Oenological Processes and Product Qualities in the Elaboration of Sparkling Wines Determine the Biogenic Amine Content

Aina Mir-Cerdà[1], Anaïs Izquierdo-Llopart[1], Javier Saurina[1*] and Sonia Sentellas[1,2]

1 Department of Chemical Engineering and Analytical Chemistry. University of Barcelona

2 Serra Húnter Lecturer, Generalitat de Barcelona, Spain

* Correspondence: xavi.saurina@ub.edu (JS)

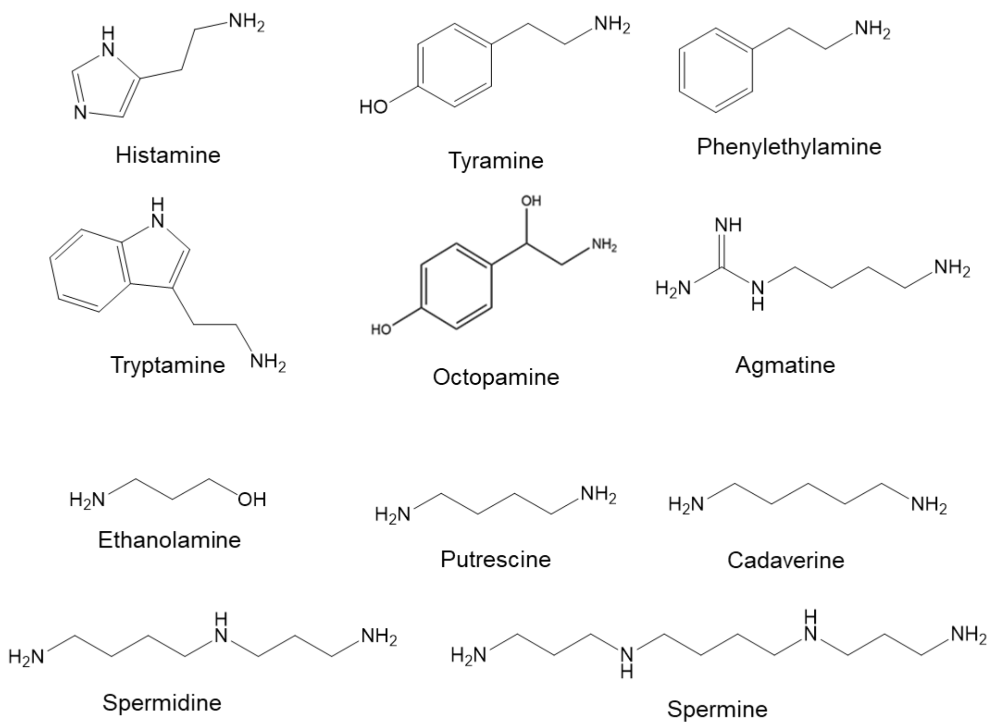

Figure S1. Structures of the most common biogenic amines in fermented foodstuffs.

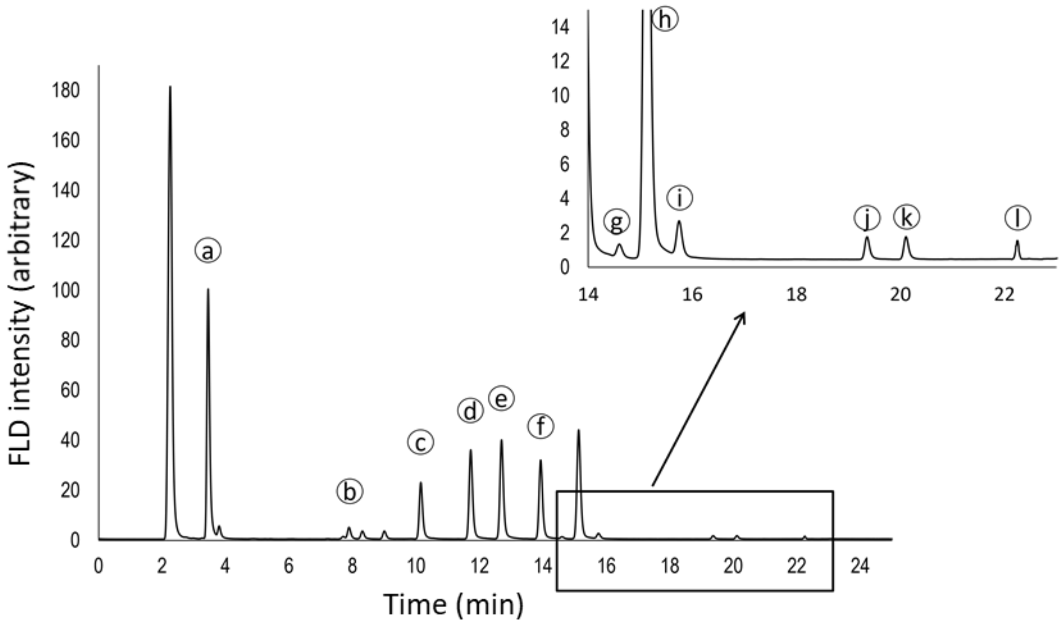

Figure S2. FLD chromatograms of a derivatized standard solution of BAs at 2 mg L^{-1} each. Peak assignment: (a) ethanolamine; (b) agmatine; (c) tryptamine; (d) phenylethylamine; (e) putrescine; (f) cadaverine; (g) histamine; (h) hexylamine (IS); (i) octopamine; (j) tyramine; (k) spermidine; (l) spermine.

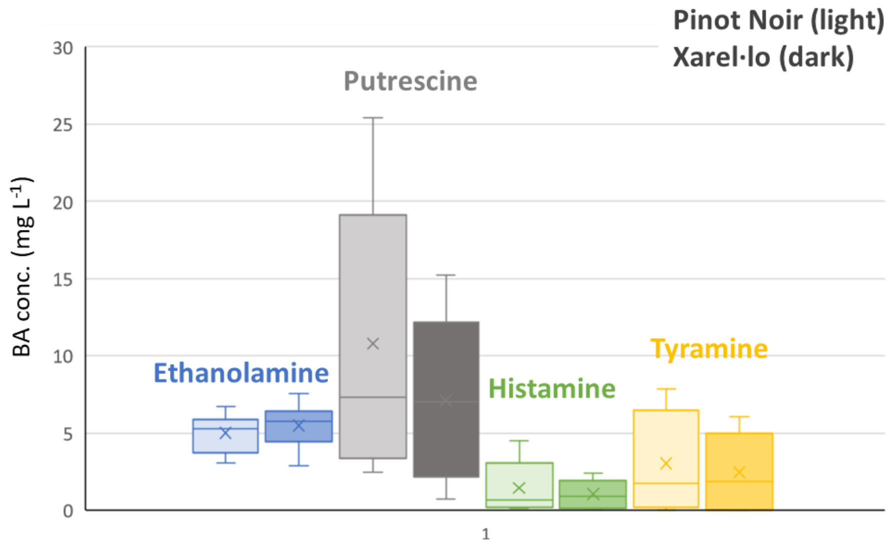

Figure S3. Boxplots with whiskers representing the concentration of ethanolamine, putrescine, histamine and tyramine in base and stabilized wines for Pinot Noir (light color) and Xarel·lo (dark color) varieties.

Table S1. MRM transitions for the detection of dansyl derivatives of biogenic amines by LC-MS/MS.

Biogenic amine	Retention time (min)	Dansyl groups	Parent ion (m/z)	Product ion (m/z)	DP (V)	CE (V)	CXP (V)
Ethanolamine	3.5	1	295.0	170.0	120	60	12
Agmatine	7.9	2	597.3	170.1	50	80	8
Tryptamine	10.2	1	394.2	234.1	60	40	10
Phenylalanine	11.7	1	355.3	170.1	90	30	10
Putrescine	12.7	2	555.3	234.0	120	60	12
Cadaverine	13.9	2	569.2	234.0	110	50	8
Histamine	14.6	2	578.3	234.0	80	40	12
Hexylamine (IS)	15.1	1	335.4	157.0	86	39	12
Octopamine	15.7	2	620.2	170.0	66	59	12
Tyramine	19.4	2	604.3	234.2	90	40	8
Spermidine	20.1	3	845.4	360.3	40	80	12
Spermine	22.4	4	1135.6	360.4	90	50	10

DP, declustering potential; CE, collision energy; CXP, cell exit potential; IS, internal standard.

Table S2. Concentration (mg L^{-1}) of biogenic amines in the different type of samples

	Eth	Agm	Tryp	Phe	Put	Cad	His	Oct	Tyr	Smd	Spm
MPA	3.0	0.16	ND	0.064	2.5	0.29	0.16	ND	ND	0.30	1.4
BWPA	3.1	0.15	ND	0.020	4.0	0.30	0.19	ND	0.017	0.20	1.4
SWPA	3.4	0.18	ND	0.026	3.8	0.31	0.20	ND	0.054	0.36	1.4
C3PA	2.9	0.16	ND	0.028	2.1	0.30	0.18	ND	0.22	0.11	1.4
C7PA	2.7	0.11	ND	0.015	1.4	0.28	0.14	ND	0.17	ND	1.4
MPB	2.7	0.13	ND	0.039	1.4	0.29	0.14	ND	0.033	0.24	1.4
BWPB	5.2	0.15	ND	0.035	3.4	0.39	0.18	ND	0.38	0.10	1.5
SWPB	5.5	0.14	ND	0.032	2.8	0.33	0.31	ND	0.31	0.36	1.5
C3PB	6.1	0.13	ND	0.031	2.7	0.32	0.30	ND	0.32	0.22	1.5
C7PB	5.5	0.13	ND	0.026	2.3	0.32	0.26	ND	0.27	0.10	1.5
MPC	3.9	0.14	ND	0.028	4.8	0.30	0.17	ND	0.014	0.40	1.4
BWPC	5.4	0.18	ND	0.29	24	0.48	4.0	ND	5.6	0.33	1.6
SWPC	4.8	0.15	ND	0.16	11	0.39	1.2	ND	3.3	ND	1.4
C3PC	4.9	0.17	ND	0.17	12	0.41	1.4	ND	3.5	0.19	1.5
C7PC	5.0	0.15	ND	0.17	11	0.40	1.4	ND	3.5	0.10	1.5
MPD	3.5	0.11	ND	0.055	2.1	0.29	0.13	ND	ND	0.10	1.4
BWPD	6.1	0.183	ND	0.47	21	0.67	3.7	ND	7.7	0.40	1.5
SWPD	6.6	0.18	ND	0.44	16	0.52	1.8	ND	7.0	0.38	1.5
C3PD	6.4	0.17	ND	0.40	16	0.50	2.3	ND	6.7	0.20	1.5
C7PD	6.7	0.18	ND	0.43	18	0.55	2.9	ND	7.2	0.22	1.5

Table S2. Cont.

	Eth	Agm	Tryp	Phe	Put	Cad	His	Oct	Tyr	Smd	Spm
MXA	2.7	0.11	ND	ND	1.3	0.28	0.11	ND	ND	0.11	1.4
BWXA	3.9	0.12	ND	ND	1.8	0.28	0.11	ND	0.015	0.20	1.4
SWXA	3.2	0.11	ND	ND	0.95	0.28	0.11	ND	0.023	ND	1.4
C3XA	3.4	0.11	ND	ND	1.1	0.28	0.13	ND	0.16	ND	1.4
C7XA	3.4	0.11	ND	ND	0.94	0.28	0.12	ND	0.16	ND	1.4
MXB	4.0	0.10	ND	ND	0.43	0.27	0.10	ND	ND	0.29	1.4
BWXB	5.1	0.12	ND	ND	3.1	0.28	0.11	ND	0.015	0.11	1.4
SWXB	6.3	0.12	ND	0.016	2.4	0.28	0.21	ND	0.35	0.25	1.4
C3XB	7.1	0.16	ND	0.031	3.1	0.31	0.26	ND	0.55	0.23	1.5
C7XB	5.6	0.14	ND	0.020	3.1	0.30	0.26	ND	0.52	0.10	1.4
MXC	5.3	0.11	ND	ND	3.3	0.28	0.11	ND	0.0024	0.33	1.4
BWXC	5.7	0.14	ND	0.38	11	0.65	1.8	ND	4.6	0.59	1.4
SWXC	5.9	0.14	ND	0.34	14	0.62	2.3	ND	5.2	0.43	1.4
C3XC	7.3	0.15	ND	0.35	18	0.72	2.6	ND	5.6	0.41	1.4
C7XC	5.9	0.15	ND	0.25	11	0.63	1.9	ND	5.4	0.49	1.4
MXD	4.1	0.13	ND	ND	2.8	0.28	0.12	ND	0.016	0.37	1.4
BWXD	6.5	0.14	ND	0.26	13	0.36	1.9	ND	3.5	0.23	1.4
SWXD	7.1	0.14	ND	0.28	10.3	0.55	1.8	ND	5.9	0.25	1.4
C3XD	6.1	0.15	ND	0.25	9.5	0.59	1.7	ND	5.4	0.31	1.4
C7XD	6.1	0.14	ND	0.33	19	0.76	2.8	ND	5.4	0.40	1.4
Average	5.0	0.14	-	0.14	7.3	0.40	0.99	-	2.2	0.24	1.4
SD	1.4	0.02	-	0.16	6.7	0.15	1.1	-	2.7	0.15	0.05
min-max	2.7-7.3	0.10-018	-	ND-0.47	0.43-24	0.27-0.76	0.10-4.0	-	ND-7.7	ND-0.59	1.4-1.6

ND: not detected

Amine identification: Agm: agmantine; Tryp: tryptamine; Phe: phenylethylamine; Put: putrescine; Cad: cadaverine; His: histamine; Oct: octopamine; Tyr: tyramine; Smd: spermidine; Spm: spermine; Eth: ethanolamine.

Table S3. ANOVA applied to the study of quality and MLF factors.

		P-value								
		Eth	**Agm**	**Phe**	**Put**	**Cad**	**His**	**Tyr**	**Smd**	**Spm**
Pinot Noir	Pre-fermentation (must)	$3.1\ 10^{-5}$	>0.05	>0.05	>0.05	>0.05	>0.05	>0.05	>0.05	>0.05
	Post-fermentation	$1.2\ 10^{-4}$	$8.6\ 10^{-4}$	$2.5\ 10^{-13}$	$8.0\ 10^{-24}$	$1.8\ 10^{-11}$	$1.9\ 10^{-20}$	$1.1\ 10^{-17}$	>0.05	>0.05
Xarel·lo	Pre-fermentation (must)	>0.05	>0.05	>0.05	$1.8\ 10^{-4}$	>0.05	>0.05	>0.05	>0.05	>0.05
	Post-fermentation	$2.4\ 10^{-5}$	$7.8\ 10^{-4}$	$3.6\ 10^{-27}$	$1.4\ 10^{-17}$	$1.6\ 10^{-16}$	$5.5\ 10^{-23}$	$8.5\ 10^{-39}$	$2.2\ 10^{-5}$	>0.05

Amine identification: Eth: ethanolamine; Agm: agmantine; Phe: phenylethylamine; Put: putrescine; Cad: cadaverine; His: histamine; Tyr: tyramine; Smd: spermidine; Spm: spermine.