convertMSP.R User Manual

(Version 1, 2020-09-25)

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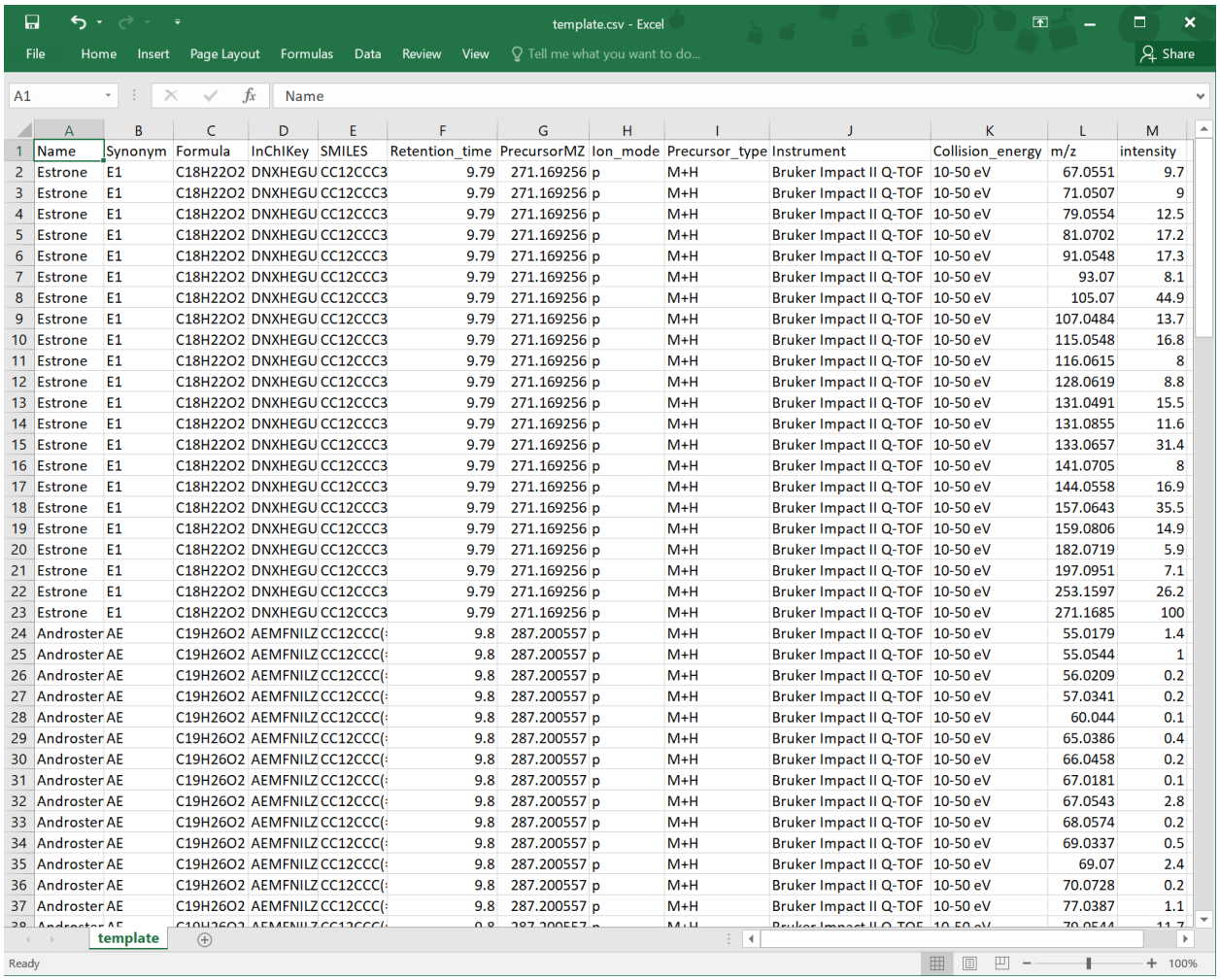
- This script constructs MS^2 spectral libraries in MSP format from a prepared csv file containing the MS^2 spectra and other related information.
- The program is written in the R language and is publicly available at https://github.com/HuanLab/DaDIA.git.
- Please see below for the code instructions.

1) Prepare the csv file following the template shown as below.
   For each MS^2 spectrum, prepare the following information and fill in the corresponding columns: 'Name', 'Synonym', 'Formula', 'InChIKey', 'SMILES', 'Retention_time', 'PrecursorMz', 'Ion_mode', 'Precursor_type', 'Instrument' and 'Collision_energy'. For each fragment ion, fill their *m/z* values and intensities into 'm/z' and 'intensity' columns.
   Note: Not all of the information is necessary other than the columns 'Name', 'm/z' and 'intensity'. Delete the unwanted columns. The columns 'm/z' and 'intensity' must be the last two columns of the csv file.



template.csv - Excel

	Name	Synonym	Formula	InChIKey	SMILES	Retention_time	PrecursorMZ	Ion_mode	Precursor_type	Instrument	Collision_energy	m/z	intensity
2	Estrone	E1	C18H22O2	DNXHEGU	CC12CCC3	9.79	271.169256	p	M+H	Bruker Impact II Q-TOF	10-50 eV	67.0551	9.7
3	Estrone	E1	C18H22O2	DNXHEGU	CC12CCC3	9.79	271.169256	p	M+H	Bruker Impact II Q-TOF	10-50 eV	71.0507	9
4	Estrone	E1	C18H22O2	DNXHEGU	CC12CCC3	9.79	271.169256	p	M+H	Bruker Impact II Q-TOF	10-50 eV	79.0554	12.5
5	Estrone	E1	C18H22O2	DNXHEGU	CC12CCC3	9.79	271.169256	p	M+H	Bruker Impact II Q-TOF	10-50 eV	81.0702	17.2
6	Estrone	E1	C18H22O2	DNXHEGU	CC12CCC3	9.79	271.169256	p	M+H	Bruker Impact II Q-TOF	10-50 eV	91.0548	17.3
7	Estrone	E1	C18H22O2	DNXHEGU	CC12CCC3	9.79	271.169256	p	M+H	Bruker Impact II Q-TOF	10-50 eV	93.07	8.1
8	Estrone	E1	C18H22O2	DNXHEGU	CC12CCC3	9.79	271.169256	p	M+H	Bruker Impact II Q-TOF	10-50 eV	105.07	44.9
9	Estrone	E1	C18H22O2	DNXHEGU	CC12CCC3	9.79	271.169256	p	M+H	Bruker Impact II Q-TOF	10-50 eV	107.0484	13.7
10	Estrone	E1	C18H22O2	DNXHEGU	CC12CCC3	9.79	271.169256	p	M+H	Bruker Impact II Q-TOF	10-50 eV	115.0548	16.8
11	Estrone	E1	C18H22O2	DNXHEGU	CC12CCC3	9.79	271.169256	p	M+H	Bruker Impact II Q-TOF	10-50 eV	116.0615	8
12	Estrone	E1	C18H22O2	DNXHEGU	CC12CCC3	9.79	271.169256	p	M+H	Bruker Impact II Q-TOF	10-50 eV	128.0619	8.8
13	Estrone	E1	C18H22O2	DNXHEGU	CC12CCC3	9.79	271.169256	p	M+H	Bruker Impact II Q-TOF	10-50 eV	131.0491	15.5
14	Estrone	E1	C18H22O2	DNXHEGU	CC12CCC3	9.79	271.169256	p	M+H	Bruker Impact II Q-TOF	10-50 eV	131.0855	11.6
15	Estrone	E1	C18H22O2	DNXHEGU	CC12CCC3	9.79	271.169256	p	M+H	Bruker Impact II Q-TOF	10-50 eV	133.0657	31.4
16	Estrone	E1	C18H22O2	DNXHEGU	CC12CCC3	9.79	271.169256	p	M+H	Bruker Impact II Q-TOF	10-50 eV	141.0705	8
17	Estrone	E1	C18H22O2	DNXHEGU	CC12CCC3	9.79	271.169256	p	M+H	Bruker Impact II Q-TOF	10-50 eV	144.0558	16.9
18	Estrone	E1	C18H22O2	DNXHEGU	CC12CCC3	9.79	271.169256	p	M+H	Bruker Impact II Q-TOF	10-50 eV	157.0643	35.5
19	Estrone	E1	C18H22O2	DNXHEGU	CC12CCC3	9.79	271.169256	p	M+H	Bruker Impact II Q-TOF	10-50 eV	159.0806	14.9
20	Estrone	E1	C18H22O2	DNXHEGU	CC12CCC3	9.79	271.169256	p	M+H	Bruker Impact II Q-TOF	10-50 eV	182.0719	5.9
21	Estrone	E1	C18H22O2	DNXHEGU	CC12CCC3	9.79	271.169256	p	M+H	Bruker Impact II Q-TOF	10-50 eV	197.0951	7.1
22	Estrone	E1	C18H22O2	DNXHEGU	CC12CCC3	9.79	271.169256	p	M+H	Bruker Impact II Q-TOF	10-50 eV	253.1597	26.2
23	Estrone	E1	C18H22O2	DNXHEGU	CC12CCC3	9.79	271.169256	p	M+H	Bruker Impact II Q-TOF	10-50 eV	271.1685	100
24	Androster	AE	C19H26O2	AEMFNILZ	CC12CCC(	9.8	287.200557	p	M+H	Bruker Impact II Q-TOF	10-50 eV	55.0179	1.4
25	Androster	AE	C19H26O2	AEMFNILZ	CC12CCC(	9.8	287.200557	p	M+H	Bruker Impact II Q-TOF	10-50 eV	55.0544	1
26	Androster	AE	C19H26O2	AEMFNILZ	CC12CCC(	9.8	287.200557	p	M+H	Bruker Impact II Q-TOF	10-50 eV	56.0209	0.2
27	Androster	AE	C19H26O2	AEMFNILZ	CC12CCC(	9.8	287.200557	p	M+H	Bruker Impact II Q-TOF	10-50 eV	57.0341	0.2
28	Androster	AE	C19H26O2	AEMFNILZ	CC12CCC(	9.8	287.200557	p	M+H	Bruker Impact II Q-TOF	10-50 eV	60.044	0.1
29	Androster	AE	C19H26O2	AEMFNILZ	CC12CCC(	9.8	287.200557	p	M+H	Bruker Impact II Q-TOF	10-50 eV	65.0386	0.4
30	Androster	AE	C19H26O2	AEMFNILZ	CC12CCC(	9.8	287.200557	p	M+H	Bruker Impact II Q-TOF	10-50 eV	66.0458	0.2
31	Androster	AE	C19H26O2	AEMFNILZ	CC12CCC(	9.8	287.200557	p	M+H	Bruker Impact II Q-TOF	10-50 eV	67.0181	0.1
32	Androster	AE	C19H26O2	AEMFNILZ	CC12CCC(	9.8	287.200557	p	M+H	Bruker Impact II Q-TOF	10-50 eV	67.0543	2.8
33	Androster	AE	C19H26O2	AEMFNILZ	CC12CCC(	9.8	287.200557	p	M+H	Bruker Impact II Q-TOF	10-50 eV	68.0574	0.2
34	Androster	AE	C19H26O2	AEMFNILZ	CC12CCC(	9.8	287.200557	p	M+H	Bruker Impact II Q-TOF	10-50 eV	69.0337	0.5
35	Androster	AE	C19H26O2	AEMFNILZ	CC12CCC(	9.8	287.200557	p	M+H	Bruker Impact II Q-TOF	10-50 eV	69.07	2.4
36	Androster	AE	C19H26O2	AEMFNILZ	CC12CCC(	9.8	287.200557	p	M+H	Bruker Impact II Q-TOF	10-50 eV	70.0728	0.2
37	Androster	AE	C19H26O2	AEMFNILZ	CC12CCC(	9.8	287.200557	p	M+H	Bruker Impact II Q-TOF	10-50 eV	77.0387	1.1

2) Get the R package “metaMS” installed by running the following code in Rstudio.

```
if (!requireNamespace("BiocManager", quietly = TRUE))
    install.packages("BiocManager")
BiocManager::install("metaMS")
```

3) Download and open the R script “convertMSP.R” in Rstudio.
4) Change the working directory. Use “/” instead of “\”.

```
# set working directory
directory <- 'E:/spectral_library'
```

5) Change the prepared csv file name.

```
# name of the prepared csv file
csv_name <- 'template.csv'
```

6) Click “Source”, and the converted spectral library named “spectral_library.msp” will be created in the working directory.