Electronic Supplementary Material (ESI) for RSC Advances.

Supporting Information

Detailed extraction procedures

The first extraction method (M1) was previously described in Abu-Reidah and co-workers[1]. Concisely, 0.5 g of sample was homogenized in 20 mL of methanol:water (80:20, v/v) using Ultra-Turrax Ika T18 basic (Ika-Werke GmbH & Co. KG, Staufen, Germany), sonicated for 30 minutes with B3510 sonicator (Branson, Danbury, CT, USA) and centrifuged at 7155 × *g* for 15 minutes and 5 °C using Sorvall ST 16 (Thermo Sci., ThermoFisher, Waltham, MA, USA). The supernatant was collected and the previous steps were repeated twice. Combined supernatants were evaporated under vacuum using a rotary evaporator at 38 °C (Rotavapor R-200, Büchi Labortechnik, AG, Switzerland).

The second extraction method (M2) was based on Aguilera and co-workers[2]. In brief, 2.5 g of sample was homogenized in 20 mL of methanol:water:hydrochloric acid (80:19:1, v/v), sonicated and centrifuged. The previous steps were repeated twice. The supernatants were combined and extracted with 7.5 mL diethyl ether (× 3) and 3.75 mL ethyl acetate (× 3). The organic phases were combined and evaporated.

The third extraction method (M3) was according to Saura-Calixto and co-workers[3], with some modifications. Succinctly, 0.5 g of sample was firstly homogenized with 25 mL methanol:water (50:50, v/v), subjected to magnetic stirrer Agimatic-N (Jp Selecta, Barcelona, Spain) at room temperature for 60 minutes, sonicated, and finally centrifuged. Residues were re-extracted with 25 mL acetone:water (70:30, v/v). The combined supernatants were evaporated.

The dry residues were dissolved in methanol:water (80:20, v/v) to obtain the same relation of the initial seed weight/volume (0.25 mg/mL). Each extraction procedure was repeated three times for 'Giza 1' chickpea seeds, and all the extracts were passed through 0.22 μm syringe filter (regenerated cellulose) and stored at -20 °C till analysis. For further analysis of the rest of chickpea seeds, two repetitions were performed for each cultivar.

References

1. I. M. Abu-Reidah, M. M. Contreras, D. Arráez-Román, A. Fernández-Gutiérrez and A. Segura-Carretero, *Electrophoresis*, 2014, **35**, 1571-1581.
2. Y. Aguilera, M. Dueñas, I. Estrella, T. Hernández, V. Benitez, R. M. Esteban and M. A. Martín-Cabrejas, *Plant foods for human nutrition*, 2011, **66**, 187-195.
3. F. Saura-Calixto, J. Serrano and I. Goñi, *Food Chemistry*, 2007, **101**, 492-501.

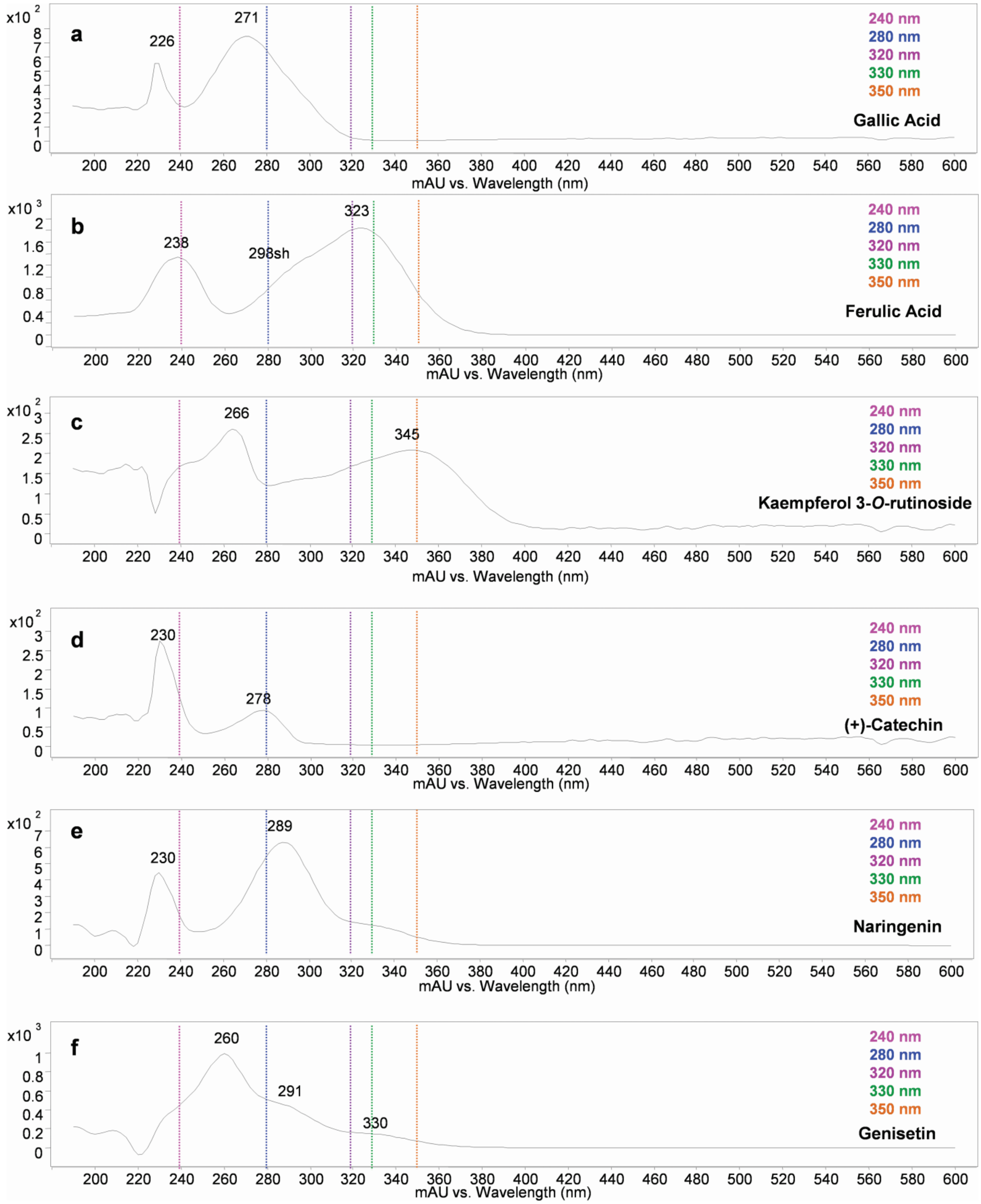


Fig. S1. UV absorbance spectra of standards of several phenolic compounds: a) gallic acid, b) ferulic acid, c) kaempferol-3-*O*-rutinoside, d) (+)-catechin, e) naringenin, and f) genistein, which belong to hydroxybenzoic acid, hydroxycinnamic acid, flavonol, flavan-3-ol, flavanone and isoflavone subclasses, respectively.

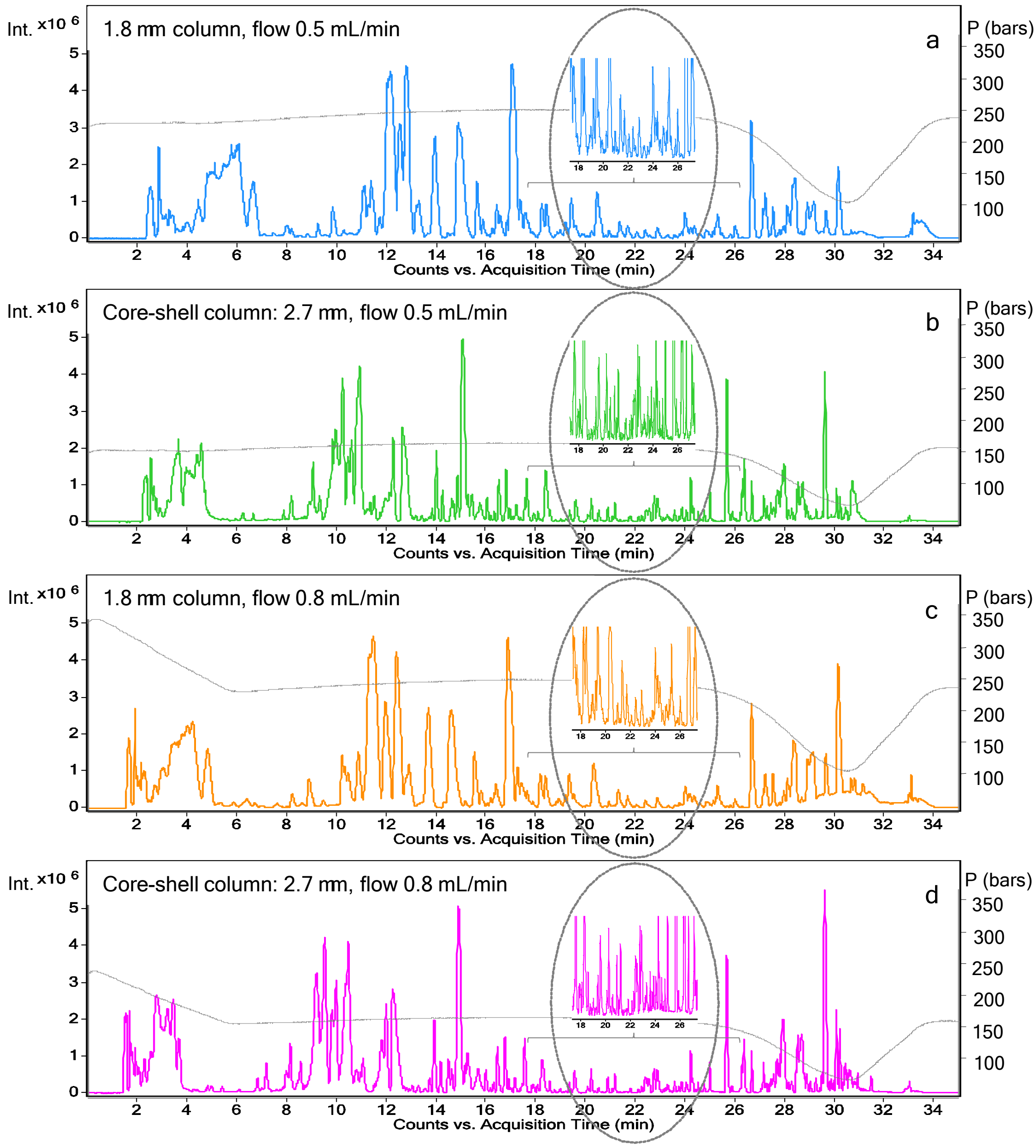
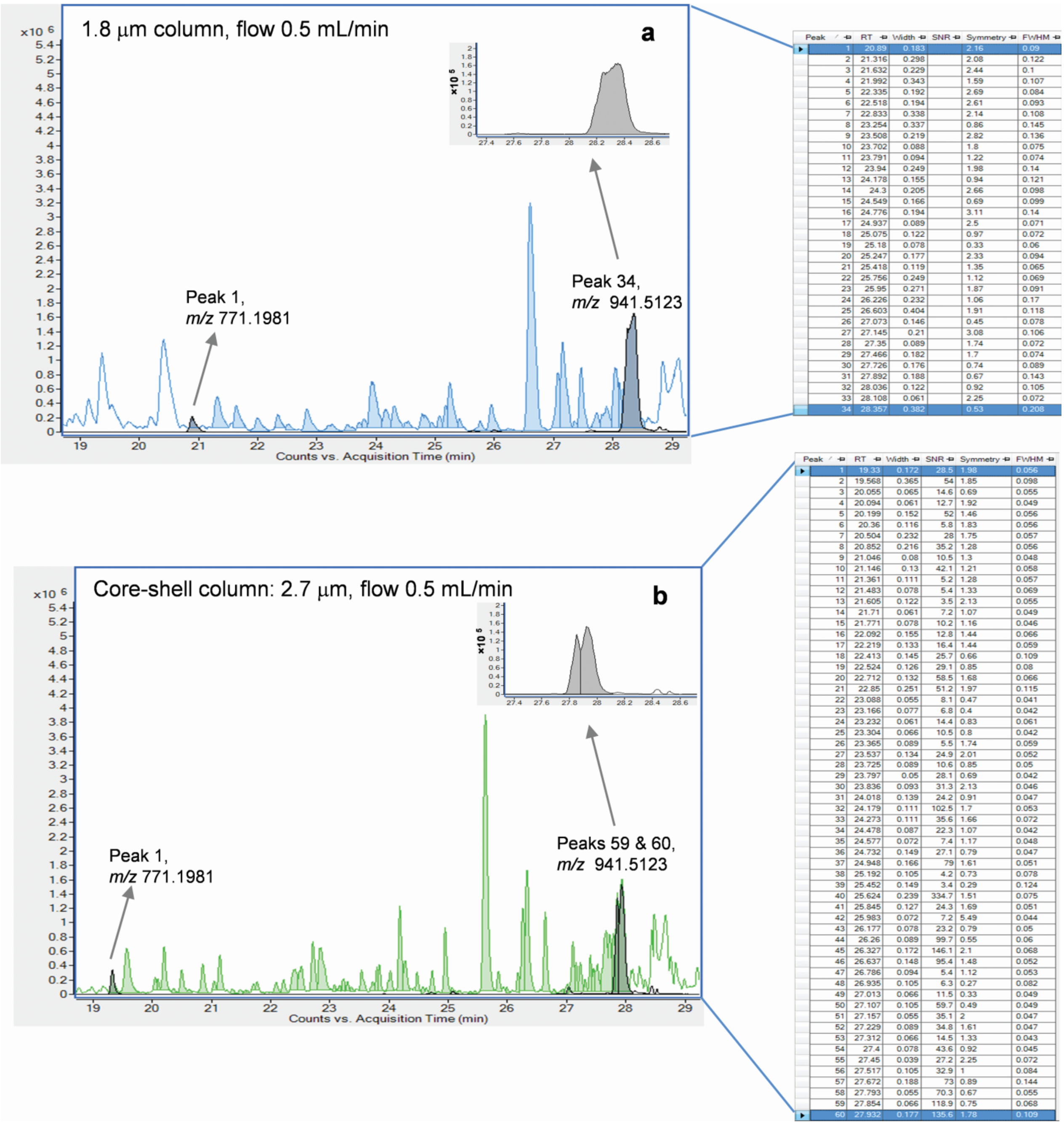


Fig. S2. Base peak chromatograms of the chickpea extract from cultivar 'Giza 1' obtained using different analytical conditions applied during the method optimization: a) flow rate at 0.5 mL/min, C18 column (4.6 × 150 mm, 1.8 µm of particle size), b) flow rate at 0.5 mL/min, C18 core-shell column (4.6 × 150 mm, 2.7 µm of particle size), c) flow rate at 0.8 mL/min, C18 column (4.6 × 150 mm, 1.8 µm of particle size), and d) flow rate at 0.8 mL/min, C18 core-shell column (4.6 × 150 mm, 2.7 µm of particle size). The mobile phases and the gradient were according to experimental section.



Peak	RT	Width	SNR	Symmetry	FWHM
1	20.89	0.183		2.16	0.09
2	21.316	0.298		2.08	0.122
3	21.632	0.229		2.44	0.1
4	21.992	0.343		1.59	0.107
5	22.335	0.192		2.69	0.084
6	22.518	0.194		2.61	0.093
7	22.833	0.338		2.14	0.108
8	23.254	0.337		0.86	0.145
9	23.508	0.219		2.82	0.136
10	23.702	0.088		1.8	0.075
11	23.791	0.094		1.22	0.074
12	23.94	0.249		1.98	0.14
13	24.178	0.155		0.94	0.121
14	24.3	0.205		2.66	0.098
15	24.549	0.166		0.69	0.099
16	24.776	0.194		3.11	0.14
17	24.937	0.089		2.5	0.071
18	25.075	0.122		0.97	0.072
19	25.18	0.078		0.33	0.06
20	25.247	0.177		2.33	0.094
21	25.418	0.119		1.35	0.065
22	25.756	0.249		1.12	0.069
23	25.95	0.271		1.87	0.091
24	26.226	0.232		1.06	0.17
25	26.603	0.404		1.91	0.118
26	27.073	0.146		0.45	0.078
27	27.145	0.21		3.08	0.106
28	27.35	0.089		1.74	0.072
29	27.466	0.182		1.7	0.074
30	27.726	0.176		0.74	0.089
31	27.892	0.188		0.67	0.143
32	28.036	0.122		0.92	0.105
33	28.108	0.061		2.25	0.072
34	28.357	0.382		0.53	0.208

Peak	RT	Width	SNR	Symmetry	FWHM
1	19.33	0.172	28.5	1.98	0.056
2	19.568	0.365	54	1.85	0.098
3	20.055	0.065	14.6	0.69	0.055
4	20.094	0.061	12.7	1.92	0.049
5	20.199	0.152	52	1.46	0.056
6	20.36	0.116	5.8	1.83	0.056
7	20.504	0.232	28	1.75	0.057
8	20.852	0.216	35.2	1.28	0.056
9	21.046	0.08	10.5	1.3	0.048
10	21.146	0.13	42.1	1.21	0.058
11	21.361	0.111	5.2	1.28	0.057
12	21.483	0.078	5.4	1.33	0.069
13	21.605	0.122	3.5	2.13	0.055
14	21.71	0.061	7.2	1.07	0.049
15	21.771	0.078	10.2	1.16	0.046
16	22.092	0.155	12.8	1.44	0.066
17	22.219	0.133	16.4	1.44	0.059
18	22.413	0.145	25.7	0.66	0.109
19	22.524	0.126	29.1	0.85	0.08
20	22.712	0.132	58.5	1.68	0.066
21	22.85	0.251	51.2	1.97	0.115
22	23.088	0.055	8.1	0.47	0.041
23	23.166	0.077	6.8	0.4	0.042
24	23.232	0.061	14.4	0.83	0.061
25	23.304	0.066	10.5	0.8	0.042
26	23.365	0.089	5.5	1.74	0.059
27	23.537	0.134	24.9	2.01	0.052
28	23.725	0.089	10.6	0.85	0.05
29	23.797	0.05	28.1	0.69	0.042
30	23.836	0.093	31.3	2.13	0.046
31	24.018	0.139	24.2	0.91	0.047
32	24.179	0.111	102.5	1.7	0.053
33	24.273	0.111	35.6	1.66	0.072
34	24.478	0.087	22.3	1.07	0.042
35	24.577	0.072	7.4	1.17	0.048
36	24.732	0.149	27.1	0.79	0.047
37	24.948	0.166	79	1.61	0.051
38	25.192	0.105	4.2	0.73	0.078
39	25.452	0.149	3.4	0.29	0.124
40	25.624	0.239	334.7	1.51	0.075
41	25.845	0.127	24.3	1.69	0.051
42	25.983	0.072	7.2	5.49	0.044
43	26.177	0.078	23.2	0.79	0.05
44	26.26	0.089	99.7	0.55	0.06
45	26.327	0.172	146.1	2.1	0.068
46	26.637	0.148	95.4	1.48	0.052
47	26.786	0.094	5.4	1.12	0.053
48	26.935	0.105	6.3	0.27	0.082
49	27.013	0.066	11.5	0.33	0.049
50	27.107	0.105	59.7	0.49	0.049
51	27.157	0.055	35.1	2	0.047
52	27.229	0.089	34.8	1.61	0.047
53	27.312	0.066	14.5	1.33	0.043
54	27.4	0.078	43.6	0.92	0.045
55	27.45	0.039	27.2	2.25	0.072
56	27.517	0.105	32.9	1	0.084
57	27.672	0.188	73	0.89	0.144
58	27.793	0.055	70.3	0.67	0.055
59	27.854	0.066	118.9	0.75	0.068
60	27.932	0.177	135.6	1.78	0.109

Fig. S3. Detail of the separation of 'Giza 1' extract achieved between 19 and 29 min (approximate), corresponding to the region between the compound with *m/z* values of 771.1981 and 941.5123, respectively, as well as the peaks found: a) flow rate at 0.5 mL/min, C18 column (4.6 × 150 mm, 1.8 µm of particle size), and b) flow rate at 0.5 mL/min, C18 core-shell column (4.6 × 150 mm, 2.7 µm of particle size). Each base peak chromatogram was integrated with the software Agilent MassHunter Qualitative Analysis B.06.00 and the Agile function. RT, retention time (min); SNR, signal-to-noise ratio; FWHM, full width of peak at the maximum height (min). The mobile phases and the gradient were according to experimental section.

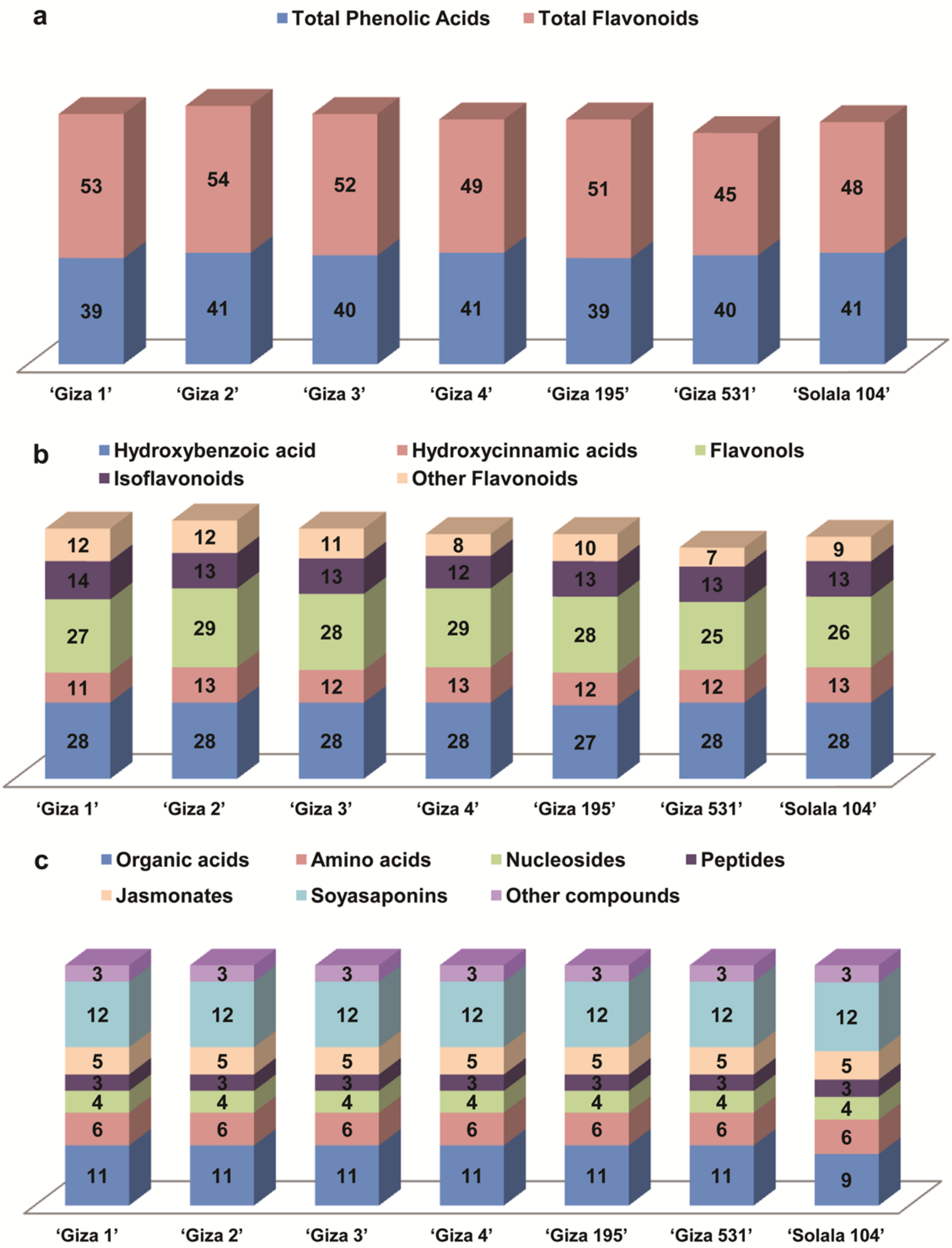


Fig. S4. Qualitative comparison of chickpea metabolites found in the seven studied Egyptian cultivars: a) main phenolic classes, b) phenolic subclasses, c) non phenolic subclasses. Other compounds: dihydrophaseic acid derivatives and a maltol.

Table S1. Phenolic compounds characterized in seven Egyptian cultivars of chickpea: ‘Giza 1’ (1), ‘Giza 2’ (2), ‘Giza 3’ (3), ‘Giza 4’ (4), ‘Giza 195’ (5), ‘Giza 531’ (6) and ‘Solala 104’ (7).

	RT (min)	Experimental *m/z*[a] [M-H]-	Theoretical mass (M)	Molecular formula	Error (ppm)	Error (mDa)	Score	Main fragments	UV (nm)	Proposed compound	Subclass	1	2	3	4	5	6	7	Species	Family	Reference
1	7.65	331.0674	332.0743	$C_{13}H_{16}O_{10}$	-0.1	0.0	90.77	313.0562, 169.0136, 168.0065, 125.0233	230, 256	Gallic acid hexoside I[b]	Hydroxybenzoic acid	+	+	+	+	+	+	+	*A. nilotica*	Fabaceae	[1]
2	8.11	169.0142	170.0215	$C_7H_6O_5$	0.7	0.1	93.82	125.0241	N.D.	Gallic acid*	Hydroxybenzoic acid	+	+	+	+	-	+	+	*C. arietinum*	Fabaceae	[2, 3]
3	8.20	329.0886	330.0951	$C_{14}H_{18}O_9$	-2.0	-0.7	82.2	167.0316, 122.0367	258	Vanillic acid-4-*O*-β-D-glucopyranoside	Hydroxybenzoic acid	+	+	+	+	+	+	+	*P. vulgaris*	Fabaceae	[4]
4	8.76	331.0673	332.0743	$C_{13}H_{16}O_{10}$	-0.4	-0.1	99.18	313.0569, 169.0138, 168.0058, 125.0242	254	Gallic acid hexoside II[b]	Hydroxybenzoic acid	+	+	+	+	+	+	+	*A. nilotica*	Fabaceae	[1]
5	9.09	299.0777	300.0845	$C_{13}H_{16}O_8$	-1.4	-0.4	98.83	137.0245, 93.0346	N.D.	Hydroxybenzoic acid hexoside I[b]	Hydroxybenzoic acid	+	+	+	+	+	+	+	*B. variegata*	Fabaceae	[5]
6	9.20	299.0777	300.0845	$C_{13}H_{16}O_8$	-1.4	-0.4	98.53	137.0245, 93.0347	248	Hydroxybenzoic acid hexoside II[b]	Hydroxybenzoic acid	+	+	+	+	+	+	+	*B. variegata*	Fabaceae	[5]
7	9.34	461.1296	462.1373	$C_{19}H_{26}O_{13}$	1.7	0.8	93.4	417.1397, 285.0992, 123.0459	N.D.	Vanillic acid hexoside pentoside I[c]	Hydroxybenzoic acid	+	+	+	+	+	+	+	*G. littoralis*	Apiaceae	[6]
8	9.90	315.0733	316.0794	$C_{13}H_{16}O_9$	-3.5	-1.1	95.55	153.0195, 152.0117, 109.0299, 108.0217	254, 314	Dihydroxybenzoic acid hexoside I[b]	Hydroxybenzoic acid	+	+	+	+	+	+	+	*V. faba/ L. sativa*	Fabaceae /Asteraceae	[7, 8]
9	9.93	331.067	332.0743	$C_{13}H_{16}O_{10}$	0.3	0.1	99.65	313.0576, 169.0148, 168.0074, 125.0250	N.D.	Gallic acid hexoside III[b]	Hydroxybenzoic acid	+	+	+	+	+	+	+	*A. nilotica*	Fabaceae	[1]
10	9.94	431.1205	432.1286	$C_{18}H_{24}O_{12}$	-2.1	-0.9	97.38	137.0244, 93.0349	N.D.	Hydroxybenzoic acid hexoside pentoside I[b]	Hydroxybenzoic acid	+	+	+	+	+	+	+	*P. vulgaris*	Fabaceae	[4]
11	10.09	315.0721	316.0794	$C_{13}H_{16}O_9$	0.4	0.1	99.17	153.0183, 152.0119, 109.0119, 108.0219	236, 314	Dihydroxybenzoic acid hexoside II[b]	Hydroxybenzoic acid	+	+	+	+	+	+	+	*V. faba/ L. sativa*	Fabaceae /Asteraceae	[7, 8]
12	10.19	461.1298	462.1373	$C_{19}H_{26}O_{13}$	1.1	0.5	97.4	315.0782, 153.0227	N.D.	**Dihydroxybenzoic acid hexoside deoxyhexoside**	Hydroxybenzoic acid	+	+	+	+	+	+	+			
13	10.39	315.0726	316.0794	$C_{13}H_{16}O_9$	-1.2	0.4	98.35	153.0195, 152.0116, 109.0297, 108.0220	240, 314	Dihydroxybenzoic acid hexoside III[b]	Hydroxybenzoic acid	+	+	+	+	+	+	+	*V. faba/ L. sativa*	Fabaceae /Asteraceae	[7, 8]
14	10.53	431.1204	432.1286	$C_{18}H_{24}O_{12}$	-1.8	-0.8	97.95	299.0795, 137.0250, 93.0353	252	Hydroxybenzoic acid hexoside pentoside II	Hydroxybenzoic acid	+	+	+	+	+	+	+	*P. vulgaris*	Fabaceae	[4]
15	11.01	431.1204	432.1286	$C_{18}H_{24}O_{12}$	-2.0	-0.9	97.08	299.0892, 137.0311, 93.0399	250	Hydroxybenzoic acid hexoside pentoside III	Hydroxybenzoic acid	+	+	+	+	+	+	+	*P. vulgaris*	Fabaceae	[4]

16	11.49	461.1295	462.1373	$C_{19}H_{26}O_{13}$	1.3	0.6	99.15	329.0879, 167.0347, 152.0111	254, 292	Vanillic acid hexoside pentoside II[c]	Hydroxybenzoic acid	+	+	+	+	+	+	+	*G. littoralis*	Apiaceae	6
17	11.65	315.0728	316.0794	$C_{13}H_{16}O_{9}$	-2.0	-0.6	97.51	153.0200, 109.0299	238, 307	Dihydroxybenzoic acid hexoside IV[b]	Hydroxybenzoic acid	+	+	+	+	+	+	+	*V. faba*/ *L. sativa*	Fabaceae /Asteraceae	7, 8
18	12.13	447.1147	448.1217	$C_{18}H_{24}O_{13}$	-0.5	-0.2	99.64	315.0729, 153.0195, 152.0119, 109.0296, 108.0221	257, 305	**Dihydroxybenzoic acid hexoside pentoside I**	Hydroxybenzoic acid	+	+	+	+	+	+	+			
19	12.35	447.1143	448.1217	$C_{18}H_{24}O_{13}$	0.4	0.2	99.15	315.0723, 153.0186, 152.0113, 109.0289, 108.0215	231, 316	**Dihydroxybenzoic acid hexoside pentoside II**	Hydroxybenzoic acid	+	+	+	+	+	+	+			
20	13.02	353.0876	354.0951	$C_{16}H_{18}O_{9}$	0.9	0.3	99.06	191.0563, 179.0354, 135.0454	230, 288, 330sh	Caffeoylquinic acid I	Hydroxycinnamic acid	-	+	-	+	-	+	+	*C. arietinum*	Fabaceae	2, 3
21	13.07	325.0926	326.1002	$C_{15}H_{18}O_{8}$	0.0	0.0	91	163.0401, 119.0501	N.D.	*p*-coumaric acid glucopyranoside	Hydroxycinnamic acid	+	+	+	+	+	+	+	*P. vulgaris*	Fabaceae	4
22	13.34	285.0616	286.0689	$C_{12}H_{14}O_{8}$	0.0	0.0	98.84	153.0182, 152.0114, 109.0927, 108.0212	268	Dihydroxybenzoic acid pentoside[b]	Hydroxybenzoic acid	+	+	+	+	+	+	+	*M. truncatula*	Fabaceae	9
23	13.64	609.1466	610.1534	$C_{27}H_{30}O_{16}$	-0.6	-0.4	97.84	447.0943, 285.0412, 284.0325, 151.0031	243, 314, 342	Kaempferol 3,7-*O*-β-D-diglucopyranoside	Flavonol	+	+	+	+	+	+	+	*V. faba*	Fabaceae	8, 10
24	14.39	355.1043	356.1107	$C_{16}H_{20}O_{9}$	-2.0	-0.7	82.29	193.0509, 149.0607	232, 291, 314	Ferulic acid hexoside I[b]	Hydroxycinnamic acid	+	+	+	+	+	+	+	*C. arietinum*	Fabaceae	11, 12
25	15.03	353.0877	354.0951	$C_{16}H_{18}O_{9}$	0.4	0.1	98.46	191.0562, 179.0344, 173.0453, 135.0449	N.D.	Caffeoylquinic acid II[b]*	Hydroxycinnamic acid	+	+	+	+	+	+	+	*C. arietinum*	Fabaceae	2, 3
26	15.14	385.1146	386.1213	$C_{17}H_{22}O_{10}$	-1.5	-0.9	90.56	223.0614, 208.0376, 191.0199, 179.0138,	258	Sinapic acid hexoside I	Hydroxycinnamic acid	+	+	+	+	+	+	+	*C. arietinum*	Fabaceae	11
27	15.32	353.0876	354.0951	$C_{16}H_{18}O_{9}$	0.6	0.2	99.11	191.0542, 173.0441, 179.0325, 161.0231, 135.0444	245, 290, 325	Caffeoylquinic acid III	Hydroxycinnamic acid	+	+	+	+	+	+	+	*C. arietinum*	Fabaceae	2, 3
28	15.42	153.0191	154.0266	$C_{7}H_{6}O_{4}$	1.2	0.2	99.51	109.0297	248, 322	Dihydroxybenzoic acid I	Hydroxybenzoic acid	+	+	+	+	+	+	+	*C. arietinum*	Fabaceae	13
29	15.72	137.0247	138.0317	$C_{7}H_{6}O_{3}$	-1.6	-0.2	99.44		256	*p*-hydroxybenzoic acid*	Hydroxybenzoic acid	+	+	+	+	+	+	+	*C. arietinum*	Fabaceae	13
30	15.79	401.0721	402.0798	$C_{16}H_{18}O_{12}$	1.4	0.6	98.33	357.0842, 315.0723, 153.0194, 152.0115, 109.0297, 108.0217	230, 279	**Dihydroxybenzoic acid malonyl hexoside I**	Hydroxybenzoic acid	+	+	+	+	+	+	+			

31	15.90	401.0740	402.0798	$C_{16}H_{18}O_{12}$	-0.3	-0.1	97.31	357.0827, 315.0730, 153.0204, 152.0125, 109.0309, 108.0230	230, 280	**Dihydroxybenzoic acid malonyl hexoside II**	Hydroxybenzoic acid	+	+	+	+	+	+	+			
32	16.03	289.0718	290.0790	$C_{15}H_{14}O_6$	0.1	0.0	97.94	245.0820, 221.0819, 203.0713, 151.0401, 123.0453, 109.0297	230, 279	(+)-Catechin*	Flavan-3-ol	+	+	+	+	+	-	+	*C. arietinum*	Fabaceae	2
33	16.05	353.0881	354.0951	$C_{16}H_{18}O_9$	-0.8	-0.3	99.19	191.0567, 179.0353, 135.0456	250, 292, 326	Caffeoylquinic acid IV	Hydroxycinnamic acid	-	+	+	+	+	-	+	*C. arietinum*	Fabaceae	2, 3
34	16.40	827.1894	828.1960	$C_{35}H_{40}O_{23}$	-0.4	0.0	99.03	783.2006, 621.1472, 447.0898, 285.0389, 284.0333, 151.0035	265, 353	**Kaempferol malonyl dihexoside pentoside I**	Flavonol	+	+	+	+	+	+	+			
35	16.60	609.1461	610.1534	$C_{27}H_{30}O_{16}$	0.6	0.4	95.74	447.0924, 285.0410, 283.0252, 151.0035	259, 324, 342	Kaempferol 3-*O*-β-D-diglucopyranoside	Flavonol	+	+	+	+	+	+	+	*G. max*	Fabaceae	10
36	16.84	355.1038	356.1107	$C_{16}H_{20}O_9$	-1.8	-0.6	90.93	193.0517	N.D.	Ferulic acid hexoside II[b]	Hydroxycinnamic acid	+	+	+	+	+	+	+	*C. arietinum*	Fabaceae	11, 12
37	17.20	167.0353	168.0426	$C_8H_8O_4$	-2.0	-0.7	98.88	152.0115, 122.0373, 108.0217	230, 260, 296	Vanillic acid*	Hydroxybenzoic acid	+	+	+	+	+	+	+	*C. arietinum*	Fabaceae	2, 3
38	17.28	445.1360	446.1424	$C_{19}H_{26}O_{12}$	-1.5	-0.7	98.04	151.0407, 137.0218, 136.0173	255	Methoxy hydroxybenzoic acid hexoside pentoside[c]	Hydroxybenzoic acid	+	+	+	+	+	+	+	*C. barbinervis*	Clethraceae	14
39	17.43	385.1138	386.1213	$C_{17}H_{22}O_{10}$	0.7	0.3	98.4	223.0616, 208.0375, 191.0198, 179.0139	256	Sinapic acid hexoside II	Hydroxycinnamic acid	+	+	+	+	+	+	+	*C. arietinum*	Fabaceae	11
40	17.46	353.0878	354.0951	$C_{16}H_{18}O_9$	-0.4	-0.2	97.55	191.0567, 179.0355, 135.0454	252, 294, 325	Caffeoylquinic acid V	Hydroxycinnamic acid	+	+	+	+	+	+	+	*C. arietinum*	Fabaceae	3, 7
41	17.53	153.0191	154.0266	$C_7H_6O_4$	1.4	0.2	99.54	109.0289	252	Dihydroxybenzoic acid II	Hydroxybenzoic acid	+	+	+	+	+	+	+	*C. arietinum*	Fabaceae	13
42	17.57	827.1887	828.1960	$C_{35}H_{40}O_{23}$	0.4	0.3	98.96	783.2003, 621.1499, 447.0977, 285.0419, 284.0337, 151.0025	348	**Kaempferol malonyl dihexoside pentoside II**	Flavonol	+	+	+	+	+	+	+			
43	17.71	695.1478	696.1538	$C_{30}H_{32}O_{19}$	-1.7	-1.2	97.69	651.1556, 489.1038, 447.0923, 446.0851, 285.0409, 151.0023, 131.0714	266, 349	Kaempferol malonyl dihexoside I[c]	Flavonol	+	+	+	+	+	+	+	*Equisetum spp*	Equisetaceae	15
44	17.94	741.1878	742.1956	$C_{32}H_{38}O_{20}$	1.1	0.8	98.66	579.1342, 447.0913, 285.0399, 284.0323, 179.0149	348	Kaempferol 3-*O*-β-D-apiofuranosyl-(1→2)-β-D-glucopyranoside-4'-*O*-β-D-glucopyranoside	Flavonol	+	+	+	+	+	+	+	*P. vulgaris*	Fabaceae	4
45	18.06	289.0717	290.0790	$C_{15}H_{14}O_6$	-1.3	-0.4	90.86	245.0815, 221.0818, 203.0712, 151.0398, 123.0450, 109.0295	230, 278	(-)-Epicatechin*	Flavan-3-ol	+	+	+	-	+	-	-	*C. arietinum*	Fabaceae	2

46	18.17	727.2097	728.2164	$C_{32}H_{40}O_{19}$	-0.8	-0.6	99.23	565.1451, 445.1034, 433.1029, 271.0577, 151.0039, 145.0297	N.D.	Naringenin dihexoside pentoside	Flavanone	+	+	+	+	+	+	+	*Capsicum spp*	Solanaceae	16
47	18.42	755.2038	756.2113	$C_{33}H_{40}O_{20}$	0.5	0.4	96.63	609.1455, 301.0342, 300.0276, 151.0028	255, 358	Quercetin -3-*O*-rutinoside-7-*O*-α-L-rhamnopyranoside	Flavonol	-	+	+	+	+	+	+	*O. viciifolia*	Fabaceae	17
48	18.54	449.1089	450.1162	$C_{21}H_{22}O_{11}$	0.2	0.1	96.96	287.0563, 269.0450, 259.0609, 153.0183, 151.0030	N.D.	Aromadendrin-3-*O*-β-*D*-glucopyranoside	Flavanonol	+	+	+	+	+	+	+	*D. sericea*	Fabaceae	18
49	18.64	609.1466	610.1534	$C_{27}H_{30}O_{16}$	-0.5	-0.3	99.34	447.0942, 446.0869, 285.0416, 283.0260, 255.0309, 151.0047	264, 346	Kaempferol-3,4'-*O*-β-D-diglucopyranoside	Flavonol	+	+	+	+	+	+	+	*A. complanatus*	Fabaceae	10
50	18.85	755.2048	756.2113	$C_{33}H_{40}O_{20}$	-0.8	-0.6	98.27	593.1517, 431.1945, 285.0409, 284.0331, 151.0029	266, 347	Kaempferol-3-*O*-rutinoside-7-*O*-β-D-glucopyranoside	Flavonol	+	+	+	+	+	+	+	*P. vulgaris*	Fabaceae	4
51	19.03	625.1413	626.1483	$C_{27}H_{30}O_{17}$	0.0	0.0	98.42	463.0909, 445.0781, 301.0352, 300.0284, 151.0037	254, 368	Quercetin-3,7-*O*-di-glucopyranoside	Flavonol	+	+	+	+	+	-	-	*V. faba*	Fabaceae	8
52	19.08	741.1880	742.1956	$C_{32}H_{38}O_{20}$	0.4	0.3	99.12	609.1450, 301.0304, 300.0279, 178.9986	256, 356	Quercetin-3-*O*-β-D-xylopyranosyl-(1→2)-rutinoside	Flavonol	+	+	+	+	+	-	+	*P. vulgaris*	Fabaceae	4
53	19.40	771.1987	772.2062	$C_{33}H_{40}O_{21}$	0.6	0.4	98.73	756.1761, 639.1565, 331.0458, 330.0375, 316.0224, 315.0149, 178.9981, 151.0033	248, 349sh, 366	**Myricetin-*O*-methyl ether hexoside deoxyhexoside pentoside**	Flavonol	+	+	+	+	+	+	+			
54	19.69	695.1475	696.1538	$C_{30}H_{32}O_{19}$	-1.5	-1.0	95.34	651.1729, 489.1049, 447.0937, 285.0411, 221.0250, 151.0031	266, 343	Kaempferol malonyl dihexoside II[c]	Flavonol	+	+	+	+	+	+	+	*Equisetum spp*	Equisetaceae	15
55	20.09	725.1935	726.2007	$C_{32}H_{38}O_{19}$	-0.1	-0.1	98.84	593.1526, 431.1001, 285.0415, 284.0337, 178.9994, 151.0042	262, 347	Kaempferol 3-*O*-lathyroside-7-*O*-α-L-rhamnopyranoside	Flavonol	+	+	+	+	+	+	+	*Lathyrus spp.*	Fabaceae	19
56	20.30	595.1664	596.1741	$C_{27}H_{32}O_{15}$	-0.6	-0.4	99.36	433.0999, 287.0559, 151.0037, 135.0451	N.D.	Aromadendrin 7-*O*-α-L-rhamnopyranosyl-(1→4)-β-D-galactopyranoside	Flavanonol	+	+	-	-	-	-	-	*C. laburnifolia*	Fabaceae	20
57	20.38	609.1466	610.1534	$C_{27}H_{30}O_{16}$	-0.7	-0.5	98.89	301.0355, 300.0287, 151.0054	256, 356	Rutin* [quercetin 3-*O*-rutinoside]	Flavonol	+	+	+	+	+	+	+	*C. arietinum*	Fabaceae	13
58	20.43	755.2045	756.2113	$C_{33}H_{40}O_{20}$	-0.8	-0.6	98.56	623.1618, 461.1259, 315.0510, 300.0275, 178.9991, 151.0086	256, 368	Isorhamnetin 3-*O*-β-D-xylopyranosyl-(1→2)-β-D-glucopyranoside-7-*O*-α-L-rhamnopyranoside	Flavonol	+	+	+	+	+	+	+	*Lathyrus spp.*	Fabaceae	21
59	20.51	639.1567	640.1639	$C_{28}H_{32}O_{17}$	-0.1	-0.1	95.92	331.0459, 316.0216	256, 368	Myricetin-*O*-methyl ether hexoside deoxyhexoside	Flavonol	+	+	+	+	+	+	+	*L. carii, G. biloba*	Chrysobalanaceae, Ginkgoaceae	22, 23
60	20.70	593.1516	594.1585	$C_{27}H_{30}O_{15}$	-0.9	-0.6	98.84	447.0922, 285.0387, 284.0318, 255.0288, 151.0030	264, 348	Kaempferol-3-*O*-β-D-glucopyranoside-7-*O*-α-L-rhamnopyranside	Flavonol	+	+	+	+	+	+	+	*O. viciifolia*	Fabaceae	17
61	20.74	163.0403	164.0473	$C_9H_8O_3$	-1.1	-0.2	99.4	119.0505, 101.0384	310	*p*-coumaric acid*	Hydroxycinnamic	+	+	+	+	+	+	+	*C. arietinum*	Fabaceae	2, 13, 24-28

											acid										
62	20.76	695.1460	696.1538	$C_{30}H_{32}O_{19}$	0.8	0.5	99.16	651.1576, 609.1458, 301.0347, 300.0248, 151.0024	N.D.	Quercetin 3-*O*-(6"-malonylneohesperidoside)	Flavonol	-	+	+	+	-	-	-	*C. ternatea*	Fabaceae	29
63	21.14	533.1665	534.1737	$C_{26}H_{30}O_{12}$	-0.6	-0.3	92.89	431.1873, 389.2187, 371.2075	N.D.	Dalpanin I	Isoflavanone	+	+	+	+	+	+	+	*P. vulgaris*	Fabaceae	4
64	21.24	463.0880	464.0955	$C_{21}H_{20}O_{12}$	0.3	0.1	99	301.0361, 300.0275, 271.0246, 255.0295, 151.0032	256, 357	Quercetin 3-*O*-β-D-glucopyranoside*	Flavonol	+	+	+	+	+	+	+	*C. arietinum*	Fabaceae	30
65	21.24	579.1352	580.1438	$C_{26}H_{28}O_{15}$	0.6	0.4	99.43	447.0949, 285.0402, 284.0329, 255.0301, 151.0193	264, 348	Kaempferol 3-*O*-β-D-apiofuranosyl-(1→2)-β-D-glucopyranoside	Flavonol	+	+	+	+	+	+	+	*C. arietinum*	Fabaceae	31
66	21.37	477.0675	478.0747	$C_{21}H_{18}O_{13}$	-0.4	-0.2	98.3	301.0359, 151.0037	N.D.	Quercetin-3-*O*-β-D-glucopyranuronic acid	Flavonol	+	+	+	+	+	-	-	*A. hypogaea*	Fabaceae	32
67	21.40	223.0615	224.0685	$C_{11}H_{12}O_5$	-1.3	-0.3	98.56	208.0378, 193.0141, 179.0146, 164.0483	254, 318	Sinapic acid*	Hydroxycinnamic acid	+	+	+	+	+	+	+	*C. arietinum*	Fabaceae	2, 3
68	21.69	593.1516	594.1585	$C_{27}H_{30}O_{15}$	-0.8	-0.5	99.22	447.0920, 285.0405, 255.0295, 151.0036	266, 345	Kaempferol 3-*O*-rutinose* [Kaempferol 3-*O*-(α-L-rhamnopyranosyl-(1→6)-β-D-glucopyranoside)]	Flavonol	+	+	+	+	+	+	+	*C. arietinum*	Fabaceae	13
69	21.71	193.0508	194.0579	$C_{10}H_{10}O_4$	1.0	0.2	96.7	134.0385	230, 286sh, 316	Ferulic acid*	Hydroxycinnamic acid	+	+	+	+	+	+	+	*C. arietinum*	Fabaceae	2
70	21.79	533.1670	534.1737	$C_{26}H_{30}O_{12}$	-2.1	-1.1	92.35	473.1567, 431.1873, 389.1829, 371.1144, 353.1062, 341.1048, 326.0762, 206.0459, 121.0300	N.D.	Dalpanin II	Isoflavanone	+	+	+	+	+	+	+	*P. vulgaris*	Fabaceae	8
71	22.27	563.1410	564.1479	$C_{26}H_{28}O_{14}$	-0.2	-0.1	97.97	431.0978, 269.0453, 175.0756	254, 323	Genistein 7-*O*-β-D-apiofuranosyl-(1→6)-β-D-glucopyranoside	Isoflavone	+	+	+	+	+	+	+	*A.inermis*	Fabaceae	33
72	22.31	665.1351	666.1432	$C_{29}H_{30}O_{18}$	1.6	1.0	98.09	621.1460, 489.1050, 327.0509, 285.0416, 284.0342, 255.0298, 151.0059	266, 348	Kaempferol-3-*O*-[6"-malonyl-β-D-apiofuranosyl-(1→2)-β-D-glucopyranoside]	Flavonol	+	+	+	+	+	+	+	*C. arietinum*	Fabaceae	30
73	22.52	121.0297	122.0368	$C_7H_6O_2$	-1.7	-0.2	99.61	77.0394	232, 284	Benzoic acid	Hydroxybenzoic acid	+	+	+	+	+	+	+	*C. obtusifolia/ S. esculentum*	Fabaceae/Solanaceae	34, 35
74	22.55	565.1562	566.1636	$C_{26}H_{30}O_{14}$	-0.1	0.0	98.07	445.1031, 433.1148, 271.0618, 151.0033, 145.0291	N.D.	Naringenin hexoside pentoside I[b]	Flavanone	+	+	+	+	+	+	+	*G. caspica*	Fabaceae	36
75	22.59	447.0935	448.1006	$C_{21}H_{20}O_{11}$	-0.3	-0.2	99.81	327.0521, 285.0406, 284.0331, 255.0299, 227.0352, 151.0033	264, 348	Kaempferol 3-*O*-β-D-glucopyarnoside*	Flavonol	+	+	+	+	+	+	+	*C. arietinum*	Fabaceae	31

76	22.70	477.1038	478.1111	$C_{22}H_{22}O_{12}$	-0.2	-0.1	97.23	315.0503, 314.0432, 300.0263, 299.0199, 285.0401, 271.0240, 179.0473, 151.0025	262, 356	Isorhamentin 3-*O*-β-D-glucopyranoside	Flavonol	+	+	+	+	+	+	+	*C. arietinum*	Fabaceae	30
77	22.80	431.0984	432.1056	$C_{21}H_{20}O_{10}$	0.0	0.0	98.76	269.045, 268.0378, 239.0345, 224.0475, 135.0215, 132.0215	257, 327	Genistin [genistein-7-*O*-β-D-glucopyranoside]	Isoflavone	+	+	+	+	+	+	+	*C. arietinum*	Fabaceae	13, 37, 38
78	22.89	565.1573	566.1636	$C_{26}H_{30}O_{14}$	-1.6	-0.9	96.69	433.1106, 271.0612, 151.0041	N.D.	Naringenin hexoside pentoside II[b]	Flavanone	+	+	+	+	+	+	+	*G. caspica*	Fabaceae	36
79	23.45	433.1144	434.1213	$C_{21}H_{22}O_{10}$	-1.2	-0.5	98.69	271.0641, 151.0035, 119.0491	N.D.	Prunin [naringenin 7-*O*-β-D-glucopyranoside]	Flavanone	+	+	+	+	+	+	+	*C. arietinum*	Fabaceae	8, 39
80	23.62	533.0940	534.1010	$C_{24}H_{22}O_{14}$	-0.4	-0.2	99.35	489.1054, 447.1205, 285.0407, 284.0326, 255.0285, 151.0026	260, 348	Kaempferol-3-*O*-(6"-malonyl-)-β-D-glucopyranoside	Flavonol	+	+	+	+	+	+	+	*C. arietinum*	Fabaceae	30
81	24.14	461.1087	462.1162	$C_{22}H_{22}O_{11}$	-0.2	-0.1	96.64	313.0566, 299.0558, 284.0321, 169.0144, 151.0031, 147.0457,107.0139, 103.0555	244, 310	Pratensein 7-*O*-β-D-glucopyranoside	Isoflavone	+	+	+	+	+	+	+	*Baptisia & Thermopsis spp.*	Fabaceae	40
82	24.52	269.0457	270.0528	$C_{15}H_{10}O_5$	-1.2	-0.3	98.01	251.0437, 241.0481	N.D.	Apigenin*	Flavone	+	+	+	+	+	+	+	*G. ephedroides*	Fabaceae	41
83	24.75	287.0566	288.0634	$C_{15}H_{12}O_6$	-2.2	-0.6	93.56	259.0617, 177.0557, 151.0031, 125.0241	290, 310sh	Dihydrokaempferol [Aromadendrin]	Flavanonol	+	+	+	+	+	+	+	*A. bella*	Fabaceae	42
84	25.00	273.0767	274.0841	$C_{15}H_{14}O_5$	0.1	0.2	99.09	167.0353, 151.0395, 137.0241, 123.0445, 121.0297, 109.0298	244, 277	(Epi)afzelechin	Flavan-3-ol	+	+	+	-	-	-	-	*V. faba*	Fabaceae	8
85	25.68	253.0506	254.0579	$C_{15}H_{10}O_4$	-0.1	0.0	92.1	225.0575, 242.0477, 209.0591, 197.0600, 135.0088, 133.0295	250, 310	Daidzein	Isoflavone	+	+	+	-	+	+	+	*C. arietinum*	Fabaceae	38
86	26.02	269.0459	270.0528	$C_{15}H_{10}O_5$	-0.9	-0.3	96.13	159.0452, 133.0294, 119.0501, 107.0139	N.D.	Genistein*	Isoflavone	+	-	-	-	-	-	-	*C. arietinum*	Fabaceae	13, 37, 38, 43
87	26.31	285.0406	286.0477	$C_{15}H_{10}O_6$	-0.3	-0.1	99.88	249.1047, 217.0515, 151.0034, 133.0259, 107.0137	278, 313	Orobol	Isoflavone	+	+	+	+	+	+	+	*M. amurensis*	Fabaceae	44
88	26.39	445.1151	446.1229	$C_{22}H_{22}O_{10}$	-3.2	-1.4	93.35	283.0618, 268.0385, 248.9730, 217.0036, 132.0202	256, 325	Biochanin A 7-*O*-β-D-glucopyranoside	Isoflavone	+	+	+	+	+	+	+	*C. arietinum*	Fabaceae	13, 45-47
89	26.67	283.0615	284.0685	$C_{16}H_{12}O_5$	-1.4	-0.4	82.07	268.0381, 250.0318, 239.0341, 164.2169, 151.0032, 132.0221, 115.0774, 107.0128	250, 311	Methyl isoflavone isomer I[d]	Isoflavone	+	+	+	+	+	+	+		Fabaceae	37
90	27.31	283.0610	284.0685	$C_{16}H_{12}O_5$	1.1	0.3	98.76	268.0342, 250.0224, 239.0324, 151.0032, 132.0215, 117.0325	258, 303	Methyl isoflavone isomer II[d]	Isoflavone	+	+	+	+	+	+	+		Fabaceae	37
91	27.74	271.0614	272.0685	$C_{15}H_{12}O_5$	-0.9	-0.2	95.1	151.0045, 119.0496, 107.0147, 93.0343	N.D.	Naringenin*	Flavanone	+	+	+	-	+	-	+	*C. arietinum*	Fabaceae	39, 48
92	27.90	285.0405	286.0477	$C_{15}H_{10}O_6$	0.3	0.1	99.09	257.0461, 239.0356, 229.0514, 185.0614, 151.0039, 107.0142, 93.0350	N.D.	Kaempferol*	Flavonol	+	+	-	+	+	+	+	*C. arietinum*	Fabaceae	3, 24, 31

93	28.02	299.0567	300.0634	$C_{16}H_{12}O_6$	-2.1	-0.6	98.52	284.0328, 255.0294, 211.0394, 151.0038, 135.0095	264, 296	Pratensein	Isoflavone	+	+	+	+	+	+	+	*C. arietinum*	Fabaceae	24, 31, 47
94	28.55	267.0651	268.0736	$C_{16}H_{12}O_4$	-1.1	-0.3	98.91	252.0430, 251.0341, 223.0403, 132.0281	252, 301	Biochanin B	Isoflavone	+	+	+	+	+	+	+	*C. arietinum*	Fabaceae	37, 45, 47
95	29.60	299.0563	300.0634	$C_{16}H_{12}O_6$	-1.7	-0.5	95.17	285.0381, 284.0332, 151.0034, 107.0148	N.D.	Kaempferide*	Flavonol	+	+	+	+	+	+	+	*A. complanatus*	Fabaceae	49
96	29.66	283.0616	284.0685	$C_{16}H_{12}O_5$	-1.3	-0.4	98.47	268.0385, 250.0246, 239.0349, 151.0028, 132.0217, 107.0131	260, 329	Biochanin A	Isoflavone	+	+	+	+	+	+	+	*C. arietinum*	Fabaceae	13, 37, 38, 43, 46, 47, 50

RT, retention time;rutinoside, rhamnopyranosyl-(1→6)-β-D-glucopyranoside; lathyroside, xylopyranosyl-(1→2)-galactopyranoside; 6''-malonylneohesperidoside, (2''-*O*-α-L-rhamnopyranosyl-6''-*O*-malonyl)-β-D-glucopyranoside

*Identification confirmed by comparison with standards; N.D., below 5 mAU or masked by compound with higher signal. Compounds in bold letter indicate new proposed structures.

Cited species from Fabaceae: *Acacia nilotica, A. nilotica; Afzelia bella , A. bella; Andira inermis, A. inermis; Arachis hypogaea, A. hypogaea; Astragalus complanatus, A. complanatus; Bauhinia variegata, B. variegata; Cassia obtusifolia, C. obtusifolia; Cicer arietinum, C. arietinum; Clitoria ternatea, C. ternatea; Crotalaria laburnifolia, C. laburnifolia; Dalbergia sericea, D. sericea; Genista ephedroides, G. ephedroides; Gleditsia caspica, G. caspica; Glycine max, G. max; Maackia amurensis, M. amurensis; Medicago truncatula, M. truncatula; Onobrychis viciifolia, O. viciifolia; Phaseolus vulgaris, P. vulgaris; Vicia faba, V. faba.* Other cited non-Fabaceae species: *Clethra barbinervis, C. barbinervis; Ginkgo biloba, G. biloba; Glehnia littoralis, G. littoralis; Licania carii, L. Cari.*

The UV data agree with [13,34, 51, 52]

[a]All detected ions were $[M-H]^-$

[b]Only the isomer corresponding to chlorogenic acid and 1-*O*-galloyl-β-D-glucopyranoside, *p*-hydroxybenzoic acid 4-*O*-β-D-glucopyranoside, primeveroside salicylic acid; protocatechuic acid hexoside, gentisic acid 5-*O*-β-D-xylopyranoside, ferulic acid-4-*O*-β-D-glucopyranoside and naringenin-7-*O*-(β-D-xylopyranosyl-(1→2))-β-D-glucopyranoside have been previously described in Fabaceae.

[c]Vanillic acid 1-*O*-[β-D-apiofuranosyl-(1 → 6)-β-D-glucopyranoside] ester, methyl salicylate β-primeveroside and Kaempferol 3-*O*-β-D-(6''-malonyl-)glucopyranoside-7-*O*-β-D-glucopyranoside have been previously identified in Apiaceae, Clethraceae and Equisetaceae, respectively.

[d]Glycitein has previously been reported in chickpea according to [37], while kakkatin, prunetin, isoprunetin, 6-hydroxyformononetin and 8-hydroxyformononetin in Fabaceae according to Reaxys database.

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Table S2. Non phenolic compounds characterized in seven Egyptian cultivars of chickpea: ‘Giza 1’ (1), ‘Giza 2’ (2), ‘Giza 3’ (3), ‘Giza 4’ (4), ‘Giza 195’ (5), ‘Giza 531’ (6) and ‘Solala 104’ (7).

	RT (min)	Experimental m/z^a $[M-H]^-$	Theoretical mass (M)	Molecular formula	Error (ppm)	Error (mDa)	Score	Main fragments	UV (nm)	Proposed compound	Subclass	1	2	3	4	5	6	7	Species	Family	Reference
1	2.67	195.0510	196.0583	$C_6H_{12}O_7$	-0.1	0.0	99.2	135.0561	N.D.	Gluconic/ galactonic acid	Organic acid	+	+	+	+	+	+	-	*C. arietinum*	Fabaceae	1, 2
2	2.98	133.0146	134.0215	$C_4H_6O_5$	-2.8	-0.4	86.6	115.0084	230, 264	Malic Acid	Organic acid	+	+	+	+	+	+	-	*C. arietinum*	Fabaceae	1, 2
3	4.31	191.0197	192.027	$C_6H_8O_7$	0.4	0.1	99.6	173.0087 , 111.0084	230, 259	Isocitric acid	Organic acid	+	+	+	+	+	+	+	*P. vulgaris*	Fabaceae	3
4	4.84	191.0206	192.027	$C_6H_8O_7$	-4.4	-0.8	96.2	173.0095 , 111.0098	238	Citric acid*	Organic acid	+	+	+	+	+	+	+	*C. arietinum*	Fabaceae	2, 4
5	4.86	167.0213	168.0283	$C_5H_4N_4O_3$	-1.7	-0.3	98.2	124.0193, 123.0136, 105.2227	284	Uric acid	Organic acid	+	+	+	+	+	+	+	*A. thaliana*	Brassicaceae	5
6	5.67	130.0876	131.0949	$C_6H_{13}NO_2$	-1.5	-0.2	98.9	112.9856	230, 270sh	Leucine/Isoleucine	Amino acid	+	+	+	+	+	+	+	*C. arietinum*	Fabaceae	4, 6, 7
7	5.71	129.0195	130.0268	$C_5H_6O_4$	-1.6	-0.2	97.9	85.0297	230, 256sh	Itaconic acid	Organic acid	+	+	+	+	+	+	+	*L. longiflorum*	Liliaceae	8
8	5.82	117.0193	118.0266	$C_4H_6O_4$	-0.1	0.0	99.7	73.0277	230, 256sh	Succinic acid	Organic acid	+	+	+	+	+	+	+	*C. arietinum*	Fabaceae	1, 2, 9, 10
9	6.23	180.0668	181.0745	$C_9H_{11}NO_3$	-1.4	-0.3	98.8	163.3854, 119.0506	224, 274	Tyrosine*	Amino acid	+	+	+	+	+	+	+	*C. arietinum*	Fabaceae	6, 7
10	6.42	243.0626	244.0699	$C_9H_{12}N_2O_6$	-1.4	-0.3	99.2	200.0570, 152.0362, 140.0350, 110.0245	261	Uridine	Nucleoside	+	+	+	+	+	+	+	*C. arietinum*	Fabaceae	4, 9, 11
11	8.27	266.0895	267.0968	$C_{10}H_{13}N_5O_4$	0.5	0.1	91.9	134.0475	258	Adenosine	Nucleoside	+	+	+	+	+	+	+	*C. arietinum*	Fabaceae	4, 11
12	8.47	282.0852	283.0917	$C_{10}H_{13}N_5O_5$	-2.0	0.6	93.3	150.042, 133.061	254	Guanosine	Nucleoside	+	+	+	+	+	+	+	*L.sativa/ S. esculentum*	Asteraceae/Solanaceae	1, 9
13	9.26	164.0718	165.0790	$C_9H_{11}NO_2$	-0.9	-0.1	99.7	147.0458, 103.0559	254	Phenylalanine*	Amino acid	+	+	+	+	+	+	+	*C. arietinum*	Fabaceae	4, 6, 7
14	10.64	309.1101	310.116486	$C_{14}H_{18}N_2O_6$	-2.7	-0.8	95.87	180.0671, 163.0405, 128.0356, 119.0507	230, 252, 270	Gamma-glutamyl-tyrosine I	Peptide	+	+	+	+	+	+	+	*G. max*	Fabaceae	12
15	10.71	218.1033	219.1107	$C_9H_{17}NO_5$	0.1	0.0	99.7	146.0818	N.D.	Pantothenic acid (Vit B5)	Organic acid	+	+	+	+	+	+	+	*C. arietinum*	Fabaceae	4, 13
16	10.77	309.1101	310.1165	$C_{14}H_{18}N_2O_6$	-2.7	-0.8	95.86	180.0656, 163.0392, 128.0350, 119.0501	230, 250,	Gamma-glutamyl-tyrosine II	Peptide	+	+	+	+	+	+	+	*G. max*	Fabaceae	12

									271												
17	11.41	380.1564	381.1635	$C_{15}H_{27}NO_{10}$	-0.1	0.0	98.5	218.1027, 146.0817	255, 293	Pantothenic acid hexoside	Organic acid	+	+	+	+	+	+	+	*S. esculentum*	Solanaceae	1
18	11.86	382.1002	383.1077	$C_{14}H_{17}N_5O_8$	0.7	0.3	98.8	266.0896, 250.546, 206.0682, 134.0473, 115.0043	256	Succinyladenosine	Nucleoside	+	+	+	+	+	+	+	*V. faba*	Fabaceae	4
19	12.74	326.1244	327.1318	$C_{15}H_{21}NO_7$	0.8	0.3	97.9	164.0718, 147.0301	260	Phenylalanine hexoside	Amino acid	+	+	+	+	+	+	+	*L.sativa/ S. esculentum*	Asteraceae/Solanaceae	1, 9
20	12.88	203.0834	204.0906	$C_{11}H_{12}N_2O_2$	-3.6	-0.7	96.2	159.0932, 142.0672, 116.0507	278	Tryptophan*	Amino acid	+	+	+	+	+	+	+	*V. faba*	Fabaceae	4
21	13.89	443.1925	444.1995	$C_{21}H_{32}O_{10}$	-0.2	-0.1	99.5	281.1399, 237.1508, 219.1339, 161.0443	260	Dihydrophaseic acid 4'-*O*-β-D-glucopyranoside	Terpenoid	+	+	+	+	+	+	+	*V. faba*	Fabaceae	4
22	14.81	175.0613	176.0685	$C_7H_{12}O_5$	-0.2	0.0	98.3	115.0394,113.0611	N.D.	Isopropylmalic acid	Organic acid	+	+	+	+	+	+	+	*L.sativa/ S. esculentum*	Asteraceae/Solanaceae	1, 9
23	15.13	293.1157	294.1216	$C_{14}H_{18}N_2O_5$	-4.5	-1.3	93.3	164.0722, 147.0497, 128.0359	258, 285	Gamma-glutamyl-phenylalanine	Peptide	+	+	+	+	+	+	+	*G. max / V. radiata*	Fabaceae	12, 14
24	16.08	431.1205	432.1268	$C_{18}H_{24}O_{12}$	-2.1	-0.9	97.58	125.0245	256	Licoagroside B [maltol 3-*O*-[6-*O*-(3-hydroxy-3-methyl-glutaroyl)]-β-D-glucopyranoside]	Maltol	+	+	+	+	+	+	+	*G. glabra*	Fabaceae	15
25	16.13	387.1668	388.1733	$C_{18}H_{28}O_9$	-2.5	-1.0	91.7	369.1579, 225.1101, 207.1026, 163.1129	N.D.	Tuberonic acid hexoside (hydroxyjasmonic acid hexose) I	Jasmonate	+	+	+	+	+	+	+	*V. faba*	Fabaceae	4
26	16.60	387.1667	388.1733	$C_{18}H_{28}O_9$	-2.0	-0.8	95.9	369.1581, 225.1114, 207.1019, 163.1152	N.D.	Tuberonic acid hexoside II	Jasmonate	+	+	+	+	+	+	+	*V. faba*	Fabaceae	4
27	17.01	519.2085	520.2156	$C_{23}H_{36}O_{13}$	-0.3	-0.1	99.0	387.1650, 225.1128, 207.1022, 163.1126	N.D.	**Tuberonic acid hexoside pentoside**	Jasmonate	+	+	+	+	+	+	+			
28	17.18	387.1667	388.1733	$C_{18}H_{28}O_9$	-1.4	-0.5	82.4	369.1551, 225.1122, 207.1031, 163.1134	N.D.	Tuberonic acid hexoside III	Jasmonate	+	+	+	+	+	+	+	*V. faba*	Fabaceae	4
29	17.66	281.1396	282.1467	$C_{15}H_{22}O_5$	-0.4	-0.1	99.9	237.1537, 219.1424, 207.1420, 189.1317, 171.1210, 153.0955, 151.0759, 139.0788	N.D.	Dihydrophaseic acid	Terpenoid	+	+	+	+	+	+	+	*V. faba*	Fabaceae	4
30	18.97	403.161	404.1682	$C_{18}H_{28}O_{10}$	-1.1	-0.4	95.7	241.1083, 225.1134, 179.0146	N.D.	Dihydroxyjasmononic hexoside	Jasmonate	+	+	+	+	+	+	+	*V. faba*	Fabaceae	4
31	22.14	245.0931	246.1004	$C_{13}H_{14}N_2O_3$	0.3	0.1	99.0	203.0833, 159.0927, 142.0664	N.D.	Acetyltryptophan	Amino acid	+	+	+	+	+	+	+	*S. esculentum*	Solanaceae	1
32	23.77	187.0985	188.1049	$C_9H_{16}O_4$	-1.5	-0.3	99.4	169.0879, 125.0976	N.D.	Azelaic acid	Organic acid	+	+	+	+	+	+	+	*P. vulgaris*	Fabaceae	9, 16

																			/ L. Sativa	/Asteraceae	
33	27.04	941.5123	942.5188	$C_{48}H_{78}O_{18}$	-0.3	-0.3	98.6	795.4499, 615.3946, 457.3681	196, 202	Soyasaponin I I	Soyasaponin	+	+	+	+	+	+	+	*C. arietinum*	Fabaceae	17-19
34	27.57	1081.5227	1082.5298	$C_{54}H_{82}O_{22}$	-0.4	-0.4	97.6	935.4680, 917.4524, 755.4041,710.4044, 579.9793	294	Lablab saponin I	Soyasaponin	+	+	+	+	+	+	+	*D. lablab*	Fabaceae	20, 21
35	27.67	1083.5393	1084.5454	$C_{54}H_{84}O_{22}$	-1.3	-1.1	95.9	1043.5481,983.5138, 895.5151, 595.2939, 571.2937, 447.2656, 279.2351	291	Soyasaponin αg I	Soyasaponin	+	+	+	+	+	+	+	*G. max*	Fabaceae	22
36	27.92	941.5123	942.5188	$C_{48}H_{78}O_{18}$	-0.7	-0.7	99.0	795.4589, 615.3942, 457.3744	196, 202	Soyasaponin I II	Soyasaponin	+	+	+	+	+	+	+	*C. arietinum*	Fabaceae	17-19
37	28.03	911.5022	912.5083	$C_{47}H_{76}O_{17}$	-1.2	-1.1	98.7	893.4905, 615.3876, 457.3690	196, 202	Soyasaponin II [astargaloside VIII]	Soyasaponin	+	+	+	+	+	+	+	*P. lobata, P. thomsonii*	Fabaceae	18
38	28.04	925.5162	926.5239	$C_{48}H_{78}O_{17}$	1.1	1.0	97.3	779.4625, 617.4048, 599.3931, 441.3698	196, 198	Kaikasaponin III[b]	Soyasaponin	+	+	+	+	+	+	+	*P. lobata, P. thomsonii*	Fabaceae	18
39	28.16	925.5161	926.5239	$C_{48}H_{78}O_{17}$	0.7	0.7	98.5	779.4499, 599.3927, 441.3687	196, 198	Kaikasaponin II[b]	Soyasaponin	+	+	+	+	+	+	+	*P. lobata, P. thomsonii*	Fabaceae	18
40	28.36	939.4966	940.5032	$C_{48}H_{76}O_{18}$	-0.8	-0.8	99.2	793.4408, 613.3761, 455.3524	196, 198	Dehydrosoyasaponin I	Soyasaponin	+	+	+	+	+	+	+	*C. arietinum*	Fabaceae	19
41	28.19	1083.5388	1084.5454	$C_{54}H_{84}O_{22}$	0.3	0.3	99.6	1043.5426, 983.5120, 921.1329, 895.5089, 595.2888, 571.2888, 447.2521, 279.2332	N.D.	Soyasaponin αg II	Soyasaponin	+	+	+	+	+	+	+	*G. max*	Fabaceae	22
42	28.27	1067.5427	1068.5505	$C_{54}H_{84}O_{21}$	1.0	1.1	97.6	1049.5325, 879.5080, 733.0341, 205.0719, 143.0358, 125.0259	296	Soyasaponin βg I	Soyasaponin	+	+	+	+	+	+	+	*C. arietinum*	Fabaceae	17, 19
43	28.64	1083.5366	1084.5454	$C_{54}H_{84}O_{22}$	1.5	1.6	97.9	897.5132, 895.4976, 595.2823, 571.2828, 447.2482, 279.2322	290	Soyasaponin αg III	Soyasaponin	+	+	+	+	+	+	+	*G. max*	Fabaceae	22
44	28.84	1067.5436	1068.5505	$C_{54}H_{84}O_{21}$	0.2	0.1	97.4	1049.5301, 879.5108, 733.4540, 205.0741, 143.0376, 125.0270	295	Soyasaponin βg II	Soyasaponin	+	+	+	+	+	+	+	*C. arietinum*	Fabaceae	17, 19

RT, retention time.

*Identification confirmed by comparison with standards; N.D., below 5 mAU or masked by compound with higher signal. Compounds in bold letter are new proposed structures.

Cited species from Fabaceae: *Cicer arietinum, C. arietinum; Dolichos lablab, D.lablab; Glycine max, G. max; Glycyrrhiza glabra, G. glabra; Phaseolus vulgaris, P. vulgaris; Pueraria lobata, P. lobata; Pueraria thomsonii,*

P.thomsonii; Vicia faba, V. faba; Vigna radiata, V. radiata. Other cited non-Fabaceae species: *Arabidopsis thaliana, A. thaliana; Lactuca sativa, L. sativa; Lilium longiflorum, L. longiflorum; Solanum esculentum, S. esculentum.*
[a]All detected ions were $[M-H]^-$
[b]The characterization is based on the elution pattern in similar conditions [18]

The UV data agree with [1, 15, 21, 23.]

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