

*Supplementary Material***Elevated α -ketoglutaric acid concentrations and a lipid-balanced signature are the key factors in long-term HIV control**

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1 Additional information

Table S1. List of the 78 metabolites identified in the study, including Human Metabolome Database ID, Retention time (RT), quantitative and qualitative ions and internal standard used. **Table S2.** List of the 114 lipid species identified in the study.

Table S2. List of the 114 lipid species identified in the study, including parental ion, m/z and retention time.

Table S3. Relative concentrations of the 45 lipid species increased in the LTEC-losing group when compared to the LTEC-extreme individuals.

Supplementary Figure 1. Overlapped extracted ion chromatograms (EIC) of metabolites analyzed by GC-EI-QTOF-MS.

Supplementary Figure 2. Overlapped extracted ion chromatograms (EIC) of lipids analyzed by LC-ESI-QTOF-MS using the accurate mass (m/z) from pseudomolecular ions. LCP, lysophosphatidylcholines; PC, phosphatidylcholines; SM, sphingomyelins; DG, diglyceride; ChoE/CE, cholesteroyl esthers; TG, triglycerides.

2 ECRIS integrated in the Spanish AIDS Research Network

1 Additional information

Table S1. List of the 78 metabolites identified in the study, including Human Metabolome Database ID, Retention time (RT), quantitative and qualitative ions and internal standard used.

Metabolite/Internal Standard	Human Metabolome Database	RT (min)	M ⁺ (m/z) (Quantitative)	M ⁺ (m/z) (Qualitative)	Internal standard
2-Hydroxybutyric acid	HMDB0000008	6.87	131.0895	205.106	Succinic-d ₄ acid
2-Hydroxyisobutyric acid	HMDB0000729	5.91	131.0895	205.106	Succinic-d ₄ acid
2-Hydroxyisovaleric acid	HMDB0000407	7.39	145.1061	147.0672	Succinic-d ₄ acid
3-hydroxybutyric acid / 3-hydroxyisobutyric acid	HMDB0000357/ HMDB0062640	7.31	117.0731	191.0925	Succinic-d ₄ acid
3-Hydroxyisovaleric acid	HMDB0000407	8.02	131.0859	205.1086	Succinic-d ₄ acid
4-Hydroxybenzoic acid	HMDB0000500	13.41	223.101	267.0912	Succinic-d ₄ acid
4-hydroxyphenyllactic acid	HMDB0000755	16.26	179.0902	308.116	Succinic-d ₄ acid
4-Hydroxyproline	HMDB0000725	12.28	230.1434	140.0919	L-Proline ¹³ C ₅
Alanine	HMDB0000161	6.45	116.0916	190.1094	L-Alanine ¹³ C ₃
alpha-Ketoglutaric acid	HMDB0000208	12.82	198.0622	288.1119	Succinic-d ₄ acid
alpha-Tocopherol	HMDB0001893	26.30	237.1337	502.4279	Glucose- ¹³ C ₆
Aspartic acid	HMDB0000191	12.23	232.13	218.1075	L-Aspartic acid ¹³ C ₄
Benzoic acid	HMDB0001870	8.51	179.0559	135.0652	Succinic-d ₄ acid
Citric acid	HMDB0000094	15.71	273.105	347.1215	Succinic-d ₄ acid
Creatinine	HMDB0000562	12.61	115.0841	329.1847	L-Proline ¹³ C ₅
d-Arabinose	HMDB0029942	14.06	307.1622	277.1497	Glucose- ¹³ C ₆
Decanoic acid	HMDB0000511	11.29	229.1615		Myristic-d ₂₇ acid
d-Fructose	HMDB0000660	16.36	307.165	103.06	Glucose- ¹³ C ₆
d-Galactitol	HMDB0000107	17.19	319.1675	307.1653	Glucose- ¹³ C ₆
d-Gluconic acid	HMDB0000625	17.35	292.1385	333.1434	Glucose- ¹³ C ₆
d-Maltose	HMDB0000163	23.72	361.179	204.1134	Glucose- ¹³ C ₆
d-Maltose (isomer)	HMDB0000163	23.81	361.179	204.1134	Glucose- ¹³ C ₆
d-Mannitol	HMDB0000765	16.95	319.1675	307.1653	Glucose- ¹³ C ₆
d-Mannonic acid	HMDB0242119	17.10	333.1434	292.1385	Glucose- ¹³ C ₆
Dodecanoic acid	HMDB0000638	13.64	257.1941		Myristic-d ₂₇ acid
d-Sucrose	HMDB0000258	23.18	361.179	204.1134	Glucose- ¹³ C ₆
d-Threitol	HMDB0004136	12.16	204.107	117.0412	Glucose- ¹³ C ₆
d-Xylose	HMDB0000098	13.89	307.1622	277.1497	Glucose- ¹³ C ₆
Erythronic acid	HMDB0000613	12.61	217.1142	117.0401	Glucose- ¹³ C ₆
Ethanolamine	HMDB0000149	8.85	174.1147	262.1472	L-Valine ¹³ C ₅
Fumaric acid	HMDB0000134	9.93	245.0752	217.0746	Succinic-d ₄ acid
Galactonic acid	HMDB0000565	17.43	292.1395		Glucose- ¹³ C ₆
Galacturonic acid	HMDB0003363	17.18	333.1434	292.1385	Glucose- ¹³ C ₆

Glutamic acid	HMDB0000148	13.41	246.1392	230.1061	L-Glutamic ¹³ C ₅
Glutamine	HMDB0000641	15.17	156.0847	245.1485	L-Glutamic ¹³ C ₅
Glyceric acid	HMDB0000139	9.79	189.0782	292.1363	Succinic-d ₄ acid
Glycerol	HMDB0000131	9.00	218.1185		Glucose- ¹³ C ₆
Glycerol-1-phosphate	HMDB0000126	15.11	299.0801	357.1222	Glucose- ¹³ C ₆
Glycine	HMDB0000123	9.41	174.1153	248.1331	Glycine ¹³ C ₂
Glycolic acid	HMDB0000115	6.04	177.0764	131.0353	Succinic-d ₄ acid
Heptanoic acid	HMDB0000666	7.34	187.1148		Myristic-d ₂₇ acid
Hexanoic acid	HMDB0000535	5.934	173.1005		Myristic-d ₂₇ acid
Hippuric acid	HMDB0000714	15.73	105.0373	206.1045	Succinic-d ₄ acid
Indole-3-propanoic acid	HMDB0002302	18.19	202.1095	333.1607	Succinic-d ₄ acid
Indolelactic acid	HMDB0000671	19.14	202.1064		Succinic-d ₄ acid
Isoleucine	HMDB0000172	9.24	158.1404	218.1063	L-Isoleucine ¹³ C ₆
Lactic acid	HMDB0144295	5.83	190.088	117.0767	Succinic-d ₄ acid
Leucine	HMDB0000687	8.94	158.1432	218.1053	L-Leucine ¹³ C ₆
Linoleic acid	HMDB0000673	19.258	117.0382	337.2654	Myristic-d ₂₇ acid
Malic acid	HMDB0000744	11.85	233.1045	245.0686	Succinic-d ₄ acid
meso-Erythritol	HMDB0002994	12.06	204.107	117.0412	Glucose- ¹³ C ₆
Methionine	HMDB0033951	12.15	128.0909	176.0949	Methionine ¹³ C ₅
myo-Inositol	HMDB0000211	18.48	318.1569	305.1495	Glucose- ¹³ C ₆
Nonanoic acid	HMDB0000847	10.04	215.1464		Myristic-d ₂₇ acid
Octanoic acid	HMDB0000482	8.72	201.1311		Myristic-d ₂₇ acid
Oleic acid	HMDB0000207	19.32	117.0382	339.2795	Myristic-d ₂₇ acid
Oleic acid (isomer)	HMDB0000207	19.3566	117.0382		Myristic-d ₂₇ acid
Ornithine	HMDB0000214	15.63	142.1063	174.1163	L-Glutamic ¹³ C ₅
Oxalic acid	HMDB0002329	6.912	131.0353	175.0616	Succinic-d ₄ acid
Oxoproline	HMDB0000267	12.21	156.0853	230.1032	L-Proline ¹³ C ₅
Palmitic acid	HMDB0000220	17.73	117.0382	313.2578	Myristic-d ₂₇ acid
Phenylalanine	HMDB0000159	13.47	218.105	192.1222	L-Phenylalanine ¹³ C ₉
Phosphoric acid	HMDB0001488	9.13	299.0788		Succinic-d ₄ acid
Pipecolic acid	HMDB0000070	10.17	156.122	230.1397	L-Serine ¹³ C ₃
Proline	HMDB0000162	9.27	142.1082	216.1261	L-Proline ¹³ C ₅
Pyruvic acid	HMDB0000243	5.68	174.0629	89.0438	Succinic-d ₄ acid
Ribonic acid	HMDB0000867	15.31	292.1424	333.1432	Glucose- ¹³ C ₆
Saccharic acid	HMDB0000663	17.68	292.1385	333.1434	Glucose- ¹³ C ₆
Sarcosine	HMDB0000271	6.95	116.0909	190.1089	L-Alanine ¹³ C ₃
Serine	HMDB0000187	10.18	204.1316	218.1084	L-Serine ¹³ C ₃
Stearic acid	HMDB0000827	19.52	117.0382	341.2983	Myristic-d ₂₇ acid
Succinic acid	HMDB0000254	9.46	247.0851	147.0702	Succinic-d ₄ acid

Tetradecanoic acid	HMDB0000806	15.776	285.2254		Myristic-d ₂₇ acid
Threonic acid	HMDB0000943	12.55	292.1383	220.098	Succinic-d ₄ acid
Threonine	HMDB0000167	10.55	218.1053	117.0738	L-Threonine ¹³ C ₄
Urea	HMDB0000294	8.45	189.0909	171.0786	Glycine ¹³ C ₂
Uric acid	HMDB0000289	18.51	441.1685	456.1901	Succinic-d ₄ acid
Valine	HMDB0000883	8.13	144.1229	218.1131	L-Valine ¹³ C ₅
L-Alanine ¹³C₃	-	6.40	119.096		-
L-Valine ¹³C₅	-	8.06	149.1347		-
L-Leucine ¹³C₆	-	8.86	164.1546		-
L-Isoleucine ¹³C₆	-	9.17	164.1573		-
L-Proline ¹³C₅	-	9.16	221.1068		-
Glycine ¹³C₂	-	9.34	176.1242		-
L-serine ¹³C₃	-	10.11	207.1323		-
L-Threonine ¹³C₄	-	10.48	222.1371		-
L-Methionine-(carboxy-¹³C, methyl-D₃)	-	12.10	132.0988		-
L-Aspartic acid ¹³C₄	-	12.16	236.1305		-
L-Glutamic ¹³C₅	-	13.34	251.1492		-
L-Phenylalanine ¹³C₉	-	13.40	201.1486		-
Succinic-d₄ acid	-	9.34	251.1121		-
Glucose-¹³C₆	-	16.64	323.1732		-
L-Alanine ¹³C₃	-	6.40	119.096		-

Table S2. List of the 114 lipid species identified in the study, including parental ion, m/z and retention time.

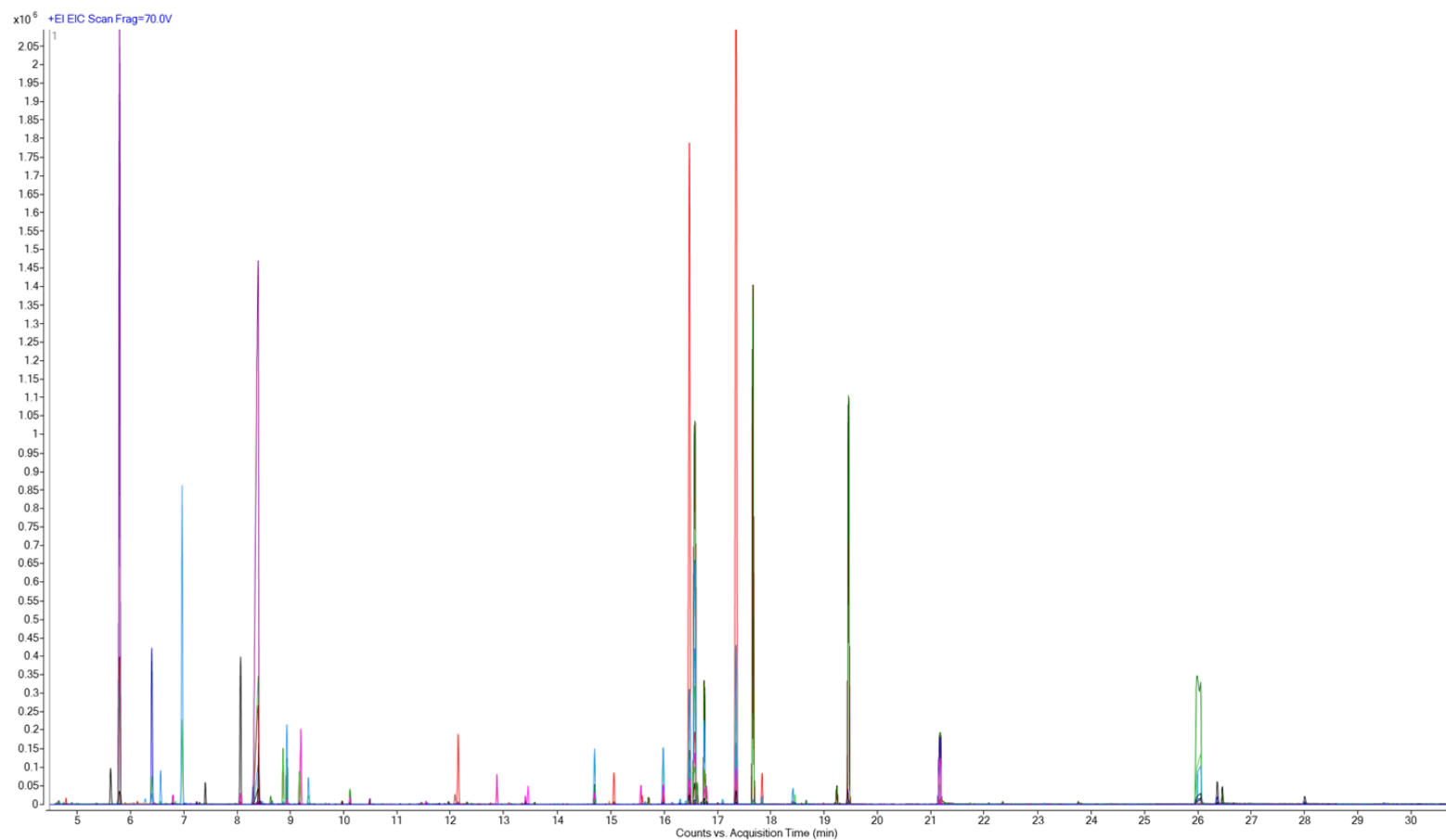
Lipid	Parent ion	m/z	Retention time (min)
CE 16:0	[M+Na] ⁺	647.5738	9.04
CE 16:1	[M+Na] ⁺	645.5581	8.62
CE 17:1	[M+Na] ⁺	659.5738	8.90
CE 18:0	[M+Na] ⁺	675.6051	9.60
CE 18:1	[M+Na] ⁺	673.5894	9.10
CE 18:2	[M+Na] ⁺	671.5738	8.80
CE 18:3	[M+Na] ⁺	669.5581	8.50
CE 20:2	[M+Na] ⁺	699.6051	9.30
CE 20:3	[M+Na] ⁺	697.5894	8.96
CE 20:4	[M+Na] ⁺	695.5738	8.65
CE 20:5	[M+Na] ⁺	693.5581	8.40
CE 22:4	[M+Na] ⁺	723.6051	9.08
CE 22:5	[M+Na] ⁺	721.5894	8.87
CE 22:6	[M+Na] ⁺	719.5738	8.59
DG 34:1	[M+Na] ⁺	617.5115	6.51
DG 34:2	[M+Na] ⁺	615.4959	6.26
DG 34:3	[M+Na] ⁺	613.4802	6.14
DG 36:1	[M+Na] ⁺	645.5434	6.70
DG 36:2	[M+Na] ⁺	643.5272	6.51
DG 36:3	[M+Na] ⁺	641.5115	6.34
DG 36:4	[M+Na] ⁺	639.4959	6.15
DG 40:4	[M+Na] ⁺	695.5591	8.26
LPC 15:0	[M+H] ⁺	482.3241	1.47
LPC 16:0	[M+H] ⁺	496.3398	1.68
LPC 16:0 e	[M+H] ⁺	482.3605	1.86
LPC 16:1 e	[M+H] ⁺	480.3449	1.86
LPC 18:0	[M+H] ⁺	524.3711	2.13
LPC 18:0 e	[M+H] ⁺	510.3918	2.35
LPC 18:1	[M+H] ⁺	522.3554	1.79
LPC 18:2	[M+H] ⁺	520.3398	1.56
LPC 20:0	[M+H] ⁺	552.4024	2.64
LPC 20:2	[M+H] ⁺	548.3711	1.94
LPC 20:3	[M+H] ⁺	546.3554	1.72
PC 30:0	[M+H] ⁺	706.5381	3.80
PC 31:0	[M+H] ⁺	720.5538	4.05
PC 32:0	[M+H] ⁺	734.5694	4.32
PC 32:1	[M+H] ⁺	732.5538	3.96
PC 32:2	[M+H] ⁺	730.5381	3.76
PC 33:0	[M+H] ⁺	748.5851	4.51

PC 33:1	[M+H] ⁺	746.5694	4.21
PC 33:2	[M+H] ⁺	730.5381	3.67
PC 34:0	[M+H] ⁺	762.6008	4.99
PC 34:1	[M+H] ⁺	760.5851	4.50
PC 34:2	[M+H] ⁺	758.5694	4.16
PC 34:3	[M+H] ⁺	756.5538	3.81
PC 34:4	[M+H] ⁺	754.5381	3.71
PC 35:1	[M+H] ⁺	774.6007	4.83
PC 35:2	[M+H] ⁺	772.5851	4.45
PC 35:4	[M+H] ⁺	768.5538	4.21
PC 36:1	[M+H] ⁺	788.6164	5.23
PC 36:2	[M+H] ⁺	786.6007	4.79
PC 36:3	[M+H] ⁺	784.5851	4.39
PC 36:4	[M+H] ⁺	782.5694	4.22
PC 36:5	[M+H] ⁺	780.5538	4.16
PC 38:2	[M+H] ⁺	814.632	5.48
PC 38:3	[M+H] ⁺	812.6164	5.09
PC 38:4	[M+H] ⁺	810.6007	4.87
PC 38:5	[M+H] ⁺	808.5851	4.36
PC 38:6	[M+H] ⁺	806.5694	4.22
PC 40:4	[M+H] ⁺	838.632	5.45
PC 40:5	[M+H] ⁺	836.6164	5.03
PC 40:6	[M+H] ⁺	834.6007	4.87
SM 32:0	[M+H] ⁺	677.5592	3.46
SM 32:1	[M+H] ⁺	675.5436	3.31
SM 32:2	[M+H] ⁺	673.5279	3.10
SM 33:1	[M+H] ⁺	689.5592	3.50
SM 34:1	[M+H] ⁺	703.5749	3.70
SM 34:2	[M+H] ⁺	701.5592	3.44
SM 35:1	[M+H] ⁺	717.5905	3.94
SM 36:0	[M+H] ⁺	733.6218	4.42
SM 36:1	[M+H] ⁺	731.6062	4.19
SM 36:2	[M+H] ⁺	729.5905	3.87
SM 38:1	[M+H] ⁺	759.6375	4.85
SM 38:2	[M+H] ⁺	757.6218	4.43
SM 39:1	[M+H] ⁺	773.6531	5.28
SM 40:1	[M+H] ⁺	787.6688	5.70
SM 40:2	[M+H] ⁺	785.6531	5.17
SM 41:1	[M+H] ⁺	801.6844	6.11
SM 41:2	[M+H] ⁺	799.6688	5.62
SM 42:1	[M+H] ⁺	815.7001	6.29
SM 42:2	[M+H] ⁺	813.6844	5.79
SM 42:3	[M+H] ⁺	811.6688	5.24

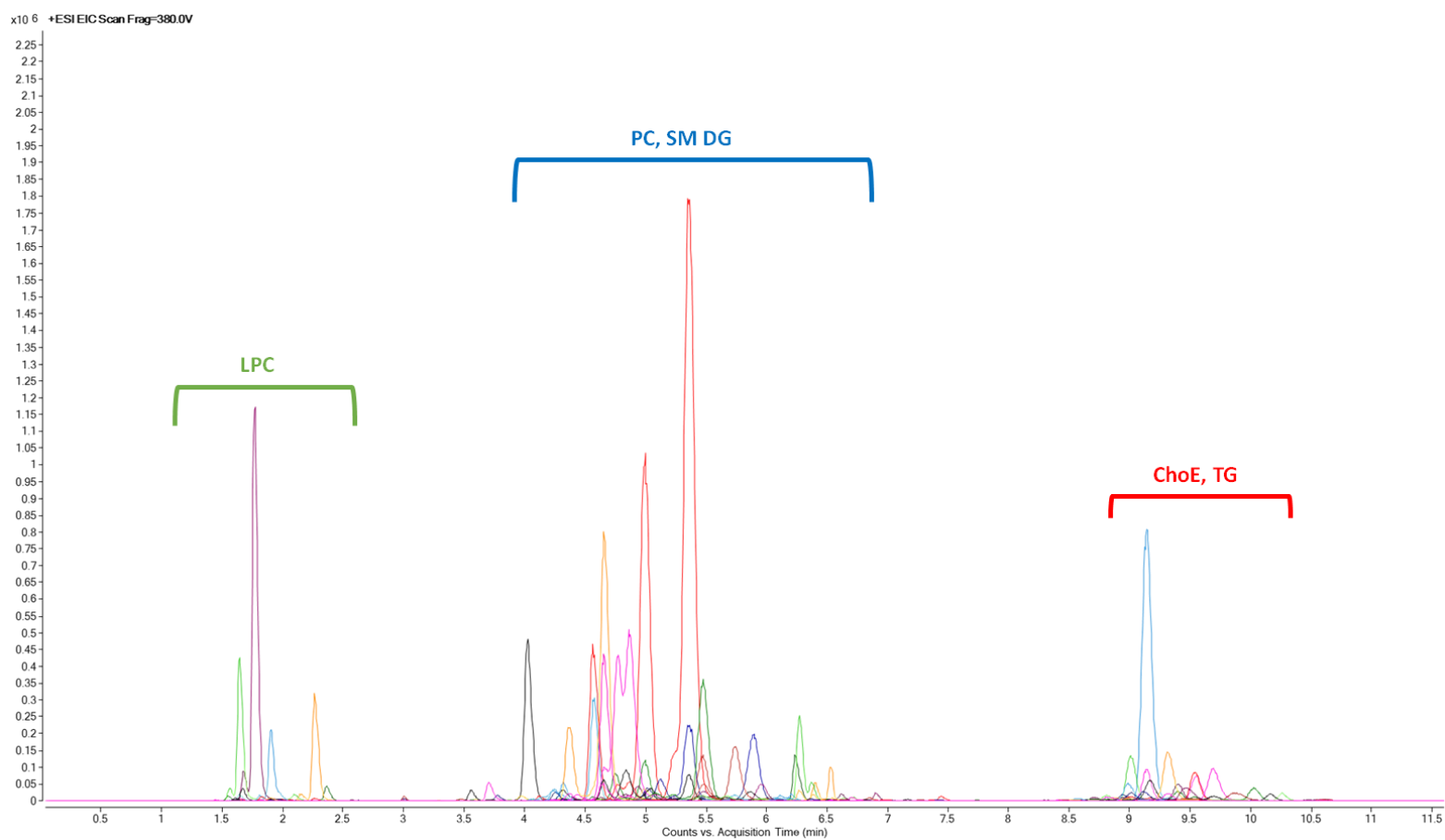
SM 43:1	[M+H] ⁺	829.7157	6.38
SM 43:2	[M+H] ⁺	827.7001	6.04
TG 46:0	[M+NH ₄] ⁺	796.7389	8.40
TG 46:1	[M+NH ₄] ⁺	794.7232	8.13
TG 46:2	[M+NH ₄] ⁺	792.7076	7.89
TG 47:0	[M+NH ₄] ⁺	810.7545	9.17
TG 47:1	[M+NH ₄] ⁺	808.7389	8.81
TG 48:0	[M+NH ₄] ⁺	824.7702	8.81
TG 48:1	[M+NH ₄] ⁺	822.7545	8.50
TG 48:2	[M+NH ₄] ⁺	820.7389	8.22
TG 48:3	[M+NH ₄] ⁺	818.7232	7.99
TG 50:0	[M+NH ₄] ⁺	852.8015	9.29
TG 50:1	[M+NH ₄] ⁺	850.7858	8.91
TG 50:2	[M+NH ₄] ⁺	848.7702	8.60
TG 50:3	[M+NH ₄] ⁺	846.7545	8.33
TG 50:4	[M+NH ₄] ⁺	844.7389	8.09
TG 51:2	[M+NH ₄] ⁺	862.7858	8.80
TG 51:3	[M+NH ₄] ⁺	860.7702	8.69
TG 52:1	[M+NH ₄] ⁺	878.8171	9.41
TG 52:2	[M+NH ₄] ⁺	876.8015	9.01
TG 52:3	[M+NH ₄] ⁺	874.7858	8.72
TG 52:4	[M+NH ₄] ⁺	872.7702	8.47
TG 52:5	[M+NH ₄] ⁺	870.7545	8.24
TG 54:2	[M+NH ₄] ⁺	904.8328	9.53
TG 54:3	[M+NH ₄] ⁺	902.8171	9.13
TG 54:4	[M+NH ₄] ⁺	900.8015	8.83
TG 54:5	[M+NH ₄] ⁺	898.7858	8.56
TG 54:6	[M+NH ₄] ⁺	896.7702	8.31
TG 54:7	[M+NH ₄] ⁺	894.7545	8.10
TG 56:6	[M+NH ₄] ⁺	924.8015	9.12
TG 56:7	[M+NH ₄] ⁺	922.7858	8.74
TG 58:8	[M+NH ₄] ⁺	948.8015	9.00

Table S3. Relative concentrations of the 45 lipid species increased in the LTEC-losing group when compared to the LTEC-extreme individuals.

Lipid compounds	LTEC-losing	SEM	LTEC-extreme	SEM	Lipid compounds	LTEC-losing	SEM	LTEC-extreme	SEM
SM (32:1)	0,2116	0,0153	0,1373	0,0161	PC (35:1)	0,0115	0,0011	0,0074	0,0011
SM (34:2)	0,3626	0,0294	0,2671	0,0299	PC (40:6)	0,1198	0,0130	0,0694	0,0125
SM (32:0)	0,0051	0,0004	0,0035	0,0004	PC (38:4)	0,4598	0,0357	0,3157	0,0355
SM (33:1)	0,0985	0,0062	0,0730	0,0063	SM (38:1)	0,2804	0,0219	0,2095	0,0222
PC (32:2)	0,0129	0,0025	0,0067	0,0025	PC (40:5)	0,0204	0,0024	0,0109	0,0023
PC (34:4)	0,0039	0,0005	0,0020	0,0005	PC (38:3)	0,1795	0,0138	0,1281	0,0135
PC (30:0)	0,0132	0,0038	0,0057	0,0038	PC (38:2)	0,0182	0,0014	0,0123	0,0014
PC (34:3)	0,0447	0,0087	0,0251	0,0087	SM (42:2)	1,8332	0,1065	1,4279	0,1067
PC (33:2)	0,0092	0,0010	0,0054	0,0010	TG (46:2)	0,0646	0,0315	0,0312	0,0315
SM (35:1)	0,0600	0,0042	0,0420	0,0043	TG (48:3)	0,0866	0,0448	0,0340	0,0448
PC (36:5)	0,0982	0,0160	0,0309	0,0135	TG (54:7)	0,0721	0,0305	0,0244	0,0305
PC (35:4)	0,0031	0,0004	0,0016	0,0004	CE (20:5)	0,4340	0,0814	0,1214	0,0767
PC (31:0)	0,0022	0,0003	0,0012	0,0003	CE (18:3)	0,3544	0,0347	0,2310	0,0289
PC (33:1)	0,0078	0,0011	0,0044	0,0011	CE (22:6)	0,3444	0,0438	0,1833	0,0423
SM (36:1)	0,4317	0,0284	0,3281	0,0282	TG (54:6)	0,2590	0,0904	0,1054	0,0905
PC (36:4)	0,8663	0,0650	0,5788	0,0680	CE (20:4)	3,1239	0,2282	2,2060	0,2279
PC (32:0)	0,0699	0,0099	0,0443	0,0101	TG (56:7)	0,2041	0,0614	0,0843	0,0617
PC (36:3)	0,8228	0,0694	0,5940	0,0704	CE (20:3)	0,2072	0,0184	0,1447	0,0181
SM (36:0)	0,0196	0,0024	0,0126	0,0024	TG (56:6)	0,2103	0,0628	0,1014	0,0631
PC (35:2)	0,0291	0,0026	0,0206	0,0027	CE (16:0)	0,2344	0,0134	0,1741	0,0133
SM (38:2)	0,0938	0,0083	0,0705	0,0084	TG (58:8)	0,0483	0,0191	0,0164	0,0192
PC (33:0)	0,0023	0,0002	0,0015	0,0002	CE (18:1)	1,3846	0,1129	1,0141	0,1112
PC (38:5)	0,0559	0,0074	0,0252	0,0056					

Supplementary Figure 1. Overlapped extracted ion chromatograms (EIC) of metabolites analyzed by GC-EI-QTOF-MS.

Supplementary Figure 2. Overlapped extracted ion chromatograms (EIC) of lipids analyzed by LC-ESI-QTOF-MS using the accurate mass (m/z) from pseudomolecular ions. LCP, lysophosphatidylcholines; PC, phosphatidylcholines; SM, sphingomyelins; DG, diglyceride; ChoE/CE, cholesteryl esters; TG, triglycerides.



2 ECRIS integrated in the Spanish AIDS Research Network

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