

Simulation of triacylglycerol ion profiles: Bioinformatics for interpretation of triacylglycerol biosyntheses

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Table S1. Mass levels of individual species of phosphatidylinositol, phosphatidic acid, and triacylglycerol determined by MDMS-SL as well as mass levels of fatty acyl chains in triacylglycerol derived from MS analysis and mass levels of acyl-CoA determined by MALDI-TOF/MS

Species	<i>m/z</i> or Mass	Mean \pm SD
Heart		
Phosphatidylinositol (PI) (nmol/mg protein)		
16:0-18:2	833.518	0.06 \pm 0.00
16:0-20:4	857.518	0.23 \pm 0.00
18:1-18:2	859.534	0.12 \pm 0.01
18:0-18:2	861.549	0.37 \pm 0.04
18:0-18:1	863.565	0.04 \pm 0.01
18:2-20:4	881.518	0.04 \pm 0.00
16:0-22:6	881.518	0.02 \pm 0.00
18:1-20:4	883.534	0.36 \pm 0.04
18:0-20:4	885.549	4.95 \pm 0.60
18:0-20:3	887.565	0.37 \pm 0.04
18:0-20:2	889.581	0.02 \pm 0.00
18:0-22:6	909.549	0.21 \pm 0.03
18:0-22:5	911.565	0.12 \pm 0.01
18:0-22:4	913.581	0.05 \pm 0.01
Sum		6.95 \pm 0.72
Phosphatidic acid (PA) (pmol/mg protein)		
16:0-16:0	647.466	11.3 \pm 1.9
16:0-18:2	671.466	11.4 \pm 0.5
16:0-18:1	673.481	47.3 \pm 0.7
18:0-18:2	699.497	5.1 \pm 0.3
18:1-18:1	699.497	5.1 \pm 0.2
18:0-18:1	701.513	0.9 \pm 0.1
Sum		81.0 \pm 1.7
Triacylglycerol (TAG) (nmol/mg protein)		
C46:2	781.690	0.08 \pm 0.00
C46:1/C47:8	783.705	0.10 \pm 0.00
C46:0/C47:7	785.721	0.06 \pm 0.01
C47:0/C48:7	799.737	0.12 \pm 0.00
C48:2/C49:9	809.721	0.17 \pm 0.05
C48:1/C49:8	811.737	0.29 \pm 0.08
C48:0/C49:7	813.752	0.22 \pm 0.06
C50:4	833.721	0.08 \pm 0.02
C50:3/C51:10	835.737	0.41 \pm 0.11
C50:2/C51:9	837.752	1.28 \pm 0.36

C50:1/C51:8	839.768	1.50±0.42
C50:0/C51:7	841.784	0.19±0.04
C51:3/C52:10	849.752	0.05±0.01
C51:2/C52:9	851.768	0.70±0.02
C51:1/C52:8	853.690	0.15±0.02
C51:0/C52:7	855.705	0.13±0.02
C52:6	857.721	0.08±0.00
C52:5	859.737	0.27±0.04
C52:4/C53:11	861.752	1.09±0.26
C52:3/C53:10	863.768	3.35±0.84
C52:2/C53:9	865.784	4.47±1.05
C52:1/C53:8	867.799	0.92±0.30
C52:0/C53:7	869.815	0.09±0.02
C53:5/C54:12	873.752	0.16±0.05
C53:4/C54:11	875.768	0.09±0.02
C53:3/C54:10	877.784	0.23±0.04
C53:2/C54:9	879.705	0.25±0.06
C53:1/C54:8	881.721	0.22±0.05
C53:0/C54:7	883.737	0.11±0.02
C54:6	885.752	0.48±0.05
C54:5/C55:12	887.768	1.65±0.20
C54:4/C55:11	889.784	3.53±0.53
C54:3/C55:10	891.799	3.76±0.72
C54:2/C55:9	893.815	1.35±0.34
C54:1/C55:8	895.831	0.21±0.06
C54:0/C55:7	897.846	0.10±0.02
C55:5/C56:12	901.784	0.09±0.01
C55:4/C56:11	903.799	0.17±0.02
C55:3/C56:10	905.721	0.22±0.03
C55:2/C56:9	907.737	0.22±0.04
C55:1/C56:8	909.752	0.29±0.04
C55:0/C56:7	911.768	0.80±0.06
C56:6	913.784	1.06±0.05
C56:5/C57:12	915.799	0.91±0.07
C56:4/C57:11	917.815	0.57±0.07
C56:3/C57:10	919.831	0.37±0.05
C56:2/C57:9	921.846	0.22±0.05
C56:1/C57:8	923.862	0.07±0.01
C56:0/C57:7/C58:14	925.784	0.03±0.00
C57:6/C58:13	927.799	0.06±0.01
C57:5/C58:12	929.815	0.16±0.08
C57:4/C58:11	931.737	0.05±0.00
C57:3/C58:10	933.752	0.10±0.01
C57:2/C58:9	935.768	0.20±0.04
C57:1/C58:8	937.784	0.42±0.05
C57:0/C58:7/C59:14	939.799	0.53±0.03
C58:6/C59:13	941.815	0.38±0.01
C58:5/C59:12	943.831	0.17±0.01
C58:4/C59:11	945.846	0.10±0.01

C58:3/C59:10	947.862	0.07±0.01
C58:2/C59:9	949.878	0.07±0.02
C58:1/C59:8/C60:15	951.893	0.11±0.07
C59:5/C60:12	957.752	0.04±0.01
C59:4/C60:11	959.768	0.05±0.01
C59:3/C60:10	961.784	0.08±0.02
C59:2/C60:9	963.799	0.09±0.02
C59:1/C60:8/C61:15	965.815	0.08±0.01
C59:0/C60:7/C61:14	967.831	0.07±0.02
C60:6/C61:13	969.846	0.04±0.00
C61:4/C62:11	987.799	0.03±0.00
C61:3/C62:10	989.815	0.03±0.00
Sum		35.89±5.72

Fatty acyl chain composition in TAG (FA)			Acyl-CoA composition
228 (14:0)	228.209	1.39±0.40	2.50±0.58
254 (16:1)	254.225	2.13±0.51	7.19±0.61
256 (16:0)	256.24	15.57±3.01	16.95±3.33
268 (17:1)	268.24	2.38±0.41	
270 (17:0)	270.256	1.93±0.40	
278 (18:3)	278.225	1.21±0.10	2.98±0.41
280 (18:2)	280.24	13.30±0.45	14.55±1.85
282 (18:1)	282.256	35.25±1.89	30.20±4.55
284 (18:0)	284.272	7.97±0.59	8.34±1.02
296 (19:1)	296.272	0.93±0.07	
298 (19:0)	298.287	0.83±0.11	
304 (20:4)	304.24	2.38±0.15	2.97±0.72
306 (20:3)	306.256	1.90±0.08	1.68±0.52
308 (20:2)	308.272	1.43±0.15	2.65±0.34
310 (20:1)	310.287	2.28±0.39	4.09±0.61
312 (20:0)	312.303	1.42±0.26	1.64±0.46
322 (21:2)	322.287	0.36±0.04	
328 (22:6)	328.24	1.41±0.43	1.96±0.38
330 (22:5)	330.256	1.10±0.27	1.58±0.31
332 (22:4)	332.272	1.09±0.14	0.72±0.42
334 (22:3)	334.287	0.98±0.24	
336 (22:2)	336.303	0.84±0.25	
338 (22:1)	338.318	0.76±0.14	
340 (22:0)	340.334	0.66±0.10	
346 (23:4)	346.287	0.24±0.03	
348 (23:3)	348.303	0.23±0.06	
Sum		100	100

Liver

Phosphatidylinositol (PI) (nmol/mg protein)		
16:0-18:2	833.518	0.18±0.03

16:0-18:1	835.534	0.03±0.01
16:0-20:4	857.518	0.62±0.08
18:1-18:2	859.534	0.19±0.03
18:0-18:2	861.549	0.19±0.02
18:2-20:4	881.518	0.04±0.00
16:0-22:6	881.518	0.02±0.00
18:1-20:4	883.534	0.48±0.07
18:0-20:4	885.549	4.79±0.48
18:0-20:3	887.565	0.27±0.04
18:1-22:6	907.534	0.01±0.00
18:0-22:6	909.549	0.06±0.00
18:0-22:5	911.565	0.03±0.00
18:0-22:4	913.581	0.02±0.00
Sum		6.92±0.73

Phosphatidic acid (PA) (pmol/mg protein)

16:0-18:2	671.466	90.0±201
16:0-18:1	673.482	35.2±7.0
18:0-18:2	699.497	20.9±6.4
18:1-18:1	699.497	20.9±6.3
18:0-18:1	701.513	3.1±1.9
18:0-20:2	727.529	1.5±1.5
Sum		172.1±41.6

Triacylglycerol (TAG) (nmol/mg protein)

C48:3	807.705	1.82±0.31
C48:2/C49:9	809.721	3.77±0.64
C48:1/C49:8	811.737	2.53±0.40
C48:0/C49:7	813.752	0.39±0.02
C50:5	831.705	1.12±0.20
C50:4	833.721	6.03±0.86
C50:3/C51:10	835.737	20.76±2.59
C50:2/C51:9	837.752	25.25±3.02
C50:1/C51:8	839.768	9.65±1.02
C51:3/C52:10	849.752	1.04±0.15
C51:2/C52:9	851.768	2.93±0.44
C51:1/C52:8	853.690	1.54±0.25
C51:0/C52:7	855.705	1.17±0.19
C52:6	857.721	3.67±0.37
C52:5	859.737	16.11±1.22
C52:4/C53:11	861.752	51.46±1.58
C52:3/C53:10	863.768	85.28±3.30
C52:2/C53:9	865.784	49.79±2.05
C52:1/C53:8	867.799	5.31±0.27
C53:4/C54:11	875.768	2.07±0.26
C53:3/C54:10	877.784	5.04±0.49
C53:2/C54:9	879.705	4.46±0.55
C53:1/C54:8	881.721	3.66±0.41
C53:0/C54:7	883.737	5.89±0.30
C54:6	885.752	14.04±0.61
C54:5/C55:12	887.768	23.55±1.48

C54:4/C55:11	889.784	29.19±3.02
C54:3/C55:10	891.799	18.18±2.07
C54:2/C55:9	893.815	4.38±0.31
C55:4/C56:11	903.799	1.79±0.28
C55:3/C56:10	905.721	1.68±0.23
C55:2/C56:9	907.737	2.85±0.11
C55:1/C56:8	909.752	7.52±0.26
C55:0/C56:7	911.768	9.29±0.24
C56:6	913.784	5.36±0.21
C56:5/C57:12	915.799	3.07±0.22
C56:4/C57:11	917.815	2.02±0.17
C56:3/C57:10	919.831	1.30±0.18
C57:3/C58:10	933.752	1.17±0.02
C57:2/C58:9	935.768	2.33±0.04
C57:1/C58:8	937.784	2.04±0.13
C57:0/C58:7/C59:14	939.799	1.29±0.05
C58:6/C59:13	941.815	0.77±0.10
Sum		442.65±28.31

Fatty acyl chain composition in TAG (FA)			Acyl-CoA composition
226(14:1)	226.193	0.28±0.05	
228(14:0)	228.209	0.94±0.08	1.31±0.21
252(16:2)	252.209	0.38±0.05	0.30±0.12
254(16:1)	254.225	7.42±0.91	9.03±1.26
256(16:0)	256.240	23.48±0.82	23.56±3.45
278(18:3)	278.225	2.77±0.20	2.55±0.43
280(18:2)	280.240	19.61±1.06	16.08±3.16
282(18:1)	282.256	29.98±0.97	28.01±4.27
284(18:0)	284.272	5.38±0.09	6.81±1.54
304(20:4)	304.240	1.66±0.06	2.96±0.88
306(20:3)	306.256	0.69±0.05	0.81±0.15
308(20:2)	308.272	0.69±0.07	1.21±0.32
310(20:1)	310.287	1.30±0.04	2.15±0.41
312(20:0)	312.303	0.74±0.08	1.05±0.27
326(21:0)	326.225	0.21±0.02	
328(22:6)	328.240	1.61±0.16	2.11±0.36
330(22:5)	330.256	0.59±0.05	0.84±0.22
332(22:4)	332.272	0.34±0.04	0.24±0.16
334(22:3)	334.287	0.94±0.09	0.98±0.32
336(22:2)	336.303	0.39±0.03	
338(22:1)	338.318	0.29±0.05	
340(22:0)	340.334	0.30±0.05	
Sum		100	100

Skeletal Muscle

Phosphatidylinositol (PI) (nmol/mg protein)		
16:0-16:0	809.518	0.05±0.00
16:0-18:2	833.518	0.08±0.00

16:0-18:1	835.534	0.11±0.01
16:0-18:0	837.549	0.06±0.01
16:0-20:4	857.518	0.11±0.01
18:1-18:2	859.534	0.04±0.01
18:0-18:2	861.549	0.16±0.01
18:0-18:1	863.565	0.02±0.00
18:2-20:4	881.518	0.06±0.00
16:0-22:6	881.518	0.03±0.00
18:1-20:4	883.534	0.19±0.01
18:0-20:4	885.549	2.49±0.06
18:0-20:3	887.565	0.25±0.06
18:0-20:2	889.581	0.03±0.01
18:0-20:0	893.612	0.01±0.00
18:1-22:6	907.534	0.06±0.00
18:0-22:6	909.549	0.88±0.02
18:0-22:5	911.565	0.21±0.01
18:0-22:4	913.581	0.02±0.01
Sum		4.84±0.12

Phosphatidic acid (PA) (pmol/mg protein)

16:1-16:1	643.434	8.8±1.3
16:0-16:0	647.466	27.1±1.9
16:0-18:2	671.466	4.5±1.3
16:0-18:1	673.481	19.6±1.8
18:0-18:2	699.497	3.9±0.4
18:1-18:1	699.497	3.9±0.3
18:0-18:1	701.513	12.9±0.7
18:0-20:4	723.497	5.3±3.0
18:0-20:2	727.528	3.1±0.6
Sum		89.1±1.4

Triacylglycerol (TAG) (nmol/mg protein)

C46:1/C47:8	783.705	0.23±0.04
C46:0/C47:7	785.721	0.12±0.01
C48:2/C49:9	809.721	1.20±0.36
C48:1/C49:8	811.737	1.04±0.24
C48:0/C49:7	813.752	0.41±0.04
C50:4	833.721	1.24±0.49
C50:3/C51:10	835.737	3.64±1.35
C50:2/C51:9	837.752	4.21±1.24
C50:1/C51:8	839.768	1.94±0.38
C50:0/C51:7	841.784	0.20±0.01
C51:3/C52:10	849.752	0.21±0.07
C51:2/C52:9	851.768	0.41±0.14
C51:1/C52:8	853.690	0.46±0.06
C51:0/C52:7	855.705	0.34±0.05
C52:6	857.721	0.43±0.10
C52:5	859.737	2.03±0.73
C52:4/C53:11	861.752	5.87±1.25
C52:3/C53:10	863.768	7.93±2.73
C52:2/C53:9	865.784	4.33±1.16

C52:1/C53:8	867.799	0.59±0.11
C53:3/C54:10	877.784	0.59±0.21
C53:2/C54:9	879.705	0.47±0.14
C53:1/C54:8	881.721	0.35±0.09
C53:0/C54:7	883.737	0.49±0.17
C54:6	885.752	1.53±0.60
C54:5/C55:12	887.768	3.89±1.56
C54:4/C55:11	889.784	5.65±2.08
C54:3/C55:10	891.799	3.81±1.20
C54:2/C55:9	893.815	0.71±0.19
C55:3/C56:10	905.721	0.33±0.11
C55:2/C56:9	907.737	0.33±0.10
C55:1/C56:8	909.752	0.46±0.15
C55:0/C56:7	911.768	0.54±0.16
C56:6	913.784	0.40±0.12
C56:5/C57:12	915.799	0.29±0.06
C57:5/C58:12	929.815	0.15±0.04
C57:4/C58:11	931.737	0.04±0.01
C57:3/C58:10	933.752	0.13±0.02
C57:2/C58:9	935.768	0.21±0.07
C57:1/C58:8	937.784	0.23±0.07
C57:0/C58:7/C59:14	939.799	0.12±0.03
C58:6/C59:13	941.815	0.05±0.01
C58:5/C59:12	943.831	0.04±0.00
C58:4/C59:11	945.846	0.04±0.01
C58:3/C59:10	947.862	0.03±0.01
C58:2/C59:9	949.878	0.05±0.01
C58:1/C59:8/C60:15	951.893	0.07±0.01
Sum		57.83±8.74

Fatty acyl chain composition in TAG (FA)			Acyl-CoA composition
226 (14:1)	226.193	0.31±0.15	
228 (14:0)	228.209	1.77±0.43	2.40±0.70
252 (16:2)	252.209	0.24±0.08	
254 (16:1)	254.225	11.83±0.82	12.07±2.01
256 (16:0)	256.240	18.45±2.43	18.78±3.26
278 (18:3)	278.225	2.34±0.57	3.55±0.82
280 (18:2)	280.240	18.09±3.61	16.95±3.47
282 (18:1)	282.256	33.70±1.32	31.14±5.32
284 (18:0)	284.272	5.80±0.78	7.22±1.58
304 (20:4)	304.240	1.59±0.52	2.34±0.61
306 (20:3)	306.256	0.73±0.18	1.08±0.31
308 (20:2)	308.272	0.55±0.09	0.61±0.22
310 (20:1)	310.287	0.80±0.23	1.21±0.26
312 (20:0)	312.303	0.49±0.15	0.49±0.16
326 (21:0)	326.225	0.18±0.12	
328 (22:6)	328.240	0.79±0.09	0.98±0.28

330 (22:5)	330.256	0.40±0.06	0.43±0.12
332 (22:4)	332.272	0.29±0.12	
334 (22:3)	334.287	0.67±0.13	0.75±0.19
336 (22:2)	336.303	0.39±0.18	
338 (22:1)	338.318	0.22±0.09	
340 (22:0)	340.334	0.37±0.14	
Sum		100	100
