

Table S1. Parameters Used in the Quantitation Assays

odorant	isotopically substituted internal standard	quantitation method	quantifier ions (<i>m/z</i>)		calibration line equation	R ²
			analyte	standard		
1	2-methyl(3,4- ² H ₂)butanal	SE, SAFE, GC-GC-MS	87	89	y = 1.2955x + 0.2150	0.999
2	3-methyl(3,4- ² H ₂)butanal	SE, SAFE, GC-GC-MS	87	89	y = 0.7010x + 0.0126	0.998
3	(¹³ C ₄)butane-2,3-dione	SE, SAFE, GC-GC-MS	87	91	y = 0.9937x - 0.0232	0.997
4	2-methyl-6-(² H ₃)methylpyrazine	SE, SAFE, GC-MS	109	112	y = 1.2480x + 0.0822	0.996
5	1-[(2-4- ² H ₂₋₅)-3,4-dihydro-2H-pyrol-5-yl]ethan-1-one	SE, SAFE, GC-GC-MS	112	114-117	y = 1.1638x - 0.0147	0.999
6	2,5-dimethyl-3-(² H ₃)methylpyrazine	SE, SAFE, GC-GC-MS	123	126	y = 0.8930x - 0.0630	1.000
7	2-(2,2,2- ² H ₃)ethyl-3,5-dimethylpyrazine	SE, SAFE, GC-GC-MS	137	140	y = 1.0732x + 0.0104	0.993
8	(² H ₃)acetic acid	SE, SAFE, GC-MS	61	64	y = 0.8949x - 0.0035	1.000
9	(² H ₅)benzaldehyde	SE, SAFE, GC-GC-MS	107	112	y = 0.9184x + 0.0574	0.999
10	1-(pyrazin-2-yl)(² H ₃)-ethan-1-one	SE, SAFE, GC-GC-MS	123	126	y = 1.1124x + 0.1421	0.994
11	(2E,4E)-(1,2,3,4- ² H ₄)deca-2,4-dienal	SE, SAFE, GC-GC-MS	153	157	y = 0.7300x + 0.0341	0.996
12	2-[² H ₃]methoxyphenol	SE, SAFE, GC-MS	113	128	y = 1.1558x + 0.0520	0.996
13	(2E)-1-(2-methyl-6,6-bis[² H ₃]methyl)cyclohexa-1,3-dien-1-yl)but-2-en-1-one	SE, SAFE, GC-GC-MS	191	197	y = 0.9682x - 0.1654	0.995
14	2-[² H ₃]methoxyphenol	SE, SAFE, GC-GC-MS	125	128	y = 0.9664x - 0.0137	0.998
15	3-hydroxy-2-(¹³ C)methyl(2- ¹³ C)-4H-pyran-4-one	SE, SAFE, GC-GC-MS	127	129	y = 1.2478x + 0.0213	1.000
16	4-(1,1,2,2- ² H ₂₋₄)ethyl-2-methoxyphenol	SE, SAFE, GC-GC-MS	153	155-157	y = 0.8621x + 0.0696	0.995
17	4-hydroxy-2,5-bis(¹³ C)methylfuran-3(2H)-one	SE, SAFE, GC-GC-MS	129	131	y = 1.3522x + 0.0530	1.000
18	5-pentyl(2,3- ¹³ C ₂)oxolan-2-one	SE, SAFE, GC-MS	157	159	y = 0.6491x + 0.1785	0.996
19	2(5)-ethyl-4-hydroxy-5(2)-(¹³ C)methyl(5(2)- ¹³ C)furan-3(2H)-one	SE, SAFE, GC-GC-MS	143	145	y = 0.8949x - 0.0602	0.996
20	4-(² H ₃)methyl(² H ₄)phenol	SE, SAFE, GC-MS	109	116	y = 1.0681x + 0.0042	1.000
21	3-hydroxy-4-methyl-5-(¹³ C)methyl(5- ¹³ C)furan-2(5H)-one	SE, SAFE, GC-GC-MS	129	131	y = 0.9196x - 0.0058	0.999
22	4-ethyl(² H ₄)phenol	SE, SAFE, GC-GC-MS	123	127	y = 0.9223x + 0.0935	1.000
23	4-ethenyl-2-[² H ₃]methoxyphenol	SE, SAFE, GC-GC-MS	151	154	y = 0.9047x + 0.3777	1.000
24	(² H ₅₋₈)2,6-dimethoxyphenol	SE, SAFE, GC-GC-MS	155	160-163	y = 0.9645x + 0.0045	0.999
25	2-[² H ₃]methoxy-4-[(1E)-prop-1-en-1-yl]phenol	SE, SAFE, GC-GC-MS	165	168	y = 1.1495x + 0.0018	1.000
26	(² H ₆₋₈)-3-methyl-1H-indole	SE, SAFE, GC-GC-MS	132	138-140	y = 0.9682x - 0.1654	0.997
27	4-hydroxy-3-[² H ₃]methoxybenzaldehyde	SE, SAFE, GC-MS	153	156	y = 1.0349x - 0.0178	1.000
28	[(² H ₃)methylsulfanyl](² H ₃)methane	Headspace-SPME GC-MS	63	69	y = 1.2731x - 0.2080	0.997
29	2-(² H ₃)methyl(3,3,3- ² H ₃)propanal	Headspace-SPME GC-MS	73	79	y = 0.9931x - 0.0771	0.997
30	3-[² H ₃]methylsulfanyl]propanal	SE, SAFE, GC-GC-MS	105	108	y = 0.9424x + 0.1132	0.997
31	[(² H ₃)methyldisulfanyl](² H ₃)methane	SE, SAFE, GC-GC-MS	95	101	y = 0.8554x - 0.0739	0.999
32	bis[² H ₃]methyl]trisulfane	SE, SAFE, GC-GC-MS	127	133	y = 1.0349x - 0.0186	1.000

Abbreviations: SE, solvent extraction; SAFE, solvent-assisted flavor evaporation; GC, gas chromatography; MS, mass spectrometry; SPME, solid phase microextraction.

Table S2. Odorant Concentrations in Naked Barley Tea and Hulled Barley Tea

odorant	naked barley tea				hulled barley tea			
	exp. 1	exp. 2	exp. 3	mean ± SD (CV)	exp. 1	exp. 2	exp. 3	mean ± SD (CV)
1	11.5	10.5	8.66	10.1 ± 1.3 (13%)	10.4	13.5	12.2	12.0 ± 1.5 (13%)
2	5.69	7.03	5.65	6.13 ± 0.79 (13%)	7.28	8.13	7.30	7.57 ± 0.49 (6%)
3	9.17	10.8	11.3	10.4 ± 1.1 (11%)	6.71	7.92	7.92	7.52 ± 0.70 (9%)
4	60.2	60.3	72.7	64.4 ± 7.2 (11%)	49.9	39.8	44.4	44.7 ± 5.1 (11%)
5	0.923	1.12		1.02 ± 0.14 (14%)	0.804	0.837	0.827	0.823 ± 0.017 (2%)
6	18.6	19.6	19.6	19.3 ± 0.6 (3%)	11.7	9.05	9.55	10.1 ± 1.4 (14%)
7	3.10	3.24	3.63	3.32 ± 0.27 (8%)	0.970	0.755	0.900	0.875 ± 0.11 (12%)
8	3660	3540	2500	3230 ± 640 (20%)	9170	8640	8970	8930 ± 268 (3%)
9	6.88	6.80	6.88	6.85 ± 0.05 (1%)	5.46	4.59	5.91	5.32 ± 0.67 (13%)
10	47.1	45.4	56.6	49.7 ± 6.03 (12%)	34.4	36.2	35.6	35.4 ± 0.9 (3%)
11	0.241	0.241	0.240	0.243 ± 0.004 (1%)	0.0954	0.103	0.102	0.100 ± 0.004 (4%)
12	59.1	61.7		60.4 ± 1.8 (3%)	40.1	48.4	46.6	45.1 ± 4.4 (10%)
13	0.0393	0.0316	0.0432	0.0380 ± 0.0059 (15%)	0.0457	0.0394	0.0378	0.0410 ± 0.0042 (10%)
14	59.3	55.9	58.5	57.9 ± 1.8 (3%)	156	130	122	136 ± 18 (13%)
15	956	816	851	874 ± 72 (8%)	770	684	894	783 ± 105 (13%)
16	18.1	20.0	19.6	19.2 ± 1.0 (5%)	29.6	22.5	27.1	26.4 ± 3.6 (13%)
17	272	286	250	269 ± 18 (7%)	130	121	100	117 ± 16 (13%)
18	9.37	11.4	10.5	10.4 ± 1.0 (10%)	10.2	11.7	10.7	10.9 ± 0.78 (7%)
19	5.70	5.43		5.56 ± 0.19 (4%)	12.0	14.6	13.1	13.2 ± 1.3 (10%)
20	2.09	2.19	1.98	2.09 ± 0.11 (5%)	2.98	3.25	2.30	2.84 ± 0.5 (17%)
21	4.74	4.74	4.01	4.50 ± 0.43 (3%)	3.61	2.95	2.78	3.11 ± 0.44 (14%)
22	2.98	3.48	3.68	3.38 ± 0.36 (11%)	49.6	44.8	41.1	45.1 ± 4.3 (9%)
23	47.1	43.1	42.4	44.2 ± 2.5 (6%)	99.8	105	99.0	101 ± 3.2 (3%)
24	12.6	13.4	13.5	13.2 ± 0.5 (4%)	56.1	46.8	45.9	49.6 ± 5.6 (11%)
25	0.946	0.970	1.06	0.993 ± 0.062 (6%)	25.8	21.1	18.6	21.8 ± 3.7 (17%)
26	0.670	0.674	0.787	0.710 ± 0.066 (9%)	0.376	0.332		0.354 ± 0.031 (9%)
27	55.3	61.8	53.2	56.8 ± 4.5 (8%)	211	281	266	253 ± 37 (15%)
28	1.40	1.38	1.25	1.34 ± 0.08 (6%)	0.625	0.778	0.549	0.650 ± 0.117 (18%)
29	0.989	1.25	1.25	1.16 ± 0.15 (13%)	0.204	0.305	0.229	0.246 ± 0.053 (21%)
30	2.63	2.61	3.46	2.90 ± 0.49 (17%)	2.85	2.34	2.50	2.57 ± 0.26 (10%)
31	0.476	0.411	0.352	0.413 ± 0.062 (15%)	0.541	0.659		0.600 ± 0.083 (14%)
32	0.107	0.0850	0.0998	0.0974 ± 0.011 (12%)	0.0735	0.0936	0.0996	0.0889 ± 0.0137 (15%)

Abbreviations: exp., experiment; SD, standard deviation; CV, coefficient of variation.