

Table S2-1. Citri Reticulatae Pericarpium

NO	Medicinal materials	ESI	Compound name	Molecular formula	Molecular weight	m/z	Retention time (min)
1	Citri Reticulatae Pericarpium/Atractylodis Rhizoma/Angelicae Dahuricae Radix	+	Methyl cinnamate	C ₁₀ H ₁₀ O ₂	162.0679	163.0752	5.005
2	Citri Reticulatae Pericarpium/Atractylodis Rhizoma	+	Chlorogenic acid	C ₁₆ H ₁₈ O ₉	354.0945	355.1018	6.081
3	Citri Reticulatae Pericarpium	+	Naringin	C ₂₇ H ₃₂ O ₁₄	580.178	581.1853	8.913
4	Citri Reticulatae Pericarpium	+	Orientin	C ₂₁ H ₂₀ O ₁₁	448.1001	449.1073	9.907
5	Citri Reticulatae Pericarpium	+	Isoorientin	C ₂₁ H ₂₀ O ₁₁	448.1002	449.1075	10.404
6	Citri Reticulatae Pericarpium	+	3',5,7-Trihydroxy-4-methylflavanone	C ₁₆ H ₁₄ O ₆	302.0786	303.0859	10.679
7	Citri Reticulatae Pericarpium	+	Vitexin-2	C ₂₇ H ₃₀ O ₁₆	610.1527	611.16	11.391
8	Citri Reticulatae Pericarpium	+	Rutin	C ₂₇ H ₃₀ O ₁₆	610.1522	611.1595	11.675
9	Citri Reticulatae Pericarpium	+	Vitexin	C ₂₁ H ₂₀ O ₁₀	432.105	433.1123	11.681

10	Citri Reticulatae Pericarpium/ Magnolia Officinalis Cortex	+	2-(3, 4-dihydroxy phenyl) ethyl 3- <i>O</i> -(6-deoxidation- beta-L-pyran mannose)-6- <i>O</i> - [(2 <i>E</i>)2-3-(3, 4-dihydroxy phenyl)- 2-propylene acyl]- beta-D-pyran glycosidase	C29 H36 O15	624.2047	642.2385	12.358
11	Citri Reticulatae Pericarpium	+	Lonicerin	C27 H30 O15	594.1576	595.1649	13.121
12	Citri Reticulatae Pericarpium	+	Naringenin-7- <i>O</i> -glucoside	C21 H22 O10	434.1206	435.1279	13.225
13	Citri Reticulatae Pericarpium	+	Naringenin	C15 H12 O5	272.068	273.0753	13.226
14	Citri Reticulatae Pericarpium	+	Kaempferol 7- <i>O</i> - neohesperidoside	C27 H30 O15	594.1575	595.1648	13.268
15	Citri Reticulatae Pericarpium	+	Isorhoifolin	C27 H30 O14	578.1625	579.1697	13.32
16	Citri Reticulatae Pericarpium	+	Isohamnetin	C16 H12 O7	316.0577	317.0649	13.364
17	Citri Reticulatae Pericarpium	+	5-hydroxy-2-(3- hydroxy-4- methoxy phenyl)-7- {[(2 <i>S</i> ,3 <i>R</i> ,4 <i>S</i> ,5 <i>S</i> ,6 <i>R</i>)-3,4,5- trihydroxy-6-({[(2 <i>R</i> ,3 <i>R</i> , 4 <i>R</i> ,5 <i>R</i> ,6 <i>S</i>)-3,4,5-trihydroxy-6- methyloxan-2- yl]oxy}methyl)oxan-2- yl]oxy}-4 <i>H</i> -chromen-4-one	C28 H32 O15	608.1735	609.1807	13.593

18	Citri Reticulatae Pericarpium	+	Naringin	C ₂₇ H ₃₂ O ₁₄	580.1786	581.1859	13.741
19	Citri Reticulatae Pericarpium	+	Hesperetin	C ₁₆ H ₁₄ O ₆	302.0787	303.086	13.848
20	Citri Reticulatae Pericarpium	+	Isorhamnetin-3-O-rutinoside	C ₂₈ H ₃₂ O ₁₆	624.1683	625.1756	13.86
21	Citri Reticulatae Pericarpium	+	Hesperidin	C ₂₈ H ₃₄ O ₁₅	610.1884	611.1957	14.04
22	Citri Reticulatae Pericarpium	+	Neohesperidin	C ₂₈ H ₃₄ O ₁₅	610.1884	611.1957	14.476
23	Citri Reticulatae Pericarpium	+	5-(2-Propenyl)-1, 3- benzodioxole	C ₁₀ H ₁₀ O ₂	162.0679	163.0752	14.7
24	Citri Reticulatae Pericarpium	+	Naringenin chalcone	C ₁₅ H ₁₂ O ₅	272.0681	273.0754	15.479
25	Citri Reticulatae Pericarpium	+	Naringenone	C ₁₅ H ₁₂ O ₅	272.0681	273.0754	19.107
26	Citri Reticulatae Pericarpium	+	Sinensetin	C ₂₀ H ₂₀ O ₇	372.1201	373.1274	20.071
27	Citri Reticulatae Pericarpium	+	Isosinensetin	C ₂₀ H ₂₀ O ₇	372.1203	373.1275	21.577
28	Citri Reticulatae Pericarpium	+	Isosinensetin isomer	C ₂₀ H ₂₀ O ₇	372.1205	373.1277	21.827
29	Citri Reticulatae Pericarpium	+	Sinensetin	C ₂₀ H ₂₀ O ₇	372.1205	373.1278	22.785
30	Citri Reticulatae	+	Nobiletin	C ₂₁ H ₂₂ O ₈	402.1305	403.1378	23.11

	Pericarpium						
31	Citri Reticulatae Pericarpium	+	5,2' -dihydroxy-6,7,8,6'- tetramethoxy-flavonoids	C19 H18 O8	374.0996	375.1069	23.622
32	Citri Reticulatae Pericarpium	+	2-(2, 6-dimethoxyphenyl)-5, 6-dimethoxy-4H-Chromen-4- one	C19 H18 O6	342.1101	343.1174	23.779
33	Citri Reticulatae Pericarpium	+	Isosinensetin	C20 H20 O7	372.1204	373.1277	24.609
34	Citri Reticulatae Pericarpium	+	Tangeretin	C20 H20 O7	372.12	373.1273	24.822
35	Citri Reticulatae Pericarpium	+	5, 6, 7, 3', 4', 5'- hexamethoxyflavone	C21 H22 O8	402.131	403.1383	25.782
36	Citri Reticulatae Pericarpium	+	Hexamethoxyflavone	C21 H22 O8	402.1308	403.1381	26.16
37	Citri Reticulatae Pericarpium	+	Dehydrocyanol	C15 H24 O	220.1825	203.1792	30.612
38	Citri Reticulatae Pericarpium/Atractylodis Rhizoma/Perilla Leaf Oil	-	4-Dicaffeoylquinic Acid	C16 H18 O9	354.0947	353.0875	4.176
39	Citri Reticulatae Pericarpium/Atractylodis Rhizoma/Perilla Leaf Oil	-	Chlorogenic acid	C16 H18 O9	354.0946	353.0873	6.089
40	Citri Reticulatae Pericarpium	-	Lucenin-2	C27 H30 O16	610.153	609.1457	7.129
41	Citri Reticulatae	-	Apigenin 6,8-C-diglucoside	C27 H30 O15	594.1579	593.1506	8.281

	Pericarpium/Radix Glycyrrhizae/Patchouli Oil						
42	Citri Reticulatae Pericarpium	–	Orientin	C21 H20 O11	448.1002	447.0929	9.914
43	Citri Reticulatae Pericarpium	–	Rutin	C27 H30 O16	610.1535	609.1462	10.739
44	Citri Reticulatae Pericarpium	–	Eriocitrin	C27 H32 O15	596.174	595.1667	11.428
45	Citri Reticulatae Pericarpium	–	Lonicerin	C27 H30 O15	594.1582	593.1509	13.124
46	Citri Reticulatae Pericarpium	–	Narirutin	C27 H32 O14	580.1789	579.1716	13.74
47	Citri Reticulatae Pericarpium	–	Hesperidin	C28 H34 O15	610.1891	609.1818	14.044
48	Citri Reticulatae Pericarpium	–	Neohesperidin	C28 H34 O15	610.1895	609.1822	14.476
49	Citri Reticulatae Pericarpium	–	Naringin	C27 H32 O14	580.1792	579.1719	14.622
50	Citri Reticulatae Pericarpium	–	Hesperetin	C16 H14 O6	302.0789	301.0716	14.895
51	Citri Reticulatae Pericarpium	–	3',5,7-trihydroxy-4'- methoxyflavanone	C16 H14 O6	302.0791	301.0718	19.739