

### Supplementary Figure Legends

Supplementary Figure 1. The OPLS-DA model and volcano map of MDR-TB/HC group in HILIC column. The OPLS-DA score scatter plots of ion mode: (a) positive, (c) negative. The permutation test results of ion mode: (b) positive, (d) negative. The differential metabolite volcano maps of ion mode: (e) positive, (f) negative. The upward trend in metabolites was indicated by red scatters, the downward trend in metabolites was indicated by blue scatters, and the non-significant trend in metabolites was indicated by black scatters.

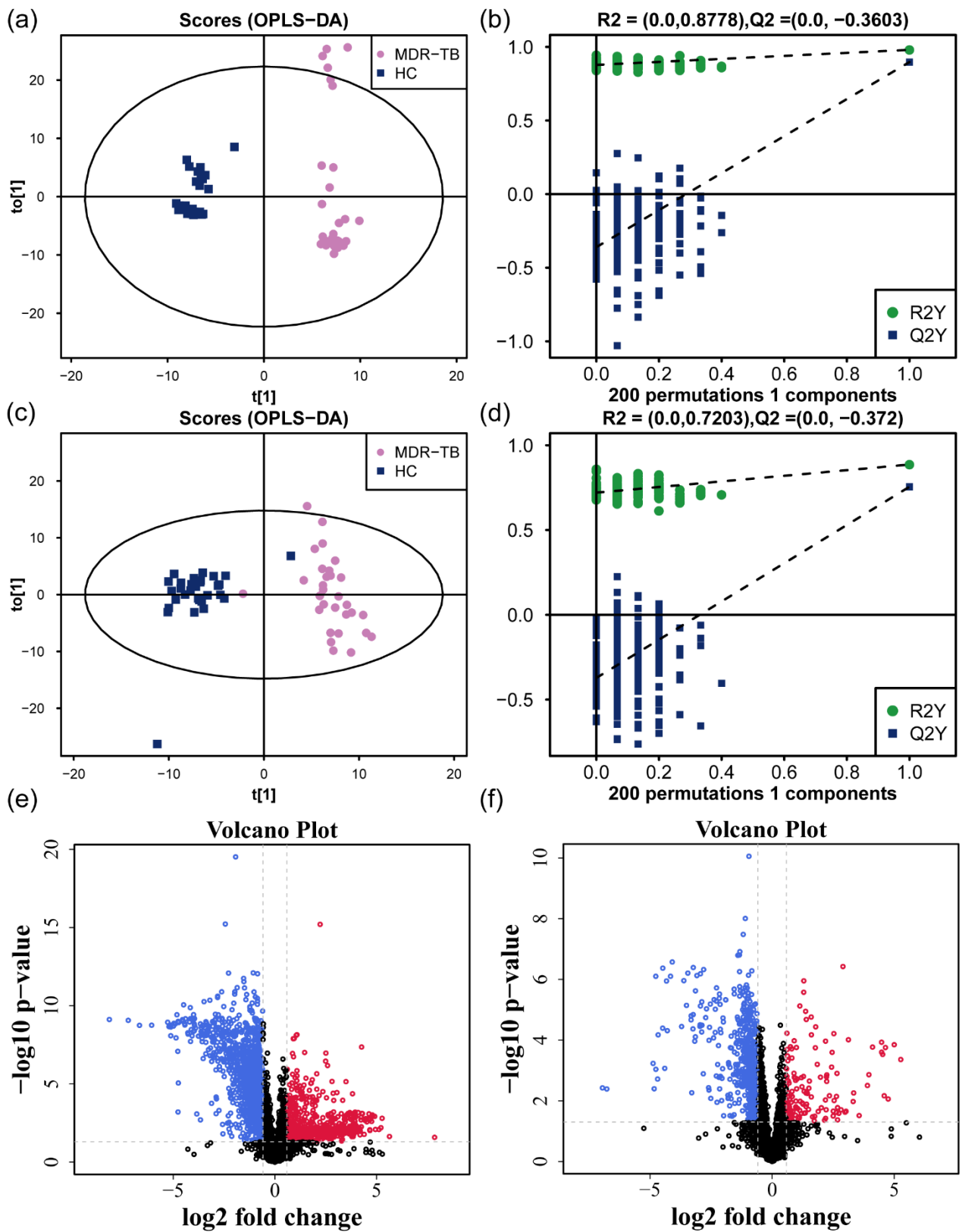
Supplementary Figure 2. The OPLS-DA model and volcano map of MDR-TB/HC group in T3 column. The OPLS-DA score scatter plots of ion mode: (a) positive, (c) negative. The permutation test results of ion mode: (b) positive, (d) negative. The differential metabolite volcano maps of ion mode: (e) positive, (f) negative. The upward trend in metabolites was indicated by red scatters, the downward trend in metabolites was indicated by blue scatters, and the non-significant trend in metabolites was indicated by black scatters.

Supplementary Figure 3. The metabolic pathway map of MDR-TB/HC group. Metabolic pathway map of HILIC column (a), metabolic pathway map of T3 column (b).

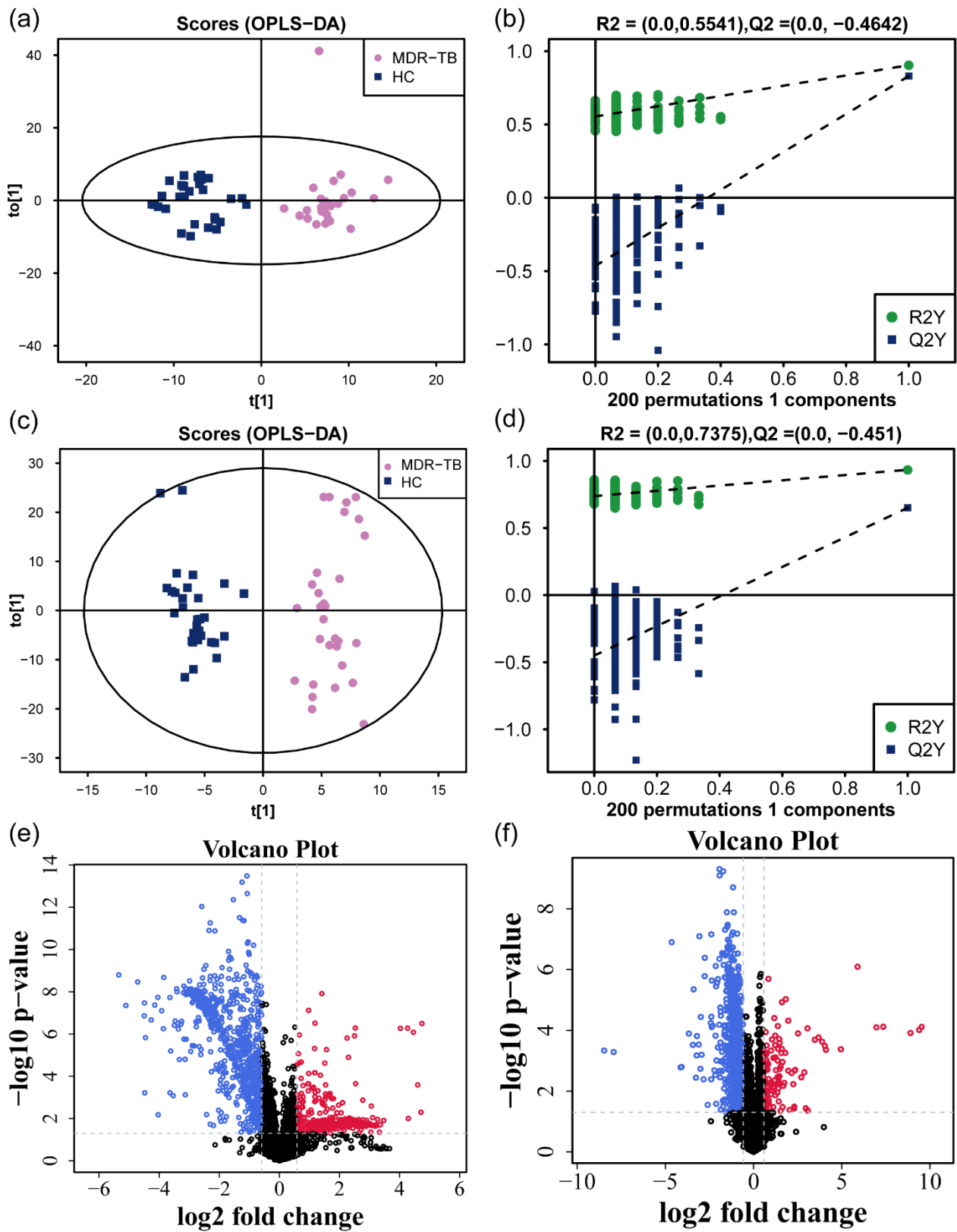
Supplementary Figure 4. The OPLS-DA model and volcano map of DS-TB/HC group in HILIC column. The OPLS-DA score scatter plots of ion mode: (a) positive, (c) negative. The permutation test results of ion mode: (b) positive, (d) negative. The differential metabolite volcano maps of ion mode: (e) positive, (f) negative. The upward trend in metabolites was indicated by red scatters, the downward trend in metabolites was indicated by blue scatters, and the non-significant trend in metabolites was indicated by black scatters.

Supplementary Figure 5. The OPLS-DA model and volcano map of DS-TB/HC group in T3 column. The OPLS-DA score scatter plots of ion mode: (a) positive, (c) negative. The permutation test results of ion mode: (b) positive, (d) negative. The differential metabolite volcano maps of ion mode: (e) positive, (f) negative. The upward trend in metabolites was indicated by red scatters, the downward trend in metabolites was indicated by blue scatters, and the non-significant trend in metabolites was indicated by black scatters.

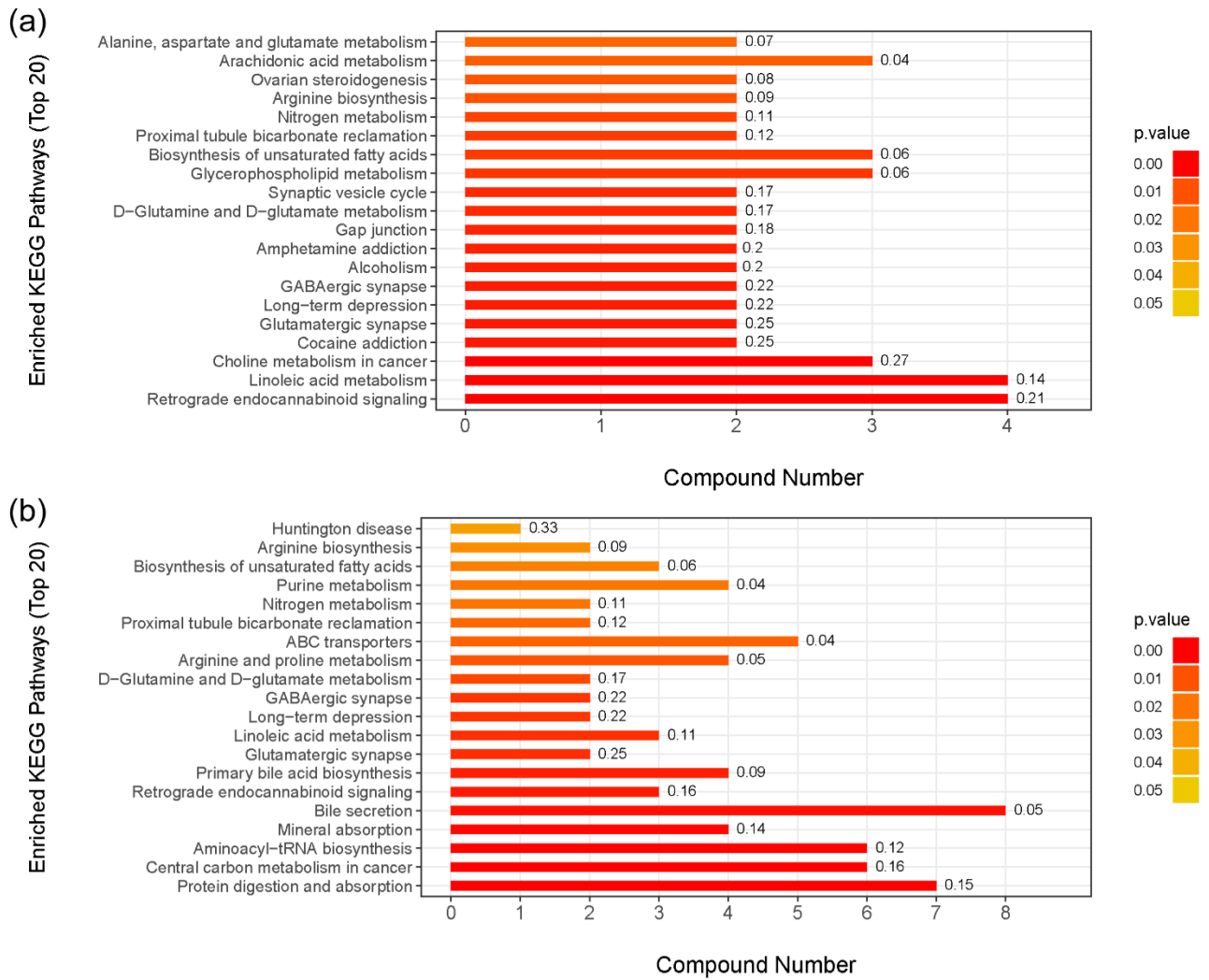
Supplementary Figure 6. The metabolic pathway map of DS-TB/HC group. Metabolic pathway map of HILIC column (a), metabolic pathway map of T3 column (b).



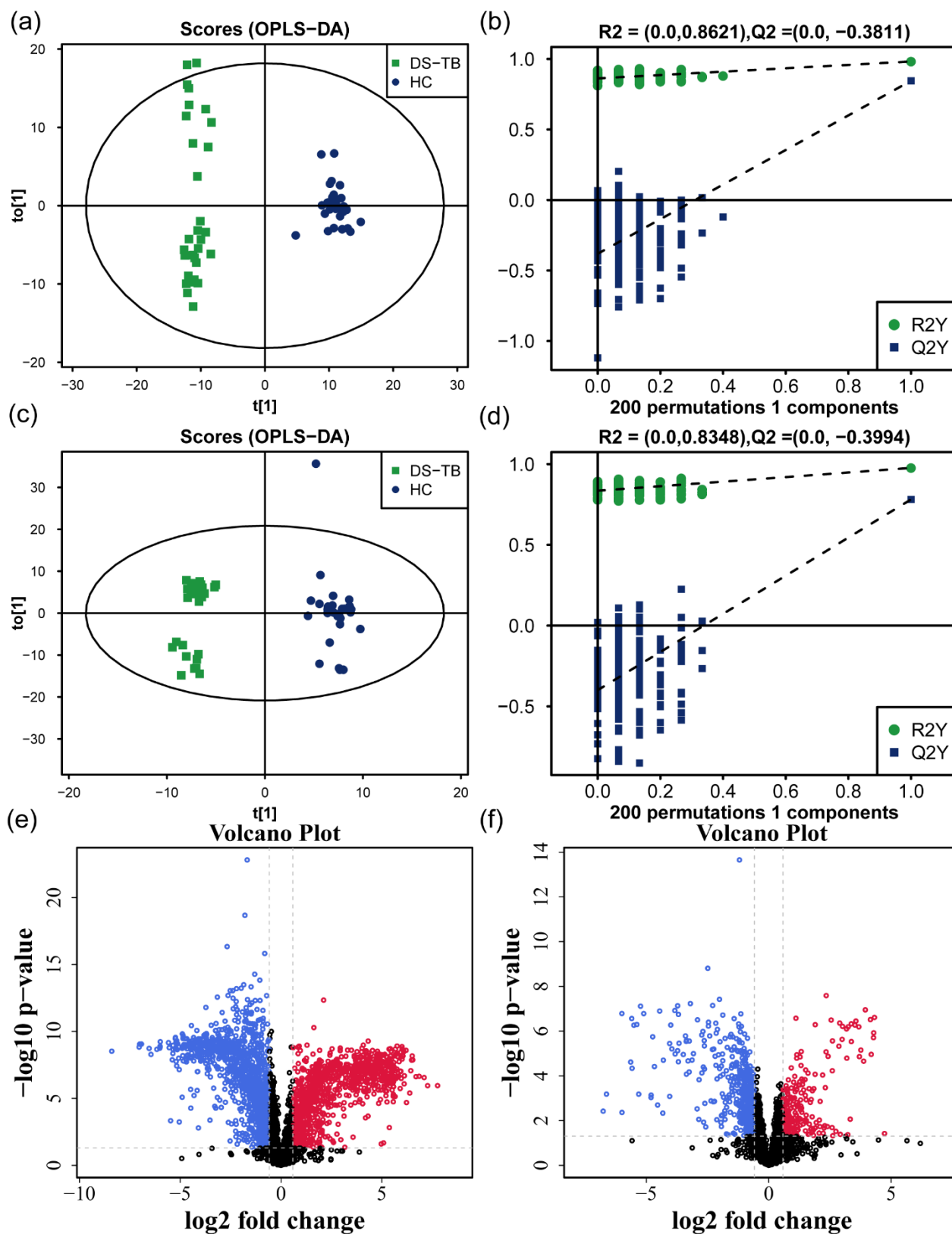
Supplementary Figure 1. The OPLS-DA model and volcano map of MDR-TB/HC group in HILIC column.



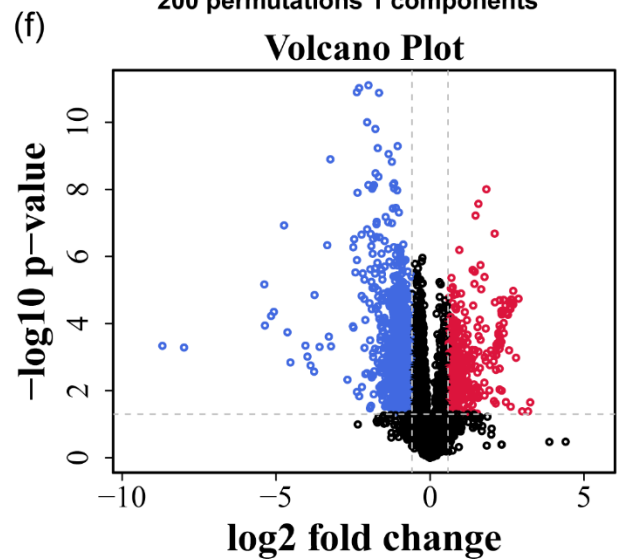
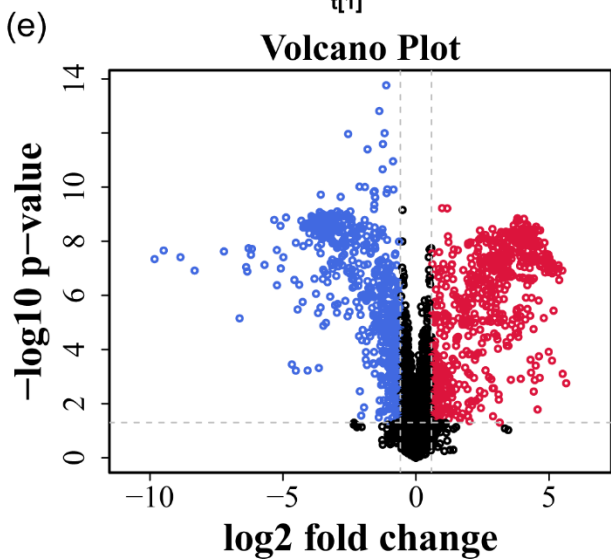
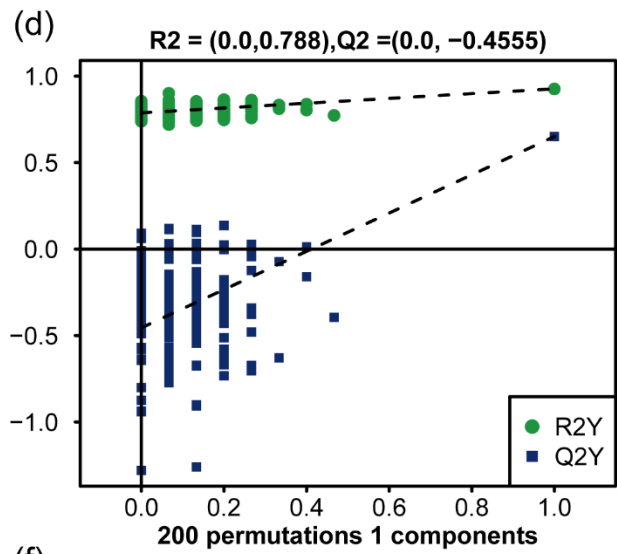
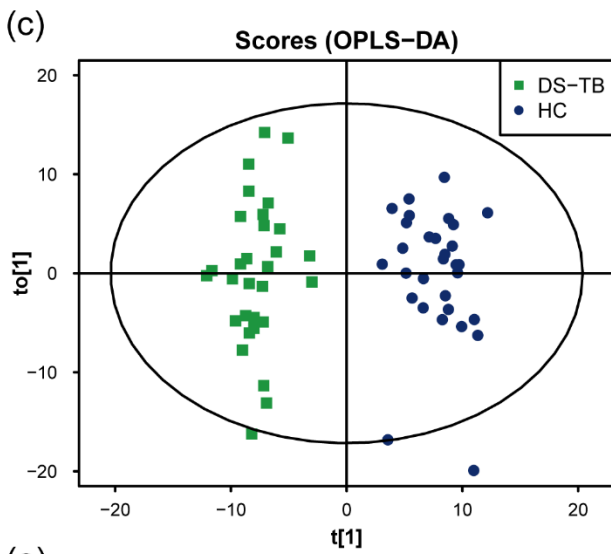
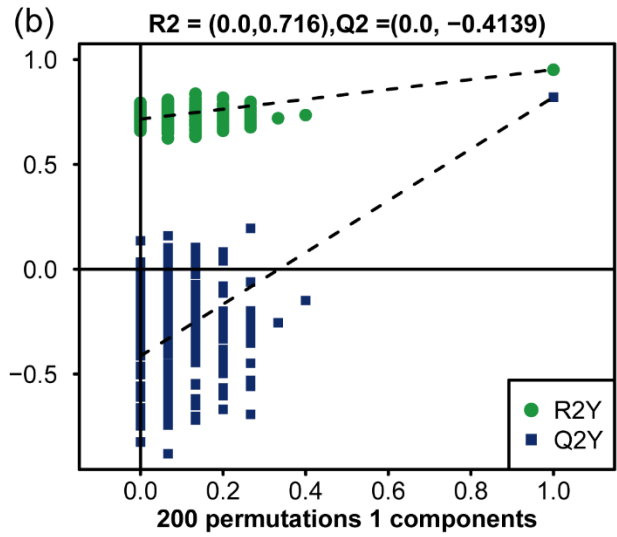
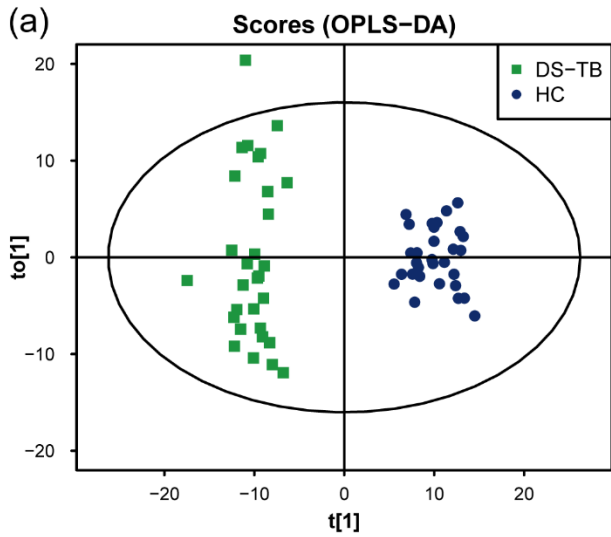
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Supplementary Figure 3. The metabolic pathway map of MDR-TB/HC group.



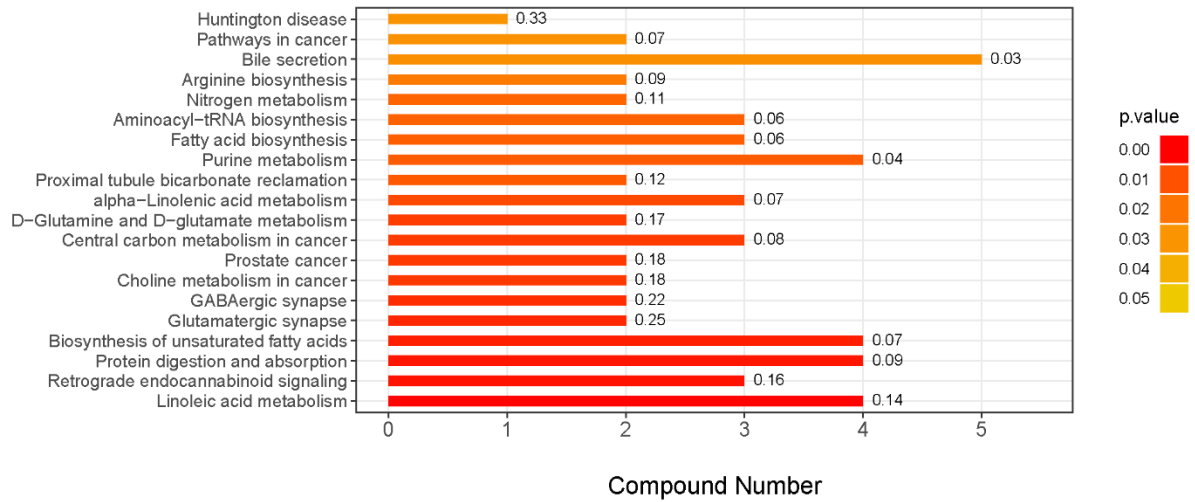
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Supplementary Figure 5. The OPLS-DA model and volcano map of DS-TB/HC group in T3 column.

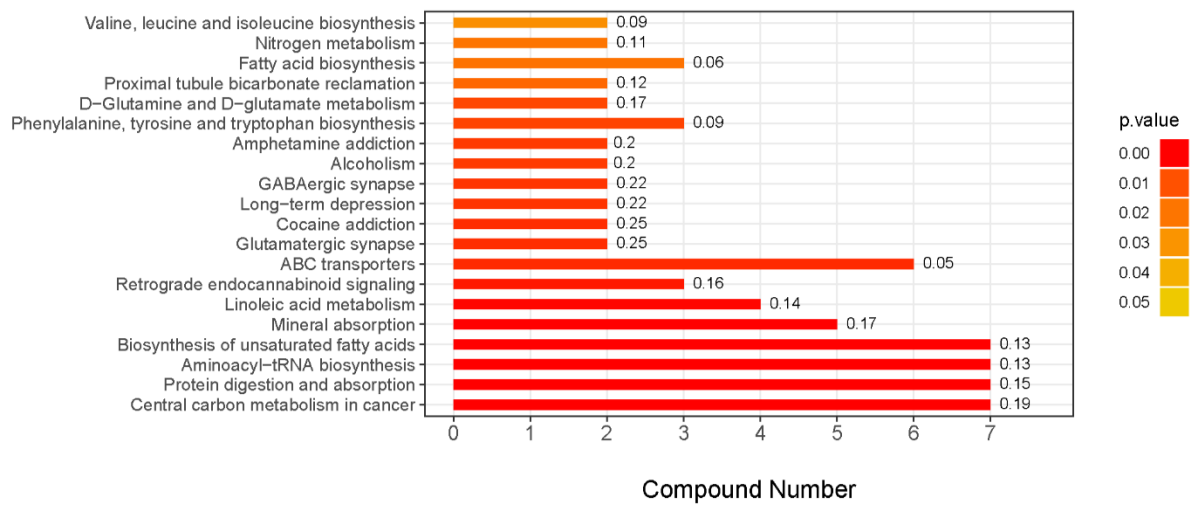
(a)

Enriched KEGG Pathways (Top 20)



(b)

Enriched KEGG Pathways (Top 20)



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