

Supplementary table 1 The contribution results of different number of PC

Component	Chromatogram		Spectra	
	Cumulative%	Eigenvalues	Cumulative%	Eigenvalues
1	0.419	107	0.36	147
2	0.608	22.8	0.504	58.5
3	0.7159	19.8	0.6473	58.3
4	0.7921	12.8	0.7523	16.3
5	0.8565	10.4	0.825	13.3
6	0.9029	8.96	0.8893	10.97
7	0.9256	7.81	0.9255	9.12
8	0.9452	7.01	0.9356	8.41