convertMSP.R User Manual

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Jian Guo[1], Sam Shen[1], Liu Min[2], Chenjingyi Wang,[1] Ying Chen[1], Shipei Xing[1], Huaxu Yu[1], Yaxi Hu[1], Yu Gao[3], Mingliang Fang[2], Tao Huan[1]*

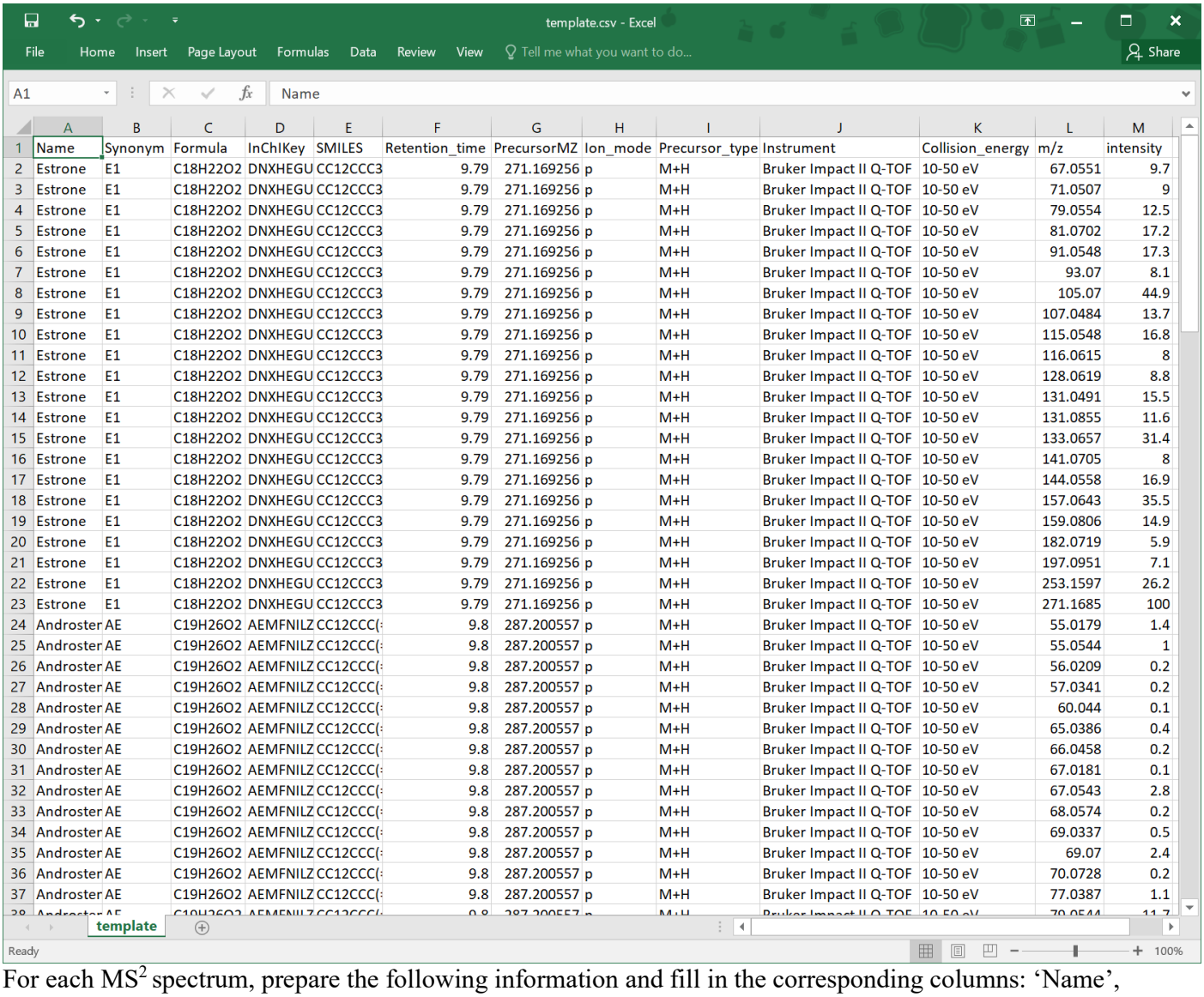
1 Department of Chemistry, Faculty of Science, University of British Columbia, Vancouver Campus, 2036 Main Mall, Vancouver, V6T 1Z1, BC, Canada

* Author to whom correspondence should be addressed:

Dr. Tao Huan
Tel: (+1)-604-822-4891
E-mail: thuan@chem.ubc.ca
Internet: https://huan.chem.ubc.ca/

• 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.



Name	Synonym	Formula	InChIKey	SMILES	Retention_time	PrecursorMZ	Ion_mode	Precursor_type	Instrument	Collision_energy	m/z	intensity
Estrone	E1	C18H22O2	DNXHEGU	CC12CCC3	9.79	271.169256	p	M+H	Bruker Impact II Q-TOF	10-50 eV	67.0551	9.7
Estrone	E1	C18H22O2	DNXHEGU	CC12CCC3	9.79	271.169256	p	M+H	Bruker Impact II Q-TOF	10-50 eV	71.0507	9
Estrone	E1	C18H22O2	DNXHEGU	CC12CCC3	9.79	271.169256	p	M+H	Bruker Impact II Q-TOF	10-50 eV	79.0554	12.5
Estrone	E1	C18H22O2	DNXHEGU	CC12CCC3	9.79	271.169256	p	M+H	Bruker Impact II Q-TOF	10-50 eV	81.0702	17.2
Estrone	E1	C18H22O2	DNXHEGU	CC12CCC3	9.79	271.169256	p	M+H	Bruker Impact II Q-TOF	10-50 eV	91.0548	17.3
Estrone	E1	C18H22O2	DNXHEGU	CC12CCC3	9.79	271.169256	p	M+H	Bruker Impact II Q-TOF	10-50 eV	93.07	8.1
Estrone	E1	C18H22O2	DNXHEGU	CC12CCC3	9.79	271.169256	p	M+H	Bruker Impact II Q-TOF	10-50 eV	105.07	44.9
Estrone	E1	C18H22O2	DNXHEGU	CC12CCC3	9.79	271.169256	p	M+H	Bruker Impact II Q-TOF	10-50 eV	107.0484	13.7
Estrone	E1	C18H22O2	DNXHEGU	CC12CCC3	9.79	271.169256	p	M+H	Bruker Impact II Q-TOF	10-50 eV	115.0548	16.8
Estrone	E1	C18H22O2	DNXHEGU	CC12CCC3	9.79	271.169256	p	M+H	Bruker Impact II Q-TOF	10-50 eV	116.0615	8
Estrone	E1	C18H22O2	DNXHEGU	CC12CCC3	9.79	271.169256	p	M+H	Bruker Impact II Q-TOF	10-50 eV	128.0619	8.8
Estrone	E1	C18H22O2	DNXHEGU	CC12CCC3	9.79	271.169256	p	M+H	Bruker Impact II Q-TOF	10-50 eV	131.0491	15.5
Estrone	E1	C18H22O2	DNXHEGU	CC12CCC3	9.79	271.169256	p	M+H	Bruker Impact II Q-TOF	10-50 eV	131.0855	11.6
Estrone	E1	C18H22O2	DNXHEGU	CC12CCC3	9.79	271.169256	p	M+H	Bruker Impact II Q-TOF	10-50 eV	133.0657	31.4
Estrone	E1	C18H22O2	DNXHEGU	CC12CCC3	9.79	271.169256	p	M+H	Bruker Impact II Q-TOF	10-50 eV	141.0705	8
Estrone	E1	C18H22O2	DNXHEGU	CC12CCC3	9.79	271.169256	p	M+H	Bruker Impact II Q-TOF	10-50 eV	144.0558	16.9
Estrone	E1	C18H22O2	DNXHEGU	CC12CCC3	9.79	271.169256	p	M+H	Bruker Impact II Q-TOF	10-50 eV	157.0643	35.5
Estrone	E1	C18H22O2	DNXHEGU	CC12CCC3	9.79	271.169256	p	M+H	Bruker Impact II Q-TOF	10-50 eV	159.0806	14.9
Estrone	E1	C18H22O2	DNXHEGU	CC12CCC3	9.79	271.169256	p	M+H	Bruker Impact II Q-TOF	10-50 eV	182.0719	5.9
Estrone	E1	C18H22O2	DNXHEGU	CC12CCC3	9.79	271.169256	p	M+H	Bruker Impact II Q-TOF	10-50 eV	197.0951	7.1
Estrone	E1	C18H22O2	DNXHEGU	CC12CCC3	9.79	271.169256	p	M+H	Bruker Impact II Q-TOF	10-50 eV	253.1597	26.2
Estrone	E1	C18H22O2	DNXHEGU	CC12CCC3	9.79	271.169256	p	M+H	Bruker Impact II Q-TOF	10-50 eV	271.1685	100
Androster	AE	C19H26O2	AEMFNILZ	CC12CCC(	9.8	287.200557	p	M+H	Bruker Impact II Q-TOF	10-50 eV	55.0179	1.4
Androster	AE	C19H26O2	AEMFNILZ	CC12CCC(	9.8	287.200557	p	M+H	Bruker Impact II Q-TOF	10-50 eV	55.0544	1
Androster	AE	C19H26O2	AEMFNILZ	CC12CCC(	9.8	287.200557	p	M+H	Bruker Impact II Q-TOF	10-50 eV	56.0209	0.2
Androster	AE	C19H26O2	AEMFNILZ	CC12CCC(	9.8	287.200557	p	M+H	Bruker Impact II Q-TOF	10-50 eV	57.0341	0.2
Androster	AE	C19H26O2	AEMFNILZ	CC12CCC(	9.8	287.200557	p	M+H	Bruker Impact II Q-TOF	10-50 eV	60.044	0.1
Androster	AE	C19H26O2	AEMFNILZ	CC12CCC(	9.8	287.200557	p	M+H	Bruker Impact II Q-TOF	10-50 eV	65.0386	0.4
Androster	AE	C19H26O2	AEMFNILZ	CC12CCC(	9.8	287.200557	p	M+H	Bruker Impact II Q-TOF	10-50 eV	66.0458	0.2
Androster	AE	C19H26O2	AEMFNILZ	CC12CCC(	9.8	287.200557	p	M+H	Bruker Impact II Q-TOF	10-50 eV	67.0181	0.1
Androster	AE	C19H26O2	AEMFNILZ	CC12CCC(	9.8	287.200557	p	M+H	Bruker Impact II Q-TOF	10-50 eV	67.0543	2.8
Androster	AE	C19H26O2	AEMFNILZ	CC12CCC(	9.8	287.200557	p	M+H	Bruker Impact II Q-TOF	10-50 eV	68.0574	0.2
Androster	AE	C19H26O2	AEMFNILZ	CC12CCC(	9.8	287.200557	p	M+H	Bruker Impact II Q-TOF	10-50 eV	69.0337	0.5
Androster	AE	C19H26O2	AEMFNILZ	CC12CCC(	9.8	287.200557	p	M+H	Bruker Impact II Q-TOF	10-50 eV	69.07	2.4
Androster	AE	C19H26O2	AEMFNILZ	CC12CCC(	9.8	287.200557	p	M+H	Bruker Impact II Q-TOF	10-50 eV	70.0728	0.2
Androster	AE	C19H26O2	AEMFNILZ	CC12CCC(	9.8	287.200557	p	M+H	Bruker Impact II Q-TOF	10-50 eV	77.0387	1.1

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.

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 “Create_library.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.