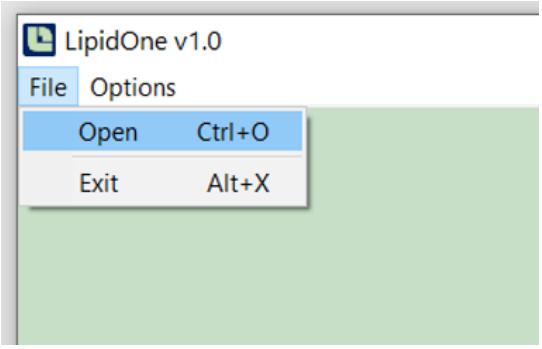
HOW TO USE

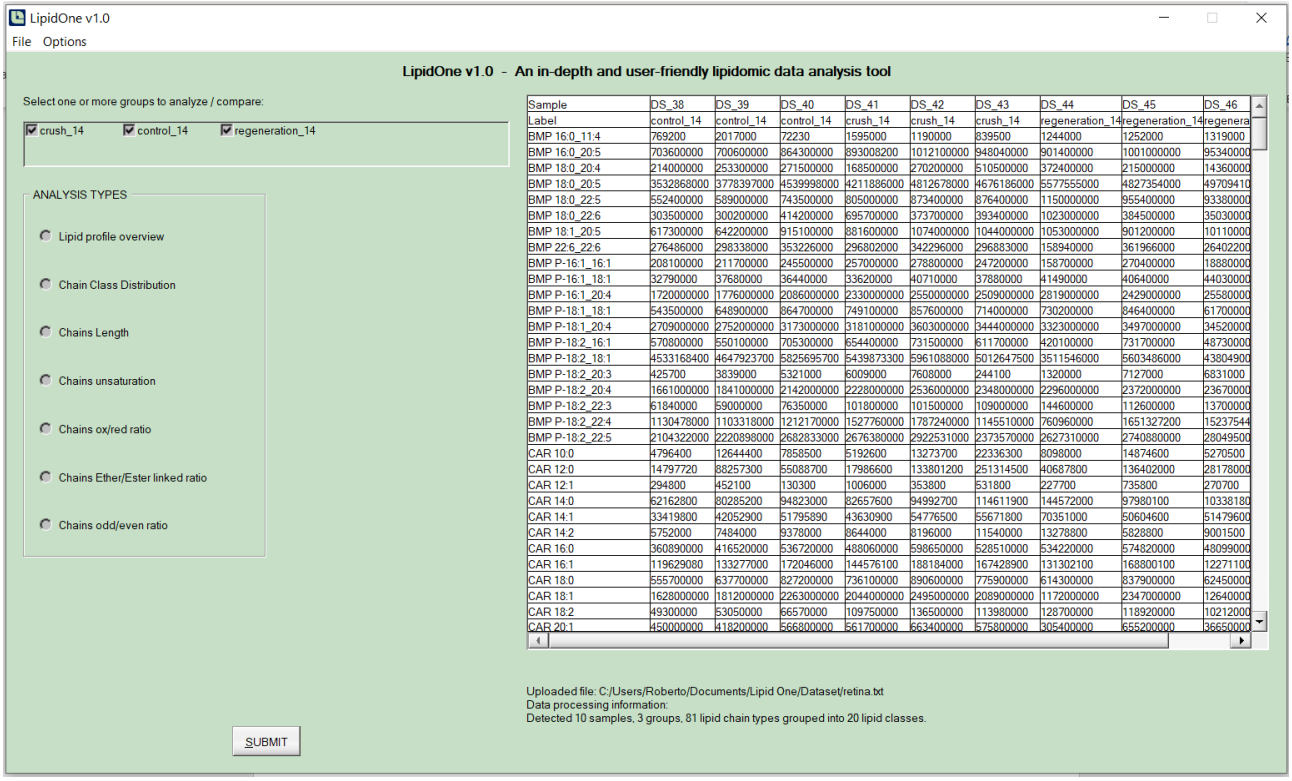
Three-step LipidOne workflow

Data upload:

First you need to upload your data. Click to File, Open. Remember that you need a matrix in txt or csv (tab delimited) format. The matrix must contain the names and concentrations in each lipid sample detected (see example dataset). Remember that the accepted lipid nomenclature is the 'molecular species level' as given in the Lipidomics Standards Initiative (LSI) guidelines.



Once the matrix has been loaded, you can view it in the window on the right:

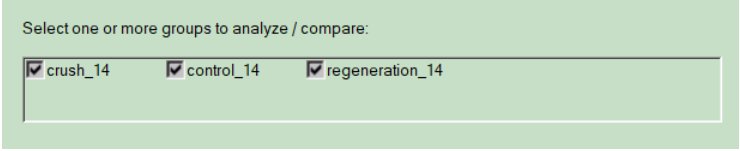


Sample	DS_38	DS_39	DS_40	DS_41	DS_42	DS_43	DS_44	DS_45	DS_46
Label	control_14	control_14	control_14	crush_14	crush_14	crush_14	regeneration_14	regeneration_14	regenera
BMP 16:0_11:4	769200	2017000	72230	1595000	1190000	839500	1244000	1252000	1319000
BMP 16:0_20:5	703600000	700600000	864300000	893008200	1012100000	948040000	901400000	1001000000	95340000
BMP 18:0_20:4	214000000	253300000	271500000	168500000	270200000	510500000	372400000	215000000	14360000
BMP 18:0_20:5	3532868000	3778397000	4539998000	4211886000	4812678000	4676186000	5577555000	4827354000	49709410
BMP 18:0_22:5	552400000	589000000	743500000	805000000	873400000	876400000	1150000000	955400000	93380000
BMP 18:0_22:6	303500000	300200000	414200000	695700000	373700000	393400000	1023000000	384500000	35030000
BMP 18:1_20:5	617300000	642200000	915100000	881600000	1074000000	1044000000	1053000000	901200000	10110000
BMP 22:6_22:6	276486000	298338000	353226000	296802000	342296000	296883000	158940000	361966000	26402200
BMP P-16:1_16:1	208100000	211700000	245500000	257000000	278800000	247200000	158700000	270400000	18880000
BMP P-16:1_18:1	32790000	37680000	36440000	33620000	40710000	37880000	41490000	40640000	44030000
BMP P-16:1_20:4	1720000000	1776000000	2086000000	2330000000	2550000000	2509000000	2819000000	2429000000	25580000
BMP P-18:1_18:1	543500000	648900000	864700000	749100000	857600000	714000000	730200000	846400000	61700000
BMP P-18:1_20:4	2709000000	2752000000	3173000000	3181000000	3603000000	3444000000	3323000000	3497000000	34520000
BMP P-18:2_16:1	570800000	550100000	705300000	654400000	731500000	611700000	420100000	731700000	48730000
BMP P-18:2_18:1	4533168400	4647923700	5825695700	5439873300	5961088000	5012647500	3511546000	5603486000	43804900
BMP P-18:2_20:3	425700	3839000	5321000	6009000	7608000	244100	1320000	7127000	6831000
BMP P-18:2_20:4	1661000000	1841000000	2142000000	2228000000	2536000000	2348000000	2296000000	2372000000	23670000
BMP P-18:2_22:3	61840000	59000000	76350000	101800000	101500000	109000000	144600000	112600000	13700000
BMP P-18:2_22:4	1130478000	1103318000	1212170000	1527760000	1787240000	1145510000	760960000	1651327200	15237544
BMP P-18:2_22:5	2104322000	2220898000	2682833000	2676380000	2922531000	2373570000	2627310000	2740880000	28049500
CAR 10:0	4796400	12644400	7858500	5192600	13273700	22336300	8098000	14874600	5270500
CAR 12:0	14797720	88257300	55088700	17986600	133801200	251314500	40687800	136402000	28178000
CAR 12:1	294800	452100	130300	1006000	353800	531800	227700	735800	270700
CAR 14:0	62162800	80285200	94823000	82657600	94992700	114611900	144572000	97980100	10338180
CAR 14:1	33419800	42052900	51795890	43630900	54776500	55671800	70351000	50604600	51479600
CAR 14:2	5752000	7484000	9378000	8644000	8196000	11540000	13278800	6828800	9001500
CAR 16:0	360890000	416520000	536720000	488060000	598650000	528510000	534220000	574820000	48099000
CAR 16:1	119629080	133277000	172046000	144576100	188184000	167428900	131302100	168800100	12271100
CAR 18:0	555700000	637700000	827200000	736100000	890600000	775900000	614300000	837900000	62450000
CAR 18:1	1628000000	1812000000	2263000000	2044000000	2495000000	2089000000	1172000000	2347000000	12640000
CAR 18:2	49300000	53050000	66570000	109750000	136500000	113980000	128700000	118920000	10212000
CAR 20:1	450000000	418200000	566800000	561700000	663400000	575800000	305400000	655200000	36650000

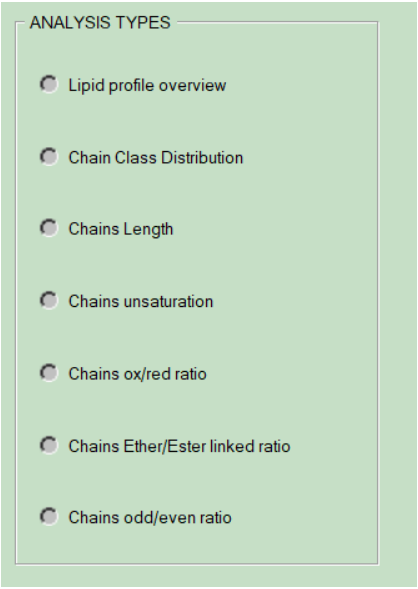
Query selection:

Now you can start exploring your data set.

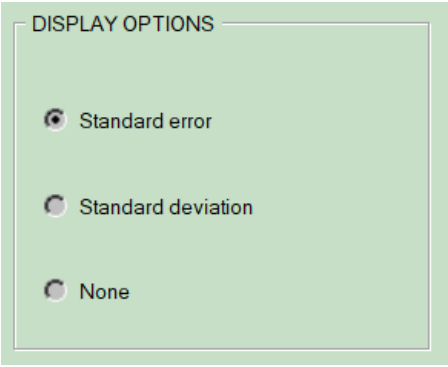
First you can decide which group of experiments to analyse:



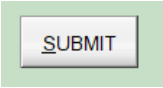
You can choose one of seven types of analysis, some using dynamic context-dependent menus.



You can also decide whether to represent the experimental error bar, the standard deviation bar or neither:

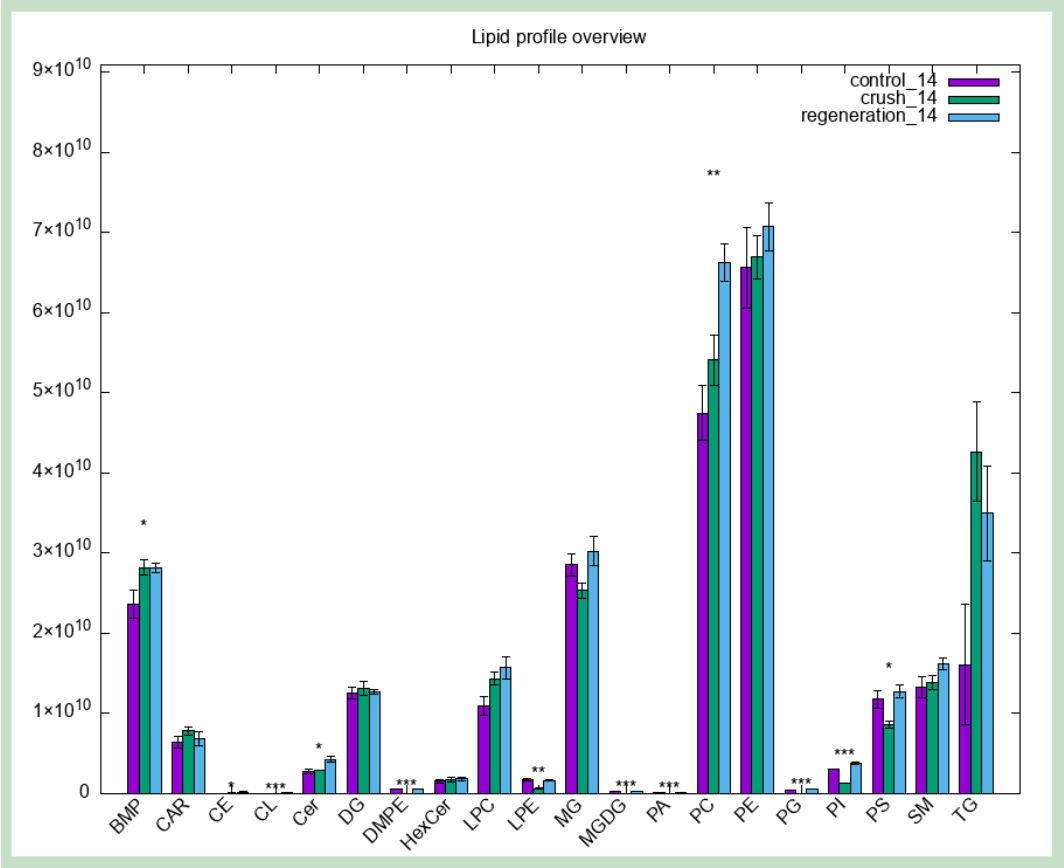


Finally, click on the submit button:



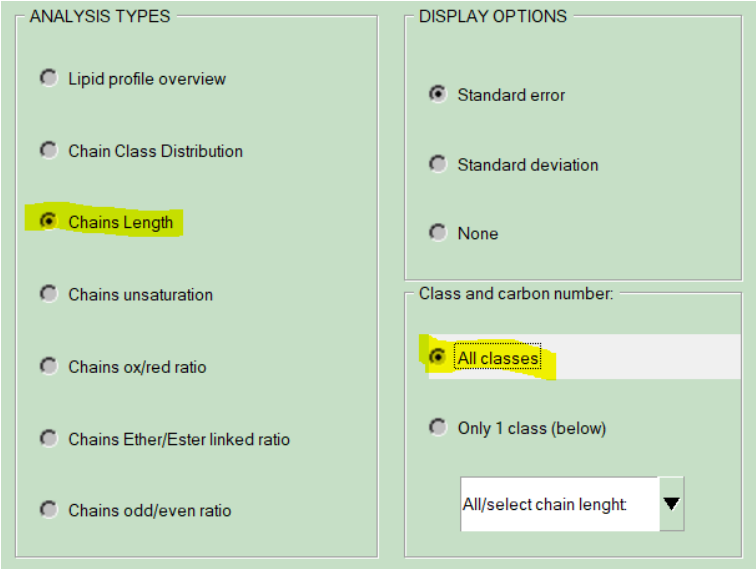
Get results:

In the right-hand window you will now find the result of your analysis. In this example we show Lipid Profile Overview.

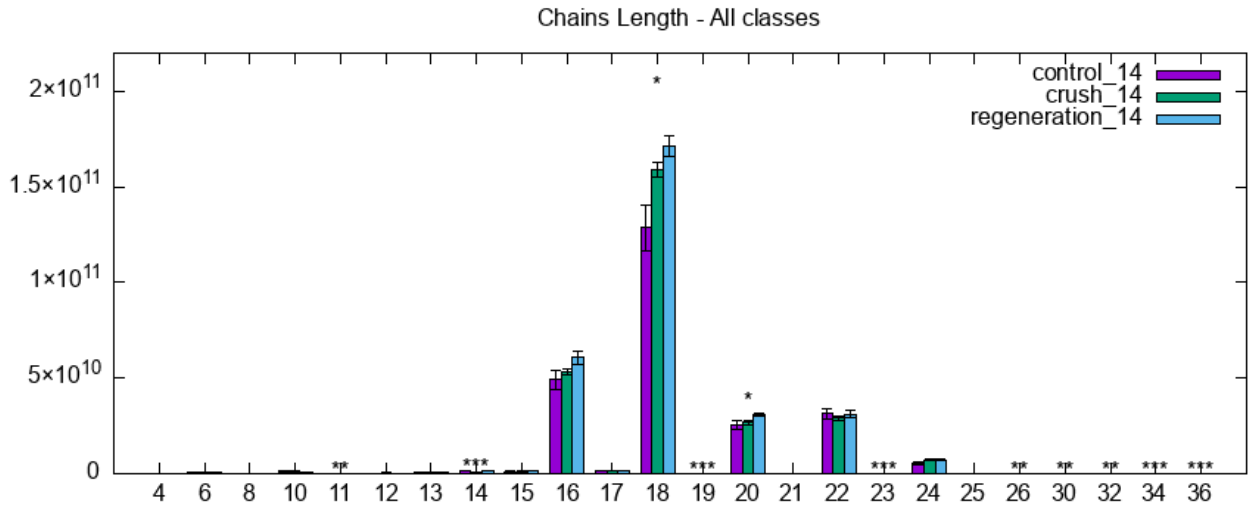


If you compare two or more groups of experiments, LipidOne calculates the significance of the differences. One, two or three asterisks correspond to p-values of less than 0.05, 0.01 and 0.001, respectively.

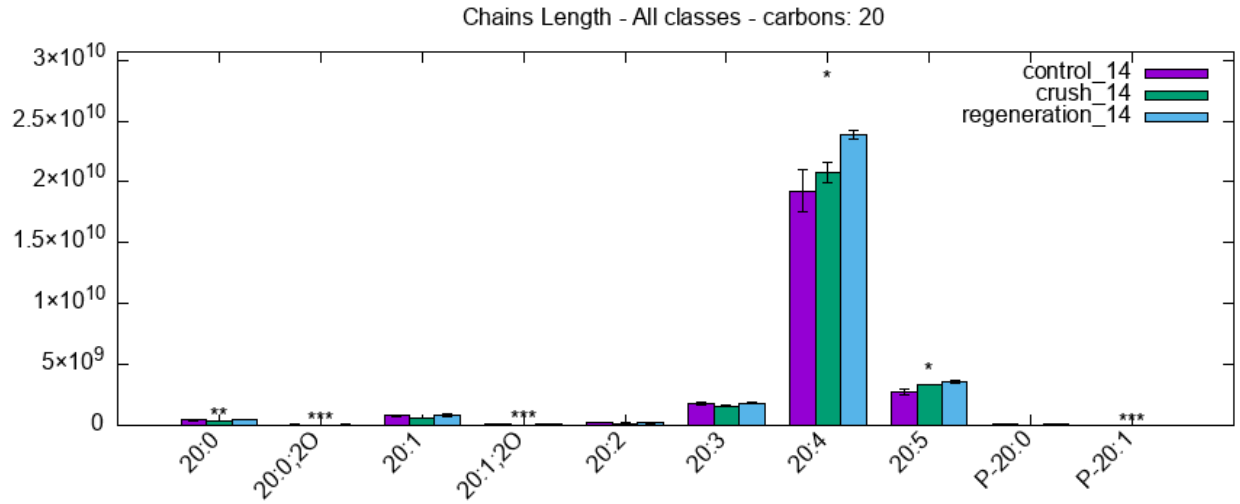
The length of the chains or the number of unsaturations can be explored for all lipid classes or for a single class:



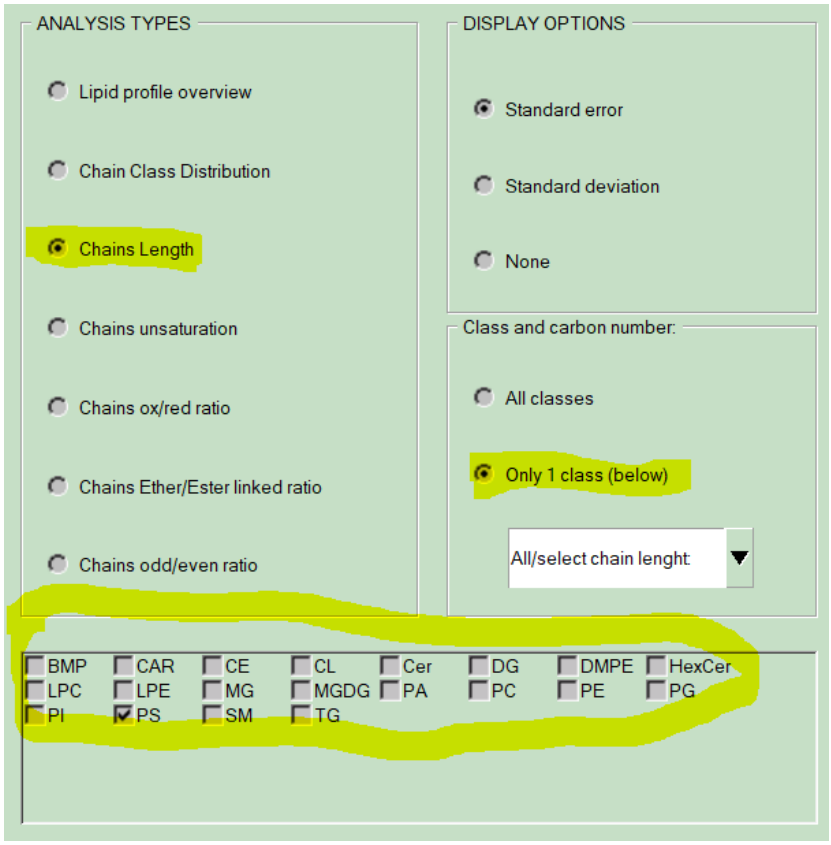
Select "All Classes" and observe the result:



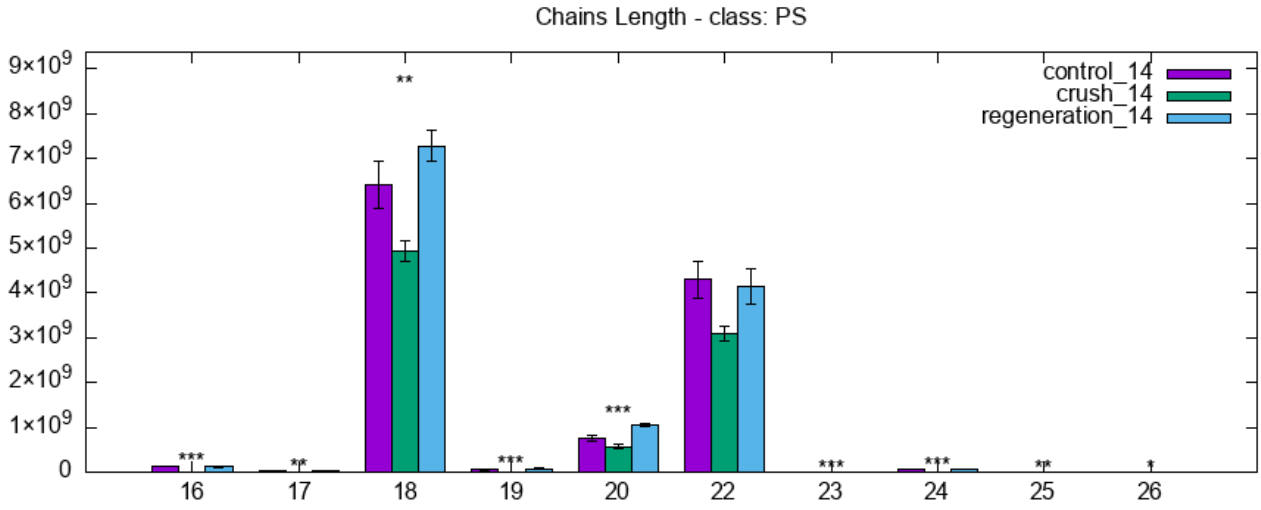
With a drop-down menu you can explore the chains according to their length. In this example we select "20": here is the result:



The same analysis can be done for every single class. If you select "single class" a window appears with all the classes in your data set.



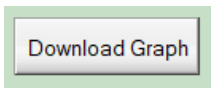
The same analysis can be done for every single class. Here we select "PS" Here is the result:



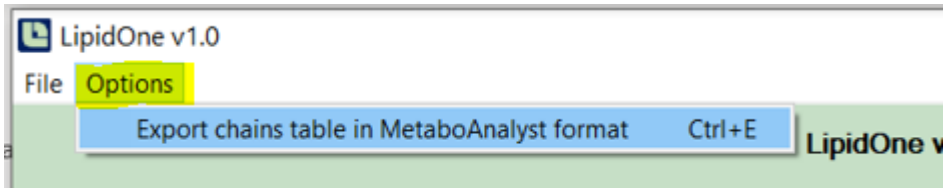
By doing this you can explore your dataset and discover many differences.

Also, remember that each graph can be downloaded (in different image formats).

To do this, click on "Download Graph":



You can also export an array with all the chain data of your set. Click to Option, Export chains table…



This file, which you find in the folder where you have saved LipidOne, can be directly loaded for statistical analysis on the MetaboAnalist platform (https://www.metaboanalyst.ca).