Supporting Information for:

Comprehensive LC-MS^E Lipidomic Analysis

using a Shotgun Approach and Its

Application to Biomarker Detection and

Identification in Osteoarthritis Patients

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Figure S1. Intraday and interday variation bar chart for all non-endogenous lipids used in the validation set.

Figure S2. Recovery for all non-endogenous lipids used in the validation set during three consecutive days.

Figure S3. High energy fragmentation for the ChoE 18:1 giving rise to the diagnostic fragment-ion at m/z 369.3504 corresponding to the cholesteryl motif which in turn can be used as a precursor ion to 'hunt' in the data set for ChoE lipids in the low energy trace.

Figure S4. High energy extracted ion precursor ion chromatograms in negative ion mode. In this figure it can be observed (from top to bottom; m/z 303.2332 FA (20:4), m/z 283.2646 FA (18:0), m/z 281.2489 FA (18:1), m/z 279.2332 FA (18:2), m/z 255.2332 FA (16:0), m/z 241.2175 FA (15:0)) the fact that fragment-ion information determining the length of the FA can be search against the low energy mode with exact mass to determine the elemental composition of the lipid and to even quantify the levels present (the low energy data is not shown in this example)

Figure S5. Low energy extracted ion chromatogram of PG 14:0/14:0 with m/z 665.4406 and the corresponding high energy extracted ion chromatogram of m/z 227.2003.

Table S1. List of all major lipids identified in the human extracted plasma; the m/z of the most abundant ion, the mass error, retention time, provisional lipid assignment and the ionization mode (positive/negative) are given.

Class	Formula	m/z Found	ppm	Time (min)	provisional assignment class		Ionization mode
ChoE	C47H77NO2	688.6016	-2.4	9.5	ChoE	20:5	[M+NH ₄] ⁺
	C49H79NO2	714.6185	-0.6	9.61	ChoE	22:6	[M+NH ₄] ⁺
	C45H77NO2	664.6057	3.6	9.67	ChoE	18:3	[M+NH ₄] ⁺
	C47H79NO2	690.6189	0.1	9.72	ChoE	20:4	[M+NH ₄] ⁺
	C45H79NO2	666.6193	0.6	9.84	ChoE	18:2	[M+NH ₄] ⁺
	C45H81NO2	668.6337	-1.3	10.14	ChoE	18:1	[M+NH ₄] ⁺
DG	C39H71NO5	634.5411	0	6.41	DG	36:4	[M+NH ₄] ⁺
FA	C18H30O2	277.2150	-6.4	1.46	FA	18:3	[M-H] ⁻
	C22H32O2	327.2301	-7.1	1.52	FA	22:6	[M-H] ⁻
	C14H28O2	227.2023	5.1	1.55	FA	14:0	[M-H] ⁻
	C16H30O2	253.2170	0.9	1.65	FA	16:1	[M-H] ⁻
	C20H32O2	303.2309	-5	1.7	FA	20:4	[M-H] ⁻
	C18H32O2	279.2319	-1.9	1.8	FA	18:2	[M-H] ⁻
	C20H34O2	305.2476	-1.6	1.98	FA	20:3	[M-H] ⁻
	C16H32O2	255.2324	-0.1	2.12	FA	16:0	[M-H] ⁻
	C22H36O2	331.2635	-0.7	2.18	FA	22:4	[M-H] ⁻
	C18H34O2	281.2479	-0.6	2.24	FA	18:1	[M-H] ⁻
	C17H34O2	269.2484	1.2	2.47	FA	17:0	[M-H] ⁻
	C18H36O2	283.2638	0.2	2.86	FA	18:0	[M-H] ⁻
	C20H38O2	309.2786	-2.5	2.95	FA	20:1	[M-H] ⁻
	C20H40O2	311.2971	6.6	3.68	FA	20:0	[M-H] ⁻
PC	C42H76NO8P	754.5411	3.2	4.89	PC	34:4	[M+H] ⁺
	C40H76NO8P	730.5409	3.1	4.4	PC	32:2	[M+H] ⁺
	C44H78NO8P	780.5551	1	4.54	PC	36:5	[M+H] ⁺
	C46H76NO8P	802.5403	2	4.54	PC	38:8	[M+H] ⁺
	C46H80NO8P	806.5709	1.2	4.55	PC	38:6	[M+H] ⁺
	C44H76NO8P	778.5371	-2.1	4.59	PC	36:6	[M+H] ⁺
	C44H80NO8P	782.5715	2	4.62	PC	36:4	[M+H] ⁺
	C42H78NO8P	756.5535	-1.1	4.71	PC	34:3	[M+H] ⁺
	C42H82NO7P	744.5935	3.8	4.71	PC-plasm	34:1	[M+H] ⁺
	C44H80NO8P	782.5718	2.4	4.78	PC	36:4	[M+H] ⁺
	C46H80NO8P	806.5729	3.7	4.78	PC	38:6	[M+H] ⁺

C40H78NO8P	732.5576	4.5	4.89	PC	32:1	[M+H] ⁺
C46H78NO8P	804.5527	-2	4.93	PC	37:0	[M+H] ⁺
C44H80NO8P	782.5728	3.6	4.94	PC	36:4	[M+H] ⁺
C35H70NO8P	664.4935	2.7	4.96	PC	28:7	[M+H] ⁺
C46H82NO8P	808.5896	4.9	4.96	PC	38:5	[M+H] ⁺
C42H80NO8P	758.5718	2.4	5.02	PC	34:2	[M+H] ⁺
C44H78NO8P	780.5545	0.2	5.04	PC	36:5	[M+H] ⁺
C44H82NO8P	784.5876	2.5	5.09	PC	36:3	[M+H] ⁺
C44H80NO7P	766.5762	1.4	5.15	PC-plasm	36:4	[M+H] ⁺
C44H82NO8P	784.5876	2.5	5.15	PC	36:3	[M+H] ⁺
C46H82NO8P	808.5851	-0.6	5.15	PC	38:5	[M+H] ⁺
C46H80NO8P	806.5684	-1.9	5.18	PC	38:6	[M+H] ⁺
C43H82NO8P	772.5861	0.6	5.22	PC	35:2	[M+H] ⁺
C46H82NO7P	792.5931	3	5.23	PC-plasm	38:5	[M+H] ⁺
C45H82NO8P	796.5875	2.4	5.23	PC	37:4	[M+H] ⁺
C46H84NO8P	810.6044	3.9	5.23	PC	38:4	[M+H] ⁺
C48H82NO8P	832.5808	-5.8	5.23	PC	39:0	[M+H] ⁺
C46H80NO7P	790.5731	-2.5	5.3	PC-plasm	38:6	[M+H] ⁺
C43H82NO8P	772.5858	0.2	5.31	PC	35:2	[M+H] ⁺
C44H78NO7P	764.5595	0.1	5.32	PC-plasm	36:5	[M+H] ⁺
C46H84NO8P	810.6016	0.4	5.35	PC	38:4	[M+H] ⁺
C48H84NO8P	834.6031	2.2	5.36	PC	40:6	[M+H] ⁺
C40H80NO8P	734.5718	2.5	5.43	PC	32:0	[M+H] ⁺
C44H84NO7P	770.6059	-0.6	5.43	PC-plasm	36:2	[M+H] ⁺
C46H84NO7P	794.6064	0	5.43	PC-plasm	38:4	[M+H] ⁺
C42H82NO8P	760.5883	3.5	5.44	PC	34:1	[M+H] ⁺
C48H86NO7P	820.6230	1.2	5.44	PC-plasm	40:5	[M+H] ⁺
C44H80NO8P	782.5695	-0.6	5.45	PC	36:4	[M+H] ⁺
C46H84NO8P	810.6037	3	5.51	PC	38:4	[M+H] ⁺
C48H82NO8P	832.5830	-3.1	5.51	PC	40:7	[M+H] ⁺
C48H86NO8P	836.6119	-6	5.51	PC	40:5	[M+H] ⁺
C46H82NO8P	808.5830	-3.2	5.58	PC	38:5	[M+H] ⁺
C44H84NO8P	786.6025	1.6	5.59	PC	36:2	[M+H] ⁺
C43H78NO8P	768.5568	3.2	5.66	PC	35:4	[M+H] ⁺
C43H84NO8P	774.6008	-0.6	5.71	PC	35:1	[M+H] ⁺
C42H84NO7P	746.6033	-4.2	5.72	PC-plasm	34:0	[M+H] ⁺
C46H86NO8P	812.6152	-2.1	5.72	PC	38:3	[M+H] ⁺
C48H84NO8P	834.5981	-3.8	5.72	PC	40:6	[M+H] ⁺
C42H84NO8P	762.6032	2.6	5.91	PC	34:0	[M+H] ⁺

	C44H82NO8P	784.5865	1.1	5.91	PC	36:3	[M+H] ⁺
	C44H86NO8P	788.6165	-0.5	5.98	PC	36:1	[M+H] ⁺
	C46H84NO8P	810.5992	-2.5	5.98	PC	38:4	[M+H] ⁺
	C46H88NO8P	814.6338	1.5	6.03	PC	38:2	[M+H] ⁺
	C41H76NO8P	742.5365	-2.9	6.06	PC	33:3	[M+H] ⁺
	C39H78NO8P	720.5533	-1.4	6.06	PC	31:0	[M+H] ⁺
	C46H92NO8P	818.6649	1.3	6.83	PC	38:0	[M+H] ⁺
	C52H96NO8P	894.6934	-2	8.44	PC	44:4	[M+H] ⁺
	C50H96NO8P	870.6982	3.5	8.57	PC	42:2	[M+H] ⁺
	C52H98NO8P	896.7118	1.1	8.6	PC	44:3	[M+H] ⁺
	C52H100NO8P	898.7225	-4.4	8.82	PC	44:2	[M+H] ⁺
	C54H102NO8P	924.7462	4.4	8.83	PC	46:3	[M+H] ⁺
	C48H94NO8P	844.6763	-3.8	8.9	PC	40:2	[M+H] ⁺
	C52H102NO8P	900.7373	-5.3	9.02	PC	44:1	[M+H] ⁺
	C54H106NO8P	928.7690	-4.8	9.21	PC	46:1	[M+H] ⁺
PE	C43H76NO8P	764.5237	0.8	5.16	PE	38:5	[M-H]-
	C39H74NO8P	714.5103	4	5.18	PE	34:2	[M-H]-
	C43H78NO8P	766.5403	2.1	5.65	PE	38:4	[M-H]-
	C41H78NO8P	742.5404	2.3	5.74	PE	36:2	[M-H]-
PG	C32H63O10P	637.4073	-1.2	2.79	PG	26:0	[M-H]-
	C36H71O10P	693.4739	4.6	4	PG	30:0	[M-H]-
	C52H99O10P	913.6851	-5.1	6.26	PG	46:2	[M-H]-
PI	C45H79O13P	857.5202	2.5	3.99	PI	36:4	[M-H]-
	C43H79O13P	833.5187	0.8	4.07	PI	34:2	[M-H]-
	C49H83O13P	909.5511	1.9	4.42	PI	40:6	[M-H]-
	C43H81O13P	835.5377	4.8	4.5	PI	34:1	[M-H]-
	C47H83O13P	885.5524	3.5	4.57	PI	38:4	[M-H]-
	C45H83O13P	861.5481	-1.4	4.64	PI	36:2	[M-H]-
	C47H85O13P	887.5643	-0.8	4.76	PI	38:3	[M-H]-
PS	C37H72NO10P	720.4839	3.2	4.11	PS	31:0	[M-H]-
	C44H80NO10P	812.5402	-4.9	4.32	PS	38:3	[M-H]-
	C42H80NO10P	788.5465	2.9	4.42	PS	36:1	[M-H]-
	C46H82NO10P	838.5621	2.7	4.42	PS	40:4	[M-H]-
	C44H82NO10P	814.5624	3.1	4.53	PS	38:2	[M-H]-
	C46H82NO10P	838.5647	5.8	4.56	PS	40:4	[M-H]-
	C48H84NO10P	864.5773	2.1	4.56	PS	42:5	[M-H]-
	C45H82NO10P	826.5618	2.4	4.66	PS	39:3	[M-H]-
	C46H84NO10P	840.5766	1.3	4.66	PS	40:3	[M-H]-
	C43H82NO10P	802.5607	1.1	4.73	PS	37:1	[M-H]-
	C48H84NO10P	864.5776	2.4	4.79	PS	42:5	[M-H]-
	C47H82NO10P	850.5644	5.4	4.81	PS	41:5	[M-H]-

	C39H72NO10P	744.4801	-2	4.96	PS	33:2	[M-H]-
	C48H86NO10P	866.5933	2.5	4.98	PS	42:4	[M-H]-
	C43H82NO10P	802.5619	2.6	5.04	PS	37:1	[M-H]-
	C44H84NO10P	816.5768	1.6	5.05	PS	38:1	[M-H]-
	C46H86NO10P	842.5944	3.9	5.11	PS	40:2	[M-H]-
	C48H86NO10P	866.5925	1.6	5.16	PS	42:4	[M-H]-
	C45H84NO10P	828.5746	-1.1	5.19	PS	39:2	[M-H]-
	C46H86NO10P	842.5911	0	5.19	PS	40:2	[M-H]-
	C45H86NO10P	830.5872	-4.7	5.26	PS	39:1	[M-H]-
	C44H84NO10P	816.5743	-1.5	5.29	PS	38:1	[M-H]-
	C45H86NO10P	830.5933	2.6	5.31	PS	39:1	[M-H]-
	C44H84NO10P	816.5790	4.3	5.37	PS	38:1	[M-H]-
	C46H86NO10P	842.5946	4.1	5.37	PS	40:2	[M-H]-
	C50H88NO10P	892.6071	0.4	5.37	PS	44:5	[M-H]-
	C44H86NO10P	818.5949	4.6	5.46	PS	38:0	[M-H]-
	C43H84NO10P	804.5775	2.5	5.48	PS	37:0	[M-H]-
	C48H88NO10P	868.6103	4	5.53	PS	42:3	[M-H]-
	C50H90NO10P	894.6236	1.3	5.54	PS	44:4	[M-H]-
	C45H86NO10P	830.5903	-1	5.61	PS	39:1	[M-H]-
	C46H88NO10P	844.6032	-4.2	5.61	PS	40:1	[M-H]-
	C50H90NO10P	894.6234	1.1	5.72	PS	44:4	[M-H]-
	C48H90NO10P	870.6227	0.3	5.74	PS	42:2	[M-H]-
	C47H88NO10P	856.6044	-2.8	5.76	PS	41:2	[M-H]-
	C45H88NO10P	832.6057	-1.3	5.77	PS	39:0	[M-H]-
	C50H92NO10P	896.6399	2	5.91	PS	44:3	[M-H]-
	C45H88NO10P	832.6039	-3.5	6	PS	39:0	[M-H]-
	C46H90NO10P	846.6190	-4.1	6.01	PS	40:0	[M-H]-
	C43H80NO10P	800.5396	-5.7	6.08	PS	37:2	[M-H]-
LPC	C24H48NO7P	494.3251	0.8	1.15	LPC	16:1	[M+H] ⁺
	C28H48NO7P	542.3225	-4.1	1.21	LPC	20:5	[M+H] ⁺
	C22H47NO7P	468.3079	-2.3	1.21	LPC	14:0	[M+H] ⁺
	C26H50NO7P	520.3397	-1.1	1.21	LPC	18:2	[M+H] ⁺
	C30H50NO7P	568.3428	4.4	1.22	LPC	22:6	[M+H] ⁺
	C28H50NO7P	544.3421	3.3	1.23	LPC	20:4	[M+H] ⁺
	C26H50NO7P	520.3394	-1.7	1.26	LPC	18:2	[M+H] ⁺
	C23H48NO7P	482.3244	-0.6	1.42	LPC	15:0	[M+H] ⁺
	C26H48NO7P	518.3246	-0.1	1.43	LPC	18:3	[M+H] ⁺
	C24H50NO7P	496.3399	-0.8	1.45	LPC	16:0	[M+H] ⁺
	C26H52NO7P	522.3538	-4.1	1.57	LPC	18:1	[M+H] ⁺
	C25H52NO7P	510.3568	1.7	1.69	LPC	17:0	[M+H] ⁺
	C27H50NO7P	532.3395	-1.5	1.69	LPC	19:3	[M+H] ⁺

	C26H54NO7P	524.3726	1.9	1.84	LPC	18:0	[M+H] ⁺
	C24H50NO6P	480.3436	-3.7	1.88	LPC	15:1	[M+H] ⁺
	C24H52NO6P	482.3603	-1.7	1.93	LPC	15:0	[M+H] ⁺
	C26H54NO7P	524.3726	1.9	1.97	LPC	18:0	[M+H] ⁺
	C28H52NO7P	546.3549	-1.9	1.99	LPC	20:3	[M+H] ⁺
	C28H52NO7P	546.3559	-0.1	2.02	LPC	20:3	[M+H] ⁺
	C26H54NO6P	508.3758	-1.8	2.06	LPC	17:1	[M+H] ⁺
	C27H56NO7P	538.3885	2.3	2.14	LPC	19:0	[M+H] ⁺
	C27H56NO7P	538.3873	0.1	2.27	LPC	19:0	[M+H] ⁺
LPE	C27H44NO7P	524.2787	1.9	1.21	LPE	22:6	[M-H] ⁻
	C25H44NO7P	500.2798	4.2	1.25	LPE	20:4	[M-H] ⁻
SM	C37H75N2O6P	675.5440	-0.1	4.7	SM	14:0	[M+H] ⁺
	C39H77N2O6P	701.5564	-4.7	4.23	SM	16:1	[M+H] ⁺
	C41H75N2O6P	723.5447	0.9	4.23	SM	18:4	[M+H] ⁺
	C38H77N2O6P	689.5617	2.9	4.45	SM	15:0	[M+H] ⁺
	C39H79N2O6P	703.5767	1.9	4.78	SM	16:0	[M+H] ⁺
	C41H77N2O6P	725.5600	0.4	4.78	SM	18:3	[M+H] ⁺
	C41H81N2O6P	729.5917	0.9	4.89	SM	18:1	[M+H] ⁺
	C43H79N2O6P	751.5771	2.3	4.89	SM	20:4	[M+H] ⁺
	C43H81N2O6P	753.5944	4.5	5.39	SM	20:3	[M+H] ⁺
	C40H81N2O6P	717.5898	-1.8	5.71	SM	17:0	[M+H] ⁺
	C47H87N2O6P	807.6346	-4.2	5.96	SM	24:4	[M+H] ⁺
	C43H87N2O6P	759.6407	3.6	5.98	SM	20:0	[M+H] ⁺
	C41H83N2O6P	731.6089	3	6	SM	18:0	[M+H] ⁺
	C47H91N2O6P	811.6653	-4.9	6.02	SM	24:2	[M+H] ⁺
	C49H89N2O6P	833.6518	-2.2	6.02	SM	26:5	[M+H] ⁺
	C47H87N2O6P	807.6377	-0.3	6.03	SM	24:4	[M+H] ⁺
	C45H89N2O6P	785.6536	0	6.06	SM	22:1	[M+H] ⁺
	C43H85N2O6P	757.6225	0.1	6.12	SM	20:1	[M+H] ⁺
	C37H63N2O6P	663.4521	2.9	6.18	SM	14:6	[M+H] ⁺
	C46H91N2O6P	799.6657	-4.5	6.2	SM	23:1	[M+H] ⁺
	C44H89N2O6P	773.6563	3.5	6.24	SM	21:0	[M+H] ⁺
	C46H91N2O6P	799.6701	1	6.3	SM	23:1	[M+H] ⁺
	C47H93N2O6P	813.6838	-1.4	6.43	SM	24:1	[M+H] ⁺
	C49H91N2O6P	835.6685	-0.9	6.43	SM	26:4	[M+H] ⁺
	C45H91N2O6P	787.6719	3.3	6.44	SM	22:0	[M+H] ⁺
	C47H89N2O6P	809.6506	-3.7	6.44	SM	24:3	[M+H] ⁺
	C47H93N2O6P	813.6871	2.7	6.54	SM	24:1	[M+H] ⁺
	C49H91N2O6P	835.6672	-2.5	6.54	SM	26:4	[M+H] ⁺

	C48H95N2O6P	827.7049	5.2	6.57	SM	25:1	[M+H] ⁺
	C46H93N2O6P	801.6882	4.1	6.68	SM	23:0	[M+H] ⁺
	C48H91N2O6P	823.6712	2.3	6.7	SM	25:3	[M+H] ⁺
	C47H95N2O6P	815.7028	2.7	6.91	SM	24:0	[M+H] ⁺
	C49H93N2O6P	837.6869	2.4	6.92	SM	26:3	[M+H] ⁺
	C45H89N2O6P	785.6570	4.3	8.38	SM	22:1	[M+H] ⁺
	C49H95N2O6P	839.7038	3.8	8.72	SM	26:2	[M+H] ⁺
	C46H93N2O6P	801.6851	0.2	8.78	SM	23:0	[M+H] ⁺
	C49H97N2O6P	841.7189	3.2	8.9	SM	26:1	[M+H] ⁺
	C53H101N2O6P	893.7510	3.9	8.92	SM	30:3	[M+H] ⁺
	C48H97N2O6P	829.7124	-4.6	8.97	SM	25:0	[M+H] ⁺
	C40H75N2O6P	711.5465	3.4	9.11	SM	17:3	[M+H] ⁺
	C50H99N2O6P	855.7324	0.6	9.21	SM	27:1	[M+H] ⁺
	C52H105N2O6P	885.7817	3.2	9.44	SM	29:0	[M+H] ⁺
	C55H109N2O6P	925.8089	-1.3	9.48	SM	32:1	[M+H] ⁺
TG	C47H89NO6	764.6807	5.1	8.03	TG	44:2	[M+NH ₄] ⁺
	C49H91NO6	790.6967	5.3	8.11	TG	46:3	[M+NH ₄] ⁺
	C53H95NO6	842.7266	3.3	8.23	TG	50:5	[M+NH ₄] ⁺
	C57H99NO6	894.7515	-4	8.23	TG	54:7	[M+NH ₄] ⁺
	C45H89NO6	740.6752	-2.1	8.24	TG	42:0	[M+NH ₄] ⁺
	C57H99NO6	894.7515	-4	8.25	TG	54:7	[M+NH ₄] ⁺
	C50H93NO6	804.7063	-2.2	8.25	TG	47:3	[M+NH ₄] ⁺
	C55H97NO6	868.7400	0.7	8.3	TG	52:6	[M+NH ₄] ⁺
	C47H91NO6	766.6937	1.6	8.3	TG	44:1	[M+NH ₄] ⁺
	C49H93NO6	792.7114	4.2	8.3	TG	46:2	[M+NH ₄] ⁺
	C61H101NO6	944.7735	3	8.31	TG	58:10	[M+NH ₄] ⁺
	C51H95NO6	818.7251	1.7	8.33	TG	48:3	[M+NH ₄] ⁺
	C51H95NO6	818.7239	0.1	8.34	TG	48:3	[M+NH ₄] ⁺
	C59H101NO6	920.7708	0.1	8.34	TG	56:8	[M+NH ₄] ⁺
	C46H91NO6	754.6968	5.8	8.36	TG	43:0	[M+NH ₄] ⁺
	C53H97NO6	844.7397	0.4	8.36	TG	50:4	[M+NH ₄] ⁺
	C53H97NO6	844.7397	0.4	8.39	TG	50:4	[M+NH ₄] ⁺
	C57H101NO6	896.7740	3.7	8.41	TG	54:6	[M+NH ₄] ⁺
	C55H99NO6	870.7558	0.8	8.42	TG	52:5	[M+NH ₄] ⁺
	C61H103NO6	946.7879	1.6	8.43	TG	58:9	[M+NH ₄] ⁺
	C50H95NO6	806.7217	-2.5	8.47	TG	47:2	[M+NH ₄] ⁺
	C52H97NO6	832.7440	5.5	8.49	TG	49:3	[M+NH ₄] ⁺
	C59H103NO6	922.7908	4.8	8.54	TG	56:7	[M+NH ₄] ⁺
	C57H101NO6	896.7720	1.5	8.55	TG	54:6	[M+NH ₄] ⁺

C49H95NO6	794.7220	-2.2	8.57	TG	46:1	[M+NH ₄] ⁺
C53H99NO6	846.7567	2	8.58	TG	50:3	[M+NH ₄] ⁺
C51H97NO6	820.7375	-2.3	8.58	TG	48:2	[M+NH ₄] ⁺
C55H101NO6	872.7720	1.5	8.62	TG	52:4	[M+NH ₄] ⁺
C53H99NO6	846.7554	0.4	8.63	TG	50:3	[M+NH ₄] ⁺
C57H103NO6	898.7861	-0.3	8.64	TG	54:5	[M+NH ₄] ⁺
C48H95NO6	782.7242	0.6	8.65	TG	45:0	[M+NH ₄] ⁺
C52H99NO6	834.7592	5	8.67	TG	49:2	[M+NH ₄] ⁺
C54H101NO6	860.7722	1.8	8.7	TG	51:3	[M+NH ₄] ⁺
C50H97NO6	808.7390	-0.5	8.7	TG	47:1	[M+NH ₄] ⁺
C59H105NO6	924.8026	0.7	8.75	TG	56:6	[M+NH ₄] ⁺
C49H97NO6	796.7368	-3.3	8.78	TG	46:0	[M+NH ₄] ⁺
C51H99NO6	822.7565	1.8	8.79	TG	48:1	[M+NH ₄] ⁺
C53H101NO6	848.7715	1	8.8	TG	50:2	[M+NH ₄] ⁺
C55H103NO6	874.7885	2.5	8.82	TG	52:3	[M+NH ₄] ⁺
C58H108NO6	916.8366	3.6	8.82	TG	55:3	[M+NH ₄] ⁺
C61H115NO6	958.8865	6.5	8.82	TG	58:3	[M+NH ₄] ⁺
C57H105NO6	900.8053	3.7	8.83	TG	54:4	[M+NH ₄] ⁺
C54H103NO6	862.7913	5.8	8.92	TG	51:2	[M+NH ₄] ⁺
C61H109NO6	952.8344	1.2	8.99	TG	58:6	[M+NH ₄] ⁺
C51H101NO6	824.7726	2.3	8.99	TG	48:0	[M+NH ₄] ⁺
C59H107NO6	926.8182	0.5	9	TG	56:5	[M+NH ₄] ⁺
C53H103NO6	850.7871	0.9	9	TG	50:1	[M+NH ₄] ⁺
C55H105NO6	876.8063	4.9	9	TG	52:2	[M+NH ₄] ⁺
C60H115NO6	946.8836	3.6	9	TG	57:2	[M+NH ₄] ⁺
C58H11NO6	918.8494	0.4	9.01	TG	55:2	[M+NH ₄] ⁺
C61H117NO6	960.8916	-4.5	9.01	TG	58:2	[M+NH ₄] ⁺
C59H109NO6	928.8317	-1.7	9.02	TG	56:4	[M+NH ₄] ⁺
C57H107NO6	902.8207	3.4	9.04	TG	54:3	[M+NH ₄] ⁺
C51H101NO6	824.7700	-0.8	9.06	TG	48:0	[M+NH ₄] ⁺
C54H105NO6	864.8056	4.2	9.07	TG	51:1	[M+NH ₄] ⁺
C56H107NO6	890.8201	2.7	9.08	TG	53:2	[M+NH ₄] ⁺
C54H105NO6	864.8061	4.8	9.12	TG	51:1	[M+NH ₄] ⁺
C59H111NO6	930.8494	0.4	9.21	TG	56:3	[M+NH ₄] ⁺
C55H109NO6	880.8375	4.8	9.21	TG	52:0	[M+NH ₄] ⁺
C55H107NO6	878.8224	5.4	9.21	TG	52:1	[M+NH ₄] ⁺
C54H99NO6	858.7546	-0.6	9.22	TG	51:4	[M+NH ₄] ⁺
C57H109NO6	904.8358	2.8	9.22	TG	54:2	[M+NH ₄] ⁺
C54H107NO6	866.8201	2.8	9.31	TG	51:0	[M+NH ₄] ⁺

C59H113NO6	932.8600	1.4	9.45	TG	56:2	[M+NH ₄] ⁺
C57H111NO6	906.8511	2.4	9.46	TG	54:1	[M+NH ₄] ⁺
C58H113NO6	920.8690	4.8	9.52	TG	55:1	[M+NH ₄] ⁺
C59H115NO6	934.8801	-0.2	9.59	TG	56:1	[M+NH ₄] ⁺
C57H113NO6	908.8682	4	9.59	TG	54:0	[M+NH ₄] ⁺
C60H117NO6	948.9012	5.6	9.7	TG	57:1	[M+NH ₄] ⁺
C61H113NO6	956.8646	2.2	9.8	TG	58:4	[M+NH ₄] ⁺
C56H109NO6	892.8337	0.4	9.9	TG	53:1	[M+NH ₄] ⁺
C63H121NO6	988.9258	-1.4	9.93	TG	60:2	[M+NH ₄] ⁺
C65H123NO6	1014.9415	-1.4	9.93	TG	62:3	[M+NH ₄] ⁺
C62H121NO6	976.9298	2.7	9.95	TG	59:1	[M+NH ₄] ⁺
C62H123NO6	978.9465	3.7	10.09	TG	59:0	[M+NH ₄] ⁺
C65H125NO6	1016.9623	3.7	10.12	TG	62:2	[M+NH ₄] ⁺
C63H123NO6	990.9436	0.7	10.12	TG	60:1	[M+NH ₄] ⁺

Table S2. 10 most abundant* lipid species found in extracted human plasma

Class	Formula	m/z Found	ppm	Time (min)	Area Abs	provisional assignment
PC	C42H80NO8P	758.5718	2.4	5.02	311	1-acyl 34:2
PC	C44H84NO8P	786.6025	1.6	5.59	210	1-acyl 36:2
PC	C42H82NO8P	760.5883	3.5	5.44	189	1-acyl 34:1
PC	C44H80NO8P	782.5728	3.6	4.94	154	1-acyl 36:4
PC	C44H82NO8P	784.5876	2.5	5.15	134	1-acyl 36:3
TG	C55H103NO6	874.7885	2.5	8.82	109	1-acyl 52:3
TG	C55H105NO6	876.8063	4.9	9	84	1-acyl 52:2
SM	C39H79N2O6P	703.5767	1.9	4.78	60	2-amido 16:0
PC	C46H80NO8P	806.5729	3.7	4.78	58	1-acyl 38:6
TG	C51H99NO6	822.7565	1.8	8.79	15	1-acyl 48:1

* Most abundant as determined by the peak area of the most abundant m/z of each lipid.