Supplements

Enantiomeric separation of very long chain fatty acids and very long-chain polyunsaturated fatty acids

Tomáš Řezanka[a], Irena Kolouchová[b], Linda Nedbalová[c], Karel Sigler[a]

[a] Institute of Microbiology of the Czech Academy of Sciences, Vídeňská 1083, 142 20 Prague 4, Czech Republic

[b] Department of Biotechnology, University of Chemistry and Technology Prague, Technická 5, 166 28 Prague, Czech Republic

[c] Charles University, Faculty of Science, Department of Ecology, Viničná 7, 128 44 Prague 2, Czech Republic

Table 1S. The number of possible TAGs from ximenia oil.

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 1S. Analysis of TAGs on reverse phase column, including retention time, equivalent carbon number (ECN), acyl carbon number (ACN), double bond(s) (DB) a formula.

tR	ACN	DB	ECN	TAG
79.0	60	6	48	24:1/18:2/18:3[a]
86.8	60	5	50	24:1/18:2/18:2[a,c]
94.8	60	4	52	24:0/18:2/18:2[b,c]
95.5	60	4	52	24:1/18:1/18:2[a,c]
97.8	60	4	52	24:1/18:2/18:1[b]
99.1	58	3	52	24:1/18:2/16:0[b]
100.4	60	4	52	24:0/18:1/18:3[b]
101.3	62	7	48	26:1/18:3/18:3[a]
101.6	58	3	52	24:0/18:3/16:0[b]
104.4	60	3	54	24:1/18:2/18:0[b]
104.8	58	2	54	24:1/18:1/16:0[b]
106.3	60	3	54	24:0/18:3/18:0[b]
106.4	58	2	54	24:0/18:2/16:0[b]
106.7	60	3	54	24:0/18:1/18:2[b,c]
107.2	58	2	54	24:0/18:1/16:1[b]
107.6	60	3	54	24:1/18:1/18:1[a,b,c]
108.2	56	1	56	24:0/16:1/16:0[b]
109.4	60	2	56	24:1/18:1/18:0[b]
110.6	64	5	54	28:1/18:2/18:2[c]
110.8	60	2	56	26:0/18:2/16:0[b]
111.0	60	2	56	24:0/18:2/18:0[b]
111.2	58	1	56	24:0/18:1/16:0[b]
112.5	60	2	56	24:0/18:1/18:1[b,c]
113.3	62	5	52	26:1/18:1/18:3[a]
114.6	62	5	52	26:1/18:2/18:2[b,c]
115.2	62	4	54	26:0/18:1/18:3[b]
117.7	62	3	56	24:1/18:1/20:1[b]
118.9	62	4	54	26:0/18:2/18:2[c]
119.8	62	4	54	26:1/18:1/18:2[c]
124.2	62	3	56	26:0/18:1/18:2[b,c]
125.4	62	3	56	26:1/18:1/18:1[a,c]
126.3	64	4	56	28:1/18:1/18:2[c]
128.7	66	5	56	30:1/18:2/18:2[c]
131.4	62	2	58	26:0/18:1/18:1[b,c]
140.3	64	3	58	28:1/18:1/18:1[c]
144.1	66	4	58	30:1/18:1/18:2[c]
160.2	66	3	60	30:1/18:1/18:1[c]

[a] present in alga

[b] present in yeast

[c] present in ximenia oil

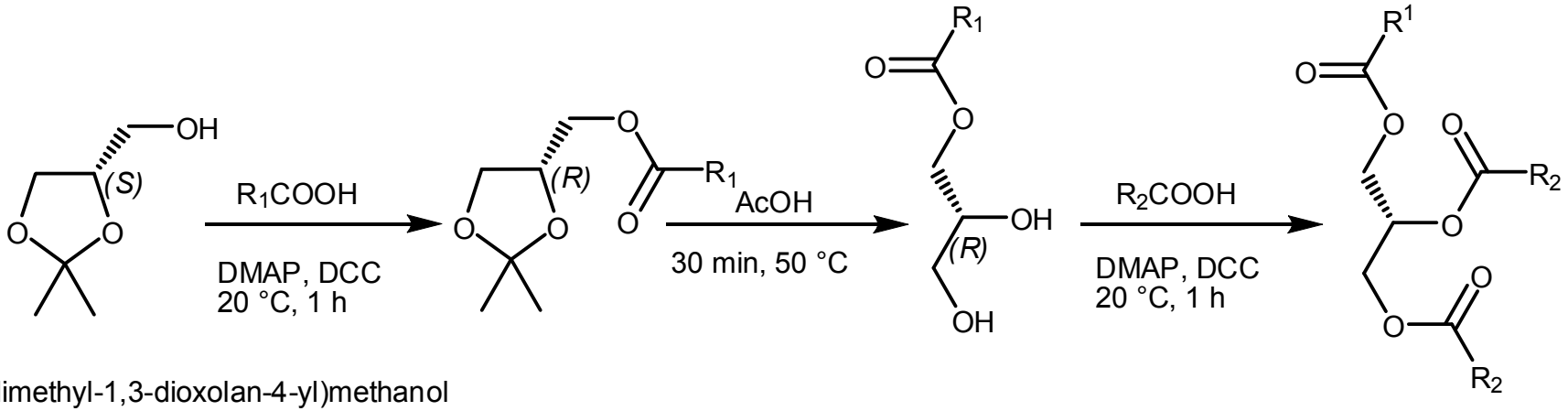
Table 2S. Description of tandem mass spectra of four TAGs (synthetic *sn*-18:1/18:1/24:1, natural *sn*-18:1/18:1/24:1, natural *sn*-24:1/18:1/18:1, and natural sn-18:1/24:1/18:1).

m/z	synthetic *sn*-18:1/18:1/24:1	natural *sn*-18:1/18:1/24:1	natural *sn*-24:1/18:1/18:1	natural *sn*-18:1/24:1/18:1	Ion Description
247.2420	8	7	8	9	sn-2 or sn-3 acyl chain ($[RC=O]^+$ with loss of H_2O)
265.2526	13	12	11	10	sn-2 or sn-3 acyl chain ($[RC=O]^+$)
321.2788	14	13	14	14	sn-2 or sn-3 acyl chain ($[RC=O+74]^+$ with loss of H_2O)
331.3359	14	15	16	15	sn-1 acyl chain ($[RC=O]^+$ with loss of H_2O)
339.2894	13	12	14	13	sn-2 or sn-3 acyl chain ($[RC=O+74]^+$)
349.3465	14	15	17	16	sn-1 acyl chain ($[RC=O]^+$)
405.3727	11	12	14	13	sn-1 acyl chain ($[RC=O+74]^+$ with loss of H_2O)
423.3833	17	18	19	21	sn-1 acyl chain ($[RC=O+74]^+$)
603.5347	66	65	63	25	Neutral loss of RCOOH (nervonic) + NH_3 from $[M+NH_4]^+$
687.6286	100	100	100	100	Neutral loss of RCOOH (oleic) + NH_3 from $[M+NH_4]^+$
951.8739	20	19	21	20	Precursor ion $[M+H]^+$ with loss of H_2O
969.8845	9	9	8	8	Precursor ion $[M+H]^+$
986.9110	33	35	33	34	Precursor ion $[M+NH_4]^+$

Table 3S. Identification of TAGs from ximenia oil.

Peak No.	RT	TAG	ACN	DB	ECN	[M+NH4]+	%
a	86.8	24:1/18:2/18:2	60	5	50	982.8797	15.4
b	94.8	24:0/18:2/18:2	60	4	52	984.8954	3.8
c	95.5	24:1/18:1/18:2	60	4	52	984.8954	23.0
d	106.7	24:0/18:1/18:2	60	3	54	986.9106	6.4
e	107.6	24:1/18:1/18:1	60	3	54	986.9106	35.8
f	110.6	28:1/18:2/18:2	64	5	54	1038.9409	70.4
g	112.5	24:0/18:1/18:1	60	2	56	988.9267	9.0
h	114.6	26:1/18:2/18:2	62	5	52	1010.9116	34.6
i	118.9	26:0/18:2/18:2	62	4	54	1012.9272	23.0
j	119.8	26:1/18:1/18:2	62	4	54	1012.9272	47.4
k	124.2	26:0/18:1/18:2	62	3	56	1014.9429	28.2
l	125.4	26:1/18:1/18:1	62	3	56	1014.9429	61.4
m	126.3	28:1/18:1/18:2	64	4	56	1040.9585	100.0
n	128.7	30:1/18:2/18:2	66	5	56	1068.9898	17.9
o(s)	131.4	26:0/18:1/18:1	62	2	58	1016.9585	38.4
p	140.3	28:1/18:1/18:1	64	3	58	1042.9721	73.0
q	144.1	30:1/18:1/18:2	66	4	58	1071.0055	26.9
r	160.2	30:1/18:1/18:1	66	3	60	1070.9993	41.0
t	171.8	26:1/26:1/18:2	70	4	62	1125.0524	9.0
u	179.6	26:1/26:1/18:1	70	3	64	1127.0681	5.1
v	192.1	28:1/26:1/18:1	72	3	66	1155.0990	2.6
w(z)	196.4	28:1/28:1/18:2	74	4	66	1181.1151	3.8
x	219.7	28:1/28:1/18:1	74	3	68	1183.1252	9.0
y	232.8	30:1/28:1/18:1	76	3	70	1211.1622	2.6

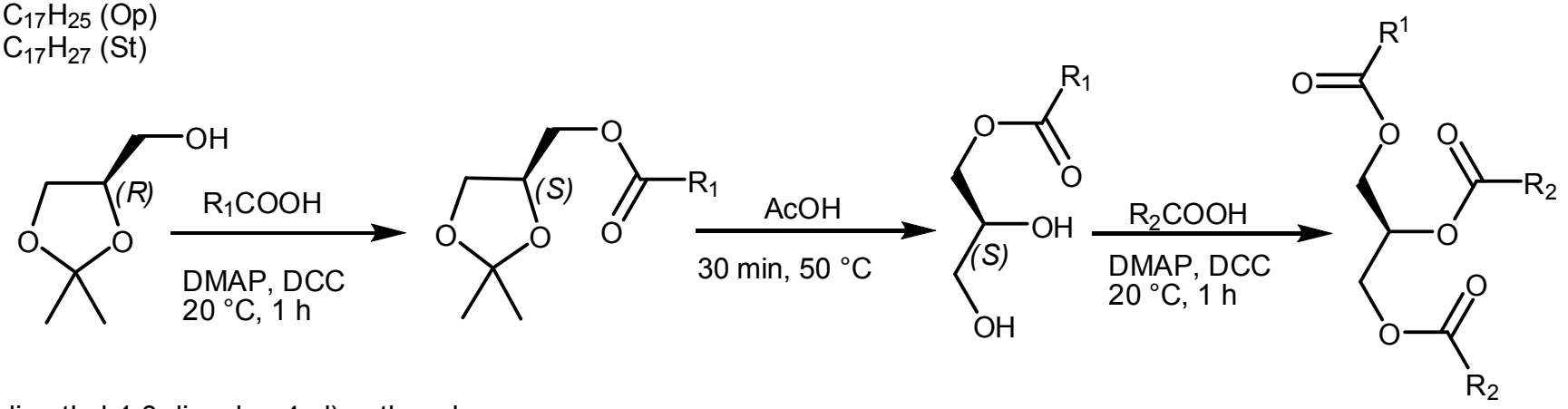
Fig. 1S. Synthesis of enantiomers by stereospecific esterification of 1,2- and 2,3-isopropylidene-*sn*-glycerols.



(*S*)-(2,2-dimethyl-1,3-dioxolan-4-yl)methanol

1,2-isopropylidene-sn-glycerol

$R_1 = C_{17}H_{25}$ (Op)
$R_2 = C_{17}H_{27}$ (St)



(*R*)-(2,2-dimethyl-1,3-dioxolan-4-yl)methanol

2,3-Isopropylidene-sn-glycerol

Fig. 2S.
Retention times of molecular species of synthetic *sn*-3-acyl-1,2-dioleins.

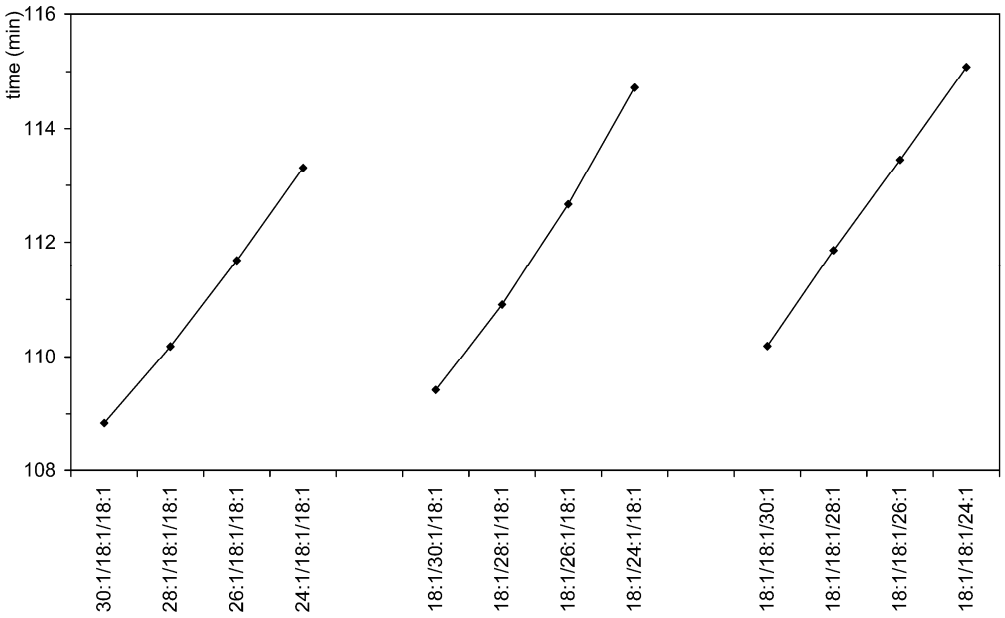


Fig. 3S.
Retention times of molecular species of synthetic *sn*-3-acyl-1,2-dilinoleins.

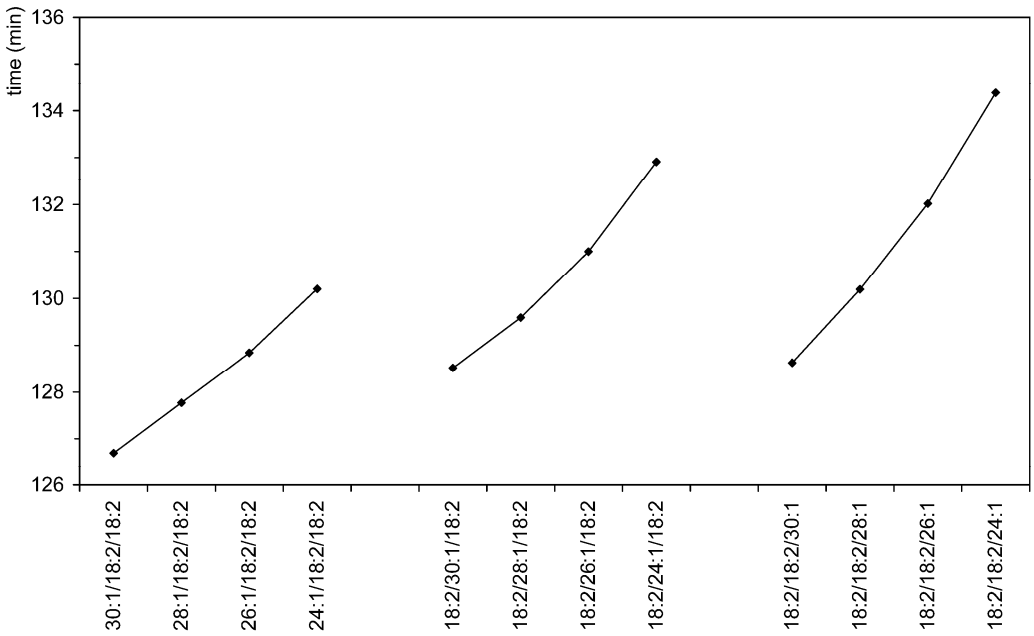


Fig. 4S.
A model of *sn*-28:8/28:8/28:7 TAG.