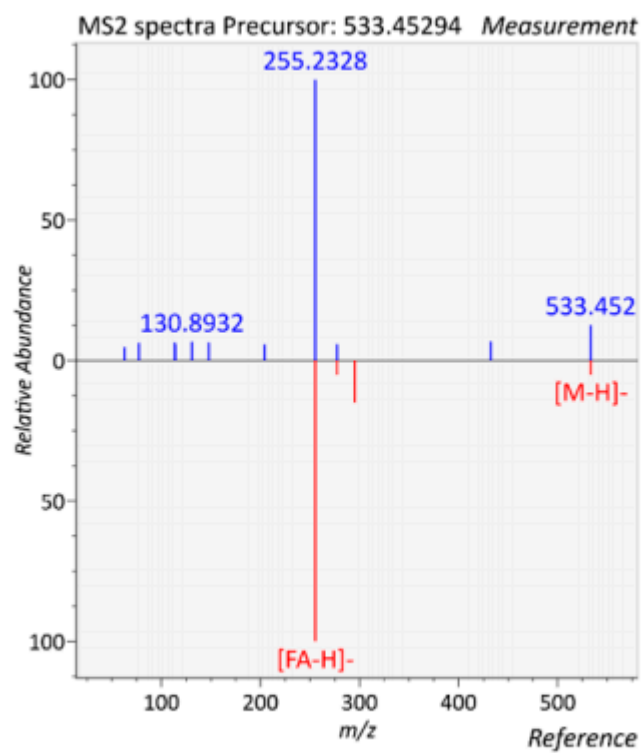
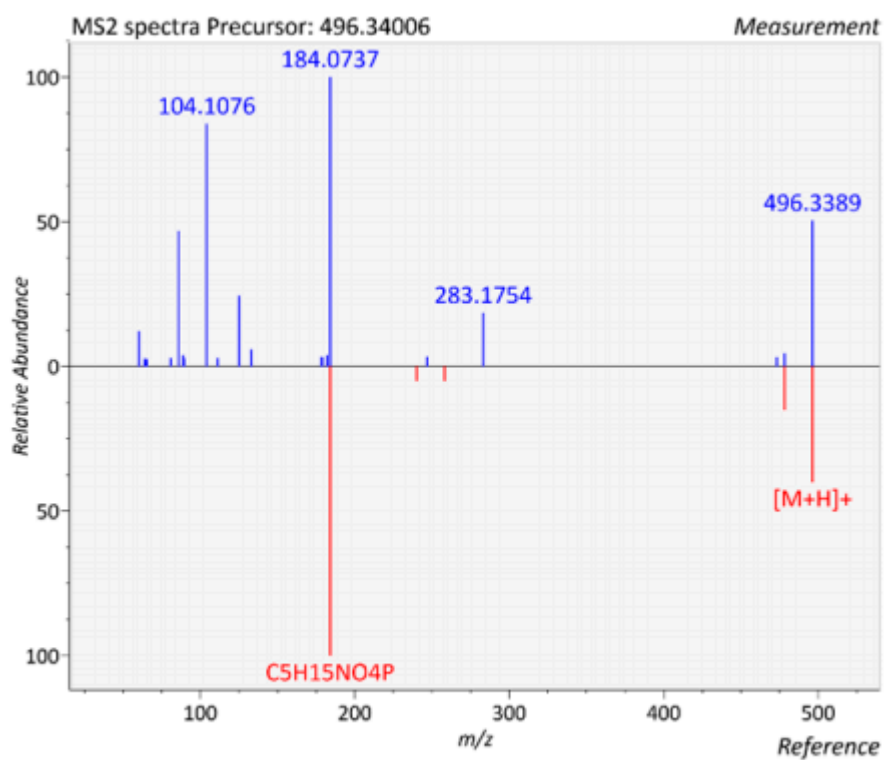


Figure S1. TICs of lipids from rat AF of QC samples in MS-DIAL software. (A) positive ion mode; (B) negative ion mode.



FAHFA 34:2



LPC 16:0

Figure S2. Selected lipids with matching fragmentation patterns to the LipidBlast library with MS-DIAL software

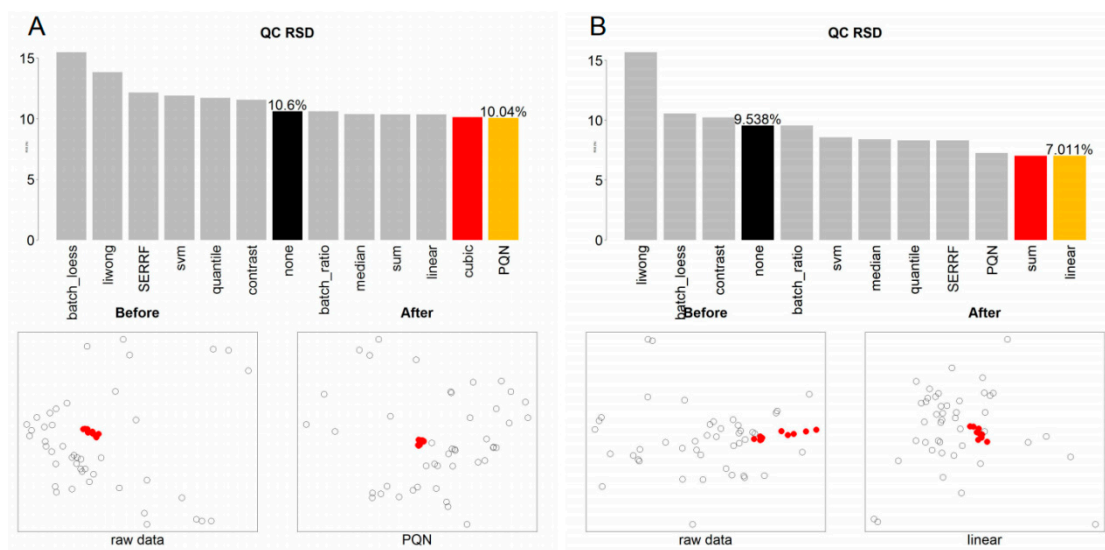


Figure S3. RSD values in QC samples obtained by different normalization methods
(A) positive ion mode; (B) negative ion mode.

Table S1. Differential lipids in AF (positive ion mode)

Significant metabolites	m/z	Rt (min)	Adduction	PPM mass error	P value	FDR	FC (CK/CP)
CAR 20:4	448.3406	1.41	[M] ⁺	-3.469	0.026	0.17	0.79
CAR 24:0	512.4688	4.91	[M] ⁺	2.877	0.002	0.08	0.67
CE 24:5	744.6622	11.43	[M+NH ₄] ⁺	-4.213	0.026	0.17	0.58
Cer 42:0;2O	652.6613	9.23	[M+H] ⁺	1.575	0.002	0.08	1.31
Cer 42:1;2O	650.6406	8.60	[M+H] ⁺	-6.074	0.002	0.08	1.35
DG O-33:1	584.5611	6.55	[M+NH ₄] ⁺	-0.233	0.004	0.08	1.29
DG O-35:1	612.5910	7.25	[M+NH ₄] ⁺	-2.508	0.004	0.08	1.24
DG O-37:1	640.6216	7.94	[M+NH ₄] ⁺	-3.429	0.004	0.08	1.25
LPC 16:1	516.3032	1.09	[M+Na] ⁺	-2.369	0.041	0.21	1.35
LPC 16:1	494.3228	1.09	[M+H] ⁺	-2.763	0.026	0.17	1.27
LPC 18:3	518.3226	0.98	[M+H] ⁺	-2.866	0.009	0.10	1.34
LPC 19:0	538.3870	3.06	[M+H] ⁺	0.565	0.015	0.13	0.46
LPC 20:2	548.3702	1.61	[M+H] ⁺	-1.506	0.004	0.08	1.43
LPC 20:3	546.3530	1.64	[M+H] ⁺	-4.367	0.002	0.08	1.56
PC 40:8	830.5715	5.26	[M+H] ⁺	2.527	0.004	0.08	0.80
PC O-40:5	822.6428	6.81	[M+H] ⁺	6.933	0.015	0.13	1.44
PI 38:6	900.5494	4.92	[M+NH ₄] ⁺	-11.409	0.009	0.10	1.81
PS 38:3	814.5660	5.97	[M+H] ⁺	8.249	0.004	0.08	1.44
SM 35:1;2O	717.5852	5.85	[M+H] ⁺	-7.374	0.026	0.17	0.71
TG 46:0	796.7399	12.75	[M+NH ₄] ⁺	0.03	0.009	0.10	1.51
TG 48:0	824.7693	12.81	[M+NH ₄] ⁺	-1.062	0.004	0.08	1.35
TG 48:3	818.7253	10.46	[M+NH ₄] ⁺	2.521	0.026	0.17	1.22
TG 51:4	858.7478	10.87	[M+NH ₄] ⁺	-7.821	0.015	0.13	0.53
TG 53:0	894.8464	12.46	[M+NH ₄] ⁺	-2.209	0.041	0.21	1.30
TG 53:6	882.7594	10.50	[M+NH ₄] ⁺	5.532	0.015	0.13	0.64
TG 54:0	908.8567	12.58	[M+NH ₄] ⁺	-8.116	0.009	0.10	1.35
TG 54:0	908.8691	12.57	[M+NH ₄] ⁺	5.582	0.009	0.10	1.30
TG 54:5	898.7811	11.12	[M+NH ₄] ⁺	-5.214	0.026	0.17	0.82
TG 54:5	903.7454	11.12	[M+Na] ⁺	4.59	0.026	0.17	0.82
TG 55:0	922.8779	12.64	[M+NH ₄] ⁺	-1.936	0.004	0.08	1.31
TG 55:1	920.8617	12.48	[M+NH ₄] ⁺	-2.581	0.041	0.21	1.37
TG 55:4	914.8077	11.64	[M+NH ₄] ⁺	-10.25	0.009	0.10	0.32
TG 55:5	912.8046	11.34	[M+NH ₄] ⁺	3.4	0.009	0.10	0.60
TG 56:0	936.8996	12.71	[M+NH ₄] ⁺	4.518	0.015	0.13	1.30
TG 56:0	936.8893	12.72	[M+NH ₄] ⁺	-6.433	0.002	0.08	1.28
TG 56:10	916.7410	9.76	[M+NH ₄] ⁺	2.295	0.002	0.08	0.36
TG 56:6	924.7965	11.18	[M+NH ₄] ⁺	-5.359	0.041	0.21	0.81
TG 56:8	925.7293	10.36	[M+Na] ⁺	-4.049	0.041	0.21	0.82
TG 57:0	950.9137	12.77	[M+NH ₄] ⁺	2.822	0.009	0.10	1.22

TG 57:1	948.9003	12.65	[M+NH ₄] ⁺	5.231	0.015	0.13	1.50
TG 57:7	936.7937	11.17	[M+NH ₄] ⁺	-8.29	0.026	0.17	0.45
TG 59:1	976.9228	12.77	[M+NH ₄] ⁺	-3.968	0.026	0.17	1.24
TG 60:1	990.9410	12.82	[M+NH ₄] ⁺	-1.349	0.041	0.21	1.20
TG 60:5	982.8842	12.11	[M+NH ₄] ⁺	4.521	0.015	0.13	0.69
TG 60:7	978.8496	11.60	[M+NH ₄] ⁺	1.158	0.041	0.21	0.82

Table S2. Differential lipids in AF (negative ion mode)

Significant metabolites	m/z	Rt (min)	Adduction	PPM mass error	p value	FDR	FC (CK/CP)
FA 22:2	335.2962	4.00	[M-H] ⁻	2.017	0.026	0.13	0.56
FA 22:4	331.2630	2.85	[M-H] ⁻	-3.694	0.002	0.04	0.62
FA 22:5	329.2481	2.26	[M-H] ⁻	-1.499	0.002	0.04	0.56
FA 24:4	359.2942	3.76	[M-H] ⁻	-3.796	0.002	0.04	0.49
FA 24:5	357.28091	3.281	[M-H] ⁻	2.817	0.002	0.04	0.62
FA 26:1	393.3745	5.81	[M-H] ⁻	1.795	0.015	0.09	0.54
FA 26:5	385.3100	3.98	[M-H] ⁻	-3.124	0.002	0.04	0.35
LPC 17:0	568.3639	1.89	[M+CH ₃ COO] ⁻	3.339	0.009	0.07	0.67
LPC 22:0	638.4384	4.21	[M+CH ₃ COO] ⁻	-2.964	0.045	0.17	0.45
LPE O-16:0	438.3000	1.80	[M-H] ⁻	2.264	0.041	0.16	0.36
PC O-34:2	802.59784	6.58	[M+CH ₃ COO] ⁻	1.367	0.015	0.09	0.39
PC O-38:4	854.6299	6.74	[M+CH ₃ COO] ⁻	2.15	0.041	0.16	0.60
PC O-39:5	866.6317	5.99	[M+CH ₃ COO] ⁻	-3.731	0.009	0.07	0.57
PE O-42:7	802.5765	7.20	[M-H] ⁻	1.154	0.041	0.16	0.52
PI 35:2	847.5294	4.87	[M-H] ⁻	-5.713	0.041	0.16	0.60
PI 37:4	871.5330	4.97	[M-H] ⁻	-1.356	0.041	0.16	0.50
PI 40:4	913.5756	5.59	[M-H] ⁻	-6.121	0.041	0.16	0.34
SM 35:1;2O	775.5988	5.81	[M+CH ₃ COO] ⁻	2.247	0.004	0.05	0.61
SM 36:1;2O	775.6005	6.14	[M+HCOO] ⁻	4.361	0.002	0.04	0.53
SM 38:2;2O	815.6271	6.25	[M+CH ₃ COO] ⁻	-1.591	0.004	0.05	0.56
SM 40:2;2O	843.6611	6.92	[M+CH ₃ COO] ⁻	1.651	0.009	0.07	0.65
SM 40:3;2O	841.6415	6.27	[M+CH ₃ COO] ⁻	-3.027	0.002	0.04	0.61

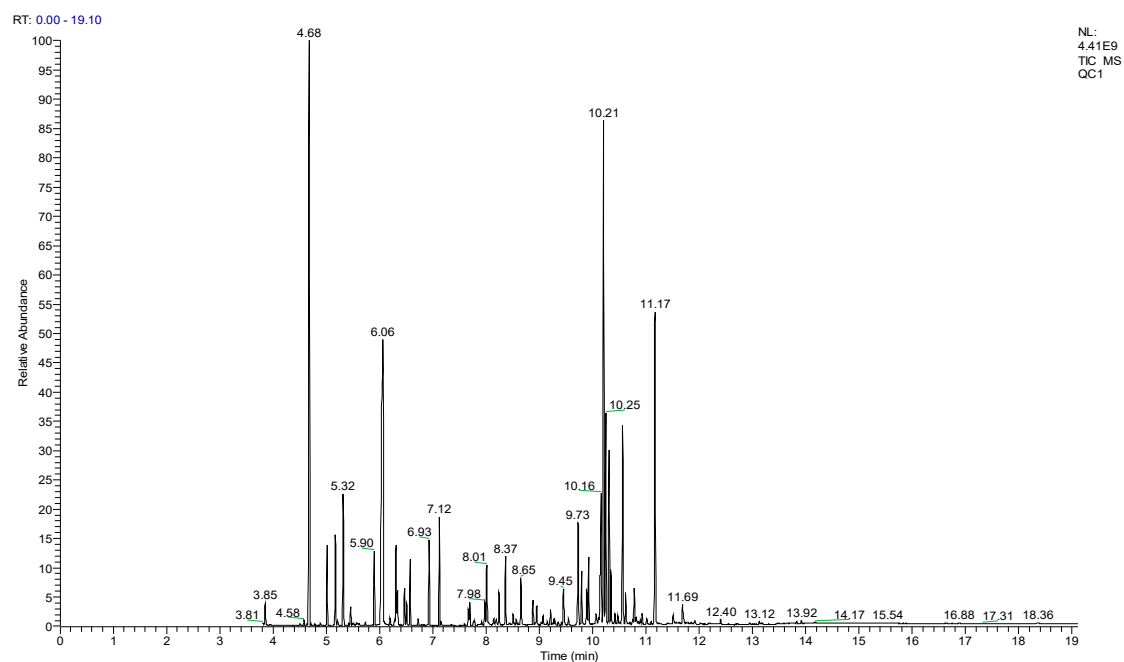


Figure S4. TICs of metabolites from rat AF of QC samples in GC-MS experiments.

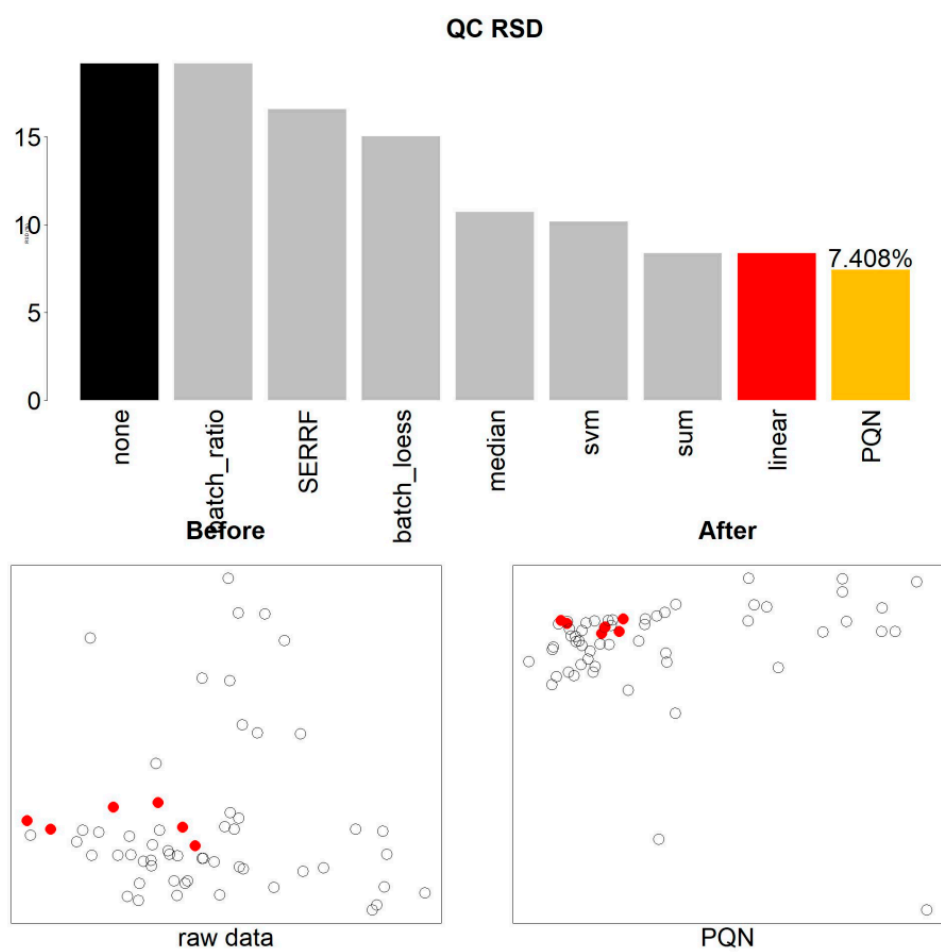


Figure S5. RSD values in QC samples obtained by different normalization methods in GC-MS experiments.

Table S3. Differential metabolites of AF detected in GC-MS

Metabolite name	FC	p value	FDR	HMDB	PubChem	KEGG
(CK/CP)						
stearic acid	1.64	0.000	0.049	HMDB0000827	5281	C01530
palmitic acid	1.60	0.000	0.049	HMDB0000220	985	C00249
tryptophan	1.54	0.009	0.155	HMDB0000929	6305	C00078
glycerol-1-phosphate	0.59	0.005	0.109	HMDB0000126	439162	C00093