

Materials List for:

Untargeted Liquid Chromatography-Mass Spectrometry-Based Metabolomics Analysis of Wheat Grain

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Materials

Name	Company	Catalog Number	Comments
13C6-sorbitol	Merck Sigma-Aldrich	605514	
2-aminoanthracene	Merck Sigma-Aldrich	A38800-1 g	
Acetonitrile	ThermoFisher Scientific	FSBA955-4	Optima LC-MS grade
Ammonium formate	Merck Sigma-Aldrich	516961-100 mL	>99.995%
Analyst TF	Sciex		Version 1.7
AnalyzerPro software	SpectralWorks Ltd.		Data processing software used for step 7.2. Version 5.7
AnalyzerPro XD software	SpectralWorks Ltd.		Data processing software used for step 7.5. Version 1.4
Balance	Sartorius. Precision Balances Pty. Ltd.		
d6-transcinnamic acid	Isotec	513962-250 mg	
Formic acid	Ajax Finechem Pty. Ltd.	A2471-500 mL	99%
Freeze dryer (Freezone 2.5 Plus)	Labconco	7670031	
Glass Schott bottles (100 mL, 500 mL, 1 L)			
Glass vials (2 mL) and screw cap lids (pre-slit)	Velocity Scientific Solutions	VSS-913 (vials), VSS-SC91191 (lids)	
Installation kit for Sciex TripleToF	Sciex	p/n 4456736	
Isopropanol	ThermoFisher Scientific	FSBA464-4	Optima LC-MS grade
Laboratory blender	Waring commercial		Model HGBTWTS3
Leucine-enkephalin	Waters	p/n 700008842	Tuning solution
Metaboanalyst	https://www.metaboanalyst.ca/MetaboAnalyst/faces/home.xhtml		Web-based analytical pipeline for high-throughput metabolomics. Free, web-based tool. Version 4.0.
Methanol	ThermoFisher Scientific	FSBA456-4	Optima LC-MS grade
Miconazole	Merck Sigma-Aldrich	M3512-1 g	
Microcentrifuge (Eppendorf 5415R)	Eppendorf (Distributed by Crown Scientific Pty. Ltd.)		5426 No. 0021716
Microcentrifuge tubes (2 mL)	SSlbio	1310-S0	
Microsoft Office Excel	Microsoft		
Peak View software	Sciex		Version 1.2 (64-bit)

Pipette tips (200 μ L, 100 μ L)	ThermoFisher Scientific	MBP2069-05-HR (200 μ L), MBP2179-05-HR (1000 μ L)	
Pipettes (200 μ L, 1000 μ L)	ThermoFisher Scientific		
Plastic centrifuge tubes (15 mL)	ThermoFisher Scientific	NUN339650	
Progenesis QI	Nonlinear Dynamics		Small molecule discovery analysis software. Version 2.3 (64-bit)
Sciex 5600 triple ToF mass spectrometer	Sciex		
Screw-cap lysis tubes (2 mL) with ceramic beads	Bertin Technologies		
Sodium formate	Merck Sigma-Aldrich	456020-25 g	
Tissue lyser/homogeniser	Bertin Technologies		Serial 0001620
Volumetric flasks (10 mL, 50 mL, 100 mL, 200 mL, 1 L)			
Vortex mixer	IKA Works Inc. (Distributed by Crown Scientific Pty. Ltd.)		001722
Water	ThermoFisher Scientific	FSBW6-4	Optima LC-MS grade
Water's Acquity LC system equipped with quaternary pumps	Waters		
Water's Aquity UPLC 100mm HSST3 C18 column	Waters	p/n 186005614	