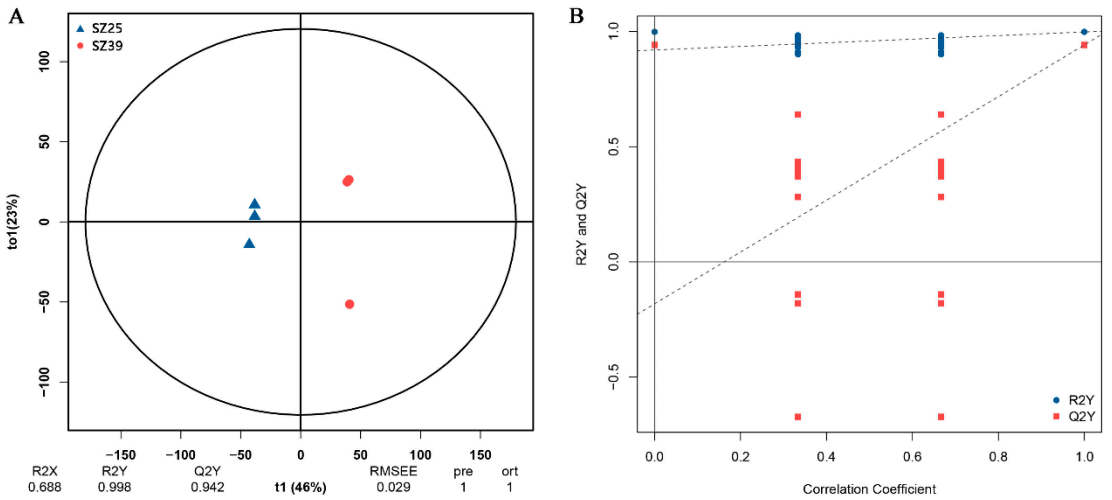
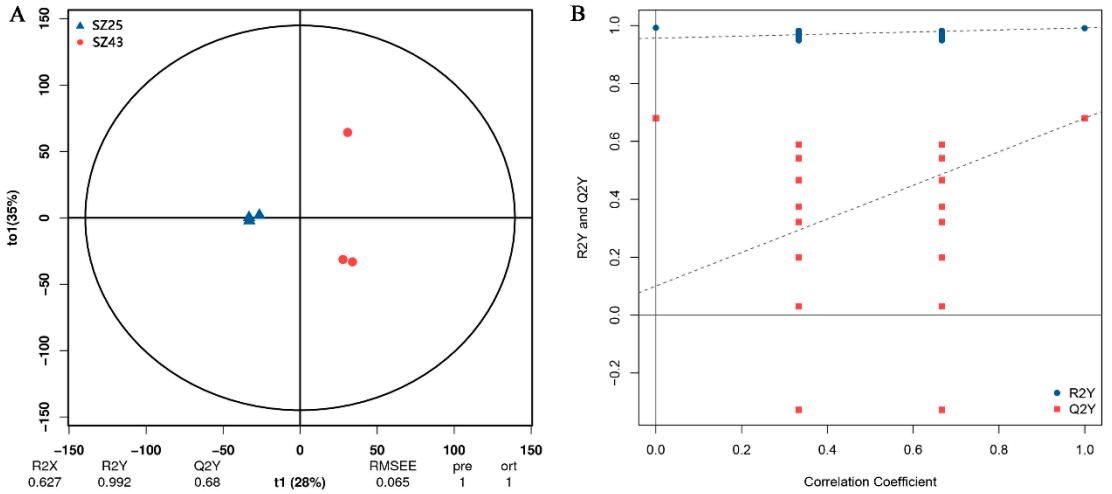
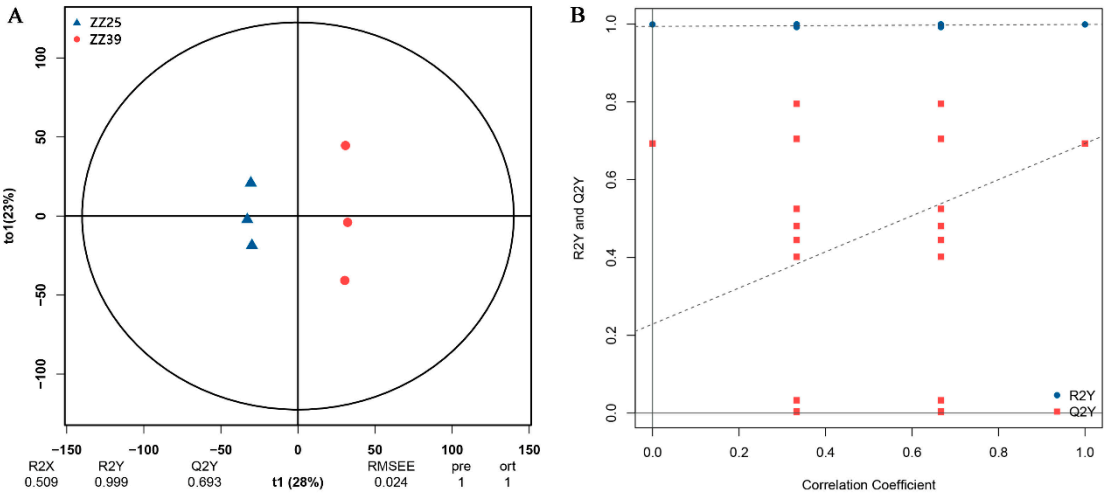


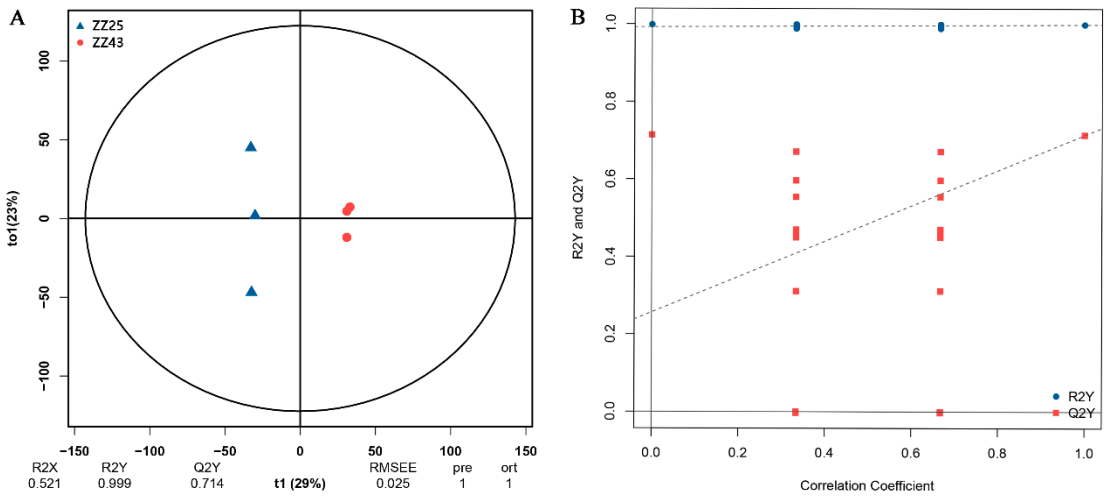
Supplementary Figure S1. OPLS-DA scores **(A)** and permutation test **(B)** plots of SZ25 vs. SZ39 comparison in positive ion mode.



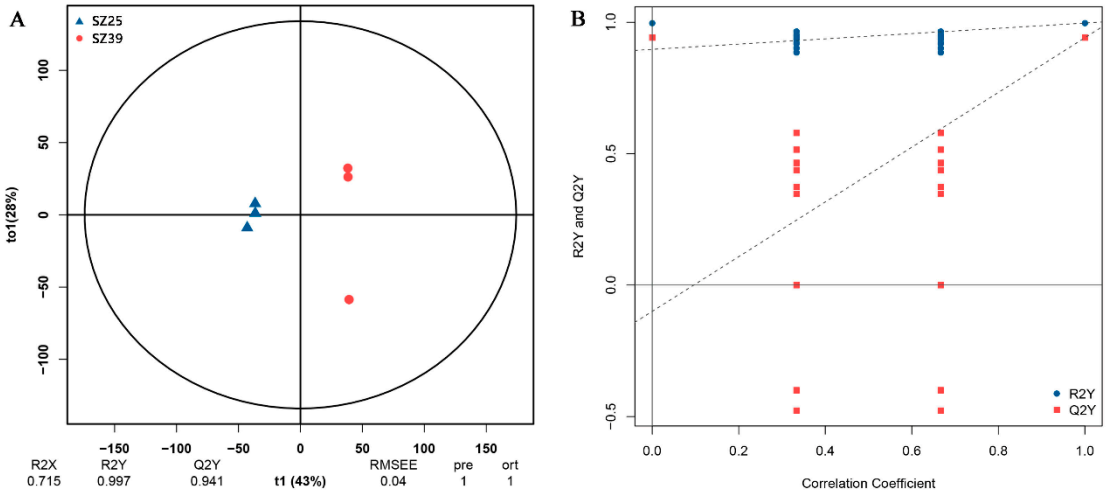
Supplementary Figure S2. OPLS-DA scores **(A)** and permutation test **(B)** plots of SZ25 vs. SZ43 comparison in positive ion mode.



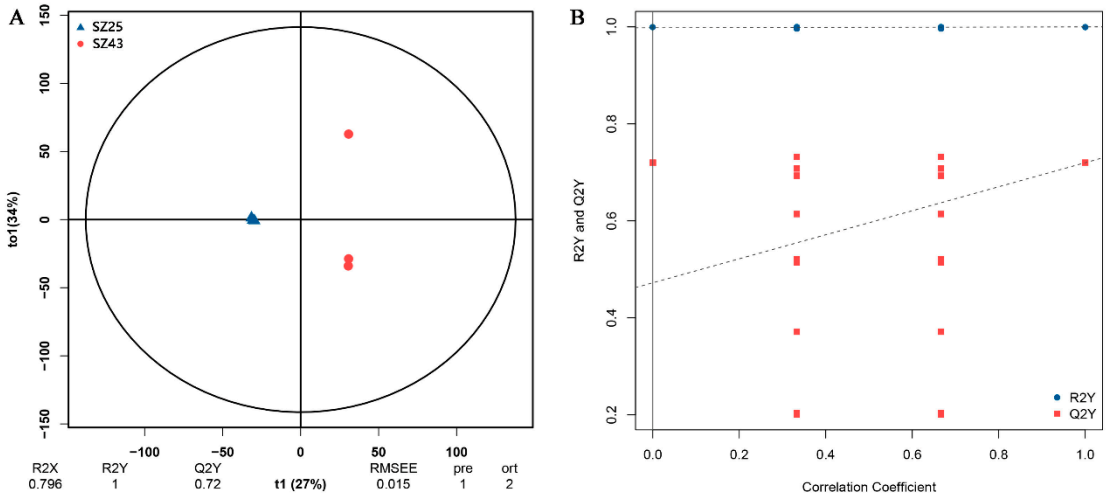
Supplementary Figure S3. OPLS-DA scores **(A)** and permutation test **(B)** plots of ZZ25 vs. ZZ39 comparison in positive ion mode.



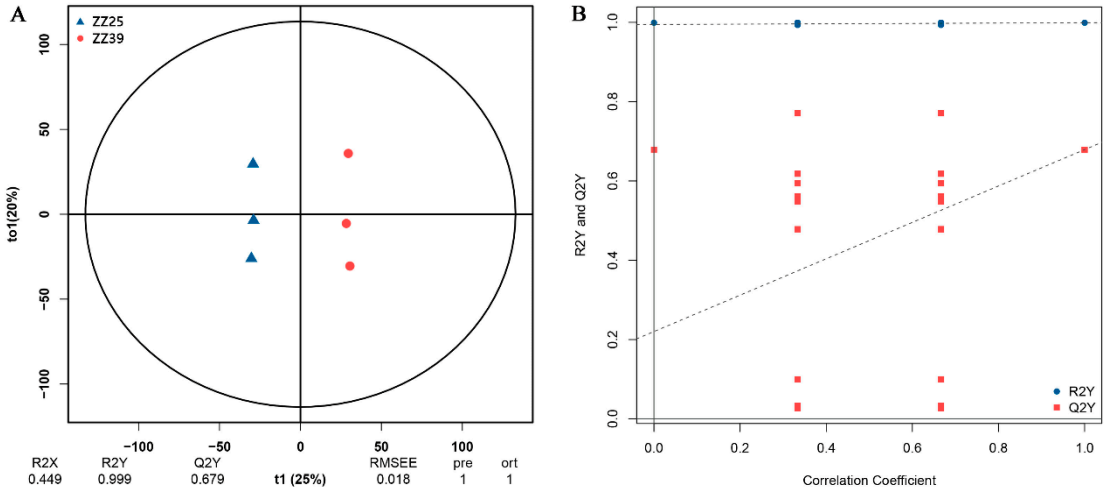
Supplementary Figure S4. OPLS-DA scores **(A)** and permutation test **(B)** plots of ZZ25 vs. ZZ43 comparison in positive ion mode.



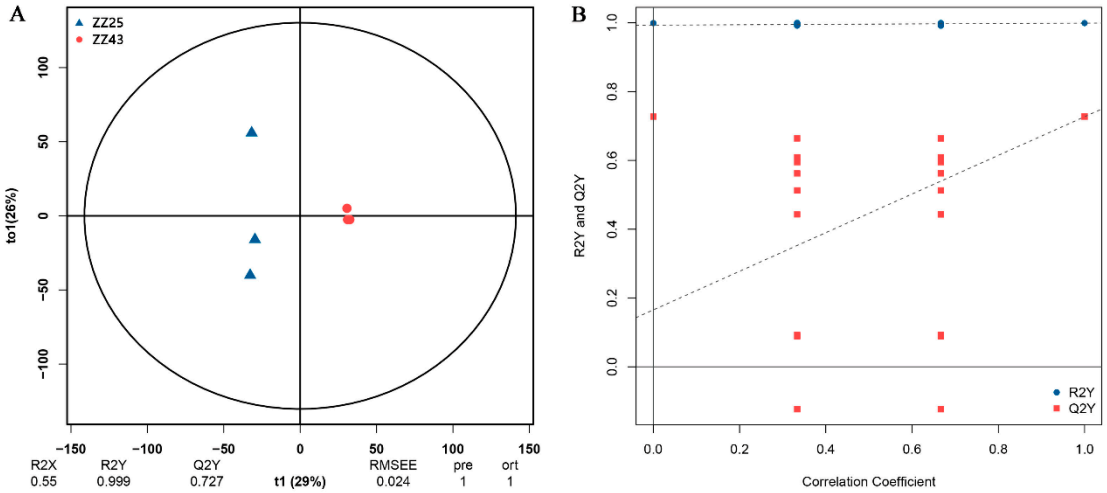
Supplementary Figure S5. OPLS-DA scores **(A)** and permutation test **(B)** plots of SZ25 vs. SZ39 comparison in negative ion mode.



Supplementary Figure S6. OPLS-DA scores **(A)** and permutation test **(B)** plots of SZ25 vs. SZ43 comparison in negative ion mode.



Supplementary Figure S7. OPLS-DA scores **(A)** and permutation test **(B)** plots of ZZ25 vs. ZZ39 comparison in negative ion mode.



Supplementary Figure S8. OPLS-DA scores **(A)** and permutation test **(B)** plots of ZZ25 vs. ZZ43 comparison in negative ion mode.