag for MW in input SDF file

/TranslateTextInput:S Y – apply character translation table from HPTRANS.TBL file to text input file(s) (Default). N – do not apply (behavior before v.1.0.4.26.)

/TranslateHexUnc=FPN In text input, replace Hexadecimal Unicode letters with ASCII (e.g. replace &03B1; with .alpha.). *FPN* is a full pathname to the translation dictionary file. An example of such a dictionary file is TransHexUnc.txt included in the package. First time implemented in v.1.0.6.6 (beta). An example of TransHexUnc.txt contents:

```
&00B1; ".+/-."
&0394; ".DELTA."
&039F; "O"
&03A9; ".OMEGA."
&03B1; ".alpha."
&03B2; ".beta."
&03B3; ".gamma."
&03B4; ".delta."
&03B5; ".epsilon."
&03B6; ".zeta."
&03B7; ".eta."
&03BA; ".kappa."
&03BB; ".lambda."
&03BC; ".mu."
&03BE; ".xi."
&03BF; "o"
&03C0; ".pi."
&03C3; ".sigma."
&03C9; ".omega."
&200B; ""
&2032; "' '"
&2192; "->"
&2206; ".DELTA."
&2212; "- "
&2265; ">="
$a     ".alpha."
$b     ".beta."
$g     ".gamma."
```

Recognized by Lib2NIST Instrument types in MS/MS spectra

| Instrument type check box in MS Search | Instrument type field in MS/MS mass spectrum |
|--|--|
| Ion Trap | "IT/ion trap" or "QQIT" or "QqLIT" |
| Ion Trap + FT | "IT-FT/ion trap with FTMS" |
| Q-TOF | Q-TOF |
| HCD | HCD |
| QqQ or Triple quadrupole | "QqQ/triple quadrupole" or "QqQ" |
| Other | any other than the above Instrument types |
| Unspecified | No instrument type specified |

Part of Instrument type starting with the slash (/) may not be omitted (e.g., IT-FT is not recognized.)

Concurrency issues

Since Lib2NIST normally reads and stores conversion parameters into the Windows Registry, two instances of Lib2NIST running simultaneously may interfere with unpredictable consequences. To avoid this, each copy of Lib2NIST may be run with its own .INI file. Lib2NIST running with .INI file does not change contents of the Windows Registry. Lib2NIST reads from the Windows Registry only if the needed conversion parameter is missing from the specified in the command line .INI file.

Windows NT/2000/XP/Vista/7/8/10 issues

If the amount of data to be converted is significant, it may be convenient to run Lib2NIST at low priority in case of a single core processor. To do that you may run it from the batch file using "START" command:

```
start /LOW /WAIT V:\Lib2NIST\lib2nist.exe <Lib2NIST command line options>
```

/LOW provides low priority

/WAIT means the next batch file line will be executed upon Lib2NIST termination.

Example

The following example shows how to transform HP/Agilent MS library C:\Mylib.L into the NIST User library Mylib.HP located in the C:\NIST98\MSSEARCH directory

Command line in the batch file:

```
lib2nist /log9 Mylib.log Mylib.ini C:\Mylib.L c:\nist98\mssearch\
```

/log9: Lib2NIST will produce the most detailed output to the logfile

Mylib.log the logfile Mylib.log will be located in the current directory

Mylib.ini Lib2NIST will read conversion options from Mylib.ini located in the current directory

C:\Mylib.L Input HP/Agilent type library location

c:\nist11\mssearch\ the result will be directed to this directory

Mylib.ini contents:

[Directory]

```

NIST=C:\NIST98\MSSEARCH
[Output]
Text=0
TextFileType=0
DB=1
CalcMW=1
IncludeSynonyms=1
KeepIDs=1
LinkMOLfile=0
MzAdd=0
MzMpy=1
NeedSubset=0

```

To create NIST User library Mylib instead of Mylib.HP, use command

```

lib2nist /log9 Mylib.log Mylib.ini C:\Mylib.L c:\nist98\mssearch\ =Mylib
or
lib2nist /log9 "Mylib.log" "Mylib.ini" "C:\Mylib.L" "=c:\nist98\mssearch\Mylib"

```

Without the .ini file the same may be accomplished by the following command line options:

```

lib2nist /log9 "Mylib.log" /OutLib /MwFromFormula:Y /IncludeSynonyms:Y /KeepIDs:Y
/StdRounding:Y /UseSubset:N "C:\Mylib.L" "=c:\nist98\mssearch\Mylib"

```

Currently, there is no command line option to set or ignore previously saved linking to molfiles

Below is a copy of Lib2NIST.INI file containing comments explaining its contents.

```

;=====
; Lib2NIST.ini contents explanations
; Lines starting with semicolons are comments.
;=====

;=====
[Directory]
;=====

; Input directory (contains libraries, datafiles).
Input=S:\INPUT

; Output directory (can be same as NIST).
Output=D:\Lib2NIST.RES

; NIST MS Search base directory (where alias.msd goes) or <None>
NIST=S:\NIST98\MSSEARCH
;NIST=<None>

; Input type: 0=>all except JCAMP, 1=>JCAMP <== do not use
;Type: 0

;=====

```

```

[Output]
;=====

; 1=>Produce NIST MS Library, 0=>No.
DB=1

; 1=>Produce MS ASCII text file, 0=>No.
Text=0

; Output MS ASCII file type: 0=>MSP, 1=>HP-JCAMP, 2=>SDF
TextFileType=0

; 1=>Calculate normalized MW from chemical formula, 0=>get MW from the input
CalcMW=1

; 1=>Include synonyms into the output, 0=>do not include
IncludeSynonyms=1

; 0=>Auto Assign IDs (1,2,3,...), 1=> get IDs from the input
KeepIDs=0

; Output structures as MOLfiles (applies to TextFileType=0 only)
;0=>No MOLfile output, 1=>MOLfile names from ID, 2=>from CAS, 3=>Both
LinkMOLfile=0

; m/z when reading text file = floor((Input m/z)*MzMpy + MzAdd + 0.5)
MzAdd=0
MzMpy=1

; 1=>treat spectra as ms/ms; 0=>No
MsmsOnly=0

; 1=>Output MS/MS library is compatible with 2008 MS Search; 0=>Compatible with newer software
Msms2008-Compat=1

; 0=>Do not use Subset, 1=>Use subset
NeedSubset=0

;=====
[Subset]
;=====

; subset type: 1=>IDs, 2=>CAS
Type=1

; 1=>apply subset to all input
; 0=>to the 1st input file or library only, then ask.
ForAll=1

; 0=>get subset string from this ini file (CasStr or IdStr)
; 1=> read subset from a separate file
FromFile=0

```

```
; pathname of file with subset containing CAS registry numbers  
CasFile=Y:\HP\Subset.CAS
```

```
; subset string containing CAS numbers  
CasStr=50362-50555
```

```
; pathname of file with subset containing input IDs  
IdFile=Y:\HP\Subset.ID
```

```
; subset string containing IDs  
IdStr=1-4500
```