

Gas Chromatography-Mass Spectrometry-Based Targeted Metabolomics of Hard Coral Samples

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Materials

Name	Company	Catalog Number	Comments
100% LC-grade methanol	Merck	439193	LC grade essential
2 mL microcentrifuge tubes, PP	Eppendorf	30121880	Polypropylene provides high resistance to chemicals, mechanical stress and temperature extremes
2030 Shimadzu gas chromatograph	Shimadzu	GC-2030	
710-1180 µm acid-washed glass beads	Merck	G1152	This size is optimal for breaking the Symbiodiniaceae cells
AOC-6000 Plus Multifunctional autosampler	Shimadzu	AOC6000	
Bradford reagent	Merck	B6916	Any protein colourimetric reagent is acceptable
Compressed air gun	Ozito	6270636	Similar design acceptable. Having a fitting to fit a 1 mL tip over is critical.
DB-5 column with 0.25 mm internal diameter column and 1 µm film thickness	Agilent	122-5013	
DMF	Merck	RTC000098	
D-Sorbitol-6- ¹³ C and/or ¹³ C ₅ - ¹⁵ N Valine	Merck	605514/ 600148	Either or both internal standards can be added to the methanol.
Flat bottom 96-well plate	Merck	CLS3614	
Glass scintillation vials	Merck	V7130	20 mL, with non-plastic seal
Immunoglobulin G	Merck	56834	if not available, Bovine Serum Albumin is acceptable
Primer		v4	
R		v4.1.2	
Shimadzu LabSolutions Insight software		v3.6	
Sodium Hydroxide	Merck	S5881	Pellets to make 1 M solution
tidyverse		v1.3.1	R package
TissueLyser LT	Qiagen	85600	Or similar

TQ8050NX triple quadrupole mass spectrometer	Shimadzu	GCMS-TQ8050 NX	
UV-96 well plate	Greiner	M3812	
Whirl-Pak sample bag	Merck	WPB01018WA	Sample collection bag; Size: big enough to house a ~5 cm coral fragment, but not too big that the water is too spread