

Supplementary table 1. Parameters for identification of bioactive compounds in the studied citrus fruits.

Compound name	Formula	Mass	RT	m/z	Deprotonated ion	Main product ions			CAS ID
						1	2	3	
Flavonoids									
Naringenin	C <sub>15</sub> H <sub>12</sub> O <sub>5</sub>	272.0680	9.76	273.0720	[M-H] <sup>-</sup>	153.0186	147.0441		480-41-1
Naringenin (isomer)	C <sub>15</sub> H <sub>12</sub> O <sub>5</sub>	272.0690	10.59	273.0720	[M-H] <sup>-</sup>	153.0156	147.0400		480-41-1
Luteolin	C <sub>15</sub> H <sub>10</sub> O <sub>6</sub>	286.0490	9.59	287.0555	[M-H] <sup>-</sup>	153.0172			491-70-3
Diosmetin	C <sub>16</sub> H <sub>12</sub> O <sub>6</sub>	300.0630	13.46	301.0728	[M-H] <sup>-</sup>	286.0408	258.0527	153.0125	520-34-3
Hesperetin	C <sub>16</sub> H <sub>14</sub> O <sub>6</sub>	302.0780	13.68	303.0867	[M-H] <sup>-</sup>	177.0549	153.0185	111.0050	
Tangeritin (isomer 1)	C <sub>20</sub> H <sub>20</sub> O <sub>7</sub>	372.1200	14.26	373.1294	[M-H] <sup>-</sup>	343.0869	312.1041	153.0205	
Tangeritin (isomer 2)	C <sub>20</sub> H <sub>20</sub> O <sub>7</sub>	372.1200	13.70	373.1296	[M-H] <sup>-</sup>	358.1058	343.0829	153.0173	
Tangeritin	C <sub>20</sub> H <sub>20</sub> O <sub>7</sub>	372.1220	15.38	373.1294	[M-H] <sup>-</sup>	358.1061	343.0826	312.1010	
Vitexin	C <sub>21</sub> H <sub>20</sub> O <sub>10</sub>	432.1060	9.44	433.1154	[M-H] <sup>-</sup>	337.0713	313.0715	283.0609	3681-93-4
Quercetin-3-arabinoside	C <sub>20</sub> H <sub>18</sub> O <sub>11</sub>	434.0970	14.32	435.1033	[M-H] <sup>-</sup>	303.0498	153.0179		22255-13-6
Homoorientin	C <sub>21</sub> H <sub>20</sub> O <sub>11</sub>	448.1020	8.92	449.1095	[M-H] <sup>-</sup>	329.0663	299.0551	127.0382	4261-42-1
Orientin	C <sub>21</sub> H <sub>20</sub> O <sub>11</sub>	448.1030	9.14	449.1053	[M-H] <sup>-</sup>	329.0543	299.0445	127.0334	28608-75-5
Quercetin-3'-glucoside	C <sub>21</sub> H <sub>20</sub> O <sub>12</sub>	464.0960	9.22	465.1030	[M-H] <sup>-</sup>	303.0499	153.0171	129.0529	482-35-9
Hesperetin 7-O-glucoside	C <sub>22</sub> H <sub>24</sub> O <sub>11</sub>	464.1318	9.97	465.1393	[M-H] <sup>-</sup>	303.0871	53.0172		114248-44-1
Isorhamnetin3-O-glucoside	C <sub>22</sub> H <sub>22</sub> O <sub>12</sub>	478.1130	10.25	479.1215	[M-H] <sup>-</sup>	317.0669	97.0274		5041-82-7
Rhoifolin	C <sub>27</sub> H <sub>30</sub> O <sub>14</sub>	578.1640	9.62	579.1718	[M-H] <sup>-</sup>	433.1151	271.0611	129.0548	17306-46-6
Vitexin-2"-O-rhamnoside	C <sub>27</sub> H <sub>30</sub> O <sub>14</sub>	578.1650	9.14	579.1677	[M-H] <sup>-</sup>	433.1191	313.0745	283.0653	64820-99-1
Naringin	C <sub>27</sub> H <sub>32</sub> O <sub>14</sub>	580.1800	8.78	581.1877	[M-H] <sup>-</sup>	273.0743	195.0272	129.0537	
Naringin (isomer)	C <sub>27</sub> H <sub>32</sub> O <sub>14</sub>	580.1820	9.88	581.1877	[M-H] <sup>-</sup>	273.0760	195.0292	129.0545	10236-47-2
Eriocitrin	C <sub>27</sub> H <sub>32</sub> O <sub>15</sub>	596.1770	9.25	597.1830	[M-H] <sup>-</sup>	289.0750	129.0566		13463-28-0
Diosmin	C <sub>28</sub> H <sub>32</sub> O <sub>15</sub>	608.1750	9.85	609.1833	[M-H] <sup>-</sup>	463.1262	301.0722	129.0544	
Rutin	C <sub>27</sub> H <sub>30</sub> O <sub>16</sub>	610.1540	9.21	611.1625	[M-H] <sup>-</sup>	303.0516	153.0176	129.0553	153-18-4
Neohesperidin	C <sub>28</sub> H <sub>34</sub> O <sub>15</sub>	610.1910	10.56	611.1986	[M-H] <sup>-</sup>	303.0852	153.0174	129.0537	13241-33-3
Hesperidin	C <sub>28</sub> H <sub>34</sub> O <sub>15</sub>	610.1920	10.05	611.1986	[M-H] <sup>-</sup>	303.0874	129.0550	153.0178	520-26-3
Isorhamnetin-3-O-rutinoside	C <sub>28</sub> H <sub>32</sub> O <sub>16</sub>	624.1650	8.66	623.1591	[M-H] <sup>-</sup>	315.0489	300.0262		604-80-8
Luteolin-Rha-Glu	C <sub>27</sub> H <sub>30</sub> O <sub>15</sub>	594.1610	9.23	595.1679	[M-H] <sup>-</sup>	449.1104	287.0564		
Apigenin-Glu-Gal	C <sub>27</sub> H <sub>30</sub> O <sub>15</sub>	594.1620	8.95	595.1679	[M-H] <sup>-</sup>	433.1130	613.0000		
Limocitrin-Hmg-Glu	C <sub>29</sub> H <sub>32</sub> O <sub>17</sub>	652.1620	10.34	651.1510	[M-H] <sup>-</sup>	549.1223	507.1116	345.0585	
Limocitrin-Rut	C <sub>29</sub> H <sub>34</sub> O <sub>17</sub>	654.1770	9.62	653.1685	[M-H] <sup>-</sup>	345.0590	303.0319	199.1116	
Limocitrol-Glu-Hmg	C <sub>30</sub> H <sub>34</sub> O <sub>18</sub>	682.1710	10.32	681.1635	[M-H] <sup>-</sup>	609.1767	537.1194	375.0663	
Eriodictyol-Glu-Rha-Glu	C <sub>33</sub> H <sub>42</sub> O <sub>20</sub>	758.2220	8.51	757.2111	[M-H] <sup>-</sup>	595.1640	449.1053	287.0725	
Limonoids									
Limonin	C <sub>26</sub> H <sub>30</sub> O <sub>8</sub>	470.1940	14.31	471.2020	[M-H] <sup>-</sup>	453.1906	425.1956	161.0595	1180-71-8
Nomilin	C <sub>28</sub> H <sub>34</sub> O <sub>9</sub>	514.2200	14.62	515.2320	[M-H] <sup>-</sup>	469.2240	187.0754	161.0595	1063-77-0
Nomilin (isomer)	C <sub>28</sub> H <sub>34</sub> O <sub>9</sub>	514.2220	13.21	515.2320	[M-H] <sup>-</sup>	499.2661	187.0735	161.0566	1063-77-0
Obacunone	C <sub>26</sub> H <sub>30</sub> O <sub>7</sub>	454.1990	14.62	455.2048	[M-H] <sup>-</sup>	409.2018	331.1342	161.0598	751-03-1
Nomilinic acid	C <sub>28</sub> H <sub>36</sub> O <sub>10</sub>	532.2340	14.13	533.2325	[M-H] <sup>-</sup>	411.2202	369.2034	161.0619	
Limonoic acid D-ring lactone	C <sub>26</sub> H <sub>32</sub> O <sub>9</sub>	488.2040	13.71	489.2119	[M-H] <sup>-</sup>	471.2005	369.3169	161.0594	
Limonoic acid A-ring lactone	C <sub>26</sub> H <sub>32</sub> O <sub>9</sub>	488.2050	9.53	489.2119	[M-H] <sup>-</sup>	471.1967	369.1640	161.0577	
Nomilinic acid glucoside	C <sub>34</sub> H <sub>48</sub> O <sub>16</sub>	712.2980	10.64	713.3008	[M-H] <sup>-</sup>	551.2486	369.2028	161.0612	
21-O-Methyllimonexic acid	C <sub>27</sub> H <sub>32</sub> O <sub>10</sub>	516.1970	14.36	515.2001	[M-H] <sup>-</sup>	480.1376	469.1934	229.1225	
Simple phenols									
4-Hydroxybenzoic acid	C <sub>7</sub> H <sub>6</sub> O <sub>3</sub>	138.0320	8.20	139.0387	[M-H] <sup>-</sup>	121.0282	93.0327	77.0389	99-96-7
2-Coumaric acid	C <sub>9</sub> H <sub>8</sub> O <sub>3</sub>	164.0480	11.46	165.0521	[M-H] <sup>-</sup>	147.0448	119.0496	91.0539	583-17-5
Shikimic acid	C <sub>7</sub> H <sub>10</sub> O <sub>5</sub>	174.0520	3.29	173.0475	[M-H] <sup>-</sup>	111.0465	93.0358	73.0309	138-59-0
Ferulic acid	C <sub>10</sub> H <sub>10</sub> O <sub>4</sub>	194.0580	8.85	195.0623	[M-H] <sup>-</sup>	177.0514	145.0253	117.0307	537-98-4
Pyrogallol	C <sub>6</sub> H <sub>6</sub> O <sub>3</sub>	126.0320	2.80	127.0370	[M-H] <sup>-</sup>	109.0294	81.0332	53.0387	87-66-1

Pyrogallol (isomer)	C <sub>6</sub> H <sub>6</sub> O <sub>3</sub>	126.0320	4.64	127.0370	[M-H] <sup>-</sup>	109.0266	81.0316	53.0367	87-66-1	<i>b</i>
<b>Carboxylic acids</b>										
Ascorbic acid	C <sub>6</sub> H <sub>8</sub> O <sub>6</sub>	176.0320	3.36	175.0231	[M-H] <sup>-</sup>	115.0023	87.0079	71.0129	50-81-7	<i>a</i>
Citric acid	C <sub>6</sub> H <sub>8</sub> O <sub>7</sub>	192.0290	3.78	191.0224	[M-H] <sup>-</sup>	111.0104	85.0513	73.0305	77-92-9	<i>a</i>
Malic acid	C <sub>4</sub> H <sub>6</sub> O <sub>5</sub>	134.0200	3.39	133.0133	[M-H] <sup>-</sup>	115.0035	89.0245	71.0139	6915-15-7	<i>a</i>

RT, retention time. Identification confirmed by standard (*a*), tentative identification by MS2 spectrum similarity to the isomer (score > 90%) (*b*), tentative identification by neutral mass losses and fragmentation pattern analysis (*c*). Glu, glucoside; Rha, rhamnoside; Rut, rutinoside; Gal, galactoside; Hmg, hydroxymethylglutaryl.