1	Feature detection (Cent wave)	ppm	10
		snthr	4
		peakwidth	10 50
		mzdiff	0.01
		prefilter peaks	4
		prefilter intensity	30000
		noise	5000
2	Grouping (Density)	bw	5
		mzwid	0.025
		minfrac	0.5
		minsamp	1
3	Retention time correction (obiwarp)	profStep	1
4	Grouping (Density)	bw	5
		mzwid	0.025
		minfrac	0.5
		minsamp	1
5	Filling peaks	/	/
6	CAMERA	annotate	isotopes + adducts
		mzabs	0.015
		ppm	15
		sigma	6
		perfwhm	0.6
		maxcharge	3
		maxiso	5
		intensity	into

Table S1. Parameters used to process the LC-HRMS data (mode + & mode –) with XCMS R package.

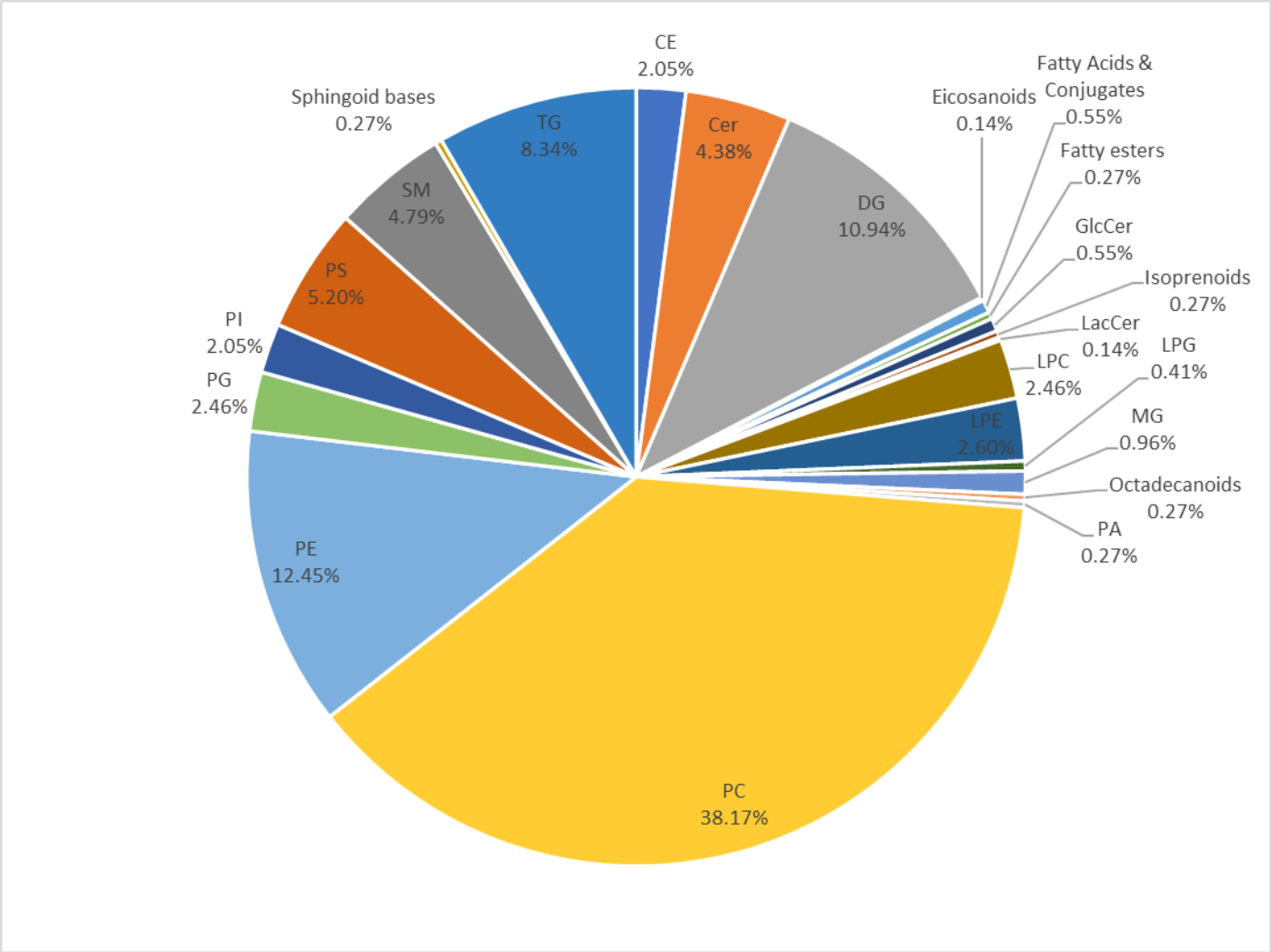

Figure S1. The classes of lipids and the percentage they represent of the background database used for the targeted identification of the lipids in the lipidome of the broilers from the pHu lines. PC = phosphatidylcholines, PE = phosphatidylethanolamines, PG = phosphatidylglycerols, PI = phosphatidylinositols, PS = phosphatidylserines, SM = sphingomyelins, TG = triacylglycerols, CE = cholesterol esters, Cer = ceramides, DG = diacylglycerols, GlcCer = glucosylceramides, LacCer = lactosylceramides, LPC = lysophosphatidylcholines, LPE = lysophosphatidylethanolamine, LPG = lysophosphatidylglycerols, MG = monoradylglycerols, PA = phosphatidic acid.

Lipid ID	Lipid	VIP	Contribution
Mode +_CE(20:4)	**CE(20:4)**	1.60485	-1.41302
Mode +_CE(22:6)	**CE(22:6)**	1.19543	-0.847395
Mode +_CE(22:4)	**CE(22:4)**	1.34957	-0.809949
Mode +_CE(22:5)	**CE(22:5)**	1.15542	-0.644901
Mode +_CE(18:2)	**CE(18:2)**	0.746702	-0.31989
Mode +_CE(18:3)	**CE(18:3)**	0.625889	-0.269798
Mode +_CE(20:3)	**CE(20:3)**	0.48525	-0.0611237
Mode +_Cer(d18:1/20:0)	**Cer(d18:1/20:0)**	0.700776	0.205177
Mode +_Cer(d18:2/23:0)	**Cer(d18:2/23:0)**	0.84626	0.345576
Mode +_Cer(d18:2/22:0)	**Cer(d18:2/22:0)**	1.13039	0.379647
Mode +_Cer(d18:0/16:0)	**Cer(d18:0/16:0)**	1.11697	0.400732
Mode +_Cer(d18:1/18:1)	**Cer(d18:1/18:1)**	1.55366	1.53696
Mode +_Cer(d18:0/18:0)	**Cer(d18:0/18:0)**	2.21729	2.54783
Mode +_Cer(d18:0/20:0)	**Cer(d18:0/20:0)**	2.29816	2.78842
Mode +_DG(18:2/20:4)	**DG(18:2/20:4)**	1.12413	-0.311501
Mode +_DG(18:0/16:0)	**DG(18:0/16:0)**	0.687238	0.21838
Mode +_DG(18:1/18:1)	**DG(18:1/18:1)**	0.978817	0.240521
Mode +_DG(16:0/16:0)	**DG(16:0/16:0)**	0.876594	0.38362
Mode +_DG(18:2/18:2)	**DG(18:2/18:2)**	1.32874	0.644907
Mode +_DG(18:1/16:0)	**DG(18:1/16:0)**	1.45766	0.891184
Mode +_DG(16:0/16:1)	**DG(16:0/16:1)**	1.48967	0.908759
Mode +_DG(16:1/18:1)	**DG(16:1/18:1)**	1.50937	0.977413
Mode +_GlcCer(d18:1/16:0)	**GlcCer(d18:1/16:0)**	0.434841	-0.0349001
Mode +_GlcCer(d18:1/22:0)	**GlcCer(d18:1/22:0)**	0.464922	0.00146593
Mode +_LPC(18:4)	**LPC(18:4)**	0.895911	-0.0208428
Mode +_LPC(20:4)	**LPC(20:4)**	0.881166	-0.00629754
Mode +_LPC(22:4)	**LPC(22:4)**	0.833625	0.00440012
Mode +_LPC(22:6)	**LPC(22:6)**	0.725501	0.0048413
Mode +_LPC(16:1)	**LPC(16:1)**	1.05932	0.0233722
Mode +_LPC(18:0)	**LPC(18:0)**	1.0736	0.11078
Mode +_LPC(18:1)	**LPC(18:1)**	1.27489	0.213744
Mode +_LPC(O-16:1)	**LPC(O-16:1)**	0.798479	0.232622
Mode +_LPC(20:5)	**LPC(20:5)**	1.07783	0.281654
Mode +_LPC(20:0)	**LPC(20:0)**	1.17612	0.321337
Mode +_LPC(O-18:1)	**LPC(O-18:1)**	1.15028	0.367344
Mode +_LPC(14:0)	**LPC(14:0)**	1.27861	0.384708
Mode +_LPC(18:2)	**LPC(18:2)**	1.25207	0.394866
Mode +_LPC(17:0)	**LPC(17:0)**	1.13631	0.422523
Mode +_LPC(20:1)	**LPC(20:1)**	1.36506	0.464815
Mode +_LPC(16:0)	**LPC(16:0)**	1.34482	0.496231
Mode +_LPC(20:2)	**LPC(20:2)**	1.42774	0.633267
Mode +_LPC(20:3)	**LPC(20:3)**	1.58845	0.860857
Mode +_LPE(22:6)	**LPE(22:6)**	0.613993	0.0230739
Mode +_LPE(18:0)	**LPE(18:0)**	0.903772	0.24393
Mode +_LPE(18:1)	**LPE(18:1)**	1.2998	0.403312
Mode +_LPE(16:1)	**LPE(16:1)**	1.37544	0.474193
Mode +_LPE(18:2)	**LPE(18:2)**	1.25041	0.564654
Mode +_LPE(16:0)	**LPE(16:0)**	1.17209	0.568239

Mode -_LysoPE(20:4)	**LPE(20:4)**	0.542205	-0.00247706
Mode -_LysoPE(22:5)	**LPE(22:5)**	0.951226	0.20762
Mode -_LysoPE(O-18:1)	**LPE(O-18:1)**	0.970371	0.294461
Mode -_LysoPE(P-16:0)	**LPE(P-16:0)**	0.96976	0.375662
Mode -_LysoPE(20:3)	**LPE(20:3)**	1.37483	0.588188
Mode +_MG(20:4)	**MG(20:4)**	0.678228	0.0799652
Mode -_PC(18:1/20:4)	**PC(18:1/20:4)**	1.51486	-1.00693
Mode -_PC(18:0/20:4)	**PC(18:0/20:4)**	1.45861	-0.948961
Mode -_PC(18:0/22:6)	**PC(18:0/22:6)**	1.19212	-0.729365
Mode -_PC(18:0/22:5)	**PC(18:0/22:5)**	1.41461	-0.700952
Mode -_PC(14:0/20:4)	**PC(14:0/20:4)**	1.42198	-0.613477
Mode -_PC(18:1/22:6)	**PC(18:1/22:6)**	0.933226	-0.530076
Mode -_PC(18:1/22:5)	**PC(18:1/22:5)**	0.960609	-0.408698
Mode -_PC(16:0/20:4)	**PC(16:0/20:4)**	1.06056	-0.286002
Mode -_PC(16:0/18:0)	**PC(16:0/18:0)**	0.707023	-0.285007
Mode +_PC(18:1/19:0)	**PC(18:1/19:0)**	0.774887	-0.249167
Mode -_PC(18:0/18:1)	**PC(18:0/18:1)**	0.997108	-0.239979
Mode +_PC(18:0/22:4)	**PC(18:0/22:4)**	0.622704	-0.156279
Mode -_PC(O-16:0/22:5)	**PC(O-16:0/22:5)**	0.768012	-0.128835
Mode +_PC(O-36:4)	**PC(O-36:4)**	1.03707	-0.10062
Mode -_PC(18:2/20:4)	**PC(18:2/20:4)**	0.593144	-0.0627586
Mode +_PC(O-34:0)	**PC(O-34:0)**	1.00231	-0.0572565
Mode +_PC(O-18:0/18:2)	**PC(O-18:0/18:2)**	0.725062	-0.0434571
Mode -_PC(16:0/22:6)	**PC(16:0/22:6)**	0.429911	-0.0422702
Mode +_PC(32:2)	**PC(32:2)**	0.958231	-0.0175031
Mode +_PC(42:11)	**PC(42:11)**	0.373417	-0.00115315
Mode +_PC(O-38:4)-1	**PC(O-38:4)-1**	0.663584	-0.00110531
Mode +_PC(34:5)	**PC(34:5)**	0.547929	0.00204551
Mode +_PC(O-44:4)	**PC(O-44:4)**	0.197956	0.0118019
Mode -_PC(16:1/18:1)	**PC(16:1/18:1)**	0.539696	0.0150597
Mode +_PC(31:0)	**PC(31:0)**	0.767773	0.0243722
Mode -_PC(O-18:1/18:2)	**PC(O-18:1/18:2)**	0.59798	0.0264139
Mode -_PC(16:0/18:1)	**PC(16:0/18:1)**	0.792878	0.0268602
Mode -_PC(18:0/20:2)	**PC(18:0/20:2)**	0.451444	0.0282559
Mode -_PC(16:1/20:4)	**PC(16:1/20:4)**	0.495245	0.115676
Mode +_PC(42:2)	**PC(42:2)**	0.650565	0.134323
Mode +_PC(O-36:1)	**PC(O-36:1)**	1.12849	0.187446
Mode +_PC(40:2)	**PC(40:2)**	0.81709	0.199052
Mode -_PC(18:0/16:2)	**PC(18:0/16:2)**	0.671714	0.199297
Mode +_PC(P-16:0/18:1)	**PC(P-16:0/18:1)**	1.05675	0.254199
Mode +_PC(O-22:0)	**PC(O-22:0)**	0.972317	0.332785
Mode -_PC(16:0/16:1)	**PC(16:0/16:1)**	1.23642	0.342025
Mode +_PC(O-18:0)	**PC(O-18:0)**	1.25076	0.387825
Mode -_PC(18:2/18:2)	**PC(18:2/18:2)**	1.08602	0.598696
Mode -_PE(P-18:0/20:4)	**PE(P-18:0/20:4)**	1.84461	-1.88698
Mode -_PE(20:1/20:4)	**PE(20:1/20:4)**	1.27511	-0.663051
Mode -_PE(18:0/20:4)	**PE(18:0/20:4)**	1.19903	-0.579199
Mode -_PE(22:6/18:1)	**PE(22:6/18:1)**	0.83121	-0.292808
Mode +_PE(18:0/22:6)	**PE(18:0/22:6)**	0.826663	-0.284938

Mode -_PE(O-18:0/22:6)	**PE(O-18:0/22:6)**	0.868883	-0.283409
Mode -_PE(P-18:0/20:2)	**PE(P-18:0/20:2)**	0.745452	-0.277779
Mode -_PE(P-16:0/20:4)	**PE(P-16:0/20:4)**	0.981789	-0.273066
Mode +_PE(P-18:0/22:4)	**PE(P-18:0/22:4)**	0.860013	-0.24005
Mode -_PE(22:4/18:0)	**PE(22:4/18:0)**	1.03667	-0.183936
Mode +_PE(P-18:0/22:6)	**PE(P-18:0/22:6)**	0.846771	-0.178836
Mode +_PE(P-18:0/18:2)	**PE(P-18:0/18:2)**	0.761173	-0.156093
Mode -_PE(P-18:1/22:6)	**PE(P-18:1/22:6)**	0.819117	-0.134644
Mode -_PE(P-16:0/22:4)	**PE(P-16:0/22:4)**	0.60781	-0.0282253
Mode -_PE(16:0/22:6)	**PE(16:0/22:6)**	0.600058	-0.0257649
Mode -_PE(P-16:0/20:3)	**PE(P-16:0/20:3)**	0.475244	-0.0194954
Mode -_PE(16:0/20:4)	**PE(16:0/20:4)**	0.545915	-0.0113733
Mode -_PE(20:5/16:0)	**PE(20:5/16:0)**	0.511122	-0.00632101
Mode -_PE(O-18:0/18:2)	**PE(O-18:0/18:2)**	0.313797	-0.00134008
Mode +_PE(P-18:0/18:1)	**PE(P-18:0/18:1)**	0.418147	-0.00126135
Mode -_PE(P-16:0/18:1)	**PE(P-16:0/18:1)**	0.366903	0.00425098
Mode +_PE(P-16:0/22:6)	**PE(P-16:0/22:6)**	0.864355	0.0463814
Mode -_PE(16:0/18:2)	**PE(16:0/18:2)**	0.805084	0.0479905
Mode -_PE(20:5/18:1)	**PE(20:5/18:1)**	0.464043	0.0970365
Mode -_PE(O-18:0/18:1)	**PE(O-18:0/18:1)**	0.76875	0.126085
Mode -_PE(16:0/18:3)	**PE(16:0/18:3)**	0.72128	0.171088
Mode +_PE(18:1/18:1)	**PE(18:1/18:1)**	0.851104	0.193085
Mode +_PE(18:1/17:0)	**PE(18:1/17:0)**	1.19235	0.226928
Mode +_PE(34:2)	**PE(34:2)**	1.05772	0.305057
Mode +_PE(16:1/16:0)	**PE(16:1/16:0)**	1.23515	0.316384
Mode -_PE(18:1/18:2)	**PE(18:1/18:2)**	0.858554	0.347899
Mode +_PE(P-16:0/18:2)	**PE(P-16:0/18:2)**	0.927682	0.364486
Mode -_PE(18:2/18:2)	**PE(18:2/18:2)**	1.37595	1.20309
Mode -_PE(O-16:0/18:1)	**PE(O-16:0/18:1)**	1.54041	1.42284
Mode -_PG(18:1/18:1)	**PG(18:1/18:1)**	0.648168	0.140006
Mode -_PI(18:1/22:4)	**PI(18:1/22:4)**	1.02442	-0.563268
Mode -_PI(18:0/20:4)	**PI(18:0/20:4)**	0.670739	-0.13245
Mode -_PI(20:4/16:0)	**PI(20:4/16:0)**	0.414641	-0.0514465
Mode -_PI(18:1/18:0)	**PI(18:1/18:0)**	0.357698	-0.0285417
Mode -_PI(18:2/16:0)	**PI(18:2/16:0)**	0.186046	-0.0181759
Mode -_PI(16:0/18:1)	**PI(16:0/18:1)**	0.575153	-0.00255493
Mode -_PS(22:0/16:0)	**PS(22:0/16:0)**	0.691227	-0.177542
Mode -_PS(20:2/20:4)	**PS(20:2/20:4)**	0.782813	-0.0855022
Mode -_PS(18:1/20:2)	**PS(18:1/20:2)**	0.671716	-0.0314262
Mode -_PS(16:0/20:0)	**PS(16:0/20:0)**	0.343293	-0.0174127
Mode -_PS(18:2/20:2)	**PS(18:2/20:2)**	0.690672	-0.00114038
Mode -_PS(18:2/18:2)	**PS(18:2/18:2)**	0.734935	0.00457329
Mode -_PS(18:2/20:3)	**PS(18:2/20:3)**	0.661247	0.00869048
Mode -_PS(18:2/18:1)	**PS(18:2/18:1)**	0.799902	0.0210943
Mode -_PS(16:1/20:0)	**PS(16:1/20:0)**	0.857765	0.431184
Mode +_SM(34:2)	**SM(34:2)**	1.28355	-0.70344
Mode +_SM(41:1)	**SM(41:1)**	1.05917	-0.299341
Mode +_SM(d18:1/24:0)	**SM(d18:1/24:0)**	1.01297	-0.297593
Mode +_SM(38:3)	**SM(38:3)**	1.05365	-0.248205

Mode +_SM(d18:2/18:0)	**SM(d18:2/18:0)**	0.866587	-0.126997
Mode +_SM(40:1)	**SM(40:1)**	1.00926	-0.100266
Mode +_SM(d18:1/18:0)	**SM(d18:1/18:0)**	1.01896	-0.0952459
Mode +_SM(30:1)	**SM(30:1)**	0.465453	-0.0816061
Mode +_SM(33:1)	**SM(33:1)**	0.96581	-0.0372163
Mode +_SM(d18:1/19:0)	**SM(d18:1/19:0)**	0.291112	-0.0141118
Mode +_SM(d18:2/25:0)	**SM(d18:2/25:0)**	0.806042	-0.00452279
Mode +_SM(d18:1/20:0)	**SM(d18:1/20:0)**	0.891011	0.000274332
Mode +_SM(41:2)	**SM(41:2)**	0.85766	0.00154643
Mode +_SM(36:3)	**SM(36:3)**	0.641322	0.00318869
Mode +_SM(d18:2/24:0)	**SM(d18:2/24:0)**	0.88299	0.00527447
Mode +_SM(42:3)	**SM(42:3)**	0.942605	0.00628839
Mode +_SM(d18:1/22:1)	**SM(d18:1/22:1)**	0.986452	0.0850724
Mode +_SM(32:0)	**SM(32:0)**	1.20336	0.496626
Mode +_SM(36:0)	**SM(36:0)**	1.68324	1.3433
Mode +_SM(34:0)	**SM(34:0)**	1.77878	1.43733
Mode +_TG(13:0/16:1/18:1)	**TG(13:0/16:1/18:1)**	0.561331	-0.0841042
Mode +_TG(15:0/15:0/17:1)	**TG(15:0/15:0/17:1)**	0.485565	-0.00982397
Mode +_TG(16:1/18:1/22:0)	**TG(16:1/18:1/22:0)**	0.435018	-0.00571819
Mode +_TG(14:0/14:0/16:0)	**TG(14:0/14:0/16:0)**	0.693073	0.00290237
Mode +_TG(15:0/16:0/18:0)	**TG(15:0/16:0/18:0)**	0.732489	0.0695474
Mode +_TG(16:0/16:0/17:1)	**TG(16:0/16:0/17:1)**	0.847747	0.0766748
Mode +_TG(16:1/17:0/18:1)	**TG(16:1/17:0/18:1)**	0.652062	0.0867277
Mode +_TG(18:0/18:1/18:2)	**TG(18:0/18:1/18:2)**	0.845864	0.11602
Mode +_TG(16:1/18:1/18:1)	**TG(16:1/18:1/18:1)**	0.402852	0.116096
Mode +_TG(16:0/18:1/19:1)	**TG(16:0/18:1/19:1)**	0.596401	0.138352
Mode +_TG(18:0/18:1/18:1)	**TG(18:0/18:1/18:1)**	0.83413	0.138426
Mode +_TG(18:0/18:0/18:1)	**TG(18:0/18:0/18:1)**	0.637459	0.156912
Mode +_TG(15:0/15:0/16:1)	**TG(15:0/15:0/16:1)**	0.982314	0.165719
Mode +_TG(16:0/18:0/18:1)	**TG(16:0/18:0/18:1)**	0.831046	0.170945
Mode +_TG(14:0/16:0/16:0)	**TG(14:0/16:0/16:0)**	1.0114	0.308247
Mode +_TG(16:0/18:1/18:1)	**TG(16:0/18:1/18:1)**	0.954098	0.310734
Mode +_TG(14:1/16:1/18:1)	**TG(14:1/16:1/18:1)**	1.15182	0.325341
Mode +_TG(16:0/16:0/18:1)	**TG(16:0/16:0/18:1)**	1.04125	0.471379
Mode +_TG(18:1/18:1/18:2)	**TG(18:1/18:1/18:2)**	1.12036	0.504664
Mode +_TG(14:0/16:0/18:1)	**TG(14:0/16:0/18:1)**	1.30893	0.637547
Mode +_TG(16:0/16:1/18:2)	**TG(16:0/16:1/18:2)**	1.39206	0.701532
Mode +_TG(16:0/16:1/16:1)	**TG(16:0/16:1/16:1)**	1.47398	0.761618
Mode +_TG(16:0/16:1/18:1)	**TG(16:0/16:1/18:1)**	1.56985	0.925374

Table S2. The 185 lipids identified in the serum of the broilers from the pHu line. The importance of each lipids in the model (VIP) and their contributions to the pHu+ (negative values) or pHu– (positive values) line modelized by OPLS-DA (M1a; 1 predictive and 3 orthogonal components, $R^2Y_{(cum)} = 0.74$ and $Q^2_{(cum)} = 0.56$) were tabulated in the third and fourth column, respectively.

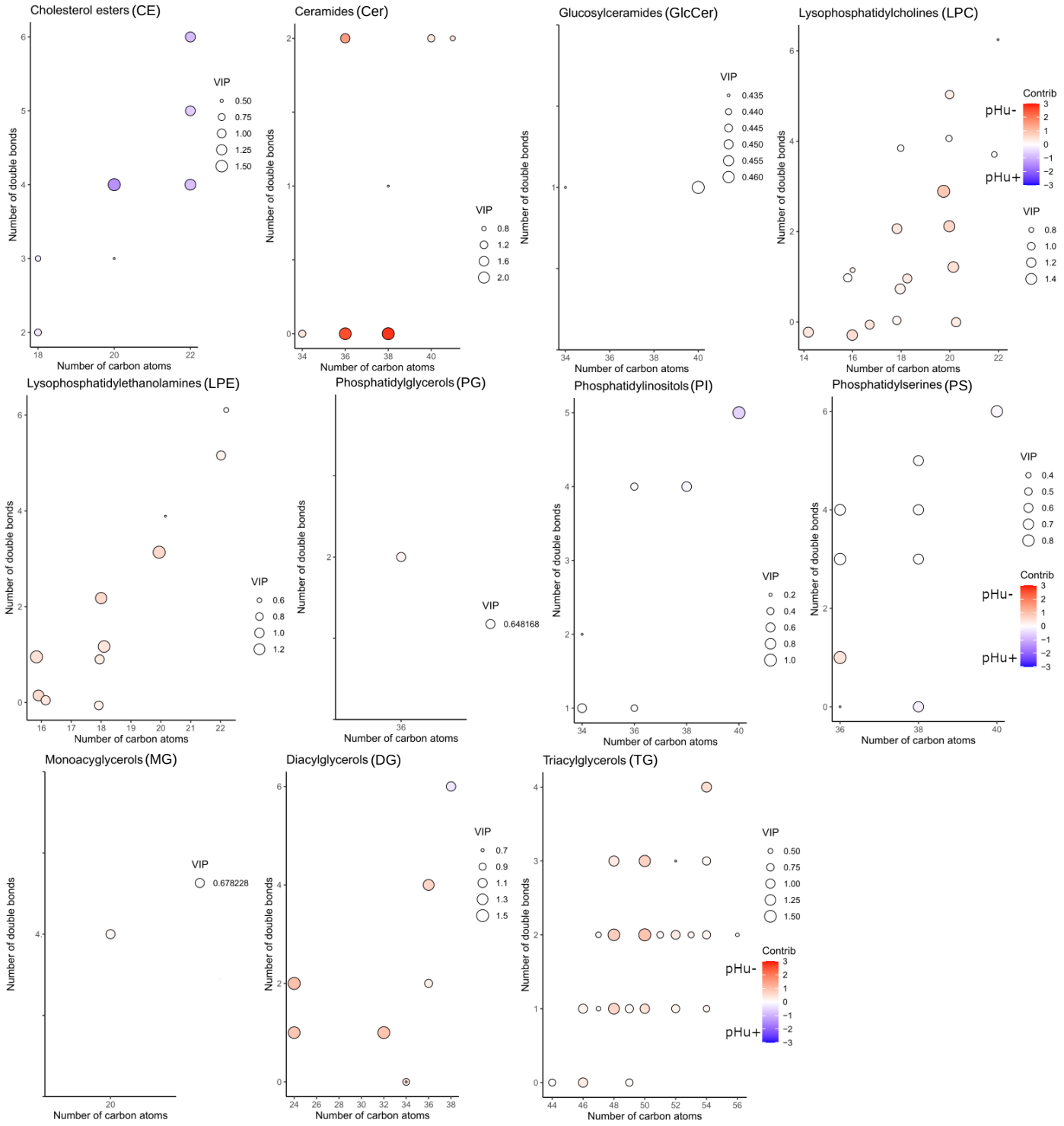

Figure S2. Relation between pHu lines, total number of carbon atoms and degree of unsaturation of acyl chains of the lipids. The importance of the lipids in the OPLS-DA model M1a (VIP) was represented by the size of the circle and the contribution to the pHu– or pHu+ lines was visualized through a gradient going from red (pHu–) to blue (pHu+). The characteristics of the M1a OPLS-DA model are 1 predictive and 3 orthogonal components, $R^2Y_{(cum)} = 0.74$ and $Q^2_{(cum)} = 0.56$. Position jitter was introduced in the LPC and LPE plots to avoid overplotting.

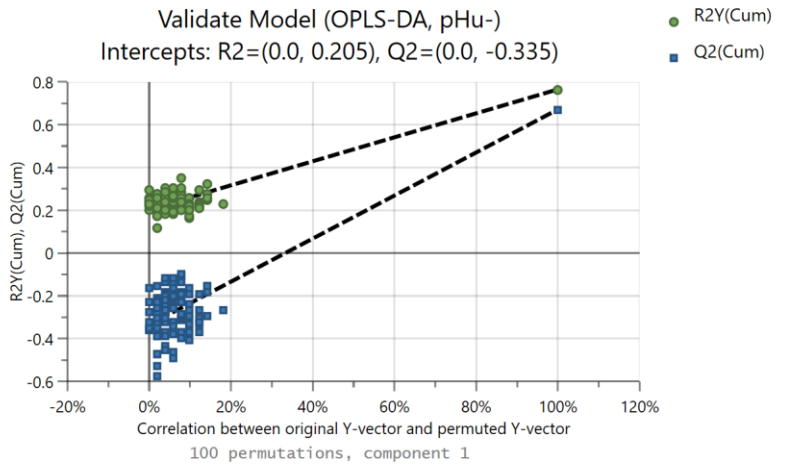

Figure S3. Permutation plot for the OPLS-DA model M1b (pHu lines). The permutation plot check the validity and the degree of overfit for the model. The plot displays the correlation coefficient between the original y-variable (i.e. pHu+ or pHu–) and the permuted y-variable on the x-axis versus the cumulative R^2 and Q^2 on the y-axis, and draws the regression line. The intercept is a measure of the overfit.

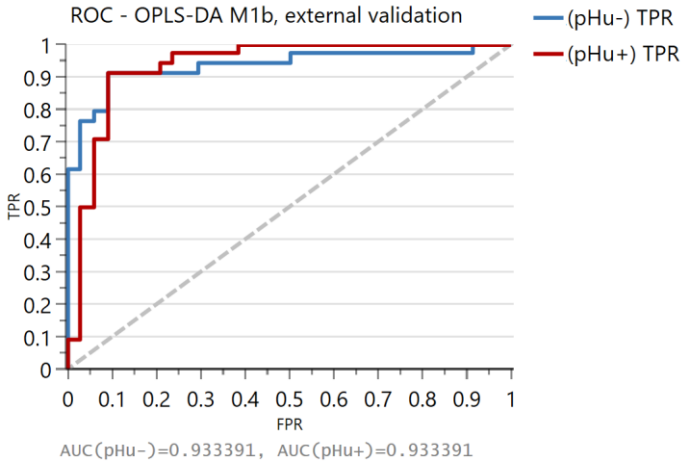

Figure S4. ROC curve external validation OPLS-DA model M1b (pHu lines). The ROC curve is a tool for visualizing and summarizing the performance of classification and discrimination models. The plot displays the true positive classification rate (TPR) of a classifier model plotted against the corresponding false positive classification rate (FPR) at various threshold settings of the criterion parameter Y predicted.
As a quantitative measure of the classification success the area under the ROC curve (AUC) is computed. This parameter ranges between 0.5 (bad classification) and 1.0 (perfect classification).

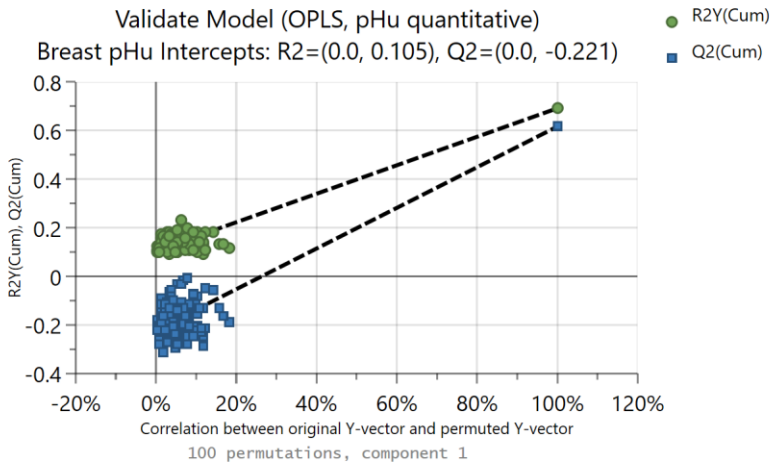

Figure S5. Permutation plot for the OPLS model M4 (pHu value). The permutation plot check the validity and the degree of overfit for the model. The plot displays the correlation coefficient between the original y-variable (i.e. pHu) and the permuted y-variable on the x-axis versus the cumulative R^2 and Q^2 on the y-axis, and draws the regression line. The intercept is a measure of the overfit.

Model OPLS-DA (Line; M1b)	VIP
Mode +_Cer(d18:0/20:0)	1.85969
Mode -_PE(P-18:0/20:4)	1.81344
Mode +_Cer(d18:0/18:0)	1.72967
Mode +_CE(20:4)	1.5651
Mode +_TG(16:0/16:1/18:1)	1.47464
Mode +_Cer(d18:1/18:1)	1.47063
Mode +_SM(34:0)	1.39926
Mode -_PE(O-16:0/18:1)	1.39021
Mode +_LPC(20:3)	1.37123
Mode +_SM(36:0)	1.26038
Mode -_PE(18:2/18:2)	1.25731
Mode +_CE(22:6)	1.235
Mode -_PE(20:1/20:4)	1.21721
Mode +_LPC(16:0)	1.2061
Mode +_SM(34:2)	1.1958
Mode +_PE(16:1/16:0)	1.18038
Mode +_LPC(18:1)	1.1636
Mode -_PI(18:1/22:4)	1.13942
Mode +_LPC(17:0)	1.12518
Mode +_TG(18:1/18:1/18:2)	1.11379
Mode +_Cer(d18:0/16:0)	1.02471
Mode -_PE(22:4/18:0)	1.01434
Mode -_PC(18:0/18:1)	1.00386
Mode +_DG(18:2/20:4)	1.00089
Mode +_LPC(16:1)	0.998122
Mode +_SM(d18:1/24:0)	0.996711
Mode +_PE(34:2)	0.983252
Mode +_SM(38:3)	0.974077
Mode +_PC(O-22:0)	0.957509
Mode +_LPC(20:4)	0.942643
Mode +_CE(18:2)	0.922736
Mode +_PC(O-34:0)	0.895652
Mode +_SM(42:3)	0.889393
Mode +_PC(32:2)	0.887753
Mode +_CE(18:3)	0.886779
Mode -_PS(18:1/20:2)	0.878176
Mode -_PC(18:1/22:6)	0.877409
Mode -_PE(16:0/18:2)	0.872093
Mode +_PC(18:1/19:0)	0.832525
Mode -_PS(16:1/20:0)	0.82469
Mode +_LPC(18:4)	0.821205
Mode +_TG(16:0/18:0/18:1)	0.818968
Mode +_SM(d18:2/18:0)	0.814218
Mode -_PE(P-18:0/20:2)	0.802684
Mode +_PE(P-18:0/18:2)	0.795111
Mode +_Cer(d18:2/23:0)	0.752075
Mode +_TG(18:0/18:1/18:1)	0.747223
Mode +_PE(P-16:0/22:6)	0.72382
Mode -_LysoPE(22:5)	0.719258
Mode +_PE(P-16:0/18:2)	0.713559
Mode -_PC(O-16:0/22:5)	0.707875
Mode -_PS(18:2/18:2)	0.706873
Mode +_TG(18:0/18:0/18:1)	0.698659
Mode +_PC(O-18:0/18:2)	0.676071
Mode -_PE(P-16:0/22:4)	0.675426
Mode +_SM(d18:1/20:0)	0.674651
Mode +_Cer(d18:1/20:0)	0.645368
Mode +_DG(18:0/16:0)	0.634939
Mode -_PC(O-18:1/18:2)	0.618063
Mode +_TG(16:0/18:1/19:1)	0.617894
Mode +_TG(13:0/16:1/18:1)	0.602118
Mode -_PC(18:0/20:2)	0.584381
Mode -_PE(16:0/20:4)	0.579373
Mode +_GlcCer(d18:1/22:0)	0.573233
Mode -_PE(20:5/18:1)	0.494819
Mode +_SM(30:1)	0.480349
Mode +_TG(16:1/18:1/18:1)	0.472926
Mode -_PS(16:0/20:0)	0.360961

Model OPLS (pHu value; M4)	VIP
Mode +_Cer(d18:0/20:0)	1.81235
Mode +_Cer(d18:0/18:0)	1.64782
Mode -_PE(P-18:0/20:4)	1.5795
Mode +_SM(34:0)	1.54753
Mode +_SM(36:0)	1.34
Mode +_LPC(20:3)	1.32623
Mode -_PE(18:2/18:2)	1.31264
Mode +_CE(20:4)	1.24836
Mode +_LPC(18:1)	1.18537
Mode +_Cer(d18:1/18:1)	1.18377
Mode +_Cer(d18:0/16:0)	1.13775
Mode +_LPC(17:0)	1.1304
Mode -_PE(O-16:0/18:1)	1.06487
Mode +_LPC(16:1)	1.06285
Mode +_TG(18:1/18:1/18:2)	1.02736
Mode +_PC(O-34:0)	0.964985
Mode +_SM(d18:2/18:0)	0.902723
Mode +_LPC(18:4)	0.898271
Mode +_PC(O-18:0/18:2)	0.891276
Mode +_SM(d18:1/20:0)	0.883637
Mode -_PE(20:1/20:4)	0.879974
Mode -_PC(18:1/22:6)	0.875134
Mode +_PC(32:2)	0.860301
Mode +_PE(P-16:0/22:6)	0.827999
Mode +_PE(P-18:0/18:2)	0.813128
Mode -_PC(18:0/18:1)	0.810042
Mode -_PS(16:1/20:0)	0.807613
Mode +_PE(P-16:0/18:2)	0.746543
Mode +_TG(18:0/18:1/18:2)	0.740285
Mode -_PE(P-16:0/20:3)	0.650669
Mode +_DG(18:0/16:0)	0.646717
Mode +_TG(16:0/18:1/19:1)	0.611252
Mode -_LysoPE(22:5)	0.59722
Mode +_PC(18:1/19:0)	0.568204
Mode +_TG(13:0/16:1/18:1)	0.543889
Mode -_PC(O-18:1/18:2)	0.543648
Mode +_CE(18:2)	0.525974
Mode -_PC(16:1/20:4)	0.505816
Mode +_CE(18:3)	0.469835
Mode +_TG(16:1/18:1/18:1)	0.410329

Table S3. Comparison between the lipid sets included in the model OPLS-DA predictive of the pHu lines (M1b) and the model OPLS predictive of the pHu value (M2). The lipids were ordered according their importance in the model (VIP) and highlighted in red when they were present in both models.