

ESM Table S14 Targeted oxylipin metabolomics method.

precursor PUFA	PUFA class	analyte	Q1	Q3	DP	EP	CE	CXP	internal standard	RT	LOD <sup>a</sup>	calibration range	ULOQ <sup>a</sup>	Reference
					[V]	[V]	[V]	[V]		[min]	[nM]	LLOQ <sup>a</sup>	[nM]	
Oleic acid (18:1 n-9)	epoxy-PUFA	9(10)-Ep-stearic acid	297.0	170.8	-120	-10	-24	-11	<sup>14</sup> H <sub>12</sub> (13)-EpOME	23.91	0.25	0.5	500	Koch (2020) Talanta
		trans-9(10)-Ep-stearic acid	297.0	170.8	-120	-10	-24	-11	<sup>14</sup> H <sub>12</sub> (13)-EpOME	24.06		relative quantification based on 9(10)-Ep-stearic acid	500	Rund (2019) POLM
	vic dihydroxy-PUFA	erythro-9,10-DiH-stearic acid	315.2	170.8	-85	-10	-35	-9	<sup>14</sup> H <sub>9</sub> ,10-DiHOME	16.34	0.25	0.50	1000	current paper
		threo-9,10-DiH-stearic acid	315.2	170.8	-85	-10	-35	-9	<sup>14</sup> H <sub>9</sub> ,10-DiHOME	17.29	0.25	0.50	1000	current paper
Linoleic Acid (LA; 18:2 n-6)	hydroxy-PUFA	9-HODE	295.2	171.1	-100	-10	-24	-7	<sup>14</sup> H <sub>9</sub> -9-HODE	19.47	0.14	0.35	348	Koch (2020) Talanta
		10-HODE	295.1	183.0	-90	-10	-25	-7	<sup>14</sup> H <sub>9</sub> -9-HODE	19.40	0.038	0.076	380	Koch (2020) Talanta
		12-HODE	295.1	183.0	-80	-10	-24	-9	<sup>14</sup> H <sub>9</sub> -12-HODE	19.02	0.025	0.05	100	Koch (2020) Talanta
		13-HODE	295.2	195.2	-100	-10	-24	-9	<sup>14</sup> H <sub>9</sub> -9-HODE	19.33	0.1	0.25	500	Koch (2020) Talanta
		15-HODE	295.2	223.0	-95	-10	-24	-9	<sup>14</sup> H <sub>9</sub> -13-HODE	18.19	0.089	0.18	177	Koch (2020) Talanta
		<sup>14</sup> H <sub>9</sub> -13-HODE	299.2	198.1	-80	-10	-24	-9	internal standard	19.21			1000	Koch (2020) Talanta
		<sup>14</sup> H <sub>9</sub> -9-HODE	299.2	172.3	-100	-10	-24	-6	internal standard	19.35			1000	Koch (2020) Talanta
	oxo-PUFA	9-oxo-ODE	293.2	185.1	-115	-10	-26	-8	<sup>14</sup> H <sub>9</sub> -13-oxo-ODE	20.90	0.25	0.5	500	Koch (2020) Talanta
		13-oxo-ODE	293.2	113.0	-100	-10	-27	-8	<sup>14</sup> H <sub>9</sub> -13-oxo-ODE	20.28	0.25	0.5	500	Koch (2020) Talanta
		<sup>14</sup> H <sub>9</sub> -13-oxo-ODE	296.2	198.2	-85	-10	-28	-8	internal standard	20.19			500	Koch (2020) Talanta
	epoxy-PUFA	9(10)-EpOME	295.2	171.1	-105	-10	-19	-8	<sup>14</sup> H <sub>12</sub> (13)-EpOME	22.50	0.081	0.2	405	Koch (2020) Talanta
		trans-9(10)-EpOME	295.2	171.1	-105	-10	-19	-8	<sup>14</sup> H <sub>12</sub> (13)-EpOME	22.65		relative quantification based on 9(10)-EpOME	185	Rund (2019) POLM
		12(13)-EpOME	295.2	195.2	-105	-10	-19	-8	<sup>14</sup> H <sub>12</sub> (13)-EpOME	22.29	0.019	0.037	185	Koch (2020) Talanta
		trans-12(13)-EpOME	295.2	195.2	-105	-10	-19	-8	<sup>14</sup> H <sub>12</sub> (13)-EpOME	22.44		relative quantification based on 12(13)-EpOME	185	Rund (2019) POLM
		<sup>14</sup> H <sub>12</sub> (13)-EpOME	299.2	198.1	-100	-10	-21	-8	internal standard	22.19			1000	Koch (2020) Talanta
	vic dihydroxy-PUFA	9,10-DiHOME	313.2	201.2	-105	-10	-28	-8	<sup>14</sup> H <sub>9</sub> ,10-DiHOME	14.94	0.0075	0.01	250	Koch (2020) Talanta
		12,13-DiHOME	313.2	183.2	-105	-10	-29	-8	<sup>14</sup> H <sub>9</sub> ,10-DiHOME	14.46	0.015	0.029	145	Koch (2020) Talanta
		<sup>14</sup> H <sub>9</sub> ,8,10-DiHOME	317.2	203.4	-105	-10	-28	-8	internal standard	14.84			145	Koch (2020) Talanta
	misc	9,10,11-TriHOME	329.1	201.1	-95	-10	-30	-8	<sup>14</sup> H <sub>9</sub> LA <sub>9</sub>	9.70	0.05	0.1	250	Koch (2020) Talanta
		9,10,13-TriHOME	329.2	171.1	-100	-10	-31	-8	<sup>14</sup> H <sub>9</sub> LA <sub>9</sub>	8.50	0.05	0.1	250	Koch (2020) Talanta
		9,12,13-TriHOME	329.2	211.1	-100	-10	-31	-10	<sup>14</sup> H <sub>9</sub> LA <sub>9</sub>	8.35	0.025	0.05	250	Koch (2020) Talanta
		8-HODE	309.2	291.1	-90	-10	-16	-6	<sup>14</sup> H <sub>9</sub> -9-HODE	17.23		relative quantification based on 12(13)-EpOME	250	Ostermann (2015) Anal Bioanal Chem
gamma-Linolenic Acid (ALA; 18:3 n-3)	hydroxy-PUFA	9-HOTIE	293.2	171.2	-85	-10	-20	-8	<sup>14</sup> H <sub>9</sub> -13-HODE	16.88	0.1	0.25	500	Koch (2020) Talanta
		13-HOTIE	293.2	195.1	-90	-10	-22	-8	<sup>14</sup> H <sub>9</sub> -13-HODE	17.24	0.25	0.5	250	Koch (2020) Talanta
	oxo-PUFA	9-oxo-OTIE	291.0	185.0	-100	-10	-24	-8	<sup>14</sup> H <sub>9</sub> -13-oxo-ODE	18.34	0.1	0.25	500	Koch (2020) Talanta
		13-oxo-OTIE	291.1	195.0	-100	-10	-27	-8	<sup>14</sup> H <sub>9</sub> -13-oxo-ODE	18.12	0.05	0.1	100	Koch (2020) Talanta
epoxy-PUFA	9(10)-EpODE	293.2	171.2	-90	-10	-16	-8	<sup>14</sup> H <sub>12</sub> (13)-EpOME	20.15	0.058	0.116	582	Koch (2020) Talanta	
	12(13)-EpODE	293.2	183.1	-90	-10	-20	-8	<sup>14</sup> H <sub>12</sub> (13)-EpOME	20.61	0.17	0.33	331	Koch (2020) Talanta	
	15(16)-EpODE	293.3	239.2	-90	-10	-16	-4	<sup>14</sup> H <sub>12</sub> (13)-EpOME	19.07	0.092	0.185	924	Koch (2020) Talanta	
	trans-9(10)-EpODE	293.2	171.2	-90	-10	-16	-8	<sup>14</sup> H <sub>12</sub> (13)-EpOME	20.30		relative quantification based on trans-9(10)-EpODE	200	Rund (2019) POLM	
	trans-12(13)-EpODE	293.2	183.1	-90	-10	-20	-8	<sup>14</sup> H <sub>12</sub> (13)-EpOME	20.76		relative quantification based on 12(13)-EpODE	200	Rund (2019) POLM	
	trans-15(16)-EpODE	293.3	235.2	-90	-10	-16	-4	<sup>14</sup> H <sub>12</sub> (13)-EpOME	20.12		relative quantification based on 15(16)-EpODE	200	Rund (2019) POLM	
vic dihydroxy-PUFA	9,10-DiHOME	311.2	201.2	-90	-10	-26	-10	<sup>14</sup> H <sub>9</sub> ,10-DiHOME	12.82	0.01	0.025	100	Koch (2020) Talanta	
	12,13-DiHOME	311.2	183.1	-105	-10	-29	-8	<sup>14</sup> H <sub>9</sub> ,10-DiHOME	12.90	0.1	0.25	250	Koch (2020) Talanta	
	15,16-DiHOME	311.2	223.2	-105	-10	-26	-10	<sup>14</sup> H <sub>9</sub> ,10-DiHOME	12.76	0.18	0.45	181	Koch (2020) Talanta	
misc	9,10,11-TriHOME	327.0	171.0	-80	-10	-25	-8	<sup>14</sup> H <sub>9</sub> LA <sub>9</sub>	8.34	0.025	0.05	250	Koch (2020) Talanta	
	9,10,13-TriHOME	327.2	201.0	-80	-10	-26	-8	<sup>14</sup> H <sub>9</sub> LA <sub>9</sub>	7.35	0.75	1	500	Koch (2020) Talanta	
	9,12,13-TriHOME	327.2	211.0	-80	-10	-29	-10	<sup>14</sup> H <sub>9</sub> LA <sub>9</sub>	7.35	0.05	0.1	250	Koch (2020) Talanta	
gamma-Linolenic Acid (GLA; 18:3 n-6)	hydroxy-PUFA	13-γ-HOTIE	293.0	193.0	-90	-10	-23	-8	<sup>14</sup> H <sub>9</sub> LTB <sub>5</sub>	17.59	1	2.5	500	Koch (2020) Talanta
delta-9-gamma-Linolenic Acid (DGLA; 20:3 n-6)	hydroxy-PUFA	8-HETE	321.2	157.1	-85	-10	-22	-9	<sup>14</sup> H <sub>9</sub> -5-HETE	21.85	0.25	0.5	500	Koch (2020) Talanta
		12-HETE	321.0	181.0	-85	-10	-24	-10	<sup>14</sup> H <sub>9</sub> -5-HETE	22.02	0.1	0.25	500	Koch (2020) Talanta
		15-HETE	321.2	221.2	-90	-10	-21	-10	<sup>14</sup> H <sub>9</sub> -5-HETE	21.47	0.05	0.1	500	Koch (2020) Talanta
	multihydroxy-PUFA	LTB <sub>5</sub>	337.2	195.2	-80	-10	-21	-8	<sup>14</sup> H <sub>11</sub> ,11,12-DiHETE	15.99	0.1	0.25	500	Koch (2020) Talanta
	epoxy-PUFA	14(15)-EpEDE	321.2	221.2	-85	-10	-19	-4	<sup>14</sup> H <sub>11</sub> ,14(15)-EpETE	23.47	0.025	0.05	100	Koch (2020) Talanta
	prostanoids	PGI <sub>1</sub>	335.4	221.0	-85	-10	-28	-7	<sup>14</sup> H <sub>9</sub> -15-deoxy-Δ <sup>12</sup> ,14-PGJ <sub>2</sub>	12.27	0.05	0.10	750	current paper
		PGD <sub>2</sub>	353.3	317.2	-80	-10	-19	-6	<sup>14</sup> H <sub>9</sub> -PGD <sub>2</sub>	9.36	0.05	0.10	250	current paper
		13,14-dihydro-15-keto-PGD <sub>2</sub>	353.3	205.0	-65	-10	-31	-7	<sup>14</sup> H <sub>9</sub> ,13,14-dihydro-15-keto-PGE <sub>2</sub>	11.68	0.25	0.50	1000	current paper
		PGE <sub>1</sub>	353.3	317.2	-80	-10	-19	-6	<sup>14</sup> H <sub>9</sub> -PGE <sub>2</sub>	9.20	0.05	0.10	250	current paper
		13,14-dihydro-PGE <sub>2</sub>	355.4	237.1	-70	-10	-37	-7	<sup>14</sup> H <sub>9</sub> ,13,14-dihydro-15-keto-PGE <sub>2</sub>	9.81	0.17	0.35	698	current paper
		13,14-dihydro-15-keto-PGE <sub>2</sub>	353.3	221.2	-70	-10	-29	-6	<sup>14</sup> H <sub>9</sub> ,13,14-dihydro-15-keto-PGE <sub>2</sub>	10.81	0.25	0.50	1000	current paper
		15-keto-PGE <sub>2</sub>	351.3	209.0	-80	-10	-31	-7	<sup>14</sup> H <sub>9</sub> -PGE <sub>2</sub>	9.96	2.50	5.00	1000	current paper
		PGF <sub>2α</sub>	355.4	293.2	-110	-10	-35	-6	<sup>14</sup> H <sub>9</sub> -PGF <sub>2α</sub>	8.60	0.025	0.05	250	Koch (2020) Talanta
		15-keto-PGF <sub>2α</sub>	353.3	193.1	-70	-10	-37	-6	theoretically <sup>14</sup> H <sub>9</sub> -PGF <sub>2α</sub> <sup>b</sup>	9.46		relative quantification based on 15-keto-PGE <sub>2</sub>	1000	current paper
		TxB <sub>2</sub>	371.3	171.2	-90	-10	-33	-10	<sup>14</sup> H <sub>9</sub> TxB <sub>2</sub>	7.37	0.40	0.80	1608	current paper
	isoprostanes	8-iso-PGE <sub>2</sub>	353.4	235.0	-80	-10	-19	-7	<sup>14</sup> H <sub>9</sub> -PGE <sub>2</sub>	8.84	0.25	0.50	500	current paper
		15-F <sub>2t</sub> -isoP (8-iso-PGF <sub>2α</sub> ) <sup>a</sup>	355.2	211.0	-100	-10	-35	-8	<sup>14</sup> H <sub>9</sub> -PGF <sub>2α</sub>	7.63	0.75	1	500	Koch (2020) Talanta
Mead acid (20:3 n-9)	hydroxy-PUFA	5-HETE	321.2	115.1	-90	-10	-17	-9	<sup>14</sup> H <sub>9</sub> -5-HETE	23.56	0.01	0.025	250	Koch (2020) Talanta
Arachidonic Acid (ARA; 20:4 n-6)	hydroperoxy-PUFA	5-HpETE	335.5	155.0	-40	-10	-23	-13	<sup>14</sup> H <sub>9</sub> -5-HETE	22.13		relative quantification based on 5-HETE	500	Meckelmann (2017) POLM
		12-HpETE	335.5	153.0	-40	-10	-23	-13	<sup>14</sup> H <sub>9</sub> -12-HETE	21.38		relative quantification based on 12-HETE	500	Meckelmann (2017) POLM
		15-HpETE	335.5	113.3	-40	-10	-23	-13	<sup>14</sup> H <sub>9</sub> -15-HETE	20.63		relative quantification based on 15-HETE	500	Meckelmann (2017) POLM
	hydroxy-PUFA	5-HETE	319.2	115.2	-80	-10	-19	-7	<sup>14</sup> H <sub>9</sub> -5-HETE	21.74	0.018	0.035	350	Koch (2020) Talanta
		8-HETE	319.2	155.2	-80	-10	-20	-6	<sup>14</sup> H <sub>9</sub> -12-HETE	21.10	0.094	0.23	468	Koch (2020) Talanta
		9-HETE	319.2	167.2	-80	-10	-21	-7	<sup>14</sup> H <sub>9</sub> -5-HETE	21.45	0.27	0.4	265	Koch (2020) Talanta
		11-HETE	319.2	167.2	-80	-10	-21	-7	<sup>14</sup> H <sub>9</sub> -12-HETE	20.68	0.022	0.044	219	Koch (2020) Talanta
		12-HETE	319.2	179.2	-80	-10	-19	-8	<sup>14</sup> H <sub>9</sub> -12-HETE	21.10	0.1	0.25	500	Koch (2020) Talanta
		15-HETE	319.2	219.2	-80	-10	-18	-8	<sup>14</sup> H <sub>9</sub> -15-HETE	20.08	0.11	0.22	220	Koch (2020) Talanta
		16-HETE	319.2	233.1	-85	-10	-18	-8	<sup>14</sup> H <sub>9</sub> -15-HETE	18.89	0.1	0.25	500	Koch (2020) Talanta
		17-HETE	319.2	247.0	-85	-10	-19	-8	<sup>14</sup> H <sub>9</sub> -15-HETE	18.71	0.1	0.25	500	Koch (2020) Talanta
		18-HETE	319.2	261.0	-85	-10	-20	-8	<sup>14</sup> H <sub>9</sub> -15-HETE	18.49	0.1	0.25	500	Koch (2020) Talanta
		19-HETE	319.3	230.9	-70	-10	-19							

	prostanoids	11P-PGE <sub>2</sub>	351.3	189.1	-40	-10	-24	-7	theoretically <sup>1</sup> H <sub>4</sub> -PGE <sub>2</sub> <sup>®</sup>	9.14		relative quantification based on PGE <sub>2</sub>	3.74		current paper
		20-OH-PGE <sub>2</sub>	340.2	198.1	-70	-10	-27	-8	<sup>1</sup> H <sub>4</sub> -PGE <sub>2</sub>	3.74	0.57	1.14	2288		current paper
		13-keto PGE <sub>2</sub>	349.2	235.1	-40	-10	-20	-7	<sup>1</sup> H <sub>4</sub> -PGE <sub>2</sub>	9.50	0.25	0.50	750		current paper
		13,14-dihydro-15-keto-PGE <sub>2</sub>	351.2	235.2	-75	-10	-18	-13	<sup>1</sup> H <sub>4</sub> -13,14-dihydro-15-keto PGE <sub>2</sub>	10.20	10.00	25.00	1000		current paper
		13,14-dihydro-15-keto-tetranor-PGE <sub>2</sub>	297.0	109.0	-70	-10	-18	-7	<sup>1</sup> H <sub>4</sub> -13,14-dihydro-15-keto PGE <sub>2</sub>	7.32	0.39	0.79	579		current paper
		1a,1b-dihomo PGE <sub>2</sub>	379.4	261.2	-70	-10	-21	-7	<sup>1</sup> H <sub>4</sub> -PGE <sub>2</sub>	11.40	0.03	0.06	451		current paper
		<sup>1</sup> H <sub>4</sub> -PGE <sub>2</sub>	355.2	275.3	-40	-10	-24	-6	internal standard	8.88					current paper
		<sup>1</sup> H <sub>4</sub> -PGE <sub>2</sub>	360.2	280.1	-45	-10	-24	-6	internal standard	8.82					Koch (2020) Talanta
		<sup>1</sup> H <sub>4</sub> -13,14-dihydro-15-keto PGE <sub>2</sub>	355.4	239.1	-45	-10	-31	-7	internal standard	10.26					current paper
		PGF <sub>2α</sub>	353.2	193.0	-40	-10	-33	-7	<sup>1</sup> H <sub>4</sub> -PGF <sub>2α</sub>	8.58	0.25	0.5	500		Koch (2020) Talanta
	isoprostanes	15(R)-PGF <sub>2α</sub>	353.3	193.0	-40	-10	-33	-7	theoretically <sup>1</sup> H <sub>4</sub> -PGF <sub>2α</sub> <sup>®</sup>	8.48		relative quantification based on PGF <sub>2α</sub>			current paper
		11β-PGE <sub>2</sub>	353.3	193.1	-70	-10	-35	-12	<sup>1</sup> H <sub>4</sub> -PGE <sub>2</sub>	7.82	0.50	0.75	1000		current paper
		20-OH-PGF <sub>2α</sub>	369.3	193.0	-70	-10	-37	-7	<sup>1</sup> H <sub>4</sub> -PGE <sub>2</sub>	9.53	1.06	1.59	2121		current paper
		13,14-dihydro-PGF <sub>2α</sub>	355.4	193.0	-40	-10	-34	-7	<sup>1</sup> H <sub>4</sub> -PGE <sub>2</sub>	9.53	5.00	10.00	1000		current paper
		15-keto-PGF <sub>2α</sub>	351.2	219.1	-40	-10	-23	-7	<sup>1</sup> H <sub>4</sub> -PGE <sub>2</sub>	9.17	0.50	0.75	750		current paper
		13,14-dihydro-15-keto-PGF <sub>2α</sub>	353.3	183.3	-100	-10	-35	-10	<sup>1</sup> H <sub>4</sub> -13,14-dihydro-15-keto PGE <sub>2</sub>	10.26	0.75	1.00	1000		current paper
		11β-13,14-dihydro-15-keto-PGF <sub>2α</sub>	353.4	195.0	-45	-10	-34	-7	<sup>1</sup> H <sub>4</sub> -13,14-dihydro-15-keto PGE <sub>2</sub>	9.83	18.25	45.62	1825		current paper
		2,3-dihydro-11β-PGF <sub>2α</sub>	325.3	163.0	-45	-10	-31	-7	<sup>1</sup> H <sub>4</sub> -PGE <sub>2</sub>	5.93	0.65	1.31	2613		current paper
		<sup>1</sup> H <sub>4</sub> -PGF <sub>2α</sub>	357.2	197.0	-40	-10	-33	-7	internal standard	8.54					Koch (2020) Talanta
		6-keto-PGF <sub>2α</sub>	369.3	163.2	-40	-10	-35	-6	<sup>1</sup> H <sub>4</sub> -6-keto-PGF <sub>2α</sub>	6.11	0.64	0.96	640		Koch (2020) Talanta
	misc	2,3-dihydro-6-keto-PGF <sub>2α</sub>	341.1	135.0	-40	-10	-31	-7	<sup>1</sup> H <sub>4</sub> -PGE <sub>2</sub>	7.34	0.15	0.25	800		current paper
		6,15-dihydro-13,14-dihydro-PGF <sub>2α</sub>	369.3	267.0	-70	-10	-31	-7	<sup>1</sup> H <sub>4</sub> -PGE <sub>2</sub>	7.72	45.49	75.82	3033		current paper
		6-keto-PGF <sub>2α</sub>	375.0	167.0	-100	-10	-35	-6	internal standard	11.93	0.014	0.027	135		Koch (2020) Talanta
		PGD <sub>2</sub>	333.3	189.2	-40	-10	-24	-8	<sup>1</sup> H <sub>4</sub> -PGE <sub>2</sub>	11.89	0.86	1.28	1712		Koch (2020) Talanta
		Δ12-PGJ <sub>2</sub>	333.3	189.2	-70	-10	-21	-8	<sup>1</sup> H <sub>4</sub> -15-deoxy-Δ12,14-PGJ <sub>2</sub>	17.73	0.75	1.00	1000		current paper
		15-deoxy-Δ <sup>11</sup> -PGJ <sub>2</sub>	315.2	203.1	-60	-10	-28	-7	<sup>1</sup> H <sub>4</sub> -15-deoxy-Δ12,14-PGJ <sub>2</sub>	17.73	0.75	1.00	1000		current paper
		<sup>1</sup> H <sub>4</sub> -15-deoxy-Δ <sup>11</sup> -PGJ <sub>2</sub>	319.4	203.0	-40	-10	-28	-7	internal standard	17.68	0.25	0.50	1000		current paper
		TxB <sub>2</sub>	369.2	169.0	-40	-10	-24	-7	<sup>1</sup> H <sub>4</sub> -Tx182	7.68	0.75	1.00	1000		current paper
		2,3-dihron-TxB <sub>2</sub>	341.2	167.0	-70	-10	-14	-8	<sup>1</sup> H <sub>4</sub> -Tx182	5.68	1.00	2.50	1000		current paper
		2,3-dihron-TxB <sub>2</sub>	343.0	142.0	-70	-10	-18	-8	<sup>1</sup> H <sub>4</sub> -Tx182	5.17	1.00	2.50	750		current paper
	hydroxy-PUFA	11-dehydro-2,3-dihron-TxB <sub>2</sub>	339.3	133.0	-55	-10	-20	-7	<sup>1</sup> H <sub>4</sub> -TxB <sub>2</sub>	6.89	0.57	0.76	762		current paper
		11-dehydro-TxB <sub>2</sub>	367.0	161.1	-70	-10	-26	-8	<sup>1</sup> H <sub>4</sub> -TxB <sub>2</sub>	9.02	0.21	0.31	412		current paper
		<sup>1</sup> H <sub>4</sub> -TxB <sub>2</sub>	373.3	173.2	-45	-10	-23	-8	internal standard	7.66					current paper
		8-iso-PGE <sub>2</sub>	351.4	271.2	-65	-10	-23	-7	<sup>1</sup> H <sub>4</sub> -PGE <sub>2</sub>	8.69	0.10	0.25	500		current paper
		8-iso-15-keto PGE <sub>2</sub>	348.4	255.0	-45	-10	-19	-7	theoretically <sup>1</sup> H <sub>4</sub> -PGE <sub>2</sub> <sup>®</sup>	9.47		relative quantification based on 15-keto PGE <sub>2</sub>			current paper
		15-F <sub>2</sub> -isoP (8-iso-PGF <sub>2α</sub> ) <sup>®</sup>	353.1	193.1	-65	-10	-34	-8	<sup>1</sup> H <sub>4</sub> -8-iso-PGF <sub>2α</sub>	7.58	0.10	0.25	500		Koch (2020) Talanta
		8-iso-15(R)-PGF <sub>2α</sub>	353.2	193.0	-40	-10	-33	-7	theoretically <sup>1</sup> H <sub>4</sub> -PGF <sub>2α</sub> <sup>®</sup>	8.48		relative quantification based on 8-iso-15(R)-PGF <sub>2α</sub>			current paper
		5(R,S)-5-F <sub>2</sub> -isoP (8,12-iso- <sup>®</sup> PGF <sub>2α</sub> -VI) <sup>®</sup>	353.2	219.2	-40	-10	-30	-8	<sup>1</sup> H <sub>4</sub> -8,12-iso- <sup>®</sup> PGF <sub>2α</sub> -VI	10.07	0.25	0.5	500		Koch (2020) Talanta
		13,14-dihydro-15-iso-15-F <sub>2</sub> -isoP <sup>®</sup>	353.2	201.1	-110	-10	-30	-8	<sup>1</sup> H <sub>4</sub> -PGF <sub>2α</sub>	8.02	0.50	0.50	500		Koch (2020) Talanta
		15-iso-15-F <sub>2</sub> -isoP <sup>®</sup>	351.2	219.0	-75	-10	-23	-8	<sup>1</sup> H <sub>4</sub> -8-iso-PGF <sub>2α</sub>	8.19	0.3	0.5	500		Koch (2020) Talanta
	Eicosapentaenoic Acid (EPA; 20:5 n-3)	2,3-dihron-15-(R,S)-15-F <sub>2</sub> -isoP <sup>®</sup>	325.2	237.0	-70	-10	-18	-8	<sup>1</sup> H <sub>4</sub> -8-iso-PGF <sub>2α</sub>	5.49	0.100	0.25	500		Koch (2020) Talanta
		5(R,S)-5-F <sub>2</sub> -isoP (8- <sup>®</sup> PGF <sub>2α</sub> -VI) <sup>®</sup>	353.3	114.8	-45	-10	-27	-8	<sup>1</sup> H <sub>4</sub> -8-iso-PGF <sub>2α</sub>	8.07	0.1	0.25	500		Koch (2020) Talanta
		<sup>1</sup> H <sub>4</sub> -8,12-iso- <sup>®</sup> PGF <sub>2α</sub> -VI	346.2	200.1	-40	-10	-30	-8	internal standard	10.01					Koch (2020) Talanta
		<sup>1</sup> H <sub>4</sub> -8-iso-PGF <sub>2α</sub>	357.2	196.8	-75	-10	-34	-8	internal standard	7.55					Koch (2020) Talanta
		20-COOH-ARA	333.2	271.0	-55	-10	-23	-6	<sup>1</sup> H <sub>4</sub> -20-HETE	17.13	0.1	0.25	500		Koch (2020) Talanta
		11,12-15-TxHETE	355.2	167.1	-100	-10	-27	-10	<sup>1</sup> H <sub>4</sub> -PGE <sub>2</sub>	10.16		relative quantification based on LX4			Rund (2018) Analytica Chimica Acta
		5-HETE	317.2	115.1	-40	-10	-18	-6	<sup>1</sup> H <sub>4</sub> -15-HETE	19.18	0.03	0.06	295		Koch (2020) Talanta
		6-HETE	317.2	155.2	-40	-10	-18	-6	<sup>1</sup> H <sub>4</sub> -15-HETE	16.30	0.03	0.06	300		Koch (2020) Talanta
		8-HETE	317.2	167.0	-70	-10	-17	-8	<sup>1</sup> H <sub>4</sub> -15-HETE	18.41	0.1	0.25	500		Koch (2020) Talanta
		11-HETE	317.2	167.0	-70	-10	-19	-8	<sup>1</sup> H <sub>4</sub> -15-HETE	18.16	0.031	0.062	310		Koch (2020) Talanta
	multihydroxy-PUFA	12-HETE	317.2	179.2	-45	-10	-18	-8	<sup>1</sup> H <sub>4</sub> -15-HETE	18.58	0.05	0.1	500		Koch (2020) Talanta
		15-HETE	317.2	219.2	-40	-10	-18	-8	<sup>1</sup> H <sub>4</sub> -15-HETE	18.04	0.05	0.1	500		Koch (2020) Talanta
		18-HETE	317.2	259.2	-75	-10	-15	-7	<sup>1</sup> H <sub>4</sub> -15-HETE	17.20	0.05	0.1	500		Koch (2020) Talanta
		19-HETE	317.2	229.3	-70	-10	-16	-8	<sup>1</sup> H <sub>4</sub> -15-HETE	16.69	0.25	0.50	1000		Rund (2018) Analytica Chimica Acta
		20-HETE	317.2	287.3	-70	-10	-18	-10	<sup>1</sup> H <sub>4</sub> -20-HETE	16.76	0.25	0.50	1000		current paper
		5(S),12(R),18(R)-TH-HEPE (RuE1)	349.3	195.0	-40	-10	-22	-10	<sup>1</sup> H <sub>4</sub> -7(S),16(R),17(S)-TH-HDHA (RuD2)	6.25	0.25	0.50	500		current paper
		5,12,12-TH-HEPE (trans-RuE2)	349.2	195.0	-40	-10	-22	-10	<sup>1</sup> H <sub>4</sub> -7(S),16(R),17(S)-TH-HDHA (RuD2)	6.03		relative quantification based on 5(S),12(R),18(R)-TH-HEPE (RuE1)			compound oil from Kutzner (2020) BBA Lipids
		5(S),18(R)-DH-HEPE (RuE2)	333.3	203.3	-40	-10	-19	-9	<sup>1</sup> H <sub>4</sub> -LTB <sub>4</sub>	11.27	4.63	8.26	1852		current paper
		17(R),18(R)-DH-HEPE (RuE3)	333.2	201.3	-40	-10	-19	-9	<sup>1</sup> H <sub>4</sub> -10-DH-OME	13.17		relative quantification based on 8,15-DH-ETE			Kutzner (2019) Frontiers in Pharmacology
		17(R),19(S)-DH-HEPE (RuE3)-RuE3)	333.2	201.3	-40	-10	-19	-9	<sup>1</sup> H <sub>4</sub> -10-DH-OME	12.56		relative quantification based on 8,15-DH-ETE			Kutzner (2019) Frontiers in Pharmacology
	apoy-PUFA	5(S),15(S)-DH-HEPE (RuE4)	333.2	150.0	-40	-10	-19	-7	<sup>1</sup> H <sub>4</sub> -LTB <sub>4</sub>	11.85	0.25	0.50	1000		current paper
		5(S),6(R),15(S)-TH-HEPE (Lx4)	349.1	215.0	-70	-10	-24	-13	<sup>1</sup> H <sub>4</sub> -5(S),6(R),15(S)-TH-HEPE (Lx4)	8.77	1.00	2.50	1000		current paper
		LTB <sub>4</sub>	333.3	195.2	-40	-10	-21	-8	<sup>1</sup> H <sub>4</sub> -LTB <sub>4</sub>	11.95	0.25	0.50	1000		current paper
		5,12-DH-HEPE	333.2	195.0	-40	-10	-19	-9	<sup>1</sup> H <sub>4</sub> -LTB <sub>4</sub>	12.32		relative quantification based on 5(S),15(S)-DH-HEPE (RuE4)			compound B/R from Kutzner (2020) BBA Lipids
		12,18-HEPE	333.3	179.0	-40	-10	-19	-8	<sup>1</sup> H <sub>4</sub> -LTB <sub>4</sub>	11.08		relative quantification based on 5(S),16(R)-DH-HEPE (RuE2)			compound oil from Kutzner (2020) BBA Lipids
		5,18-18-HEPE 1	349.2	215.0	-40	-10	-22	-10	<sup>1</sup> H <sub>4</sub> -5(S),6(R),15(S)-TH-HEPE (Lx4)	7.92		relative quantification based on 5(S),6(R),15(S)-TH-HEPE (Lx4)			compound oil from Kutzner (2020) BBA Lipids
		5,18-18-HEPE 2	349.3	145.0	-40	-10	-22	-10	<sup>1</sup> H <sub>4</sub> -5(S),6(R),15(S)-TH-HEPE (Lx4)	8.4		relative quantification based on 5(S),6(R),15(S)-TH-HEPE (Lx4)			compound H from Kutzner (2020) BBA Lipids
		8/9-EpETE	317.2	189.1	-40	-10	-16	-6	<sup>1</sup> H <sub>4</sub> -8/9-EpETE	21.98		relative quantification based on 8/9-EpETE			synthesized using MCPBA as described Newman (2002) J. Lipid Res
		8/9-EpETE	317.2	127.2	-40	-10	-16	-6	<sup>1</sup> H <sub>4</sub> -8/9-EpETE	21.32	0.5	0.75	500		Koch (2020) Talanta
		11(12)-EpETE	317.2	167.0	-40	-10	-16	-6	<sup>1</sup> H <sub>4</sub> -14(15)-EpETE	21.14	0.1	0.25	500		Koch (2020) Talanta
	vic hydroxy-PUFA	14(15)-EpETE	317.2	207.2	-40	-10	-16	-6	<sup>1</sup> H <sub>4</sub> -14(15)-EpETE	20.97	0.1	0.25	500		Koch (2020) Talanta
		17(18)-EpETE	317.2	215.2	-40	-10	-16	-6	<sup>1</sup> H <sub>4</sub> -14(15)-EpETE	20.21	0.5	0.75	500		Koch (2020) Talanta
		trans-8/9-EpETE	317.2	189.1	-40	-10	-16	-6	<sup>1</sup> H <sub>4</sub> -8/9-EpETE	21.71		relative quantification based on 8/9-EpETE			Koch (2020) Talanta
		trans-8/9-EpETE	317.2	127.2	-40	-10	-16	-6	<sup>1</sup> H <sub>4</sub> -8/9-EpETE	21.47		relative quantification based on 8/9-EpETE			Koch (2020) Talanta
		trans-11(12)-EpETE	317.2	167.0	-40	-10	-16	-6	<sup>1</sup> H <sub>4</sub> -14(15)-EpETE	21.29		relative quantification based on 11(12)-EpETE			Koch (2020) Talanta
		trans-14(15)-EpETE	317.2	207.2	-40	-10	-16	-6	<sup>1</sup> H <sub>4</sub> -14(15)-EpETE	21.12		relative quantification based on 14(15)-EpETE			Koch (2020) Talanta
		trans-17(18)-EpETE	317.2	215.2	-40	-10	-16	-6	<sup>1</sup> H <sub>4</sub> -14(15)-EpETE	20.36		relative quantification based on 17(18)-EpETE			Koch (2020) Talanta
		5,6-DH-DHTE	335.2	115.1	-45	-10	-20	-8	<sup>1</sup> H <sub>4</sub> -LTB <sub>4</sub>	15.43	0.23	0.3	15		Koch (2020) Talanta
		8,9-DH-DHTE	335.2	127.1	-40	-10	-20	-8	<sup>1</sup> H <sub>4</sub> -LTB <sub>4</sub>	14.68	0.05	0.100	500		Koch (2020) Talanta
		11,12-DH-DHTE	335.2	167.1	-40	-10	-25	-6	<sup>1</sup> H <sub>4</sub> -LTB <sub>4</sub>	14.27	0.025	0.05	250		Koch (2020) Talanta
	prostanoids	14,15-DH-DHTE	335.3	207.2	-40	-10	-24	-10	<sup>1</sup> H <sub>4</sub> -LTB <sub>4</sub>	14.04	0.025	0.05	250		Koch (2020) Talanta
		17,18-DH-DHTE	335.3	247.2	-40	-10	-23	-8	<sup>1</sup> H <sub>4</sub> -LTB <sub>4</sub>	13.44	0.063	0.11	55		Koch (2020) Talanta
		PGD <sub>2</sub>	341.3	223.0											

Legend

- <sup>1)</sup> limit of detection (LOD) set to lowest concentration with a signal to noise ratio ≥3  
<sup>2)</sup> lower limit of quantification (LLOQ) set to lowest calibration standards with a signal to noise ratio ≥5 and accuracy ±20%  
<sup>3)</sup> upper limit of quantification (ULOQ) set to calibration of the highest injected standard  
<sup>4)</sup> other isoprostanes, isofuranes and phytyprostanes can be included as described in Rund et al., 2017 (Anal Chim Acta 1037, 63-74)  
<sup>5)</sup> preparation of independent calibration necessary due to interferences

Abbreviations

AdA	adrenic acid
ALA	alpha-linolenic acid
ARA	arachidonic acid
CE	collision energy
CXP	collision cell exit potential
DGLA	dihomo-gamma linolenic acid
DHA	docosahexaenoic acid
DH	dihydroxy
DHDHA	dihydroxydocosahexaenoic acid
DHDPE	dihydroxydocosapentaenoic acid
DHNEPE	dihydroxyecosapentaenoic acid
DHETE	dihydroxyicosatetraenoic acid
DHETE	dihydroxyicosatetraenoic acid
DHODE	dihydroxyoctadecadienoic acid
DHOMe	dihydroxyoctadecamonoenoic acid/ dihydroxyoctadecenoic acid
DP	decalustering potential
DPA	docosapentaenoic acid
EKODE	epoxy-keto-octadecadienoic acid
Ep	epoxy
EP	entrance potential
EPA	ecosapentaenoic acid
EpDoTfE	epoxydocosatrienoic acid
EpDPE	epoxydocosapentaenoic acid
EpEDE	epoxyecosadienoic acid
EpETE	epoxyecosatetraenoic acid
EpETfE	epoxyicosatrienoic acid
EpETfE	epoxyicosatrienoic acid
EpODE	epoxyoctadecadienoic acid
EpOMe	epoxyoctadecamonoenoic acid/ epoxyoctadecenoic acid
ETE	icosatetraenoic acid
FA	fatty acid
GLA	gamma-linolenic acid
HDHA	hydroxydocosahexaenoic acid
HEPE	hydroxyecosapentaenoic acid
HETE	hydroxyicosatetraenoic acid
HETE	hydroxyicosatetraenoic acid
HHTfE	hydroxyheptatrienoic acid
HOTfE	hydroxyoctadecatrienoic acid
HbETE	hydroperoxyicosatetraenoic acid
IsOP IP	isoprostane
LA	linoleic acid
LLOQ	lower limit of quantification
LOD	limit of detection
LT	leukotriene
Lx	lipxin
Mar	marish
ODE	octadecadienoic acid
Oleic	oleic acid
OTfE	octadecatrienoic acid
P	protein
PG	prostaglandin
Rv	resolin
TriHDHA	trihydroxydocosahexaenoic acid
TriHNEPE	trihydroxyecosapentaenoic acid
TriHETE	trihydroxyicosatetraenoic acid
TriHETfE	trihydroxyicosatetraenoic acid
TriHODE	trihydroxyoctadecadienoic acid
TriHOMe	trihydroxyoctadecamonoenoic acid/ trihydroxyoctadecenoic acid
Tx	thromboxane
ULOQ	upper limit of quantification

References

Koch, E., et al., Talanta 2020, 217, 121074.  
Kützner, L., et al., Biochimica et Biophysica Acta (BBA) - Molecular and Cell Biology of Lipids 2020, 1865 (12), 158806.  
Kützner, L., et al., Frontiers in Pharmacology 2019, 10 (169).  
Lundström, S. L., et al., PLoS ONE 2011, 6 (6), e23864.  
Mochelmann, S. W., et al., Prostaglandins & Other Lipid Mediators 2017, 130, 8-15.  
Newman, J. W., et al., Journal of Lipid Research 2002, 43 (9), 1563-1578.  
Ostermann, A. L., et al., Anal Bioanal Chem 2015, 407, 1403-1414.  
Rund, K. M., et al., Analytica Chimica Acta 2016, 1037, 63-74.  
Rund, K. M., et al., Prostaglandins Other Lipid Mediators 2019, 144, 106334.  
Yang, J., et al., Analytical Chemistry 2009, 81 (19), 8085-8093.  
Zikovic, A. M., et al., Metabolomics 2012, 8 (6), 1102-1113.