

Supplementary information

Regioisomeric Characterization of Triacylglycerols Using Silver-Ion HPLC/MS and Randomization Synthesis of Standards

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Number of tables: 1

Number of figures: 3

Table S1. Basic retention characteristics of all TGs identified in analyzed plant oils (sunflower, blackcurrant, olive and palm) and animal fat (lard) ^a

TG	DB ^b	[M+H] ⁺	Retention time	Relative retention ^c
			[min]	
ASP ^d	0	891	17.6	0.861
SSP ^d		863	17.9	0.899
SPP ^d		835	18.3	0.949
PPP		807	18.7	1.000
SPM ^d		807	18.7	1.000
LgOP	1	945	36.6	0.945
BOS		945	36.6	0.945
BOP		917	36.9	0.956
AOS		917	36.9	0.956
AOP		889	37.3	0.971
SOS		889	37.3	0.971
SOMa		875	37.5	0.978
SOP		861	37.7	0.985
POMa		847	37.9	0.993
POP		833	38.1	1.000
LgPO ^d		945	38.3	1.007
BSO ^d		945	38.3	1.007
POM		805	38.4	1.011
BPO ^d		917	38.6	1.018
ASO ^d		917	38.6	1.018
APO ^d		889	38.9	1.029
SSO		889	38.9	1.029
SMaO ^d		875	39.1	1.037
SPO ^d		861	39.3	1.044
SPMo ^d		847	39.6	1.055
OPMa ^d		847	39.7	1.059
OPP		833	39.7	1.059
OSM ^d		833	39.7	1.059
OPM ^d		805	40.0	1.070
LgLS		2	971	50.5
BLS	943		50.8	0.939
LgLP	943		50.8	0.939
ALS	915		51.1	0.946
BLP	915		51.1	0.946
SLS	887		51.4	0.953
ALP	887		51.4	0.953
LgSL ^d	971		51.6	0.958
SLP	859		51.7	0.960
BSL ^d	943		51.9	0.965
LgPL ^d	943		51.9	0.965

PLP		831	52.0	0.967
ASL ^d		915	52.2	0.972
BPL ^d		915	52.2	0.972
PLM		803	52.3	0.974
LgOO		971	52.4	0.977
SSL		887	52.5	0.979
APL ^d		887	52.5	0.979
C23:0OO		957	52.5	0.979
BOO		943	52.6	0.981
SPL ^d		859	52.8	0.986
AOO		915	52.8	0.986
LPP		831	53.0	0.991
SOO		887	53.1	0.993
OOMa		873	53.2	0.995
LPM ^d		803	53.2	0.995
OLgO		971	53.2	0.995
OC23:0O		957	53.4	1.000
OOP		859	53.4	1.000
OBO		943	53.6	1.005
OOM		831	53.7	1.007
OAO		915	53.8	1.009
OSO		887	54.0	1.014
OMaO		873	54.2	1.019
OPO		859	54.3	1.021
OPMo		845	54.5	1.026
OMO		831	54.6	1.028
OPPo		831	54.6	1.028
LgLO		969	57.5	0.919
C23:0LO		955	57.7	0.923
BLO		941	58.0	0.929
LgOL		969	58.0	0.929
C23:0OL		955	58.2	0.933
GLP		885	58.2	0.933
GOO		913	58.4	0.937
ALO		913	58.6	0.941
BOL		941	58.6	0.941
SLO		885	59.2	0.953
AOL		913	59.2	0.953
OLMa	3	871	59.4	0.957
OLgL		969	59.5	0.959
PLnP		829	59.8	0.965
OLP		857	59.8	0.965
SOL		885	59.8	0.965
OC23:0L		955	59.8	0.965
LOMa		871	60.2	0.972
OBL		941	60.2	0.972
LOP		857	60.5	0.978
OLM		829	60.5	0.978
OAL		913	60.7	0.982

LOM		829	61.1	0.990
OSL		885	61.2	0.992
OMaL		871	61.5	0.998
OOO		885	61.6	1.000
GOG		941	61.6	1.000
OPL		857	61.8	1.004
OOMo		871	61.9	1.006
LnPP		829	61.9	1.006
OPoO		857	62.2	1.012
OML		829	62.5	1.018
LgLL	4	967	67.9	0.965
C23:0LL		953	68.0	0.966
BLL		939	68.2	0.970
ALL		911	68.6	0.976
GLO		911	68.8	0.980
C20:2PL		883	68.9	0.981
SLL		883	69.0	0.983
LLgL		967	69.1	0.985
GOL		911	69.2	0.986
LLMa		869	69.2	0.986
LC23:0L		955	69.3	0.988
LLP		855	69.4	0.990
LBL		939	69.5	0.992
LLC15:0		841	69.7	0.995
OLO		883	70.0	1.000
LLM		827	70.0	1.000
LAL		911	70.0	1.000
OOL		883	70.4	1.007
LSL		883	70.4	1.007
OLMo		869	70.5	1.008
LMaL		869	70.6	1.010
LPL		855	70.8	1.014
OLnP		855	70.9	1.015
LC15:0L		841	71.1	1.019
OPoL		855	71.1	1.019
LML		827	71.3	1.022
LnOP		855	71.4	1.024
SOLn		883	71.4	1.024
OPLn	855	72.2	1.037	
γ LnOP	855	72.2	1.037	
C20:2LO	5	909	74.9	0.968
C20:2OL		909	75.3	0.974
GLL		909	75.3	0.974
LGL		909	76.2	0.988
OLL		881	77.0	1.000
SLnL		881	77.1	1.002
LOL		881	77.4	1.006
SL γ Ln		881	77.8	1.012
LPoL		853	78.2	1.018

LLnP		853	79.3	1.035	
LnLP		853	79.5	1.038	
OLnO		881	79.7	1.041	
OOLn		881	80.4	1.051	
LPLn		853	80.9	1.059	
γ LnLP		853	81.2	1.063	
OO γ Ln		881	81.3	1.065	
StOP		853	82.9	1.089	
C20:2LL		6	907	83.2	0.971
GLLn	907		85.3	0.999	
LLL	879		85.4	1.000	
GL γ Ln	907		86.6	1.016	
OLnL	881		86.7	1.017	
GLLn	907		86.7	1.017	
OLLn	879		86.8	1.019	
LOLn	879		87.2	1.024	
LnLnP	851		88.2	1.038	
OL γ Ln	879		88.3	1.039	
LO γ Ln	879		88.6	1.043	
LnPLn	851		89.7	1.058	
γ LnPLn	851		91.1	1.076	
StLP	851		91.3	1.079	
γ Ln γ LnP	851		91.5	1.082	
SLSt	879		91.5	1.082	
LLnL	7		877	92.1	1.000
LLLn			877	92.3	1.002
LL γ Ln			877	93.7	1.020
OLnLn			877	94.1	1.025
LnOLn			877	94.5	1.030
γ LnOLn		877	95.2	1.038	
γ LnO γ Ln		877	95.8	1.046	
OLSt		877	96.6	1.055	
LOSt		877	97.0	1.060	
LnPSt		849	98.1	1.074	
γ LnPSt		849	98.5	1.079	
LLnLn	8	875	101.6	1.000	
LnLLn		875	101.8	1.002	
γ LnLLn		875	102.6	1.011	
LLSt		875	104.3	1.030	
γ LnL γ Ln		875	104.4	1.031	
LnOSt		875	105.4	1.042	
γ LnOSt		875	106.0	1.048	
StPSt		847	108.5	1.076	
LnLnLn	9	873	110.1	1.000	
LnLSt		873	111.0	1.009	
γ LnLnLn		873	111.4	1.013	
γ LnLSt		873	112.5	1.024	
γ Ln γ LnLn		873	112.9	1.028	
γ Ln γ Ln γ Ln		873	114.3	1.042	

LnLnSt	10	871	120.2	1.102
γ LnLnSt		871	121.9	1.119
γ Ln γ LnSt		871	123.1	1.131
StLnSt	11	869	131.8	1.219

^a Chromatographic conditions are described in the Experimental section. ^b DB, number of double bonds. ^c Relative retention is defined as $r = (t_R - t_M) / (t_S - t_M)$, where t_M is 10.8 minutes and t_S are retention times of standards for particular DB groups, i. e., PPP (DB = 0), POP (1), OOP (2), OOO (3), OLO (4), OLL (5), LLL (6), LLnL (7), LLnLn (8) and LnLnLn (9 and more). ^d Regioisomers of XYO / YXO and XYL / YXL types (X and Y are saturated fatty acids) and saturated TGs are not differentiated.