

SUPPLEMENTARY MATERIAL

Supplementary table 1. Characteristics of the study population

	Healthy controls n = 46	Only AD n = 30	AD with FA n = 82	P value	P value		
					Healthy controls vs only AD	Healthy controls vs AD with FA	only AD vs AD with FA
Male (%)	27 (58.7%)	19 (63.3%)	55 (67.1%)	0.637‡	0.686	0.343	0.711
Parental history of allergic disease (%)	19 (41.3%)	19 (63.3%)	63 (76.8%)	< 0.001‡	0.060‡	< 0.001‡	0.153‡
Feeding type (%)							
Breast feeding	3 (6.5%)	4 (13.3%)	38 (46.3%)	<0.001 ^a	0.049 ^a	< 0.010 ^a	<0.001 ^a
Mixed Feeding	43 (93.5%)	23 (76.7%)	33 (40.3%)				
Bottle feeding	0	3 (10%)	11 (13.4%)				
Delivery mode (%)							
Vaginal	26 (56.5%)	25 (83.3%)	52 (63.4%)	0.050‡	0.015‡	0.443‡	0.044‡
Cesarean section	20 (43.5%)	5 (16.7%)	30 (36.6%)				
SCORAD index	-	15.28 ± 2.24	26.33 ± 1.65	-	-	-	< 0.001†
Total IgE (kU/L)	27.62 ± 5.79	114.65 ± 66.82	245.75 ± 85.95	< 0.001*	0.120	< 0.001	< 0.001
Specific IgE to egg white (kU/L)	0.07 ± 0.01	2.64 ± 1.87	14.60 ± 2.35	< 0.001*	0.048	< 0.001	< 0.001
Specific IgE to cow's milk (kU/L)	0.09±0.01	0.15±0.04	4.87±1.82	< 0.001*	0.307	< 0.001	< 0.001
Eosinophil (%)	2.32±0.21	4.74±0.78	6.4±0.43	< 0.001*	0.001	< 0.001	0.013

*Kruskal-Wallis test, ‡chi square test, †Mann-Whitney *U* test, ^aFisher's exact test

Supplementary table 2. MRM transitions and ion source conditions for target lipidome

LC-MS/MS	Lipids	LC	MRM transitions		MS parameters			
		RT (min)	Q1 (Da)	Q3 (Da)	DP(V)	EP(V)	CE(V)	CXP(V)
Agilent1290 /Qtrap5500	C14 Ceramide	11.6	510.324	492.4	66	10	15	30
	C16 Ceramide	13.2	538.356	520.4	66	10	15	34
	C18 Ceramide	15.4	566.288	548.4	66	10	17	36
	C18:1 Ceramide	13.6	564.417	546.4	66	10	15	34
	C20 Ceramide	18.0	594.379	576.5	66	10	17	42
	C24 Ceramide	22.0	650.471	632.5	66	10	19	34
	C24:1 Ceramide	20.0	648.475	630.5	66	10	19	46
	C17 Ceramide (IS)	14.2	552.362	534.4	66	10	15	36
	18:0 Sphingomyelin	11.3	731.521	184.1	66	10	31	12
	18:1 Sphingomyelin	10.3	729.497	85.9	66	10	85	10
	16:0 Sphingomyelin	10.0	703.466	86.1	66	10	87	10
	24:0 Sphingomyelin	17.2	815.667	184.1	66	10	37	18
	24:1 Sphingomyelin	14.5	813.709	184.1	66	10	35	16
	Sphinganine	3.6	302.218	284.2	66	10	19	22
	Sphingosine	3.4	300.195	282.3	66	10	15	20
	C16:0/16:0 DAG	4.2	569.341	313.1	80	8	15	15
	C16:0/18:1 DAG	4.2	595.333	339.1	80	8	15	20
	C18:0/C18:0 DAG	5.2	625.447	341.2	80	8	13	28
	C18:1/18:1 DAG	4.1	621.367	339.2	80	8	15	15
	C18:0/18:2 DAG	4.2	621.34	337.2	80	8	25	15
C18:0/20:4 DAG	4.3	645.396	341.1	80	8	25	10	
C19:0/19:0 DAG (IS)	6.0	658.578	640.5	80	8	15	15	
Ultimate3000 /LTQ-Orbtrap XL		LC	PRM transitions		MS parameters			
	Lipids	RT (min)	Q1 (Da)	Q3 (Da)	HCD	Mass accuracy (ppm)		
	S1P	4.71	378.2409	78.9585	50	10		
	S1P-C17 (IS)	4.48	364.2253	78.9585	50	10		

MRM, multiple reaction monitoring; DP, declustering potential; EP, entrance potential; CE, collision energy; CXP, collision exit potential; PRM, parallel reaction monitoring; HCD, high energy collision dissociation; DAG, diacylglycerol; S1P, sphingosine 1-phosphate; IS, internal standard