

Table S1a Summary of Pre-processing methods and wavenumber regions selected for ATR-FT-MIR

<i>Component</i>	<i>Sample Treatment</i>	<i>Rank</i>	<i>Pre-processing Method</i>	<i>Wavenumber Regions</i>
Anthocyanins (mg/L)	Filtered	7	Log10	(1100-2500) (2700-4000)
Anthocyanins (mg/L)	Untreated	8	Autoscale	4000 - 400
Colour Density	Filtered	6	Baseline (Automatic Whittaker Filter)	4000 - 400
Colour Density	Untreated	4	Glog	4000 - 400
Polymeric Pigments (mg/L)	Filtered	8	Multiway Scaling	(1500 - 1700) (2500 - 3500)
Polymeric Pigments (mg/L)	Untreated	7	Autoscale	(1400 - 1500) (2500 - 2600) (3100 - 3500)
Tannins (mg/L)	Filtered	5	Normalising	4000 - 400
Tannins (mg/L)	Untreated	3	GLog	4000 - 400
Total polyphenol index	Filtered	9	Autoscale	(1000 - 1500) (2700 - 3000) (3500 - 3700)
Total polyphenol index	Untreated	8	Baseline (Automatic Weighted Least Squares)	(1400 - 2000) (2700 - 3000)

Table S1b Summary of Pre-processing methods and wavenumber regions selected for T-FT-NIR

<i>Component</i>	<i>Sample Treatment</i>	<i>Rank</i>	<i>Pre-processing Method</i>	<i>Wavenumber Regions</i>
Anthocyanins (mg/L)	Filtered	4	Baseline (Automatic Weighted Least Squares)	(5800-6000) (7000 - 7050)
Anthocyanins (mg/L)	Untreated	4	Baseline (Automatic Weighted Least Squares)	5800 -6000
Colour Density	Filtered	5	Baseline (Automatic Whittaker Filter)	(5800-6200) (7000 -8000)
Colour Density	Untreated	5	Median Centering	(5800 - 6200) (8000 - 8400) (10000 - 11400)
Polymeric Pigments (mg/L)	Filtered	3	Min-Max Scaling	(5800 -6200)
Polymeric Pigments (mg/L)	Untreated	4	Median Centering	(5800 - 6200) (8000 - 8400)
Tannins (mg/L)	Filtered	2	Baseline (Automatic Weighted Least Squares)	(6000 -6200) (8500 - 9500) (10000 -10200)
Tannins (mg/L)	Untreated	7	MSC	(5800 -6200)
Total polyphenol index	Filtered	4	Baseline (Automatic Weighted Least Squares)	(5800 - 6200) (7000 -8000)
Total polyphenol index	Untreated	3	Baseline (Automatic Weighted Least Squares)	4000 - 11400

Table S1c Summary of Pre-processing methods and wavenumber regions selected for DR-FT-NIR

<i>Component</i>	<i>Sample Treatment</i>	<i>Rank</i>	<i>Pre-processing Method</i>	<i>Wavenumber Regions</i>
Anthocyanins (mg/L)	Filtered	9	Multiway Scale	4100 - 12000
Anthocyanins (mg/L)	Turbid	8	Multiway Scale	4000-12000
Colour Density	Filtered	7	Baseline (Automatic Whittaker Filter)	4100 - 12000
Colour Density	Turbid	7	Multiway Scale	4000-12000
Polymeric Pigments (mg/L)	Filtered	7	Autoscale	4000-12000
Polymeric Pigments (mg/L)	Turbid	3	2nd Derivative	4000-12000
Tannins (mg/L)	Filtered	6	Detrend	4000-12000
Tannins (mg/L)	Turbid	6	Detrend	4000-12000
Total polyphenol index	Filtered	8	Multiway Scale	4100 - 12000
Total polyphenol index	Turbid	7	Min-Max Scaling	4100 - 12000