

Figure S1 PCA score plot of <sup>1</sup>H-NMR. Each point is each sample. Different groups are in different colors, with circles representing the 95% confidence interval.

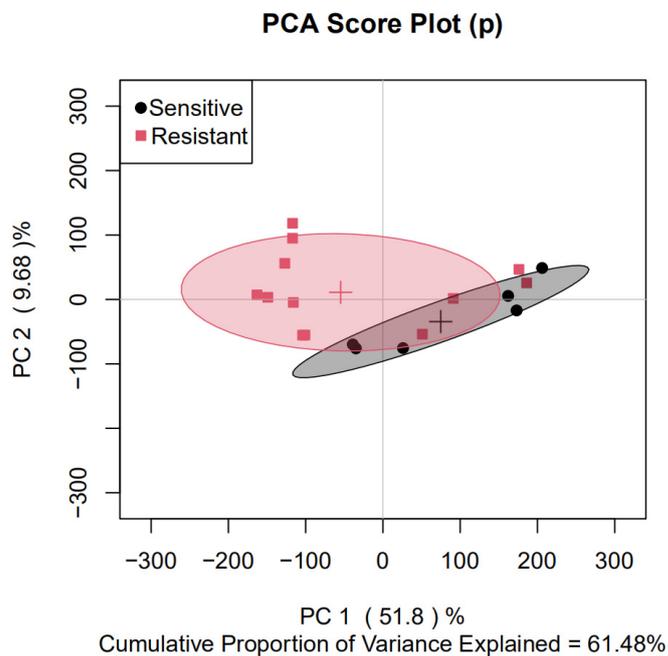


Figure S2 PCA(A) and OPLS-DA(B) analysis of the data achieved from UPLC-MS. Each point is each sample. Different groups are in different colors, with circles representing the 95% confidence interval.

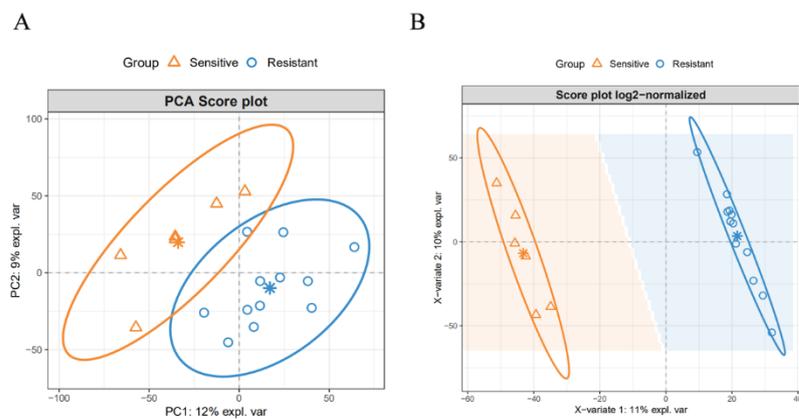
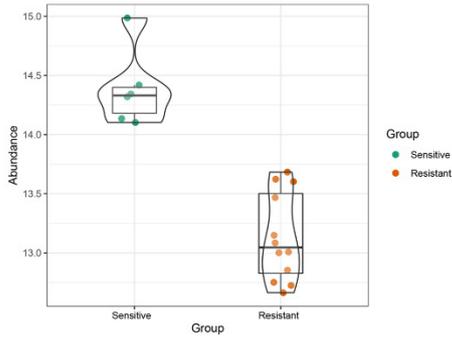


Figure S3 Other significant metabolites identified by UPLC-MS between the two groups.

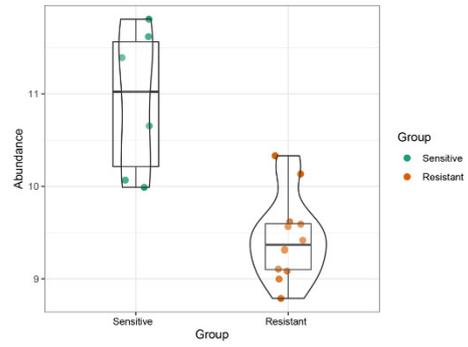
ID05858\_6.37\_249.05

$W_{\text{Mann-Whitney}} = 72.00$ ,  $p = 8.85e-04$ ,  $\rho_{\text{rank}}^{\text{biserial}} = 1.00$ ,  $CI_{95\%} [1.00, 1.00]$ ,  $n_{\text{obs}} = 18$



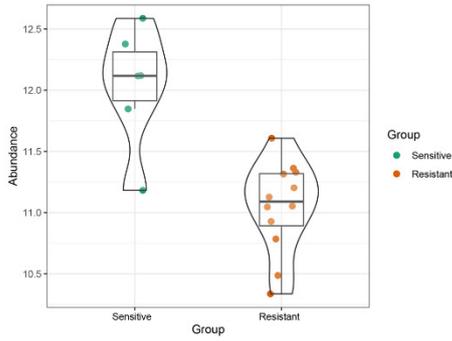
ID00863\_2.8\_113.03

$W_{\text{Mann-Whitney}} = 68.00$ ,  $p = 0.003$ ,  $\rho_{\text{rank}}^{\text{biserial}} = 0.89$ ,  $CI_{95\%} [0.68, 0.96]$ ,  $n_{\text{obs}} = 18$



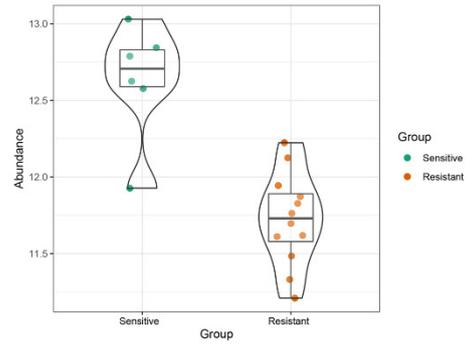
ID00274\_5.18\_72.99

$W_{\text{Mann-Whitney}} = 67.00$ ,  $p = 0.004$ ,  $\rho_{\text{rank}}^{\text{biserial}} = 0.86$ ,  $CI_{95\%} [0.61, 0.95]$ ,  $n_{\text{obs}} = 18$



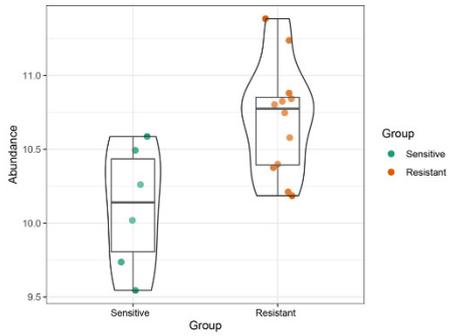
ID00736\_6.79\_104.03

$W_{\text{Mann-Whitney}} = 69.00$ ,  $p = 0.002$ ,  $\rho_{\text{rank}}^{\text{biserial}} = 0.92$ ,  $CI_{95\%} [0.76, 0.97]$ ,  $n_{\text{obs}} = 18$



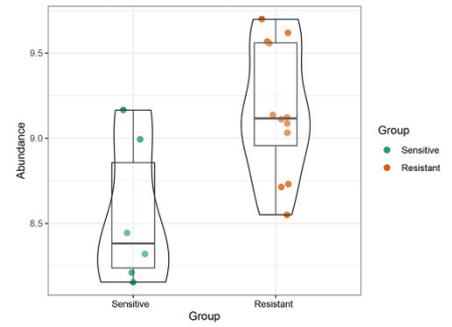
ID02077\_6.14\_145.05

$W_{\text{Mann-Whitney}} = 11.00$ ,  $p = 0.022$ ,  $\rho_{\text{rank}}^{\text{biserial}} = -0.69$ ,  $CI_{95\%} [-0.89, -0.27]$ ,  $n_{\text{obs}} = 18$



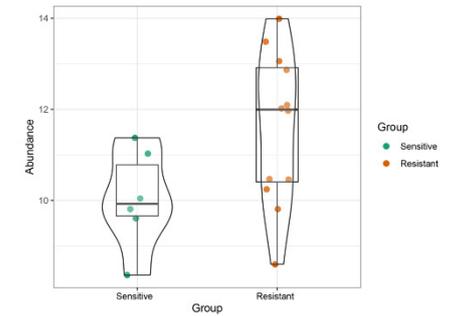
ID02814\_6.78\_169.01

$W_{\text{Mann-Whitney}} = 11.00$ ,  $p = 0.022$ ,  $\rho_{\text{rank}}^{\text{biserial}} = -0.69$ ,  $CI_{95\%} [-0.89, -0.27]$ ,  $n_{\text{obs}} = 18$



ID09298\_8.72\_329.03

$W_{\text{Mann-Whitney}} = 14.00$ ,  $p = 0.044$ ,  $\rho_{\text{rank}}^{\text{biserial}} = -0.61$ ,  $CI_{95\%} [-0.86, -0.13]$ ,  $n_{\text{obs}} = 18$



ID02428\_1.24\_157.12

$W_{\text{Mann-Whitney}} = 71.00$ ,  $p = 0.001$ ,  $\rho_{\text{rank}}^{\text{biserial}} = 0.97$ ,  $CI_{95\%} [0.91, 0.99]$ ,  $n_{\text{obs}} = 18$

