

Supplements:

Impaired β -oxidation and altered complex lipid fatty acid partitioning with advancing chronic kidney disease

Authors:

Farsad Afshinnia¹, Thekkelnaycke M. Rajendiran^{2,3}, Tanu Soni², Jaeman Byun¹, Stefanie Wernisch¹, Kelli M. Sas¹, Jennifer Hawkins¹, Keith Bellovich⁴, Debbie Gipson⁵, George Michailidis^{2,6}, Subramaniam Pennathur^{1,2,7}, and the Michigan Kidney Translational Core CPROBE Investigator Group*

¹University of Michigan, Department of Internal Medicine-Nephrology, Ann Arbor, MI

²University of Michigan, Michigan Regional Comprehensive Metabolomics Resource Core, Ann Arbor, MI

³University of Michigan, Department of Pathology, Ann Arbor, MI

⁴ St. Clair Nephrology Research, Detroit, MI

⁵University of Michigan, Department of Pediatrics, Ann Arbor, MI

⁶University of Florida, Gainesville, FL

⁷University of Michigan, Department of Molecular and Integrative Physiology, Ann Arbor, MI

Journal: Journal of American Society of Nephrology

Supplement Table 1: Identified lipids by adducts, mass, and retention time in positive and negative modes. The mass accuracy was ± 0.001 Da in positive mode and ± 0.005 Da in negative mode, with overall mass error of less than 2 parts per million. CE: Cholesterol Esters; DAG: Diacylglycerol; LPC: Lysophosphatidylcholine; LPE: Lysophosphatidylethanolamine; MAG: Monoacylglycerol; PC: Phosphatidylcholine; pPC: Plasmeyl-Phosphatidylcholine; PE: Phosphatidylethanolamine; pPE: Plasmeyl-Phosphatidylethanolamine; PA: Phosphatidic Acid; SM: Sphingomyelin; TAG: Triacylglycerol; FFA: Free Fatty Acid; CerP: Ceramide-Phosphates; CL: Cardiolipin; PG: Phosphatidylglycerol; PI: Phosphatidylinositol

Lipids in Positive Mode				
Class	Compound name	Type of Adducts	m/z	RT/min
CE	CE(16:0)	[M+NH ₄] ⁺	642.6189	10.94
	CE(16:1)	[M+NH ₄] ⁺	640.6032	10.68
	CE(16:2)	[M+NH ₄] ⁺	638.5876	10.51
	CE(17:1)	[M+NH ₄] ⁺	654.6189	10.87
	CE(18:0)	[M+NH ₄] ⁺	670.6502	11.38
	CE(18:1)	[M+NH ₄] ⁺	668.6345	10.92
	CE(18:2)	[M+NH ₄] ⁺	666.6189	10.74
	CE(18:3)	[M+NH ₄] ⁺	664.6032	10.49
	CE(20:1)	[M+NH ₄] ⁺	696.6659	11.3
	CE(20:2)	[M+NH ₄] ⁺	694.6502	11.09
	CE(20:3)	[M+NH ₄] ⁺	692.6345	10.76
	CE(20:4)	[M+NH ₄] ⁺	690.6189	10.55
	CE(20:5)	[M+NH ₄] ⁺	688.6032	10.43
	CE(22:1)	[M+NH ₄] ⁺	724.6972	11.74
	CE(22:4)	[M+NH ₄] ⁺	718.6502	10.87
	CE(22:5)	[M+NH ₄] ⁺	716.6345	10.69
	CE(22:6)	[M+NH ₄] ⁺	714.6189	10.48
	DAG	DAG 28:1	[M+NH ₄] ⁺	528.4625
DAG 30:0		[M+NH ₄] ⁺	558.5094	7.36
DAG 30:1		[M+NH ₄] ⁺	556.4938	6.87
DAG 32:0		[M+NH ₄] ⁺	586.5407	7.89
DAG 32:1		[M+NH ₄] ⁺	584.5251	7.43
DAG 32:2		[M+NH ₄] ⁺	582.5094	7.02
DAG 32:3		[M+NH ₄] ⁺	580.4938	6.55
DAG 33:0		[M+NH ₄] ⁺	600.5564	8.13
DAG 33:1		[M+NH ₄] ⁺	598.5407	7.72
DAG 34:0		[M+NH ₄] ⁺	614.572	8.37
DAG 34:2		[M+NH ₄] ⁺	610.5407	7.54
DAG 34:3		[M+NH ₄] ⁺	608.5251	7.18
DAG 34:4		[M+NH ₄] ⁺	606.5094	6.85
DAG 34:5		[M+NH ₄] ⁺	604.4938	6.49

	DAG 35:1	[M+NH4] ⁺	626.572	8.21
	DAG 35:2	[M+NH4] ⁺	624.5564	7.83
	DAG 35:3	[M+NH4] ⁺	622.5407	7.45
	DAG 36:0	[M+NH4] ⁺	642.6033	8.85
	DAG 36:1	[M+NH4] ⁺	640.5877	8.42
	DAG 36:2	[M+NH4] ⁺	638.572	8.02
	DAG 36:3	[M+NH4] ⁺	636.5564	7.66
	DAG 36:4	[M+NH4] ⁺	634.5407	7.33
	DAG 36:5	[M+NH4] ⁺	632.5251	6.94
	DAG 36:6	[M+NH4] ⁺	630.5094	6.65
	DAG 38:0	[M+NH4] ⁺	670.6346	8.94
	DAG 38:1	[M+NH4] ⁺	668.6189	8.73
	DAG 38:2	[M+NH4] ⁺	666.6033	8.49
	DAG 38:3	[M+NH4] ⁺	664.5877	8.20
	DAG 38:4	[M+NH4] ⁺	662.572	7.92
	DAG 38:5	[M+NH4] ⁺	660.5564	7.57
	DAG 38:6	[M+NH4] ⁺	658.5407	7.27
	DAG 38:7	[M+NH4] ⁺	656.5251	6.88
	DAG 40:0	[M+NH4] ⁺	698.6659	9.56
	DAG 40:5	[M+NH4] ⁺	688.5877	8.03
	DAG 40:6	[M+NH4] ⁺	686.572	7.74
	DAG 40:7	[M+NH4] ⁺	684.5564	7.51
	DAG 40:8	[M+NH4] ⁺	682.5407	7.13
LPC	LPC 14:0	[M+H] ⁺	468.309	1.08
	LPC 14:0	[M+Na] ⁺	490.291	1.05
	LPC 15:0	[M+H] ⁺	482.3246	1.20
	LPC 15:0	[M+Na] ⁺	504.3066	1.21
	LPC 16:0	[M+H] ⁺	496.3403	1.46
	LPC 16:0	[M+Na] ⁺	504.343	1.82
	LPC 16:1	[M+Na] ⁺	516.3066	1.14
	LPC 17:0	[M+Na] ⁺	532.3379	2.20
	LPC 17:1	[M+H] ⁺	508.3403	1.40
	LPC 18:0	[M+H] ⁺	524.3716	2.30
	LPC 18:0	[M+Na] ⁺	530.3586	2.03
	LPC 18:1	[M+Na] ⁺	544.3379	1.81
	LPC 18:2	[M+Na] ⁺	542.3223	1.09
	LPC 18:3	[M+H] ⁺	518.3246	1.09
	LPC 18:3	[M+Na] ⁺	540.3066	1.05
	LPC 19:0	[M+H] ⁺	538.3873	2.73
	LPC 19:0	[M+Na] ⁺	560.3692	2.76
	LPC 20:0	[M+H] ⁺	552.4029	3.22

	LPC 20:0	[M+Na] ⁺	574.3848	3.17
	LPC 20:1	[M+H] ⁺	550.3873	2.48
	LPC 20:1	[M+Na] ⁺	572.3692	2.47
	LPC 20:2	[M+H] ⁺	548.3716	1.86
	LPC 20:3	[M+Na] ⁺	568.3379	1.42
	LPC 20:5	[M+H] ⁺	542.3246	1.01
	LPC 22:0	[M+H] ⁺	580.4342	4.13
	LPC 22:4	[M+H] ⁺	572.3716	1.76
	LPC 22:4	[M+Na] ⁺	594.3535	1.82
	LPC 22:5	[M+H] ⁺	570.356	1.47
	LPC 22:5	[M+Na] ⁺	592.3379	1.45
	LPC 24:0	[M+H] ⁺	608.4655	5.03
	LPC 24:1	[M+H] ⁺	606.4498	4.18
	LPC 26:1	[M+H] ⁺	634.4812	5.02
LPE	LPE 16:0	[M+H] ⁺	454.2934	1.62
	LPE 18:0	[M+H] ⁺	482.3246	2.45
	LPE 18:0	[M+Na] ⁺	504.3066	2.46
	LPE 18:1	[M+H] ⁺	480.309	1.76
	LPE 18:2	[M+H] ⁺	478.2934	1.32
	LPE 18:3	[M+H] ⁺	476.2777	1.08
	LPE 20:3	[M+H] ⁺	504.309	1.55
	LPE 20:4	[M+H] ⁺	502.2934	1.25
	LPE 22:5	[M+H] ⁺	528.309	1.46
	LPE 22:6	[M+H] ⁺	526.2933	1.19
MAG	MAG 17:0	[M+Li] ⁺	351.3087	3.12
	MAG 18:1	[M+NH ₄] ⁺	374.327	2.90
	MAG 18:2	[M+NH ₄] ⁺	372.3114	2.26
PA	PA 34:0	[M+Na] ⁺	699.4941	13.75
PC	PC 28:0	[M+Na] ⁺	700.4893	5.11
	PC 30:0	[M+Na] ⁺	728.5206	5.85
	PC 30:1	[M+Na] ⁺	726.505	5.33
	PC 32:0	[M+H] ⁺	734.57	5.36
	PC 32:1	[M+Na] ⁺	754.5363	5.99
	PC 32:2	[M+Na] ⁺	752.5206	5.51
	PC 33:3	[M+H] ⁺	742.5387	5.39
	PC 34:0	[M+Na] ⁺	784.5832	7.07
	PC 34:3	[M+Na] ⁺	778.5363	5.65
	PC 34:4	[M+H] ⁺	754.5387	6.02
	PC 34:4	[M+Na] ⁺	776.5206	5.49
	PC 35:5	[M+H] ⁺	766.5387	5.41
	PC 36:1	[M+Na] ⁺	810.5989	7.18

	PC 36:3	[M+H] ⁺	784.5856	7.10
	PC 36:4	[M+H] ⁺	782.57	4.68
	PC 36:4	[M+Na] ⁺	804.5519	5.85
	PC 36:5	[M+H] ⁺	780.5543	4.28
	PC 36:5	[M+Na] ⁺	802.5363	5.58
	PC 36:6	[M+Na] ⁺	800.5206	5.31
	PC 36:7	[M+H] ⁺	776.523	5.25
	PC 38:4	[M+Na] ⁺	832.5832	6.75
	PC 38:5	[M+H] ⁺	808.5856	5.06
	PC 38:6	[M+H] ⁺	806.57	4.85
	PC 38:6	[M+Na] ⁺	828.5519	5.99
	PC 38:7	[M+H] ⁺	804.5543	5.87
	PC 38:7	[M+Na] ⁺	826.5363	5.46
	PC 38:8	[M+H] ⁺	802.5387	5.41
	PC 40:10	[M+H] ⁺	826.5387	5.55
	PC 40:8	[M+Na] ⁺	852.5519	5.70
	PC 40:9	[M+H] ⁺	828.5543	5.86
	PC 42:10	[M+H] ⁺	854.57	5.63
	PC 42:11	[M+H] ⁺	852.5543	5.68
	PC 42:9	[M+H] ⁺	856.5856	6.69
PE	PE 34:1	[M+H] ⁺	718.5387	6.74
	PE 34:2	[M+H] ⁺	716.523	6.29
	PE 34:3	[M+H] ⁺	714.5074	5.94
	PE 35:1	[M+H] ⁺	732.5543	6.99
	PE 35:2	[M+H] ⁺	730.5387	6.66
	PE 36:0	[M+H] ⁺	748.5856	7.76
	PE 36:1	[M+H] ⁺	746.57	7.35
	PE 36:2	[M+H] ⁺	744.5543	6.89
	PE 36:4	[M+H] ⁺	740.523	6.31
	PE 36:5	[M+H] ⁺	738.5074	5.88
	PE 37:6	[M+H] ⁺	750.5074	5.86
	PE 38:3	[M+H] ⁺	770.57	7.15
	PE 38:4	[M+H] ⁺	768.5543	6.90
	PE 38:6	[M+H] ⁺	764.523	6.10
	PE 40:6	[M+H] ⁺	792.5543	6.86
	PE 40:7	[M+H] ⁺	790.5387	6.27
pPC	pPC 18:0	[M+Na] ⁺	544.3379	1.73
	pPC 20:0	[M+Na] ⁺	572.3692	2.45
	pPC 36:1	[M+Na] ⁺	794.604	7.48
	pPC 36:4	[M+Na] ⁺	788.557	6.45
	pPC 40:4	[M+Na] ⁺	844.6196	7.40

	pPC 44:4	[M+Na] ⁺	900.6822	8.16
pPE	pPE 34:0	[M+H] ⁺	704.5594	7.55
	pPE 34:1	[M+H] ⁺	702.5438	7.10
	pPE 34:2	[M+H] ⁺	700.5281	6.65
	pPE 36:1	[M+H] ⁺	730.5751	7.62
	pPE 36:2	[M+H] ⁺	728.5594	7.20
	pPE 36:4	[M+H] ⁺	724.5281	6.58
	pPE 36:5	[M+H] ⁺	722.5125	6.25
	pPE 38:1	[M+H] ⁺	758.6063	8.08
	pPE 38:2	[M+H] ⁺	756.5907	7.81
	pPE 38:3	[M+H] ⁺	754.5751	7.42
	pPE 38:4	[M+H] ⁺	752.5594	7.21
	pPE 38:5	[M+H] ⁺	750.5438	6.71
	pPE 38:6	[M+H] ⁺	748.5281	6.49
	pPE 40:4	[M+H] ⁺	780.5907	7.70
	pPE 40:6	[M+H] ⁺	776.5594	7.12
SM	SM 21:1	[M] ⁺	521.3719	1.26
	SM 28:0	[M] ⁺	621.4971	3.83
	SM 30:1	[M+Na] ⁺	669.4948	4.26
	SM 31:1	[M] ⁺	661.5284	4.66
	SM 32:0	[M+Na] ⁺	699.5417	5.36
	SM 32:1	[M+Na] ⁺	697.5261	4.99
	SM 32:2	[M] ⁺	673.5284	4.50
	SM 32:2	[M+Na] ⁺	695.5104	4.43
	SM 33:1	[M+Na] ⁺	711.5417	5.37
	SM 33:2	[M] ⁺	687.5441	4.85
	SM 33:2	[M+Na] ⁺	709.5261	4.82
	SM 34:0	[M+Na] ⁺	727.573	6.03
	SM 34:1	[M] ⁺	703.5754	5.73
	SM 34:1	[M+Na] ⁺	725.5573	5.72
	SM 34:2	[M+Na] ⁺	723.5417	5.17
	SM 35:0	[M] ⁺	719.6067	6.56
	SM 35:1	[M+Na] ⁺	739.573	6.07
	SM 35:2	[M+Na] ⁺	737.5573	5.59
	SM 36:1	[M+Na] ⁺	753.5886	6.46
	SM 36:2	[M] ⁺	729.5911	5.89
	SM 36:2	[M+Na] ⁺	751.573	5.94
	SM 37:1	[M] ⁺	745.6224	6.81
	SM 37:2	[M] ⁺	743.6067	6.29
SM 38:0	[M] ⁺	761.6536	7.33	
SM 38:1	[M+Na] ⁺	781.6199	7.07	

	SM 38:4	[M] ⁺	753.5911	5.57
	SM 38:5	[M] ⁺	751.5754	5.12
	SM 39:1	[M+Na] ⁺	795.6356	7.40
	SM 39:2	[M] ⁺	771.638	6.84
	SM 40:1	[M+Na] ⁺	809.6513	7.59
	SM 40:2	[M] ⁺	785.6536	6.88
	SM 40:2	[M+Na] ⁺	807.6356	7.18
	SM 40:4	[M] ⁺	781.6224	6.24
	SM 41:0	[M] ⁺	803.7006	8.09
	SM 41:1	[M+Na] ⁺	823.6669	7.87
	SM 41:2	[M+Na] ⁺	821.6513	7.42
	SM 41:4	[M] ⁺	795.638	6.50
	SM 42:1	[M+Na] ⁺	837.6826	8.12
	SM 42:2	[M] ⁺	813.6849	7.64
	SM 42:2	[M+Na] ⁺	835.6669	7.64
	SM 42:4	[M] ⁺	809.6536	6.81
	SM 42:5	[M] ⁺	807.638	6.45
	SM 43:1	[M] ⁺	829.7163	8.43
	SM 43:1	[M+Na] ⁺	851.6982	8.31
	SM 43:2	[M] ⁺	827.7006	8.05
	SM 43:2	[M+Na] ⁺	849.6826	7.79
	SM 43:4	[M] ⁺	823.6693	7.01
	SM 44:1	[M] ⁺	843.7319	8.60
	SM 44:2	[M] ⁺	841.7163	8.13
TAG	TAG 40:0	[M+NH ₄] ⁺	712.6451	9.49
	TAG 42:0	[M+Na] ⁺	745.6318	9.77
	TAG 42:0	[M+NH ₄] ⁺	740.6764	9.76
	TAG 42:1	[M+NH ₄] ⁺	738.6608	9.50
	TAG 44:1	[M+NH ₄] ⁺	766.6921	9.82
	TAG 44:2	[M+NH ₄] ⁺	764.6764	9.53
	TAG 46:0	[M+NH ₄] ⁺	796.739	10.31
	TAG 46:1	[M+NH ₄] ⁺	794.7233	10.07
	TAG 46:2	[M+NH ₄] ⁺	792.7077	9.83
	TAG 46:3	[M+NH ₄] ⁺	790.6921	9.59
	TAG 48:0	[M+NH ₄] ⁺	824.7702	10.54
	TAG 48:1	[M+Na] ⁺	827.71	8.98
	TAG 48:1	[M+NH ₄] ⁺	822.7546	10.31
	TAG 48:2	[M+NH ₄] ⁺	820.739	10.09
	TAG 48:3	[M+NH ₄] ⁺	818.7233	9.86
	TAG 49:0	[M+NH ₄] ⁺	838.7859	10.68
	TAG 49:1	[M+NH ₄] ⁺	836.7702	10.48

TAG 49:2	[M+NH4] ⁺	834.7546	10.24
TAG 50:0	[M+NH4] ⁺	852.8015	10.80
TAG 50:1	[M+Na] ⁺	855.7413	9.29
TAG 50:1	[M+NH4] ⁺	850.7859	10.54
TAG 50:2	[M+NH4] ⁺	848.7702	10.34
TAG 50:3	[M+NH4] ⁺	846.7546	10.13
TAG 50:4	[M+NH4] ⁺	844.739	9.93
TAG 50:5	[M+NH4] ⁺	842.7233	9.74
TAG 51:1	[M+NH4] ⁺	864.8015	10.71
TAG 51:2	[M+NH4] ⁺	862.7859	10.51
TAG 51:3	[M+NH4] ⁺	860.7702	10.31
TAG 51:4	[M+NH4] ⁺	858.7546	10.11
TAG 52:0	[M+NH4] ⁺	880.8328	11.04
TAG 52:1	[M+Na] ⁺	883.7726	10.68
TAG 52:1	[M+NH4] ⁺	878.8172	10.82
TAG 52:2	[M+NH4] ⁺	876.8015	10.57
TAG 52:3	[M+Na] ⁺	879.7413	10.40
TAG 52:3	[M+NH4] ⁺	874.7859	10.38
TAG 52:4	[M+Na] ⁺	877.7257	10.22
TAG 52:4	[M+NH4] ⁺	872.7702	10.19
TAG 52:5	[M+Na] ⁺	875.71	10.01
TAG 52:5	[M+NH4] ⁺	870.7546	9.99
TAG 52:6	[M+Na] ⁺	873.6944	9.80
TAG 52:6	[M+NH4] ⁺	868.739	9.81
TAG 52:7	[M+NH4] ⁺	866.7233	9.61
TAG 53:0	[M+NH4] ⁺	894.8484	11.16
TAG 53:1	[M+NH4] ⁺	892.8328	10.93
TAG 53:2	[M+NH4] ⁺	890.8172	10.74
TAG 53:3	[M+NH4] ⁺	888.8015	10.54
TAG 53:4	[M+NH4] ⁺	886.7859	10.35
TAG 53:5	[M+NH4] ⁺	884.7702	10.17
TAG 53:6	[M+NH4] ⁺	882.7546	9.96
TAG 53:7	[M+NH4] ⁺	880.739	9.77
TAG 54:0	[M+Na] ⁺	913.8195	11.28
TAG 54:0	[M+NH4] ⁺	908.8641	11.28
TAG 54:1	[M+Na] ⁺	911.8038	11.03
TAG 54:1	[M+NH4] ⁺	906.8484	11.06
TAG 54:2	[M+Na] ⁺	909.7882	10.87
TAG 54:2	[M+NH4] ⁺	904.8328	10.85
TAG 54:3	[M+Na] ⁺	907.7726	10.69
TAG 54:3	[M+NH4] ⁺	902.8172	10.66

TAG 54:4	[M+NH4] ⁺	900.8015	10.44
TAG 54:5	[M+Na] ⁺	903.7413	10.33
TAG 54:5	[M+NH4] ⁺	898.7859	10.24
TAG 54:6	[M+Na] ⁺	901.7257	10.06
TAG 54:6	[M+NH4] ⁺	896.7702	10.06
TAG 54:7	[M+Na] ⁺	899.71	9.85
TAG 54:7	[M+NH4] ⁺	894.7546	9.90
TAG 54:8	[M+NH4] ⁺	892.739	9.71
TAG 55:0	[M+NH4] ⁺	922.8797	11.39
TAG 55:1	[M+NH4] ⁺	920.8641	11.17
TAG 55:3	[M+NH4] ⁺	916.8328	10.77
TAG 55:5	[M+NH4] ⁺	912.8015	10.46
TAG 55:6	[M+NH4] ⁺	910.7859	10.29
TAG 56:0	[M+NH4] ⁺	936.8954	11.54
TAG 56:1	[M+NH4] ⁺	934.8797	11.30
TAG 56:2	[M+NH4] ⁺	932.8641	11.09
TAG 56:3	[M+NH4] ⁺	930.8484	10.88
TAG 56:4	[M+NH4] ⁺	928.8328	10.71
TAG 56:5	[M+Na] ⁺	931.7726	10.57
TAG 56:5	[M+NH4] ⁺	926.8172	10.55
TAG 56:6	[M+NH4] ⁺	924.8015	10.38
TAG 56:7	[M+Na] ⁺	927.7413	10.20
TAG 56:7	[M+NH4] ⁺	922.7859	10.20
TAG 56:8	[M+NH4] ⁺	920.7702	10.02
TAG 56:9	[M+Na] ⁺	923.71	9.87
TAG 56:9	[M+NH4] ⁺	918.7546	9.82
TAG 57:2	[M+NH4] ⁺	946.8797	11.23
TAG 57:3	[M+NH4] ⁺	944.8641	11.00
TAG 57:6	[M+NH4] ⁺	938.8172	10.50
TAG 57:7	[M+NH4] ⁺	936.8015	10.36
TAG 57:8	[M+NH4] ⁺	934.7859	10.17
TAG 58:0	[M+NH4] ⁺	964.9267	11.85
TAG 58:1	[M+NH4] ⁺	962.911	11.57
TAG 58:10	[M+NH4] ⁺	944.7702	9.95
TAG 58:11	[M+NH4] ⁺	942.7546	9.77
TAG 58:12	[M+NH4] ⁺	940.739	9.57
TAG 58:2	[M+NH4] ⁺	960.8954	11.32
TAG 58:3	[M+NH4] ⁺	958.8797	11.12
TAG 58:4	[M+NH4] ⁺	956.8641	10.93
TAG 58:5	[M+NH4] ⁺	954.8484	10.80
TAG 58:6	[M+NH4] ⁺	952.8328	10.60

	TAG 58:7	[M+NH4] ⁺	950.8172	10.50
	TAG 58:8	[M+NH4] ⁺	948.8015	10.29
	TAG 58:9	[M+NH4] ⁺	946.7859	10.14
	TAG 60:10	[M+NH4] ⁺	972.8015	10.18
	TAG 60:11	[M+NH4] ⁺	970.7859	10.09
	TAG 60:12	[M+NH4] ⁺	968.7702	9.90
	TAG 60:15	[M+NH4] ⁺	962.7233	9.31
	TAG 60:3	[M+NH4] ⁺	986.911	11.24
	TAG 60:8	[M+NH4] ⁺	976.8328	10.53
	TAG 62:12	[M+NH4] ⁺	996.8015	10.17
	TAG 62:14	[M+NH4] ⁺	992.7702	9.84
	TAG 62:3	[M+NH4] ⁺	1014.942	11.58

Lipids in Negative Mode				
Class	Sample.Name	Adducts	m/z	RT/min
FFA	FFA (16:0)		255.2329	2.30
	FFA(18:0)		283.2642	3.27
	FFA(18:1)		281.2486	2.50
	FFA(18:2)		279.2329	1.92
	FFA(20:0)		311.2955	4.30
	FFA(20:1)		309.2799	3.45
	FFA(20:2)		307.2642	2.82
	FFA (20:4)		303.2329	1.85
	FFA(22:0)		339.3268	5.29
	FFA(22:1)		337.3112	4.43
	FFA(22:2)		335.2955	3.76
	FFA(22:3)		333.2799	3.18
	FFA(24:0)		367.3581	6.21
	FFA(24:1)		365.3425	5.36
	FFA(24:2)		363.3268	4.70
FFA(24:3)		361.3112	4.07	
CerP	CerP 32:1	[M-H] ⁻	588.4393	5.02
	CerP 34:1	[M-H] ⁻	616.4706	5.75
CL	CL 66:1	[M-2H](2 ⁻)	688.4861	6.17
	CL 70:5	[M-2H](2 ⁻)	712.4861	5.95
	CL 72:3	[M-2H](2 ⁻)	728.5174	7.52
	CL 74:1	[M-2H](2 ⁻)	744.5487	6.75
	CL 74:3	[M-2H](2 ⁻)	742.5331	5.67
	CL 74:5	[M-2H](2 ⁻)	740.5174	5.83
	CL 74:7	[M-2H](2 ⁻)	738.5018	6.03
	CL 76:11	[M-2H](2 ⁻)	748.4861	5.88

	CL 78:3	[M-2H](2-)	770.5644	7.41
	CL 78:5	[M-2H](2-)	768.5487	6.31
	CL 82:13	[M-2H](2-)	788.5174	6.32
	CL 82:9	[M-2H](2-)	792.5487	7.01
LPE	LPE 16:0	[M-H]-	452.2777	1.60
	LPE 17:0	[M-H]-	466.2934	1.92
	LPE 18:0	[M-H]-	480.309	2.34
	LPE 18:1	[M-H]-	478.2934	1.76
	LPE 18:2	[M-H]-	476.2777	1.31
	LPE 20:3	[M-H]-	502.2934	1.59
	LPE 20:4	[M-H]-	500.2777	1.29
	LPE 20:5	[M-H]-	498.2621	1.05
	LPE 22:4	[M-H]-	528.309	1.85
	LPE 22:5	[M-H]-	526.2934	1.49
	LPE 22:6	[M-H]-	524.2777	1.26
	LPE 24:0	[M-H]-	564.403	5.18
PA	PA 34:1	[M-H]-	673.4808	6.58
	PA 34:2	[M-H]-	671.4652	6.15
	PA 36:4	[M-H]-	695.4652	6.08
	PA 38:6	[M-H]-	719.4652	6.03
PC	PC 24:0	[M-Ac-H]-	680.4503	3.58
	PC 26:0	[M-Ac-H]-	708.4816	4.38
	PC 28:0	[M-Ac-H]-	736.5129	5.15
	PC 29:0	[M-Ac-H]-	750.5285	5.48
	PC 30:0	[M-Ac-H]-	764.5442	5.87
	PC 30:1	[M-Ac-H]-	762.5285	5.31
	PC 31:0	[M-Ac-H]-	778.5598	6.03
	PC 32:0	[M-Ac-H]-	792.5754	6.50
	PC 32:1	[M-Ac-H]-	790.5598	6.01
	PC 32:2	[M-Ac-H]-	788.5442	5.51
	PC 32:3	[M-Ac-H]-	786.5285	5.06
	PC 33:0	[M-Ac-H]-	806.5911	6.71
	PC 33:1	[M-Ac-H]-	804.5754	6.33
	PC 33:2	[M-Ac-H]-	802.5598	5.87
	PC 33:3	[M-Ac-H]-	800.5442	5.43
	PC 34:0	[M-Ac-H]-	820.6068	7.06
	PC 34:1	[M-Ac-H]-	818.5911	6.56
	PC 34:2	[M-Ac-H]-	816.5754	4.60
	PC 34:3	[M-Ac-H]-	814.5598	5.69
	PC 34:4	[M-Ac-H]-	812.5442	5.46
	PC 34:5	[M-Ac-H]-	810.5285	5.05

	PC 35:1	[M-Ac-H]-	832.6068	6.91
	PC 35:2	[M-Ac-H]-	830.5911	6.45
	PC 35:3	[M-Ac-H]-	828.5754	6.02
	PC 35:4	[M-Ac-H]-	826.5598	5.85
	PC 35:5	[M-Ac-H]-	824.5442	5.42
	PC 36:1	[M-Ac-H]-	846.6224	7.16
	PC 36:2	[M-Ac-H]-	844.6068	6.72
	PC 36:3	[M-Ac-H]-	842.5911	4.71
	PC 36:4	[M-Ac-H]-	840.5754	4.96
	PC 36:5	[M-Ac-H]-	838.5598	5.57
	PC 36:6	[M-Ac-H]-	836.5442	5.34
	PC 37:1	[M-Ac-H]-	860.6381	7.39
	PC 37:2	[M-Ac-H]-	858.6224	7.06
	PC 37:3	[M-Ac-H]-	856.6068	6.65
	PC 37:4	[M-Ac-H]-	854.5911	6.44
	PC 37:5	[M-Ac-H]-	852.5754	5.96
	PC 37:6	[M-Ac-H]-	850.5598	5.71
	PC 38:1	[M-Ac-H]-	874.6537	7.6
	PC 38:2	[M-Ac-H]-	872.6381	7.32
	PC 38:3	[M-Ac-H]-	870.6224	6.97
	PC 38:4	[M-Ac-H]-	868.6068	6.65
	PC 38:5	[M-Ac-H]-	866.5911	6.27
	PC 38:6	[M-Ac-H]-	864.5754	5.92
	PC 38:7	[M-Ac-H]-	862.5598	5.45
	PC 39:4	[M-Ac-H]-	882.6224	6.98
	PC 39:5	[M-Ac-H]-	880.6068	6.53
	PC 39:6	[M-Ac-H]-	878.5911	6.32
	PC 40:1	[M-Ac-H]-	902.685	8.19
	PC 40:2	[M-Ac-H]-	900.6694	7.94
	PC 40:3	[M-Ac-H]-	898.6537	7.42
	PC 40:4	[M-Ac-H]-	896.6381	7.19
	PC 40:5	[M-Ac-H]-	894.6224	6.94
	PC 40:6	[M-Ac-H]-	892.6068	6.58
	PC 40:7	[M-Ac-H]-	890.5911	6.10
	PC 40:8	[M-Ac-H]-	888.5754	5.70
	PC 40:9	[M-Ac-H]-	886.5598	5.30
	PC 42:10	[M-Ac-H]-	912.5754	5.63
	PC 42:2	[M-Ac-H]-	928.7007	8.38
	PC 42:4	[M-Ac-H]-	924.6694	7.84
	PC 42:5	[M-Ac-H]-	922.6537	7.32
	PC 42:7	[M-Ac-H]-	918.6224	6.73

	PC 44:2	[M-Ac-H]-	956.7319	8.86
	PC 44:4	[M-Ac-H]-	952.7007	8.37
	PC 44:5	[M-Ac-H]-	950.685	7.86
PE	PE 30:0	[M-H]-	662.4761	6.03
	PE 32:0	[M-H]-	690.5074	6.65
	PE 32:1	[M-H]-	688.4917	6.18
	PE 32:2	[M-H]-	686.4761	5.65
	PE 33:1	[M-H]-	702.5074	6.47
	PE 33:2	[M-H]-	700.4917	6.02
	PE 34:1	[M-H]-	716.5231	6.78
	PE 34:2	[M-H]-	714.5074	5.02
	PE 34:2	[M-H]-	714.5074	6.31
	PE 34:3	[M-H]-	712.4917	5.98
	PE 34:4	[M-H]-	710.4761	5.64
	PE 35:0	[M-H]-	732.5543	7.49
	PE 35:1	[M-H]-	730.5387	7.05
	PE 35:2	[M-H]-	728.5231	6.60
	PE 35:3	[M-H]-	726.5074	6.17
	PE 35:4	[M-H]-	724.4917	6.00
	PE 36:0	[M-H]-	746.57	7.77
	PE 36:1	[M-H]-	744.5543	7.35
	PE 36:2	[M-H]-	742.5387	6.91
	PE 36:3	[M-H]-	740.5231	6.46
	PE 36:4	[M-H]-	738.5074	6.14
	PE 36:5	[M-H]-	736.4917	5.88
	PE 37:2	[M-H]-	756.5543	6.15
	PE 37:3	[M-H]-	754.5387	6.74
	PE 37:4	[M-H]-	752.5231	6.62
	PE 37:5	[M-H]-	750.5074	6.03
	PE 38:1	[M-H]-	772.5856	7.82
	PE 38:2	[M-H]-	770.57	7.41
	PE 38:3	[M-H]-	768.5543	7.15
	PE 38:4	[M-H]-	766.5387	6.89
	PE 38:5	[M-H]-	764.5231	6.45
	PE 38:6	[M-H]-	762.5074	6.09
	PE 39:4	[M-H]-	780.5543	7.04
PE 39:5	[M-H]-	778.5387	6.60	
PE 39:6	[M-H]-	776.5231	6.46	
PE 40:3	[M-H]-	796.5856	6.99	
PE 40:4	[M-H]-	794.57	7.35	
PE 40:5	[M-H]-	792.5543	7.05	

	PE 40:6	[M-H]-	790.5387	6.81
	PE 40:7	[M-H]-	788.5231	6.32
	PE 40:8	[M-H]-	786.5074	5.91
	PE 42:8	[M-H]-	814.5387	6.43
	PE 42:9	[M-H]-	812.5231	6.00
PG	PG 33:0	[M-H]-	735.5176	6.08
	PG 34:1	[M-H]-	747.5176	5.88
	PG 34:2	[M-H]-	745.5019	5.47
	PG 36:0	[M-H]-	777.5646	6.90
	PG 36:1	[M-H]-	775.5489	6.47
	PG 36:2	[M-H]-	773.5333	6.04
	PG 36:3	[M-H]-	771.5176	5.41
	PG 36:4	[M-H]-	769.5019	5.46
	PG 38:4	[M-H]-	797.5333	6.07
PI	PI 34:1	[M-H]-	835.5337	5.72
	PI 34:2	[M-H]-	833.518	5.28
	PI 36:1	[M-H]-	863.5649	6.33
	PI 36:2	[M-H]-	861.5493	5.91
	PI 36:3	[M-H]-	859.5337	5.43
	PI 36:4	[M-H]-	857.518	5.27
	PI 38:3	[M-H]-	887.5649	6.12
	PI 38:4	[M-H]-	885.5493	5.89
	PI 38:5	[M-H]-	883.5337	5.41
	PI 40:6	[M-H]-	909.5493	5.83
pPE	pPE 32:0	[M-H]-	674.5124	7.04
	pPE 32:1	[M-H]-	672.4968	6.51
	pPE 34:0	[M-H]-	702.5438	7.25
	pPE 34:1	[M-H]-	700.5281	7.08
	pPE 34:2	[M-H]-	698.5124	6.64
	pPE 34:3	[M-H]-	696.4968	6.28
	pPE 36:0	[M-H]-	730.5751	8.04
	pPE 36:1	[M-H]-	728.5594	7.64
	pPE 36:2	[M-H]-	726.5438	7.24
	pPE 36:3	[M-H]-	724.5281	6.83
	pPE 36:4	[M-H]-	722.5124	6.59
	pPE 36:5	[M-H]-	720.4968	6.26
	pPE 38:1	[M-H]-	756.5907	8.14
	pPE 38:2	[M-H]-	754.5751	7.78
	pPE 38:3	[M-H]-	752.5594	7.42
	pPE 38:4	[M-H]-	750.5438	7.15
	pPE 38:5	[M-H]-	748.5281	6.66

	pPE 38:6	[M-H]-	746.5124	6.48
	pPE 40:3	[M-H]-	780.5907	7.70
	pPE 40:4	[M-H]-	778.5751	7.68
	pPE 40:5	[M-H]-	776.5594	7.24
	pPE 40:5	[M-H]-	776.5594	7.48
	pPE 40:6	[M-H]-	774.5438	7.10
	pPE 42:5	[M-H]-	804.5907	7.80
	pPE 42:6	[M-H]-	802.5751	7.68

Supplement Table 2: Alignment of various lipid species in to different principle components using principle component analysis.

TAG			DAG		SM			CE		CL	
Short LDB	Long LDB	Long HDB	Short LDB	Long HDB	Short LDB	Long LDB	Long HDB	Short LDB	Long HDB	LDB	HDB
TAG 40:0	TAG 54:0	TAG 52:7	DAG 30:0	DAG 34:2	SM 30:1	SM 38:1	SM 34:1	CE 16:1	CE 20:4	CL 74:3	CL 66:1
TAG 42:0	TAG 54:1	TAG 54:8	DAG 30:1	DAG 34:3	SM 32:1	SM 40:1	SM 36:2	CE 16:2	CE 22:4	CL 78:3	CL 70:5
TAG 42:1	TAG 54:2	TAG 56:6	DAG 32:0	DAG 34:4	SM 32:2	SM 42:1	SM 38:0	CE 18:1	CE 22:5	CL 78:5	CL 74:1
TAG 44:1	TAG 54:3	TAG 56:7	DAG 32:1	DAG 36:4	SM 34:2		SM 38:4	CE 20:2	CE 22:6		CL 74:7
TAG 44:2	TAG 54:4	TAG 56:8	DAG 32:2	DAG 36:5			SM 40:4	CE 20:3			CL 76:11
TAG 46:0	TAG 56:1	TAG 56:9	DAG 34:0	DAG 36:6			SM 42:2				CL 82:13
TAG 46:1	TAG 56:2	TAG 58:10	DAG 36:0	DAG 38:5			SM 42:4				CL 82:9
TAG 46:2	TAG 56:3	TAG 58:11		DAG 38:6			SM 42:5				
TAG 46:3	TAG 56:4	TAG 58:12		DAG 38:7			SM 44:1				
TAG 48:0	TAG 58:0	TAG 58:6		DAG 40:7			SM 44:2				
TAG 48:1	TAG 58:1	TAG 58:7		DAG 40:8							
TAG 48:2	TAG 58:2	TAG 58:8									
TAG 48:3	TAG 58:3	TAG 58:9									
TAG 50:0	TAG 58:4	TAG 60:10									
TAG 50:1	TAG 60:3	TAG 60:11									
TAG 50:2	TAG 62:3	TAG 60:12									
TAG 50:3		TAG 60:8									
TAG 52:0		TAG 62:12									
TAG 52:1		TAG 62:14									

PE				pPE		pPC		PI	
Short LDB	Intermediate LDB	Long LDB	Long HDB	Short LDB	Long HDB	Short LDB	Long HDB	Short LDB	Long HDB
PE 30:0	PE 34:1	PE 32:2	PE 38:6	pPE 32:0	pPE 38:4	pPC 18:0	pPC 36:1	PI 34:1	PI 36:4
PE 32:0	PE 34:2	PE 34:4	PE 40:6	pPE 32:1	pPE 38:5	pPC 20:0	pPC 40:4	PI 34:2	PI 38:3
PE 32:1	PE 34:3	PE 38:1	PE 40:7	pPE 36:0	pPE 38:6		pPC 44:4	PI 36:1	PI 38:4
PE 38:5	PE 36:1	PE 38:2	PE 38:4		pPE 40:5			PI 36:2	PI 38:5
	PE 36:2	PE 40:3	PE 40:8		pPE 40:6			PI 36:3	PI 40:6
	PE 36:3	PE 40:4			pPE 42:5				
	PE 36:4				pPE 42:6				
	PE 38:3								

Note: LDB=Low Double Bond, HDB=High Double Bond; CE: Cholesterol Esters; DAG: Diacylglycerol; PE: Phosphatidylethanolamine; pPC: Plasmeyl-Phosphatidylcholine; pPE: Plasmeyl-Phosphatidylethanolamine; SM: Sphingomyelin; TAG: Triacylglycerol; CL: Cardiolipin; PI: Phosphatidylinositol

Supplement Table 3: Free fatty acids (FFA) subtypes independently associated with complex lipid sub-classes of cholesterol ester (CE), lysophosphatidylcholine (LPC), Lysophosphatidylethanolamine (LPE), plasmeyl-phosphatidylethanolamine (pPE), plasmeyl-phosphatidylcholine (pPC), sphingomyelin (SM), and phosphatidylinositol (PI) using multiple linear regression models adjusted for age, sex, and race. Complex lipid sub-classes as well as FFA cutoff for acyl chain length are defined by principle component analysis. Acyl chain >20 carbons (>C-20), Acyl chain ≤20 (≤C-20).

Complex lipid Sub-Classes (Dependent variable)	Independent FFA associates	B	SE	r	P.Val
Short, low-double-bond CE	Length >C-20	0.441	0.137	0.321	0.001
	Length ≤C-20	-0.275	0.133	-0.209	0.040
Low-double-bond-Cardiolipins	Length >C-20	0.658	0.134	0.478	<0.001
	Length ≤C-20	-0.266	0.130	-0.202	0.043
low-double-bond LPC	Length >C-20	0.455	0.141	0.331	0.001
	Length ≤C-20	-0.323	0.137	-0.246	0.019
Long, high-double-bond LPE	Length ≤C-20	0.211	0.089	0.161	0.018
Long, low-double-bond pPE	Length >C-20	0.319	0.090	0.232	<0.001
Short, low-double-bond pPE	Length >C-20	0.262	0.092	0.190	0.005
Long, high-double-bond SM	Length ≤C-20	0.166	0.081	0.126	0.042
Long, Low-double-bond SM	Length >C-20	0.209	0.093	0.152	0.026
Short, low-double-bond PI	Length >C-20	0.558	0.138	0.406	<0.001
	Length ≤C-20	-0.439	0.133	-0.335	0.001
Short, low-double-bond pPC	Length ≤C-20	0.489	0.081	0.373	<0.001

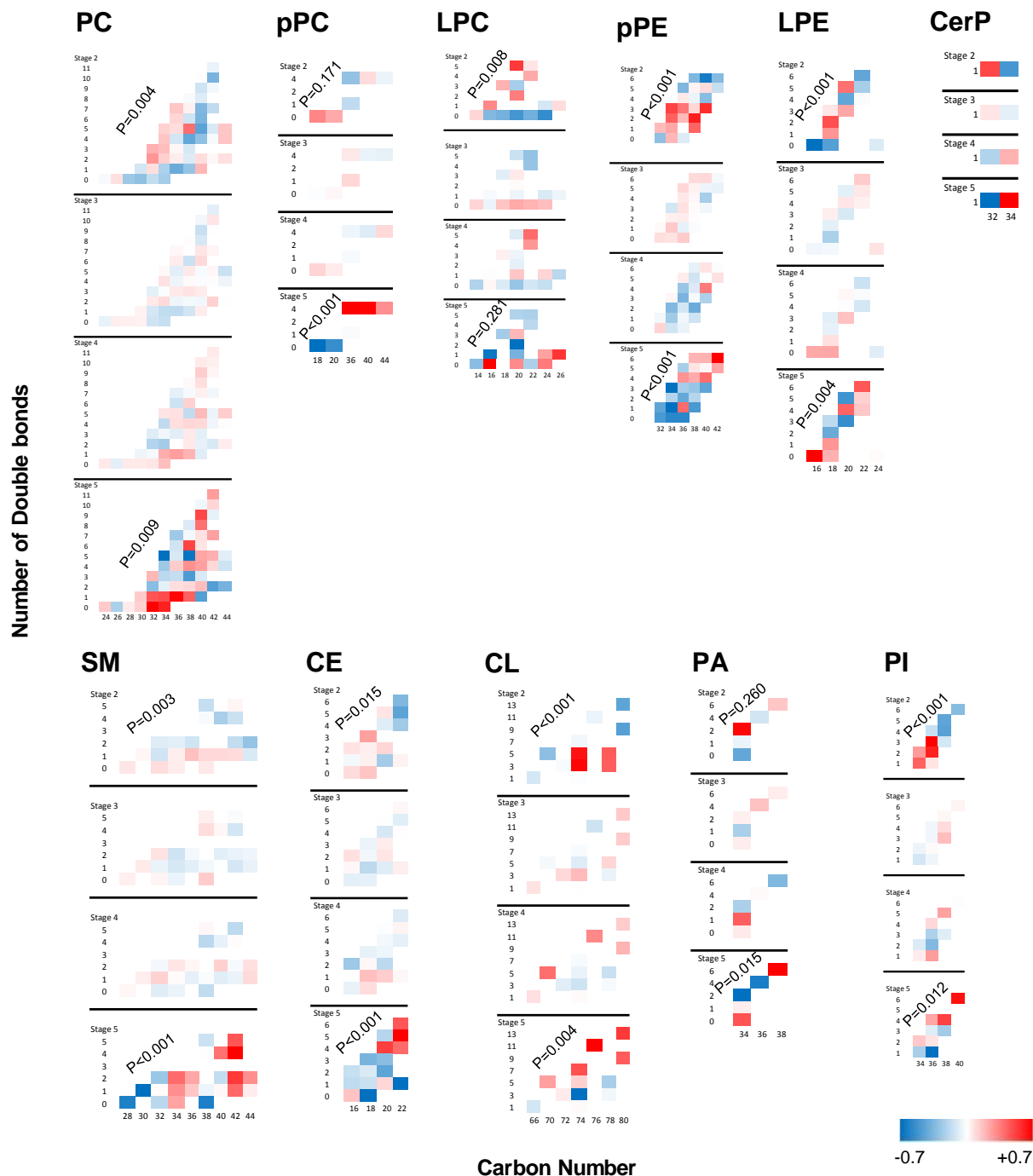
Supplement Table 4: Comparing the patients' characteristics and backgrounds in selected sub-cohort as compared to the rest of the cohort shows that overall the selected patients are similar to the rest of the unselected patients suggesting that the selected sub-cohort is an unbiased representative of the entire cohort.

	GFR\geq60 (Stage 1&2)	GFR 30-59 (Stage 3)	GFR 15-29 (Stage 4)	GFR<15 (Stage 5)	P value
N: Selected/Unselected	36/374	99/471	61/162	18/14	
Age: Selected	46 \pm 15 ^a	62 \pm 14	62 \pm 14	66 \pm 18	0.032
Age: Unselected	44 \pm 15	59 \pm 13	60 \pm 15	59 \pm 13	
Male Sex (%): Selected	17 (47.2)	49 (49.5)	36 (59.0)	8 (44.4)	0.702
Male Sex (%): Unselected	155 (41.4)	215 (45.6)	81 (50.0)	10 (71.4)	
White race (%): Selected	27 (75.0)	68 (68.7)	43 (70.5)	12 (66.7)	0.205
White race (%): Unselected	206 (55.1)	228 (48.4)	93 (57.4)	10 (71.4)	
SBP (mmHg): Selected	132 \pm 21	133 \pm 21	139 \pm 21	146 \pm 26	0.896
SBP (mmHg): Unselected	130 \pm 18	136 \pm 20	138 \pm 22	145 \pm 25	
DBP (mmHg): Selected	77 \pm 10	72 \pm 10	76 \pm 13	78 \pm 13	0.779
DBP (mmHg): Unselected	77 \pm 12	76 \pm 12	75 \pm 13	74 \pm 10	
Height (m): Selected	1.7 \pm 0.1	1.7 \pm 0.1	1.7 \pm 0.2	1.7 \pm 0.1	0.363
Height (m): Unselected	1.7 \pm 0.1	1.7 \pm 0.1	1.7 \pm 0.1	1.7 \pm 0.1	
Weight (kg): Selected	83 \pm 19	93 \pm 23	91 \pm 20	84 \pm 16	0.635
Weight (kg): Unselected	89 \pm 25	92 \pm 26	91 \pm 25	82 \pm 18	
BMI (kg/m²): Selected	28.1 \pm 5.5 ^b	32.5 \pm 7.3	30.9 \pm 6.9	29.6 \pm 4.2	0.316
BMI (kg/m²): Unselected	31.3 \pm 7.9	32.8 \pm 8.6	32.0 \pm 9.6	27.9 \pm 5.2	
Comorbidities					
Hypertension (%): Selected	27 (75.0)	79 (79.8)	53 (86.9)	17 (94.0)	0.937
Hypertension (%): Unselected	253 (67.6)	412 (88.0)	138 (86.3)	13 (92.9)	
Diabetes (%): Selected	5 (13.9)	41 (41.4)	35 (57.4)	8 (44.4)	0.651
Diabetes (%): Unselected	95 (25.5)	207 (44.2)	75 (46.9)	7 (50.0)	
Heart Failure (%): Selected	1 (2.8)	16 (16.2)	12 (19.7)	2 (11.1)	0.578
Heart Failure (%): Unselected	15 (4.0)	56 (12.0)	20 (12.5)	4 (28.6)	
PVD (%): Selected	1 (2.8)	14 (14.1)	12 (19.7)	2 (11.1)	0.043
PVD (%): Unselected	15 (4.0)	56 (12.0)	20 (12.5)	4 (28.6)	
Nephrotic syndrome (%): Selected	1 (2.8)	11 (11.1)	4 (6.6)	1 (5.6)	0.760
Nephrotic syndrome (%): Unselected	47 (12.6)	17 (3.6)	10 (6.2)	1 (7.1)	
Medications					
Statins (%): Selected	14 (38.9)	54 (54.5)	36 (59.0)	10 (55.6)	0.328
Statins (%): Unselected	114 (30.5)	227 (48.2)	83 (51.2)	8 (57.1)	
Fibrates (%): Selected	0 (0)	10 (10.1)	8 (13.1)	0 (0)	0.151
Fibrates (%): Unselected	12 (3.2)	17 (3.6)	6 (3.7)	0 (0)	
Niacin (%): Selected	1 (2.8)	5 (5.1)	1 (1.6)	0 (0)	0.306
Niacin (%): Unselected	2 (0.5)	3 (0.6)	5 (3.1)	0 (0)	
Steroids (%): Selected	9 (25.0)	14 (14.1)	5 (8.2)	2 (11.1)	0.279
Steroids (%): Unselected	98 (26.2)	40 (8.5)	12 (7.4)	0 (0)	
Mycophenolate (%): Selected	6 (16.7)	8 (8.1)	3 (4.9)	1 (5.6)	0.167
Mycophenolate (%): Unselected	53 (14.2)	17 (3.6)	3 (1.9)	0 (0)	
Albumin (g/dL): Selected	4.1 \pm 0.5	4.1 \pm 0.5	4.0 \pm 0.4	3.9 \pm 0.3	<0.001
Albumin (g/dL): Unselected	3.8 \pm 0.7	4.0 \pm 0.5	3.9 \pm 0.6	3.4 \pm 0.4	
UPCR: Selected	0.5 [0.2-1.6]	0.4 [0.1-1.7]	0.8 [0.2-3.0]	1.4 [0.3-3.3]	0.051
UPCR: Unselected	0.9 [0.2-2.2]	0.4 [0.1-1.6]	1.0 [0.3-3.3]	4.5 [2.9-10.9]	
WBC (1000/μL): Selected	6.8 \pm 2.5	7.4 \pm 3.1	7.1 \pm 3.2	6.5 \pm 1.8	0.060

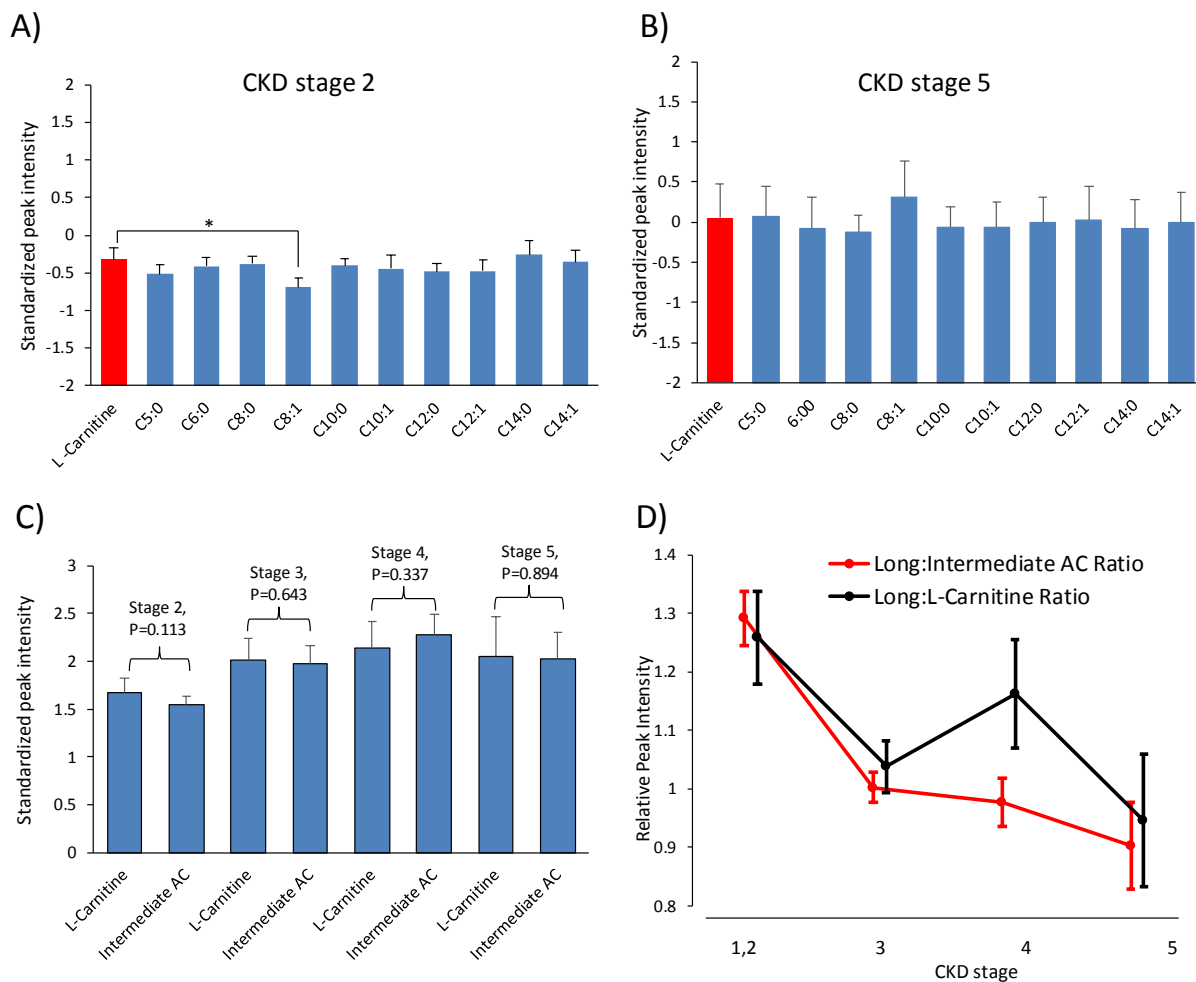
WBC (1000/μL): Unselected	7.4 \pm 2.8	7.6 \pm 2.9	7.8 \pm 2.7	7.4 \pm 2.1	
eGFR (mL/min): Selected	82 \pm 15	41 \pm 8	23 \pm 4	14 \pm 10	0.180
eGFR (mL/min): Unselected	91 \pm 24	44 \pm 8	23 \pm 4	14 \pm 11	

Serum albumin in unselected cohort is measured in 333, 364, 126, and 13 patients from CKD stage 2 to 5, respectively, in the unselected cohort. Urine protein: creatinine ratio is measured in 236, 222, 103, and 10 patients in patients from CKD stage 2 to 5, respectively, in the unselected cohort. The p values are the product of the main effect comparison of the selected versus unselected cohorts for each variable using a 2-way analysis of variance in generalized linear models, except for that of UPCR which is product of the Mann-Whitney test. SBP: Systolic blood pressure; DBP: Diastolic blood pressure; BMI: Body mass index; PVD: Peripheral vascular disease; UPCR: Urine protein: creatinine ratio; WBC: White blood cell count; eGFR: Estimated glomerular filtration rate. Values are mean \pm SD, count (%), or median [interquartile range].

Supplement Figure 1: Comparing standardized mean values of other complex lipids by carbon number and number of double bonds in CKD stages 2 to 5. The significance of the interaction term of change in abundance of lipid by carbon number and number of double bonds from CKD stage 2 to 5 is shown by p values in the diagonal of each lipid class, using mixed linear model. CE: Cholesterol Esters; LPC: Lysophosphatidylcholine; LPE: Lysophosphatidylethanolamine; PC: Phosphatidylcholine; pPC: Plasmeyl-Phosphatidylcholine; pPE: Plasmeyl-Phosphatidylethanolamine; PA: Phosphatidic Acid; SM: Sphingomyelin; CerP: Ceramide-Phosphates; CL: Cardiolipin; PI: Phosphatidylinositol

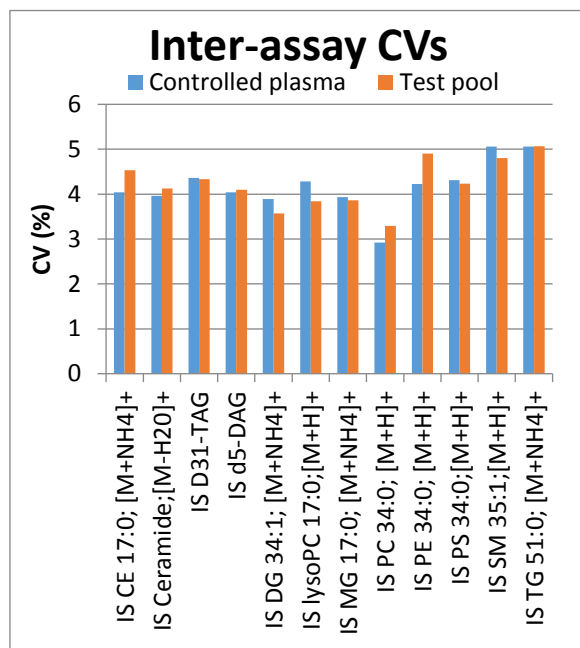


Supplement Figure 2: Comparing mean standardized values of medium chain acylcarnitines compared with L-Carnitine in CKD stage 2 (panel A) and CKD stage 5 (panel B). The lower level of C8:1 acylcarnitine compared with L-carnitine ($p < 0.001$) in CKD stage 2 reached statistical significance. Corresponding values of no other medium chain acylcarnitine were significantly different from L-Carnitine in CKD stage 2 and stage 5. Mean of intermediate acylcarnitines (AC) as compared with L-carnitine was not different within each stage of CKD (panel C). Overall, the trend of long-intermediate acylcarnitine ratio from stage 2 to stage 5 was similar to trend of long acylcarnitine-L-Carnitine ratio (panel D).

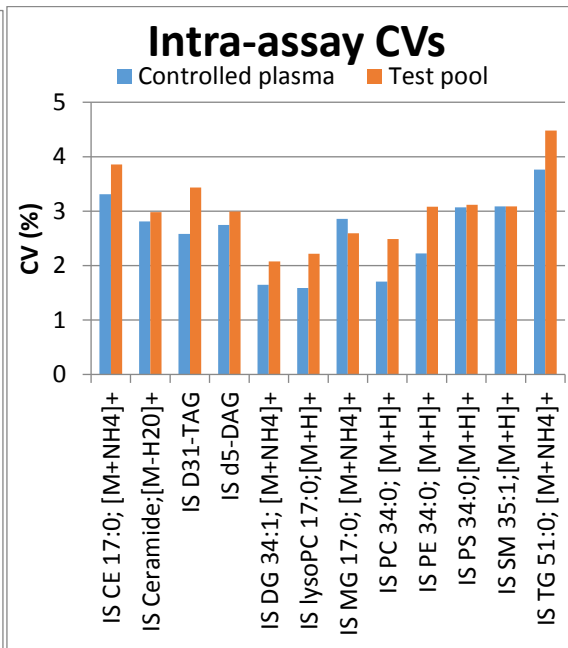


Supplement Figure 3: Comparing inter- (Panel A) and intra-assay (Panel B) coefficient of variation (CV) of different internal standards in test pool and control plasma in the lipidomic platform on log2 scale. Control plasma is reference sample obtained from American Red Cross. Test pool is pool of study samples. IS: internal standard; CE: Cholesterol Esters; TAG: Triacylglycerol; DG: Diacylglycerol; PC: Phosphatidylcholine; MG: Monoacylglycerol; PE: Phosphatidylethanolamine; PS: Phosphatidylserine; SM: Sphingomyelin

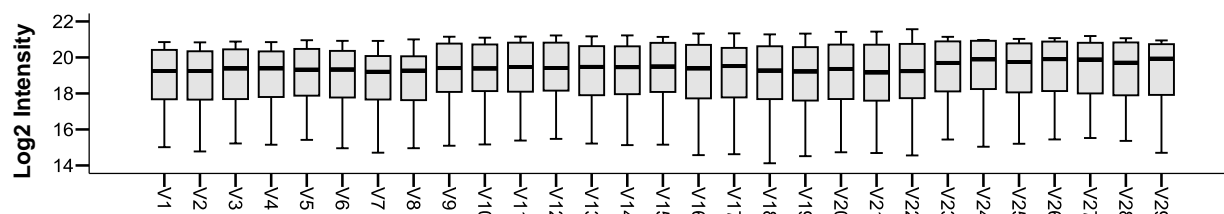
A)



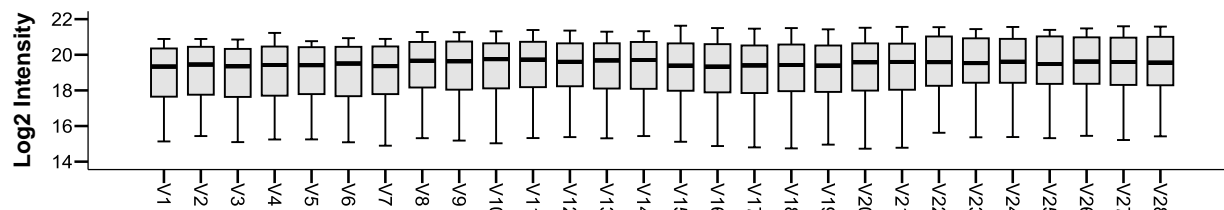
B)



Supplement Figure 4: Negligible batch to batch variability of internal standards in reference pools



Panel A) Batch variability of internal standards in test pools



Panel B: Batch variability of internal standards in pooled plasma