



# Supplementary Information

## Quantitative Chemical Profile and Multivariate Statistical Analysis of Alembic Distilled Sugarcane Spirit Fractions

Felipe A. T. Serafim,<sup>a</sup> Carlos A. Galinaro,<sup>a</sup> Alexandre A. da Silva,<sup>a</sup> Silmara F. Buchviser,<sup>a</sup>  
 Eduardo S. P. do Nascimento,<sup>a</sup> Fernando V. Novaes<sup>b</sup> and Douglas W. Franco<sup>\*a</sup>

<sup>a</sup>Instituto de Química de São Carlos, Universidade de São Paulo,  
 Avenida Trabalhador São-Carlense 400, CP 780, 13560-970 São Carlos-SP, Brazil

<sup>b</sup>Escola Superior de Agricultura “Luiz de Queiroz” (ESALQ), Universidade de São Paulo,  
 Av. Pádua Dias, 11, 13418-900 Piracicaba-SP, Brazil

**Table S1.** Secondary composition concentration (mg L<sup>-1</sup>) of alembic fractions

Compounds	Head fraction samples (HCA code)													
	S01 (37)	S05 (25)	S08 (34)	S09 (31)	S20 (19)	S22 (23)	S25 (28)	S29 (10)	S30 (16)	S31 (1)	S32 (7)	S33 (4)	S34 (13)	S35 (40)
Ethyl acetate	632	42.3	286	443	772	1477	209	1370	262	2177	465	401	367	1080
Ethyl butanoate	4.7	<LOD	8.0 × 10 <sup>-1</sup>	6.4 × 10 <sup>-1</sup>	5.36	5.64	<LOD	<LOD	9.1 × 10 <sup>-1</sup>	9.4 × 10 <sup>-1</sup>	1.04	1.40	1.23	2.27
Ethyl hexanoate	2.24	<LOD	<LOD	9.8 × 10 <sup>-1</sup>	7.19	12.4	1.0	<LOD	1.39	9.5 × 10 <sup>-1</sup>	2.07	6.96	4.87	3.03
Ethyl lactate	3.8	34.6	21.9	196	11.6	9.3	162	338	10.3	295	15.3	12.3	19	5.3
Ethyl octanoate	13.1	1.52	8.4 × 10 <sup>-1</sup>	2.55	17.8	27.7	6.0	8.3 × 10 <sup>-1</sup>	4.38	2.58	12.0	40.2	42.1	9.74
Ethyl nonanoate	3.9 × 10 <sup>-1</sup>	<LOD	<LOD	<LOD	3.1 × 10 <sup>-1</sup>	2.3 × 10 <sup>-1</sup>	<LOD	<LOD	<LOD	1.6 × 10 <sup>-1</sup>	7.4 × 10 <sup>-1</sup>	6.1 × 10 <sup>-1</sup>	5.3 × 10 <sup>-1</sup>	<LOD
Ethyl decanoate	24.2	6.4	3.1	11	17.1	27.3	8.87	1.09	6.17	3.47	16.7	43.6	46.8	19.1
Isoamyl octanoate	7.0 × 10 <sup>-2</sup>	<LOD	<LOD	7.0 × 10 <sup>-2</sup>	3.4 × 10 <sup>-1</sup>	1.2 × 10 <sup>-1</sup>	<LOD	<LOD	6.0 × 10 <sup>-2</sup>	1.2 × 10 <sup>-1</sup>	1.5 × 10 <sup>-1</sup>	5.1 × 10 <sup>-1</sup>	3.1 × 10 <sup>-1</sup>	9.0 × 10 <sup>-2</sup>
Ethyl dodecanoate	5.26	1.86	6.0 × 10 <sup>-1</sup>	4.88	3.13	2.54	1.76	7.4 × 10 <sup>-1</sup>	9.0 × 10 <sup>-1</sup>	2.62	1.84	7.23	10.2	2.69
Acetylacetone	<LOD	<LOD	<LOD	<LOD	<LOD	<LOD	4.7 × 10 <sup>-1</sup>	1.35	<LOD	<LOD	<LOD	5.0 × 10 <sup>-1</sup>	<LOD	8.3 × 10 <sup>-1</sup>
Formaldehyde	1.3 × 10 <sup>-1</sup>	5.0 × 10 <sup>-2</sup>	1.9 × 10 <sup>-1</sup>	1.5 × 10 <sup>-1</sup>	1.0 × 10 <sup>-1</sup>	2.3 × 10 <sup>-1</sup>	7.0 × 10 <sup>-2</sup>	1.3 × 10 <sup>-1</sup>	9.0 × 10 <sup>-2</sup>	3.4 × 10 <sup>-1</sup>	1.0 × 10 <sup>-1</sup>	2.5 × 10 <sup>-1</sup>	9.0 × 10 <sup>-2</sup>	2.6 × 10 <sup>-1</sup>
5-HMF	<LOD	3.0 × 10 <sup>-2</sup>	5.9 × 10 <sup>-1</sup>	1.8 × 10 <sup>-1</sup>	<LOD	1.1 × 10 <sup>-1</sup>	5.0 × 10 <sup>-1</sup>	<LOD	9.0 × 10 <sup>-2</sup>	<LOD	3.0 × 10 <sup>-2</sup>	1.0 × 10 <sup>-2</sup>	1.0 × 10 <sup>-2</sup>	<LOD
Acetaldehyde	50.8	1.8	23.0	15.5	51.1	66.6	14.9	7.6	28.9	24.5	29.0	12.7	12.4	9.5
Acrolein	6.0 × 10 <sup>-2</sup>	<LOD	3.0 × 10 <sup>-2</sup>	<LOD	9.0 × 10 <sup>-2</sup>	1.1 × 10 <sup>-1</sup>	<LOD	<LOD	<LOD	9.0 × 10 <sup>-2</sup>	4.5 × 10 <sup>-1</sup>	1.4 × 10 <sup>-1</sup>	1.1 × 10 <sup>-1</sup>	1.1 × 10 <sup>-1</sup>
Propionaldehyde	2.8 × 10 <sup>-1</sup>	1.2 × 10 <sup>-1</sup>	2.5 × 10 <sup>-1</sup>	5.0 × 10 <sup>-1</sup>	1.2 × 10 <sup>-1</sup>	2.1 × 10 <sup>-1</sup>	5.0 × 10 <sup>-2</sup>	5.0 × 10 <sup>-2</sup>	9.0 × 10 <sup>-2</sup>	1.1 × 10 <sup>-1</sup>	3.5 × 10 <sup>-1</sup>	4.0 × 10 <sup>-2</sup>	2.8 × 10 <sup>-1</sup>	1.4 × 10 <sup>-1</sup>
Butiral/Isobutiraldehyde	4.3 × 10 <sup>-1</sup>	1.1 × 10 <sup>-1</sup>	8.0 × 10 <sup>-2</sup>	3.43	4.9 × 10 <sup>-1</sup>	4.5 × 10 <sup>-1</sup>	2.0 × 10 <sup>-1</sup>	1.1 × 10 <sup>-1</sup>	4.8 × 10 <sup>-1</sup>	4.0 × 10 <sup>-2</sup>	5.7 × 10 <sup>-1</sup>	4.9 × 10 <sup>-1</sup>	1.7 × 10 <sup>-1</sup>	<LOD
Furfuraldehyde	<LOD	<LOD	<LOD	<LOD	<LOD	<LOD	1.5 × 10 <sup>-1</sup>	9.0 × 10 <sup>-2</sup>	<LOD	<LOD	<LOD	<LOD	1.0 × 10 <sup>-2</sup>	3.0 × 10 <sup>-2</sup>
Benzaldehyde	3.2 × 10 <sup>-1</sup>	1.4 × 10 <sup>-1</sup>	<LOD	1.25	5.0 × 10 <sup>-1</sup>	4.7 × 10 <sup>-1</sup>	9.7 × 10 <sup>-1</sup>	1.2 × 10 <sup>-1</sup>	<LOD	<LOD	3.3 × 10 <sup>-1</sup>	4.7 × 10 <sup>-1</sup>	1.0 × 10 <sup>-1</sup>	4.8 × 10 <sup>-1</sup>
Valeraldehyde	7.7 × 10 <sup>-1</sup>	<LOD	1.9 × 10 <sup>-1</sup>	<LOD	1.13	1.03	3.8 × 10 <sup>-1</sup>	<LOD	5.3 × 10 <sup>-1</sup>	<LOD	2.64	7.6 × 10 <sup>-1</sup>	1.15	<LOD
Diacetyl	<LOD	1.0 × 10 <sup>-2</sup>	<LOD	2.0 × 10 <sup>-2</sup>	2.0 × 10 <sup>-2</sup>	4.0 × 10 <sup>-2</sup>	<LOD	<LOD	6.8 × 10 <sup>-1</sup>	3.0 × 10 <sup>-2</sup>	1.00	2.0 × 10 <sup>-2</sup>	4.8 × 10 <sup>-1</sup>	<LOD
Lactic acid	24.3	1.50	32.5	89.5	8.42	19.2	74.1	145	10.3	131	11.4	15.6	63.3	9.17
Glycolic acid	<LOD	<LOD	<LOD	<LOD	<LOD	1.61	<LOD	<LOD	3.3 × 10 <sup>-1</sup>	<LOD	4.9 × 10 <sup>-1</sup>	8.9 × 10 <sup>-1</sup>	<LOD	<LOD
Pyruvic acid	<LOD	<LOD	<LOD	<LOD	<LOD	<LOD	<LOD	<LOD	<LOD	<LOD	<LOD	1.0 × 10 <sup>-1</sup>	<LOD	<LOD
Succinic acid	<LOD	<LOD	1.0 × 10 <sup>-1</sup>	7.0 × 10 <sup>-2</sup>	3.0 × 10 <sup>-1</sup>	2.1 × 10 <sup>-1</sup>	1.1 × 10 <sup>-1</sup>	<LOD	1.0 × 10 <sup>-1</sup>	<LOD	<LOD	1.0 × 10 <sup>-1</sup>	1.6 × 10 <sup>-1</sup>	7.0 × 10 <sup>-2</sup>
Capric acid	6.05	<LOD	7.1 × 10 <sup>-1</sup>	5.41	11.70	9.8 × 10 <sup>-1</sup>	1.1	<LOD	3.52	2.15	5.65	18.3	54.85	<LOD
Lauric acid	1.04	<LOD	2.5 × 10 <sup>-1</sup>	1.93	1.07	2.1 × 10 <sup>-1</sup>	3.3 × 10 <sup>-1</sup>	<LOD	2.9 × 10 <sup>-1</sup>	1.46	6.4 × 10 <sup>-1</sup>	1.47	8.54	6.6 × 10 <sup>-1</sup>
Myristic acid	4.3 × 10 <sup>-1</sup>	<LOD	3.0 × 10 <sup>-1</sup>	1.03	1.8 × 10 <sup>-1</sup>	1.4 × 10 <sup>-1</sup>	2.8 × 10 <sup>-1</sup>	<LOD	5.7 × 10 <sup>-1</sup>	6.9 × 10 <sup>-1</sup>	9.3 × 10 <sup>-1</sup>	6.3 × 10 <sup>-1</sup>	2.16	<LOD
Palmitic acid	1.04	<LOD	1.01	2.57	1.13	4.2 × 10 <sup>-1</sup>	1.54	<LOD	1.95	3.31	3.14	1.99	8.44	1.78
Citramalic acid	<LOD	<LOD	4.0 × 10 <sup>-1</sup>	2.9 × 10 <sup>-1</sup>	<LOD	<LOD	<LOD	<LOD	<LOD	<LOD	<LOD	1.0 × 10 <sup>-1</sup>	2.6 × 10 <sup>-1</sup>	<LOD
Acetic acid	123	40.7	257	49.7	95	23	153	2783	21	1139	84	48	42	35
Methanol	<LOD	19.7	<LOD	5.25	414	270	<LOD	<LOD	<LOD	13.2	<LOD	<LOD	<LOD	<LOD
2-Butanol	44.6	<LOD	<LOD	<LOD	<LOD	<LOD	<LOD	<LOD	<LOD	<LOD	<LOD	<LOD	<LOD	<LOD
Propanol	623	142	202	169	239	1097	<LOD	116	219	80	224	192	372	523
Isobutanol	380	108	376	536	555	315	<LOD	517	409	464	433	346	398	475
Butanol	17.6	8.6	17.2	3.3	16.1	7.3	<LOD	3.04	3.43	1.72	3.44	2.83	5.06	23.2
Isoamyl alcohol	1776	1175	1659	1549	2943	929	<LOD	1903	1867	1466	1851	1950	1276	2071
Ethyl carbamate	<LOD	1.7 × 10 <sup>-1</sup>	1.7 × 10 <sup>-1</sup>	<LOD	<LOD	<LOD	<LOD	2.4 × 10 <sup>-1</sup>	<LOD	6.0 × 10 <sup>-2</sup>	1.0 × 10 <sup>-1</sup>	5.8 × 10 <sup>-1</sup>	4.0 × 10 <sup>-1</sup>	7.0 × 10 <sup>-2</sup>
Alcoholic content	61.1	52.1	49.7	53.1	59.7	69.9	55	41.8	47.6	43.0	49.1	52.4	52.7	65.9

\*e-mail: douglas@iqsc.usp.br

Table S1. Continuation

Compounds	Heart fraction samples (HCA code)													
	S01 (38)	S05 (26)	S08 (35)	S09 (32)	S20 (20)	S22 (23)	S25 (29)	S29 (11)	S30 (17)	S31 (2)	S32 (8)	S33 (5)	S34 (14)	S35 (41)
Ethyl acetate	26.8	27.5	78.0	48.9	37.8	14.6	53	1363	17.5	1404	37.7	17.3	35.2	46.2
Ethyl butanoate	<LOD	<LOD	<LOD	<LOD	<LOD	<LOD	<LOD	<LOD	<LOD	9.7 × 10 <sup>-1</sup>	<LOD	<LOD	<LOD	<LOD
Ethyl hexanoate	<LOD	<LOD	<LOD	<LOD	<LOD	<LOD	<LOD	<LOD	<LOD	3.8 × 10 <sup>-1</sup>	<LOD	<LOD	<LOD	<LOD
Ethyl lactate	7.02	46.3	24.9	261	23.40	48.2	211	384	16.4	207	27.0	24.0	38.2	18.3
Ethyl octanoate	<LOD	5.5 × 10 <sup>-1</sup>	<LOD	3.8 × 10 <sup>-1</sup>	5.5 × 10 <sup>-1</sup>	3.2 × 10 <sup>-1</sup>	5.0 × 10 <sup>-1</sup>	6.4 × 10 <sup>-1</sup>	2.8 × 10 <sup>-1</sup>	9.6 × 10 <sup>-1</sup>	1.13	6.0 × 10 <sup>-1</sup>	5.0 × 10 <sup>-1</sup>	<LOD
Ethyl nonanoate	<LOD	<LOD	<LOD	<LOD	<LOD	<LOD	<LOD	<LOD	<LOD	<LOD	<LOD	<LOD	<LOD	<LOD
Ethyl decanoate	1.18	3.98	6.9 × 10 <sup>-1</sup>	3.05	4.58	1.81	2.12	1.35	7.1 × 10 <sup>-1</sup>	1.74	3.20	2.92	1.51	8.5 × 10 <sup>-1</sup>
Isoamyl octanoate	<LOD	<LOD	<LOD	<LOD	1.0 × 10 <sup>-1</sup>	<LOD	<LOD	<LOD	<LOD	2.0 × 10 <sup>-2</sup>	<LOD	<LOD	<LOD	<LOD
Ethyl dodecanoate	9.5 × 10 <sup>-1</sup>	1.45	2.4 × 10 <sup>-1</sup>	1.96	2.21	1.40	4.6 × 10 <sup>-1</sup>	1.63	<LOD	7.6 × 10 <sup>-1</sup>	3.2 × 10 <sup>-1</sup>	5.2 × 10 <sup>-1</sup>	<LOD	7.9 × 10 <sup>-1</sup>
Acetylacetone	<LOD	<LOD	<LOD	<LOD	<LOD	<LOD	3.5 × 10 <sup>-1</sup>	3.1 × 10 <sup>-1</sup>	<LOD	<LOD	<LOD	2.2 × 10 <sup>-1</sup>	<LOD	2.2 × 10 <sup>-1</sup>
Formaldehyde	3.0 × 10 <sup>-2</sup>	5.0 × 10 <sup>-2</sup>	8.0 × 10 <sup>-2</sup>	4.0 × 10 <sup>-2</sup>	4.0 × 10 <sup>-2</sup>	5.0 × 10 <sup>-2</sup>	3.0 × 10 <sup>-2</sup>	1.8 × 10 <sup>-1</sup>	3.0 × 10 <sup>-2</sup>	1.9 × 10 <sup>-1</sup>	4.0 × 10 <sup>-2</sup>	3.0 × 10 <sup>-2</sup>	2.0 × 10 <sup>-2</sup>	1.3 × 10 <sup>-1</sup>
5-HMF	1.1 × 10 <sup>-1</sup>	3.0 × 10 <sup>-2</sup>	6.6 × 10 <sup>-1</sup>	1.8 × 10 <sup>-1</sup>	1.8 × 10 <sup>-1</sup>	1.37	1.19	<LOD	1.2 × 10 <sup>-1</sup>	1.0 × 10 <sup>-2</sup>	8.0 × 10 <sup>-2</sup>	5.0 × 10 <sup>-2</sup>	2.0 × 10 <sup>-2</sup>	2.0 × 10 <sup>-2</sup>
Acetaldehyde	1.43	5.9 × 10 <sup>-1</sup>	6.96	2.95	2.74	6.6 × 10 <sup>-1</sup>	1.78	10.74	3.53	10.98	2.46	1.38	3.4 × 10 <sup>-1</sup>	4.03
Acrolein	4.0 × 10 <sup>-2</sup>	<LOD	3.0 × 10 <sup>-2</sup>	<LOD	2.0 × 10 <sup>-2</sup>	<LOD	<LOD	<LOD	<LOD	5.0 × 10 <sup>-2</sup>	6.0 × 10 <sup>-1</sup>	4.0 × 10 <sup>-2</sup>	2.0 × 10 <sup>-2</sup>	6.0 × 10 <sup>-2</sup>
Propionaldehyde	9.0 × 10 <sup>-2</sup>	8.0 × 10 <sup>-2</sup>	1.6 × 10 <sup>-1</sup>	2.4 × 10 <sup>-1</sup>	1.0 × 10 <sup>-1</sup>	7.0 × 10 <sup>-2</sup>	2.0 × 10 <sup>-2</sup>	2.1 × 10 <sup>-1</sup>	1.0 × 10 <sup>-2</sup>	1.6 × 10 <sup>-1</sup>	1.1 × 10 <sup>-1</sup>	<LOD	7.0 × 10 <sup>-2</sup>	<LOD
Butiral/Isobutiraldehyde	<LOD	1.2 × 10 <sup>-1</sup>	4.0 × 10 <sup>-2</sup>	2.1 × 10 <sup>-1</sup>	8.0 × 10 <sup>-2</sup>	1.2 × 10 <sup>-1</sup>	<LOD	1.5 × 10 <sup>-1</sup>	5.0 × 10 <sup>-2</sup>	1.0 × 10 <sup>-1</sup>	5.0 × 10 <sup>-2</sup>	<LOD	3.0 × 10 <sup>-2</sup>	1.3 × 10 <sup>-1</sup>
Furfuraldehyde	<LOD	<LOD	<LOD	4.0 × 10 <sup>-2</sup>	1.0 × 10 <sup>-2</sup>	1.0 × 10 <sup>-2</sup>	2.0 × 10 <sup>-1</sup>	3.1 × 10 <sup>-1</sup>	<LOD	<LOD	<LOD	1.0 × 10 <sup>-2</sup>	2.0 × 10 <sup>-2</sup>	6.0 × 10 <sup>-2</sup>
Benzaldehyde	<LOD	5.0 × 10 <sup>-2</sup>	<LOD	<LOD	<LOD	<LOD	5.6 × 10 <sup>-1</sup>	1.0 × 10 <sup>-1</sup>	<LOD	1.2 × 10 <sup>-1</sup>	4.0 × 10 <sup>-2</sup>	2.2 × 10 <sup>-1</sup>	<LOD	2.6 × 10 <sup>-1</sup>
Valeraldehyde	<LOD	<LOD	8.0 × 10 <sup>-2</sup>	<LOD	<LOD	<LOD	<LOD	<LOD	<LOD	<LOD	9.0 × 10 <sup>-2</sup>	<LOD	<LOD	<LOD
Diacetyl	<LOD	1.0 × 10 <sup>-2</sup>	<LOD	1.0 × 10 <sup>-2</sup>	1.0 × 10 <sup>-2</sup>	2.0 × 10 <sup>-2</sup>	<LOD	1.0 × 10 <sup>-2</sup>	4.4 × 10 <sup>-1</sup>	3.0 × 10 <sup>-2</sup>	6.8 × 10 <sup>-1</sup>	<LOD	4.0 × 10 <sup>-2</sup>	<LOD
Lactic acid	5.60	3.30	40.9	73.5	34.0	41.0	99.0	326	13.0	150	36.6	48.3	116	16.6
Glycolic acid	<LOD	<LOD	4.5 × 10 <sup>-1</sup>	9.3 × 10 <sup>-1</sup>	<LOD	<LOD	<LOD	<LOD	1.6 × 10 <sup>-1</sup>	2.7 × 10 <sup>-1</sup>	8.0 × 10 <sup>-1</sup>	8.5 × 10 <sup>-1</sup>	2.3	<LOD
Pyruvic acid	<LOD	<LOD	<LOD	<LOD	<LOD	<LOD	9.0 × 10 <sup>-1</sup>	<LOD	1.61	22.2	<LOD	<LOD	<LOD	<LOD
Succinic acid	<LOD	<LOD	1.0 × 10 <sup>-1</sup>	5.0 × 10 <sup>-2</sup>	5.8 × 10 <sup>-1</sup>	5.2 × 10 <sup>-1</sup>	2.3 × 10 <sup>-1</sup>	2.1 × 10 <sup>-1</sup>	8.0 × 10 <sup>-2</sup>	<LOD	1.6 × 10 <sup>-1</sup>	7.0 × 10 <sup>-2</sup>	7.0 × 10 <sup>-2</sup>	1.0 × 10 <sup>-1</sup>
Capric acid	5.3 × 10 <sup>-1</sup>	<LOD	1.10	2.16	<LOD	<LOD	<LOD	<LOD	<LOD	1.6 × 10 <sup>-1</sup>	1.03	1.71	<LOD	<LOD
Lauric acid	2.6 × 10 <sup>-1</sup>	<LOD	3.0 × 10 <sup>-1</sup>	1.16	<LOD	<LOD	1.8 × 10 <sup>-1</sup>	1.9 × 10 <sup>-1</sup>	<LOD	2.7 × 10 <sup>-1</sup>	2.0 × 10 <sup>-1</sup>	4.8 × 10 <sup>-1</sup>	2.0 × 10 <sup>-1</sup>	3.4 × 10 <sup>-1</sup>
Myristic acid	4.0 × 10 <sup>-1</sup>	<LOD	3.5 × 10 <sup>-1</sup>	5.8 × 10 <sup>-1</sup>	<LOD	<LOD	2.7 × 10 <sup>-1</sup>	<LOD	2.8 × 10 <sup>-1</sup>	2.7 × 10 <sup>-1</sup>	3.2 × 10 <sup>-1</sup>	2.6 × 10 <sup>-1</sup>	1.3 × 10 <sup>-1</sup>	<LOD
Palmitic acid	1.32	<LOD	9.0 × 10 <sup>-1</sup>	9.6 × 10 <sup>-1</sup>	6.1 × 10 <sup>-1</sup>	7.1 × 10 <sup>-1</sup>	1.40	6.7 × 10 <sup>-1</sup>	9.2 × 10 <sup>-1</sup>	1.71	8.0 × 10 <sup>-1</sup>	1.26	1.31	2.67
Citramalic acid	9.0 × 10 <sup>-2</sup>	<LOD	7.5 × 10 <sup>-1</sup>	3.0 × 10 <sup>-1</sup>	<LOD	<LOD	<LOD	<LOD	<LOD	5.4 × 10 <sup>-1</sup>	1.6 × 10 <sup>-1</sup>	3.0 × 10 <sup>-1</sup>	2.0 × 10 <sup>-1</sup>	<LOD
Acetic acid	136	68.7	324	32.2	162.8	39.1	251	2942	24.0	1797	95.4	57.5	120	91.2
Methanol	13.2	21.8	<LOD	25.5	<LOD	22.0	<LOD	17.7	18.8	13.5	11.2	3.08	43.3	<LOD
2-Butanol	4.90	<LOD	<LOD	<LOD	<LOD	<LOD	<LOD	<LOD	<LOD	1.01	<LOD	<LOD	<LOD	<LOD
Propanol	155	212	187	122	183	762	<LOD	70.6	200	61.9	120	93.5	270	421
Isobutanol	147	107	271	179	308	50.7	<LOD	359	182	238	155.	77.2	80.7	183
Butanol	2.91	8.40	3.45	13.8	8.87	3.13	<LOD	1.92	2.89	1.52	1.87	<LOD	2.36	12.8
Isoamyl alcohol	508	735	881	1468	1225	215	<LOD	1254	831	778	680	394	156	834
Ethyl carbamate	<LOD	7.0 × 10 <sup>-2</sup>	8.0 × 10 <sup>-2</sup>	8.0 × 10 <sup>-2</sup>	<LOD	5.0 × 10 <sup>-2</sup>	<LOD	8.0 × 10 <sup>-2</sup>	<LOD	<LOD	<LOD	6.0 × 10 <sup>-2</sup>	1.0 × 10 <sup>-1</sup>	<LOD
Alcoholic content	44.0	45.4	44.7	47	38.0	47.4	45.1	39.5	40.1	38.9	39.7	37.01	32.8	48.5
Compounds	Tail fraction samples (HCA code)													
	S01 (39)	S05 (27)	S08 (36)	S09 (33)	S20 (21)	S22 (24)	S25 (30)	S29 (12)	S30 (18)	S31 (3)	S32 (9)	S33 (6)	S34 (15)	S35 (42)
Ethyl acetate	35.0	26.0	53.0	16.0	36.0	15.0	80.0	766	7.0	1057	26.0	15.0	29.0	12.0
Ethyl butanoate	<LOD	<LOD	<LOD	<LOD	<LOD	<LOD	<LOD	<LOD	<LOD	6.5 × 10 <sup>-1</sup>	<LOD	<LOD	<LOD	<LOD
Ethyl hexanoate	<LOD	<LOD	<LOD	<LOD	<LOD	<LOD	<LOD	<LOD	<LOD	<LOD	<LOD	<LOD	<LOD	<LOD
Ethyl lactate	8.6	61.9	29.7	270	29.2	53.9	159	228	24.6	75.9	39.7	19.7	27.9	28.5
Ethyl octanoate	<LOD	3.0 × 10 <sup>-1</sup>	<LOD	<LOD	<LOD	3.0 × 10 <sup>-1</sup>	<LOD	<LOD	<LOD	<LOD	<LOD	<LOD	<LOD	<LOD
Ethyl nonanoate	<LOD	<LOD	<LOD	<LOD	<LOD	<LOD	<LOD	<LOD	<LOD	<LOD	<LOD	<LOD	<LOD	<LOD
Ethyl decanoate	<LOD	2.0	<LOD	<LOD	<LOD	1.1	<LOD	<LOD	<LOD	<LOD	<LOD	<LOD	<LOD	<LOD
Isoamyl octanoate	<LOD	<LOD	<LOD	<LOD	<LOD	<LOD	<LOD	<LOD	<LOD	<LOD	<LOD	<LOD	<LOD	<LOD
Ethyl dodecanoate	<LOD	6.6 × 10 <sup>-1</sup>	<LOD	<LOD	<LOD	1.0	<LOD	<LOD	<LOD	<LOD	<LOD	<LOD	<LOD	<LOD
Acetylacetone	<LOD	<LOD	<LOD	<LOD	<LOD	<LOD	<LOD	1.0 × 10 <sup>-1</sup>	<LOD	<LOD	<LOD	5.0 × 10 <sup>-2</sup>	<LOD	2.0 × 10 <sup>-1</sup>
Formaldehyde	<LOD	3.0 × 10 <sup>-2</sup>	7.0 × 10 <sup>-2</sup>	1.0 × 10 <sup>-2</sup>	2.0 × 10 <sup>-2</sup>	5.0 × 10 <sup>-2</sup>	6.0 × 10 <sup>-2</sup>	6.0 × 10 <sup>-2</sup>	<LOD	2.3 × 10 <sup>-1</sup>	1.0 × 10 <sup>-2</sup>	2.0 × 10 <sup>-2</sup>	<LOD	1.0 × 10 <sup>-1</sup>
5-HMF	2.0 × 10 <sup>-1</sup>	3.0 × 10 <sup>-2</sup>	7.6 × 10 <sup>-1</sup>	2.0 × 10 <sup>-1</sup>	6.0 × 10 <sup>-1</sup>	1.50	1.23	<LOD	1.8 × 10 <sup>-1</sup>	5.0 × 10 <sup>-2</sup>	7.0 × 10 <sup>-2</sup>	9.0 × 10 <sup>-2</sup>	4.0 × 10 <sup>-2</sup>	1.0 × 10 <sup>-1</sup>
Acetaldehyde	2.0 × 10 <sup>-1</sup>	3.5 × 10 <sup>-1</sup>	1.54	2.1 × 10 <sup>-1</sup>	3.9 × 10 <sup>-1</sup>	7.7 × 10 <sup>-1</sup>	1.5 × 10 <sup>-1</sup>	1.9 × 10 <sup>-1</sup>	6.0 × 10 <sup>-2</sup>	9.3	1.6 × 10 <sup>-1</sup>	4.6 × 10 <sup>-1</sup>	7.0 × 10 <sup>-2</sup>	2.33
Acrolein	1.0 × 10 <sup>-2</sup>	<LOD	1.0 × 10 <sup>-2</sup>	<LOD	2.0 × 10 <sup>-2</sup>	<LOD	5.0 × 10 <sup>-2</sup>	<LOD	<LOD	8.0 × 10 <sup>-2</sup>	5.0 × 10 <sup>-2</sup>	1.0 × 10 <sup>-2</sup>	6.0 × 10 <sup>-2</sup>	2.0 × 10 <sup>-2</sup>
Propionaldehyde	4.0 × 10 <sup>-2</sup>	6.0 × 10 <sup>-2</sup>	8.0 × 10 <sup>-2</sup>	5.0 × 10 <sup>-2</sup>	3.0 × 10 <sup>-2</sup>	7.0 × 10 <sup>-2</sup>	1.0 × 10 <sup>-2</sup>	1.2 × 10 <sup>-1</sup>	<LOD	<LOD	4.0 × 10 <sup>-2</sup>	<LOD	2.0 × 10 <sup>-2</sup>	<LOD

**Table S1.** Continuation

Compounds	Tail fraction samples (HCA code)													
	S01 (39)	S05 (27)	S08 (36)	S09 (33)	S20 (21)	S22 (24)	S25 (30)	S29 (12)	S30 (18)	S31 (3)	S32 (9)	S33 (6)	S34 (15)	S35 (42)
Butiral/Isobutiraldehyde	$5.0 \times 10^{-2}$	$9.0 \times 10^{-2}$	$2.0 \times 10^{-2}$	$3.0 \times 10^{-2}$	$5.0 \times 10^{-2}$	$1.5 \times 10^{-1}$	$9.0 \times 10^{-2}$	$2.0 \times 10^{-2}$	$1.0 \times 10^{-2}$	$8.0 \times 10^{-2}$	$2.0 \times 10^{-2}$	<LOD	$1.0 \times 10^{-2}$	$9.0 \times 10^{-2}$
Furfuraldehyde	$1.8 \times 10^{-1}$	$1.0 \times 10^{-2}$	<LOD	1.55	$7.0 \times 10^{-2}$	$5.0 \times 10^{-2}$	$2.8 \times 10^{-2}$	$1.6 \times 10^{-1}$	$6.0 \times 10^{-2}$	$6.0 \times 10^{-2}$	$1.0 \times 10^{-2}$	$5.0 \times 10^{-2}$	$1.5 \times 10^{-1}$	$4.3 \times 10^{-1}$
Benzaldehyde	<LOD	$1.0 \times 10^{-1}$	$3.0 \times 10^{-2}$	<LOD	$3.0 \times 10^{-2}$	$4.0 \times 10^{-2}$	<LOD	<LOD	<LOD	<LOD	$1.0 \times 10^{-2}$	$4.0 \times 10^{-2}$	<LOD	$1.5 \times 10^{-1}$
Valeraldehyde	<LOD	<LOD	$4.0 \times 10^{-2}$	<LOD	<LOD	<LOD	<LOD	<LOD	<LOD	<LOD	<LOD	<LOD	<LOD	<LOD
Diacetyl	<LOD	$9.0 \times 10^{-2}$	<LOD	$4.0 \times 10^{-2}$	$8.0 \times 10^{-2}$	$1.0 \times 10^{-2}$	<LOD	<LOD	$6.0 \times 10^{-2}$	$2.0 \times 10^{-2}$	$1.2 \times 10^{-1}$	<LOD	<LOD	<LOD
Lactic acid	26.9	14.3	41.9	89.5	97.4	64.0	175	451	57.8	125	25.6	105	151	31.5
Glycolic acid	<LOD	<LOD	$4.0 \times 10^{-1}$	<LOD	$6.0 \times 10^{-1}$	$1.0 \times 10^{-1}$	<LOD	<LOD	<LOD	18.4	<LOD	1.8	2.3	<LOD
Pyruvic acid	<LOD	<LOD	$9.0 \times 10^{-1}$	<LOD	1.42	<LOD	<LOD	<LOD	2.32	11.4	<LOD	<LOD	<LOD	$1.6 \times 10^{-1}$
Succinic acid	1.52	<LOD	$8.0 \times 10^{-2}$	<LOD	1.67	$2.8 \times 10^{-1}$	$9.8 \times 10^{-1}$	<LOD	$5.0 \times 10^{-2}$	$1.1 \times 10^{-1}$	<LOD	$8.0 \times 10^{-2}$	$8.0 \times 10^{-2}$	$1.9 \times 10^{-1}$
Capric acid	<LOD	<LOD	$6.4 \times 10^{-1}$	<LOD	$3.6 \times 10^{-1}$	<LOD	<LOD	<LOD	<LOD	$2.3 \times 10^{-1}$	$7.6 \times 10^{-1}$	1.10	<LOD	<LOD
Lauric acid	<LOD	<LOD	$1.5 \times 10^{-1}$	<LOD	$6.0 \times 10^{-2}$	<LOD	<LOD	<LOD	<LOD	$1.4 \times 10^{-1}$	$1.9 \times 10^{-1}$	$1.6 \times 10^{-1}$	$1.7 \times 10^{-1}$	$8.0 \times 10^{-2}$
Myristic acid	<LOD	<LOD	$3.0 \times 10^{-1}$	<LOD	$1.0 \times 10^{-1}$	$2.6 \times 10^{-1}$	<LOD	<LOD	<LOD	$1.4 \times 10^{-1}$	$3.0 \times 10^{-1}$	$3.0 \times 10^{-1}$	$2.8 \times 10^{-1}$	<LOD
Palmitic acid	$7.2 \times 10^{-1}$	<LOD	$4.5 \times 10^{-1}$	<LOD	$4.2 \times 10^{-1}$	1.50	$9.0 \times 10^{-2}$	<LOD	$4.8 \times 10^{-1}$	$5.0 \times 10^{-2}$	$3.5 \times 10^{-1}$	$5.9 \times 10^{-1}$	$2.0 \times 10^{-1}$	$3.5 \times 10^{-1}$
Citramalic acid	<LOD	<LOD	$5.3 \times 10^{-1}$	<LOD	$1.0 \times 10^{-1}$	<LOD	$2.2 \times 10^{-1}$	<LOD	<LOD	$5.0 \times 10^{-2}$	$1.3 \times 10^{-1}$	$5.4 \times 10^{-1}$	$2.8 \times 10^{-1}$	<LOD
Acetic acid	94.7	85.2	191	68.5	266	30.0	328	5448	77	2587	98.0	87.0	116	40.0
Methanol	20.0	19.8	<LOD	16.9	<LOD	22.7	<LOD	21.8	12.1	20.0	10.9	10.8	16.12	8.8
2-Butanol	44.0	<LOD	<LOD	<LOD	<LOD	<LOD	<LOD	<LOD	<LOD	<LOD	<LOD	<LOD	<LOD	<LOD
Propanol	122	175	78.0	52.0	45	530	<LOD	25.0	47.0	38.0	39.0	29.0	49.0	530
Isobutanol	127	60.0	75.0	42.0	11.0	20.0	<LOD	42.0	13.0	62.0	19.0	5.0	6.0	530
Butanol	2.7	6.5	1.10	<LOD	<LOD	1.7	<LOD	<LOD	<LOD	<LOD	<LOD	<LOD	<LOD	3.4
Isoamyl alcohol	103	378	286	168	59.0	93.0	<LOD	152	50.0	171	71.0	21.0	41.0	167
Ethyl carbamate	<LOD	$1.6 \times 10^{-1}$	<LOD	$9.0 \times 10^{-2}$	<LOD	$5.0 \times 10^{-2}$	<LOD	$1.5 \times 10^{-1}$	<LOD	$6.0 \times 10^{-2}$	<LOD	$2.2 \times 10^{-1}$	$1.5 \times 10^{-1}$	<LOD
Alcoholic content	27.7	39.7	37.7	29.4	20.9	44.16	22.3	18.8	17.8	23.0	21.6	16.4	15.5	31.5

LOD = Limit of Detection

**Table S2.** Median values (mg L<sup>-1</sup>) of secondary composition of head, heart and tail fractions from alembic distilled

Compounds	Boiling point <sup>a</sup> / °C	Head	Heart	Tail
<b>Esters</b>				
Ethyl acetate	77	454	37.8	27.5
Ethyl butanoate	121	1.0	<LOD	<LOD
Ethyl hexanoate	168	1.7	<LOD	<LOD
Ethyl lactate	118	17.2	32.6	34.7
Ethyl octanoate	172	7.87	0.5	<LOD
Ethyl nonanoate	186	0.082	<LOD	<LOD
Ethyl decanoate	200	13.85	1.775	<LOD
Isoamyl octanoate	198	0.078	<LOD	<LOD
Ethyl dodecanoate	228	2.58	0.77	<LOD
<b>Aldehydes</b>				
Acetylacetone	140	<LOD	<LOD	<LOD
Formaldehyde	20	0.13	0.04	0.01
5-HMF	115/1 mm Hg	0.05	0.13	0.08
Acetaldehyde	21	19.3	2.60	0.28
Acrolein	53	0.07	0.02	0.01
Propionaldehyde	48	0.13	0.08	0.03
Butiral/Isobutiraldehyde	75/ 63	0.31	0.07	0.04
Furfuraldehyde	162	0.06	<LOD	0.01
Benzaldehyde	179	0.33	0.02	0.01
Valeraldehyde	103	0.46	<LOD	<LOD
Diacetyl	88	0.018	0.010	0.007
<b>Organic acids</b>				
Lactic acid	122/15 mm Hg	17.4	41.0	76.8
Glycolic acid	112	<LOD	0.08	0.04
Pyruvic acid	165	<LOD	<LOD	<LOD

**Table S2.** Continuation

Compounds	Boiling point <sup>a</sup> / °C	Head	Heart	Tail
Organic acids				
Succinic acid	235	0.10	0.09	0.11
Capric acid	269	4.47	0.08	< LOD
Lauric acid	225	0.87	0.23	0.11
Myristic acid	250	0.50	0.27	0.12
Palmitic acid	271	1.87	1.11	0.35
Citramalic acid		< LOD	< LOD	0.1
Acetic acid	118	66.8	107.9	96.1
Alcohols				
Methanol	65	< LOD	14.4	16.0
2-Butanol	99.6	< LOD	< LOD	< LOD
Propanol	97	222	185	51
Isobutanol	108	415	180	42
Butanol	117	6.16	3.02	0.00
Isoamyl alcohol	129	1770	770	117
Ethyl carbamate / ppb	186	65.0	26.0	24.0
Alcoholic content	-	52.6	42.9	26.0

<sup>a</sup>Weast, R.C.; 53<sup>rd</sup> ed., *Handbook of Chemistry and Physics*; Chemical Rubber: Cleveland, 1986. LOD = Limit of Detection

**Table S3.** Select chemical data (mg L<sup>-1</sup>) for cachaça, bagaceira, orujo, grappa and rums distilled spirits

	Bagaceira <sup>14</sup>			Cachaça <sup>a</sup>			Bagaceira <sup>15</sup>	Orujo <sup>15</sup>	Grappa <sup>15</sup>	Cuban rum <sup>26</sup>	Non Cuban rum <sup>26</sup>
	Head	Heart	Tail	Head	Heart	Tail					
Decanoic acid	0.348	4.54	3.46	4.47	0.08	< LOD	3.7 ± 2.3	3.0	15.8	-	-
Dodecanoic acid	1.45	0.56	0.45	0.87	0.23	0.11	1.1 ± 0.7	4.1	3.3	-	-
Ethyl acetate	1325	321	403	454	37.8	27.5	209.2 ± 157.3	849	784.5 ± 149	40.5	57
Ethyl butyrate	0.152	0.202	0.019	1.0	< LOD	< LOD	1.2 ± 0.4	1.6	< LOD	-	-
Ethyl hexanoate	9.84	4.36	1.71	1.7	< LOD	< LOD	4.3 ± 2.9	9.1	5.1 ± 2.8	-	-
Ethyl octanoate	13.2	7.35	4.52	7.87	0.5	< LOD	11.0 ± 9.5	22.8	12.6 ± 8.3	-	-
Ethyl decanoate	3.95	4.18	2.27	13.85	1.775	< LOD	10.7 ± 6.2	19.1	39.6 ± 13.6	-	-
Ethyl dodecanoate	2.05	1.20	0.87	2.58	0.77	< LOD	2.3 ± 1.3	8.6	16.2 ± 13.2	-	-
Methanol	4554	2637	2981	< LOD	14.4	16.0	3389.2 ± 1279	5169	8869 ± 4338	22.3	16.7
Acetaldehyde	142	5.93	13.8	19.3	2.60	0.28	283 ± 212	58	< LOD	42.5	26.7
2-Butanol	< LOD	5.05	5.22	< LOD	< LOD	< LOD	53 ± 36.8	4.7	206 ± 33	1.62	10.3
Propanol	352	163	263	222	185	51	253 ± 75	304	1160 ± 113	49.9	36.5
1-Butanol	10.5	5.33	6.22	6.16	3.02	< LOD	22.7 ± 7.1	9.3	17.0 ± 14.1	96.9	33.2
Ethyl lactate	-	-	-	17.2	32.6	34.7	189.9	9.7	152 ± 31.1	-	-
Alcohol content	-	-	-	52.6	42.9	22.6	45 ± 4.5	58.1	72.9 ± 7.7	-	-

<sup>a</sup>This work. For commercial products, only the heart fraction is considered. LOD = Limit of Detection

**Table S4.** ANOVA (p-value) test, mean (mg L<sup>-1</sup>), and standard deviation values of secondary composition and among head, heart and tail fractions from alembic distilled

	ANOVA (p-value)			Standard deviation			Mean values		
	Between head and heart fractions	Between heart and tail fractions	Between head and tail fractions	Head	Heart	Tail	Head	Heart	Tail
Ester									
Ethyl acetate	0.028	0.642	0.005	604.1	489.4	326.0	713.	229.1	155.2
Ethyl butanoate	0.003	0.782	0.003	1.971	0.260	0.173	1.779	0.069	0.046
Ethyl hexanoate	0.004	0.327	0.004	3.597	0.102	0.000	3.079	0.027	0.000
Ethyl lactate	0.748	0.610	0.885	116.6	119.1	82.7	81.0	95.5	75.5
Ethyl octanoate	0.003	0.000	0.002	14.16	0.34	0.11	12.95	0.46	0.04
Ethyl nanoate	0.006	-	0.006	0.261	0.00	0.000	0.211	0.00	0.000
Ethyl decanoate	0.001	0.000	0.000	14.46	1.24	0.59	16.78	2.12	0.22
Isoamyl octanoate	0.007	0.251	0.003	0.152	0.0278	0.000	0.131	0.009	0.000
Ethyl dodecanoate	0.004	0.001	0.000	2.732	0.717	0.309	3.303	0.906	0.119
Aldehydes									
Formaldehyde	0.004	0.199	0.000	0.086	0.056	0.061	0.156	0.068	0.038
Acetaldehyde	0.000	0.041	0.000	19.01	3.51	2.43	24.89	3.61	1.15
Valeraldehyde	0.005	0.299	0.005	0.734	0.0296	0.010	0.613	0.011	0.003
Propionaldehyde	0.035	0.019	0.001	0.13	0.075	0.04	0.184	0.093	0.037
Benzaldehyde	0.018	0.136	0.002	0.371	0.158	0.04	0.367	0.095	0.03
Organic acids									
Lactic acid	0.151	0.281	0.038	40.54	66.96	111.4	34.78	65.78	104.1
Acetic acid	0.661	0.787	0.539	757.7	967.9	1461	349.7	495.2	623
Myristic acid	0.028	0.170	0.007	0.57	0.175	0.14	0.59	0.22	0.14
Palmitic acid	0.048	0.000	0.001	1.986	0.543	0.380	2.338	1.196	0.395
Alcohols									
Isobutanol	0.000	0.025	0.000	111.9	89.6	134.6	409.4	180.0	77.4
Butanol	0.100	0.006	0.001	6.973	4.322	1.905	8.641	4.903	1.166
Isoamyl alcohol	0.000	0.000	0.000	477.6	377.3	99.0	1727	765.8	135.2
Alcoholic content	0.000	0.000	0.000	8.322	4.526	9.151	53.6	42.1	26.2

**Table S5.** Secondary composition concentration (mg L<sup>-1</sup>) of sample tested in LDA

Organic compounds	Sample tested in LDA												
	SA	SB	SC	SD	SE	SF	SG	SH	SI	SJ	SK	SL	SM
Ethyl acetate	144	< LOD	189	161	80.8	68.4	95.5	63.4	513	226	50.9	99.1	987
Ethyl butanoate	< LOD	< LOD	< LOD	< LOD	0.440	< LOD	< LOD	0.550	0.610	< LOD	< LOD	< LOD	< LOD
Ethyl hexanoate	1.180	< LOD	0.635	0.562	0.618	0.579	< LOD	1.290	0.756	0.766	< LOD	< LOD	0.644
Ethyl lactate	< LOD	226	32	75.9	11.6	26.2	41.2	< LOD	64.4	157	32.4	26.4	559
Ethyl octanoate	5.57	1.91	1.99	1.87	1.82	1.82	1.42	3.59	2.31	1.77	1.53	1.23	1.71
Ethyl nonanoate	< LOD	< LOD	< LOD	< LOD	< LOD	< LOD	< LOD	< LOD	< LOD	< LOD	< LOD	< LOD	< LOD
Ethyl decanoate	13.1	3.74	3.66	4.42	3.4	3.47	2.88	6.13	4.81	2.54	3.18	< LOD	3.01
Isoamyl octanoate	0.950	< LOD	< LOD	< LOD	< LOD	< LOD	< LOD	< LOD	< LOD	< LOD	< LOD	< LOD	< LOD
Ethyl dodecanoate	6.24	2.05	< LOD	2.37	< LOD	1.92	< LOD	2.41	2.47	< LOD	< LOD	< LOD	1.88
Acetylacetone	< LOD	< LOD	< LOD	< LOD	< LOD	< LOD	< LOD	< LOD	< LOD	< LOD	< LOD	< LOD	< LOD
Formaldehyde	2.6	7.0	20.4	1.16	1.21	1.33	3.46	2.9	3.5	2.2	1.3	1.5	2.1
5-HMF	0.81	0.316	1.92	1.08	0.28	0.78	0.109	0.9	1.6	0.9	0.5	0.3	3.6
Acetaldehyde	236	61.8	200	123	98.5	100	123	127	101	172	45.2	89.5	133
Acrolein	0.3	0.126	0.218	< LOD	0.187	0.258	< LOD	< LOD	0.49	1.37	< LOD	< LOD	0.04
Propionaldehyde	0.01	0.057	0.074	0.045	0	0.06	0.1	< LOD	< LOD	< LOD	< LOD	< LOD	< LOD
Butiraldehyde	0.4	0.31	< LOD	0.456	0.74	0.61	< LOD	< LOD	< LOD	0.78	22	4.78	0.53
Furfuraldehyde	< LOD	< LOD	< LOD	< LOD	< LOD	< LOD	< LOD	< LOD	0.65	< LOD	< LOD	< LOD	< LOD
Benzaldehyde	9.1	8.55	1.89	5.71	8.57	1.72	1.9	2.3	2.1	< LOD	2.1	3.9	3.1
Valeraldehyde	< LOD	< LOD	5.75	< LOD	< LOD	< LOD	< LOD	< LOD	< LOD	2.65	< LOD	< LOD	< LOD
Diacetyl	< LOD	< LOD	< LOD	< LOD	< LOD	< LOD	< LOD	< LOD	< LOD	< LOD	< LOD	0.26	< LOD
Lactic acid	0.2	401	71.3	883	0.32	596	135	174	332	849	214	2.14	232.67
Glycolic acid	< LOD	< LOD	< LOD	< LOD	< LOD	< LOD	0.13	< LOD	0.16	0.02	< LOD	< LOD	< LOD
Pyruvic acid	< LOD	< LOD	< LOD	< LOD	< LOD	< LOD	0.4	< LOD	< LOD	< LOD	< LOD	< LOD	< LOD
Succinic acid	< LOD	< LOD	0.03	< LOD	< LOD	< LOD	0.03	< LOD	0.05	< LOD	0.02	< LOD	< LOD
Capric acid	0.79	0.18	0.11	< LOD	< LOD	< LOD	0.69	0.91	< LOD	0.09	0.13	< LOD	< LOD
Lauric acid	0.65	0.07	0.06	0.15	0.05	0.02	0.48	0.23	0.32	0.04	0.09	0.06	0.06
Myristic acid	0.08	0.15	0.37	0.11	0.06	0.09	0.11	0.01	0.21	0.1	0.28	0.05	0.04
Palmitic acid	0.24	0.47	0.21	0.73	0.5	0.58	0.17	0.03	0.31	0.15	0.16	0.11	1.22
Citramalic acid	< LOD	0.1	0.05	< LOD	< LOD	0.05	< LOD	< LOD	0.04	0.04	0.1	< LOD	0.06
Acetic acid	103	1752	171	136	100	67	129	14.6	1211	140	86.9	44.4	524
Methanol	239	1.1	7.85	14.6	21.1	14.5	15.6	66	17.2	130	21.7	50.9	519
2-Butanol	< LOD	0.5	< LOD	< LOD	33	< LOD	< LOD	< LOD	< LOD	< LOD	< LOD	78.2	< LOD
Propanol	118	1330	329	126	215	124	232	157	140	432	118	185	237
Isobutanol	323	115	171	189	196	111	187	256	249	145	234	219	131
Butanol	3.6	0.58	10.3	0	4.26	4.26	4.64	4.12	4.54	< LOD	< LOD	< LOD	< LOD
Isoamyl alcohol	1190	476	462	827	779	780	368	642	754	433	937	549	455
Ethyl carbamate / ppb	< LOD	60	50	70	40	< LOD	< LOD	< LOD	< LOD	< LOD	< LOD	< LOD	100
Alcoholic content	42.6	40.6	41.3	41.7	41.9	35.4	41.3	40.3	38.7	40.3	41	38.7	44.2

LOD = Limit of Detection

**Table S6.** Mean values of relative standard deviation - RSD (%) for analytical data analyzed

Compounds	RSD / %	Compounds	RSD / %
Ethyl acetate	3.4	Acetylacetone	8.7
Ethyl butyrate	2.5	Formaldehyde	2.9
Ethyl hexanoate	0.7	5-HMF	4.8
Ethyl lactate	2.0	Acetaldehyde	2.4
Ethyl octanoate	1.9	Acrolein	4.5
Ethyl nonanoate	2.6	Propionaldehyde	2.5
Ethyl decanoate	3.0	Butiral/ Isobutiraldehyde	6.2
Isoamyl octanoate	5.1	Furfuraldehyde	5.9
Ethyl laurate	4.1	Benzaldehyde	2.1
Ethyl carbamate	5.0	Valeraldehyde	3.8
Lactic acid	2.9	Diacetyl	9.1
Glycolic acid	7.6	Methanol	1.9
Pyruvic acid	8.8	2-Butanol	1.0
Succinic acid	3.7	Propanol	1.2
Capric acid	4.3	Isobutanol	3.2
Lauric acid	2.6	Butanol	4.2
Myristic acid	2.9	Isoamyl alcohol	1.6
Palmitic acid	1.3		
Citramalic acid	8.4		
Acetic acid	3.9		