

Supplementary Materials

Table 3 R² and Q² intercept values for the OPLS-DA mode

Name	R ²	Q ²
RP	0.640	0.604
HI	0.752	0.669
RP+HI	0.909	0.869
VDS	0.718	0.674
GEM	0.791	0.715
BCNU	0.682	0.638
MIT	0.819	0.727
API	0.838	0.762
DIO	0.618	0.589

Note: RP are the database from RPLC method, HI are the database from HILIC method, RP+HI means that the RP and HI data was combined together.

Table 4 CV-ANOVA parameters derived from cross-validation of OPLS-DA model

	SS	df	MS	F	P	SD
Total corr.	360	360	1			1
Regression	239.189	42	5.695	14.990	4.01E-20	2.386
Residual	120.811	318	0.380			0.616

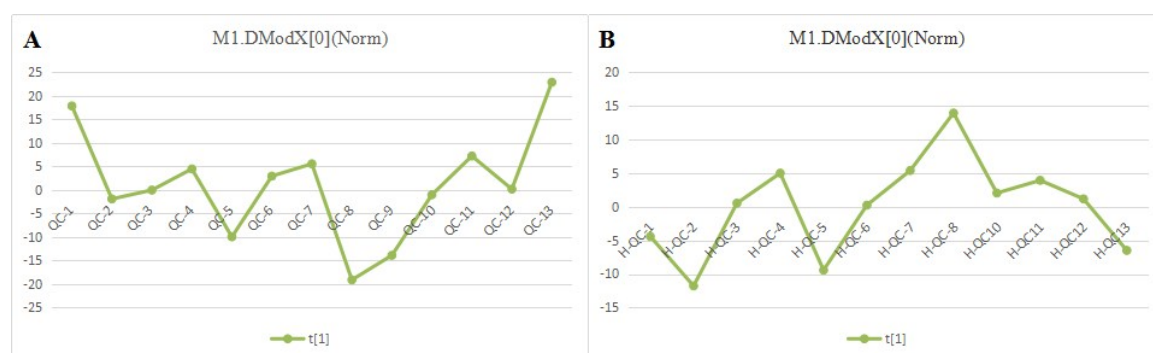


Fig.7 Stability of UPLC-MS system in analysis

A:RPLCmethod; B:HILIC method

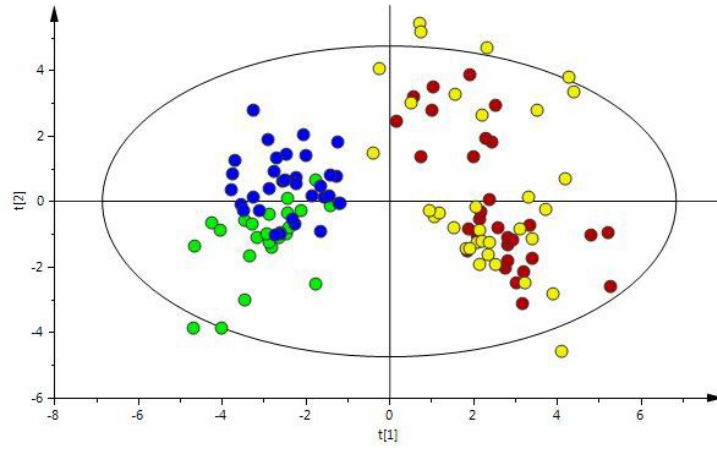


Fig.8 The PCA score plot of cells in drug-treated groups of four classes
 $R^2=0.426$ $Q^2=0.147$