

Table S1. PLS-DA cross-validation details

Measure	1 comps	2 comps	3 comps	4 comps	5 comps
Accuracy	1.0	1.0	1.0	1.0	1.0
R2	0.90656	0.96898	0.993	0.99824	0.99941
Q2	0.8572	0.94947	0.96161	0.96433	0.96826