Supporting information

Isolation and metabolic assessment of cancer cell mitochondria

Nguyen Phuoc Long[1,#], Jung Eun Min[1,#], Nguyen Hoang Anh[1], Sun Jo Kim[1], Seongoh Park[2], Hyung Min Kim[1], Sang Jun Yoon[1], Johan Lim[3], Seul Ji Lee[1], Sung Won Kwon[1,4,*]

[1]College of Pharmacy, Seoul National University, Seoul, 08826, Republic of Korea

[2]Department of Statistics, Sungshin Women's University, Seoul, 02844, Republic of Korea

[3]Department of Statistics, Seoul National University, Seoul, 08826, Republic of Korea

[4]Plant Genomics and Breeding Institute, Seoul National University, Seoul 08826, Republic of Korea

[#]These authors contributed equally to this work.

[*]To whom correspondence should be addressed: S.W.K. (swkwon@snu.ac.kr)

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Table S1: Metabolite composition of mitochondria as compared to that of bulk cancer cells.

Significantly compartmentalized species[#]	KEGG ID	HMDB ID	A549			MDA-MB-231			PANC1		
			P-value	FDR	Fold change[^]	*P*-value	FDR	Fold change	*P*-value	FDR	Fold change
1-methylhistidine	C01152	HMDB0000001	0.0004357	0.0031524	0.64226	0.00011651	0.0016959	0.057509	0.001417	0.0076004	0.068508
(DL)-2-aminooctanoic acid		HMDB0000991	0.00018553	0.0017554	0.085595	7.0587E-05	0.0011947	0.039536			
3-methylphenylacetic acid		HMDB0002222				0.0071085	0.022172	3.2268			
DL-O-phosphoserine	C01005	HMDB0001721	0.0033117	0.0106	0.32724						
L-acetylcarnitine	C02571	HMDB0000201				1.8102E-05	0.00059285	0.31426	1.1871E-05	0.00039121	0.20179
Adenosine	C00212	HMDB0000050	3.1699E-05	0.00063204	62.043	0.00015018	0.0017884	1535.3			
L-alanine	C00041	HMDB0000161	0.018459	0.039833	3.3582	0.010572	0.030104	2.8844	0.0051429	0.015354	3.1408
AMP	C00020	HMDB0000045	2.1052E-05	0.00056382	201.66	0.0011942	0.0059742	79.679	6.2407E-05	0.00097652	287.7
L-arginine	C00062	HMDB0000517	3.9427E-06	0.00016165	10.627	7.2961E-05	0.0011947	11.446	0.0016838	0.0082787	4.1668
L-aspartic acid	C00049	HMDB0000191				0.003826	0.012851	3.2109			
Betaine	C00719	HMDB0000043	0.0026409	0.009023	2.9761	0.0012307	0.0059742	1.7276	6.7751E-05	0.00097652	2.063
Biotin	C00120	HMDB0000030	0.0000616	0.00075768	65.188						
Carbamoyl phosphate	C00169	HMDB0001096				0.012977	0.034545	0.311			
L-carnitine	C00318	HMDB0000062	0.018134	0.039833	0.32266	0.00027027	0.002529	0.53396	7.9976E-06	0.00039121	0.23756
Cholesterol sulfate	C18043	HMDB0000653	0.013288	0.030837	67.298						
Choline	C00114	HMDB0000097				0.00076725	0.0047994	0.089895	0.00007448	0.00097652	0.064635
Citric acid	C00158	HMDB0000094	0.001826	0.0072452	0.15021	0.0014716	0.0066475	0.08974	0.012413	0.028596	0.077278
Cytidine monophosphate	C00055	HMDB0000095	0.0034041	0.0106	3.1559				0.0018901	0.008921	12.577
Creatine	C00300	HMDB0000064	0.021556	0.043466	0.42879				0.012516	0.028596	2.4728
Creatinine	C00791	HMDB0000562							0.01264	0.028596	0.45795
Cytidine triphosphate (neg)	C00063	HMDB0000082	0.00011099	0.0012411	0.077154	0.0030379	0.011054	0.11478	0.0004138	0.0034878	0.073413
L-cystathionine	C02291	HMDB0000099	0.0017384	0.0071276	0.041502				0.0020732	0.0090607	0.044002

Cytidine	C00475	HMDB0000089	0.0019661	0.0073284	10.649						
Cytosine	C00380	HMDB0000630	0.0007634	0.0044713	1.4481	0.0039468	0.012926	9.9949			
dCMP	C00239	HMDB0001202							0.0012767	0.0071739	14.316
Deoxyadenosine	C00559	HMDB0000101				0.015032	0.037153	4.4506			
Glyceraldehyde 3-phosphate	C00661	HMDB0001112							0.010426	0.025108	0.17925
dGMP	C00362	HMDB0001044	0.0065675	0.017283	2.8315				0.0074513	0.020935	29.152
dGTP	C00286	HMDB01440	0.00017677	0.0017554	0.032272	0.00020972	0.0021133	0.051328	0.0095206	0.024422	0.046158
Dimethylglycine	C01026	HMDB0000092	0.0002201	0.0018048	2.9691						
Ethanolamine	C00189	HMDB0000149				0.0037648	0.012851	2.3178			
FAD	C00016	HMDB0001248	0.009621	0.022757	3.4337	0.013185	0.034545	6.6938	0.00015017	0.0014767	11.443
Fumaric acid	C00122	HMDB0000134	0.0056747	0.015511	0.36404	0.0017729	0.007038	0.09228	0.0015052	0.0077224	0.13329
Guanosine diphosphate (neg)	C00035	HMDB0001201	0.020395	0.04325	0.49671				0.018332	0.037296	0.44715
Glucosamine	C00329	HMDB0001514	0.0041807	0.012243	6.327	0.0012313	0.0059742	8.3653	0.019114	0.038228	4.4973
L-glutamic acid	C00025	HMDB0000148	0.021486	0.043466	1.756				0.0035567	0.012344	0.45762
L-glutamine	C00064	HMDB0000641	0.01477	0.033642	0.69545	0.014091	0.035498	1.632	0.00063344	0.0044442	0.30336
Oxidized glutathione (neg)	C00127	HMDB0003337				0.00044378	0.0034197	0.38492			
Oxidized glutathione (pos)	C00127	HMDB0003337	0.0014772	0.0064889	4.1723				0.017479	0.036184	2.7323
Glutathione (neg)	C00051	HMDB0000125	0.0018969	0.0072912	0.056641	0.016875	0.040194	0.1061	0.010372	0.025108	0.14597
Glycerophosphocholine	C00670	HMDB0000086	0.0010612	0.0056751	2.0936						
Glycine	C00037	HMDB0000123	0.0085423	0.021443	0.21493				0.003187	0.011691	0.16386
Guanosine triphosphate (neg)	C00044	HMDB0001273	0.00002292	0.00056382	0.048887	0.00073566	0.0047994	0.09636	0.0023439	0.009878	0.095995
Guanine	C00242	HMDB0000132				0.010157	0.029633	0.3167			
Guanosine	C00387	HMDB0000133							0.0052048	0.015354	0.09916
L-homoserine	C00263	HMDB0000719	0.00021687	0.0018048	0.36522						
4-hydroxyproline	C01157	HMDB0000725	0.00048386	0.0033064	0.13216				0.022475	0.043538	0.20325
Imidazoleacetic acid	C02835	HMDB0002024							0.0029018	0.011587	20.089
Inosine	C00294	HMDB0000195				0.0028274	0.010582	0.037887			

Lactic acid	C00186	HMDB0000190	0.0025801	0.009023	0.17959	0.0036889	0.012851	0.2548			
L-leucine	C00123	HMDB0000687	0.00034937	0.0026858	0.020292	2.125E-06	0.00010802	0.021592	1.3262E-05	0.00039121	0.010231
Malic acid	C00149	HMDB0000156	0.0014098	0.0064889	3.5187						
Maleic acid	C01384	HMDB0000176							0.00090016	0.0053109	43.802
L-methionine	C00073	HMDB0000696	5.0352E-07	3.0966E-05	0.016299	0.00098718	0.0054199	0.046979	6.5509E-06	0.00039121	0.015418
Methionine sulfoxide	C02989	HMDB0002005	0.00052565	0.0034029	38.112	0.0017256	0.007038	52.496	0.00071945	0.0046888	25.066
1-methylnicotinamide	C02918	HMDB0000699	0.0091977	0.022183	0.10971	0.0093841	0.028589	0.10159	0.0051601	0.015354	0.053379
Myo-inositol	C00137	HMDB0000211							0.010003	0.025108	0.40343
N-acetylputrescine	C02714	HMDB0002064							0.001987	0.0090179	6.7473
NAD (neg)	C00003	HMDB0000902							0.0067107	0.019314	8.5007
NAD (pos)	C00003	HMDB0000902	4.6247E-05	0.00063204	9.8006	0.00059524	0.004332	2.7744	0.00013532	0.0014516	12.88
Asymmetric dimethylarginine	C03626	HMDB0001539	0.0047949	0.013404	8.8148				0.00010167	0.0011997	9.2401
Nicotinamide	C00153	HMDB0001406				3.8175E-07	5.0009E-05	2.6344			
Nicotinamide ribotide	C00455	HMDB0000229	0.0014696	0.0064889	0.27147						
O-acetylserine	C00979	HMDB0003011	0.003791	0.011373	8.9209	0.0015773	0.0066656	5.4506	0.0136	0.029719	5.7883
Ornithine	C00077	HMDB0000214	0.0066039	0.017283	6.7983	0.00076937	0.0047994	7.8217	0.00075498	0.0046888	4.983
Oxaloacetic acid	C00036	HMDB0000223				0.0019005	0.0073226	2.7799			
Pantothenic acid	C00864	HMDB0000210	1.8497E-08	2.2751E-06	0.010814	4.1322E-05	0.0010443	0.004819	0.00064027	0.0044442	0.02153
L-phenylalanine	C00079	HMDB0000159	3.6174E-05	0.00063204	0.015089	0.00017639	0.0019256	0.021513	0.00046014	0.0036198	0.011666
Phosphoenolpyruvic acid	C00074	HMDB0000263							0.012844	0.028596	9.494
L-proline	C00148	HMDB0000162	0.0030984	0.0103	0.5263	2.4737E-06	0.00010802	0.33541	0.014051	0.030145	0.40524
Purine	C15587	HMDB0001366							0.003044	0.011587	2.8961
Pyridoxamine	C00534	HMDB0001431				0.021029	0.049193	3.5676			
Pyridoxine	C00314	HMDB0000239							0.004461	0.01504	0.00792
Pyroglutamic acid	C01879	HMDB0000267	0.021075	0.043466	0.21879						
Pyruvic acid	C00022	HMDB0000243				0.0013609	0.0063673	0.22911			
Quinolinic acid	C03722	HMDB0000232				0.01352	0.034728	4.3866			

S-adenosylhomocysteine (pos)	C00021	HMDB0000939	4.3068E-05	0.00063204	80.196						
S-adenosylmethionine	C00019	HMDB0001185	0.01819	0.039833	0.64257	0.010179	0.029633	0.40304	0.023976	0.045632	0.54147
L-serine	C00065, C00740	HMDB0000187				0.011031	0.030104	2.9809			
Spermidine	C00315	HMDB0001257	0.00075994	0.0044713	17.486				0.008664	0.022719	12.428
Succinic acid/Methylmalonic acid	C00042/C02170	HMDB0000254/HMDB0000202	0.0013883	0.0064889	15.092	4.7831E-05	0.0010443	17.161	0.022507	0.043538	3.282
Taurine	C00245	HMDB0000251	0.0010563	0.0056751	0.023534	0.00088203	0.0052521	0.036295	0.0047317	0.015354	0.045481
Thiamine	C00378	HMDB0000235				0.00033317	0.0027278	0.047073	0.0076751	0.021062	0.065683
Thiamine monophosphate	C01081	HMDB0002666							0.0080457	0.021577	8.538
Thymine	C00178	HMDB0000262				0.015597	0.037838	9.6961	6.9652E-05	0.00097652	6.9419
L-tryptophan	C00078	HMDB0000929	0.0025324	0.009023	0.024412	0.0015447	0.0066656	0.044388	2.7163E-05	0.00064104	0.054614
L-tyrosine	C00082	HMDB0000158	0.0069895	0.017911	0.33606	0.010923	0.030104	0.56868			
Uridine 5'-diphosphate (neg)	C00015	HMDB0000295	0.001537	0.0065191	0.068079				0.0050519	0.015354	0.13568
Uridine diphosphate glucose	C00029	HMDB0000286				0.0002935	0.0025632	0.012843	0.0032695	0.011691	0.037383
Uridine diphosphate glucuronic acid	C00167	HMDB0000935	0.0034473	0.0106	0.22834	0.00013411	0.0017568	0.039309	0.0030143	0.011587	0.062934
Uridine diphosphate-N-acetylglucosamine	C00043	HMDB0000290	0.0013379	0.0064889	0.17082	0.00099296	0.0054199	0.027664	0.016317	0.034382	0.096348
Uridine 5'-monophosphate	C00105	HMDB0000288							0.00039998	0.0034878	229.98
Uracil	C00106	HMDB0000300	0.0087882	0.021619	0.3074	0.0056444	0.018035	0.070756			
L-valine	C00183	HMDB0000883	0.0043793	0.012527	2.8996						

[#]: Significant differences in metabolite composition as deduced from the univariate test. The original tracked metabolites of the experiment were adopted from a previous study.[18]

^ Fold change: fold change of concentration in mitochondrial fraction was calculated with respect to net concentration in the whole cell. Some metabolites were tracked in two ion modes but could be detected in one ion mode.

Table S2: Differentially expressed lipids among the three indicated cell lines.

Significantly compartmentalized species	A549			MDA-MB-231			PANC1		
	P-value	FDR	Fold change	*P*-value	FDR	Fold change	*P*-value	FDR	Fold change
ACar 14:0	0.0010026	0.024449	0.36888	0.00032274	0.034862	0.15579	7.6041E-05	0.01172	0.21531
ACar 16:0	0.0081174	0.044815	0.58668				0.0076746	0.10769	0.28766
ACar 18:1	0.006112	0.037672	0.49465	0.0021726	0.034862	0.23663	0.00036413	0.023149	0.95334
BMP 44:12	0.001899	0.024449	2.9902				0.0024584	0.069757	1.9134
CE 22:6	0.012164	0.059695	0.57673	0.018802	0.086576	0.38613	0.0073495	0.10769	0.51849
Cer-NDS d40:0	0.014268	0.063696	1.7021				0.02845	0.1957	1.2982
Cer-NS d40:1	0.033611	0.097944	1.67						
DAG 36:0				0.0021855	0.034862	4.2009	0.030217	0.19931	14.073
DAG 36:2	0.01931	0.074317	0.46459	0.011739	0.063939	0.28566			
DAG 38:3	0.0018436	0.024449	0.17505				0.0022418	0.069757	0.16331
DAG 38:4	3.0083E-05	0.003986	0.090595	0.00052724	0.034862	0.26811	0.00010326	0.01172	0.14557
DAG 40:6	0.0010625	0.024449	0.171				0.00040791	0.023149	0.21905
HexCer-NS d42:1	0.0074191	0.04274	2.1925						
LPC 14:0-SN1	0.0062875	0.037672	3.3322						
LPC 16:0e	0.0053956	0.037627	1.715						
LPC 16:1-SN1	0.0039051	0.035133	2.9852				0.0013972	0.059164	2.3932
LPC 18:0-SN1	0.0029317	0.03137	0.50172	0.027332	0.10236	1.7571	0.025279	0.17932	2.234
LPC 18:1-SN1							0.02512	0.17932	1.4867
LPC 20:1e	0.00026726	0.011804	1.8071						
LPC 20:3e	0.031364	0.097714	0.51771						
LPC 20:4-SN2							0.020435	0.17181	2.6746
LPC 22:6-SN2							0.0015638	0.059164	2.3396
LPC 26:0-SN1	0.036872	0.10621	1.5922						

LPC 26:1-SN1	0.031711	0.097714	2.9297						
PC 28:5e	0.0061907	0.037672	1.8651						
PC 30:0e	0.042551	0.11996	1.5005						
PC 30:1				0.032641	0.10777	0.57069			
PC 30:3				0.0084613	0.057537	0.38809			
PC 32:2				0.047191	0.13569	0.52801			
PC 32:4							0.021552	0.17473	0.65877
PC 32:8e	0.013754	0.063696	8.8888						
PC 34:0e	0.005358	0.037627	1.9196						
PC 34:3				0.031784	0.10777	0.56973			
PC 34:4							0.017651	0.16077	2.1689
PC 34:4e	0.025193	0.087583	0.71184						
PC 34:5				0.014723	0.073614	0.46637			
PC 36:0e	0.00088369	0.024449	1.8581						
PC 36:1				0.0022558	0.034862	3.393			
PC 36:1e	0.033634	0.097944	1.5833						
PC 36:3				0.010835	0.061398	0.69339	0.016723	0.16077	0.79924
PC 36:3e	0.045503	0.12431	1.4304						
PC 36:4e							0.015496	0.16077	2.2204
PC 36:5				0.018695	0.086576	0.44707			
PC 36:6_1				0.0046853	0.048941	0.45836			
PC 36:6_2	0.014245	0.063696	0.8165	0.0051639	0.048941	0.51204			
PC 36:7	0.04908	0.12931	0.69155						
PC 38:1e	0.02519	0.087583	1.1833						
PC 38:2e	0.00026162	0.011804	1.4507						
PC 38:3				0.019316	0.086576	0.59384			
PC 38:5				0.039767	0.1186	0.81607			

PC 38:5e	0.026906	0.088975	1.3708						
PC 38:6	0.014065	0.063696	0.81773	0.037823	0.11585	0.54342			
PC 38:7				0.023188	0.09518	0.37236			
PC 38:7e_1	0.042005	0.11969	1.172						
PC 38:7e_2	0.014422	0.063696	0.66471						
PC 38:8				0.010141	0.061398	0.44965			
PC 40:1				0.026445	0.10217	0.60524			
PC 40:10	0.00036395	0.013778	0.69919						
PC 42:10	0.012489	0.060175	0.54579						
PC 40:2				0.038163	0.11585	0.53026			
PC 40:3				0.0018126	0.034862	0.37241			
PC 40:5				0.010804	0.061398	0.58709			
PC 40:6				0.04789	0.13569	0.58234			
PC 40:7				0.020654	0.087781	0.5347			
PC 40:9_1				0.0079052	0.057537	0.52062	0.0056335	0.10769	13.188
PC 40:9_2				0.0081749	0.057537	0.44522			
PC 40:9_3				0.005679	0.048941	8.7721			
PC 42:0				0.0049958	0.048941	0.50533			
PC 42:1				0.033961	0.10777	0.57473			
PC 42:11				0.033632	0.10777	0.50686			
PC 42:2				0.020332	0.087781	0.46839			
PC 42:3	0.049418	0.12931	1.0868	0.0083774	0.057537	0.43294			
PC 42:4	0.0048643	0.037627	0.66304						
PC 42:4e	0.033558	0.097944	1.9001						
PC 42:6e_1	0.011307	0.056535	1.7962						
PC 42:6e_2	0.024129	0.087583	1.4597						
PC 42:7e	0.019311	0.074317	1.7077						

PC 44:12				0.012776	0.065813	0.56105			
PC 44:2				0.029381	0.10523	0.45885			
PC 44:2e				0.0081811	0.057537	0.49029			
PC 44:4				0.012036	0.063939	0.4926			
PC 44:5	0.0018674	0.024449	0.62245						
PC 44:5e	0.027757	0.089703	1.8252						
PC 44:7e							0.011318	0.13522	0.61418
PC 44:8e	0.002104	0.024449	1.8523						
PC 46:2				0.027697	0.10236	0.56773			
PC 46:3				0.019352	0.086576	0.40358			
PC 46:4				0.034232	0.10777	0.37668			
PC 46:5				0.0057577	0.048941	0.4391			
PC 46:8e							0.030731	0.19931	0.63222
PC 48:4				0.0025317	0.034958	0.39053			
PE 34:0							0.0050042	0.10769	2.4781
PE 36:3e	0.046346	0.12516	1.2487						
PE 38:2e	0.017783	0.0725	1.3085						
PE 38:4				0.044815	0.13135	1.2561			
PS 34:1	0.0452	0.12431	1.4486						
PS 34:2	0.020573	0.077884	1.4481						
PS 38:3	0.016539	0.069413	1.384						
SM d32:0	0.018868	0.074317	1.9044						
SM d32:1	0.0095361	0.050541	1.9616						
SM d34:0	0.0041745	0.035685	1.2144				0.022544	0.17647	1.5739
SM d34:2	0.0057371	0.037672	1.4213						
SM d34:4	0.024523	0.087583	1.9042						
SM d36:1	0.0013873	0.024449	1.8331						

SM d36:5	0.0019498	0.024449	1.4356						
SM d38:0	0.0057631	0.037672	1.3818						
SM d38:1	0.0030778	0.03137	1.6109						
SM d40:0	0.0052908	0.037627	2.2769						
SM d40:1	0.0001779	0.011804	1.8956						
SM d40:2	0.00020249	0.011804	1.6673						
SM d42:3				0.032733	0.10777	1.2653			
SM d42:4	0.044785	0.12431	1.5759						
SM d44:1	0.016764	0.069413	1.8812						
SM d44:2	0.015276	0.066363	1.9408						
Sphingosine 18:1	0.027185	0.088975	2.6606						
TAG 42:0				0.0026733	0.034958	6.1598	0.0071527	0.10769	4.3777
TAG 42:2				0.024426	0.096569	4.8557			
TAG 44:1				0.0019621	0.034862	12.995	0.0091787	0.11575	7.8306
TAG 44:2				0.0030416	0.036934	11.969			
TAG 46:2				0.0016061	0.034862	24.895	0.003835	0.096727	10.155
TAG 46:3				0.001729	0.034862	7.4508			
TAG 48:2				0.0097435	0.061398	7.3714			
TAG 48:3				0.002083	0.034862	15.569	0.017438	0.16077	6.6312
TAG 50:1	0.0083195	0.044993	0.60802						
TAG 50:1e	0.0029696	0.03137	0.40855						
TAG 50:3	0.03359	0.097944	0.55375	0.023515	0.09518	5.8064			
TAG 50:4				0.010753	0.061398	4.3765			
TAG 50:6	0.0015472	0.024449	0.41487						
TAG 52:2	0.0014769	0.024449	0.58535				0.00707	0.10769	0.45122
TAG 52:2e	0.0037642	0.035133	0.39177						
TAG 52:5	0.0019079	0.024449	0.57618						

TAG 52:6	0.02326	0.085609	0.46878				0.018414	0.16077	0.67571
TAG 52:7	0.0049417	0.037627	0.48074						
TAG 52:8	0.0038601	0.035133	0.40784						
TAG 54:1e	0.0039773	0.035133	0.432						
TAG 54:2	0.027196	0.088975	0.44514						
TAG 54:3	0.0013427	0.024449	0.42564				0.0080647	0.10769	0.44381
TAG 54:4							0.017435	0.16077	0.54122
TAG 54:5	0.0010157	0.024449	0.50254						
TAG 54:6				0.029713	0.10523	0.47248			
TAG 54:7	0.0015405	0.024449	0.43655				0.018397	0.16077	0.63942
TAG 56:4	0.010421	0.053108	0.41986				0.024269	0.17932	0.37805
TAG 56:5	0.010258	0.053108	0.40489						
TAG 56:6	0.0049476	0.037627	0.40478	0.001004	0.034862	0.29135	0.0061669	0.10769	0.42497
TAG 56:7				0.0054187	0.048941	0.40139			
TAG 56:7e	0.025525	0.087583	0.38905						
TAG 56:9	2.9909E-05	0.003986	0.49838						
TAG 58:1	0.046758	0.12516	0.5995						
TAG 58:11	0.032625	0.097944	0.45124						
TAG 58:2	0.015698	0.067096	0.47342						
TAG 58:4	0.01935	0.074317	0.49617						
TAG 58:5	0.005045	0.037627	0.4357						
TAG 60:2	0.029029	0.092682	0.44475						
TAG 60:4	0.031377	0.097714	0.42856						
TAG 60:5	0.025779	0.087583	0.41155						
TAG 62:14	0.022064	0.082353	0.43879						
TAG 62:3	0.0063911	0.037672	0.40495						
TAG 62:4	0.0063972	0.037672	0.40213						

TAG 64:3	0.0076961	0.043393	0.45891						
TAG 64:4	0.002122	0.024449	0.37692						
LPC 16:0e	0.0053956	0.037627	1.715						
LPC 20:1e	0.00026726	0.011804	1.8071						
LPC 20:3e	0.031364	0.097714	0.51771						
PC 28:5e	0.0061907	0.037672	1.8651						
PC 30:0e	0.042551	0.11996	1.5005						
PC 32:8e	0.013754	0.063696	8.8888						
PC 34:0e	0.005358	0.037627	1.9196						
PC 34:4e	0.025193	0.087583	0.71184						
PC 36:0e	0.00088369	0.024449	1.8581						
PC 36:1e	0.033634	0.097944	1.5833						
PC 36:3e	0.045503	0.12431	1.4304						
PC 36:4e							0.015496	0.16077	2.2204
PC 38:1e	0.02519	0.087583	1.1833						
PC 38:2e	0.00026162	0.011804	1.4507						
PC 38:5e	0.026906	0.088975	1.3708						
PC 38:7e_1	0.042005	0.11969	1.172						
PC 38:7e_2	0.014422	0.063696	0.66471						
PC 42:4e	0.033558	0.097944	1.9001						
PC 42:6e_1	0.011307	0.056535	1.7962						
PC 42:6e_2	0.024129	0.087583	1.4597						
PC 42:7e	0.019311	0.074317	1.7077						
PC 44:2e				0.0081811	0.057537	0.49029			
PC 44:5e	0.027757	0.089703	1.8252						
PC 44:7e							0.011318	0.13522	0.61418
PC 44:8e	0.002104	0.024449	1.8523						

PC 46:8e				0.030731	0.19931	0.63222
PE 36:3e	0.046346	0.12516	1.2487			
PE 38:2e	0.017783	0.0725	1.3085			
TAG 50:1e	0.0029696	0.03137	0.40855			
TAG 52:2e	0.0037642	0.035133	0.39177			
TAG 54:1e	0.0039773	0.035133	0.432			
TAG 56:7e	0.025525	0.087583	0.38905			

* Fold change: concentration in mitochondrial fraction vs concentration in whole cell. Reported lipids are sum compositions unless the fatty acyl constituents can be confidently determined.

Table S3: MS-DIAL lipid data alignment and processing.

MS-DIAL: Analysis parameter setting	
Data collection	
MS1 tolerance	0.03 Da
MS2 tolerance	0.05 Da
Retention time begin	0.3 min
Retention time end	12.6 min
Mass range begin	280 Da
Mass range end	1200 Da
Maximum charged number	2
Peak detection	
Minimum peak height	500 amplitude
Mass slice width	0.05 Da
Smoothing method	Savitzky-Golay filter
Smoothing level	3 scan
Minimum peak width	5 scan
MS2 Dec	
Sigma window value	0.5
MS/MS abundance cut off	0 amplitude
Exclude after precursor ion	checked
Keep the isotopic ions until	0.5 Da
Identification	
Retention time tolerance	0.15 min
Accurate mass tolerance (MS1)	0.03 Da
Accurate mass tolerance (MS2)	0.05 Da
Identification score cut off	70%
Adduct	[M+H]+, [M+NH4]+, [M+Na]+, [M+CH3OH+H]+ and [M+H-H2O]+
Alignment	
Reference file	A working QC sample in the sequence
Retention time tolerance	0.1 min
MS1 tolerance	0.025 Da
Advanced	Default

Figure S1. The expression level of FASH, ACC, SCL25A1, and ACLY in the three indicated cancer cell lines.

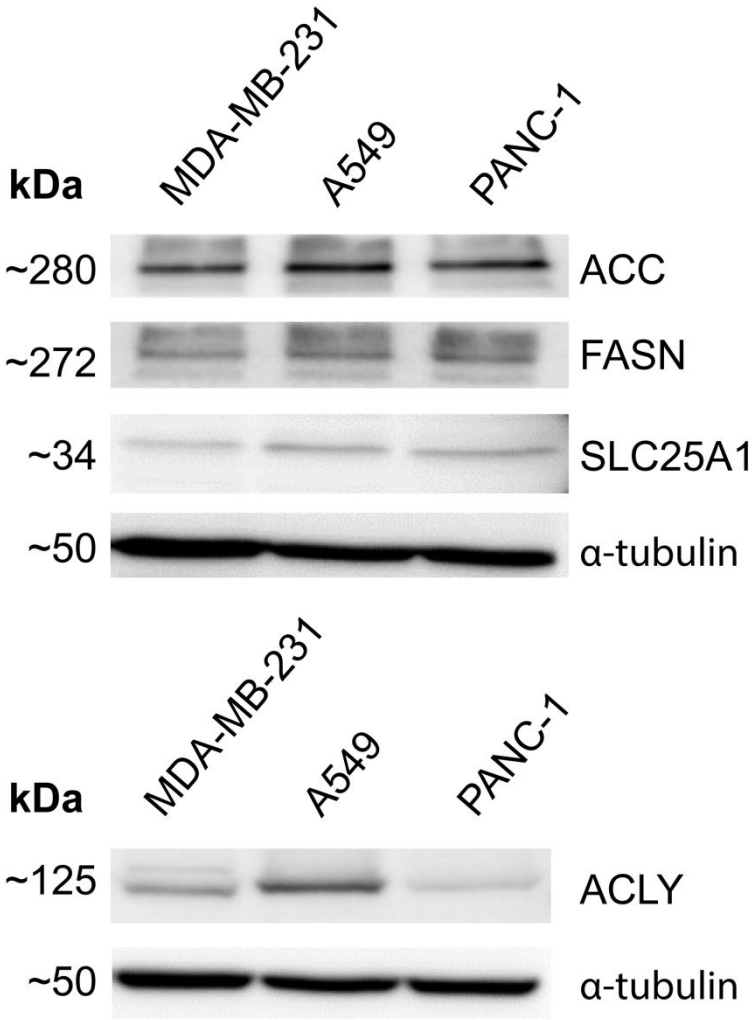

Figure S2: Lipid compositions of mitochondria and bulk A549 cells.

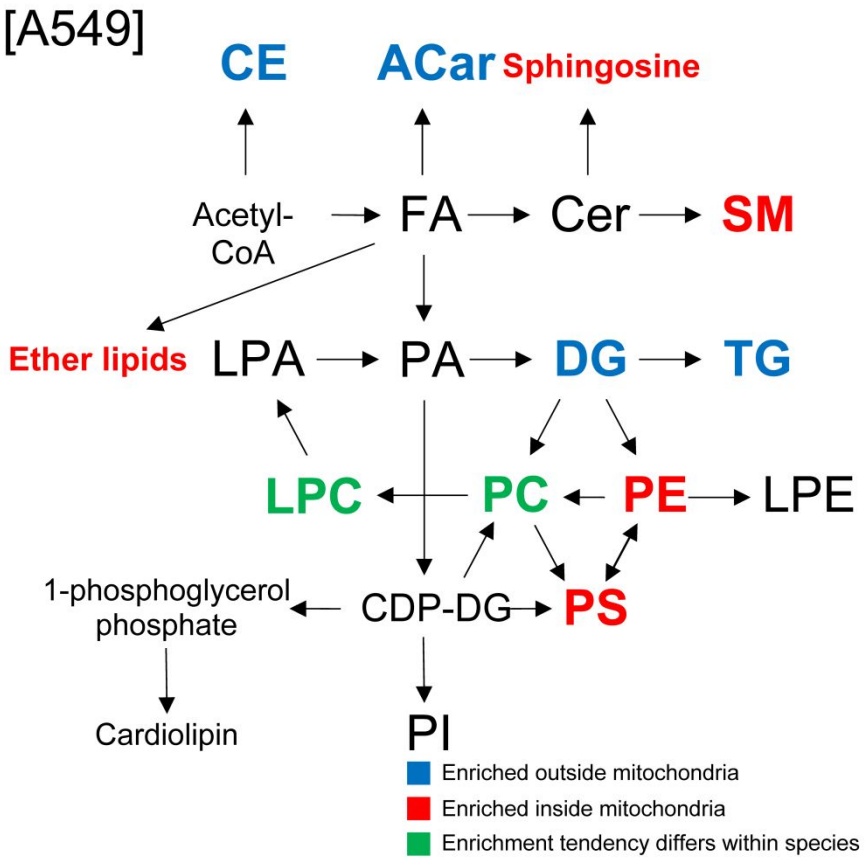

Figure S3: Lipid compositions of mitochondria and bulk MDA-MB-231 cells.

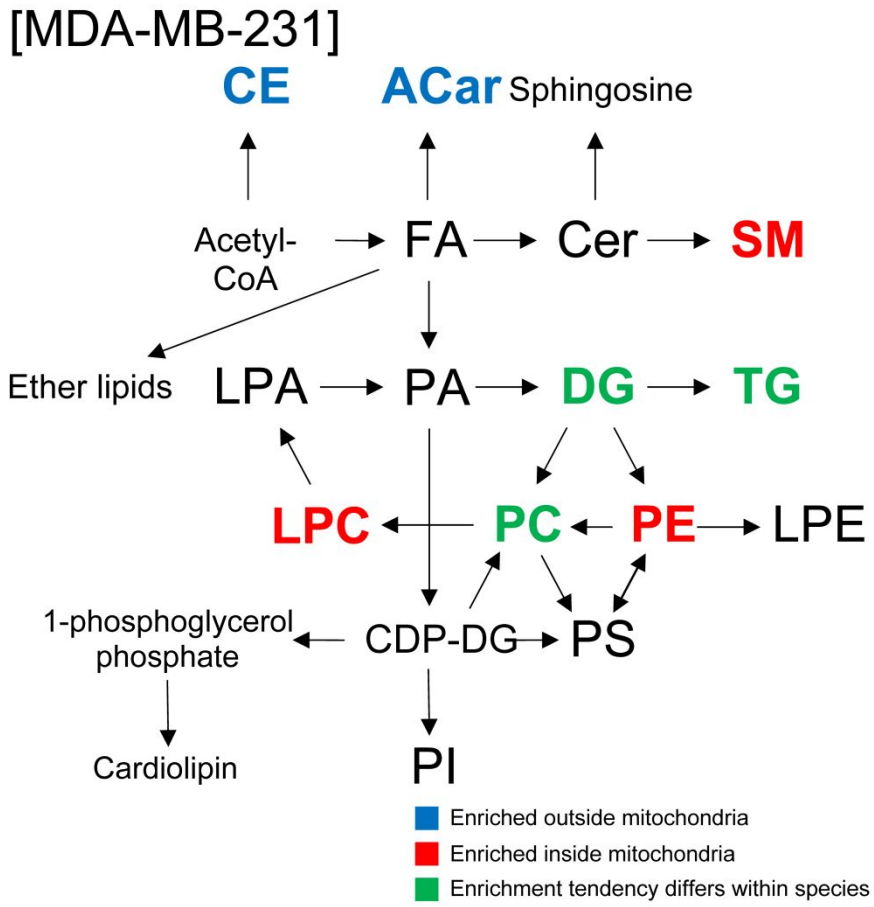

Figure S4: Lipid compositions of mitochondria and bulk PANC1 cells.