

Table S2 Differences in lipid species in CD patients before EEN and healthy controls

Lipid ion	Classes	Ion formula	Fold change	P value	VIP
ChE(18:2)+NH ₄	ChE	C45 H80 O2 N1	0.59	<0.001	2.35
SM(d34:1)+H	SM	C39 H80 O6 N2 P1	0.85	0.025	2.09
PC(34:2p)+H	PC	C42 H81 O7 N1 P1	0.45	<0.001	2.02
PC(33:2)+H	PC	C41 H79 O8 N1 P1	0.36	<0.001	1.01
PC(34:2e)+H	PC	C42 H83 O7 N1 P1	0.27	<0.001	2.49
PE(18:0p/20:4)+H	PE	C43 H79 O7 N1 P1	0.32	<0.001	1.25
PC(34:2)+H	PC	C42 H81 O8 N1 P1	0.74	<0.001	5.20
PC(36:4p)+H	PC	C44 H81 O7 N1 P1	0.66	0.001	1.46
PC(36:4e)+H	PC	C44 H83 O7 N1 P1	0.47	<0.001	1.31
PC(36:4e)+H	PC	C44 H83 O7 N1 P1	0.53	<0.001	2.49
PC(36:2p)+H	PC	C44 H85 O7 N1 P1	0.40	<0.001	1.22
PC(35:2)+H	PC	C43 H83 O8 N1 P1	0.45	<0.001	1.48
PC(36:2e)+H	PC	C44 H87 O7 N1 P1	0.33	<0.001	1.17
PC(36:4)+H	PC	C44 H81 O8 N1 P1	0.38	<0.001	1.61
PC(36:4)+H	PC	C44 H81 O8 N1 P1	0.22	<0.001	4.26
SM(d40:2)+H	SM	C45 H90 O6 N2 P1	0.53	<0.001	1.75
PC(36:2)+H	PC	C44 H85 O8 N1 P1	0.66	<0.001	6.28
SM(d40:1)+H	SM	C45 H92 O6 N2 P1	0.64	<0.001	1.91
LPC(16:0)+H	LPC	C24 H51 O7 N1 P1	0.55	<0.001	3.28
PC(38:4p)+H	PC	C46 H85 O7 N1 P1	0.75	0.011	1.25
PC(36:1e)+Na	PC	C44 H88 O7 N1 P1 Na1	0.61	0.001	1.10
SM(d41:1)+H	SM	C46 H94 O6 N2 P1	0.51	<0.001	1.19
PC(16:0/22:6)+H	PC	C46 H81 O8 N1 P1	0.71	0.017	1.89
PC(38:6)+H	PC	C46 H81 O8 N1 P1	0.36	<0.001	1.74
SM(d42:2)+H	SM	C47 H94 O6 N2 P1	1.25	0.017	3.56
SM(d42:1)+H	SM	C47 H96 O6 N2 P1	0.53	<0.001	1.77
PC(40:7)+H	PC	C48 H83 O8 N1 P1	1.25	0.003	1.15
SM(d44:6)+H	SM	C49 H90 O6 N2 P1	1.29	0.001	1.33
SM(d44:5)+H	SM	C49 H92 O6 N2 P1	1.17	<0.001	1.63
SM(d42:2)+Na	SM	C47 H93 O6 N2 P1 Na1	0.58	<0.001	1.10
SM(d44:4)+H	SM	C49 H94 O6 N2 P1	0.55	<0.001	1.15
LPC(18:2)+H	LPC	C26 H51 O7 N1 P1	0.32	<0.001	3.16
LPC(18:1)+H	LPC	C26 H53 O7 N1 P1	0.57	<0.001	1.44
LPC(18:0)+H	LPC	C26 H55 O7 N1 P1	0.48	<0.001	2.38
TG(18:1/18:1/20:3)+NH ₄	TG	C59 H108 O6 N1	1.48	0.030	1.50
LPC(18:2)+Na	LPC	C26 H50 O7 N1 P1 Na1	0.31	<0.001	1.42

LPE(18:2)-H	LPE	C23 H43 O7 N1 P1	0.47	<0.001	1.07
LPC(16:0)+HCOO	LPC	C25 H51 O9 N1 P1	0.60	<0.001	3.53
LPC(18:2)+HCOO	LPC	C27 H51 O9 N1 P1	0.35	<0.001	4.51
LPC(18:1)+HCOO	LPC	C27 H53 O9 N1 P1	0.60	<0.001	1.67
LPC(18:0)+HCOO	LPC	C27 H55 O9 N1 P1	0.52	<0.001	3.30
Cer(d18:1/16:0)+HCOO	Cer	C35 H68 O5 N1	1.20	0.020	1.38
LPC(20:3)+H	LPC	C28 H53 O7 N1 P1	0.44	<0.001	1.17
Cer(d18:1/24:0)+HCOO	Cer	C43 H84 O5 N1	0.53	<0.001	2.28
PE(34:2p)-H	PE	C39 H73 O7 N1 P1	0.24	<0.001	1.78
SM(d16:0/16:1)+HCOO	SM	C38 H76 O8 N2 P1	0.49	<0.001	1.41
PE(36:4p)-H	PE	C41 H73 O7 N1 P1	0.37	<0.001	2.70
PE(36:3p)-H	PE	C41 H75 O7 N1 P1	0.33	<0.001	1.30
PE(36:2p)-H	PE	C41 H77 O7 N1 P1	0.26	<0.001	2.40
PE(16:0/20:4)-H	PE	C41 H73 O8 N1 P1	1.63	<0.001	1.66
PE(18:0/18:1)-H	PE	C41 H79 O8 N1 P1	1.52	0.007	1.02
PE(16:0p/22:6)-H	PE	C43 H73 O7 N1 P1	0.44	<0.001	1.60
PE(18:0p/20:5)-H	PE	C43 H75 O7 N1 P1	0.34	<0.001	2.71
PE(16:0p/22:5)-H	PE	C43 H75 O7 N1 P1	0.33	<0.001	1.29
PE(38:4p)-H	PE	C43 H77 O7 N1 P1	0.33	<0.001	3.60
PE(18:0/20:4)-H	PE	C43 H77 O8 N1 P1	1.61	0.001	2.96
PE(18:1p/22:6)-H	PE	C45 H75 O7 N1 P1	0.43	<0.001	1.16
PC(14:0/18:2)+HCOO	PC	C41 H77 O10 N1 P1	0.32	0.001	1.28
PE(18:0p/22:6)-H	PE	C45 H77 O7 N1 P1	0.40	<0.001	1.57
SM(d20:0/16:0)+HCOO	SM	C42 H86 O8 N2 P1	1.71	0.007	1.02
PC(16:0p/18:2)+HCOO	PC	C43 H81 O9 N1 P1	0.48	<0.001	1.82
PC(16:0e/18:2)+HCOO	PC	C43 H83 O9 N1 P1	0.31	<0.001	2.22
PS(37:1)-H	PS	C43 H81 O10 N1 P1	0.72	<0.001	1.52
PC(16:0p/20:3)+HCOO	PC	C45 H83 O9 N1 P1	0.58	<0.001	1.80
PS(38:1)-H	PS	C44 H83 O10 N1 P1	0.49	<0.001	1.36
SM(d39:1)+HCOO	SM	C45 H90 O8 N2 P1	0.50	<0.001	1.07
PC(18:2/18:2)+HCOO	PC	C45 H81 O10 N1 P1	0.41	<0.001	1.37
PS(39:3)-H	PS	C45 H81 O10 N1 P1	0.27	<0.001	4.31
SM(d20:0/20:3)+HCOO	SM	C46 H88 O8 N2 P1	1.50	<0.001	1.11
SM(d22:0/18:2)+HCOO	SM	C46 H90 O8 N2 P1	0.59	<0.001	1.92
PC(18:1/18:1)+HCOO	PC	C45 H85 O10 N1 P1	0.65	<0.001	5.04
SM(d22:0/18:1)+HCOO	SM	C46 H92 O8 N2 P1	0.68	<0.001	1.65
SM(d41:2)+HCOO	SM	C47 H92 O8 N2 P1	0.57	<0.001	1.24
SM(d41:1)+HCOO	SM	C47 H94 O8 N2 P1	0.56	<0.001	1.67
PC(18:2/20:4)+HCOO	PC	C47 H81 O10 N1 P1	0.41	<0.001	1.84
SM(d24:0/18:2)+HCOO	SM	C48 H94 O8 N2 P1	1.26	0.002	6.46
SM(d42:1)+HCOO	SM	C48 H96 O8 N2 P1	0.61	<0.001	2.05
PI(18:1/18:1)-H	PI	C45 H82 O13 N0 P1	0.66	0.022	1.52

MGDG(43:10)-H	MG DG	C52 H79 O10	0.38	<0.001	1.36
PI(18:0/20:4)-H	PI	C47 H82 O13 N0 P1	0.81	0.044	1.67

CD, Crohn's disease; Cer, ceramide; ChE, cholesterol ester; EEN, exclusive enteral nutrition; LPC, lysophosphatidylcholine; MGDG, monogalactosyldiacylglycerol; PC, phosphatidylcholine; PE, phosphatidylethanolamine; PI, phosphatidylinositol; PS, phosphatidylserine; SM, sphingomyelin; TG, triglyceride; VIP, variable importance in the projection.