Supplementary tables

Table S1. UHPLC program. Solvent A consisted of 0.1% formic acid in water, solvent B consisted of 0.1% formic acid in acetonitrile, solvent C consisted of methanol and solvent D consisted of 2-propanol. The column oven temperature was set to 50 °C.

time [min]	flow [mL/min]	solvent A concentration [%]	solvent B concentration [%]	solvent C concentration [%]	solvent D concentration [%]	solvent B and C curve*
primary metabolites						
0.01	0.25	100				
2.00	0.25	100				
5.00	0.25	75				
11.00	0.25	65				
15.00	0.25	5				
20.00	0.25	5				
20.01	0.25	100				
25.00	stop					
lipid mediators						
0	0.2	90	10			
10.0	0.2	75	25			
20.0	0.2	65	35			
40.0	0.2	25	75			
40.2	0.2	5	95			
50.0	0.2	5	90			
50.2	0.2	90	10			
59.0	Stop					
phospholipids						
0.0	0.15	80	10		10	
2.0	0.15	80	10		10	

4.0	0.15	60	20	20	-3
50.0	0.15	7.6	46.2	46.2	
52.0	0.15	0	50	50	
70.0	0.15	0	50	50	
70.2	0.15	80	10	10	
80.0	stop				

sphingosine-1-phosphate and sphingosine

0	0.4	90	10
0.01	0.4	0	100
3.00	0.4	0	100
5.00	0.8	0	100
7.00	0.8	0	100
7.01	0.8	90	10
7.80	0.8	90	10
8.30	0.3	90	10
9.50	0.3	90	10
9.51	Stop		

*sets the gradient curve of the solvent (-10 to 10)

Table S2. Mass spectrometer (LCMS 8050) settings.

source conditions	parameters
nebulizing gas flow rate	3.0 L/min
heating gas flow rate	10.0 L/min
drying gas flow rate	10.0 L/min
collision-induced dissociation gas pressure	230 kPa
interface temperature	300 °C
desolvation line temperature	250 °C
block heater temperature	400 °C
ionization mode	electrospray ionisation (ESI)

Table S3: Mass transitions for identified significantly changed primary metabolites. The target ion shows the multiple reaction monitoring (MRM) transitions, the ionization polarity (IP) shows the ionization mode of the electrospray ionization (ESI) source and the internal standard (IS) column assigns the number of the internal standard to the compounds with which they were evaluated. The internal standard is marked in bold letters. Injection volume of 10 µl sample.

no.	compound	target ion	IP	IS
1	4-hydroxyproline	132.10>86.05	+	1
2	adenine	136.00>119.05	+	1
3	adenosine monophosphate	348.00>136.05	+	1
4	adenylsuccinic acid	464.10>252.10	+	1
5	alanine	89.90>89,90	+	1
6	arginine	175.10>70.10	+	1
7	argininosuccinic acid	291.00>70.10	+	1
8	asparagine	133.10>87.15	+	1
9	bilirubin	583.30>285.25	-	1
10	carnitine	162.10>103.05	+	1
11	carnosine	227.10>110.05	+	1
12	choline†	104.10>60.05	+	1
13	cholesterol	369.40>161.30	+	1
14	citrulline	176.10>70.05	+	1
15	creatine	132.10>44.05	+	1
16	creatinine	114.10>44.05	+	1
17	cystathionine	223.00>88.05	+	1
18	cystine	241.00>151.95	+	1
19	cytidine	244.10>112.05	+	1
20	cytidine 3',5'-cyclic monophosphate (cAMP)	306.00>112.10	+	1
21	cytidine monophosphate	324.00>112.05	+	1
22	cytosine	112.00>95.10	+	1

23	dihydroxyphenylalanine (DOPA)	198.10>152.10	+	1
24	dimethylarginine (symmetric/asymmetric)	203.10>70.15	+	1
25	dimethylglycine	104.10>58.05	+	1
26	flavin adenine dinucleotide	786.15>136.10	+	1
27	flavin mononucleotide	455.00>97.00	-	1
28	glutamic acid	147.90>84.10	+	1
29	glutamine	147.10>84.15	+	1
30	glutathione	308.00>179.10	+	1
31	guanosine 3',5'-cyclic monophosphate (cGMP)	346.00>152.05	+	1
32	guanosine monophosphate	364.00>152.05	+	1
33	histamine	112.10>95.05	+	1
34	histidine	155.90>110.10	+	1
35	isoleucine	132.10>69.15	+	1
36	kynurenine	209.10>192.05	+	1
37	leucine	132.10>30.05	+	1
38	lysine	147.10>84.10	+	1
39	niacinamide	123.10>80.05	+	1
40	nicotinic acid	124.05>80.05	+	1
41	ophthalmic acid	290.10>58.10	+	1
42	ornithine	133.10>70.10	+	1
43	phenylalanine	166.10>120.10	+	1
44	proline	116,10>70,15	+	1
45	oxidized glutathione	611.10>306.00	-	1
46	s-adenosylmethionine	399.10>250.05	+	1
47	serotonin	177.10>160.10	+	1
48	threonine	120.10>74.15	+	1

49	thymidine	243.10>127.10	+	1
50	thymidine monophosphate	322.90>81.10	+	1
51	tyrosine	182.10>136.10	+	1
52	uracil	113.00>70.00	+	1
53	uric acid	167.10>123.95	-	1
54	uridine	245.00>113.05	+	1
55	valine	118.10>72.15	+	1
56	**2-morpholinoethanesulfonic acid (IS)**	**194.00>80.15**	**-**	**1**

†illustrated in heatmaps of phospholipids

Table S4: Mass transitions for identified significantly changed phospholipids. The target ion shows the multiple reaction monitoring (MRM) transitions, the ionization polarity (IP) shows the ionization mode of the ESI source and the internal standard (IS) column assigns the number of the internal standard to the lipid species with which they were evaluated. The internal standard is marked in bold letters. (LPC: lysophosphatidylcholine, PC: phosphatidylcholine, LPE: lysophosphatidylethanolamine, PE: phosphatidylethanolamine, LPG: lysophosphatidylglycerol, LPI: lysophosphatidylinositol, PI: phosphatidylinsitol, LPS: lysophosphatidylserine, PS: phosphatidylserine, SM: sphingomyelin)

no.	lipid species	target ion	IP	IS
1	LPC(16:1)	494.3>184.10	+	1
2	LPC(18:1)*	522.4>184.10	+	1
3	LPC(18:3)	518.3>184.10	+	1
4	LPC(20:0)	552.4>184.10	+	1
5	LPC(20:1)	550.4>184.10	+	1
6	LPC(20:2)	548.4>184.10	+	1
7	LPC(20:3)	546.4>184.10	+	1
8	LPC(20:4)*	544.4>184.10	+	1
9	LPC(20:5)	542.3>184.10	+	1
10	LPC(22:0)	580.5>184.10	+	1
11	LPC(22:1)	578.4>184.10	+	1
12	LPC(22:6)*	568.4>184.10	+	1
13	PC(30:0)	706.6>184.10	+	1
14	PC(30:1)*	704.5>184.10	+	1
15	PC(30:2)*	702.5>184.10	+	1
16	PC(32:0)*	734.6>184.10	+	1
17	PC(32:1)*	732.6>184.10	+	1
18	PC(32:2)	730.6>184.10	+	1
19	PC(34:3)*	756.6>184.10	+	1
20	PC(36:0)	790.7>184.10	+	1
21	PC(36:1)*	788.6>184.10	+	1

22	PC(36:3)*	784.6>184.10	+	1
23	PC(36:5)*	780.6>184.10	+	1
24	PC(38:1)	816.7>184.10	+	1
25	PC(38:2)*	814.7>184.10	+	1
26	PC(38:3)*	812.6>184.10	+	1
27	PC(38:5)*	808.6>184.10	+	1
28	PC(38:7)*	804.6>184.10	+	1
29	PC(38:8)	802.6>184.10	+	1
30	PC(40:0)	846.7>184.10	+	1
31	PC(40:1)	844.7>184.10	+	1
32	PC(40:2)	842.7>184.10	+	1
33	PC(40:3)	840.7>184.10	+	1
34	PC(40:4)	838.7>184.10	+	1
35	PC(40:5)*	836.6>184.10	+	1
36	PC(40:7)*	832.6>184.10	+	1
37	PC(40:8)	830.6>184.10	+	1
38	PC(42:0)	874.8>184.10	+	1
39	PC(42:1)	872.7>184.10	+	1
40	PC(42:2)	870.7>184.10	+	1
41	PC(42:3)	868.7>184.10	+	1
42	PC(42:4)	866.7>184.10	+	1
43	PC(42:5)	864.7>184.10	+	1
44	PC(42:6)	862.7>184.10	+	1
45	PC(42:7)	860.6>184.10	+	1
46	PC(42:8)	858.6>184.10	+	1
47	PC(44:1)	900.8>184.10	+	1

48	PC(44:6)	890.7>184.10	+	1
49	PC(44:7)	888.7>184.10	+	1
50	LPE(14:0)	426.3>285.24	+	1
51	LPE(14:1)	424.3>283.23	+	1
52	LPE(16:0)	454.3>313.27	+	1
53	LPE(16:1)	452.3>311.26	+	1
54	LPE(18:0)	482.3>341.30	+	1
55	LPE(18:1)	480.3>339.29	+	1
56	LPE(18:2)	478.3>337.27	+	1
57	LPE(18:3)	476.3>335.26	+	1
58	LPE(20:0)	510.4>369.34	+	1
59	LPE(20:2)	506.3>365.30	+	1
60	LPE(20:3)	504.3>363.29	+	1
61	LPE(20:4)	502.3>361.27	+	1
62	LPE(20:5)	500.3>359.26	+	1
63	LPE(22:0)	538.4>397.37	+	1
64	LPE(22:1)	536.4>395.35	+	1
65	LPE(22:6)	526.3>385.27	+	1
66	PE(32:0)	692.5>551.50	+	1
67	PE(32:1)	690.5>549.49	+	1
68	PE(32:2)	688.5>547.47	+	1
69	PE(34:1)	718.6>577.52	+	1
70	PE(34:2)	716.5>575.50	+	1
71	PE(34:3)	714.5>573.49	+	1
72	PE(36:1)	746.6>605.55	+	1
73	PE(36:2)	744.6>603.53	+	1

74	PE(36:3)	742.6>601.52	+	1
75	PE(36:4)	740.5>599.50	+	1
76	PE(36:5)	738.5>597.49	+	1
77	PE(38:0)	776.6>635.60	+	1
78	PE(38:1)	774.6>633.58	+	1
79	PE(38:2)	772.6>631.57	+	1
80	PE(38:3)	770.6>629.55	+	1
81	PE(38:4)	768.6>627.53	+	1
82	PE(38:5)*	766.6>625.52	+	1
83	PE(38:7)	762.5>621.49	+	1
84	PE(40:0)	804.7>663.63	+	1
85	PE(40:4)	796.6>655.57	+	1
86	PE(40:5)	794.6>653.55	+	1
87	PE(40:6)	792.6>651.53	+	1
88	PE(40:7)	790.6>649.52	+	1
89	PE(40:8)	788.5>647.50	+	1
90	PE(42:0)	832.7>691.66	+	1
91	PE(42:1)	830.7>689.64	+	1
92	PE(44:0)	860.7>719.69	+	1
93	LPG(14:1)	455.3>283.14	+	1
94	LPG(16:0)	485.3>313.19	+	1
95	LPG(16:1)	483.3>311.17	+	1
96	LPG(18:1)	511.3>339.20	+	1
97	LPG(18:2)	509.3>337.19	+	1
98	LPI(16:0)	571.3>241.01	-	1
99	LPI(18:0)	599.3>241.01	-	1

100	LPI(18:1)	597.3>241.01	-	1
101	LPI(18:2)	595.3>241.01	-	1
102	LPI(20:4)	619.3>241.01	-	1
103	LPI(22:6)	643.3>241.01	-	1
104	PI(34:1)	835.6>241.01	-	1
105	PI(34:2)	833.5>241.01	-	1
106	PI(36:1)	863.6>241.01	-	1
107	PI(36:2)	861.6>241.01	-	1
108	PI(36:3)	859.6>241.01	-	1
109	PI(36:4)	857.5>241.01	-	1
110	PI(36:5)	855.5>241.01	-	1
111	PI(38:4)	885.6>241.01	-	1
112	PI(38:5)	883.6>241.01	-	1
113	PI(38:6)	881.5>241.01	-	1
114	PI(40:6)	909.6>241.01	-	1
115	LPS(16:0)	498.3>313.26	+	1
116	LPS(18:0)	526.3>341.29	+	1
117	LPS(18:1)	524.3>339.28	+	1
118	LPS(18:2)	522.3>337.26	+	1
119	LPS(20:4)	546.3>361.26	+	1
120	LPS(22:6)	570.3>385.26	+	1
121	PS(34:1)	762.6>577.51	+	1
122	PS(36:1)	790.6>605.54	+	1
123	PS(36:2)	788.6>603.52	+	1
124	PS(36:4)	784.5>599.49	+	1
125	PS(36:5)	782.5>597.48	+	1

126	PS(36:6)	780.5>595.46	+	1
127	PS(38:3)	814.6>629.54	+	1
128	PS(38:4)	812.6>627.52	+	1
129	PS(38:6)	808.5>623.49	+	1
130	PS(38:8)	804.5>619.46	+	1
131	PS(40:4)	840.6>655.56	+	1
132	PS(40:5)	838.6>653.54	+	1
133	PS(40:6)	836.6>651.52	+	1
134	PS(40:7)	834.6>649.51	+	1
135	SM(32:1)	675.6>184.10	+	1
136	SM(32:2)	673.6>184.10	+	1
137	SM(34:2)	701.6>184.10	+	1
138	SM(36:1)	731.6>184.10	+	1
139	SM(36:2)	729.6>184.10	+	1
140	SM(36:3)	727.6>184.10	+	1
141	SM(36:4)	725.6>184.10	+	1
142	SM(38:2)*	757.6>184.10	+	1
143	SM(38:6)	749.6>184.10	+	1
144	SM(40:2)*	785.7>184.10	+	1
145	**sphingosine-1-phosphate (17:0) IS**	**366.3>250.4**	**+**	**1**

*0.5 µl sample injection volume

Table S5: Mass transitions for identified significantly changed lipid mediators. The target ion shows the multiple reaction monitoring (MRM) transitions, the ionization polarity (IP) shows the ionization mode of the ESI source and the internal standard (IS) column assigns the number of the internal standard to the lipid mediators with which they were evaluated. The internal standard is marked in bold letters.

no.	compound		target ion	IP	IS
1	9,10-DiHOME	9,10-dihydroxy-octadecenoic acid	313,2>201,2	-	1
2	14-HDoHE	14-hydroxy-docosahexaenoic acid	343,2>205,2	-	1
3	19-HETE	19-hydroxyeicosatetraenoic acid	319,2>275,2	-	1
4	AA	arachidonic acid	303,2>303,2	-	1
5	cholic acid†		407.25>407.25	-	1
6	DCA†	deoxycholic acid	391.30>391.30	-	1
7	DHA	docosahexaenoic acid	327,2>283,2	-	1
8	EPA	eicosapentaenoic acid	301,2>257,2	-	1
9	GLCA†	glycolithocholic acid	432.30>432.30	-	1
10	Lyso-PAF	lyso-platelet activating factor	482,3>184,1	-	1
11	OEA	oleoylethanolamine	326,2>62,1	+	1
12	TCDCA†	taurochenodeoxycholic acid	498.40>498.40	-	1
13	TDCA†	taurodeoxycholic acid	498.40>498.40	-	1
14	UDCA†	ursodeoxycholic acid	391.30>391.30	-	1
15	**S1P (17:0) IS**	**sphingosine-1-phosphate (17:0) IS**	**366.3>250.4**	+	**1**

†illustrated in heatmap of primary metabolites

Table S6: Mass transitions for sphingosine-1-phosphate and sphingosine. The target ion shows the multiple reaction monitoring (MRM) transitions, the ionization polarity (IP) shows the ionization mode of the ESI source and the internal standard (IS) column assigns the number of the internal standard to the compounds with which they were evaluated. The internal standard is marked in bold letters.

no.	compound	target ion	IP	IS
1	sphingosine-1-phosphate†	380.3>264.4	+	1
2	sphingosine†	300.4>282.4	+	1
3	**sphingosine-1-phosphate (17:0) IS**	**366.3>250.4**	**+**	**1**

†illustrated in heatmap of phospholipids II

Table S7. Average concentration of cytokines in serum. Mice underwent sham or CLP surgery, 24 h later 31 cytokines and chemokines were assessed in serum. Data are expressed as mean ± SEM (pg/ml). The following groups were studied WT sham (n = 5), *Xid* sham (n = 5), WT-CLP (n = 10), *Xid*-CLP (n = 10), WT-CLP + ibrutinib (n = 8), *Xid*-CLP + ibrutinib (n = 6).

	WT Sham		***Xid* Sham**		**WT CLP**		***Xid* CLP**		**WT CLP + ibrutinib**		***Xid* CLP + ibrutinib**	
	Mean	SEM +/-	Mean	SEM +/-	Mean	SEM +/-	Mean	SEM +/-	Mean	SEM +/-	Mean	SEM +/-
BCA-1/CXCL13	7034.2	3097.9	8937.8	2330.0	83810.3	4310.6	77435.3	2269.3	85285.5	3220.6	80840.9	1375.5
CTACK/CCL27	1872.3	202.1	2327.4	398.1	3886.4	339.4	8395.2	1781.0	7661.8	1191.3	7369.2	1032.9
ENA-78/CXCL5	1980.0	772.6	2831.5	987.5	45770.7	5248.7	8462.4	969.7	11727.6	2524.8	7210.7	982.8
Eotaxin/CCL11	420.6	151.2	733.3	171.2	6869.6	356.5	1952.5	224.5	2690.1	465.2	1907.8	179.3
Eotaxin-2/CCL24	13102.7	4999.2	18708.2	3000.5	56736.3	5714.4	25735.7	2079.7	11983.1	1876.6	29652.0	3562.5
Fractalkine/CXCL1	264.5	9.1	279.7	17.5	1181.9	109.7	322.8	12.2	457.7	47.5	352.9	20.4
GM-CSF	5.4	0.8	5.4	0.7	346.2	58.6	7.5	1.1	14.7	3.2	7.7	0.7
I-309/CCL1	45.6	4.9	58.4	14.0	198.7	66.5	799.7	190.5	80.1	15.6	11691.8	9593.7
IFN-γ	133.8	11.1	155.5	17.5	134.0	16.2	102.3	15.1	98.1	28.8	191.6	14.4
IL-1β	680.0	57.0	706.3	72.6	1536.3	184.7	674.6	31.4	611.0	43.8	768.9	28.0
IL-2	11.7	2.6	15.9	4.0	38.3	7.8	102.6	25.8	72.8	15.4	57.4	18.7
IL-6	45.5	4.8	52.6	6.7	524272.8	43243.2	6380.9	1557.2	29367.0	18095.0	4296.7	1827.7
IL-4	74.7	3.6	87.5	8.0	65.2	3.9	76.0	8.0	52.3	9.2	92.0	3.5
IL-10	1296.5	84.4	1677.4	159.6	23882.5	2465.0	2077.0	370.9	3485.3	947.8	2252.3	362.6
IL-16	978.4	68.9	1048.3	87.4	2836.1	207.4	1313.4	86.9	1814.6	200.3	1462.5	95.6
IP-10/CXClL10	4561.3	205.3	4994.1	536.0	4837.9	327.2	4547.3	583.3	4036.2	420.8	5182.1	157.5
I-TAC/CXCL11	4666.7	272.0	5570.1	490.2	3217.0	291.5	3372.9	340.1	2991.7	826.7	5569.5	376.0
KC/CXCL1	298.0	24.0	337.9	24.5	158693.9	35967.2	9014.0	1570.5	16952.6	6344.1	8912.3	2432.5
MCP-1/CCL2	515.8	36.3	601.9	59.7	262035.2	117148.0	9660.5	3217.7	10558.8	3887.3	3100.1	531.8
MCP-5/CCL12	24.0	4.9	31.6	4.5	5348.5	785.1	935.7	129.2	1020.6	157.1	758.3	70.1
MDC/CCL22	190.9	41.0	210.3	35.3	1869.7	235.7	494.0	48.3	515.9	36.1	717.8	69.6
MIP-1α/CCL3	27.5	2.1	34.0	3.7	4994.4	1664.0	175.4	56.9	81.7	24.5	56.1	2.2
MIP1-β/CCL4	123.9	6.9	141.1	12.9	51791.1	19413.9	1445.3	372.8	2859.4	1022.9	509.2	68.5
MIP-3α/CCL20	38.8	3.4	41.7	4.4	893.8	117.3	691.2	157.2	549.9	176.4	1134.8	163.6
MIP-3β/CCL19	2285.8	104.5	2520.6	204.6	3622.2	350.3	3830.6	351.0	2933.2	242.3	4925.1	465.9
Rantes/CCL5	28.8	5.4	33.4	5.9	2647.5	421.4	80.0	10.3	487.9	148.7	110.0	24.3
SCYB16/CXCL16	601.1	133.4	748.4	91.0	4588.5	467.1	2250.7	317.4	2440.4	447.1	1851.1	266.6
SDF-1α/CXCL12	929.5	197.3	1263.0	218.9	447.7	63.0	1612.0	177.7	1113.3	341.6	2304.9	389.7
TARC/CCL17	115.6	16.7	146.8	21.6	3293.6	376.2	2269.2	441.2	755.4	114.8	5268.3	1862.4
TNF-α	311.2	16.7	310.6	28.0	471.7	42.9	205.1	16.5	208.5	38.7	330.8	27.1