

Table 1S – Peak attributions of lipid extracts ¹H NMR spectra.

Chemical shift assignments of ¹H NMR signals indicated in Figure 5. Abbreviations: s, singlet; d, doublet; t, triplet; m, multiplet.

Peak	Chemical shift, δ (ppm)	Multiplicity	Proton/ Functional group	Attribution	Reference
a, a'	0.07	s	CH ₃ [Si(CH ₃) ₂ O] _n Si(CH ₃) ₃	Silicone grease: Polydimethylsiloxane (PDMS)	Gottlieb et al., 1997
b, b'	0.50-0.60	m			
C, c'	0.60-0.69	Broad signal			
D, d'	0.88	t	-CH ₃	Terminal methyl protons in every acyl chain	Vlahov 1999
E, e'	0.92-0.99	Broad signal	-CH ₃	¹³ C satellite of signal at 0.88 ppm	Alonso-Salces et al., 2012
F, f'	1.00-1.16	Broad signal			
G, g'	1.25		-CH ₂ -	Methylene envelop of various compounds	Vlahov 1999
h	1.36				

i, i'	1.59		-OCO-CH ₂ -CH ₂ -	H-3 protons of acyl moieties in acylglyceric or ester compounds	Vlahov 1999
j, j'	2.01	Broad signal	=CH-CH ₂ -	Allylic methylenes	Vlahov 1999
k, k'	2.29	m	i) HOOC-CH ₂ - ii) -CO-CH ₂ -	i) Methylene protons adjacent to a carboxylic group ii) H-2 protons of acyl moieties in acylglyceric or ester compounds	Alonso-Salces et al., 2012 Vlahov 1999
l, l'	3.22/3.28/3.18	Broad signal			
m	3.65	d	-CH ₂ OH	Glyceryl group in DAGs	Alonso-Salces et al., 2012
n, n'	3.90-4.04	Broad signal			
o, o'	4.05-4.23	m	CH-OH -CH ₂ -OR	Glycerol group in DAGs H-1/H-3 proton of glycerol group TAG	Almoselhy 2014 Vlahov 1999
p, p'	4.30-4.44	d	-CH ₂ -OR	H-1/H-3 proton of glycerol group TAG	Vlahov 1999
q	5.10	m			

r, r'	5.16-5.26	Broad signal	>CH-OR	H-2 proton in TAGs	Vlahov 1999
s, s'	5.29	t	=CH-	All UFA	Vlahov 1999
t, t'	7.26 (not shown)			CDCl ₃ solvent residual peak	Gottlieb et al., 1997
