

Supplementary Information

Chemical Profiles and Simultaneous Quantification of *Aurantii Fructus* by Use of HPLC-Q-TOF-MS Combined with GC-MS and HPLC Methods

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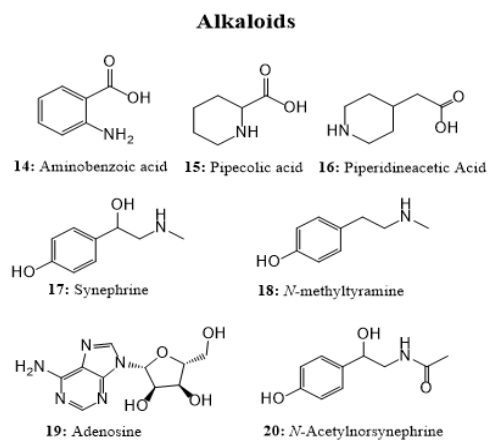
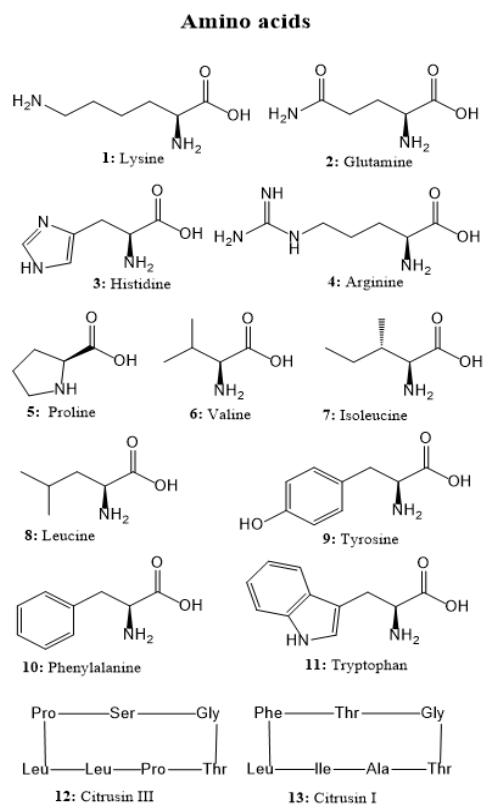
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Flavanones

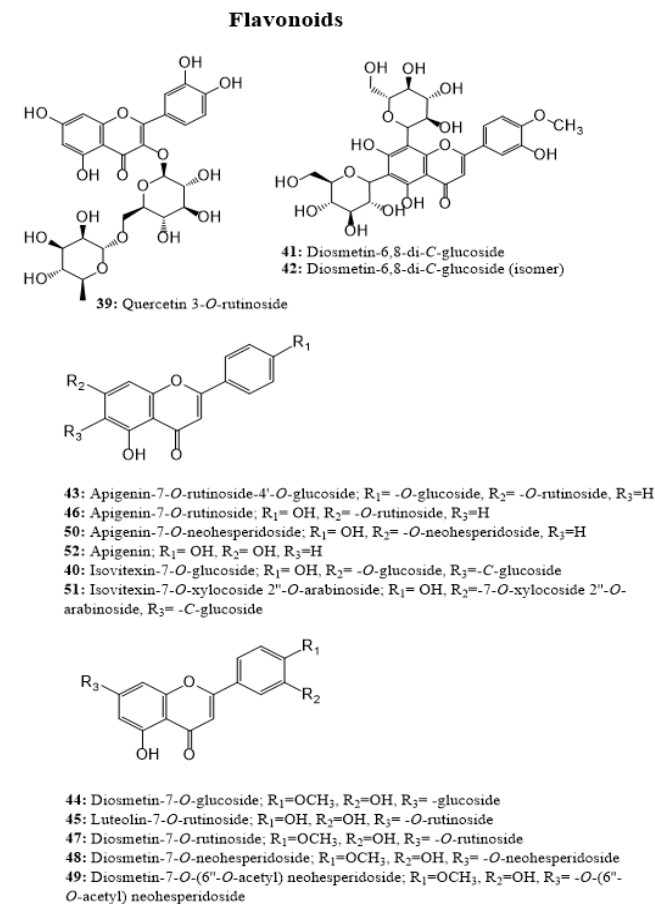
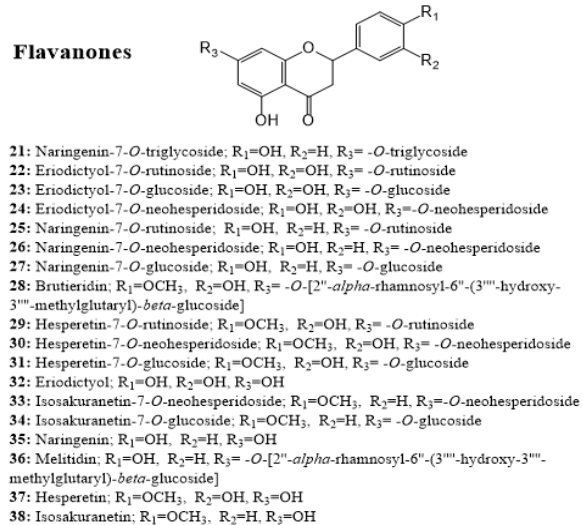
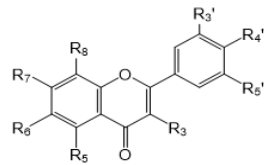


Figure S1. Structures of 86 compounds form ethanol extract of *Aurantii fructus*.

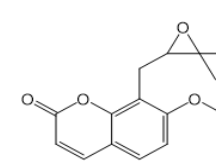
Figure S1. Cont.

Polymethoxyflavonoids

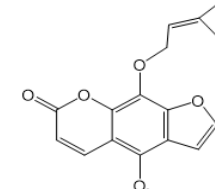


- 53: 3-Hydroxy-5,7,8-trimethoxyflavone; $R_3=OH, R_5=OCH_3, R_6=H, R_7=OCH_3, R_8=OCH_3, R_3'=H, R_4'=H, R_5'=H$
 54: 5-Hydroxy-6,7,3',4'-tetramethoxyflavone; $R_3=H, R_5=OH, R_6=OCH_3, R_7=OCH_3, R_8=H, R_3'=OCH_3, R_4'=OCH_3, R_5'=H$
 55: 5-Hydroxy-6,7,3',4',5'-pentamethoxyflavone; $R_3=H, R_5=OH, R_6=OCH_3, R_7=OCH_3, R_8=H, R_3'=OCH_3, R_4'=OCH_3, R_5'=OCH_3$
 56: 5,7,8,3',4'-Pentamethoxyflavone; $R_3=H, R_5=OCH_3, R_6=H, R_7=OCH_3, R_8=OCH_3, R_3'=OCH_3, R_4'=OCH_3, R_5'=H$
 57: 5,6,7,3',4'-Pentamethoxyflavone; $R_3=H, R_5=OCH_3, R_6=OCH_3, R_7=OCH_3, R_8=H, R_3'=OCH_3, R_4'=OCH_3, R_5'=H$
 58: 5-Hydroxy-6,7,8,3',4'-pentamethoxyflavone; $R_3=H, R_5=OH, R_6=OCH_3, R_7=OCH_3, R_8=OCH_3, R_3'=OCH_3, R_4'=OCH_3, R_5'=H$
 59: 5,6,7,8,3',4'-Hexamethoxyflavone; $R_3=H, R_4=OCH_3, R_6=OCH_3, R_7=OCH_3, R_8=OCH_3, R_3'=OCH_3, R_4'=OCH_3, R_5'=H$
 60: 3,5,6,7,8,3',4'-Heptamethoxyflavone; $R_3=OCH_3, R_5=OCH_3, R_6=OCH_3, R_7=OCH_3, R_8=OCH_3, R_3'=OCH_3, R_4'=OCH_3, R_5'=H$
 61: 5,6,7,4'-Tetramethoxyflavone; $R_3=H, R_5=OCH_3, R_6=OCH_3, R_7=OCH_3, R_8=H, R_3'=H, R_4'=OCH_3, R_5'=H$
 62: 5-Hydroxy-3,6,7,8,3',4'-hexamethoxyflavone; $R_3=OCH_3, R_5=OH, R_6=OCH_3, R_7=OCH_3, R_8=OCH_3, R_3'=OCH_3, R_4'=OCH_3, R_5'=H$
 63: 5-Hydroxy-3,6,7,8-tetramethoxyflavone; $R_3=OCH_3, R_5=OH, R_6=OCH_3, R_7=OCH_3, R_8=OCH_3, R_3'=H, R_4'=H, R_5'=H$
 64: 5,7,8,4'-Tetramethoxyflavone; $R_3=H, R_5=OCH_3, R_6=H, R_7=OCH_3, R_8=OCH_3, R_3'=H, R_4'=OCH_3, R_5'=H$
 65: 5,6,7,8,4'-Pentamethoxyflavone; $R_3=H, R_5=OCH_3, R_6=OCH_3, R_7=OCH_3, R_8=OCH_3, R_3'=H, R_4'=OCH_3, R_5'=H$
 66: 3-Hydroxy-5,6,7,8,3',4'-hexamethoxyflavone; $R_3=OH, R_5=OCH_3, R_6=OCH_3, R_7=OCH_3, R_8=OCH_3, R_3'=OCH_3, R_4'=OCH_3, R_5'=H$
 67: 5-Hydroxy-6,7,8,4'-tetramethoxyflavone; $R_3=H, R_5=OH, R_6=OCH_3, R_7=OCH_3, R_8=OCH_3, R_3'=H, R_4'=OCH_3, R_5'=H$

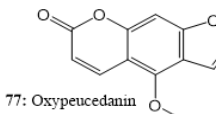
Coumarins



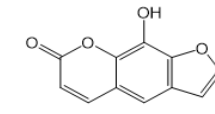
75: Meranzin
80: Meranzin isomer



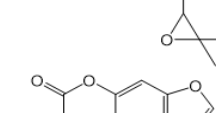
74: Pellopterin



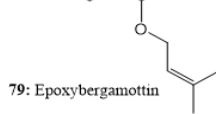
77: Oxypeucedanin



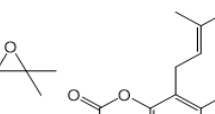
76: Xanthotoxol



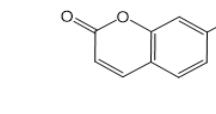
78: Scopoletin



79: Epoxybergamottin

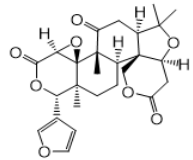


81: Osthol

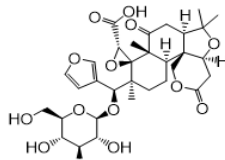


82: Auraptene

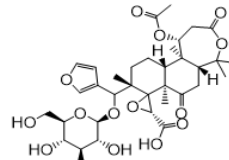
Triterpenoids



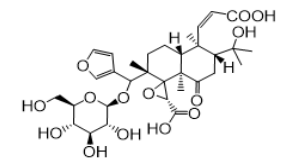
68: Limonin



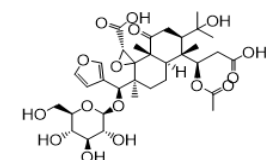
69: Limonin-17-beta-D-glucoside



70: Nominin-17-beta-D-glucoside

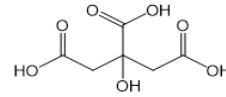


71: Obacunonic acid-17-beta-D-glucoside

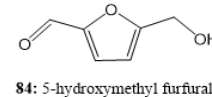


72: Nomialic acid-17-beta-D-glucoside

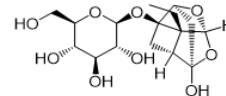
Other compounds



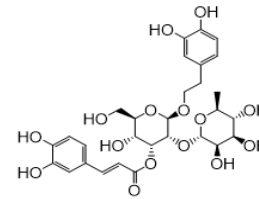
83: Citric acid



84: 5-hydroxymethyl furfural



85: Paeoniflorin



86: Magnolioside A

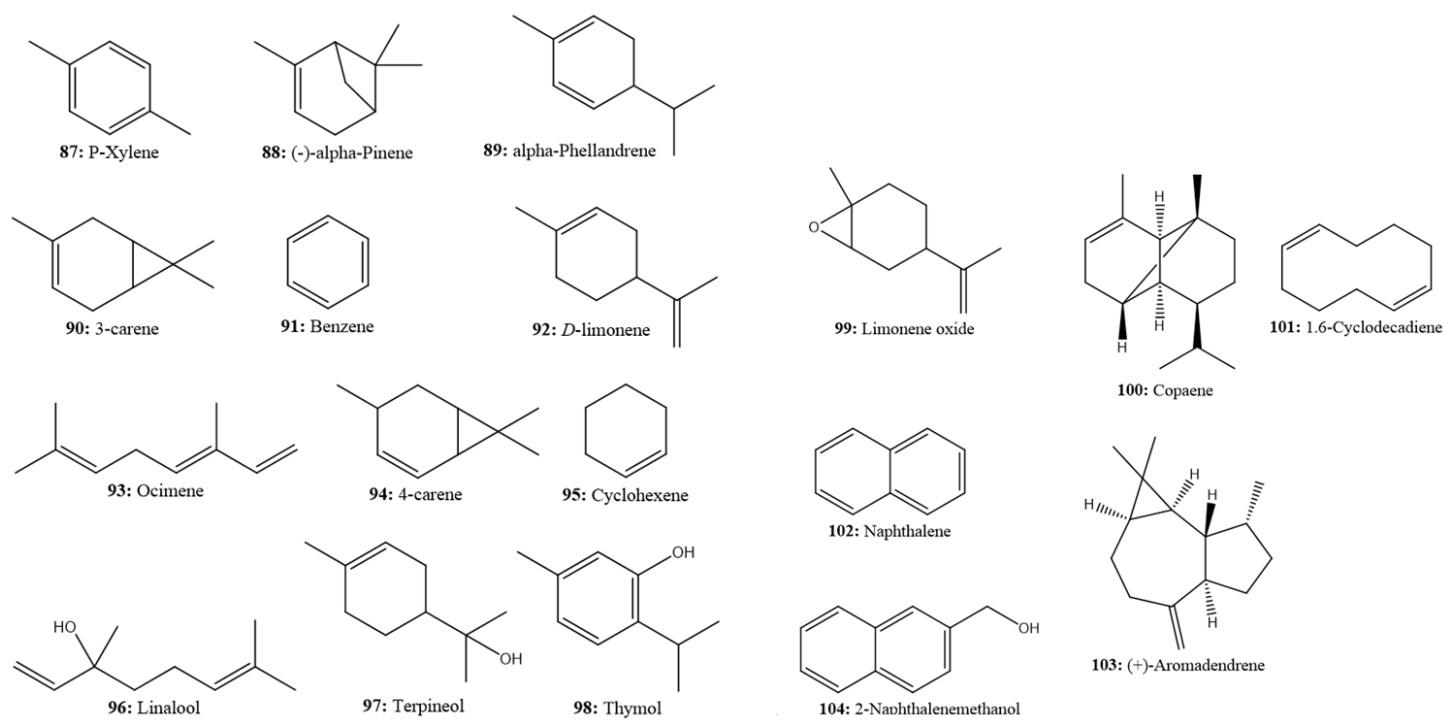


Figure S2. Structures of 18 compounds in volatile oils of *Aurantii fructus*.

Table S1. The 11 batches of *Aurantii fructus* obtained from different regions.

Sample	Region	Variety	Geographical location (approximate)	Collection date
S-1	Sanyantang, Yuanjiang, Hunan	<i>Citrus aurantium</i> L.	N28°45', E112°21', 30m	2016.06.30
S-2	Fuqiushan, Taojiang, Hunan	<i>Citrus aurantium</i> L.	N28°28', E112°01', 30m	2016.07.25
S-3	Hesanqu, Yiyang, Hunan	<i>Citrus aurantium</i> L.	N28°34', E112°22', 100m	2017.07.10
S-4	Yangjixiang, Anren, Hunan	<i>Citrus aurantium</i> L.	N26°38', E113°13', 80m	2016.07.06
S-5	Yangjixiang, Anren, Hunan	<i>Citrus aurantium</i> L.	N26°38', E113°13', 80m	2016.07.06
S-6	Hunan agricultural university	<i>Citrus aurantium</i> L.	N28°11', E113°05', 60m	2016.07.25
S-7	Fenglinzheng, Zhuzhou, Hunan	<i>Citrus aurantium</i> L.	N27°47', E113°25', 70m	2016.07.24
S-8	Shenzhengqiao, Xingan, Jiangxi	<i>Citrus aurantium</i> L.	N27°42', E115°28', 30m	2016.07.11
S-9	Shenzhengqiao, Xingan, Jiangxi	<i>Citrus aurantium</i> L.	N27°42', E115°28', 30m	2016.07.11
S-10	Zhangshu, Jiangxi	<i>Citrus aurantium</i> L.	N28°03', E115°32', 30m	2016.08.25
S-11	Changsha, Hunan	<i>Citrus aurantium</i> L. (variant)	N28°13', E112°56', 45m	2016.07.03

Table S2. Contents of chemical markers in *Aurantii fructus* from 11 different samples (mg/g)

Batches	S1	S2	S3	S4	S5	S6	S7	S8	S9	S10	S11
Eriocitrin	2.07	1.56	1.35	2.13	2.10	0.82	0.76	0.08	1.13	1.33	0.98
Neoeriocitrin	4.34	3.82	4.36	5.13	4.86	2.09	4.77	1.27	6.48	4.65	4.04
Narirutin	9.15	7.15	6.40	7.10	7.12	6.98	3.78	2.90	2.87	5.44	8.40
Naringin	106.81	101.97	97.59	96.91	98.44	82.35	96.13	100.68	89.98	92.35	80.40
Hesperidin	6.51	8.44	6.79	5.60	6.03	9.77	5.68	7.37	5.10	7.98	38.14
Neohesperidin	35.99	48.37	37.53	37.99	40.43	74.13	102.3	96.20	70.4	37.85	26.97
Poncirin	5.32	8.22	8.09	6.25	7.35	9.23	7.59	9.40	3.73	7.35	1.80
Naringenin	0.56	0.26	0.73	0.12	0.14	0.22	0.02	0.76	0.44	0.68	1.17
Hesperetin	0.13	0.12	0.20	0.18	0.19	0.15	0.05	0.38	0.24	0.28	0.57
Nobiletin	1.16	1.95	2.71	1.64	1.76	2.71	0.81	1.02	0.8	1.95	0.59
Tangeretin	1.39	2.29	2.90	1.81	1.85	1.90	0.78	1.30	0.81	2.28	0.43
Auraptene	1.22	1.71	2.13	1.36	1.67	0.42	0.43	0.15	0.35	2.00	0.36
Total (mg/g)	174.65	185.86	170.78	166.22	171.94	190.77	223.1	221.51	182.33	164.14	163.85