SUPPLEMENTAL MATERIAL:

Oral ibuprofen differentially affects plasma and sweat lipid mediator profiles in healthy adult males

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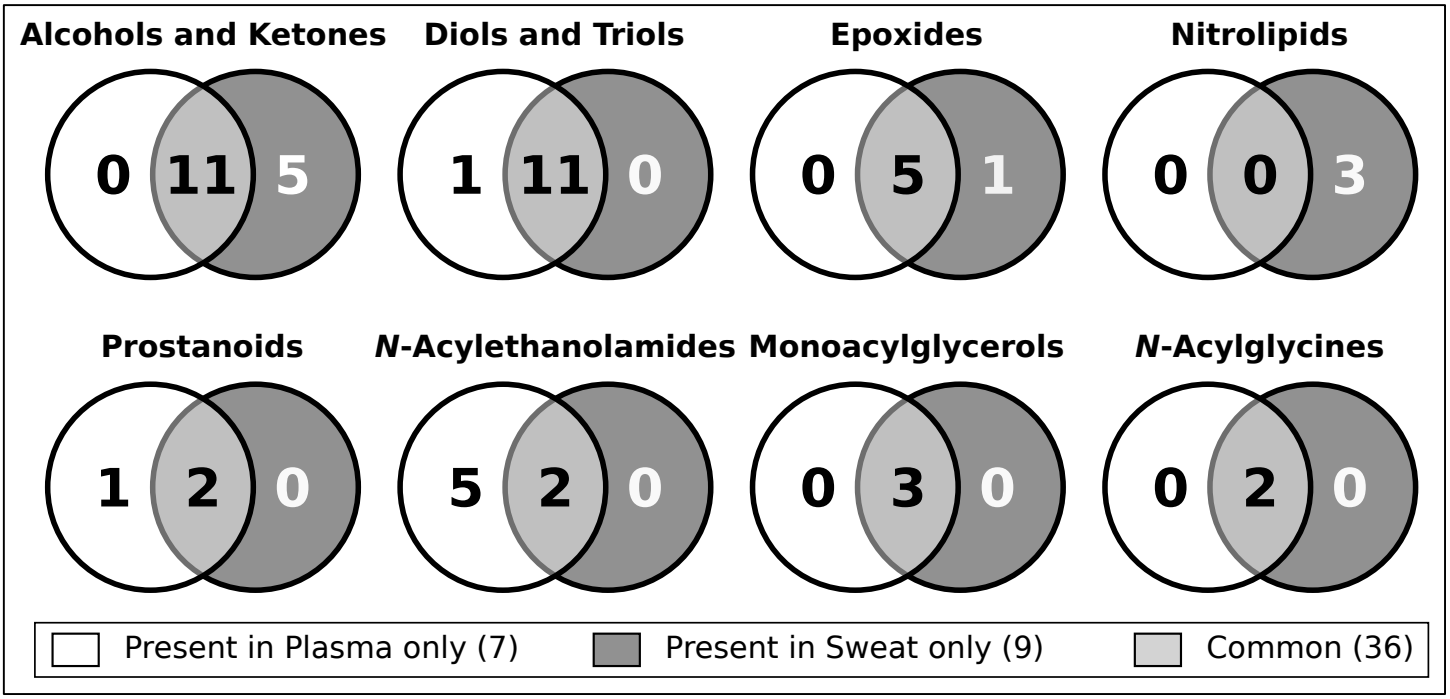
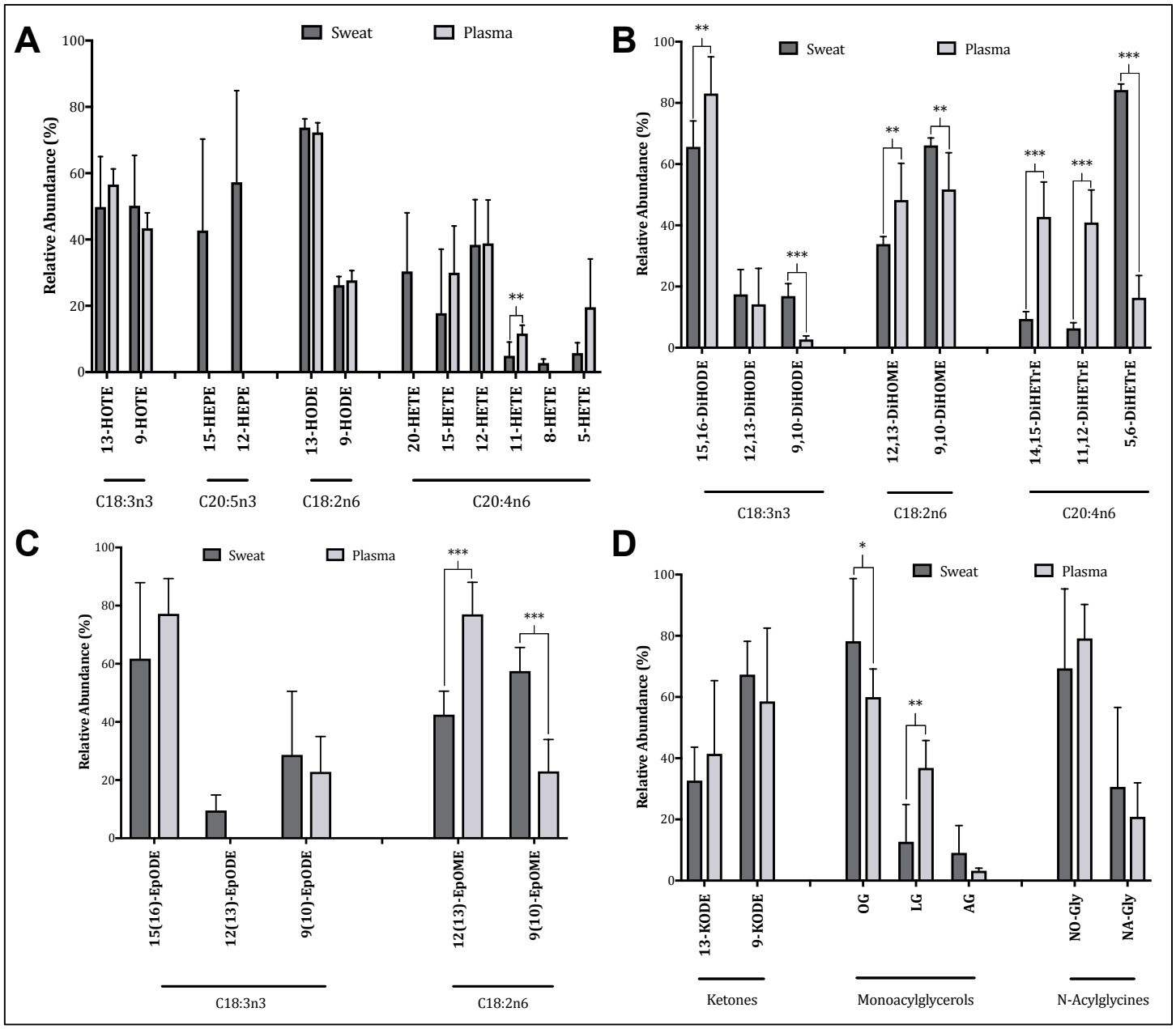
Supplemental Figure S1



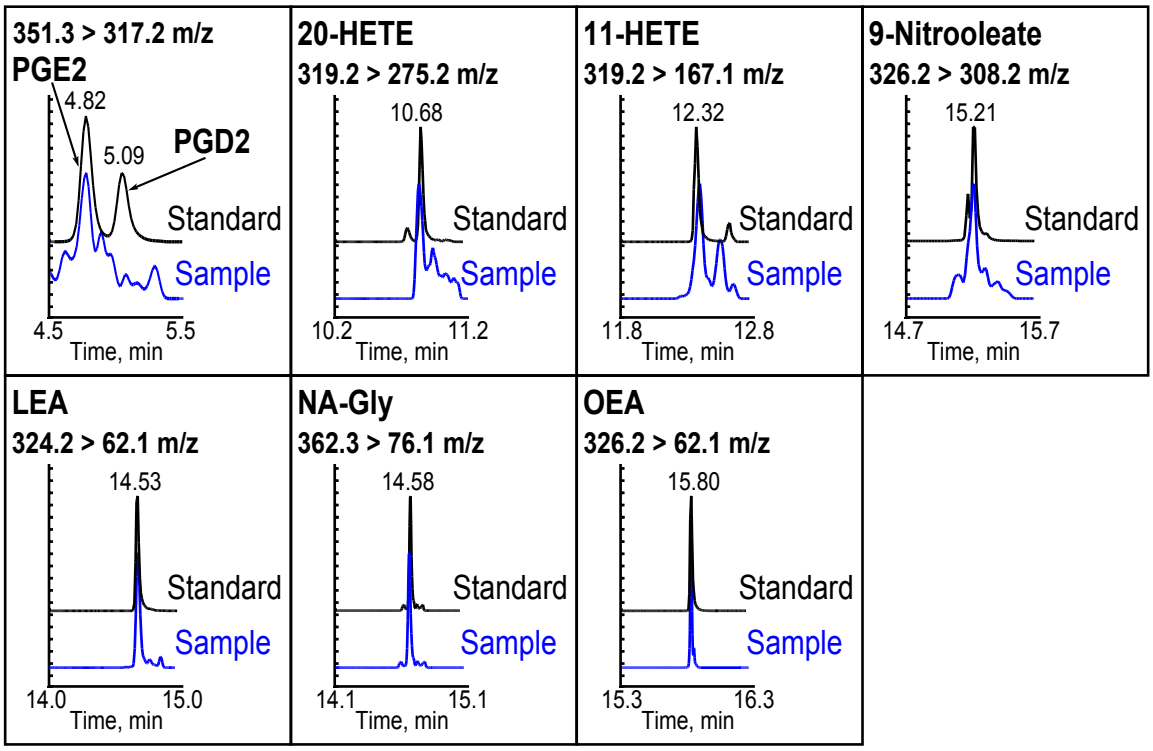
Supplemental Fig. S1. Plasma and sweat demonstrate different lipid mediator profiles. Of the 43 lipid mediators detected in plasma and 45 lipid mediators detected in sweat, 36 are common to both matrices and 16 are unique. Despite this considerable overlap in lipid mediator profiles, individual plasma and sweat lipid mediators do not appear to be correlated, and relative abundances of lipid mediator classes as well as class-specific relative abundances of individual lipid mediator isomers derived from the same fatty acid precursor are different, which suggests the origins of lipid mediators are different in each matrix.

Supplemental Figure S2



Supplemental Fig. S2. Class-specific relative abundances of lipid mediator isomers derived from the same fatty acid precursor demonstrate differences at baseline. (A) Alcohols derived from arachidonate demonstrate increased proportions of 11-hydroxyeicosatetraenoic acid (HETE) in plasma, and 20-HETE and 8-HETE are detectable in sweat but not plasma. (B) Diols derived from a-linolenate, linoleate and arachidonate demonstrate isomeric differences in sweat and plasma. (C) Epoxides derived from linoleate demonstrate isomeric differences in sweat and plasma. (D) While no differences were observed in plasma and sweat ketone or N-acylglycine proportions, plasma was enriched in oleoylglycerol whereas sweat was enriched in linoleoylglceryol. Data are reported as arithmetic mean ± standard deviation (n = 8), and matrix differences were evaluated using Wilcoxon's rank-sum exact tests. * $P < 0.05$; ** $P < 0.005$; *** $P < 0.0005$.

Supplemental Figure S3



Supplemental Fig. S3. Representative chromatograms of sweat lipid mediators affected by oral consumption of 400 mg ibuprofen. Extracted ion chromatograms acquired following UPLC-MS/MS analysis indicate detected analytes in a representative sweat sample obtained from a subject and are overlaid with extracted ion chromatograms from the representative standard to demonstrate appropriateness of peak selection in the samples.

Supplemental Table S1

Supplemental Table S1. Baseline physiological characteristics and exercise parameters of study participants. Values are reported as either Arithmetic Mean ± SD or Geometric Mean [Range].

Parameter	Observed Value (n = 9)
Age (yr)	27.6 ± 2.9
Height (cm)	180.6 ± 6.9
Weight (kg)	82.4 ± 14.0
Body Mass Index (kg/m^2)	25.3 ± 4.6
Sweat Volume Collected (μL)	
Baseline (0 hr)	45 [9 - 105]
0.5 hr after Ibuprofen intake	43 [14 - 93]
2 hr after Ibuprofen intake	75 [44 - 95]
4 hr after Ibuprofen intake	48 [11 - 137]

Supplemental Table S2

Supplemental Table S2A. 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 S2

Supplemental Table S2B. 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)
Aspirin	NSAID		d4-Aspirin	2.84	Negative	178.8 > 137.2	-18	-35
d4-Aspirin	SSTD		PHAU -esi	2.85	Negative	182.9 > 140.9	-18	-45
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
Naproxen	NSAID		d3-Naproxen	5.50	Negative	229.0 > 185.0	-12	-35
d3-Naproxen	SSTD		PHAU -esi	5.50	Negative	232.0 > 188.0	-9	-35
Resolvin D1	Triol	C22:6n3	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 S2

Supplemental Table S2B. 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
Diclofenac	NSAID		d4-Diclofenac	7.78	Negative	294.1 > 250.1	-18	-35
d4-Diclofenac	SSTD		CUDA -esi	7.78	Negative	300.1 > 256.1	-18	-35
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
Ibuprofen	NSAID		d3-Ibuprofen	8.88	Negative	205.1 > 161.1	-9	-50
d3-Ibuprofen	SSTD		CUDA -esi	8.88	Negative	208.0 > 164.0	-9	-55
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

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Supplemental Table S2

Supplemental Table S2B. 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
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

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

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Supplemental Table S2

Supplemental Table S2B. 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)
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
Acetaminophen	NSAID		d4-Acetaminophen	1.81	Positive	152.1 > 110.1	21	60
d4-Acetaminophen	SSTD		PHAU +esi	1.81	Positive	156.1 > 114.1	21	60
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

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

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Supplemental Table S2

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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)
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
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 S3

Supplemental Table S3. List of 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 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

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[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 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	C22:6n3	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

[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 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
ASA	Aspirin	2-(acetyloxy)benzoic acid	Non-Steroidal Anti-Inflammatory Drug		HMDB0001879	2244	BSYNRYMUTXBXSQ-UHFFFAOYSA-N
APAP	Acetaminophen / Paracetamol	N-(4-hydroxyphenyl)acetamide	Non-Steroidal Anti-Inflammatory Drug		HMDB0001859	1983	RZVAJINKPMORJF-UHFFFAOYSA-N
DIC	Diclofenac	2-{2-[(2,6-dichlorophenyl)amino]phenyl}acetic acid	Non-Steroidal Anti-Inflammatory Drug		HMDB0014724	3033	DCOPUUMXTXDBNB-UHFFFAOYSA-N
IBU / IBP	Ibuprofen	2-[4-(2-methylpropyl)phenyl]propanoic acid	Non-Steroidal Anti-Inflammatory Drug		HMDB0001925	3672	HEFNNWSXXWATRW-UHFFFAOYSA-N
NAP / NP	Naproxen	(2S)-2-(6-methoxynaphthalen-2-yl)propanoic acid	Non-Steroidal Anti-Inflammatory Drug		HMDB0001923	156391	CMWTZPSULFXXJA-VIFPVBQESA-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 S4

Supplemental Table S4. Ibuprofen and detected lipid mediator concentrations in plasma and sweat at baseline and at three timepoints after oral administration of 400 mg ibuprofen to healthy male adult subjects (n = 9). All values are expressed as Geometric Mean [Range] and upper-case superscript letters indicate differences between group means as determined by linear mixed models with Tukey's post-hoc HSD.

Lipid Mediator	Units	Concentration in Plasma						Concentration in Sweat						Baseline (0 h) Concentration Correlation [a]	
		0 h [a]	0.5 h [a]	2 h [b]	4 h [a]	*P* [c]	q [d]	0 h	0.5 h	2 h	4h	*P* [c]	q [d]	Kendall's τ	*P* [e]
Ibuprofen	µg/mL	ND[A]	18.8 [3.4 - 65.3][B]	48.3 [39.1 - 75.9][C]	33.8 [14.9 - 90.1][B,C]	< 0.0001	< 0.0001	ND	ND	ND	ND				
Oxylipin - Prostaglandin															
PGE1	pmol/mL or nM	0.126 [0.04 - 0.421]	0.0867 [0.02 - 0.17]	0.152 [0.01 - 0.9]	0.158 [0.02 - 1.2]	0.6	0.7	0.453 [0.12 - 4.91]	0.343 [0.09 - 1.95]	0.394 [0.14 - 1.41]	0.413 [0.2 - 0.92]	0.9	0.6	0.296	0.3
PGE2	pmol/mL or nM	0.159 [0.06 - 0.6]	0.145 [0.02 - 0.51]	0.0893 [0.02 - 1.23]	0.219 [0.02 - 2.73]	0.6	0.7	2.71 [0.34 - 51.6][A]	2.01 [0.67 - 22.2][A,B]	1.28 [0.15 - 12.9][A,B]	0.848 [0.37 - 3.24][B]	0.04	0.15	0.473	0.1
PGF2a	pmol/mL or nM	5.47 [1.43 - 23.7]	5.02 [1.13 - 22.7]	3.95 [0.07 - 18.3]	2.52 [0.08 - 17.2]	0.8	0.7	ND	ND	ND	ND				
Oxylipin - Alcohol															
13-HODE	pmol/mL or nM	23 [11.7 - 40.7]	19.2 [11.9 - 26.1]	22.9 [12.9 - 51.8]	32.6 [17.6 - 98.6]	0.1	0.3	21.9 [3.72 - 69.6]	23.6 [1.3 - 60.1]	24.7 [0.62 - 86]	26 [0.62 - 135]	0.5	0.5	0.214	0.5
9-HODE	pmol/mL or nM	8.77 [5.38 - 16]	6.91 [3.83 - 10.5]	8.48 [5.41 - 18.1]	12.8 [6.97 - 41.1]	0.07	0.3	7.72 [1.69 - 23.4]	8.16 [0.46 - 23.3]	8.04 [0.22 - 29.7]	9.24 [0.23 - 44.2]	0.5	0.5	0	1
13-HOTE	pmol/mL or nM	1.56 [0.92 - 4.65]	1.36 [0.36 - 2.44]	1.37 [0.36 - 8.46]	2.94 [1.16 - 19.5]	0.1	0.3	1.08 [0.29 - 3.23]	0.988 [0.01 - 4.65]	1.38 [0.15 - 3.13]	1.84 [0.06 - 11]	0.2	0.4	-0.214	0.5
9-HOTE	pmol/mL or nM	1.19 [0.71 - 2.43]	0.916 [0.36 - 2.06]	1.14 [0.64 - 6.12]	1.45 [0.54 - 3.94]	0.5	0.6	1.08 [0.53 - 3.25]	1.11 [0.31 - 3.52]	0.957 [0.3 - 1.64]	1.4 [0.13 - 7.98]	0.7	0.6	-0.473	0.1
20-HETE	pmol/mL or nM	ND	ND	ND	ND			0.742 [0.25 - 1.74][A]	0.675 [0.23 - 1.3][A,B]	0.242 [0.02 - 0.76][B]	0.792 [0.2 - 1.93][A]	0.006	0.04		
15-HETE	pmol/mL or nM	0.861 [0.14 - 3.56]	0.828 [0.28 - 2.92]	1.15 [0.62 - 9.01]	1.75 [0.96 - 6.62]	0.2	0.4	0.311 [0.06 - 4.05]	0.302 [0.04 - 1.07]	0.541 [0.05 - 6.31]	0.352 [0.02 - 1.49]	0.2	0.3	0.074	0.8
12-HETE	pmol/mL or nM	1.31 [0.66 - 6.38]	1.45 [0.54 - 3.18]	1.4 [0.81 - 2.92]	2.02 [1.05 - 6.66]	0.4	0.6	0.965 [0.52 - 1.7]	0.481 [0.11 - 1.8]	0.717 [0.27 - 1.61]	0.611 [0.17 - 1.49]	0.07	0.19	0.214	0.5
11-HETE	pmol/mL or nM	0.408 [0.2 - 0.88]	0.276 [0.11 - 0.67]	0.324 [0.07 - 1.57]	0.305 [0.02 - 0.82]	0.8	0.7	0.0882 [0.01 - 0.39][A]	0.136 [0.01 - 0.34][A,B]	0.152 [0.01 - 0.52][A,B]	0.239 [0.11 - 0.81][B]	0.006	0.04	0	1
8-HETE	pmol/mL or nM	ND	ND	ND	ND			0.0618 [0.01 - 0.18]	0.0596 [0.02 - 0.15]	0.0708 [0.01 - 0.27]	0.0772 [0.04 - 0.15]	0.5	0.5		
5-HETE	pmol/mL or nM	0.425 [0.02 - 1.86]	0.73 [0.12 - 3.49]	0.693 [0.37 - 1.41]	1.16 [0.42 - 2.19]	0.2	0.4	0.138 [0.04 - 0.36]	0.0932 [0.02 - 0.2]	0.138 [0.06 - 0.42]	0.0747 [0.01 - 0.49]	0.5	0.5	-0.327	0.3
15-HEPE	pmol/mL or nM	ND	ND	ND	ND			0.0576 [0.00136 - 0.3]	0.0763 [0.03 - 0.13]	0.0934 [0.04 - 0.39]	0.0863 [0.02 - 0.3]	0.7	0.6		
12-HEPE	pmol/mL or nM	ND	ND	ND	ND			0.0781 [0.01 - 0.23]	0.0885 [0.02 - 0.25]	0.0801 [0.01 - 0.23]	0.0761 [0.01 - 0.27]	1	0.6		
17-HDoHE	pmol/mL or nM	2.55 [0.1 - 34.7]	1.71 [0.32 - 9.84]	3.08 [0.72 - 8.59]	3.9 [0.22 - 75]	0.7	0.7	0.46 [0.09 - 7.41]	0.212 [0.13 - 0.9]	0.308 [0.05 - 1.59]	0.257 [0.03 - 0.7]	0.3	0.4	0.286	0.3

[a] Due to LC-MS/MS injection failures in plasma samples, reported data are based on $n = 8$.

[b] Due to LC-MS/MS injection failures in plasma samples, reported data are based on $n = 7$.

[c] *P* value calculated by repeated measures linear mixed model ANOVA. Values are not adjusted for multiple comparisons.

[d] False discovery rate calculated according to the procedures of Storey and Tibshirani (2003). Q < 0.2 was considered acceptable for this study.

[e] Reported *P* values are not adjusted for multiple comparisons.

[f] 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.

[g] Sum of the 1- and 2- isomers of each monoacylglyceride.

Supplemental Table S4

Supplemental Table S4. Ibuprofen and detected lipid mediator concentrations in plasma and sweat at baseline and at three timepoints after oral administration of 400 mg ibuprofen to healthy male adult subjects (n = 9). All values are expressed as Geometric Mean [Range] and upper-case superscript letters indicate differences between group means as determined by linear mixed models with Tukey's post-hoc HSD.

Lipid Mediator	Units	Concentration in Plasma						Concentration in Sweat						Baseline (0 h) Concentration Correlation [a]	
		0 h [a]	0.5 h [a]	2 h [b]	4 h [a]	*P* [c]	q [d]	0 h	0.5 h	2 h	4h	*P* [c]	q [d]	Kendall's τ	*P* [e]
Oxylipin - Diol															
9,10-e-DiHO	pmol/mL or nM	10.4 [5.76 - 34.1]	8.34 [4.37 - 27.8]	9.82 [4.88 - 47.7]	14.6 [6.5 - 89]	0.5	0.6	58.4 [39 - 135]	63.5 [28.1 - 196]	50.4 [24.9 - 97.7]	64.7 [9.99 - 256]	0.8	0.6	-0.500	0.08
12,13-DiHOME	pmol/mL or nM	4.13 [2.24 - 10.4]	3.81 [2.08 - 7.22]	4.87 [2.36 - 13.8]	6.35 [3.26 - 19.2]	0.09	0.3	1.89 [0.9 - 3.6]	1.95 [0.92 - 3.16]	1.61 [0.54 - 3.72]	1.68 [0.21 - 5.64]	0.8	0.6	-0.071	0.8
9,10-DiHOME	pmol/mL or nM	4.44 [1.44 - 12]	3.94 [1.71 - 8.71]	4.23 [2.46 - 9.76]	6.21 [3.22 - 16.9]	0.3	0.5	3.61 [1.85 - 7.66]	4.15 [2.79 - 8.1]	3.2 [1.25 - 7.56]	3.17 [0.56 - 10.5]	0.7	0.6	-0.286	0.3
15,16-DiHODE	pmol/mL or nM	15 [6.96 - 37.5]	12.3 [6.37 - 30.6]	16.5 [10.7 - 57.5]	17.1 [8.77 - 54.7]	0.2	0.4	1.49 [0.43 - 5.65]	1.65 [0.42 - 4.04]	1.04 [0.18 - 3.3]	1.12 [0.12 - 7.01]	0.4	0.5	-0.286	0.3
12,13-DiHODE	pmol/mL or nM	1.77 [0.3 - 7.52]	2.11 [0.43 - 8.95]	1.58 [0.3 - 27.6]	2.14 [0.85 - 35]	0.9	0.8	0.332 [0.12 - 1.34]	0.512 [0.1 - 1.53]	0.382 [0.09 - 0.91]	0.417 [0.04 - 3.55]	0.6	0.5	-0.357	0.2
9,10-DiHODE	pmol/mL or nM	0.458 [0.2 - 1.04]	0.409 [0.22 - 1.45]	0.434 [0.2 - 3.16]	0.463 [0.11 - 1.22]	1	0.8	0.35 [0.1 - 0.87]	0.416 [0.1 - 0.86]	0.319 [0.07 - 0.75]	0.327 [0.03 - 2]	0.8	0.6	-0.473	0.1
14,15-DiHETrE	pmol/mL or nM	1.17 [0.7 - 2.77]	1.18 [0.76 - 1.67]	1.29 [0.85 - 2.24]	1.45 [1.01 - 2.3]	0.4	0.6	0.341 [0.09 - 1.09]	0.479 [0.06 - 1.44]	0.396 [0.08 - 1.08]	0.433 [0.03 - 2.12]	0.5	0.5	-0.286	0.3
11,12-DiHETrE	pmol/mL or nM	1.11 [0.56 - 3.09]	1.04 [0.69 - 1.8]	1.25 [0.62 - 4.92]	1.42 [0.71 - 4.52]	0.7	0.7	0.231 [0.07 - 1.02]	0.285 [0.06 - 0.99]	0.203 [0.08 - 0.51]	0.301 [0.02 - 1.37]	0.5	0.5	0.036	0.9
5,6-DiHETrE	pmol/mL or nM	0.406 [0.06 - 1.04]	0.674 [0.26 - 1.84]	0.507 [0.18 - 1.3]	0.871 [0.48 - 3.15]	0.06	0.3	3.29 [1.28 - 10.7]	4.45 [0.83 - 11.9]	3.63 [1.65 - 7.42]	4.21 [0.42 - 17.3]	0.5	0.5	-0.255	0.4
17,18-DiHETE	pmol/mL or nM	20.2 [7.4 - 33.2]	21.3 [10.7 - 47.4]	21.6 [10.2 - 82.4]	23.1 [12 - 116]	1	0.8	1.76 [0.31 - 6.72]	2.05 [0.32 - 6.38]	1.55 [0.48 - 4.67]	2.34 [0.14 - 8.72]	0.3	0.4	-0.214	0.5
19,20-DiHDoPA	pmol/mL or nM	1.91 [0.76 - 4.13]	2.55 [1.34 - 4.13]	2.51 [1.52 - 5.23]	2.3 [0.99 - 5.61]	0.6	0.7	ND	ND	ND	ND				
Oxylipin - Triol															
Sum TriHOMEs [f]	pmol/mL or nM	7.88 [4.64 - 12.2]	6.2 [4.66 - 9.33]	6.58 [3.96 - 14.1]	11.3 [4.71 - 115]	0.2	0.4	31.7 [11.4 - 93.5]	39.4 [8.65 - 100]	21.7 [9.23 - 55.6]	25.3 [7.25 - 71.6]	0.07	0.19	0.071	0.8
Oxylipin - Epoxide															
9(10)-EpO	pmol/mL or nM	9.96 [2.37 - 45.8]	8.28 [3.87 - 16.6]	4.92 [2.02 - 58.3]	13.2 [3.81 - 107]	0.1	0.3	2.81 [0.89 - 6.54]	2.35 [0.99 - 6.43]	1.55 [0.17 - 5.52]	3.07 [0.73 - 6.59]	0.2	0.4	-0.214	0.5
12(13)-EpOME	pmol/mL or nM	4.1 [1.14 - 11.8]	3.49 [1.93 - 7.28]	3.68 [2.09 - 10.3]	4.73 [2.59 - 33.4]	0.9	0.8	0.485 [0.08 - 1.31]	0.822 [0.38 - 1.89]	0.759 [0.12 - 1.86]	0.831 [0.03 - 2.24]	0.2	0.3	-0.445	0.1
9(10)-EpOME	pmol/mL or nM	1.12 [0.26 - 4.7]	1.05 [0.22 - 3.35]	1.28 [0.57 - 7.99]	2.11 [0.57 - 19.1]	0.5	0.6	0.657 [0.16 - 1.93]	0.778 [0.08 - 2.47]	0.749 [0.04 - 2.92]	1.21 [0.08 - 4.49]	0.07	0.2	-0.143	0.6
15(16)-EpODE	pmol/mL or nM	3.95 [0.95 - 11.3]	3.67 [1.22 - 9.12]	3.49 [1.36 - 14.1]	5.83 [2.53 - 56.5]	0.5	0.7	0.491 [0.04 - 4.5]	0.908 [0.16 - 2.55]	0.694 [0.21 - 4.97]	0.625 [0.04 - 2.62]	0.6	0.5	-0.143	0.6
12(13)-EpODE	pmol/mL or nM	ND	ND	ND	ND			0.0703 [0.02 - 0.14]	0.0696 [0.02 - 0.21]	0.0959 [0.02 - 0.35]	0.128 [0.04 - 0.5]	0.06	0.17		
9(10)-EpODE	pmol/mL or nM	1.02 [0.35 - 10.2]	0.926 [0.35 - 2.47]	0.909 [0.25 - 13.9]	1.37 [0.15 - 40.4]	0.9	0.8	0.194 [0.04 - 0.51]	0.302 [0.08 - 0.74]	0.172 [0.01 - 0.57]	0.278 [0.01 - 1.92]	0.4	0.5	0	1

[a] Due to LC-MS/MS injection failures in plasma samples, reported data are based on $n = 8$.

[b] Due to LC-MS/MS injection failures in plasma samples, reported data are based on $n = 7$.

[c] P value calculated by repeated measures linear mixed model ANOVA. Values are not adjusted for multiple comparisons.

[d] False discovery rate calculated according to the procedures of Storey and Tibshirani (2003). Q < 0.2 was considered acceptable for this study.

[e] Reported P values are not adjusted for multiple comparisons.

[f] 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.

[g] Sum of the 1- and 2- isomers of each monoacylglyceride.

Supplemental Table S4

Supplemental Table S4. Ibuprofen and detected lipid mediator concentrations in plasma and sweat at baseline and at three timepoints after oral administration of 400 mg ibuprofen to healthy male adult subjects (n = 9). All values are expressed as Geometric Mean [Range] and upper-case superscript letters indicate differences between group means as determined by linear mixed models with Tukey's post-hoc HSD.

Lipid Mediator	Units	Concentration in Plasma						Concentration in Sweat						Baseline (0 h) Concentration Correlation [a]	
		0 h [a]	0.5 h [a]	2 h [b]	4 h [a]	*P* [c]	q [d]	0 h	0.5 h	2 h	4h	*P* [c]	q [d]	Kendall's τ	*P* [e]
Oxylipin - Ketone															
13-KODE	pmol/mL or nM	1.89 [0.13 - 19.3]	1.66 [0.12 - 9.12]	2.16 [0.43 - 51.1]	3.79 [0.35 - 37.2]	0.7	0.7	2.17 [0.3 - 13.2]	3.32 [1.56 - 16.8]	2.62 [0.05 - 12.3]	2.69 [0.06 - 13.3]	0.8	0.6	-0.214	0.5
9-KODE	pmol/mL or nM	3.09 [0.67 - 15.7]	1.32 [0.02 - 5.24]	1.62 [0.23 - 15.8]	3.42 [0.96 - 33.2]	0.4	0.6	5.35 [0.64 - 38.5]	4.93 [0.45 - 30.5]	3.89 [0.04 - 16.7]	5.14 [0.11 - 24.3]	0.8	0.6	0.071	0.8
12(13)-Ep-9-KODE	pmol/mL or nM	ND	ND	ND	ND			1.82 [0.72 - 3.64]	1.82 [0.53 - 5.54]	1.05 [0.34 - 1.94]	2.38 [0.5 - 12.9]	0.2	0.3		
Nitrolipid															
10-Nitrooleate	pmol/mL or nM	ND	ND	ND	ND			1.78 [0.36 - 6.24]	2.47 [0.13 - 31.5]	0.839 [0.09 - 6.06]	1.6 [0.24 - 9.37]	0.2	0.4		
9-Nitrooleate	pmol/mL or nM	ND	ND	ND	ND			0.729 [0.09 - 3.76] [A,B]	1.68 [0.2 - 14.6] [B]	0.224 [0.05 - 2.57] [A]	0.751 [0.08 - 4.71] [A,B]	0.007	0.04		
10-Nitrolinoleate	pmol/mL or nM	ND	ND	ND	ND			0.297 [0.16 - 0.6]	0.234 [0.05 - 2.32]	0.142 [0.04 - 0.44]	0.175 [0.01 - 0.89]	0.4	0.5		
Endocannabinoid - Acylethanolamide															
OEA	pmol/mL or nM	4.14 [2.83 - 8.65] [A]	4.33 [2.57 - 7.49] [A]	5.58 [3.71 - 8.99] [A,B]	7.78 [3.42 - 21] [B]	0.004	0.04	0.586 [0.09 - 2.7] [A]	0.058 [0.01 - 0.81] [B]	0.0381 [0.01 - 0.13] [B]	0.127 [0.01 - 0.25] [B]	< 0.0001	< 0.0001	-0.214	0.5
LEA	pmol/mL or nM	1.19 [0.67 - 1.95]	1.24 [0.65 - 1.78]	1.26 [0.77 - 2.55]	1.95 [0.96 - 4.4]	0.06	0.2	0.0447 [0.01 - 0.22] [A]	0.0122 [0.01 - 0.03] [B]	0.0177 [0.01 - 0.03] [B]	0.0161 [0.01 - 0.04] [B]	< 0.0005	0.002	0.429	0.1
aLEA	pmol/mL or nM	0.0968 [0.04 - 0.29]	0.0949 [0.04 - 0.29]	0.113 [0.06 - 0.81]	0.166 [0.08 - 0.62]	0.3	0.5	ND	ND	ND	ND				
Dihomo GLA EA	pmol/mL or nM	0.168 [0.05 - 0.39] [A]	0.204 [0.13 - 0.33] [A,B]	0.174 [0.09 - 0.43] [A]	0.315 [0.22 - 0.43] [B]	0.02	0.13	ND	ND	ND	ND				
AEA	pmol/mL or nM	0.627 [0.29 - 0.92] [A]	0.632 [0.41 - 0.95] [A]	0.653 [0.34 - 0.98] [A]	1 [0.62 - 2.58] [B]	0.004	0.04	ND	ND	ND	ND				
DEA	pmol/mL or nM	0.298 [0.21 - 0.48]	0.276 [0.17 - 0.5]	0.259 [0.13 - 0.45]	0.355 [0.17 - 1.14]	0.5	0.6	ND	ND	ND	ND				
DHEA	pmol/mL or nM	0.76 [0.28 - 1.46]	0.837 [0.39 - 2.05]	0.942 [0.41 - 1.82]	1.23 [0.46 - 3.01]	0.07	0.3	ND	ND	ND	ND				
Endocannabinoid - Acylglycine															
NO-Gly	pmol/mL or nM	3.5 [1.62 - 9.44]	3.65 [1.68 - 5.93]	5.09 [3.2 - 9]	5.43 [2.81 - 21.9]	0.1	0.3	0.156 [0.01 - 0.55]	0.132 [0.02 - 1.64]	0.0757 [0.02 - 0.23]	0.0918 [0.02 - 0.4]	0.5	0.5	0.036	0.9
NA-Gly	pmol/mL or nM	0.833 [0.34 - 1.63]	0.55 [0.03 - 2.71]	0.593 [0.41 - 0.87]	1.32 [0.51 - 5.7]	0.09	0.3	0.0627 [0.01 - 0.23] [A,B]	0.103 [0.01 - 0.97] [B]	0.0222 [0.01 - 0.1] [A]	0.0486 [0.01 - 0.16] [A,B]	0.05	0.16	0.109	0.7
Endocannabinoid - Monoacylglycerol															
OG[g]	pmol/mL or nM	393 [212 - 702]	365 [204 - 595]	384 [173 - 1020]	543 [185 - 8150]	0.7	0.7	61.5 [2.67 - 5620]	33.1 [4.61 - 3170]	26.3 [4.33 - 238]	16.6 [1.14 - 406]	0.3	0.4	0.071	0.8
LG[g]	pmol/mL or nM	238 [67.6 - 820]	215 [78.5 - 579]	229 [126 - 661]	243 [104 - 494]	0.9	0.7	4.11 [0.46 - 21.2]	4.09 [0.76 - 17.1]	4.55 [1.39 - 18.4]	2.16 [0.04 - 10.7]	0.4	0.5	0.071	0.8
AG[g]	pmol/mL or nM	20.7 [10 - 51.2]	18.2 [10.6 - 46.5]	17.7 [5.67 - 57.7]	18.6 [5.39 - 41]	0.9	0.8	4.2 [0.15 - 836]	3.5 [0.47 - 287]	2.89 [0.26 - 22.4]	2.24 [0.08 - 33]	0.8	0.6	0.143	0.6

[a] Due to LC-MS/MS injection failures in plasma samples, reported data are based on $n = 8$.

[b] Due to LC-MS/MS injection failures in plasma samples, reported data are based on $n = 7$.

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