Supplementary Table 1. Examples of published data describing the separation and identification of archaeal lipids by LC-MS.

Column	Stat. phase	Mobil. phase	Detection	Interval (m/z)	Type of Compounds	Sample	Ref.
150 mm × 2.1 mm, 3 µm	cyano	linear gradient, 45 min, hexane to propanol	$APCI^+$	950–1450	GDGTs	sediment	[146]
150 mm × 3.9 mm	C18	isocratic 95:5 methanol:0.1M ammonium acetate	ESI^-, $APCI^-$	700–1200	archaeol phosphatidylglycerol, phosphatidylglycerylsulphate, phosphatidylglycerylphosphate, etc	*Halorubrum lacusprofundi*	[168]
150 mm × 2.1 mm, 3 µm	cyano	linear gradient A (n-hexane/isopropanol, 99:1, v/v) to B (n-hexane/isopropanol, 90:10, v/v) in 55 min	$APCI^+$	100–2000	di- and tetraethers	*Methanococcus thermolithotrophicus, Methanopyrus kandleri,* peat bog, marine sediments	[156]
150 mm × 2.1 mm, 3 µm	C18	gradient A (MeOH/HCOOH/14.8 M NH3) to B propan-2-ol/HCOOH/14.8 M NH3 (~1 h)	ESI^+	100–2000	GDGTs of PC, PG, PS, 1G, 2G, P1G	sediments: Mediterranean Sea, the Black Sea, the Sea of Marmara, the Peruvian margin and a cold seep off Pakistan	[145]
150 mm × 2.1 mm, 5 µm	diol	A=hexane/propan-2-ol/HCO2H/14.8 M NH3 to B=propan-2-ol/water/HCO2H/14.8 M NH3	ESI^+	100–2000	GDGTs of PC, PG, PS, 1G, 2G, P1G	sediments: Mediterranean Sea, the Black Sea, the Sea of Marmara, the Peruvian margin and a cold seep off Pakistan	[145]
150 mm × 2.1 mm, 3 µm	cyano	gradient A=hexane/propan-2-ol (99:1) to B=hexane/propan-2-ol (90:10)	ESI^+	100–2000	GDGTs of PC, PG, PS, 1G, 2G, P1G	sediments: Mediterranean Sea, the Black Sea, the Sea of Marmara, the Peruvian margin and a cold seep off Pakistan	[145]

150 mm × 2.1 mm, 3 µm	cyano	linear gradient A to B, A (n-hexane) and B (n-hexane/ isopropanol, 55 min	APCI$^+$	100–1700	GDGTs	expression tetraether synthase, *Sulfolobus acidocaldarius, Methanococcus maripaludis*	[228]
150 mm × 2.1 mm, 1.7 µm	C18	linear gradient, A (5 mM ammonium formate in water/acetonitrile 40:60, v/v) to B (5 mM ammonium formate in acetonitrile/1-butanol, 10:90, v/v), 25 min	ESI$^-$	probably to 2000?	mixed cardiolipins (glycerol-archaetidylphosphatidyl-, glycerol-diphosphatidyl-, glycerol-di-archaetidyl)	overexpressed cardiolipin synthase from *Methanospirillum hungatei* to *E. coli*	[227]
250 mm × 4.6 mm, 5 µm	NH_2	linear gradient hexane-propan-2-ol (99/1 v/v)	APCI$^+$	1280–1320	tetraether lipid cores	*Methanobacter thermautotrophicus*	[226]
250 mm × 4.6 mm, 5 µm	NH_2	gradient hexane:isopropanol	APCI$^+$	900–1500	GDGTs	*Sulfolobus acidocalarius, S. shibatae, S. solfataricus, Ignisphaera, Pyrobaculum, Desulfurococcus* sp. + sediments	[218]
150 mm × 2.1 mm, 1.7 µm 150 mm × 2.1 mm, 1.7 µm 150 mm × 2.1 mm, 1.7 µm 150 mm × 2.1	C18 C8 pentafluorophenyl phenyl-hexyl	A: MeOH with 0.04% HCOOH B: propan-2-ol with 0.04% HCOOH gradient 60%:40% A:B to 50% B at 20 min.	APCI+, ESI	?	GDGT isomers	marine and lacustrine sediments, peat bog soils	[275]

mm, 1.7 µm							
150 mm × 2.1 mm, 3 µm	cyano	linear gradient A (hexane/propanol (99:1, v/v)) to B (hexane/propanol (90:10, v/v), 1 h	APCI+, ESI	SIM at different *m/z* 741.2-744.8, 1016.5-1023.5, 1030.5-1037.5, 1044.5-1051.1, 1287.2-1304.8, etc.	GDGT isomers	marine and lacustrine sediments, peat bog soils	[275]
150 mm × 2.1 mm, 3 µm	cyano	linear gradient A (n-hexane) to B (isopropanol) 99% A and 1% B to 10% B, 40 min	$APCI^{+}$	SIM at different *m/z* 1295.0, 1302.1, 1049.5, 1035.5, 1021.5, 654.2	GDGTs	early Miocene terrestrial to lacustrine sediments	[276]
125 mm × 2 mm, 5µm	diol	linear gradient A (n-hexane:isopropanol:formic acid:ammonia (25% in water) 79:20:1.2:0.04 v/v to B (isopropanol:water:formic acid:ammonia (25% in water) 88:10:1.2:0.04 v/v), 20 min	ESI^{-}	400–2,000	intact polar lipids	early Miocene terrestrial to lacustrine sediments	[276]
150 mm × 2.1 mm, 3 µm	cyano	linear gradient A (hexane) and B (propanol), A:B (99:1) to (98.2:1.8), 45 min	$APCI^{+}$	950–1450	GDGTs	sediment Congo River	[180]

150 mm × 2.1 mm, 1.7 µm	C18	A was MeOH:H2O 85:15 (v:v), 0.04% formic acid, 0,1% NH4OH, mobile phase B isopropanol:- MeOH 50:50 (v:v), 0.04% formic acid, 0.1% NH4OH	ESI^+	?	geranylgeranylglycerol (GGG), acetylated Ac-GGG, double acetylated Ac2-GGG	*Haloferax volcanii* and *Halobacterium salinarum*	[185]
150 mm × 3.9 mm	C18	95% methanol and 5% 0.1M ammonium acetate	ESI^-	700–1200	archaeol and hydroxyarchaeol phosphatidylglycerol and phosphatidylinositol	*Methanococcoides burtonii*	[158]
250 mm × 2.1 mm, 5 µm	diol	nonlinear gradient, see paper	ESI^+, ESI^-	650–2000	GDGTs with polar heads-phosphatidyl inositol, glycosylated phosphatidyl hexose, dihexose, etc.	*Pyrococcus furiosus, P. yayanosii, Thermococcus kodakarensis*	[165]
150 mm × 2.1 mm, 3 µm	cyano	linear gradient A:B (99:1) to 1.8% B (98.2:1.8), 45 min A (hexane) and B (2-propanol)	$APCI^+$	SIM at *m/z* 950–1450	GDGTs	sediment core from the Arabian Sea	[159]
250 mm × 2.1 mm, 5 µm	diol	gradient A:B (100:0) to A:B (35:65), 20 min A (hexane-isopropanol-formic acid-14.8M NH3, 79:20:0.12:0.04) B (isopropanol-water-formic acid-aqueous 14.8 M NH3, 88:10:0.12:0.04)	ESI^+	1000–2000	GDGTs and GDGTs with polar heads: hexose, dihexose, phosphohexose, hexose+phosphohexose	candidatus *Nitrosopumilus maritimus*	[169]
?	C18	linear gradient, ethyl acetate and acetonitrile/water, 9:1 v/v, 35 min	ESI^+, HPLC–diode array detector	300–900	bisanhydrobacterioruberin, bacterioruberin, monoanydrobacterioruberine, etc.	*Halogeometricum borinquense, Haloferax volcanii, Haloarcula marismortui* hypersaline lakes in Algeria	[244]

PC, phosphocholine; PG, phosphoglycerol; PS, phosphoserine; 1G, monoglycosyl; 2G, diglycosyl; P1G, phosphomonoglycosyl of GDGTs

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