

Materials List for:

Single-throughput Complementary High-resolution Analytical Techniques for Characterizing Complex Natural Organic Matter Mixtures

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Materials

Name	Company	Catalog Number	Comments
methoxyamine hydrochloride	Sigma Aldrich	226904	derivitization agent
5 mm triple resonance salt-tolerant cold probe	Bruker		instrumentation
capillary GC column HP-5MS column (30 m × 0.25 mm × 0.25 μm)	Agilent	AG19091S-433	instrumentation
reversed phase charged surface hybrid column (3.0 mm × 150 mm × 1.7 μm particle size)	ThermoFisher		instrumentation
2 mL glass vials	VWR International	46610-722	sample vials
autosampler vials	VWR International	97055-324; 9467671	sample vials
Chloroform	VWR International	JT9174-3	solvent
Ethanol	VWR International	BDH67002.400	solvent
methanol	VWR International	BDH85681.400	solvent
pyridine	VWR International	BDH67007.400	solvent
2,2-dimethyl-2-silapentane-5-sulfonate-d6	Sigma Aldrich	178837	standard
C8-C24 fatty acid methyl ester	Sigma Aldrich	CRM18918	standard
N-methyl-N-(trimethylsilyl)trifluoroacetamide	Sigma Aldrich	24589-78-4	standard
Suwanee River Fulvic Acid standard	International Humic Substances Society	2S101F	standard
trimethylchlorosilane	Sigma Aldrich	89595	standard
Tuning Solution	Agilent		
FTICR-MS analysis software	Bruker	Compass DataAnalysis 4.1	
Formularity Software	Pacific Northwest National Laboratory	Formularity	available for download at: https://omics.pnl.gov/software/formularity
GC-MS	Agilent	Agilent GC 7890A with MSD 5975C	
silica-based sorbent	Phenomenex (Torrance, CA)	Strata C18-E (PN 8E-S001-DAK)	
NMR TUBE 3MM 8 150 CS5	VWR International	KT897820-0008	NMR tube
Varian Direct Drive 600-MHz NMR spectrometer	Varian Inova	Varian Direct Drive 600-MHz	NMR spectrometer

Chenomx NMR Suite 8.3	Chenomx	Chenomx NMR Suite	NMR software
ultra-performance liquid chromatograph	waters	Aquity UPLC H	liquid chromatograph
Velos-ETD Orbitrap mass spectrometer	ThermoFisher	Thermo Scientific LTQ Orbitrap Velos	mass spectrometer