

Supplementary Material

Simultaneous Determination of Amino Acids and Biogenic Amines by Liquid Chromatography Coupled to Mass Spectrometry for Assessing Wine Quality

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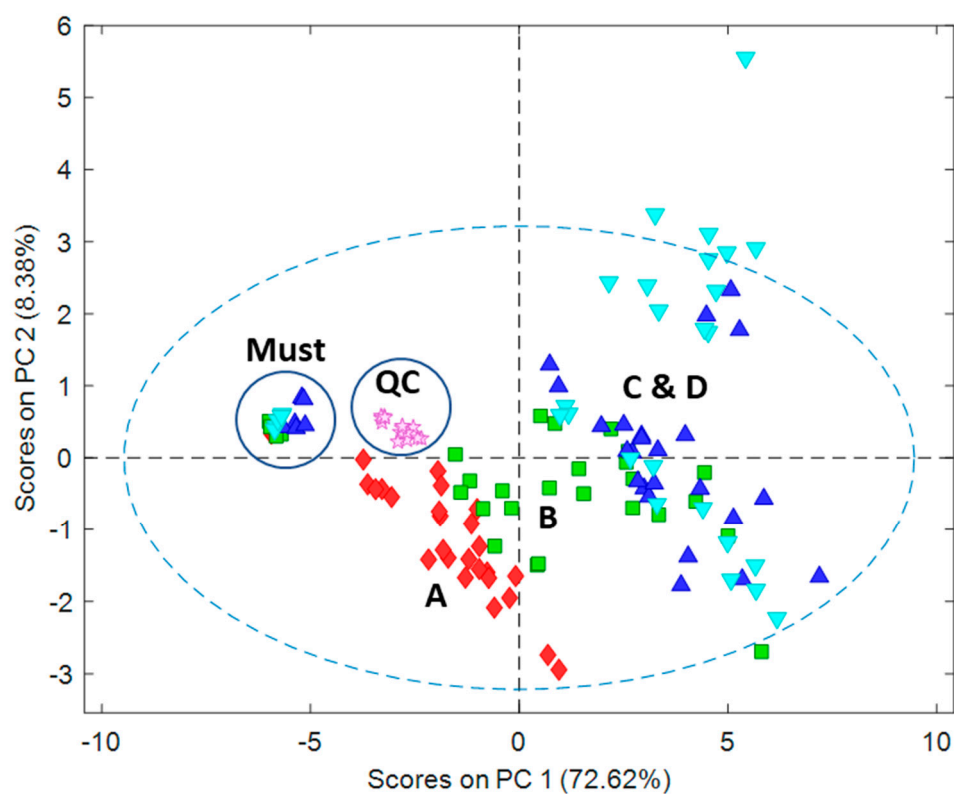


Figure S1. PCA score plot of PC1 vs. PC2 for the exploratory evaluation of samples using AA profiles as the data. Sample assignment: Star, QC; Rhombus, Quality A; Square, Quality B; Triangle (vertex up), Quality C; Triangle (vertex down), Quality D.

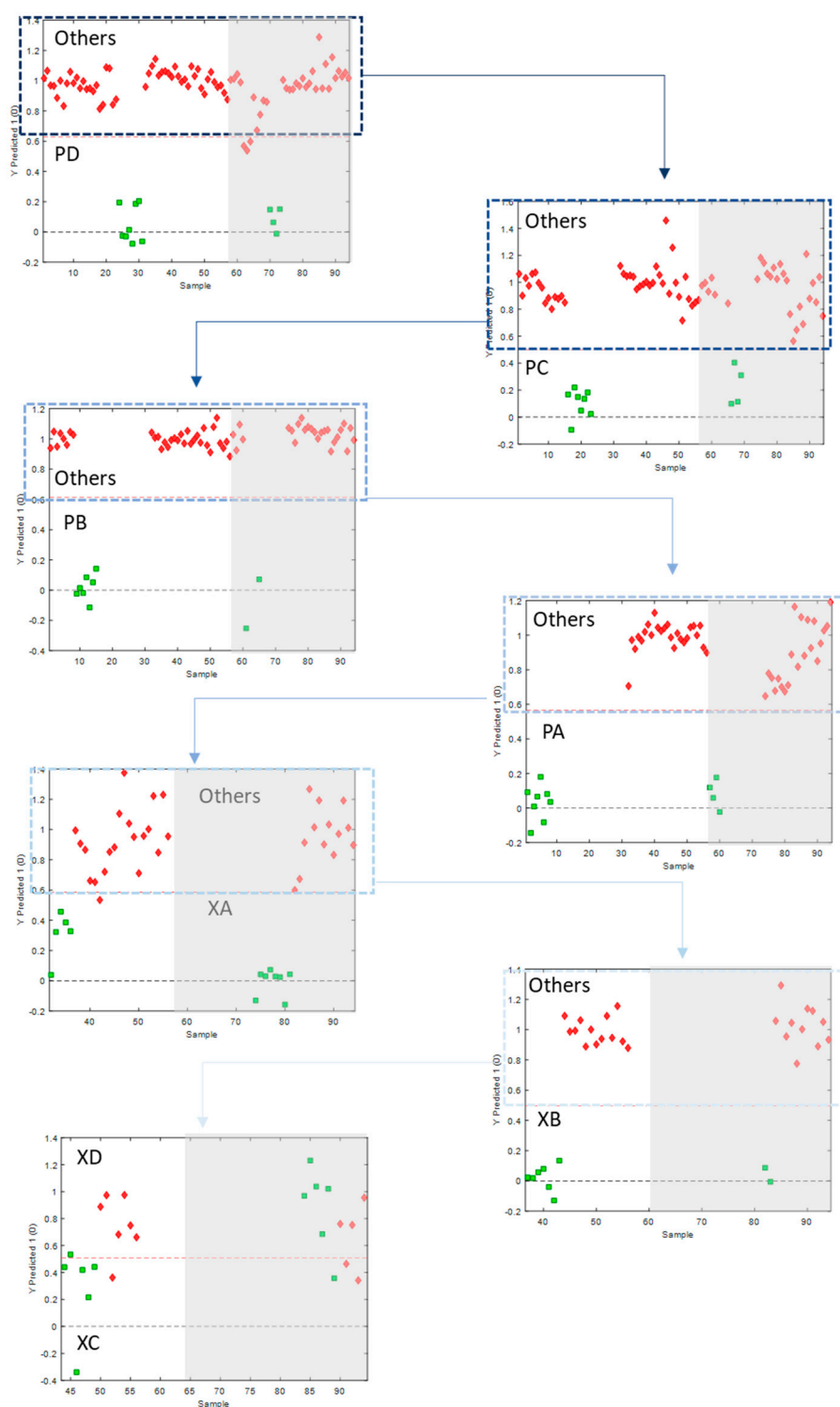


Figure S2. Two-class classification models obtained by PLS-DA according to the calibration tree shown in Figure 6. The calibration set comprises the 60% of all samples randomly chosen and the prediction set the 40% remaining samples.

Table S1. Parameters of the MS instruments for the set of analytes under study. DP, declustering potential; CE, collision energy, CXP, cell exit potential.

Analyte	Dansyl units	Q1 mass (Da)	Q3 mass (Da)	DP (V)	CE (V)	CXP (V)	Retention time (min)
Arginine	1	408	170	100	50	12	5.1
Asparagine	1	366	170	100	50	12	5.3
Glutamine	1	380	170	100	50	12	5.8
Serine	1	339	170	100	50	12	6.6
Agmatine	2	597	170	50	80	8	6.8
Glutamic acid	1	381	170	100	50	12	7.1
Aspartic acid	1	367	170	100	50	12	7.3
Hydroxyproline	1	365	170	100	50	12	7.3
Threonine	1	353	170	100	50	12	7.7
Ethanolamine	1	295	170	100	50	12	8.0
Glycine	1	309	170	100	50	12	8.6
Alanine	1	323	170	100	50	12	9.6
Proline	1	349	170	100	50	12	12.2
Valine	1	351	170	100	50	12	12.6
Methionine	1	383	170	100	50	12	12.7
Triptan	1	438	170	100	50	12	13.1
Ethylamine	1	279	170	100	50	12	13.7
Phenylalanine	1	399	170	100	50	12	14.1
Isoleucine	1	365	170	100	50	12	14.4
Leucine	1	365	170	100	50	12	14.6
Cysteine	1	355	170	90	30	10	15.1
Ornithine	2	599	170	100	50	12	16.5
Lysine	2	613	170	100	50	12	17.2
Histidine	2	622	170	100	50	12	17.5
Tryptamine	1	394	234	60	40	10	17.7
Phenylethylamine	1	355	170	90	30	10	18.8
Putrescine	2	555	234	120	60	12	19.6
Cadaverine	2	569	234	100	50	12	20.5
Tyrosine	2	648	170	100	50	12	20.5
Histamine	2	578	234	100	50	12	20.9
Hexylamine	1	335	157	86	39	12	21.3
Octopamine	2	620	170	66	59	12	21.6
Tyramine	1	604	234	100	50	12	23.8
Spermidine	3	845	360	40	80	12	24.3
Spermine	4	1135	360	90	50	12	27.3

Taula S2. Figures of merit of the proposed HPLC-MS/MS method.

Compound	Linear range (mg L ⁻¹)	Sensitivity (counts per min)	R ²	Repeatability (Retention time) RSD%	Repeatability at 0.2 mg L ⁻¹ (peak area) RSD%	Repeatability at 2 mg L ⁻¹ (peak area) RSD%	LOD (mg L ⁻¹)
Arginine	0.1 - 4	2.80 × 10 ⁵	0.9944	0.17	4.39	8.52	0.05
Asparagine	0.1 - 5	3.08 × 10 ⁴	0.9979	0.15	1.21	7.73	0.07
Glutamine	0.1 - 5	9.92 × 10 ⁴	0.9906	0.13	8.89	8.57	0.05
Serine	0.2 - 5	3.28 × 10 ⁴	0.9909	0.14	8.89	8.04	0.16
Agmatine	0.1 - 0.5	1.14 × 10 ⁶	0.9932	0.29	2.67	7.85	0.05
Glutamic acid	0.1 - 5	3.51 × 10 ⁵	0.9968	0.35	4.84	5.03	0.04
Aspartic acid	0.1 - 5	1.15 × 10 ⁵	0.9974	0.35	4.58	6.57	0.08
Hydroxyproline	0.2 - 5	2.88 × 10 ⁵	0.9903	0.16	8.23	7.80	0.06
Threonine	0.1 - 2	4.88 × 10 ⁴	0.9989	0.12	8.27	8.18	0.08
Ethanolamine	0.1 - 2	7.07 × 10 ⁴	0.9980	0.13	7.93	9.25	0.05
Glycine	0.1 - 4	9.66 × 10 ⁴	0.9983	0.10	6.42	5.02	0.11
Alanine	0.1 - 2	1.46 × 10 ⁵	0.9991	0.11	7.53	6.73	0.06
Proline	0.5 - 10	3.32 × 10 ⁵	0.9984	0.07	8.92	7.29	0.09
Valine	0.2 - 10	3.11 × 10 ⁵	0.9979	0.06	5.34	7.04	0.05
Methionine	0.2 - 10	2.82 × 10 ⁵	0.9979	0.04	1.24	8.26	0.01
Tryptophan	0.05 - 10	1.01 × 10 ⁶	0.9976	0.12	5.36	6.44	0.05
Ethylamine	0.1 - 5	5.54 × 10 ⁵	0.9977	0.06	6.72	4.95	0.05
Phenylalanine	0.2 - 5	4.85 × 10 ⁵	0.9990	0.06	8.88	3.14	0.07
Isoleucine	0.2 - 5	6.06 × 10 ⁵	0.9941	0.04	2.40	4.35	0.02
Leucine	0.1 - 5	5.54 × 10 ⁵	0.9977	0.06	6.72	4.95	0.05
Cysteine	0.05 - 10	6.93 × 10 ⁵	0.9982	0.06	2.42	2.66	0.02
Ornithine	0.5 - 5	7.87 × 10 ⁵	0.9978	0.08	2.71	8.51	0.21
Lysine	0.2 - 10	6.80 × 10 ⁵	0.9996	0.08	3.21	9.02	0.10
Histidine	0.5 - 5	1.21 × 10 ⁶	0.9991	0.10	2.97	7.20	0.15
Tryptamine	0.05 - 10	6.03 × 10 ⁴	0.9987	0.07	2.70	6.16	0.04
Phenylethylamine	0.2 - 4	6.11 × 10 ⁵	0.9990	0.04	8.48	5.30	0.13
Putrescine	0.1 - 2	5.53 × 10 ⁴	0.9961	0.04	5.73	8.68	0.03
Cadaverine	0.2 - 2	1.93 × 10 ⁵	0.9992	0.03	4.68	7.14	0.04
Tyrosine	0.05 - 10	4.07 × 10 ⁵	0.9985	0.12	4.20	8.70	0.04
Histamine	0.1 - 2	1.60 × 10 ⁵	0.9957	0.03	8.54	9.14	0.06
Octopamine	0.05 - 10	7.62 × 10 ⁵	0.9991	0.06	2.54	4.83	0.03
Tyramine	0.1 - 2	2.96 × 10 ⁵	0.9914	0.02	7.83	6.94	0.07
Spermidine	0.5 - 2	5.08 × 10 ⁵	0.9993	0.05	4.92	3.66	0.14
Spermine	0.5 - 5	1.66 × 10 ⁴	0.9961	0.04	n.d.	4.43	0.40