

**Chemical Fingerprint and Simultaneous Determination of
Flavonoids in Flos Sophorae Immaturus by HPLC-DAD and HPLC-
ESI-MS/MS Coupled with Chemometrics Analysis**

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Supporting information

Figure S1 Extraction efficiencies of the three compounds by different solvent (A), different methanol concentration (B), different solvent volume (C), and different extraction time (D). Extraction efficiencies were evaluated by comparing the peak areas of the target compounds when samples were fixed at the same weight.

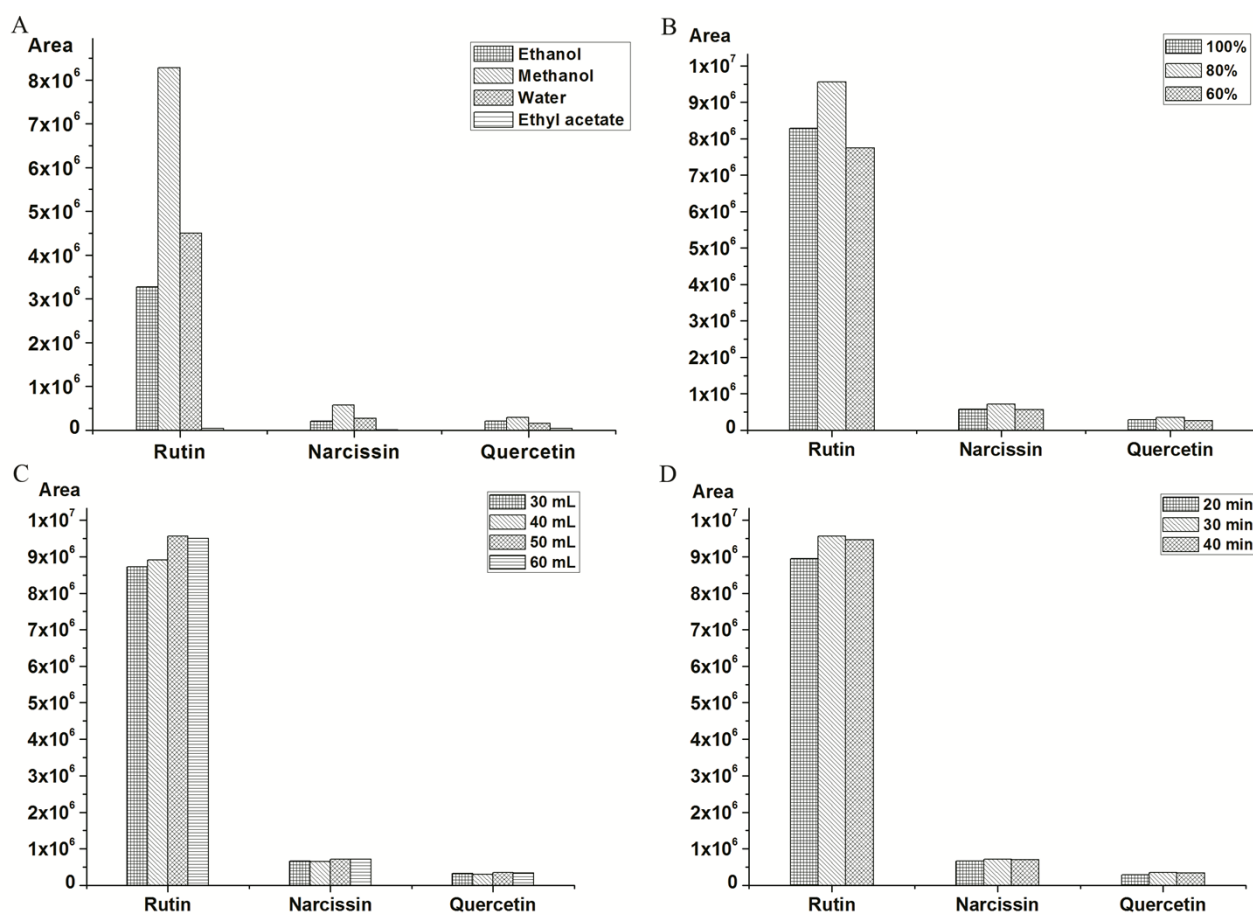


Figure S2 Proposal desolation path way of typical quercetin and isorhamnetin glycoside (A: rutin, B: narcissin).

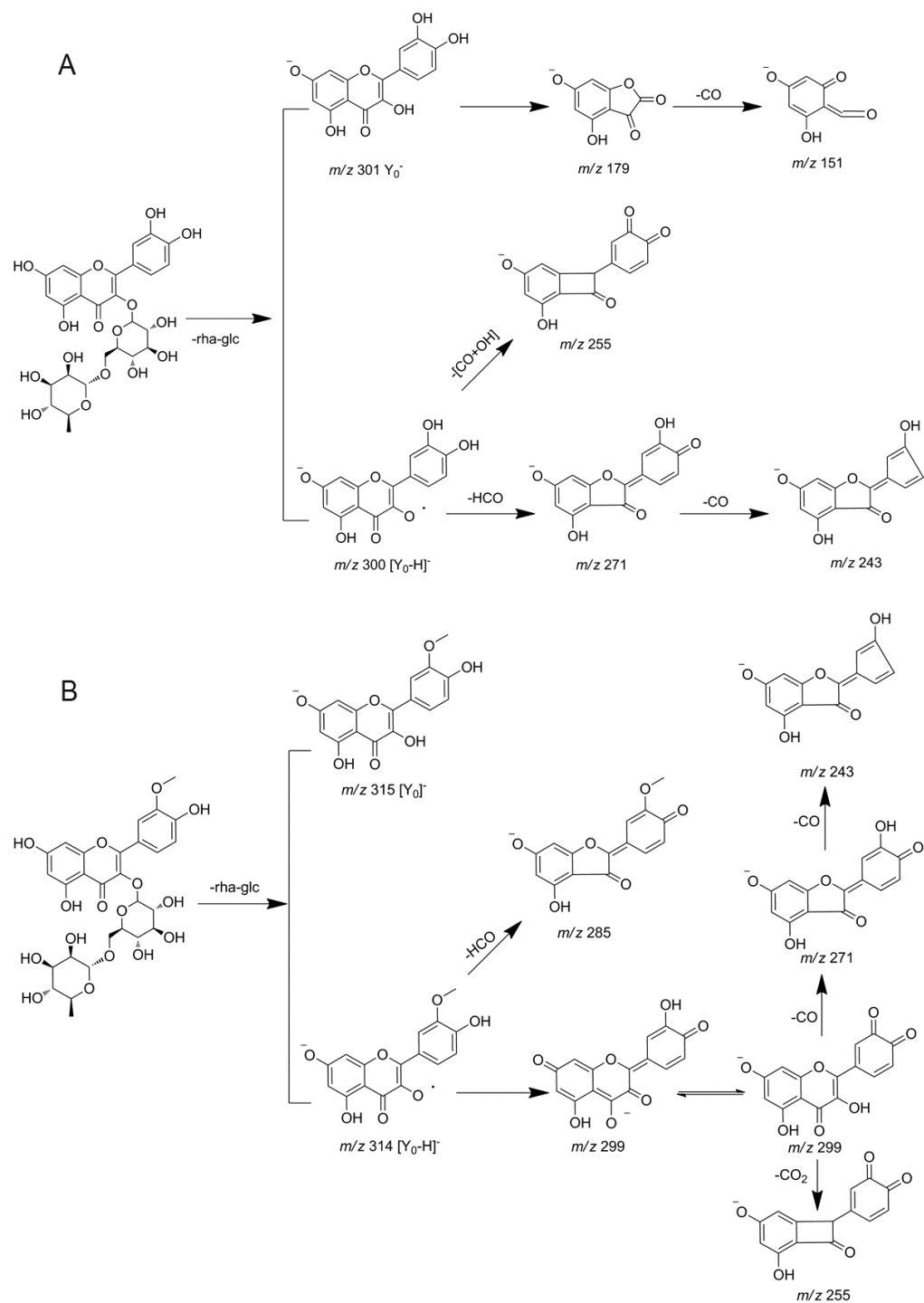


Figure S3 The command for the calculation of Mahalanobis distance of all samples by

Matlab 7.0

A =

```
      0      0
    0.6936 -0.3886
   -0.7326  1.3129
   -0.5015 -0.0756
   -0.8739 -2.1585
    0.0539  0.4368
   -0.1218  1.5601
   -1.0589  0.8244
   -0.6559  0.1853
   -0.9876  0.1615
    1.2813  0.6610
    0.1895 -1.4100
    0.0926 -0.6078
    0.0260 -0.5470
    2.5953  0.0456
```

```
>> X = A(:,1);
Y = A(:,2);
N = length(X);
D = zeros(N,N);
for I = 2:N
for J = 1:I-1
D(I,J) = sqrt((X(I) - X(J))*(X(I) - X(J)) + (Y(I) - Y(J))*(Y(I) - Y(J)));
end
end
D%
D1 = D+D' %
```

Figure S4 The output for the calculation of Mahalanobis distance of all samples by Matlab 7.0. The first column represents the Mahalanobis distance between each sample point and the origin (radius) and the field included by the blue box represents the Mahalanobis distance between each sample point.

D1 =

0	0.7950	1.5035	0.5072	2.3287	0.4401	1.5648	1.3420	0.6815	1.0007	1.4417	1.4227	0.6148	0.5476	2.5957
0.7950	0	2.2201	1.2354	2.3642	1.0442	2.1124	2.1313	1.4664	1.7689	1.2029	1.1391	0.6397	0.6861	1.9507
1.5035	2.2201	0	1.4076	3.4743	1.1773	0.6589	0.5875	1.1303	1.1793	2.1167	2.8748	2.0904	2.0087	3.5610
0.5072	1.2354	1.4076	0	2.1159	0.7556	1.6792	1.0586	0.3031	0.5408	1.9290	1.5027	0.7976	0.7075	3.0992
2.3287	2.3642	3.4743	2.1159	0	2.7561	3.7939	2.9886	2.3539	2.3229	3.5488	1.3004	1.8273	1.8458	4.1102
0.4401	1.0442	1.1773	0.7556	2.7561	0	1.1370	1.1784	0.7530	1.0772	1.2477	1.8517	1.0452	0.9842	2.5714
1.5648	2.1124	0.6589	1.6792	3.7939	1.1370	0	1.1914	1.4749	1.6448	1.6664	2.9863	2.1784	2.1122	3.1107
1.3420	2.1313	0.5875	1.0586	2.9886	1.1784	1.1914	0	0.7556	0.6667	2.3459	2.5595	1.8377	1.7487	3.7363
0.6815	1.4664	1.1303	0.3031	2.3539	0.7530	1.4749	0.7556	0	0.3325	1.9947	1.8054	1.0905	1.0006	3.2542
1.0007	1.7689	1.1793	0.5408	2.3229	1.0772	1.6448	0.6667	0.3325	0	2.3232	1.9635	1.3261	1.2367	3.5848
1.4417	1.2029	2.1167	1.9290	3.5488	1.2477	1.6664	2.3459	1.9947	2.3232	0	2.3412	1.7386	1.7421	1.4510
1.4227	1.1391	2.8748	1.5027	1.3004	1.8517	2.9863	2.5595	1.8054	1.9635	2.3412	0	0.8081	0.8784	2.8119
0.6148	0.6397	2.0904	0.7976	1.8273	1.0452	2.1784	1.8377	1.0905	1.3261	1.7386	0.8081	0	0.0901	2.5866
0.5476	0.6861	2.0087	0.7075	1.8458	0.9842	2.1122	1.7487	1.0006	1.2367	1.7421	0.8784	0.0901	0	2.6368
2.5957	1.9507	3.5610	3.0992	4.1102	2.5714	3.1107	3.7363	3.2542	3.5848	1.4510	2.8119	2.5866	2.6368	0