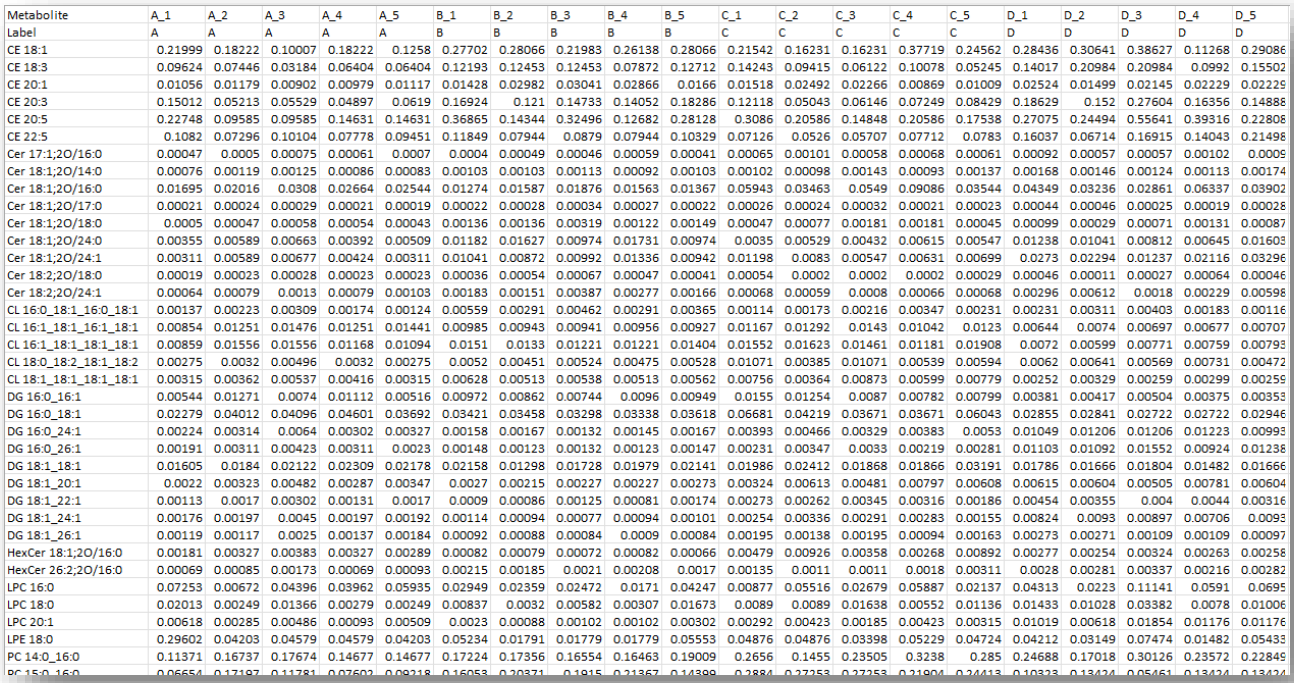
How to prepare data for LipidOne 2.0

We recommend preparing the data table using a spreadsheet such as Excel. Please look at the example below:



Metabolite	A_1	A_2	A_3	A_4	A_5	B_1	B_2	B_3	B_4	B_5	C_1	C_2	C_3	C_4	C_5	D_1	D_2	D_3	D_4	D_5
Label	A	A	A	A	A	B	B	B	B	B	C	C	C	C	C	D	D	D	D	D
CE 18:1	0.21999	0.18222	0.10007	0.18222	0.1258	0.27702	0.28066	0.21983	0.26138	0.28066	0.21542	0.16231	0.16231	0.37719	0.24562	0.28436	0.30641	0.38627	0.11268	0.29086
CE 18:3	0.09624	0.07446	0.03184	0.06404	0.06404	0.12193	0.12453	0.12453	0.07872	0.12712	0.14243	0.09415	0.06122	0.10078	0.05245	0.14017	0.20984	0.20984	0.0992	0.15502
CE 20:1	0.01056	0.01179	0.00902	0.00979	0.01117	0.01428	0.02982	0.03041	0.02866	0.0166	0.01518	0.02492	0.02266	0.00869	0.01009	0.02524	0.01499	0.02145	0.02229	0.02229
CE 20:3	0.15012	0.05213	0.05529	0.04897	0.0619	0.16924	0.121	0.14733	0.14052	0.18286	0.12118	0.05043	0.06146	0.07249	0.08429	0.18629	0.152	0.27604	0.16356	0.14888
CE 20:5	0.22748	0.09585	0.09585	0.14631	0.14631	0.36865	0.14344	0.32496	0.12682	0.28128	0.3086	0.20586	0.14848	0.20586	0.17538	0.27075	0.24494	0.55641	0.39316	0.22808
CE 22:5	0.1082	0.07296	0.10104	0.07778	0.09451	0.11849	0.07944	0.0879	0.07944	0.10329	0.07126	0.0526	0.05707	0.07712	0.0783	0.16037	0.06714	0.16915	0.14043	0.21498
Cer 17:1;2O/16:0	0.00047	0.0005	0.00075	0.00061	0.0007	0.0004	0.00049	0.00046	0.00059	0.00041	0.00065	0.00101	0.00058	0.00068	0.00061	0.00092	0.00057	0.00057	0.00102	0.0009
Cer 18:1;2O/14:0	0.00076	0.00119	0.00125	0.00086	0.00083	0.00103	0.00103	0.00113	0.00092	0.00103	0.00102	0.00098	0.00143	0.00093	0.00137	0.00168	0.00146	0.00124	0.00113	0.00174
Cer 18:1;2O/16:0	0.01695	0.02016	0.0308	0.02664	0.02544	0.01274	0.01587	0.01876	0.01563	0.01367	0.05943	0.03463	0.0549	0.09086	0.03544	0.04349	0.03236	0.02861	0.06337	0.03902
Cer 18:1;2O/17:0	0.00021	0.00024	0.00029	0.00021	0.00019	0.00022	0.00028	0.00034	0.00027	0.00022	0.00026	0.00024	0.00032	0.00021	0.00023	0.00044	0.00046	0.00025	0.00019	0.00028
Cer 18:1;2O/18:0	0.0005	0.00047	0.00058	0.00054	0.00043	0.00136	0.00136	0.00319	0.00122	0.00149	0.00047	0.00077	0.00181	0.00181	0.00045	0.00099	0.00029	0.00071	0.00131	0.00087
Cer 18:1;2O/24:0	0.00355	0.00589	0.00663	0.00392	0.00509	0.01182	0.01627	0.00974	0.01731	0.00974	0.0035	0.00529	0.00432	0.00615	0.00547	0.01238	0.01041	0.00812	0.00645	0.01603
Cer 18:1;2O/24:1	0.00311	0.00589	0.00677	0.00424	0.00311	0.01041	0.00872	0.00992	0.01336	0.00942	0.01198	0.0083	0.00547	0.00631	0.00699	0.0273	0.02294	0.01237	0.02116	0.03296
Cer 18:2;2O/18:0	0.00019	0.00023	0.00028	0.00023	0.00023	0.00036	0.00054	0.00067	0.00047	0.00041	0.00054	0.0002	0.0002	0.0002	0.00029	0.00046	0.00011	0.00027	0.00064	0.00046
Cer 18:2;2O/24:1	0.00064	0.00079	0.0013	0.00079	0.00103	0.00183	0.00151	0.00387	0.00277	0.00166	0.00068	0.00059	0.0008	0.00066	0.00068	0.00296	0.00612	0.0018	0.00229	0.00598
CL 16:0_18:1_16:0_18:1	0.00137	0.00223	0.00309	0.00174	0.00124	0.00559	0.00291	0.00462	0.00291	0.00365	0.00114	0.00173	0.00216	0.00347	0.00231	0.00231	0.00311	0.00403	0.00183	0.00116
CL 16:1_18:1_16:1_18:1	0.00854	0.01251	0.01476	0.01251	0.01441	0.00985	0.00943	0.00941	0.00956	0.00927	0.01167	0.01292	0.0143	0.01042	0.0123	0.00644	0.0074	0.00697	0.00677	0.00707
CL 16:1_18:1_18:1_18:1	0.00859	0.01556	0.01556	0.01168	0.01094	0.0151	0.0133	0.01221	0.01221	0.01404	0.01552	0.01623	0.01461	0.01181	0.01908	0.0072	0.00599	0.00771	0.00759	0.00793
CL 18:0_18:2_18:1_18:2	0.00275	0.0032	0.00496	0.0032	0.00275	0.0052	0.00451	0.00524	0.00475	0.00528	0.01071	0.00385	0.01071	0.00539	0.00594	0.0062	0.00641	0.00569	0.00731	0.00472
CL 18:1_18:1_18:1_18:1	0.00315	0.00362	0.00537	0.00416	0.00315	0.00628	0.00513	0.00538	0.00513	0.00562	0.00756	0.00364	0.00873	0.00599	0.00779	0.00252	0.00329	0.00259	0.00299	0.00259
DG 16:0_16:1	0.00544	0.01271	0.0074	0.01112	0.00516	0.00972	0.00862	0.00744	0.0096	0.00949	0.0155	0.01254	0.0087	0.00782	0.00799	0.00381	0.00417	0.00504	0.00375	0.00353
DG 16:0_18:1	0.02279	0.04012	0.04096	0.04601	0.03692	0.03421	0.03458	0.03298	0.03338	0.03618	0.06681	0.04219	0.03671	0.03671	0.06043	0.02855	0.02841	0.02722	0.02722	0.02946
DG 16:0_24:1	0.00224	0.00314	0.0064	0.00302	0.00327	0.00158	0.00167	0.00132	0.00145	0.00167	0.00393	0.00466	0.00329	0.00383	0.0053	0.01049	0.01206	0.01206	0.01223	0.00993
DG 16:0_26:1	0.00191	0.00311	0.00423	0.00311	0.0023	0.00148	0.00123	0.00132	0.00123	0.00147	0.00231	0.00347	0.0033	0.00219	0.00281	0.01103	0.01092	0.01552	0.00924	0.01238
DG 18:1_18:1	0.01605	0.0184	0.02122	0.02309	0.02178	0.02158	0.01298	0.01728	0.01979	0.02141	0.01986	0.02412	0.01868	0.01866	0.03191	0.01786	0.01666	0.01804	0.01482	0.01666
DG 18:1_20:1	0.0022	0.00323	0.00482	0.00287	0.00347	0.0027	0.00215	0.00227	0.00227	0.00273	0.00324	0.00613	0.00481	0.00797	0.00608	0.00615	0.00604	0.00505	0.00781	0.00604
DG 18:1_22:1	0.00113	0.0017	0.00302	0.00131	0.0017	0.0009	0.00086	0.00125	0.00081	0.00174	0.00273	0.00262	0.00345	0.00316	0.00186	0.00454	0.00355	0.004	0.0044	0.00316
DG 18:1_24:1	0.00176	0.00197	0.0045	0.00197	0.00192	0.00114	0.00094	0.00077	0.00094	0.00101	0.00254	0.00336	0.00291	0.00283	0.00155	0.00824	0.0093	0.00897	0.00706	0.0093
DG 18:1_26:1	0.00119	0.00117	0.0025	0.00137	0.00184	0.00092	0.00088	0.00084	0.0009	0.00084	0.00195	0.00138	0.00195	0.00094	0.00163	0.00273	0.00271	0.00109	0.00109	0.00097
HexCer 18:1;2O/16:0	0.00181	0.00327	0.00383	0.00327	0.00289	0.00082	0.00079	0.00072	0.00082	0.00066	0.00479	0.00926	0.00358	0.00268	0.00892	0.00277	0.00254	0.00324	0.00263	0.00258
HexCer 26:2;2O/16:0	0.00069	0.00085	0.00173	0.00069	0.00093	0.00215	0.00185	0.0021	0.00208	0.0017	0.00135	0.0011	0.0011	0.0018	0.00311	0.0028	0.00281	0.00337	0.00216	0.00282
LPC 16:0	0.07253	0.00672	0.04396	0.03962	0.05935	0.02949	0.02359	0.02472	0.0171	0.04247	0.00877	0.05516	0.02679	0.05887	0.02137	0.04313	0.0223	0.11141	0.0591	0.0695
LPC 18:0	0.02013	0.00249	0.01366	0.00279	0.00249	0.00837	0.0032	0.00582	0.00307	0.01673	0.0089	0.0089	0.01638	0.00552	0.01136	0.01433	0.01028	0.03382	0.0078	0.01006
LPC 20:1	0.00618	0.00285	0.00486	0.00093	0.00509	0.0023	0.00088	0.00102	0.00102	0.00302	0.00292	0.00423	0.00185	0.00423	0.00315	0.01019	0.00618	0.01854	0.01176	0.01176
LPE 18:0	0.29602	0.04203	0.04579	0.04579	0.04203	0.05234	0.01791	0.01779	0.01779	0.05553	0.04876	0.04876	0.03398	0.05229	0.04724	0.04212	0.03149	0.07474	0.01482	0.05433
PC 14:0_16:0	0.11371	0.16737	0.17674	0.14677	0.14677	0.17224	0.17356	0.16554	0.16463	0.19009	0.2656	0.1455	0.23505	0.3238	0.285	0.24688	0.17018	0.30126	0.23572	0.22849
PC 15:0_16:0	0.06654	0.17187	0.11781	0.07602	0.09218	0.16053	0.20371	0.1815	0.21367	0.14389	0.2884	0.27253	0.27153	0.21804	0.24413	0.10333	0.13424	0.05461	0.13424	0.13424

There are some rules to follow:

1) The first column should show the names of the lipids.
2) Samples should occur in columns starting with the second column.
3) The first row must show the names of the samples.
4) The second row must show the names of the groups to which the samples belong.
5) Sample and group names must be simple, formatted as a character (not numeric), without spaces or special characters.
6) Pay attention: the second row starts with "**Label**".
7) The lipid nomenclature must comply with the "**Molecular species level**" of Lipidomics Standards Initiative (LSI) Guidelines [1]. If the lipid nomenclature is at the 'sum composition' level, you cannot use the building block analysis section of LipidOne 2.0.
8) Ensure that the data in the table is represented in numeric format with decimals, and not in scientific notation.

When you have prepared the table, save it in **CSV** (comma separated) or **TXT** (tab separated) format.

You should know that:

- Two or more lines with the same lipid name are not allowed. If there are duplicate names, an error message will appear telling you which names are duplicate.
- Numeric values that are absent or have a value of "0" (zero) are automatically replaced with a number equal to one-tenth of the lowest value in the same row.
- Quantitative data can be reported either as concentration or as peak area or ion intensity.

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[1] Update on LIPID MAPS classification, nomenclature, and shorthand notation for MS-derived lipid structures, Liebisch, Gerhard et al., Journal of Lipid Research, 2020, Volume 61, Issue 12, 1539 - 1555.

Note that there are some free tools available that translate the name of the lipids into the standardized form:

a) Goslin webapplication - A Parser, Validator and Normalizer for Shorthand Lipid Nomenclature: https://apps.lifs-tools.org/goslin/
b) LipidMaps Tools: https://lipidmaps.org/resources/tools/nomenclature
c) You can also use excel to edit the nomenclature, below you have an example of how the names of some of the major lipid classes should be translated:

This type of lipid nomenclature…	**Must be reported as**
PC(16:0/18:1) or PC(16:0/18:1)[H+]+ or (16:0/18:1) PC or PC(16:0/18:1(9Z))	PC 16:0_18:1
DG(16:0/18:2/0:0)	DG 16:0_18:2
LPE(18:1)	LPE 18:1
SM(d16:1/18:2)	SM 16:0;O2/18:2
Mixed forms such as PC 36:1|PC 16:0_18:1	PC 16:0_18:1