SUPPLEMENTARY DATA
Espinase Nandorfy, D., Likos, D., Lewin, S., Barter, S., Kassara, S., Wang, S., Kulcasar, A., Williamson, P., Bindon, K., Bekker, M., Gledhill, J., Siebert, T., Shellie, R.A., Keast, R., & Francis, L. (2023).
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https://doi.org/10.20870/oeno-one.2023.57.3.7651

Supplementary Material

Table S1. Component proportions of each blend treatment produced in duplicate.

Wine (n=2)	CAS-1 (%)	CAS-2 (%)	LGR (%)
1	0.00	0.00	100.00
2	0.00	70.00	30.00
3	0.00	85.00	15.00
4	0.00	100.00	0.00
5	21.25	56.25	22.50
6	21.25	71.25	7.50
7	35.00	35.00	30.00
8	42.50	42.50	15.00
9	50.00	50.00	0.00
10	56.25	21.25	22.50
11	71.25	21.25	7.50
12	70.00	0.00	30.00
13	85.00	0.00	15.00
14	100.00	0.00	0.00

SUPPLEMENTARY DATA
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Table S2. Demographic and consumption characteristics of the consumers (n = 126).

Overview of consumers	Percentage
Gender	
Male	49.2
Female	50.0
Prefer not to say	0.0
Non-binary	0.8
Age	
18-35	34.9
36-50	28.6
51-65	36.5
Education	
High school	8.7
TAFE, Cert., diploma, apprenticeship	16.7
Bachelor's degree	39.7
Postgraduate degree	33.3
Other	1.6
Household income per year ($AUD)	
Less than 20,000	3.2
20-39,999	7.9
40-59,999	8.7
60-79,999	11.9
80-99,999	14.3
100-149,999	19.8
more than 150 000	34.1
How long drinking wine (years)	
Less than 2	2.4
2-5	10.3
6-10	26.2
11-20	25.4
More than 20	35.7
Frequency of red wine consumption (per week)	
A few times a week	48.4
Once a week	51.6
Once a fortnight	0.0
Once a month	0.0
Consumption of Cabernet Sauvignon	
Never tried	0.8
Don't drink that wine	0.8
1-2 times per year	7.1
3-4 times per year	13.5
Once a month	27.8
Once a fortnight	22.2
Once a week	14.3
A few times per week	13.5

SUPPLEMENTARY DATA
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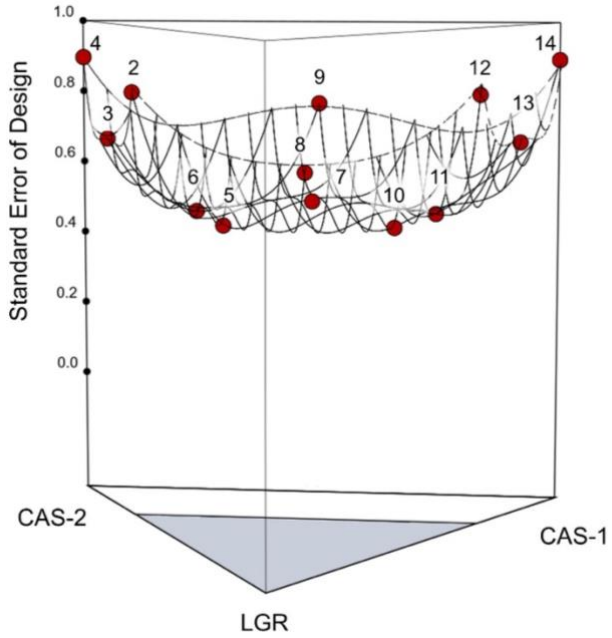

Figure S1. Response surface plot of constrained mixture model standard error.

SUPPLEMENTARY DATA
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Table S3. Mean liking and consumer cluster scores for each blend.

Blend	Liking	Cluster 1	Cluster 2	Cluster 3
1	5.1	4.5	4.3	7.5
2	6.3	6.4	5.4	7.6
3	6.4	7.1	5.5	7.0
4	6.3	6.4	5.5	7.5
5	6.2	6.6	5.2	7.2
6	6.2	6.2	5.9	6.9
7	6.1	6.8	4.9	7.3
8	6.2	6.5	5.3	7.5
9	6.1	6.6	5.0	7.3
10	5.9	5.8	5.5	6.9
11	6.2	6.7	5.3	7.1
12	5.9	6.2	4.9	7.2
13	5.7	6.2	4.6	6.7
14	5.5	5.8	4.5	7.0

SUPPLEMENTARY DATA
Espinase Nandorfy, D., Likos, D., Lewin, S., Barter, S., Kassara, S., Wang, S., Kulcasar, A., Williamson, P., Bindon, K., Bekker, M., Gledhill, J., Siebert, T., Shellie, R.A., Keast, R., & Francis, L. (2023).
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Table S4. Mean blend replicate scores for consumer liking scores and appearance and aroma ratings.

Blend	Blend Rep	Liking	Opacity	Purple Hue	Red Hue	Dark Berries A	Red Berries A	Cassis A	Vegetal A	Cedar A	Vanilla A	Dried Fruit A	Leather A	Pungency
1	1	5.1	8.0	7.2	2.3	5.5	2.5	2.6	2.2	2.4	0.6	1.0	3.6	4.7
1	2	5.1	7.9	7.2	2.4	5.4	2.5	2.5	1.8	2.7	0.5	1.5	3.7	4.7
2	1	6.5	6.8	4.9	4.2	5.0	3.9	1.7	1.2	2.0	0.7	2.4	1.0	4.7
2	2	6.0	6.9	5.4	4.0	5.0	3.9	1.9	1.7	1.7	0.8	1.8	1.2	4.5
3	1	6.2	6.5	4.2	4.7	4.8	4.3	1.8	1.4	1.7	0.7	2.1	0.9	4.4
3	2	6.6	6.4	4.1	4.9	4.7	4.6	1.6	1.1	1.6	0.6	2.8	1.2	4.5
4	1	6.5	5.5	2.7	5.4	4.4	4.8	1.5	1.9	1.8	0.4	3.0	1.4	4.5
4	2	6.1	5.6	2.2	5.7	4.3	4.9	1.5	1.3	1.7	0.6	3.0	1.2	4.4
5	1	6.3	6.7	4.6	4.4	5.2	4.1	1.8	1.6	1.6	0.5	2.5	1.3	4.5
5	2	6.1	6.6	4.9	4.2	5.0	3.7	1.7	2.1	2.1	0.2	2.2	1.3	4.5
6	1	6.3	5.6	3.0	5.1	4.6	4.8	1.2	1.5	1.5	0.4	2.6	1.0	4.6
6	2	6.1	5.9	2.9	5.3	4.5	4.5	1.5	1.4	1.8	0.6	2.5	1.2	4.4
7	1	6.3	6.9	5.1	4.0	5.5	3.4	1.7	1.9	2.0	0.7	1.7	1.9	4.6
7	2	6.0	6.9	5.0	4.3	5.0	3.5	1.2	1.3	1.9	0.5	2.0	2.4	4.6
8	1	6.3	5.9	3.7	4.8	4.7	4.1	1.3	1.6	1.8	0.7	1.9	1.7	4.6
8	2	6.2	6.3	3.7	5.0	5.2	4.0	1.7	1.9	1.9	0.3	1.6	1.6	4.6
9	1	6.1	5.2	1.8	5.6	4.1	5.2	1.0	1.7	1.7	0.6	2.3	1.2	4.5
9	2	6.1	5.2	2.2	5.6	4.4	4.9	0.9	1.6	1.9	0.3	2.6	1.4	4.4
10	1	5.8	6.3	4.5	4.5	4.9	3.7	2.3	1.7	1.8	0.3	1.5	1.8	4.6
10	2	6.0	6.6	4.4	4.6	5.1	3.5	1.6	2.2	1.5	0.4	1.5	2.7	4.8
11	1	6.3	5.2	2.4	5.5	4.2	4.6	1.0	1.6	1.9	0.4	2.1	1.1	4.7
11	2	6.1	5.6	2.7	5.4	4.5	4.3	1.6	1.9	1.6	0.6	1.9	1.8	4.6
12	1	5.9	6.7	5.0	4.3	5.0	3.1	2.0	2.4	1.9	0.0	1.2	3.2	4.7
12	2	5.9	6.8	4.9	4.3	5.0	3.7	1.9	1.6	1.8	0.7	1.6	1.7	4.6
13	1	5.5	5.9	3.4	5.1	4.4	3.2	0.8	2.4	1.7	0.0	0.9	4.1	4.9
13	2	5.8	6.0	3.7	5.1	4.6	3.4	1.5	2.9	1.7	0.1	1.1	3.2	4.8
14	1	5.2	4.9	1.8	5.8	4.1	3.9	1.4	2.4	2.0	0.2	1.9	3.0	4.8
14	2	5.8	4.7	1.8	5.6	3.7	4.1	0.8	2.6	1.9	0.0	1.8	3.5	4.8

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Table S5. Mean blend replicate intensity ratings for taste, mouthfeel and flavour terms.

Blend	Blend Rep	Sourness	Sweetness	Viscosity	Astringency	Bitterness	Hotness	Dark Berries F	Red Berries F	Cassis F	Dried Fruit F	Cedar F	Vanilla F
1	1	4.0	1.1	2.7	6.1	3.1	3.8	5.3	2.3	2.4	1.1	2.1	0.3
1	2	3.9	1.2	2.6	6.2	3.0	3.6	5.3	2.1	2.4	1.7	2.4	0.3
2	1	3.1	2.6	3.1	4.3	2.3	4.1	5.2	3.9	1.5	2.8	1.2	0.4
2	2	2.9	2.9	3.1	4.3	2.3	4.0	5.5	3.7	2.2	1.8	1.4	0.5
3	1	2.8	3.1	3.2	3.9	2.3	4.0	4.8	4.2	1.5	2.7	1.4	0.6
3	2	2.9	3.0	3.1	3.8	2.3	4.1	5.0	4.6	1.7	2.7	1.2	0.8
4	1	2.8	3.3	3.2	3.4	2.2	4.1	4.6	4.5	1.4	2.9	1.4	0.6
4	2	2.6	3.4	3.1	3.3	2.1	3.9	4.6	4.8	1.4	3.0	1.2	1.0
5	1	2.9	2.8	3.0	4.0	2.3	4.0	5.4	4.0	1.5	2.2	1.0	0.6
5	2	3.2	2.5	3.1	3.9	2.3	4.2	5.5	3.9	1.7	2.2	1.8	0.3
6	1	2.8	3.1	3.1	3.7	1.9	3.7	4.8	4.9	1.4	2.7	1.0	0.6
6	2	2.8	3.1	3.2	3.6	2.5	4.1	4.8	4.5	1.3	2.8	1.4	0.5
7	1	3.1	2.5	2.9	4.3	2.7	3.9	5.7	3.4	1.6	2.0	1.7	0.6
7	2	2.9	2.5	3.1	4.1	2.5	4.2	5.4	3.5	1.3	2.2	1.5	0.4
8	1	2.8	2.8	3.1	3.8	2.6	4.2	4.8	3.9	1.0	2.2	1.7	0.4
8	2	2.9	2.6	3.0	3.8	2.5	4.1	5.4	3.6	1.6	2.0	1.8	0.3
9	1	2.8	3.5	3.2	3.5	2.4	4.0	4.4	4.9	1.1	2.7	1.4	0.7
9	2	3.0	2.8	3.0	3.6	2.4	4.1	4.5	4.8	1.0	2.8	1.6	0.5
10	1	3.2	2.1	3.0	4.2	2.4	4.2	5.2	3.5	2.2	1.5	1.6	0.3
10	2	3.1	2.7	3.0	4.2	2.6	4.0	5.5	3.5	1.8	1.8	1.4	0.4
11	1	2.8	2.8	3.1	3.8	2.3	4.0	4.4	4.6	1.0	2.0	1.4	0.7
11	2	3.0	2.7	2.9	4.0	2.5	4.0	4.7	4.3	1.5	2.3	1.5	0.6
12	1	3.2	1.8	2.8	4.8	2.7	4.2	5.2	3.1	1.9	1.4	1.8	0.1
12	2	3.1	2.1	2.7	4.6	2.6	4.3	5.2	3.3	1.8	1.9	1.5	0.4
13	1	3.1	2.4	2.9	4.5	2.6	4.2	4.9	3.8	1.3	1.9	1.9	0.1
13	2	3.3	2.1	2.7	4.4	2.6	4.0	4.8	3.7	1.4	1.7	1.7	0.2
14	1	3.0	2.3	2.9	4.0	2.5	4.3	4.4	4.2	1.4	2.0	1.7	0.3
14	2	3.0	2.1	2.7	4.1	2.5	4.0	4.2	4.5	0.9	2.3	1.7	0.1

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Table S6. Summary of the compounds and physical properties quantified in the 28 wines.

					Range	
Variable	**CAS registry number**	**Code**	**Unit**	**Mean**	**Minimum**	**Maximum**
Fermentation-derived volatiles						
2-Methylbutanoic acid	116-53-0	2MeBuAc	µg/L	1067	599	1555
2-Methylbutanol	137-32-6	2MeBuOH	mg/L	73	64	90
2-Methylbutyl acetate	624-41-9	2MeBuOAc	µg/L	74	56	111
2-Methylpropanoic acid	79-31-2	2MePrAc	µg/L	1109	874	1269
2-Methylpropanol	78-83-1	2MePrOH	mg/L	47	38	53
2-Methylpropyl acetate	110-19-0	2MePrOAc	µg/L	22	14	30
2-Phenylethanol	60-12-8	2PhEtOH	mg/L	96	83	107
2-Phenylethyl acetate	103-45-7	2PhEtOAc	µg/L	119	72	204
3-Methylbutanoic acid	503-74-2	3MeBuAc	µg/L	1558	1014	1967
3-Methylbutanol	123-51-3	3MeBuOH	mg/L	274	262	291
3-Methylbutyl acetate	123-92-2	3MeBuOAc	µg/L	633	442	950
Acetic acid	64-19-7	AcAc	mg/L	414	341	449
Butanoic acid	107-92-6	BuAc	µg/L	672	601	859
Butanol	71-36-3	BuOH	µg/L	1847	1698	2002
Decanoic acid	334-48-5	DecAc	µg/L	370	321	530
Ethyl 2-methylbutanoate	7452-79-1	Et2MeBu	µg/L	21	15	29
Ethyl 2-methylpropanoate	97-62-1	Et2MePr	µg/L	95	84	105
Ethyl 3-methylbutanoate	108-64-5	Et3MeBu	µg/L	28	22	37
Ethyl acetate	141-78-6	EtOAc	mg/L	55	51	58
Ethyl butanoate	105-54-4	EtBu	µg/L	141	128	161
Ethyl decanoate	110-38-3	EtDec	µg/L	100	69	153
Ethyl hexanoate	123-66-0	EtHex	µg/L	320	255	351
Ethyl octanoate	106-32-1	EtOct	µg/L	322	268	364
Ethyl propanoate	105-37-3	EtPr	µg/L	167	152	175
Hexanoic acid	142-62-1	HexAc	µg/L	1751	1340	1940
Hexanol	111-27-3	HexOH	µg/L	2749	1392	3296
Hexyl acetate	142-92-7	HexOAc	µg/L	8	7	9
Octanoic acid	124-07-2	OctAc	µg/L	1311	1042	1551
Propanoic acid	79-09-4	PrAc	µg/L	1112	853	1445
Monoterpenes						
Geraniol	106-24-1	Geran	µg/L	5.3	2.6	7.1
1,8-Cineole	470-82-6	Cineole	µg/L	2.3	0.3	7.8

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					Range	
Variable	**CAS registry number**	**Code**	**Unit**	**Mean**	**Minimum**	**Maximum**
cis-Rose oxide	876-17-5	cisROx	µg/L	0.05	0.02	0.06
Linalool	78-70-6	Linal	µg/L	6.8	5.8	7.6
Nerol	106-25-2	Ner	µg/L	1.2	0.9	1.5
Terpinolene	586-62-9	Terpino	µg/L	0.1	0.0	0.2
α-Terpineol	98-55-5	aTerp	µg/L	5.9	5.1	6.3
β-Citronellol	106-22-9	bCitron	µg/L	8.3	5.2	12.7
Norisoprenoids						
Vitispirane	99881-85-3	CisViti	µg/L	1.9	1.3	3.2
β-Damascenone	23726-93-4	bDam	µg/L	5.8	3.2	8.3
1,1,6-Trimethyl-1,2-dihydronapthalene	30364-38-6	TDN	µg/L	0.33	0.14	0.51
C6-Alcohols						
(*E*)-2-Hexenol	928-95-0	E2Hex	µg/L	9.2	6.7	12.3
(*Z*)-3-Hexenol	928-96-1	Z3Hex	µg/L	117	69	159
Low molecular weight sulfur volatiles						
Hydrogen sulfide	7783-06-4	H2S	µg/L	2.4	1.6	3.4
2-Furylmethanethiol	98-02-2	2FMT	ng/L	0.3	0.0	0.8
3-Sulfanylhexanol	51755-83-0	3SH	ng/L	391	252	600
3-Sulfanylhexyl acetate	136954-20-6	3SHA	ng/L	1.6	0.9	2.7
Carbon disulfide	75-15-0	CS2	µg/L	1.6	0.9	2.8
Dimethyl sulfide	75-18-3	DMS	µg/L	44.0	12.5	62.2
Methanethiol	74-93-1	MeSH	µg/L	1.7	1.4	2.1
Methyl thioacetate	1534-08-3	MeSAc	µg/L	9.7	5.5	17.4
Phenylmethanethiol	100-53-8	PMT	ng/L	0.4	0.2	0.8
Oak volatiles						
Furfural	98-01-1	Furf	µg/L	117.7	68.0	191.0
4-Ethylphenol	123-07-9	4EP	µg/L	6.5	5.0	27.0
4-Methylguaiacol	93-51-6	4MeG	µg/L	1.6	1.0	2.0
cis-Oak lactone	55013-32-6	cisOak	µg/L	12.9	5.0	45.0
Guaiacol	90-05-1	Guaiac	µg/L	4.3	4.0	6.0
Vanillin	121-33-5	Vanil	µg/L	13.3	5.0	32.0
Pyrazines						
Isobutylmethoxypyrazine	24683-00-9	IBMP	ng/L	3.4	2.5	6.0
Tannin concentration and composition						
Tannin concentration[a]	-	MCPT	mg/L	1529	1156	2605
Tannin mass conversion[b]		%MC	%	30.5	20.9	40.6
Tannin molecular mass (by subunit composition)[c]	-	MM	g/mol	2427	1723	4508

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					Range	
Variable	**CAS registry number**	**Code**	**Unit**	**Mean**	**Minimum**	**Maximum**
Tannin molecular mass (by GPC)[d]		50% GPC	g/mol	2038	1609	2316
Mean degree of polymerisation[e]	-	mDP	no unit	8.1	5.8	15.0
Degree of galloylation[f]		%gall	%	2.8	2.2	3.4
(-)-Epigallocatechin (extension)[g]	970-74-1	%Tri-OH or epigallocatechin-phlor-	%	31	24	45
(+)-Catechin (extension)[h]	7295-85-4	cat-phlor	%	3.6	2.4	4.7
(-)-Epicatechin (extension [h]	490-46-0	epicat-phlor	%	49.6	43.8	52.1
(-)-Epicatechin-3-*O*-gallate (extension) [h]	1257-08-5	epicat-gall-phlor	%	2.7	2.0	3.2
(+)-Catechin (terminal)[i]	7295-85-4	Cat	%	8.0	3.7	10.6
(-)-Epicatechin (terminal)[i]	490-46-0	Epi	%	4.8	2.8	6.5
(-)-Epicatechin-3-*O*-gallate (terminal) [i]	1257-08-5	EpiGal	%	0.2	0.1	0.2
Amnio Acids						
Alanine	56-41-7	ALA	mg/L	9.4	6.1	12.4
Arginine	74-79-3	ARG	mg/L	10.3	6.8	13.1
Aspartic acid	56-84-8	ASP	mg/L	12.0	11.0	12.7
Glutamate	56-86-0	GLU	mg/L	12.3	8.0	17.5
Glycine	56-40-6	GLY	mg/L	7.1	3.5	9.0
Histidine	71-00-1	HIS	mg/L	6.7	5.9	7.4
Isoleucine	73-32-5	ISO	mg/L	1.7	1.4	2.0
Leucine	61-90-5	LEU	mg/L	3.9	3.3	5.0
Lysine	56-87-1	LYS	mg/L	8.4	7.7	8.7
Methionine	63-68-3	METH	mg/L	7.1	3.2	9.1
Phenylalanine	63-91-2	PHE	mg/L	3.7	2.5	4.6
Proline	147-85-3	PRO	mg/L	3531	1959	4847
Serine	56-45-1	SER	mg/L	2.8	2.4	3.4
Threonine	72-19-5	THREO	mg/L	3.7	3.0	4.9
Tyrosine	60-18-4	TYR	mg/L	3.4	2.4	4.4
Valine	72-18-4	VAL	mg/L	1.8	1.4	2.3
Metals						
Aluminium	7429-90-5	Al	ug/L	328	106	466
Arsenic	7440-38-2	Ar	ug/L	1.5	1.0	2.4
Calcium	7440-70-2	Ca	mg/L	51.2	46.0	64.0
Chromium	7440-47-3	Cr	ug/L	15.6	13.0	19.0
Chloride	16887-00-6	Cl	mg/L	193.3	99.4	267.0
Cobalt	7440-48-4	Co	ug/L	3.9	1.0	5.0
Copper	7440-50-8	Co	mg/L	0.2	0.1	0.2
Iron	7439-89-6	Fe	mg/L	2.1	0.8	3.5

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					Range	
Variable	**CAS registry number**	**Code**	**Unit**	**Mean**	**Minimum**	**Maximum**
Lead	7439-92-1	Pb	ug/L	5.7	3.0	12.5
Lithium	7439-93-2	Li	ug/L	11.9	5.1	17.6
Magnesium	7439-95-4	Mg	mg/L	139.9	114.0	158.0
Manganese	7439-96-5	Mn	mg/L	1.8	0.8	2.3
Nickel	7440-02-0	Ni	ug/L	11.8	10.2	15.4
Potassium	7440-09-7	K	mg/L	1437	1279	1597
Sodium	7440-23-5	Na	mg/L	34.3	19.0	46.0
Strontium	7440-24-6	Sr	ug/L	1970	1534	2464
Tin	7440-31-5	Ti	ug/L	5.8	4.0	7.0
Zinc	7440-66-6	Zn	ug/L	1006	656	1287
Physical measurements						
Dynamic Viscosity	-	DyVisc	Pa s	1.57	1.55	1.59
Kinematic Viscosity	-	KinVisc	m2s-1	1.59	1.57	1.61
Conductivity	-	Cond	S	2711	2644	2779
General wine and non-volatile composition						
Fructose	57-48-7	Fru	g/L	0.3	0.2	0.6
Glycerol	56-81-5	Glyc	g/L	9.7	9.4	10.0
Ethanol	64-17-5	EtOH	% v/v	14.9	14.7	15.0
Lactic acid	50-21-5	Lact	g/L	1.8	1.2	2.5
Succinic acid	110-15-6	Succ	g/L	1.3	1.2	1.6
Tartaric acid	87-69-4	Tart	g/L	2.3	2.0	2.5
pH	-	pH		3.69	3.64	3.75
Specific gravity	-	SG	kg/m-3	0.9929	0.9925	0.9936
Titratable acid pH 7.0	-	TA7.0	tartaric equiv.	5.0	4.6	5.8
Titratable acid pH 8.2	-	TA8.2	tartaric equiv.	5.7	5.3	6.4

[a]Tannin concentration determined by methyl cellulose precipitation as epicatechin equivalents; [b]Mass conversion is the recovery of tannin as its component subunits by phloroglucinolysis, as a proportion of the total tannin concentration by methyl cellulose precipitation; [c]Molecular mass determined from subunit composition by phloroglucinolysis; [d]Molecular mass as determined by gel permeation chromatography (GPC) at 50% elution; [e]Mean degree of tannin polymerisation; [f]Galloylated subunits, molar proportion of extension and terminal (-)-epicatechin-3-*O*-gallate; [g]Trihydroxylated subunits, molar proportion of extension (-)-epigallocatechin; [h]Molar proportion of extension proanthocyanidin subunits; [i]Molar proportion of terminal proanthocyanidin subunits.

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Table S7. F-ratios, probability values from preliminary ANOVA and subsequent RSM and probability values for suggested higher order model effects. Statistically significant ($P < 0.05$) probability values in bold.

			Quadratic			Cubic	Special cubic			Special Quadratic		
Variable	Model	Linear	AB	AC	BC	ABC	AB(A-B)	AC(A-C)	BC(B-C)	A^2BC	AB^2C	ABC^2
Volatiles												
4-Methylguaiacol	15.04***	15.04***										
cis-Oak lactone	26.50***	26.50***										
Furfural	553.30***	553.30***										
Guaiacol	16.91**	22.32**	0.001	27.93**	21.84**					5.79†	1.55	23.77**
Vanillin	23.28***	81.88***	3.19	0.7682	0.3344					1.21	4.04	0.8767
Isobutylmethoxypyrazine	7.08*	7.08*										
Hydrogen sulfide	4.50*	5.94*	2.56	0.3863	0.0175							
Methanethiol	19.75***	19.75***										
Dimethyl sulfide	69.63***	69.63***										
Carbon disulfide	20.26***	20.26***										
Methyl thioacetate	7.80**	7.80**										
Hexanol	276.71***	276.71***										
(*Z*)-3-Hexenol	158.09***	158.09***										
(*E*)-2-Hexenol	95.57***	391.03***	1.38	5.87†	7.01†	7.47†	23.22*	4.76	7.97†			
Ethyl acetate	29.41***	29.41***										
2-Methylpropanol	345.45***	345.45***										
Acetic acid	21.09***	21.09***										
Butanol	24.07***	24.07***										
Ethyl propanoate	7.46**	7.46**										
Ethyl 2-methylpropanoate	37.40**	138.74***	2.68	31.48†	29.77†	28.95†	2.56	32.82†	25.23†			
3-Methylbutanol	NS											
2-Methylbutanol	12.19***	12.19***										
Propanoic acid	4.97*	7.06*	3.33	4.31†	5.35†							
2-Methylpropyl acetate	136.94***	136.94***										
Ethyl butanoate	28.44***	28.44***										
2-Methylpropanoic acid	NS	4.79*	1.24	0.2246	0.0049							
Ethyl 2-methylbutanoate	304.14***	753.55***	12.42**	0.0389	0.0004							
Ethyl 3-methylbutanoate	296.82***	733.62***	16.57***	1.51	1.37							
Butanoic acid	22.69***	19.97***	12.85*	9.46*	7.71*	10.53*						
3-Methylbutyl acetate	154.96***	154.96***										
2-Methylbutyl acetate	109.32***	109.32***										
3-Methylbutanoic acid	205.51***	205.51***										
2-Methylbutanoic acid	394.78***	977.64***	1.37	0.7825	0.0524							

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			Quadratic			Cubic	Special cubic			Special Quadratic		
Variable	Model	Linear	AB	AC	BC	ABC	AB(A-B)	AC(A-C)	BC(B-C)	A^2BC	AB^2C	ABC^2
Ethyl hexanoate	20.66***	20.66***										
Hexyl acetate	24.49***	24.49***										
Hexanoic acid	22.74***	51.34***	0.9412	6.90*	6.58*	6.21*						
2-Phenylethanol	114.32***	114.32***										
Ethyl octanoate	75.13***	75.13***										
Octanoic acid	218.69***	218.69***										
2-Phenylethyl acetate	325.07***	325.07***										
Ethyl decanoate	70.05***	246.35***	1.68	15.49*	7.44†	17.44*	0.4217	18.36*				
Decanoic acid	NS											
1,8-Cineole	466.92***	466.92***										
Terpinoline	NS	3.95	0.1829	6.36†	4.78†					4.85†	1.93	7.27†
Linalool	168.03***	168.03***										
cis-Rose oxide	8.14*	6.5†	2.17	15.00*	12.78*					3.19	1.19	17.20*
α-Terpineol	8.55**	8.55**										
β-Citronellol	NS											
Nerol	8.02**	8.02**										
Geraniol	6.72*	13.39**	0.5478	4.16†	3.34	4.65†						
Vitispirane	323.96***	1430.25***	13.71*	37.48**	37.77**	36.66**	0.0317	36.31**	38.02**			
1,1,6-Trimethyl-1,2-dihydronapthalene	407.88***	1009.95***	0.0012	0.2981	2.89							
β-Damascenone	1091.33***	4804.57***	0.51	10.07†	12.03*	12.26*	60.71***	7.81†	11.98*			
3-Sulfanylhexanol	72.26***	72.26***										
3-Sulfanylhexyl acetate	32.94***	32.94***										
Phenylmethanethiol	25.59***	25.59***										
2-Furylmethanethiol	29.35***	65.68***	9.87*	2.03	0.6581							
Acetic acid	21.00***	51.62***	0.5815	8.71*	4.77†	8.85*						
Alcohol	10.88***	10.88***										
Non-volatiles												
Aspartic acid	4.17*	4.17*										
Glutamate	353.43***	1390.54***	1.19	5.49†	7.62†					15.49*	0.0093	2.03
Serine	30.90***	108.64***	12.11*	0.4038	1.06					16.2*	0.4384	2.6
Glycine	19.70***	19.70***										
Histidine	4.68*	1.38	12.73*	1.31	3.96†	6.94*						
Threonine	NS											
Arginine	11.25*	23.79**	0.8859	7.02†	4.46					3.91	0.0233	8.70†
Alanine	6.15*	11.20*	2.14	0.2101	0.0348					2.95	0.8945	3.88
Proline	360.32***	360.32***										

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			Quadratic			Cubic	Special cubic			Special Quadratic		
Variable	Model	Linear	AB	AC	BC	ABC	AB(A-B)	AC(A-C)	BC(B-C)	A^2BC	AB^2C	ABC^2
Tyrosine	8.21**	8.21**										
Valine	5.81*	5.81*										
Methionine	5.68*	5.68*										
Isoleucine	4.16*	0.285	8.88*	1.02	3.54							
Leucine	15.83***	30.80***	15.75**	0.1758	0.0324							
Phenylalanine	18.14***	18.14***										
Lysine	48.37***	145.24***	8.46*	0.0283	1.21					3.85	3.13	2.62
Methylcellulose precipitable tannin	45.72***	45.72***										
Molecular mass	79.17***	79.17***										
Mean degree of polymerisation	79.51***	79.51***										
%Tri-OH	98.83***	98.83***										
%gall	4.71*	4.71*										
%MC	5.70*	5.70*										
Epigallocatechin-phlor	98.83***	98.83***										
Cat-phlor	22.33***	22.33***										
Epicat-phlor	18.11***	18.11***										
Catechin	87.31***	87.31***										
Epicat-gall-phlor	4.52*	6.54*	5.26†	1.51	2.89							
Epicatechin	38.63***	87.74***	16.84***	0.0285	0.0363							
Epicatechin gallate	NS											
Fructose	NS											
Glycerol	44.84***	44.84***										
Lactic acid	644.20***	644.20***										
pH	2004.48***	8887.14***	9.5†	51.13**	47.72**	36.69**	6.11	47.65**	40.45**			
Specific gravity	161.05***	626.64***	1.33	4.65†	3.25					5.24	2.75	2.57
Succinic acid	41.56***	164.77***	5.52	18.76*	18.70*	19.97*	6.37†	21.21*	18.80*			
Tartaric acid	67.65***	67.65***										
Titratable acid pH 7	216.45***	216.45***										
Titratable acid pH 8.2	146.99***	146.99***										
Chloride	1648.12***	1648.12***										
Aluminium	499.97***	499.97***										
Arsenic	19.00***	19.00***										
Calcium	NS											
Chromium	38.10***	38.10***										
Cobalt	80.25***	80.25***										
Copper	15.61***	15.61***										
Iron	1380.78***	1380.78***										

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			Quadratic		Cubic	Special cubic			Special Quadratic		
Variable	Model	Linear	AB	AC	BC	ABC	AB(A-B)	AC(A-C)	BC(B-C)	A²BC	AB²C	ABC²
Lead	23.90***	23.90***										
Lithium	163.16***	163.16***										
Magnesium	47.96***	47.96***										
Manganese	472.24***	472.24***										
Nickel	9.83*	25.13**	1.5	0.0127	0.191					7.81*	1.34	2.41
Potassium	202.78***	202.78***										
Sodium	911.30***	911.30***										
Strontium	777.44***	777.44***										
Tin	NS											
Zinc	553.06***	1374.99***	9.91*	1.2	0.357							
Physical measurements												
Kinematic Viscosity	NS											
Dynamic Viscosity	NS											
Conductivity	146.96***	355.30***	0.0346	14.62**	8.19*							
Consumer and Sensory scores												
Liking	15.84***	15.84***										
Opacity	200.07***	492.12***	0.4834	7.97*	3.84							
Purple hue	651.47***	2891.42***	5.39	31.72*	30.41*	26.04*	0.7216	29.57*	25.47*			
Red hue	830.01***	3682.10***	0.0133	32.00*	31.42*	31.42*	10.49*	37.83**	31.70*			
Dark Berries aroma	98.89***	267.32***	1.86	3.02	1.01	14.35**						
Red Berries aroma	29.55***	29.55***										
Cassis aroma	8.46**	8.46**										
Vegetal aroma	55.15***	180.41***	31.55*	28.46*	31.21*	26.98*	31.12*	22.71*	36.01**			
Cedar aroma	NS											
Vanilla aroma	56.30***	162.91***	12.21*	71.70***	73.25***	67.31***	65.95***	64.47***	75.19***			
Dried Fruit aroma	30.96***	30.96***										
Leather aroma	12.48***	12.48***										
Pungency aroma	17.70***	17.70***										
Sourness	20.77***	20.77***										
Sweetness	60.83***	60.83***										
Viscosity	83.94***	292.53***	25.48**	1.11	2.22					6.90†	9.61*	0.157
Astringency	252.76***	677.47***	18.46**	0.0001	0.0025	34.47***						
Bitterness	19.94***	19.94***										
Hotness	4.81*	4.81*										
Dark Berries flavour	1976.27***	8033.55***	2.13	193.52***	204.03***	143.29***	195.20***	167.08***	220.80***			
Red Berries flavour	40.28***	40.28***										
Cassis flavour	8.96**	8.96**										

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				Quadratic		Cubic		Special cubic			Special Quadratic	
Variable	Model	Linear	AB	AC	BC	ABC	AB(A-B)	AC(A-C)	BC(B-C)	A^2BC	AB^2C	ABC^2
Dried Fruit flavour	52.26***	52.26***										
Cedar flavour	9.18**	9.18**										
Vanilla flavour	11.49***	11.49***										