

Gradient Elution and operating conditions by RP-HPLC-DAD-ESI-QTOF-MS/MS

The gradient elution was conducted according [10,22] with two mobile phases, 0.5% acetic acid, *v/v* (phase A) and acetonitrile (phase B), with a constant flow rate of 0.5 mL min⁻¹. The gradient program was as follows: 0 min 99% A and 1% B, 5.50 min 93% A and 7% B, 11 min 86% A and 14% B, 17.5 min 76% A and 24% B, 22.50 min 60% A and 40% B, 27.50 min 0% A and 100% B, 28.5 min 0% A and 100% B, 29.5 min. For column equilibration, initial conditions were finally maintained for 5.50 min. (total run 35 min). The injection volume was 15 µL. Briefly, the operating conditions were: drying nitrogen gas temperature 325 °C with a flow of 10 L min⁻¹; nebulizer pressure 20 psig; sheath gas temperature 400 °C with a flow 12 L min⁻¹; capillary voltage 4000 V; nozzle voltage 500 V; fragmentor voltage 130 V; skimmer voltage 45 V; octapole radiofrequency voltage 750 V.

Data acquisition (2.5 Hz) in profile mode was governed via MassHunter Workstation software (Agilent technologies). The spectra were acquired in the negative ionization mode, over a mass-to-charge (*m/z*) range from 70 to 1100. The detection window was set to 100 ppm. Reference mass correction on each sample was performed with a continuous infusion of Agilent TOF biopolymer analysis mixture containing trifluoroacetic acid ammonium salt (*m/z* 112.9856) and hexakis (1H, 1H, 3H-tetrafluoropropoxy) phosphazine (*m/z* 980.0164 corresponding to the acetic adduct).

Table S1. Phenolic compounds characterized in SG32 oil.

Number	RT (min)	Experimental m/z^a [M-H] ⁺	Theoretical mass (M)	Molecular formula	Error (ppm)	Error (mDa)	Score	Main fragments	DBE	UV (nm)	Proposed compound	Subclass	Species	Family	Reference	Oil	Cake
9	4.70	151.0402	152.0473	C ₈ H ₈ O ₃	−0.26	0.0	99	123.0450, 122.0372	5	267	Vanillin	Phenolic aldehyde	<i>Olea europaea</i>	Oleaceae	[47]	+	-
16	7.31	169.0140	170.0215	C ₇ H ₆ O ₅	1.25	0.20	87	125.0247	5	N.D.	Gallic acid*	Hydroxybenzoic acid	<i>Sesamum indicum</i>	Pedaliaceae	[10]	+	+
20	8.74	137.0243	138.0316	C ₇ H ₆ O ₃	0.34	0.05	94	N.D.	5	N.D.	Sesamol	Phenol derivative	<i>Sesamum indicum</i>	Pedaliaceae	[10]	+	+
21	9.19	147.0447	148.0524	C ₉ H ₈ O ₂	3.0	0.5	96	103.0556	6	N.D.	Cinnamic acid	Hydroxycinnamic acid	<i>Sesamum indicum</i>	Pedaliaceae	[10]	+	+
24	10.64	329.0879	330.0951	C ₁₄ H ₁₈ O ₉	−0.24	−0.08	99	167.0347, 152.0114, 123.0450, 108.0218	6	255, 286	Vanillic acid hexoside	Hydroxybenzoic acid	<i>Sesamum indicum</i>	Pedaliaceae	[10]	+	+
25	11.33	153.0192	154.0266	C ₇ H ₆ O ₄	1.02	0.16	99	137.0244, 109.0293, 108.0213	5	258, 288	3,4-Dihydroxybenzoic acid* (protocatechuic acid)	Hydroxybenzoic acid	<i>Sesamum indicum</i>	Pedaliaceae	[10]	+	+
26	11.83	359.0978	360.1057	C ₁₅ H ₂₀ O ₁₀	1.2	0.4	97	197.0474, 182.0213, 153.0544, 138.0318	6	N.D.	Syringic acid hexoside	Hydroxybenzoic acid	<i>Sesamum indicum</i>	Pedaliaceae	[10]	+	+
27	12.47	325.0932	326.1002	C ₁₅ H ₁₈ O ₈	0.4	0.1	94	163.0398, 119.0502	7	287	<i>p</i> -Coumaric acid hexoside I	Hydroxycinnamic acid	<i>Cicer arietinum</i> / <i>Sesamum indicum</i>	Fabaceae /Pedaliaceae	[10,21]	+	+
28	12.72	325.0931	326.1002	C ₁₅ H ₁₈ O ₈	−0.5	−0.16	99	163.0400, 119.0502	7	288	<i>p</i> -Coumaric acid hexoside II	Hydroxycinnamic acid	<i>Cicer arietinum</i> / <i>Sesamum indicum</i>	Fabaceae /Pedaliaceae	[10,21]	+	+
30	13.95	355.1035	356.1107	C ₁₆ H ₂₀ O ₉	−0.1	−0.03	99	193.0505, 178.0271, 149.0607	7	279	Ferulic acid hexoside I	Hydroxycinnamic acid	<i>Cicer arietinum</i> / <i>Sesamum indicum</i>	Fabaceae /Pedaliaceae	[10,21]	+	+
31	14.01	355.1037	356.1107	C ₁₆ H ₂₀ O ₉	−0.69	−0.25	100	N.D.	7	282	Ferulic acid hexoside II	Hydroxycinnamic acid	<i>Cicer arietinum</i> / <i>Sesamum indicum</i>	Fabaceae /Pedaliaceae	[10,21]	+	+

32	14.36	137.0240	138.0317	C ₇ H ₆ O ₃	−1.1	−0.15	99	119.0142, 109.0293, 108.0218, 93.0344, 92.0269	5	273	Hydroxybenzoic acid	Hydroxybenzoic acid	<i>Sesamum indicum</i>	Pedaliaceae	[10]	+	+
33	14.49	151.0401	152.0473	C ₈ H ₈ O ₃	−0.88	−0.13	97	137.0245, 107.0506	5	237, 274	Hydroxybenzoic acid methyl ester	Hydroxybenzoic acid			[25]	+	+
35	14.99	353.0879	354.0951	C ₁₆ H ₁₈ O ₉	−0.45	−0.16	99	191.0559, 179.0344, 173.0457, 161.0246, 135.0452	8	238, 279	Caffeoylquinic acid I* (Chlorogenic acid)	Hydroxycinnamic acid	<i>Cicer arietinum</i> / <i>Sesamum indicum</i>	Fabaceae /Pedaliaceae	[10,21]	+	+
36	15.10	385.1137	386.1213	C ₁₇ H ₂₂ O ₁₀	−0.6	−0.23	88	223.0611, 208.0373, 193.0141, 179.0703, 164.0472, 149.0242	7	290	Sinapic acid hexoside	Hydroxycinnamic acid	<i>Cicer arietinum</i> / <i>Sesamum indicum</i>	Fabaceae /Pedaliaceae	[10,21]	+	+
37	15.53	325.0928	326.1002	C ₁₅ H ₁₈ O ₈	−0.15	−0.05	98	163.0397, 119.0503	7	277	<i>p</i> -Coumaric acid hexo- side III	Hydroxycinnamic acid	<i>Cicer arietinum</i> / <i>Sesamum indicum</i>	Fabaceae /Pedaliaceae	[10,21]	+	+
38	16.61	325.0929	326.1002	C ₁₅ H ₁₈ O ₈	−1.1	−0.36	89	N.D.	7	N.D.	<i>p</i> -Coumaric acid hexo- side IV	Hydroxycinnamic acid	<i>Cicer arietinum</i> / <i>Sesamum indicum</i>	Fabaceae /Pedaliaceae	[10,21]	+	+
39	16.68	355.1033	356.1107	C ₁₆ H ₂₀ O ₉	0.5	0.18	100	193.0500, 178.0272, 149.0609	7	282	Ferulic acid hexoside III	Hydroxycinnamic acid	<i>Cicer arietinum</i> / <i>Sesamum indicum</i>	Fabaceae /Pedaliaceae	[10,21]	+	+
40	16.73	167.0346	168.0426	C ₈ H ₈ O ₄	1.29	0.22	98	152.0144, 123.0449, 108.0251	5	258	Vanillic acid*	Hydroxybenzoic acid	<i>Sesamum indicum</i>	Pedaliaceae	[10]	+	+
41	17.11	593.1510	594.1585	C ₂₇ H ₃₀ O ₁₅	0.3	0.15	99	503.1188, 473.1085, 443.0981, 413.0872, 383.0767, 353.0667, 135.0457, 119.0357, 117.0367	13	267, 320	Luteolin C-deoxyhexo- side C-hexoside I	Flavone	<i>Sesamum indicum</i>	Pedaliaceae	[10]	+	+
42	17.23	353.0876	354.0951	C ₁₆ H ₁₈ O ₉	0.3	0.1	96	191.0556, 179.0327, 173.0450, 161.0233, 135.0445	8	274	Caffeoylquinic acid II	Hydroxycinnamic acid	<i>Cicer arietinum</i> / <i>Sesamum indicum</i>	Fabaceae /Pedaliaceae	[10,21]	+	+

43	17.36	593.1590	594.1585	C ₂₇ H ₃₀ O ₁₅	0.3	0.15	99	533.1285, 503.1193, 473.1085, 443.0989, 413.0873, 383.0771, 353.0665	13	270, 325	Luteolin C-deoxyhexo- side C-hexoside II	Flavone	<i>Sesamum indicum</i>	Pedaliaceae	[10]	+	+
44	17.34	197.0453	198.05282	C ₉ H ₁₀ O ₅	0.6	0.1	97	N.D.	5		Syringic acid*	Hydroxybenzoic acid	<i>Cicer arietinum</i> / <i>Sesamum indicum</i>	Fabaceae /Pedaliaceae	[10,21]	+	-
45	17.47	355.1034	356.1107	C ₁₆ H ₂₀ O ₉	0.4	0.16	96	N.D.	7	287	Ferulic acid hexoside IV	Hydroxycinnamic acid	<i>Cicer arietinum</i> / <i>Sesamum indicum</i>	Fabaceae /Pedaliaceae	[10,21]	+	-
46	17.78	289.0718	290.0790	C ₁₅ H ₁₄ O ₆	0.79	0.02	93	253.0334, 245.1390, 217.0027, 131.0712, 123.0450	9	N.D.	(-)-Epicatechin*	Flavan-3-ol	<i>Sesamum indicum</i>	Pedaliaceae	[10]	+	+
47	17.78	531.1719	532.1792	C ₂₃ H ₃₂ O ₁₄	-0.53	-0.28	89	179.0140, 165.0554, 150.0317	8	283	Sinapic acid deoxyhexo- side hexoside	Hydroxycinnamic acid	<i>Sesamum indicum</i>	Pedaliaceae	[10]	+	+
48	17.96	681.2400	682.2473	C ₃₂ H ₄₂ O ₁₆	0.54	0.37	100	357.1302, 151.0384	12	242, 275	Pinoresinol dihexoside I	Lignan	<i>Sesamum indicum</i>	Pedaliaceae	[10]	+	+
49	18.21	563.1411	564.1479	C ₂₆ H ₂₈ O ₁₄	-0.57	-0.32	99	545.1297, 503.1189, 473.1087, 443.0979, 413.0872, 383.0771, 353.0664, 117.0343	13	274, 330	Apigenin C-pentoside C-hexoside I	Flavone	<i>Sesamum indicum</i>	Pedaliaceae	[10]	+	+
50	18.27	121.0293	122.0368	C ₇ H ₆ O ₂	1.20	0.15	100	92.0269	5	278	Benzoic acid	Hydroxybenzoic acid	<i>Sesamum indicum</i>	Pedaliaceae	[10]	+	+
51	18.63	563.1405	564.1479	C ₂₆ H ₂₈ O ₁₄	0.08	0.05	99	545.1323, 503.1179, 473.1083, 443.0976, 413.0871, 383.0767, 353.0666, 117.0335	13	272, 327	Apigenin C-pentoside C-hexoside II	Flavone	<i>Sesamum indicum</i>	Pedaliaceae	[10]	+	+
52	18.89	563.1408	564.1479	C ₂₆ H ₂₈ O ₁₄	0.08	0.05	99	545.1298, 503.1191, 473.1087, 443.0976, 413.0878, 383.0769, 353.0666, 117.0336	13	269, 331	Apigenin C-pentoside C-hexoside III	Flavone	<i>Sesamum indicum</i>	Pedaliaceae	[10]	+	+
53	18.87	447.0935	448.1006	C ₂₁ H ₂₀ O ₁₁	-0.46	-0.21	99	327.0515, 179.0141, 135.0447	12	268, 325	Luteolin C-hexoside I	Flavone	<i>Sesamum indicum</i>	Pedaliaceae	[10]	+	+

54	19.50	447.0930	448.1006	C ₂₁ H ₂₀ O ₁₁	0.28	0.21	92	327.0539, 179.0138, 135.0450	12	N.D.	Luteolin C-hexoside II	Flavone	<i>Sesamum indicum</i>	Pedaliaceae	[10]	+	+
55	20.34	151.0400	152.0473	C ₈ H ₈ O ₃	−0.28	0.0	98	136.0167, 92.0269	5	256	Methoxybenzoic acid I	Hydroxybenzoic acid			[25]	+	−
56	20.40	163.0399	164.0473	C ₉ H ₈ O ₃	0.47	0.08	97	N.D.	6	N.D.	<i>p</i> -Coumaric acid*	Hydroxycinnamic acid	<i>C. arietinum</i>	Fabaceae	[21]	+	+
57	20.46	609.1472	610.1534	C ₂₇ H ₃₀ O ₁₆	−1.41	−0.86	96	300.0267, 151.0033	13	255, 355	Quercetin 3- <i>O</i> -rutinoside (rutin)*	Flavonol	<i>Cicer arietinum</i> / <i>Sesamum indicum</i>	Fabaceae/ Pedaliaceae	[10,21]	+	+
58	20.59	593.1510	594.1585	C ₂₇ H ₃₀ O ₁₅	0.3	0.16	99	447.0897, 285.0396, 133.0281	13	267, 320	Luteolin deoxyhexoside hexoside	Flavone	<i>Sesamum indicum</i>	Pedaliaceae	[10]	+	−
59	20.93	300.9988	302.00627	C ₁₄ H ₆ O ₈	0.82	0.25	95	N.D.	12	N.D.	Ellagic acid*	Hexahydroxydiphenic acid dilactone	<i>Sesamum indicum</i>	Pedaliaceae	[6]	+	−
60	21.06	463.0874	464.09548	C ₂₁ H ₂₀ O ₁₂	0.25	0.12	85	300.9980, 151.0030	12	N.D.	Quercetin 3- <i>O</i> -β-D-galactopyranoside*	Flavonol	<i>Cicer arietinum</i> / <i>Sesamum indicum</i>	Fabaceae/ Pedaliaceae	[10,21]	+	+
61	21.18	623.1972	624.2054	C ₂₉ H ₃₆ O ₁₅	1.52	0.95	94	461.1649, 387.1502, 315.1074, 297.0957, 179.0347, 161.0239, 153.0543, 135.0447, 113.0233	12	N.D.	Verbascoside	Hydroxycinnamic acid	<i>Sesamum indicum</i>	Pedaliaceae	[10]	+	+
62	21.18	681.2402	682.2473	C ₃₂ H ₄₂ O ₁₆	−0.12	−0.08	99	519.1525, 357.1333, 179.0529, 151.0382, 149.0467	12	N.D.	Pinoresinol dihexoside II	Lignan	<i>Sesamum indicum</i>	Pedaliaceae	[10]	+	+
63	21.30	463.0883	464.09548	C ₂₁ H ₂₀ O ₁₂	−0.02	−0.01	99	301.0324, 300.0248, 271.02228, 255.0276, 178.9974, 151.0027, 136.0172, 135.0447	12	250, 352	Quercetin 3- <i>O</i> -β-D-glucopyranoside*	Flavonol	<i>Cicer arietinum</i> / <i>Sesamum indicum</i>	Fabaceae/ Pedaliaceae	[10,21]	+	+
64	21.36	447.0936	448.1006	C ₂₁ H ₂₀ O ₁₁	−0.84	−0.38	97	285.0402, 151.0026, 133.0284	12	N.D.	Luteolin 7- <i>O</i> -β-D-glucopyranoside*	Flavone	<i>Sesamum indicum</i>	Pedaliaceae	[10]	+	+
65	21.87	575.1189	576.1268	C ₃₀ H ₂₄ O ₁₂	0.51	0.30	93	N.D.	19	N.D.	Procyanidin A2*	Proanthocyanidin	<i>Vaccinium macrocarpon</i>	Ericaceae	[37]	+	+

66	21.79	1017.3111	1018.3165	C ₄₄ H ₅₈ O ₂₇	-1.71	-1.74	97	855.2573, 693.2019, 369.0973, 323.0977, 221.0642, 219.0663, 179.0559, 161.0452, 149.0451, 143.0349	16	280	Sesaminol tetrahexo-side I	Lignan	<i>Sesamum indicum</i>	Pedaliaceae	[10]	+	+
67	22.27	1017.3095	1018.3165	C ₄₄ H ₅₈ O ₂₇	-0.15	-0.15	98	855.2556, 693.2026, 369.0971, 323.0973, 221.0682, 179.0555, 161.0459, 149.0443, 143.0342	16	280	Sesaminol tetrahexo-side II	Lignan	<i>Sesamum indicum</i>	Pedaliaceae	[10]	+	+
68	22.39	593.1504	594.1585	C ₂₇ H ₃₀ O ₁₅	0.84	0.50	96	N.D.	13	N.D.	Kaempferol 3-O-rutino-side* [Kaempferol 3-O-(α-L-rhamnopyranosyl-(1→6)-β-D-glucopyranoside)]	Flavonol	<i>Cicer arietinum</i>	Fabaceae	[21]	+	-
69	22.52	841.2775	842.2857	C ₃₈ H ₅₀ O ₂₁	-0.04	-0.04	99	679.2225, 485.1504, 355.1176, 323.0978, 221.0665, 179.0548, 161.0454, 149.0450, 143.0352, 121.0288, 89.0245	14	286	Xanthoxylol trihexo-side	Lignan	<i>Sesamum indicum</i>	Pedaliaceae	[10]	+	+
70	22.54	163.0404	164.0473	C ₉ H ₈ O ₃	-1.97	-0.32	84	N.D.	6	284	<i>m</i> -Coumaric acid*	Hydroxycinnamic acid	<i>Sesamum indicum</i>	Pedaliaceae	[10]	+	+
71	22.60	193.0505	194.0579	C ₁₀ H ₁₀ O ₄	0.5	0.1	100	178.0270, 134.0371, 119.0503	6	230, 282, 310	Ferulic acid*	Hydroxycinnamic acid	<i>Sesamum indicum</i>	Pedaliaceae	[10]	+	+
72	22.73	855.2582	856.2637	C ₃₈ H ₄₈ O ₂₂	-1.18	-1.55	97	693.2036, 485.1494, 369.0963, 323.0999, 221.0663, 179.0556, 161.0456, 149.0446, 143.0346, 119.0348	15	278	Sesaminol trihexoside I	Lignan	<i>Sesamum indicum</i>	Pedaliaceae	[10]	+	+
73	23.18	609.1822	610.1898	C ₂₈ H ₃₄ O ₁₅	0.49	0.3	98	447.1293, 301.0713, 259.0811, 175.0023, 151.0031	12	281	Hesperetin hexoside deoxyhexoside	Flavanone		Several families	[26]	+	-
74	23.20	447.0943	448.1006	C ₂₁ H ₂₀ O ₁₁	-2.07	-0.93	97	285.0404, 135.0452, 127.0764	12	N.D.	Kaempferol 3-O-β-D-glucopyranoside*	Flavonol	<i>Cicer arietinum</i>	Fabaceae	[21]	+	-

75	23.30	855.2572	856.2637	C ₃₈ H ₄₈ O ₂₂	−0.62	−0.53	98	693.2060, 485.1514, 369.0970, 323.0983, 221.0667, 179.0560, 161.0453, 149.0452, 143.0352, 119.0351	15	277	Sesaminol trihexoside II	Lignan	<i>Sesamum indicum</i>	Pedaliaceae	[10]	+	+
76	23.49	855.2568	856.2637	C ₃₈ H ₄₈ O ₂₂	−0.28	−0.24	100	693.2029, 485.1508, 369.0981, 323.0980, 221.0660, 179.0563, 161.0457, 149.0451, 143.0351, 119.0349	15	287	Sesaminol trihexoside III	Lignan	<i>Sesamum indicum</i>	Pedaliaceae	[10]	+	+
78	24.21	871.2521	872.2586	C ₃₈ H ₄₈ O ₂₃	−0.7	−0.61	95	709.1983, 691.1938, 485.1527, 385.0925, 323.0985, 221.0664, 179.0556, 161.0447, 143.0354, 137.0245, 119.0354, 89.0245	15	277	Hydroxysesamolol trihexoside	Lignan	<i>Sesamum indicum</i>	Pedaliaceae	[10]	+	+
79	24.27	539.1775	540.1843	C ₂₅ H ₃₂ O ₁₃	−0.8	−0.43	99	377.1240, 359.1192, 333.0842, 327.0880, 275.0918, 223.0641, 209.0455, 191.0349, 179.0697, 171.0293, 161.0473, 153.0559, 127.0400	10	235, 273	Sinapoyl-3-dehydroshikimic acid hexoside I	Hydroxycinnamic acid				+	−
80	24.24	135.0451	136.0525	C ₈ H ₈ O ₂	−0.17	−0.02	85	77.0400	5	273	Methyl benzoic acid	Hydroxybenzoic acid	<i>Sesamum indicum</i>	Pedaliaceae	[10]	+	−
81	24.43	679.2248	680.2319	C ₃₂ H ₄₀ O ₁₆	−0.35	−0.24	99	517.2748, 485.1429, 355.1176, 323.0964, 221.0661, 179.0566, 161.0453, 149.0449, 143.0342, 121.0288, 89.0244	13	282	Xanthoxylol dihexoside	Lignan				+	−
82	24.76	539.1775	540.1843	C ₂₅ H ₃₂ O ₁₃	0.52	0.28	99	333.0854, 327.0889, 223.0609, 209.0446, 191.0340, 171.0299, 161.0482, 153.0537, 127.0399	10	230, 277	Sinapoyl-3-dehydroshikimic acid hexoside II	Hydroxycinnamic acid				+	−

83	24.82	161.0249	162.0322	C ₉ H ₆ O ₃	−3.38	−0.19	76	N.D.	7	N.D.	7-Hydroxycoumarin (umbelliferone)*	Coumarin	<i>Sesamum indicum</i>	Pedaliaceae	[10]	+	+
84	24.97	151.0400	152.0473	C ₈ H ₈ O ₃	−0.13	0.0	100	136.0167, 92.0270	5	N.D.	Methoxybenzoic acid II	Hydroxybenzoic acid			[25]	+	−
85	26.45	285.0408	286.0477	C ₁₅ H ₁₀ O ₆	−1.18	−0.34	99	227.1288, 135.0450	11	287, 325	Luteolin*	Flavone	<i>Sesamum indicum</i>	Pedaliaceae	[10]	+	+
86	28.32	271.0614	272.0685	C ₁₅ H ₁₂ O ₅	−0.73	−0.2	99	N.D.	10	N.D.	Naringenin*	Flavanone	<i>Cicer arietinum</i> / <i>Sesamum indicum</i>	Fabaceae /Pedaliaceae	[10,21]	+	+

^a Detected ions were [M-H][−]. * Identification confirmed by comparison with standards; N.D., below 5 mAU or masked by compound with higher signal. Isomers are denoted with letter codes I, II, etc. Compounds in bold letter indicate new proposed structures.

Table 2. Non-phenolic compounds characterized in Sg32 oil.

Number	RT (min)	Experimental m/z^a [M-H] ⁺	Theoretical mass (M)	Molecular formula	Error (ppm)	Error (mDa)	Score	Main fragments	DBE	UV (nm)	Proposed compound	Subclass	Species	Family	Reference	Oil	Cake
1	2.65	195.0506	196.0583	C ₆ H ₁₂ O ₇	2.33	0.046	98	165.0398	1	N.D.	Gluconic/ galactonic acid	Organic acid	<i>Cicer arietinum</i> / <i>Sesamum indicum</i>	Fabaceae /Pedaliaceae	[21,10]	+	+
2	3.09	191.0201	192.027	C ₆ H ₈ O ₇	−1.72	−0.33	99	173.0094, 111.0089	3	N.D.	Citric acid I	Organic acid	<i>Cicer arietinum</i> / <i>Sesamum indicum</i>	Fabaceae /Pedaliaceae	[21,10]	+	+
3	3.15	133.0142	134.0215	C ₄ H ₆ O ₅	0.29	0.04	99	115.0039	2	N.D.	Malic acid I	Organic acid	<i>Cicer arietinum</i> / <i>Sesamum indicum</i>	Fabaceae /Pedaliaceae	[21,10]	+	+
4	3.40	133.0141	134.0215	C ₄ H ₆ O ₅	1.37	0.18	99	115.004	2	N.D.	Malic acid II	Organic acid	<i>Cicer arietinum</i> / <i>Sesamum indicum</i>	Fabaceae /Pedaliaceae	[21,10]	+	+
5	4.02	191.0203	192.027	C ₆ H ₈ O ₇	−2.91	−0.56	98	173.0096, 111.0092	3	N.D.	Citric acid II	Organic acid	<i>Cicer arietinum</i> / <i>Sesamum indicum</i>	Fabaceae /Pedaliaceae	[21,10]	+	+
6	4.08	128.0358	129.0426	C ₅ H ₇ NO ₃	−2.98	−0.38	96	111.0092	3	N.D.	Pyroglutamic acid I	Amino acid		Several families	[26]	+	+
7	4.27	191.0191	192.027	C ₆ H ₈ O ₇	3.25	0.62	97	173.0081, 111.0088	3	N.D.	Citric acid III	Organic acid	<i>Cicer arietinum</i> / <i>Sesamum indicum</i>	Fabaceae /Pedaliaceae	[21,10]	+	+
8	4.58	128.0353	129.0426	C ₅ H ₇ NO ₃	−0.83	−0.11	98	111.0092	3	N.D.	Pyroglutamic acid II	Amino acid		Several families	[26]	+	+
10	5.01	130.0869	131.0949	C ₆ H ₁₃ NO ₂	3.76	0.49	96	112.9856	1	N.D.	Leucine/Isoleucine I	Amino acid	<i>Cicer arietinum</i> / <i>Sesamum indicum</i>	Fabaceae /Pedaliaceae	[21,10]	+	+
11	5.45	117.0193	118.0266	C ₄ H ₆ O ₄	0	0	98	73.0298	2	N.D.	Succinic acid	Organic acid	<i>C. arietinum</i>	Fabaceae	[21]	+	+
12	5.51	130.087	131.0949	C ₆ H ₁₃ NO ₂	2.59	0.34	99	112.9856	1	N.D.	Leucine/Isoleucine II	Amino acid	<i>Cicer arietinum</i> / <i>Sesamum indicum</i>	Fabaceae /Pedaliaceae	[21,10]	+	+

13	5.82	180.0668	181.0745	C ₉ H ₁₁ NO ₃	1.73	0.31	96	163.097	5	265	Tyrosine*	Amino acid	<i>Cicer arietinum</i> / <i>Sesamum indi-</i> <i>cum</i>	Fabaceae /Peda- liaceae	[21,10]	+	+
14	6.01	130.087	131.0949	C ₆ H ₁₃ NO ₂	2.98	0.39	86	112.9856	1	N.D.	Leucine/Isoleucine III	Amino acid	<i>Cicer arietinum</i> / <i>Sesamum indi-</i> <i>cum</i>	Fabaceae /Peda- liaceae	[21,10]	+	+
15	6.01	611.1444	612.152	C ₂₀ H ₃₂ N ₆ O ₁₂ S ₂	0.25	0.016	98	306.0731, 305.0671, 128.0366	8	N.D.	Oxidized Glutathione (glutathione disulfide)	Peptide	<i>Sesamum indi-</i> <i>cum</i>	Pedaliaceae	[10]	+	+
17	7.75	171.0293	172.0372	C ₇ H ₈ O ₅	3.2	0.6	84	127.0402	4	230	(-)-3-dehydroshikimic acid	Organic acid	<i>Sesamum indi-</i> <i>cum</i>	Pedaliaceae	[10]	+	+
18	7.87	191.0563	192.0634	C ₇ H ₁₂ O ₆	-0.77	-0.15	100	147.0665, 129.0556, 101.0608	2	N.D.	Quinic acid I	Organic acid	<i>Sesamum indi-</i> <i>cum</i>	Pedaliaceae	[10]	+	+
19	8.18	191.0562	192.0634	C ₇ H ₁₂ O ₆	-0.33	-0.06	99	147.0660, 129.0556, 101.0607	2	N.D.	Quinic acid II	Organic acid	<i>Sesamum indi-</i> <i>cum</i>	Pedaliaceae	[10]	+	+
22	9.20	164.0718	165.0790	C ₉ H ₁₁ NO ₂	-0.26	0.0	100	147.049	5	N.D.	Phenylalanine*	Amino acid	<i>Sesamum indi-</i> <i>cum</i>	Pedaliaceae	[10]	+	+
23	10.61	218.1031	219.1107	C ₉ H ₁₇ NO ₅	1.33	0.3	98	146.0819	2	N.D.	Pantothenic acid (Vit B5)	Organic acid	<i>Cicer arietinum</i> / <i>Sesamum indi-</i> <i>cum</i>	Fabaceae /Peda- liaceae	[21,10]	+	+
29	13.05	203.0834	204.0906	C ₁₁ H ₁₂ N ₂ O ₂	-1.94	-0.4	87	142.0663, 116.0507	7	277	Tryptophan*	Amino acid	<i>Cicer arietinum</i> <i>Cicer arietinum</i> / <i>Sesamum indi-</i> <i>cum</i>	Fabaceae Fabaceae /Peda- liaceae	[21] [21,10]	+	+
34	14.49	175.0612	176.0685	C ₇ H ₁₂ O ₅	0.19	0.03	100	115.0402	2	N.D.	Isopropylmalic acid	Organic acid	<i>Cicer arietinum</i> / <i>Sesamum indi-</i> <i>cum</i>	Fabaceae /Peda- liaceae	[21,10]	+	+
77	24.05	187.0979	188.1049	C ₉ H ₁₆ O ₄	-1.75	-0.33	99	125.097	2	N.D.	Azelaic acid	Organic acid	<i>Cicer arietinum</i> / <i>Sesamum indi-</i> <i>cum</i>	Fabaceae /Peda- liaceae	[21,10]	+	+

^a Detected ions were [M-H]⁻. * Identification confirmed by comparison with standards; N.D., below 5 mAU or masked by compound with higher signal. Isomers are denoted with letter codes I, II, etc.