

Supplementary Materials

Table S1. The detailed results of differential lipid molecules in BF vs. PM, PM vs. LD and LD vs. BF

Lipid molecules	Formula	RT (min)	CalMz	FC	p-value	VIP
BF vs. PM						
PC (16:0/16:1)	C39H75O8N1P1	9.968	716.523	0.662	0.045	2.270
PC (18:0e/18:2)	C45H87O9N1P1	10.409	816.612	0.746	0.048	1.501
PS (17:1/18:0)	C41H77O10N1P1	9.148	774.529	0.732	0.041	1.104
PS (18:1e/18:1)	C42H79O9N1P1	10.179	772.550	0.559	0.034	1.618
PS (18:0/20:3)	C44H79O10N1P1	11.100	812.545	0.641	0.044	2.432
PS (18:0/22:5)	C46H79O10N1P1	8.687	836.545	1.339	0.013	1.735
Hex1Cer (d32:2)	C39H72O10N1	9.059	714.516	0.720	0.035	1.026
LPC (18:1)	C27H53O9N1P1	1.947	566.346	0.725	0.013	2.167
LPE (18:1)	C23H45O7N1P1	2.076	478.294	0.759	0.048	1.565
PC (15:0/22:6)	C46H79O10N1P1	8.687	836.545	1.362	0.005	1.350
PC (16:0/22:5)	C47H83O10N1P1	9.178	852.576	7.202	0.012	5.603
PE (17:0/18:1)	C40H77O8N1P1	10.536	730.539	0.626	0.025	1.427
PE (18:0/18:1)	C41H79O8N1P1	11.102	744.555	0.582	0.026	5.759
PE (18:1/18:1)	C41H77O8N1P1	10.071	742.539	0.563	0.016	4.221
PE (18:2/18:2)	C41H73O8N1P1	8.340	738.508	0.556	0.031	1.036
PG (16:0/18:1)	C40H76O10N0P1	8.629	747.518	0.766	0.017	1.757
PI (16:0/20:4)	C45H78O13N0P1	7.339	857.519	1.694	0.009	1.004
PC (25:0/11:3)	C44H82O8N1P1Na1	7.805	806.567	2.653	0.014	1.789
PE (16:1e/18:1)	C39 H76 O7 N1 P1 Na1	9.657	724.525	0.168	0.001	7.808
PC (31:1)	C39H77O8N1P1	9.991	718.538	0.611	0.028	1.011
PM vs. LD						
PC (36:4e)	C44H83O7N1P1	8.422	768.590	0.633	0.012	1.587
PE (8:1e/12:3)	C25H45O7N1P1	1.619	502.293	1.362	0.034	1.029
SM (t37:2)	C42H84O7N2P1	9.646	759.601	0.074	0.009	1.085
TG (12:0e/12:0/12:1)	C39H74O5Na1	12.953	645.542	1.558	0.002	1.068
TG (12:0e/10:1/14:1)	C39H72O5Na1	11.939	643.527	1.902	0.002	1.076
TG (18:3e/6:0/12:1)	C39H69O5	11.87	617.514	1.571	0.014	1.062
TG (18:2e/6:0/14:2)	C41H73O5	12.953	645.545	1.565	0.002	1.076
TG (16:0/10:0/14:0)	C43H86O6N1	5.09	712.644	1.952	0.019	2.263
TG (16:0/10:0/16:0)	C45H90O6N1	15.534	740.676	1.937	0.016	2.889
DG (26:2e)	C29H55O4	15.540	467.409	2.264	0.010	1.196
DG (28:2e)	C31H59O4	16.028	495.441	1.908	0.020	1.048
DG (32:3e)	C35H65O4	16.019	549.488	1.725	0.036	1.026
DG (34:1e)	C37H72O4Na1	17.019	603.532	1.554	0.006	1.593

Table S1. The detailed results of differential lipid molecules in BF vs. PM, PM vs. LD and LD vs. BF (continued)

Lipid molecules	Formula	RT (min)	CalMz	FC	p-value	VIP
DG (34:3e)	C37H69O4	16.701	577.519	1.244	0.031	1.304
DG (34:4e)	C37H67O4	16.474	575.503	1.396	0.009	1.416
DG (22:0/14:2)	C39H76O5N1	11.938	638.572	1.815	0.004	1.149
Hex1Cer (d32:1)	C38H77O8N2	14.177	689.567	2.172	0.009	1.385
Hex1Cer (d40:3)	C46H89O8N2	15.556	797.661	1.364	0.027	1.589
Hex1Cer (d22:0/22:0+O)	C50H103O9N2	14.798	875.765	2.123	0.028	1.398
Hex1Cer (d21:2_23:0+O)	C50H99O9N2	15.103	871.734	1.828	0.047	1.624
LD vs. BF						
CL (18:2/16:1/18:2/18:2)	C79H139O17P2	14.809	1,421.949	1.742	0.017	4.765
CL (18:3/18:2/16:1/18:2)	C79H137O17P2	14.308	1,419.933	0.891	0.026	3.343
LPC (16:0)	C25H51O9N1P1	1.957	540.330	1.341	0.001	1.106
PE (18:0/18:1)	C41H79O8N1P1	11.101	744.554	1.172	0.036	3.378
PI (16:0/20:4)	C45H78O13N0P1	7.338	857.518	0.986	0.011	2.607
PI (18:0/20:1)	C47H88O13N0P1	10.444	891.596	0.685	0.024	1.072
Co (Q10)	C59H94O4N1	15.460	880.717	1.639	0.032	5.571
PI (18:0/22:1)	C49H92O13N0P1	11.412	919.628	2.315	0.022	1.427
PI (18:0/24:1)	C51H96O13N0P1	12.370	947.659	0.779	0.047	2.607
PI (18:0/17:0)	C44H84O13N0P1	9.691	851.565	0.985	0.012	1.072
CL (18:3/16:1/20:4/16:1)	C79H135O17P2	13.773	1,417.918	1.441	0.042	3.421
CL (18:3/18:2/20:3/15:0)	C80H139O17P2	14.653	1,433.949	1.726	0.037	1.025
PI (18:0/23:1)	C50H94O13N0P1	11.887	933.643	1.662	0.008	3.915
CL (82:4)	C91H171O17P2	10.787	1,598.198	1.448	0.049	1.103
CL (82:6)	C91H167O17P2	9.771	1,594.167	2.567	0.025	2.341
SM (t36:0)	C41H86O7N2P1	8.975	749.616	2.317	0.012	1.892
SM (t37:2)	C42H84O7N2P1	9.646	759.601	1.809	0.005	5.351
SM (t38:4)	C43H82O7N2P1	8.722	769.585	1.646	0.016	1.037
SM (t38:5)	C43H80O7N2P1	9.45	767.569	0.985	0.033	4.647
SM (t41:6)	C46H84O7N2P1	9.646	807.601	1.758	0.032	1.327

OPLS-DA VIP>1 and p-value<0.05.

RT, retention time; FC, fold change; VIP, variable importance in projection.