SUPPLEMENTAL MATERIAL:

Effects of atopic dermatitis and gender on sebum lipid mediator and fatty acid profiles

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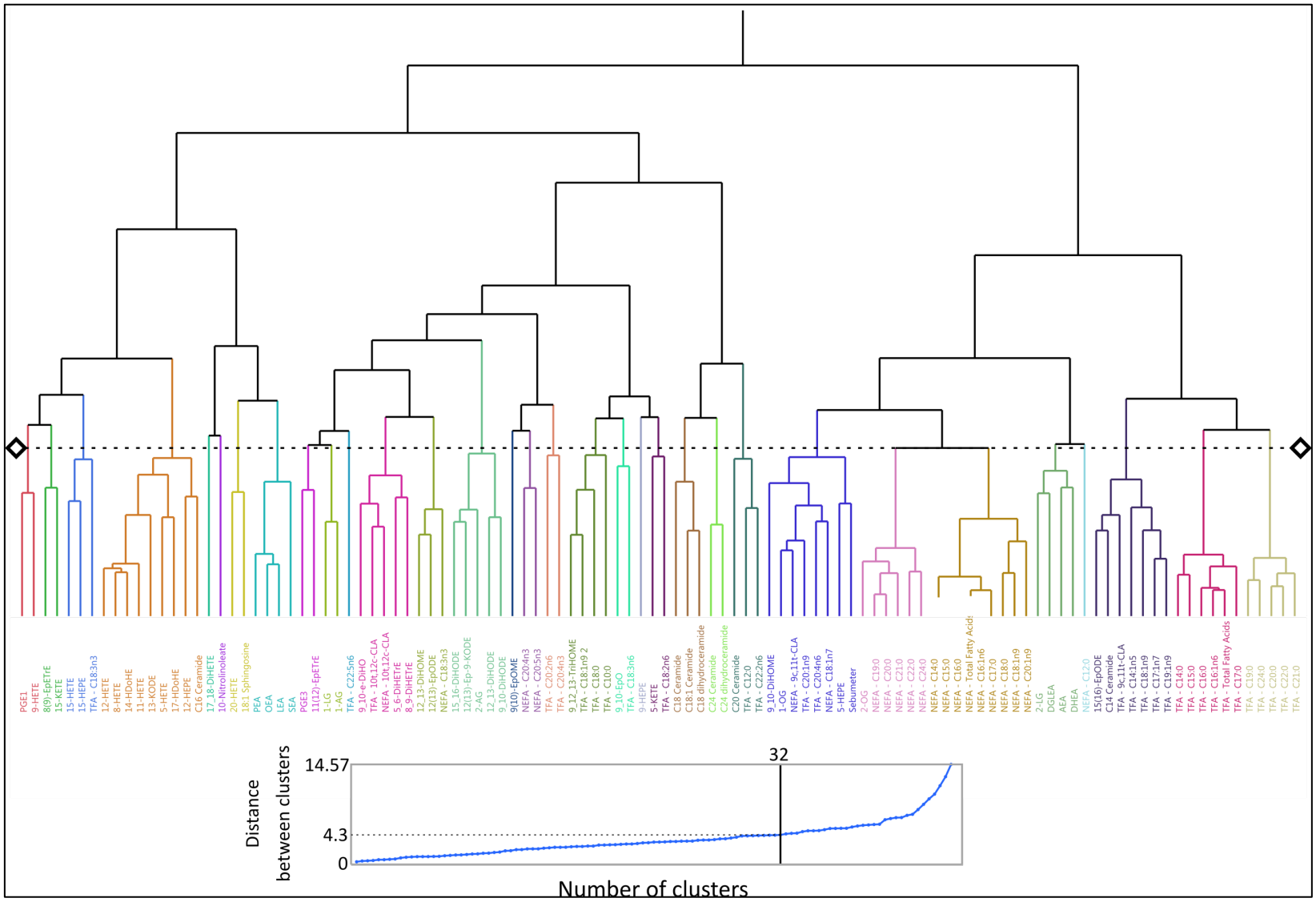
Supplemental Figure S1

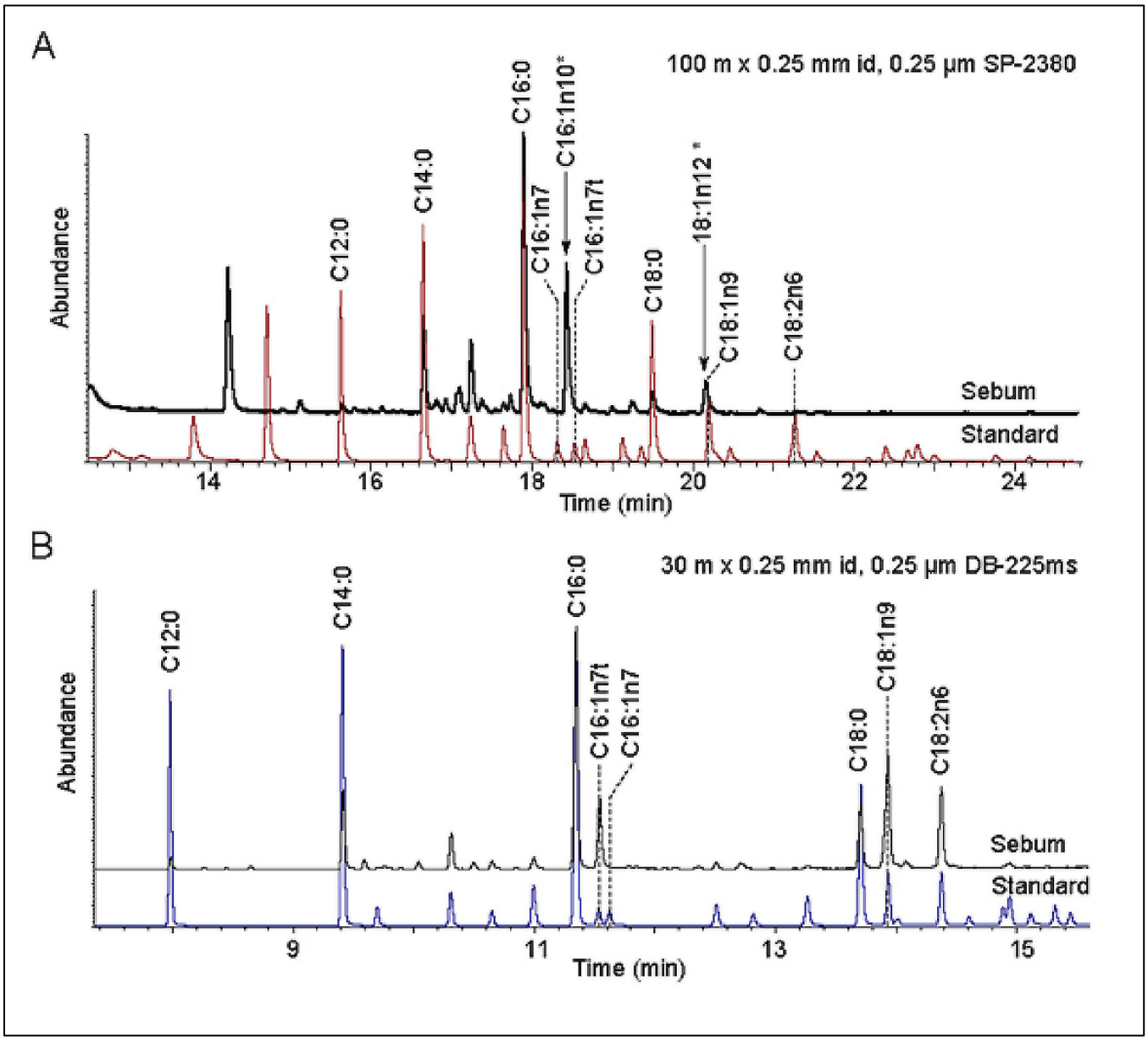
Supplemental Fig. S1. Sebutape® patches were used to collect sebum for analysis in this study. Patches consist of a lipid-absorbing polymeric film with adhesive that was placed on the bilateral cheeks for one hour and then placed on manufacturer-supplied plastic cards and stored at –80 °C until analysis. As sebum is absorbed onto the Sebutape® patch, the patch changes from opaque to translucent, which provides a semi-quantitative estimation of the amount of sebum collected.

Supplemental Figure S2



Supplemental Fig. S2. Hierarchical clustering of variables based on Ward's method. Upper panel: Hierarchical clustering tree. Lower panel: Distance between clusters calculated based on ANOVA sum of squares v/s the number of clusters.

Supplemental Figure S3



Supplemental Fig. S3. Sebum lipids separated on two distinct gas chromatography columns demonstrates unique isomeric composition of sebum. A: Lipids separated on a 90% biscyanopropyl/10% cyanopropylphenyl polysiloxane column designed for cis/trans isomer resolution. B: Lipids separated on a (50%-cyanopropylphenyl)-methylpolysiloxane used for quantification. Where different, calibration standards lipids are indicated with dashed lines and sebum lipids are indicated with arrows.

Supplemental Table S1

Supplemental Table S1A. Mobile phase gradient conditions for the analysis of oxylipins, nitrolipids, free fatty acids, endocannabinoids and endocannabinoid-like compounds by UPLC-MS/MS. A Waters Acquity UPLC® BEH C18 2.1 x 150 mm, 1.7 µm column was used to separate analytes and column temperature was maintained at 60°C.

Time (min)	Mobile Phase A [a] (%)	Mobile Phase B [b] (%)	Flow Rate (mL/min)
0.00	75	25	0.25
1.00	60	40	0.25
2.50	58	42	0.25
4.50	50	50	0.25
10.50	35	65	0.25
12.50	25	75	0.25
13.25	20	80	0.25
17.25	15	85	0.25
18.25	5	95	0.25
18.75	0	100	0.25
19.00	0	100	0.25
19.10	75	25	0.25
20.00	75	25	0.25

[a] Mobile Phase A: 0.1% Acetic Acid in Water

[b] Mobile Phase B: 90:10 Acetonitrile:Isopropanol

Supplemental Table S1

Supplemental Table S1B. UPLC/electrospray ionization QTrap analyte and instrument specific parameters for assayed oxylipins, nitrolipids, free fatty acids, endocannabinoids, and endocannabinoid-like compounds

Lipid Mediator	Analyte Class	Fatty Acid Precursor	Internal Standard	Retention Time (min)	Electrospray Ionization Mode	Q1 > Q3 Transition (m/z)	Collision Energy (V)	Declustering Potential (V)
PHAU -esi	ISTD			3.07	Negative	249.2 > 130.1	-18	-30
6-keto PGF1a	Prostanoid	C20:4n6	d4-PGF2a	3.43	Negative	369.3 > 163.1	-33	-70
d4-6-Keto PGF1a	SSTD		PHAU -esi	3.45	Negative	373.3 > 167.1	-36	-70
PGF3a	Prostanoid	C20:5n3	d4-PGF2a	4.03	Negative	351.3 > 307.4	-24	-60
PGE3	Prostanoid	C20:5n3	d4-PGF2a	4.18	Negative	349.3 > 269.2	-21	-35
TXB2	Prostanoid	C20:4n6	d4-TXB2	4.48	Negative	369.3 > 169.1	-21	-50
d4-TXB2	SSTD		PHAU -esi	4.55	Negative	373.3 > 173.1	-45	-50
Sum TriHOMEs	Triol	C18:2n6	d4-PGF2a	4.73	Negative	329.2 > 211.2	-30	-60
d4-PGF2a	SSTD		PHAU -esi	4.77	Negative	357.3 > 197.2	-33	-70
PGF2a	Prostanoid	C20:4n6	d4-PGF2a	4.78	Negative	353.3 > 193.2	-33	-70
PGE2	Prostanoid	C20:4n6	d4-PGD2	4.89	Negative	351.302 > 271.2	-21	-40
PGE1	Prostanoid	C20:3n6	d4-PGD2	5.06	Negative	353.3 > 317.2	-18	-40
d4-PGD2	SSTD		PHAU -esi	5.17	Negative	355.3 > 275.2	-27	-40
PGD2	Prostanoid	C20:4n6	d4-PGD2	5.18	Negative	351.303 > 271.2	-24	-40
15-Keto PGE2	Prostanoid	C20:4n6	d4-PGF2a	5.22	Negative	349.2 > 331.3	-15	-50
Resolvin D1	Triol	C20:4n6	d4-PGF2a	5.69	Negative	375.3 > 121.1	-39	-60
Lipoxin A4	Triol	C20:4n6	d4-PGF2a	5.80	Negative	351.3 > 217.2	-27	-45
LTB5	Leukotriene	C20:5n3	d4-PGF2a	6.89	Negative	333.3 > 195.2	-21	-50
15,16-DiHODE	Diol	C18:3n3	d11-14,15-DiHETrE	7.38	Negative	311.2 > 235.2	-27	-55
12,13-DiHODE	Diol	C18:3n3	d11-14,15-DiHETrE	7.47	Negative	311.2 > 183.2	-27	-60
8,15-DiHETE	Diol	C20:5n3	d11-14,15-DiHETrE	7.48	Negative	335.3 > 235.2	-21	-65
9,10-DiHODE	Diol	C18:3n3	d11-14,15-DiHETrE	7.52	Negative	311.2 > 201.2	-27	-65
d4-LTB4	SSTD		CUDA -esi	7.62	Negative	339.3 > 163.1	-33	-70
17,18-DiHETE	Diol	C20:5n3	d11-14,15-DiHETrE	7.75	Negative	335.3 > 247.2	-24	-70

ISTD - Internal Standard. This compound is added to the samples at the reconstitution step

SSTD - Surrogate. This compound is added to the samples prior to extraction

Supplemental Table S1

Supplemental Table S1B. UPLC/electrospray ionization QTrap analyte and instrument specific parameters for assayed oxylipins, nitrolipids, free fatty acids, endocannabinoids, and endocannabinoid-like compounds

Lipid Mediator	Analyte Class	Fatty Acid Precursor	Internal Standard	Retention Time (min)	Electrospray Ionization Mode	Q1 > Q3 Transition (m/z)	Collision Energy (V)	Declustering Potential (V)
5,15-DiHETE	Diol	C20:5n3	d11-14,15-DiHETrE	7.75	Negative	335.3 > 173.1	-18	-40
6-trans-LTB4	Leukotriene	C20:4n6	d11-14,15-DiHETrE	7.79	Negative	335.301 > 195.2	-21	-85
14,15-DiHETE	Diol	C20:5n3	d11-14,15-DiHETrE	8.42	Negative	335.3 > 207.2	-24	-40
CUDA -esi	ISTD			8.45	Negative	339.4 > 214.2	-30	-70
LTB4	Leukotriene	C20:4n6	d11-14,15-DiHETrE	8.50	Negative	335.302 > 195.2	-24	-50
10,11-DHHep	SSTD		CUDA -esi	8.80	Negative	301.2 > 283.2	-30	-90
12,13-DiHOME	Diol	C18:2n6	d11-14,15-DiHETrE	8.81	Negative	313.3 > 183.2	-30	-70
9,10-DiHOME	Diol	C18:2n6	d11-14,15-DiHETrE	9.23	Negative	313.3 > 201.2	-27	-65
d11-14,15-DiHETrE	SSTD		CUDA -esi	9.42	Negative	348.4 > 207.2	-24	-65
19,20-DiHDoPE	Diol	C22:6n3	d11-14,15-DiHETrE	9.46	Negative	361.3 > 273.2	-24	-80
14,15-DiHETrE	Diol	C20:4n6	d11-14,15-DiHETrE	9.49	Negative	337.3 > 207.2	-24	-60
11,12-DiHETrE	Diol	C20:4n6	d11-14,15-DiHETrE	10.10	Negative	337.3 > 167.1	-27	-55
9,10-e-DiHO	Diol	C18:0	d11-14,15-DiHETrE	10.23	Negative	315.2 > 297.2	-30	-110
12,13-Ep-9-KODE	Ketone	C18:3n3	d11-14,15-DiHETrE	10.39	Negative	309.2 > 291.2	-21	-90
9-HOTrE	Alcohol	C18:3n3	d4-9(S)-HODE	10.42	Negative	293.2 > 171.1	-21	-60
13-HOTrE	Alcohol	C18:3n3	d4-9(S)-HODE	10.50	Negative	293.2 > 195.2	-24	-70
8,9-DiHETrE	Diol	C20:4n6	d11-14,15-DiHETrE	10.59	Negative	337.3 > 127.1	-27	-65
15-deoxy PGJ2	Prostanoid	C20:4n6	d11-14,15-DiHETrE	10.66	Negative	315.2 > 271.2	-21	-50
d6-20-HETE	SSTD		CUDA -esi	10.81	Negative	325.3 > 281.2	-21	-80
20-HETE	Alcohol	C20:4n6	d6-20-HETE	10.85	Negative	319.2 > 275.2	-24	-95
15-HEPE	Alcohol	C20:5n3	d8-12(S)-HETE	10.95	Negative	317.2 > 219.2	-18	-55
12-HEPE	Alcohol	C20:5n3	d8-12(S)-HETE	11.22	Negative	317.2 > 179.1	-18	-45
5,6-DiHETrE	Diol	C20:4n6	d11-14,15-DiHETrE	11.37	Negative	337.3 > 145.1	-24	-55
9-HEPE	Alcohol	C20:5n3	d4-9(S)-HODE	11.43	Negative	317.201 > 167.2	-18	-45

ISTD - Internal Standard. This compound is added to the samples at the reconstitution step

SSTD - Surrogate. This compound is added to the samples prior to extraction

Supplemental Table S1

Supplemental Table S1B. UPLC/electrospray ionization QTrap analyte and instrument specific parameters for assayed oxylipins, nitrolipids, free fatty acids, endocannabinoids, and endocannabinoid-like compounds

Lipid Mediator	Analyte Class	Fatty Acid Precursor	Internal Standard	Retention Time (min)	Electrospray Ionization Mode	Q1 > Q3 Transition (m/z)	Collision Energy (V)	Declustering Potential (V)
13-HODE	Alcohol	C18:2n6	d4-9(S)-HODE	11.72	Negative	295.201 > 195.2	-24	-90
5-HEPE	Alcohol	C20:5n3	d8-5(S)-HETE	11.91	Negative	317.2 > 115.1	-21	-40
9-HODE	Alcohol	C18:2n6	d4-9(S)-HODE	11.91	Negative	295.201 > 171.1	-24	-70
d4-9,S-HODE	SSTD		CUDA -esi	11.94	Negative	299.2 > 172.1	-27	-85
15,16-EpODE	Epoxide	C18:3n3	d4-12,13-EpOME	12.00	Negative	293.201 > 275.2	-18	-75
15-HETE	Alcohol	C20:4n6	d8-12(S)-HETE	12.10	Negative	319.201 > 219.2	-18	-55
13-KODE	Ketone	C18:2n6	d4-9(S)-HODE	12.18	Negative	293.2 > 179.1	-27	-80
9,10-EpODE	Epoxide	C18:3n3	d4-12,13-EpOME	12.19	Negative	293.202 > 275.2	-18	-65
17,18-EpETE	Epoxide	C20:5n3	d4-12,13-EpOME	12.21	Negative	317.2 > 259.2	-15	-55
17-HDoHE	Alcohol	C22:6n3	d8-12(S)-HETE	12.31	Negative	343.301 > 281.2	-18	-55
12,13-EpODE	Epoxide	C18:3n3	d4-12,13-EpOME	12.40	Negative	293.2 > 183.2	-24	-50
14-HDoHE	Alcohol	C22:6n3	d8-12(S)-HETE	12.52	Negative	343.302 > 281.2	-18	-60
15-HpETE screen	Hydroperoxide	C20:4n6	d8-12(S)-HETE	12.55	Negative	335.2 > 113.1	-24	-55
11-HETE	Alcohol	C20:4n6	d8-12(S)-HETE	12.55	Negative	319.201 > 167.1	-21	-45
14,15-EpETE	Epoxide	C20:5n3	d4-12,13-EpOME	12.57	Negative	317.2 > 247.2	-18	-35
15-KETE	Ketone	C20:4n6	d8-12(S)-HETE	12.58	Negative	317.2 > 273.2	-18	-60
13-HpODE screen	Hydroperoxide	C18:2n6	d4-9(S)-HODE	12.62	Negative	311.2 > 179.1	-24	-55
9-KODE	Ketone	C18:2n6	d4-9(S)-HODE	12.62	Negative	293.2 > 185.2	-27	-100
d8-12(S)-HETE	SSTD		CUDA -esi	12.67	Negative	327.2 > 184.2	-21	-60
11,12-EpETE	Epoxide	C20:5n3	d4-12,13-EpOME	12.70	Negative	317.202 > 167.2	-18	-40
9-HpODE screen	Hydroperoxide	C18:2n6	d4-9(S)-HODE	12.72	Negative	311.2 > 185.2	-24	-55
12-HETE	Alcohol	C20:4n6	d8-12(S)-HETE	12.87	Negative	319.2 > 179.1	-21	-60
12-HpETE screen	Hydroperoxide	C20:4n6	d8-12(S)-HETE	12.95	Negative	335.2 > 153.1	-27	-55
8-HETE	Alcohol	C20:4n6	d8-12(S)-HETE	12.96	Negative	319.201 > 155.1	-21	-45

ISTD - Internal Standard. This compound is added to the samples at the reconstitution step

SSTD - Surrogate. This compound is added to the samples prior to extraction

Supplemental Table S1

Supplemental Table S1B. UPLC/electrospray ionization QTrap analyte and instrument specific parameters for assayed oxylipins, nitrolipids, free fatty acids, endocannabinoids, and endocannabinoid-like compounds

Lipid Mediator	Analyte Class	Fatty Acid Precursor	Internal Standard	Retention Time (min)	Electrospray Ionization Mode	Q1 > Q3 Transition (m/z)	Collision Energy (V)	Declustering Potential (V)
9-HETE	Alcohol	C20:4n6	d8-12(S)-HETE	13.08	Negative	319.202 > 167.1	-18	-60
d8-5(S)-HETE	SSTD		CUDA -esi	13.29	Negative	327.2 > 116.1	-18	-70
5-HpETE screen	Hydroperoxide	C20:4n6	d8-5(S)-HETE	13.44	Negative	335.2 > 155.1	-24	-55
19,20-EpDPE	Epoxide	C22:6n3	d4-12,13-EpOME	13.47	Negative	343.303 > 281.2	-18	-60
5-HETE	Alcohol	C20:4n6	d8-5(S)-HETE	13.48	Negative	319.2 > 115.1	-18	-50
d4-12,13-EpOME	SSTD [c]		CUDA -esi	13.54	Negative	299.2 > 198.1	-24	-90
12,13-EpOME	Epoxide	C18:2n6	d4-12,13-EpOME	13.63	Negative	295.202 > 195.2	-21	-85
4-HDoHE	Alcohol	C22:6n3	d8-5(S)-HETE	13.65	Negative	343.304 > 281.2	-18	-60
14,15-EpETrE	Epoxide	C20:4n6	d4-12,13-EpOME	13.67	Negative	319.202 > 219.2	-18	-50
9,10-EpOME	Epoxide	C18:2n6	d4-12,13-EpOME	13.79	Negative	295.202 > 171.1	-21	-75
16,17-EpDPE	Epoxide	C22:6n3	d4-12,13-EpOME	13.83	Negative	343.3 > 273.5	-15	-45
5-KETE	Ketone	C20:4n6	d8-5(S)-HETE	14.09	Negative	317.2 > 203.2	-27	-75
11,12-EpETrE	Epoxide	C20:4n6	d4-12,13-EpOME	14.13	Negative	319.203 > 167.1	-21	-40
8,9-EpETrE	Epoxide	C20:4n6	d4-12,13-EpOME	14.25	Negative	319.202 > 155.1	-18	-40
10-Nitrolinoleate	Nitrolipid	C18:2n6	d17-10-Nitrooleate	14.45	Negative	324.3 > 277.2	-18	-40
d17-10-Nitrooleate	SSTD [c]		CUDA -esi	15.21	Negative	343.2 > 307.5	-18	-65
10-Nitrooleate	Nitrolipid	C18:1n9	d17-10-Nitrooleate	15.30	Negative	326.2 > 279.5	-24	-40
EPA screen	Fatty Acid		d8-Arachidonic Acid	15.38	Negative	301.4 > 257.2	-15	-60
9-Nitrooleate	Nitrolipid	C18:1n9	d17-10-Nitrooleate	15.40	Negative	326.2 > 308.2	-18	-50
ALA screen	Fatty Acid		d8-Arachidonic Acid	15.55	Negative	277.4 > 259.2	-24	-115
DHA screen	Fatty Acid		d8-Arachidonic Acid	16.16	Negative	327.2 > 283.2	-15	-45
d8-Arachidonic Acid	SSTD		CUDA -esi	16.43	Negative	311.3 > 267.1	-18	-60
Arachidonate screen	Fatty Acid		d8-Arachidonic Acid	16.50	Negative	303.4 > 259.2	-18	-40
Linoleate screen	Fatty Acid		d8-Arachidonic Acid	16.89	Negative	279.4 > 261.2	-38	-185

ISTD - Internal Standard. This compound is added to the samples at the reconstitution step

SSTD - Surrogate. This compound is added to the samples prior to extraction

Supplemental Table S1

Supplemental Table S1B. UPLC/electrospray ionization QTrap analyte and instrument specific parameters for assayed oxylipins, nitrolipids, free fatty acids, endocannabinoids, and endocannabinoid-like compounds

Lipid Mediator	Analyte Class	Fatty Acid Precursor	Internal Standard	Retention Time (min)	Electrospray Ionization Mode	Q1 > Q3 Transition (m/z)	Collision Energy (V)	Declustering Potential (V)
PHAU +esi	ISTD			3.02	Positive	251.2 > 114.1	21	65
d4-PGF2a EA	SSTD		PHAU +esi	3.56	Positive	384.3 > 62.1	42	50
PGF2a EA	Acylethanolamide	C20:4n6	d4-PGF2a EA	3.56	Positive	380.3 > 62.1	39	45
PGE2 EA	Acylethanolamide	C20:4n6	d4-PGF2a EA	3.59	Positive	378.301 > 62.1	39	65
PGD2 EA	Acylethanolamide	C20:4n6	d4-PGF2a EA	3.91	Positive	378.302 > 62.1	42	65
PGF2a 1G	Monoacylglycerol	C20:4n6	d4-PGF2a EA	4.19	Positive	411.3 > 301.2	21	40
PGE2 1G	Monoacylglycerol	C20:4n6	d4-PGF2a EA	4.26	Positive	409.3 > 317.2	21	75
CUDA +esi	ISTD			8.45	Positive	341.3 > 216.2	24	50
15-HETE EA	Acylethanolamide	C20:4n6	d8-AEA	9.55	Positive	346.3 > 62.1	21	75
11,12-EpETre EA	Acylethanolamide	C20:4n6	d8-AEA	11.66	Positive	364.3 > 62.1	45	75
aLEA	Acylethanolamide	C18:3n3	d8-AEA	13.33	Positive	322.2 > 62.1	21	60
DHEA	Acylethanolamide	C22:6n3	d8-AEA	14.50	Positive	372.3 > 62.1	45	55
d8-NA-Gly	SSTD		CUDA +esi	14.58	Positive	370.3 > 76.1	21	45
d8-AEA	SSTD		CUDA +esi	14.62	Positive	356.3 > 63.1	45	50
NA-Gly	Acylgylcine	C20:4n6	d8-NA-Gly	14.64	Positive	362.3 > 76.1	21	65
AEA	Acylethanolamide	C20:4n6	d8-AEA	14.68	Positive	348.3 > 62.1	39	70
LEA	Acylethanolamide	C18:2n6	d8-AEA	14.79	Positive	324.2 > 62.1	21	70
Dihomo GLA EA	Acylethanolamide	C18:3n6	d4-PEA	15.36	Positive	350.3 > 62.1	36	35
d5-2-AG	SSTD		CUDA +esi	15.42	Positive	384.3 > 287.2	21	60
2-AG	Monoacylglycerol	C20:4n6	d5-2-AG	15.43	Positive	379.301 > 287.2	24	110
2-LG	Monoacylglycerol	C18:2n6	d8-NA-Gly	15.49	Positive	355.301 > 263.2	12	25
d4-PEA	SSTD		CUDA +esi	15.60	Positive	304.2 > 62.1	18	90
PEA	Acylethanolamide	C16:0	d4-PEA	15.62	Positive	300.2 > 62.1	18	70
1-AG	Monoacylglycerol	C20:4n6	d5-2-AG	15.66	Positive	379.302 > 287.2	21	95

ISTD - Internal Standard. This compound is added to the samples at the reconstitution step

SSTD - Surrogate. This compound is added to the samples prior to extraction

Supplemental Table S1

Supplemental Table S1B. UPLC/electrospray ionization QTrap analyte and instrument specific parameters for assayed oxylipins, nitrolipids, free fatty acids, endocannabinoids, and endocannabinoid-like compounds

Lipid Mediator	Analyte Class	Fatty Acid Precursor	Internal Standard	Retention Time (min)	Electrospray Ionization Mode	Q1 > Q3 Transition (m/z)	Collision Energy (V)	Declustering Potential (V)
1-LG	Monoacylglycerol	C18:2n6	d5-2-AG	15.81	Positive	355.302 > 263.2	12	40
NO-Gly	Acylgylcine	C18:1n9	d8-NA-Gly	15.95	Positive	340.2 > 76.2	21	60
DEA	Acylethanolamide	C22:4n6	d5-2-AG	16.02	Positive	376.3 > 62.1	45	105
OEA	Acylethanolamide	C18:1n9	d4-PEA	16.04	Positive	326.2 > 62.1	21	105
2-OG	Monoacylglycerol	C18:1n9	d5-2-AG	16.87	Positive	357.301 > 265.2	15	50
1-OG	Monoacylglycerol	C18:1n9	d5-2-AG	17.19	Positive	357.302 > 265.2	15	55
SEA	Acylethanolamide	C18:0	d4-PEA	17.67	Positive	328.2 > 62.1	21	100

ISTD - Internal Standard. This compound is added to the samples at the reconstitution step

SSTD - Surrogate. This compound is added to the samples prior to extraction

Supplemental Table S2

Supplemental Table S2A. Mobile phase gradient conditions for the analysis of ceramides and sphingoid bases by UPLC-MS/MS. A Waters Acquity UPLC® BEH C8 2.1 x 100 mm, 1.7 µm column was used to separate analytes and column temperature was maintained at 60°C.

Time (min)	Mobile Phase A [a] (%)	Mobile Phase B [b] (%)	Flow Rate (mL/min)
0.00	30	70	0.25
2.00	20	80	0.25
5.00	15	85	0.25
5.50	10	90	0.25
13.50	5	95	0.25
13.75	1	99	0.25
14.50	1	99	0.25
14.70	30	70	0.25
16.00	30	70	0.25

[a] Mobile Phase A: 5 mM Ammonium Formate and 0.2% Formic Acid in Water

[b] Mobile Phase B: 5 mM Ammonium Formate and 0.2% Formic Acid in Methanol

Supplemental Table S2

Supplemental Table S2B. UPLC/electrospray ionization QTRAP analyte and instrument specific parameters for assayed ceramides and sphingoid bases.

Lipid Mediator	Analyte Class	Fatty Acid Precursors [a]	Internal Standard	Retention Time (min)	Electrospray Ionization Mode	Q1 > Q3 Transition (m/z)	Collision Energy (V)	Declustering Potential (V)
CUDA	ISTD [b]			3.24	Positive	341.3 > 216.2	24.00	60
17:1 Sphingosine	SSTD [c]		CUDA	3.64	Positive	286.4 > 268.3	15.00	40
17:1 Sphingosine-1P	SSTD [c]		CUDA	3.96	Positive	366.4 > 250.3	24.00	65
18:1 Sphingosine	Sphingoid Base		17:1 Sphingosine	4.00	Positive	300.4 > 282.4	15.00	40
18:0 Sphinganine-1P	Sphingoid Base		17:1 Sphingosine-1P	4.32	Positive	382.4 > 266.4	24.00	70
18:1 Sphingosine-1P	Sphingoid Base		17:1 Sphingosine-1P	4.32	Positive	380.4 > 264.4	24.00	70
C14 Ceramide	[NS] Ceramide	d C18:1/C14:0	C17 Ceramide	10.09	Positive	510.7 > 492.6	18.00	65
C16 Ceramide	[NS] Ceramide	d C18:1/C16:0	C17 Ceramide	11.04	Positive	538.8 > 264.4	36.00	50
C18:1 Ceramide	[NS] Ceramide	d C18:1/C18:1	C17 Ceramide	11.40	Positive	564.5 > 546.4	18.00	50
C17 Ceramide	SSTD [c]		CUDA	11.52	Positive	552.8 > 534.5	18.00	55
C18 Ceramide	[NS] Ceramide	d C18:1/C18:0	C17 Ceramide	12.01	Positive	566.7 > 264.4	42.00	50
C18 dihydroceramide	[NdS] Ceramide	d C18:0/C18:0	C17 Ceramide	12.27	Positive	568.7 > 266.4	45.00	45
C20 Ceramide	[NS] Ceramide	d C18:1/C20:0	C17 Ceramide	13.06	Positive	594.4 > 576.5	21.00	60
C24 Ceramide	[NS] Ceramide	d C18:1/C24:0	C17 Ceramide	15.32	Positive	650.9 > 264.4	48.00	60
C24 dihydroceramide	[NdS] Ceramide	d C18:0/C24:0	C17 Ceramide	15.50	Positive	652.9 > 266.4	48.00	35

[a] Ceramides are synthesized by the addition of a fatty acid chain (represented by the carbon chain to the right of the slash) to a sphingoid base (represented by the carbon chain to the left of the slash)

[b] ISTD = Internal Standard. This compound is added to the samples at the reconstitution step

[c] SSTD = Surrogate. This compound is added to the samples prior to extraction

Supplemental Table S3

Supplemental Table S3. List of lipid mediator and fatty acid analytes with common database identifiers.

Common Abbreviation	Common Name	IUPAC Name	Analyte Class	Fatty Acid Precursor	HMDB ID [a]	PubChem CID [b]	InChI Key [c]
9-HODE	9-hydroxyoctadecanoic acid	(10E,12E)-9-hydroxyoctadeca-10,12-dienoic acid	Oxylipin – Alcohol	C18:2n6	HMDB10223	5282945	NPDSHTNEKLQQIJ-SIGMCMEVSA-N
13-HODE	13-hydroxyoctadecadienoic acid	(9Z,11E)-13-hydroxyoctadeca-9,11-dienoic acid	Oxylipin – Alcohol	C18:2n6	HMDB04667	6443013	HNICUWMFWZBIFP-IRQZEAMPSA-N
9-HOTrE	9-hydroxyoctadecatrienoic acid	(9E,11E,15Z)-9-hydroxyoctadeca-9,11,15-trienoic acid	Oxylipin – Alcohol	C18:3n3	HMDB10224	53480359	YUPHIKSLGBATJK-OBKPXJAFSA-N
13-HOTrE	13-hydroxyoctadecatrienoic acid	(9Z,11E,15Z)-13-hydroxyoctadeca-9,11,15-trienoic acid	Oxylipin – Alcohol	C18:3n3	HMDB10203	10469728	KLLGGGQNRTVBSU-JDTPQGGVSA-N
5-HETE	5-hydroxyeicosatetraenoic acid	(6E,8Z,11Z,14Z)-5-hydroxyicosa-6,8,11,14-tetraenoic acid	Oxylipin – Alcohol	C20:4n6	HMDB11134	5280733	KGIJOOYOSFUGPC-JGKLHWIESA-N
8-HETE	8-hydroxyeicosatetraenoic acid	(5Z,9E,11Z,14Z)-8-hydroxyicosa-5,9,11,14-tetraenoic acid	Oxylipin – Alcohol	C20:4n6	HMDB04679	5283154	NLUNAYAEIJYXRB-VYOQERLCSA-N
9-HETE	9-hydroxyeicosatetraenoic acid	(5E,7Z,11Z,14Z)-9-hydroxyicosa-5,7,11,14-tetraenoic acid	Oxylipin – Alcohol	C20:4n6	HMDB10222	5312978	KATOYYZUTNAWSA-DLJQHUEDSA-N
11-HETE	11-hydroxyeicosatetraenoic acid	(5E,8Z,12Z,14Z)-11-hydroxyicosa-5,8,12,14-tetraenoic acid	Oxylipin – Alcohol	C20:4n6	HMDB04682	5312981	GCZRCCHPLVMMJE-RSPKXIRXSA-N
12-HETE	12-hydroxyeicosatetraenoic acid	(5E,8Z,10Z,14Z)-12-hydroxyicosa-5,8,10,14-tetraenoic acid	Oxylipin – Alcohol	C20:4n6	HMDB06111	5312983	ZNHVWPKMFKADKW-FYMOKONMSA-N
15-HETE	15-hydroxyeicosatetraenoic acid	(5Z,8Z,11Z,13E)-15-hydroxyicosa-5,8,11,13-tetraenoic acid	Oxylipin – Alcohol	C20:4n6	HMDB03876	5280724	JSFATNQSLKRBCI-VAEKSGALSA-N
20-HETE	20-hydroxyeicosatetraenoic acid	(5Z,8Z,11Z,14Z)-20-hydroxyicosa-5,8,11,14-tetraenoic acid	Oxylipin – Alcohol	C20:4n6	HMDB05998	5283157	NNDIXBJHNLFJJP-DTLRTWKJSA-N
5-HEPE	5-Hydroxyeicosapentaenoic acid	(6E,8Z,11Z,14Z,17Z)-5-hydroxyicosa-6,8,11,14,17-pentaenoic acid	Oxylipin – Alcohol	C20:5n3	HMDB05081	6439678	FTAGQROYQYQRHF-FCWZHQICSA-N
9-HEPE	9-Hydroxyeicosapentaenoic acid	(5Z,7E,11Z,14Z,17Z)-9-hydroxyicosa-5,7,11,14,17-pentaenoic acid	Oxylipin – Alcohol	C20:5n3	HMDB60053	5283187	OXOPDAZWPWFJEW-FPRWAWDYSA-N
12-HEPE	12-Hydroxyeicosapentaenoic acid	(5Z,8Z,10E,14Z,17Z)-12-hydroxyicosa-5,8,10,14,17-pentaenoic acid	Oxylipin – Alcohol	C20:5n3	HMDB10202	10041593	MCRJLMXYVFDXLS-QGQBRVLBSA-N
15-HEPE	15-Hydroxyeicosapentaenoic acid	(5Z,8Z,11Z,13E,17Z)-16-hydroxyicosa-5,8,11,13,17-pentaenoic acid	Oxylipin – Alcohol	C20:5n3	HMDB10209	53480357	UDXLGBLAJBYLSZ-XBCQTNLFSA-N
4-HDoHE	4-hydroxydocosahexaenoic acid	(5E,7Z,10Z,13Z,16Z,19Z)-4-hydroxydocosa-5,7,10,13,16,19-hexaenoic acid	Oxylipin – Alcohol	C22:6n3	HMDB60049	53394255	IFRKCNPQVIJFAQ-UHFFFAOYSA-N
14-HDoHE	14-hydroxydocosahexaenoic acid	(4Z,7Z,10Z,12E,16Z,19Z)-14-hydroxydocosa-4,7,10,12,16,19-hexaenoic acid	Oxylipin – Alcohol	C22:6n3	HMDB60044	11566378	ZNEBXONKCYFJAF-BGKMTWLOSA-N
17-HDoHE	17-hydroxydocosahexaenoic acid	(4Z,7Z,10Z,13Z,15E,19Z)-17-hydroxydocosa-4,7,10,13,15,19-hexaenoic acid	Oxylipin – Alcohol	C22:6n3	HMDB10213	6439179	SWTYBBUBEPPYCX-VIIQGJSXSA-N
9,10-e-DiHO	9,10-dihydroxyoctadecanoic acid	9,10-dihydroxyoctadecanoic acid	Oxylipin – Diol	C18:0	–	441460	VACHUYIREGFMSP-SJORKVTESA-N
9,10-DiHOME	9,10-dihydroxyoctadecenoic acid	(Z)-9,10-dihydroxyoctadec-12-enoic acid	Oxylipin – Diol	C18:2n6	HMDB04704	9966640	XEBKSQSGNGRGDW-YFHOEESVSA-N
12,13-DiHOME	12,13-dihydroxyoctadecenoic acid	(Z)-12,13-dihydroxyoctadec-9-enoic acid	Oxylipin – Diol	C18:2n6	HMDB04705	10236635	CQSLTKIXAJTQGA-FLIBITNWSA-N
9,10-DiHODE	9,10-dihydroxyoctadecadienoic acid	(12Z,15Z)-9,10-dihydroxyoctadeca-12,15-dienoic acid	Oxylipin – Diol	C18:3n3	HMDB10221	16061066	QRHSEDZBZMZPOA-ZJSQCTGTSA-N
12,13-DiHODE	12,13-dihydroxyoctadecadienoic acid	(9Z,15Z)-12,13-dihydroxyoctadeca-9,15-dienoic acid	Oxylipin – Diol	C18:3n3	HMDB10201	16061067	RGRKFKRAFZJQMS-OOHFSOINSA-N
15,16-DiHODE	15,16-dihydroxyoctadecadienoic acid	(9Z,12Z)-15,16-dihydroxyoctadeca-9,12-dienoic acid	Oxylipin – Diol	C18:3n3	HMDB10208	16061068	LKLLJYJTYPVCID-OHPMOLHNSA-N
5,6-DiHETrE	5,6-dihydroxyeicosatrienoic acid	(8Z,11Z,14Z)-5,6-dihydroxyicosa-8,11,14-trienoic acid	Oxylipin – Diol	C20:4n6	HMDB02343	5283142	GFNYAPAJUNPMGH-QNEBEIHSSA-N
8,9-DiHETrE	8,9-dihydroxyeicosatrienoic acid	(5Z,11Z,14Z)-8,9-dihydroxyicosa-5,11,14-trienoic acid	Oxylipin – Diol	C20:4n6	HMDB02311	5283144	DCJBINATHQHPKO-TYAUOURKSA-N
11,12-DiHETrE	11,12-dihydroxyeicosatrienoic acid	(5Z,8Z,14Z)-11,12-dihydroxyicosa-5,8,14-trienoic acid	Oxylipin – Diol	C20:4n6	HMDB02314	5283146	LRPPQRCHCPFBPE-KROJNAHFSA-N
14,15-DiHETrE	14,15-dihydroxyeicosatrienoic acid	(5Z,8Z,11Z)-14,15-dihydroxyicosa-5,8,11-trienoic acid	Oxylipin – Diol	C20:4n6	HMDB02265	5283147	SYAWGTIVOGUZMM-ILYOTBPNSA-N
5,15-DiHETE	5,15-dihydroxyeicosatetraenoic acid	(6E,8Z,11Z,13E)-5,15-dihydroxyicosa-6,8,11,13-tetraenoic acid	Oxylipin – Diol	C20:5n3	HMDB10216	5283158	UXGXCGPWGSUMNI-BVHTXILBSA-N
8,15-DiHETE	8,15-dihydroxyeicosatetraenoic acid	(5Z,9E,11Z,13E)-8,15-dihydroxyicosa-5,9,11,13-tetraenoic acid	Oxylipin – Diol	C20:5n3	HMDB10219	53480358	NNPWRKSGORGTIM-RCDCWWQHSA-N
14,15-DiHETE	14,15-dihydroxyeicosatetraenoic acid	(5Z,8Z,11Z,17Z)-14,15-dihydroxyicosa-5,8,11,17-tetraenoic acid	Oxylipin – Diol	C20:5n3	HMDB10204	16061119	BLWCDFIELVFRJY-QXBXTPPVSA-N
17,18-DiHETE	17,18-dihydroxyeicosatetraenoic acid	(5Z,8Z,11Z,14Z)-17,18-dihydroxyicosa-5,8,11,14-tetraenoic acid	Oxylipin – Diol	C20:5n3	HMDB10211	16061120	XYDVGNAQQFWZEF-JPURVOHMSA-N

[a] Compound identification number for the Human Metabolome Database (http://www.hmdb.ca/). Analytes not listed in the Human Metabolome Database are designated with "–"

[b] Compound identification number for the National Center for Biotechnology Information's PubChem database (https://pubchem.ncbi.nlm.nih.gov/)

[c] IUPAC International Chemical Identifier

[d] This analyte represents the sum of the peaks of all observed isomers of the linoleate-derived triols. Concentrations are calculated relative to concentrations of authentic 9,12,13-TriHOME standards, the nomenclature of which is shown here

Supplemental Table S3

Supplemental Table S3. List of lipid mediator and fatty acid analytes with common database identifiers.

Common Abbreviation	Common Name	IUPAC Name	Analyte Class	Fatty Acid Precursor	HMDB ID [a]	PubChem CID [b]	InChI Key [c]
19,20-DiHDoPE	19,20-dihydroxydocosapentaenoic acid	(4Z,7Z,10Z,13Z,16Z)-19,20-dihydroxydocosa-4,7,10,13,16-pentaenoic acid	Oxylipin – Diol	C22:6n3	HMDB10214	16061148	FFXKPSNQCPNORO-MBYQGORISA-N
9,10-EpOME	9,10-epoxyoctadecenoic acid	8-[3-[(E)-oct-2-enyl]oxiran-2-yl]octanoic acid	Oxylipin – Epoxide	C18:2n6	HMDB04704	5283018	FBUKMFOXMZRGRB-JXMROGBWSA-N
12,13-EpOME	12,13-epoxyoctadecenoic acid	(Z)-11-(3-pentyloxiran-2-yl)undec-9-enoic acid	Oxylipin – Epoxide	C18:2n6	HMDB04702	5356421	CCPPLLJZDQAOHD-FLIBITNWSA-N
9,10-EpODE	9,10-epoxyoctadecadienoic acid	8-[3-[(2Z,5Z)-octa-2,5-dienyl]oxiran-2-yl]octanoic acid	Oxylipin – Epoxide	C18:3n3	HMDB10220	16061060	JTEGNNHWOIJBJZ-ZJSQCTGTSA-N
12,13-EpODE	12,13-epoxyoctadecadienoic acid	(Z)-11-[3-[(Z)-pent-2-enyl]oxiran-2-yl]undec-9-enoic acid	Oxylipin – Epoxide	C18:3n3	HMDB10200	16061061	BKKGUKSHPCTUGE-OOHFSOINSA-N
15,16-EpODE	15,16-epoxyoctadecadienoic acid	(9Z,12Z)-14-(3-ethyloxiran-2-yl)tetradeca-9,12-dienoic acid	Oxylipin – Epoxide	C18:3n3	HMDB10206	16061062	HKSDVVJONLXYKL-OHPMOLHNSA-N
8,9-EpETrE	8,9-epoxyeicosatrienoic acid	(Z)-7-[3-[(2Z,5Z)-undeca-2,5-dienyl]oxiran-2-yl]hept-5-enoic acid	Oxylipin – Epoxide	C20:4n6	HMDB02232	5283203	DBWQSCSXHFNTMO-TYAUOURKSA-N
11,12-EpETrE	11,12-epoxyeicosatrienoic acid	(5E,8Z)-10-[3-[(E)-oct-2-enyl]oxiran-2-yl]deca-5,8-dienoic acid	Oxylipin – Epoxide	C20:4n6	HMDB10409	53480479	DXOYQVHGIODESM-IQCOFVSKSA-N
14,15-EpETrE	14,15-epoxyeicosatrienoic acid	(5Z,8Z,12E)-11-hydroxy-13-(3-pentyloxiran-2-yl)trideca-5,8,12-trienoic acid	Oxylipin – Epoxide	C20:4n6	HMDB04693	11954058	WLMZMBKVRPUYIG-LTCHCNGXSA-N
11,12-EpETE	11,12-epoxyeicosatetraenoic acid	(5Z,8Z)-10-[3-[(2Z,5Z)-octa-2,5-dienyl]oxiran-2-yl]deca-5,8-dienoic acid	Oxylipin – Epoxide	C20:5n3	–	16061087	QHOKDYBJJBDJGY-BVILWSOJSA-N
14,15-EpETE	14,15-epoxyeicosatetraenoic acid	(5Z,8Z,11Z)-13-[3-[(Z)-pent-2-enyl]oxiran-2-yl]trideca-5,8,11-trienoic acid	Oxylipin – Epoxide	C20:5n3	HMDB10205	16061088	RGZIXZYRGZWDMI-QXBXTPPVSA-N
17,18-EpETE	17,18-epoxyeicosatetraenoic acid	(5Z,8Z,11Z,14Z)-16-(3-ethyloxiran-2-yl)hexadeca-5,8,11,14-tetraenoic acid	Oxylipin – Epoxide	C20:5n3	HMDB10212	16061089	GPQVVJQEBXAKBJ-JPURVOHMSA-N
16,17-EpDPE	16,17-epoxydocosapentaenoic acid	(4Z,7Z,10Z,13Z)-15-[3-[(Z)-pent-2-enyl]oxiran-2-yl]pentadeca-4,7,10,13-tetraenoic acid	Oxylipin – Epoxide	C22:6n3	HMDB13621	14392758	BCTXZWCPBLWCRV-ZYADFMMDSA-N
19,20-EpDPE	19,20-epoxydocosapentaenoic acid	(4Z,7Z,10Z,13Z,16Z)-18-(3-ethyloxiran-2-yl)octadeca-4,7,10,13,16-pentaenoic acid	Oxylipin – Epoxide	C22:6n3	HMDB13620	11631565	OSXOPUBJJDUAOJ-MBYQGORISA-N
9-HpODE	9-hydroperoxyoctadecadienoic acid	(10E,12Z)-9-hydroperoxyoctadeca-10,12-dienoic acid	Oxylipin – Hydroperoxide	C18:2n6	HMDB06940	6439847	JGUNZIWGNMQSBM-ZJHFMPGASA-N
13-HpODE	13-hydroperoxyoctadecadienoic acid	(9Z,11E)-13-hydroperoxyoctadeca-9,11-dienoic acid	Oxylipin – Hydroperoxide	C18:2n6	HMDB03871	5280720	JDSRHVWSAMTSSN-IRQZEAMPSA-N
5-HpETE	5-hydroperoxyicosatetraenoic acid	(6E,8Z,11Z,14Z)-5-hydroperoxyicosa-6,8,11,14-tetraenoic acid	Oxylipin – Hydroperoxide	C20:4n6	HMDB11135	5283171	JNUUNUQHXIOFDA-XTDASVJISA-N
12-HpETE	12-hydroperoxyicosatetraenoic acid	(5Z,8Z,10E,14Z)-12-hydroperoxyicosa-5,8,10,14-tetraenoic acid	Oxylipin – Hydroperoxide	C20:4n6	HMDB04243	5280892	ZIOZYRSDNLNNNJ-LQWMCKPYSA-N
15-HpETE	15-hydroperoxyicosatetraenoic acid	(5Z,8Z,11Z,13E)-15-hydroperoxyicosa-5,8,11,13-tetraenoic acid	Oxylipin – Hydroperoxide	C20:4n6	HMDB04244	5280893	BFWYTORDSFIVKP-VAEKSGALSA-N
9-KODE	9-oxo-octadecadienoic acid	(10E,12Z)-9-oxooctadeca-10,12-dienoic acid	Oxylipin – Ketone	C18:2n6	HMDB04669	9839084	LUZSWWYKKLTDHU-ZJHFMPGASA-N
13-KODE	13-oxo-octadecadienoic acid	(9Z,11E)-13-oxooctadeca-9,11-dienoic acid	Oxylipin – Ketone	C18:2n6	HMDB04668	6446027	JHXAZBBVQSRKJR-BSZOFBHHSA-N
12,13-Ep-9-KODE	9-oxo-12,13-epoxy-10-octadecenoic acid	(E)-9-oxo-11-(3-pentyloxiran-2-yl)undec-10-enoic acid	Oxylipin – Ketone	C18:3n3	HMDB13623	5283007	RCMABBHQYMBYKV-BUHFOSPRSA-N
5-KETE	5-oxo-eicosatetraenoic acid	(6E,8Z,11Z,14Z)-5-oxoicosa-6,8,11,14-tetraenoic acid	Oxylipin – Ketone	C20:4n6	HMDB10217	5283159	MEASLHGILYBXFO-XTDASVJISA-N
15-KETE	15-oxo-eicosatetraenoic acid	(5Z,8Z,11Z,13E)-15-oxoicosa-5,8,11,13-tetraenoic acid	Oxylipin – Ketone	C20:4n6	HMDB10210	5280701	YGJTUEISKATQSM-USWFWKISSA-N
6-trans-LTB4	6-trans-Leukotriene B4	(5S,6E,8E,10E,12R,14Z)-5,12-dihydroxyicosa-6,8,10,14-tetraenoic acid	Oxylipin – Leukotriene	C20:4n6	HMDB05087	5283128	VNYSSYRCGWBHLG-UKNWISKWSA-N
LTB4	Leukotriene B4	(5S,6Z,8E,10E,12R,14Z)-5,12-dihydroxyicosa-6,8,10,14-tetraenoic acid	Oxylipin – Leukotriene	C20:4n6	HMDB02886	5280492	VNYSSYRCGWBHLG-AMOLWHMGSA-N
LTB5	Leukotriene B5	(5S,6Z,8E,10E,12R,14Z,17Z)-5,12-dihydroxyicosa-6,8,10,14,17-pentaenoic acid	Oxylipin – Leukotriene	C20:5n3	HMDB05073	5283125	BISQPGCQOHLHQK-HDNPQISLSA-N
PGE1	Prostaglandin E1	7-[(1R,2R,3R)-3-hydroxy-2-[(E,3S)-3-hydroxyoct-1-enyl]-5-oxocyclopentyl]heptanoic acid	Oxylipin – Prostanoid	C20:3n6	HMDB01442	5280723	GMVPRGQOIOIIMI-DWKJAMRDSA-N
PGD2	Prostaglandin D2	(Z)-7-[(1R,2R,5S)-5-hydroxy-2-[(E,3S)-3-hydroxyoct-1-enyl]-3-oxocyclopentyl]hept-5-enoic acid	Oxylipin – Prostanoid	C20:4n6	HMDB01403	448457	BHMBVRSPMRCCGG-OUTUXVNYSA-N
PGE2	Prostaglandin E2	(Z)-7-[(1R,2R,3R)-3-hydroxy-2-[(E,3S)-3-hydroxyoct-1-enyl]-5-oxocyclopentyl]hept-5-enoic acid	Oxylipin – Prostanoid	C20:4n6	HMDB01220	5280360	XEYBRNLFEZDVAW-ARSRFYASSA-N
15-keto PGE2	15-keto Prostaglandin E2	(Z)-7-[(1R,2R,3R)-3-hydroxy-5-oxo-2-[(E)-3-oxooct-1-enyl]cyclopentyl]hept-5-enoic acid	Oxylipin – Prostanoid	C20:4n6	HMDB03175	5280719	YRTJDWROBKPZNV-KMXMBPPJSA-N
6-keto PGF1a	6-keto Prostaglandin F1alpha	7-[(1R,2R,3R,5S)-3,5-dihydroxy-2-[(E,3S)-3-hydroxyoct-1-enyl]cyclopentyl]-6-oxoheptanoic acid	Oxylipin – Prostanoid	C20:4n6	HMDB02886	5280888	KFGOFTHODYBSGM-ZUNNJUQCSA-N

[a] Compound identification number for the Human Metabolome Database (http://www.hmdb.ca/). Analytes not listed in the Human Metabolome Database are designated with "–"

[b] Compound identification number for the National Center for Biotechnology Information's PubChem database (https://pubchem.ncbi.nlm.nih.gov/)

[c] IUPAC International Chemical Identifier

[d] This analyte represents the sum of the peaks of all observed isomers of the linoleate-derived triols. Concentrations are calculated relative to concentrations of authentic 9,12,13-TriHOME standards, the nomenclature of which is shown here

Supplemental Table S3

Supplemental Table S3. List of lipid mediator and fatty acid analytes with common database identifiers.

Common Abbreviation	Common Name	IUPAC Name	Analyte Class	Fatty Acid Precursor	HMDB ID [a]	PubChem CID [b]	InChI Key [c]
PGF2a	Prostaglandin F2alpha	(Z)-7-[(1R,2R,3R,5S)-3,5-dihydroxy-2-[(E,3S)-3-hydroxyoct-1-enyl]cyclopentyl]hept-5-enoic acid	Oxylipin – Prostanoid	C20:4n6	HMDB01139	5280363	PXGPLTODNUVGFL-YNNPMVKQSA-N
15-deoxy PGJ2	15-deoxy Prostaglandin J2	(Z)-7-[(1S,5E)-5-[(E)-oct-2-enylidene]-4-oxocyclopent-2-en-1-yl]hept-5-enoic acid	Oxylipin – Prostanoid	C20:4n6	HMDB05079	5311211	VHRUMKCAEVRUBK-GODQJPCRSA-N
TXB2	Thromboxane B2	(Z)-7-[(2R,3S,4S)-4,6-dihydroxy-2-[(E,3S)-3-hydroxyoct-1-enyl]oxan-3-yl]hept-5-enoic acid	Oxylipin – Prostanoid	C20:4n6	HMDB03252	5283137	XNRNNGPBEPRNAR-JQBLCGNGSA-N
PGE3	Prostaglandin E3	(Z)-7-[(1R,2R,3R)-3-hydroxy-2-[(1E,3S,5Z)-3-hydroxyocta-1,5-dienyl]-5-oxocyclopentyl]hept-5-enoic acid	Oxylipin – Prostanoid	C20:5n3	HMDB02664	5280937	CBOMORHDRONZRN-QLOYDKTKSA-N
PGF3a	Prostaglandin F3alpha	(Z)-7-[(1R,2R,3R,5S)-3,5-dihydroxy-2-[(1E,3S,5Z)-3-hydroxyocta-1,5-dienyl]cyclopentyl]hept-5-enoic acid	Oxylipin – Prostanoid	C20:5n3	–	5280940	SAKGBZWJAIABSY-SAMSIYEGSA-N
Sum TriHOMEs [d]	9,12,13-Trihydroxyoctadecenoic acid	(10E)-9,12,13-trihydroxyoctadec-10-enoic acid	Oxylipin – Triol	C18:2n6	HMDB04708	9858729	MDIUMSLCYIJBQC-MVFSOIOZSA-N
LXA4	Lipoxin A4	(5S,6R,7E,9E,11Z,13E,15S)-5,6,15-trihydroxyicosa-7,9,11,13-tetraenoic acid	Oxylipin – Triol	C20:4n6	HMDB04385	5280914	IXAQOQZEOGMIQS-SSQFXEBMSA-N
RvD1	Resolvin D1	(4Z,7S,9E,11E,13Z,15E,17S,19Z)-7,8,17-trihydroxydocosa-4,9,11,13,15,19-hexaenoic acid	Oxylipin – Triol	C20:4n6	HMDB03733	16061135	OIWTWACQMDFHJG-NJIQAZPPSA-N
9-Nitrooleate	9-Nitrooleic acid	9-nitrooctadec-9-enoic acid	Nitrolipid	C18:1n9	–	53412232	CQOAKBVRRVHWKV-UHFFFAOYSA-M
10-Nitrooleate	10-Nitrooleic acid	10-nitrooctadec-9-enoic acid	Nitrolipid	C18:1n9	–	53394576	WRADPCFZZWXOTI-UHFFFAOYSA-N
10-Nitrolinoleate	10-Nitrolinoleic acid	(9E,12Z)-10-nitrooctadeca-9,12-dienoic acid	Nitrolipid	C18:2n6	–	5282259	LELVHAQTWXTCLY-XYWKCAQWSA-N
C18:2n6	Linoleic Acid	(9Z,12Z)-octadeca-9,12-dienoic acid	Free Fatty Acid		HMDB00673	5280450	OYHQOLUKZRVURQ-HZJYTTRNSA-N
C18:3n3	alpha-Linolenic Acid	(9Z,12Z,15Z)-octadeca-9,12,15-trienoic acid	Free Fatty Acid		HMDB01388	5280934	DTOSIQBPPRVQHS-PDBXOOCHSA-N
C20:4n6	Arachidonic Acid	(5Z,8Z,11Z,14Z)-icosa-5,8,11,14-tetraenoic acid	Free Fatty Acid		HMDB01043	444899	YZXBAPSDXZZRGB-DOFZRALJSA-N
C20:5n3	Eicosapentaenoic Acid	(5Z,8Z,11Z,14Z,17Z)-icosa-5,8,11,14,17-pentaenoic acid	Free Fatty Acid		HMDB01999	446284	JAZBEHYOTPTENJ-JLNKQSITSA-N
C22:6n3	Docosahexanoic Acid	(4Z,7Z,10Z,13Z,16Z,19Z)-docosa-4,7,10,13,16,19-hexaenoic acid	Free Fatty Acid		HMDB62579	445580	MBMBGCFOFBJSGT-KUBAVDMBSA-N
PEA	Palmitoylethanolamide	N-(2-hydroxyethyl)hexadecanamide	Acylethanolamide	C16:0	HMDB02100	4671	HXYVTAGFYLMHSO-UHFFFAOYSA-N
SEA	Stearoylethanolamide	N-(2-hydroxyethyl)octadecanamide	Acylethanolamide	C18:0	HMDB13078	27902	OTGQIQQTPXJQRG-UHFFFAOYSA-N
OEA	Oleoylethanolamide	(Z)-N-(2-hydroxyethyl)octadec-9-enamide	Acylethanolamide	C18:1n9	HMDB02088	5283454	BOWVQLFMWHZBEF-KTKRTIGZSA-N
LEA	Linoleoylethanolamide	(9Z,12Z)-N-(2-hydroxyethyl)octadeca-9,12-dienamide	Acylethanolamide	C18:2n6	HMDB12252	5283446	KQXDGUVSAAQARU-HZJYTTRNSA-N
aLEA	alpha-Linolenoylethanolamide	(9Z,12Z,15Z)-N-(2-hydroxyethyl)octadeca-9,12,15-trienamide	Acylethanolamide	C18:3n3	HMDB13624	5283449	HBJXRRXWHSHZPU-PDBXOOCHSA-N
Dihomo GLA EA	Dihomo-gamma-linolenoylethanolamide	(8Z,11Z,14Z)-N-(2-hydroxyethyl)icosa-8,11,14-trienamide	Acylethanolamide	C18:3n6	HMDB13625	5282272	ULQWKETUACYZLI-QNEBEIHSSA-N
11,12-EpETre EA	11,12-epoxyeicosatrienoic acid ethanolamide	(5Z,8Z)-N-(2-hydroxyethyl)-10-[3-[(Z)-oct-2-enyl]oxiran-2-yl]deca-5,8-dienamide	Acylethanolamide	C20:4n6	HMDB13652	16061183	TYRRSRADDAROSO-KROJNAHFSA-N
15-HETE EA	15-hydroxyeicosatetraenoic acid ethanolamide	(5Z,8Z,11Z,13E,15S)-15-hydroxy-N-(2-hydroxyethyl)icosa-5,8,11,13-tetraenamide	Acylethanolamide	C20:4n6	–	91886095	XZQKRCUYLKDPEK-BPVVGZHASA-N
AEA	Arachidonoylethanolamide / Anandamide	(5Z,8Z,11Z,14Z)-N-(2-hydroxyethyl)icosa-5,8,11,14-tetraenamide	Acylethanolamide	C20:4n6	HMDB04080	5281969	LGEQQWMQCRIYKG-DOFZRALJSA-N
PGD2 EA	Prostaglandin D2 ethanolamide	(Z)-N-(2-hydroxyethyl)-7-[(1R,2R,5S)-5-hydroxy-2-[(E,3S)-3-hydroxyoct-1-enyl]-3-oxocyclopentyl]hept-5-enamide	Acylethanolamide	C20:4n6	HMDB13629	5283120	KEYDJKSQFDUAGF-YIRKRNQHSA-N
PGE2 EA	Prostaglandin E2 ethanolamide	(Z)-N-(2-hydroxyethyl)-7-[(1R,2R,3R)-3-hydroxy-2-[(E,3S)-3-hydroxyoct-1-enyl]-5-oxocyclopentyl]hept-5-enamide	Acylethanolamide	C20:4n6	–	5283119	GKKWUSPPIQURFM-IGDGGSTLSA-N
PGF2a EA	Prostaglandin F2alpha ethanolamide	(E)-7-[(1R,2R,3R,5S)-3,5-dihydroxy-2-[(E,3S)-3-hydroxyoct-1-enyl]cyclopentyl]-N-(2-hydroxyethyl)hept-5-enamide	Acylethanolamide	C20:4n6	HMDB13628	53481911	XCVCLIRZZCGEMU-FPLRWIMGSA-N
DEA	Docosatetraenoylethanolamine	(7Z,10Z,13Z,16Z)-N-(2-hydroxyethyl)docosa-7,10,13,16-tetraenamide	Acylethanolamide	C22:4n6	HMDB13626	5282273	FMVHVRYFQIXOAF-DOFZRALJSA-N
DHEA	Docosahexanoylethanolamide	2-hydroxyethyl (4Z,7Z,10Z,13Z,16Z,19Z)-docosa-4,7,10,13,16,19-hexaenoate	Acylethanolamide	C22:6n3	HMDB13627	53245830	CXWASNUDKUTFPQ-KUBAVDMBSA-N
1-OG	1-oleoylglycerol	2,3-dihydroxypropyl (Z)-octadec-9-enoate	Monoacylglycerol	C18:1n9	HMDB11567	12178130	RZRNAYUHWVFMIP-QJRAZLAKSA-N
2-OG	2-oleoylglycerol	1,3-dihydroxypropan-2-yl (Z)-octadec-9-enoate	Monoacylglycerol	C18:1n9	HMDB11537	5319879	UPWGQKDVAURUGE-KTKRTIGZSA-N

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[d] This analyte represents the sum of the peaks of all observed isomers of the linoleate-derived triols. Concentrations are calculated relative to concentrations of authentic 9,12,13-TriHOME standards, the nomenclature of which is shown here

Supplemental Table S3

Supplemental Table S3. List of lipid mediator and fatty acid analytes with common database identifiers.

Common Abbreviation	Common Name	IUPAC Name	Analyte Class	Fatty Acid Precursor	HMDB ID [a]	PubChem CID [b]	InChI Key [c]
1-LG	1-linoleoylglycerol	2,3-dihydroxypropyl (9Z,12Z)-octadeca-9,12-dienoate	Monoacylglycerol	C18:2n6	HMDB11568	6436630	WECGLUPZRHILCT-GSNKCQISSA-N
2-LG	2-linoleoylglycerol	1,3-dihydroxypropan-2-yl (9Z,12Z)-octadeca-9,12-dienoate	Monoacylglycerol	C18:2n6	HMDB11538	5365676	IEPGNWMPIFDNSD-HZJYTTRNSA-N
1-AG	1-arachidonoylglycerol	2,3-dihydroxypropyl (5Z,8Z,11Z,14Z)-icosa-5,8,11,14-tetraenoate	Monoacylglycerol	C20:4n6	HMDB11578	16019980	DCPCOKIYJYGMDN-HUDVFFLJSA-N
2-AG	2-arachidonoylglycerol	1,3-dihydroxypropan-2-yl (5Z,8Z,11Z,14Z)-icosa-5,8,11,14-tetraenoate	Monoacylglycerol	C20:4n6	HMDB04666	5282280	RCRCTBLIHCHWDZ-DOFZRALJSA-N
PGE2 1G	Prostaglandin E2 1-glycerol	[(2R)-2,3-dihydroxypropyl] (Z)-7-[(1R,2R,3S)-3-hydroxy-2-[(E,3S)-3-hydroxyoct-1-enyl]-5-oxocyclopentyl]hept-5-enoate	Monoacylglycerol	C20:4n6	HMDB13043	52193688	RJXVYMMSQBYEHN-SDTVLRMPSA-N
PGF2a 1G	Prostaglandin F2alpha 1-glycerol	2,3-dihydroxypropyl (Z)-7-[(1R,2R,3R,5S)-3,5-dihydroxy-2-[(E,3S)-3-hydroxyoct-1-enyl]cyclopentyl]hept-5-enoate	Monoacylglycerol	C20:4n6	–	24778485	NWKPOVHSHWJQNI-OMVDPNNKSA-N
NO-Gly	N-oleoylglycine	2-[[(Z)-octadec-9-enoyl]amino]acetic acid	Acylglycine	C18:1n9	HMDB13631	6436908	HPFXACZRFJDURI-KTKRTIGZSA-N
NA-Gly	N-arachidonoylglycine	2-[[(5Z,8Z,11Z,14Z)-icosa-5,8,11,14-tetraenoyl]amino]acetic acid	Acylglycine	C20:4n6	HMDB05096	5283389	YLEARPUNMCCKMP-DOFZRALJSA-N
C18 dihydroceramide	Ceramide (d18:0/18:0)	N-[(2S,3R)-1,3-dihydroxyoctadecan-2-yl]octadecanamide	Sphingolipid – [NdS] Ceramide		HMDB11761	5283573	KZTJQXAANJHSCE-OIDHKYIRSA-N
C24 dihydroceramide	Ceramide (d18:0/24:0)	N-[(2S,3R)-1,3-dihydroxyoctadecan-2-yl]tetracosanamide	Sphingolipid – [NdS] Ceramide		HMDB11768	5283577	BPLYVSYSBPLDOA-WVILEFPPSA-N
C14 Ceramide	Ceramide (d18:1/14:0)	N-[(E,2S,3R)-1,3-dihydroxyoctadec-4-en-2-yl]tetradecanamide	Sphingolipid – [NS] Ceramide		HMDB11773	5282310	ZKRPGPZHULJLKJ-JHRQRACZSA-N
C16 Ceramide	Ceramide (d18:1/16:0)	N-[(E,2S,3R)-1,3-dihydroxyoctadec-4-en-2-yl]hexadecanamide	Sphingolipid – [NS] Ceramide		HMDB04949	5283564	YDNKGFDKKRUKPY-TURZORIXSA-N
C18 Ceramide	Ceramide (d18:1/18:0)	N-[(E,2S,3R)-1,3-dihydroxyoctadec-4-en-2-yl]octadecanamide	Sphingolipid – [NS] Ceramide		HMDB04950	5283565	VODZWWMEJITOND-NXCSZAMKSA-N
C18:1 Ceramide	Ceramide (d18:1/18:1)	(Z)-N-[(E,2S,3R)-1,3-dihydroxyoctadec-4-en-2-yl]octadec-9-enamide	Sphingolipid – [NS] Ceramide		HMDB04948	5283563	OBFSLMQLPNKVRW-RHPAUOISSA-N
C20 Ceramide	Ceramide (d18:1/20:0)	N-[(E,2S,3R)-1,3-dihydroxyoctadec-4-en-2-yl]icosanamide	Sphingolipid – [NS] Ceramide		HMDB04951	5283566	XWBWIAOWSABHFI-NUKVNZTCSA-N
C24 Ceramide	Ceramide (d18:1/24:0)	N-[(E,2S,3R)-1,3-dihydroxyoctadec-4-en-2-yl]tetracosanamide	Sphingolipid – [NS] Ceramide		HMDB04956	5283571	ZJVVOYPTFQEGPH-AUTSUKAISA-N
	18:0 Sphinganine-1P	[(2S,3R)-2-amino-3-hydroxyoctadecyl] dihydrogen phosphate	Sphingolipid – Sphingosine		HMDB01383	644260	YHEDRJPUIRMZMP-ZWKOTPCHSA-N
	18:1 Sphingosine	(E)-2-aminooctadec-4-ene-1,3-diol	Sphingolipid – Sphingosine		HMDB00252	5353955	WWUZIQQURGPMPG-CCEZHUSRSA-N
	18:1 Sphingosine-1P	[(E)-2-amino-3-hydroxyoctadec-4-enyl] dihydrogen phosphate	Sphingolipid – Sphingosine		HMDB00277	5353956	DUYSYHSSBDVJSM-CCEZHUSRSA-N
C12:0	Lauric Acid	Dodecanoic Acid	Saturated Fatty Acid (SFA)		HMDB00638	3893	POULHZVOKOAJMA-UHFFFAOYSA-N
C14:0	Myristic Acid	Tetradecanoic Acid	Saturated Fatty Acid (SFA)		HMDB00806	11005	TUNFSRHWOTWDNC-UHFFFAOYSA-N
C15:0		Pentadecanoic Acid	Saturated Fatty Acid (SFA)		HMDB00826	13849	WQEPLJUUGTLDZJY-UHFFFAOYSA-N
C16:0	Palmitic Acid	Hexadecanoic Acid	Saturated Fatty Acid (SFA)		HMDB00220	985	IPCSVZSSVZVIGE-UHFFFAOYSA-N
C17:0	Margaric Acid	Heptadecanoic Acid	Saturated Fatty Acid (SFA)		HMDB02259	10465	KEMQGTRYUADPNZ-UHFFFAOYSA-N
C18:0	Stearic Acid	Octadecanoic Acid	Saturated Fatty Acid (SFA)		HMDB00827	5281	QIQXTHQIDYTFRH-UHFFFAOYSA-N
C20:0	Arachidic Acid	Icosanoic Acid	Saturated Fatty Acid (SFA)		HMDB02212	10467	VKOBVWXKNCXXDE-UHFFFAOYSA-N
C22:0	Behenic Acid	Docosanoic Acid	Saturated Fatty Acid (SFA)		HMDB00944	8215	UKMSUNONTOPOIO-UHFFFAOYSA-N
C24:0	Lignoceric Acid	Tetracosanoic Acid	Saturated Fatty Acid (SFA)		HMDB02003	11197	QZZGJDVWLFXDLK-UHFFFAOYSA-N
C16:1n7t	Palmitelaidic Acid	(E)-hexadec-9-enoic acid	Monounsaturated Fatty Acid (MUFA)		HMDB12328	5282745	SECPZKHBENQXJG-BQYQJAHWSA-N
C16:1n7	Palmitoleic Acid	(Z)-hexadec-9-enoic acid	Monounsaturated Fatty Acid (MUFA)		HMDB03229	445638	SECPZKHBENQXJG-FPLPWBNLSA-N
C18:1n9	Oleic Acid	(Z)-octadec-9-enoic acid	Monounsaturated Fatty Acid (MUFA)		HMDB00207	445639	ZQPPMHVWECSIRJ-KTKRTIGZSA-N
C18:1n7	Vaccenic Acid	(Z)-octadec-11-enoic acid	Monounsaturated Fatty Acid (MUFA)		HMDB03231	5282761	UWHZIFQPPBDJPM-FPLPWBNLSA-N
C19:1n9	10-Nonadecenoic acid	(Z)-nonadec-10-enoic acid	Monounsaturated Fatty Acid (MUFA)		HMDB13622	5312513	BBOWBNGUEWHNQZ-KTKRTIGZSA-N

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Supplemental Table S3

Supplemental Table S3. List of lipid mediator and fatty acid analytes with common database identifiers.

Common Abbreviation	Common Name	IUPAC Name	Analyte Class	Fatty Acid Precursor	HMDB ID [a]	PubChem CID [b]	InChI Key [c]
C20:1n9	11-Eicosenoic acid	(Z)-icos-11-enoic acid	Monounsaturated Fatty Acid (MUFA)		HMDB02231	5282768	BITHHVVYSMSWAG-KTKRTIGZSA-N
C18:2n6	Linoleic Acid	(9Z,12Z)-octadeca-9,12-dienoic acid	Polyunsaturated Fatty Acid (PUFA)		HMDB00673	5280450	OYHQOLUKZRVURQ-HZJYTTRNSA-N
C18:3n6	gamma-Linolenic acid	(6Z,9Z,12Z)-octadeca-6,9,12-trienoic acid	Polyunsaturated Fatty Acid (PUFA)		HMDB03073	5280933	VZCCETWTMQHEPK-QNEBEIHSSA-N
C18:2(9c,11t)-CLA	Bovinic Acid	(9Z,11E)-octadeca-9,11-dienoic acid	Polyunsaturated Fatty Acid (PUFA)		HMDB03797	5280644	JBYXPOFIGCOSSB-GOJKSUSPSA-N
C18:3n3	alpha-Linolenic Acid	(9Z,12Z,15Z)-octadeca-9,12,15-trienoic acid	Polyunsaturated Fatty Acid (PUFA)		HMDB01388	5280934	DTOSIQBPPRVQHS-PDBXOOCHSA-N
C20:2n6	Dihomo-Linoleic Acid	(11Z,14Z)-icosa-11,14-dienoate	Polyunsaturated Fatty Acid (PUFA)		–	40846588	XSXIVVZCUAHUJO-HZJYTTRNSA-M
C20:3n6	Dihomo-gamma-Linolenic Acid	(8Z,11Z,14Z)-icosa-8,11,14-trienoic acid	Polyunsaturated Fatty Acid (PUFA)		HMDB02925	5280581	HOBAELRKJCKHQD-QNEBEIHSSA-N
C20:3n9	Mead Acid	(5Z,8Z,11Z)-icosa-5,8,11-trienoic acid	Polyunsaturated Fatty Acid (PUFA)		HMDB10378	5312531	UNSRRHDPHVZAHH-YOILPLPUSA-N
C20:4n6	Arachidonic Acid	(5Z,8Z,11Z,14Z)-icosa-5,8,11,14-tetraenoic acid	Highly Unsaturated Fatty Acid (HUFA)		HMDB01043	444899	YZXBAPSDXZZRGB-DOFZRALJSA-N
C22:4n6	Adrenic Acid	(7Z,10Z,13Z,16Z)-docosa-7,10,13,16-tetraenoic acid	Highly Unsaturated Fatty Acid (HUFA)		HMDB02226	5497181	TWSWSIQAPQLDBP-DOFZRALJSA-N
C22:5n6	Osbond Acid (Docosapentaenoic Acid)	(4Z,7Z,10Z,13Z,16Z)-docosa-4,7,10,13,16-pentaenoic acid	Highly Unsaturated Fatty Acid (HUFA)		–	6441454	AVKOENOBFIYBSA-WMPRHZDHSA-N
C18:4n3	Stearidonic Acid (Moroctic Acid)	(6Z,9Z,12Z,15Z)-octadeca-6,9,12,15-tetraenoic acid	Highly Unsaturated Fatty Acid (HUFA)		HMDB06547	5312508	JIWBIWFOSCKQMA-LTKCOYKYSA-N
C20:4n3		(4Z,7Z,10Z,13Z)-eicosatetraenoic acid	Highly Unsaturated Fatty Acid (HUFA)		–	–	–
C20:5n3	Timnodonic Acid (Eicosapentaenoic Acid, EPA)	(5Z,8Z,11Z,14Z,17Z)-icosa-5,8,11,14,17-pentaenoic acid	Highly Unsaturated Fatty Acid (HUFA)		HMDB01999	446284	JAZBEHYOTPTENJ-JLNKQSITSA-N
C22:5n3	Clupanodonic Acid (Docosapentaenoic Acid, DP	(7Z,10Z,13Z,16Z,19Z)-docosa-7,10,13,16,19-pentaenoic acid	Highly Unsaturated Fatty Acid (HUFA)		HMDB06528	5497182	YUFFSWGQGVEMMI-JLNKQSITSA-N
C22:6n3	Cervonic Acid (Docosahexaenoic Acid, DHA)	(4Z,7Z,10Z,13Z,16Z,19Z)-docosa-4,7,10,13,16,19-hexaenoic acid	Highly Unsaturated Fatty Acid (HUFA)		HMDB02183	445580	MBMBGCFOFBJSGT-KUBAVDMBSA-N

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Supplemental Table S4. Effects of atopic dermatitis and gender on detected sebum lipid mediators and fatty acids.

Cluster [a]	Metabolite	Unit	Concentration in Blank Sebutapes	Blank-Corrected Concentration in Samples [b]				$P (P_{adj})$ [c]		
				Control Female (n = 4)	AD Female (n = 5)	Control Male (n = 5)	AD Male (n = 6)	Disease	Gender	Disease*Gender
1	9-HETE	pmol/tape	0.009	0.0103 [0.00414 - 0.0259]	0.0161 [0.00324 - 0.0308]	0.0203 [0.00494 - 0.0344]	0.0397 [0.0176 - 0.0746]	0.7 (0.9)	0.1 (0.3)	0.9 (0.9)
	PGE1	pmol/tape	0.002	0.00199 [0.00138 - 0.00356]	0.00174 [0.00028 - 0.00705]	0.00676 [0.00122 - 0.19]	0.00202 [0.00043 - 0.0096]			
2	15-KETE	pmol/tape	0.084	0.319 [0.264 - 0.381]	0.254 [0.116 - 0.507]	0.41 [0.0409 - 2.06]	0.493 [0.178 - 0.686]	0.4 (0.7)	0.02 (0.16)	0.4 (0.9)
	8,9-EpETrE	pmol/tape	ND	0.675 [0.101 - 3.24]	1.03 [0.79 - 1.31]	2.79 [0.379 - 34.5]	3.65 [1.01 - 10.5]			
3	15-HEPE	pmol/tape	0.007	0.0104 [0.00487 - 0.0212]	0.0146 [0.00667 - 0.0194]	0.0367 [0.00837 - 0.134]	0.0186 [0.0133 - 0.03]	0.9 (1)	0.01 (0.11)	0.2 (0.8)
	15-HETE	pmol/tape	0.01	0.185 [0.122 - 0.284]	0.107 [0.0324 - 0.406]	0.797 [0.181 - 3.25]	0.489 [0.309 - 0.73]			
	TFA - C18:3n3	µmol/tape	1.212	0.616 [0.337 - 1.26]	1.16 [0.35 - 1.96]	1.55 [0.946 - 4.38]	0.75 [0.325 - 1.37]			
4	11-HETE	pmol/tape	0.005	0.011 [0.00544 - 0.0146]	0.00708 [0.00198 - 0.0276]	0.0291 [0.00734 - 0.137]	0.0186 [0.0005 - 0.0709]	0.5 (0.9)	0.01 (0.11)	0.8 (0.9)
	12-HEPE	pmol/tape	0.003	0.00318 [0.00147 - 0.00901]	0.00313 [0.0003 - 0.0182]	0.0163 [0.00696 - 0.0337]	0.0118 [0.00487 - 0.0607]			
	12-HETE	pmol/tape	0.002	0.0835 [0.0339 - 0.323]	0.153 [0.0462 - 0.456]	0.354 [0.0772 - 2.25]	0.469 [0.0662 - 1.76]			
	13-KODE	pmol/tape	11.5	6.97 [4.29 - 17.2]	1.48 [0.1 - 3.82]	3.56 [1.3 - 25.5]	7.31 [4.4 - 12.4]			
	14-HDoHE	pmol/tape	ND	0.0225 [0.0043 - 0.0566]	0.0202 [0.00374 - 0.0583]	0.1 [0.0497 - 0.395]	0.0647 [0.00717 - 0.29]			
	17-HDoHE	pmol/tape	ND	0.0639 [0.0469 - 0.112]	0.105 [0.0446 - 0.147]	0.292 [0.0473 - 0.903]	0.165 [0.0941 - 0.399]			
	5-HETE	pmol/tape	0.011	0.0852 [0.0516 - 0.134]	0.0236 [0.007 - 0.0689]	0.079 [0.0303 - 0.424]	0.0312 [0.0078 - 0.0714]			
	8-HETE	pmol/tape	0.007	0.00499 [0.0011 - 0.0119]	0.0143 [0.00122 - 0.059]	0.0292 [0.0037 - 0.272]	0.0556 [0.0308 - 0.178]			
	C16 Ceramide	pmol/tape	0.4	13 [9.57 - 15.9]	5.79 [2.65 - 11.7]	16.9 [10.3 - 25.5]	15.1 [8.19 - 25.8]			
5	17,18-DiHETE	pmol/tape	0.12	0.09 [0.045 - 0.311]	0.205 [0.109 - 0.3]	0.155 [0.124 - 0.189]	0.121 [0.008 - 0.372]	0.2 (0.7)	0.8 (0.9)	0.5 (0.9)
6	10-Nitrolinoleate	pmol/tape	0.088	0.0598 [0.0199 - 0.165]	0.0545 [0.0209 - 0.209]	0.101 [0.0669 - 0.15]	0.0474 [0.0021 - 0.199]	0.8 (1)	0.8 (0.9)	0.6 (0.9)
7	18:1 Sphingosine	pmol/tape	2.6	14 [11.3 - 16.4]	15.7 [10.5 - 21.4]	15.1 [11.9 - 18.7]	14.5 [9.37 - 23.6]	1 (1)	0.8 (0.9)	0.4 (0.9)
	20-HETE	pmol/tape	0.122	0.195 [0.078 - 0.501]	0.24 [0.081 - 0.506]	0.241 [0.098 - 0.403]	0.169 [0.076 - 0.285]			
8	LEA	pmol/tape	2.19	1.42 [0.07 - 6.51]	1.95 [0.16 - 15.5]	2.53 [0.27 - 8.21]	0.991 [0.27 - 5.34]	0.6 (0.9)	0.8 (0.9)	0.2 (0.8)
	OEA	pmol/tape	1	2.76 [0.549 - 28.6]	2.92 [0.499 - 61.1]	9.68 [1.35 - 42]	4.45 [0.959 - 22.1]			
	PEA	pmol/tape	18.4	34.2 [16.3 - 82.6]	48 [28.5 - 160]	59.5 [22.8 - 149]	16.8 [4.6 - 79.1]			
	SEA	pmol/tape	19.8	25.2 [8.5 - 49.1]	35.5 [20.5 - 74.1]	34.5 [20.4 - 60]	19.4 [3.47 - 35.6]			
9	11,12-EpETrE	pmol/tape	0.008	0.0105 [0.00375 - 0.0199]	0.00635 [0.00132 - 0.0221]	0.00397 [0.00035 - 0.0202]	0.00353 [0.00137 - 0.00875]	0.7 (0.9)	0.6 (0.9)	0.9 (1)
	PGE3	pmol/tape	ND	0.0134 [0.00653 - 0.0271]	0.0145 [0.00819 - 0.0201]	0.0163 [0.00873 - 0.025]	0.016 [0.0125 - 0.0211]			
10	1-AG	pmol/tape	0.256	0.327 [0.175 - 0.68]	0.357 [0.041 - 2.27]	0.821 [0.256 - 3.68]	0.642 [0.161 - 1.72]	0.7 (0.9)	0.5 (0.8)	0.3 (0.9)
	1-LG	pmol/tape	127	116 [73 - 194]	143 [23 - 322]	170 [44 - 443]	96.4 [26 - 196]			
11	TFA - C22:5n6	µmol/tape	0.236	1.56 [0.347 - 5.36]	1.09 [0.166 - 5.03]	1.64 [0.896 - 5.13]	0.591 [0.29 - 2.99]	0.3 (0.7)	0.9 (0.9)	0.5 (0.9)
12	5,6-DiHETrE	pmol/tape	0.001	0.00116 [0.000539 - 0.00333]	0.00157 [0.000499 - 0.00664]	0.00121 [0.000192 - 0.00584]	0.00157 [0.000669 - 0.00316]	0.9 (1)	0.8 (0.9)	0.03 (0.5)
	8,9-DiHETrE	pmol/tape	5.68	1.17 [0.59 - 1.95]	2.32 [0.76 - 5.62]	2.1 [0.47 - 5.52]	1.71 [0.48 - 6.22]			
	9,10-e-DiHO	pmol/tape	0.55	1.61 [1.18 - 1.98]	1.74 [1.24 - 2.39]	1.99 [1.51 - 3.54]	1.42 [0.976 - 2.14]			
	NEFA - 10t,12c-CLA	µmol/tape	0.045	0.0171 [0.011 - 0.024]	0.0447 [0.024 - 0.107]	0.0622 [0.032 - 0.204]	0.0258 [0.006 - 0.341]			
	TFA - 10t,12c-CLA	µmol/tape	0.051	0.0266 [0.006 - 0.099]	0.0878 [0.0608 - 0.136]	0.0867 [0.0153 - 0.233]	0.0438 [0.014 - 0.101]			
13	12,13-EpODE	pmol/tape	0.175	0.0465 [0.02 - 0.136]	0.241 [0.129 - 0.845]	0.109 [0.046 - 0.306]	0.0471 [0.008 - 0.145]	0.2 (0.7)	0.7 (0.9)	0.03 (0.5)
	12,13-DiHOME	pmol/tape	0.66	0.457 [0.3 - 0.69]	0.799 [0.41 - 2.64]	0.585 [0.109 - 3.7]	0.468 [0.246 - 0.83]			
	NEFA - C18:3n3	µmol/tape	0.607	0.381 [0.243 - 0.455]	0.592 [0.349 - 1.91]	0.576 [0.34 - 0.785]	0.543 [0.314 - 1.07]			

[a] Analytes were subjected to heirarchical cluster analysis using the method of Ward (1965)

[b] Data reported as Geometric Mean [Range]

[c] The reported p-values are also adjusted for multiple comparisons by the Benjamini-Hochberg procedure at q = 0.2

[d] This analyte represents the sum of the peaks of all observed isomers of the linoleate-derived triols. Concentrations were calculated relative to concentrations of authentic 9,12,13-TriHOME standards

[e] Analyte quantified using the response of the coeluting C16:1n7t standards

[f] Analyte quantified using the response of the coeluting C18:1n9 standards

Supplemental Table S4. Effects of atopic dermatitis and gender on detected sebum lipid mediators and fatty acids.

Cluster [a]	Metabolite	Unit	Concentration in Blank Sebutapes	Blank-Corrected Concentration in Samples [b]				$P (P_{adj})$ [c]		
				Control Female (n = 4)	AD Female (n = 5)	Control Male (n = 5)	AD Male (n = 6)	Disease	Gender	Disease*Gender
14	12,13-Ep-9-KODE	pmol/tape	0.34	2.34 [1.96 - 2.74]	2.85 [2.45 - 3.32]	2.57 [1.43 - 4.29]	2.83 [1.94 - 4.67]	0.9 (1)	0.8 (0.9)	1 (1)
	12,13-DiHODE	pmol/tape	0.064	0.0527 [0.0427 - 0.0667]	0.0549 [0.0209 - 0.4]	0.0433 [0.0264 - 0.125]	0.0358 [0.019 - 0.0827]			
	15,16-DiHODE	pmol/tape	0.321	0.11 [0.091 - 0.15]	0.135 [0.008 - 7.41]	0.137 [0.082 - 0.365]	0.0952 [0.015 - 0.759]			
	2-AG	pmol/tape	0.34	0.808 [0.218 - 2.24]	0.901 [0.22 - 2.78]	2.04 [0.779 - 10.8]	1.42 [0.54 - 4.93]			
	9,10-DiHODE	pmol/tape	0.075	0.0394 [0.0317 - 0.0527]	0.0727 [0.0164 - 2.65]	0.0319 [0.0191 - 0.0627]	0.0292 [0.0137 - 0.0637]			
15	9,10-EpOME	pmol/tape	1.34	1.03 [0.32 - 3.26]	7.74 [4.1 - 21]	1.01 [0.29 - 4.43]	0.999 [0.15 - 2.79]	0.1 (0.3)	0.1 (0.3)	0.1 (0.7)
16	NEFA - C20:4n3	µmol/tape	0.239	0.306 [0.205 - 0.503]	0.406 [0.331 - 0.486]	0.339 [0.217 - 0.617]	0.368 [0.188 - 0.645]	0.2 (0.7)	0.6 (0.9)	0.4 (0.9)
	NEFA - C20:5n3	µmol/tape	0.002	0.349 [0.228 - 0.419]	0.48 [0.384 - 0.557]	0.36 [0.204 - 0.705]	0.355 [0.247 - 0.992]			
17	TFA - C20:2n6	µmol/tape	0.064	0.0492 [0.008 - 0.158]	0.129 [0.055 - 0.21]	0.082 [0.0271 - 0.176]	0.0699 [0.016 - 0.151]	0.6 (0.9)	0.7 (0.9)	0.1 (0.7)
	TFA - C20:4n3	µmol/tape	0.031	0.333 [0.258 - 0.478]	0.37 [0.229 - 0.537]	0.486 [0.288 - 0.739]	0.368 [0.228 - 0.517]			
18	Sum TriHOMEs [d]	pmol/tape	1.6	0.683 [0.23 - 2.79]	0.33 [0.1 - 1.07]	0.487 [0.07 - 4.65]	0.781 [0.16 - 4.05]	0.7 (0.9)	0.9 (0.9)	0.5 (0.9)
	TFA - C10:0	µmol/tape	0.21	6.98 [0.558 - 120]	1.87 [1.32 - 3.6]	2.22 [0.419 - 52.6]	3.1 [0.657 - 69.5]			
	TFA - C18:0	µmol/tape	21.473	47.9 [29.4 - 65.4]	34.8 [18.9 - 51.6]	30.4 [11.7 - 89.2]	32.6 [17.2 - 69.1]			
	TFA - C18:1n7	µmol/tape	0.281	2.12 [1.42 - 3.02]	1.86 [1.02 - 3.59]	2.82 [0.897 - 8.77]	1.63 [0.248 - 11.3]			
19	9,10-EpO	pmol/tape	1.1	10.9 [5.6 - 49.4]	7.94 [6.21 - 10.7]	7.96 [6.04 - 9.85]	8.68 [6.61 - 10.8]	0.4 (0.7)	0.2 (0.5)	0.8 (0.9)
	TFA - C18:3n6	µmol/tape	0.013	0.0661 [0.027 - 0.123]	0.0957 [0.043 - 0.21]	0.121 [0.049 - 0.227]	0.134 [0.0527 - 0.408]			
20	9-HEPE	pmol/tape	0.005	0.00637 [0.00276 - 0.0138]	0.00515 [0.00161 - 0.00935]	0.00632 [0.00259 - 0.0134]	0.00274 [0.00013 - 0.0144]	0.5 (0.8)	0.7 (0.9)	0.8 (0.9)
21	5-KETE	pmol/tape	0.004	0.00742 [0.00357 - 0.0147]	0.00359 [0.00055 - 0.0116]	0.00785 [0.00417 - 0.0144]	0.00344 [0.00092 - 0.008]	0.04 (0.3)	0.3 (0.7)	0.4 (0.9)
	TFA - C18:2n6	µmol/tape	8.689	16.7 [13.2 - 20.2]	15.7 [6.7 - 34.9]	22.1 [5.3 - 107]	9.27 [2.78 - 104]			
22	C18 Ceramide	pmol/tape	0.608	0.818 [0.351 - 1.3]	0.152 [0.007 - 0.662]	0.529 [0.372 - 0.982]	0.323 [0.136 - 0.732]	0 (0.12)	0.1 (0.3)	0.3 (0.9)
	C18 dihydroceramide	pmol/tape	ND	2.65 [1.84 - 4.02]	1.59 [1.13 - 2.36]	1.93 [1.11 - 2.99]	1.53 [0.99 - 1.94]			
	C18:1 Ceramide	pmol/tape	0.1	39.8 [32.6 - 61.4]	28.2 [18.8 - 36.2]	29.6 [24.9 - 33.2]	23.5 [17.3 - 30.6]			
23	C24 Ceramide	pmol/tape	0.19	6.93 [5.55 - 8.23]	6.04 [3.54 - 7.86]	2.8 [1.26 - 9.76]	3.11 [1.42 - 10.9]	0.9 (1)	0 (0.11)	0.6 (0.9)
	C24 dihydroceramide	pmol/tape	ND	6.53 [5.34 - 7.96]	5.41 [3.72 - 8.5]	1.7 [0.89 - 6.11]	2.04 [1.06 - 4.03]			
24	C20 Ceramide	pmol/tape	1.84	2.34 [0.7 - 8.14]	2.05 [0.43 - 3.97]	2.33 [1.36 - 3.12]	1.27 [0.91 - 1.65]	0.02 (0.3)	0.7 (0.9)	0.7 (0.9)
	TFA - C12:0	µmol/tape	0.923	30.1 [12.8 - 129]	11.1 [5.89 - 23.2]	19.1 [5.99 - 83.9]	13.6 [2.92 - 113]			
	TFA - C22:2n6	µmol/tape	0.124	1.94 [1.31 - 3.22]	0.84 [0.343 - 1.25]	2.62 [1.16 - 8.07]	1 [0.159 - 1.78]			
25	1-OG	pmol/tape	68	270 [122 - 421]	96 [58.8 - 166]	615 [175 - 1770]	202 [44.8 - 539]	0.04 (0.3)	0.1 (0.3)	0.9 (1)
	5-HEPE	pmol/tape	0.012	0.0227 [0.007 - 0.0502]	0.0044 [0.0001 - 0.0319]	0.0239 [0.0055 - 0.0872]	0.00901 [0.00073 - 0.0434]			
	9,10-DiHOME	pmol/tape	0.66	0.852 [0.716 - 0.936]	1.39 [0.816 - 6.54]	0.942 [0.506 - 1.81]	0.91 [0.726 - 1.24]			
	NEFA - 9c,11t-CLA	µmol/tape	0.083	0.0631 [0.027 - 0.132]	0.0466 [0.013 - 0.102]	0.295 [0.14 - 0.738]	0.0625 [0.008 - 0.486]			
	NEFA - C18:1n7	µmol/tape	0.19	0.347 [0.207 - 0.516]	0.178 [0.013 - 1.53]	0.864 [0.334 - 3.95]	0.915 [0.346 - 2.39]			
	Sebumeter Reading	µg/cm^2		0.0783 [0.047 - 0.111]	0.0274 [0.012 - 0.148]	0.076 [0.013 - 0.199]	0.0694 [0.029 - 0.133]			
	TFA - C20:1n9	µmol/tape	0.123	5.25 [4.62 - 5.99]	2.19 [0.713 - 3.8]	7.37 [3.24 - 23.6]	4.07 [0.523 - 11.2]			
	TFA - C20:4n6	µmol/tape	0.264	0.163 [0.0432 - 0.377]	0.236 [0.164 - 0.415]	0.358 [0.074 - 1.05]	0.125 [0.038 - 0.282]			

[a] Analytes were subjected to heirarchical cluster analysis using the method of Ward (1965)

[b] Data reported as Geometric Mean [Range]

[c] The reported p-values are also adjusted for multiple comparisons by the Benjamini-Hochberg procedure at q = 0.2

[d] This analyte represents the sum of the peaks of all observed isomers of the linoleate-derived triols. Concentrations were calculated relative to concentrations of authentic 9,12,13-TriHOME standards

[e] Analyte quantified using the response of the coeluting C16:1n7t standards

[f] Analyte quantified using the response of the coeluting C18:1n9 standards

Supplemental Table S4. Effects of atopic dermatitis and gender on detected sebum lipid mediators and fatty acids.

Cluster [a]	Metabolite	Unit	Concentration in Blank Sebutapes	Blank-Corrected Concentration in Samples [b]				P (P_{adj}) [c]		
				Control Female (n = 4)	AD Female (n = 5)	Control Male (n = 5)	AD Male (n = 6)	Disease	Gender	Disease*Gender
26	2-OG	pmol/tape	11	130 [38.2 - 221]	77.6 [21.6 - 152]	239 [46.5 - 769]	179 [81.2 - 268]	0.3 (0.7)	0.04 (0.19)	0.8 (0.9)
	NEFA - C19:0	µmol/tape	0.115	0.23 [0.079 - 0.595]	0.2 [0.113 - 0.332]	0.716 [0.244 - 1.76]	0.498 [0.067 - 4.09]			
	NEFA - C20:0	µmol/tape	0.368	0.949 [0.611 - 1.52]	0.768 [0.448 - 1.08]	2.28 [0.873 - 5.62]	1.84 [0.537 - 14.7]			
	NEFA - C21:0	µmol/tape	0.088	0.103 [0.069 - 0.214]	0.079 [0.05 - 0.12]	0.218 [0.083 - 0.641]	0.191 [0.063 - 1.32]			
	NEFA - C22:0	µmol/tape	0.307	1.5 [1.02 - 1.8]	1.49 [1.28 - 1.92]	2.59 [1.38 - 5.32]	2.45 [1.09 - 13.5]			
	NEFA - C24:0	µmol/tape	0.301	2.41 [1.27 - 3.76]	1.92 [0.917 - 3.13]	3.51 [0.702 - 11.2]	4.32 [1.34 - 29.1]			
27	NEFA - C14:0	µmol/tape	1.024	10.1 [4.14 - 24.3]	7.35 [2.34 - 20.6]	30.8 [9.48 - 90]	17.9 [2.65 - 62.8]	0.3 (0.7)	0.02 (0.16)	0.8 (0.9)
	NEFA - C15:0	µmol/tape	0.343	8.37 [5.33 - 20.8]	4.42 [1.33 - 11.2]	20.9 [4.19 - 68.5]	15.1 [2.57 - 58]			
	NEFA - C16:0	µmol/tape	12.717	37.3 [23.8 - 76.9]	28 [10.4 - 44.5]	106 [34.1 - 290]	57.6 [10.7 - 218]			
	NEFA - C16:1n10 [e]	µmol/tape	0.443	28.7 [16.3 - 72]	12.5 [3.52 - 46.5]	84.8 [14.7 - 318]	41.7 [4.88 - 273]			
	NEFA - C17:0	µmol/tape	0.385	1.88 [0.978 - 4.92]	1.28 [0.503 - 2.23]	5.52 [1.76 - 16.4]	3.68 [0.75 - 19]			
	NEFA - C18:0	µmol/tape	18.828	8.76 [3.36 - 13.4]	10.5 [5.92 - 16.7]	23.5 [15.2 - 42.3]	15.1 [5.13 - 58.6]			
	NEFA - C18:1n12 [f]	µmol/tape	3.424	19.8 [9.18 - 44.4]	17.5 [6.43 - 47.8]	59 [19.7 - 203]	36 [5.6 - 193]			
	NEFA - C20:1n9	µmol/tape	0.84	0.524 [0.146 - 1.43]	0.487 [0.175 - 1.5]	3.17 [1.16 - 14.4]	1.44 [0.2 - 11.3]			
	NEFA - Total Fatty Acids	µmol/tape		127 [74.8 - 270]	96.4 [38.7 - 163]	365 [113 - 1070]	211 [40 - 968]			
28	2-LG	pmol/tape	27.8	11.8 [2.8 - 50.4]	11.1 [7.88 - 16.3]	19.9 [9.41 - 72.1]	8.21 [1.7 - 28.3]	0.1 (0.3)	0.2 (0.6)	0.7 (0.9)
	AEA	pmol/tape	ND	0.00699 [0.00551 - 0.0104]	0.00267 [0.0018 - 0.00532]	0.0112 [0.00433 - 0.0666]	0.00363 [0.00108 - 0.0132]			
	DGLEA	pmol/tape	ND	0.0257 [0.0106 - 0.0547]	0.0119 [0.00386 - 0.0583]	0.0694 [0.00792 - 0.39]	0.0394 [0.0138 - 0.0952]			
	DHEA	pmol/tape	0.001	0.00216 [0.000687 - 0.00532]	0.00119 [0.000231 - 0.00492]	0.0086 [0.00277 - 0.039]	0.00165 [0.000507 - 0.00586]			
29	NEFA - C12:0	µmol/tape	1.1	0.962 [0.127 - 2.67]	2.43 [1.02 - 4.85]	5.14 [0.931 - 11.7]	2.78 [0.77 - 6.04]	0.9 (1)	0.04 (0.19)	0.1 (0.6)
30	15,16-EpODE	pmol/tape	0.1	17.2 [9.86 - 24.6]	6.62 [4.65 - 14.2]	12.1 [3.23 - 27.4]	9.03 [1.98 - 22.3]	0.04 (0.3)	0.4 (0.8)	0.5 (0.9)
	C14 Ceramide	pmol/tape	0.3	3.3 [2.63 - 5.15]	2.14 [1.28 - 4.76]	4.08 [2.16 - 7.57]	2.64 [1.11 - 4.14]			
	TFA - 9c,11t-CLA	µmol/tape	0.119	0.801 [0.725 - 0.901]	0.292 [0.098 - 0.647]	0.924 [0.525 - 1.64]	0.411 [0.149 - 0.899]			
	TFA - C14:1n5	µmol/tape	0.181	3.2 [2.08 - 4.38]	1.55 [0.551 - 3.62]	2.22 [0.913 - 6.48]	2.09 [0.274 - 5.85]			
	TFA - C17:1n7	µmol/tape	0	48 [33.6 - 60.5]	21 [12.1 - 31.6]	47.2 [23 - 93.6]	36.9 [7.52 - 80.8]			
	TFA - C18:1n12 [f]	µmol/tape	4.67	178 [141 - 291]	86.1 [59.7 - 128]	171 [109 - 358]	122 [28.1 - 314]			
	TFA - C19:1n9	µmol/tape	0.299	3.38 [2.75 - 5.11]	1.69 [0.861 - 3.2]	3.43 [1.23 - 10.2]	1.78 [0.106 - 6.21]			
31	TFA - C14:0	µmol/tape	1.211	117 [101 - 154]	61.9 [35.1 - 127]	95.7 [46.6 - 158]	83.3 [17.8 - 416]	0.2 (0.7)	0.6 (0.9)	0.3 (0.9)
	TFA - C15:0	µmol/tape	0.192	75.9 [58 - 93.7]	36.5 [21 - 60.1]	59.7 [23.8 - 109]	66.8 [17.5 - 274]			
	TFA - C16:0	µmol/tape	14.935	298 [261 - 362]	171 [116 - 254]	258 [124 - 501]	215 [53.8 - 712]			
	TFA - C16:1n10 [e]	µmol/tape	0.374	403 [349 - 477]	186 [97.6 - 342]	350 [159 - 708]	299 [46.5 - 1100]			
	TFA - C17:0	µmol/tape	0.432	13.6 [9.98 - 17.8]	6.41 [3.44 - 9.87]	13.9 [6.74 - 27.6]	13.2 [3.43 - 34.8]			
	TFA - Total Fatty Acids	µmol/tape		1340 [1180 - 1510]	678 [459 - 1030]	1200 [729 - 2200]	974 [217 - 3360]			
32	TFA - C19:0	µmol/tape	0.098	1.66 [1.33 - 1.89]	0.815 [0.401 - 1.16]	1.85 [0.967 - 3.32]	1.74 [0.419 - 3.73]	0.3 (0.7)	0.2 (0.5)	0.4 (0.9)
	TFA - C20:0	µmol/tape	0.631	5.62 [4.94 - 6.28]	2.97 [1.62 - 4.12]	5.91 [3.54 - 9.62]	5.02 [1.08 - 13.7]			
	TFA - C21:0	µmol/tape	0.087	0.462 [0.421 - 0.486]	0.252 [0.082 - 0.464]	0.521 [0.176 - 1.07]	0.526 [0.137 - 1.29]			
	TFA - C22:0	µmol/tape	0.521	4.78 [4.19 - 5.55]	3.1 [2.19 - 4.32]	5.13 [2.75 - 8.52]	4.53 [1.08 - 12.9]			
	TFA - C24:0	µmol/tape	0.348	13 [9.58 - 15.3]	7.44 [5.01 - 12.9]	13.8 [7.96 - 24.7]	11.5 [1.42 - 35.8]			

[a] Analytes were subjected to heirarchical cluster analysis using the method of Ward (1965)

[b] Data reported as Geometric Mean [Range]

[c] The reported p-values are also adjusted for multiple comparisons by the Benjamini-Hochberg procedure at q = 0.2

[d] This analyte represents the sum of the peaks of all observed isomers of the linoleate-derived triols. Concentrations were calculated relative to concentrations of authentic 9,12,13-TriHOME standards

[e] Analyte quantified using the response of the coeluting C16:1n7t standards

[f] Analyte quantified using the response of the coeluting C18:1n9 standards

Supplemental Table S5

Supplemental Table S5A. Effects of various standardizing strategies on sebum lipid mediator concentrations in individuals with atopic dermatitis (n = 11 in all cases).

Lipid Mediator	Coefficient of Variance (%) [a]				
	Per Sebutape Patch	Per NEFA	Per Total TFA	Per Sebumeter Reading	P [b]
Oxylipins and Nitrolipids					
PGE1	96.1	189	200	161	0.013
PGE3	25	111	99.2	95.5	0.07
Sum TriHOMEs [c]	124	74.4	102	97.7	< 0.001
9,10-e-DiHO	30.7	68.4	67.5	103	< 0.001
12,13-DiHOME	88.5	113	129	87	< 0.001
9,10-DiHOME	117	119	158	84	< 0.001
15,16-DiHODE	271	275	303	180	< 0.001
12,13-DiHODE	154	150	205	78.7	< 0.001
9,10-DiHODE	291	286	307	194	< 0.001
5,6-DiHETrE	85	122	141	108	0.15
8,9-DiHETrE	74.1	92.7	94	76.7	< 0.001
17,18-DiHETE	53.6	109	84.5	86.4	< 0.001
20-HETE	55.9	116	79.5	108	< 0.001
15-HETE	67.1	103	104	114	< 0.001
12-HETE	111	221	215	146	< 0.001
11-HETE	91.6	199	178	131	< 0.001
9-HETE	80.9	162	156	100	0.006
8-HETE	98	224	213	136	< 0.001
5-HETE	69.2	66.8	103	150	< 0.001
15-HEPE	35.7	115	117	89.5	0.22
12-HEPE	128	231	235	174	< 0.001
9-HEPE	71.9	146	151	121	0.02
5-HEPE	98.3	99.3	119	91.5	< 0.001
17-HDoHE	59.9	154	166	94.2	< 0.001
14-HDoHE	116	236	228	164	< 0.001
9,10-EpO	20.7	84.7	87.9	96.7	< 0.001
12,13-EpODE	128	123	167	140	< 0.001
9,10-EpOME	118	114	142	156	< 0.001
12,13-Ep-9-KODE	25.7	76.9	66.5	90.2	< 0.001
15,16-EpODE	69.6	54	44.4	117	< 0.001
11,12-EpETrE	97.2	110	133	174	0.004
8,9-EpETrE	105	77	105	63.8	< 0.001
13-KODE	72.5	92.2	93.7	56.7	< 0.001
15-KETE	51.1	46.6	53.4	103	< 0.001
5-KETE	69.7	94.4	116	125	0.008
10-Nitrolinoleate	88.5	111	117	156	< 0.001

[a] Coefficient of Variance calculated as the ratio of the standard deviation of all subject's lipid mediator concentrations when standardized using the appropriate denominator to the mean of the same values

[b] The reported p-values are adjusted for multiple comparisons by the Benjamini-Hochberg procedure at q = 0.2

[c] This analyte represents the sum of the peaks of all observed isomers of the linoleate-derived triols. Concentrations were calculated relative to concentrations of authentic 9,12,13-TriHOME standards

Supplemental Table S5

Supplemental Table S5A. Effects of various standardizing strategies on sebum lipid mediator concentrations in individuals with atopic dermatitis (n = 11 in all cases).

Lipid Mediator	Coefficient of Variance (%) [a]				
	Per Sebutape Patch	Per NEFA	Per Total TFA	Per Sebumeter Reading	p [b]
Endocannabinoids					
1-OG	79.6	91.3	97.4	74.4	< 0.001
2-OG	54.1	67.2	73.6	79.4	0.8
1-LG	62.3	139	95.9	139	0.051
2-LG	104	203	208	163	0.053
1-AG	86.7	206	130	144	< 0.001
2-AG	86.2	95.9	79.2	133	< 0.001
PEA	101	146	93.8	112	< 0.001
SEA	59.8	103	88.7	107	< 0.001
OEA	173	216	168	184	< 0.001
LEA	144	172	127	155	< 0.001
AEA	86.8	141	138	108	0.046
DGLEA	82.3	114	115	139	< 0.001
DHEA	87.6	95.7	80.5	169	0.012
Sphingolipids					
18:1 Sphingosine	29.6	103	82	89.2	< 0.001
C14 Ceramide	46	55.4	50.2	129	< 0.001
C16 Ceramide	63.9	147	157	84	< 0.001
C18 Ceramide	68.7	154	155	139	< 0.001
C18:1 Ceramide	25	82.2	55.2	106	< 0.001
C20 Ceramide	58.6	115	84.4	138	< 0.001
C24 Ceramide	59.5	130	141	107	< 0.001
C18 dihydroceramide	28.4	82.5	52.2	94.3	< 0.001
C24 dihydroceramide	59.9	113	78.3	111	< 0.001

[a] Coefficient of Variance calculated as the ratio of the standard deviation of all subject's lipid mediator concentrations when standardized using the appropriate denominator to the mean of the same values

[b] The reported p-values are adjusted for multiple comparisons by the Benjamini-Hochberg procedure at q = 0.2

[c] This analyte represents the sum of the peaks of all observed isomers of the linoleate-derived triols. Concentrations were calculated relative to concentrations of authentic 9,12,13-TriHOME standards

Supplemental Table S5

Supplemental Table S5B. Effects of various standardizing strategies on sebum lipid mediator concentrations in individuals without atopic dermatitis (n = 9 in all cases).

Lipid Mediator	Coefficient of Variance (%) [a]				
	Per Sebutape Patch	Per NEFA	Per Total TFA	Per Sebumeter Reading	p [b]
Oxylipins and Nitrolipids					
PGE1	263	265	278	294	0.002
PGE3	42.5	96.4	34.5	113	0.002
Sum TriHOMEs [c]	130	171	102	91.7	< 0.001
9,10-e-DiHO	35.9	73.4	39.2	135	< 0.001
12,13-DiHOME	132	86.2	88.7	59.5	< 0.001
9,10-DiHOME	37.3	71.9	30.7	73.7	< 0.001
15,16-DiHODE	63.5	73.1	48.7	100	< 0.001
12,13-DiHODE	56.7	79.4	30.4	73.8	< 0.001
9,10-DiHODE	37.7	82.4	41.7	115	0.007
5,6-DiHETrE	101	88	100	195	0.02
8,9-DiHETrE	75.6	80.9	73.3	171	< 0.001
17,18-DiHETE	57.3	57.7	64.3	141	< 0.001
20-HETE	55.2	83.2	64.5	149	< 0.001
15-HETE	134	52.2	95.6	170	< 0.001
12-HETE	163	81	122	196	< 0.001
11-HETE	133	76.4	109	206	< 0.001
9-HETE	61.9	60.6	77.2	181	< 0.001
8-HETE	191	114	152	217	< 0.001
5-HETE	105	99.6	93.2	195	< 0.001
15-HEPE	118	79.7	100	199	< 0.001
12-HEPE	89.7	77.1	73.4	156	< 0.001
9-HEPE	57.4	118	61.9	165	0.012
5-HEPE	80.3	125	52.2	48.9	< 0.001
17-HDoHE	122	125	128	222	0.02
14-HDoHE	129	51.7	84	152	< 0.001
9,10-EpO	115	142	117	148	< 0.001
12,13-EpODE	107	133	75	110	0.011
9,10-EpOME	95.1	158	69.6	134	0.9
12,13-Ep-9-KODE	31.3	80.2	42.1	76.4	< 0.001
15,16-EpODE	54.1	75.1	53.5	53.9	< 0.001
11,12-EpETrE	74.7	124	69	145	0.001
8,9-EpETrE	210	98.1	163	126	< 0.001
13-KODE	105	131	79.3	143	< 0.001
15-KETE	107	54.4	71.2	134	< 0.001
5-KETE	48.5	83	54.8	104	0.013
10-Nitrolinoleate	50.1	82.7	72.9	128	< 0.001

[a] Coefficient of Variance calculated as the ratio of the standard deviation of all subject's lipid mediator concentrations when standardized using the appropriate denominator to the mean of the same values

[b] The reported p-values are adjusted for multiple comparisons by the Benjamini-Hochberg procedure at q = 0.2

[c] This analyte represents the sum of the peaks of all observed isomers of the linoleate-derived triols. Concentrations were calculated relative to concentrations of authentic 9,12,13-TriHOME standards

Supplemental Table S5

Supplemental Table S5B. Effects of various standardizing strategies on sebum lipid mediator concentrations in individuals without atopic dermatitis (n = 9 in all cases).

Lipid Mediator	Coefficient of Variance (%) [a]				
	Per Sebutape Patch	Per NEFA	Per Total TFA	Per Sebumeter Reading	p [b]
Endocannabinoids					
1-OG	92.1	31.5	60.1	93.7	< 0.001
2-OG	94	64.9	67.1	95.3	< 0.001
1-LG	68.8	63.9	54	112	< 0.001
2-LG	96.9	149	64.6	88.2	< 0.001
1-AG	123	56.8	89.9	174	< 0.001
2-AG	178	181	166	139	0.011
PEA	73.1	49.4	69.6	175	< 0.001
SEA	45.1	81.6	47.9	129	< 0.001
OEA	120	132	136	233	< 0.001
LEA	76.3	113	102	211	< 0.001
AEA	142	47.8	90.1	115	< 0.001
DGLEA	133	54.1	98.2	80.9	< 0.001
DHEA	178	176	165	113	0.02
Sphingolipids					
18:1 Sphingosine	16.8	62.9	44	143	< 0.001
C14 Ceramide	46.8	52.3	30	83.8	< 0.001
C16 Ceramide	33.1	56.7	55.3	168	< 0.001
C18 Ceramide	50	90.9	63.7	100	< 0.001
C18:1 Ceramide	30.2	77.7	39.6	98.3	< 0.001
C20 Ceramide	74.7	138	66.3	125	< 0.001
C24 Ceramide	59.2	93.8	78.9	90.5	< 0.001
C18 dihydroceramide	37.3	80	46.2	84.5	< 0.001
C24 dihydroceramide	68.1	100	77.2	83.7	< 0.001

[a] Coefficient of Variance calculated as the ratio of the standard deviation of all subject's lipid mediator concentrations when standardized using the appropriate denominator to the mean of the same values

[b] The reported p-values are adjusted for multiple comparisons by the Benjamini-Hochberg procedure at q = 0.2

[c] This analyte represents the sum of the peaks of all observed isomers of the linoleate-derived triols. Concentrations were calculated relative to concentrations of authentic 9,12,13-TriHOME standards

Supplemental Table S6

Supplemental Table S6. Lipid mediator concentrations in analytes detected in both sweat and sebum collected from the same subjects (n = 19). Analyte concentrations are reported per representative sample of each matrix. Sweat concentrations were obtained from data previously published in Journal of Lipid Research. Agrawal, K., L.A. Hassoun, N. Foolad, T.L. Pedersen, R.K. Sivamani, and J.W. Newman. Sweat lipid mediator profiling: a noninvasive approach for cutaneous research. Journal of Lipid Research. 2017; 58:188-195. © the American Society for Biochemistry and Molecular Biology.

Lipid Mediator	Concentration (pmol/sample) [a]		*P* [b]	Fold Difference [c]	Spearman's p (*P*)
	Sweat	Sebum			
Oxylipins and Nitrolipids					
5-HETE	0.00551 ± 0.00565	0.155 ± 0.199	4.60E-09	23.5 [3.4 - 214]	0.25 (0.3)
8-HETE	0.00711 ± 0.00704	0.088 ± 0.14	0.87	6.9 [0.4 - 87]	0.42 (0.08)
11-HETE	0.00602 ± 0.00472	0.0555 ± 0.0658	1.00E-05	6.2 [0.2 - 62]	0.45 (0.05)
12-HETE	0.0232 ± 0.0338	0.951 ± 1.23	2.40E-08	45.7 [3 - 1582]	0.25 (0.3)
15-HETE	0.0166 ± 0.0243	1.09 ± 1.42	4.10E-11	65.3 [8.2 - 588]	0.41 (0.09)
9-HEPE	0.00184 ± 0.00123	0.0119 ± 0.0083	5.10E-05	5.9 [0.1 - 79]	0.11 (0.7)
12-HEPE	0.00395 ± 0.00256	0.0284 ± 0.0286	2.00E-04	5.3 [0.2 - 55]	-0.02 (0.9)
9,10-e-DiHO	25.2 ± 82.9	3.42 ± 1.17	0.7	0.9 [0.01 - 7.4]	-0.01 (1)
9,10-DiHOME	0.166 ± 0.203	1.88 ± 0.529	4.10E-11	16.4 [1.9 - 62]	0.39 (0.1)
12,13-DiHOME	0.246 ± 1.04	1.38 ± 1.53	8.70E-05	261.9 [0.2 - 2560]	-0.04 (0.9)
9,10-DiHODE	0.00591 ± 0.00465	0.0701 ± 0.0299	4.60E-09	15.2 [3.7 - 111]	-0.05 (0.8)
15,16-DiHODE	0.029 ± 0.0447	0.291 ± 0.334	8.00E-08	12.9 [1.6 - 185]	0.19 (0.4)
5,6-DiHETrE	0.154 ± 0.11	0.00914 ± 0.026	2.10E-03	0.04 [0.003 - 2.2]	0.18 (0.5)
8,9-DiHETrE	0.0339 ± 0.022	4.37 ± 3.21	4.90E-14	119.4 [34 - 574]	0.28 (0.2)
17,18-DiHETE	0.0418 ± 0.0393	0.341 ± 0.21	9.90E-06	9.9 [0.3 - 81]	-0.26 (0.3)
9,10-EpOME	0.0783 ± 0.126	4.72 ± 5.87	0.15	70.8 [0.5 - 2001]	-0.11 (0.6)
11,12-EpETrE	0.00102 ± 0.00112	0.0155 ± 0.0134	7.60E-06	18.9 [1.1 - 3885]	-0.04 (0.9)
13-KODE	0.157 ± 0.304	12.1 ± 12.3	2.00E-09	113.5 [1.4 - 4273]	0.23 (0.3)
12,13-Ep-9-KODE	0.103 ± 0.154	5.47 ± 1.57	1.40E-12	101 [11 - 567]	0.29 (0.2)
5-KETE	0.00199 ± 0.00139	0.0124 ± 0.00804	1.90E-05	7.3 [0.6 - 153]	-0.01 (1)
10-Nitrolinoleate	0.00893 ± 0.0133	0.19 ± 0.136	2.40E-08	29.2 [1.2 - 357]	0.21 (0.4)
PGE1	0.0167 ± 0.0139	0.024 ± 0.0881	0.15	0.5 [0.03 - 17]	0.34 (0.2)
Sum TriHOMEs [a]	1.66 ± 1.85	1.87 ± 2.54	0.72	0.9 [0.1 - 4.8]	0.41 (0.09)

[a] Values are reported as Mean ± SD.

[b] P values are adjusted for multiple comparisons using the Benjamini-Hochberg procedure (q = 0.2).

[c] Ratio of each individual's sebum lipid mediator concentrations to that individual's sweat lipid mediator concentrations. Data are presented as geometric mean [range].

[d] This analyte represents the sum of the peaks of all observed isomers of the linoleate-derived triols. Concentrations were calculated relative to concentrations of authentic 9,12,13-TriHOME standards

Supplemental Table S6

Supplemental Table S6. Lipid mediator concentrations in analytes detected in both sweat and sebum collected from the same subjects (n = 19). Analyte concentrations are reported per representative sample of each matrix. Sweat concentrations were obtained from data previously published in Journal of Lipid Research. Agrawal, K., L.A. Hassoun, N. Foolad, T.L. Pedersen, R.K. Sivamani, and J.W. Newman. Sweat lipid mediator profiling: a noninvasive approach for cutaneous research. Journal of Lipid Research. 2017; 58:188-195. © the American Society for Biochemistry and Molecular Biology.

Lipid Mediator	Concentration (pmol/sample) [a]		*P* [b]	Fold Difference [c]	Spearman's p (*P*)
	Sweat	Sebum			
Endocannabinoids					
PEA	0.203 ± 0.499	104 ± 88.3	2.70E-13	1008.8 [74 - 6195]	0.38 (0.1)
OEA	0.0234 ± 0.0501	25.4 ± 35.1	3.30E-13	1234.4 [25 - 15169]	0.57 (0.01)
SEA	0.219 ± 0.533	63.5 ± 35.1	2.70E-13	745.4 [41 - 6605]	0.18 (0.5)
LEA	0.0025 ± 0.00196	5.31 ± 8.2	0.16	1273.9 [147 - 18128]	0.06 (0.8)
AEA	0.00106 ± 0.000648	0.0177 ± 0.0287	2.30E-08	12.5 [3.6 - 419]	0.34 (0.2)
2-OG	53.2 ± 208	416 ± 388	6.60E-08	276.5 [0.3 - 21794]	0.38 (0.1)
1-OG	412 ± 1590	777 ± 873	1.80E-05	45 [0.1 - 3041]	0.24 (0.3)
2-LG	6.58 ± 22.5	24 ± 33.3	0.83	31.1 [0.03 - 4553]	0.49 (0.03)
1-LG	72.6 ± 253	300 ± 230	0.06	69.2 [0.2 - 3053]	0.34 (0.2)
2-AG	1.88 ± 6.66	3.75 ± 4.87	2.00E-04	11.6 [0.1 - 708]	-0.03 (0.9)
1-AG	13.2 ± 48.9	1.17 ± 3.24	0.41	1.1 [0.01 - 136]	0.37 (0.1)
Sphingolipids					
18:1 Sphingosine	0.457 ± 0.422	31 ± 7.37	6.60E-12	101.9 [15 - 3056]	-0.06 (0.8)
C14 Ceramide	0.0321 ± 0.0333	6.81 ± 3.32	5.40E-13	343.4 [46 - 17633]	0.41 (0.08)
C16 Ceramide	0.221 ± 0.155	27.8 ± 13.8	2.70E-13	148.8 [33 - 1290]	0.23 (0.4)
C18 Ceramide	0.0446 ± 0.0349	1.07 ± 0.693	1.60E-07	22.9 [0.3 - 727]	-0.14 (0.6)
C20 Ceramide	0.0651 ± 0.0496	4.25 ± 3.5	5.00E-11	69.5 [9.7 - 1549]	-0.17 (0.5)
C24 Ceramide	0.163 ± 0.137	10.5 ± 6.11	5.00E-11	70.7 [5.6 - 1570]	-0.33 (0.2)
C18 dihydroceramide	0.0333 ± 0.057	3.98 ± 1.55	2.70E-13	203.8 [14 - 1502]	0.06 (0.8)
C24 dihydroceramide	0.131 ± 0.126	7.96 ± 5.12	3.10E-11	69.3 [5.5 - 641]	-0.1 (0.7)

[a] Values are reported as Mean ± SD.

[b] P values are adjusted for multiple comparisons using the Benjamini-Hochberg procedure (q = 0.2).

[c] Ratio of each individual's sebum lipid mediator concentrations to that individual's sweat lipid mediator concentrations. Data are presented as geometric mean [range].

[d] This analyte represents the sum of the peaks of all observed isomers of the linoleate-derived triols. Concentrations were calculated relative to concentrations of authentic 9,12,13-TriHOME standards.