

**Table S1.** Peak areas (n = 3) of selected volatiles detected by HS-SPME-GC-MS in the coffee samples. Rows that share the same letter are not significantly different by Tukey's post-hoc means comparison ( $p < 0.05$ ) (freezer storage "F"; room temperature storage "R"; and newly roasted "N").

Sample	RI <sub>calc</sub>	RI <sub>lit</sub>	"City" Roast			"Vienna" Roast								
			N	F	R	N	F	R						
1-acetoxy-2-butanone	1510.8	1521 <sup>WB</sup>	7.29E+07	ab	7.54E+07	a	7.61E+07	a	6.75E+07	c	7.04E+07	bc	6.80E+07	c
1-furfurylpyrrole	1789.5	1815 <sup>WB</sup>	3.30E+07	b	N.D.	c	N.D.	c	5.30E+07	a	N.D.	c	N.D.	c
1-methylpyrrole	1116.1	1127 <sup>WB</sup>	7.87E+06	b	9.35E+06	b	8.30E+06	b	2.02E+07	a	1.93E+07	a	2.12E+07	a
2,2-bifuran	1562.8	1564 <sup>N14</sup>	4.12E+06	b	N.D.	c	N.D.	c	5.89E+06	a	N.D.	c	N.D.	c
2,3-dimethylpyrazine	1315.2	1318 <sup>WB</sup>	4.20E+07	c	4.26E+07	c	4.43E+07	c	5.08E+07	b	5.24E+07	bc	5.91E+07	a
2,3-pentanedione	1047.4	1042 <sup>WB</sup>	6.07E+07	a	6.80E+07	a	5.14E+07	b	2.82E+07	c	3.18E+07	c	2.55E+07	c
2,5-dimethylfuran	943.9	943 <sup>WB</sup>	5.22E+06	b	6.12E+06	b	4.93E+06	b	1.23E+07	a	1.36E+07	a	1.41E+07	a
2,5-dimethylpyrazine	1292.7	1293 <sup>WB</sup>	2.65E+08	a	2.35E+08	b	2.42E+08	b	2.21E+08	c	2.02E+08	d	2.23E+08	c
2,6-diethylpyrazine	1409.0	1410 <sup>WB</sup>	1.33E+07	bc	1.28E+07	c	1.34E+07	bc	1.35E+07	bc	1.40E+07	b	1.74E+07	a
2,6-dimethylpyrazine	1299.8	1300 <sup>WB</sup>	2.77E+08	a	2.55E+08	b	2.60E+08	b	2.52E+08	b	2.38E+08	c	2.63E+08	b
2-acetylpyrrole	1930.4	1933 <sup>WB</sup>	2.64E+07	b	N.D.	c	N.D.	c	5.00E+07	a	N.D.	c	N.D.	c
2-acetylfuran	1470.3	1475 <sup>WB</sup>	2.79E+08	ab	2.61E+08	cd	2.47E+08	de	2.85E+08	a	2.64E+08	bc	2.39E+08	e
2-ethyl 3,5-dimethylpyrazine	1419.0	1415 <sup>WB</sup>	5.50E+07	b	5.07E+07	bc	5.37E+07	bc	4.94E+07	c	5.30E+07	bc	6.32E+07	a
2-ethyl 3-methylpyrazine	1375.8	1383 <sup>WB</sup>	3.68E+07	c	3.65E+07	c	3.83E+07	bc	3.71E+07	bc	3.94E+07	b	4.61E+07	a
2-ethyl 5-methylpyrazine	1363.0	1356 <sup>WB</sup>	8.80E+07	ab	8.46E+07	b	9.05E+07	a	7.33E+07	c	7.58E+07	c	8.87E+07	ab
2-ethyl 6-methylpyrazine	1358.1	1350 <sup>WB</sup>	1.44E+08	bc	1.42E+08	bc	1.48E+08	b	1.32E+08	d	1.36E+08	cd	1.59E+08	a
2-ethylpyrazine	1305.1	1306 <sup>WB</sup>	6.93E+07	ab	6.80E+07	bc	6.85E+07	bc	6.67E+07	bc	6.50E+07	c	7.25E+07	a
2-furfurylfuran	1577.8	1583 <sup>WB</sup>	4.11E+07	b	N.D.	c	N.D.	c	4.82E+07	a	N.D.	c	N.D.	c
2-furanmethanol	1632.1	1631 <sup>WB</sup>	1.93E+08	b	1.76E+08	bc	1.62E+08	c	2.34E+08	a	1.97E+08	b	1.71E+08	c
2-furfurylacetate	1514.8	1515 <sup>WB</sup>	2.25E+08	d	2.37E+08	cd	2.44E+08	c	3.62E+08	b	3.61E+08	b	3.77E+08	a
2-furfurylmethylsulfide	1456.9	1460 <sup>WB</sup>	2.02E+07	b	N.D.	c	N.D.	c	7.21E+07	a	N.D.	c	N.D.	c
2-methoxy 4-vinylphenol	>2000	2188 <sup>N14</sup>	1.02E+07	d	1.49E+07	c	1.63E+07	bc	1.39E+07	c	1.87E+07	ab	2.06E+07	a
2-methylbutanal	908.7	910 <sup>FN</sup>	2.16E+07	a	2.55E+07	a	2.05E+07	a	2.12E+07	a	2.30E+07	a	2.38E+07	a
2-propionylfuran	1543.5	1557 <sup>WB</sup>	4.75E+07	b	2.87E+07	c	1.85E+07	d	5.80E+07	a	4.71E+07	b	2.03E+07	d
benzenemethanethiol	1600.9	1615 <sup>WB</sup>	3.20E+06	b	N.D.	c	N.D.	c	1.53E+06	a	N.D.	c	N.D.	c
3-methylbutanoic acid	1639.3	1638 <sup>WB</sup>	9.08E+07	b	8.80E+07	b	1.10E+08	a	7.09E+07	d	7.84E+07	c	8.14E+07	c
3-methylbutanal	912.2	912 <sup>FN</sup>	8.48E+06	a	1.18E+07	a	8.53E+06	a	9.22E+06	a	9.63E+06	a	8.86E+06	a
3-pentanone	964.5	958 <sup>WB</sup>	4.70E+06	b	5.46E+06	b	4.75E+06	b	6.60E+06	a	7.11E+06	a	6.67E+06	a
3-propyl 2-methylpyrazine	1434.7	1438 <sup>WB</sup>	1.70E+07	b	1.81E+07	b	1.89E+07	b	2.09E+07	a	2.15E+07	a	2.27E+07	c
5-methylfurfural	1538.1	1540 <sup>WB</sup>	5.63E+08	a	3.77E+08	b	3.00E+08	b	3.12E+08	b	1.53E+08	c	1.50E+08	c
acetaldehyde	< 800	714 <sup>FN</sup>	1.13E+07	a	1.27E+07	a	5.25E+06	b	1.10E+07	a	1.10E+07	a	6.24E+06	b
acetic acid	1408.9	1410 <sup>WB</sup>	3.62E+08	a	2.72E+08	b	2.67E+08	b	2.28E+08	c	1.61E+08	d	1.46E+08	d
decanoic acid	>2000	2276 <sup>N14</sup>	4.54E+05	a	N.D.	b	N.D.	b	3.78E+05	a	N.D.	b	N.D.	b
2,3-butanedione	968.7	970 <sup>FN</sup>	6.83E+07	a	N.D.	b	N.D.	b	7.09E+07	a	N.D.	b	N.D.	b
2,2-propenylfuran	1186.5	1181 <sup>WB</sup>	8.17E+06	c	7.23E+06	c	7.58E+06	c	1.84E+07	a	1.63E+07	a	1.77E+07	b
Furaneol <sup>TM</sup>	1999.5	1997 <sup>WB</sup>	8.85E+06	a	6.46E+06	b	4.72E+06	c	4.56E+06	c	3.98E+06	c	2.14E+06	d
furfural	1433.0	1433 <sup>WB</sup>	6.66E+08	a	N.D.	c	N.D.	c	2.85E+08	b	N.D.	c	N.D.	c
furfuryl formate	1471.3	1472 <sup>WB</sup>	6.18E+07	d	6.72E+07	c	6.53E+07	c	8.34E+07	a	7.51E+07	b	7.54E+07	b
guaiaicol	1814.5	1815 <sup>WB</sup>	6.62E+06	c	6.48E+06	c	6.80E+06	c	2.52E+07	a	2.28E+07	b	2.39E+07	b
methanethiol	< 800	696 <sup>FN</sup>	3.08E+06	b	1.32E+06	d	N.D.	e	5.84E+06	a	2.24E+06	c	N.D.	e

2-methylpyrazine	1235.9	1238 <sup>WB</sup>	4.00E+08	a	3.35E+08	b	3.10E+08	c	4.07E+08	a	3.30E+08	bc	3.31E+08	b
nonanoic acid	>2000	2171 <sup>N14</sup>	8.19E+05	a	9.43E+05	a	1.20E+06	a	1.72E+06	a	7.64E+05	a	7.44E+05	a
phenol	1977.1	1978 <sup>WB</sup>	7.09E+06	c	6.69E+06	c	6.75E+06	c	2.55E+07	a	2.50E+07	a	2.26E+07	b
propanal	< 800	571 <sup>FN</sup>	1.25E+06	a	1.21E+06	a	5.09E+05	c	1.28E+06	a	9.00E+05	b	4.75E+05	c
pyridine	1151.3	1156 <sup>WB</sup>	2.22E+08	b	4.05E+07	c	5.28E+07	c	4.63E+08	a	N.D.	d	N.D.	d

WB ... NIST Chemistry WebBook Standard Reference Database Number 69 <https://webbook.nist.gov/chemistry/>

FN ... Acree, T.; Arn, H. (2004) Flavornet and human odor space. Available online <https://flavornet.org/>.

N14 ... NIST Mass-Spectral Database 14