

Quantification of organic acids in wine and grape by electrospray ionization mass spectrometry

Quantification of organic acids in wine and grape by direct infusion electrospray mass spectrometry

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Supplementary Material

Table S1. Results of the evaluation of method selectivity for malic, tartaric and citric acids at concentrations of 1.25 µg/mL

	malic acid		tartaric acid		citric acid	
	standard	blank	standard	blank	standard	blank
mean area	39,275,447	32,137,030	8,126,197	6,433,442	12,724,429	10,743,383
variance	3,452,670	1,260,729	166,591	214,953	315,201	381,724
number of observations	3	3	3	3	3	3
F _{calculated}		7.5		0.60		0.68
F _{critical 95%}		19.0		19.0		19.0

*Acceptance Criteria: $F < F_{crit}$

Table S2. Analytical parameters obtained for quantitative analysis of the acids in wine.

compound	Data linearity curve Equation	R	(µg/mL)			Accuracy (recovery%) ± SD		
			LOD	LOQ		1	2	3
Malic acid	Y= -2,72E6+3,36E7X	0.999	0.278	0.843	95.30±0.60	107.58±0.67	117.63±0.74	
Tartaric acid	Y= -9,23E6+1,41EX	0.997	0.456	1.383	93.15±3.59	98.87±3.81	103.01±3.97	
Citric acid	Y= -6,55E6+1,40EX	0.993	0.711	2.157	45.59±1.77	82.41±3.20	87.25±3.39	

* Acceptance Criteria: 70% < Recovery < 120%. Concentrations used (1)1.25 µg/mL; (2) 2.5 µg/mL; (3) 5.0 µg/mL; LOD = limits of detection; LOQ = limits of quantification; SD = standard deviation relative to triplicate.

Table S3. Repeatability and intermediate precision of the method.

acids	Instrument repeatability (CV%)			Method repeatability (CV%)								
	1	2	3	1			2			3		
				1 ^o day	2 ^o day	3 ^o day	1 ^o day	2 ^o day	3 ^o day	1 ^o day	2 ^o day	3 ^o day
malic	0.82	1.20	1.24	0.87	0.82	1.84	1.20	1.93	1.96	3.17	3.10	1.24
tartaric	2.99	0.93	1.04	3.38	2.99	3.74	1.83	1.50	0.93	1.04	2.77	2.09
citric	2.20	1.76	1.12	4.26	4.21	2.20	1.76	2.89	2.51	1.40	1.12	2.77

*(1) tartaric acid, malic acid and citric acids at concentrations of : (1) 2 µg/mL; (2) 4 µg/mL ; (3) 8 µg/mL.

Table S4. Analytical parameters obtained for linearity, limit of detection and quantification and accuracy for the analytes studied.

Compound	Equation	R	LOD/LOQ (µg/mL)		Accuracy (recovery %)		
			LOD	LOQ	1	2	3
tartaric acid	Y= 2.88E6+4.98E6X	0.998	0.65	1.98	114%	91%	84%
malic acid	Y= 9.08E6+2.07E6X	0.992	1.50	4.55	89%	90%	91%

* Acceptance Criteria: 70% < Recovery < 120%; malic, tartaric and citric (1) 1.0 µg/mL; (2) 2.0 µg/mL; (3) 3.0 µg/mL; LOD = limits of detection; LOQ = limits of quantification.