

Table S2-2. Atractylodis Rhizoma

NO	Medicinal materials	ESI	Compound name	Molecular formula	Molecular weight	m/z	Retention time (min)
1	Atractylodis Rhizoma	+	5-Hydroxymethylfurfural	C ₆ H ₆ O ₃	126.0315	127.0388	2.346
2	Atractylodis Rhizoma/ Perilla Leaf Oil	+	Isovanillic Acid	C ₈ H ₈ O ₄	168.042	169.0493	4.179
3	Atractylodis Rhizoma	+	Methyl caffeate	C ₁₀ H ₁₀ O ₄	194.0577	177.0544	4.987
4	Atractylodis Rhizoma/ Citri Reticulatae Pericarpium/Angelicae Dahuricae Radix	+	Methyl cinnamate	C ₁₀ H ₁₀ O ₂	162.0679	163.0752	5.005
5	Atractylodis Rhizoma/ Citri Reticulatae Pericarpium	+	Chlorogenic acid	C ₁₆ H ₁₈ O ₉	354.0945	355.1018	6.081
6	Atractylodis Rhizoma/ Perilla Leaf Oil	+	Ferulic acid	C ₁₀ H ₁₀ O ₄	194.0576	177.0543	6.081
7	Atractylodis Rhizoma	+	4-O-Feruloylquinic acid	C ₁₇ H ₂₀ O ₉	368.1103	369.1176	9.295
8	Atractylodis Rhizoma/ Perilla Leaf Oil	+	Isoferulic acid	C ₁₀ H ₁₀ O ₄	194.0576	177.0543	10.837
9	Atractylodis Rhizoma /Pinellia Rhizoma	+	3-phenyl-L-alanine	C ₉ H ₁₁ N O ₂	165.0788	166.0861	11.178
10	Atractylodis Rhizoma	+	Safrole	C ₁₀ H ₁₀ O ₂	162.0679	163.0752	11.189

11	Atractylodis Rhizoma	+	Isochlorogenic acid A	C25 H24 O12	516.1264	517.1335	13.663
12	Atractylodis Rhizoma	+	9,10-Dehydroisolongifolene	C15 H22 O	218.1667	219.174	18.638
13	Atractylodis Rhizoma	+	Atractylenolide III	C15 H20 O3	248.1408	249.1481	24.75
14	Atractylodis Rhizoma	+	(9Z,11E,15Z)-13-hydroxy-9,11,15- calendic acid	C18 H30 O3	294.2192	295.2264	26.999
15	Atractylodis Rhizoma	+	Atractylodin	C13 H10 O	182.073	183.0802	28.581
16	Atractylodis Rhizoma	+	Atractyline	C15 H22 O	218.1669	219.1742	29.397
17	Atractylodis Rhizoma	+	Dibutyl phthalate	C16 H22 O4	278.1513	279.1586	32.954
18	Atractylodis Rhizoma /Pinellia Rhizoma/ Perilla Leaf Oil	—	3-phenyl-L-alanine	C9 H11 N O2	165.0789	164.0717	2.326
19	Atractylodis Rhizoma /Perilla Leaf Oil	—	Vanillic acid	C8 H8 O4	168.0422	167.0349	3.073
20	Atractylodis Rhizoma /Perilla Leaf Oil/Citri Reticulatae Pericarpium	—	Cryptochlorogenic acid	C16 H18 O9	354.0947	353.0875	4.176
21	Atractylodis Rhizoma /Perilla Leaf Oil	—	3-Hydroxy-4-methoxybenzoic acid	C8 H8 O4	168.0421	167.0348	4.342
22	Atractylodis Rhizoma /Perilla Leaf Oil/Citri Reticulatae Pericarpium	—	Chlorogenic acid	C16 H18 O9	354.0946	353.0873	6.089
23	Atractylodis Rhizoma	—	Ferulic acid	C10 H10 O4	194.0578	193.0505	7.36

	/Perilla Leaf Oil						
24	Atractylodis Rhizoma	–	3-Feruloylquinic acid	C17 H20 O9	368.1104	367.1031	9.29
25	Atractylodis Rhizoma /Perilla Leaf Oil	–	Isoferulic acid	C10 H10 O4	194.0578	193.0506	10.142
26	Atractylodis Rhizoma	–	Isochlorogenic acid B	C25 H24 O12	516.1266	515.1193	13.807
27	Atractylodis Rhizoma	–	Isochlorogenic acid C	C25 H24 O12	516.1266	515.1193	14.413
28	Atractylodis Rhizoma	–	Isochlorogenic acid A	C25 H24 O12	516.1268	515.1195	15.686
29	Atractylodis Rhizoma	–	atractyloside A	C21 H36 O10	448.2309	493.2291	16.368
30	Atractylodis Rhizoma	–	(10 <i>E</i> ,15 <i>Z</i>)-9,12,13-trihydroxy-10,15-octadecadienoic acid	C18 H34 O5	330.2406	329.2334	19.671
31	Atractylodis Rhizoma/ Patchouli Oil	GC-MS	Terpinen-4-ol	C10H18O	/	/	13.3
32	Atractylodis Rhizoma/ Perilla Leaf Oil/ Angelicae Dahuricae Radix	GC-MS	α -Pinene	C10H16	/	/	14.795
33	Atractylodis Rhizoma	GC-MS	5-Hydroxymethyl-2-furaldehyde	C6H6O3	/	/	15.98
34	Atractylodis Rhizoma	GC-MS	Guaiol	C15H26O	/	/	26.735
35	Atractylodis Rhizoma	GC-MS	Beta-Eudesmol	C15H26O	/	/	27.27
36	Perilla Leaf Oil/Atractylodis Rhizoma	GC-MS	Caryophyllene oxide	C15H24O	/	/	30.25

37	Atractylodis Rhizoma/ Perilla Leaf Oil	GC-MS	Linolenic acid	C18H32O2	/	/	35.35
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