

Analysis	Min. volume	Method	Instrument	Matrix types
Esters, alcohols, acetates	20 mL	Targeted	GCMS	Wine, Yeast slurry, Bacteria (broth/OJ)
Esters, alcohols, acetates + other unknown volatiles detected	20 mL	Non-targeted (Volatile profiling)		
Amino acids, Biogenic amines	2 mL	Targeted	LC-MS/MS	Wine/juice, Fruit extracts
Resveratrol	5 mL	Targeted	LC-MS/MS	Plasma
Organic acids	500 uL	Targeted	LC-MS/MS	Fruit extracts, Plant extracts
Acetaldehyde, acetoin	20 mL	Targeted	GCMS	Wine, Yeast slurry
Volatile fatty acids	20 mL	Targeted	GCMS	Wine, Yeast slurry
Raspberry ketone and intermediates	10 mL	Targeted	LC-MS/MS	Ferment media
Oak/guaiacol glyconjugates	2 mL/5g	Targeted	LC-MS/MS	Grape, Juice, Wine, Leaf, stem
Phenolics (non-polar metabolites)	10 mL	Non-targeted	LC-MS/MS	Wine, Juice, Microalgae, Macroalgae (seaweed),
Carbohydrates, amino acids, TCA intermediates, nucleotides, lipids	5 mL	Non-targeted	GCMS	Wine, Juice, Urine, Microalgae
	5 mL	Non-targeted	LC-MS/MS	Wine, Juice, Urine, Microalgae
High Resolution Accurate mass	200uL 1mg/L	Direct infusion	MS (QTOF)	Isolated compound