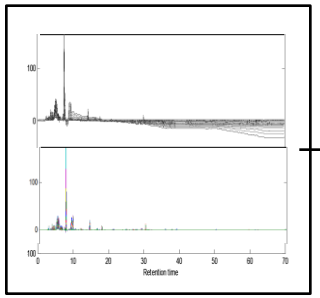
MEASURING DEVICES

TRAINING SET HERB A

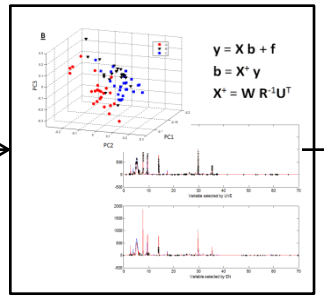
TRAINING SET CHEMICAL FINGERPRINT

TRAINING SET BIOLOGICAL ACTIVITY

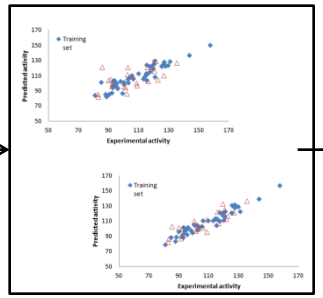
DATA PRE-PROCESSING



DIMENSIONALITY REDUCTION



MODEL REFINEMENT

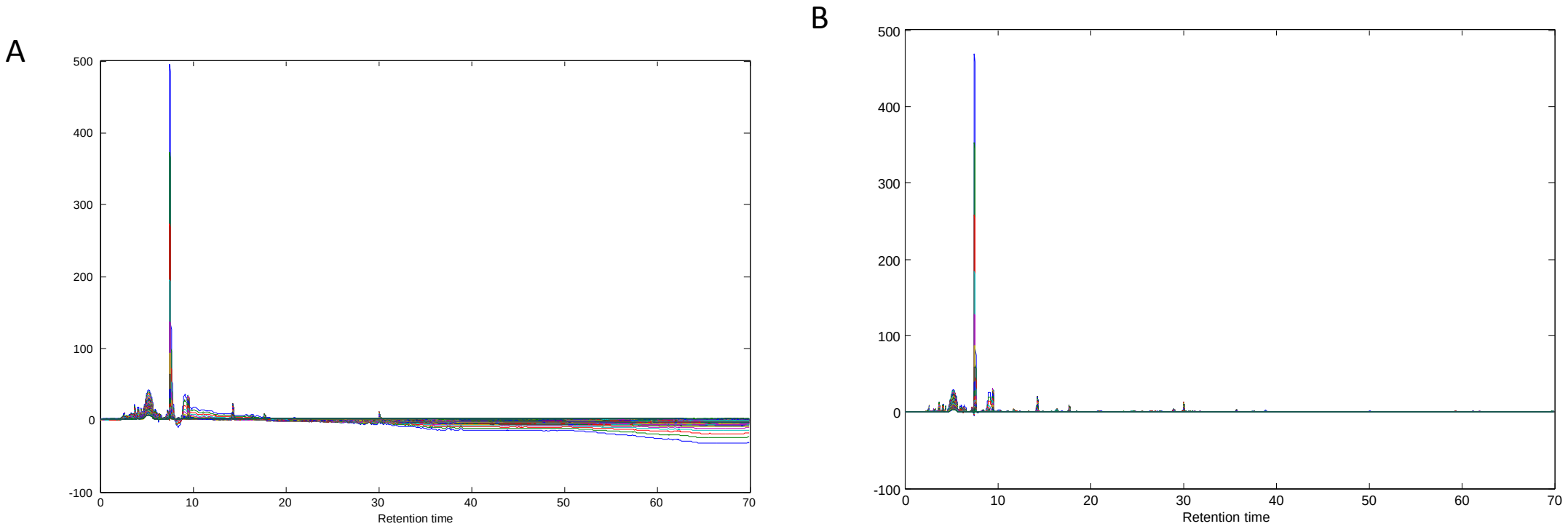


TEST SET HERB A CHEMICAL FINGERPRINT

QPAR model

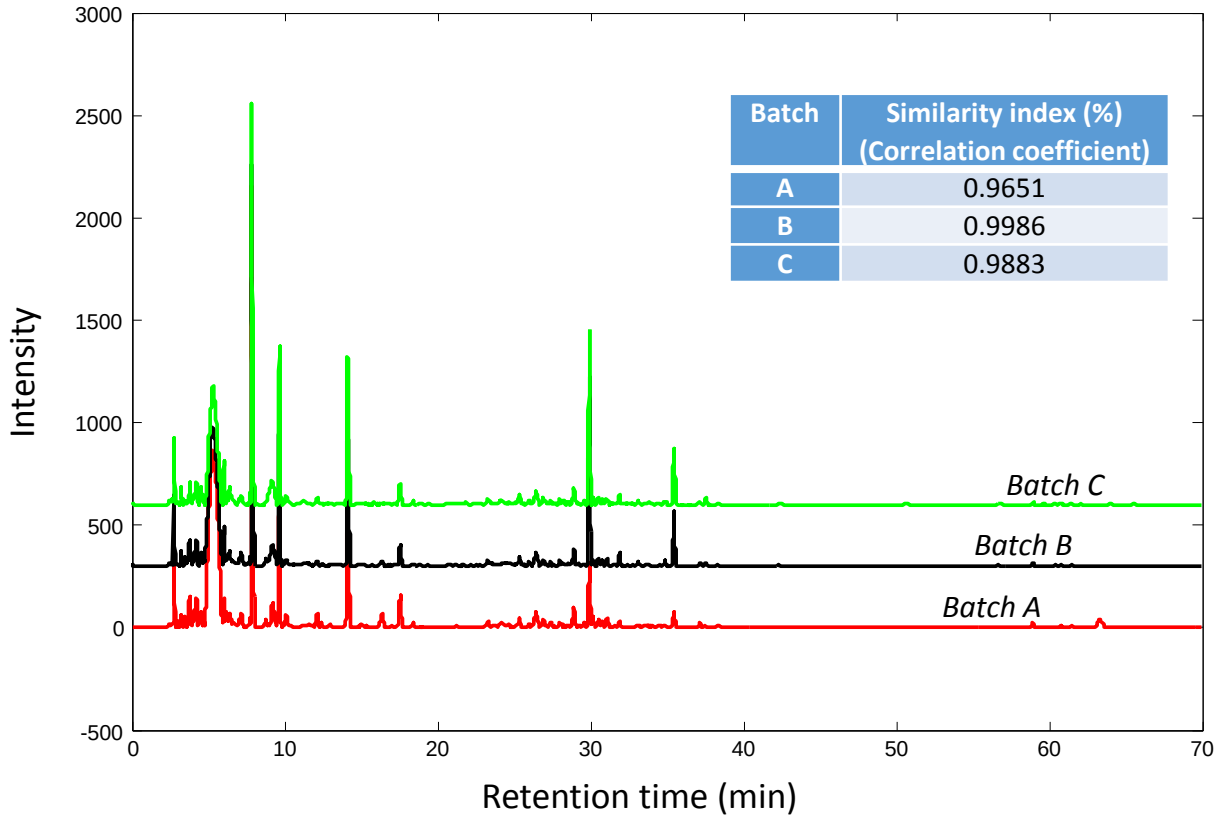
PREDICTION BIOLOGICAL ACTIVITY

Supplementary Figure 1. The schematic diagram of the development of the CD80-QPAR chemometric model.

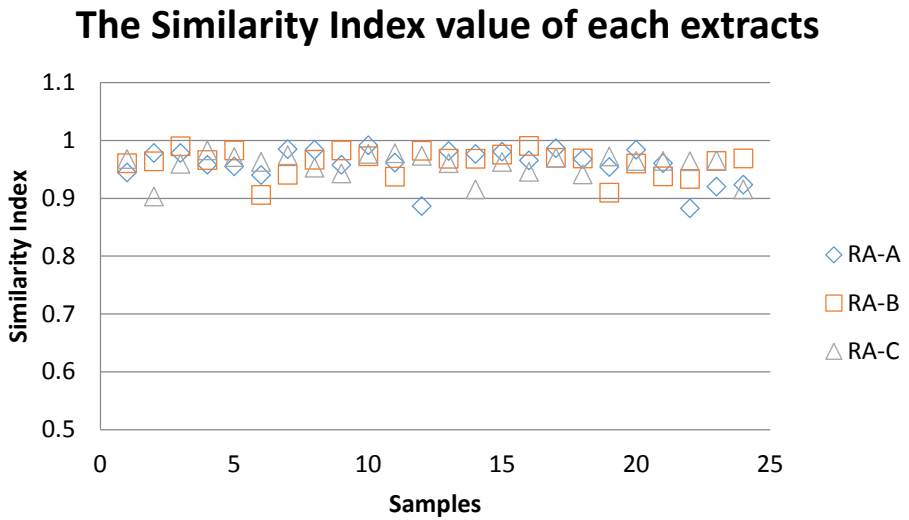


Supplementary Figure 2: The HPLC chromatograms of RA-A (A) before and (B) after data pre-processing were illustrated for the importance of applying the data pre-processing such as background correction and peaks alignment.

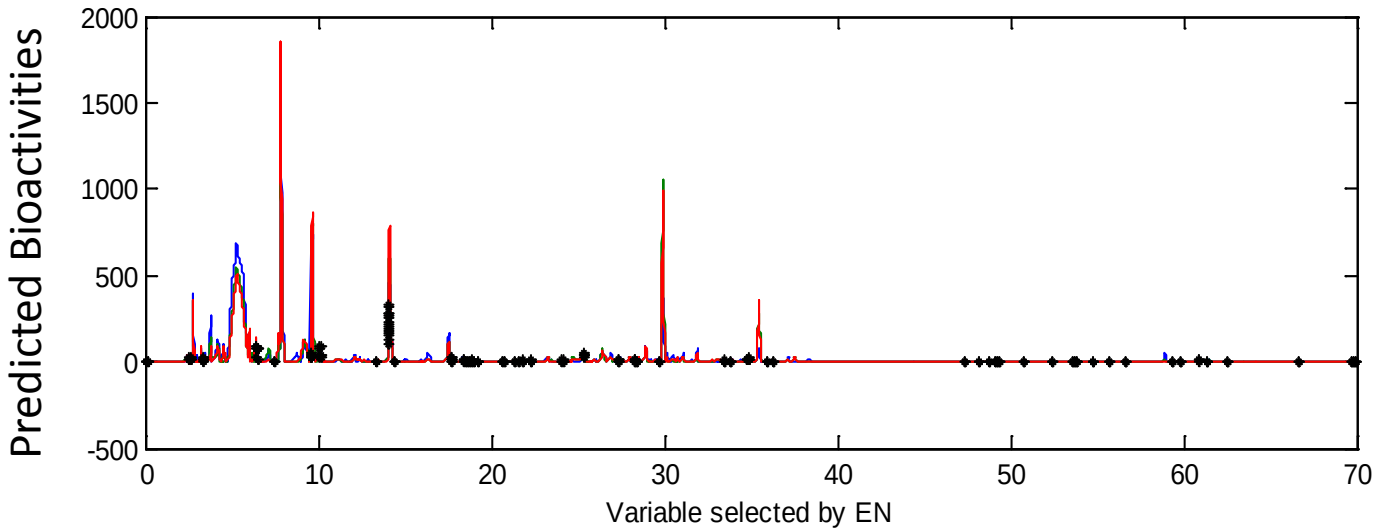
a.


Batch
Similarity index (%) (Correlation coefficient)
A
0.9651
B
0.9986
C
0.9883
Batch C
Batch B
Batch A
Intensity
Retention time (min)
3000
2500
2000
1500
1000
500
0
-500
0
10
20
30
40
50
60
70

b.


The Similarity Index value of each extracts
Similarity Index
1.1
1
0.9
0.8
0.7
0.6
0.5
0
5
10
15
20
25
Samples
RA-A
RA-B
RA-C

Supplementary Figure 3: (a) HPLC-DAD mean chromatogram (common pattern) of 72 extracts which from three batches (Red: RA-A; Black: RA-B; Green: RA-C). The table in the right top corner showed the value of the similarity indices of the three median chromatographic modes of the extracts from A, B and C with respect to their median; (b) The distribution, the mean and standard derivation of the similarity indices of each extract from three batches.


Predicted Bioactivities
2000
1500
1000
500
0
-500
0
10
20
30
40
50
60
70
Variable selected by EN

Supplementary Figure 4: The variables selected by Elastic Net (EN) PLS (lower) algorithm for models building in QPAR studies of Radix Astragali (RA).

Supplementary Table 1: A table of the result from uniform design by varying the two extraction factors (reflux time and solvent volume) for the preparation of 24 RA extracts from each batch.

Extract	Level	
	Reflux Time	**Volume of solvent used**
1	2 (2 hr)	4 (250 ml)
2	4 (4 hr)	2 (150 ml)
3	2 (2 hr)	4 (250 ml)
4	4 (4 hr)	3 (200 ml)
5	3 (3 hr)	1 (100 ml)
6	1 (1 hr)	2 (150 ml)
7	2 (2 hr)	3 (200 ml)
8	2 (2 hr)	1 (100 ml)
9	1 (1 hr)	4 (250 ml)
10	3 (3 hr)	1 (100 ml)
11	3 (3 hr)	2 (150 ml)
12	2 (2 hr)	2 (150 ml)
13	4 (4 hr)	3 (200 ml)
14	4 (4 hr)	1 (100 ml)
15	3 (3 hr)	4 (250 ml)
16	3 (3 hr)	3 (200 ml)
17	1 (1 hr)	2 (150 ml)
18	4 (4 hr)	4 (250 ml)
19	1 (1 hr)	3 (200 ml)
20	1 (1 hr)	1 (100 ml)
21	0 (0 hr)	4 (250 ml)
22	0 (0 hr)	1 (100 ml)
23	0 (0 hr)	3 (200 ml)
24	0 (0 hr)	2 (150 ml)

Uniform design based on CD_2 Discrepancy: $U_n(q^s)$;
n = number of runs, s = number of factors, q = number of levels

Supplementary Table 2: Similarity indices (SI) correlation coefficient (mean ± SD) of each extract from the three batches with respect to their batch means chemical fingerprints.

SI	Batch A	Batch B	Batch C
Avg	0.9583	0.9610	0.9576
SD	0.0297	0.0226	0.0210

Supplementary Table 3: The t-test and ANOVA results of the difference of the immunomodulatory effect among Batch A, B and C on THP-1 cells.

CD80			
	Batch A	**Batch B**	**Batch C**
Mean	106.23	95.83	122.75
S^2	115.47	116.17	160.37
t-test			
Group	**A and B**	**A and C**	**B and C**
t	3.28	-4.77	-7.77
***p* value**	0.002	1.9e-5	0.000