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Supplementary Information

Correlation between Chemical Composition and Sensory Properties of Brazilian Sugarcane Spirits (*Cachaças*)

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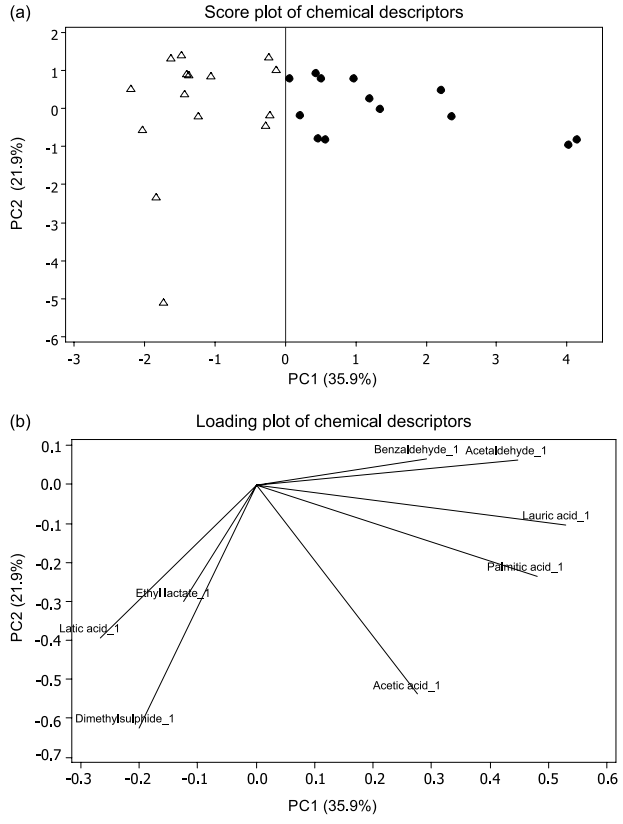

Figure S1. PCA of the chemical data, (a) score plot and (b) loading plot.

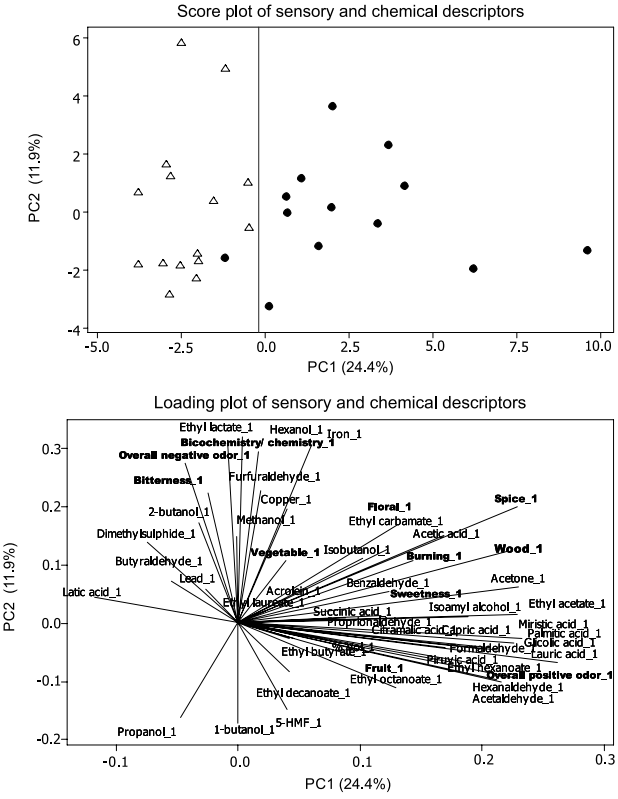

Figure S2. PCA of the sensory and chemical data, (a) score plot and (b) loading plot.

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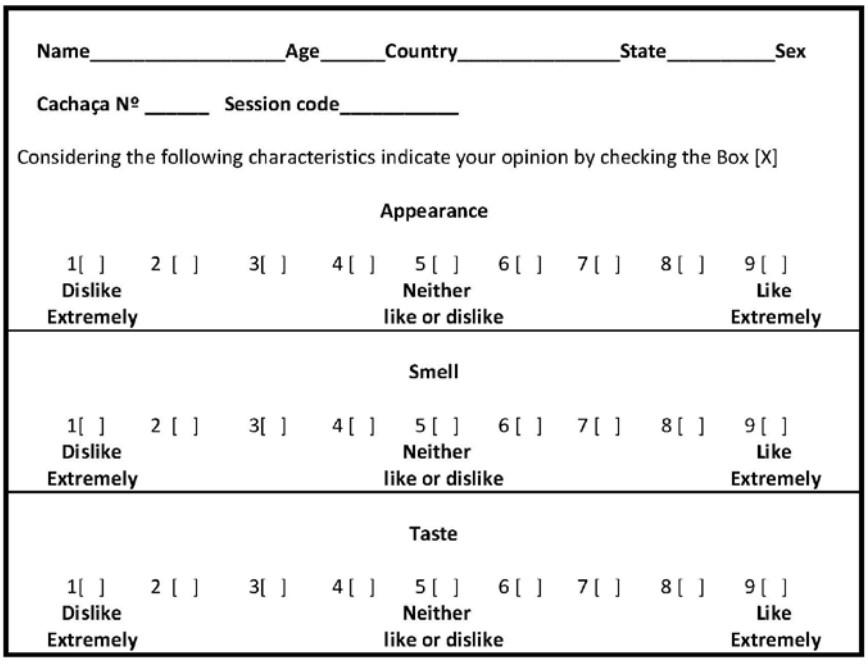

Figure S3. Form used in the consumer hedonic test of *cachaça*.

Table S1 Aging times and nature of the aging material for the *cachaças*

Cachaça sample	Aging time	Recipient
D3	8 months	Stainless steel
D4	6 months	Freijó (*Cordia goeldiana*)
D5	8 months	Amendoim (*Pterogyne nitens*)
D6	2 months	Amendoim (*Pterogyne nitens*)
D7	6 months	Oak (*Quercus*)
D8	3 years	Stainless steel
D9	6 months	Oak (*Quercus*)
D11	3 months	Jequitibá (*Cariniana estrellensis*)
D12	3 months	Jequitibá (*Cariniana estrellensis*)
E1	1 year	Oliveira (*Olea europaea* L.)
E3	2 years	Oak (*Quercus*)
E4	4years	Oak (*Quercus*)
E6	1 year and 6 months	Oak (*Quercus*)
E7	1 year	Jequitibá (*Cariniana estrellensis*), Grapia (*Apuleia Leiocarpa*)
E8	1 year	Grapia (*Apuleia Leiocarpa*)
E10	4 years	Oak (*Quercus*)
E11	2 years	Oak (*Quercus*)
E13	10 years	Oak (*Quercus*)
E14	2 years	Oak (*Quercus*)
E15	4 years	Oak (*Quercus*)
E18	2 years	Oak (*Quercus*)
E21	2 years	Oak (*Quercus*)
E22	3 years	Oak (*Quercus*)
E23	4 years	Oak (*Quercus*)
E24	2 years	Louro canela (*Lauraceae*)
E28	1 year and 6 months	Oak (*Quercus*)
E29	1 year and 6 months	Oak (*Quercus*)
E31	2 year	Oak (*Quercus*)

Table S2. Descriptive sensory vocabulary for *cachaças*

Aroma	Appearance	Taste
Floral	intensity of the yellow color	burnt
Fruity	transparency	sweetness
Vegetable		bitterness
Spicy		
Biochemistry/Chemistry (fermented, plastic, fusel oil, sulfide, solvent)		
Woody		
Overall positive odor		
Overall negative odor		

Table S3. Median and average concentrations for organic compounds according to the HI values of the *cachaças*

Sample	Average (HI < 6)	Average (HI > 6)	Median (HI < 6)	Median (HI > 6)
Hedonic index	5.38	6.3	5.3	6.3
% vol.	40.3	40.2	41	40.3
Methanol / (mg L^{-1})	31	38	21	29
Propanol / (mg L^{-1})	179	188	157	163
Isobutanol / (mg L^{-1})	196	199	193	204
Isoamyl alcohol / (mg L^{-1})	627	810	642	669
1-Butanol / (mg L^{-1})	3.48	3.3	4.26	4.19
2-Butanol / (mg L^{-1})	25.3	2.9	< LOD	< LOD
Hexanol / (mg L^{-1})	5.6	5.5	5.5	3.7
Acetaldehyde / (mg L^{-1})	127	232	123	212
Benzaldehyde / (mg L^{-1})	3.3	5.6	2.1	5.55
Butyraldehyde / (mg L^{-1})	2.1	0.5	0.35	0.41
Formaldehyde / (mg L^{-1})	3.79	9.7	2.74	9.3
Hexanaldehyde / (mg L^{-1})	0.07	0.3	< LOD	0.23
5-HMF / (mg L^{-1})	1.49	4.0	1.01	2.43
Proprionaldehyde / (mg L^{-1})	0.15	0.3	0.06	0.16
Acetone / (mg L^{-1})	< LOD	2.5	< LOD	< LOD
Ethyl acetate / (mg L^{-1})	228	526	164	479
Ethyl butyrate / (mg L^{-1})	0.11	8.8	< LOD	0.52
Ethyl hexanoate / (mg L^{-1})	0.57	1.0	0.62	0.93
Ethyl lactate / (mg L^{-1})	45.0	41.8	35.7	30
Dimethylsulfide / (mg L^{-1})	1.69	0.0	0.42	0.04
Ethyl carbamate / (mg L^{-1})	43	66	46	60
Copper / (mg L^{-1})	2.1	1.9	1.2	1.7
Iron / (mg L^{-1})	0.4	0.6	< LOD	0.3
Lead / (mg L^{-1})	0.05	< LOD	0.03	0.02
Acetic acid / (mg L^{-1})	277	484	129	417
Latic acid / (mg L^{-1})	173	29	65	29
Glicolic acid / (mg L^{-1})	0.07	1.0	< LOD	0.5
Piruvic acid / (mg L^{-1})	0.07	0.4	< LOD	< LOD
Succinic acid / (mg L^{-1})	0.1	0.2	< LOD	0.14
Citramalic acid / (mg L^{-1})	< LOD	0.2	< LOD	0.11
Capric acid / (mg L^{-1})	0.3	1.1	0.13	1.06
Lauric acid / (mg L^{-1})	0.19	1.1	0.15	0.93
Miristic acid / (mg L^{-1})	0.18	1.4	0.11	0.71
Palmitic acid / (mg L^{-1})	0.30	0.7	0.23	0.52

LOD: limit of detection