

Supplementary Table S1. Yeasts present in *Agave* distilled beverages and the most prominent volatile and non-volatile compounds.

Yeasts	Volatile and non-volatile compounds	Distilled beverage	<i>Agave species</i>	(Bibliographic reference)
<i>Candida spp.</i> <i>Candida magnolia</i> <i>Hanseniaspora guilliermondii</i> <i>Hanseniaspora uvarum</i> <i>Hanseniaspora vineae</i> <i>Kluyveromyces marxianus</i> <i>Pichia membranifaciens</i> <i>Torulaspora delbrueckii</i> <i>Saccharomyces cerevisiae</i>	acetals (24 different) organic acids (11 different) alcohols (22 different) aldehydes (49 different) furans (14 different) ketones (12 different) phenols (8 different) pyrazines (5 different) sulfur compounds (3 different) terpenes (25 different) miscellaneous compounds (5 different)	Tequila. Jalisco.	<i>A. tequilana.</i>	Lachance, 1995; Benn & Peppard, 1996; López, 1999
<i>Clavispora lusitaniae</i> <i>Kluyveromyces marxianus</i> <i>Pichia fermentans</i> <i>Saccharomyces cerevisiae</i>	ethyl acetate methanol ethanol 2-butanol n-propanol 2-methyl-propanol 2,3-methyl-1-butanol ethyl-2-hydroxypropionate acetic acid high alcohol	Mezcal. S.L.P.	<i>A. salmiana.</i>	De León-Rodríguez <i>et al.</i> 2006
<i>Candida spp.</i> <i>Hanseniaspora spp.</i> <i>Saccharomyces cerevisiae</i>	ethanol organic acids fusel oil esters terpenes aldehydes	Mezcal. Oaxaca.	<i>A. angustifolia</i>	(Andrade Meneses & Ruíz Terán, 2004)
<i>Candida parapsilosis</i> <i>Clavispora lusitaniae</i> <i>Debaryomyces hansenii</i> <i>Kluyveromyces marxianus</i> <i>Pichia caribbica</i> <i>Pichia guilliermondii</i> <i>Torulaspora delbrueckii</i>	ethanol	Mezcal. Yucatán.	<i>A. fourcroydes.</i>	Lappe <i>et al.</i> 2004

<i>Saccharomyces cerevisiae</i>				
<i>Clavispora lusitaniae</i> <i>Kluyveromyces marxianus</i> <i>Saccharomyces cerevisiae</i>	ethanol, organic acids, fusel oil esters aldehydes terpenes (31 different types) 2-fenil etanol acetaldehyde ethyl-acetate 2-methyl-propanol amil alcoholes 1-propanol	Raicilla. Jalisco.	A. <i>angustifolia</i> , A. <i>inaequidens</i> , A. <i>maximiliana</i>	Arrizon <i>et al.</i> 2007
<i>Saccharomyces cerevisiae</i> <i>Zygosaccharomyces rouxii</i> <i>Zygosaccharomyces bisporus</i> <i>Torulaspora delbrueckii</i> <i>Pichia membranifaciens</i>	ethyl lactate ethyl acetate methanol acetaldehyde isobutanol propanol amyl alcohols ethanol higher alcohols esters	Mezcal. Oaxaca.	A. <i>angustifolia</i> .	(Kirchmayr <i>et al.</i> 2017)
<i>Hanseniaspora uvarum</i> <i>Kluyveromyces marxianus</i> <i>Saccharomyces cerevisiae</i> <i>Torulaspora delbrueckii</i>	2-methyl-1-propanol 3-methyl-1-butanol acetic acid 1-(2-furanyl)-ethenone Furfural $\alpha$ -terpineol ethyl phenyl acetate phenyl ethyl alcohol esters (15 different types)	Mezcal. Durango.	A. <i>duranguensis</i> .	Martell Nevárez <i>et al.</i> , 2011

Supplementary Table S2. Data used to generate the heatmap in figure 4.

Variable	Palenque (Categorical and scalar values) *			
	1	2	3	4
Earth oven	0.5	-1.5	0.5	0.5
Stone oven	-0.5	1.5	-0.5	-0.5
Tahona	0.5	-1.5	0.5	0.5
Shredder	-0.5	1.5	-0.5	-0.5
Wooden fermentation container	0.5	0.5	-1.5	0.5
Plastic fermentation container	-0.5	-0.5	1.5	-0.5
Copper distiller	0.5	-1.5	0.5	0.5
Pottery distiller	-0.5	1.5	-0.5	-0.5
River water	0.5	-1.5	0.5	0.5
Tap water	-0.5	1.5	-0.5	-0.5
<i>Agave angustifolia</i>	0.5	0.5	-1.5	0.5
<i>Agave potatorum</i>	-0.5	-0.5	1.5	-0.5
pH	-0.68	-0.75	-0.68	1.43
Total soluble solutes	-0.15	1.44	-0.78	-0.50
Temperature	-1.08	-0.39	0.08	1.31

\*A categorical and scalar values used in scale function in Rstudio to generate standardized values with a common scale to compare and recognize clustering in the multiple analyzed variables.

Supplementary Table S3. Table where is grouped the corresponding data from the the correlation matrix used to generate the PCA analysis. This table is the result to apply the “corr” R function, originated in the “corr” and the “ggcorrplot” packages. All the data is escalated and to use this table as a matrix, the table present the variable in the first line and in the first column.

	Earth oven	Stone oven	Tahona	Shredder	Wooden fermentation container	Plastic fermentation container	Copper distiller	Pottery distiller
Earth oven	1.00	-1.00	1.00	-1.00	-0.33	0.33	1.00	-1.00
Stone oven	-1.00	1.00	-1.00	1.00	0.33	-0.33	-1.00	1.00
Tahona	1.00	-1.00	1.00	-1.00	-0.33	0.33	1.00	-1.00
Shredder	-1.00	1.00	-1.00	1.00	0.33	-0.33	-1.00	1.00
Wooden fermentation container	-0.33	0.33	-0.33	0.33	1.00	-1.00	-0.33	0.33
Plastic fermentation container	0.33	-0.33	0.33	-0.33	-1.00	1.00	0.33	-0.33
Copper distiller	1.00	-1.00	1.00	-1.00	-0.33	0.33	1.00	-1.00
Pottery distiller	-1.00	1.00	-1.00	1.00	0.33	-0.33	-1.00	1.00
River water	1.00	-1.00	1.00	-1.00	-0.33	0.33	1.00	-1.00
Tap water	-1.00	1.00	-1.00	1.00	0.33	-0.33	-1.00	1.00
<i>Agave angustifolia</i>	-0.33	0.33	-0.33	0.33	1.00	-1.00	-0.33	0.33
<i>Agave potatorum</i>	0.33	-0.33	0.33	-0.33	-1.00	1.00	0.33	-0.33
pH	0.05	-0.05	0.05	-0.05	0.45	-0.45	0.05	-0.05
Total soluble solutes	-0.96	0.96	-0.97	0.97	0.53	-0.53	-0.97	0.97
Temperature	0.21	-0.21	0.21	-0.21	-0.05	0.05	0.21	-0.21

	River water	Tap water	<i>Agave angustifolia</i>	<i>Agave potatorum</i>	pH	Total soluble solutes	Temperature
Earth oven	1.00	-1.00	-0.33	0.33	0.05	-0.97	0.21
Stone oven	-1.00	1.00	0.33	-0.33	-0.05	0.97	-0.21
Tahona	1.00	-1.00	-0.33	0.33	0.05	-0.97	0.21
Shredder	-1.00	1.00	0.33	-0.33	-0.05	0.97	-0.21
Wooden fermentation container	-0.33	0.33	1.00	-1.00	0.45	0.53	-0.05
Plastic fermentation container	0.33	-0.33	-1.00	1.00	-0.45	-0.53	0.05
Copper distiller	1.00	-1.00	-0.33	0.33	0.05	-0.97	0.21
Pottery distiller	-1.00	1.00	0.33	-0.33	-0.05	0.97	-0.21
River water	1.00	-1.00	-0.33	0.33	0.05	-0.97	0.21
Tap water	-1.00	1.00	0.33	-0.33	-0.05	0.97	-0.21
<i>Agave angustifolia</i>	-0.33	0.33	1.00	-1.00	0.45	0.53	-0.05
<i>Agave potatorum</i>	0.33	-0.33	-1.00	1.00	-0.45	-0.53	0.05
pH	0.05	-0.05	0.45	-0.45	1.00	-0.07	0.86
Total soluble solutes	-0.97	0.97	0.53	-0.53	-0.07	1.00	-0.34
Temperature	0.21	-0.21	-0.05	0.05	0.86	-0.34	1.00

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