1. HeapMS files format and export tutorial

2023/03/20

2023/10/22 Revised

2024/06/20 Revised

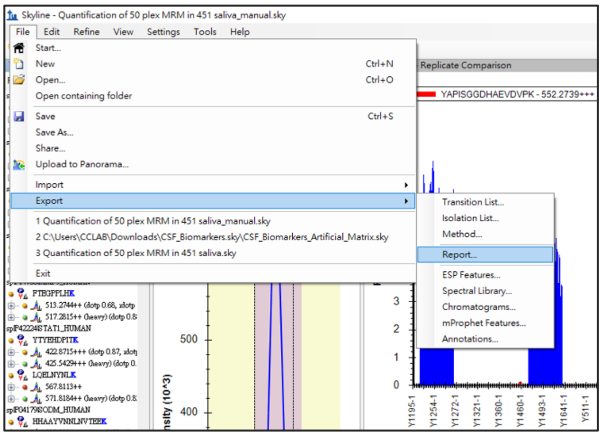
File Definitions

1. Skyline.csv: Peak boundary selection data exported from skyline.
2. Human.csv: Peak boundary selection data revised by human in skyline.
3. Time_intensity.tsv: Peak boundary data includes time, intensity and area information.

1.1 Skyline.csv file format and export

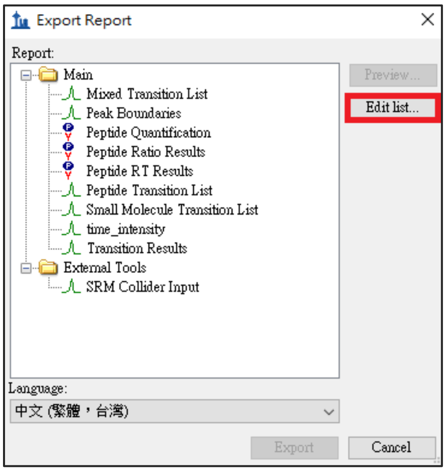
Step 1.

After running the data in Skyline software[1], please click **File** → **Export** → **Report** to save the file.



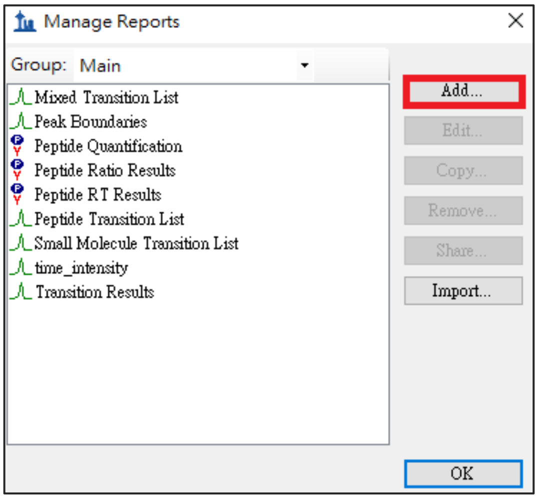
Step 2.

Click **Edit list...**



Step 3.

Click **Add...**



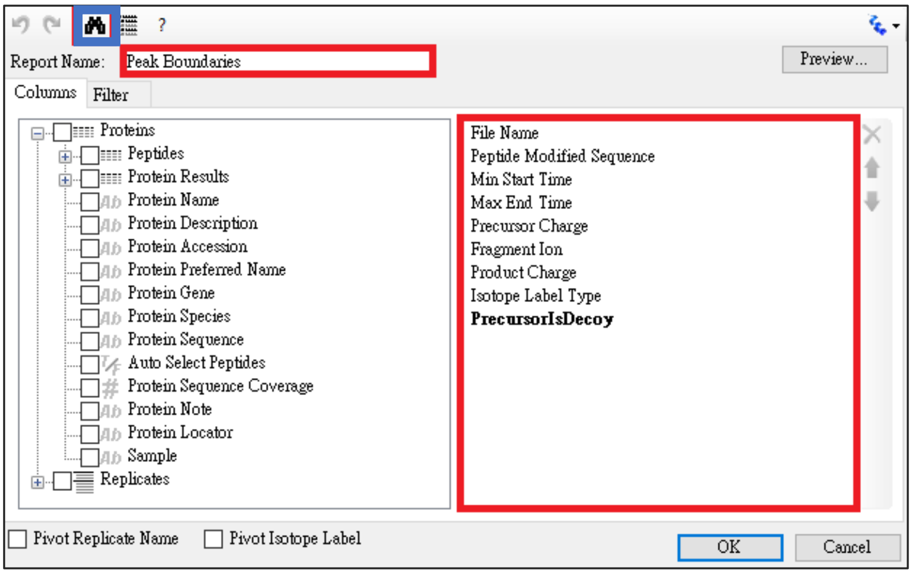
Group: Main

Step 4.

(A) Use the search engine(blue box in the figure) on the upper left and search for the fields on the lower right as shown in the red box.

(B) Remember to type "**Report Name**", such as Peak Boundaries.

(C) Click **OK**.

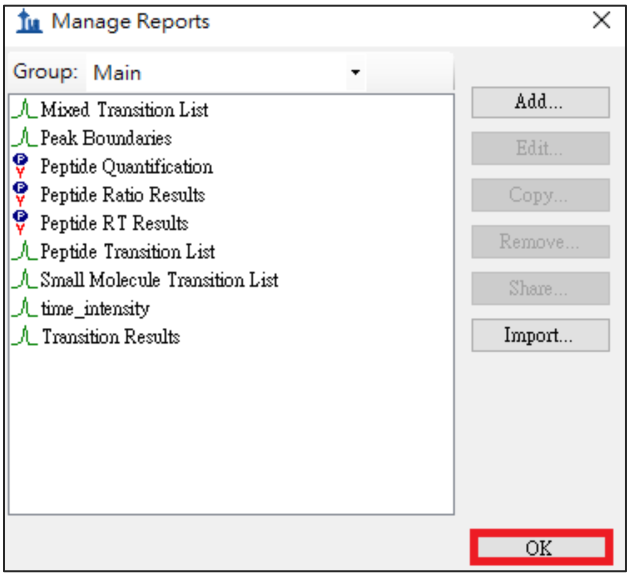


Report Name: Peak Boundaries

File Name
Peptide Modified Sequence
Min Start Time
Max End Time
Precursor Charge
Fragment Ion
Product Charge
Isotope Label Type
PrecursorIsDecoy

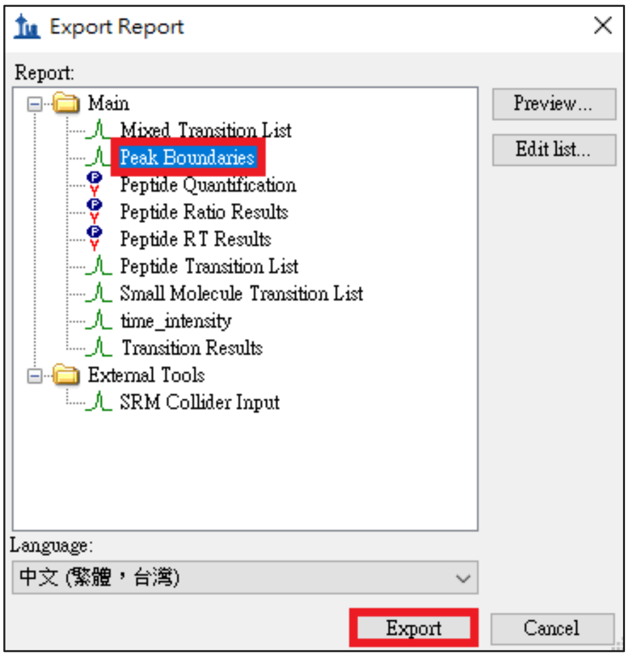
Step 5.

Click **OK**.



Step 6.

Select the named report file(e.g. Peak Boundaries) and select **Export**.

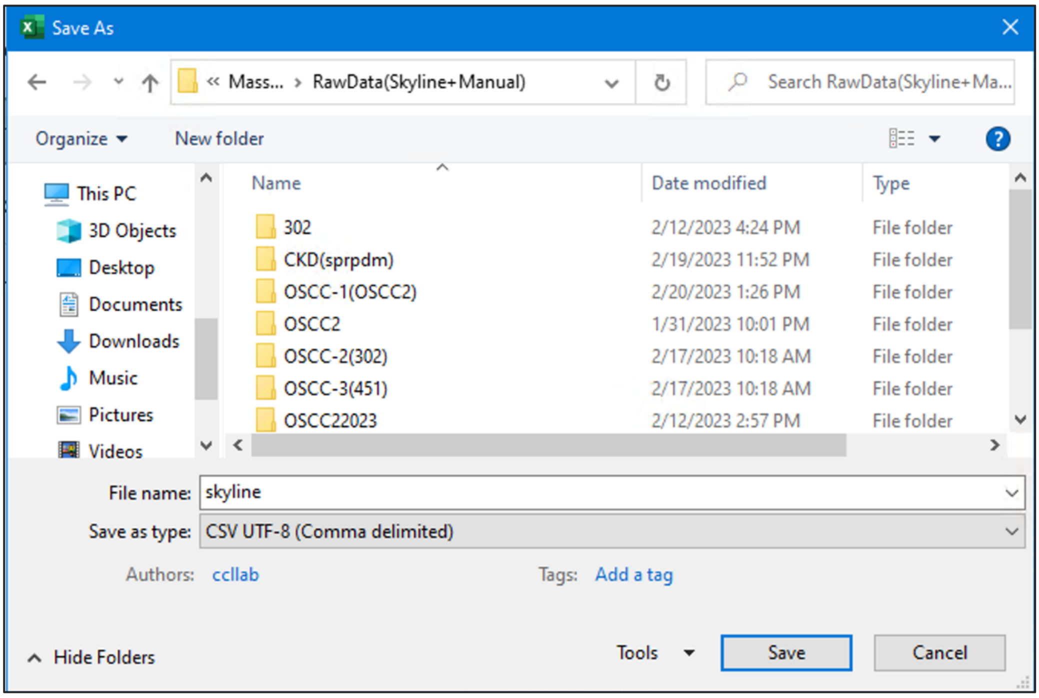


Step 7.

(A) File name can be arbitrary, just remember if it is Skyline.csv or Human.csv (next section).

(B) Please make sure the file format is CSV or CSV UTF-8.

(C) Click the file and save it, it can be used as the input file for HeapMS.



Name	Date modified	Type
302	2/12/2023 4:24 PM	File folder
CKD(sprpdm)	2/19/2023 11:52 PM	File folder
OSCC-1(OSCC2)	2/20/2023 1:26 PM	File folder
OSCC2	1/31/2023 10:01 PM	File folder
OSCC-2(302)	2/17/2023 10:18 AM	File folder
OSCC-3(451)	2/17/2023 10:18 AM	File folder
OSCC22023	2/12/2023 2:57 PM	File folder

File name: skyline

Save as type: CSV UTF-8 (Comma delimited)

Authors: ccllab

Tags: Add a tag

1.2 Human.csv file format and export

After running the data in skyline software and select the boundary manually, follow **Step 1** to **Step 7** in 1.1 section.

***** Skyline.csv and Human.csv file final format *****

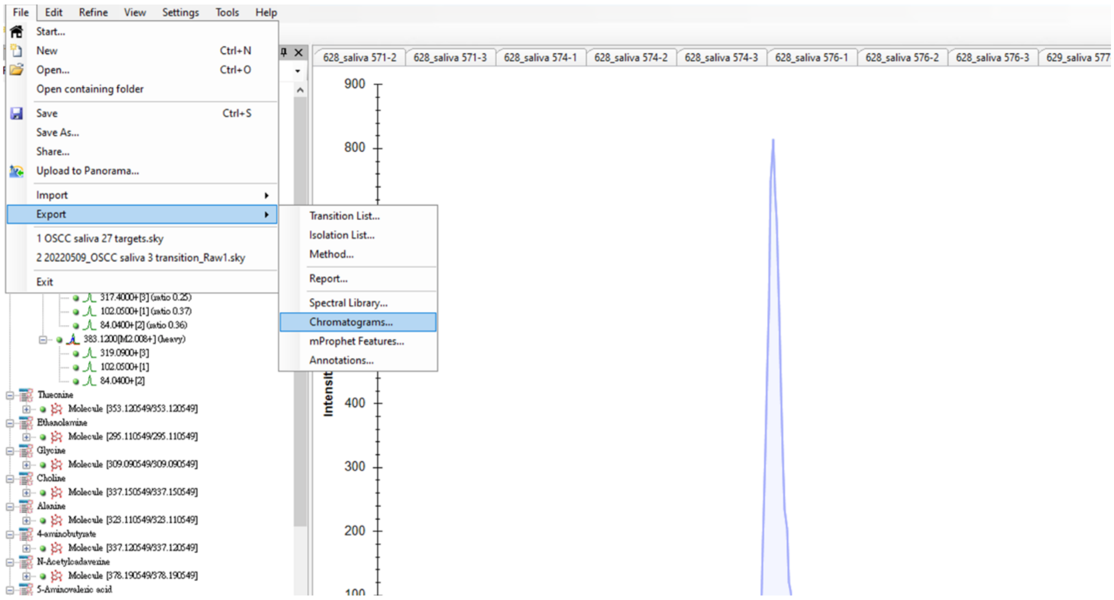
Final file format for both skyline.csv and human.csv will be look like the figure below. Required columns:

File Name, **Peptide Modified Sequence**, **Min Start Time**, **Max End Time**, **Precursor Charge**, **Fragment Ion**, **Product Charge** and **Isotope Label Type**

1.3 Time_intensity.tsv file format

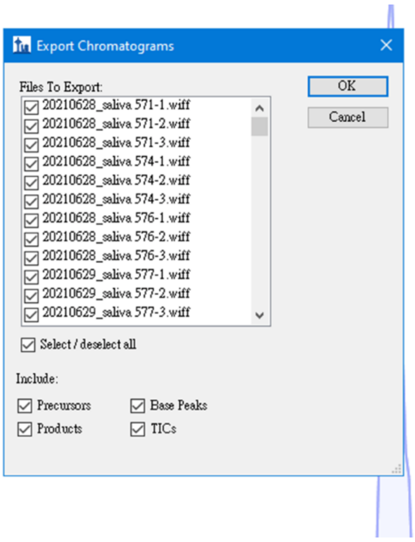
Step 1.

In Skyline software[1], please click **File** → **Export** → **Chromatograms** to save the file.



Step 2.

Depending on your choices and check the items here. Then click **OK**.



Files To Export:

☑ 20210628_saliva 571-1.wiff
☑ 20210628_saliva 571-2.wiff
☑ 20210628_saliva 571-3.wiff
☑ 20210628_saliva 574-1.wiff
☑ 20210628_saliva 574-2.wiff
☑ 20210628_saliva 574-3.wiff
☑ 20210628_saliva 576-1.wiff
☑ 20210628_saliva 576-2.wiff
☑ 20210628_saliva 576-3.wiff
☑ 20210629_saliva 577-1.wiff
☑ 20210629_saliva 577-2.wiff
☑ 20210629_saliva 577-3.wiff

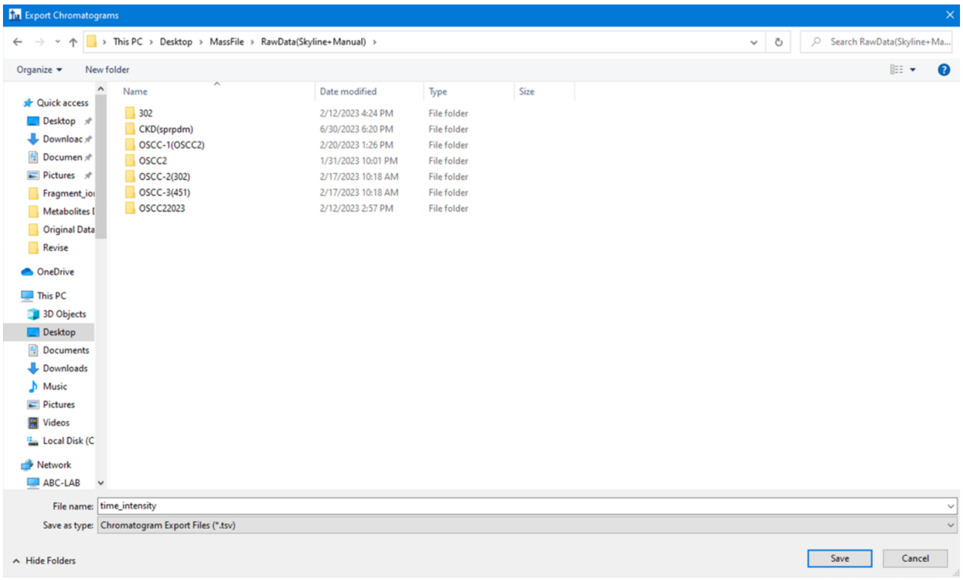
☑ Select / deselect all

Include:

☑ Precursors ☑ Base Peaks
☑ Products ☑ TICs

Step 3.

Naming your tsv file and click **Save**.



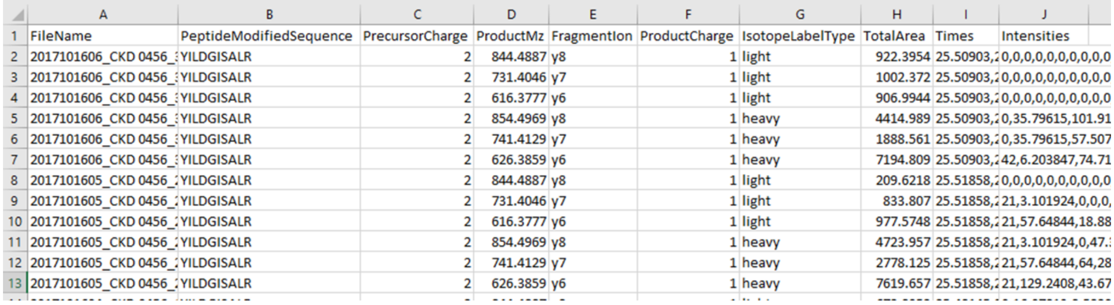
Name	Date modified	Type	Size
302	2/12/2023 4:24 PM	File folder	
CKD(sprpdm)	6/30/2023 6:20 PM	File folder	
OSCC-1(OSCC2)	2/20/2023 1:26 PM	File folder	
OSCC2	1/31/2023 10:01 PM	File folder	
OSCC-2(302)	2/17/2023 10:18 AM	File folder	
OSCC-3(451)	2/17/2023 10:18 AM	File folder	
OSCC22023	2/12/2023 2:57 PM	File folder	

File name: time_intensity

Save as type: Chromatogram Export Files (*.tsv)

***Notes:**

Please make sure that the tsv format and column names are exactly the same as in the picture.



	A	B	C	D	E	F	G	H	I	J
1	FileName	PeptideModifiedSequence	PrecursorCharge	ProductMz	FragmentIon	ProductCharge	IsotopeLabelType	TotalArea	Times	Intensities
2	2017101606_CKD 0456_	YILDGISALR	2	844.4887	y8	1	light	922.3954	25.50903,	0,0,0,0,0,0,0,0,0
3	2017101606_CKD 0456_	YILDGISALR	2	731.4046	y7	1	light	1002.372	25.50903,	0,0,0,0,0,0,0,0,0
4	2017101606_CKD 0456_	YILDGISALR	2	616.3777	y6	1	light	906.9944	25.50903,	0,0,0,0,0,0,0,0,0
5	2017101606_CKD 0456_	YILDGISALR	2	854.4969	y8	1	heavy	4414.989	25.50903,	0,35.79615,101.91
6	2017101606_CKD 0456_	YILDGISALR	2	741.4129	y7	1	heavy	1888.561	25.50903,	0,35.79615,57.507
7	2017101606_CKD 0456_	YILDGISALR	2	626.3859	y6	1	heavy	7194.809	25.50903,	42,6.203847,74.71
8	2017101605_CKD 0456_	YILDGISALR	2	844.4887	y8	1	light	209.6218	25.51858,	0,0,0,0,0,0,0,0,0
9	2017101605_CKD 0456_	YILDGISALR	2	731.4046	y7	1	light	833.807	25.51858,	21,3.101924,0,0,0,
10	2017101605_CKD 0456_	YILDGISALR	2	616.3777	y6	1	light	977.5748	25.51858,	21,57.64844,18.88
11	2017101605_CKD 0456_	YILDGISALR	2	854.4969	y8	1	heavy	4723.957	25.51858,	21,3.101924,0,47.
12	2017101605_CKD 0456_	YILDGISALR	2	741.4129	y7	1	heavy	2778.125	25.51858,	21,57.64844,64,28
13	2017101605_CKD 0456_	YILDGISALR	2	626.3859	y6	1	heavy	7619.657	25.51858,	21,129.2408,43.67

**** Required Column Names (from left to right)** :

FileName, PeptideModifiedSequence, PrecursorCharge, ProductMZ, FragmentIon, ProductCharge, IsotopeLabelType, TotalArea, Times, Intensities.

REFERENCES

[1] MacLean, B., Tomazela, D. M., Shulman, N., Chambers, M., Finney, G. L., Frewen, B., ... & MacCoss, M. J. (2010). Skyline: an open source document editor for creating and analyzing targeted proteomics experiments. *Bioinformatics*, 26(7), 966-968.