

Table S3 Differences in lipid species in CD patients after EEN and healthy controls

Lipid ion	Class	Ion formula	Fold change	P value	VIP
ChE(18:2)+NH4	ChE	C45 H80 O2 N1	0.52	<0.001	2.43
ChE(20:4)+NH4	ChE	C47 H80 O2 N1	0.59	<0.001	1.25
SM(d34:1)+H	SM	C39 H80 O6 N2 P1	0.88	0.010	1.81
PC(32:1)+H	PC	C40 H79 O8 N1 P1	4.49	0.001	4.16
PC(32:0)+H	PC	C40 H81 O8 N1 P1	1.16	0.026	1.04
PC(34:2p)+H	PC	C42 H81 O7 N1 P1	0.40	<0.001	1.88
PC(34:2e)+H	PC	C42 H83 O7 N1 P1	0.34	<0.001	1.90
PC(33:1)+H	PC	C41 H81 O8 N1 P1	2.55	0.017	1.09
PE(18:0p/20:4)+H	PE	C43 H79 O7 N1 P1	0.24	<0.001	1.16
PC(34:3)+H	PC	C42 H79 O8 N1 P1	2.76	0.030	1.26
PC(34:2)+H	PC	C42 H81 O8 N1 P1	0.81	<0.001	4.92
SM(d38:1)+H	SM	C43 H88 O6 N2 P1	0.72	<0.001	1.01
PC(34:1)+H	PC	C42 H83 O8 N1 P1	1.28	0.034	4.71
PC(36:4p)+H	PC	C44 H81 O7 N1 P1	0.48	<0.001	1.90
PC(36:4e)+H	PC	C44 H83 O7 N1 P1	0.47	<0.001	1.15
PC(36:4e)+H	PC	C44 H83 O7 N1 P1	0.53	<0.001	2.23
PC(35:2)+H	PC	C43 H83 O8 N1 P1	0.57	<0.001	1.11
PC(34:1)+Na	PC	C42 H82 O8 N1 P1 Na1	0.84	0.018	3.43
PC(36:4)+H	PC	C44 H81 O8 N1 P1	0.29	<0.001	3.25
PC(36:3)+H	PC	C44 H83 O8 N1 P1	5.11	0.001	4.59
SM(d40:2)+H	SM	C45 H90 O6 N2 P1	0.55	<0.001	1.66
PC(36:2)+H	PC	C44 H85 O8 N1 P1	0.66	<0.001	5.85
SM(d40:1)+H	SM	C45 H92 O6 N2 P1	0.62	<0.001	2.00
PC(36:1)+H	PC	C44 H87 O8 N1 P1	1.52	0.033	3.04
LPC(16:0)+H	LPC	C24 H51 O7 N1 P1	0.82	0.030	1.70
PC(38:6e)+H	PC	C46 H83 O7 N1 P1	0.48	<0.001	1.03
PC(18:1p/18:0)+Na	PC	C44 H86 O7 N1 P1 Na1	0.37	<0.001	1.03
PC(38:4p)+H	PC	C46 H85 O7 N1 P1	0.58	<0.001	1.74
PC(36:1e)+Na	PC	C44 H88 O7 N1 P1 Na1	0.50	<0.001	1.30
SM(d41:1)+H	SM	C46 H94 O6 N2 P1	0.49	<0.001	1.16
PC(16:0/22:6)+H	PC	C46 H81 O8 N1 P1	4.76	0.001	1.13
PC(16:0/22:6)+H	PC	C46 H81 O8 N1 P1	0.55	<0.001	3.44
PC(38:6)+H	PC	C46 H81 O8 N1 P1	0.36	<0.001	1.49
PC(38:5)+H	PC	C46 H83 O8 N1 P1	0.83	0.017	1.55
PC(38:3)+H	PC	C46 H87 O8 N1 P1	5.12	0.003	2.80
SM(d42:1)+H	SM	C47 H96 O6 N2 P1	0.53	<0.001	1.70
TG(16:0/14:0/18:2)+NH4	TG	C51 H98 O6 N1	3.03	0.017	2.72
TG(16:0/16:0/16:1)+NH4	TG	C51 H100 O6 N1	2.96	0.033	3.30
TG(16:0/16:0/16:0)+NH4	TG	C51 H102 O6 N1	2.43	0.023	1.57
PC(40:6)+H	PC	C48 H85 O8 N1 P1	0.54	0.002	1.98

PC(40:6)+H	PC	C48 H85 O8 N1 P1	5.82	0.001	1.14
SM(d42:2)+Na	SM	C47 H93 O6 N2 P1 Na1	0.62	<0.001	1.04
SM(d44:4)+H	SM	C49 H94 O6 N2 P1	0.56	<0.001	1.09
TG(16:0/16:1/18:1)+NH4	TG	C53 H102 O6 N1	2.78	0.004	5.47
TG(16:0/16:0/18:1)+NH4	TG	C53 H104 O6 N1	2.00	0.014	4.24
LPC(18:2)+H	LPC	C26 H51 O7 N1 P1	0.30	<0.001	2.72
LPC(18:0)+H	LPC	C26 H55 O7 N1 P1	0.57	<0.001	1.83
TG(18:1/18:1/20:3)+NH4	TG	C59 H108 O6 N1	1.76	0.015	1.04
LPC(18:2)+Na	LPC	C26 H50 O7 N1 P1 Na1	0.29	<0.001	1.22
LPC(16:1)+HCOO	LPC	C25 H49 O9 N1 P1	2.81	0.003	1.40
LPC(16:0)+HCOO	LPC	C25 H51 O9 N1 P1	0.85	0.043	1.46
LPC(18:2)+HCOO	LPC	C27 H51 O9 N1 P1	0.36	<0.001	3.96
LPC(18:0)+HCOO	LPC	C27 H55 O9 N1 P1	0.61	<0.001	2.46
LPC(20:4)+HCOO	LPC	C29 H51 O9 N1 P1	0.58	<0.001	1.13
Cer(d18:1/24:0)+HCOO	Cer	C43 H84 O5 N1	0.64	<0.001	1.94
PE(34:2p)-H	PE	C39 H73 O7 N1 P1	0.36	<0.001	1.26
PE(16:1/18:1)-H	PE	C39 H73 O8 N1 P1	2.66	<0.001	1.83
PE(16:0/18:1)-H	PE	C39 H75 O8 N1 P1	3.49	0.003	1.42
PE(36:4p)-H	PE	C41 H73 O7 N1 P1	0.37	<0.001	2.31
PE(36:2p)-H	PE	C41 H77 O7 N1 P1	0.31	<0.001	1.89
PE(16:0/20:4)-H	PE	C41 H73 O8 N1 P1	3.71	<0.001	2.19
PE(18:1/18:2)-H	PE	C41 H75 O8 N1 P1	1.83	0.016	1.04
PE(18:0/18:2)-H	PE	C41 H77 O8 N1 P1	1.47	0.019	1.65
PE(16:0p/22:6)-H	PE	C43 H73 O7 N1 P1	0.39	<0.001	1.58
SM(d16:0/18:1)+HCOO	SM	C40 H80 O8 N2 P1	0.91	0.025	2.07
PE(18:0p/20:5)-H	PE	C43 H75 O7 N1 P1	0.33	<0.001	2.39
PE(16:0p/22:5)-H	PE	C43 H75 O7 N1 P1	0.35	<0.001	1.09
PE(38:4p)-H	PE	C43 H77 O7 N1 P1	0.24	<0.001	3.58
PE(18:1/20:4)-H	PE	C43 H75 O8 N1 P1	2.42	0.001	1.11
PE(18:0/20:4)-H	PE	C43 H77 O8 N1 P1	1.89	0.001	2.32
PE(18:1p/22:6)-H	PE	C45 H75 O7 N1 P1	0.32	<0.001	1.18
PE(18:0p/22:6)-H	PE	C45 H77 O7 N1 P1	0.26	<0.001	1.68
PC(16:0/16:1)+HCOO	PC	C41 H79 O10 N1 P1	4.71	0.001	4.48
PC(16:0/16:0)+HCOO	PC	C41 H81 O10 N1 P1	1.16	0.016	1.55
PC(16:0p/18:2)+HCOO	PC	C43 H81 O9 N1 P1	0.41	<0.001	1.88
PC(16:0e/18:2)+HCOO	PC	C43 H83 O9 N1 P1	0.38	<0.001	1.68
PC(17:1/16:0)+HCOO	PC	C42 H81 O10 N1 P1	2.63	0.014	1.27
PS(37:1)-H	PS	C43 H81 O10 N1 P1	0.76	<0.001	5.16
SM(d20:0/18:1)+HCOO	SM	C44 H88 O8 N2 P1	0.75	<0.001	1.20
PC(16:0/18:1)+HCOO	PC	C43 H83 O10 N1 P1	1.40	0.015	7.48
PI(16:0/16:1)-H	PI	C41 H76 O13 N0 P1	11.25	<0.001	1.78
PC(16:0p/20:4)+HCOO	PC	C45 H81 O9 N1 P1	0.50	<0.001	1.73
PC(16:0p/20:3)+HCOO	PC	C45 H83 O9 N1 P1	0.55	<0.001	2.06

PS(38:1)-H	PS	C44 H83 O10 N1 P1	0.56	<0.001	1.12
PS(39:3)-H	PS	C45 H81 O10 N1 P1	0.34	<0.001	3.34
PS(39:2)-H	PS	C45 H83 O10 N1 P1	5.75	0.001	5.45
SM(d22:0/18:2)+HCOO	SM	C46 H90 O8 N2 P1	0.62	<0.001	2.06
PC(18:1/18:1)+HCOO	PC	C45 H85 O10 N1 P1	0.66	<0.001	5.74
SM(d22:0/18:1)+HCOO	SM	C46 H92 O8 N2 P1	0.67	<0.001	2.49
PC(18:0/18:1)+HCOO	PC	C45 H87 O10 N1 P1	1.58	0.022	4.17
PI(16:0/18:1)-H	PI	C43 H80 O13 N0 P1	2.51	0.005	2.38
PC(18:0p/20:4)+HCOO	PC	C47 H85 O9 N1 P1	0.61	<0.001	1.45
PC(18:0p/20:4)+HCOO	PC	C47 H85 O9 N1 P1	0.38	<0.001	1.07
PC(18:0p/20:3)+HCOO	PC	C47 H87 O9 N1 P1	0.52	<0.001	1.37
SM(d41:2)+HCOO	SM	C47 H92 O8 N2 P1	0.61	<0.001	1.16
SM(d41:1)+HCOO	SM	C47 H94 O8 N2 P1	0.56	<0.001	1.94
PC(18:2/20:4)+HCOO	PC	C47 H81 O10 N1 P1	0.40	<0.001	1.64
PC(16:0/22:6)+HCOO	PC	C47 H81 O10 N1 P1	0.58	<0.001	3.05
PI(16:0/20:3)-H	PI	C45 H80 O13 N0 P1	12.83	0.001	1.26
SM(d42:1)+HCOO	SM	C48 H96 O8 N2 P1	0.61	<0.001	2.50
PS(43:5)-H	PS	C49 H85 O10 N1 P1	0.60	0.008	1.65
PI(18:0/20:4)-H	PI	C47 H82 O13 N0 P1	0.77	0.018	1.59
PI(18:0/20:3)-H	PI	C47 H84 O13 N0 P1	11.35	0.007	2.24

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.