

1. HeapMS result predictions

2023/03/20

2023/06/01 Revised

File Definitions

(Please see the Demo page on HeapMS website)

a. Peak Boundary

1. **AI.csv**: Peak boundary data are of good quality for further research after determined by HeapMS.
2. **Uncertain.csv**: Peak boundary data should be re-picked by human after determined by HeapMS.
3. **Deletion.csv**: Peak boundary data should be deleted or re-picked by human after determined by HeapMS.

b. Intensity

1. **AI.tsv**: Peak boundary data includes time, intensity and area information after determined by HeapMS.
2. **Uncertain.tsv**: Peak boundary data should be re-picked by human includes time, intensity and area information after determined by HeapMS.
3. **Deletion.tsv**: Peak boundary data should be deleted or re-picked by human includes time, intensity and area information after determined by HeapMS.

c. Peak Boundaries Files

1. **Skyline.csv**: Peak boundary selection data exported from skyline[1].
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.

d. AI Prediction Summary

1. **Summary.csv**: This file contains the predicted results for each peptide and each sample with the quality indications by HeapMS.

Reference

- [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.