Electronic Supplementary Material (ESI) for Analytical Methods.

Supportment materials

Table S1 Total variance explained of AAs

	Initial eigenvalues			Extraction sums of squared loadings		
Component	Total	% of variance	% of percent	Total	% of variance	% of percent
1	7.872	56.229	56.229	5.803	41.447	41.447
2	3.949	28.204	84.432	5.498	39.270	80.718
3	1.399	9.993	94.425	1.919	13.707	94.425
4	0.781	5.575	100.000			

1: the first factor; 2: the second factor; 3: the third factor; 4: the forth factor.

Table S2 Extraction compound matrix of AAs

	Compound		
	1	2	3
Phenylalanine	-0.188	-0.959	0.141
Leucine	-0.455	0.889	-0.030
Methionine	0.037	-0.239	0.739
Valine	0.954	-0.096	0.273
Proline	-0.334	-0.941	0.053
Alanine	0.297	0.458	0.757
Glycine	-0.455	0.889	-0.030
Serine	0.810	-0.334	0.481

Glutamic acid	-0.455	0.889	-0.030
Aspartic acid	-0.456	0.888	-0.035
Arginine	0.999	-0.039	-0.013
Histidine	0.857	-0.132	0.442
Lysine	0.799	-0.349	0.488
Tyrosine	0.893	-0.066	-0.183

Table S3 Total variance explained of NNs

	Initial eigenvalues			Extraction sums of squared loadings		
Component	Total	% of variance	% of percent	Total	% of variance	% of percent
1	4.688	52.083	52.083	4.597	51.076	51.076
2	2.359	26.216	78.300	2.276	25.294	76.370
3	1.228	13.640	91.940	1.401	15.570	91.940
4	0.725	8.060	100.000			

Table S4 Extraction compound matrix of NNs

	Compound		
	1	2	3
Thymidine	0.488	0.488	0.162
Adenine	-0.015	0.180	0.983
Hypoxanthine	-0.929	-0.225	0.275
Uridine	0.965	0.140	0.208
Inosine	-0.159	0.888	0.145

Adenosine	0.210	0.977	0.020
Guanosine	0.991	0.119	-0.055
Uracil	0.877	-0.422	-0.146
Guanine	0.862	-0.006	0.495