

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