

EASY-FIA: A Readably Usable Standalone Tool for High-Resolution Mass Spectrometry Metabolomics Data Pre-Processing

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Supplementary materials

Supplementary figure 1: Graphic User Interface of EASY-FIA

Supplementary figure 2: Case study 1-Multiple plots of 100 random m/z intensities (y axis) through the runs (x axis) for positive (A) and negative (B) ionization modes.

Supplementary figure 3: Case study 2-Multiple plots of 100 random m/z intensities (y axis) through the runs (x axis) for positive (A) and negative (B) ionization modes.

Supplementary Table 1: Matrix of intensities of case study 1 in positive ionization.

<https://github.com/AMrbt20/SupplementaryMaterials>

Supplementary Table 2: Matrix of intensities of case study 1 in negative ionization.

<https://github.com/AMrbt20/SupplementaryMaterials>

Supplementary Table 3: Matrix of intensities of case study 2 in positive ionization.

<https://github.com/AMrbt20/SupplementaryMaterials>

Supplementary Table 4: Matrix of intensities of case study 2 in negative ionization.

<https://github.com/AMrbt20/SupplementaryMaterials>

Supplementary table 5: Summary of the number of m/z identified, not identified, and correctly aligned by EASY-FIA after discarding the m/z detected in a single sample.

Supplementary table 6: Number of m/z acquired in the samples and blanks, in accordance with the acquisition mode. Table also reports the percentage of shared m/z between samples and blanks in both case studies.

Supplementary Figure S1: Graphic User Interface of EASY-FIA.

EASY-FIA

Parameters	
Delta mass (ppm)	6
Intensity cut-off	0
Sample cut-off	1

Adduct definition	
M-Na+	22.9892
M-K+	38.9632

Output Folder
Alignment-22-Feb-2022

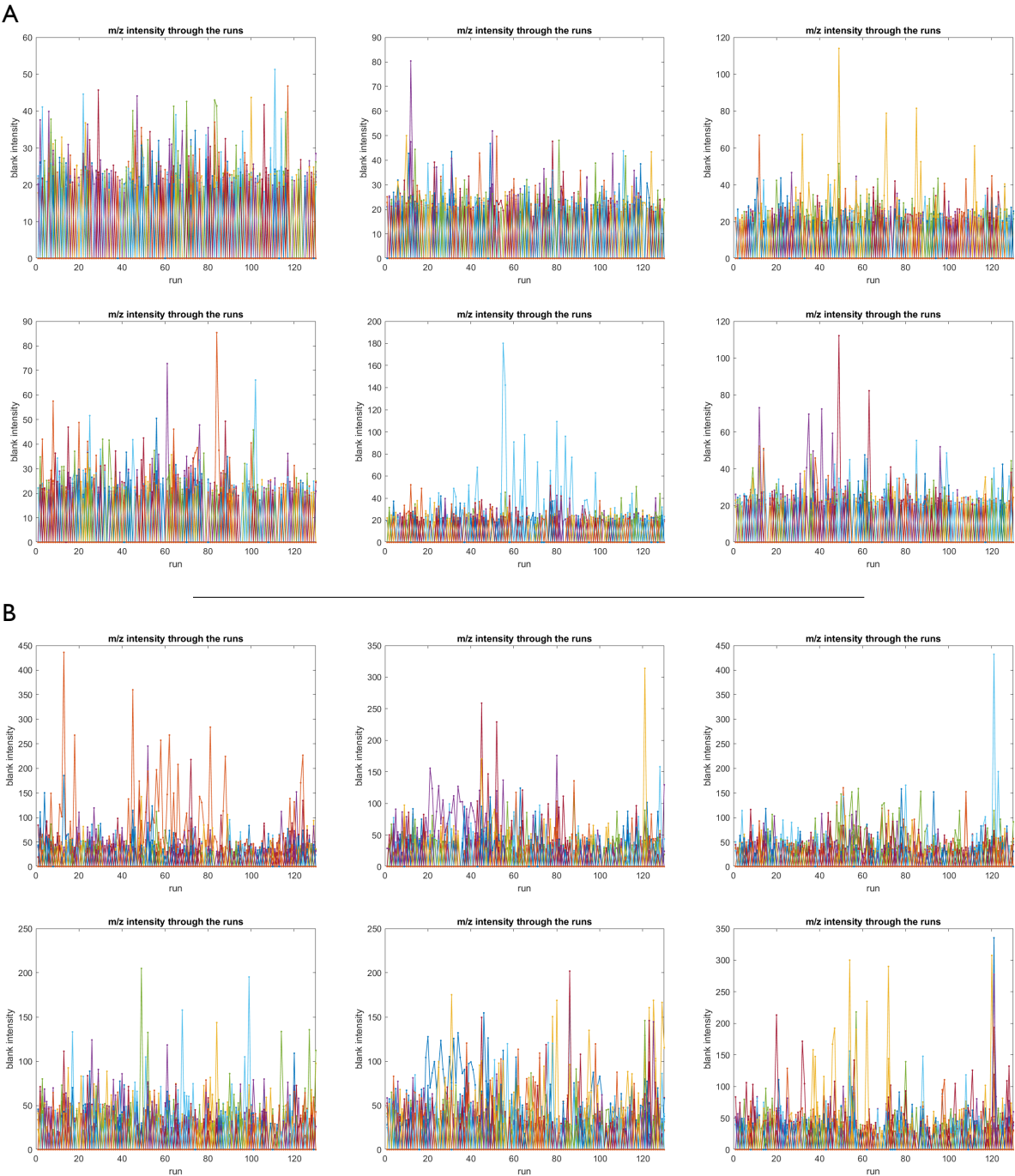
☐ Sort matrix by adducts

ALIGNMENT

HMDB ANNOTATION

- Waiting -

Supplementary Figure S2: Case study 1-Multiple plots of 100 random m/z intensities (y axis) through the runs (x axis) for positive (A) and negative (B) ionization modes.



Supplementary Figure S3: Case study 2-Multiple plots of 100 random m/z intensities (y axis) through the runs (x axis) for positive (A) and negative (B) ionization modes.



Supplementary Table S5: Summary of the number of m/z identified and not identified, correctly aligned by EASY-FIA after discarding the m/z detected in a single sample.

Case Study	Acquisition mode	Identified m/z	Not identified m/z	Tot. m/z	Tot. identified m/z
1	Positive	25.134	222.866	248.000	35.017
1	Negative	9.883	241.674	251.557	
2	Positive	12.024	26.339	38.363	20.084
2	Negative	8.060	66.509	74.569	

Supplementary Table S6: Number of m/z acquired in the samples and blanks, in accordance with the acquisition mode. Table also reports the percentage of shared m/z between samples and blanks in both case studies.

Case Study	Acquisition mode	Sample m/z	Blank m/z	Sample/Blank m/z match (%)
1	Positive	263.122	262.933	21,43
1	Negative	262.943	262.726	27,47
2	Positive	54.885	35.687	38,19
2	Negative	74.799	74.866	96,54