

Table S1. Identified compounds from the gas chromatography mass-spectroscopy analysis showing the mean values of the peak area

Label	RT	Coffee I4	Coffee I5	Coffee I6	Coffee I8	Coffee I9	Coffee I10	Coffee I11	Coffee I12	Coffee I13
C1	2.304	1053765 ^c	1227054 ^c	2134968 ^a	1737572 ^{abc}	1060691 ^c	1946113 ^{ab}	1627479 ^{abc}	1998353 ^{ab}	1311814 ^{bc}
		±291991	±120896	±137599	±159278	±200418	±93434	±236631	±509691	±84050
C2 ^{NS}	3.763	327810	314824	437281	357825	247115	353378	331812	373511	216431
		±112227	±44491	±24534	±33742	±95329	±120312	±36877	±98986	±15910
C3	4.157	193841 ^{bc}	219241 ^{bc}	233863 ^a	213637 ^{ab}	151040 ^{bc}	167024 ^{ab}	135208 ^{bc}	0 ^c	0 ^c
		±64614	±73080	±15727	±71512	±50347	±14771	±45069	±0	±0
C4	4.653	2007006 ^c	1600609 ^d	2273003 ^c	2061787 ^c	2589969 ^b	2696908 ^b	3392361 ^a	3329210 ^a	3535933 ^a
		±125299	±21346	±42662	±80816	±63680	±47734	±164671	±202558	±29725
C5 ^{NS}	5.421	0	256442	256502	223321	0	186816	323193	308720	117050
		±0	±85481	±85501	±74440	±0	±62272	±147590	±77730	±4575
C6	5.583	120276 ^d	143614 ^{bcd}	162337 ^{ab}	144670 ^{bcd}	145138 ^{cd}	153928 ^{abc}	207336 ^{ab}	256717 ^a	165139 ^{ab}
		±40092	±50631	±10720	±48268	±48379	±4899	±18219	±58560	±8888
C7 ^{NS}	7.243	1785674	1633842	1460163	1546575	1538904	1339267	1602119	1639911	1644665
		±595225	±30077	±11018	±37786	±30647	±16479	±44174	±50151	±22261
C8 ^{NS}	7.540	218608	208291	295893	255649	238271	338154	274664	277236	300148
		±13837	±6918	±1175	±881	±10495	±4798	±93060	±35041	±5095
C9	7.626	3414080 ^{ab}	4151779 ^a	3250383 ^{ab}	3126573 ^{ab}	2637467 ^{bc}	3283118 ^{bcd}	1456729 ^{cde}	1397122 ^e	1257113 ^{de}
		±379364	±123706	±19170	±56987	±28521	±1101658	±41108	±465803	±17213
C10	8.344	6788562 ^a	5811678 ^{bc}	5981577 ^b	5740074 ^{bc}	6717083 ^a	5815504 ^{bc}	5817353 ^{bc}	5466434 ^{cd}	5123077 ^d
		±130376	±113125	±107428	±115401	±124089	±167451	±248483	±261034	±98864
C11	9.299	0 ^b	0 ^b	0 ^b	0 ^b	0 ^b	130133 ^{ab}	200858 ^{ab}	216329 ^a	139713 ^a
		±0	±0	±0	±0	±0	±43377.67	±67425	±83860.56	±5511.048
C12 ^{NS}	9.886	1628381	1625811	1726694	1581779	1744358	1710289	1262429	1082072	1064173
		±77709	±13507	±575729	±13246	±53675	±570096	±29829	±44467	±354756
C13	9.953	1642057 ^{ab}	1601205 ^{ab}	1486332 ^{bc}	1522647 ^{bc}	1516707 ^{bc}	1369429 ^c	1649144 ^{ab}	1627378 ^{ab}	1712270 ^a
		±108712	±41704	±57931	±63778	±21698	±39819	±66684	±63504	±16342
C14	11.043	266466 ^a	250106 ^{ab}	288032 ^a	269329 ^a	246102 ^b	248656 ^{ab}	162581 ^c	0 ^c	0 ^c
		±23716	±6060	±11329	±9663	±82452	±8520	±54194	±0	±0
C15	11.156	608613 ^c	729479 ^d	826432 ^{cd}	862998 ^c	1108060 ^a	986752 ^b	992259 ^b	1164075 ^a	1065226 ^{ab}
		±79344	±12128	±33873	±16757	±24445	±5260	±15399	±37535	±28400
C16	11.249	5855313 ^c	7096012 ^a	6761174 ^{ab}	6658752 ^{abc}	6275168 ^{bc}	6113317 ^{bc}	3287250 ^d	2906720 ^d	2615782 ^d

		±75535	±61886	±93131	±60520	±218249	±17650	±147179	±36973	±49268
C17	11.723	229712 ^{ef}	242610 ^f	325062 ^{ef}	317257 ^{ef}	559170 ^{cd}	527139 ^{de}	779232 ^{bc}	1176831 ^a	844466 ^b
		±76610	±80870	±108363	±5204	±29590	±175713	±12020	±32159	±37002
C18	12.046	10478104 ^c	9964917 ^c	12929237 ^a	11960177 ^b	13156807 ^a	13007757 ^a	10262411 ^c	9668104 ^c	9655968 ^c
		±451659	±252543	±178240	±222318	±572930	±219927	±110333	±357730	±17367
C19	12.067	1103864 ^{de}	1044390 ^e	1105476 ^{de}	1248787 ^{bc}	1176886 ^{cd}	1169914 ^{cd}	1368238 ^{ab}	1410032 ^a	1367150 ^{ab}
		±73415	±35653	±10994	±14306	±72959	±13036	±11967	±38821	±27613
C20	12.124	1309043 ^a	1254666 ^a	0 ^b	1401484 ^a	0 ^b	0 ^b	0 ^b	0 ^b	0 ^b
		±32036.17	±419422.3	±0	±478359.3	±0	±0	±0	±0	±0
C21	12.205	0 ^c	0 ^c	0 ^c	0 ^c	0 ^c	0 ^c	0 ^c	934328 ^a	862015 ^b
		±0	±0	±0	±0	±0	±0	±0	±17226.06	±15494.85
C22	12.241	1235885 ^{bcd}	1199322 ^{cde}	1352693 ^{ab}	1344330 ^{ab}	1380534 ^a	1325751 ^{abc}	1172956 ^{de}	1002786 ^f	1101308 ^{ef}
		±73574	±28636	±24840	±41317	±69217	±14448	±34195	±39424	±13751
C23	12.342	492455 ^{bc}	551638 ^c	666609 ^{ab}	639165 ^{ab}	708901 ^a	721076 ^a	568415 ^{ab}	562243 ^{bc}	496220 ^{ab}
		±57187	±183888	±7444	±13599	±25039	±3385	±17041	±9209	±2879
C24	12.978	0 ^d	97316 ^{cd}	0 ^d	0 ^d	154948 ^a	137905 ^a	115030 ^{ab}	124825 ^{ab}	109786 ^{bc}
		±0	±32439	±0	±0	±11942	±3060	±2966	±41677	±4125
C25	13.031	168261 ^{bc}	217799 ^{ab}	287265 ^a	229958 ^{ab}	181211 ^{bc}	214905 ^{bc}	143650 ^c	146111 ^c	113831 ^c
		±56149	±11106	±3698	±14045	±60421	±74919	±47883	±48704	±38042
C26	13.473	0 ^b	416784 ^a	522434 ^a	540592 ^a	712542 ^a	631768 ^a	609928 ^a	652542 ^a	572111 ^a
		±0	±3663	±8281	±6332	±240830	±14545	±203314	±16460	±19816
C27 ^{NS}	13.556	0	103754	140336	125525	153055	162593	165567	177469	137361
		±0	±34585	±46779	±41842	±4308	±54200	±4119	±59156	±45996
C28	13.800	668580 ^e	708023 ^{de}	860823 ^{bc}	841317 ^{bc}	1102637 ^a	948175 ^b	925532 ^{bc}	850016 ^{bc}	817329 ^{cd}
		±74916	±16593	±8276	±6838	±59746	±29835	±19585	±43147	±7418
C29	13.888	1003104 ^{cd}	1098025 ^{bcd}	1147563 ^d	1392439 ^{abc}	1310453 ^d	1316760 ^{cd}	1485687 ^{abc}	1919063 ^{ab}	1785775 ^a
		±98905	±24511	±382521	±21768	±436818	±438941	±8317	±43641	±23483
C30	13.916	190089 ^s	231318 ^{fg}	294787 ^{def}	255760 ^{efg}	319476 ^{cde}	357757 ^{cd}	392785 ^{bc}	628924 ^a	473549 ^b
		±18433	±17072	±6610	±12071	±17828	±18993	±13225	±76641	±4968
C31 ^{NS}	14.014	1429050	2419757	3081367	2574165	2437543	3264639	3864495	4519789	3187485
		±584802	±160188	±1027797	±68873	±334795	±163911	±1288809	±795008	±119815
C32	14.076	711526 ^f	748129 ^{ef}	941187 ^{abc}	891487 ^{bcd}	987862 ^{ab}	1057238 ^a	813647 ^{def}	858396 ^{cde}	845404 ^{cde}
		±66405	±67601	±21682	±28184	±37756	±9730	±12197	±58572	±18082
C33	14.121	0 ^d	651529 ^{cd}	0 ^d	583035 ^{cd}	1247061 ^{bcd}	1324742 ^{bcd}	2656167 ^{abc}	3401537 ^{ab}	2847172 ^a

		±0	±217940	±0	±232048	±53170	±12422	±885658	±1136186	±84739
C34	14.523	0 ^c	134537 ^{ab}	185623 ^a	168595 ^a	160138 ^{bc}	174365 ^a	180291 ^{ab}	141980 ^{bc}	152018 ^a
		±0	±3057	±7113	±3491	±53379	±14591	±60190	±47327	±3829
C35	14.964	0 ^b	108770 ^b	0 ^b	0 ^b	169956 ^a	156408 ^a	134192 ^b	0 ^b	117647 ^b
		±0	±36257	±0	±0	±18442	±3262	±44731	±0	±39216
C36	15.160	0 ^d	0 ^d	0 ^d	0 ^d	0 ^d	0 ^d	146981 ^c	214785 ^a	173947 ^b
		±0	±0	±0	±0	±0	±0	±5344	±9926	±4663
C37	15.952	0 ^c	0 ^c	867443 ^{ab}	700442 ^c	807607 ^c	936482 ^{ab}	981023 ^{ab}	1141178 ^a	712406 ^b
		±0	±0	±13565	±233481	±269202	±26059	±18901	±211130	±39099
C38	15.998	1459498 ^d	1832398 ^{cd}	2079813 ^{bc}	1909384 ^{bcd}	1851550 ^{cd}	1888357 ^{cde}	2085829 ^{bc}	2841068 ^a	2343388 ^b
		±248665	±29718	±39368	±78675	±88584	±160571	±121417	±334340	±52831
C39	16.246	0 ^c	153974 ^{ab}	135732 ^b	0 ^c	161911 ^{ab}	145174 ^b	0 ^c	134175 ^b	220520 ^a
		±0	±2996	±45265	±0	±1966	±48403	±0	±45169	±9325
C40	16.578	0 ^b	0 ^b	0 ^b	0 ^b	0 ^b	0 ^b	133399 ^a	152210 ^a	102739 ^b
		±0	±0	±0	±0	±0	±0	±6791	±50756	±34246
C41	16.695	0 ^d	103791 ^{cd}	163695 ^{bc}	124257 ^{cd}	149239 ^{ab}	211378 ^a	188224 ^{ab}	230121 ^a	223775 ^a
		±0	±34597	±55224	±41419	±8253	±18481	±4116	±27470	±3598
C42	16.746	0 ^f	124204 ^e	157150 ^{de}	174338 ^d	167661 ^{de}	186167 ^{cd}	226569 ^{bc}	272664 ^a	252841 ^{ab}
		±0	±5029	±8631	±4775	±17417	±5770	±5980	±37107	±7732
C43	17.770	188811 ^f	352948 ^{ef}	453686 ^e	472696 ^e	758849 ^d	926466 ^d	1895337 ^c	3703017 ^a	3050747 ^b
		±34532	±13245	±9556	±58444	±12275	±41109	±88263	±166000	±81227
C44	18.159	196534 ^g	284241 ^f	433956 ^e	447959 ^e	675638 ^d	742902 ^d	836121 ^c	1235111 ^a	1049600 ^b
		±29190	±5727	±18578	±16052	±5652	±33698	±17505	±53823	±16645
C45	18.381	126538 ^c	209608 ^c	186368 ^c	207068 ^c	170703 ^c	171157 ^c	211068 ^{bc}	422079 ^a	321126 ^{ab}
		±42276	±69887	±6027	±69285	±57444	±57062	±4198	±11735	±7327

^{a-g} Different letters depict the significant differences ($p < 0.05$) between samples (columns) based on the ANOVA and Least Significant Difference *post hoc* test. ^{NS} Non-significant differences.

Table S2. Factor loadings of the main two components of the principal component analysis. Abbreviations of the compounds are found in Table 3; PC1 and PC2: Principal component one and two.

Compound	PC1	PC2
C1	0.07	-0.17
C2	-0.04	-0.10
C3	-0.18	-0.09
C4	0.18	-0.01
C5	0.09	-0.06
C6	0.17	<-0.01
C7	<-0.01	0.30
C8	0.10	-0.18
C9	-0.18	-0.05
C10	-0.14	<0.01
C11	0.18	0.01
C12	-0.18	-0.14
C13	0.07	0.27
C14	-0.18	-0.11
C15	0.17	-0.12
C16	-0.18	-0.11
C17	0.20	0.01
C18	-0.09	-0.27
C19	0.18	0.04
C20	-0.14	0.15
C21	0.17	0.11
C22	-0.15	-0.19
C23	-0.04	-0.30
C24	0.12	-0.08
C25	-0.13	-0.18
C26	0.13	-0.22
C27	0.14	-0.21
C28	0.06	-0.24
C29	0.19	0.02
C30	0.20	-0.01
C31	0.18	-0.09
C32	0.03	-0.29
C33	0.19	0.04
C34	0.08	-0.24
C35	0.03	-0.11
C36	0.19	0.11
C37	0.14	-0.19
C38	0.18	-0.02
C39	0.07	-0.08
C40	0.18	0.10
C41	0.17	-0.15
C42	0.18	-0.10
C43	0.20	0.06
C44	0.20	-0.03
C45	0.18	0.06

Data in straight bold depict the main compounds that represent the principal components on the positive side of the axis, while data in bold and italics are the compounds that represent the principal components on the negative side of the axis.