Supplements

Table 1S. The number of possible TAGs.

Description	Number of possible TAGs	Number of possible TAGs for y = 11
without isomers	$x = (y^3 + 3y^2 + 2y)/6$	286
without enantiomers	$x = (y^2 + y^3)/2$	726
all isomers	$x = y^3$	1331

where x is the number of TAGs, y is the number of FAs in TAGs

Table 2S. Survey of literature data on the separation of TAGs on chiral columns. References not listed in the main article text are given below.

Reference	Column type	Mobile phase; temperature/infusion solvent/ matrix	Ion source analyzer	Mass range(m/z)	Samples matrix
[28]	Chiracel OF cellulose-tris-(4-chlorphenylcarbamate)	hexane/iPrOH(200/1 or 400/1)	UV, 210 nm		
	Chiracel OD cellulose-tris-(3,5-dimethylphenylcarbamate)	hexane/iPrOH(200/1 or 400/1)	UV, 210 nm		
[11]	Two chiral Lux Cellulose-1	gradient 90% hexane and 10% hexane/iPrOH(99/1, *v*/*v*)	positive-ion APCI mode	50-1200	TAG-regioisomers + enantiomers of hazelnut oil + human plasma
[29]	Chiralpak IA amylose tris-(3,5-dimethylphenyl carbamate)	hexane/ethanol (100/0.5, *v*/*v*); or hexane/iPrOH(100/0.5, *v*/*v*) or methanol or acetonitrile	positive ion APCI mode	500-1000	TAG-enantiomers
[10]	Chiracel OD-RH (or OD-H) cellulose tris-(3,5-dimethylphenylcarbamate)	methanol	positive ion APCI mode	500-1000	TAG-enantiomers from marine fish and mammals
[30]	CYCLOBOND™ I 2000 DMP 3,5-dimethylphenyl carbamate modified β-cyclodextrin	99:1 methanol:10 mM ammonium acetate	positive ion APCI mode	200-1000	diatom *Phaeodactylum tricornutum* + synthetic standards
[31]	two CYCLOBOND™ I 2000 DMP 3,5-dimethylphenyl carbamate modified β-cyclodextrin	gradient 90% hexane and 10% hexane/iPrOH (99:2, *v*/*v*) to 50% hexane and 50% hexane/iPrOH 120 min	positive ion APCI mode	200-1100	11 yeast strains
[32]	two Astec CYCLOBOND™ I 2000 DMP (3,5-dimethylphenyl carbamate modified β-cyclodextrin)	gradient 90% hexane and 10% hexane/iPrOH(99:2, *v*/*v*) to 50% hexane and 50% hexane/iPrOH 180 min	positive ion APCI mode	200-1100	microalgae
[33]	Astec CYCLOBOND™ I 2000 DMP (3,5-dimethylphenyl carbamate modified β-cyclodextrin)	gradient 90% hexane and 10% hexane/iPrOH(99:2, *v*/*v*) to 50% hexane and 50% hexane/iPrOH 120 min	positive-ion APCI mode	200-1100	TAGs in different strains of the green alga *Stichococcus bacillaris*
[17]	two Astec cyclobondTM I 2000 DMP (3,5-dimethyl-phenyl-carbamate modified β-	gradient 90% hexane and 10% hexane/iPrOH(99:2, *v*/*v*) to 50% hexane and 50% hexane/iPrOH	positive-ion APCI mode	200-1100	TAG-regioisomers + enantiomers of C16, C18 and C20 PUFAs

	cyclodextrin)	180 min			
[19]	two Astec cyclobond™ I 2000 DMP (3,5-dimethyl-phenyl-carbamate modified β-cyclodextrin)	gradient 90% hexane and 10% hexane/iPrOH(99:2, *v*/*v*) to 50% hexane and 50% hexane/iPrOH 180 min	positive-ion APCI mode	200-1000	TAG-regioisomers + enantiomers of *Trachydiscus minutus* (PUFAs)
[18]	Astec cyclobond™ I 2000 DMP (3,5-dimethyl-phenyl-carbamate modified β-cyclodextrin)	gradient 90% hexane and 10% hexane/iPrOH(99:2, *v*/*v*) to 50% hexane and 50% hexane/iPrOH 180 min	positive-ion APCI mode	200-1100	Odd-TAG regioisomers + enantiomers of *Khawkinea quartana* + *Mortierella alpina*

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Table 3S. The effect of salinity on the representation of FAs in *Coccolithophora* sp.

FA	Abbreviations	7.5‰	15‰	30‰	45‰	60‰
14:0	M	7.5	2.6	1.4	6.3	11.0
16:1ω-7	Po	4.9	9.2	9.6	4.9	2.0
16:0	P	23.2	13.7	15.1	21.7	26.6
18:5ω-3	Op	8.3	11.2	12.3	10.6	8.3
18:4ω-3	St	21.1	26.0	18.3	14.8	10.7
18:3ω-3	Ln	4.0	6.4	5.0	3.7	2.7
18:2ω-6	L	2.2	2.4	7.0	5.3	3.7
18:1ω-9	O	3.7	7.2	8.6	6.0	4.4
18:0	S	13.0	4.6	2.6	12.5	19.1
20:5ω-3	E	3.1	4.3	5.1	2.9	3.2
22:5ω-3	Dp	2.1	3.2	4.1	3.1	2.2
22:6ω-3	D	6.9	9.2	10.9	8.2	6.1