Supplementary Information (SI) for Sustainable Food Technology.
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Electronic Supplementary Information

An assessment of spent coffee grounds as a replacement for peat in the production of Scotch Whisky: chemical and sensory analysis of new make spirits.

FT-ICR-MS

Spectral processing was carried out with CoreMS 2.5.2.beta in Python 3.11.4 starting with an intrinsic error investigation (Corilo et al., 2021, Van Rossum et al., 2009). Peaks were picked according to a signal to noise threshold based on the logarithmic intensity of each peak, including noise and analyte peaks (Zhurov et al., 2014) using standard deviations of 10 and the number of bins used in the histogram was set to 500. The minimum relative intensity required for a peak to be picked was set to 1%. Initial formula assignments were made with the elemental limits $C_{0\text{-}100}H_{0\text{-}200}O_{0\text{-}26}$ and a maximum/minimum error threshold of ±5 ppm. For each spectrum, the m/z and m/z error of each picked peak were then plotted to examine the intrinsic error distribution of the instrument. From this a ppm error range was generated from which only peaks within the range were calibrated using a polynomial function and a calibration list of known whisky compounds (Kew, 2018). Final formula assignments were made using the elemental limits $C_{1\text{-}90}H_{4\text{-}200}O_{0\text{-}26}S_{0\text{-}5}N_{0\text{-}5}$ for m/z between 100 and 800 and a maximum/minimum error threshold of ± 0.25 ppm. Formula assignments were also made on each blank spectrum to identify any potential contaminants, which were defined as any assigned peaks with a peak height greater than 5% of the highest assigned peak in each blank spectrum. The formulae corresponding to these peaks were removed from sample mass lists.

Python was used to apply a mass filter to the triplicate samples where any formula that appeared in only one replicate was removed. Average mass lists were produced from triplicate samples with each mass given an average peak height form the triplicate samples. These mass lists were analysed in Python, using PyKrev 1.2.4, and UpSet Plot 0.8.0 (Kitson et al., 2021; Seabold et al., 2010). Pykrev automatically removes isotopologues from mass lists. Attributes for each sample were determined, including average numbers of individual elements compound classes determined using both constituent elements and multidimensional stoichiometric compound classification (MSCC) (Rivas-Ubach et al., 2018).

Sample	Assigned Formula	Mean Mz	Mean C	Mean H	Mean N	Mean O	Mean S	OC	HC	DBE	AI	NOSC
Coffee-Average	3795	399.4012	20.8424	31.8403	0.2403	6.8941	0.1431	0.3740	1.5278	6.0424	0.0889	-0.7050
Industrial-Average	2700	368.7842	19.0863	30.2252	0.2037	6.4204	0.1485	0.3845	1.5702	5.0756	0.0665	-0.7291
Laboratory-Average	3225	382.4957	19.6102	30.1150	0.2738	6.8536	0.1367	0.3951	1.5276	5.6896	0.0795	-0.6533

Sample	Lipid %	Carbohydrate %	Amino sugar %	Peptide %	Tannin/Lignin like %	CHO %	CHOS %	CHON %	CHNS %	CHS %
Coffee-Average	57.3386	2.6350	0.3689	5.8235	27.1146	75.5731	13.7549	10.0922	0.2635	0.2899
Industrial-Average	60.8889	3.1481	0.3333	5.1852	23.0000	76.7037	14.5556	8.3703	0.1852	0.1111
Laboratory-Average	56.2791	2.5116	1.0853	6.8217	25.8605	75.4729	13.2093	10.7907	0.2171	0.2481

Table S1. Summary of attributes for the average spectra determined using PyKrev. Assigned formula excludes isotopologues. Mean elemental counts are the average amount per formula. OC and HC are elemental ratios. DBE = Double bond equivalents, AI = Aromaticity index calculated using 'rAImod' in PyKrev. NOSC = Nominal oxidative state of carbon. Lipid, Carbohydrate, Amino sugar, and Oxy-aromatic classes are assigned with MSCC.

Sample	Calibration Points	Calibration RMS	Assigned Peaks	Percentage Relative Abundance	Assignment RMS	Contaminants Removed
Coffee-1	32	0.110157	5808	70.96166	0.123024	33
Coffee-2	32	0.119478	5917	66.98768	0.125417	28
Coffee-3	34	0.180006	5792	63.74303	0.125594	28
Industrial-1	31	0.171134	3378	69.8346	0.12198	33
Industrial-2	28	0.129888	4393	71.1742	0.121812	33
Industrial-3	29	0.156082	5116	72.52873	0.119098	31
Laboratory-1	34	0.132897	6454	56.43949	0.128581	26
Laboratory-2	21	0.192144	2924	73.22707	0.128287	29
Laboratory-3	33	0.166098	5788	55.04218	0.129861	27

Table S2. Summary of assignments. Calibration points are the number of matched calibration points with the spectrum. RMS = Root Mean Square Error, assigned peaks include isotopologues.

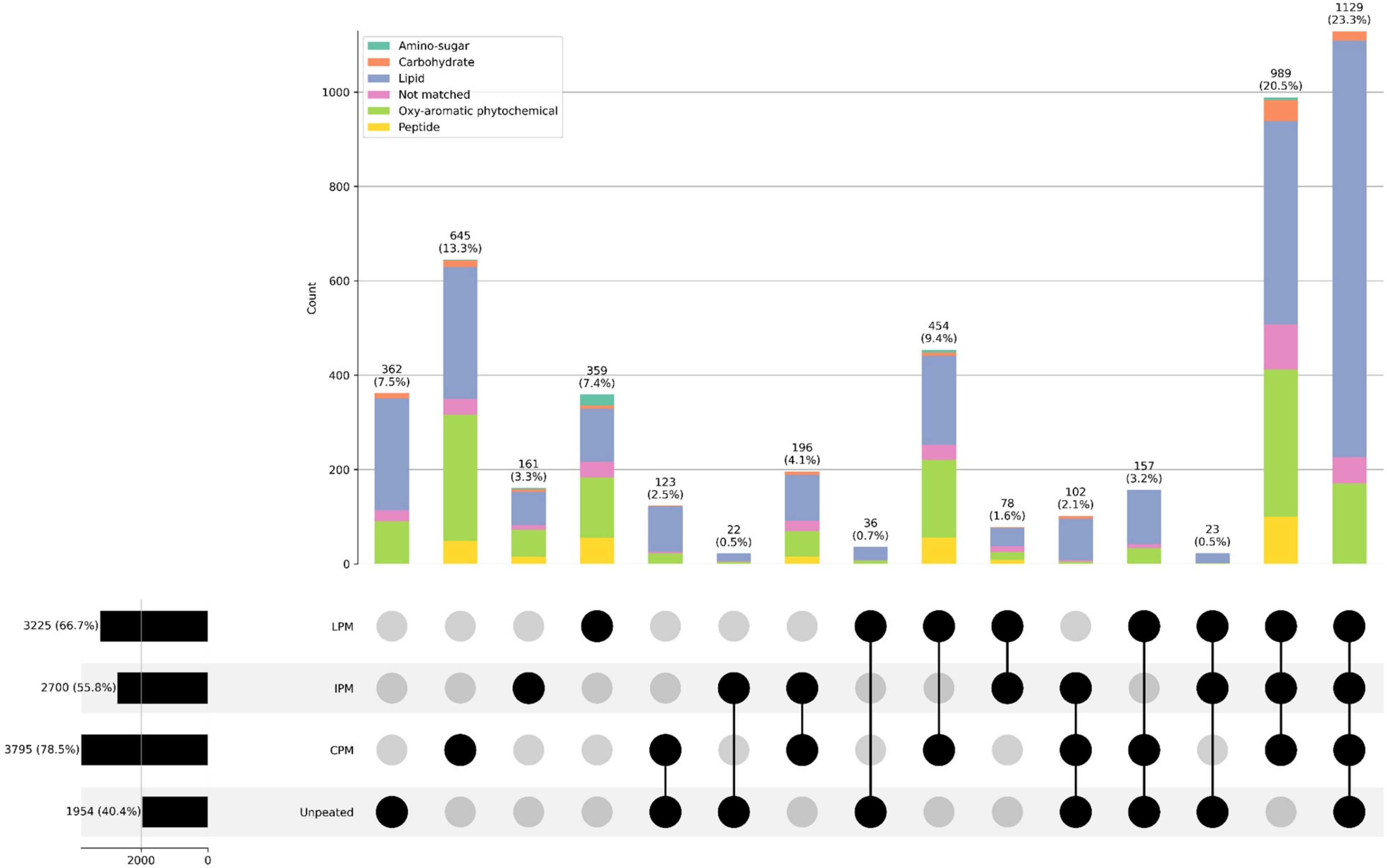

Figure S1. Upset analysis of the smoked NMS plus non-peated NMS. Lipid, Carbohydrate, Amino sugar, and Oxy-aromatic classes are assigned with MSCC.

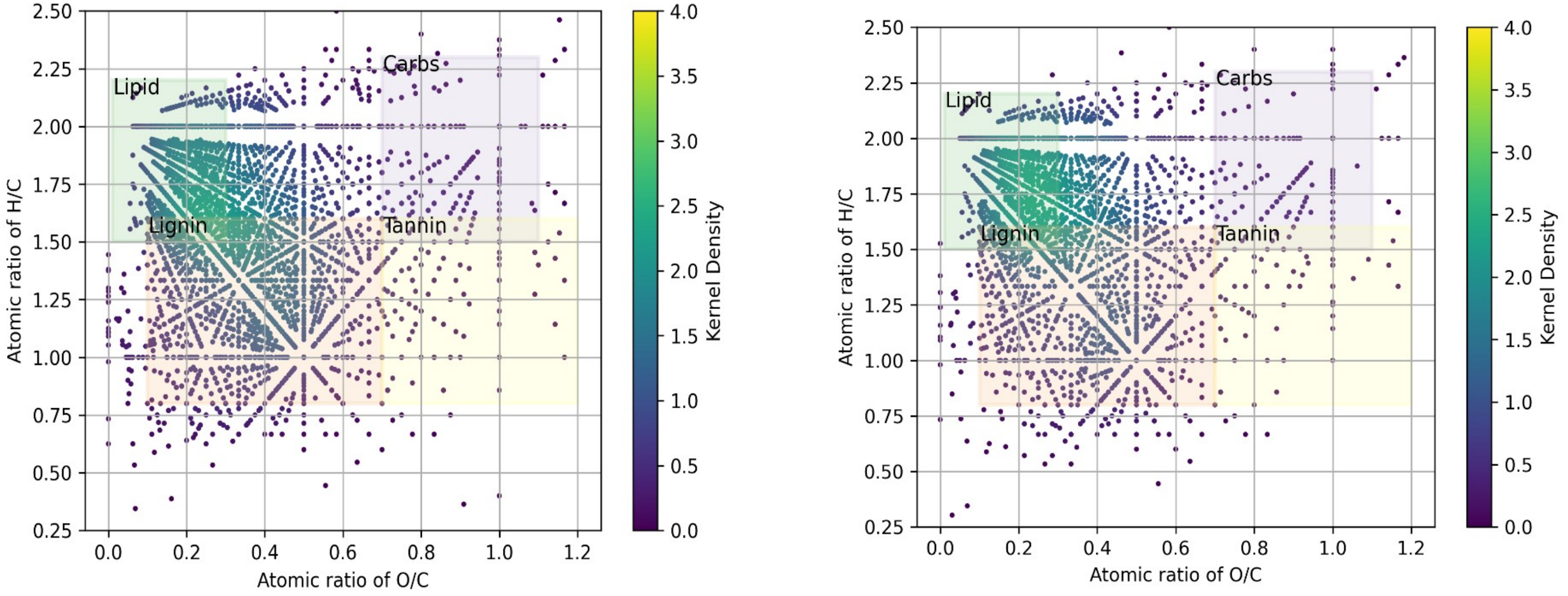

Figure S2. Van Krevelen diagrams of laboratory peated NMS (left) vs industrial peated NMS (right)

id	assigned formula	mean mz	dbe	ai	nosc	gfe	CHO %	CHOS %	CHNS %	CHS %	CHON %
Coffee	768	495.5765	8.727865	0.132895	-0.67203	79.45295	65.36458	17.31771	0.520833	0.911458	15.88542
Industrial	183	443.7086	7.081967	0.074667	-0.56086	76.28457	53.00546	25.68306	0.546448	0	20.76503
Laboratory	395	460.0991	8.017722	0.081597	-0.27449	68.12284	53.67089	17.21519	0.506329	1.012658	27.59494

Table S3. Summary of attributes for the average spectra determined using PyKrev. Assigned formula excludes isotopologues. DBE = Double bond equivalents, AI = Aromaticity index calculated using ‘rAImod’ in PyKrev. NOSC = Nominal oxidative state of carbon.

New make spirit production

Green malt

A bulk supply of KWS Sassy barley was supplied by a maltings. This bulk sample of barley was steeped and germinated in the laboratory to produce green malt. The steeping and germination conditions are shown in Table X. After the end of the last germination step the green malt was stored in a freezer.

Step	**Time (h)**	**Temperature (°C)**
1st Steep	8	17
1st Rest	16	17
2nd Steep	24	17
Germination	96	17

Table S4. Steeping and germination conditions to produce green malt.

Peat or Coffee grounds smoking of malt

Frozen green malt was thawed overnight in a fridge and then allowed to equilibrate to ambient temperature prior to use in peating experiments. 35g of peat (provided by a maltsters who had sourced it from Peterhead) or coffee grounds was used to smoke 350g of green malt until smoking was complete (1.5 h) using a Carbolite EHA 12/150B horizontal tube oven (Fig. 1). Peat or coffee grounds samples were placed inside the oven via a quartz glass sample boat. The oven has been modified at the chimney end to have a 90° elbow pipe attached to a quartz glass tube which holds the green malt. Air passes into the system via an air inlet from a benchtop air tap. The flow of air can be controlled from this tap and is measured by using an anemometer. The combustions were carried out at the same settings across all peatings; 550°C with an air flow of 5.5 m/s. Once the green malt had been peated they were kilned at 50°C for 24hr. To produce enough malt for processing into spirit, these peatings were carried out for a total of 4 times for the laboratory coffee smoked malt, and the laboratory peated malt.

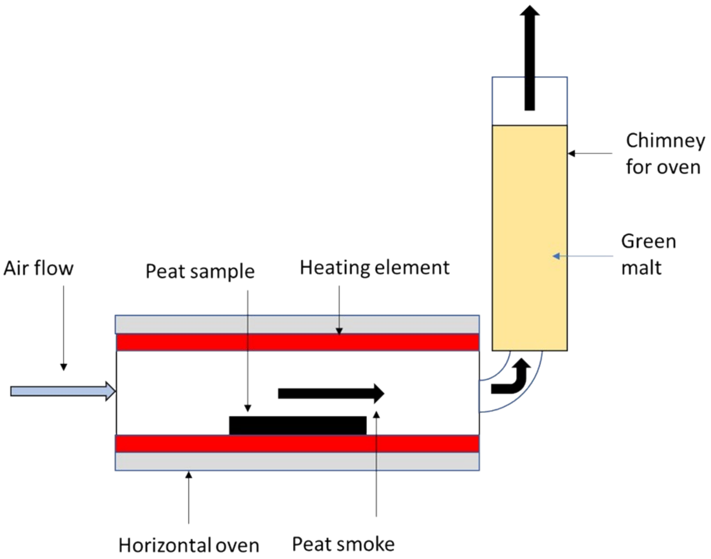

Figure S3. Diagram of the SWRI laboratory scale peating apparatus.

Mashing

A 128 g sample of malt was weighed into a milling beaker and milled using a Buhler Miag Universal Laboratory Disc Mill (Buhler GmbH, Braunschweig, Germany, Post fach 3369, D-38023) set at 0.2 mm gap width using a feeler gauge. The resultant grist was immediately placed into a tared container and 125 g (± 0.001 g) weighed out. This process was repeated three times to obtain a total of 500 g of grist from each malt sample.

Each 125 g aliquot of grist was transferred as quantitatively as possible to a mashing beaker and placed in a 1-Cube R8 Mashing Bath at 65 °C. Distilled water was heated to 68 °C and 325 mL added to the grist in the mashing beaker, carefully rinsing any excess flour in the grist container. Each mash was stirred thoroughly using a glass rod to eliminate any lumps and covered with aluminium foil. The mash temperature was maintained at 65 °C for 1 h with regular stirring.

The mash was then transferred to a polypropylene centrifuge bottle and spun at 1200 g (2000 rpm) for 6 min in a Sanyo MSE Mistral 3000E centrifuge (MSE (UK) Limited, London, UK, SE26 5AZ). The supernatant was decanted and filtered under vacuum through a Buchner filter fitted with an unbleached Classic Calico cotton filter (John Lewis plc., London, UK, SW1E 5NN) into a 2-L Buchner flask. The residual grains were then transferred to the filter funnel and filtered under vacuum to apparent dryness. A glass reagent bottle stopper was used to tamp down the bed and maintain the vacuum. The resulting filtrate was cooled to ambient temperature and transferred to a 3L round bottom flask. The dried grains were returned to the mashing beaker and placed in the water bath which had been heated to 80 °C. The centrifuge bottle was rinsed with 200 mL boiling distilled water and the hot washings added to the grains as second water. The grains were extracted at 80 °C for 30 min, and then filtered under vacuum through the Buchner apparatus as described previously. The resulting filtrate was cooled and added to the 3L round bottom flask. The grains were returned to the mashing beaker and the beaker placed in a water bath at 100 °C and allowed to equilibrate for 5 min. Subsequently, 150 mL boiling water was added to the grains and extracted at 100 °C for 10 min. The grains were then filtered as quickly as possible in order to maximise elution of wort sugars before cooling. An appropriate volume was added to the wort in the fermenter in order to achieve a total wort volume of 2200 mL.

Fermentation

Once all the wort had been collected, the fermentation flask was sealed with a fermentation lock and placed in a water bath programmed from 19 °C to 33 °C over 72 hours).

Distillation

The fermented wash was distilled using copper stills. Prior to distillation, the frozen wash was rapidly thawed in a sink of hot water. The still was then charged with 1.65 L of wash and 550 mL of low wines were collected. 50ml of the low wines was retained for analysis. The remaining 500 mL was charged to the spirit still and the following cut-points were used; 100 mL new make spirit, 2 consecutive 100 mL feints fractions. For both the wash, and spirit distillations, 10 drops of Foamdoctor F2887 were added to the still to reduce foaming.

Sensory Analysis

Sensory Panel

All sensory evaluations were carried out by the trained sensory panel at The Scotch Whisky Research Institute (SWRI). This panel comprises a pool of 22 panellists (SWRI employees, over 18 years of age, mixed gender) who have training and expertise in the evaluation of Scotch whisky. Panellists are prescreened using an odour recognition test which uses everyday odours to test their ability to recognise and describe aromas. Selected panellists are then trained on specific whisky flavours based on the SWRI Scotch Whisky Flavour Wheel. Trainee panellists are exposed to a number of different spirits and sensory techniques during their period of training. Their performance as compared to the trained panel average is tracked across tests and overall performance of both trainee and trained panellists is regularly assessed using the Whisky Sensory Proficiency Scheme (FlavorActiV™; Flavoractiv Ltd., Watlington, UK). Trainees join the expert panel when the SWRI sensory scientist decides they have reached the required level of expertise based on these criteria. There was only sufficient volume for 15 trained panellists to assess the samples. Those who were available on each test day took part in the sensory evaluations.

Preparation of samples for sensory

The duplicates of each type of both the new make spirit (NMS) and feints sample were nosed by the SWRI sensory scientist and determined to be similar enough to composite them to increase the sample volume available for sensory analysis. The low wines samples were not assessed by the sensory panel because the available volume was low. The feints samples were assessed on separate day to the NMS samples. Samples were diluted to 20% abv using distilled water on the day of testing. 20 mL of each sample was presented in blue nosing glasses covered with a watch glass and identified only with a 3-digit random code.

Sensory profiling

Quantitative Descriptive Profiling (QDP) conducted in accordance with ISO 13299:2016 was used to assess the peaty characteristics (burnt, smoky, medicinal and overall peat intensity) of the samples. The intensity of each of these attributes was scored using a 0-3 continuous line scale marked at 0.5 intervals.

A monadic design (one sample presented at a time and rated for all attributes) was used for QDP with the sample presentation order balanced across all panellists. Compusense® cloud based sensory software (Compusense Inc., Guelph, ON, Canada) was used for the design and presentation of the test. All sensory testing took place in the SWRI sensory laboratory as per our standard protocol.

Analysis of sensory data

Mean scores for each attribute were calculated and analysis of variance (ANOVA) used to find any statistically significant ($p<0.05$) differences between the samples followed by Tukey’s post hoc test to determine sample groupings for any significant result. Unistat® 10.0 for Excel (Unistat Ltd., London, UK) was used for statistical analysis of the sensory data.

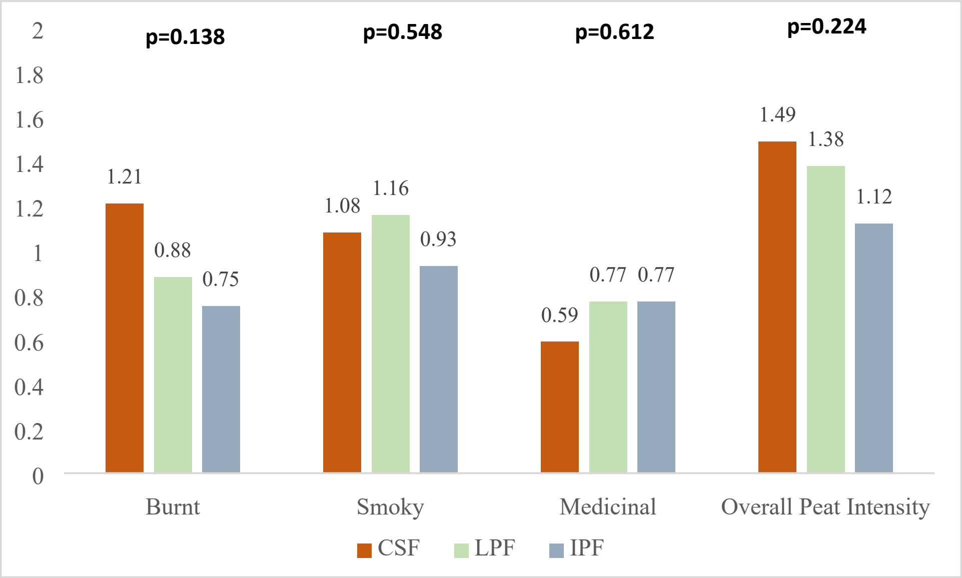

Figure S4. Average panel scores and results of the statistical analysis ($p<0.05$) for the feints samples. CSF – coffee smoked feints; LPF – laboratory peated feints; IPF – industrially peated feints.

NMR spectra

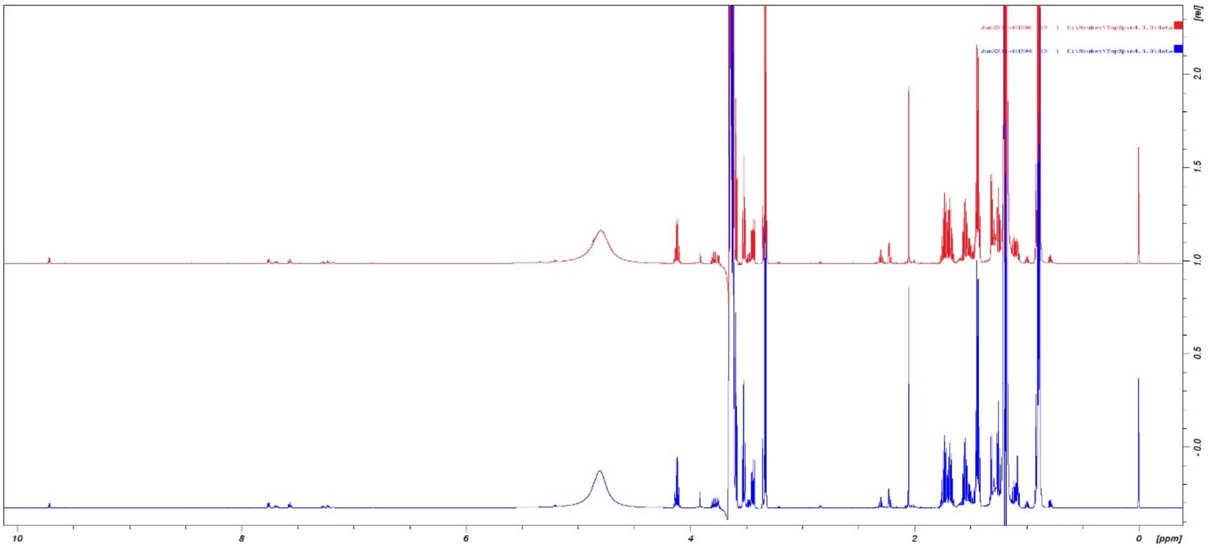

Figure S5. ^{1}H NMR spectra of IPNMS1 (bottom), IPNMS2 (top) recorded at 600 MHz.

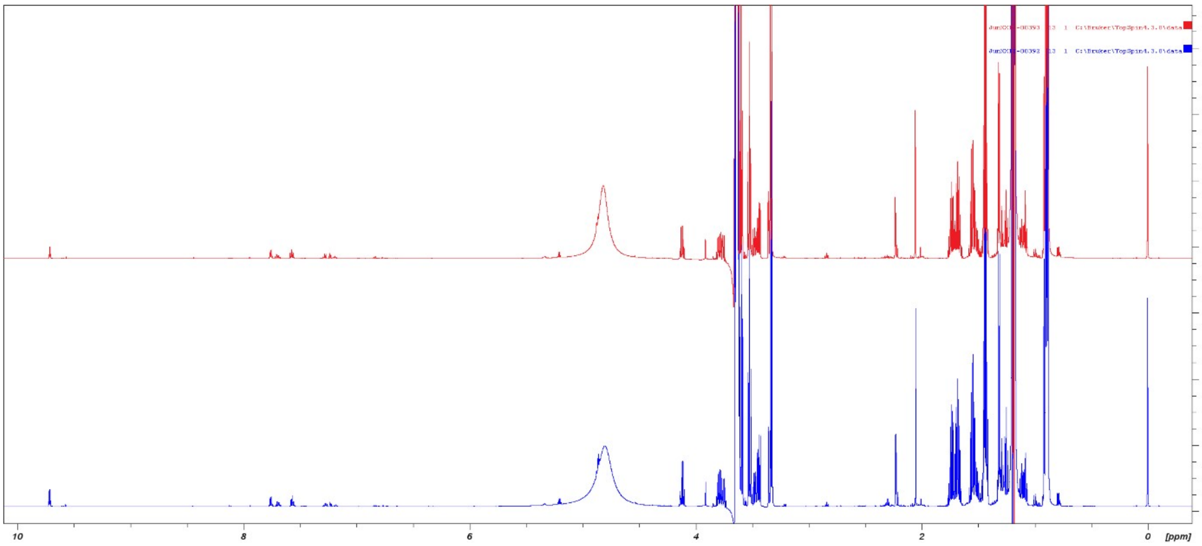

Figure S6. ^{1}H NMR spectra of LPNMS1 (bottom), LPNMS2 (top)

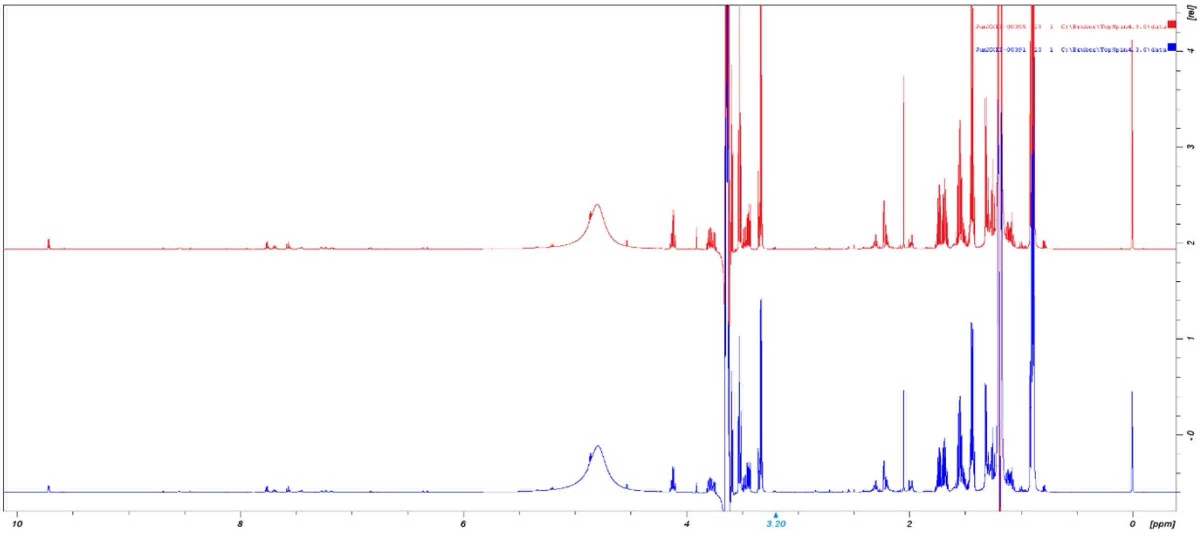

Figure S7. ^{1}H NMR spectra of CSNMS1 (bottom) and CSNMS2 (top) recorded at 600 MHz.

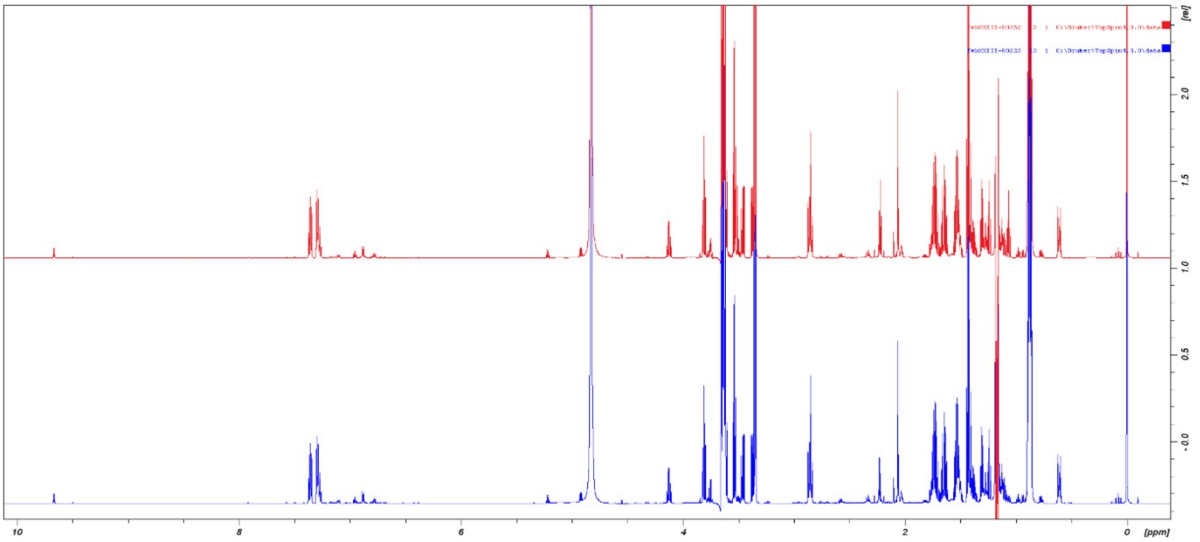

Figure S8. ^{1}H NMR spectra of IPLW1 (bottom), IPLW2 (top) recorded at 600 MHz.

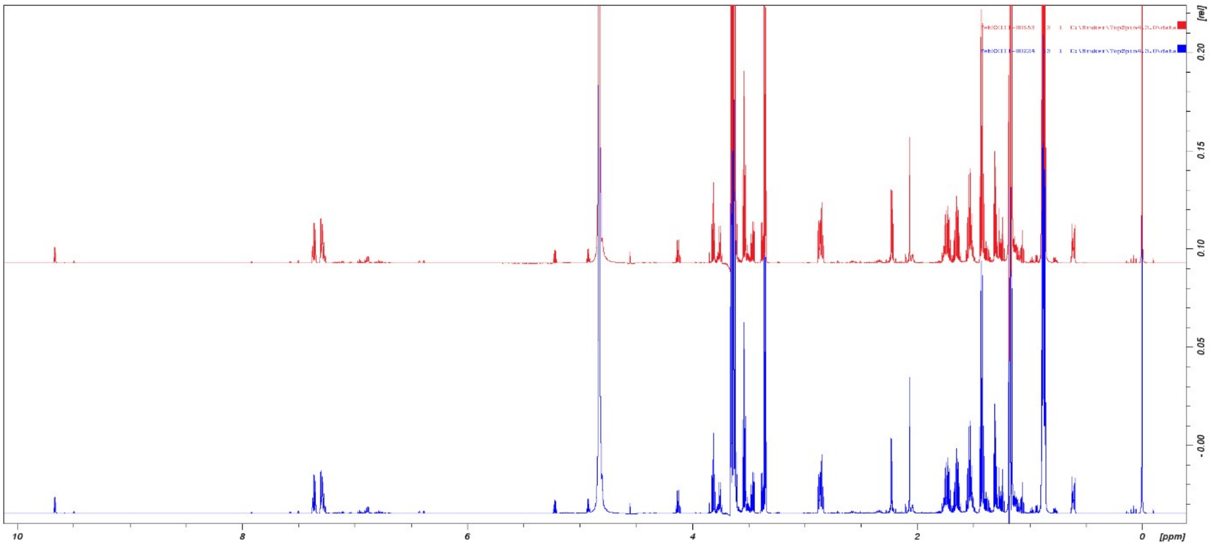

Figure S9. ^{1}H NMR spectra of LPLW1 (bottom), LPLW2 (top)

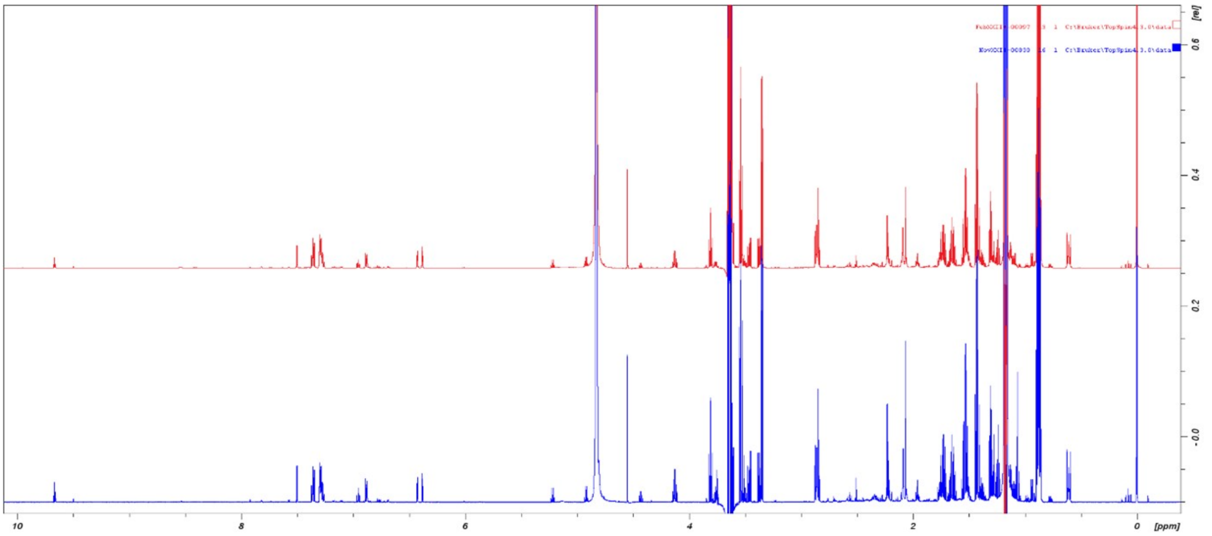

Figure S10. ^{1}H NMR spectra of CSLW1 (bottom) and CSLW2 (top) recorded at 600 MHz.

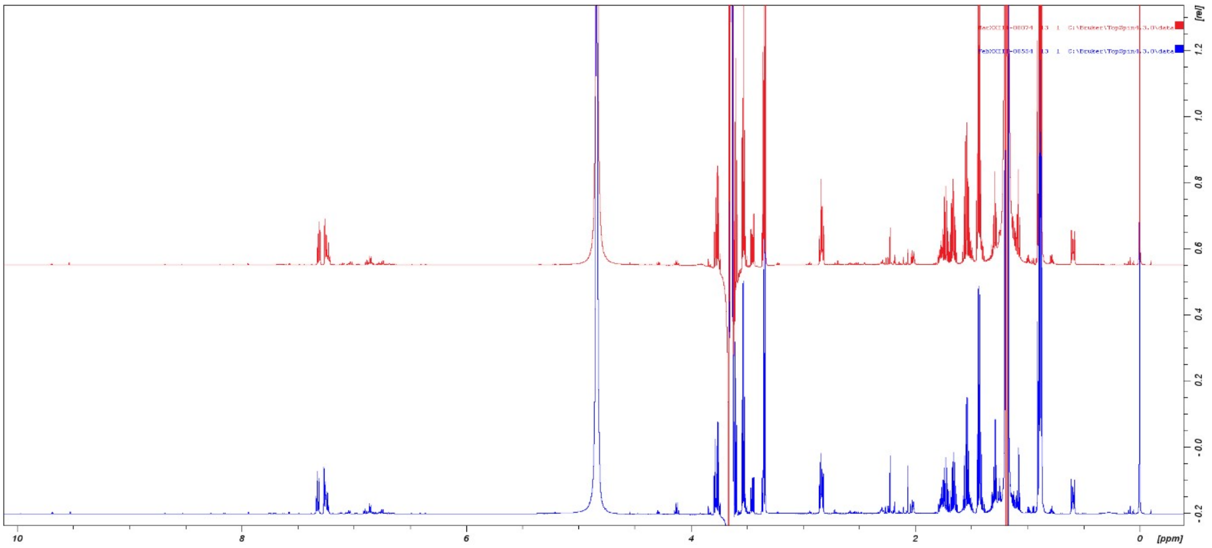

Figure S11. ^{1}H NMR spectra of IPF1 (bottom), IPF2 (top) recorded at 600 MHz.

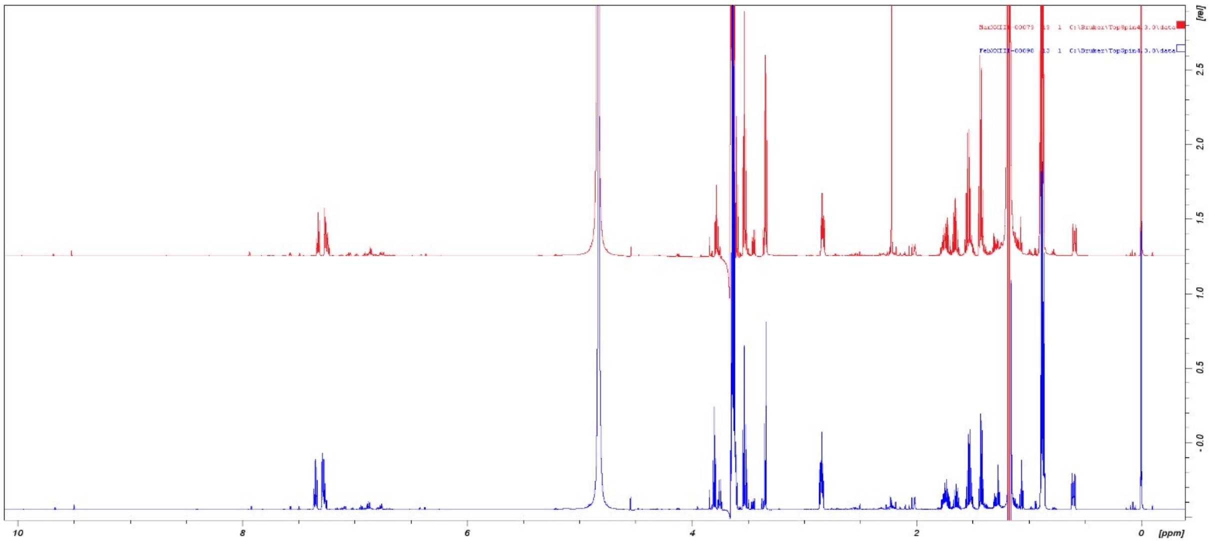

Figure S12. ^{1}H NMR spectra of LPF1 (bottom), LPF2 (top)

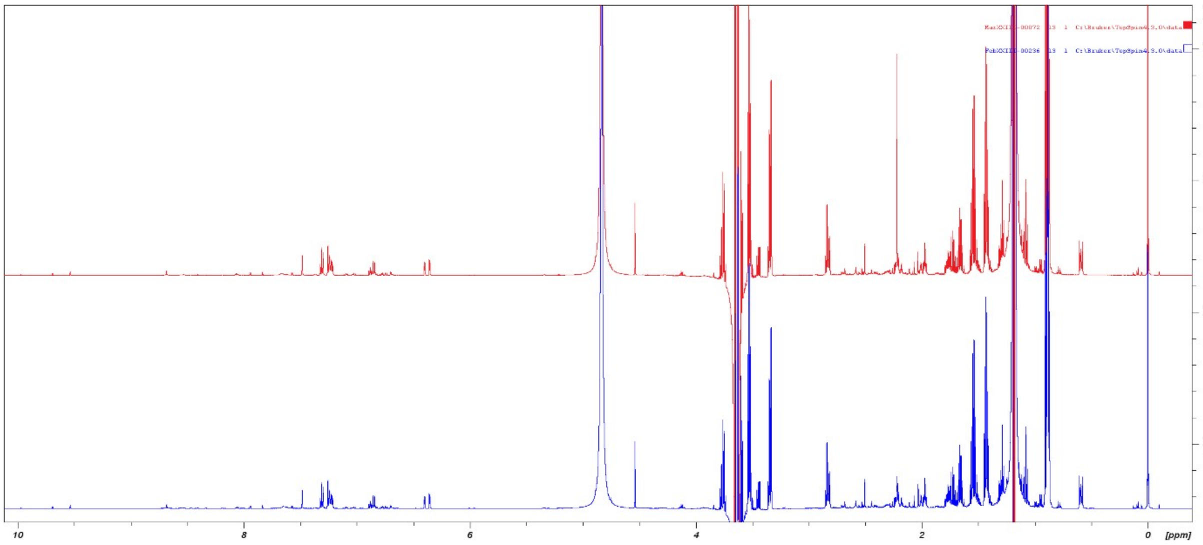

Figure S13. ^{1}H NMR spectra of CSF1 (bottom) and CSF2 (top) recorded at 600 MHz.

Signal assignments

δ_H / ppm	Multiplicity	Integration	Inferences	Concentration / mmol L^{-1}
0	Singlet	10	DSS 3xCH_3	1.00
0.79	Multiplet	2.55	Fusel alcohols CH_3 groups carbon satellites	-
0.89	Multiplet	434.1	Fusel alcohols CH_3 groups	-
1.00	Multiplet	2.06	Fusel alcohols CH_3 groups carbon satellites	-
1.10	Multiplet	-	Fusel alcohols ethyl esters CH_3 groups	-
1.19	Distorted	-	Ethanol CH_3 group, suppressed	-
1.25	Triplet, J = 7.1 Hz	30.8	Ethyl acetate CH_3 next to CH_2	9.24
1.29	Triplet, J = 7.1 Hz	-	Ethanol CH_3 carbon satellite	-
1.31	Doublet, J = 5.2 Hz	14.4	1,1-diethoxyethane CH_3 next to CH	4.33

1.43	Quartet, J = 7.0 Hz	67.7	3-methylbutanol CH_2 next to CH and CH_2	30.5
1.54	Sextet, J = 7.2 Hz	32.9	*n*-propanol CH_2 next to CH_2 and CH_3	14.8
1.68	Nonet, J = 6.7 Hz	-	3-methylbutanol CH next to 2xCH_3 and CH_2	-
1.73	Nonet, J = 6.7 Hz	-	2-methylpropanol CH next to 2xCH_3 and CH_2	-
1.94	Singlet	0.11	Acetic acid CH_3 carbon satellite	-
2.05	Singlet	16.7	Acetic acid CH_3	5.01
2.08	Singlet	0.17	Ethyl acetate isolated CH_3	0.052
2.16	Singlet	0.13	Acetic acid CH_3 carbon satellite	-
2.18	Singlet	0.16	*ortho*-cresol CH_3 group	0.048
2.23	Doublet, J = 3.0 Hz	2.73	Acetaldehyde CH_3 next to CH	0.82
2.27	Singlet	0.22	*para*-cresol CH_3 group	0.066
2.84	Triplet, J = 7.4 Hz	0.65	2-phenylethanol CH_2 next to CH_3	0.29
3.21	Doublet, J = 6.6 Hz	0.30	Isobutanol CH_2 carbon satellite	-
3.22	Part of DD, J =6.8 Hz	0.046	2-methylbutanol CH_2 carbon satellite	-
3.23	Singlet	0.019	Methanol CH_3 carbon satellite	-
3.33	Doublet, J = 6.6 Hz	54.3	2-methylpropanol CH_2 next to CH_2	24.4
3.34	Part of DD, J = 6.5 Hz	8.81	2-methylbutanol part of diastereotopic CH_2	-
3.35	Singlet	4.46	Methanol CH_3	1.34
3.44	DD, J = 10.6 Hz, 5.9 Hz	14.3	2-methylbutanol part of diastereotopic CH_2	12.9
3.48	Quartet, J = 7.1 Hz	-	Ethanol CH_2 carbon satellite	-
3.52	Triplet, J = 6.8 Hz	23.7	*n*-propanol CH_2 next to CH_2	10.7
3.59	Triplet, J = 7.1 Hz	45.0	3-methylbutanol CH_2 next to CH_2	20.2
3.63	Distorted	-	Ethanol CH_2, suppressed	-
3.78	Quartet, J = 7.1 Hz	-	Ethanol CH_2 carbon satellite	-
3.81	Singlet	0.21	Guaiacol OCH_3	0.063
4.12	Quartet, J = 7.1 Hz	-	Lactic acid CH next to CH_3	-
4.22	Quartet, J = 6.9 Hz	-	Ethyl acetate CH_2 next to CH_3	-
4.80	Broad singlet	-	Water, suppressed	-
5.20	Quartet, J = 5.2 Hz	-	Acetaldehyde water hemiacetal	-
6.73	Doublet, J = 8.5 Hz	0.075	*para*-cresol 2xCH next to CH, overlap with *ortho*-cresol	0.034
6.76	DD, J = 3.6 Hz, 1.6 Hz	0.046	Furfural aromatic CH	0.041
6.83	Doublet, J = 8.3 Hz	0.28	Phenol 2x CH next to CH	0.13
6.97	Doublet, J = 7.8 Hz	0.042	*para*-cresol 2xCH next to CH	0.020
7.18	Multiplet	0.48	Phenol 2xCH next to 2xCH	0.22
7.22	Doublet, J = 7.0 Hz	0.81	2-phenylethanol aromatic	-
7.27	Doublet, J = 7.4 Hz	0.52	2-phenylethanol aromatic	-
7.94	Multiplet	0.046	Furfural aromatic CH	0.041
8.12	Singlet	0.098	Ethyl formate CH	0.088
8.44	Singlet	0.039	Formic acid CH	0.035
9.57	Singlet	0.051	Furfural CHO	0.046

9.71	Quartet, J =2.9 Hz	0.83	Acetaldehyde CHO	0.75

Table S5. Signal assignment for NMR spectrum of new make spirit produced using industrially peated malt, recorded at the University of Edinburgh using a 600 MHz spectrometer, IPNMS1.

δ_H / ppm	Multiplicity	Integration	Inferences	Concentration / mmol L^{-1}
0	Singlet	10	DSS 3xCH_3	1.00
0.79	Multiplet	2.69	Fusel alcohols CH_3 groups carbon satellites	-
0.89	Multiplet	438.2	Fusel alcohols CH_3 groups	-
1.00	Multiplet	2.43	Fusel alcohols CH_3 groups carbon satellites	-
1.10	Multiplet	-	Fusel alcohols ethyl esters CH_3 groups	-
1.18	Distorted	-	Ethanol CH_3 group, suppressed	-
1.25	Triplet, J = 7.2 Hz	24.1	Ethyl acetate CH_3 next to CH_2	7.23
1.29	Triplet, J = 7.1 Hz	-	Ethanol CH_3 carbon satellite	-
1.31	Doublet, J = 5.0 Hz	18.3	1,1-diethoxyethane CH_3 next to CH	5.49
1.43	Quartet, J = 7.0 Hz	64.2	3-methylbutanol CH_2 next to CH and CH_2	28.9
1.55	Sextet, J = 7.2 Hz	30.7	*n*-propanol CH_2 next to CH_2 and CH_3	13.8
1.68	Nonet, J = 6.9 Hz	-	3-methylbutanol CH next to 2xCH_3 and CH_2	-
1.73	Nonet, J = 6.7 Hz	-	2-methylpropanol CH next to 2xCH_3 and CH_2	-
1.94	Singlet	0.10	Acetic acid CH_3 carbon satellite	-
2.05	Singlet	16.0	Acetic acid CH_3	4.80
2.08	Singlet	0.15	Ethyl acetate isolated CH_3	0.046
2.16	Singlet	0.11	Acetic acid CH_3 carbon satellite	-
2.18	Singlet	0.12	*ortho*-cresol CH_3 group	0.036
2.23	Doublet, J = 3.0 Hz	3.77	Acetaldehyde CH_3 next to CH	1.13
2.26	Singlet	0.16	*para*-cresol CH_3 group	0.048
2.84	Triplet, J = 7.4 Hz	0.51	2-phenylethanol CH_2 next to CH_3	0.23
3.21	Doublet, J = 6.6 Hz	0.34	Isobutanol CH_2 carbon satellite	-
3.22	Part of DD, J =6.8 Hz	0.068	2-methylbutanol CH_2 carbon satellite	-
3.23	Singlet	0.031	Methanol CH_3 carbon satellite	-
3.32	Doublet, J =6.6 Hz	56.6	2-methylpropanol CH_2 next to CH_2	25.5
3.34	Part of DD, J = 6.7 Hz	8.58	2-methylbutanol part of diastereotopic CH_2	-
3.35	Singlet	4.45	Methanol CH_3	1.34
3.44	DD, J = 10.6 Hz, 6.0 Hz	15.6	2-methylbutanol part of diastereotopic CH_2	14.1
3.47	Quartet, J = 7.1 Hz	-	Ethanol CH_2 carbon satellite	-
3.52	Triplet, J = 6.9 Hz	21.5	*n*-propanol CH_2 next to CH_2	9.68
3.59	Triplet, J = 7.0 Hz	28.8	3-methylbutanol CH_2 next to CH_2	13.0
3.63	Distorted	-	Ethanol CH_2, suppressed	-
3.78	Quartet, J = 7.1 Hz	-	Ethanol CH_2 carbon satellite	-

3.81	Singlet	0.21	Guaiacol OCH_3	0.065
4.12	Quartet, J = 7.0 Hz	-	Lactic acid CH next to CH_3	-
4.22	Quartet, J = 7.1 Hz	-	Ethyl acetate CH_2 next to CH_3	-
4.79	Broad singlet	-	Water, suppressed	-
5.20	Quartet, J = 5.2 Hz	-	Acetaldehyde water hemiacetal	-
6.72	Doublet, J = 8.2 Hz	0.056	*para*-cresol 2xCH next to CH, overlap with *ortho*-cresol	0.025
6.76	DD, J = 3.4 Hz, 1.5 Hz	0.042	Furfural aromatic CH	0.037
6.83	Doublet, J = 8.2 Hz	0.18	Phenol 2xCH next to CH	0.08
6.97	Doublet, J = 8.4 Hz	0.029	*para*-cresol 2xCH next to CH	0.013
7.18	Multiplet	0.40	Phenol 2xCH next to 2xCH	0.18
7.22	Doublet, J = 7.0 Hz	0.66	2-phenylethanol aromatic	-
7.27	Doublet, J = 7.4 Hz	0.44	2-phenylethanol aromatic	-
7.94	Multiplet	0.039	Furfural aromatic CH	0.038
8.12	Singlet	0.087	Ethyl formate CH	0.083
8.44	Singlet	0.047	Formic acid CH	0.038
9.57	Singlet	0.046	Furfural CHO	0.041
9.71	Quartet, J =2.9 Hz	1.15	Acetaldehyde CHO	1.03

Table S6. Signal assignment for NMR spectrum of new make spirit produced using industrially peated malt, recorded at the University of Edinburgh using a 600 MHz spectrometer, IPNMS2

δ_H / ppm	Multiplicity	Integration	Inferences	Concentration / mmol L^{-1}
0	Singlet	10	DSS $3xCH_3$	1.00
0.79	Multiplet	2.81	Fusel alcohols CH_3 groups carbon satellites	-
0.89	Multiplet	439.0	Fusel alcohols CH_3 groups	-
1.00	Multiplet	2.42	Fusel alcohols CH_3 groups carbno satellites	-
1.08	Triplet, J = 7.1 Hz	-	Ethanol CH_3 carbon satellite	-
1.10	Multiplet	-	Fusel alcohols ethyl esters CH_3 groups	-
1.19	Distorted	-	Ethanol CH_3, suppressed	
1.25	Triplet, J = 7.2 Hz	17.2	Ethyl acetate CH_3 next to CH_2	5.16
1.29	Triplet, J = 7.0 Hz	13.3	Ethanol CH_3 carbon satellite	-
1.31	Doublet, J = 5.2 Hz	28.4	1,1-diethoxyethane CH_3 next to CH	8.52
1.43	Quartet, J = 7.0 Hz	71.9	3-methylbutanol CH_2 next to CH and CH_2	32.4
1.55	Sextet, J = 7.2 Hz	39.0	n-propanol CH_2 next to CH_2 and CH_3	17.6
1.68	Nonet, J = 6.7 Hz	-	3-methylbutanol CH next to $2xCH_3$ and CH_2	-
1.73	Nonet, J = 6.7 Hz	-	2-methylpropanol CH next to $2xCH_3$ and CH_2	-
1.94	Singlet	0.036	Acetic acid CH_3 carbon satellite	-
2.05	Singlet	9.36	Acetic acid CH_3	2.81
2.08	Singlet	0.12	Ethyl acetate isolated CH_3	0.036
2.16	Singlet	0.11	Acetic acid CH_3 carbon satellite	-
2.18	Singlet	0.17	*para*-cresol CH_3	0.051

2.21	Singlet	0.83	Acetone 2xCH_3	0.12
2.23	Doublet, J = 2.9 Hz	6.38	Acetaldehyde CH_3 next to CH	1.91
2.27	Singlet	0.21	*ortho*-cresol CH_3 group	0.063
2.84	Triplet, J = 7.4 Hz	0.72	2-phenylethanol CH_2 next to CH_2	0.32
3.21	Doublet, J = 6.5 Hz	0.32	Isobutanol CH_2 carbon satellite	-
3.22	Doublet, J = 6.8 Hz	0.096	Part of 2-methylbutanol CH_2 carbon satellite	-
3.23	Singlet	0.031	Methanol CH_3 carbon satellite	-
3.33	Doublet, J = 6.6 Hz	46.9	Isobutanol CH_2 next to CH	21.1
3.34	Doublet, J = 6.7 Hz	7.72	Part of 2-methylbutanol diastereotopic CH_2	-
3.35	Singlet	3.22	Methanol CH_3	0.97
3.44	DD, J = 10.6 Hz, 5.9 Hz	13.9	Part of 2-methylbutanol diastereotopic CH_2	12.5
3.48	Quartet, J = 7.1 Hz	-	Ethanol CH_2 carbon satellite	-
3.52	Triplet, J = 6.8 Hz	30.7	n-propanol CH_2 next to CH_2	13.8
3.59	Triplet, J = 7.0 Hz	41.5	3-methylbutanol CH_2 next to CH_2	18.7
3.63	Distorted	-	Ethanol CH_2, suppressed	-
3.75	Quartet, J = 7.1 Hz	-	Ethanol CH_2 carbon satellite	-
3.81	Singlet	0.53	Guaiacol OCH_3	0.16
4.12	Quartet, J = 7.1 Hz	-	Lactic acid CH next to CH_3	-
4.22	Quartet, J = 6.9 Hz	-	Ethyl acetate CH_2 next to CH_3	-
4.80	Broad singlet	-	Water suppressed	-
5.20	Quartet, J =5.2 Hz	-	Acetaldehyde water hemiacetal	-
6.32	Doublet, J = 3.4 Hz	0.030	2-methylfuran aromatic CH	0.027
6.36	Multiplet	0.028	2-methylfuran aromatic CH	0.025
6.68	Multiplet	0.017	5-Hydroxymethylfurural CH	0.015
6.73	Multiplet	0.10	*para*-cresol 2x CH next to CH, overlap with *ortho*-cresol	0.045
6.76	DD, J = 3.7 Hz, 1.6 Hz	0.15	Furfural CH next to 2xCH	0.13
6.83	Doublet, J = 8.4 Hz	0.22	Phenol 2x CH next to CH	0.10
6.97	Doublet, J = 8.4 Hz	0.05	*para*-cresol 2xCH next to CH	0.022
7.04	Multiplet	0.026	*ortho*-cresol aromatic CH	0.024
7.18	Triplet, J = 7.1 Hz	0.48	Phenol 2xCH next to CH	0.21
7.22	Multiplet	0.80	2-phenylethanol aromatic	-
7.27	Multiplet	0.78	2-phenylethanol aromatic	-
7.94	Multiplet	0.13	Furfural CH next to CH	0.12
8.12	Singlet	0.090	Ethyl formate CH	0.081
8.44	Singlet	0.041	Formic acid CH	0.037
9.57	Singlet	0.13	Furfural CHO	0.12
9.59	Doublet, J = 2.0 Hz	0.031	5-Hydroxymethylfurfural CHO	0.028
9.71	Quartet, J = 2.9 Hz	1.94	Acetaldehyde CHO	1.74
9.99	Singlet	0.0065	Vanillin CHO	0.0058

Table S7. Signal assignment for NMR spectrum of new make spirit produced using laboratory peated malt, recorded at the University of Edinburgh using a 600 MHz spectrometer, LPNMS1.

δ_H / ppm	Multiplicity	Integration	Inferences	Concentration / mmol L^{-1}
0	Singlet	10	DSS 3xCH_3	1.00
0.79	Multiplet	2.94	Fusel alcohols CH_3 groups carbon	-

			satellites	
0.89	Multiplet	340.5	Fusel alcohols CH_3 groups	-
1.00	Multiplet	2.47	Fusel alcohols CH_3 groups carbno satellites	-
1.08	Triplet, J = 7.2 Hz	-	Ethanol CH_3 carbon satellite	-
1.10	Multiplet	-	Fusel alcohols ethyl esters CH_3 groups	-
1.19	Distorted	-	Ethanol CH_3, suppressed	
1.25	Triplet, J = 7.2 Hz	12.2	Ethyl acetate CH_3 next to CH_2	3.65
1.29	Triplet, J = 6.8 Hz	9.31	Ethanol CH_3 carbon satellite	-
1.31	Doublet, J = 5.2 Hz	20.9	1,1-diethoxyethane CH_3 next to CH	6.27
1.43	Quartet, J = 7.0 Hz	57.1	3-methylbutanol CH_2 next to CH and CH_2	25.7
1.55	Sextet, J = 7.2 Hz	28.9	n-propanol CH_2 next to CH_2 and CH_3	13.0
1.68	Nonet, J = 6.7 Hz	-	3-methylbutanol CH next to 2xCH_3 and CH_2	-
1.73	Nonet, J = 6.7 Hz	-	2-methylpropanol CH next to 2xCH_3 and CH_2	-
1.94	Singlet	0.036	Acetic acid CH_3 carbon satellite	-
2.05	Singlet	6.70	Acetic acid CH_3	2.01
2.08	Singlet	0.11	Ethyl acetate isolated CH_3	0.033
2.16	Singlet	0.054	Acetic acid CH_3 carbon satellite	-
2.18	Singlet	0.16	*para*-cresol CH_3	0.049
2.21	Singlet	0.77	Acetone 2xCH_3	0.11
2.23	Doublet, J = 2.9 Hz	5.43	Acetaldehyde CH_3 next to CH	1.63
2.27	Singlet	0.18	*ortho*-cresol CH_3 group	0.054
2.84	Triplet, J = 7.4 Hz	0.89	2-phenylethanol CH_2 next to CH_2	0.40
3.21	Doublet, J = 6.6 Hz	0.37	Isobutanol CH_2 carbon satellite	-
3.23	Doublet, J = 6.8 Hz	0.18	Part of 2-methylbutanol CH_2 carbon satellite	-
3.24	Singlet	0.060	Methanol CH_3 carbon satellite	-
3.33	Doublet, J = 6.6 Hz	36.2	Isobutanol CH_2 next to CH	16.3
3.34	Doublet, J = 6.8 Hz	6.00	Part of 2-methylbutanol diastereotopic CH_2	-
3.35	Singlet	2.87	Methanol CH_3	0.86
3.44	DD, J = 10.6 Hz, 5.8 Hz	5.84	Part of 2-methylbutanol diastereotopic CH_2	5.25
3.48	Quartet, J = 7.0 Hz	-	Ethanol CH_2 carbon satellite	-
3.52	Triplet, J = 6.8 Hz	24.3	n-propanol CH_2 next to CH_2	10.9
3.60	Triplet, J = 7.0 Hz	29.3	3-methylbutanol CH_2 next to CH_2	13.2
3.63	Distorted	-	Ethanol CH_2, suppressed	-
3.75	Quartet, J = 7.3 Hz	-	Ethanol CH_2 carbon satellite	-
3.81	Singlet	0.25	Guaiacol OCH_3	0.075
4.12	Quartet, J = 7.1 Hz	-	Lactic acid CH next to CH_3	-
4.23	Quartet, J = 6.7 Hz	-	Ethyl acetate CH_2 next to CH_3	-
4.82	Broad singlet	-	Water suppressed	-
5.20	Quartet, J =5.2 Hz	-	Acetaldehyde water hemiacetal	-
6.33	Doublet, J = 3.1 Hz	0.033	2-methylfuran aromatic CH	0.029

6.37	Multiplet	0.025	2-methylfuran aromatic CH	0.024
6.69	DD, J = 3.4 Hz, 1.5 Hz	0.021	5-Hydroxymethylfurfural CH	0.019
6.73	Multiplet	0.043	*para*-cresol 2x CH next to CH, overlap with *ortho*-cresol	0.019
6.77	DD, J = 3.6 Hz, 1.7 Hz	0.15	Furfural CH next to 2xCH	0.14
6.84	Doublet, J = 8.1 Hz	0.26	Phenol 2x CH next to CH	0.12
6.98	Doublet, J = 8.1 Hz	0.053	*para*-cresol 2xCH next to CH	0.024
7.04	Multiplet	0.031	*ortho*-cresol aromatic CH	0.028
7.19	Triplet, J = 7.2 Hz	0.56	Phenol 2xCH next to CH	0.25
7.23	Multiplet	0.91	2-phenylethanol aromatic	-
7.28	Multiplet	0.86	2-phenylethanol aromatic	-
7.94	Multiplet	0.14	Furfural CH next to CH	0.12
8.13	Singlet	0.067	Ethyl formate CH	0.060
8.44	Singlet	0.082	Formic acid CH	0.074
9.57	Singlet	0.14	Furfural CHO	0.12
9.59	Doublet, J = 2.0 Hz	0.025	5-Hydroxymethylfurfural CHO	0.023
9.71	Quartet, J = 2.8 Hz	1.54	Acetaldehyde CHO	1.38
9.99	Singlet	0.0068	Vanillin CHO	0.0061

Table S8. Signal assignment for NMR spectrum of new make spirit produced using laboratory peated malt, recorded at the University of Edinburgh using a 600 MHz spectrometer, LPNMS2.

δ_H / ppm	Multiplicity	Integration	Inferences	Concentration / mmol L^{-1}
0	Singlet	10	DSS 3xCH$_3$	1.00
0.79	Multiplet	2.37	Fusel alcohols CH$_3$ groups carbon satellites	-
0.89	Multiplet	342.3	Fusel alcohols CH$_3$ groups	-
1.00	Multiplet	2.10	Fusel alcohols CH$_3$ groups carbon satellites	-
1.08	Triplet, J = 7.1 Hz	-	Ethanol CH$_3$ carbon satellite	-
1.10	Multiplet	-	Fusel alcohols ethyl esters CH$_3$ groups	-
1.19	Distorted	-	Ethanol CH$_3$, suppressed	-
1.25	Triplet, J = 7.3 Hz	19.2	Ethyl acetate CH$_3$ next to CH$_2$	5.76
1.29	Triplet, J = 7.1 Hz	16.1	Ethanol CH$_3$ carbon satellite	-
1.31	Doublet, J = 5.1 Hz	23.0	1,1-diethoxyethane CH$_3$ next to CH	6.91
1.43	Quartet, J = 7.0 Hz	55.2	3-methylbutanol CH$_2$ next to CH and CH$_2$	24.8
1.55	Sextet, J = 7.3 Hz	40.0	n-propanol CH$_2$ next to CH$_2$ and CH$_3$	18.0
1.68	Nonet, J = 6.8 Hz	-	3-methylbutanol CH next to 2xCH$_3$ and CH$_2$	-
1.73	Nonet, J = 6.7 Hz	-	2-methylpropanol CH next to 3xCH$_3$ and CH$_2$	-
1.94	Singlet	0.12	Acetic acid CH$_3$ carbon satellite	-
1.97	Multiplet	3.78	3-Methylpyridine CH$_3$	1.13
2.05	Singlet	9.21	Acetic acid CH$_3$	2.76
2.08	Singlet	0.30	Ethyl acetate isolated CH$_3$	0.09

2.18	Singlet	0.54	*para*-cresol CH$_3$	0.16
2.21	Singlet	1.57	Acetone 2xCH$_3$	0.24
2.22	Doublet, J = 2.9 Hz	5.52	Acetaldehyde CH$_3$ next to CH	1.66
2.25	Singlet	0.31	*ortho*-cresol CH$_3$	0.092
2.54	Singlet	0.43	2-methylpyridine CH$_3$	0.13
2.84	Triplet, J =7.3 Hz	0.55	2-phenylethanol CH$_2$ next to CH$_2$	0.25
3.21	Doublet, J = 6.6 Hz	0.31	Isobutanol carbon satellite	-
3.22	Doublet, J = 7.0 Hz	0.097	2-methylbutanol part of CH$_2$ carbon satellite	-
3.23	Singlet	0.056	Methanol CH$_3$ carbon satellite	-
3.32	Doublet, J = 6.6 Hz	36.2	Isobutanol CH$_2$ next to CH	16.3
3.34	Doublet, J = 6.9 Hz	5.97	2-methylbutanol part of diastereotopic CH$_2$	-
3.35	Singlet	3.66	Methanol CH$_3$	1.10
3.44	DD, J = 10.8 Hz, 5.8 Hz	11.6	2-methylbutanol part of diastereotopic CH$_2$	10.4
3.47	Quartet, J = 7.2 Hz	-	Ethanol CH$_2$ carbon satellite	-
3.52	Triplet, J = 6.8 Hz	31.1	n-propanol CH$_2$	14.0
3.59	Triplet, J = 7.1 Hz	17.1	3-methylbutanol CH$_2$ next to CH$_2$	7.70
3.63	Distorted	-	Ethanol CH$_2$, suppressed	-
3.75	Quartet, J = 7.0 Hz	-	Ethanol CH$_2$ carbon satellite	-
3.81	Singlet	0.33	Guaiacol OCH$_3$	0.10
4.12	Quartet, J = 7.0 Hz	-	Lactic acid CH next to CH$_3$	-
4.22	Quartet, J = 7.1 Hz	-	Ethyl acetate CH$_2$ next to CH$_3$	-
4.79	Broad singlet	-	Water suppressed	-
5.20	Quartet, J = 5.2 Hz	-	Acetaldehyde water hemiacetal	-
6.32	Doublet, J = 3.1 Hz	0.26	2-methylfuran CH	0.23
6.36	Multiplet	0.27	2-methylfuran CH	0.24
6.68	DD, J = 3.7 Hz, 1.7 Hz	0.074	5-HMF CH next to CH and coupling to CHO	0.067
6.72	Multiplet	0.038	o-cresol, overlap with p-cresol	0.034
6.76	DD, J = 3.7 Hz, J = 1.7 Hz	0.072	Furfural CH coupling to 2xCH	0.065
6.83	Doublet, J = 8.0 Hz	0.30	Phenol 2xCH next to CH	0.14
6.97	Multiplet	0.034	o-cresol, overlap with p-cresol	0.031
7.03	Doublet, J = 8.7 Hz	0.032	o-cresol	0.029
7.17	Triplet, J = 7.7 Hz	-	Phenol CH next to 2xCH	-
7.22	Multiplet	0.43	2-phenylethanol aromatic	-
7.27	Multiplet	0.51	2-phenylethanol aromatic	-
7.32	Doublet, J = 8.1 Hz	0.13	2-methylpyridine CH	0.12
7.44	Multiplet	-	Pyridine	-
7.54	Doublet, J = 3.8 Hz	0.11	Furfural CH next to CH	0.10
7.88	Multiplet	0.26	Pyridine, overlap with methylpyridine	-
8.12	Singlet	0.090	Ethyl formate CH	0.081
8.41	Doublet, J =4.6 Hz	0.066	2-methylpyridine CH	0.059
8.44	Singlet	0.17	Formic acid CH	0.16
8.54	Singlet	0.55	Pyridine 2xCH	0.25
9.57	Singlet	0.083	Furfural CHO	0.075
9.59	Doublet, J = 1.9 Hz	0.050	5-Hydroxymethylfurfural CHO	0.045

9.71	Quartet, J = 2.7 Hz	1.50	Acetaldehyde CHO	1.34
10.0	Singlet	0.010	Vanillin CHO	0.0090

Table S9. Signal assignment for NMR spectrum of new make spirit produced using malt smoked using spent coffee grounds, recorded at the University of Edinburgh using a 600 MHz spectrometer, CSNMS1.

δ_H / ppm	Multiplicity	Integration	Inferences	Concentration / mmol L^{-1}
0	Singlet	10	DSS 3xCH_3	1.00
0.79	Multiplet	1.87	Fusel alcohols CH_3 groups carbon satellites	-
0.89	Multiplet	283.1	Fusel alcohols CH_3 groups	-
1.00	Multiplet	1.87	Fusel alcohols CH_3 groups carbon satellites	-
1.08	Triplet, J = 7.2 Hz	-	Ethanol CH_3 carbon satellite	-
1.10	Multiplet	-	Fusel alcohols ethyl esters CH_3 groups	-
1.19	Distorted	-	Ethanol CH_3, suppressed	-
1.25	Triplet, J = 7.1 Hz	16.9	Ethyl acetate CH_3 next to CH_2	5.07
1.29	Triplet, J = 7.0 Hz	14.2	Ethanol CH_3 carbon satellite	-
1.31	Doublet, J = 5.2 Hz	17.8	1,1-diethoxyethane CH_3 next to CH	5.34
1.43	Quartet, J = 7.0 Hz	43.9	3-methylbutanol CH_2 next to CH and CH_2	19.7
1.55	Sextet, J = 7.2 Hz	33.3	n-propanol CH_2 next to CH_2 and CH_3	15.0
1.68	Nonet, J = 6.7 Hz	-	3-methylbutanol CH next to 2xCH_3 and CH_2	-
1.73	Nonet, J = 6.7 Hz	-	2-methylpropanol CH next to 3xCH_3 and CH_2	-
1.94	Singlet	0.12	Acetic acid CH_3 carbon satellite	-
1.97	Multiplet	3.12	3-Methylpyridine CH_3	0.94
2.05	Singlet	7.76	Acetic acid CH_3	2.33
2.08	Singlet	0.24	Ethyl acetate isolated CH_3	0.071
2.18	Singlet	0.54	*para*-cresol CH_3	0.10
2.21	Singlet	1.20	Acetone 2xCH_3	0.18
2.22	Doublet, J = 2.9 Hz	4.07	Acetaldehyde CH_3 next to CH	1.22
2.25	Singlet	0.22	*ortho*-cresol CH_3	0.065
2.54	Singlet	0.33	2-methylpyridine CH_3	0.10
2.84	Triplet, J =7.3 Hz	0.39	2-phenylethanol CH_2 next to CH_2	0.18
3.21	Doublet, J = 6.6 Hz	0.31	Isobutanol carbon satellite	-
3.22	Doublet, J = 6.7 Hz	0.057	2-methylbutanol part of CH_2 carbon satellite	-
3.23	Singlet	0.025	Methanol CH_3 carbon satellite	-
3.32	Doublet, J = 6.6 Hz	29.6	Isobutanol CH_2 next to CH	13.3
3.34	Doublet, J = 6.6 Hz	2.60	2-methylbutanol part of diastereotopic CH_2	-
3.35	Singlet	3.14	Methanol CH_3	0.94
3.44	DD, J = 10.7 Hz, 5.9 Hz	8.91	2-methylbutanol part of diastereotopic CH_2	8.02
3.47	Quartet, J = 7.1 Hz	-	Ethanol CH_2 carbon satellite	-
3.52	Triplet, J = 6.8 Hz	25.9	n-propanol CH_2	11.6

3.59	Triplet, J = 7.0 Hz	13.4	3-methylbutanol CH$_2$ next to CH$_2$	6.04
3.63	Distorted	-	Ethanol CH$_2$, suppressed	-
3.75	Quartet, J = 7.1 Hz	-	Ethanol CH$_2$ carbon satellite	-
3.81	Singlet	0.26	Guaiacol OCH$_3$	0.079
4.12	Quartet, J = 7.0 Hz	-	Lactic acid CH next to CH$_3$	-
4.22	Quartet, J = 7.1 Hz	-	Ethyl acetate CH$_2$ next to CH$_3$	-
4.79	Broad singlet	-	Water suppressed	-
5.20	Quartet, J = 5.2 Hz	-	Acetaldehyde water hemiacetal	-
6.32	Doublet, J = 3.2 Hz	0.24	2-methylfuran CH	0.22
6.36	DD, J = 3.1 Hz, 1.8 Hz	0.23	2-methylfuran CH	0.21
6.68	DD, J = 3.6 Hz, 1.7 Hz	0.069	5-HMF CH next to CH and coupling to CHO	0.062
6.72	Multiplet	0.024	o-cresol, overlap with p-cresol	0.022
6.76	DD, J = 3.6 Hz, J = 1.7 Hz	0.099	Furfural CH coupling to 2xCH	0.089
6.83	Doublet, J = 7.6 Hz	0.27	Phenol 2xCH next to CH	0.12
6.97	Multiplet	0.043	o-cresol, overlap with p-cresol	0.039
7.03	Doublet, J = 8.1 Hz	0.033	o-cresol	0.029
7.17	Multiplet	-	Phenol CH next to 2xCH	-
7.22	Multiplet	0.36	2-phenylethanol aromatic	-
7.27	Multiplet	0.44	2-phenylethanol aromatic	-
7.33	Doublet, J = 8.2 Hz	0.12	2-methylpyridine CH	0.10
7.44	DD, J = 1.8 Hz, 0.8 Hz	-	Pyridine	-
7.54	Doublet, J = 3.5 Hz	0.12	Furfural CH next to CH	0.11
7.88	Multiplet	0.22	Pyridine, overlap with methylpyridine	-
8.12	Singlet	0.074	Ethyl formate CH	0.066
8.41	Doublet, J =3.8 Hz	0.049	2-methylpyridine CH	0.044
8.44	Singlet	0.086	Formic acid CH	0.078
8.54	Singlet	0.44	Pyridine 2xCH	0.20
9.57	Singlet	0.089	Furfural CHO	0.080
9.59	Doublet, J = 1.9 Hz	0.036	5-Hydroxymethylfurfural CHO	0.032
9.71	Quartet, J = 2.9 Hz	1.14	Acetaldehyde CHO	1.02
10.0	Singlet	0.0061	Vanillin CHO	0.0055

Table S10. Signal assignment for NMR spectrum of new make spirit produced using malt smoked using spent coffee grounds, recorded at the University of Edinburgh using a 600 MHz spectrometer, CSNMS2.

δ_H / ppm	Multiplicity	Integration	Inferences	Concentration / mmol L^{-1}
0	Singlet	10	DSS 3xCH$_3$	1.00
0.61	Multiplet	2.39	DSS CH$_2$	1.08
0.77	Multiplet	0.34	Fusel alcohols CH$_3$ groups carbon satellites	-
0.88	Multiplet	69.0	Fusel alcohols CH$_3$ groups	-
0.98	Multiplet	0.37	Fusel alcohols CH$_3$ groups carbon satellites	-
1.06	Triplet, J = 7.1 Hz	0.31	Ethanol CH$_3$ carbon satellite	-
1.13	Triplet, J = 7.5 Hz	-	2-methylbutanol CH$_3$ next to CH$_2$	-
1.17	Distorted	-	Ethanol CH$_3$, suppressed	

1.24	Triplet, J = 7.2 Hz	1.59	Ethyl acetate CH_3 next to CH_2	0.48
1.27	Triplet, J =7.0 Hz	1.14	Ethanol CH_3 carbon satellite	-
1.33	Doublet, J = 8.0 Hz	0.18	Lactic acid CH_3 next to CH	0.056
1.37	Sextet, J = 7.4 Hz	-	n-butanol CH_2 next to CH_2 and CH_3	-
1.39	Quintet, J = 7.7 Hz	-	n-butanol CH_2 next to 2xCH_2	-
1.42	Quartet, J = 6.9 Hz	9.15	3-methylbutanol CH_2 next to CH and CH_2	4.12
1.53	Sextet, J = 7.1 Hz	-	n-propanol CH_2 next to CH_2 and CH_3	-
1.65	Nonet, J = 6.7 Hz	4.62	3-methylbutanol CH next to 2xCH_3 and CH_2	4.16
1.72	Nonet, J = 6.6 Hz	6.34	2-methylpropanol CH next to 2xCH_3 and CH_2	5.70
2.06	Singlet	1.35	Acetic acid CH_3	0.41
2.10	Singlet	0.21	Ethyl acetate CH_3 isolated	0.063
2.15	Singlet	0.037	Acetic acid CH_3 carbon satellite	-
2.19	Singlet	0.12	*p*-cresol CH_3	0.036
2.22	Singlet	0.11	Acetone 2xCH_3	0.016
2.23	Doublet, J = 3.0 Hz	0.74	Acetaldehyde CH_3 next to CH	0.22
2.27	Singlet	0.11	*o*-cresol CH_3	0.033
2.84	Triplet, J = 7.0 Hz	3.31	Phenylethanol CH_2 next to CH_2	1.49
2.85	Doublet, J = 8.2 Hz	1.50	DSS	0.68
3.22	Singlet	0.0080	Methanol CH_3 carbon satellite	-
3.23	Doublet, J = 6.6 Hz	0.046	Isobutanol CH_2 carbon satellite	-
3.25	Doublet, J = 3.9 Hz	0.010	2-methylbutanol part of CH_2 carbon satellite	-
3.34	Singlet	1.13	Methanol CH_3	0.34
3.35	Doublet, J = 6.5 Hz	8.01	Isobutanol CH_2 next to CH	3.61
3.36	Part of DD	0.47	2-methylbutanol part of diastereotopic CH_2	-
3.38	Part of DD	1.31	2-methylbutanol part of diastereotopic CH_2	-
3.46	DD, J = 10.8 Hz, J = 6.0 Hz	2.17	2-methylbutanol part of diastereotopic CH_2	1.95
3.54	Triplet, J = 6.7 Hz	3.80	n-propanol CH_2 next to CH_2	1.71
3.61	Triplet, J = 7.0 Hz	-	3-methylbutanol CH_2 next to CH_2	-
3.64	Distorted	-	Ethanol CH_2 suppressed	-
3.75	Quartet, J = 7.1 Hz	0.49	Ethanol CH_2 carbon satellite	-
3.81	Triplet, J = 6.9 Hz	2.31	2-phenylethanol CH_2 and CH_2	1.04
3.84	Singlet	0.054	Guaiacol OCH_3	0.016
4.12	Quartet, J = 7.2 Hz	1.03	Ethyl acetate CH_2 next to CH_3	0.46
4.83	Broad Singlet	-	Water suppressed	-
4.92	Quartet, J = 5.2 Hz	-	Acetaldehyde ethyl hemiacetal	-
5.22	Quartet, J = 5.2 Hz	0.21	Acetaldehyde water hemiacetal	-
6.38	Doublet, J = 3.4 Hz	0.019	2-methylfuran CH	0.017
6.42	DD, J = 3.2 Hz, 1.8 Hz	0.020	2-methylfuran CH	0.018
6.68	Doublet, J = 8.9 Hz	0.038	*p*-cresol 2xCH next to CH	0.017
6.72	Multiplet	0.039	*o*-cresol CH	0.035

6.76	DD, J = 3.6 Hz J = 1.7 Hz	0.029	Furfural CH coupling to 2xCH	0.026
6.80	Doublet, J = 8.5 Hz	0.057	*p*-cresol 2xCH next to CH	0.026
6.88	Doublet, J = 7.7 Hz	0.45	Phenol 2xCH next to CH	0.20
6.95	Triplet, J = 7.4 Hz	0.20	Phenol CH coupling to 2xCH	0.18
7.03	Doublet, J = 8.0 Hz	0.022	*o*-cresol CH	0.020
7.10	Doublet, J = 8.4 Hz	0.14	4-ethylphenol 2xCH next to CH	0.062
7.17	Triplet, J = 7.9 Hz	0.082	2-ethylphenol CH	0.074
7.26	Multiplet	-	Phenol 2xCH next to 2xCH	-
7.28	Multiplet	3.10	2-phenylethanol	-
7.36	Multiplet	2.26	2-phenylethanol	-
7.50	Doublet, J = 1.2 Hz	0.022	Furfural CH	0.020
7.92	Singlet	0.016	Furfural CH	0.015
9.49	Singlet	0.015	Furfural CHO	0.014
9.66	Quartet, J = 3.0 Hz	0.20	Acetaldehyde CHO	0.18
9.94	Singlet	-	Vanillin CHO	-

Table S11. Signal assignment for NMR spectrum of low wines sample produced using industrially peated malt, recorded at the University of Edinburgh using a 600 MHz spectrometer, IPLW1.

δ_H / ppm	Multiplicity	Integration	Inferences	Concentration / mmol L^{-1}
0	Singlet	10	DSS 3xCH_3	1.00
0.61	Multiplet	2.39	DSS CH_2	1.08
0.77	Multiplet	0.38	Fusel alcohols CH_3 groups carbon satellites	-
0.88	Multiplet	68.5	Fusel alcohols CH_3 groups	-
0.98	Multiplet	0.33	Fusel alcohols CH_3 groups carbon satellites	-
1.06	Triplet, J = 7.0 Hz	1.09	Ethanol CH_3 carbon satellite	-
1.13	Triplet, J = 7.5 Hz	-	2-methylbutanol CH_3 next to CH_2	-
1.17	Distorted	-	Ethanol CH_3, suppressed	
1.24	Triplet, J = 7.1 Hz	1.52	Ethyl acetate CH_3 next to CH_2	0.46
1.27	Triplet, J =7.0 Hz	1.40	Ethanol CH_3 carbon satellite	-
1.33	Doublet, J = 8.4 Hz	0.17	Lactic acid CH_3 next to CH	0.052
1.37	Sextet, J = 7.6 Hz	-	n-butanol CH_2 next to CH_2 and CH_3	-
1.39	Quintet, J = 7.7 Hz	-	n-butanol CH_2 next to 2xCH_2	-
1.42	Quartet, J = 6.9 Hz	8.90	3-methylbutanol CH_2 next to CH and CH_2	4.01
1.53	Sextet, J = 7.1 Hz	-	n-propanol CH_2 next to CH_2 and CH_3	-
1.65	Nonet, J = 6.7 Hz	4.48	3-methylbutanol CH next to 2xCH_3 and CH_2	4.04
1.72	Nonet, J = 6.6 Hz	6.20	2-methylpropanol CH next to 2xCH_3 and CH_2	5.58
2.06	Singlet	1.35	Acetic acid CH_3	0.40
2.10	Singlet	0.21	Ethyl acetate CH_3 isolated	0.063
2.15	Singlet	0.031	Acetic acid CH_3 carbon satellite	-
2.19	Singlet	0.11	*p*-cresol CH_3	0.033
2.22	Singlet	0.55	Acetone 2xCH_3	0.082
2.23	Doublet, J = 2.9 Hz	0.72	Acetaldehyde CH_3 next to CH	0.22

2.27	Singlet	0.10	*o*-cresol CH_3	0.032
2.84	Triplet, J = 6.9 Hz	3.27	Phenylethanol CH_2 next to CH_2	1.47
2.87	Doublet, J = 8.0 Hz	1.47	DSS	0.66
3.22	Singlet	0.0056	Methanol CH_3 carbon satellite	-
3.23	Doublet, J = 6.5 Hz	0.041	Isobutanol CH_2 carbon satellite	-
3.25	Doublet, J = 4.3 Hz	0.0029	2-methylbutanol part of CH_2 carbon satellite	-
3.34	Singlet	1.28	Methanol CH_3	0.38
3.35	Doublet, J = 6.6 Hz	7.84	Isobutanol CH_2 next to CH	3.53
3.36	Part of DD	0.43	2-methylbutanol part of diastereotopic CH_2	-
3.38	Part of DD	1.25	2-methylbutanol part of diastereotopic CH_2	-
3.46	DD, J = 10.8 Hz, J = 5.9 Hz	2.14	2-methylbutanol part of diastereotopic CH_2	1.93
3.54	Triplet, J = 6.7 Hz	3.84	n-propanol CH_2 next to CH_2	1.73
3.61	Triplet, J = 7.0 Hz	-	3-methylbutanol CH_2 next to CH_2	-
3.64	Distorted	-	Ethanol CH_2 suppressed	-
3.75	Quartet, J = 6.8 Hz	0.49	Ethanol CH_2 carbon satellite	-
3.81	Triplet, J = 6.9 Hz	2.22	2-phenylethanol CH_2 and CH_2	1.00
3.84	Singlet	0.050	Guaiacol OCH_3	0.015
4.12	Quartet, J = 7.1 Hz	1.01	Ethyl acetate CH_2 next to CH_3	0.46
4.83	Broad Singlet	-	Water suppressed	-
4.92	Quartet, J = 5.2 Hz	-	Acetaldehyde ethyl hemiacetal	-
5.22	Quartet, J = 5.2 Hz	0.18	Acetaldehyde water hemiacetal	-
6.38	Doublet, J = 3.1 Hz	0.016	2-methylfuran CH	0.014
6.42	DD, J = 3.1 Hz, 1.8 Hz	0.016	2-methylfuran CH	0.014
6.68	Doublet, J = 8.3 Hz	0.036	*p*-cresol 2xCH next to CH	0.016
6.72	Multiplet	0.036	*o*-cresol CH	0.032
6.76	DD, J = 3.8 Hz J = 1.7 Hz	0.023	Furfural CH coupling to 2xCH	0.021
6.80	Doublet, J = 8.6 Hz	0.051	*p*-cresol 2xCH next to CH	0.023
6.88	Doublet, J = 7.6 Hz	0.42	Phenol 2xCH next to CH	0.19
6.95	Triplet, J = 7.4 Hz	0.19	Phenol CH coupling to 2xCH	0.17
7.03	Doublet, J = 8.2 Hz	0.018	*o*-cresol CH	0.016
7.10	Doublet, J = 8.3 Hz	0.13	4-ethylphenol 2xCH next to CH	0.059
7.17	Triplet, J = 7.9 Hz	0.074	2-ethylphenol CH	0.067
7.26	Multiplet	-	Phenol 2xCH next to 2xCH	-
7.28	Multiplet	3.04	2-phenylethanol	-
7.36	Multiplet	2.22	2-phenylethanol	-
7.50	Doublet, J = 1.6 Hz	0.021	Furfural CH	0.019
7.92	Singlet	0.016	Furfural CH	0.015
9.49	Singlet	0.015	Furfural CHO	0.014
9.66	Quartet, J = 3.0 Hz	0.20	Acetaldehyde CHO	0.18
9.94	Singlet	-	Vanillin CHO	-

Table S12. Signal assignment for NMR spectrum of low wines sample produced using industrially peated malt, recorded at the University of Edinburgh using a 600 MHz spectrometer, IPLW2.

δ_H / ppm	Multiplicity	Integration	Inferences	Concentration / mmol L^{-1}

0	Singlet	10	DSS 3xCH_3	1.00
0.61	Multiplet	2.17	DSS	0.98
0.77	Multiplet	0.30	Fusel alcohols CH_3 groups carbon satellites	-
0.88	Multiplet	54.1	Fusel alcohols CH_3 groups	-
0.98	Multiplet	0.30	Fusel alcohols CH_3 groups carbon satellites	-
1.06	Triplet, J = 7.3 Hz	0.66	Ethanol CH_3 carbon satellite	-
1.13	Triplet, J = 7.5 Hz	-	2-methylbutanol CH_2	-
1.17	Distorted	-	Ethanol CH_3 suppressed	-
1.24	Triplet, J = 7.1 Hz	1.01	Ethyl acetate CH_3 next to CH_2	0.30
1.27	Triplet, J = 7.1 Hz	1.29	Ethanol CH_3 carbon satellite	-
1.33	Doublet, J = 7.6 Hz	0.19	Lactic acid CH_3 next to CH	0.057
1.37	Sextet, J = 7.4 Hz	-	n-butanol CH_2 next to CH_2 and CH_3	-
1.38	Quintet, J = 7.5 Hz	-	n-butanol CH_2 next to 2xCH_2	-
1.42	Quartet, J = 6.9 Hz	8.08	3-methylbutanol CH_2 next to CH_2 and CH	3.64
1.53	Sextet, J = 7.1 Hz	-	n-propanol CH_2 next to CH_2 and CH_3	-
1.65	Nonet, J = 6.8 Hz	4.06	3-methylbutanol CH next to 2xCH_3 and CH_2	3.65
1.74	Nonet, J = 6.6 Hz	-	2-methylpropanol next to 2xCH_3 and CH_2	-
1.96	Singlet	0.030	Acetic acid CH_3 carbon satellite	-
2.06	Singlet	2.00	Acetic acid CH_3	0.60
2.10	Singlet	0.13	Ethyl acetate isolated CH_3	0.040
2.15	Singlet	0.041	Acetic acid CH_3 carbon satellite	-
2.19	Singlet	0.091	*p*-cresol CH_3	0.027
2.22	Singlet	0.14	Acetone 2xCH_3	0.021
2.23	Doublet, J = 3.1 Hz	1.37	Acetaldehyde CH_3 next to CH	0.41
2.27	Singlet	0.072	*o*-cresol CH_3	0.022
2.50	Singlet	0.024	5-methylfurfural CH_3	0.0073
2.85	Triplet, J = 6.9 Hz	-	Phenylethanol CH_2 next to CH_2	-
2.86	Multiplet	-	DSS	-
3.22	Singlet	0.0053	Methanol CH_3 carbon satellite	-
3.23	Doublet, J = 6.5 Hz	0.038	Isobutanol CH_2 carbon satellite	
3.26	Doublet, J = 6.6 Hz	0.018	2-methylbutanol part of CH_2 carbon satellite	-
3.34	Singlet	0.64	Methanol CH_3	0.19
3.35	Doublet, J = 6.5 Hz	5.35	Isobutanol CH_2 next to CH	2.41
3.37	Singlet	0.33	2-methylbutanol part of diastereotopic CH_2	-
3.38	Doublet, J = 6.6 Hz	0.94	2-methylbutanol part of diastereotopic CH_2	-
3.46	DD, J = 10.8 Hz, 5.9 Hz	1.63	2-methylbutanol part of diastereotopic CH_2	1.47
3.51	Quartet, J = 7.1 Hz	-	Ethanol CH_2 carbon satellite	-
3.54	Triplet, J = 6.7 Hz	4.23	n-propanol CH_2 next to CH_2	1.90
3.61	Triplet, J = 6.9 Hz	-	3-methylbutanol CH_2 next to CH_2	-

3.64	Quartet, J = 7.1 Hz	-	Ethanol CH_2 suppressed	-
3.75	Quartet, J = 7.0 Hz	-	Ethanol CH_2 carbon satellite	-
3.81	Triplet, J = 6.9 Hz	1.83	Phenylethanol CH_2 next to CH_2	0.82
3.84	Singlet	0.12	Guaiacol OCH_3	0.035
4.12	Quartet, J = 7.0 Hz	0.75	Ethyl acetate CH_2 next to CH_3	0.34
4.82	Broad singlet	-	Water suppressed	-
4.92	Quartet, J = 5.2 Hz	-	Acetaldehyde ethyl hemiacetal	-
5.22	Quartet, J = 5.2 Hz	0.38	Acetaldehyde water hemiacetal	-
6.38	Doublet, J = 3.2 Hz	0.068	2-methylfuran CH	0.061
6.42	DD, J = 3.1 Hz, 1.9 Hz	0.066	2-methylfuran CH	0.059
6.68	Doublet, J = 8.0 Hz	0.026	*p*-cresol 2xCH	0.012
6.73	Multiplet	0.021	*o*-cresol CH	0.019
6.75	DD, J = 3.7 Hz, 1.7 Hz	0.051	Furfural CH next to 2xCH	0.046
6.81	Doublet, J = 8.0 Hz	0.026	*p*-cresol 2xCH	0.022
6.88	Multiplet	0.30	Phenol 2xCH next to CH	0.14
6.96	Triplet, J = 7.7 Hz	0.14	Phenol CH next to 2xCH	0.12
7.04	Doublet, J = 7.9 Hz	0.039	*o*-cresol CH	0.035
7.10	Doublet, J = 8.1 Hz	0.11	4-ethylphenol 2xCH	0.049
7.17	Multiplet	-	2-ethylphenol	-
7.27	Multiplet	-	Phenol CH next to 2xCH	-
7.29	Multiplet	-	2-phenylethanol	-
7.36	Multiplet	-	2-phenylethanol	-
7.50	DD, J = 1.8 Hz, 0.8 Hz	0.070	Furfural aromatic CH	0.063
7.57	Doublet, J = 3.7 Hz	0.041	5-Hydroxymethylfurfural	0.037
7.91	Multiplet	0.042	Furfural CH	0.038
9.49	Doublet, J = 0.8 Hz	0.039	Furfural CHO	0.035
9.56	Doublet, J = 2.0 Hz	0.0035	5-hydroxymethylfurfural CHO	0.0032
9.66	Quartet, J = 3.0 Hz	0.40	Acetaldehyde CHO	0.36
9.94	Singlet	0.0012	Vanillin CHO	0.0011

Table S13. Signal assignment for NMR spectrum of low wines sample produced using laboratory peated malt, recorded at the University of Edinburgh using a 600 MHz spectrometer, LPLW1.

δ_H / ppm	Multiplicity	Integration	Inferences	Concentration / mmol L^{-1}
0	Singlet	10	DSS $3xCH_3$	1.00
0.61	Multiplet	2.18	DSS	0.98
0.77	Multiplet	0.32	Fusel alcohols CH_3 groups carbon satellites	-
0.88	Multiplet	51.6	Fusel alcohols CH_3 groups	-
0.98	Multiplet	0.24	Fusel alcohols CH_3 groups carbon satellites	-
1.06	Triplet, J = 7.2 Hz	0.67	Ethanol CH_3 carbon satellite	-
1.13	Triplet, J = 7.5 Hz	-	2-methylbutanol CH_2	-
1.17	Distorted	-	Ethanol CH_3 suppressed	-
1.24	Triplet, J = 7.2 Hz	1.05	Ethyl acetate CH_3 next to CH_2	0.32
1.27	Triplet, J = 7.0 Hz	1.35	Ethanol CH_3 carbon satellite	-
1.33	Doublet, J = 8.4 Hz	0.17	Lactic acid CH_3 next to CH	0.050
1.37	Sextet, J = 7.5 Hz	-	n-butanol CH_2 next to CH_2 and	-

			CH_3	
1.38	Quintet, J = 7.6 Hz	-	n-butanol CH_2 next to $2xCH_2$	-
1.42	Quartet, J = 6.9 Hz	7.64	3-methylbutanol CH_2 next to CH_2 and CH	3.44
1.53	Sextet, J = 7.1 Hz	-	n-propanol CH_2 next to CH_2 and CH_3	-
1.65	Nonet, J = 6.7 Hz	3.78	3-methylbutanol CH next to $2xCH_3$ and CH_2	3.40
1.72	Nonet, J = 6.6 Hz	-	2-methylpropanol next to $2xCH_3$ and CH_2	-
1.96	Singlet	0.020	Acetic acid CH_3 carbon satellite	-
2.06	Singlet	1.85	Acetic acid CH_3	0.56
2.10	Singlet	0.11	Ethyl acetate isolated CH_3	0.033
2.15	Singlet	0.030	Acetic acid CH_3 carbon satellite	-
2.19	Singlet	0.086	*p*-cresol CH_3	0.026
2.22	Singlet	0.64	Acetone $2xCH_3$	0.009
2.23	Doublet, J = 3.0 Hz	1.28	Acetaldehyde CH_3 next to CH	0.38
2.27	Singlet	0.057	*o*-cresol CH_3	0.017
2.50	Singlet	0.020	5-methylfurfural CH_3	0.0061
2.85	Triplet, J = 6.9 Hz	-	Phenylethanol CH_2 next to CH_2	-
2.86	Multiplet	-	DSS	-
3.22	Singlet	0.0027	Methanol CH_3 carbon satellite	-
3.23	Doublet, J = 6.5 Hz	0.027	Isobutanol CH_2 carbon satellite	
3.26	Doublet, J = 6.7 Hz	0.0055	2-methylbutanol part of CH_2 carbon satellite	-
3.34	Singlet	0.66	Methanol CH_3	0.20
3.35	Doublet, J = 6.6 Hz	5.07	Isobutanol CH_2 next to CH	2.28
3.37	Singlet	0.30	2-methylbutanol part of diastereotopic CH_2	-
3.38	Doublet, J = 6.7 Hz	0.94	2-methylbutanol part of diastereotopic CH_2	-
3.46	DD, J = 10.8 Hz, 5.9 Hz	1.51	2-methylbutanol part of diastereotopic CH_2	1.36
3.51	Quartet, J = 7.1 Hz	-	Ethanol CH_2 carbon satellite	-
3.54	Triplet, J = 6.7 Hz	4.00	n-propanol CH_2 next to CH_2	1.80
3.61	Triplet, J = 7.0 Hz	-	3-methylbutanol CH_2 next to CH_2	-
3.64	Quartet, J = 7.1 Hz	-	Ethanol CH_2 suppressed	-
3.75	Quartet, J = 7.0 Hz	-	Ethanol CH_2 carbon satellite	-
3.81	Triplet, J = 6.9 Hz	1.72	Phenylethanol CH_2 next to CH_2	0.77
3.84	Singlet	0.10	Guaiacol OCH_3	0.031
4.12	Quartet, J = 7.1 Hz	0.70	Ethyl acetate CH_2 next to CH_3	0.32
4.82	Broad singlet	-	Water suppressed	-
4.92	Quartet, J = 5.3 Hz	-	Acetaldehyde ethyl hemiacetal	-
5.22	Quartet, J = 5.2 Hz	0.32	Acetaldehyde water hemiacetal	-
6.38	Doublet, J = 3.2 Hz	0.061	2-methylfuran CH	0.055
6.42	DD, J = 3.1 Hz, 1.8 Hz	0.060	2-methylfuran CH	0.054
6.68	Doublet, J = 8.1 Hz	0.019	*p*-cresol 2xCH	0.0085
6.72	Multiplet	0.017	*o*-cresol CH	0.015
6.76	DD, J = 3.7 Hz, 1.6	0.046	Furfural CH next to 2xCH	0.041

	Hz			
6.81	Doublet, J = 8.5 Hz	0.041	*p*-cresol 2xCH	0.018
6.88	Multiplet	0.28	Phenol 2xCH next to CH	0.13
6.96	Triplet, J = 7.4 Hz	0.14	Phenol CH next to 2xCH	0.11
7.04	Doublet, J = 8.0 Hz	0.039	*o*-cresol CH	0.032
7.10	Doublet, J = 8.2 Hz	0.097	4-ethylphenol 2xCH	0.044
7.18	Multiplet	-	2-ethylphenol	-
7.27	Multiplet	-	Phenol CH next to 2xCH	-
7.29	Multiplet	-	2-phenylethanol	-
7.36	Multiplet	-	2-phenylethanol	-
7.50	DD, J = 1.8 Hz, 0.7 Hz	0.064	Furfural aromatic CH	0.058
7.57	Doublet, J = 3.8 Hz	0.038	5-Hydroxymethylfurfural	0.034
7.91	Multiplet	0.039	Furfural CH	0.035
9.49	Singlet	0.036	Furfural CHO	0.032
9.56	Doublet, J = 2.1 Hz	0.0027	5-hydroxymethylfurfural CHO	0.0024
9.66	Quartet, J = 3.0 Hz	0.38	Acetaldehyde CHO	0.33
9.94	Singlet	0.0013	Vanillin CHO	0.0012

Table S14. Signal assignment for NMR spectrum of low wines sample produced using laboratory peated malt, recorded at the University of Edinburgh using a 600 MHz spectrometer, LPLW2.

δ_H / ppm	Multiplicity	Integration	Inferences	Concentration / mmol L^{-1}
0	Singlet	10	DSS 3xCH_3	1.00
0.61	Multiplet	2.26	DSS	1.02
0.77	Multiplet	0.21	Fusel alcohols CH_3 groups carbon satellites	-
0.88	Multiplet	45.9	Fusel alcohols CH_3 groups	-
0.98	Multiplet	0.31	Fusel alcohols CH_3 groups carbon satellites	-
1.06	Triplet, J = 7.1 Hz	1.42	Ethanol CH_3 carbon satellite	-
1.13	Triplet, J = 7.6 Hz	-	2-methylbutanol CH_2	-
1.17	Distorted	-	Ethanol CH_3 suppressed	-
1.24	Triplet, J = 7.2 Hz	1.57	Ethyl acetate CH_3 next to CH_2	0.47
1.27	Triplet, J = 7.1 Hz	1.59	Ethanol CH_3 carbon satellite	-
1.37	Sextet, J = 7.5 Hz	-	n-butanol CH_2 next to CH_2 and CH_3	-
1.39	Quintet, J = 7.8 Hz	-	n-butanol CH_2 next to 2xCH_2	-
1.42	Quartet, J = 6.9 Hz	6.50	3-methylbutanol CH_2 next to CH and CH_2	2.92
1.53	Sextet, J = 7.1 Hz	6.68	n-propanol CH_2 next to CH_2 and CH_3	3.01
1.65	Nonet, J = 6.7 Hz	3.44	3-methylbutanol CH next to 2xCH_3 and CH_2	3.10
1.72	Nonet, J = 6.7 Hz	4.80	2-methylpropanol CH next to 2xCH_3 and CH_2	4.32
1.96	Multiplet	0.78	3-methylpyridine CH_3	0.23
2.06	Singlet	1.08	Acetic acid CH_3	0.32
2.10	Singlet	0.11	Ethyl acetate isolated CH_3	0.032
2.19	Singlet	0.25	*p*-cresol CH_3	0.076
2.22	Singlet	0.30	Acetone 2xCH_3	0.045

2.23	Doublet, J = 2.7 Hz	1.14	Acetaldehyde CH$_3$ next to CH	0.34
2.27	Singlet	0.1178	*o*-cresol CH$_3$	0.035
2.50	Singlet	0.14	5-methylfurfural CH$_3$	0.042
2.84	Triplet, J = 8.2 Hz	-	2-phenylethanol CH$_2$ next to CH$_2$	-
2.86	Multiplet	-	Singlet	-
3.22	Singlet	0.0043	Methanol CH$_3$ carbon satellite	-
3.23	Doublet, J = 6.5 Hz	0.022	Isobutanol CH$_2$ carbon satellite	-
3.34	Singlet	0.78	Methanol CH$_3$	0.23
3.35	Doublet, J = 6.6 Hz	3.96	Isobutanol CH$_2$ next to CH	1.78
3.37	DD, J = 10.8 Hz, 6.6 Hz	1.19	2-methylbutanol part of diastereotopic CH$_2$	1.08
3.46	DD, J = 10.8 Hz, 5.9 Hz	1.24	2-methylbutanol part of diastereotopic CH$_2$	1.12
3.51	Quartet, J = 7.6 Hz	-	Ethanol CH$_2$ carbon satellite	-
3.53	Triplet, J = 6.7 Hz	4.71	n-propanol CH$_2$ next to CH$_2$	2.12
3.61	Triplet, J = 7.0 HZ	-	3-methylbutanol CH$_2$ next to CH$_2$	-
3.64	Distorted	-	Ethanol CH$_2$ suppressed	-
3.75	Quartet, J = 6.9 Hz	-	Ethanol CH$_2$ carbon satellite	-
3.81	Triplet, J = 6.9 Hz	1.36	2-phenylethanol CH$_2$ next to CH$_2$	0.61
3.84	Singlet	0.019	Guaiacol OCH$_3$	0.0058
4.12	Quartet, J = 7.2 Hz	0.81	Ethyl acetate CH$_2$ next to CH$_3$	0.36
4.82	Broad singlet	-	Water suppressed	-
4.92	Quartet, J = 5.2 Hz	0.33	Acetaldehyde ethyl hemiacetal	-
5.22	Quartet, J = 5.2 Hz	0.22	Acetaldehyde water hemiacetal	-
6.38	Doublet, J = 3.2 Hz	0.70	2-methylfuran CH	0.63
6.42	DD, J = 3.3 Hz, 1.9 Hz	0.40	2-methylfuran CH	0.36
6.69	DD, J = 3.7 Hz, 1.7 Hz	0.047	5-hydroxymethylfurfural CH	0.042
6.72	Multiplet	0.029	*o*-cresol CH$_3$	0.026
6.76	DD, J = 3.7 Hz, 1.7 Hz	0.043	Furfural CH coupling to 2xCH	0.038
6.88	Multiplet	0.72	Phenol 2xCH coupling to CH	0.32
6.95	Triplet, J = 7.4 Hz	0.32	Phenol CH coupling to 2xCH	0.28
7.10	Multiplet	-	4-ethylphenol	-
7.17	Triplet, J = 7.9 Hz	-	2-ethylphenol	-
7.28	Multiplet	-	2-phenylethanol	-
7.36	Multiplet	-	2-phenylethanol	-
7.50	DD, J = 1.9 Hz, 0.8 Hz	0.67	2-methylfuran CH	0.60
7.57	DD, J = 3.8 Hz, 0.7 Hz	0.044	5-hydroxymethylfurfural CH	0.040
7.92	Multiplet	0.040	Furfural aromatic CH	0.036
9.50	Doublet, J = 0.9 Hz	0.039	Furfural CHO	0.035
9.56	Doublet, J = 2.2 Hz	-	5-hydroxymethylfurfural CHO	-
9.66	Quartet, J = 3.0 Hz	0.27	Acetaldehyde CHO	0.24

Table S15. Signal assignment for NMR spectrum of low wines sample produced using malt smoked using spent coffee grounds, recorded at the University of Edinburgh using a 600 MHz spectrometer, CSLW1.

δ_H / ppm	Multiplicity	Integration	Inferences	Concentration / mmol L^{-1}

0	Singlet	10	DSS 3xCH_3	1.00
0.61	Multiplet	2.42	DSS	1.09
0.77	Multiplet	0.26	Fusel alcohols CH_3 groups carbon satellites	-
0.88	Multiplet	49.9	Fusel alcohols CH_3 groups	-
0.98	Multiplet	0.25	Fusel alcohols CH_3 groups carbon satellites	-
1.06	Triplet, J = 7.1 Hz	-	Ethanol CH_3 carbon satellite	-
1.13	Triplet, J = 7.6 Hz	-	2-methylbutanol CH_2	-
1.17	Distorted	-	Ethanol CH_3 suppressed	-
1.24	Triplet, J = 7.2 Hz	1.32	Ethyl acetate CH_3 next to CH_2	0.40
1.27	Triplet, J = 7.1 Hz	1.20	Ethanol CH_3 carbon satellite	-
1.37	Sextet, J = 7.5 Hz	-	n-butanol CH_2 next to CH_2 and CH_3	-
1.39	Quintet, J = 7.8 Hz	-	n-butanol CH_2 next to 2xCH_2	-
1.42	Quartet, J = 6.9 Hz	6.92	3-methylbutanol CH_2 next to CH and CH_2	3.11
1.53	Sextet, J = 7.1 Hz	7.08	n-propanol CH_2 next to CH_2 and CH_3	3.19
1.65	Nonet, J = 6.7 Hz	3.78	3-methylbutanol CH next to 2xCH_3 and CH_2	3.40
1.72	Nonet, J = 6.7 Hz	4.77	2-methylpropanol CH next to 2xCH_3 and CH_2	4.29
1.96	Multiplet	0.82	3-methylpyridine CH_3	0.25
2.06	Singlet	1.09	Acetic acid CH_3	0.33
2.10	Singlet	0.14	Ethyl acetate isolated CH_3	0.042
2.19	Singlet	0.29	*p*-cresol CH_3	0.088
2.22	Singlet	0.31	Acetone 2xCH_3	0.046
2.23	Doublet, J = 2.7 Hz	1.23	Acetaldehyde CH_3 next to CH	0.37
2.27	Singlet	0.18	*o*-cresol CH_3	0.055
2.50	Singlet	0.14	5-methylfurfural CH_3	0.042
2.84	Triplet, J = 8.2 Hz	-	2-phenylethanol CH_2 next to CH_2	-
2.86	Multiplet	-	Singlet	-
3.22	Singlet	0.0051	Methanol CH_3 carbon satellite	-
3.23	Doublet, J = 6.5 Hz	0.027	Isobutanol CH_2 carbon satellite	-
3.34	Singlet	0.81	Methanol CH_3	0.24
3.35	Doublet, J = 6.6 Hz	4.41	Isobutanol CH_2 next to CH	1.99
3.37	DD, J = 10.8 Hz, 6.6 Hz	1.29	2-methylbutanol part of diastereotopic CH_2	1.16
3.46	DD, J = 10.8 Hz, 5.9 Hz	1.34	2-methylbutanol part of diastereotopic CH_2	1.21
3.51	Quartet, J = 7.6 Hz	-	Ethanol CH_2 carbon satellite	-
3.53	Triplet, J = 6.7 Hz	5.05	n-propanol CH_2 next to CH_2	2.27
3.61	Triplet, J = 7.0 HZ	-	3-methylbutanol CH_2 next to CH_2	-
3.64	Distorted	-	Ethanol CH_2 suppressed	-
3.75	Quartet, J = 6.9 Hz	-	Ethanol CH_2 carbon satellite	-
3.81	Triplet, J = 6.9 Hz	1.56	2-phenylethanol CH_2 next to CH_2	0.70
3.84	Singlet	0.031	Guaiacol OCH_3	0.0092
4.12	Quartet, J = 7.2 Hz	0.73	Ethyl acetate CH_2 next to CH_3	0.33
4.82	Broad singlet	-	Water suppressed	-

4.92	Quartet, J = 5.2 Hz	0.64	Acetaldehyde ethyl hemiacetal	-
5.22	Quartet, J = 5.2 Hz	0.30	Acetaldehyde water hemiacetal	-
6.38	Doublet, J = 3.2 Hz	0.71	2-methylfuran CH	0.64
6.42	DD, J = 3.3 Hz, 1.9 Hz	0.71	2-methylfuran CH	0.64
6.69	DD, J = 3.7 Hz, 1.7 Hz	0.053	5-hydroxymethylfurfural CH	0.048
6.72	Multiplet	0.030	*o*-cresol CH$_3$	0.027
6.76	DD, J = 3.7 Hz, 1.7 Hz	0.032	Furfural CH coupling to 2xCH	0.029
6.88	Multiplet	0.75	Phenol 2xCH coupling to CH	0.34
6.95	Triplet, J = 7.4 Hz	0.34	Phenol CH coupling to 2xCH	0.30
7.10	Multiplet	-	4-ethylphenol	-
7.17	Triplet, J = 7.9 Hz	-	2-ethylphenol	-
7.28	Multiplet	-	2-phenylethanol	-
7.36	Multiplet	-	2-phenylethanol	-
7.50	DD, J = 1.9 Hz, 0.8 Hz	0.69	2-methylfuran CH	0.62
7.57	DD, J = 3.8 Hz, 0.7 Hz	0.033	5-hydroxymethylfurfural CH	0.030
7.92	Multiplet	0.027	Furfural aromatic CH	0.024
9.50	Doublet, J = 0.9 Hz	0.028	Furfural CHO	0.025
9.56	Doublet, J = 2.2 Hz	-	5-hydroxymethylfurfural CHO	-
9.66	Quartet, J = 3.0 Hz	0.30	Acetaldehyde CHO	0.27

Table S16. Signal assignment for NMR spectrum of low wines sample produced using malt smoked using spent coffee grounds, recorded at the University of Edinburgh using a 600 MHz spectrometer, CSLW2.

δ_H / ppm	Multiplicity	Integration	Inferences	Concentration / mmol L^{-1}
0	Singlet	10	DSS	1
0.59	Multiplet	2.44	DSS	1.10
0.78	Multiplet	0.39	Fusel alcohols CH$_3$ groups carbon satellites	-
0.88	Multiplet	58.0	Fusel alcohols CH$_3$ groups	-
0.98	Multiplet	0.31	Fusel alcohols CH$_3$ groups carbon satellites	-
1.08	Triplet, J = 7.2 Hz	2.93	Ethanol CH$_3$ carbon satellite	-
1.18	Distorted	-	Ethanol CH$_3$ suppressed	-
1.25	Triplet, J = 7.1 Hz	-	Ethyl acetate CH$_3$ next to to CH$_2$	-
1.29	Triplet, J = 7.0 Hz	4.09	Ethanol CH$_3$ carbon satellite	-
1.31	Doublet, J = 5.0 Hz	1.10	1,1-diethoxyethane CH$_3$ next to CH	0.33
1.40	Quintet, J = 5.3 Hz	-	n-butanol	-
1.43	Quartet, J = 7.0 Hz	9.39	3-methylbutanol CH$_2$ next to CH$_2$ and CH$_3$	4.23
1.54	Sextet, J = 7.2 Hz	11.3	n-propanol CH$_2$ next to CH$_2$ and CH$_3$	5.08
1.66	Nonet, J = 6.7 Hz	4.94	3-methylbutanol CH next to 2xCH$_3$ and CH$_2$	4.44
1.73	Nonet, J = 6.6 Hz	3.89	Isobutanol CH next to 2xCH$_3$ and CH$_2$	3.50

2.06	Singlet	0.18	Acetic acid CH_3	0.053
2.08	Singlet	0.055	Ethyl acetate CH_3 isolated	0.016
2.18	Singlet	0.24	*p*-cresol CH_3	0.071
2.22	Singlet	0.64	2-methylfuran CH_3	0.19
2.22	Singlet	-	Acetone 2xCH_3	-
2.24	Doublet, J = 3.0 Hz	0.30	Acetaldehyde CH_3 next to CH	0.089
2.26	Singlet	0.15	*o*-cresol CH_3	0.046
2.51	Singlet	0.34	5-methylfurfural	0.10
2.68	Singlet	0.14	2-methylpyridine	-
2.85	Triplet, J = 7.0 Hz	0.35	2-phenylethanol CH_2 next to CH_2	0.16
3.34	Doublet, J =6.6 Hz	4.87	Isobutanol CH_2 next to CH	2.19
3.35	Singlet	1.31	Methanol CH_3	0.39
3.45	DD, J = 10.7 Hz, 6.0 Hz	1.09	2-methylbutanol part of diastereotopic CH_2	0.98
3.52	Quartet, J = 7.1 Hz	-	Ethanol CH_2 carbon satellite	-
3.53	Triplet, J = 6.8 Hz	-	*n*-propanol CH_2 next to CH_2	-
3.60	Triplet, J = 7.0 Hz	-	3-methylbutanol CH_2 next to CH_2	-
3.64	Distorted	-	Ethanol CH_2 suppressed	-
3.76	Quartet, J = 7.2 Hz	3.20	Ethanol CH_2 carbon satellites	-
3.77	Triplet, J = 7.4 Hz		2-phenylethanol CH_2 next to CH_2	-
3.84	Singlet	0.028	Guaiacol OCH_3	0.0082
4.12	Quartet, J = 7.1 Hz		Ethyl acetate CH_2 next to CH_3	-
4.83	Singlet	-	Water OH suppressed	-
5.21	Quartet, J = 5.3 Hz	0.082	Acetaldehyde water hemiacetal	0.074
6.36	Doublet, J = 3.2 Hz	0.54	2-methylfuran	0.48
6.40	DD, J = 3.1 Hz, 1.9 Hz	0.52	2-methylfuran	0.47
6.68	Multiplet	-	*o*-cresol CH	-
6.74	Doublet, J = 8.5 Hz	0.091	*p*-cresol 2xCH next to CH	0.041
6.77	DD, J = 3.7 Hz, 1.7 Hz	0.10	Furfural CH next to 2xCH	0.090
6.80	Doublet, J = 1.0 Hz	0.018	5-methylfurfural CH	0.016
6.85	Doublet, J = 7.6 Hz	0.69	Phenol 2xCH next to CH	0.31
6.88	Triplet, J = 7.4 Hz	0.36	Phenol CH coupling to 2xCH	0.33
7.03	Multiplet	0.17	*p*-cresol	0.077
7.10	Triplet, J = 7.6 Hz	0.12	Ethyl phenol	0.055
7.22	Multiplet	1.31	Phenol 2xCH next to 2xCH	0.59
7.25	Doublet, J = 6.9 Hz	1.55	2-phenylethanol 2xCH	0.70
7.31	Triplet	1.46	2-phenylethanol 2xCH	0.66
7.48	DD, J = 1.8 Hz, 0.8 Hz	0.60	2-methylfuran	0.54
7.57	Doublet, J = 3.6 Hz	-	Furfural aromatic CH	-
7.64	Multiplet	-	2-methylpyridine	-
7.83	DD, J = 1.7 Hz, 0.5 Hz	0.099	5-methylfurfural	0.089
7.94	Multiplet	0.085	Furfural aromatic CH	0.076
8.18	TD, J = 7.8 Hz, 1.4 Hz	0.041	2-methylpyridine	0.012
8.53	Singlet	-	Pyridine	-
9.54	Singlet	0.068	Furfural CHO	0.061

9.69	Quartet, J = 2.9 Hz	0.054	Acetaldehyde CHO	0.048
9.97	Singlet	0.0097	Vanilin CHO	0.0088

Table S17. Signal assignment for NMR spectrum of feints sample produced using malt smoked using spent coffee grounds, recorded at the University of Edinburgh using a 600 MHz spectrometer, CSF1.

δ_H / ppm	Multiplicity	Integration	Inferences	Concentration / mmol L^{-1}
0	Singlet	10	DSS	1
0.59	Multiplet	2.54	DSS	1.14
0.78	Multiplet	0.60	Fusel alcohols CH$_3$ groups carbon satellites	-
0.89	Multiplet	59.3	Fusel alcohols CH$_3$ groups	-
0.99	Multiplet	0.69	Fusel alcohols CH$_3$ groups carbon satellites	-
1.08	Triplet, J = 7.2 Hz	3.59	Ethanol CH$_3$ carbon satellite	-
1.18	Distorted	-	Ethanol CH$_3$ suppressed	-
1.25	Triplet, J = 7.1 Hz	-	Ethyl acetate CH$_3$ next to to CH$_2$	-
1.29	Triplet, J = 7.0 Hz	4.44	Ethanol CH$_3$ carbon satellite	-
1.31	Doublet, J = 5.2 Hz	1.05	1,1-diethoxyethane CH$_3$ next to CH	0.31
1.40	Quintet, J = 5.3 Hz	-	n-butanol	-
1.43	Quartet, J = 7.0 Hz	9.56	3-methylbutanol CH$_2$ next to CH$_2$ and CH$_3$	4.30
1.54	Sextet, J = 7.2 Hz	11.3	n-propanol CH$_2$ next to CH$_2$ and CH$_3$	5.08
1.66	Nonet, J = 6.7 Hz	4.89	3-methylbutanol CH next to 2xCH$_3$ and CH$_2$	4.40
1.73	Nonet, J = 6.6 Hz	3.82	Isobutanol CH next to 2xCH$_3$ and CH$_2$	3.44
2.03	Singlet	0.38	Acetic acid CH$_3$	0.053
2.06	Singlet	0.18	Ethyl acetate CH$_3$ isolated	0.016
2.18	Singlet	0.27	*p*-cresol CH$_3$	0.080
2.22	Singlet	0.56	2-methylfuran CH$_3$	0.17
2.22	Singlet	-	Acetone 2xCH$_3$	-
2.24	Doublet, J = 3.0 Hz	0.27	Acetaldehyde CH$_3$ next to CH	0.080
2.26	Singlet	0.14	*o*-cresol CH$_3$	0.043
2.51	Singlet	0.34	5-methylfurfural	0.10
2.68	Singlet	0.12	2-methylpyridine	0.035
2.84	Triplet, J = 7.0 Hz	1.26	2-phenylethanol CH$_2$ next to CH$_2$	0.16
3.34	Doublet, J =6.6 Hz	4.98	Isobutanol CH$_2$ next to CH	2.24
3.35	Singlet	1.39	Methanol CH$_3$	0.42
3.45	DD, J = 10.6 Hz, 6.0 Hz	1.04	2-methylbutanol part of diastereotopic CH$_2$	0.94
3.52	Quartet, J = 7.1 Hz	-	Ethanol CH$_2$ carbon satellite	-
3.53	Triplet, J = 6.8 Hz	-	*n*-propanol CH$_2$ next to CH$_2$	-
3.60	Triplet, J = 7.0 Hz	-	3-methylbutanol CH$_2$ next to CH$_2$	-
3.64	Distorted	-	Ethanol CH$_2$ suppressed	-
3.75	Quartet, J = 7.0 Hz	2.88	Ethanol CH$_2$ carbon satellites	-
3.77	Triplet, J = 7.3 Hz	-	2-phenylethanol CH$_2$ next to CH$_2$	-
3.84	Singlet	-	Guaiacol OCH$_3$	-
4.12	Quartet, J = 7.1 Hz	-	Ethyl acetate CH$_2$ next to CH$_3$	-

4.83	Singlet	-	Water OH suppressed	-
5.21	Quartet, J = 5.2 Hz	0.049	Acetaldehyde water hemiacetal	0.044
6.36	Doublet, J = 3.2 Hz	0.55	2-methylfuran	0.50
6.40	DD, J = 3.2 Hz, 1.8 Hz	0.53	2-methylfuran	0.58
6.68	Multiplet	-	*o*-cresol CH	-
6.74	Doublet, J = 8.5 Hz	0.093	*p*-cresol 2xCH next to CH	0.042
6.77	DD, J = 3.6 Hz, 1.7 Hz	0.10	Furfural CH next to 2xCH	0.091
6.80	Multiplet	0.017	5-methylfurfural CH	0.015
6.85	Doublet, J = 7.7 Hz	0.70	Phenol 2xCH next to CH	0.32
6.88	Triplet, J = 7.3 Hz	0.37	Phenol CH coupling to 2xCH	0.33
7.03	Multiplet	0.17	*p*-cresol	0.076
7.10	Triplet, J = 7.7 Hz	0.12	Ethyl phenol	0.056
7.22	Multiplet	1.34	Phenol 2xCH next to 2xCH	0.60
7.25	Doublet, J = 7.0 Hz	1.56	2-phenylethanol 2xCH	0.70
7.31	Triplet, J = 7.6 Hz	1.47	2-phenylethanol 2xCH	0.66
7.48	DD, J = 1.8 Hz, 0.8 Hz	0.62	2-methylfuran	0.56
7.57	Doublet, J = 3.7 Hz	-	Furfural aromatic CH	-
7.64	Multiplet	-	2-methylpyridine	-
7.83	DD, J = 1.6 Hz, 0.6 Hz	0.096	5-methylfurfural	0.086
7.94	Multiplet	0.082	Furfural aromatic CH	0.074
8.18	TD, J = 7.8 Hz, 1.6 Hz	0.034	2-methylpyridine	0.010
8.53	Singlet	-	Pyridine	-
9.54	Singlet	0.070	Furfural CHO	0.063
9.69	Quartet, J = 3.0 Hz	0.050	Acetaldehyde CHO	0.045
9.97	Singlet	0.010	Vanilin CHO	0.0091

Table S18. Signal assignment for NMR spectrum of feints sample produced using malt smoked using spent coffee grounds, recorded at the University of Edinburgh using a 600 MHz spectrometer, CSF2.

δ_H / ppm	Multiplicity	Integration	Inferences	Concentration / mmol L^{-1}
0	Singlet	10	DSS	1
0.59	Multiplet	2.42	DSS	1.09
0.78	Multiplet	-	Fusel alcohols CH_3 groups carbon satellites	-
0.88	Multiplet	-	Fusel alcohols CH_3 groups	-
0.98	Multiplet	-	Fusel alcohols CH_3 groups carbon satellites	-
1.08	Triplet, J = 7.1 Hz	-	Ethanol CH_3 carbon satellite	-
1.18	Distorted	-	Ethanol CH_3 suppressed	-
1.25	Triplet, J = 7.1 Hz	2.62	Ethyl acetate CH_3 next to CH_2	0.79
1.28	Triplet, J = 7.0 Hz	3.83	Ethanol CH_3 carbon satellite	-
1.31	Doublet, J = 5.3 Hz	0.73	1,1-diethoxyethane CH_3 next to CH	0.22
1.43	Quartet, J = 7.0 Hz	9.00	3-methylbutanol CH_2 next to CH and CH_2	4.05
1.54	Sextet, J = 7.1 Hz	7.58	n-propanol CH_2 next to CH_2 and	3.41

			CH_3	
1.66	Nonet, J = 6.8 Hz	4.35	3-methylbutanol CH next to 2xCH_3 and CH_2	3.92
1.73	Nonet, J = 7.0 Hz	-	Isobutanol CH next to 2xCH_3 and CH_2	-
2.07	Singlet	0.50	Acetic acid CH_3	0.15
2.10	Singlet	0.070	Ethyl acetate CH_3	0.021
2.18	Singlet	0.22	*o*-cresol CH_3	0.068
2.22	Singlet	0.81	Acetone 2xCH_3	0.12
2.24	Doublet, J = 2.9 Hz	0.16	Acetaldehyde CH_3 next to CH	0.050
2.26	Singlet	0.15	*p*-cresol CH_3	0.045
2.72	Singlet	0.10	2-methylpyridine	0.031
2.84	Triplet, J = 5.0 Hz	-	Phenylethanol CH_2 next to CH_2	0.49
3.22	Doublet, J = 6.6 Hz	0.061	Isobutanol CH_2 carbon satellite	-
3.23	Singlet	0.017	Methanol CH_3 carbon satellite	-
3.34	Doublet, J = 6.6 Hz	6.55	Isobutanol CH_2 next to CH	2.95
3.35	Singlet	1.93	Methanol CH_3	0.58
3.36	Doublet, J = 6.9 Hz	-	2-methylbutanol part of diastereotopic CH_2	-
3.45	DD, J = 10.7 Hz, 5.9 Hz	2.05	2-methylbutanol part of diastereotopic CH_2	1.40
3.52	Quartet, J = 7.0 Hz	-	Ethanol CH_2 carbon satellite	-
3.53	Triplet, J = 6.7 Hz	6.04	n-propanol CH_2 next to CH_2	2.72
3.60	Triplet, J = 7.0 Hz	-	3-methylbutanol CH_2 next to CH_2	-
3.64	Quartet, J = 7.0 Hz	-	Ethanol CH_2 suppressed	-
3.75	Quartet, J = 7.1 Hz	-	Ethanol CH_2 carbon satellite	-
3.78	Triplet, J = 7.1 Hz	-	2-phenylethanol CH_2 next to CH_3	-
3.84	Singlet	0.069	Guaiacol OCH_3	0.021
4.12	Quartet, J =7.1 Hz	0.36	Ethyl acetate CH_2 next to CH_3	0.16
4.83	Singlet	-	Water OH, suppressed	-
5.21	Quartet, J = 5.2 Hz	-	Acetaldehyde water hemiacetal	-
6.36	Doublet, J = 3.1 Hz	0.017	2-methylfuran CH	0.015
6.41	DD, J = 3.2 Hz, 1.9 Hz	0.016	2-methylfuran CH	0.014
6.75	Doublet, J = 8.5 Hz	0.20	*p*-cresol 2xCH next to CH	0.091
6.76	Doublet, J = 1.9 Hz	-	Furfural CH	-
6.85	Doublet, J = 7.6 Hz	0.50	Phenol 2xCH next to CH	0.23
6.90	Triplet, J = 7.4 Hz	0.23	Phenol CH coupling to 2xCH	0.20
6.98	Multiplet	-	*o*-cresol	-
7.04	Doublet, J = 8.2 Hz	0.18	*p*-cresol 2xCH next to CH	0.082
7.26	Multiplet	3.94	2-phenylethanol 2xCH	1.18
7.32	Multiplet	2.27	2-phenylethanol 2xCH	1.02
7.49	Multiplet	0.018	2-methylfuran	0.016
7.58	Doublet, J = 3.7 Hz	0.045	Furfural aromatic CH	0.040
7.94	Multiplet	0.045	Furfural aromatic CH	0.041
8.52	Singlet	-	Formic acid CH	-
8.56	Multiplet	-	Pyridine	-
9.52	Singlet	0.041	Furfural CHO	0.037
9.68	Quartet, J = 3.0 Hz	0.046	Acetaldehyde CHO	0.041
9.97	Singlet	0.0031	Vanilin CHO	0.0028

Table S19. Signal assignment for NMR spectrum of feints sample produced using malt smoked industrially, recorded at the University of Edinburgh using a 600 MHz spectrometer, IPF1.

δ_H / ppm	Multiplicity	Integration	Inferences	Concentration / mmol L^{-1}
0	Singlet	10	DSS	1
0.59	Multiplet	2.46	DSS	1.09
0.79	Multiplet	-	Fusel alcohols CH_3 groups carbon satellites	-
0.89	Multiplet	-	Fusel alcohols CH_3 groups	-
0.99	Multiplet	-	Fusel alcohols CH_3 groups carbon satellites	-
1.08	Triplet, J = 7.2 Hz	-	Ethanol CH_3 carbon satellite	-
1.18	Distorted	-	Ethanol CH_3 suppressed	-
1.25	Triplet, J = 7.2 Hz	3.95	Ethyl acetate CH_3 next to CH_2	1.19
1.29	Triplet, J = 7.0 Hz	4.60	Ethanol CH_3 carbon satellite	-
1.31	Doublet, J = 5.2 Hz	0.89	1,1-diethoxyethane CH_3 next to CH	0.27
1.43	Quartet, J = 7.0 Hz	13.4	3-methylbutanol CH_2 next to CH and CH_2	6.02
1.54	Sextet, J = 7.2 Hz	9.44	n-propanol CH_2 next to CH_2 and CH_3	4.25
1.66	Nonet, J = 6.8 Hz	6.13	3-methylbutanol CH next to $2xCH_3$ and CH_2	5.52
1.73	Nonet, J = 6.5 Hz	-	Isobutanol CH next to $2xCH_3$ and CH_2	-
2.06	Singlet	0.17	Acetic acid CH_3	0.051
2.10	Singlet	0.082	Ethyl acetate CH_3	0.024
2.18	Singlet	0.19	*o*-cresol CH_3	0.056
2.22	Singlet	0.50	Acetone $2xCH_3$	0.076
2.24	Doublet, J = 2.9 Hz	0.16	Acetaldehyde CH_3 next to CH	0.043
2.26	Singlet	0.14	*p*-cresol CH_3	0.043
2.71	Singlet	0.044	2-methylpyridine	0.013
2.84	Triplet, J = 7.0 Hz	1.54	Phenylethanol CH_2 next to CH_2	0.69
3.22	Doublet, J = 6.6 Hz	0.053	Isobutanol CH_2 carbon satellite	-
3.23	Singlet	-	Methanol CH_3 carbon satellite	-
3.34	Doublet, J = 6.6 Hz	9.39	Isobutanol CH_2 next to CH	4.23
3.35	Singlet	2.03	Methanol CH_3	0.61
3.36	Doublet, J = 6.9 Hz	-	2-methylbutanol part of diastereotopic CH_2	-
3.45	DD, J = 10.7 Hz, 5.9 Hz	2.05	2-methylbutanol part of diastereotopic CH_2	1.84
3.52	Quartet, J = 7.1 Hz	-	Ethanol CH_2 carbon satellite	-
3.53	Triplet, J = 6.8 Hz	3.87	n-propanol CH_2 next to CH_2	3.09
3.60	Triplet, J = 7.0 Hz	-	3-methylbutanol CH_2 next to CH_2	-
3.64	Quartet, J = 6.9 Hz	-	Ethanol CH_2 suppressed	-
3.75	Quartet, J = 7.3 Hz	-	Ethanol CH_2 carbon satellite	-
3.78	Triplet, J = 7.3 Hz	-	2-phenylethanol CH_2 next to CH_3	-
3.84	Singlet	0.052	Guaiacol OCH_3	0.011
4.12	Quartet, J =7.1 Hz	0.16	Ethyl acetate CH_2 next to CH_3	0.073
4.83	Singlet	-	Water OH, suppressed	-

5.21	Quartet, J = 5.2 Hz	-	Acetaldehyde water hemiacetal	-
6.36	Doublet, J = 3.1 Hz	0.013	2-methylfuran CH	0.012
6.40	DD, J = 3.1 Hz, 1.8 Hz	0.012	2-methylfuran CH	0.010
6.74	Doublet, J = 8.5 Hz	0.17	*p*-cresol 2xCH next to CH	0.075
6.76	Doublet, J = 2.0 Hz	-	Furfural CH	-
6.85	Doublet, J = 7.7 Hz	0.57	Phenol 2xCH next to CH	0.26
6.88	Triplet, J = 7.4 Hz	0.25	Phenol CH coupling to 2xCH	0.22
6.98	Multiplet	-	*o*-cresol	-
7.02	Doublet, J = 8.4 Hz	0.16	*p*-cresol 2xCH next to CH	0.073
7.25	Multiplet	3.97	2-phenylethanol 2xCH	1.19
7.31	Multiplet	2.30	2-phenylethanol 2xCH	1.04
7.48	Multiplet	0.020	2-methylfuran	0.018
7.57	Doublet, J = 3.5 Hz	0.048	Furfural aromatic CH	0.043
7.94	Multiplet	0.049	Furfural aromatic CH	0.044
9.53	Singlet	0.044	Furfural CHO	0.039
9.69	Quartet, J = 3.0 Hz	0.035	Acetaldehyde CHO	0.031
9.97	Singlet	0.0023	Vanilin CHO	0.0021

Table S20. Signal assignment for NMR spectrum of feints sample produced using malt smoked industrially, recorded at the University of Edinburgh using a 600 MHz spectrometer, IPF2.

δ_H / ppm	Multiplicity	Integration	Inferences	Concentration / mmol L^{-1}
0	Singlet	10	DSS	1
0.59	Multiplet	2.41	DSS	1.08
0.78	Multiplet	-	Fusel alcohols CH_3 groups carbon satellites	-
0.89	Multiplet	-	Fusel alcohols CH_3 groups	-
0.98	Multiplet	-	Fusel alcohols CH_3 groups carbon satellites	-
1.07	Triplet, J = 6.9 Hz	1.56	Ethanol CH_3 carbon satellite	-
1.18	Distorted	-	Ethanol CH_3 suppressed	-
1.25	Triplet, J = 7.1 Hz	-	Ethyl acetate CH_3 next to CH_2	-
1.28	Triplet, J = 7.0 Hz	-	Ethanol CH_3 carbon satellite	-
1.31	Doublet, J = 5.5 Hz	0.89	1,1-diethoxyethane CH_3	0.27
1.39	Multiplet	-	*n*-butanol	-
1.43	Quartet, J = 7.0 Hz	8.77	3-methylbutanol CH_2 next to CH and CH_2	3.95
1.54	Sextet, J = 7.2 Hz	8.67	*n*-propanol CH_2 next to CH_2 and CH_3	3.90
1.66	Nonet, J = 6.7 Hz	4.25	3-methylbutanol CH next to 2xCH_3 and CH_2	1.91
1.73	Nonet, J = 6.7 Hz	-	Isobutanol CH next to 2xCH_3 and CH_2	-
2.07	Singlet	0.059	Acetic acid CH_3	0.039
2.08	Singlet	-	Ethyl acetate CH_3 isolated	-
2.14	Singlet	0.059	Acetic acid CH_3 carbon satellite	-
2.18	Singlet	0.23	*o*-cresol CH_3	0.068
2.22	Singlet	6.74	Acetone 2xCH_3	1.01
2.24	Doublet, J = 3.0 Hz	0.25	Acetaldehyde CH_3 next to CH	0.074
2.26	Singlet	0.095	*p*-cresol CH_3	0.028

2.72	Singlet	-	2-methylpyridine CH_3	-
2.84	Triplet, J = 7.2 Hz	-	Phenylethanol CH_2 next to CH_2	-
3.22	Doublet, J = 6.7 Hz	0.056	Isobutanol CH_2 carbon satellite	-
3.34	Doublet, J = 6.7 Hz	5.32	Isobutanol CH_2 next to CH	2.40
3.36	Doublet, J = 6.7 Hz	0.82	2-methylbutanol part of diastereotopic CH_2	-
3.45	DD, J = 10.7 Hz, J = 5.9 Hz	1.29	2-methylbutanol part of diastereotopic CH_2	1.16
3.52	Quartet, J = 7.0 Hz	-	Ethanol CH_2 carbon satellite	-
3.53	Triplet, J = 6.7 Hz	3.96	*n*-propanol CH_2 next to CH_2	3.44
3.60	Triplet, J = 7.1 Hz	4.05	3-methylbutanol CH_2 next to CH_2	1.82
3.64	Distorted	-	Ethanol CH_2	-
3.76	Multiplet	-	Ethanol CH_2 carbon satellite	-
3.78	Triplet, J = 7.1 Hz	2.17	2-phenylethanol CH_2 next to CH_2	0.98
3.84	Singlet	0.24	Guaiacol OCH_3	0.071
4.12	Quartet, J = 7.1 Hz	0.037	Ethyl acetate CH_2 next to CH_3	0.016
4.84	Singlet	-	Water OH suppressed	-
5.21	Quartet, J = 5.2 Hz	0.091	Acetaldehyde water hemiacetal	0.082
6.36	Doublet, J = 3.2 Hz	0.074	2-methylfuran	0.066
6.41	DD, J = 3.2 Hz, 1.9 Hz	0.070	2-methylfuran	0.063
6.75	Doublet, J = 8.4 Hz	-	*p*-cresol 2xCH next to CH	-
6.77	DD, J = 3.4 Hz, J = 1.5 Hz	-	Furfural CH next to 2xCH	-
6.86	Doublet, J = 7.7 Hz	-	Phenol 2xCH next to CH	-
6.91	Triplet, J = 7.5 Hz	0.21	Phenol CH coupling to 2xCH	0.19
7.05	Doublet, J = 8.3 Hz	0.18	*p*-cresol 2xCH next to CH	0.079
7.24	Multiplet	0.66	Phenol 2xCH next to 2xCH	0.30
7.26	Multiplet	3.08	2-phenylethanol 2xCH, overlapping with CH	0.92
7.33	Triplet, J = 7.5 Hz	2.39	2-phenylethanol 2xCH	1.08
7.49	Doublet, J = 1.1 Hz	0.083	2-methylfuran	0.074
7.58	Doublet, J = 3.7 Hz	0.12	Furfural aromatic CH	0.11
7.73	Multiplet	-	2-methylpyridine	-
7.83	Doublet, J = 1.4 Hz	0.020	5-HMF	0.018
7.94	Singlet	0.12	Furfural aromatic CH	0.10
8.30	Multiplet	0.0063	2-methylpyridine	0.0019
9.52	Singlet	0.11	Furfural CHO	0.10
9.68	Quartet, J = 2.9 Hz	0.058	Acetaldehyde CHO	0.052
9.96	Singlet	0.005	Vanilin CHO	0.0045

Table S21. Signal assignment for NMR spectrum of feints sample produced using laboratory smoked malt, recorded at the University of Edinburgh using a 600 MHz spectrometer, LPF1.

δ_H / ppm	Multiplicity	Integration	Inferences	Concentration / mmol L^{-1}
0	Singlet	10	DSS	1
0.60	Multiplet	2.41	DSS	1.08
0.78	Multiplet	-	Fusel alcohols CH_3 groups carbon satellites	-
0.89	Multiplet	-	Fusel alcohols CH_3 groups	-
0.99	Multiplet	-	Fusel alcohols CH_3 groups carbon	-

			satellites	
1.06	Triplet, J = 7.2 Hz	1.33	Ethanol CH_3 carbon satellite	-
1.17	Distorted	-	Ethanol CH_3 suppressed	-
1.24	Triplet, J = 7.2 Hz	-	Ethyl acetate CH_3 next to CH_2	-
1.27	Triplet, J = 7.0 Hz	-	Ethanol CH_3 carbon satellite	-
1.30	Doublet, J = 5.4 Hz	0.51	1,1-diethoxyethane CH_3	0.15
1.39	Multiplet	-	*n*-butanol	-
1.42	Quartet, J = 6.9 Hz	3.34	3-methylbutanol CH_2 next to CH and CH_2	1.51
1.53	Sextet, J = 7.1 Hz	4.80	*n*-propanol CH_2 next to CH_2 and CH_3	2.16
1.65	Nonet, J = 6.7 Hz	3.03	3-methylbutanol CH next to 2xCH_3 and CH_2	0.81
1.74	Nonet, J = 6.6 Hz	-	Isobutanol CH next to 2xCH_3 and CH_2	-
2.06	Singlet	0.056	Acetic acid CH_3	0.017
2.10	Singlet	-	Ethyl acetate CH_3 isolated	-
2.14	Singlet	0.057	Acetic acid CH_3 carbon satellite	-
2.18	Singlet	0.16	*o*-cresol CH_3	0.047
2.22	Singlet	0.059	Acetone 2xCH_3	0.0088
2.23	Doublet, J = 3.1 Hz	0.24	Acetaldehyde CH_3 next to CH	0.072
2.26	Singlet	0.093	*p*-cresol CH_3	0.028
2.71	Singlet	-	2-methylpyridine CH_3	-
2.85	Triplet, J = 7.9 Hz	-	Phenylethanol CH_2 next to CH_2	-
3.23	Doublet, J = 6.8 Hz	0.013	Isobutanol CH_2 carbon satellite	-
3.34	Doublet, J = 6.7 Hz	2.99	Isobutanol CH_2 next to CH	1.35
3.36	DD, J = 10.7 Hz, 6.6 Hz	-	2-methylbutanol part of diastereotopic CH_2	-
3.46	DD, J = 10.7 Hz, J = 5.9 Hz	0.45	2-methylbutanol part of diastereotopic CH_2	0.40
3.51	Quartet, J = 7.1 Hz	-	Ethanol CH_2 carbon satellite	-
3.53	Triplet, J = 6.7 Hz	3.96	*n*-propanol CH_2 next to CH_2	1.78
3.61	Triplet, J = 7.0 Hz	-	3-methylbutanol CH_2 next to CH_2	-
3.63	Distorted	-	Ethanol CH_2	-
3.75	Quartet, J = 6.9 Hz	-	Ethanol CH_2 carbon satellite	-
3.80	Triplet, J = 6.9 Hz	2.56	2-phenylethanol CH_2 next to CH_2	1.15
3.84	Singlet	0.22	Guaiacol OCH_3	0.068
4.12	Quartet, J = 7.1 Hz	0.072	Ethyl acetate CH_2 next to CH_3	0.033
4.83	Singlet	-	Water OH suppressed	-
4.91	Quartet, J = 5.2 Hz	-	Acetaldehyde ethyl hemiacetal	-
5.21	Quartet, J = 5.2 Hz	0.066	Acetaldehyde water hemiacetal	0.059
6.38	Doublet, J = 3.2 Hz	0.091	2-methylfuran	0.082
6.42	DD, J = 3.2 Hz, 1.9 Hz	0.086	2-methylfuran	0.078
6.76	DD, J = 3.9 Hz, 1.7 Hz	-	Furfural CH next to 2xCH	-
6.77	Doublet, J = 8.4 Hz	-	*p*-cresol 2xCH next to CH	-
6.87	Doublet, J = 7.7 Hz	-	Phenol 2xCH next to CH	-
6.94	Triplet, J = 7.4 Hz	0.19	Phenol CH coupling to 2xCH	0.17
7.09	Doublet, J = 8.3 Hz	0.16	*p*-cresol 2xCH next to CH	0.072

7.27	Multiplet	0.72	Phenol 2xCH next to 2xCH	0.32
7.28	Multiplet	3.32	2-phenylethanol 2xCH, overlapping with CH	1.00
7.35	Triplet, J = 7.6 Hz	2.59	2-phenylethanol 2xCH	1.16
7.50	DD, J = 1.8 Hz, 0.8 Hz	0.094	2-methylfuran	0.085
7.57	Doublet, J = 3.7 Hz	0.101	Furfural aromatic CH	0.091
7.74	Multiplet	-	2-methylpyridine	-
7.82	DD, J = 1.6 Hz, 0.5 Hz	0.018	5-HMF	0.017
7.92	Singlet	0.10	Furfural aromatic CH	0.091
9.50	Singlet	0.096	Furfural CHO	0.086
9.67	Quartet, J = 3.0 Hz	0.046	Acetaldehyde CHO	0.041
9.95	Singlet	0.0029	Vanilin CHO	0.0026

Table S22. Signal assignment for NMR spectrum of feints sample produced using laboratory smoked malt, recorded at the University of Edinburgh using a 600 MHz spectrometer, LPF2.

ABV measurements

ABV measurements were performed for low wines and feints through comparison of integration values of the OH and CH_3 signals, accounting for the overlap of ethanol and water OH signals. Each measurement was performed in triplicate.

CSLW1	OH signal integration	CH_3 signal integration	mol%	w%	Density (g/mL)	ABV
Sample 1	6.59	1	9.62	21.40	0.9667	26.79
Sample 2	6.62	1	9.59	21.34	0.9668	26.71
Sample 3	6.60	1	9.62	21.39	0.9667	26.78
Average						26.76 ± 0.04
CSLW2						
Sample 1	6.66	1	9.54	21.23	0.9669	26.59
Sample 2	6.64	1	9.56	21.27	0.9668	26.64
Sample 3	6.64	1	9.56	21.27	0.9668	26.64
Average						26.62 ± 0.03
LPLW1						
Sample 1	7.47	1	8.54	19.27	0.9696	24.20
Sample 2	7.47	1	8.54	19.28	0.9695	24.21
Sample 3	7.48	1	8.53	19.25	0.9696	24.17
Average						24.20 ± 0.02
LPLW2						
Sample 1	9.99	1	6.46	15.00	0.9751	18.94
Sample 2	9.99	1	6.46	15.00	0.9751	18.95
Sample 3	10.0	1	6.44	14.98	0.9751	18.92
						18.94 ± 0.01
IPLW1						
Sample 1	6.88	1	9.24	20.66	0.9677	25.90
Sample 2	6.88	1	9.24	20.65	0.9677	25.89
Sample 3	6.89	1	9.22	20.62	0.9678	25.85

						25.88 ± 0.02
IPLW 2						
Sample 1	7.38	1	8.64	19.48	0.9693	24.45
Sample 2	7.38	1	8.65	19.49	0.9693	24.46
Sample 3	7.40	1	8.62	19.43	0.9694	24.39
						24.44 ± 0.04
CSF1						
Sample 1	2.36	1	24.78	45.71	0.9231	54.65
Sample 2	2.36	1	24.74	45.67	0.9232	54.61
Sample 3	2.36	1	24.79	45.73	0.9231	54.67
						54.64 ± 0.03
CSF2						
Sample 1	2.26	1	25.74	46.98	0.9204	56.00
Sample 2	2.26	1	25.73	46.97	0.9204	55.99
Sample 3	2.26	1	25.69	46.91	0.9205	55.93
						55.97 ± 0.04
LPF1						
Sample 1	3.13	1	19.23	37.84	0.9394	46.03
Sample 2	3.13	1	19.23	37.84	0.9394	46.04
Sample 3	3.14	1	19.18	37.76	0.9395	45.95
						46.01 ± 0.05
LPF2						
Sample 1	5.43	1	11.57	25.07	0.9615	31.22
Sample 2	5.45	1	11.53	24.99	0.9617	31.12
Sample 3	5.43	1	11.57	25.07	0.9615	31.22
						31.19 ± 0.06
IPF1						
Sample 1	2.44	1	24.00	44.67	0.9254	53.53
Sample 2	2.44	1	24.06	44.75	0.9252	53.63
Sample 3	2.43	1	24.13	44.84	0.9250	53.73
						53.63 ± 0.10
IPF2						
Sample 1	2.90	1	20.62	39.91	0.9353	48.35
Sample 2	2.89	1	20.67	39.98	0.9352	48.43
Sample 3	2.89	1	20.67	39.98	0.9352	48.43
						48.40 ± 0.04

Table S23. ABV measurements performed for low wines and feints samples using ^{1}H NMR.