

Supplementary material

Effects of cadmium stress on growth, physiological characteristics, and metabolic profiling in rice (*Oryza sativa* L.) by using HPLC-QTOF/MS.

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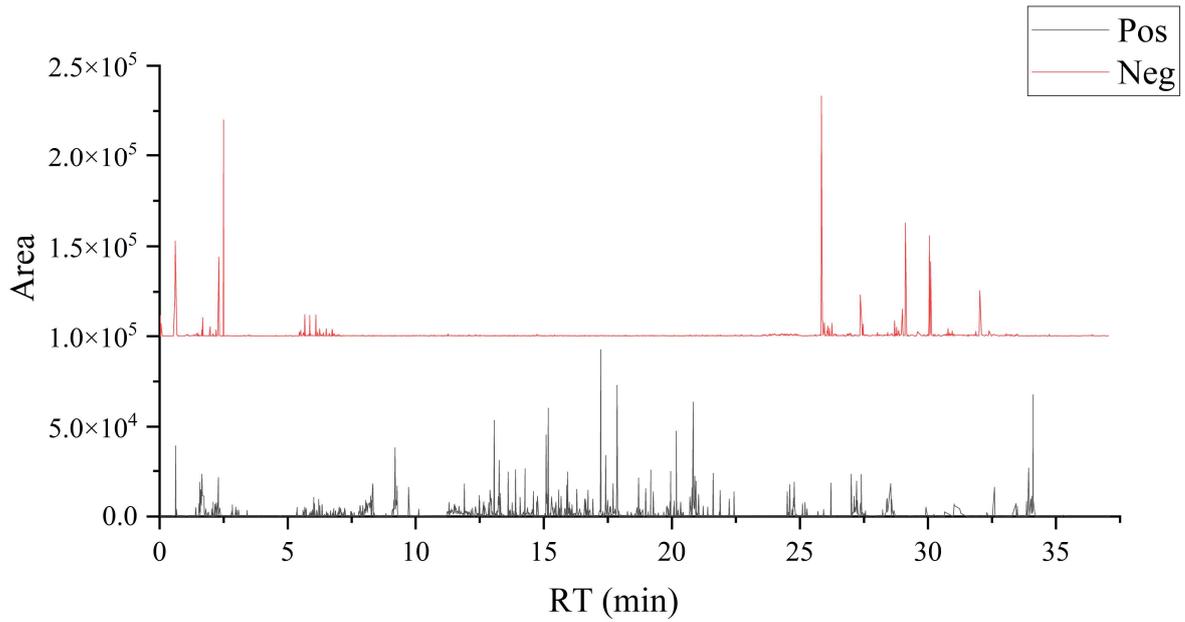


Figure S1. Total ion flow chromatogram of QC samples.

A

Analysis parameter setting

Molecular species	Charge	Accurate mass [Da]	Included
[M+H] ⁺	1	1.0078250207	<input checked="" type="checkbox"/>
[M+NH4] ⁺	1	18.03437413	<input checked="" type="checkbox"/>
[M+Na] ⁺	1	22.989792809	<input checked="" type="checkbox"/>
[M+CH3OH+H] ⁺	1	33.03403978207	<input type="checkbox"/>
[M+K] ⁺	1	38.96370668	<input type="checkbox"/>
[M+H] ₂ O ⁺	1	77.016045	<input type="checkbox"/>
[M+ACN+H] ⁺	1	42.03437413207	<input type="checkbox"/>
[M+H+H2O] ⁺	1	-17.00273964793	<input type="checkbox"/>
[M+H+H2O] ₂ ⁺	1	-35.013042793	<input type="checkbox"/>
[M+2Na+H] ⁺	1	44.9717132973	<input type="checkbox"/>
[M+isoProp+H] ⁺	1	61.06533991207	<input type="checkbox"/>
[M+ACN+Na] ⁺	1	64.0161183809	<input type="checkbox"/>
[M+2K+H] ⁺	1	76.9195832793	<input type="checkbox"/>
[M+DMSO+H] ⁺	1	79.02176103207	<input type="checkbox"/>
[M+2ACN+H] ⁺	1	83.06292323207	<input type="checkbox"/>
[M+isoProp+Na+H] ⁺	1	84.0510919297	<input type="checkbox"/>
[M+CGH1004+H] ⁺	1	-145.05008376687	<input type="checkbox"/>
[M+CGH1005+H] ⁺	1	-161.04499838643	<input type="checkbox"/>
[M+CGH906+H] ⁺	1	-175.02426294185	<input type="checkbox"/>
[2M+H] ⁺	1	1.0078250207	<input checked="" type="checkbox"/>
[2M+NH4] ⁺	1	18.03437413	<input type="checkbox"/>
[2M+Na] ⁺	1	22.989792809	<input type="checkbox"/>
[2M+3H2O+2H] ⁺	1	56.0473410414	<input type="checkbox"/>
[2M+K] ⁺	1	38.96370668	<input type="checkbox"/>

Analysis parameter setting

Result name: alignmentRun_2023_10_25_19_37_11

Reference file:

Retention time tolerance: 0.1 min

MS1 tolerance: 0.025 Da

Analysis parameter setting

Minimum peak height: 10 amplitude

Mass slice width: 0.1 Da

Analysis parameter setting

MS1 tolerance: 0.05 Da

MS2 tolerance: 0.1 Da

Analysis parameter setting

MSP file:

Retention time tolerance: 1000 min

Accurate mass tolerance (MS1): 0.015 Da

Accurate mass tolerance (MS2): 0.075 Da

Identification score cut off: 60 %

Use retention time for scoring:

Use retention time for filtering:

B

Analysis parameter setting

Molecular species	Charge	Accurate mass [Da]	Included
[M-H] ⁻	1	-1.0078250207	<input checked="" type="checkbox"/>
[M-H2O-H] ⁻	1	-150.038971207	<input checked="" type="checkbox"/>
[M+Na-2H] ⁻	1	20.97411921676	<input type="checkbox"/>
[M+Cl] ⁻	1	34.9688268	<input type="checkbox"/>
[M+K-2H] ⁻	1	36.9409661598	<input type="checkbox"/>
[M+FA-H] ⁻	1	44.99765396793	<input type="checkbox"/>
[M+Hac-H] ⁻	1	59.01330396793	<input type="checkbox"/>
[M+CH3N+Na-2H] ⁻	1	62.00066831777	<input type="checkbox"/>
[M+Br] ⁻	1	78.9183371	<input type="checkbox"/>
[M+TFA-H] ⁻	1	112.9801896793	<input type="checkbox"/>
[M+CGH1004-H] ⁻	1	-147.0657338101	<input type="checkbox"/>
[M+CGH1005-H] ⁻	1	-163.06064845057	<input type="checkbox"/>
[M+CGH906-H] ⁻	1	-177.03951300599	<input type="checkbox"/>
[M+CH3COONa-H] ⁻	1	80.99524996793	<input type="checkbox"/>
[2M-H] ⁻	1	-1.0078250207	<input checked="" type="checkbox"/>
[2M+FA-H] ⁻	1	44.99765396793	<input type="checkbox"/>
[2M+Hac-H] ⁻	1	59.01330396793	<input type="checkbox"/>
[3M-H] ⁻	1	-1.0078250207	<input type="checkbox"/>
[M-2H] ⁻	2	-2.0156500414	<input type="checkbox"/>
[M-3H] ⁻	3	-3.0234750621	<input type="checkbox"/>

Analysis parameter setting

Result name: alignmentRun_2023_10_25_19_37_11

Reference file:

Retention time tolerance: 0.1 min

MS1 tolerance: 0.025 Da

Analysis parameter setting

Minimum peak height: 10 amplitude

Mass slice width: 0.1 Da

Analysis parameter setting

MS1 tolerance: 0.05 Da

MS2 tolerance: 0.1 Da

Analysis parameter setting

MSP file:

Retention time tolerance: 1000 min

Accurate mass tolerance (MS1): 0.015 Da

Accurate mass tolerance (MS2): 0.075 Da

Identification score cut off: 60 %

Use retention time for scoring:

Use retention time for filtering:

Figure S2. MSDIAL data processing parameter settings for positive (A) and negative (B) ions.

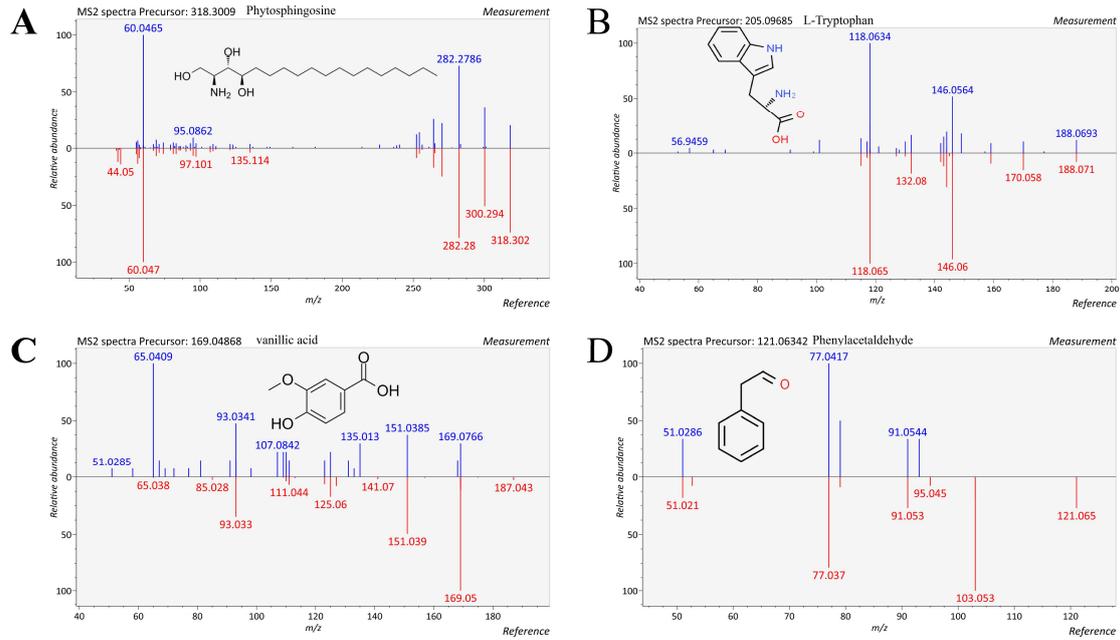


Figure S3. Identification information for the four metabolites with the highest (A, B) and lowest (C, D) matching degrees to the references. The red and blue colors represent references and measurements, respectively.

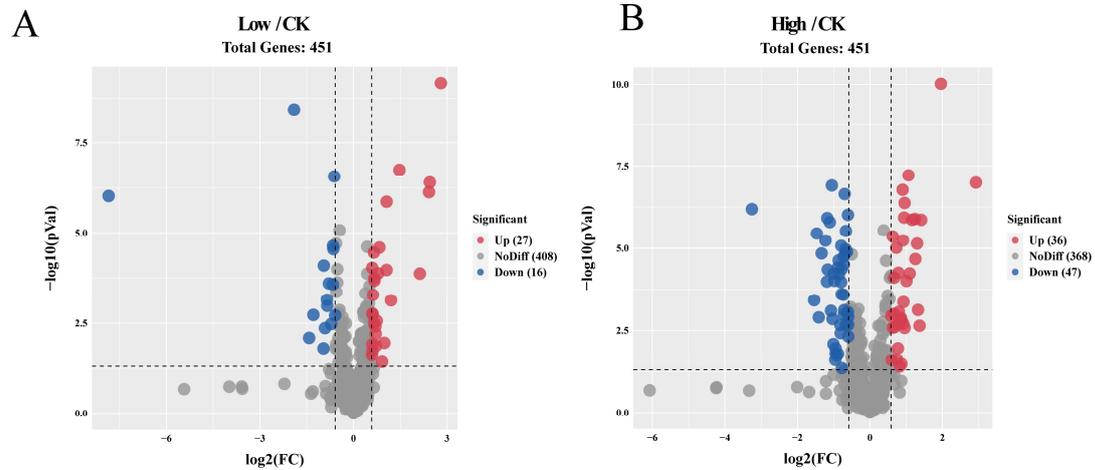


Figure S4. Rice root tissue differential metabolites volcano plots in the Low-group (A) and High-group (B) compared with the CK group. CK: control; Low: 2 mg kg⁻¹; High: 10 mg kg⁻¹, respectively.

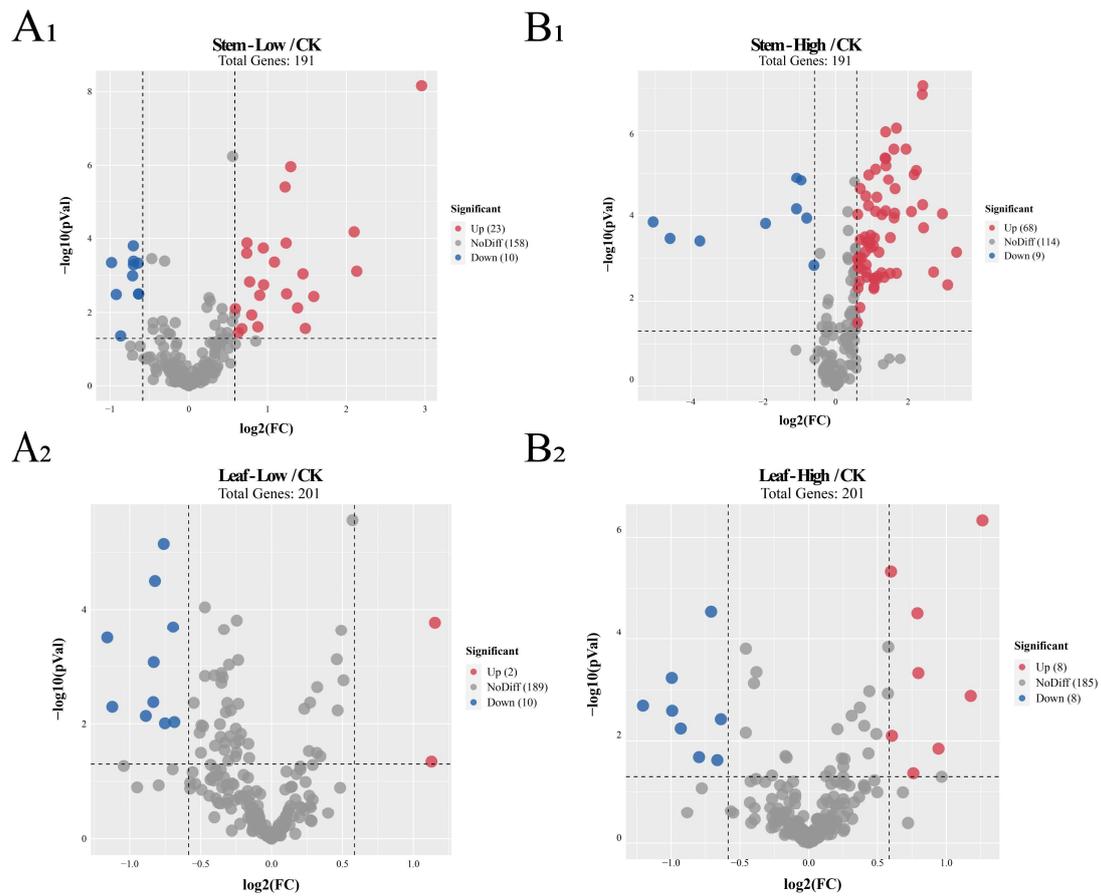


Figure S5. Differential metabolites volcano plots in the Low-group (A) and High-group (B) compared with the CK group, CK: control; Low: 2 mg kg⁻¹; High: 10 mg kg⁻¹; 1 and 2 represent stems and leaves respectively.