SUPPORTING INFORMATION

Sample list names:

Cachaça samples: Cachaça 21 (São Paulo); Caninha da Roça (São Paulo); Catedral (São Paulo); Jequity (São Paulo); Pitú (Pernambuco); Santo Antônio (Rio Grande do Sul); Velho Barreiro (São Paulo); Verita Silver (Rio de Janeiro); Ypioca Prata (Ceará); Catedral (São Paulo); Colonial (Ceará) (Ceará); Guaramiranga (Pernambuco); Pitú Gold (Pernambuco); Tiquara (São Paulo); Velho Barreiro Gold (São Paulo); Veritas Gold (Rio de Janeiro); Vila Velha (São Paulo);Ypioca Ouro(Ceará).

Rum samples: Anivesario Pampero (Venezuela); Appleton Estate (Jamaica); Bacardi Carta Blanca (Brazil); Bacardi Carta de Oro (Brazil); Bacardi Premium Black (Brazil); Bacardi 1873 Solera (Mexico); Captain Morgan "White rum" (Canada); Cartain Morgan "Dark rum" (Canada); El Dorado "Golden rum" (Guyana); Havana Club Añejo 7 años (Cuba); Havana Club Añejo Reserve (Cuba); Havana Club Silver Dry (Cuba); Montila Carta Branca (Brazil); Montila Carta Ouro (Brazil); Myers's "Original Dark" (Jamaica-USA); Negrita Bardinet "Dry and Light" (France); Negrita Bardinet "Bardinet S. A. Bordeaux" (France); Negrita Bardinet Old Reserve (France); Selecto (Venezuela); Soccaron (France); XK Solera (Mexico).

Table 1. Concentration of acetaldehyde. ethyl acetate and alcohols in cachaça (C) and rum (R) samples (mg L^{-1}).

Sample	acetaldehyde	ethyl acetate	methanol	propanol	isobutanol	butanol	isopentanol
C01	36.9	64.9	10.7	136	181	6.60	571
C02	43.9	69.9	11.8	172	220	6.43	572
C03	40.5	28.8	25.7	309	11.2	8.76	559
C04	56.9	90.5	3.48	247	222	7.96	786
C05	28.7	32.4	28.5	123	133	5.76	584
C06	36.5	442	22.8	352	133	5.69	485
C07	74.3	78.1	21.7	198	205	7.52	654
C08	43.2	187	25.7	137	250	6.67	604
C09	107	120	17.9	137	195	6.43	549
C10	60.5	83.3	10.1	319	176	7.83	596
C11	43.4	71.6	17.2	138	a	6.33	774
C12	37.6	75.7	16.3	124	221	6.29	621
C13	17.6	15.5	28.7	159	165	6.96	669
C14	62.5	181	26.4	175	277	a	938
C15	53.4	66.4	22.6	184	187	6.69	669
C16	38.2	163	34.4	177	262	6.03	588
C17	33.9	45.5	8.28	126	169	7.07	524
C18	114	116	18.7	129	194	5.83	505

R01	96.9	428	68.0	30.4	12.8	a	36.6
R02	36.7	107	19.6	104	83.4	5.91	156
R03	58.3	54.2	9.55	47.1	40.9	5.00	120
R04	35.1	60.8	10.7	50.1	37.3	5.49	122
R05	60.1	148	18.8	115	111	7.43	347
R06	60.8	91.7	9.74	181	73.1	9.42	287
R07	25.3	12.6	2.92	15.3	21.7	a	6.86
R08	31.9	36.9	30.2	74.9	67.1	a	112
R09	83.2	64.1	15.9	35.4	9.79	a	1.35
R10	56.9	129	21.9	69.9	106	5.00	293
R11	44.9	65.1	20.4	74.0	104	5.06	259
R12	16.2	11.6	11.4	24.2	20.9	a	45.7
R13	18.6	28.2	a	17.4	27.9	4.37	73.4
R14	18.2	24.2	11.1	17.7	24.2	a	65.5
R15	40.4	183	17.9	40.4	212	128.3	207
R16	20.0	16.4	13.5	28.8	11.3	a	17.2
R17	40.8	109	37.7	274	149	8.93	295
R18	44.3	85.5	23.9	77.1	79.9	5.09	247
R19	49.0	81.1	19.8	18.8	11.8	8.44	19.2
R20	28.4	13.7	3.68	46.9	13.0	a	3.84
R21	23.3	24.3	11.1	a	a	a	a

a = not detected <0.05 mg L^{-1}

Table 2. Concentration of metals in cachaça (C) and rum (R) samples (mg L^{-1}).

Sample	Na	Ca	Mg	Cr	Mn	Fe	Co	Ni	Cu	Zn	Pb	Cd
C01	9.81	6.37	0.013	b	0.80	0.051	b	b	3.3	0.06	b	0.014
C02	33.8	6.06	0.032	b	1.2	0.10	b	b	3.1	0.04	b	0.021
C03	c	4.72	0.026	b	1.3	0.061	b	b	0.021	0.59	b	0.018
C04	14.5	1.92	0.002	b	1.4	b	b	0.0060	0.036	b	b	b
C05	10.6	0.30	0.004	b	0.035	0.061	b	b	0.067	0.03	b	0.023
C06	3.69	2.14	0.004	b	0.38	0.087	b	b	4.0	0.16	0.054	0.017
C07	27.2	6.74	0.028	b	0.65	0.075	b	0.017	2.6	0.07	b	0.008
C08	7.47	2.75	0.052	b	0.38	0.77	b	0.015	2.8	0.12	b	0.013
C09	107	1.87	0.048	b	1.9	0.078	b	b	1.4	0.04	b	0.014
C10	0.33	3.20	0.043	b	0.79	0.053	b	b	0.24	0.51	b	0.019
C11	19.2	3.61	0.034	b	2.7	1.2	b	b	5.2	0.17	b	0.009
C12	18.6	3.10	0.028	b	2.4	0.95	b	b	4.9	0.15	b	0.008
C13	27.9	2.93	0.016	b	0.24	0.42	b	b	0.68	0.08	b	0.018
C14	c	1.88	0.072	b	0.54	b	b	b	1.4	0.03	b	b
C15	36.2	2.87	0.053	b	0.48	0.43	b	b	4.1	0.08	b	0.014
C16	7.47	1.62	0.023	b	0.48	0.10	b	b	0.59	0.19	0.0060	0.021
C17	14.4	10.7	0.21	b	1.6	0.07	b	b	0.36	0.15	b	0.023
C18	11.5	1.37	0.023	b	0.60	0.19	b	b	1.5	0.04	0.016	0.023

R01	14.5	0.16	0.0040	b	0.072	0.54	b	0.0060	0.050	b	b	b
R02	5.87	4.94	0.083	b	0.67	0.010	b	0.0090	c	0.030	b	b
R03	0.0650	0.49	0.0010	b	0.020	0.020	b	b	0.015	0.060	b	0.023
R04	0.388	0.62	0.0020	b	0.018	0.070	b	b	0.030	0.041	b	b
R05	2.44	0.49	0.0020	b	0.035	0.13	b	b	0.097	0.068	b	0.017
R06	0.500	0.14	0.0010	b	B	0.030	b	0.0070	c	0.03	b	b
R07	2.13	2.06	0.0050	b	0.44	0.010	b	b	c	0.010	b	b
R08	30.9	1.20	0.0080	b	0.23	0.05	b	b	0.40	0.11	0.03	b
R09	12.8	3.56	0.069	b	1.6	b	b	0.0080	0.066	0.09	b	b
R10	30.2	1.13	0.0050	b	0.054	1.2	b	b	0.15	0.12	b	0.026
R11	35.2	0.59	0.0040	b	0.033	2.6	b	b	0.30	0.12	b	0.024
R12	2.36	1.10	0.0050	b	0.069	0.040	b	b	0.032	0.06	b	0.023
R13	3.29	1.12	0.026	b	0.12	0.080	b	b	0.12	0.08	b	0.019
R14	5.99	1.48	0.012	b	0.21	0.23	b	b	0.17	0.15	b	0.011
R15	3.79	0.35	0.0040	b	0.027	0.030	b	b	0.075	b	b	b
R16	5.96	1.49	0.019	b	0.21	0.23	b	b	0.17	0.15	b	0.011
R17	105	0.78	0.0010	0.008	0.11	b	b	0.0070	0.22	b	b	b
R18	10.1	0.88	0.0020	b	0.10	0.010	b	b	0.015	0.037	b	0.018
R19	25.4	2.71	0.055	b	0.47	0.090	b	0.0080	c	0.006	b	b
R20	c	0.54	0.0020	b	0.11	b	b	b	c	b	b	b
R21	8.27	1.08	0.0050	b	0.10	0.11	b	b	0.24	0.093	b	b

b = concentração < 0.005 mg L^{-1}

c = concentração <0.05 mg L^{-1}

Table 3. Concentration of organic acids in cachaça (C) and rum (R) samples (mg L^{-1}).

Sample	octanoic acid	decanoic acid	dodecanoic acid
C01	0.066	0.19	0.07
C02	0.065	0.16	0.046
C03	0.045	0.13	0.069
C04	0.071	0.19	0.053
C05	0.058	0.14	0.04
C06	0.057	0.109	0.048
C07	0.065	0.15	0.049
C08	0.094	0.16	0.056
C09	0.039	0.13	0.055
C10	0.041	0.072	0.035
C11	0.057	0.11	0.047
C12	0.066	0.17	0.051
C13	0.054	0.13	0.049
C14	0.29	11.4	0.29
C15	0.13	0.55	0.22
C16	d	d	d
C17	0.11	0.067	0.035
C18	0.12	0.048	0.031

R01	0.033	0.036	0.03
R02	0.033	0.036	0.032
R03	0.038	0.045	d
R04	0.037	0.038	d
R05	0.03	0.03	d
R06	0.031	0.035	d
R07	0.033	0.04	0.031
R08	d	0.036	0.04
R09	0.033	0.04	0.033
R10	0.046	0.077	0.048
R11	0.04	0.046	0.042
R12	0.04	0.071	0.036
R13	0.037	0.061	0.048
R14	d	0.049	d
R15	0.037	0.062	0.039
R16	d	d	d
R17	0.041	0.15	0.13
R18	0.10	0.054	0.032
R19	0.14	0.24	0.11
R20	0.042	0.07	0.033
R21	0.073	0.15	0.034

d = concentração < 0.001 mg L^{-1}

Table 4. Concentration of polyphenols in cachaça (C) and rum (R) samples (mg L^{-1}).

Sample	protocatechuic acid	gallic acid	epicatechin	vanillic acid	syringic acid	syringaldehyde
C01	e	0.55	e	e	0.18	e
C02	e	0.57	e	e	e	0.30
C03	e	0.18	e	e	0.10	e
C04	e	0.17	e	e	0.12	e
C05	e	0.41	e	e	e	e
C06	e	0.66	e	e	0.10	e
C07	e	0.62	e	e	0.41	e
C08	e	0.84	e	e	0.29	e
C09	e	1.1	e	0.64	1.3	1.1
C10	e	0.72	e	0.50	0.44	0.78
C11	e	0.88	0.18	0.72	0.64	1.4
C12	e	1.3	0.20	0.80	0.34	1.2
C13	e	1.1	0.29	0.50	1.2	1.6
C14	e	1.1	0.16	0.60	1.6	1.2
C15	e	1.1	e	0.49	0.82	0.92
C16	e	1.6	e	1.2	1.0	1.2
C17	e	0.55	e	0.39	0.62	0.87

C18	e	1.1	0.21	0.49	1.6	2.1
R01	2.1	6.3	0.49	0.62	1.3	2.5
R02	2.2	5.3	0.18	3.8	6.0	6.5
R03	0.19	1.4	e	1.2	1.2	0.19
R04	0.18	0.33	e	0.16	0.20	0.55
R05	0.30	1.8	0.18	0.62	1.5	2.0
R06	1.9	1.1	0.26	2.7	3.1	4.7
R07	0.17	2.5	e	0.84	1.5	0.35
R08	1.9	3.1	0.27	0.90	1.9	2.4
R09	0.16	1.4	e	0.10	0.10	0.67
R10	2.7	6.1	0.38	4.0	4.8	6.8
R11	1.1	4.2	e	2.5	3.6	2.9
R12	0.17	1.3	e	e	0.12	e
R13	0.20	0.62	e	0.10	0.24	0.11
R14	0.14	0.49	e	0.42	0.62	1.1
R15	1.4	1.5	0.35	1.1	e	1.6
R16	0.19	2.2	e	1.6	1.8	1.1
R17	1.4	1.7	0.30	4.6	5.5	5.9
R18	1.9	6.5	0.44	3.2	3.9	7.6
R19	1.9	5.9	0.52	2.2	3.4	4.4
R20	0.10	0.58	e	e	1.1	e

R21	1.2	2.6	e	0.69	1.4	2.3

e = not detected <0.08 µg L^{-1}

Table 5. Concentration of polyphenols in cachaça (C) and rum (R) samples (mg L^{-1}).

Sample	vanillin	p-cumaric acid	coniferylaldehyde	synapaldehyde	ellagic acid
C01	e	e	e	e	e
C02	e	e	e	e	e
C03	e	e	e	e	e
C04	e	e	e	e	e
C05	e	e	0.10	e	e
C06	e	e	e	e	e
C07	e	e	e	e	e
C08	e	e	0.10	e	e
C09	0.90	e	0.11	e	e
C10	1.3	e	e	e	e
C11	1.4	e	e	e	e
C12	1.6	0.14	e	e	e
C13	1.5	e	0.25	1.2	0.40
C14	1.9	0.18	e	0.51	0.87
C15	1.4	e	0.18	e	0.11
C16	1.3	e	e	e	e
C17	0.99	e	0.12	0.87	0.19
C18	1.0	e	e	e	e

R01	4.6	0.90	0.26	1.3	1.7
R02	8.6	1.0	0.18	0.79	1.4
R03	0.62	e	e	e	e
R04	0.62	0.41	e	1.1	0.22
R05	3.9	0.55	e	1.9	0.62
R06	7.2	1.6	e	1.8	1.6
R07	e	e	0.28	e	e
R08	4.9	0.55	0.15	1.4	2.1
R09	0.30	e	e	e	0.25
R10	7.9	1.0	0.10	2.1	0.41
R11	3.2	0.41	e	0.62	0.52
R12	e.	e	e	e	e
R13	0.14	e	e	e	e
R14	0.86	e	e	1.2	0.62
R15	1.7	1.3	0.10	2.6	1.9
R16	e	e	0.14	e	e
R17	5.1	0.86	0.28	1.5	1.3
R18	6.4	1.5	0.16	1.6	1.2
R19	7.7	1.3	e	1.8	1.3
R20	e.	e	0.35	e	e
R21	3.3	e	e	0.65	1.2

e = not detected <0.08 µg L^{-1}

Note: - Protocatechuic. and kaempferol do not present in either of cachaça sample analyzed.

- Coniferyl alchool was found only in sample: C08 (0.12 mg L^{-1})

- p-cumaric acid was found only in sample: C13 (0.14 mg L^{-1}).

- synapaldehyde was found in two samples: C15 (1.2 mg L^{-1}) and C19 (0.87 mg L^{-1}).

- Kaempferol do not present in either of rum samples analyzed.

- Quercetin was found only in sample: R16 (0.10 mg L^{-1}).

Coniferyl alchool was found only in sample: R09 (0.18 mg L^{-1}).