

### Supplemental Materials (Tables)

Table S1. Detailed information of target metabolites and ISs

NO.	Analytes	Formula	CAS	Common Name
□	□	□	□	□
1	dhkPGE2	C20H32O5	363-23-5	13,14-dihydro-15-keto PGE2
2	dhkPGF2	C20H34O5	27376-76-7	13,14-dihydro-15-keto Prostaglandin F2 $\alpha$
3	dhkPGD2	C20H32O5	59894-07-4	13,14-dihydro-15-keto Prostaglandin D2
4	15dPGD2	C20H30O4	85235-11-6	15-deoxy- $\Delta$ 12,14-Prostaglandin D2
5	15kPGE2	C20H30O5	26441-05-4	15-keto Prostaglandin E2
6	15dPGJ2	C20H28O3	87893-55-8	15-deoxy- $\Delta$ 12,14-Prostaglandin J2
7	20oh PGF2 $\alpha$	C20H34O6	57930-92-4	20-hydroxy Prostaglandin F2 $\alpha$
8	20oh PGE2	C20H32O6	57930-95-7	20-hydroxy Prostaglandin E2
9	19oh PGE2	C20H32O6	64625-54-3	19(R)-hydroxy Prostaglandin E2
10	12-OxoETE	C20H30O3	108437-64-5	12-oxo-5Z,8Z,10E,14Z-eicosatetraenoic acid
11	12(S)-HETE	C20H32O3	54397-83-0	12S-hydroxy-5Z,8Z,10E,14Z-eicosatetraenoic acid
12	11-HETE	C20H32O3	73804-65-6	11-hydroxy-eicosatetraenoic acid
13	11,12-EET	C20H32O3	123931-40-8	(12)-epoxy-5Z,8Z,14Z-eicosatrienoic acid
14	5-oxoETE	C20H30O3	106154-18-1	5-oxo-6E,8Z,11Z,14Z-eicosatetraenoic acid
15	5(S)-HETE	C20H32O3	70608-72-9	5S-hydroxy-6E,8Z,11Z,14Z-eicosatetraenoic acid
16	LTB4	C20H32O4	71160-24-2	Leukotriene B4
17	6t LTB4	C20H32O4	71652-82-9	6-trans Leukotriene B4
18	12epi LTB4	C20H32O4	83709-73-3	5S,12S-dihydroxy-6Z,8E,10E,14Z-eicosatetraenoic acid
19	6t,12epi LTB4	C20H32O4	71548-19-1	5S,12S-dihydroxy-6E,8E,10E,14Z-eicosatetraenoic acid
20	12-oxoLTB4	C20H30O4	136696-10-1	5S-hydroxy-12-oxo-6Z,8E,10E,14Z-eicosatetraenoic acid

21	20-HETE	C20H32O3	79551-86-3	20-hydroxy Arachidonic Acid
22	12-HHT	C17H28O3	54397-84-1	12S-hydroxy-5Z,8E,10E-heptadecatrienoic acid
23	LTD4	C25H40N2O6S	73836-78-9	Leukotriene D4
24	5(S),15(S)-DiHETE	C20H32O4	82200-87-1	5S,15S-dihydroxy-6E,8Z,10Z,13E-eicosatetraenoic acid
25	15(S)-HETE	C20H32O3	54845-95-3	15S-hydroxy-5Z,8Z,11Z,13E-eicosatetraenoic acid
26	20-hydroxy Leukotriene B4	C20H32O5	79516-82-8	5S,12R,20-trihydroxy-6Z,8E,10E,14Z-eicosatetraenoic acid
27	6k PGF1a	C20H34O6	58962-34-8	6-keto Prostaglandin F1 $\alpha$
28	TxB2	C20H34O6	54397-85-2	Thromboxane B2
29	PGF2a	C20H34O5	551-11-1	Prostaglandin F2 $\alpha$
30	PGE2	C20H32O5	363-24-6	Prostaglandin E2
31	PGD2	C20H32O5	41598-07-6	Prostaglandin D2
32	11 $\beta$ PGE2	C20H32O5	38310-90-6	11-beta-Prostaglandin E2
33	13-HDoHE	C22H32O3	90780-53-3	13- hydroxy-docosahexaenoic acid
34	PGJ2	C20H30O4	60203-57-8	Prostaglandin J2
35	5-iso PGF2a VI	C20H34O5	180469-63-0	Isoprostane F2 $\alpha$ -VI
36	LTE4	C23H37NO5S	75715-89-8	Leukotriene E4
37	13-HOTrE	C18H30O3	87984-82-5	13-hydroxy-octadecatrienoic acid
38	15-oxoETE	C20H30O3	81416-72-0	15-oxo-eicosatetraenoic acid
39	12,13-EpOME	C18H32O3	none	12(13)-epoxy-octadecenoic acid
40	9,10-diHOME	C18H34O4	263399-34-4	( $\pm$ )9,10-dihydroxy-12Z-octadecenoic acid
41	AA	C20H32O2	506-32-1	Arachidonic acid
42	Adrenic Acid	C22H36O2	28874-58-0	Adrenic acid
43	EPA	C20H30O2	10417-94-4	Eicosapentaenoic acid
44	DHA	C22H32O2	6217-54-5	Docosahexaenoic acid
45	14:0 PC (DMPC)	C36H72NO8P	18194-24-6	1,2-dimyristoyl-sn-glycero-3-phosphocholine
46	16:0 PC (DPPC)	C40H80NO8P	63-89-8	1,2-dipalmitoyl-sn-glycero-3-phosphocholine

47	16:0-18:0 PC	C42H84NO8P	59403-51-9	1-palmitoyl-2-stearoyl-sn-glycero-3-phosphocholine
48	16:0-18:1 PC	C42H82NO8P	26853-31-6	1-palmitoyl-2-oleoyl-sn-glycero-3-phosphocholine
49	16:0-20:4 PC	C44H80NO8P	35418-58-7	1-palmitoyl-2-arachidonoyl-sn-glycero-3-phosphocholine
50	18:0 PC (DSPC)	C44H88NO8P	816-94-4	1,2-distearoyl-sn-glycero-3-phosphocholine
51	18:0-18:1 PC	C44H86NO8P	56421-10-4	1-stearoyl-2-oleoyl-sn-glycero-3-phosphocholine
52	18:0-22:6 PC	C48H84NO8P	59403-52-0	1-stearoyl-2-docosahexaenoyl-sn-glycero-3-phosphocholine
53	20:0 PC	C48H96NO8P	61596-53-0	1,2-diarachidoyl-sn-glycero-3-phosphocholine
54	16:0 LPC	C24H50NO7P	17364-16-8	1-palmitoyl-2-hydroxy-sn-glycero-3-phosphocholine
55	18:1 Lyso PC	C26H52NO7P	19420-56-5	1-oleoyl-2-hydroxy-sn-glycero-3-phosphocholine
56	18:0 Lyso PC	C26H54NO7P	19420-57-6	1-stearoyl-2-hydroxy-sn-glycero-3-phosphocholine
57	20:0 LPC	C28H58NO7P	108341-80-6	1-heptadecanoyl-2-hydroxy-sn-glycero-3-phosphocholine
58	16:0 PA	C35H68NaO8P	169051-60-9	1,2-dipalmitoyl-sn-glycero-3-phosphate (sodium salt)
59	16:0-18:1 PA	C37H70O8PNa	169437-35-8	1-palmitoyl-2-oleoyl-sn-glycero-3-phosphate (sodium salt)
60	16:0 Lyso PA	C19H38O7PNa	17618-08-5	1-palmitoyl-2-hydroxy-sn-glycero-3-phosphate (sodium salt)
61	16:0 PS	C38H73NO10PNa	145849-32-7	1,2-dipalmitoyl-sn-glycero-3-phospho-L-serine (sodium salt)
62	18:0-18:1 PS	C42H79NO10PNa	321883-23-2	1-stearoyl-2-oleoyl-sn-glycero-3-phospho-L-serine (sodium salt)
63	18:0 Lyso PS	C24H47NPO9Na	1246298-16-7	1-stearoyl-2-hydroxy-sn-glycero-3-phospho-L-serine
64	16:0 PI	C41H82NO13P	34290-57-8	1,2-dipalmitoyl-sn-glycero-3-phospho-(1'-myo-inositol)
65	18:0 PI	C45H90NO13P	849412-67-5	1,2-distearoyl-sn-glycero-3-phosphoinositol
66	16:0-18:1 PI	C43H84NO13P	50730-13-7	1-palmitoyl-2-oleoyl-sn-glycero-3-phosphoinositol
67	18:0-20:4 PI	C47H86NO13P	1331751-28-0	1-stearoyl-2-arachidonoyl-sn-glycero-3-phosphoinositol
68	18:0 Lyso PI	C27H56NO12P	849412-49-3	1-stearoyl-2-hydroxy-sn-glycero-3-phosphoinositol
69	14:0 PG	C34H66O10PNa	200880-40-6	1,2-dimyristoyl-sn-glycero-3-phospho-(1'-rac-glycerol)
70	16:0-18:1 PG	C40H76O10PNa	268550-95-4	1-palmitoyl-2-oleoyl-sn-glycero-3-phospho-(1'-rac-glycerol)
71	18:0 PG	C42H82O10PNa	200880-42-8	1,2-distearoyl-sn-glycero-3-phospho-(1'-rac-glycerol)
72	14:0 PE	C33H66NO8P	998-07-2	1,2-dimyristoyl-sn-glycero-3-phosphoethanolamine

73	16:0 PE	C37H74NO8P	923-61-5	1,2-dipalmitoyl-sn-glycero-3-phosphoethanolamine
74	18:0 PE	C41H82NO8P	1069-79-0	1,2-distearoyl-sn-glycero-3-phosphoethanolamine
75	16:0 Lyso PE	C21H44NO7P	53862-35-4	1-palmitoyl-2-hydroxy-sn-glycero-3-phosphoethanolamine
76	18:0 Lyso PE	C23H48NO7P	69747-55-3	1-Stearoyl-2-Hydroxy-sn-Glycero-3-Phosphoethanolamine
77	Cho	C27H46O	57-88-5	Cholesterol
78	253Hy	C27H45NaO5S	884905-07-1	25-hydroxycholesterol-3-sulfate (sodium salt)
79	24EC	C27H44O2	72542-49-5	24(S),25-EPOXYCHOLESTEROL
80	22Hy	C27H46O2	22348-64-7	22 $\beta$ -hydroxycholesterol
81	27Hy	C27H46O2	20380-11-4	27-hydroxycholesterol
82	25HY	C27H46O2	2140-46-7	25-hydroxycholesterol
83	CS	C27H46O4S	1256-86-6	cholesterol 3-sulfate
84	4bHY	C27H46O2	17320-10-4	4-beta-hydroxycholesterol
85	24sHY	C27H46O2	474-73-7	24s-hydroxycholesterol
86	3bHY	C27H44O2	566-28-9	3beta-hydroxy-5-cholesten-7-one(7-ketocholesterol)
87	7ahy	C27H46O2	566-26-7	7alpha-hydroxycholesterol
88	7bhy	C27H46O2	566-27-8	7beta-hydroxycholesterol
89	7ahc	C27H44O2	3862-25-7	7alpha-hydroxy-4-cholesterol-3-one
90	GCDA	C26H43NO5	640-79-9	Glycoursodeoxycholic acid
91	TCDA	C26H45NO6S	516-35-8	Taurochenodesoxycholic acid
92	GCDCDA	C26H43NO5	64480-66-6	Chenodeoxycholic acid glycine conjugate
93	GDCA	C26H43NO5	360-65-6	Deoxycholic acid glycine conjugate
94	DCA	C24H40O4	83-44-3	Desoxycholic acid
95	GCA	C26H43NO6	475-31-0	Glycocholic acid
96	TCA	C26H45NO7S	81-24-3	Taurocholic acid
97	CDCA	C24H40O4	474-25-9	Chenodeoxycholic acid
98	CA	C24H40O5	81-25-4	Cholic acid

99	LCA	C24H40O3	434-13-9	Lithocholic acid
100	UDCA	C24H40O3	128-13-2	Ursodeoxycholic acid
101	GLCA	C26H43NO4	474-74-8	Lithocholic acid glycine conjugate
102	TDCA	C26H45NO6S	207737-97-1	Taurodeoxycholic acid
103	TLCA	C26H45NO5S	6042-32-6	Taurolithocholic acid
104	TUDCA	C26H45NO6S	14605-22-2	Tauroursodeoxycholic acid
105	(d4) TXB2	C20H30D4O6	1346112-79-5	(d4) Thromboxane B2
106	(d4) PGD2	C20H28D4O5	211105-29-2	(d4) Prostaglandin D2
107	(d4) 15d PGJ2	C20H24D4O3	1542166-82-4	(d4) 15-deoxy-Prostaglandin J2
108	(d4) LTB4	C20H28D4O4	124629-74-9	(d4) Leukotriene B4
109	(d4) 13-HODE	C18H28D4O3	139408-39-2	(d4) 13-hydroxy-octadecadienoic acid
110	(d7) 5-oxoETE	C20H23D7O3	none	(d7) 5-oxo-eicosatetraenoic acid
111	(d11) 11,12 EET	C20H21D11O3	none	(d11) 11(12)-epoxy-eicosatrienoic acid
112	(d8) Arachidonic Acid	C20H24D8O2	69254-37-1	(d8) Arachidonic acid
113	(d8) 5(s)-HETE	C20H24D8O3	330796-62-8	(d8)5S-hydroxy-6E,8Z,11Z,14Z-eicosatetraenoic acid
114	(d6) 20-HETE	C20H26D6O3	none	(d6)20-hydroxy Arachidonic Acid
115	(d8) 15(S)-HETE	C20H24D8O3	54845-95-3	(d8)15S-hydroxy-5Z,8Z,11Z,13E-eicosatetraenoic acid
116	17:0 Lyso PC	C25H52NO7P	50930-23-9	1-heptadecanoyl-2-hydroxy-sn-glycero-3-phosphocholine
117	17:0 Lyso PA	C20H40O7PNa	799268-66-9	1-heptadecanoyl-2-hydroxy-sn-glycero-3-phosphate
118	17:1 Lyso PS	C23H43NNaO9P	1246298-15-6	1-(10Z-heptadecenoyl)-2-hydroxy-sn-glycero-3-[phospho-L-serine]
119	17:1 Lyso PI	C26H52NO12P	1246353-39-8	1-(10Z-heptadecenoyl)-2-hydroxy-sn-glycero-3-phospho-(1'-myo-inositol)
120	15:0 PG	C36H70O10PNa	322647-32-5	1,2-dipentadecanoyl-sn-glycero-3-phospho-(1'-rac-glycerol)
121	17:1 Lyso PE	C22H44NO7P	1246298-09-8	1-(10Z-heptadecenoyl)-sn-glycero-3-phosphoethanolamine
122	(d7)7ahc	C27H37D7O2	2260669-17-6	(d7)7alpha-hydroxy-4-cholesterol-3-one
123	(C13)GCA	C25H43NO6C13	none	Glycocholic acid-C13

