

Supporting information: Results of the quantitative determination of substances by NMR

Brand	Sample <sup>1</sup>	Caffeine (mg/L)	Acesulfame -K (mg/L)	Aspartame <sup>2</sup> (mg/L)	Cyclamate (mg/L)	Benzoate (mg/L)	E 150D (g/L)	HMF (mg/L)	Vanillin (mg/L)
Brand 1	Sample 1 G	98	ND	ND	ND	ND	2.14	4.9	ND
	Sample 2 G	96	ND	ND	ND	ND	2.05	3.9	ND
	Sample 3 F	95	ND	ND	ND	ND	2.68	4.9	ND
	Sample 4 F	106	ND	ND	ND	ND	1.95	5.8	ND
	Sample 5 F	105	ND	ND	ND	ND	2.05	5.8	ND
	Sample 6 F	101	ND	ND	ND	ND	2.09	5.8	ND
	Sample 7 F	103	ND	ND	ND	ND	1.86	5.8	ND
	Sample 8 F	96	ND	ND	ND	ND	2.55	4.9	ND
	Sample 9 F	105	ND	ND	ND	ND	1.91	4.9	ND
	Sample 10 G	100	ND	ND	ND	ND	2.05	3.9	ND
	Sample 11 G	100	ND	ND	ND	ND	2.05	3.9	ND
	Sample 12 G	100	ND	ND	ND	ND	2.18	3.9	ND
	Sample 13 G	99	ND	ND	ND	ND	2.00	3.9	ND
	Sample 14 G	103	ND	ND	ND	ND	3.05	3.9	ND
	Sample 15 G	104	ND	ND	ND	ND	2.27	2.9	ND
	Sample 16 G	104	ND	ND	ND	ND	2.09	4.9	ND
	Sample 17 G	99	ND	ND	ND	ND	2.14	3.9	ND
Brand 1 light	Sample 1 F	125	158	243	ND	ND	2.32	3.9	ND
	Sample 2 F	124	158	249	ND	ND	1.64	3.9	ND
	Sample 3 F	124	160	249	ND	ND	1.68	3.9	ND
	Sample 4 F	126	160	255	ND	ND	1.68	3.9	ND
	Sample 5 F	125	160	255	ND	ND	1.73	3.9	ND
	Sample 6 F	125	156	249	ND	ND	1.68	3.9	ND
	Sample 7 G	130	156	146	254	ND	2.00	3.9	ND
	Sample 8 G	125	154	143	254	ND	1.86	3.9	ND
	Sample 9 G	129	153	153	254	ND	2.23	2.9	ND
	Sample 10 G	133	153	146	260	ND	2.00	3.9	ND
	Sample 11 G	121	156	156	244	ND	2.91	1.0	ND
Brand 1 zero	Sample 1 F	98	44	430	ND	ND	1.82	3.9	ND
	Sample 2 F	96	41	423	ND	ND	1.86	2.9	ND
	Sample 3 F	98	43	419	ND	ND	1.95	2.9	ND
	Sample 4 F	96	44	416	ND	ND	1.91	2.9	ND
	Sample 5 F	96	44	427	ND	ND	1.95	2.9	ND
	Sample 6 F	94	41	434	ND	ND	1.95	2.9	ND
	Sample 7 F	99	41	Overlap	250	ND	2.09	2.9	ND
	Sample 8 G	100	164	Overlap	247	ND	3.00	ND	ND

	Sample 9 G	94	150	Overlap	247	ND	1.55	3.9	ND
	Sample 10 G	90	146	Overlap	247	ND	1.55	2.9	ND
	Sample 11 G	89	148	Overlap	255	ND	1.91	2.9	ND
	Sample 12 G	99	155	Overlap	247	ND	2.14	4.9	ND
	Sample 13 G	98	148	Overlap	Interference	ND	2.14	3.9	ND
Brand 1 without caffeine	Sample 1 F	ND	ND	ND	ND	ND	1.82	3.9	ND
Brand 1 light without caffeine	Sample 1 F	ND	170	224	ND	ND	1.82	2.9	ND
	Sample 2 F	ND	166	255	ND	ND	2.05	3.9	ND
	Sample 3 F	ND	168	231	ND	ND	1.86	2.9	ND
	Sample 4 F	ND	156	237	ND	ND	1.99	3.9	ND
	Sample 5 F	ND	156	237	ND	ND	1.99	2.9	ND
Brand 1 Vanilla	Sample 1 G	105	ND	ND	ND	ND	2.91	1.9	16.3
	Sample 2 G	103	ND	ND	ND	ND	3.14	1.0	17.3
Brand 2	Sample 1 F	108	ND	ND	ND	ND	1.27	1.9	ND
	Sample 2 G	104	ND	ND	ND	ND	1.82	1.9	ND
	Sample 3 G	113	ND	ND	ND	ND	1.45	1.9	ND
	Sample 4 G	108	ND	ND	ND	ND	1.45	1.9	ND
	Sample 5 G	111	ND	ND	ND	ND	1.41	1.9	ND
	Sample 6 G	113	ND	ND	ND	ND	1.68	2.9	ND
	Sample 7 G	113	ND	ND	ND	ND	1.23	2.9	ND
	Sample 8 G	113	ND	ND	ND	ND	1.68	1.9	ND
	Sample 9 G	111	ND	ND	ND	ND	1.86	2.9	ND
	Sample 10 G	113	ND	ND	ND	ND	1.50	1.9	ND
Brand 2 light	Sample 1 G	125	93	Overlap	ND	143	1.32	1.9	ND
	Sample 2 G	123	94	Overlap	ND	145	1.32	1.9	ND
	Sample 3 G	129	93	Overlap	ND	143	1.27	1.9	ND
	Sample 4 G	130	93	Overlap	ND	145	1.27	1.9	ND
	Sample 5 G	126	98	Overlap	ND	151	1.32	1.9	ND
	Sample 6 G	126	96	Overlap	ND	149	1.14	1.9	ND
	Sample 7 G	131	93	Overlap	ND	148	1.27	1.9	ND
	Sample 8 G	139	96	Overlap	ND	149	1.32	1.9	ND
Brand 2 zero	Sample 1 F	130	41	601	ND	ND	2.23	1.9	ND
Brand 3 discount	Sample 1 F	116	ND	ND	ND	ND	2.36	1.9	ND
	Sample 2 F	114	ND	ND	ND	ND	1.82	1.9	ND
	Sample 3 F	119	ND	ND	ND	ND	2.32	1.9	ND
	Sample 4 F	124	ND	ND	ND	ND	2.14	1.9	ND
	Sample 5 F	136	ND	ND	ND	ND	1.95	1.9	ND

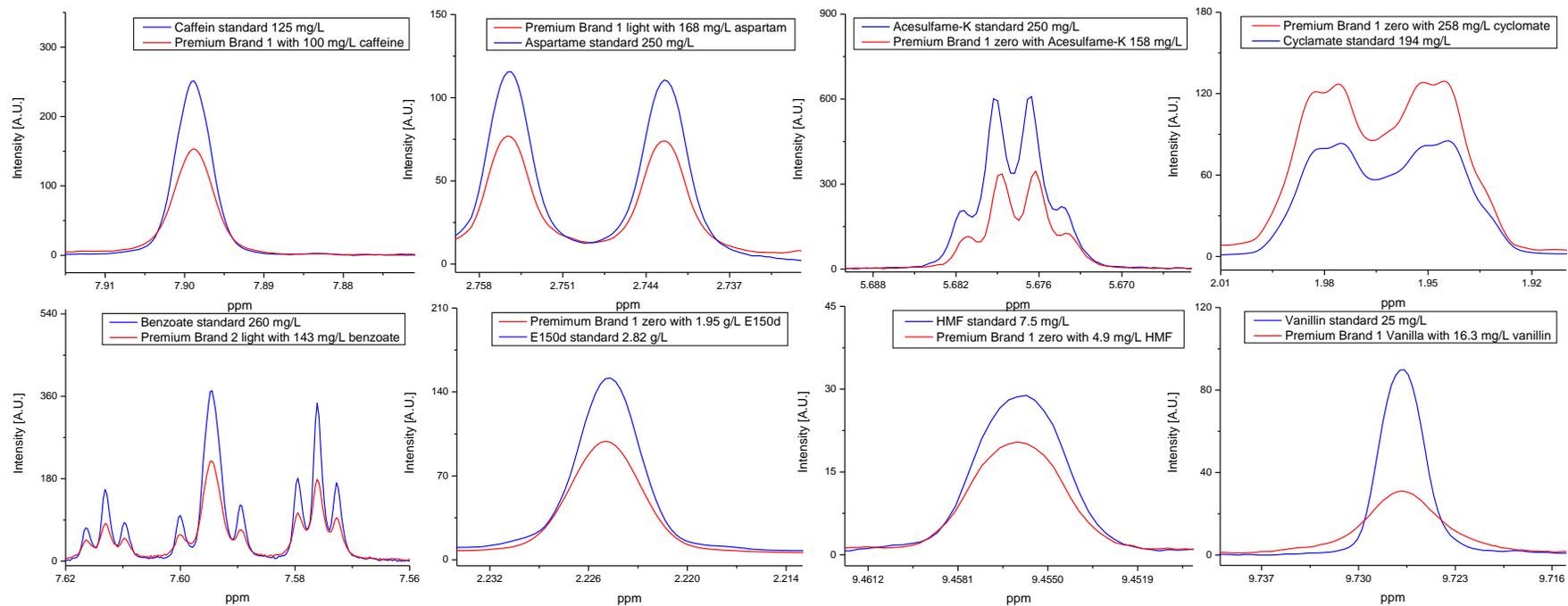
	Sample 6 F	115	ND	ND	ND	ND	2.59	1.9	ND
	Sample 7 F	115	ND	ND	ND	ND	2.64	1.9	ND
Brand 4 discount	Sample 1 G	69	ND	ND	ND	ND	2.50	1.9	ND
	Sample 2 G	71	ND	ND	ND	ND	2.18	1.0	ND
	Sample 3 G	71	ND	ND	ND	ND	2.18	1.9	ND
	Sample 4 G	73	ND	ND	ND	ND	2.23	1.0	ND
	Sample 5 G	74	ND	ND	ND	ND	2.27	1.0	ND
Brand 4 discount zero	Sample 1 G	63	104	168	278	ND	1.55	2.9	ND
	Sample 2 G	61	88	137	230	ND	1.55	1.0	ND
	Sample 3 G	63	96	115	225	ND	1.45	1.0	ND
	Sample 4 G	61	89	134	228	ND	1.50	1.0	ND
	Sample 5 G	65	91	137	231	ND	1.59	1.0	ND
Brand 5 discount	Sample 1 F	86	ND	ND	ND	ND	1.27	4.9	ND
	Sample 2 F	86	ND	ND	ND	ND	1.32	3.9	ND
	Sample 3 F	84	ND	ND	ND	ND	1.50	4.9	ND
	Sample 4 F	91	ND	ND	ND	ND	1.18	5.8	ND
	Sample 5 F	88	ND	ND	ND	ND	1.23	4.9	ND
	Sample 6 F	86	ND	ND	ND	ND	1.45	3.9	ND
Brand 5 discount zero	Sample 1 F	81	109	388	ND	117	1.41	3.9	ND
	Sample 2 F	78	108	373	ND	115	1.41	3.9	ND
	Sample 3 F	81	105	386	ND	116	1.41	3.9	ND
	Sample 4 F	80	115	349	ND	120	1.27	3.9	ND
	Sample 5 F	65	106	330	ND	116	1.18	3.9	ND
	Sample 6 F	80	108	375	ND	116	1.41	3.9	ND
Brand 6 discount	Sample 1 G	104	ND	ND	ND	ND	4.05	ND	ND
	Sample 2 G	98	ND	ND	ND	ND	3.86	ND	ND
	Sample 3 G	101	ND	ND	ND	ND	3.95	ND	ND
	Sample 4 G	100	ND	ND	ND	ND	3.50	ND	ND
	Sample 5 G	96	ND	ND	ND	ND	3.95	ND	ND
	Sample 6 G	105	ND	ND	ND	ND	4.14	ND	ND
	Sample 7 G	95	ND	ND	ND	ND	2.14	1.9	ND
	Sample 8 G	94	ND	ND	ND	ND	3.68	ND	ND
Brand 6 discount light	Sample 1 G	89	150	Overlap	264	ND	2.73	1.0	ND
	Sample 2 G	88	139	Overlap	251	ND	2.73	ND	ND
	Sample 3 G	91	156	Overlap	249	ND	2.64	ND	ND
	Sample 4 G	86	144	Overlap	260	ND	2.73	ND	ND
	Sample 5 G	81	135	Overlap	247	ND	2.59	1.9	ND
Brand 6	Sample 1 G	95	154	Overlap	276	ND	1.50	1.9	ND

discount zero	Sample 2 G	106	158	Overlap	271	ND	1.82	1.0	ND
	Sample 3 G	103	160	Overlap	265	ND	2.64	ND	ND
	Sample 4 G	104	158	Overlap	266	ND	1.91	1.0	ND
	Sample 5 G	104	154	Overlap	264	ND	1.91	1.0	ND
Brand 6 discount strong	Sample 1 G	235	ND	ND	ND	ND	2.59	3.9	ND
Brand 7 discount	Sample 1 G	96	ND	ND	ND	ND	4.09	ND	ND
	Sample 2 G	93	ND	ND	ND	ND	4.23	ND	ND
	Sample 3 G	91	ND	ND	ND	ND	4.14	ND	ND
	Sample 4 G	95	ND	ND	ND	ND	4.23	ND	ND
	Sample 5 G	100	ND	ND	ND	ND	4.14	ND	ND
Brand 7 discount light	Sample 1 G	84	130	Overlap	222	ND	3.27	ND	ND
	Sample 2 G	83	139	Overlap	244	ND	3.32	1.0	ND
	Sample 3 G	80	139	Overlap	246	ND	3.05	1.0	ND
	Sample 4 G	81	133	Overlap	231	ND	3.09	1.0	ND
	Sample 5 G	81	143	Overlap	216	ND	2.91	ND	ND
Brand 8 strong	Sample 1 G	243	ND	ND	ND	ND	2.95	7.8	ND
Brand 9 strong	Sample 1 G	252	ND	ND	ND	ND	1.73	2.9	ND

<sup>1</sup> G and F means that the samples were produced in Germany and France, respectively

<sup>2</sup> For the brand 1 light, brand 1 light without caffeine and brand 4 discount zero (containing small amount of citric acid), the doublet between 2.73 and 2.76 ppm was integrated while for the brand 1 zero, brand 2 zero and brand 5 discount zero, the multiplet between 3.03 and 3.11 ppm was integrated

# 1 Supporting information: NMR resonances of selected compounds in standard solutions and cola samples



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