The Yeast-Extract Spectral Lineup

· love it, hate it, assign it

Sixteen suspects, two interrogation rooms — one dimension of ^{1}H where everybody talks at once, and a second dimension of ^{13}C where the alibis get checked — and five jars from three countries, each booked as a spoonful dissolved in D_2O. Every spread confesses somewhere between 9 and 0.8 ppm; the lineup walks downfield to upfield, room by room, sorted by the δ of each suspect's most incriminating signal, and every confession is graded on how much of it would survive cross-examination. The headline charge: the star witness of version 1.1, a "nucleotide" singlet at 8.6 ppm, was histidine all along, and the umami-synergy story that rested on it has been withdrawn. The rest of the room is trehalose, glucan and sucrose, three trimethylammonium compounds under one singlet, and a vegetable that never claimed to be yeast.

PROCESS NMR ASSOCIATES

^{1}H / ^{13}C NMR field guide · yeast-extract edition

Five retail spreads, one lot each: Marmite L0308A1795 · Marmite XO L2276A1795 · Vegemite K15SEP21B · Sanitarium Marmite (NZ) · Promite

300 MHz, JCE-PNA-MVX300 · D_2O, unbuffered, apparent pH ≈ 5 · ^{1}H, ^{13}C{^{1}H}, DEPT, gHSQC, gHMBC, 2D J-resolved

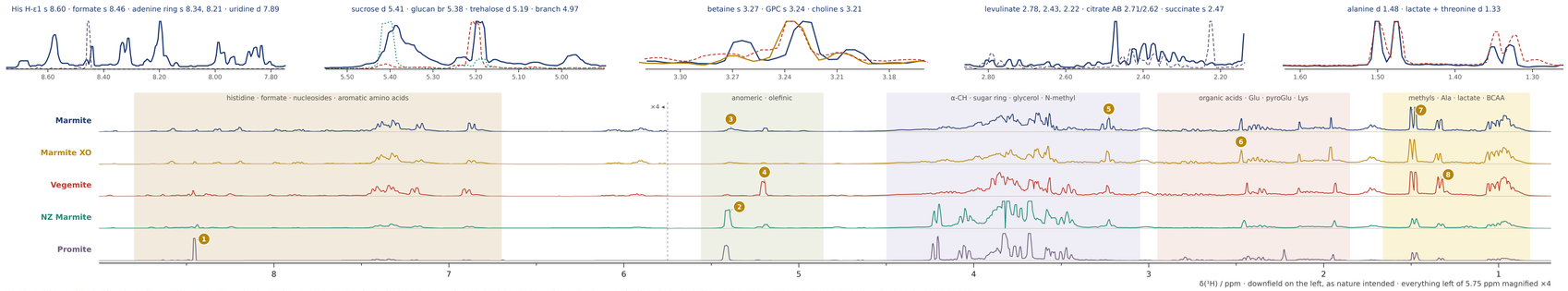
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Shifts: ^{1}H vs. the internal reference at 0.00 ppm; ^{13}C on the DSS scale after axis correction (see fine print)

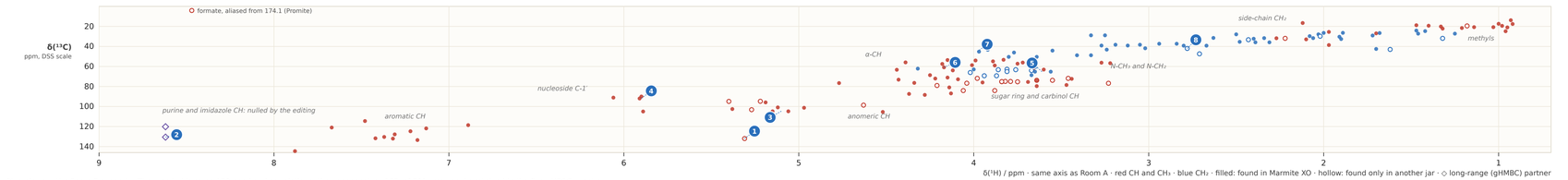
Where the bodies are buried

Room A — the proton room (^{1}H). Not instrument records: five printed traces redrawn column by column from the figures of the paper, each jar scaled to its own tallest in-frame signal, so heights are shares of a jar, not concentrations.



navy Marmite · **gold** Marmite XO · **red** Vegemite · **teal** New Zealand Marmite · **purple** Promite · in the insets every trace is scaled to its own tallest line and the second jar is dashed · gold pins are the Room A suspects, placed on the jar where each speaks loudest.

Room B — the carbon room (gHSQC, with gHMBC and ^{13}C in support). Not a contour plot: one dot for each one-bond correlation of the assignment table at its tabulated position, on the same ^{1}H axis as Room A.



Blue pins are the Room B suspects. The map holds some 150 one-bond correlations; the paper assigns 155, of 591 cross-peaks retained in the five gHSQC spectra.

Reading the lineup

Confirmed	Three or more one-bond correlations, one of them unique, or one-bond correlations backed by a long-range, J-resolved or ^{13}C observation.
Probable	Two correlations, or one unique correlation with ^{13}C support.
Tentative	A single correlation, or a coincidence of shift.
Withdrawn	A reading of version 1.1 that the numerical data overturned.
Blind spot	The experiments as run cannot decide it; absence proves nothing.

Grades are the paper's own (Table 12), one square per jar in the order **M** Marmite · **X** Marmite XO · **V** Vegemite · **N** New Zealand Marmite · **P** Promite; a hollow square is "not found", a dotted one "not assessable". Nothing has been spiked, so every grade stops short of proof.

Mugshots are schematic multiplets drawn at 300 MHz from δ and J — the shape to look for, not a measured spectrum. **Multiplicity:** s singlet · d doublet · t triplet · dd doublet of doublets · m multiplet · br broad · AB two-spin system. **Sort key** is the δ of the headline signal: δ(^{1}H) in Room A, δ(^{13}C) in Room B.

The arithmetic

Molecules per molecule of free alanine from the ^{1}H spectra (90° pulse, 8.3 s recycle): the mean of a two-Lorentzian fit on a straight local baseline and a direct integral over the same limits, set 4 Hz beyond the outer lines; in parentheses, the range when the limits are moved to 3 and 5 Hz.

	Marmite	Marmite XO	Vegemite	NZ Marmite	Promite
trehalose per alanine	**0.29 (0.27–0.33)**	**0.08 (0.08–0.09)**	**1.25 (1.15–1.37)**	**0.68 (0.64–0.73)**	**none**
α-glucan residues per alanine	2.3	1.2	≤ 0.8	≈ 0.8	not measured
α-glucan residues per trehalose	≈ 9	≈ 15	≤ 0.6	≈ 1.2	—
the same, from gHSQC volumes	12	19	1.7	1.9	—
sucrose per alanine	trace	none	none	6.5	7.9
choline relative to GPC	0.3–0.4	0.3–0.4	0.3	0.25	no signal
betaine relative to GPC	0.6	≈ 0.25	< 0.2	< 0.2	no signal

Each ^{1}H ratio is good to about one part in ten. Alanine is a ruler that stretches: it rises as autolysis proceeds, so the Marmite XO figures are not losses of that size. In the New Zealand jar there is one trehalose for every ten sucrose, and ^{1}H and ^{13}C agree on it.

Chain of custody

Five workspaces written by the PNA NMR Processor (v2.6.4), one per jar, each carrying its MestReNova 14.1.1 document unaltered. The workspaces' own 2D entries were unusable (one-dimensional transforms of the 2D time-domain data; none at all for two jars), so the processed spectra were decoded from the JPEG 2000 codestreams inside the MestReNova documents. Nothing was re-phased, apodized or baseline-corrected: MestReNova remains the engine of record. Checks: the reference at 0.0000 ± 0.0001 ppm in all five ^{1}H spectra; compression error near 10^{-5} of full scale, below the noise. The ^{1}H spectra of Marmite and Vegemite date from March 2021; Vegemite's ^{13}C and 2D data are from a fresh dissolution of the same lot in February 2023. No ^{31}P, no DOSY, no TOCSY, no spike yet: the evidence is consistent, not closed.

The booking sheet — by jar

jar	made in · lot	experiments	C / P / T of 50	carbohydrate signature	class
Marmite	UK · L0308A1795	^{1}H, gHSQC	25 / 8 / 6	glucan ≫ trehalose	brewer's-yeast autolysate
Marmite XO	UK · L2276A1795	^{1}H, ^{13}C, DEPT, gHSQC, gHMBC, 2D-J	34 / 2 / 4	glucan; trehalose nearly gone	extended-maturation autolysate
Vegemite	Australia · K15SEP21B	^{1}H, ^{13}C, DEPT, gHSQC, gHMBC	20 / 9 / 4	trehalose ≫ glucan	trehalose-rich autolysate
NZ Marmite	New Zealand · Sanitarium	^{1}H, ^{13}C, DEPT, gHSQC, gHMBC	25 / 8 / 5	sucrose ≫ trehalose ≈ glucan	yeast extract under sucrose
Promite	Australia · Mars Food	^{1}H, ^{13}C, gHSQC	17 / 8 / 4	sucrose, glucose syrup	acid-HVP and sugar spread

Confirmed / probable / tentative constituents out of the 50 graded. In all: 591 gHSQC cross-peaks retained and 447 assigned; 155 one-bond, 83 long-range (Marmite XO 67, Vegemite 30, New Zealand Marmite 33) and 33 J-resolved assignments. The grading favors Marmite XO, which had six experiments; Marmite had two.

A Room A — the proton room · ^{1}H · sorted downfield → upfield

what one dimension will admit to

#	SUSPECT	MUGSHOT	HEADLINE SIGNAL	FULL SIGNATURE	HOW IT GIVES ITSELF AWAY · CROSS-EXAMINATION	EVIDENCE	CASE FILE
1	**Formate** *the loudest voice in the jar with no yeast*	8.62 8.30	**δ 8.46 ppm** s, $H\text{-}COO^-$ — in Promite the strongest signal downfield of 5.5 ppm	A singlet in the ^{1}H spectra of all five jars (8.44–8.47); in Promite it stands over an almost empty aromatic window. Its carbon (173.9 ppm) lies outside the 170 ppm F1 window of the gHSQC, and its ^{1}J(C,H) of 195 Hz falls near the null of the multiplicity editing.	Formate and levulinate are the paired end-products of hexoses degraded by hot acid, so a loud formate beside sucrose and a quiet amino-acid region is the first hint that the protein was made with hydrochloric acid and not with yeast enzymes. In the yeast jars it is a minor singlet and convicts nobody. In the carbon room it comes in through the wrong door: an aliased response at an apparent 4.1 ppm that unfolds to 174.1.	M X V N P **Confirmed** ^{1}H singlet in all five; aliased gHSQC response in Promite only	§8.7, §8.11; Table 9; Figs 19, 26
2	**Sucrose** *the sugar coat — declared, deliberate, dominant*	5.57 5.25	**δ 5.41 ppm** d, glucosyl H-1 (J 3.9 Hz) — with 4.22 d, 4.05 t and 3.67 s of the fructosyl ring	New Zealand Marmite 6.5 and Promite 7.9 molecules per alanine. All eleven protonated carbons at their database positions; quaternary C-2′ at 106.36 ppm, missing from DEPT as it must be; gHMBC from H-1 across the glycosidic oxygen to C-2′. About one-eighth inverted in the New Zealand jar (glucose ≈ fructose ≈ 13–15 % of sucrose by ^{13}C), 5–6 % in Promite. A trace in Marmite (5.42/94.8), tentative.	Declared as sugar on both labels, so nothing is hidden; the charge is dilution, with the yeast signals compressed underneath. Sweetness is the most effective single suppressor of bitterness, and the New Zealand recipe also swaps part of its salt for potassium chloride, whose off-notes sucrose repairs. The low invert fraction says the sugar went in after the hot steps, or that they are mild: a candidate thermal-history marker, on one lot.	M X V N P **Confirmed** **Withdrawn** **Blind spot** grades shown for GPC; choline P C P P –, betaine P C – – –; v1.1 "choline" withdrawn; phosphocholine unseen	§8.11–8.13; Tables 9–11, 13; Figs 22, 29
3	**α-Glucan** *the starch-like hump — wort dextrin, glycogen stub, or both*	5.52 4.88	**δ 5.38 ppm** br, α-(1→4) H-1 (C-1 102.5) — with the α-(1→6) branch H-1 at 4.97 (C-1 101.1)	In all five jars. Per alanine: 2.3 glucose residues in Marmite, 1.2 in Marmite XO, 0.8 at most in Vegemite, about 0.8 in New Zealand Marmite. Branch residues are 0.12–0.13 of the anomeric total by ^{1}H and 0.20–0.24 by gHSQC in the yeast jars, 0.14 in Promite. 4-O-substituted C-4 at 3.65/80.1; non-reducing ends at 3.71/75.6.	A branched dextrin with many chain ends; probably the limit dextrin of wort and of the yeast's own glucoside, but intact glycogen is not excluded without DOSY or SEC, and the two sources cannot be told apart at all. The maltodextrin declared on the New Zealand label hides inside the same signal. The HSQC over-counts branches, because the internal residues of a polymer relax faster than its ends: read the ^{1}H figure as the floor and the HSQC figure as the ceiling.	M X V N P **Confirmed** a reference signal, not a concentration	§8.11–8.12, §9.3; Tables 9, 10, 13; Fig. 22
4	**Trehalose** *the yeast's own sugar — on no label*	5.35 5.03	**δ 5.19 ppm** d, H-1 of both rings (J 3.8 Hz; C-1 95.9–96.0)	Per alanine: 0.29 (0.27–0.33) in Marmite, 0.08 (0.08–0.09) in Marmite XO, 1.25 (1.15–1.37) in Vegemite, 0.68 (0.64–0.73) in New Zealand Marmite; absent from Promite. gHMBC from H-1 to C-1′ of the partner ring, across the glycosidic oxygen, which only a symmetric non-reducing disaccharide can give. One molecule per ten of sucrose in the New Zealand jar.	Listed on no label, and the 5 % compound-ingredient loophole cannot deliver a dominant sugar: the working reading is the yeast's reserve disaccharide, kept by a process that spares it (the condition of the yeast at intake, or an early heat kill of the trehalases). Both mechanisms are hypotheses. Commercial trehalose is made from C_4 maize starch and the yeast's own from C_3 wort, so ^{13}C IRMS on the isolated sugar would settle added against retained.	M X V N P **Confirmed** identity confirmed in four jars; origin argued, not proven	§8.5, §8.9, §8.11–8.12; Tables 9, 10, 13; Figs 12, 13, 25, 27
5	**The trimethylammonium three** *betaine, glycerophosphocholine, choline — three suspects in one trench coat*	3.34 3.14	**δ 3.27 / 3.24 / 3.21 ppm** three s, $N(CH_3)_3$ — betaine, glycerophosphocholine (GPC) and choline	GPC is the tall one in all four yeast jars ($N\text{-}CH_3$ 3.22–3.23/56.7; $N\text{-}CH_2$ 3.67/68.6; O-CH_2 4.32/62.2). Choline is 0.25–0.4 of it everywhere (gHMBC to 70.2). Betaine is in the British jars only: 0.6 of GPC in Marmite, about 0.25 in Marmite XO ($N\text{-}CH_3$ carbon 56.2–56.3; gHMBC to 68.8; DEPT line 56.03), and below about 0.2 in Vegemite and New Zealand Marmite. Promite: nothing at all.	Version 1.1 booked the whole singlet as choline and cleared betaine. The carbon room reversed both: the CH_2–O–P carbon of GPC is a 6 Hz doublet at 69.2 ppm, split by phosphorus, which free choline cannot produce. GPC is membrane phospholipid stripped of its fatty acids, so the trio records lipid breakdown during autolysis. Betaine's CH_2 and its link to the carboxylate were not seen, its source is undecided (cereal wort, vegetable juice concentrate, beet molasses), and phosphocholine would hide under the 3.24 line until someone runs ^{31}P.	M X V N P **Confirmed** **Withdrawn** **Blind spot** grades shown for GPC; choline P C P P –, betaine P C – – –; v1.1 "choline" withdrawn; phosphocholine unseen	§8.11–8.13; Tables 9–11, 13; Figs 22, 29
6	**Succinate** *the pH snitch*	2.63 2.31	**δ 2.47 ppm** s, both CH_2 groups — 2.39 at neutral pH (C 35.4–35.8, not 36.9)	An isolated singlet at 2.46–2.48 in the four yeast jars; not found in Promite. gHMBC to its carboxylate (183.6–183.9) and to its own symmetry-related CH_2 at 35.4, the mark of a $-CH_2\text{–}CH_2-$ unit. Acetate (1.95–1.97 s) is displaced the same way.	Succinate sits downfield of its neutral-pH address in ^{1}H and upfield in ^{13}C because part of it is protonated: the solutions were unbuffered, at an apparent pH near 5. That makes it a free pH meter, and a warning that every comparison with a pH 7.4 database on this poster carries the same displacement. Histidine in its imidazolium form tells the same story from the other end of the spectrum.	M X V N P **Confirmed** and absent from the acid hydrolysate	§8.11–8.12; Tables 9, 10; Tredwell 2016
7	**Alanine** *the ruler that stretches*	1.64 1.32	**δ 1.48 ppm** d, β-CH_3 (J 7.2 Hz; C 18.8) — the denominator of every ratio here	The tallest signal in the ^{1}H spectra of the yeast jars. gHMBC from the methyl protons to C-α (53.3) and to the carboxylate (178.5). Peptide-bound alanine stands beside it: internal residues at 1.41/19.4 in all five jars, C-terminal at 1.34/20.1 in the British jars, N-terminal at 1.58 (d) in Marmite XO.	A convenient ruler, because the doublet is sharp and fully relaxed, and a treacherous one, because free alanine rises as autolysis proceeds: Marmite XO shows a quarter of Marmite's trehalose per alanine, but part of that is the denominator growing. The three resolved alanine methyls (free, internal, terminal) are a ready-made degree-of-hydrolysis index that nobody has calibrated yet.	M X V N P **Confirmed** a reference signal, not a concentration	§8.11–8.12, §9.3; Tables 9, 10, 13; Fig. 22
8	**Lactate and threonine** *two suspects, one doublet*	1.49 1.17	**δ 1.33 ppm** d + d superposed — lactate CH_3 (J 6.9) on threonine γ-CH_3 (J 6.4)	One doublet in ^{1}H and one cross-peak in the gHSQC (1.33/22.5). The gHMBC splits it: correlations to 68.6 and 63.0 (threonine C-β, C-α) dominate in Marmite XO, those to 185.5 and 71.0 (lactate) dominate in Vegemite. Lactate methine at 4.13–4.15/71.1–71.2 in the British jars.	The doublet cannot be integrated as either compound. The long-range correlations say which one is talking in each jar, and they say something different in Burton and in Melbourne. Any lactate number read from 1.33 ppm in a yeast extract is a lactate-plus-threonine number until the 4.1 ppm methine or a 2D experiment says otherwise.	M X V N P **Confirmed** grades shown for lactate; threonine confirmed in all five	§8.4, §8.5, §8.12; Table 10; Figs 29, 30

B Room B — the carbon room · gHSQC, gHMBC, ^{13}C · sorted downfield → upfield in δ(^{13}C)

what the second dimension confirmed, overturned or could not see

#	SUSPECT	MUGSHOT	HEADLINE SIGNAL	FULL SIGNATURE	HOW IT GIVES ITSELF AWAY · CROSS-EXAMINATION	EVIDENCE	CASE FILE
1	**Monounsaturated fatty acyl chains** *the only jar with grease on its hands*	5.47 5.15	**δC 132.0 ppm** olefinic CH at δH 5.31 — with allylic CH_2 2.02/29.8 and $(CH_2)_n$ 1.32/31.9	Vegemite only. The chain methylene is among the stronger CH_2 cross-peaks of that spectrum; there is no bis-allylic CH_2, so the chains are monounsaturated. In ^{1}H the olefinic multiplet sits on the glucan envelope, which is why Vegemite's glucan is only an upper bound.	Version 1.1 flagged a weak oleifinic cross-peak as tentative and predicted the allylic and chain signals that should accompany it; the numerical data found both. Monounsaturated chains are the only kind Saccharomyces makes, so this is yeast lipid that stayed mobile through the process and not an added oil. Why only the Melbourne jar keeps it is not known, and one lot cannot say.	M X V N P **Confirmed** one jar, one lot: identifies, does not generalize	§8.5, §8.11; Tables 9, 12, 14; Fig. 27
2	**Histidine** *the alibi that broke the nucleotide case*	8.78 8.46	**δC 130.6 and 120.2 ppm** gHMBC from the 8.60–8.64 ppm singlet (H-ε1) to C-γ and C-δ2 of the imidazolium ring	β-CH_2 at 3.35/28.7 and 3.28/29.1, the positions of the protonated ring (3.13–3.22/30.7 at neutral pH); β-protons to the same C-γ at 131.1; ^{13}C lines at 136.86, 131.17, 120.24 and 28.63 in Marmite XO. The ring CH carbons themselves are nulled by the gHSQC editing.	Version 1.1 read the 8.6 ppm singlet as H-8 of an adenine nucleotide and built an umami-synergy argument on it. An adenine H-8 would reach C-4 and C-5 near 151 and 121 ppm; this proton reaches 130.6 and 120.2, and nothing at 151. It is free histidine and should not be counted as RNA. Same shift, same sharp singlet, different molecule: the textbook reason to check a 1D assignment in the second dimension.	M X V N P **Confirmed** **Withdrawn** confirmed in Marmite XO; the v1.1 adenine H-8 reading is withdrawn	§8.12, §8.15; Tables 10, 14; Fig. 29
3	**Mannan** *cell wall that came through the filter*	5.27 4.95	**δC 104.7 ppm** terminal α-mannose H-1/C-1 at δH 5.06–5.16 — with the 2,6-substituted backbone at 5.10–5.15/100.6–101.0	Anomeric and C-2 correlations in the ranges established for Saccharomyces mannan: 2-O-substituted C-2 at 3.98–4.14/80.5–80.9, unsubstituted H-2/C-2 at 4.10/72.8. Clearest in Marmite and Marmite XO, weak in Vegemite and New Zealand Marmite, absent from Promite.	Soluble mannoprotein survives the separation that is meant to remove the cell walls, and only a yeast can supply it: a vegetable hydrolysate has none. A weak response at 4.54/105.4 in Marmite XO, with two partners, may be a fragment of β-glucan from the same wall; it has no HMBC or ^{13}C support and stays tentative. The shifts are from the literature, not from an authentic standard run in this laboratory.	M X V N P **Confirmed** β-linked glucosyl residue in XO: tentative	§8.11; Tables 9, 12; Figs 23–25; Vinogradov 1998
4	**Uridine and the purine nucleosides** *RNA debris, one phosphate short of a flavor enhancer*	6.06 5.74	**δC 91.8 ppm** uridine H-1′/C-1′ at δH 5.90 — adenosine-type 6.04/91.0, guanosine-type 5.88/90.4	Uridine by six correlations in Marmite XO (H-6 7.85/144.6, H-5 5.90/105.1, ribose 4.14/87.0, 4.35/76.2, 4.23/72.2) and gHMBC from H-6 to C-2 and C-4 (154.3, 168.7). Adenine ring: 8.33 → 150.9 and 8.17 → 158.0; guanine ring: 8.00 → 153.7. One weak uridine-type response in Vegemite and New Zealand Marmite; none in Promite.	These are nucleoside positions. A 5′-nucleotide would put C-1′ near 89.6–90.1 with H-1′ at 6.1 and, decisively, a 5′-CH_2 near 66 ppm; no methylene is found at 4.03/66.2. Nucleosides have none of the glutamate synergy of 5′-IMP and 5′-GMP, so the version 1.1 claim that the British jars exploit umami synergy is withdrawn until ^{31}P NMR shows the nucleotides. A weak methine at 4.39/87.4 is the only hint of one. Cytidine, cytosine and uracil were sought and not found.	M X V N P **Confirmed** **Withdrawn** **Blind spot** grades shown for uridine; 5′-nucleotides T T – – –; synergy inference withdrawn	§8.9, §8.11–8.12; Tables 9, 10, 14; Fig. 24
5	**Glycerol** *the tallest carbon in the room*	3.76 3.44	**δC 65.18 ppm** CH_2OH, the tallest ^{13}C line of Marmite XO — CHOH at 74.66 at half the height	gHSQC methylene pair at 3.65 and 3.57/65.2, methine at 3.77–3.79/74.8–75.0, gHMBC between them; in the 2D-J spectrum the 3.56 ppm proton is a doublet of doublets (11.6 and 6.9 Hz). Confirmed in the British jars, probable in Vegemite and New Zealand Marmite; in Promite its carbons coincide with sucrose C-6′ and C-5 and cannot be assessed.	Version 1.1 gave the tallest ^{13}C line of Marmite XO to C-6 of the glucan and trehalose, which in fact sit at 63.2. It is glycerol: the main by-product of yeast fermentation, arriving with the brewery yeast and topped up by the same lipid hydrolysis that makes glycerophosphocholine. A carbon axis misread by 2 ppm was enough to hide it.	M X V N P **Confirmed** **Withdrawn** v1.1 "glucan C-6" reading withdrawn; Promite not assessable	§8.11–8.13, §8.15; Tables 9–11, 14; Fig. 23
6	**Pyroglutamate** *the umami that got away*	4.33 4.01	**δC 60.9 ppm** α-CH at δH 4.17 — with γ-CH_2 2.40/32.3 and β-CH_2 2.51 and 2.03/27.9	Its γ-CH_2 cross-peak is as tall as glutamate's in Marmite (signal-to-noise 34 against 35) and Marmite XO (75 against 69), and about half as tall in Vegemite (16 against 28) and New Zealand Marmite (42 against 78). ^{13}C height ratio to glutamate 0.9–1.2 in XO, 0.45–0.8 in the other two. Glutamine itself is established in no jar.	Glutamine cyclizes to pyroglutamate on heating and on storage, and the cyclized product carries none of glutamate's umami: abundant pyroglutamate with no glutamine is the signature of that conversion, and a candidate record of thermal history. The assignment rests on three one-bond and two long-range correlations and on database values for the anion that were not re-measured; a spike is the proper confirmation. Version 1.1 listed it among the minor multiplets.	M X V N P **Confirmed** internally consistent; not yet spiked	§8.11–8.12, §8.14; Tables 9, 10, 13; Fig. 22
7	**Peptide-bound residues** *the hydrolysis that never finished*	4.04 3.72	**δC 45.2 ppm** internal glycyl CH_2 at δH 3.98 — N-terminal at 3.92/43.3, C-terminal at 3.79/46.1	A second population of amino-acid signals at random-coil positions: alanyl CH_3 1.41/19.4 (internal) and 1.34/20.1 (C-terminal), threonyl 1.21/21.7, valyl 0.96/21.0, isoleucyl 0.92/17.7, lysyl 1.42/24.7, prolyl α-CH 4.45/63.3; in Promite a leucyl β-CH_2 at 1.61/43.2. gHMBC confirms the threonyl (1.21 → 70.0–70.3) and N-terminal alanyl (1.58 → 51.8, 173.3) residues.	Every jar still contains small peptides, and hydrophobic peptides are the principal source of bitterness in a yeast extract. The free-to-bound ratio of one residue is therefore a degree-of-hydrolysis index and, plausibly, a bitterness index; neither has been calibrated. The positions come from a random-coil compilation, not from sequenced peptides: the residue type is identified, the peptide is not.	M X V N P **Confirmed** residue types only; no peptide is sequenced	§8.11–8.12, §9.3; Tables 9, 10; Fig. 22; Wishart 1995
8	**Levulinate** *fingerprints of hydrochloric acid*	2.86 2.12	**δC 42.0, 33.3 and 32.0 ppm** $CH_2C{=}O$ at δH 2.78, CH_2COO^- at 2.43, CH_3 at 2.22 (s) — Promite only	Three one-bond correlations of similar intensity, the pattern of $CH_3\text{–}CO\text{–}CH_2\text{–}CH_2\text{–}COO^-$, and three matching ^{13}C lines (31.95, 42.00, 33.49); none of the three in any yeast jar. Beside it citrate, a declared ingredient (AB 2.71/2.62 on 47.4; C-3 at 78.46), and no asparagine or tryptophan, which hot acid deamidates and destroys.	Version 1.1 had only a methyl singlet and could not exclude acetone; acetone has no CH_2 carbons and cannot make this pattern. But the ketone carbon was sought out to 271 ppm, and nothing rises above 3.5 times the noise between 195 and 235 ppm, as expected of a slow-relaxing carbonyl at this signal-to-noise. So the grade is probable, not confirmed: a spike, or an HMBC reaching 220 ppm, would finish it. Levulinate is the established marker of acid-hydrolyzed vegetable protein in soy sauce.	M X V N P **Probable** three correlations, three ^{13}C lines; ketone carbon not detected	§8.7, §8.11; Tables 9, 12, 14; Fig. 26; Wang 1999; Sano 2007

1. The ruler was wrong

Version 1.1 took the gHSQC carbon axes to be on the TMS scale. Measured against alanine, leucine, valine, lysine and the sugar anomerics, every axis was off by its own amount: +2.40 to +2.55 ppm for the five gHSQC spectra, +2.85 to +5.05 for the gHMBC, −0.04 to +3.11 for the 1D ^{13}C. Parameter sets still named CDCl₃ at 85 °C and DMSO. Set one internal carbon reference at acquisition.

2. An address is not a GPS fix

Unbuffered, at an apparent pH near 5: succinate at 2.47 instead of 2.39, acetate at 1.96 instead of 1.91, histidine as its imidazolium ion. Anything with a carboxyl or an imidazole drifts with pH. Vegemite's 2021 ^{1}H spectrum even disagrees with its own 2023 gHSQC, run on a fresh dissolution: succinate at 2.41 against 2.46.

3. Volumes are not moles

gHSQC cross-peak volumes (1.0 s relaxation delay) compare like with like only. Against the fully relaxed ^{1}H ratios, trehalose-to-alanine volumes run 2.2× high in Marmite, 3.0× in Marmite XO, 1.2× in Vegemite and 1.0× in New Zealand Marmite; N-methyl against alanine 1.3–2.0×; sucrose against alanine 0.57–0.69×. Cause not established. Take mole ratios from ^{1}H.

4. The baseline that flattered

A first fit of the trehalose and alanine doublets let the local baseline curve. It returned values 10 to 30 % higher, by driving the fitted baseline below zero under the doublets of Vegemite and New Zealand Marmite. It was rejected, and it is on record so that nobody reuses it. A straight baseline and a matched direct integral agree to about one part in ten.

5. What the editing cannot see

The gHSQC is multiplicity-edited and tuned to 146 Hz. Carbons with ^{1}J(C,H) of 195–220 Hz — purine C-8 and C-2, the imidazolium C-ε1 of histidine, formate — fall into the null of the editing and give little or nothing. Their absence from the map is a property of the experiment, not of the jar. A non-edited HSQC is on the list.

6. One jar is an anecdote

One lot of each product, nothing spiked, and grades uneven because the experiments were uneven. Every between-jar difference on this poster is a difference between two jars, not yet between two brands or two countries. Replicate lots, a buffered re-acquisition with one carbon reference, and spikes of betaine, GPC, pyroglutamate and levulinate come first.

🕵 The confession we withdrew

Version 1.1 and the October 2026 post said the British jars reach palatability through glutamate–nucleotide synergy, because their 8.0–8.75 ppm band was "nucleotides". The band is histidine plus, mainly, nucleosides. Nucleosides do not synergize with glutamate; 5′-IMP and 5′-GMP do, and neither has been shown. Pyroglutamate as abundant as glutamate points the same way. On present evidence the British route to palatability is salt and glutamate. ^{31}P NMR could reinstate the charge.

📜 What the labels admit

Marmite: yeast extract, salt, vegetable juice concentrate, vitamins, natural flavoring; 10.8 g salt per 100 g, no sweetener. Vegemite: yeast extract, salt, mineral salt (potassium chloride), malt extract, color 150c. New Zealand Marmite: yeast, sugar, salt, potassium chloride, caramel III, corn maltodextrin, iron. Promite: vegetable protein extract (39 %), sugar, yeast extract, glucose syrup, citric acid. Every sugar the spectra found in bulk is declared, except trehalose, which no label lists.

🔍 Two that don't fit the script

New Zealand Marmite was booked in version 1.1 as a trace-trehalose jar; it carries 0.68 per alanine, more than twice the British Marmite, underneath 6.5 of sucrose. And Vegemite's trehalose, the loudest sugar signal in its spectrum, is loud partly because the glucan behind it is small: at most 0.6 glucose residues per trehalose, against 9 in Marmite and 15 in Marmite XO. A dominant peak is a statement about a ratio, not about an amount.

🔒 Still at large, or released for lack of evidence

Unassigned: a methine at 5.15/74.1 (New Zealand Marmite, Promite), a methylene at 2.37/34.1 (yeast jars), sharp ^{1}H lines at 8.63, 8.55 and 8.49 with no 2D partner, a doublet at 5.24 in Vegemite; 144 of 591 gHSQC cross-peaks have no name, none above about 11 % of the largest. Released: free glucose in Marmite XO (no ^{13}C anomeric line), intact glycogen (needs DOSY or SEC), added maltodextrin in the New Zealand jar (indistinguishable from yeast glucan), phosphocholine (needs ^{31}P), 2,3-butanediol and niacin (tentative).

⚖ Salt is evidence the magnet cannot hear

About a tenth of every jar is salt, and two recipes replace part of it with potassium chloride. Neither has a proton, so neither appears anywhere on this poster, yet both drive the taste, and the ionic strength moves the shifts. Sodium suppresses bitterness; potassium adds some; sucrose and trehalose mask it. The sensory reasoning here rests on the published taste literature and the declared recipes, not on a panel that tasted these jars.

Fine print. Chemical shifts are the positions found in these unbuffered D_2O solutions at 300 MHz — ^{1}H against the internal reference at 0.00 ppm, ^{13}C on the DSS scale after the axis corrections of Table B — street addresses, not GPS coordinates; they drift with pH, ionic strength and temperature. Room A is five ^{1}H envelopes digitized from the printed figures of the paper, each scaled to its own tallest in-frame signal, with everything left of 5.75 ppm magnified four times and off-scale sugar signals clipped; the insets are scaled trace by trace. Room B is drawn from the assignment table (reference positions, or the positions found where the paper quotes them), not from the data matrix. Ratios are ^{1}H line fits made on the MestReNova-processed traces and should be repeated in MestReNova. Evidence grades are those of Table 12 of the white paper; "withdrawn" marks a version 1.1 reading that the numerical data overturned. Reference shifts come from the BMRB (132 entries), the HMDB (pyroglutamate, glycerophosphocholine, levulinate, tyrosine; not re-verified numerically), the random-coil compilation and the carbohydrate literature; nothing was run against authentic standards in this laboratory. Product names belong to their owners and are used only to identify the retail samples analyzed; this guide is not affiliated with or endorsed by any of them.

Case files. Hoch et al., Nucleic Acids Res. 51, D368 (2023) · Wishart et al., J. Biomol. NMR 5, 67 (1995); 6, 135 (1995) · Boyer et al., J. Magn. Reson. 165, 253 (2003) · Bax & Summers, J. Am. Chem. Soc. 108, 2093 (1986) · Bajstrup et al., Anal. Chem. 85, 8802 (2013) · Petersen et al., Food Chem. 150, 65 (2014) · Vinogradov et al., Carbohydr. Res. 307, 177 (1998) · Gidley, Carbohydr. Res. 139, 85 (1985) · Zang et al., Carbohydr. Res. 220, 1 (1991) · Tredwell et al., Metabolomics 12, 152 (2016) · Govindaraju et al., NMR Biomed. 13, 129 (2000) · Fernández-Murray & McMaster, J. Biol. Chem. 280, 38290 (2005) · Zeisel et al., J. Nutr. 133, 1302 (2003) · Wang et al., J. Food Drug Anal. 7, 133 (1999) · Sano et al., Food Chem. 105, 1242 (2007) · François & Parrou, FEMS Microbiol. Rev. 25, 125 (2001) · Lillie & Pringle, J. Bacteriol. 143, 1384 (1980) · Somani et al., J. Am. Soc. Brew. Chem. 70, 123 (2012) · Nwaka & Holzer, Prog. Nucleic Acid Res. Mol. Biol. 58, 197 (1997) · Higashiyama, Pure Appl. Chem. 74, 1263 (2002) · Keast & Breslin, Food Qual. Prefer. 14, 111 (2003) · Breslin & Beauchamp, Nature 387, 563 (1997) · Sinopoli & Lawless, J. Food Sci. 77, S319 (2012) · Yamaguchi, J. Food Sci. 32, 473 (1967) · Zhang et al., Proc. Natl Acad. Sci. USA 105, 20930 (2008) · Ludwig & Viant, Phytochem. Anal. 21, 22 (2010) · Process NMR Associates, Yeast-Extract Spreads by Multinuclear NMR, white paper PNA-WP-2026-YE01 v1.2 (November 2026).

Purely for entertainment — no jar was harmed beyond dissolution in D_2O, and no ratio was rounded in a flattering direction.