**Supplement 1.** Workflow of spectra analysis using MZMine 3.4

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**Supplement 2.** Permutation validation test was carried out through MetaboAnalyst v6.0 on PLS-DA result confirming the validity of the analysis with data overfitting



**Supplement 3.** Permutation validation test was carried out through MetaboAnalyst v6.0 on OPLS-DA result confirming the validity of the analysis with no data overfitting with the valid model

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**Supplement 4.** Heatmap of all 12 *H. itama* bee bread samples (ungrouped)