Supplementary Information for

Archeochemistry reveals the first steps into modern industrial brewing

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Supplementary tables

Supplementary Table S1. Regular beer attributes and folate contents of Barre Pilsener from 1885 and 2019 compared to Vienna, Böhmisch and Bayerisch beer from 1888.

Beer attribute	Unit	Barre Pilsner 1885	Vienna Beer [a]	Bohemian Beer [a]	Bavarian Beer [a]	Barre Pilsner 2019
Original gravity	w/w%	10.36	10.39-13.26	12.45	14.71	11.195
Alcohol	w/w%	3.12	2.9-3.7	3.43	3.94	3.94
Real extract	w/w%	4.26	4.4-5.7	5.4	6.7	3.6
Attenuation limit, real	%	58.8	57	56.2	54.3	68
pH	-	4.42	-	-	-	4.21
Bitter units	IBU [b]	18.4	-	-	-	28.7
Color	EBC [c]	12.5	-	-	-	7.7
Folate analysis						
PteGlu	[µg/100g]	n.d.	-	-	-	n.d. [d]
H_4Holate	[µg/100g]	n.d.	-	-	-	n.d.
5-CH_3-H_4Folate	[µg/100g]	0.58	-	-	-	1.10
5-CHO-H_4Folate	[µg/100g]	n.d.	-	-	-	2.06
10-CHO-PteGlu	[µg/100g]	n.d.	-	-	-	3.91
Total Folates	[µg/100g]	0.58	-	-	-	7.08

[a] Thausing, J.E. (1888), Die Theorie und Praxis der Malzbereitung und Bierfabrikation, Gebhardt's

[b] International Bitter Units

[c] European Brewery Convention (value)

[d] not detected

Supplementary Table S2. ^{1}H and ^{13}C chemical Shifts, Proton Multiplicities for identified metabolites in the beer samples.

Compound (No.)	Assigned group	δ ^{1}H	Multiplicity [a]	δ ^{13}C
2-Methyl-1-propanol (1)	2xCH_3	0.88	d	21.0
	$(CH_3)_2CHCH_2OH$	1.76	m	27.0
	$(CH_3)_2CHCH_2OH$	3.38		
3-Methyl-1-butanol (2)	2xCH_3	0.89	d	24.8
	$(CH_3)_2CH(CH_2)_2OH$	1.44	m	43.0
	$(CH_3)_2CHCH_2CH_2O$	1.66	m	27.2
	H	3.64		
Propanol (3)	$CH_3CH_2CH_2OH$	0.89	t	n.d. [b]
	$CH_3CH_2CH_2OH$	1.56	m	
	$CH_3CH_2CH_2OH$	3.57	t	
Valine (4)	2xCH_3	1.05, 0.99 2.27	d, d	19.7
	$(CH_3)_2CH$		m	
Lactic acid (5)	CH_3(CHOH)COOH	1.33	d	19.33
	CH_3(CHOH)COOH	4.11	q	71.6
Alanine (6)	CH_3	1.48	d	19.4
	CH	3.79	q	
Acetic acid (7)	CH_3	1.92	s	26.3
Proline (8)	γ-CH_2	2.00	m	26.6
	β-CH_2	2.06	m	31.7
	β-CH_2	2.33	m	31.7
	σ-CH_2	3.32	m	48.9
	σ-CH_2	3.41	m	48.9
	α-CH	4.11	dd	64.1
GABA (9)	CH_2COO	2.30	t	37.3
	$(CH_2)CH_2(CH_2$	1.90	m	26.7
	NH_2CH_2	3.02	t	42.3
Pyruvate (10)	CH_3	2.37	s	29.5
Succinic acid (11)	$(CH_2)_2$	2.40	s	37.4
Citrate (12)	CH'_2	2.53	d	48.8
	CH''_2	2.66	d	48.8
(13) – (20)	Compound classes			
Uridine (21)	2x C=CH	5.92, 7.88	d, d	90.7,144.8
Adenosin/ Inosine (22)	N=CH′	8.27	s	155.7
	N=CH′′	8.36	s	143.5
	OCHN	6.07	d	91.3
Tyrosol (23)	2x C=CH′	6.87	m	118.6
	2x C=CH′′	7.19	m	133.4
Tyrosine (24)	2x C=CH′	6.91	m	119.0
	2x C=CH′′	7.20	m	133.7
Phenylalanine (25)	$CH'_{aromatic}$	7.34	m	132.1
	$CH''_{aromatic}$	7.43	m	131.1
Histidine (26)	N=CH	8.00	s	140.7
	C=CH	7.06	s	119.5
Cytidine (27)	C=CH′	6.07	d	99.2
	C=CH′′	7.85	d	144.7
Formic acid (28)	HCOOH	8.46	s	174.0
Niacin (29)	4x C=CH	8.95, 8.62 8.27,	m	n.d.

Supplementary Table S2 (continued). ^{1}H and ^{13}C chemical Shifts, Proton Multiplicities for identified metabolites in the beer samples.

Compound (No.)	Assigned group	σ ^{1}H	Multiplicity [a]	σ ^{13}C
HMF (30)	C**H**O	9.46	s	183.7
	2x C=C**H**	7.55	d	n.d.
	C**H**$_2$OH	6.69	m	n.d.
Furfural (31)	C**H**O	9.50	s	n.d.
	3x C=C**H**	7.94, 7.60, 6.78	m	n.d.
Acetaldehyde (32)	C**H**O	9.68	q	n.d.
	C**H**$_3$	2.21	d	n.d.

[a] singlet (s), doublet (d), triplet (t), quartet (q), doublet of doublets (dd), multiplet (m)

[b] not detected

Supplementary Table S3. General statistical and model parameters of the multivariate data analysis.

Parameter	
Missing values	Random noise imputation within the range of (average noise level – σ ± σ)
Data normalization	UV-scaling
Outlier detection	Hotelling's T^2 (95 %)
7-fold Cross validation	R^2Y (cum)
	Q^2 (cum)
Additional CV	CV-ANOVA
Significant features	95th percentile of features with most characteristic loadings (385 compositions)
Metadata	As given on the beers' label. The UV/Vis measurements were executed for 221 samples as described in Pieczonka et al. (2021), Food Chem., 361 (130112), 1-9
Sample exclusion	For the grain and Purity Law model, 23 samples were excluded due to ambiguous information of the grains used ("rice and/or corn", "cereals")
Statistics software	SIMCA 13.0.3.0 (Umetrics, Umeå, Sweden)

Statistical model	**n**	**A**	**R^2Y**	**R^2X**	**Q^2**	**ANOVA**	
						F	**p**
Beer type (OPLS-DA)	400	2+5+0	0.865	0.294	0.752	83.27	<< 0.05
Fermentation (OPLS-DA)	400	1+5+0	0.936	0.274	0.792	122.75	<< 0.05
Purity Law (OPLS-DA)	377	1+8+0	0.971	0.325	0.569	26.26	<< 0.05
Grain (OPLS-DA)	377	2+9+0	0.858	0.363	0.579	16.64	<< 0.05
Maillard (OPLS) 294 nm	221	1+3+0	0.941	0.239	0.806	108.60	<< 0.05

Supplementary Table S4. Instrumental parameters and reagents used for FTICR-MS, UPLC-ToF-MS and HPLC-Triple Quad (Folates) measurements.

Reagent	**Source**
Methanol (MeOH)	FLUKA, Sigma-Aldrich (LC-MS grade, CHROMASOLV, St Louis, MO, USA)
Acetonitrile (ACN)	FLUKA, Sigma-Aldrich (LC-MS grade, CHROMASOLV, St Louis, MO, USA)
	Honeywell CHROMASOLV® (LC-MS grade)
Ultrapure water	Milli-Q Integral Water Purification System (Millipore, MA, Billerica, USA)
	CHEMSOLUTE® (LC-MS grade)
L-arginine	Sigma-Aldrich (reagent grade >98%, St Louis, MO, USA)
Formic acid (FA)	VWR HiPerSolv CHROMANORM® (LC-MS grade; ≥99%)

FTICR-MS	**Value**
Sample preparation	Degassing by ultrasonification (10 °C, 5min.); dilution 1:500 in methanol (v:v); separation of precipitated proteins by centrifugation (10,000 rpm, 3min.)
Spectrometer	Bruker solariX
ICR-cell	Infinity Cell
Direct injection flowrate	120 µL.h^{-1}.
ESI capillary voltage	3600 V (negative ionization) (APOLO II ESI source (Bruker Daltonics GmbH, Bremen, Germany)
Magnetic field	12 T superconducting magnet (Magnex Scientific Inc., Yarton, GB)
Time domain	4 mega words
Accumulation time	0.25 ms
Mass range	*m/z* 120 to 1000
Accumulated scans	400 (for all samples), 2000 (additionally for Samples B1855 and B2019)
Measurement time	10 min.
External calibration	clusters of arginine (5 mg.L^{-1} in methanol)
Internal calibration	in-house calibration list containing 2000 sum formulae, which are highly abundant in beers
Timeframe of analyses	2018 to 2020
Quality Control	Representative beer sample measured as QC within the course of the batches

UPLC-ToF-MS	**Value**
Sample preparation	SPE: Bond Elut PPL, 1 mL and 100 mg (Agilent Santa Clara, CA, USA); conditioning: 100 µL MeOH, 2x1000µL Mili-Q-Water + 2% Formic acid (FA); 1000 µL acidified sample (2% FA); washing: 500 µL Mili-Q-Water + 2%FA; dry vacuum; elution: 2x500µL MeOH)
Spectrometer	Shimadzu LCMS-9030 Q ToF
Column	RP (C18: 1.7 µm, 2.1 x 100 mm, Acquity™ UPLC BEH™)
Flow rate	400 µL min^{-1}

Supplementary Table S4 (continued). Instrumental parameters and reagents used for FTICR-MS, UPLC-ToF-MS and HPLC-Triple Quad (Folates) measurements.

UPLC-ToF-MS	**Value**
ESI ionization mode	negative
Column temperature	40 °C
Injection volume	5 µL (partial loop)
Gradient profile	95 % A (0.1 % formic acid in water) and 5 % B (0.1 % formic acid in acetonitrile) for 1 min; decreasing to 0.5 % A in 5 min; held for 4 min.
Measurement time	10 min.
External calibration	Sodium iodide solution clusters
Internal calibration	ESI-L Low Concentration Tuning Mix
Nitrogen flowrate	10 L min^{-1}
Interface temperature	300°C
Nebulizer gas flow	1 L min^{-1}
Interface voltage	-4 kV
DL temperature	250 °C
Heat block temperature	400 °C
Drying gas flow	10 L min^{-1}
Detector voltage	2 kV
MS^1 parameters	5 Hz event cycle time
	Ion accumulation on
MS^2 fragmentation parameters	DDA (3 dependent events)
	CE spread 20 eV ± 15 eV

UHPLC-Triple Quad-MS (Folates)	**Value**
Sample preparation	The sample preparation of Striegel et al. (2018), *Front. Chem*., 6(11) was modified by adding the suitable $^{13}C_5$ labelled isotopologue standard of 10-CHO-PteGlu for quantification. As described in Pferdemenges et al. (2021), *J. Food Compos. Anal.*
Spectrometer	Shimadzu Nexera X2
Column	Raptor™ ARC-18 (2.7 µm, 100 x 2.1 mm)
Precolumn	Raptor™ EXP Guard Column (2.7 µm, 5 x 2.1 mm)
Flow rate	400 µL min^{-1}
Column temperature	30 °C
Injection volume	10 µL
Gradient profile	97 % A (0.1 % formic acid in water) and 3 % B (0.1 % formic acid in acetonitrile) for 1 min; increasing to 10% B in 2 min; held for 2.5 min; increasing to 15 % B in 5 min; increasing to 50 % B in 1 min; held for 1 min; decrease to 3 % B in 1 min; equilibrate for 4 min.
Measurement time	17.5 min
ESI ionization mode	Positive (MRM-multiple reaction monitoring)

Supplementary Table S4 (continued). Instrumental parameters and reagents used for FTICR-MS, UPLC-ToF-MS and HPLC-Triple Quad (Folates) measurements.

UHPLC-Triple Quad-MS (Folates)	**Value**
Interface temperature	300 °C
Nebulizer gas flow	3 L min^{-1}
Heating gas flow	10 L min^{-1}
Interface voltage	4 kV
DL temperature	250 °C
Heat block temperature	400 °C
Drying gas flow	10 L min^{-1}
CID gas	270 kPa

Supplementary Table S5. Instrumental parameters, reagents and standards used for NMR-measurements.

Reagent	Source (Purity)
D_2O	Armar chemicals (99.8 atom%, Döttingen, CH)
Di-sodiumhydrogenphosphate dodecahydrate	Merck Millipore (99 %, Billerica, MA, USA)
3-(trimethylsilyl)propionic-2,2,3,3-d4 acid sodium salt	Sigma Aldrich (98 atom%, MO, St Louis, USA)
Standard	**Source (Purity)**
Furfural	Sigma Aldrich (99 %, MO, St Louis, USA)
Niacin	Sigma Aldrich (≥ 98 %, MO, St Louis, USA)
Histidine	Merck Millipore (≥ 98 %, MA, Billerica, USA)
Xylose	Sigma Aldrich (≥ 99 %, MO, St Louis, USA)
NMR	**Value**
Spectrometer	800 MHz Bruker AVANCE lll
Probehead	5 mm QCI-probehead
Temperature	300 K
Pusle calibration	Calibrated for each acquisition
Processing	Sine bell with shift 2 in all dimensions
1D-NOE-experiment	
Pulse sequence	90° pulse (12.4 µs), mixing time (100 ms), relaxation delay (16 s), t1 measured by inversion recovery and based on slowest relaxing hydrogen, presaturation for 2.4 sec prior to the first pulse
Cycle time	20 s (AQ = 4 s)
Data acquisition	32 transients, 102562 data points
Spectral width	12,820 Hz
2D-TOCSY (^{1}H, ^{1}H)	
Pulse program	dipsi2gpph
Pulse sequence	90° pulse (12.4 µs), mixing time (70 ms), relaxation delay (2.4 s), t1 (42.5 ms), t2 (2 s)
Data acquisition	16 transients, 1024 increments, 48074 data points
Spectral width	12,000 Hz (both dimensions)

Supplementary Table S5. Instrumental parameters, reagents and standards used for NMR-measurements.

NMR	Value
2-D HSQC (^{1}H, ^{13}C)	
Pulse program	Hsqcetgppssisp2.2
Pulse sequence	90° pulse (^{1}H 12.4 µs, ^{13}C 11.5 µs), relaxation delay (1.25 s), t1 (3.2 ms), t2 (0.25 s)
Data acquisition	128 transients, 300 increments
Spectral width	12,000 Hz (F2), 46,300 Hz (F1)

Supplementary Table S6. Metadata of the analyzed beer samples.

Sample	Beer style	Fermen-tation	PurityLaw	Grain	Abs. 294 nm	Origin	Sample	Beer style	Fermen-tation	Purity Law	Grain	Abs. 294nm	Origin
1	Wheat	top	yes	Wheat	0.048	GER	**238**	Lager	bottom	yes	Barley	0.330	GER
2	Lager	bottom	yes	Barley	0.083	GER	**239**	Lager	bottom	no	Rice	-	ESP
3	Lager	bottom	yes	Barley	0.105	GER	**241**	Lager	bottom	no	Rice	-	ESP
4	Craft	top	no	Barley	0.069	BEL	**242**	Lager	bottom	yes	Barley	0.166	GER
5	Wheat	top	yes	Wheat	0.081	GER	**243**	Lager	bottom	yes	Barley	0.133	GER
6	Wheat	top	yes	Wheat	0.07	GER	**244**	Lager	bottom	yes	Barley	0.145	GER
7	Wheat	top	yes	Wheat	-	GER	**245**	Lager	bottom	yes	Barley	0.115	GER
8	Lager	bottom	yes	Barley	0.077	GER	**246**	Lager	bottom	yes	Barley	0.129	GER
9	Lager	bottom	yes	Barley	0.162	GER	**247**	Lager	bottom	yes	Barley	0.186	GER
10	Lager	bottom	yes	Barley	0.14	GER	**248**	Lager	bottom	yes	Barley	0.111	GER
11	Wheat	top	yes	Wheat	-	GER	**249**	Lager	bottom	yes	Barley	0.172	GER
12	Wheat	top	yes	Wheat	0.168	GER	**250**	Wheat	top	yes	Wheat	0.158	GER
13	Lager	top	yes	Barley	0.17	GER	**251**	Wheat	top	yes	Wheat	0.18	GER
15	Lager	bottom	yes	Barley	0.067	GER	**252**	Lager	bottom	yes	Barley	0.129	GER
16	Lager	bottom	yes	Barley	0.053	GER	**253**	Wheat	top	yes	Wheat	0.137	GER
19	Wheat	top	yes	Wheat	0.136	GER	**254**	Lager	bottom	no	Barley	0.122	CZE
20	Wheat	top	yes	Wheat	0.149	GER	**255**	Wheat	top	yes	Wheat	0.159	GER
21	Wheat	top	yes	Wheat	0.144	GER	**256**	Wheat	top	yes	Wheat	0.137	GER
22	Lager	bottom	yes	Barley	0.138	GER	**257**	Wheat	top	yes	Wheat	0.156	GER
23	Lager	bottom	yes	Barley	0.298	GER	**258**	Wheat	top	yes	Wheat	0.185	GER
24	Lager	bottom	no	Barley	0.267	IRL	**259**	Wheat	top	yes	Wheat	0.235	GER
25	Wheat	top	yes	Wheat	0.2	GER	**260**	Lager	bottom	yes	Barley	0.177	GER
26	Lager	bottom	yes	Barley	0.356	GER	**261**	Lager	bottom	yes	Barley	0.167	GER
27	Lager	bottom	yes	Barley	0.142	GER	**262**	Lager	bottom	yes	Barley	-	GER
28	Wheat	top	yes	Wheat	0.243	GER	**263**	Wheat	top	yes	Wheat	-	GER
29	Wheat	top	yes	Wheat	0.224	GER	**264**	Lager	bottom	no	Corn	-	ESP
30	Lager	bottom	yes	Barley	0.138	GER	**265**	Lager	bottom	no	Corn	-	ESP
31	Wheat	top	yes	Wheat	-	GER	**266**	Lager	bottom	no	Corn	-	ESP
32	Craft	top	no	Barley	0.127	BEL	**267**	Lager	bottom	no	Corn	-	ESP
33	Wheat	top	yes	Wheat	0.264	GER	**268**	Lager	bottom	no	-	-	ESP
34	Wheat	top	yes	Wheat	0.074	GER	**269**	Lager	bottom	no	Corn	-	ESP
35	Lager	top	yes	Barley	0.136	GER	**270**	Lager	bottom	no	Corn	-	ESP
36	Lager	bottom	yes	Barley	0.126	GER	**271**	Lager	bottom	no	Corn	-	ESP
37	Lager	bottom	yes	Barley	0.42	GER	**272**	Lager	bottom	no	Rice	0.358	ESP
38	Wheat	top	yes	Wheat	0.124	GER	**273**	Craft	top	yes	Barley	-	ESP
39	Lager	bottom	yes	Barley	0.145	GER	**274**	Lager	bottom	no	Rice	-	ESP
41	Wheat	top	yes	Wheat	0.139	GER	**275**	Lager	bottom	no	Corn	0.139	ESP
43	Craft	top	yes	Barley	0.129	BEL	**276**	Lager	bottom	no	Corn	-	ESP
44	Lager	bottom	yes	Barley	0.122	GER	**277**	Lager	bottom	no	Corn	-	ESP
45	Wheat	top	yes	Wheat	0.13	GER	**278**	Craft	top	yes	Barley	-	ESP
46	Lager	bottom	yes	Barley	0.099	GER	**279**	Lager	bottom	yes	Barley	-	ESP
47	Lager	bottom	yes	Wheat	0.113	GER	**280**	Lager	bottom	no	Corn	-	ESP
48	Lager	bottom	yes	Barley	0.399	GER	**281**	Craft	top	yes	Barley	-	ESP
49	Craft	top	yes	Barley	0.203	GER	**282**	Craft	top	yes	Barley	0.386	ESP
50	Lager	bottom	yes	Barley	0.121	GER	**283**	Lager	bottom	no	Corn	-	ESP
51	Wheat	top	yes	Wheat	0.197	GER	**284**	Craft	top	yes	Barley	0.222	ESP
52	Wheat	top	yes	Wheat	0.149	GER	**285**	Lager	bottom	no	Corn	0.16	ESP
53	Lager	bottom	yes	Barley	-	GER	**286**	Craft	top	yes	Barley	-	ESP
54	Craft	top	no	Barley	-	BEL	**287**	Craft	top	yes	Barley	-	ESP
55	Craft	top	no	Wheat	0.187	LTU	**288**	Craft	top	no	Barley	-	BEL
56	Wheat	top	yes	Wheat	0.169	GER	**289**	Craft	top	no	Wheat	-	BEL
57	Craft	top	yes	Barley	0.421	GER	**290**	Wheat	top	no	Wheat	0.169	NLD
58	Wheat	top	yes	Wheat	0.156	GER	**291**	Lager	top	no	Barley	-	BEL
59	Craft	top	no	Barley	-	BEL	**292**	Craft	top	no	Barley	0.13	BEL
60	Craft	top	yes	Barley	0.282	GER	**293**	Lager	bottom	yes	Barley	0.27	HRV
61	Craft	top	yes	Wheat	0.191	GER	**294**	Lager	bottom	yes	Barley	-	SLO
62	Craft	top	yes	Wheat	-	GER	**295**	Lager	bottom	yes	Barley	-	HRV
63	Wheat	top	yes	Wheat	-	GER	**296**	Lager	bottom	no	Corn	-	HRV
64	Craft	top	yes	Barley	0.174	GER	**297**	Lager	bottom	yes	-	-	HRV
65	Craft	top	no	Barley	0.296	BEL	**298**	Craft	top	yes	Barley	-	HRV
66	Craft	top	no	Barley	0.33	BEL	**299**	Craft	top	yes	Wheat	-	HRV
67	Wheat	top	no	Wheat	0.167	GER	**300**	Lager	bottom	yes	Barley	0.252	HRV
68	Lager	bottom	yes	Barley	0.218	GER	**301**	Craft	top	yes	Barley	-	HRV
69	Wheat	top	no	Wheat	0.095	BEL	**302**	Lager	bottom	no	Barley	-	HRV
70	Lager	bottom	yes	Barley	0.048	NAM	**303**	Wheat	top	yes	Wheat	-	HRV
71	Lager	bottom	yes	Barley	-	DNK	**304**	Lager	bottom	yes	Barley	-	HRV
72	Lager	bottom	yes	Barley	-	GER	**305**	Wheat	top	yes	Wheat	-	HRV
73	Lager	bottom	yes	Barley	-	GER	**306**	Lager	bottom	yes	Barley	-	JPN
76	Wheat	top	yes	Wheat	0.279	GER	**307**	Lager	bottom	no	Rice	-	JPN
78	Craft	top	yes	Barley	0.275	GER	**308**	Lager	top	yes	Wheat	-	JPN
80	Lager	bottom	no	Rice	0.112	GER	**309**	Lager	bottom	no	Rice	-	JPN
81	Craft	top	yes	Barley	0.222	GER	**310**	Craft	top	yes	Barley	-	USA
83	Lager	bottom	yes	Barley	0.243	GER	**311**	Lager	bottom	no	Rice	-	JPN
85	Craft	top	yes	Wheat	-	GER	**312**	Lager	bottom	no	Rice	-	JPN
86	Craft	top	yes	Barley	0.238	GER	**313**	Lager	bottom	no	Rice	-	JPN
90	Craft	top	yes	Barley	0.136	GER	**314**	Wheat	top	no	Wheat	-	FRA
91	Lager	bottom	no	Barley	0.099	CUB	**315**	Lager	top	no	Barley	-	FRA
92	Lager	bottom	no	Barley	0.063	CUB	**317**	Lager	bottom	no	-	-	ESP
93	Lager	bottom	yes	Barley	0.232	MEX	**318**	Lager	bottom	no	Rice	-	ESP
94	Lager	bottom	yes	Barley	0.134	MEX	**319**	Lager	bottom	no	Corn	-	ESP
95	Lager	bottom	no	Rice	0.086	CHN	**320**	Lager	bottom	no	Corn	-	ESP
96	Lager	bottom	yes	Barley	0.16	PER	**321**	Lager	bottom	no	Rice	-	ESP
97	Lager	bottom	no	Corn	0.1	ARG	**322**	Lager	bottom	no	-	-	ESP
98	Lager	bottom	yes	Barley	-	PER	**323**	Lager	bottom	no	Corn	-	ESP

Supplementary Table S6 (continued). Metadata of the analyzed beer samples.

Sample	Beer style	Fermen -tation	Purity Law	Grain	Abs. 294 nm	Origin	Sample	Beer style	Fermen -tation	Purity Law	Grain	Abs. 294nm	Origin
99	Lager	bottom	no	Barlev	0.137	ESP	**324**	Lager	bottom	no	Rice	-	ESP
100	Craft	top	no	-	-	BRA	**325**	Lager	bottom	no	-	-	ESP
101	Craft	top	no	Rice	0.189	JPN	**326**	Lager	bottom	yes	Barley	-	ESP
102	Wheat	top	no	Wheat	0.116	NDL	**327**	Lager	bottom	no	Rice	-	ESP
103	Lager	bottom	no	Barley	0.104	KOR	**328**	Lager	bottom	no	Corn	-	ESP
104	Craft	top	yes	Barley	-	GER	**329**	Lager	bottom	no	Corn	-	ESP
105	Craft	top	no	Wheat	0.121	BEL	**330**	Lager	bottom	no	Corn	-	ESP
106	Craft	top	yes	Wheat	0.36	BEL	**331**	Lager	bottom	no	Rice	-	ESP
107	Craft	top	no	Barley	0.192	BEL	**333**	Lager	bottom	yes	Barley	-	ESP
108	Craft	top	no	Wheat	0.107	BEL	**334**	Lager	bottom	no	Rice	-	PHL
109	Craft	top	yes	Barley	0.368	BEL	**335**	Lager	bottom	no	Rice	-	THA
110	Craft	top	yes	Barley	0.204	NDL	**336**	Lager	bottom	no	Rice	-	TWN
111	Lager	bottom	yes	Barley	0.134	NDL	**337**	Lager	bottom	no	Rice	-	SGP
112	Craft	top	yes	Barley	0.219	NDL	**357**	Craft	top	yes	Wheat	-	GER
113	Lager	bottom	yes	Barley	0.167	GER	**358**	Lager	bottom	yes	Barley	-	GER
114	Lager	bottom	yes	Barley	0.127	SGP	**360**	Craft	top	no	-	-	MEX
116	Craft	top	no	Barley	0.238	BEL	**361**	Lager	bottom	no	-	-	MEX
117	Craft	top	yes	Wheat	0.167	BEL	**362**	Lager	bottom	no	-	-	MEX
118	Craft	top	yes	Wheat	-	BEL	**363**	Lager	bottom	yes	-	-	MEX
119	Craft	top	yes	Barley	0.709	NDL	**364**	Craft	top	no	Wheat	-	ZAF
121	Craft	top	yes	Wheat	-	BEL	**365**	Craft	top	no	Barley	-	USA
123	Craft	top	no	Wheat	0.132	NDL	**366**	Lager	bottom	no	-	-	EGY
124	Craft	top	yes	Wheat	0.418	GER	**367**	Wheat	top	yes	Wheat	-	NAM
125	Craft	top	no	Barley	0.276	BEL	**368**	Craft	top	yes	Barley	-	ZAF
126	Craft	top	yes	Wheat	-	BEL	**369**	Lager	bottom	yes	Barley	-	ZAF
127	Lager	bottom	yes	Barley	0.334	GER	**370**	Craft	top	yes	Barley	-	USA
128	Craft	top	yes	Barley	0.657	GER	**371**	Wheat	top	yes	Wheat	-	GER
129	Lager	bottom	yes	Barley	0.197	NDL	**372**	Wheat	top	yes	Wheat	-	ZAF
130	Craft	top	no	Barley	0.353	BEL	**373**	Lager	bottom	no	-	-	ARG
131	Craft	top	yes	Barley	0.144	BEL	**374**	Lager	bottom	no	-	-	ARG
132	Craft	top	no	Barley	0.183	BEL	**375**	Lager	bottom	yes	Barley	-	ZAF
133	Craft	top	no	Wheat	0.187	BEL	**376**	Lager	bottom	yes	Barley	-	BRA
134	Craft	top	no	Barley	-	BEL	**377**	Lager	bottom	no	-	-	BRA
136	Lager	bottom	yes	Barley	0.095	FRA	**378**	Lager	bottom	no	-	-	MEX
137	Wheat	top	yes	Wheat	-	GER	**379**	Lager	bottom	no	Corn	-	MEX
138	Craft	top	no	Wheat	0.076	BEL	**380**	Craft	top	yes	Barley	-	USA
139	Lager	bottom	no	Barley	0.128	IND	**381**	Lager	bottom	no	Rice	-	JPN
140	Lager	bottom	yes	Barley	0.288	GER	**382**	Lager	bottom	no	Rice	-	CHN
141	Lager	bottom	yes	Barley	0.409	GER	**383**	Lager	bottom	no	Corn	-	BRA
142	Lager	bottom	yes	Barley	0.177	GER	**385**	Lager	bottom	yes	Barley	-	CHE
143	Lager	bottom	yes	Barley	0.137	GER	**386**	Craft	top	yes	-	-	CHN
144	Lager	bottom	yes	Barley	0.086	GER	**387**	Craft	top	yes	Barley	-	USA
145	Lager	bottom	no	Barley	0.102	MEX	**388**	Lager	bottom	no	-	-	BRA
146	Lager	bottom	yes	Barley	0.095	BEL	**389**	Craft	top	no	Barley	0.627	ESP
147	Lager	bottom	yes	Barley	0.326	GER	**390**	Craft	top	no	Barley	-	ESP
148	Lager	bottom	yes	Barley	0.153	GER	**391**	Lager	bottom	no	Rice	-	MEX
149	Craft	top	no	Barley	0.19	BEL	**392**	Lager	bottom	yes	Barley	-	FRA
151	Craft	top	no	Corn	0.189	FRA	**393**	Craft	top	yes	Barley	-	ITA
152	Wheat	top	yes	Wheat	0.118	GER	**394**	Craft	top	no	Rice	0.709	ITA
153	Lager	bottom	yes	Barley	0.147	GER	**395**	Craft	top	no	Wheat	-	ITA
154	Lager	bottom	yes	Barley	0.146	GER	**396**	Craft	top	yes	Barley	-	ITA
155	Wheat	top	yes	Wheat	0.349	GER	**397**	Craft	top	yes	Wheat	-	ITA
156	Craft	top	no	Corn	0.287	FRA	**398**	Craft	top	yes	Barley	0.46	ESP
157	Lager	bottom	yes	Barley	0.184	GER	**399**	Craft	top	yes	Barley	-	CRO
159	Lager	bottom	yes	Barley	0.123	GER	**400**	Craft	top	no	Wheat	-	ESP
160	Lager	bottom	no	Corn	-	CHN	**401**	Craft	top	yes	Barley	-	GRE
161	Lager	bottom	no	-	0.118	ITA	**402**	Craft	top	no	Wheat	-	EST
162	Lager	bottom	no	Barley	0.12	PHL	**404**	Craft	top	no	Wheat	-	GRE
163	Lager	bottom	yes	Barley	0.112	GER	**405**	Craft	top	no	Wheat	-	CAT
164	Lager	bottom	no	-	0.115	GBR	**406**	Craft	top	yes	Barley	-	POR
165	Lager	bottom	yes	Barley	0.137	GER	**407**	Lager	bottom	no	Rice	-	CHN
166	Lager	bottom	no	Rice	0.126	THA	**408**	Lager	bottom	no	-	-	ITA
167	Lager	bottom	no	Corn	0.124	ITA	**409**	Craft	top	no	Wheat	-	FRA
168	Lager	bottom	no	Rice	0.114	CHN	**410**	Lager	bottom	no	Rice	-	VAT
169	Lager	bottom	no	Corn	0.132	ITA	**411**	Lager	bottom	no	Corn	-	CHN
170	Lager	bottom	no	Rice	0.088	GTM	**412**	Lager	bottom	no	Wheat	-	NLD
171	Lager	bottom	no	Rice	0.088	GTM	**413**	Lager	bottom	no	Rice	-	CHN
172	Lager	bottom	no	Corn	0.089	CRI	**414**	Lager	bottom	yes	Barley	-	GER
173	Lager	bottom	no	Rice	0.084	NIC	**416**	Craft	top	yes	Barley	0.247	GER
174	Craft	top	yes	Barley	0.153	FIN	**417**	Craft	top	yes	Barley	0.685	NDL
175	Lager	bottom	no	Barley	0.103	FIN	**418**	Craft	top	yes	Barley	0.456	GBR
177	Craft	top	yes	Barley	0.331	FIN	**419**	Craft	top	yes	Barley	0.457	GBR
178	Lager	bottom	yes	Barley	0.108	LUX	**420**	Craft	top	no	Barley	0.367	GER
179	Lager	bottom	yes	Barley	0.123	FRA	**421**	Craft	top	no	Barley	0.435	GBR
180	Lager	bottom	yes	Barley	0.188	LUX	**422**	Craft	top	no	Barley	0.613	GER
182	Craft	top	yes	Barley	0.183	NZL	**424**	Craft	top	no	Barley	0.687	BEL
191	Lager	bottom	no	Corn	0.135	BEL	**425**	Craft	top	no	Barley	0.432	GBR
192	Lager	bottom	yes	Barley	-	GER	**426**	Craft	top	yes	Barley	-	GER
193	Lager	bottom	yes	Barley	0.121	GER	**427**	Craft	top	yes	Barley	0.804	GER
194	Lager	bottom	yes	Wheat	0.525	GER	**428**	Craft	top	yes	Barley	0.196	GER
197	Craft	top	no	Barley	0.262	GER	**429**	Lager	bottom	yes	Barley	0.18	GER
198	Craft	top	no	Wheat	-	POL	**430**	Craft	top	yes	Barley	0.393	GBR
199	Craft	top	no	Barley	-	POL	**431**	Craft	top	yes	Barley	0.466	BEL
200	Wheat	top	yes	Wheat	0.152	GER	**432**	Craft	top	yes	Barley	0.679	GER
201	Lager	bottom	yes	Barley	0.098	CHE	**433**	Lager	bottom	yes	Barley	-	GER

Supplementary Table S6 (continued). Metadata of the analyzed beer samples.

Sample	Beer style	Fermen -tation	Purity Law	Grain	Abs. 294 nm	Origin	Sample	Beer style	Fermen -tation	Purity Law	Grain	Abs. 294nm	Origin
202	Craft	top	no	Wheat	0.155	POL	**434**	Lager	bottom	yes	Barley	-	GER
203	Lager	bottom	yes	Barley	0.168	ZAF	**435**	Lager	bottom	yes	Barley	-	GER
205	Lager	bottom	yes	Barley	0.127	CHE	**436**	Lager	bottom	yes	Barley	-	GER
206	Lager	bottom	no	Barley	0.966	POL	**437**	Craft	top	no	Rice	-	BEL
207	Craft	top	no	Wheat	0.781	POL	**438**	Craft	top	yes	Barley	-	BEL
208	Lager	bottom	yes	Barley	0.163	GER	**439**	Craft	top	no	Wheat	-	BEL
209	Lager	bottom	yes	Barley	0.193	POL	**440**	Craft	top	yes	Barley	-	NLD
210	Craft	top	no	Barley	-	POL	**441**	Craft	top	no	Wheat	-	NLD
211	Craft	top	yes	Barley	0.89	POL	**442**	Wheat	top	no	Wheat	-	NLD
212	Craft	top	yes	Barley	0.155	HUN	**443**	Lager	bottom	yes	Barley	-	NLD
213	Lager	bottom	no	Rice	0.145	ESP	**444**	Lager	bottom	yes	Barley	-	BEL
214	Lager	bottom	yes	Barley	0.168	GER	**445**	Craft	top	yes	Barley	-	NLD
215	Craft	top	yes	Barley	0.185	GER	**446**	Craft	top	no	Wheat	-	BEL
216	Lager	bottom	yes	Barley	0.157	GER	**447**	Craft	top	yes	Barley	-	GER
217	Wheat	top	yes	Wheat	0.249	GER	**448**	Craft	top	yes	Barley	-	NLD
218	Craft	top	yes	Barley	0.134	GER	**449**	Craft	top	no	Wheat	-	BEL
219	Craft	top	yes	Barley	0.27	GER	**450**	Lager	bottom	yes	Wheat	-	GER
220	Craft	top	yes	Barley	0.208	GER	**451**	Craft	top	no	Barley	-	BEL
221	Craft	top	yes	Wheat	0.132	GER	**452**	Craft	top	no	Rice	-	BEL
222	Lager	bottom	no	-	0.114	JPN	**453**	Wheat	top	yes	Wheat	-	GER
223	Lager	bottom	yes	Barley	0.569	GER	**454**	Craft	top	no	Barley	-	BEL
224	Lager	bottom	yes	Barley	0.211	GER	**455**	Lager	bottom	no	Barley	-	IRL
226	Lager	bottom	yes	Barley	0.238	GER	**456**	Craft	top	no	Barley	-	BEL
227	Wheat	top	yes	Wheat	0.207	GER	**457**	Lager	bottom	yes	Barley	-	GER
228	Lager	bottom	no	Corn	0.14	ESP	**458**	Lager	bottom	yes	Barley	-	GER
229	Lager	bottom	no	Corn	0.158	ESP	**459**	Lager	bottom	yes	Barley	-	ISR
230	Lager	bottom	no	Corn	0.143	ESP	**460**	Lager	bottom	yes	-	-	ISR
231	Lager	bottom	no	Corn	0.096	ESP	**464**	Lager	bottom	no	Rice	-	THA
232	Lager	bottom	no	-	0.193	ESP	**465**	Lager	bottom	no	Rice	-	THA
235	Lager	bottom	no	Corn	-	ESP	**467**	Lager	bottom	no	Rice	-	THA
236	Lager	bottom	no	Corn	-	ESP	**B1885**	-	-	-	-	-	GER
237	Lager	bottom	no	Corn	-	ESP	**B2019**	Lager	bottom	no	Barley	-	GER

Supplementary Table S7. Score values of the samples.

Sample	Beer style		Fermentation		Purity Law		Grain			Abs. 294nm	
	PC1	PC2	PC1	PC2	PC1	PC2	PC1	PC2	PC3	PC1	PC2
1	-2.49	18.71	8.09	19.04	10.21	37.73	-10.17	-15.51	-2.89	-23.81	-27.70
2	-12.73	-3.39	-10.99	12.35	9.92	14.49	12.52	3.04	-3.47	-21.97	8.11
3	-12.17	-4.88	-10.78	10.09	8.98	12.79	12.51	2.05	-3.08	-18.21	7.10
4	7.31	-1.20	9.23	22.08	-11.14	22.15	6.82	3.37	-2.66	-15.56	-11.13
5	-4.45	38.37	15.09	20.97	9.73	17.99	-9.66	-21.02	1.51	-19.03	2.17
6	-0.45	37.37	16.56	27.06	8.07	20.35	-12.96	-19.25	1.08	-19.08	-4.65
7	0.23	33.60	12.43	16.11	6.86	6.03	-13.62	-15.55	-1.76	-	-
8	-11.47	-0.62	-9.81	8.70	10.17	10.93	12.91	4.77	-4.67	-12.76	7.19
9	-11.93	-1.82	-7.94	12.82	8.74	8.83	13.78	4.32	-4.56	-14.46	15.44
10	-6.12	-5.86	-5.67	16.65	11.82	22.02	13.24	0.79	1.53	-16.11	-3.10
11	-4.87	16.82	7.72	24.42	6.92	56.56	-11.85	-15.11	-3.19	-	-
12	-3.01	22.54	9.88	31.99	7.25	43.59	-6.94	-12.22	0.18	-12.31	-34.56
13	-3.71	-0.12	8.86	13.28	7.1	5.14	10.69	2.44	-1.17	-6.44	12.25
15	-11.67	-3.13	-11.46	14.76	10.72	35.14	9.63	0.54	-2.98	-14.69	-25.25
16	-8.58	-3.32	-8.04	13.01	10.81	23.79	13.28	-0.06	-1.19	-15.27	-11.26
19	-2.69	30.88	13.74	22.81	12.02	22.16	-8.94	-20.70	-1.25	-16.06	-9.15
20	-2.83	19.92	7.45	26.28	8.81	41.92	-8.29	-13.93	-0.91	-9.33	-37.09
21	-4.69	16.65	4.44	29.15	8.31	48.9	-5.72	-11.01	-0.84	-10.77	-44.02
22	-9.52	0.92	-9.08	21.46	6.83	46.27	5.59	2.60	-1.54	-8.76	-40.99
23	-8.54	0.15	-9.53	20.43	8.83	37.36	10.77	2.02	-1.73	5.03	-32.73
24	-2.70	0.61	-4.22	18.73	-12.6	10.23	6.21	0.44	-0.81	4.31	-41.97
25	1.37	14.36	8.32	17.12	8.91	36.83	-8.52	-9.14	-0.51	-2.84	-35.34
26	-7.95	2.08	-7.10	-5.85	9.56	14.23	11.81	2.94	0.07	15.86	-14.37
27	-10.64	-0.43	-10.67	17.31	10.49	40.15	11.68	1.50	-0.93	-13.04	-30.83
28	-0.74	15.59	7.07	29.31	8.29	49.96	-3.74	-10.63	-0.47	-5.76	-49.19
29	3.23	19.77	11.63	27.09	8.2	40.03	-6.59	-16.52	2.29	-2.76	-40.17
30	-7.55	0.74	-6.40	23.19	7.84	44.88	7.55	0.96	-0.91	-8.95	-39.33
31	-3.77	19.29	5.48	22.72	7.86	42.17	-5.18	-12.49	-0.94	-	-
32	7.89	-0.18	8.09	12.46	-10.38	15.85	1.61	2.12	-2.80	-1.88	-15.79
33	4.99	26.91	18.02	9.88	9	3.35	-8.42	-18.95	1.37	2.32	0.87
34	1.49	26.47	14.26	25.64	7.94	31.34	-8.56	-15.34	0.73	-15.55	-23.69
35	-1.97	-3.74	6.78	12.85	6.38	3.7	11.10	1.40	-1.66	-15.67	11.34
36	-7.11	-1.89	-6.28	15.89	7.49	30.83	11.28	-0.62	0.93	-13.08	-22.63
37	-9.70	-4.30	-9.55	-43.99	8.86	-22.05	11.82	0.07	-3.80	26.69	14.41
38	-4.10	21.09	8.05	16.41	9.85	28.66	-4.43	-14.77	0.92	-7.65	-23.43
39	-13.38	0.77	-11.25	13.37	9.72	32.69	8.18	0.82	-2.30	-9.73	-23.64
41	2.66	23.31	12.59	21.74	6.61	28.66	-8.66	-15.30	-1.60	-9.36	-26.09
43	5.53	2.23	8.31	22.83	8.67	-23.58	1.12	0.01	-1.47	-10.17	-22.29
44	-9.24	-0.42	-8.54	16.77	10.45	39.04	10.74	-0.49	-0.77	-13.01	-31.16
45	-2.76	25.17	10.93	23.33	9.5	29.8	-5.70	-16.65	0.41	-13.30	-21.83
46	-4.10	0.60	-7.18	19.67	8.26	54.12	4.31	-2.46	-1.22	-14.38	-51.72
47	0.27	1.67	-2.86	19.98	7.59	54.02	-1.26	-9.82	-1.79	-12.16	-54.36
48	-5.43	4.40	-5.55	1.98	8.28	30.96	5.37	-0.88	0.19	12.43	-36.68
49	12.35	-4.37	9.19	25.73	7.98	39.96	6.75	-0.21	0.41	-5.39	-37.84
50	-8.37	-0.53	-6.27	20.81	8.49	33.3	11.93	4.27	-0.35	-14.11	-17.22
51	-4.16	30.37	11.54	24.81	6.93	25.99	-11.96	-15.43	-0.48	-10.74	-13.69
52	-0.31	30.03	14.26	25.42	8.21	25.46	-10.10	-17.32	1.61	-9.98	-17.49
53	-12.59	-7.15	-9.17	5.91	9.9	-17.51	10.06	2.68	-4.19	-	-
54	12.35	4.06	9.89	17.73	-6.77	37.4	1.92	-2.42	-0.51	-	-
55	16.90	-3.53	12.23	28.42	-13.1	-12.56	1.71	-10.12	0.45	-4.31	-51.46
56	-3.20	29.92	12.31	16.32	11.21	15.23	-7.74	-17.72	-2.61	-11.90	-2.91
57	20.63	-8.00	17.04	-0.56	7.75	-8.37	8.26	0.26	0.81	24.15	2.90
58	-1.36	21.58	10.60	24.09	6.97	29.61	-6.63	-16.50	0.35	-12.79	-22.32
59	19.47	-4.47	11.01	6.11	-12.62	20.23	3.16	0.01	-1.76	-	-
60	16.95	-10.89	13.97	5.44	10.84	-4.37	11.52	1.58	-1.34	7.90	7.91
61	12.47	-2.92	8.22	14.03	10.13	37.72	-3.40	-13.26	-2.84	-5.00	-37.91
62	17.28	2.41	13.95	15.51	9.8	16.62	-9.37	-18.90	-2.35	-	-
63	1.95	38.48	8.99	19.05	8.6	2	-8.04	-21.04	3.15	-	-
64	10.88	-5.03	9.99	16.79	9.15	17.82	11.89	-1.60	1.09	-6.50	-11.08
65	22.76	-5.07	18.52	19.54	-13.98	10.38	9.29	-0.12	0.73	7.67	-13.49
66	21.18	-2.42	16.33	20.51	-9.03	31.95	9.30	2.13	-0.63	16.03	-41.61
67	2.54	18.29	11.88	17.72	-13.96	5.19	-6.47	-15.98	3.09	-11.22	-13.44
68	-7.48	4.30	-8.37	-2.92	7.84	26	5.74	0.03	-0.18	10.33	-30.25
69	6.32	12.31	13.12	21.92	-5.89	17.11	-3.11	-11.65	0.29	-11.67	-12.10
70	-8.38	-0.90	-6.92	17.51	10.2	29.75	13.47	-0.21	0.69	-16.96	-17.33
71	-9.69	0.03	-7.87	15.80	5.01	28.84	7.36	3.29	1.51	-	-
72	-13.46	-0.58	-12.35	16.73	7.22	35.93	7.49	3.97	-1.99	-	-
73	-11.69	-0.29	-11.41	12.10	9.22	35.9	6.77	-0.09	0.13	-	-
76	2.47	23.28	13.95	20.77	6.94	27.51	-6.77	-17.28	0.80	-1.61	-25.14
78	15.57	-4.52	12.33	13.58	8.83	18.92	8.18	1.00	3.24	7.10	-19.26
80	-6.51	1.53	-8.55	22.47	-8.81	41.04	-6.24	9.88	5.59	-13.73	-34.93
81	18.50	-5.15	13.07	22.02	7.33	32.54	3.03	-1.42	0.85	0.29	-35.04
83	-0.91	-1.04	-5.08	7.10	9.22	25.71	7.43	0.08	0.52	0.66	-23.88
85	8.48	1.52	8.58	20.20	8.19	36.46	-2.96	-8.99	-0.42	-	-
86	12.85	-6.87	9.67	24.77	10.41	33.05	11.70	-0.15	0.00	-4.88	-29.43
90	21.13	-8.34	15.99	5.82	7.87	22.74	11.99	0.92	-5.30	-7.23	-12.27
91	-9.52	-5.74	-9.07	-20.94	-11.07	-54.1	11.55	2.63	-5.10	-11.47	91.02
92	-12.89	-5.46	-11.22	-16.75	-12.74	-44.83	10.77	1.89	-0.03	-13.31	83.30
93	-17.47	-4.68	-13.26	-75.35	9.65	-87.94	6.00	3.35	-2.48	4.71	115.1
94	-13.40	-1.88	-10.28	-23.77	8.87	-53.57	3.62	0.19	-1.35	-10.99	98.66
95	-16.81	-4.29	-14.50	-13.73	-12.55	-29.81	-14.49	15.68	21.56	-18.96	62.05
96	-11.74	-8.64	-10.40	-19.03	9.06	-52.37	9.06	0.08	-2.87	-4.52	97.57
97	-9.67	-4.26	-11.80	-9.41	-12.01	-31.78	-24.39	13.00	-14.70	-13.51	59.39

Supplementary table S7 (continued). Score values of the samples.

Sample	Beer style		Fermentation		Purity Law			Grain		Abs. 294nm	
	PC1	PC2	PC1	PC2	PC1	PC2	PC1	PC2	PC3	PC1	PC2
98	-6.23	-4.21	-11.15	-32.93	9.65	-11.11	6.07	1.04	-2.13	-	-
99	-21.19	-1.34	-20.06	-40.91	-10.62	-96.16	13.66	8.35	-0.52	-22.13	120.4
100	21.90	-5.67	13.86	19.87	-11.28	36.31	-	-	-	-	-
101	23.45	-4.20	14.83	-26.95	-11.26	-81.44	-18.30	18.25	26.14	-11.44	95.13
102	5.70	23.88	14.56	13.88	-11.88	-17.9	-13.43	-19.55	1.58	-23.96	33.81
103	-7.59	-5.73	-12.96	11.03	-13.21	-11.83	10.37	-1.35	-2.45	-18.51	41.82
104	23.15	-8.47	16.18	8.85	6.03	27.6	11.51	2.16	-6.88	-	-
105	20.77	5.00	16.62	20.73	-14.26	-2.84	-7.88	-17.88	-0.44	-15.50	12.74
106	21.41	-2.24	13.30	-46.70	11	-44.98	-7.41	-16.59	-1.48	23.71	30.93
107	14.14	-7.99	13.14	4.18	-12.5	-16.67	8.99	1.26	-2.46	-2.53	28.73
108	20.62	9.49	17.98	20.29	-11.49	-8.57	-9.76	-18.63	1.97	-19.78	22.44
109	20.27	-8.74	11.81	-38.07	9.24	-26.19	7.39	2.91	-2.80	30.66	8.53
110	14.91	-10.65	12.05	-6.72	8.2	-28.12	9.67	-2.63	0.83	-3.80	39.01
111	-10.62	-6.53	-10.85	-8.40	7.64	-26.6	12.12	-0.35	-4.84	-16.64	55.60
112	21.24	-11.42	14.68	4.49	9.23	-14.94	6.44	0.04	3.26	-1.97	24.84
113	-9.09	-6.27	-10.10	-19.08	9.2	-21.14	9.44	-2.37	1.11	-6.36	33.97
114	-9.41	-5.82	-9.82	10.38	6.59	20.65	3.20	3.05	-1.83	-13.86	-0.22
116	10.96	-4.08	11.34	9.72	-9.74	3.61	8.62	-0.29	-1.57	0.21	1.68
117	22.81	-2.24	14.00	12.41	8.68	17.16	-9.03	-18.22	1.82	-8.82	13.30
118	19.85	-2.24	11.02	22.26	10.26	25.39	-8.42	-15.82	1.77	-	-
119	23.64	-7.28	15.28	-51.34	10.7	-39.59	5.09	-0.66	-0.43	65.38	6.25
121	22.04	-4.52	13.03	8.73	7.44	24.18	-7.53	-11.73	-1.18	-	-
123	10.61	-6.65	8.18	8.02	-11.82	-0.15	-3.10	-7.00	-0.23	-10.17	3.90
124	13.98	4.70	12.53	-46.04	9.23	-29.77	-7.25	-13.71	-0.73	42.16	3.04
125	25.04	-6.73	19.27	15.39	-13.35	-1.87	13.47	1.49	2.76	7.81	2.60
126	25.91	-7.60	12.24	-2.90	10.37	10.18	-7.98	-16.55	-0.03	-	-
127	-7.66	-7.68	-11.38	-59.61	8.6	-54.21	11.73	2.54	-2.62	18.61	51.27
128	18.38	-4.93	18.46	-	8.6	-	11.24	-2.33	0.81	59.31	63.90
129	-4.21	-1.11	-9.26	-3.63	11.74	23.02	9.33	-3.86	-1.26	-4.02	-17.39
130	25.35	-3.73	14.98	-8.19	-12.03	-5.14	9.75	1.07	-0.19	25.45	-13.53
131	11.93	-4.37	9.16	14.54	7.93	-31.16	4.16	-1.38	2.16	-8.50	-8.64
132	20.36	-8.44	13.77	5.28	-14.2	-0.56	10.36	0.48	1.06	0.54	-4.60
133	22.58	0.29	18.52	16.60	-9.59	-1.13	-1.99	-16.74	4.15	-6.35	1.14
134	27.70	-10.25	13.69	-15.80	-13.88	-26.37	12.90	4.48	-4.32	-	-
136	-10.51	-8.68	-12.67	11.12	9.86	13.22	5.58	2.42	-5.36	-11.34	10.41
137	10.40	28.94	15.78	-	8.32	-124.5	-5.15	-17.09	-3.08	-	-
138	12.32	5.29	11.82	25.05	-11.27	14.21	-4.78	-16.36	3.84	-19.21	1.70
139	-17.01	-7.52	-13.57	-24.49	-14.69	-28.51	13.74	-3.22	-0.44	-11.68	50.97
140	-8.56	-4.24	-10.70	-26.77	8.17	-16.66	14.51	1.68	-2.39	12.70	29.44
141	-18.12	-7.64	-17.34	-75.98	5.72	-50.19	11.58	0.72	-5.31	26.87	47.36
142	-9.20	-2.81	-8.28	-9.62	5.77	7.21	10.11	2.96	1.34	7.39	-0.99
143	-13.07	-5.51	-12.07	15.84	11.82	20.39	15.90	0.31	-1.23	-8.98	6.68
144	-15.29	-4.86	-14.69	13.60	7.36	32.13	10.23	3.85	-0.46	-14.60	-18.97
145	-11.92	-4.66	-13.46	11.93	-12.52	21.61	4.53	2.71	1.64	-11.46	-14.60
146	-6.93	-5.35	-9.40	17.72	7.62	-9.68	6.76	1.44	-0.38	-18.19	-7.67
147	-9.96	-1.97	-9.49	-29.86	8.67	-13.9	10.92	0.71	-2.59	17.54	14.65
148	-13.71	-3.42	-12.43	2.48	8.9	10.86	9.12	0.00	-1.85	-10.45	3.31
149	18.16	-6.68	14.70	20.24	-12.11	22.18	4.98	-1.50	-1.68	-0.74	-25.19
151	6.29	-4.09	5.59	13.36	-11.52	23.27	-13.99	7.89	-11.48	0.48	-23.95
152	8.04	24.93	15.37	18.04	7.7	15.43	-7.77	-18.24	4.39	-8.55	-14.59
153	-16.49	-5.03	-16.12	-3.16	7.49	24.17	4.09	2.67	-2.73	-10.22	-0.65
154	-10.98	-5.60	-10.69	12.71	5.3	26.19	7.68	5.30	-2.03	-9.67	-12.10
155	5.08	32.30	16.50	5.95	9.85	-7.06	-13.21	-21.20	3.11	8.94	9.10
156	12.42	-3.18	11.09	6.79	-10.05	16.82	-13.20	6.74	-11.84	11.27	-23.09
157	-11.53	-4.61	-10.16	6.35	5.4	14.5	9.92	3.12	-1.17	-8.77	-0.99
159	-14.18	-6.38	-13.05	-13.03	11.48	-36.2	16.03	0.63	-5.86	-18.25	70.40
160	-15.14	-2.41	-16.52	-29.24	-10.75	-56.76	-22.79	12.01	-18.87	-	-
161	-12.10	-7.33	-11.91	-15.52	-12.49	-87.17	-	-	-	-9.62	35.76
162	-14.64	-4.68	-12.65	-3.69	-13.02	-18.4	12.62	0.13	2.43	-10.64	43.18
163	-16.50	-4.40	-11.53	13.99	9.23	27.76	10.66	1.75	-0.25	-14.64	-5.94
164	-5.81	-0.45	-6.23	19.14	-12.63	26.88	-	-	-	-11.53	-17.07
165	-16.99	-7.57	-13.88	0.23	5.56	-2.25	5.99	5.31	0.68	-13.07	26.77
166	-17.99	-4.19	-15.74	7.34	-13.13	12.03	-12.87	17.61	11.63	-13.69	6.15
167	-14.19	-4.29	-13.19	13.32	-11.06	21.33	-16.64	13.28	-4.16	-12.80	-5.68
168	-10.33	-6.41	-11.73	12.89	-12.66	19.14	-10.77	12.65	13.34	-10.41	-8.20
169	-15.61	-2.63	-13.24	15.16	-7.59	28.01	-13.20	12.15	-8.45	-14.33	-12.67
170	-13.48	-1.59	-12.03	17.79	-7.97	32.5	-3.89	10.07	5.34	-15.40	-23.30
171	-15.24	-2.64	-11.95	12.71	-10.73	16.23	-7.03	13.15	6.27	-17.97	-0.79
172	-14.39	-2.50	-14.89	14.42	-9.05	33.67	-14.62	13.55	-8.73	-13.35	-26.43
173	-12.03	0.68	-10.88	13.62	-11.83	19.92	-11.25	12.81	4.86	-18.96	-8.87
174	12.41	-9.62	9.99	-4.51	9.71	-18.52	9.87	0.80	3.86	-4.74	25.71
175	-7.48	0.43	-8.08	19.96	-8.08	30.55	4.61	1.46	0.81	-13.02	-23.40
177	21.50	-9.50	17.15	-26.26	8.24	-25.61	10.19	-1.01	2.80	24.15	12.80
178	-10.72	-3.55	-11.03	14.24	4.77	33.66	7.37	4.22	-0.11	-17.43	-23.85
179	-8.99	0.09	-7.91	16.90	8.17	39.19	3.79	3.96	0.57	-8.93	-29.61
180	-4.50	-5.14	-8.14	2.28	9.42	22.05	6.84	0.26	-4.08	-3.74	-17.58
182	14.68	-7.56	10.78	-39.48	10.15	-62.65	9.41	3.02	4.40	-12.81	73.81
191	-10.47	-4.69	-8.56	5.02	-12.51	-6.63	-13.70	11.39	-12.70	-11.41	27.72
192	-8.46	-6.77	-9.44	7.60	8.78	10.76	13.19	2.03	3.89	-	-
193	-17.01	-5.40	-	-	5.91	-79.49	10.37	-0.50	-3.57	-22.50	80.91
194	-19.78	-6.80	-	-	-	-	-10.53	-15.45	-4.21	36.33	73.14
197	12.11	-0.75	12.36	-8.03	-9.95	-17.68	4.59	0.53	-0.75	6.64	18.76
198	12.83	-4.34	7.73	21.50	-10.96	30.61	-6.23	-8.59	-0.74	-	-
199	18.29	-5.17	11.09	5.36	-10	2.13	12.61	1.55	2.35	-	-
200	0.99	36.42	17.57	18.50	7.16	12.05	-15.86	-21.90	0.21	-16.19	-1.67

Supplementary table S7 (continued). Score values of the samples.

Sample	Beer style		Fermentation		Purity Law			Grain		Abs. 294nm	
	PC1	PC2	PC1	PC2	PC1	PC2	PC1	PC2	PC3	PC1	PC2
201	-11.68	-7.04	-11.96	9.82	5	5.37	8.63	5.08	-1.72	-17.52	17.00
202	22.36	-0.21	15.61	15.90	-11.77	-8.14	-12.53	-20.72	4.45	-11.37	8.31
203	-14.17	-8.17	-11.16	-7.52	9.89	-9.1	10.40	3.99	1.49	-6.57	30.79
205	-13.42	-4.14	-11.62	11.62	3.4	15.3	4.91	5.83	2.46	-13.32	1.99
206	-11.35	-5.19	-15.40	-	-11.55	-74.66	5.92	0.71	-2.09	106.76	9.93
207	10.61	0.02	15.55	-	-12.81	-92.85	-6.77	-17.18	4.71	73.99	8.55
208	-9.40	-5.42	-9.79	8.42	6.77	19.53	10.39	4.06	0.52	-7.46	-8.92
209	-2.06	-3.79	-3.57	-8.04	8.68	-8.43	5.74	2.54	2.11	-1.73	15.53
210	19.24	-5.80	9.74	-28.22	-11.66	-16.41	13.12	7.44	-1.10	-	-
211	18.50	-4.96	16.40	-	10.4	-64.07	13.72	3.06	1.74	93.77	-14.44
212	13.53	-8.31	12.19	10.65	7.97	-5.84	4.96	-2.26	1.92	-8.56	21.95
213	-9.55	-5.38	-11.78	4.98	-12.22	3.27	-12.88	19.82	17.69	-4.58	13.00
214	-5.05	-5.38	-7.89	7.37	8.19	14.19	6.87	2.54	-3.27	-3.96	-1.85
215	14.02	-11.11	11.87	-5.64	8.89	-26.37	12.25	1.89	0.52	1.88	42.92
216	-11.17	-6.04	-9.75	-18.62	5.57	-22.89	9.76	2.12	-2.14	-6.89	40.03
217	8.06	33.98	18.20	0.19	8.26	-7.28	-12.08	-19.90	2.43	4.41	9.45
218	17.29	-9.08	14.00	11.63	9.26	3.57	11.81	1.46	-0.90	-6.56	5.20
219	17.34	-9.09	13.93	11.60	9	3.52	11.69	1.35	-0.79	-6.70	5.23
220	11.38	-8.10	11.22	-2.19	8.25	-16.85	11.00	-0.35	-3.86	1.61	25.86
221	18.53	5.13	16.41	0.52	9.58	-14.29	-7.45	-13.45	-1.66	-11.62	21.16
222	-8.77	-6.28	-11.56	1.28	-14.44	-3.22	-	-	-	-8.93	16.63
223	-10.25	-0.68	-12.37	-44.28	8.75	-28.6	10.33	3.44	-4.12	47.42	20.14
224	-9.51	-5.99	-11.14	-4.24	9.14	-2.16	10.64	3.28	1.18	0.37	18.65
226	-14.63	-1.73	-13.42	-22.99	8.99	-15.11	8.56	1.12	-4.46	5.77	23.35
227	2.00	36.92	15.28	-0.85	9.63	-6.03	-13.81	-20.03	1.48	1.20	10.08
228	-13.47	-3.57	-14.38	5.79	-13.42	10.52	-19.75	12.60	-15.16	-10.23	-0.25
229	-10.95	-4.50	-13.37	9.35	-12.52	21.41	-18.34	11.72	-12.58	-8.59	-14.96
230	-12.65	-4.93	-13.69	11.41	-9.1	19.69	-8.36	9.60	-9.01	-9.09	-10.10
231	-15.00	-3.65	-11.91	19.59	-13.19	28.86	-18.73	14.39	-16.69	-7.99	-11.93
232	-12.62	-3.65	-13.90	2.92	-10.74	4.77	-	-	-	-0.86	3.08
235	-6.74	0.26	-8.36	12.61	-14.36	25.02	-20.27	10.05	-13.60	-	-
236	-11.93	-2.31	-12.83	12.06	-12.76	17.02	-24.31	12.45	-17.40	-	-
237	-15.15	-3.01	-14.02	8.54	-12.47	13.27	-22.00	13.69	-19.97	-	-
238	-18.11	-5.41	-13.60	-79.36	5.93	-56.08	10.52	2.65	-4.97	13.15	57.65
239	-11.47	-5.67	-13.34	15.87	-11.18	29.27	-12.59	14.95	2.21	-	-
241	-12.90	-2.49	-13.34	14.06	-11.12	29.43	-14.15	15.10	4.54	-	-
242	-13.59	-3.96	-12.06	13.22	8.69	24.2	10.23	4.35	-3.22	-14.09	-9.01
243	-11.32	-10.21	-9.56	17.38	10.1	14.16	12.32	1.20	-3.64	-9.06	9.63
244	-6.87	-3.78	-6.41	8.29	7.18	4.12	9.94	-0.01	-4.07	-15.64	9.88
245	-15.11	-2.29	-14.95	14.95	8.21	35.53	6.98	2.75	-1.56	-19.12	-21.47
246	-15.19	-4.80	-15.18	10.65	8.95	19.72	11.09	2.66	-1.81	-16.01	-3.42
247	-12.30	-1.96	-12.88	11.21	6.94	27.77	4.44	2.31	-2.85	-9.22	-19.27
248	-9.03	-2.06	-10.52	19.71	7.73	42.13	7.12	1.09	0.79	-14.95	-34.29
249	-9.42	-1.93	-10.81	13.93	7.96	21.91	8.45	2.16	-2.83	-9.58	-10.74
250	-1.03	25.17	11.26	21.13	8.41	24.95	-10.91	-15.63	-1.58	-10.93	-17.70
251	1.49	21.83	13.35	14.88	6.83	13.02	-4.11	-14.67	0.77	-6.08	-5.75
252	-14.04	-3.08	-12.72	14.71	8.98	29.19	11.06	2.68	0.88	-16.04	-13.59
253	-1.00	32.68	13.70	20.57	11.1	18.88	-7.29	-21.55	3.42	-13.19	-11.25
254	-9.54	-0.13	-9.14	12.32	7.42	20.17	1.65	3.04	1.81	-7.38	-29.57
255	-1.52	23.26	9.30	20.15	8.05	29.25	-8.84	-14.53	0.45	-6.64	-26.61
256	-3.28	20.25	7.86	25.59	6.68	34.92	-9.50	-11.05	-0.38	-13.28	-28.41
257	-3.06	25.55	11.97	30.14	9.28	35.18	-7.11	-18.75	1.59	-12.54	-23.97
258	-1.45	26.89	12.73	19.68	9.47	26.56	-6.13	-16.23	3.18	-8.38	-21.51
259	3.68	23.03	13.68	8.17	8.4	20.06	-5.89	-15.65	1.40	6.03	-25.07
260	-7.18	-2.84	-8.07	12.29	8.7	30.56	6.65	-0.04	2.13	-8.45	-23.79
261	-14.05	0.01	-11.26	6.57	9.7	23.62	8.70	1.69	-0.05	-5.96	-15.42
262	-14.69	-5.75	-16.19	9.40	7.88	17.16	8.90	3.73	-0.92	-	-
263	-5.29	35.14	11.22	18.46	8.87	16.83	-14.09	-19.62	-0.87	-	-
264	-13.75	-6.84	-14.89	9.81	-13.25	5.93	-18.04	16.07	-13.07	-	-
265	-11.13	-4.97	-13.57	11.38	-13.17	18.26	-18.25	15.63	-7.33	-	-
266	-3.39	-1.34	-6.40	19.41	-11.69	36.69	-19.50	10.38	-7.71	-	-
267	-11.83	-4.74	-14.08	6.64	-13.77	13.49	-22.09	13.46	-8.36	-	-
268	-9.52	-5.15	-11.59	-0.56	-11.86	-3.05	-	-	-	-	-
269	-9.18	-0.42	-8.53	8.86	-11.76	12.22	-15.07	7.01	-7.50	-	-
270	-7.47	-1.85	-10.36	19.55	-12.37	37.55	-18.38	11.25	-11.27	-	-
271	-4.89	1.33	-6.79	22.18	-8.27	55.42	-13.62	8.49	-9.38	-	-
272	-3.59	-0.83	-8.10	-1.00	-10.84	6.85	-13.05	14.52	5.69	13.66	-7.59
273	23.21	-9.32	15.78	-71.77	10.01	-85.37	9.04	1.41	-0.96	-	-
274	-4.67	-0.55	-11.04	-11.45	-12.37	-11.29	-14.59	19.35	13.50	-	-
275	-16.02	-3.71	-15.97	10.63	-11.86	20.39	-19.59	17.30	-4.08	-12.94	-8.29
276	-13.83	-5.48	-12.55	5.39	-9.04	6.12	-17.75	15.12	-15.38	-	-
277	-12.16	-3.39	-12.25	7.23	-10.14	14.28	-13.69	13.55	-9.19	-	-
278	23.55	-7.65	17.09	-15.95	7.55	-27.51	4.31	2.80	2.08	-	-
279	-4.32	-3.41	-5.99	19.52	6.42	28.42	2.03	5.58	-1.27	-	-
280	-12.41	-2.65	-13.26	11.12	-10.13	22.87	-16.13	12.93	-8.09	-	-
281	13.17	-5.33	11.90	7.85	6.43	8.59	8.57	1.49	0.65	-	-
282	16.47	-3.74	10.60	-32.89	11.51	-22.61	11.96	3.77	-1.13	32.12	-0.53
283	-10.94	-5.74	-11.40	9.36	-9.59	16.51	-8.18	11.86	-6.99	-	-
284	12.41	-4.99	9.90	11.44	5.7	22.79	6.75	2.50	-0.07	9.90	-30.05
285	-9.72	-2.55	-9.68	5.55	-10.11	12.75	-13.94	12.29	-10.30	-3.05	-7.19
286	7.87	-6.35	7.10	8.77	7.12	12.11	8.14	2.27	2.19	-	-
287	12.31	-4.92	10.21	11.05	10.51	21.5	6.20	0.83	0.18	-	-
288	13.58	-4.43	10.05	18.82	-12.13	24.67	2.87	0.95	-0.59	-	-
289	7.61	6.38	8.79	24.42	-11.85	29.51	-13.96	-8.64	-2.65	-	-
290	8.88	15.73	14.27	13.16	-7.79	11.59	-7.47	-12.76	4.01	1.76	-13.91
291	0.52	-2.36	6.39	14.31	-10.43	10.62	4.15	1.00	1.80	-	-

Supplementary table S7 (continued). Score values of the samples.

Sample	Beer style		Fermentation		Purity Law			Grain		Abs. 294nm	
	PC1	PC2	PC1	PC2	PC1	PC2	PC1	PC2	PC3	PC1	PC2
292	7.76	-7.16	6.34	17.72	-10.94	10.9	10.22	2.35	1.84	-13.80	-0.77
293	-11.21	-1.60	-11.26	-23.09	6.57	-12.61	6.47	3.31	-1.90	12.45	15.12
294	-2.88	-8.51	-5.50	1.61	7.92	7.49	6.19	2.17	1.11	-	-
295	-6.26	-2.70	-7.18	2.58	9.24	15.35	4.80	1.29	0.87	-	-
296	-6.73	-0.03	-7.45	18.93	-13.31	31.44	-16.08	9.57	-6.27	-	-
297	-8.54	-2.81	-10.12	14.14	8.06	40.19	-	-	-	-	-
298	19.51	-8.88	11.65	-16.89	9.75	-42.06	2.58	1.79	3.13	-	-
299	16.77	-2.25	15.40	-10.21	7.84	-19.3	-3.28	-9.13	1.20	-	-
300	-8.53	-1.11	-11.69	-48.24	9.53	-24.51	9.72	2.18	-0.03	22.71	13.42
301	8.95	-3.78	9.74	0.06	10.04	6.84	13.75	2.65	3.39	-	-
302	-7.99	-2.79	-8.92	-5.12	-9.53	-3.28	2.10	5.39	-0.98	-	-
303	1.81	40.99	7.94	-20.29	9.62	-36.63	-7.36	-17.79	2.39	-	-
304	-11.65	-7.12	-12.11	-18.87	8.48	-35.23	15.52	3.11	-0.48	-	-
305	1.16	36.72	14.86	-8.65	7.98	-27.76	-10.36	-18.80	2.24	-	-
306	-16.42	-9.54	-14.64	-8.95	7.87	-11.12	9.92	4.81	3.83	-	-
307	-4.78	-7.49	-8.06	-6.94	-10.81	-14.48	-6.02	13.42	6.21	-	-
308	-17.80	-9.48	24.75	48.75	12.91	9.42	-15.13	-24.82	7.12	-	-
309	-13.94	-8.09	-1.55	28.73	-10.09	8.87	-16.87	7.67	18.03	-	-
310	15.33	-11.03	15.06	-27.40	9.09	-50.14	8.56	1.59	2.23	-	-
311	-7.69	-2.94	-8.18	14.34	-6.08	29.87	-3.01	9.01	2.04	-	-
312	-10.34	-4.04	-9.76	9.24	-5.64	21.79	-1.14	8.32	3.64	-	-
313	-10.85	-5.10	-11.50	7.15	-9.15	15.7	-5.85	13.48	2.55	-	-
314	9.81	30.03	13.26	29.97	-11.28	30.59	-11.41	-22.25	-0.10	-	-
315	-3.30	-3.59	9.43	6.67	-13.52	-15.46	11.94	1.34	-2.65	-	-
317	-13.70	-6.46	-13.72	4.21	-11.53	5.4	-	-	-	-	-
318	-12.80	-7.88	-11.91	7.82	-10.91	5.45	-14.19	19.57	19.00	-	-
319	-19.15	-8.17	-16.97	-7.83	-12.3	-8.66	-24.18	17.38	-18.15	-	-
320	-9.77	-3.60	-13.27	10.47	-13.9	20.7	-22.83	15.17	-9.88	-	-
321	-10.88	-5.28	-12.19	13.59	-8.63	26.02	-7.26	12.50	5.68	-	-
322	-14.14	-4.68	-14.42	11.73	-13	21.3	-	-	-	-	-
323	-11.49	-8.16	-10.38	-1.76	-12.14	-14.7	-19.29	13.68	-15.29	-	-
324	-14.01	-5.77	-14.48	9.52	-13.95	18.38	-19.93	21.34	13.25	-	-
325	-8.27	-5.64	-12.41	-0.15	-11.77	15.1	-	-	-	-	-
326	-13.82	-0.69	-12.67	18.49	8.31	50.39	4.65	1.47	-3.18	-	-
327	-11.07	-4.57	-11.69	7.57	-13.82	15.44	-16.93	19.47	9.50	-	-
328	-5.54	-2.75	-9.35	14.94	-12.94	28.59	-24.98	13.26	-10.93	-	-
329	-13.56	-4.55	-14.69	9.76	-12.79	11.77	-20.38	14.34	-12.91	-	-
330	-14.28	-3.12	-14.13	10.57	-15.14	18.49	-25.39	16.05	-14.58	-	-
331	-12.64	-2.74	-13.71	5.99	-12.41	8.42	-10.67	16.73	17.68	-	-
333	-15.99	-6.89	-14.35	-1.98	-13.19	19.86	2.03	7.34	-1.75	-	-
334	-6.11	-2.71	-10.76	-2.05	-11.4	-18.75	-14.52	18.71	21.59	-	-
335	-14.27	-3.37	-13.17	10.23	-10.96	-2.41	-19.21	19.18	24.29	-	-
336	-7.59	0.97	-15.12	1.57	-13.91	-24.55	-12.99	14.46	19.36	-	-
337	-12.46	-3.52	-13.48	4.00	-9.97	-17.13	-15.92	19.22	23.25	-	-
357	19.40	13.52	14.04	13.18	7.42	2.19	-13.40	-19.18	3.30	-	-
358	-10.38	-6.24	-12.47	-30.71	9.09	-41.97	8.75	3.20	-0.77	-	-
360	17.57	-4.91	9.70	12.76	-13.45	8.46	-	-	-	-	-
361	-7.74	-3.55	-12.59	-9.17	-11.01	-26.53	-	-	-	-	-
362	-6.42	-2.43	-12.55	4.02	-9.98	-15.61	-	-	-	-	-
363	-7.60	0.84	-12.59	12.98	8.49	-19.42	-	-	-	-	-
364	18.93	7.41	5.20	-13.77	-7.79	-81.12	-9.00	-8.69	7.60	-	-
365	17.17	-5.18	11.96	-40.16	-11.28	-80.56	10.60	1.37	0.56	-	-
366	-8.37	-0.76	-13.17	5.40	-12.91	-26.23	-	-	-	-	-
367	7.34	35.10	15.51	19.24	8.75	-7.28	-11.53	-17.33	5.13	-	-
368	20.00	-7.62	15.50	-22.80	9.27	-96.44	9.30	6.87	-6.00	-	-
369	-13.58	-4.79	-13.62	-13.07	9.61	-42.94	9.96	3.89	-0.58	-	-
370	16.05	-2.26	10.84	-61.43	10.15	-99.04	13.14	-0.16	0.87	-	-
371	0.54	60.45	12.83	-3.56	4.88	-35.26	-7.97	-18.90	3.10	-	-
372	1.76	42.19	12.57	3.61	9.71	-28.21	-14.11	-19.18	4.57	-	-
373	-16.56	-2.54	-13.74	12.04	-9.83	-1.91	-	-	-	-	-
374	-11.72	-2.00	-12.74	14.10	-13.09	7.47	-	-	-	-	-
375	-12.69	-4.46	-13.71	0.93	11.13	-17.45	12.13	4.14	-1.52	-	-
376	-9.23	-4.56	-12.34	-5.15	8.24	-38.97	8.95	0.28	-7.38	-	-
377	-9.50	-3.59	-10.95	17.54	-12.52	20.48	-	-	-	-	-
378	-12.93	-2.97	-12.16	11.42	-11.79	5.47	-	-	-	-	-
379	-17.78	-7.18	-8.55	4.77	-12.63	-33.09	-24.06	15.98	-21.73	-	-
380	19.59	-8.22	13.64	-30.64	7.71	-40.61	14.42	4.03	-0.11	-	-
381	-6.82	-4.16	-9.74	8.99	-10.39	22.03	-11.35	14.83	13.09	-	-
382	-11.65	-0.65	-11.63	7.21	-9.33	11.53	-9.97	13.37	15.02	-	-
383	-12.04	-3.71	-12.66	19.32	-12.57	28.68	-21.36	16.40	-10.11	-	-
385	-3.77	-2.55	-15.32	-7.51	7.89	-46.39	17.54	-2.41	-7.86	-	-
386	21.40	-8.33	13.68	-13.28	9.97	-15.6	-	-	-	-	-
387	19.84	-4.93	12.92	-77.69	10.55	-96.34	13.67	2.95	-2.59	-	-
388	-11.05	-4.30	-13.62	16.24	-10.82	11.49	-	-	-	-	-
389	19.50	-6.16	14.38	-10.16	-7.55	5.01	10.63	3.91	0.88	49.60	-33.06
390	20.13	-5.27	15.77	-27.31	-11.57	-15.49	9.44	4.00	1.33	-	-
391	-11.54	-4.68	-13.07	-12.06	-13.62	-22.36	-15.60	16.05	13.59	-	-
392	-14.91	-3.05	-11.51	-14.52	9.35	-27.07	12.10	3.02	3.06	-	-
393	11.38	-5.59	9.31	17.69	6.46	28.81	6.72	0.34	0.63	-	-
394	23.90	-4.10	17.01	-27.68	-14.73	-27.58	-9.00	10.52	9.36	63.23	-4.26
395	20.14	-2.30	14.25	17.35	-13.11	-12.34	-12.37	-17.87	-0.90	-	-
396	16.41	-6.87	13.23	-3.29	8.97	4.14	9.02	3.26	2.59	-	-
397	14.68	-0.10	16.21	42.16	6.48	10.49	-7.40	-16.13	2.27	-	-
398	19.33	-6.02	14.37	-6.18	9.31	4.65	9.61	1.26	0.30	31.98	-18.31
399	11.87	-2.07	12.39	16.91	9.16	16.11	10.69	-2.68	2.02	-	-

Supplementary table S7 (continued). Score values of the samples.

Sample	Beer style		Fermentation		Purity Law		Grain			Abs. 294nm	
	PC1	PC2	PC1	PC2	PC1	PC2	PC1	PC2	PC3	PC1	PC2
400	24.26	3.84	11.05	16.86	-12.14	-9.56	-9.85	-20.28	5.49	-	-
401	19.57	-9.41	13.32	-4.03	9.68	-14.44	7.38	-2.79	2.23	-	-
402	23.68	-6.70	17.38	6.70	-12.83	-14.12	-9.82	-15.69	2.45	-	-
404	21.82	-5.47	15.29	-0.87	-12.72	6.49	-1.33	-7.90	0.53	-	-
405	21.51	-10.77	14.24	12.71	-11.03	-5.73	-9.34	-13.19	3.55	-	-
406	20.08	-9.04	16.62	16.78	5.98	15.64	8.65	-1.72	2.57	-	-
407	-8.81	4.35	-7.30	11.85	-13.21	15.81	-13.66	14.27	13.77	-	-
408	-15.83	-4.66	-15.76	-20.48	-13.02	-29.84	-	-	-	-	-
409	20.53	-6.37	12.33	-88.67	-11.55	-95.92	-13.37	-23.69	-0.99	-	-
410	-18.88	-6.53	-13.92	-15.58	-11.17	-27.15	-13.06	17.89	20.86	-	-
411	-9.76	-7.07	-14.21	-18.77	-11.31	-34.72	-25.87	13.57	-18.47	-	-
412	-10.82	0.81	-14.32	-19.88	-11.29	-52.56	-12.11	-16.23	4.34	-	-
413	-10.02	-7.67	-13.10	-0.28	-14.16	-8.08	-12.62	16.33	17.63	-	-
414	-20.22	-5.81	-14.19	-14.99	7.85	-33.57	11.63	2.17	-1.84	-	-
416	12.86	-0.48	13.39	-1.56	10.28	1.68	9.41	-1.47	-0.23	13.97	-5.52
417	21.73	-5.58	15.92	-14.67	6.45	-0.69	7.80	1.33	1.51	48.73	-24.17
418	18.50	-6.55	14.19	-33.78	8.27	-12.36	12.42	4.72	0.82	46.64	-13.90
419	11.19	-2.76	8.51	-2.18	6.6	16.61	8.57	4.09	1.11	31.06	-30.57
420	19.82	-6.39	14.13	-28.94	-11.67	-36.26	10.35	2.25	-2.12	29.20	16.49
421	16.57	-4.95	10.76	3.05	8.06	32.48	7.86	-0.69	-2.28	27.16	-33.86
422	14.01	0.17	13.02	-31.53	-11.41	-32.06	6.91	1.13	1.47	51.61	10.79
424	26.03	-7.54	15.71	-65.94	-11.14	-49.78	6.87	1.49	4.28	71.43	-4.75
425	19.30	-6.36	13.52	-57.59	-11.67	-41.25	6.28	1.54	1.85	32.73	12.70
426	21.94	-13.26	-	-	-	-	19.33	-0.64	-3.71	-	-
427	12.57	-2.88	9.86	-10.87	7.4	6.92	9.24	3.69	0.75	50.94	-28.36
428	8.85	-3.31	8.44	16.64	7.41	30.09	8.73	0.75	1.76	4.23	-32.21
429	-9.42	-4.42	-9.70	8.20	3.85	18.16	5.78	5.34	-0.68	-6.53	-7.96
430	17.03	-4.63	13.13	12.82	5.27	32.86	9.81	1.43	0.33	23.26	-48.90
431	10.87	-0.64	9.87	0.92	-14.09	18.42	4.95	1.52	-0.15	29.76	-29.98
432	21.71	-8.60	15.29	-73.04	8.91	-56.37	9.38	1.65	-0.95	67.59	10.76
433	-12.92	-4.28	-14.09	-40.52	7.48	-56.75	16.87	6.85	-5.87	-	-
434	-14.03	-11.99	-13.64	-3.34	7.67	-18.25	14.37	3.77	3.53	-	-
435	-8.14	-10.48	-12.58	1.76	7.62	0.52	10.42	-1.48	1.29	-	-
436	-7.07	-11.17	-9.78	0.77	8.04	-1.01	10.74	-0.94	1.62	-	-
437	27.92	-8.77	18.48	17.04	-12.6	-19.78	-12.37	17.13	18.95	-	-
438	23.77	-16.78	18.63	37.91	7.2	-14.95	12.49	4.63	-3.96	-	-
439	15.22	1.62	14.23	23.87	-6.42	20.45	-1.64	-11.50	0.67	-	-
440	15.03	-3.66	10.03	-43.85	9.72	-41.63	7.11	2.96	-4.13	-	-
441	18.43	1.30	11.23	-11.80	-10.93	-29.95	-14.15	-21.57	2.26	-	-
442	6.24	18.99	15.13	22.81	-8.68	16.82	-11.55	-14.12	-0.68	-	-
443	-1.78	-5.44	-6.28	-30.63	6.94	-23.53	8.27	2.67	-2.84	-	-
444	-2.00	-3.43	-6.68	10.65	10.53	31.22	5.46	-1.93	-1.57	-	-
445	29.00	-9.42	20.25	-27.16	9.27	-75.19	13.72	4.17	-5.14	-	-
446	21.44	-4.15	9.89	-70.99	-10.2	-83.34	-9.56	-13.93	-1.58	-	-
447	16.64	-7.29	12.08	2.11	8.15	-6.59	9.14	1.58	1.14	-	-
448	18.60	-7.28	15.73	5.97	9.17	-100.2	7.70	0.46	-0.44	-	-
449	11.27	6.46	12.54	31.45	-9.29	12.08	-6.07	-13.26	3.26	-	-
450	-7.05	5.12	-8.90	3.44	7.73	-7.3	-8.42	-15.81	3.65	-	-
451	27.53	-1.93	14.19	-9.90	-11.37	-6.76	7.74	5.49	-3.52	-	-
452	9.55	-3.80	6.70	24.23	-12.16	19.01	-8.67	9.82	13.53	-	-
453	3.63	24.35	14.72	17.80	9.9	20.92	-6.69	-16.87	5.69	-	-
454	10.83	-2.05	8.81	13.28	-13.82	12.2	6.08	3.42	2.69	-	-
455	-1.54	-5.20	-5.76	-4.39	-9.9	6.25	10.54	8.25	3.55	-	-
456	18.37	-3.45	14.68	9.91	-12.35	9.89	5.42	2.35	0.10	-	-
457	-13.03	-3.52	-11.92	-16.90	9.68	-19.33	13.21	1.41	2.34	-	-
458	-11.68	-4.61	-12.98	-31.08	8.98	-27.63	7.66	0.81	2.74	-	-
459	-14.86	-7.19	-13.27	-5.11	7.5	-5.26	9.85	6.32	2.27	-	-
460	-13.73	-4.25	-11.45	15.76	7.38	25.43	-	-	-	-	-
464	-15.30	-2.52	-12.67	12.67	-10.15	22.77	-8.90	14.38	14.69	-	-
465	-7.41	-2.32	-9.22	18.33	-12.76	37.03	-5.39	13.22	9.88	-	-
467	-16.88	-6.17	-15.94	-1.55	-8.72	5.29	-5.40	14.15	13.61	-	-
B1885	-9.28	2.74	-5.54	10.89	3.82	12.14	-14.17	-2.56	4.19	-16.69	20.60
B2019	-12.41	-1.52	-10.01	14.94	5.38	20.19	8.57	6.63	0.29	-18.08	3.41

Supplementary figures

A

(I)

(II)

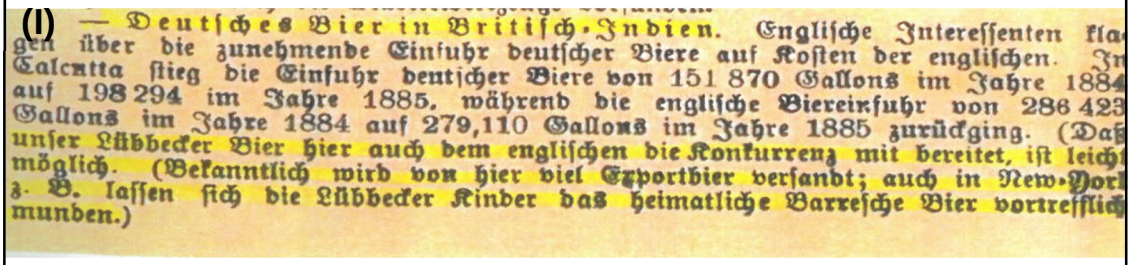
(III)

Newspaper article (19th June 1978): An original find. Beer from the German Empire era.

Beer label:
This beer is brewed from the very finest hops and malt and excellent brewing water, represented in all Lloyd-steamers, whose annual purchase is over 300,000 bottles. Purity guaranteed. Ernst Barre successor brewery, Lübbecke in Westphalia. Original brewery filling.

B

(I)

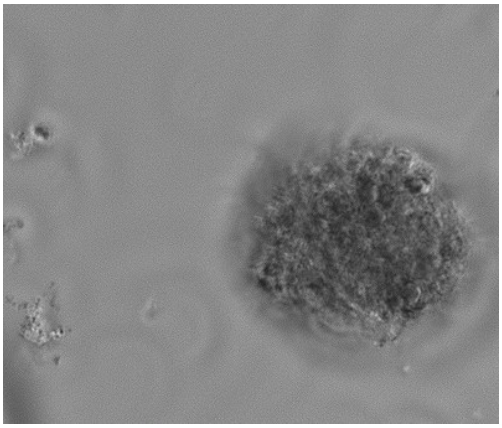


— Deutſches Bier in Britiſch-Indien. Engliſche Intereſſenten kla
gen über die zunehmende Einfuhr deutſcher Biere auf Koſten der engliſchen. In
Calcutta ſtieg die Einfuhr deutſcher Biere von 151 870 Gallons im Jahre 1884
auf 198 294 im Jahre 1885, während die engliſche Biereinfuhr von 286 423
Gallons im Jahre 1884 auf 279,110 Gallons im Jahre 1885 zurückging. (Daß
unſer Lübbecker Bier hier auch dem engliſchen die Konkurrenz mit bereitet, iſt leicht
möglich. (Bekanntlich wird von hier viel Exportbier verſandt; auch in New-York
z. B. laſſen ſich die Lübbecker Kinder das heimatliche Barreſche Bier vortrefflich
munden.)

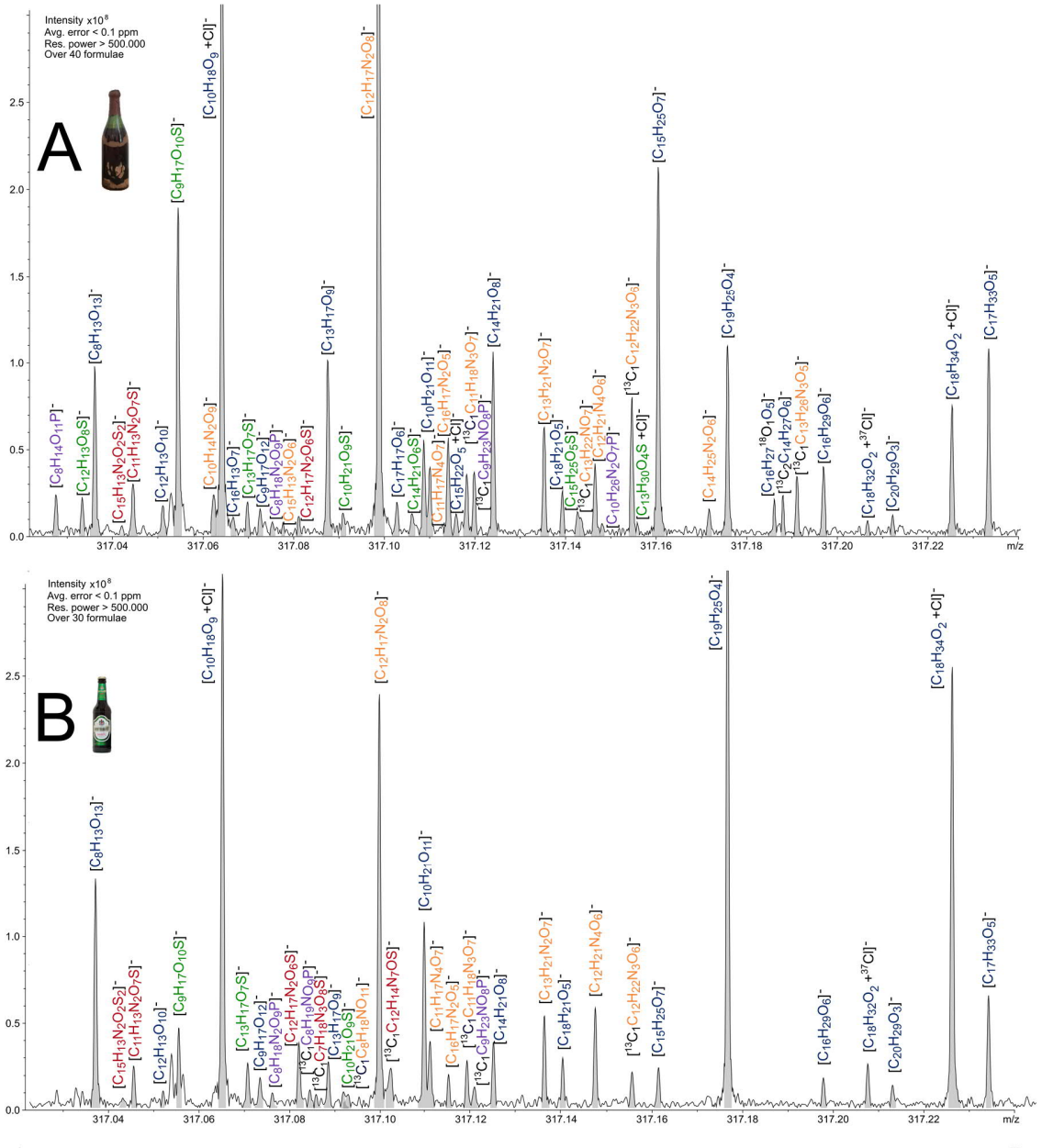
(II)

German beer in British India.
English interests complain of increasing imports of German beers at the expense of English ones. In Kolkata, imports of German beers increased from 151,870 gallons in 1884 to 198,294 in 1885, while English beer imports decreased from 286,423 gallons in 1884 to 279,110 gallons in 1885. It is quite possible that the Lübbecker beer here is now competing with the English beer. (As is well known, a lot of export beer is shipped from here; even in New York, for example, the children of Lübbecke enjoy the local Barre beer).

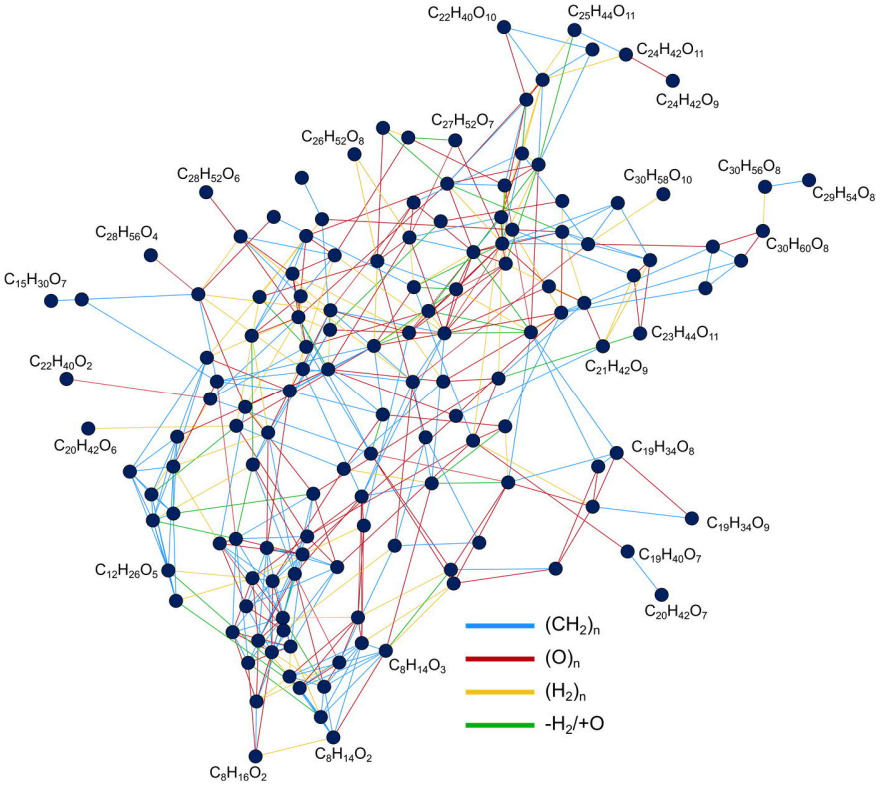
Supplementary Figure S1. Historical sources about the discovery and origin of the beer. A Newspaper article of June 1978 (**A-I**) describes the finding of the unique sample from the German Empire era. The historical beer sample and a replica are shown in **A-II**. The German heading of the newspaper article and the beer's label are translated in **A-III**. Another article refers to the export of Barre beers beginning with the year 1885 and the resulting new competition on the world market (**B-I**). It is translated in **B-II**. The pictures of the beer bottles, the newspaper article and the historical article are used under explicit permission of Privatbrauerei Ernst Barre GmbH.



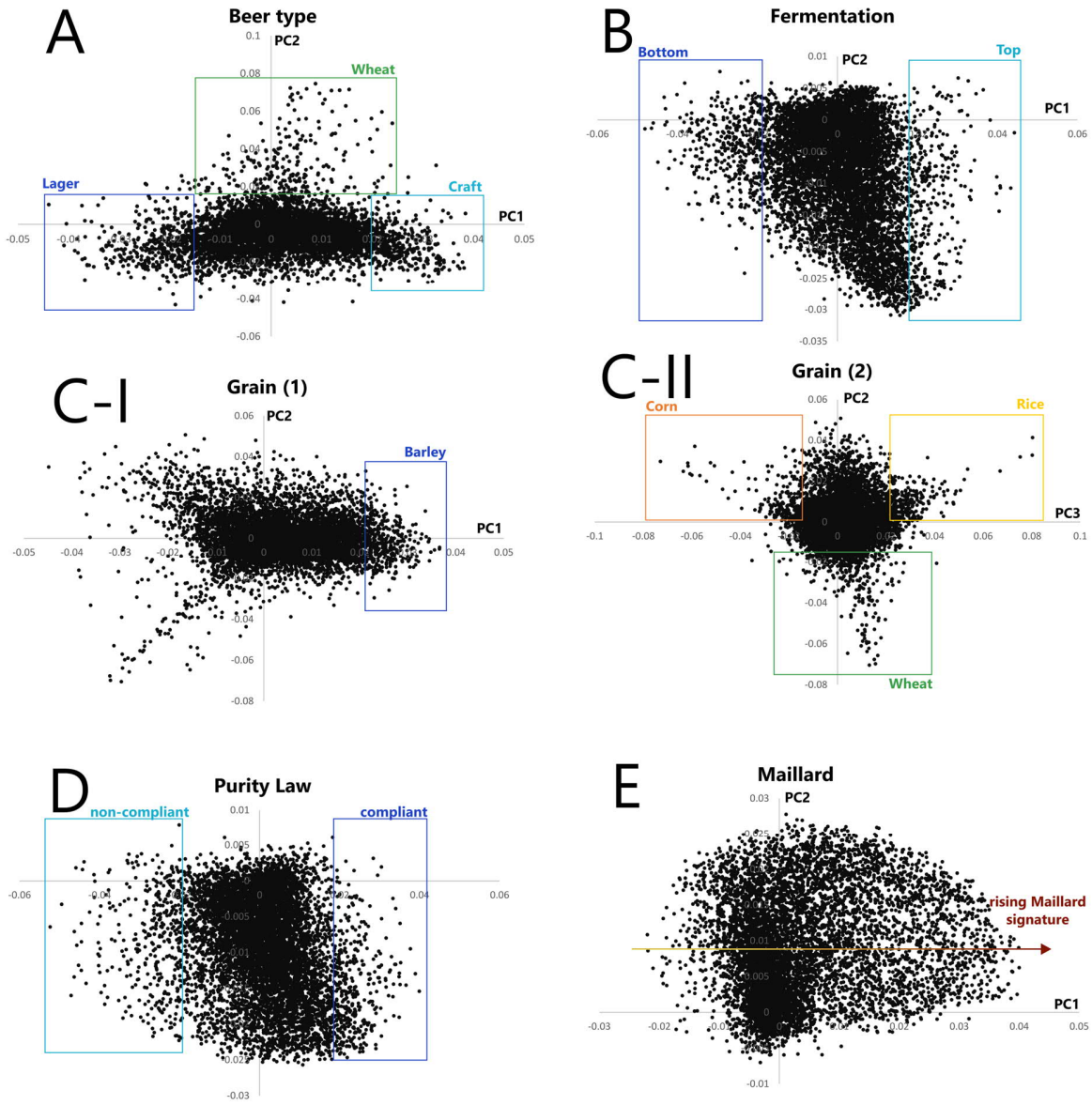
Supplementary Figure S2. Phase-contrast microscopy of amorphous organic particles of 1885 beer. Typical particles that occur during the aging of filtered beers due to polyphenol-protein complexation.



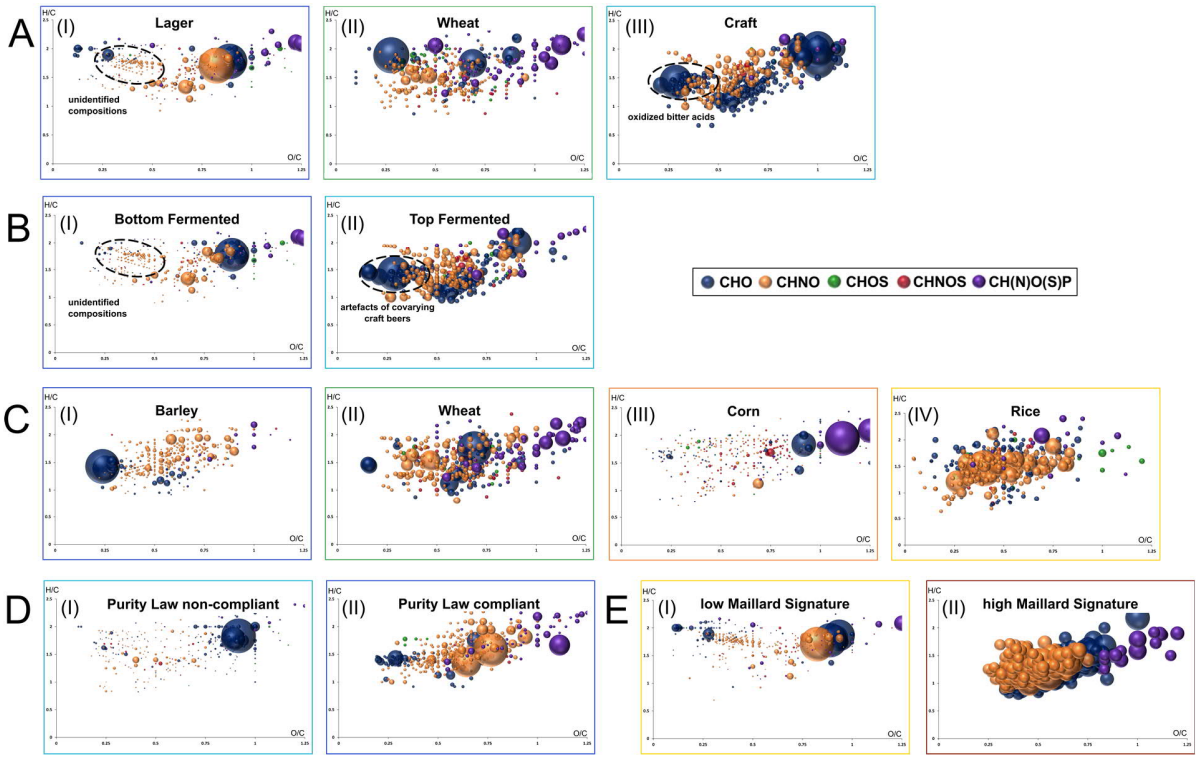
Supplementary Figure S3. FTICR mass spectrum excerpt of beer B1885 (A) and B2019 (B) showing over 40 different compositions in the nominal mass m/z 317. Chemical space color code: CHO (blue), CHNO (orange), CHOS (green), CHNOS (red), CH(N)O(S)P (violet). The pictures of the beer bottles are used under explicit permission of Privatbrauerei Ernst Barre GmbH.



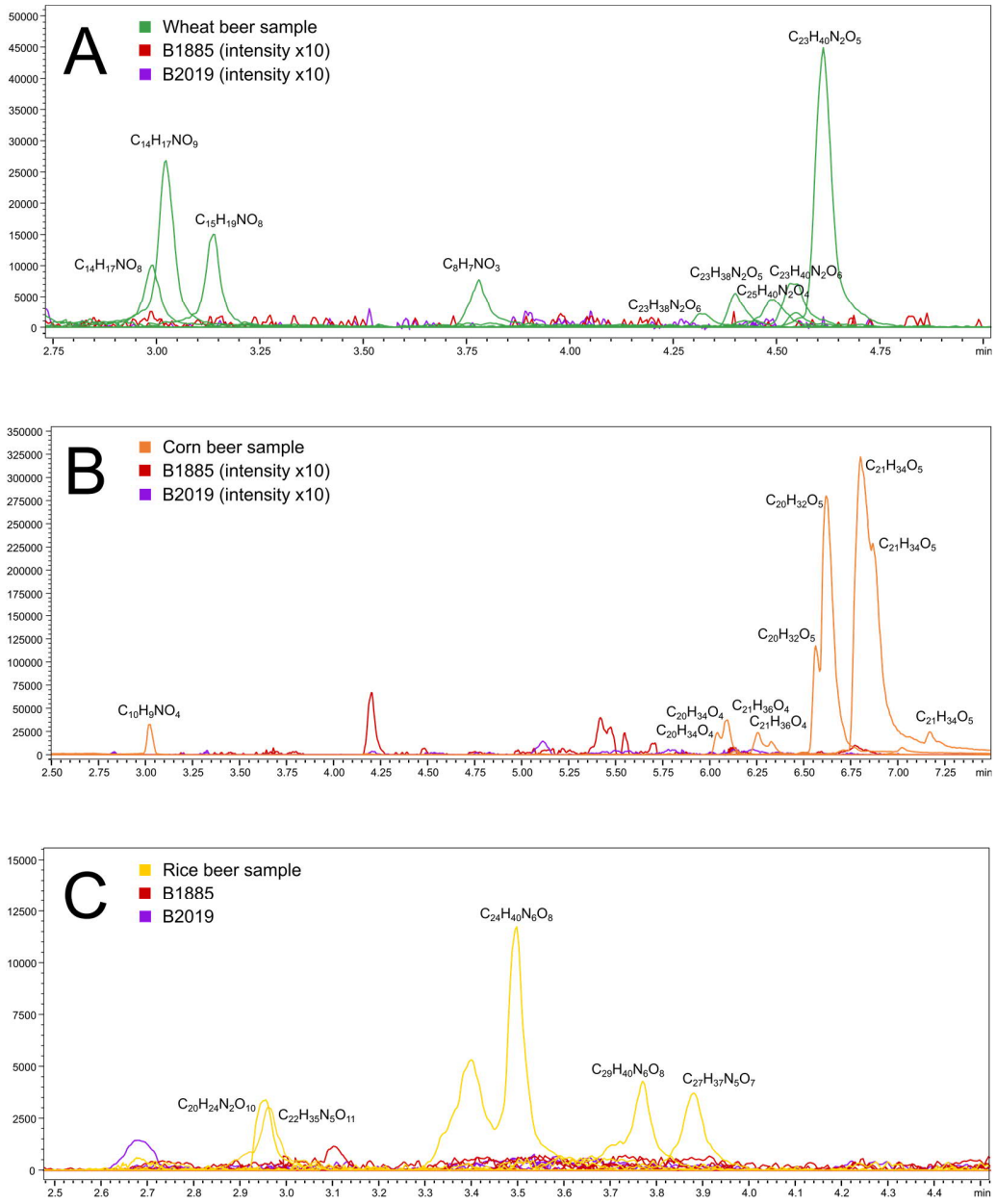
Supplementary Figure S4. Mass difference network of specific lipid-type compositions (as specified by their compositional area in the van Krevelen diagram) for the historical beer. The compositions are represented as nodes that are connected by edges, representing changes in the molecular formula equivalent to (bio-)chemical redox processes.



Supplementary Figure S5. Loading plots including 7,700 compositions for the OPLS-DA differentiating beer types (A), fermentation types (B), grains used (C), compliance with the German purity Law (D) and Maillard signatures by the absorption at 294 nm (E). The features specific for an attribute (unique or significantly more abundant) are highlighted. The 95th percentile is highlighted.



Supplementary Figure S6. Van Krevelen diagrams of the characteristic compositional profiles for beer types (A), fermentation types (B), grains used (C), compliance with the German Purity Law (D) and Maillard signatures (E). Color code: CHO (blue), CHNO (orange), CHOS (green), CHNOS (red), CH(N)O(S)P (violet). Neutral compositions are depicted. Specific areas are highlighted. Bubble size indicates relative signal intensities.



Supplementary Figure S7. Extracted Ion chromatograms of compound masses found to be specific for wheat (A), corn (B) and rice (C) including a respective grain-containing sample, sample B1885 and sample B2019. The EIC mass range is the respective exact *m/z* –value ± 10 ppm**.** No overlap of reported marker molecules (Pieczonka et al. (2021), Front. Chem., 9 (715372), 1-12) between the grain-containing samples and samples B1885 and B2019 was observed.