

Table S1 Samples used in present study

Sample	Species	Voucher ID	Harvest Years	Collection Location
Cp-1	<i>Citrus reticulata</i> ‘Tangerina’	cpt1601	2016	Lukou Town, Zhuzhou, Hunan
Cp-2	<i>Citrus reticulata</i> ‘Tangerina’	cpt1602	2016	Lukou Town, Zhuzhou, Hunan
Cp-3	<i>Citrus reticulata</i> ‘Tangerina’	cpt1603	2016	Lukou Town, Zhuzhou, Hunan
Cp-4	<i>Citrus reticulata</i> ‘Tangerina’	cpt1701	2017	Lukou Town, Zhuzhou, Hunan
Cp-5	<i>Citrus reticulata</i> ‘Tangerina’	cpt1702	2017	Lukou Town, Zhuzhou, Hunan
Cp-6	<i>Citrus reticulata</i> ‘Tangerina’	cpt1604	2016	Nanchang, Jiangxi
Cp-7	<i>Citrus reticulata</i> ‘Tangerina’	cpt1605	2016	Nanchang, Jiangxi
Cp-8	<i>Citrus reticulata</i> ‘Tangerina’	cpt1606	2016	Nanchang, Jiangxi
Cp-9	<i>Citrus reticulata</i> ‘Tangerina’	cpt1607	2016	Nanchang, Jiangxi
Cp-10	<i>Citrus reticulata</i> ‘Tangerina’	cpt1703	2017	Nanchang, Jiangxi
Cp-11	<i>Citrus reticulata</i> ‘Tangerina’	cpt1704	2017	Nanchang, Jiangxi
Cp-12	<i>Citrus reticulata</i> ‘Tangerina’	cpt1705	2017	Nanchang, Jiangxi
Cp-13	<i>Citrus reticulata</i> ‘Tangerina’	cpt1706	2017	Nanchang, Jiangxi
Cp-14	<i>Citrus reticulata</i> ‘Unshiu’	cpu1601	2016	Huangyan District, Taizhou Zhejiang
Cp-15	<i>Citrus reticulata</i> ‘Unshiu’	cpu1602	2016	Huangyan District, Taizhou Zhejiang
Cp-16	<i>Citrus reticulata</i> ‘Unshiu’	cpu1701	2017	Huangyan District, Taizhou Zhejiang
Cp-17	<i>Citrus reticulata</i> ‘Unshiu’	cpu1702	2017	Huangyan District, Taizhou Zhejiang
Cp-18	<i>Citrus reticulata</i> ‘Unshiu’	cpu1703	2017	Huangyan District, Taizhou Zhejiang
Cp-19	<i>Citrus reticulata</i> ‘Unshiu’	cpu1704	2017	Huangyan District, Taizhou Zhejiang
Cp-20	<i>Citrus reticulata</i> ‘Unshiu’	cpu1705	2017	Huangyan District, Taizhou Zhejiang
Cp-21	<i>Citrus reticulata</i> ‘Unshiu’	cpu1706	2017	Huangyan District, Taizhou Zhejiang
Cp-22	<i>Citrus reticulata</i> ‘Unshiu’	cpu1707	2017	Huangyan District, Taizhou Zhejiang
Cp-23	<i>Citrus reticulata</i> ‘Unshiu’	cpu1708	2017	Huangyan District, Taizhou Zhejiang
Cp-24	<i>Citrus reticulata</i> ‘Unshiu’	cpu1709	2017	Huangyan District, Taizhou Zhejiang
Cp-25	<i>Citrus reticulata</i> ‘Unshiu’	cpu1710	2017	Huangyan District, Taizhou Zhejiang
Cp-26	<i>Citrus reticulata</i> ‘Unshiu’	cpu1711	2017	Yichang, Hubei
Cp-27	<i>Citrus reticulata</i> ‘Unshiu’	cpu1712	2017	Yichang, Hubei
Cp-28	<i>Citrus reticulata</i> ‘Unshiu’	cpu1713	2017	Yichang, Hubei
Cp-29	<i>Citrus reticulata</i> ‘Dahongpao’	cpd1601	2016	Zigong, Sichuan
Cp-30	<i>Citrus reticulata</i> ‘Dahongpao’	cpd1602	2016	Zigong, Sichuan
Cp-31	<i>Citrus reticulata</i> ‘Dahongpao’	cpd1701	2017	Zigong, Sichuan
Gcp-1	<i>Citrus reticulata</i> ‘Chachi’	gcp1601	2016	Xinhui, Guangdong
Gcp-2	<i>Citrus reticulata</i> ‘Chachi’	gcp1602	2016	Xinhui, Guangdong
Gcp-3	<i>Citrus reticulata</i> ‘Chachi’	gcp1603	2016	Xinhui, Guangdong
Gcp-4	<i>Citrus reticulata</i> ‘Chachi’	gcp1604	2016	Xinhui, Guangdong
Gcp-5	<i>Citrus reticulata</i> ‘Chachi’	gcp1605	2016	Xinhui, Guangdong

Gcp-6	<i>Citrus reticulata</i> 'Chachi'	gcp1606	2016	Xinhui, Guangdong
Gcp-7	<i>Citrus reticulata</i> 'Chachi'	gcp1701	2017	Xinhui, Guangdong
Gcp-8	<i>Citrus reticulata</i> 'Chachi'	gcp1702	2017	Xinhui, Guangdong
Gcp-9	<i>Citrus reticulata</i> 'Chachi'	gcp1703	2017	Xinhui, Guangdong
Gcp-10	<i>Citrus reticulata</i> 'Chachi'	gcp1704	2017	Xinhui, Guangdong
Gcp-11	<i>Citrus reticulata</i> 'Chachi'	gcp1705	2017	Xinhui, Guangdong
Gcp-12	<i>Citrus reticulata</i> 'Chachi'	gcp1710	2017	Xinhui, Guangdong
Gcp-13	<i>Citrus reticulata</i> 'Chachi'	gcp1711	2017	Xinhui, Guangdong
Gcp-14	<i>Citrus reticulata</i> 'Chachi'	gcp1712	2017	Xinhui, Guangdong
Gcp-15	<i>Citrus reticulata</i> 'Chachi'	gcp1620	2016	Xinhui, Guangdong
Gcp-16	<i>Citrus reticulata</i> 'Chachi'	gcp1621	2016	Xinhui, Guangdong
Gcp-17	<i>Citrus reticulata</i> 'Chachi'	gcp1501	2015	Xinhui, Guangdong
Gcp-18	<i>Citrus reticulata</i> 'Chachi'	gcp1502	2015	Xinhui, Guangdong
Gcp-19	<i>Citrus reticulata</i> 'Chachi'	gcp1503	2015	Sihui, Guangdong
Gcp-20	<i>Citrus reticulata</i> 'Chachi'	gcp1504	2015	Sihui, Guangdong

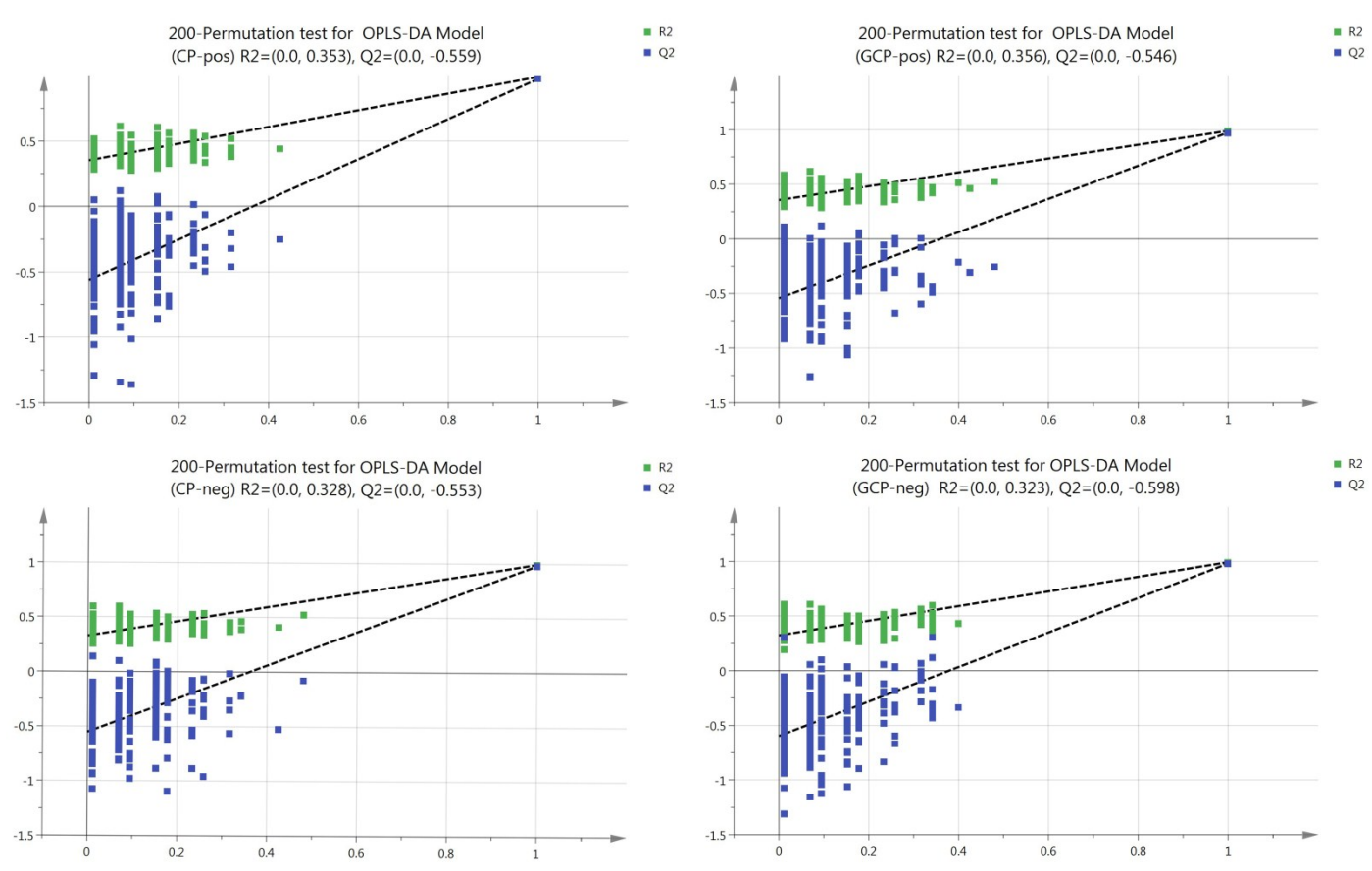


Figure S1 Permutations test plot for OPLS-DA (200 tests) in positive and negative mode.

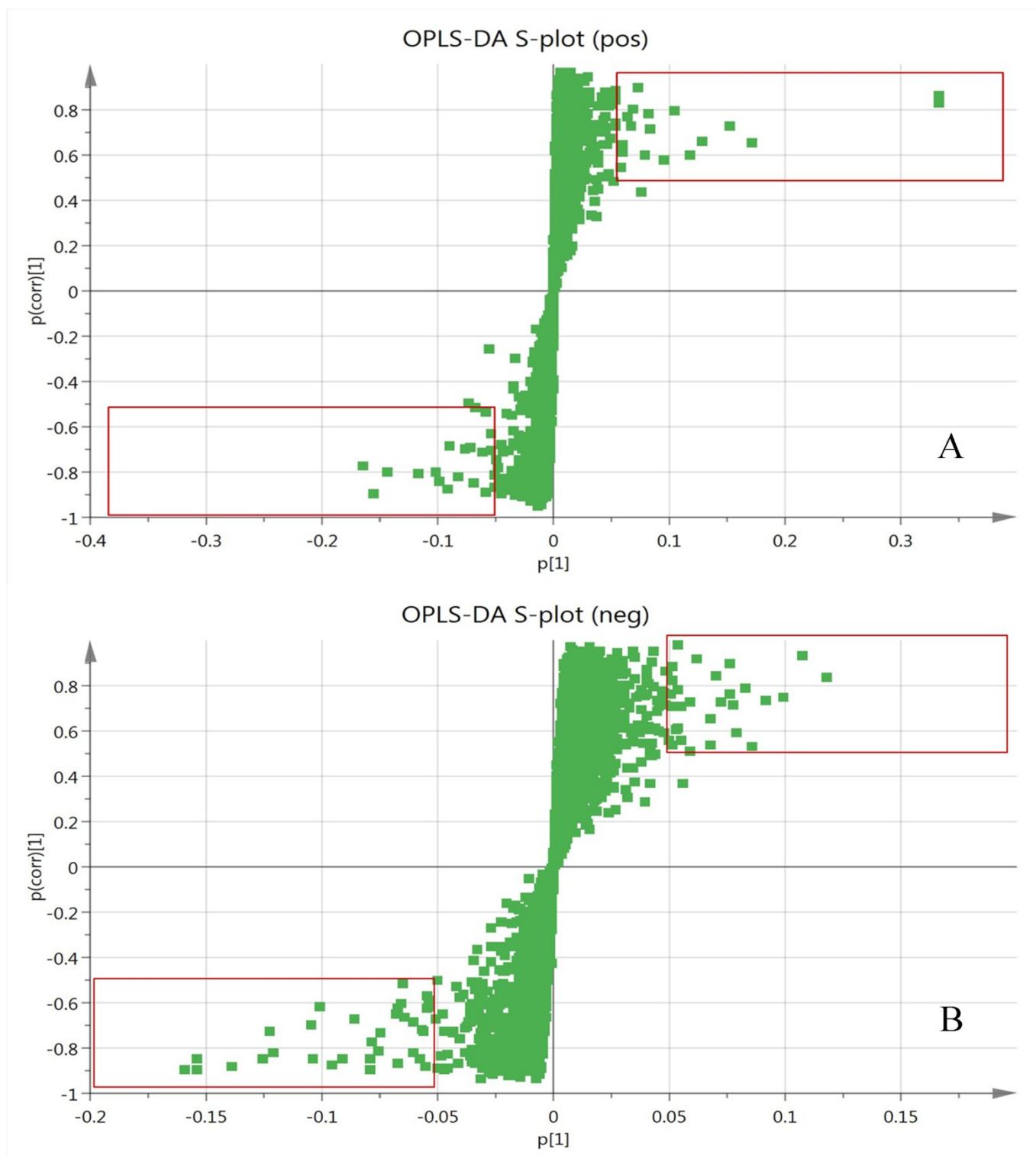


Figure S2 The S-plots of OPLS-DA both positive and negative mode.

Table S2. The classified and predicted results obtained by SVM model.

Training Set Accuracy: 100%			Test Set Accuracy: 100%		
Samples	Actual	Predict	Samples	Actual	Predict
Cp-27	CP	CP	Cp-26	CP	CP
Cp-28	CP	CP	Cp-5	CP	CP
Cp-1	CP	CP	Cp-8	CP	CP
Cp-2	CP	CP	Cp-11	CP	CP
Cp-3	CP	CP	Cp-22	CP	CP
Cp-4	CP	CP	Gcp-4	GCP	GCP

Cp-6	CP	CP	Gcp-5	GCP	GCP
Cp-7	CP	CP	Gcp-11	GCP	GCP
Cp-9	CP	CP	Gcp-20	GCP	GCP
Cp-10	CP	CP	Gcp-14	GCP	GCP
Cp-12	CP	CP	Gcp-17	GCP	GCP
Cp-13	CP	CP	QC-1	QC	QC
Cp-29	CP	CP	QC-9	QC	QC
Cp-30	CP	CP			
Cp-31	CP	CP			
Gcp-19	GCP	GCP			
Gcp-13	GCP	GCP			
Gcp-15	GCP	GCP			
Gcp-16	GCP	GCP			
Gcp-18	GCP	GCP			
QC-2	QC	QC			
QC-3	QC	QC			
QC-4	QC	QC			
QC-5	QC	QC			
Cp-14	CP	CP			
Cp-15	CP	CP			
Cp-16	CP	CP			
Cp-17	CP	CP			
Cp-18	CP	CP			
Cp-19	CP	CP			
Cp-20	CP	CP			
Cp-21	CP	CP			
Cp-23	CP	CP			
Cp-24	CP	CP			
Cp-25	CP	CP			
Gcp-1	GCP	GCP			
Gcp-2	GCP	GCP			
Gcp-3	GCP	GCP			
Gcp-6	GCP	GCP			
Gcp-7	GCP	GCP			
Gcp-8	GCP	GCP			
Gcp-9	GCP	GCP			
Gcp-10	GCP	GCP			
Gcp-12	GCP	GCP			
QC-6	QC	QC			
QC-7	QC	QC			
QC-8	QC	QC			

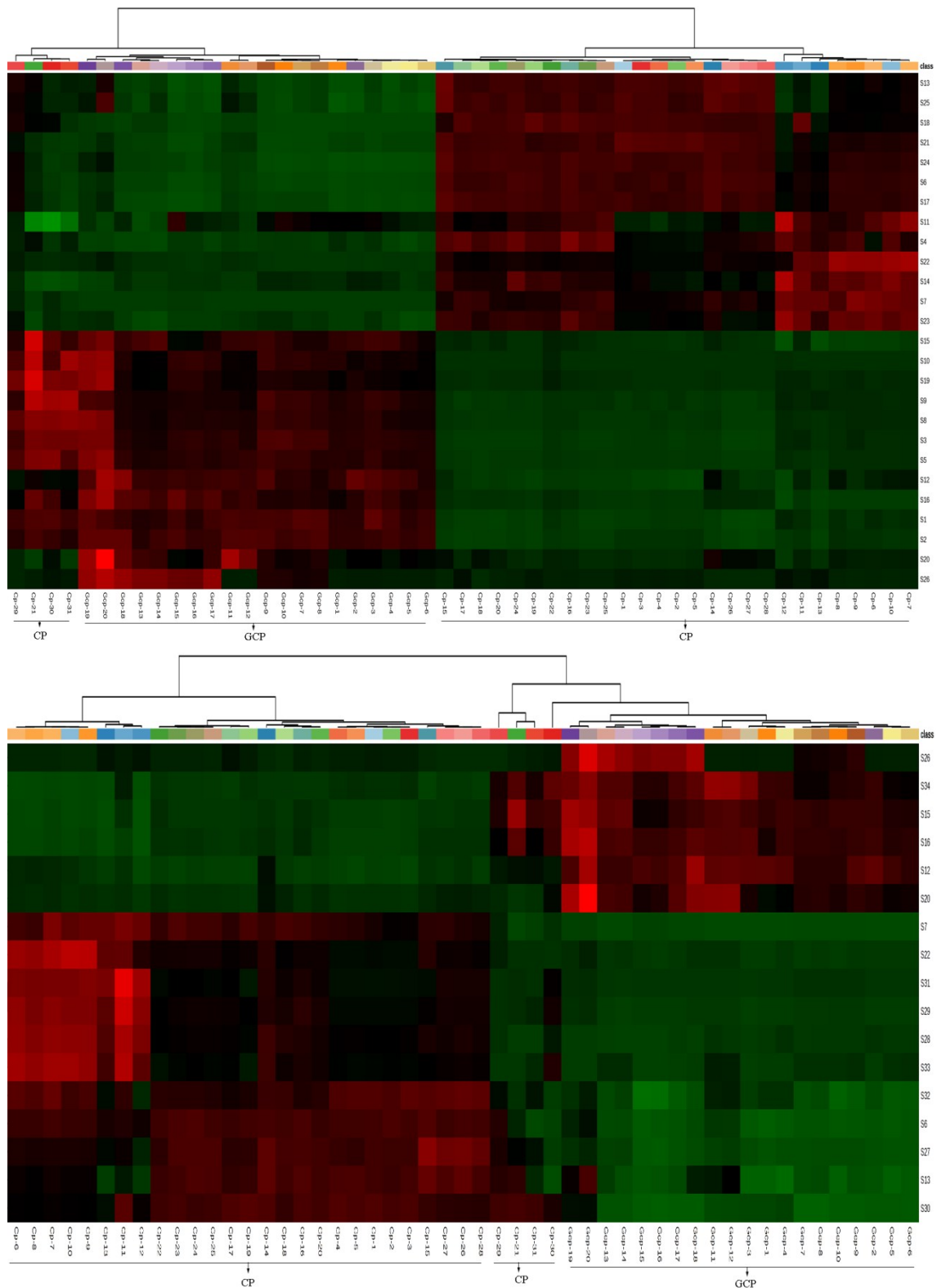


Figure S3 The heatmap of the differences of chemical markers in GCP and CP (Up: positive;Down: negative)

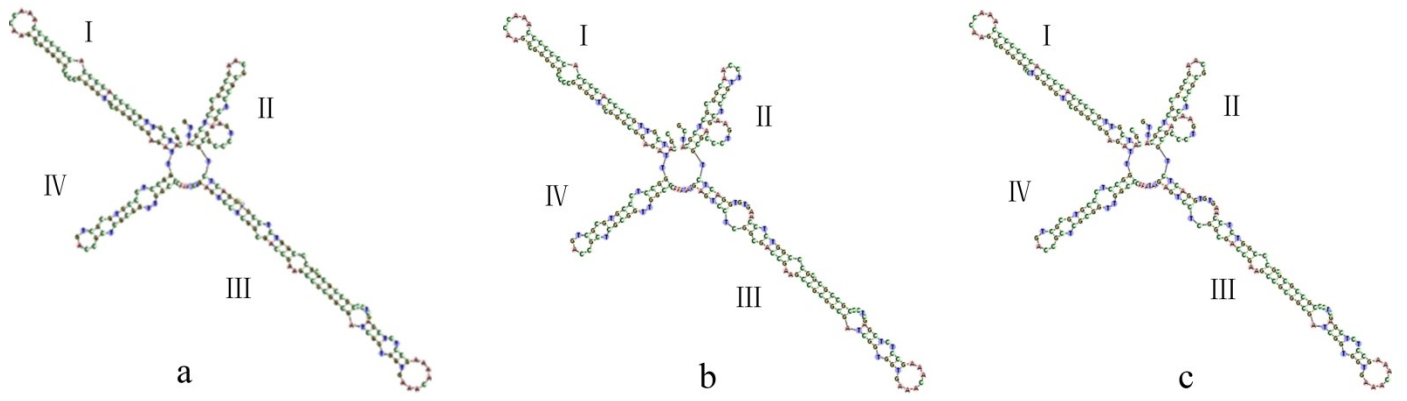


Figure S4 The secondary structures of: (a) *Citrus reticulata* ‘Chachi’; (b) *Citrus limon* (L.) Burm.; (c) *Citrus maxima* (Burm.) Merr