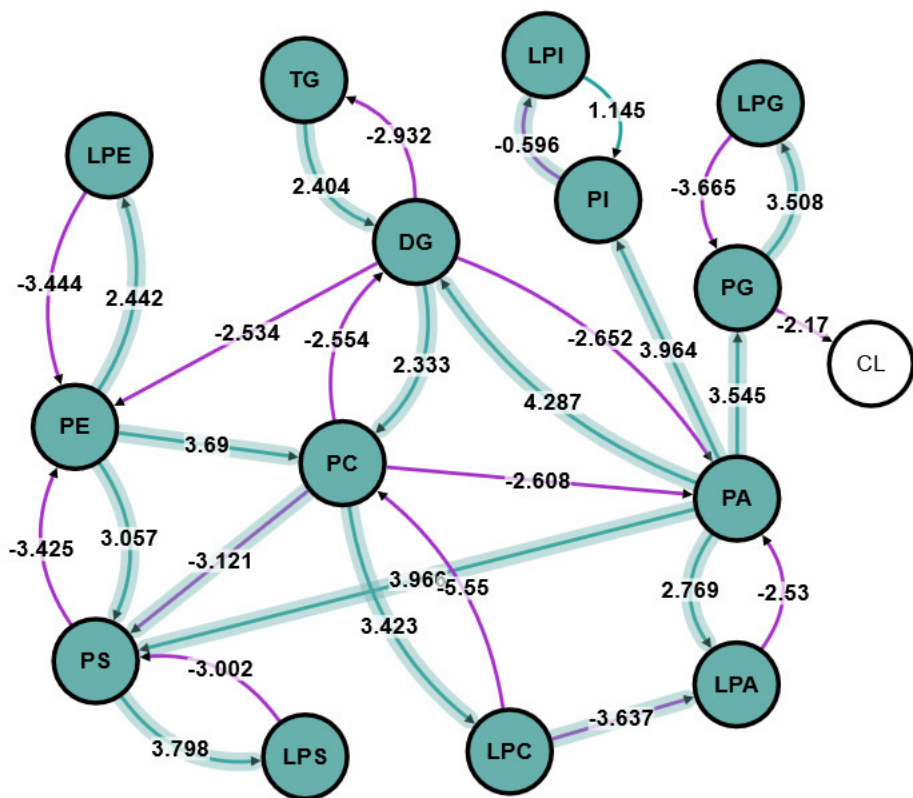




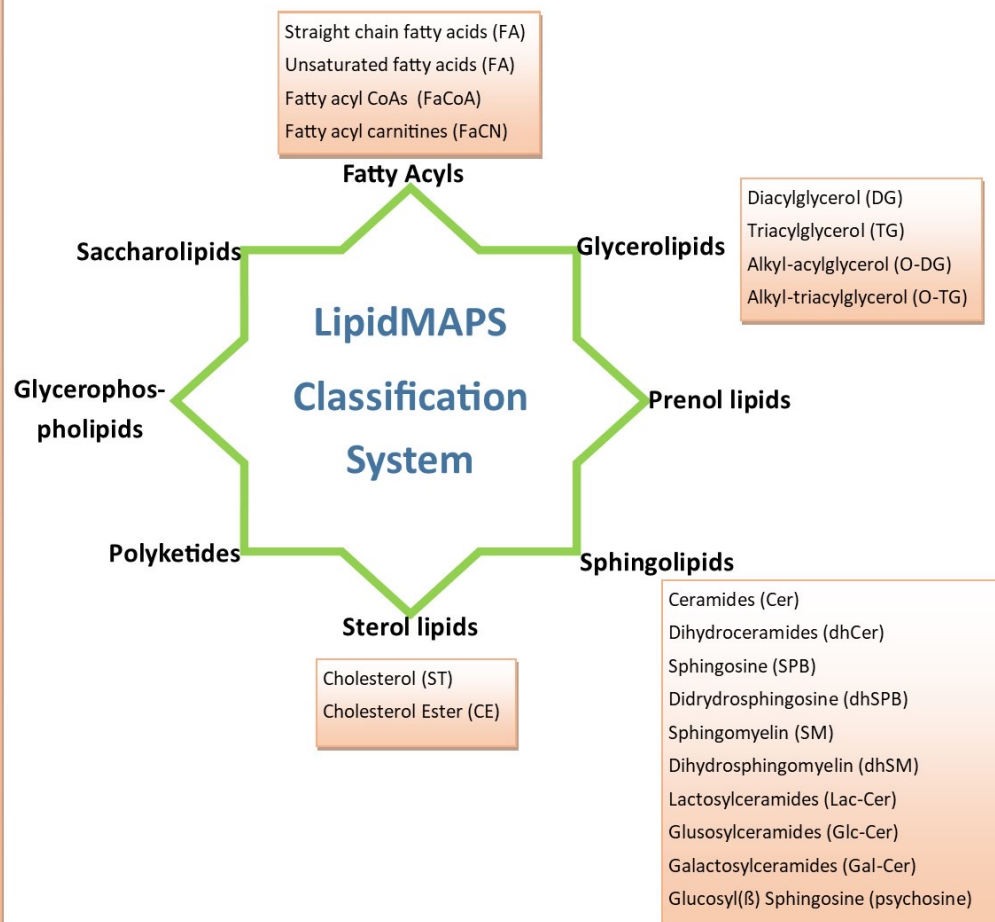
BioPAN

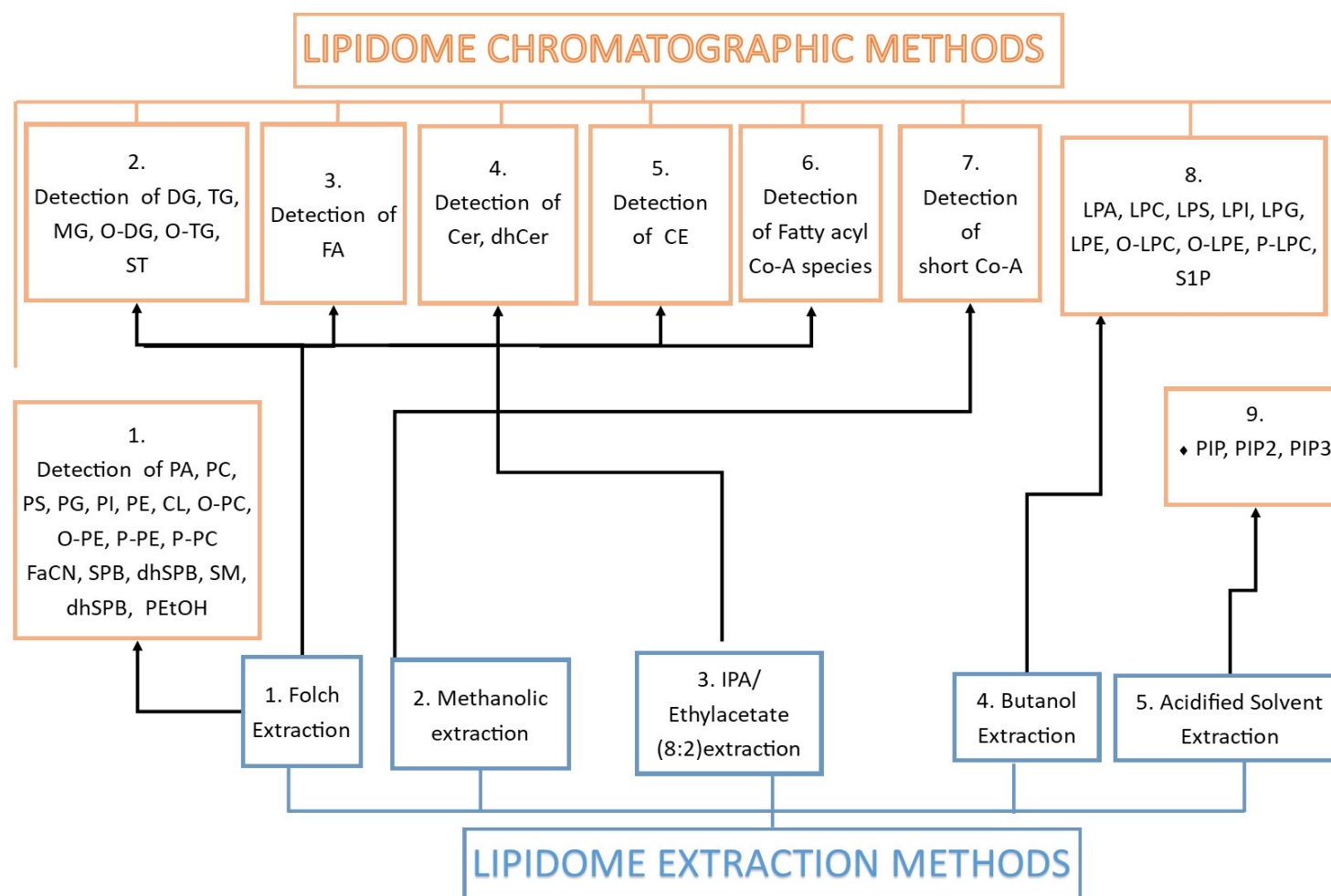
Biosynthetic Pathway Analysis

Dr. Andrea Lopez
Resolian



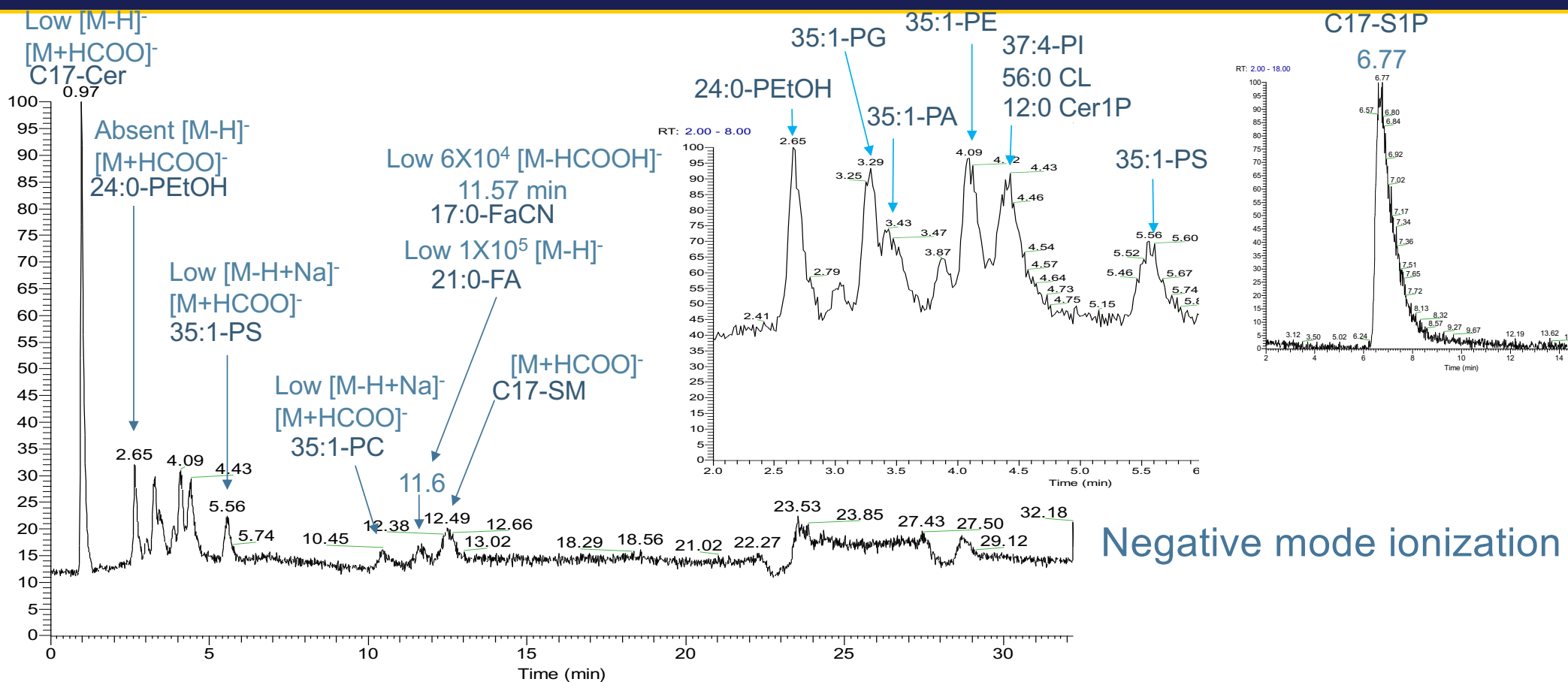
Phosphatidic acid (PA)
 Phosphatidylcholine (PC)
 Phosphatidylethanolamine (PE)
 Phosphatidylinositol (PI)
 Phosphatidylserine (PS)
 Phosphatidylglycerol (PG)
 Alkyl-cylphosphatidylcholine (O-PC)
 Alkenyl-acylphosphatidylcholine (P-PC)
 Alkyl-acylphosphatidylethanolamine (O-PE)
 Alkenyl-acylphosphatidylethanolamine (P-PE)
 Lysophosphatidic acid (LPA)
 Lysophosphatidylcholine (LPC)
 Lysophosphatidylethanolamine (LPE)
 Lysophosphatidylinositol (LPI)
 Lysophosphatidylserine (LPS)
 Lysophosphatidylglycerol (LPG)
 Alkyl-lysophosphatidic acid (O-LPA)
 Alkenyl-lysophosphatidic acid (P-LPA)
 Alkyl-lysophosphatidylcholine (O-LPC)
 Alkenyl-lysophosphatidylcholine (P-LPC)
 Alkyl-lysophosphatidylethanolamine (O-LPE)
 Alkenyl-lysophosphatidylethanolamine (P-LPE)
 Diacylglycerophosphoglycerophosphodiradyl-
 glycerols -Cardiolipin (CL)-
 Phosphatidylinositol monophosphate (PIP)
 Phosphatidylinositol diphosphate (PIP2)
 Phosphatidylinositol triphosphate (PIP3)







Lipid subclasses abundances

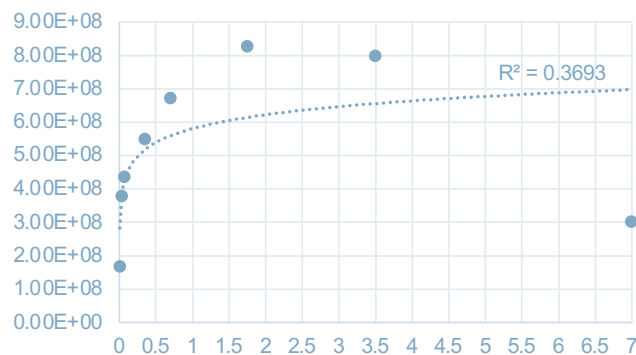


Negative mode ionization

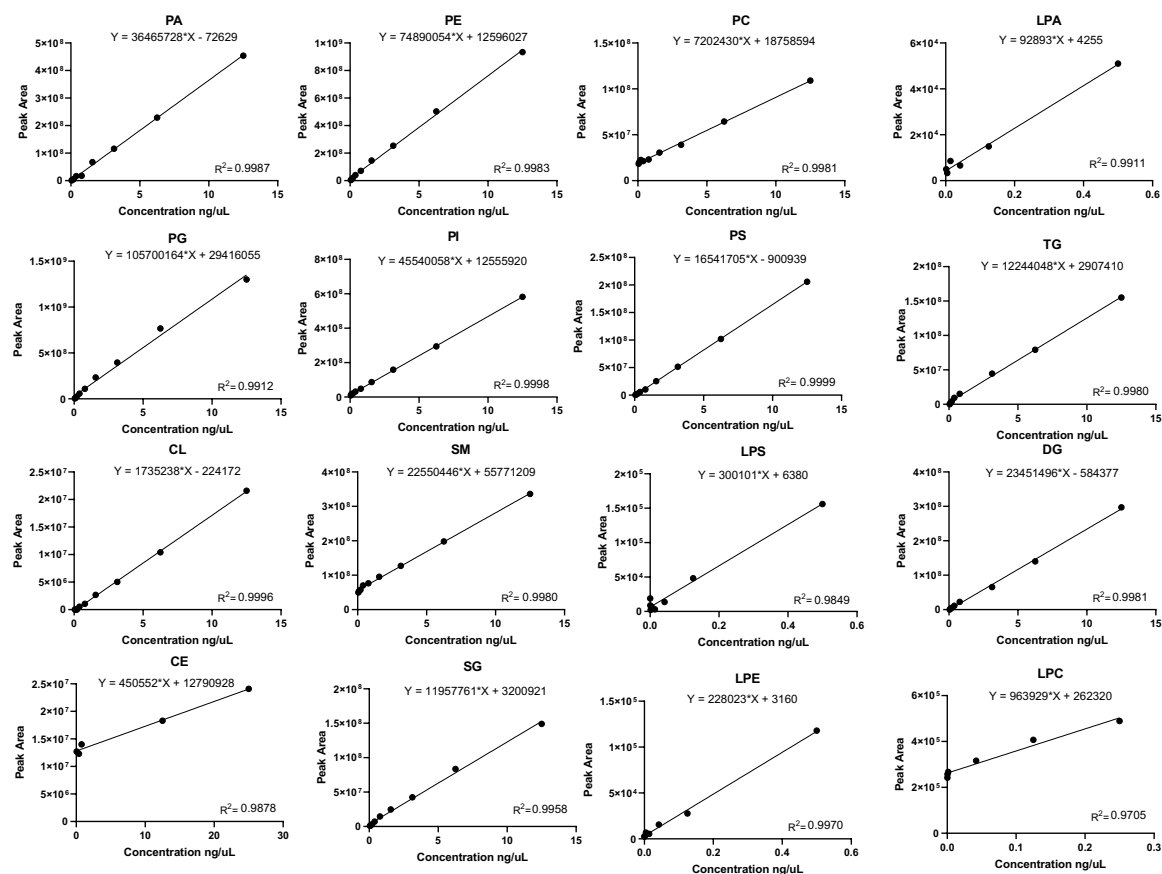
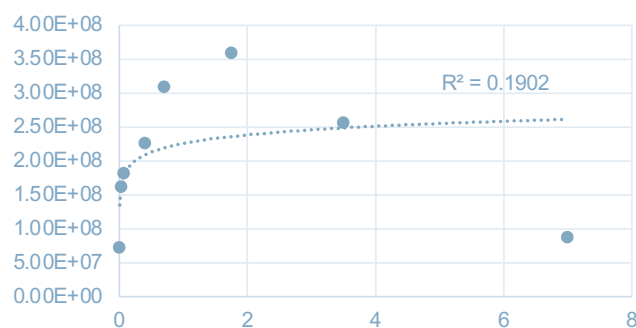


Lipid analysis good practice

PC area [M+H]⁺



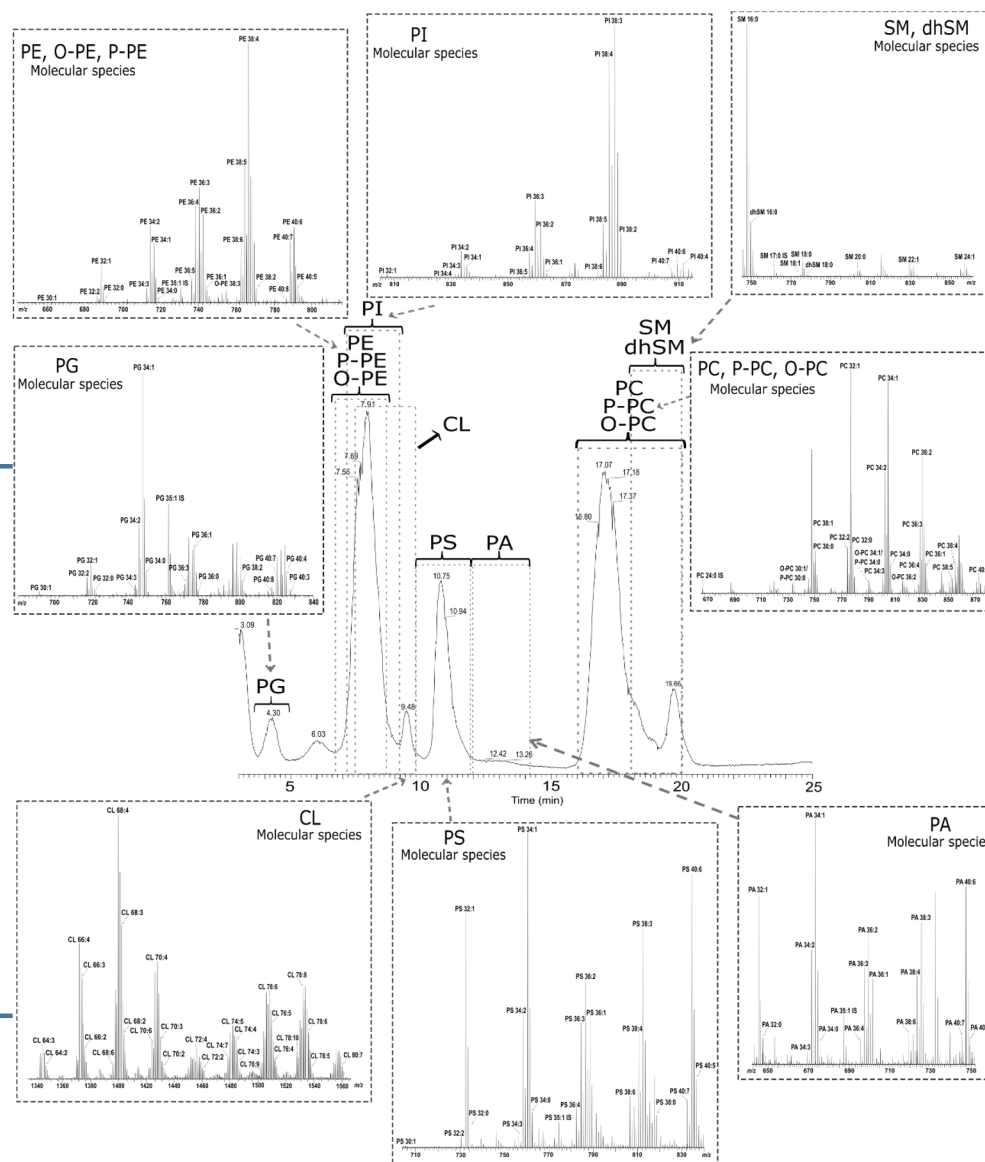
PC area [M+Na]⁺





CL(64:3)
CL(64:4)
CL(66:3)
CL(66:4)
CL(66:5)
CL(66:6)
CL(68:3)
CL(68:4)
CL(68:5)
CL(68:6)
CL(68:7)
CL(68:8)
CL(70:4)
CL(70:5)
CL(70:6)
CL(70:7)
CL(70:8)
CL(70:9)
CL(72:5)
CL(72:6)
CL(72:7)
CL(72:8)
CL(72:9)
CL(74:7)
CL(74:8)
CL(74:9)
CL(74:10)

PG(14:0/16:0)
PG(14:0/16:1)
PG(16:0/16:0)
PG(16:0/16:1)
PG(16:0/18:0)
PG(16:0/18:1)
PG(16:0/18:2)
PG(16:0/18:3)
PG(18:0/18:0)
PG(18:0/18:1)
PG(18:0/18:2)
PG(18:0/18:3)
PG(18:0/18:4)
PG(18:0/18:5)
PG(18:0/18:6)
PG(18:0/20:1)
PG(18:0/20:2)
PG(18:0/20:3)
PG(18:0/20:4)
PG(18:0/20:5)
PG(18:0/20:6)
PG(18:0/20:7)
PG(18:0/22:2)
PG(18:0/22:3)
PG(18:0/22:6)
PG(18:0/22:7)

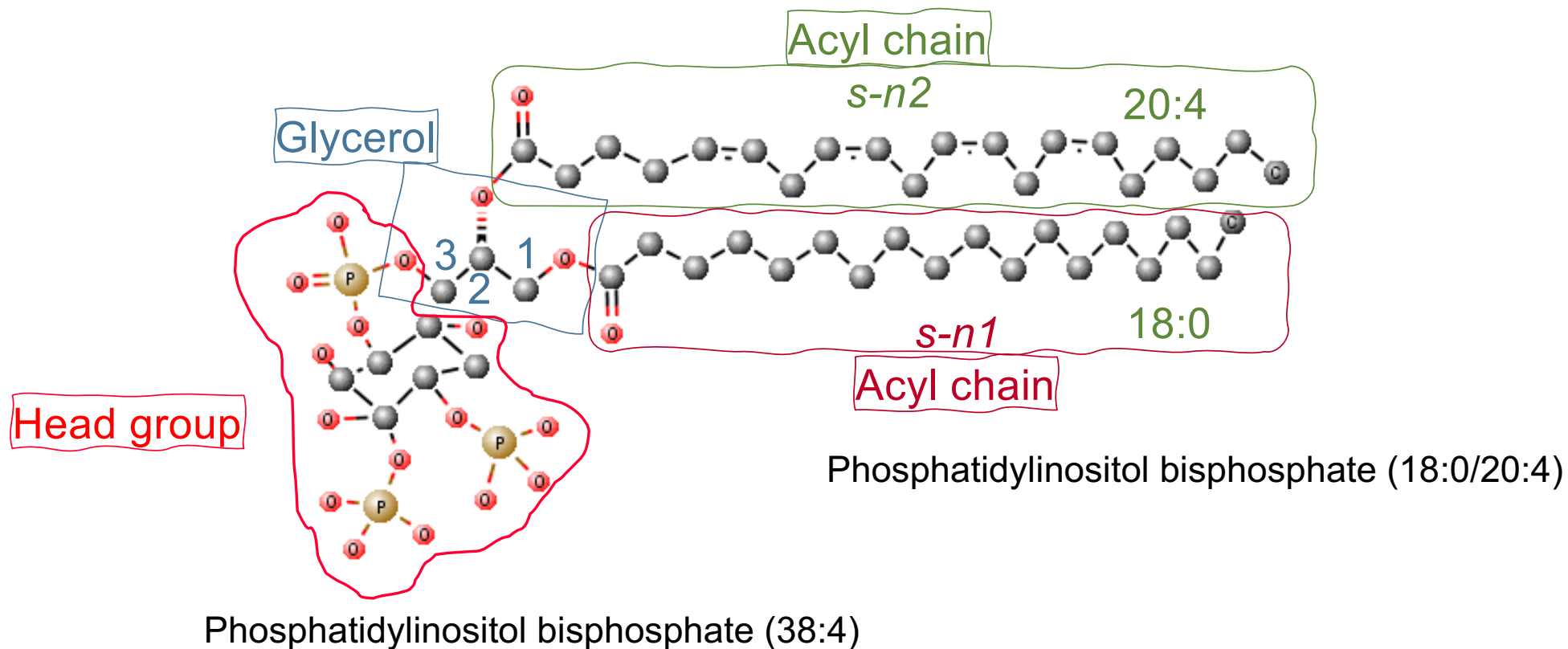


PA(14:0/16:0)
PA(16:0/16:0)
PA(16:0/16:1)
PA(16:0/18:0)
PA(16:0/18:1)
PA(16:0/18:2)
PA(16:0/18:3)
PA(18:0/18:0)
PA(18:0/18:1)
PA(18:0/18:2)
PA(18:0/18:3)
PA(18:0/18:4)
PA(18:0/18:5)
PA(18:0/20:0)
PA(18:0/20:1)
PA(18:0/20:2)
PA(18:0/20:3)
PA(18:0/20:4)
PA(18:0/20:5)
PA(18:0/20:6)
PA(18:0/22:6)

PC(14:0/16:0)
PC(16:0/16:0)
PC(16:0/16:1)
PC(16:0/18:0)
PC(16:0/18:1)
PC(16:0/18:2)
PC(18:0/18:1)
PC(18:0/18:2)
PC(18:0/18:1)
PC(18:0/18:2)
PC(18:0/18:3)
PC(18:0/18:4)
PC(18:0/20:2)
PC(18:0/20:3)
PC(18:0/20:1)
PC(18:0/20:2)
PC(18:0/20:3)
PC(18:0/20:4)
PC(18:0/20:5)
PC(18:0/20:6)
PC(18:0/22:0)
PC(18:0/22:1)
PC(18:0/22:2)
PC(18:0/22:3)
PC(18:0/22:4)
PC(18:0/22:5)
PC(18:0/22:6)
PC(18:0/22:7)



Lipid sum composition





Lipid Levels



	C_1	C_2	C_3	C_4	C_5	C_6	K_1	K_2	K_3	K_4	K_5	K_6
PA(14:0/16:0)	0.33790039	0.44108444	0.48404661	0.44326571	0.46048721	0.44001775	3.20203158	3.24872244	3.048198	2.29536984	2.79269603	2.52959502
PA(16:0/16:0)	0.7120343	0.83923648	0.96866359	1.08917546	0.80505818	0.80489856	12.4873504	12.3401085	11.8541033	8.49340596	10.3383459	9.15887851
PA(16:0/16:1)	1.11536432	1.42400929	1.87602945	1.50024152	1.42646769	1.79288723	2.5146545	2.54986936	2.51845419	2.0803469	2.37200143	2.19626168
PA(16:0/18:0)	0	0	0	0	0	0	6.24367518	6.09450257	5.29743812	3.59088303	4.83351235	4.29906542
PA(16:0/18:1)	1.36904489	1.64610248	2.40422587	1.94954017	1.52111044	2.18967375	4.17581578	4.51421316	4.64611377	3.6177609	4.26065163	3.95638629
PA(16:0/18:2)	0.4824174	0.67653999	0.79096986	0.64886506	0.5514389	0.83122126	0.72174594	0.72403698	0.77290491	0.5859375	0.67132116	0.62616822
PA(16:0/18:3)	0	0.06745928	0	0	0	0.08190843	0.03528189	0.03201794	0.03951405	0.03380383	0.02808138	0.0314179
PA(18:0/18:0)	0	0	0	0	0	0	0.36435074	0.32799279	0.28968292	0.15531679	0.26428133	0.21940816
PA(18:0/18:1)	0.097936	0.15104432	0.34966064	0.21699571	0.14566773	0.35036975	0.75611479	0.8625484	0.83803734	0.59668865	0.76083065	0.68847352
PA(18:0/18:2)	0.30100288	0.39197552	0.56874151	0.46360364	0.30760048	0.62823155	0.60718309	0.63589335	0.71211463	0.52571472	0.61761547	0.57943925
PA(18:0/18:3)	0	0.12200037	0.30266676	0.15801394	0	0.42225482	0.12509406	0.11734662	0.13517946	0.09688837	0.11259994	0.0993919
PA(18:0/18:4)	0	0.05435181	0	0	0	0.17023162	0.07845473	0.08379599	0.07882808	0.05423411	0.05881945	0.04459746
PA(18:0/18:5)	0	0	0	0	0	0	0	0	0	0	0	0.01075936
PA(18:0/20:0)	0	0	0	0	0	0	0.0351271	0.03161691	0.0239107	0	0.01667808	0.02138582
PA(18:0/20:1)	0	0	0	0	0	0	0.02944392	0.0307213	0	0.01998904	0.02017228	0.02231521
PA(18:0/20:2)	0	0	0	0	0	0	0	0.0345066	0.02893352	0.01849278	0.02578623	0.02546129
PA(18:0/20:3)	0	0.17524507	0.60929526	0.26892309	0.15819282	0.65690167	0.10993808	0.12509093	0.14582942	0.09095571	0.07640452	0.05972865
PA(18:0/20:4)	0	0.12871998	0.45427141	0.16186077	0.11431649	0.47544597	0.13445953	0.15785482	0.1522482	0.10934583	0.09645144	0.09857225
PA(18:0/20:5)	0	0	0	0	0	0.1167109	0.03922891	0.04649056	0.04976563	0.03550365	0.0330387	0.02447303
PA(18:0/20:6)	0	0	0	0	0	0.27693551	0.13887713	0.14133846	0.1349456	0.10420646	0.11453984	0.10306472
PA(18:0/22:6)	0.15990904	0.29413299	1.09733132	0.5677377	0.27863193	1.39394782	0.2270065	0.23074403	0.21359217	0.17755657	0.11605811	0.05448125
DG(14:0/16:0)	0.20175683	0.16651616	0.22249522	0.21353515	0.19269859	0.19825614	0.5911592	0.67602779	0.84858686	0.54270578	0.68609023	0.72848789
DG(16:0/16:0)	0.62988668	0.47819167	0.67955182	0.64541214	0.4683128	0.46386327	2.12907248	2.86745754	2.56273113	1.81263585	2.51607064	3.17600612
DG(16:0/16:1)	1.65282862	1.54146459	1.96068874	1.83382056	1.57573023	1.61152735	2.1404475	2.41227644	3.15379959	2.02610401	2.57612915	2.56708533
DG(16:0/18:0)	0.17457116	0.13728425	0.17865233	0.18660062	0.13163669	0.08909864	1.10025303	1.59073639	1.59506522	1.11935521	1.49877984	1.85276642
DG(16:0/18:1)	2.99643495	2.46927213	3.38309728	3.27598382	2.41602261	2.43205784	5.39705252	7.80031422	6.72717955	4.81740563	6.71629949	8.21797338
DG(16:0/18:2)	2.43565578	2.26109123	2.90872243	2.63286857	2.20997492	2.26416966	1.61991951	1.85427048	2.36317431	1.58474415	1.97586948	1.92302431
DG(18:0/18:1)	0.51524148	0.45874629	0.61305715	0.58809137	0.47763507	0.40720567	1.45872251	2.05576965	2.23411765	1.5209789	1.95988175	2.3560997
DG(18:0/18:2)	2.18209242	1.89771187	2.58799746	2.53855247	2.12041001	2.27785404	2.09864983	3.17887513	2.99097742	2.12760883	2.76308022	3.45190801
DG(18:0/18:3)	0.97158873	0.84711791	1.22577123	1.13223288	0.75850257	0.83389831	0.52570213	0.83960625	0.79248194	0.456562	0.78007519	0.83876358
DG(18:0/18:4)	0.28282447	0.25231658	0.34660627	0.33661458	0.205175	0.23930765	0.37622221	0.49786299	0.53272934	0.25223081	0.39925694	0.42593777
DG(18:0/20:2)	0	0	0	0	0	0	0	0	0	0	0	0
DG(18:0/20:3)	0	0	0	0	0	0	0	0	0	0	0	0
DG(18:0/20:4)	0	0	0	0	0	0	0	0	0	0	0	0
DG(18:0/20:5)	0	0	0	0	0	0	0	0	0	0	0	0
DG(18:0/20:6)	0	0	0	0	0	0	0	0	0	0	0	0
DG(18:0/22:4)	0	0	0	0	0	0	0	0	0	0	0	0
DG(18:0/22:5)	0.05819521	0.03165168	0.07341543	0.07393383	0.02114928	0.02871064	0.07468442	0.11601932	0.1118308	0.05425519	0.07716067	0.09351623
DG(18:0/22:6)	0.24007935	0.22995088	0.27846028	0.28901734	0.20961499	0.24514545	0.33342197	0.59785756	0.61364752	0.32871432	0.43703008	0.48955723

PA(38:4) →

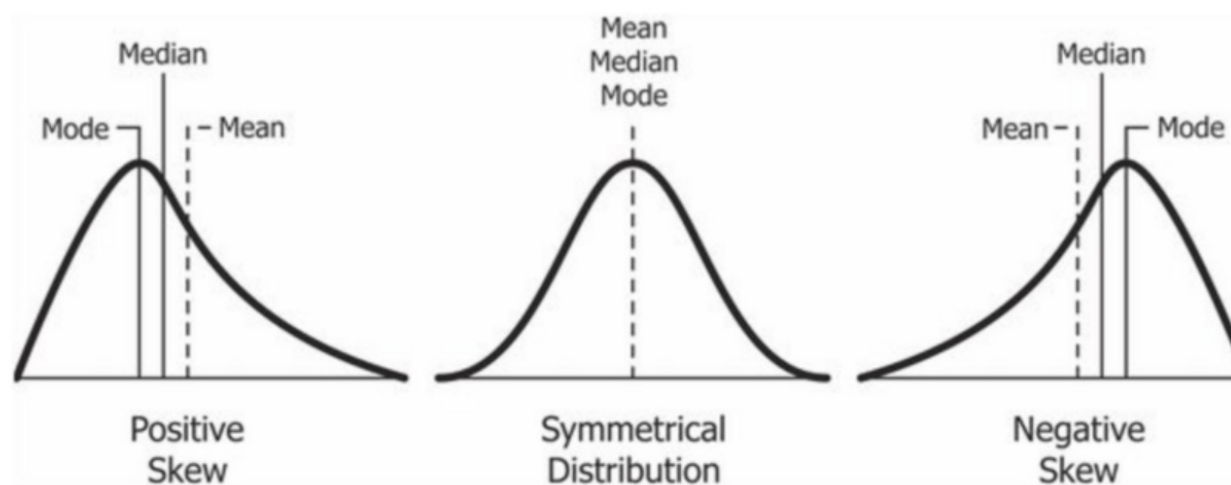
Do I have the same sample size in C as in K?

}

<https://www.lipidmaps.org/biopan/>



Skeweness



A general relationship of mean and median under differently skewed unimodal distribution.



Skewness



	C_1	C_2	C_3	C_4	C_5	C_6	K_1	K_2	K_3	K_4	K_5	K_6	Mean C	Skewness C	Mean K
PA(14:0/16:0)	0.33790039	0.44108444	0.48404661	0.44326571	0.46048721	0.44001775	3.20203158	3.24872244	3.048198	2.29536984	2.79269603	2.52959502	0.43446702	-1.7993634	2.852768818
PA(16:0/16:0)	0.7120343	0.83923648	0.96866359	1.08917546	0.80505818	0.80489856	12.4873504	12.3401085	11.8541033	8.49340596	10.3383459	9.15887851	0.86984443	0.84101553	10.77869875
PA(16:0/16:1)	1.11536432	1.42400929	1.87602945	1.50024152	1.42646769	1.79288723	2.5146545	2.54986936	2.51845419	2.0803469	2.37200143	2.19626168	1.52249992	-0.0761289	2.371931344
PA(16:0/18:0)	0	0	0	0	0	0	6.24367518	6.09450257	5.29743812	3.59088303	4.83351235	4.29906542	0	0	5.059846111
PA(16:0/18:1)	1.36904489	1.64610248	2.40422587	1.94954017	1.52111044	2.18967375	4.17581578	4.51421316	4.64611377	3.6177609	4.26065163	3.95638629	1.84661627	0.28970677	4.195156921
PA(16:0/18:2)	0.4824174	0.67653999	0.79096986	0.64886506	0.5514389	0.83122126	0.72174594	0.72403698	0.77290491	0.5859375	0.67132116	0.62616822	0.66357541	-0.0715603	0.683685785
PA(16:0/18:3)	0	0.06745928	0	0	0	0.08190843	0.03528189	0.03201794	0.03951405	0.03380383	0.02808138	0.0314179	0.02489462	1.02806947	0.03335283
PA(18:0/18:0)	0	0	0	0	0	0	0.36435074	0.32799279	0.28968292	0.15531679	0.26428133	0.21940816	0	0	0.270172122
PA(18:0/18:1)	0.097936	0.15104432	0.34966064	0.21699571	0.14566773	0.35036975	0.75611479	0.8625484	0.83803734	0.59668865	0.76083065	0.68847352	0.21861236	0.48790339	0.750448892
PA(18:0/18:2)	0.30100288	0.39197552	0.56874151	0.46360364	0.30760048	0.62823155	0.60718309	0.63589335	0.71211463	0.52571472	0.61761547	0.57943925	0.44352593	0.32998227	0.612993419
PA(18:0/18:3)	0	0.12200037	0.30266676	0.15801394	0	0.42225482	0.12509406	0.11734662	0.13517946	0.09688837	0.11259994	0.0993919	0.16748931	0.59986893	0.114416725
PA(18:0/18:4)	0	0.05435181	0	0	0	0.17023162	0.07845473	0.08379599	0.07882808	0.05423411	0.05881945	0.04459746	0.03743057	1.98644224	0.06645497
PA(18:0/18:5)	0	0	0	0	0	0	0	0	0	0	0	0.01075936	0	0	0.001793226
PA(18:0/20:0)	0	0	0	0	0	0	0.0351271	0.03161691	0.0239107	0	0.01667808	0.02138582	0	0	0.021453101
PA(18:0/20:1)	0	0	0	0	0	0	0.02944392	0.0307213	0	0.01998904	0.02017228	0.02231521	0	0	0.020440293
PA(18:0/20:2)	0	0	0	0	0	0	0	0.0345066	0.02893352	0.01849278	0.02578623	0.02546129	0	0	0.022196735
PA(18:0/20:3)	0	0.17524507	0.60929526	0.26892309	0.15819282	0.65690167	0.10993808	0.12509093	0.14582942	0.09095571	0.07640452	0.05972865	0.31142632	0.50873111	0.101324552
PA(18:0/20:4)	0	0.12871998	0.45427141	0.16186077	0.11431649	0.47544597	0.13445953	0.15785482	0.1522482	0.10934583	0.09645144	0.09857225	0.22243577	0.6146248	0.124822013
PA(18:0/20:5)	0	0	0	0	0	0.1167109	0.03922891	0.04649056	0.04976563	0.03550365	0.0330387	0.02447303	0.01945182	2.44948974	0.038083415
PA(18:0/20:6)	0	0	0	0	0	0.27693551	0.13887713	0.14133846	0.1349456	0.10420646	0.11453984	0.10306472	0.04615592	2.44948974	0.122828699
PA(18:0/22:6)	0.15990904	0.29413299	1.09733132	0.56777377	0.27863193	1.39394782	0.2270065	0.23074403	0.21359217	0.17755657	0.11605811	0.05448125	0.63194847	0.83909269	0.169906436
DG(14:0/16:0)	0.20175683	0.16651616	0.22249522	0.21353515	0.19269859	0.19825614	0.5911592	0.67602779	0.84858686	0.54270578	0.68609023	0.72848789	0.1	If skewness value lies above +1 or below -1, data is highly skewed. If it lies between +0.5 to -0.5, it is moderately skewed. If the value is 0, then the data is symmetric	
DG(16:0/16:0)	0.62988668	0.47819167	0.67955182	0.64541214	0.4683128	0.46386327	2.12907248	2.86745754	2.56273113	1.81263585	2.51607064	3.17600612	0.5		
DG(16:0/16:1)	1.65282862	1.54146459	1.96068874	1.83382056	1.57573023	1.61152735	2.1404475	2.41227644	3.15379959	2.02610401	2.57612915	2.56708533	1.6		
DG(16:0/18:0)	0.17457116	0.13728425	0.17865233	0.18660062	0.13163669	0.08909864	1.10025303	1.59073639	1.59506522	1.11935521	1.49877984	1.85276642	0.1		
DG(16:0/18:1)	2.99643495	2.46927213	3.38309728	3.27598382	2.41602261	2.43205784	5.39705252	7.80031422	6.72717955	4.81740563	6.71629949	8.21797338	2.8	0.28891001	0.012704151
DG(16:0/18:2)	2.43565578	2.26109123	2.90872243	2.63286857	2.20997492	2.26416966	1.61991951	1.85427048	2.36317431	1.58474415	1.97586948	1.92302431	2.45208043	1.08458835	1.886833705
DG(18:0/18:1)	0.51524148	0.45874629	0.61305715	0.58809137	0.47763507	0.40720567	1.45872251	2.05576965	2.23411765	1.5209789	1.95988175	2.3560997	0.50999617	0.19463073	1.930928359
DG(18:0/18:2)	2.18209242	1.89771187	2.58799746	2.53855247	2.12041001	2.27785404	2.09864983	3.17887513	2.99097742	2.12760883	2.76308022	3.45190801	2.26743638	-0.0246536	2.768516573
DG(18:0/18:3)	0.97158873	0.84711791	1.22577123	1.13223288	0.75850257	0.83389831	0.52570213	0.83960625	0.79248194	0.456562	0.78007519	0.83876358	0.9615186	0.55124738	0.705531849
DG(18:0/18:4)	0.28282447	0.25231658	0.34660627	0.33661458	0.205175	0.23930765	0.37622221	0.49786299	0.53272934	0.25223081	0.39925694	0.42593777	0.27714076	0.17795039	0.41404001



Handling skewness (Normalisation or Data transformation)



$$z = \frac{x - \min(x)}{\max(x) - \min(x)} \quad z = \frac{x - \mu}{\sigma} \quad \begin{matrix} \mu = \text{Mean} \\ \sigma = \text{Standard Deviation} \end{matrix}$$

	Mean C	Skewness C	Min	Max	Min-Max normalisation_1	Min-Max normalisation_2	Min-Max normalisation_3	Min-Max normalisation_4	Min-Max normalisation_5	Min-Max normalisation_6	Z-score_1	Z-score_2	Z-score_3	Z-score_4	Z-score_5	Z-score_6
PA(14:0/16:0)	0.43446702	-1.7993634	0.33790039	3.24872244	0.00000	0.03545	0.05021	0.03620	0.04211	0.03508	-1.92271	0.13176	0.98717	0.17519	0.51808	0.11052
PA(16:0/16:0)	0.86984443	0.84101553	0.7120343	12.4873504	0.00000	0.01080	0.02179	0.03203	0.00790	0.00789	-1.16259	-0.22549	0.72800	1.61581	-0.47728	-0.47846
PA(16:0/16:1)	1.52249992	-0.0761289	1.11536432	2.54986936	0.00000	0.21516	0.53026	0.26830	0.21687	0.47230	-1.47052	-0.35574	1.27690	-0.08039	-0.34686	0.97661
PA(16:0/18:0)	0	0	0	6.24367518	0.00000	0.00000	0.00000	0.00000	0.00000	0.00000	#DIV/0!	#DIV/0!	#DIV/0!	#DIV/0!	#DIV/0!	#DIV/0!
PA(16:0/18:1)	1.84661627	0.28970677	1.36904489	4.64611377	0.00000	0.08454	0.31589	0.17714	0.04640	0.25042	-1.18402	-0.49712	1.38246	0.25517	-0.80701	0.85053
PA(16:0/18:2)	0.66357541	-0.0715603	0.4824174	0.77290491	0.00000	0.66826	1.06219	0.57299	0.23761	1.20075	-1.34943	0.09657	0.94895	-0.10958	-0.83530	1.24878
PA(16:0/18:3)	0.02489462	1.02806947	0	0.03951405	0.00000	1.70722	0.00000	0.00000	0.00000	2.07289	-0.64101	1.09600	-0.64101	-0.64101	-0.64101	1.46805
PA(18:0/18:0)	0	0	0	0.36435074	0.00000	0.00000	0.00000	0.00000	0.00000	0.00000	#DIV/0!	#DIV/0!	#DIV/0!	#DIV/0!	#DIV/0!	#DIV/0!
PA(18:0/18:1)	0.21861236	0.48790339	0.097936	0.8625484	0.00000	0.06946	0.32922	0.15571	0.06243	0.33015	-1.11105	-0.62209	1.20655	-0.01488	-0.67159	1.21308
PA(18:0/18:2)	0.44352593	0.32998227	0.30100288	0.71211463	0.00000	0.22128	0.65126	0.39551	0.01605	0.79596	-1.05273	-0.38077	0.92489	0.14830	-1.00400	1.36431
PA(18:0/18:3)	0.16748931	0.59986893	0	0.13517946	0.00000	0.90251	2.23900	1.16892	0.00000	3.12366	-0.99582	-0.27046	0.80371	-0.05634	-0.99582	1.51473
PA(18:0/18:4)	0.03743057	1.98644224	0	0.08379599	0.00000	0.64862	0.00000	0.00000	0.00000	2.03150	-0.54567	0.24668	-0.54567	-0.54567	-0.54567	1.93601
PA(18:0/18:5)	0	0	0	0.01075936	0.00000	0.00000	0.00000	0.00000	0.00000	0.00000	#DIV/0!	#DIV/0!	#DIV/0!	#DIV/0!	#DIV/0!	#DIV/0!
PA(18:0/20:0)	0	0	0	0.0351271	0.00000	0.00000	0.00000	0.00000	0.00000	0.00000	#DIV/0!	#DIV/0!	#DIV/0!	#DIV/0!	#DIV/0!	#DIV/0!
PA(18:0/20:1)	0	0	0	0.0307213	0.00000	0.00000	0.00000	0.00000	0.00000	0.00000	#DIV/0!	#DIV/0!	#DIV/0!	#DIV/0!	#DIV/0!	#DIV/0!
PA(18:0/20:2)	0	0	0	0.0345066	0.00000	0.00000	0.00000	0.00000	0.00000	0.00000	#DIV/0!	#DIV/0!	#DIV/0!	#DIV/0!	#DIV/0!	#DIV/0!
PA(18:0/20:3)	0.31142632	0.50873111	0	0.14582942	0.00000	1.20171	4.17814	1.84409	1.08478	4.50459	-1.17894	-0.51553	1.12762	-0.16090	-0.58008	1.30783
PA(18:0/20:4)	0.22243577	0.6146248	0	0.15785482	0.00000	0.81543	2.87778	1.02538	0.72419	3.01192	-1.13695	-0.47901	1.18499	-0.30962	-0.55263	1.29322
PA(18:0/20:5)	0.01945182	2.44948974	0	0.04976563	0.00000	0.00000	0.00000	0.00000	0.00000	2.34521	-0.40825	-0.40825	-0.40825	-0.40825	-0.40825	2.04124
PA(18:0/20:6)	0.04615592	2.44948974	0	0.14133846	0.00000	0.00000	0.00000	0.00000	0.00000	1.95938	-0.40825	-0.40825	-0.40825	-0.40825	-0.40825	2.04124
PA(18:0/22:6)	0.63194847	0.83909269	0.15990904	0.23074403	0.00000	1.89488	13.23389	5.75745	1.67605	17.42132	-0.93916	-0.67211	0.92582	-0.12775	-0.70295	1.51606
DG(14:0/16:0)	0.19920968	-0.8171683	0.16651616	0.84858686	0.05167	0.00000	0.08207	0.06894	0.03839	0.04653	0.13185	-1.69231	1.20533	0.74153	-0.33703	-0.04936
DG(16:0/16:0)	0.56086973	0.09774951	0.46386327	3.17600612	0.06121	0.00528	0.07953	0.06694	0.00164	0.00000	0.68465	-0.82017	1.17734	0.83867	-0.91817	-0.96231
DG(16:0/16:1)	1.69601001	1.00168524	1.54146459	3.15379959	0.06907	0.00000	0.26001	0.18132	0.02125	0.04345	-0.26144	-0.93569	1.60250	0.83437	-0.72823	-0.51150
DG(16:0/18:0)	0.14964062	-0.8022624	0.08909864	1.85276642	0.04846	0.02732	0.05078	0.05528	0.02412	0.00000	0.66766	-0.33091	0.77696	0.98982	-0.48216	-1.62137
DG(16:0/18:1)	2.82881144	0.28891601	2.41602261	8.21797338	0.10004	0.00918	0.16668	0.14822	0.00000	0.00276	0.37626	-0.80704	1.24418	1.00374	-0.92657	-0.89057
DG(16:0/18:2)	2.45208043	1.08458835	2.20997492	2.36317431	1.47312	0.33366	4.56103	2.76041	0.00000	0.35375	-0.06023	-0.70031	1.67440	0.66291	-0.88775	-0.68903
DG(18:0/18:1)	0.50999617	0.19463073	0.40720567	2.3560997	0.05543	0.02645	0.10562	0.09281	0.03614	0.00000	0.06663	-0.65100	1.30914	0.99201	-0.41107	-1.30570
DG(18:0/18:2)	2.26743638	-0.0246536	1.89771187	3.45190801	0.18298	0.00000	0.44414	0.41233	0.14329	0.24459	-0.32634	-1.41374	1.22575	1.03669	-0.56220	0.03983
DG(18:0/18:3)	0.9615186	0.55124738	0.75850257	0.83960625	2.62733	1.09262	5.76137	4.60806	0.00000	0.92962	0.05467	-0.62104	1.43453	0.92674	-1.10210	-0.69280
DG(18:0/18:4)	0.27714076	0.17795039	0.205175	0.53272934	0.23706	0.14392	0.43178	0.40128	0.00000	0.10420	0.10168	-0.44412	1.24277	1.06402	-1.28750	-0.67685



Handling skewness (Normalisation or Data transformation)



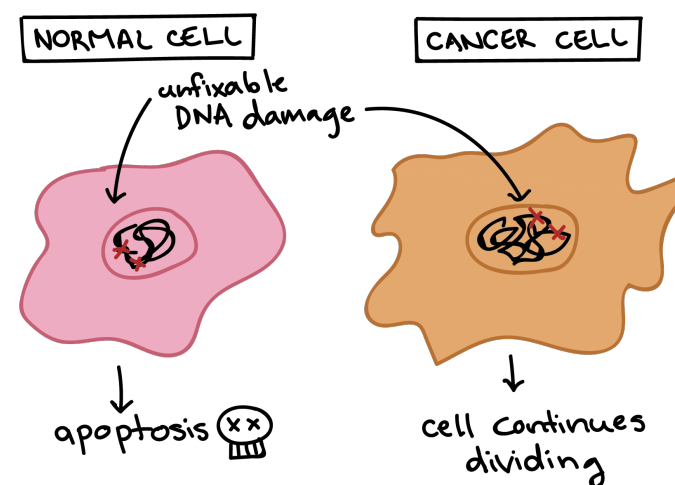
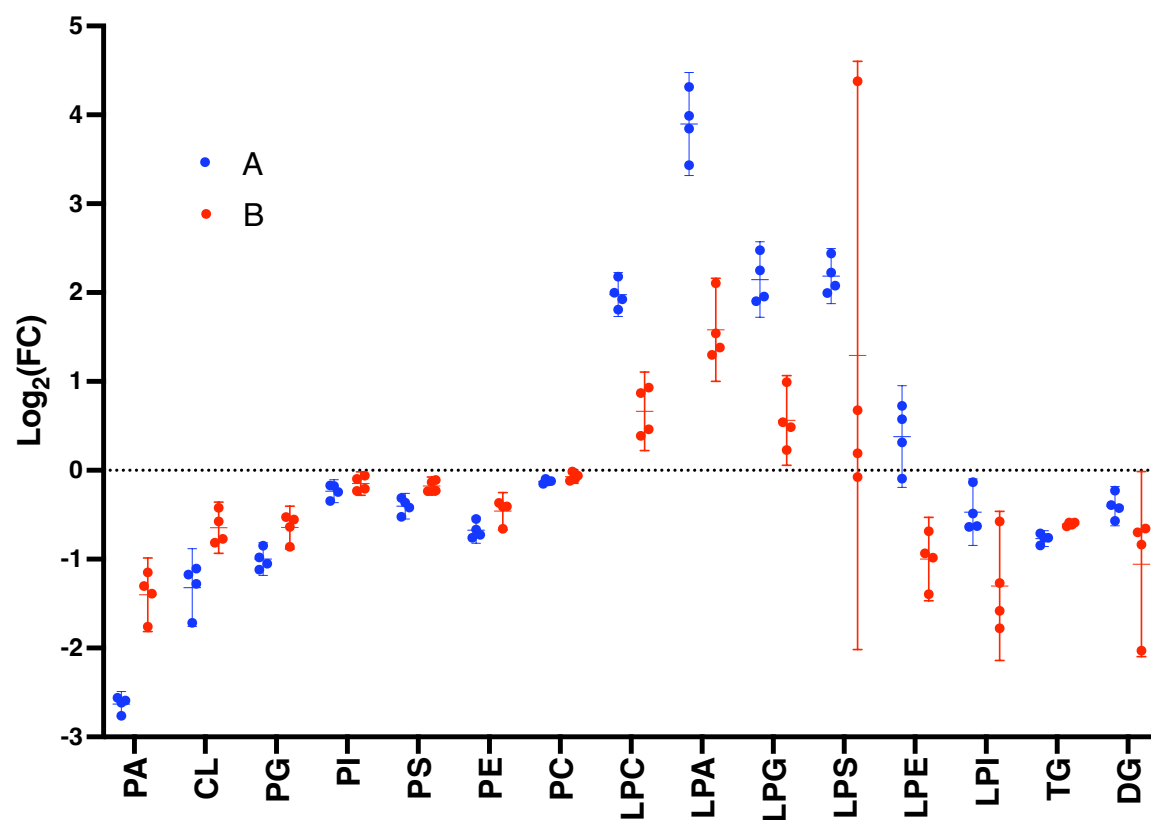
	Log2 C_1	Log2 C_2	Log2 C_3	Log2 C_4	Log2 C_5	Log2 C_6	Log2 K_1	Log2 K_2	Log2 K_3	Log2 K_4	Log2 K_5	Log2 K_6
PA(14:0/16:0)	-1.5653301	-1.1808732	-1.0467821	-1.1737563	-1.118767	-1.1843664	1.67898754	1.69987249	1.60795662	1.19872663	1.48165855	1.33890643
PA(16:0/16:0)	-0.4899813	-0.2528507	-0.0459324	0.12323638	-0.3128351	-0.3131211	3.64239548	3.62528317	3.56731463	3.08634321	3.36993347	3.19517095
PA(16:0/16:1)	0.15751502	0.50995856	0.90768247	0.58519477	0.51244707	0.84228475	1.33036019	1.35042333	1.33253849	1.05682412	1.24610488	1.13504996
PA(16:0/18:0)	#NUM!	#NUM!	#NUM!	#NUM!	#NUM!	#NUM!	2.64239548	2.60750847	2.40529483	1.84433866	2.27307193	2.10402306
PA(16:0/18:1)	0.45316976	0.71905416	1.26557244	0.96313388	0.6051249	1.13071593	2.06205807	2.17447454	2.21602448	1.85509706	2.09107409	1.98418329
PA(16:0/18:2)	-1.0516462	-0.5637529	-0.3383054	-0.6240096	-0.8587271	-0.2666955	-0.470437	-0.4658647	-0.3716372	-0.7711813	-0.574925	-0.6753778
PA(16:0/18:3)	#NUM!	-3.8898392	#NUM!	#NUM!	#NUM!	-3.6098443	-4.8249283	-4.9649758	-4.6614906	-4.8866696	-5.1542424	-4.9922694
PA(18:0/18:0)	#NUM!	#NUM!	#NUM!	#NUM!	#NUM!	#NUM!	-1.4566002	-1.608264	-1.7874535	-2.6867143	-1.9198536	-2.1883109
PA(18:0/18:1)	-3.352017	-2.7269562	-1.5159727	-2.2042616	-2.7792467	-1.5130499	-0.4033228	-0.2133227	-0.2549136	-0.7449498	-0.3943527	-0.5385269
PA(18:0/18:2)	-1.7321508	-1.3511646	-0.814155	-1.1090362	-1.7008703	-0.6706317	-0.7197965	-0.6531433	-0.4898186	-0.927648	-0.6952192	-0.7872707
PA(18:0/18:3)	#NUM!	-3.0350426	-1.7241979	-2.6618763	#NUM!	-1.2438142	-2.9989148	-3.0911518	-2.8870522	-3.3675327	-3.150722	-3.3307278
PA(18:0/18:4)	#NUM!	-4.2015281	#NUM!	#NUM!	#NUM!	-2.554429	-3.6719958	-3.576975	-3.6651465	-4.2046556	-4.087563	-4.4868948
PA(18:0/18:5)	#NUM!	#NUM!	#NUM!	#NUM!	#NUM!	#NUM!	#NUM!	#NUM!	#NUM!	#NUM!	#NUM!	-6.5382646
PA(18:0/20:0)	#NUM!	#NUM!	#NUM!	#NUM!	#NUM!	#NUM!	-4.8312718	-4.98316	-5.3861998	#NUM!	-5.905903	-5.5472014
PA(18:0/20:1)	#NUM!	#NUM!	#NUM!	#NUM!	#NUM!	#NUM!	-5.0858862	-5.024617	#NUM!	-5.6446469	-5.631482	-5.4858285
PA(18:0/20:2)	#NUM!	#NUM!	#NUM!	#NUM!	#NUM!	#NUM!	#NUM!	-4.8569841	-5.1111144	-5.7568941	-5.2772554	-5.2955507
PA(18:0/20:3)	#NUM!	-2.5125542	-0.7147866	-1.8947345	-2.660244	-0.6062507	-3.1852369	-2.9989509	-2.7776463	-3.458692	-3.7101981	-4.0654331
PA(18:0/20:4)	#NUM!	-2.9576921	-1.1383736	-2.6271747	-3.1288945	-1.0726467	-2.8947561	-2.6633298	-2.7155029	-3.1930299	-3.3740534	-3.3426746
PA(18:0/20:5)	#NUM!	#NUM!	#NUM!	#NUM!	#NUM!	-3.0989888	-4.6719389	-4.4269184	-4.3287064	-4.8158888	-4.9196992	-5.3526632
PA(18:0/20:6)	#NUM!	#NUM!	#NUM!	#NUM!	#NUM!	-1.852378	-2.8481191	-2.822774	-2.8895502	-3.2624834	-3.1260787	-3.2783776
PA(18:0/22:6)	-2.6446766	-1.7654595	0.13399918	-0.8167036	-1.8435675	0.47917656	-2.1391945	-2.1156348	-2.2270694	-2.4936494	-3.1070808	-4.1980964
DG(14:0/16:0)	-2.3093106	-2.5862659	-2.1681537	-2.2274545	-2.3755821	-2.3345625	-0.7583814	-0.5648455	-0.2368658	-0.8817578	-0.5435298	-0.4570231
DG(16:0/16:0)	-0.6668358	-1.0643391	-0.5573445	-0.6317074	-1.0944556	-1.1082285	1.09022507	1.51977212	1.35768213	0.85808912	1.33117243	1.66721369
DG(16:0/16:1)	0.72493714	0.62430175	0.97136052	0.87485248	0.65602056	0.68842867	1.09791245	1.27039525	1.65709099	1.01870823	1.36520492	1.36013125
DG(16:0/18:0)	-2.5181128	-2.864762	-2.4847733	-2.4219743	-2.9253664	-3.4884528	0.13783535	0.66969478	0.67361542	0.16266793	0.58378848	0.88968101
DG(16:0/18:1)	1.58324705	1.30408584	1.75834466	1.71192823	1.27263395	1.28217754	2.43217173	2.96353224	2.75000176	2.2682564	2.74766656	3.03878266
DG(16:0/18:2)	1.28431026	1.1770192	1.54038563	1.39663551	1.14402999	1.17898207	0.69592213	0.8908517	1.24072605	0.66424994	0.98248765	0.943377
DG(18:0/18:1)	-0.9566794	-1.1242316	-0.7059065	-0.7658878	-1.0660193	-1.2961705	0.54470546	1.03967862	1.15970516	0.60500014	0.97076661	1.23640059
DG(18:0/18:2)	1.12571221	0.92426096	1.3718362	1.34400608	1.08434325	1.1876753	1.06946146	1.66851635	1.58061702	1.08923293	1.46627745	1.78739402
DG(18:0/18:3)	-0.0415823	-0.2393653	0.29368974	0.17917073	-0.398774	-0.2620566	-0.9276825	-0.2522152	-0.33555	-1.1311173	-0.3583149	-0.2536639
DG(18:0/18:4)	-1.8220212	-1.9866931	-1.5286303	-1.5708304	-2.2850731	-2.0630616	-1.4103431	-1.0061793	-0.9085254	-1.9871836	-1.3246106	-1.2312854

Square root = $x^{1/2}$
(only applied to positive values)

Cube root = $x^{1/3}$

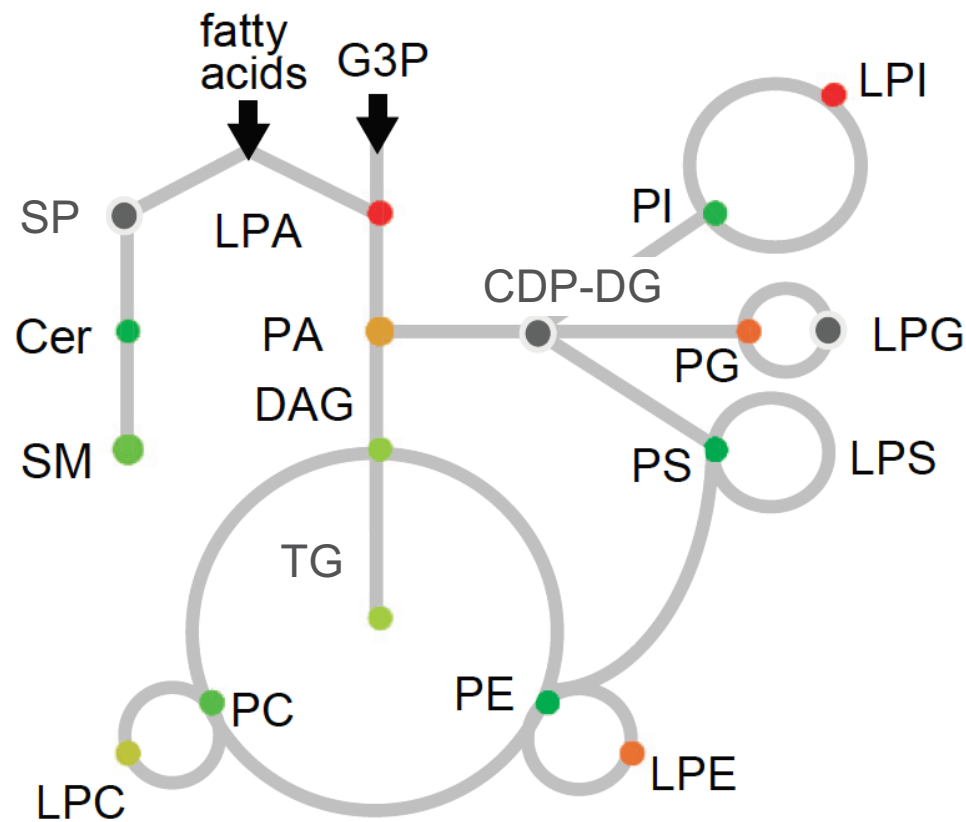


Handling skewness (Normalisation or Data transformation)



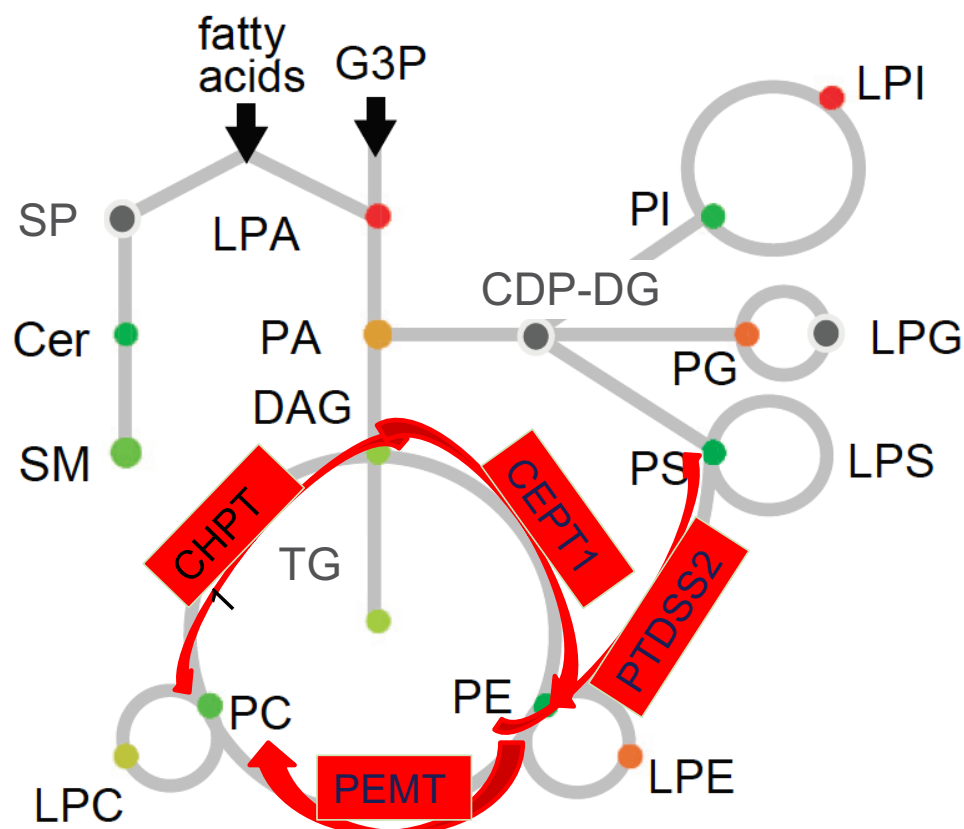


Lipid biosynthetic pathways





Lipid biosynthetic pathways





Automated pathway analysis



LIPID MAPS®

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BioPAN: Bioinformatics Methodology For Pathway Analysis

BioPAN for **Bioinformatics Methodology For Pathway Analysis** is a tool that allows users to upload their own mammalian lipidomics dataset and perform a pathway analysis.

In this analysis, you can explore systematic changes in lipid pathways at different levels: lipid subclass and lipid molecular species. Those pathways will be highlighted and changes in gene activity will also be predicted.

BioPAN is fully integrated with LipidLynxX¹ to allow the user to upload dataset from different naming conventions and levels of structural information.

LipidLynxX - LipidLynxX is available on the LIPID MAPS website.

Resources

Documentation - We recommend the user to read the detailed about BioPAN before using.

Video Tutorial - Watch our tutorial video on YouTube.

Start analysis

Load a data file
CSV file
Quantitative data



<https://www.lipidmaps.org/biopan/>



Automated pathway analysis



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BioPAN's Workflow

STEP 1 - Load a data file

There are guidelines on how prepare your data [here](#).

After loading a file, LipidLynxX¹ will be firstly launched in the background to convert the lipid molecular species naming used in the file to the BioPAN nomenclature.

- Option 1: select a data file for analysis

Choose the file to import

Choose File



Example.csv

What's the annotation level* of your dataset?

Sum composition

☒ Run LipidLynxX

Launch BioPAN

- Option 2: try BioPAN with a demonstration file

Small dataset



Load demo file

The small demonstration file is downloadable [here](#) and the complete dataset² [here](#).



Automated pathway analysis



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BioPAN's Workflow

STEP 1 - Load a data file

There are guidelines on how prepare your data [here](#).

After loading a file, LipidLynx¹ will be firstly launched in the background to convert the lipid molecular species naming used in the file to the BioPAN nomenclature.

- Option 1: select a data file for analysis

Choose the file to import

Choose File  Example.csv

Launch BioPAN

What's the annotation level* of your dataset?

- ✓ Sum composition
- Full structure
- Both

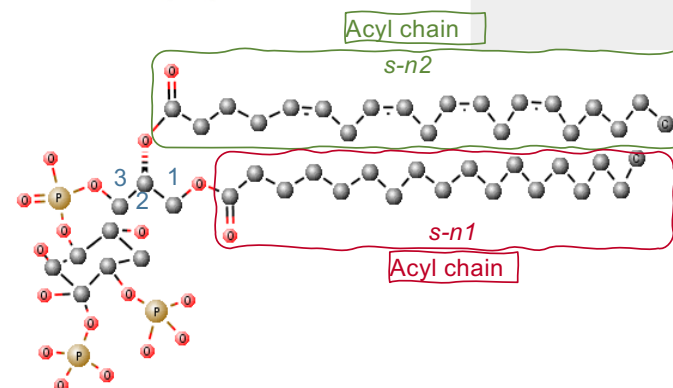
☐ Run LipidLynx

- Option 2: try BioPAN with a demonstration file

Small dataset 

Load demo file

The small demonstration file is downloadable [here](#) and the complete dataset² [here](#).





Automated pathway analysis



Information:

- There are no FAcOA in your dataset, BioPAN generated some based on the FA molecular species it contains. Look at the [documentation](#) to understand.

BioPAN's Workflow

The data file **other** has been successfully uploaded.

Here is your data summary:

	Number
Unrecognised molecular species	8
Processed molecular species	410
Unprocessed molecular species	79
Total	496

There are guidelines on how interpret the data summary [here](#).

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Unprocessed molecular species

Here is a table of the Unprocessed molecular species with a mapping between the nomenclature used by BioPAN and the nomenclature of dataset.

BioPAN nomenclature	Dataset nomenclature
PC(28:0)	PC(28:0)
PI(30:0)	PI(30:0)
PI(30:1)	PI(30:1)
SM(16:1)	SM(16:1)
SM(18:0)	SM(18:0)
SM(20:1)	SM(20:1)
SM(22:1)	SM(22:1)
SM(22:2)	SM(22:2)
SM(24:2)	SM(24:2)
SM(24:3)	SM(24:3)
dhSM(14:0)	dhSM(14:0)
TG(36:0)	TG(36:0)
TG(42:0)	TG(42:0)
TG(44:0)	TG(44:0)
TG(44:1)	TG(44:1)
TG(44:2)	TG(44:2)
TG(46:0)	TG(46:0)
TG(46:1)	TG(46:1)
TG(46:2)	TG(46:2)
TG(46:3)	TG(46:3)
TG(48:3)	TG(48:3)
TG(50:5)	TG(50:5)
Cer(22:3)	Cer(22:3)
Cer(26:1)	Cer(26:1)
FA(22:2)	FA(22:2)
FA(22:6)	FA(22:6)

FA(22:2)	FA(22:2)
FA(22:6)	FA(22:6)
FA(24:2)	FA(24:2)
ST(14:0)	CE(14:0)
ST(16:0)	CE(16:0)
ST(16:1)	CE(16:1)
ST(18:0)	CE(18:0)
ST(18:1)	CE(18:1)
ST(18:2)	CE(18:2)
ST(18:3)	CE(18:3)
ST(20:1)	CE(20:1)
ST(20:2)	CE(20:2)
ST(20:3)	CE(20:3)
ST(20:4)	CE(20:4)
ST(20:5)	CE(20:5)
ST(22:1)	CE(22:1)
ST(22:2)	CE(22:2)
ST(22:3)	CE(22:3)
ST(22:4)	CE(22:4)
ST(22:5)	CE(22:5)
ST(22:6)	CE(22:6)
ST(24:1)	CE(24:1)
ST(24:2)	CE(24:2)
ST(26:2)	CE(26:2)
ST(26:3)	CE(26:3)
ST(27:0)	ST(27:0)
O-PC(30:0)	O-PC(30:0)
O-PC(30:1)	O-PC(30:1)
O-PC(32:2)	O-PC(32:2)
O-PC(32:3)	O-PC(32:3)
O-PC(36:6)	O-PC(36:6)
O-PC(38:7)	O-PC(38:7)
O-PC(40:7)	O-PC(40:7)
P-PC(40:0)	P-PC(40:0)
O-PE(30:1)	O-PE(30:1)



Automated pathway analysis



Information:

- There are no FAcOA in your dataset, BioPAN generated some based on the FA molecular species it contains. Look at the [documentation](#) to understand.

BioPAN's Workflow

The data file **other** has been successfully uploaded.

Here is your data summary:

	Number
Unrecognised molecular species	8
Processed molecular species	410
Unprocessed molecular species	79
Total	496

There are guidelines on how interpret the data summary [here](#).

STEP 2 - Assign conditions to different samples

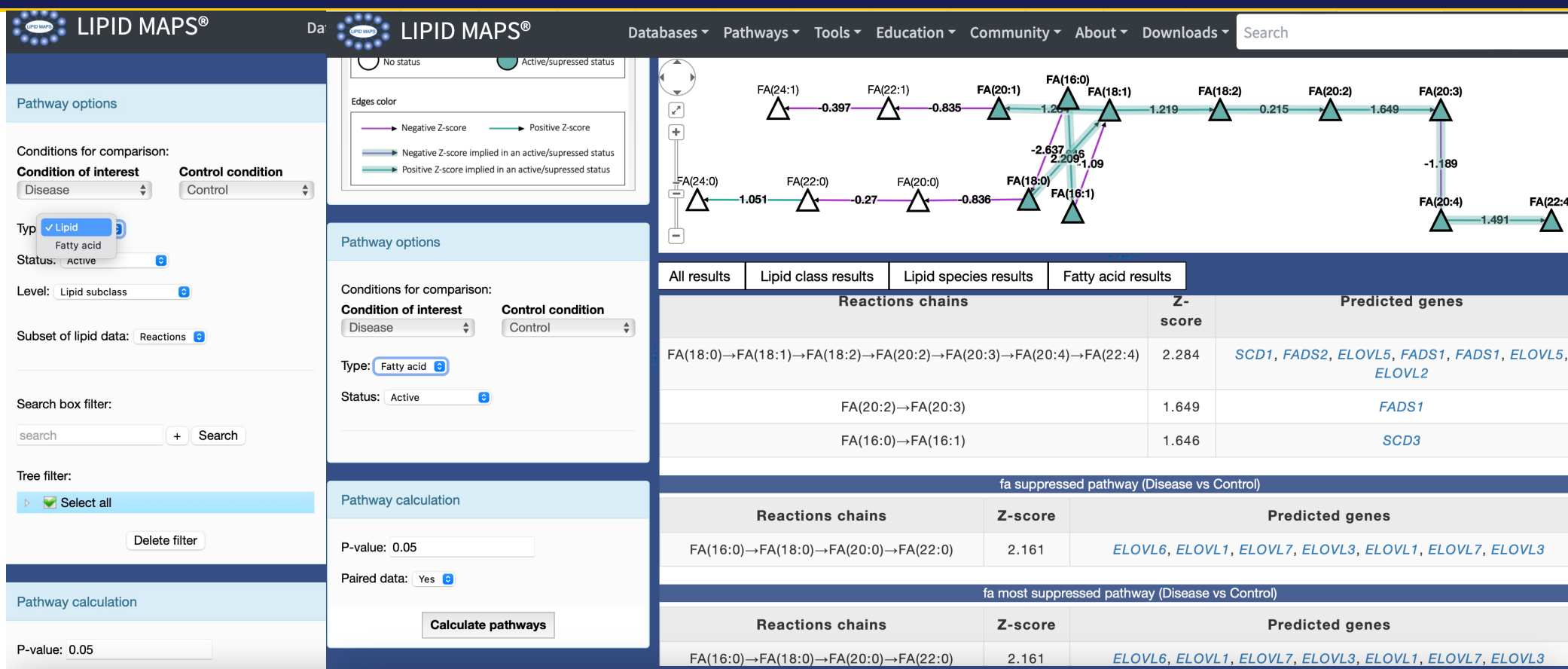
In this step you have a chance to assign a condition to each sample.

Sample name	Sample condition
Control_1	Control
Control_2	Control
Control_3	Control
Control_4	Control
Disease_1	Disease
Disease_2	Disease
Disease_3	Disease
Disease_4	Disease

Assign conditions



Reactions chains	Z-score	Predicted genes
PIP2→DG→TG	3.225	<i>PLCB1, PLCB2, PLCB3, PLCB4, PLCD1, PLCD3, PLCD4, PLCE1, PLCG1, PLCG2, DGAT2</i>
PIP2→PIP→PI→LPI	2.939	<i>FIG4, OCRL, INPP5E, PTEN, SYNJ1, SYNJ2, SACM1L, MTMR1, MTMR2, MTMR3, MTMR4, MTMR6, MTMR7, MTMR8, MTMR9, MTMR14, PTEN, PLA2G4D, PLA2G4E</i>
DG→TG	2.512	<i>DGAT2</i>
PIP2→DG→PE→LPE	2.431	<i>PLCB1, PLCB2, PLCB3, PLCB4, PLCD1, PLCD3, PLCD4, PLCE1, PLCG1, PLCG2, CEPT1,</i>





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Pathway options

Conditions for comparison:

Condition of interest
Disease ▾

Control condition
Control ▾

Type: Lipid ▾

Status: Active ▾

Active

Level: Most active ▾

Suppressed

Subset of lipid data: Reactions ▾

Search box filter:
 +

Tree filter:

Select all

Pathway options

Conditions for comparison:

Condition of interest
Disease ▾

Control condition
Control ▾

Type: Lipid ▾

Status: Active ▾

Lipid subclass

Level: Lipid molecular species ▾

Subset of lipid data: Reactions ▾

Search box filter:
 +

Tree filter:

Select all

Pathway calculation

P-value: 0.05

Pathway calculation

P-value: 0.05

All results	Lipid class results	Lipid species results	Fatty acid results
lipid subclass active reaction (Disease vs Control)			
Reactions chains	Z-score	Predicted genes	
PIP2→DG→TG	3.225	<i>PLCB1, PLCB2, PLCB3, PLCB4, PLCD1, PLCD3, PLCD4, PLCE1, PLCG1, PLCG2, PLCG3, PLCG4, PLCG5, PLCG6, PLCG7, PLCG8, PLCG9, PLCG10, PLCG11, PLCG12, PLCG13, PLCG14, PLCG15, PLCG16, PLCG17, PLCG18, PLCG19, PLCG20, PLCG21, PLCG22, PLCG23, PLCG24, PLCG25, PLCG26, PLCG27, PLCG28, PLCG29, PLCG30, PLCG31, PLCG32, PLCG33, PLCG34, PLCG35, PLCG36, PLCG37, PLCG38, PLCG39, PLCG40, PLCG41, PLCG42, PLCG43, PLCG44, PLCG45, PLCG46, PLCG47, PLCG48, PLCG49, PLCG50, PLCG51, PLCG52, PLCG53, PLCG54, PLCG55, PLCG56, PLCG57, PLCG58, PLCG59, PLCG60, PLCG61, PLCG62, PLCG63, PLCG64, PLCG65, PLCG66, PLCG67, PLCG68, PLCG69, PLCG70, PLCG71, PLCG72, PLCG73, PLCG74, PLCG75, PLCG76, PLCG77, PLCG78, PLCG79, PLCG80, PLCG81, PLCG82, PLCG83, PLCG84, PLCG85, PLCG86, PLCG87, PLCG88, PLCG89, PLCG90, PLCG91, PLCG92, PLCG93, PLCG94, PLCG95, PLCG96, PLCG97, PLCG98, PLCG99, PLCG100</i>	
PIP2→PIP→PI→LPI	2.939	<i>FIG4, OCRL, INPP5E, PTEN, SYNJ1, SYNJ2, SACM1L, MTMR1, MTMR2, MTMR3, MTMR4, MTMR5, MTMR6, MTMR7, MTMR8, MTMR9, MTMR10, MTMR11, MTMR12, MTMR13, MTMR14, MTMR15, MTMR16, MTMR17, MTMR18, MTMR19, MTMR20, MTMR21, MTMR22, MTMR23, MTMR24, MTMR25, MTMR26, MTMR27, MTMR28, MTMR29, MTMR30, MTMR31, MTMR32, MTMR33, MTMR34, MTMR35, MTMR36, MTMR37, MTMR38, MTMR39, MTMR40, MTMR41, MTMR42, MTMR43, MTMR44, MTMR45, MTMR46, MTMR47, MTMR48, MTMR49, MTMR50, MTMR51, MTMR52, MTMR53, MTMR54, MTMR55, MTMR56, MTMR57, MTMR58, MTMR59, MTMR60, MTMR61, MTMR62, MTMR63, MTMR64, MTMR65, MTMR66, MTMR67, MTMR68, MTMR69, MTMR70, MTMR71, MTMR72, MTMR73, MTMR74, MTMR75, MTMR76, MTMR77, MTMR78, MTMR79, MTMR80, MTMR81, MTMR82, MTMR83, MTMR84, MTMR85, MTMR86, MTMR87, MTMR88, MTMR89, MTMR90, MTMR91, MTMR92, MTMR93, MTMR94, MTMR95, MTMR96, MTMR97, MTMR98, MTMR99, MTMR100</i>	
DG→TG	2.512	<i>DGAT2</i>	
PIP2→DG→PE→LPE	2.431	<i>PLCB1, PLCB2, PLCB3, PLCB4, PLCD1, PLCD3, PLCD4, PLCE1, PLCE2, PLCE3, PLCE4, PLCE5, PLCE6, PLCE7, PLCE8, PLCE9, PLCE10, PLCE11, PLCE12, PLCE13, PLCE14, PLCE15, PLCE16, PLCE17, PLCE18, PLCE19, PLCE20, PLCE21, PLCE22, PLCE23, PLCE24, PLCE25, PLCE26, PLCE27, PLCE28, PLCE29, PLCE30, PLCE31, PLCE32, PLCE33, PLCE34, PLCE35, PLCE36, PLCE37, PLCE38, PLCE39, PLCE40, PLCE41, PLCE42, PLCE43, PLCE44, PLCE45, PLCE46, PLCE47, PLCE48, PLCE49, PLCE50, PLCE51, PLCE52, PLCE53, PLCE54, PLCE55, PLCE56, PLCE57, PLCE58, PLCE59, PLCE60, PLCE61, PLCE62, PLCE63, PLCE64, PLCE65, PLCE66, PLCE67, PLCE68, PLCE69, PLCE70, PLCE71, PLCE72, PLCE73, PLCE74, PLCE75, PLCE76, PLCE77, PLCE78, PLCE79, PLCE80, PLCE81, PLCE82, PLCE83, PLCE84, PLCE85, PLCE86, PLCE87, PLCE88, PLCE89, PLCE90, PLCE91, PLCE92, PLCE93, PLCE94, PLCE95, PLCE96, PLCE97, PLCE98, PLCE99, PLCE100</i>	



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Export Documentation

No status

Active/supressed status

Edges color

Negative Z-score

Positive Z-score

Negative Z-score implied in an active/supressed status

Positive Z-score implied in an active/supressed status

Pathway options

Conditions for comparison:

Condition of interest

Disease

Control condition

Control

Type: Lipid

Status: Most active

Level: Lipid subclass

Subset of lipid data: Pathways

Search box filter:

search + Search

Tree filter:

All resultsLipid class resultsLipid species resultsFatty acid results

lipid subclass active pathway (Disease vs Control)

Pathways	Classification(s) of the pathways	Z-score	Predicted genes
PIP2→PIP→PI	Biosynthesis of PIPs (Glycerolipids and Glycerophospholipids)	3.044	FIG4, OCRL, INPP5E, PTEN, SYNJ1, SYNJ2, SACM1L, MTMR1, MTMR2, MTMR3, MTMR4, MTMR6, MTMR7, MTMR8, MTMR9, MTMR14, PTEN
DG→TG	Triglycerol biosynthesis (Triglycerol metabolism)	2.285	DGAT2
PIP→PI	Biosynthesis of PIPs (Glycerolipids and Glycerophospholipids)	2.218	SYNJ1, SYNJ2, SACM1L, MTMR1, MTMR2, MTMR3, MTMR4, MTMR6, MTMR7, MTMR8, MTMR9, MTMR14, PTEN
DG→PC	Biosynthesis of PS (Glycerolipids and Glycerophospholipids), Biosynthesis of PE (Glycerolipids and Glycerophospholipids), Biosynthesis of PC (Glycerolipids and Glycerophospholipids)	2.213	CHPT1




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Documentation

☐ No status
☒ Active/supressed status

Edges color

- Negative Z-score
- Positive Z-score
- Negative Z-score implied in an active/supressed status
- Positive Z-score implied in an active/supressed status

Pathway options

Conditions for comparison:
Condition of interest **Control condition**

Type:

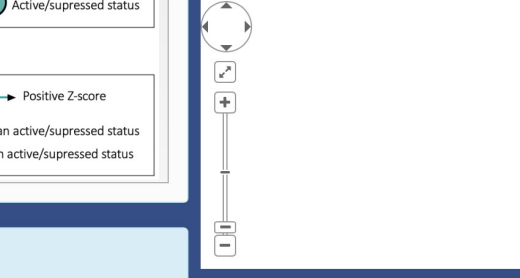
Status:

Level:

Subset of lipid data:

Search box filter:

Tree filter:



All results
Lipid class results
Lipid species results
Fatty acid results

lipid species active pathway (Disease vs Control)

Pathways	Classification(s) of the pathways	Z-score	Predicted genes
DG(36:1)→TG(58:7)	Triglycerol biosynthesis (Triglycerol metabolism)	3.598	<i>DGAT2</i>
DG(34:2)→TG(56:8)	Triglycerol biosynthesis (Triglycerol metabolism)	3.469	<i>DGAT2</i>
PIP2(36:3)→PIP(36:3)→PI(36:3)	Biosynthesis of PIPs (Glycerolipids and Glycerophospholipids)	3.405	<i>FIG4, OCRL, INPP5E, PTEN, SYNJ1, SYNJ2, SACM1L, MTMR1, MTMR2, MTMR3, MTMR4, MTMR6, MTMR7, MTMR8, MTMR9, MTMR14, PTEN</i>




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 Positive Z-score implied in an active/suppressed status

Pathway options

Conditions for comparison:

Condition of interest
Disease ▾

Control condition
Control ▾

Type: Lipid 

Status: Most active 

Level: Lipid molecular species 

Subset of lipid data: Pathways 

Search box filter:

Tree filter:

  Select all

Pathway calculation





All results
Lipid class results
Lipid species results
Fatty acid results

PIP(38:4)→PI(38:4)	Biosynthesis of PIPs (Glycerolipids and Glycerophospholipids)	2.509	SYNJ1 , SYNJ2 , SACM1L , MTMR1 , MTMR2 , MTMR3 , MTMR4 , MTMR6 , MTMR7 , MTMR8 , MTMR9 , MTMR14 , PTEN
DG(32:0)→TG(52:4)	Triglycerol biosynthesis (Triglycerol metabolism)	2.505	DGAT2
PIP2(34:2)→PIP(34:2)→PI(34:2)	Biosynthesis of PIPs (Glycerolipids and Glycerophospholipids)	2.496	FIG4 , OCRL , INPP5E , PTEN , SYNJ1 , SYNJ2 , SACM1L , MTMR1 , MTMR2 , MTMR3 , MTMR4 , MTMR6 , MTMR7 , MTMR8 , MTMR9 , MTMR14



Automated pathway analysis



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Search

Condition of interest

Disease ▾

Control condition

Control ▾

Type:

Lipid ▾

Status:

Most active ▾

Level:

Lipid molecular species ▾

Subset of lipid data:

Reactions ▾

Search box filter:

36:1 + Search

Tree filter:

Select all

Delete filter

Pathway calculation

P-value: 0.05

Paired data: Yes ▾

Calculate pathways

PIP2(36:1) → DG(36:1) → TG(58:7)

4.107

PLCB1, PLCB2, PLCB3, PLCB4, PLCD1, PLCD3, PLCD4, PLCE1, PLCG1, PLCG2, DGAT2

PIP2(34:2) → DG(34:2) → TG(56:8)

4.034

PLCB1, PLCB2, PLCB3, PLCB4, PLCD1, PLCD3, PLCD4, PLCE1, PLCG1, PLCG2, DGAT2

PIP2(34:2) → DG(34:2) → PC(34:2) → PA(34:2) → PS(34:2) → LPS(18:2)

3.873

PLCB1, PLCB2, PLCB3, PLCB4, PLCD1, PLCD3, PLCD4, PLCE1, PLCG1, PLCG2, CHPT1, PLD1, PLD2, CDS1, PTDSS1, PLA2G2E, PLA2G2A, PLA2G2F

PIP2(34:1) → DG(34:1) → TG(56:5)

3.858

PLCB1, PLCB2, PLCB3, PLCB4, PLCD1, PLCD3, PLCD4, PLCE1, PLCG1, PLCG2, DGAT2

O-DG(36:2) → O-PC(36:2)

3.778

CHPT1

PIP2(34:2) → DG(34:2) → PC(34:2) → PA(34:2) → PS(34:2) → PE(34:2) → LPE(18:2)

3.755

PLCB1, PLCB2, PLCB3, PLCB4, PLCD1, PLCD3, PLCD4, PLCE1, PLCG1, PLCG2, CHPT1, PLD1, PLD2, CDS1, PTDSS1, PISD, PLA2G4C

PIP2(36:1) → DG(36:1) → TG(58:7)

4.107

PLCB1, PLCB2, PLCB3, PLCB4, PLCD1, PLCD3, PLCD4, PLCE1, PLCG1, PLCG2, DGAT2

PIP2(34:2) → DG(34:2) → TG(56:8)

4.034

PLCB1, PLCB2, PLCB3, PLCB4, PLCD1, PLCD3, PLCD4, PLCE1, PLCG1, PLCG2, DGAT2

PIP2(34:2) → DG(34:2) → PC(34:2) → PA(34:2) → PS(34:2) → LPS(18:2)

3.873

PLCB1, PLCB2, PLCB3, PLCB4, PLCD1, PLCD3, PLCD4, PLCE1, PLCG1, PLCG2, CHPT1, PLD1, PLD2, CDS1, PTDSS1, PLA2G2E, PLA2G2A, PLA2G2F

PIP2(34:1) → DG(34:1) → TG(56:5)

3.858

PLCB1, PLCB2, PLCB3, PLCB4, PLCD1, PLCD3, PLCD4, PLCE1, PLCG1, PLCG2, DGAT2

O-DG(36:2) → O-PC(36:2)

3.778

CHPT1

PIP2(34:2) → DG(34:2) → PC(34:2) → PA(34:2) → PS(34:2) → PE(34:2) → LPE(18:2)

3.755

PLCB1, PLCB2, PLCB3, PLCB4, PLCD1, PLCD3, PLCD4, PLCE1, PLCG1, PLCG2, CHPT1, PLD1, PLD2, CDS1, PTDSS1, PISD, PLA2G4C

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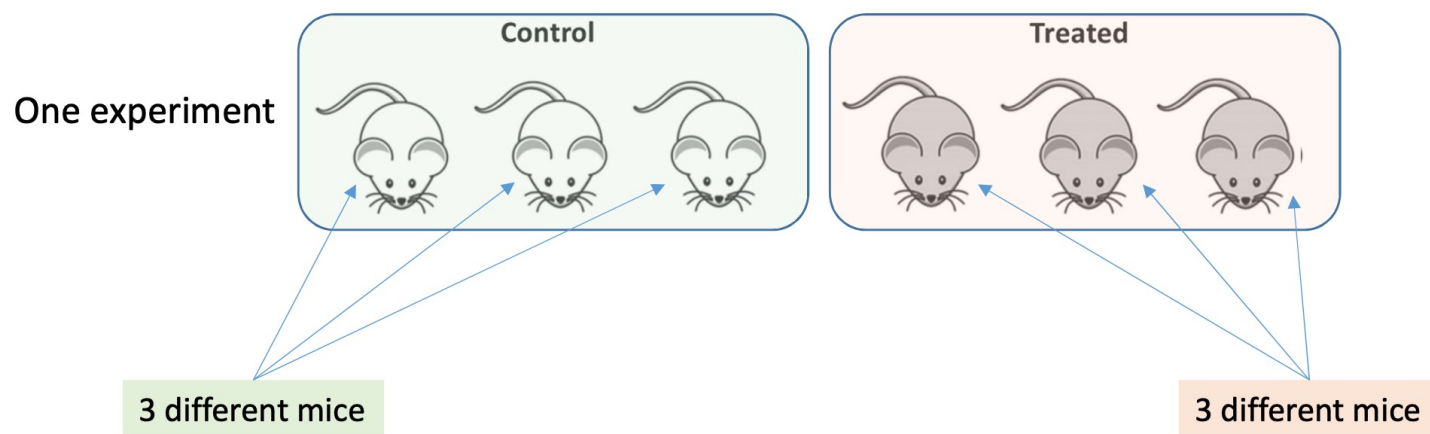
27



Independent or matched experiment

Independent: 2 or more groups in an experiment.

- **Example 1**: 2 groups with $n=3$ in the control group and $n=3$ in the treated group

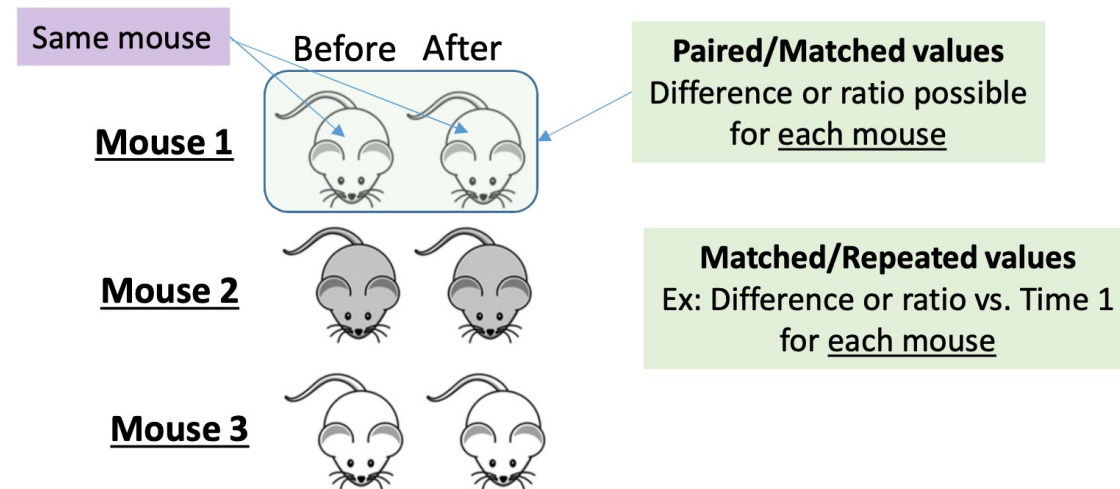




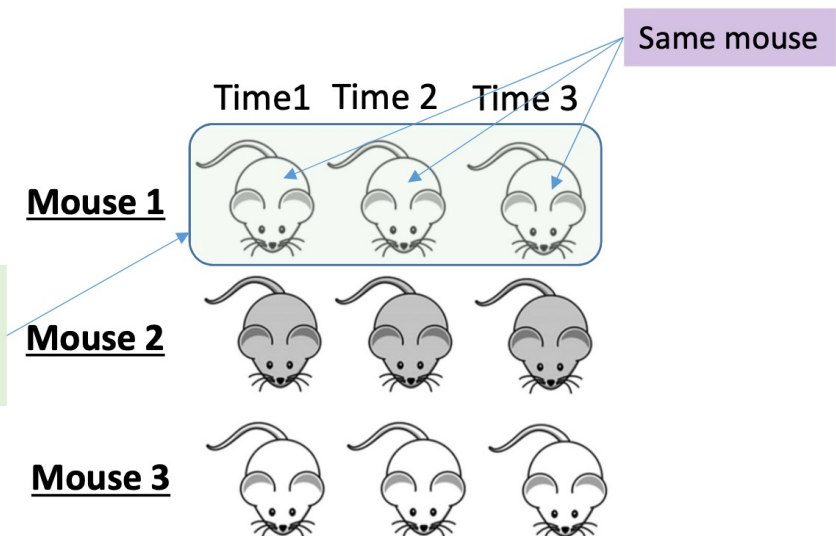
Independent or matched experiment

- **Matched** = repeated = dependent = paired (if 2 groups)
 - Design 1: 2 or more measures per animal/subject/petri dish

Example 1: before/after treatment measures

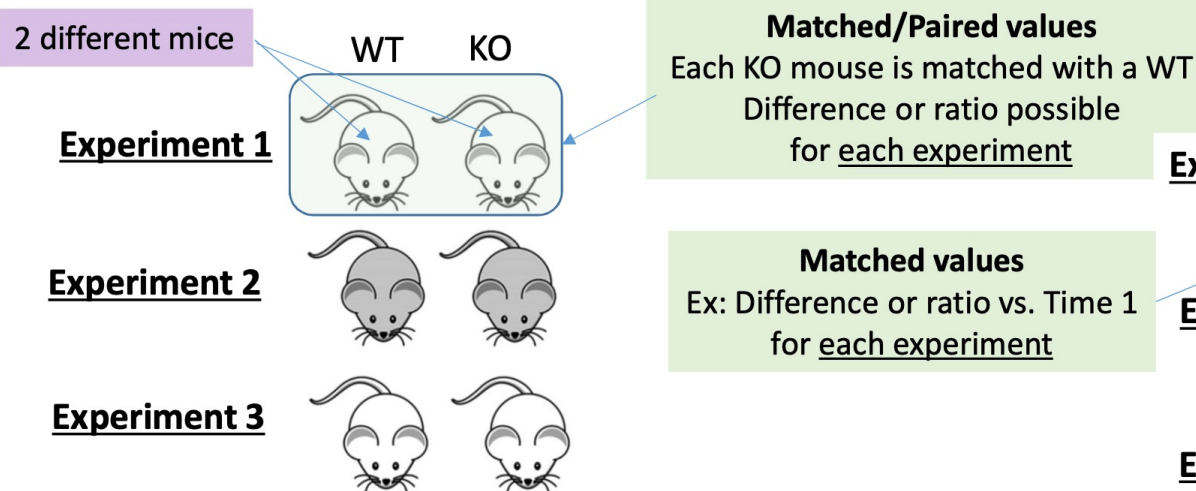


Example 2: 3 time points

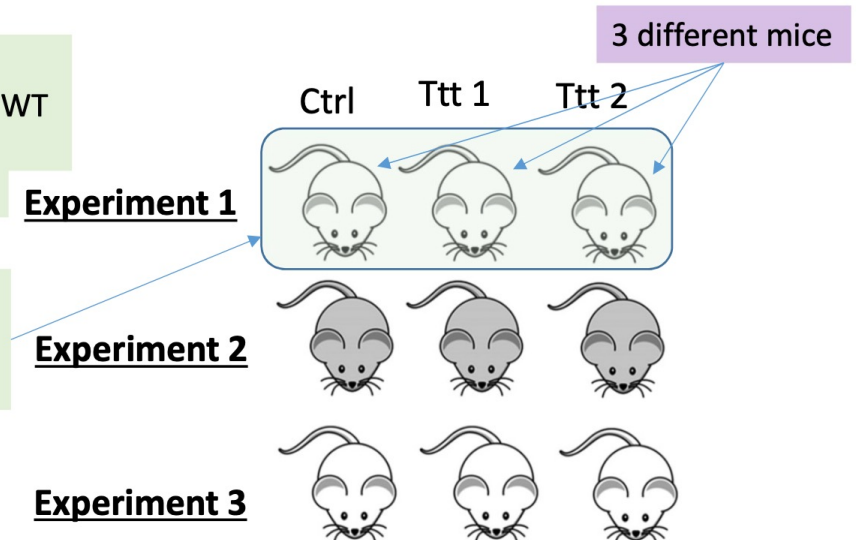


- **Matched** = repeated = dependent = paired (if 2 groups)
 - Design2: Within each experiment: same conditions (e.g. genotype, treatment ...)

Example 1: 3 independent experiments
2 mice within each: WT and KO



Example 2: 3 independent experiments
3 mice within each: control and 2 treatments





Troubleshooting BioPAN



JZ80 X Jx

	A	B	C	D	E	F	G	H	I
270	FA(22:2)	0.00313638	0.0054266	0.00493609	0.00398024	0.04164963	0.0387246	0.04168935	0
271	FA(22:4)	0.0048644	0.00254595	0.00392452	0.00351096	0.0596262	0.12531578	0.06504756	0
272	FA(22:6)	0.00418783	0.00255945	0.0060003	0.00348447	0.04688447	0.13050733	0.04135058	0
273	FA(24:0)	0.10975759	0.05565333	0.53235198	0.09161583	0.30559911	0.10357591	0.18663144	0
274	FA(24:1)	0.07566379	0.04829846	0.0518793	0.04894499	0.19817337	0.13690983	0.15505402	0
275	FA(24:2)	0.00100919	0.00147702	9.83E-04	0.00109628	0.0070951	0.00812438	0.00813063	0
276	CE(14:0)	0.96362252	0.97260545	0.77075764	0.36294344	0	0.25205009	0	0.30452047
277	CE(16:0)	3.11657995	9.17511151	4.95666541	3.26237235	0	0	0	3.49493047
278	CE(16:1)	6.07776747	12.2368209	7.69006144	4.91535084	1.62102737	6.84487973	6.75793443	5.51744635
279	CE(18:0)	3.0742855	3.29628897	1.84351714	1.15867431	1.39918774	6.96764991	4.24824545	3.91769849
280	CE(18:1)	30.7022897	56.6729792	31.9320967	17.816749	18.3323947	97.3554646	93.4610826	65.1117051
281	CE(18:2)	6.57003731	22.4546532	12.8557392	8.88096739	4.28400979	18.3268077	23.9752455	14.7009532
282	CE(18:3)	0.44580585	3.76542205	1.55780569	1.22151133	0.18002399	1.30055696	1.54726899	1.1320092
283	CE(20:1)	4.13527624	1.5970568	1.42240937	0.32546194	5.12853367	26.6864106	27.2065676	9.51749017
284	CE(20:2)	8.27572007	6.84933986	5.33634392	1.88023779	15.1124878	68.4705885	79.7194223	38.1513897
285	CE(20:3)	5.28646017	3.05402307	2.96541042	1.70411265	10.9386209	71.2529125	54.0347392	26.9603154
286	CE(20:4)	3.97984211	17.0037058	9.17985269	5.73417201	0	13.9626863	29.955857	12.2148596
287	CE(20:5)	1.84798491	8.82151458	4.12635026	3.04130926	1.53434838	4.82682033	7.12375891	4.50792338
288	CE(22:1)	1.17997215	0.59640706	0.47127696	0.13802231	1.80608645	7.747185	9.94861925	2.32129333



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Error: ×

- The input file must contain at least 2 conditions and each group must contain at least 2 samples.

Export Documentation

Graph legend

Nodes shape

☐ Glycerolipids and Glycerophospholipids

☐ Sphingolipids

☐ Fatty acids

Nodes color

☐ No status

☒ Active/supressed status

Edges color

→

Negative Z-score

→

Positive Z-score

→

Negative Z-score implied in an active/supressed status

→

Positive Z-score implied in an active/supressed status

Pathway options

Conditions for comparison:

Condition of interest

Control condition

Type: Lipid

↻

+

−

All results

Lipid class results

Lipid species results

Fatty acid results



Troubleshooting BioPAN



29	291	CE(22:4)	1.05375036	0	0.17637001	0	0.66273329	4.89026364	10.0359784	4.54621371
	292	CE(22:5)	4.25440223	1.84461751	2.55700389	0.77090103	8.12755866	33.1298371	71.4169769	20.5454772
	293	CE(22:6)	11.3712184	20.4293142	12.9762383	6.39447186	14.7567919	65.9548069	73.3694124	60.0248532
	294	CE(24:1)	2.22709909	1.44248535	0.85225516	0.39261636	2.46147867	7.93412292	26.1867889	4.01345801
	295	CE(24:2)	1.03898842	1.42145122	0.54467354	0.33012762	3.84203698	10.6654115	18.5548419	3.82822911
	296	CE(26:2)	0.60582561	0.83553803	0.18052744	0.30234104	1.50443904	4.91140638	15.8641685	2.58533902
	297	CE(26:3)	0.32022838	0.26311093	0.15810204	0.09202442	2.30662135	6.9317395	10.9507919	1.9279316
30	298	ST(27:0)	358.065849	272.584699	235.867633	217.517318	456.488472	918.324634	685.38561	1290.03164
	299	O-PC(29:0)	0.23138494	0.19701208	0.10283525	0.16264436	0.37910262	0.95984591	0.34730558	0.43705534
	300	O-PC(30:1)	0.04302948	0.06000144	0.02712594	0.04693831	0.09867804	0.24831112	0.10883309	0.13022465
	301	O-PC(32:0)	0.96207422	1.33718609	0.53403714	1.19995397	1.53718322	3.38342054	1.20036491	1.64118738
	302	O-PC(32:1)	1.59533827	1.64028161	0.83415719	1.4312704	1.72413793	3.79001185	1.43243546	1.97120876
	303	O-PC(32:2)	0.16481103	0.26654576	0.11828261	0.23059356	0.28458662	0.60407852	0.25847858	0.38175446
	304	O-PC(32:3)	0.00686036	0.00586579	0.00277611	0.0057034	0.00596178	0.01524717	0.00652198	0.00909789

¹ **LipidLynxX: a data transfer hub to support integration of large scale lipidomics datasets.** Zhixu Ni, Maria Fedorova.
[bioRxiv, 2020.04.09.033894.](#)

² **BioPAN: a web-based tool to explore mammalian lipidome metabolic pathways on LIPID MAPS.** Caroline Gaud, Bebiana C. Sousa, *et al.*
[F1000Research 2021, 10:4.](#)

Thank You

www.bmss.org.uk

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