

Supplemental Table 1. Primers for quantitative real-time PCR.

Gene		Sequence 5'----3'(Mouse)
β-actin	Foward	GGCTGTATTCCCCTCCATCG
	Reverse	CCAGTTGGTAACAATGCCATGT
IDO1	Foward	GCTTTGCTCTACCACATCCAC
	Reverse	CAGGCGCTGTAACCTGTGT
TDO2	Foward	ATGAGTGGGTGCCCGTTTG
	Reverse	GGCTCTGTTTACACCAGTTTGAG
TPH	Foward	AACAAAGACCATTCTCCGAAAG
	Reverse	TGTAACAGGCTCACATGATTCTC
AADC	Foward	TAGCTGACTATCTGGATGGCAT
	Reverse	GTCCTCGTATGTTTCTGGCTC
SCD1	Foward	TTCTTGCGATACTCTGGTGC
	Reverse	CGGGATTGAATGTTCTTGTCGT
FASN	Foward	GGAGGTGGTGATAGCCGGTAT
	Reverse	TGGGTAATCCATAGAGCCCAG
IL-17A	Foward	TTTAACTCCCTTGGCGCAAAA

Reverse

CTTCCCTCCGCATTGACAC

Supplemental Table 2. Upregulated differential metabolites between the control group and the *Pneumocystis*-infected WT mice group under ESI- and ESI+ modes.

No.	Compounds	Class.I	Class.II	VIP	p_value	Fold_Change	Log2FC	Type
Positive ion (ESI+)								
1	PE-NMe(14:0/18:1(11Z))	Lipids and lipid-like molecules	Glycerophospholipids	1.54	0.00	2.58	1.37	up
2	PC(16:0/18:1(11Z))	Lipids and lipid-like molecules	Glycerophospholipids	1.35	0.01	4.39	2.13	up
3	1,2-Dipentadecanoyl-sn-glycero-3-phosphocholine	Lipids and lipid-like molecules	Glycerophospholipids	1.54	0.00	2.87	1.52	up
4	PC(14:0/22:2(13Z,16Z))	Lipids and lipid-like molecules	Glycerophospholipids	1.79	0.00	6.22	2.64	up
5	PC(20:2(11Z,14Z)/16:0)	Lipids and lipid-like molecules	Glycerophospholipids	1.38	0.01	3.72	1.89	up
6	9,10-Dihydroxystearate	Lipids and lipid-like molecules	Fatty Acyls	1.36	0.01	2.07	1.05	up
7	PC(14:0/20:1(11Z))	Lipids and lipid-like molecules	Glycerophospholipids	1.32	0.02	4.86	2.28	up
8	11-HpODE; (9Z,12Z)-(11S)-11-Hydroperoxy octadeca-9,12-dienoate	Lipids and lipid-like molecules	Fatty Acyls	1.40	0.01	2.19	1.13	up
9	Toluene-cis-dihydrodiol;(1S,2R)- 3-Methylcyclohexa-3,5-diene-1,2 -diol	Organic oxygen compounds	Organooxygen compounds	1.44	0.01	2.03	1.02	up
10	PC(20:0/14:1(9Z))	Lipids and lipid-like molecules	Glycerophospholipids	1.33	0.01	2.03	1.02	up
11	5alpha-Androstane-3alpha,17beta -diol	Lipids and lipid-like molecules	Steroids and steroid derivatives	1.30	0.01	2.48	1.31	up
12	PA(20:2(11Z,14Z)/15:0)	Lipids and lipid-like molecules	Glycerophospholipids	1.49	0.00	2.55	1.35	up
13	11,14,15-THETA	Lipids and lipid-like molecules	Fatty Acyls	1.27	0.02	2.83	1.50	up
14	PC(18:1(11Z)/18:0)	Lipids and lipid-like molecules	Glycerophospholipids	1.23	0.03	2.66	1.41	up

	DG(22:1(13Z)/20:5(5Z,8Z,11Z,1								
15	4Z,17Z)/0:0)	Lipids and lipid-like molecules	Glycerolipids	1.76	0.00	5.45	2.45	up	
16	PC(14:1(9Z)/22:0)	Lipids and lipid-like molecules	Glycerophospholipids	1.32	0.01	2.29	1.20	up	
17	Adenosine 5'-Monophosphate	Nucleotide And Its metabolomics	Nucleotide and Its metabolomics	1.36	0.01	3.07	1.62	up	
18	PE-NMe(16:0/20:0)	Lipids and lipid-like molecules	Glycerophospholipids	1.10	0.03	2.55	1.35	up	
	DG(20:4(5Z,8Z,11Z,14Z)/22:5(4								
19	Z,7Z,10Z,13Z,16Z)/0:0)	Lipids and lipid-like molecules	Glycerolipids	1.27	0.02	2.11	1.08	up	
20	Choline	Tryptamines,Cholines,Pigments	Cholines	1.31	0.01	2.22	1.15	up	
21	Inosine	Nucleotide And Its metabolomics	Nucleotide and Its metabolomics	1.71	0.00	2.13	1.09	up	
22	3-Hydroxybutyrylcarnitine	Lipids and lipid-like molecules	Fatty Acyls	1.42	0.01	2.24	1.17	up	
	DG(20:1(11Z)/20:5(5Z,8Z,11Z,1								
23	4Z,17Z)/0:0)	Lipids and lipid-like molecules	Glycerolipids	1.32	0.02	2.72	1.44	up	
24	PA(21:0/12:0)	Lipids and lipid-like molecules	Glycerophospholipids	1.40	0.02	2.08	1.06	up	
25	Crotonoside	Nucleosides, nucleotides, and analogues	Purine nucleosides	1.69	0.00	3.35	1.75	up	
		Hormones and hormone related	Hormones and hormone related						
26	Progesterone	compunds	compunds	1.24	0.02	2.34	1.23	up	
27	Allopurinol	Nucleotide And Its metabolomics	Nucleotide and Its metabolomics	1.71	0.00	2.02	1.01	up	
28	Cytidine	Nucleotide And Its metabolomics	Nucleotide and Its metabolomics	1.52	0.00	2.27	1.18	up	
29	Cumaroylspermidine	Phenylpropanoids and polyketides	Cinnamic acids and derivatives	1.35	0.01	2.64	1.40	up	
30	(R)-Pantetheine	Organic acids and derivatives	Carboxylic acids and derivatives	1.73	0.00	2.14	1.10	up	
31	Tyr Ser Leu	--	--	1.29	0.02	8.85	3.15	up	
32	Pro Pro Ile	--	--	1.58	0.00	2.81	1.49	up	
	Indole-3-acetaldehyde								
	oxime;Indole-3-acetaldoxime;3-I								
	ndoleacetaldoxime;(E)-Indol-3-yl								
33	acetaldoxime	Organoheterocyclic compounds	Indoles and derivatives	1.18	0.03	2.06	1.04	up	

34	Formyl-5-hydroxykynurenamine	Organic oxygen compounds	Organooxygen compounds	1.19	0.05	2.58	1.37	up
35	Propamocarb	Organic acids and derivatives	Carboxylic acids and derivatives	1.18	0.03	2.35	1.24	up
			Benzene and substituted					
36	Benzamidine	Benzenoids	derivatives	1.25	0.04	2.13	1.09	up
37	LysoPA(16:0/0:0)	Lipids and lipid-like molecules	Glycerophospholipids	1.23	0.04	4.45	2.16	up
	1-Stearoyl-2-linoleoyl-sn-glycero							
38	-3-phosphocholine	Lipids and lipid-like molecules	Glycerophospholipids	1.16	0.03	2.79	1.48	up
39	Phosphite	Homogeneous non-metal compounds	Non-metal oxoanionic compounds	1.50	0.00	2.67	1.42	up
40	Prostaglandin E2-1-glyceryl ester	Lipids and lipid-like molecules	Fatty Acyls	1.23	0.03	2.42	1.27	up
41	7-(Methylthio)heptanenitrile	Organic nitrogen compounds	Organonitrogen compounds	1.22	0.01	2.02	1.01	up
42	5-Geranoxy-7-methoxycoumarin	Lipids and lipid-like molecules	Prenol lipids	1.45	0.00	2.52	1.33	up
	Phosphonic acid, P-[[[(1R,2S)-2-aminocyclohexyl]							
43	amino]carbonyl]-, rel-	Organic nitrogen compounds	Organonitrogen compounds	1.67	0.00	2.41	1.27	up
44	Noroxymorphone	Benzenoids	Phenanthrenes and derivatives	1.15	0.04	2.03	1.02	up
45	Leu-Gly	Amino acid and Its metabolomics	Small Peptide	1.40	0.01	2.14	1.10	up
46	Trimethylamine oxide	Organic nitrogen compounds	Organonitrogen compounds	1.39	0.01	8.27	3.05	up
47	Pro Ile	--	--	1.65	0.00	2.78	1.48	up
48	Farnesylthiosalicylic acid	Lipids and lipid-like molecules	Prenol lipids	1.45	0.01	2.77	1.47	up
49	Sitagliptin	Organic acids and derivatives	Carboxylic acids and derivatives	1.50	0.00	2.50	1.32	up
50	Pro Leu Val	--	--	1.63	0.00	2.46	1.30	up
51	8-Cyclopentyltheophylline	Organoheterocyclic compounds	Imidazopyrimidines	1.44	0.00	2.04	1.03	up
			Benzene and substituted					
52	Hydroxyzine	Benzenoids	derivatives	1.79	0.00	2.10	1.07	up
53	Tyr Tyr Asp	--	--	1.11	0.04	4.00	2.00	up
54	Trp Phe Arg	--	--	1.20	0.04	2.20	1.14	up

	2'-Deoxyguanosine							
2	5'-monophosphate	Nucleosides, nucleotides, and analogues	Purine nucleotides	1.32	0.01	2.49	1.31	up
3	Dihydroxyacetone	Organic oxygen compounds	Organooxygen compounds	1.24	0.02	3.45	1.79	up
4	2-Aminoethanesulfonic Acid	Organic acid And Its derivatives	Sulfonic acids	1.35	0.01	2.22	1.15	up
5	L-Lactic Acid	Organic acid And Its derivatives	Organic acid and Its derivatives	1.25	0.02	3.17	1.66	up
6	Guanosine	Nucleotide And Its metabolomics	Nucleotide and Its metabolomics	1.54	0.00	2.03	1.02	up
7	4-hydroxybenzenesulfonic acid	Organic acid And Its derivatives	Sulfonic acids	1.36	0.01	2.09	1.06	up
8	Hexanoyl Glycine	Amino acid and Its metabolomics	Amino acid derivatives	1.60	0.00	2.51	1.33	up
9	3'-Aenylic Acid	Nucleotide And Its metabolomics	Nucleotide and Its metabolomics	1.43	0.01	2.43	1.28	up
10	PG(16:0/0:0)[U]	--	--	1.32	0.01	2.11	1.08	up
11	alpha-Bisabolol oxide C	Organoheterocyclic compounds	Oxanes	1.57	0.00	4.68	2.23	up
12	Uridine	Nucleotide And Its metabolomics	Nucleotide and Its metabolomics	1.71	0.00	2.63	1.40	up
13	Fast green FCF	--	--	1.43	0.00	4.02	2.01	up
			Benzene and substituted					
14	Glucotropaeolin	Benzene and substituted derivatives	derivatives	1.33	0.01	2.45	1.29	up
15	(±)13-HpODE	Oxidized lipid	Oxidized lipid	1.35	0.02	2.19	1.13	up
16	2-Hydroxy-2-methylbutyric acid	Organic acids	Organic acids	1.37	0.01	2.69	1.43	up
17	4-Hydroxybenzoic Acid	Phenolic acids	Phenolic acids	1.35	0.01	2.03	1.02	up
18	Lys Thr Gln Lys	--	--	1.72	0.00	2.36	1.24	up
	Diethylstilbestrol diphosphate; Fosfestrol; Diethylstil							
19	bestrol bisphosphate	Phenylpropanoids and polyketides	Stilbenes	1.32	0.01	2.85	1.51	up
			Benzene and substituted					
20	Darunavir	Benzenoids	derivatives	1.62	0.00	2.80	1.49	up
21	N6-Succinyl Adenosine	Nucleotide And Its metabolomics	Nucleotide and Its metabolomics	1.22	0.03	2.92	1.54	up

Supplemental Table 3. Downregulated differential metabolites between the control group and *Pneumocystis*-infected WT mice group under ESI- and ESI+ modes.

No.	Compounds	Class.I	Class.II	VIP	p_value	Fold_Change	Log2FC	Type
Positive ion (ESI+)								
1	PE-NMe2(20:5(5Z,8Z,11Z,14Z,17Z)/22:6(4Z,7Z,10Z,13Z,16Z,19Z))	Lipids and lipid-like molecules	Glycerophospholipids	1.73	0.00	0.46	-1.13	down
2	(6E)-8-Oxogeraniol	Lipids and lipid-like molecules	Prenol lipids	1.73	0.00	0.49	-1.04	down
3	MG(0:0/18:1(9Z)/0:0)	Lipids and lipid-like molecules	Glycerolipids	1.47	0.01	0.38	-1.39	down
4	Atrazine	Heterocyclic compounds	Heterocyclic compounds	1.72	0.00	0.41	-1.29	down
5	2-Succinyl-5-enolpyruvyl-6-hydroxy-3-cyclohexene-1-carboxylate;5-Enolpyruvyl-6-hydroxy-2-succinylcyclohex-3-ene-1-carboxylate	Organic acids and derivatives	Carboxylic acids and derivatives	1.40	0.01	0.48	-1.06	down
6	2-acetamido-N-[(2S,4R)-4-hydroxy-2-(hydroxymethyl)-5-[6-(methylamino)purin-9-yl]oxolan-3-yl]-3-(4-hydroxyphenyl)propanamide	Nucleosides, nucleotides, and analogues	Purine nucleosides	1.39	0.01	0.44	-1.18	down
7	20-oxo-leukotriene B4	Lipids and lipid-like molecules	Fatty Acyls	1.53	0.00	0.34	-1.54	down
8	(-)-endo-Fenchol;(-)-alpha-Fenchyl alcohol	Lipids and lipid-like molecules	Prenol lipids	1.21	0.02	0.39	-1.34	down
9	1,2,3,4,4a,7,7a,13-octahydro-4,12-methanobenzofuro[3,2-e]isoquinoline-7,9-diol	Alkaloids and derivatives	Morphinans	1.16	0.02	0.49	-1.04	down

10	Bufotenine	Organoheterocyclic compounds	Indoles and derivatives	1.62	0.00	0.36	-1.48	down
11	TG(18:2(9Z,12Z)/20:5(5Z,8Z,11Z,14Z,17Z)/18:4(6Z,9Z,12Z,15Z))	Lipids and lipid-like molecules	Glycerolipids	1.78	0.00	0.22	-2.18	down
12	10,16-Dihydroxyhexadecanoic acid	Lipids and lipid-like molecules	Fatty Acyls Benzene and substituted derivatives	1.41	0.01	0.48	-1.05	down
13	Phenylacetic acid	Benzenoids	derivatives	1.65	0.00	0.45	-1.15	down
14	3-Methyl-2-Oxobutanoic Acid	Organic acid And Its derivatives	Organicacid and Its derivatives	1.51	0.00	0.41	-1.28	down
15	Aflatoxin B1	Phenylpropanoids and polyketides	Coumarins and derivatives	1.73	0.00	0.33	-1.58	down
16	(E)-2-Methylbutanal oxime	Organic nitrogen compounds	Organonitrogen compounds	1.72	0.00	0.47	-1.08	down
17	2-Iminopropanoate (1R,6R)-6-Hydroxy-2-succinylcyclohexa-2,4-diene-1-carboxylate;(1R,6R)-2-Succinyl-6-hydroxy-2,4-cyclohexadiene-1-carboxylate;SHCHC	Organic nitrogen compounds	Organonitrogen compounds	1.29	0.01	0.48	-1.06	down
18	oxylate;SHCHC	Organic acids and derivatives	Keto acids and derivatives	1.57	0.00	0.44	-1.18	down
19	N-Formylidemecolcine	Hydrocarbon derivatives	Tropones	1.77	0.00	0.32	-1.63	down
20	Caffeine	Alkaloids	Alkaloids	1.73	0.00	0.25	-2.01	down
21	Val-Pro (2S)-4-(2-aminophenyl)-2-azaniumyl-4-oxobutanoate	Organic acids and derivatives	Carboxylic acids and derivatives	1.64	0.00	0.32	-1.63	down
22	iumyl-4-oxobutanoate	Organic oxygen compounds	Organooxygen compounds	1.26	0.03	0.36	-1.49	down
23	2'-O-methyladenosine	Nucleotide And Its metabolomics	Nucleotide and Its metabolomics	1.40	0.01	0.45	-1.14	down
24	3'-Adenylic acid	Nucleosides, nucleotides, and analogues	Ribonucleoside 3'-phosphates	1.33	0.01	0.39	-1.34	down
25	Enoxolone	Lipids and lipid-like molecules	Prenol lipids	1.69	0.00	0.42	-1.24	down
26	3"-Deamino-3"-hydroxykanamycin	Organic oxygen compounds	Organooxygen compounds	1.56	0.00	0.29	-1.81	down

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			Benzene and substituted						
27	Bisphenol A diglycidyl ether	Benzenoids	derivatives	1.74	0.00	0.36	-1.46	down	
28	Gly Leu Arg Asn Gln	--	--	1.71	0.00	0.36	-1.49	down	
29	Lys Lys Thr	--	--	1.52	0.01	0.24	-2.09	down	
30	Asiatic acid	Lipids and lipid-like molecules	Prenol lipids	1.68	0.00	0.49	-1.02	down	
31	4,6-Dihydroxyquinoline	Alkaloids	Quinoline alkaloids	1.42	0.02	0.05	-4.28	down	
	4-(2-Aminophenyl)-2,4-dioxob								
32	utanoic acid	Organic oxygen compounds	Organooxygen compounds	1.37	0.00	0.40	-1.34	down	
	Diphenylphosphine isopropyl								
33	ester	--	--	1.70	0.00	0.33	-1.62	down	
34	Pro Arg Trp	--	--	1.66	0.00	0.25	-2.00	down	
35	Ammelide	Organoheterocyclic compounds	Triazines	1.71	0.00	0.43	-1.20	down	
36	Val Ser Ser Ser Leu	--	--	1.71	0.00	0.44	-1.18	down	
	2-methoxy-1,7,9-trimethylpurin								
37	e-6,8-dione	Organoheterocyclic compounds	Imidazopyrimidines	1.37	0.02	0.30	-1.73	down	
38	Propylparaben	Benzene and substituted derivatives	Phenolic acids	1.53	0.00	0.37	-1.44	down	
39	3 β -Hydroxy-5-cholenoic acid	Lipids and lipid-like molecules	Steroids and steroid derivatives	1.72	0.00	0.47	-1.09	down	
40	2-Oxoglutaric acid	Organic acids and derivatives	Keto acids and derivatives	1.31	0.01	0.47	-1.08	down	
41	Chenodeoxycholic acid	Lipids and lipid-like molecules	Steroids and steroid derivatives	1.69	0.00	0.49	-1.04	down	
			Benzene and substituted						
42	4-Anisaldehyde	Benzenoids	derivatives	1.68	0.00	0.46	-1.12	down	
43	L-Homoarginine	Amino acids and derivatives	Amino acids and derivatives	1.69	0.00	0.47	-1.08	down	
44	Carnitine C5:0	FA	CAR	1.67	0.00	0.38	-1.38	down	
45	Kynurenine	Amino acid and Its metabolomics	Amino acid derivatives	1.55	0.00	0.46	-1.13	down	
46	PA(i-21:0/a-15:0)	Lipids and lipid-like molecules	Glycerophospholipids	1.77	0.00	0.42	-1.25	down	

			Benzene and substituted						
47	Fenobucarb	Benzenoids	derivatives	1.33	0.03	0.28	-1.83	down	
48	Leu Ser Asn (1R,2S,3S,4S,5S,8R,9R,12R)-5 -hydroxy-4-methyl-13-methyl denetetracyclo[10.2.1.01,9.03,8]pentadecane-2,4,8-tricarboxyli c acid	--	--	1.72	0.00	0.43	-1.22	down	
49	Asp Gln Asn Asp	Lipids and lipid-like molecules	Prenol lipids	1.49	0.01	0.31	-1.70	down	
50	Cortisone	--	--	1.67	0.00	0.41	-1.27	down	
51	Retinoic Acid	Lipids and lipid-like molecules	Steroids and steroid derivatives	1.64	0.00	0.48	-1.05	down	
52	Butyl Phosphorotrithioate	Lipids and lipid-like molecules	Prenol lipids	1.07	0.04	0.49	-1.04	down	
53	Val His Ile	Organophosphorus compounds	Organothiophosphorus compounds	1.35	0.02	0.31	-1.68	down	
54	PE-NMe(15:0/18:4(6Z,9Z,12Z, 15Z))	--	--	1.64	0.00	0.30	-1.75	down	
55	Ile Pro Tyr	Lipids and lipid-like molecules	Glycerophospholipids	1.43	0.01	0.50	-1.01	down	
56	Feruloylcholine	--	--	1.65	0.00	0.49	-1.02	down	
57	Ser Gly Ala Asn Lys	Alkaloids	Alkaloids	1.65	0.00	0.47	-1.09	down	
58	benzyl 4-(1,3-dioxoisindolin-2-yl)-2', 2'-dimethyl-3',5-dioxo-2',3',4,5- tetrahydro-3H-spiro[furan-2,9'- imidazo[1,2-a]indole]-1'(9a'H)- carboxylate	--	--	1.66	0.00	0.29	-1.77	down	
59	Carpropamid	--	--	1.61	0.00	0.42	-1.25	down	
60		Benzenoids	Benzene and substituted	1.65	0.00	0.40	-1.32	down	

			derivatives						
61	PA(21:0/i-15:0) 4-Coumaroylshikimate;trans-5-	Lipids and lipid-like molecules	Glycerophospholipids	1.81	0.00	0.32	-1.65	down	
62	O-(4-Coumaroyl)shikimate	Phenylpropanoids and polyketides	Cinnamic acids and derivatives	1.68	0.00	0.26	-1.93	down	
63	Goshonoside F2	Lipids and lipid-like molecules	Prenol lipids	1.21	0.03	0.50	-1.01	down	
64	1,24-Dihydroxyvitamin D3	Lipids and lipid-like molecules	Steroids and steroid derivatives	1.38	0.02	0.19	-2.38	down	
65	Leu Ala Tyr Hydroxyspirilloxanthin;Monod	--	--	1.57	0.00	0.41	-1.28	down	
66	emethyl spirilloxanthin	Lipids and lipid-like molecules	Prenol lipids	1.67	0.00	0.31	-1.69	down	
67	Normeperidine (4S,4aS,12aR)-4-azaniumyl-2-c arbamoyl-10,11,12a-trihydroxy -6-methyl-3,12-dioxo-4a,5-dihy	Organoheterocyclic compounds	Piperidines	1.40	0.02	0.05	-4.20	down	
68	dro-4H-tetracen-1-olate	--	--	1.67	0.00	0.42	-1.24	down	
69	N-Acetyl-5-Hydroxytryptamine	Tryptamines,Cholines,Pigments	Tryptamines	1.62	0.00	0.30	-1.74	down	
70	Fluazifop-butyl N-[4-[3,5-Bis(trifluoromethyl)p yrazol-1-yl]phenyl]-4-methylth	Benzenoids	Benzene and substituted derivatives	1.64	0.00	0.45	-1.15	down	
71	iadiazole-5-carboxamide N,N-Diethyl-3-methylbenzami	Benzenoids	Benzene and substituted derivatives	1.45	0.00	0.48	-1.06	down	
72	de 20-Hydroxy-3,7,11,15,23-penta	Benzenoids	derivatives	1.74	0.00	0.43	-1.22	down	
73	oxolanost-8-en-26-oic acid	Lipids and lipid-like molecules	Prenol lipids	1.69	0.00	0.41	-1.30	down	
74	D-Pantothenoyl-L-cysteine	Organic acids and derivatives	Peptidomimetics	1.62	0.00	0.30	-1.73	down	
75	Thr His Ala	--	--	1.72	0.00	0.48	-1.07	down	

76	Isonicotinamide	Organoheterocyclic compounds	Pyridines and derivatives	1.66	0.00	0.38	-1.40	down
77	Ritalinic acid	Organic acid And Its derivatives	Organicacid and Its derivatives	1.53	0.00	0.43	-1.23	down
78	Carbinoxamine	Benzenoids	Benzene and substituted derivatives	1.72	0.00	0.46	-1.12	down
	5-(Methylthio)-N-(3-pyridyl)-6-(trifluoromethyl)indoline-1-carboxamide							
79	boxamide	Organoheterocyclic compounds	Indoles and derivatives	1.35	0.01	0.40	-1.34	down
80	Ala Asp Arg Arg	--	--	1.69	0.00	0.43	-1.22	down
	Coumarin-suberoylanilide							
81	hydroxamic acid	Phenylpropanoids and polyketides	Coumarins and derivatives	1.73	0.00	0.41	-1.29	down
82	Albendazole oxide	Organoheterocyclic compounds	Benzimidazoles	1.71	0.00	0.50	-1.00	down
83	Monoethyl phthalate	Benzenoids	Benzene and substituted derivatives	1.64	0.00	0.45	-1.16	down
84	Aflatoxin B2	Phenylpropanoids and polyketides	Coumarins and derivatives	1.69	0.00	0.46	-1.12	down
	N-Cbz-L-phenylalanyl-chloromethane		Benzene and substituted derivatives					
85	ethane	Benzenoids	derivatives	1.58	0.00	0.31	-1.69	down
86	Phosphamidon	Organic acids and derivatives	Organic phosphoric acids and derivatives	1.68	0.00	0.41	-1.30	down
			Benzene and substituted derivatives					
87	Bezafibrate	Benzenoids	derivatives	1.61	0.00	0.23	-2.10	down
88	4-Pyridylthioamide	Organoheterocyclic compounds	Pyridines and derivatives	1.71	0.00	0.40	-1.34	down
89	Tiotropium	--	--	1.35	0.02	0.33	-1.61	down
	N5-(1-Imino-3-butenyl)-L-ornithine							
90	hine	Organic acids and derivatives	Carboxylic acids and derivatives	1.48	0.01	0.43	-1.23	down
91	Citrinin	Organoheterocyclic compounds	Benzopyrans	1.63	0.00	0.41	-1.28	down
92	Flufenacet	Benzenoids	Benzene and substituted	1.35	0.01	0.34	-1.54	down

			derivatives						
93	Ala Thr Ile Lys	--	--	1.61	0.00	0.37	-1.42	down	
94	2-Aminobenzimidazole	Organoheterocyclic compounds	Benzimidazoles	1.49	0.01	0.36	-1.46	down	
95	Nifurtimox	Organoheterocyclic compounds	Furans	1.50	0.00	0.42	-1.24	down	
			Benzene and substituted						
96	4,5-diphenyl-1,2,3-Thiadiazole	Benzenoids	derivatives	1.22	0.03	0.33	-1.59	down	
97	Trp Val Arg	--	--	1.35	0.01	0.47	-1.08	down	
98	9-Phenanthrol	Benzenoids	Phenanthrenes and derivatives	1.55	0.00	0.47	-1.09	down	
	(2E)-3-(4-hydroxyphenyl)-1-ph								
99	enylprop-2-en-1-one	Phenylpropanoids and polyketides	Linear 1,3-diarylpropanoids	1.40	0.02	0.33	-1.61	down	
100	Pseudoephedrine	Alkaloids	Amphetamine alkaloids	1.65	0.00	0.44	-1.19	down	
101	4-pentyn-1-ol	Acetylides	--	1.59	0.00	0.40	-1.32	down	
			Benzene and substituted						
102	Norsufentanil	Benzenoids	derivatives	1.73	0.00	0.39	-1.35	down	
103	Val Val Leu	--	--	1.67	0.00	0.45	-1.16	down	
	Aniline; LC-ESI-QTOF; MS2;								
104	CE	--	--	1.70	0.00	0.49	-1.04	down	
			Benzene and substituted						
105	Ethiofencarb	Benzenoids	derivatives	1.61	0.00	0.29	-1.78	down	
	(5-Amino-1H-1,2,4-triazol-3-yl								
106)methanol	Organoheterocyclic compounds	Azoles	1.33	0.01	0.43	-1.22	down	
			Triazole ribonucleosides and						
107	Ribavirin	Nucleosides, nucleotides, and analogues	ribonucleotides	1.51	0.00	0.42	-1.26	down	
108	Pro Glu Tyr	--	--	1.69	0.00	0.42	-1.25	down	
			Organic sulfonic acids and						
109	Acamprosate	Organic acids and derivatives	derivatives	1.46	0.01	0.41	-1.30	down	

110	Val Asn Asp Myristyltrimethylaminium bromide;Tetradecyltrimethylam monium bromide;MTAB	--	--	1.71	0.00	0.46	-1.12	down
111		Organic nitrogen compounds	Organonitrogen compounds	1.63	0.00	0.48	-1.05	down
112	Bispyribac	Organic oxygen compounds	Organooxygen compounds	1.54	0.01	0.22	-2.19	down
113	Fentrazamide	Organoheterocyclic compounds	Azoles	1.68	0.00	0.45	-1.14	down
114	Gly Phe Asp	--	--	1.47	0.01	0.31	-1.69	down
115	Bensultap	Benzenoids	Benzene and substituted derivatives	1.56	0.00	0.27	-1.92	down
116	P-Aminohippuric Acid	Amino acid and Its metabolomics	Amino acid derivatives	1.74	0.00	0.37	-1.45	down
117	TyrMe-Asp-OH	--	--	1.52	0.00	0.29	-1.77	down
118	Picoxystrobin	Benzenoids	Benzene and substituted derivatives	1.34	0.01	0.33	-1.58	down
119	Leu-Tyr	Organic acids and derivatives	Carboxylic acids and derivatives	1.48	0.00	0.43	-1.23	down
120	Nocodazole	Organoheterocyclic compounds	Benzimidazoles	1.66	0.00	0.19	-2.39	down
121	Westiellamide	Organic acids and derivatives	Carboxylic acids and derivatives	1.71	0.00	0.49	-1.03	down
122	Pro Pro Gly	--	--	1.55	0.00	0.48	-1.06	down
123	Ser Phe Lys 2-Methylamino-1-(3,4-methyle nedioxyphenyl)butan-1-one	--	--	1.64	0.00	0.50	-1.01	down
124		Benzenoids	Benzene and substituted derivatives	1.77	0.00	0.44	-1.19	down
125	D-Arginine	Organic acids and derivatives	Carboxylic acids and derivatives	1.69	0.00	0.42	-1.26	down
126	BUTACAINE	--	--	1.70	0.00	0.48	-1.06	down
127	Seneciophyllin	Alkaloids and derivatives	--	1.71	0.00	0.42	-1.27	down
128	Pro Val Phe	--	--	1.24	0.01	0.46	-1.11	down
129	Asp His Met	--	--	1.16	0.02	0.48	-1.05	down
130	Treprostinil	Benzenoids	Benzene and substituted	1.64	0.00	0.40	-1.31	down

			derivatives					
131	Bromopride	Benzenoids	Phenol ethers	1.66	0.00	0.31	-1.67	down
132	Monoethylglycinexylidide	Organic acids and derivatives	Carboxylic acids and derivatives	1.53	0.01	0.25	-2.02	down
133	Carnosine	Organic acids and derivatives	Peptidomimetics	1.70	0.00	0.47	-1.09	down
			Benzene and substituted					
134	Formetanate	Benzenoids	derivatives	1.79	0.00	0.34	-1.55	down
135	Carminic acid	--	--	1.56	0.00	0.36	-1.46	down
136	Gly Leu Arg Val Phe	--	--	1.74	0.00	0.49	-1.02	down
137	2-Butyl-4-methylphenol	Benzenoids	Phenols	1.52	0.00	0.38	-1.40	down
138	Tacrine	Organoheterocyclic compounds	Quinolines and derivatives	1.70	0.00	0.36	-1.46	down
139	Trehalose 6-phosphate	Others	Saccharides and Alcohols	1.64	0.00	0.31	-1.67	down
140	Hexobarbital	Organoheterocyclic compounds	Diazines	1.50	0.00	0.44	-1.18	down
141	Arg Gln Arg	--	--	1.65	0.00	0.49	-1.03	down
			Benzene and substituted					
142	Tebufenpyrad	Benzenoids	derivatives	1.66	0.00	0.20	-2.34	down
143	Asp His Phe	--	--	1.44	0.01	0.47	-1.08	down
144	His Tyr Ile Asp	--	--	1.10	0.03	0.48	-1.06	down
145	Cys Glu Lys	--	--	1.61	0.00	0.32	-1.62	down
			Benzene and substituted					
146	(4-Chlorophenyl)biguanide	Benzenoids	derivatives	1.46	0.00	0.35	-1.53	down
147	Ala Pro Met	--	--	1.56	0.01	0.22	-2.17	down
	L-Threonylcarbamoyladenylate ;L-Threonylcarbamoyl-AMP;T							
148	C-AMP	Nucleosides, nucleotides, and analogues	Purine nucleotides	1.40	0.02	0.27	-1.89	down
			Benzene and substituted					
149	Dexmedetomidine	Benzenoids	derivatives	1.73	0.00	0.36	-1.48	down

150	Cys Tyr Thr	--	--	1.53	0.00	0.44	-1.17	down
151	Carnitine C14:1	FA	CAR	1.55	0.01	0.22	-2.19	down
			Benzene and substituted					
152	Emopamil 1H-1,4-Diazepine, 4-(aminoacetyl)hexahydro-2-m ethyl-1-[(4-methyl-5-isoquinoli nyl)sulfonyl]-, (2S)-	Benzenoids	derivatives	1.72	0.00	0.48	-1.06	down
153	Demethoxykanugin	Organic acids and derivatives	Carboxylic acids and derivatives	1.49	0.01	0.24	-2.03	down
154	Tyr Cys Leu	Phenylpropanoids and polyketides	Flavonoids	1.69	0.00	0.45	-1.15	down
155	Genistein	--	--	1.50	0.00	0.45	-1.15	down
156	Iprovalicarb	Flavonoids	Isoflavones	1.60	0.00	0.34	-1.55	down
			Benzene and substituted					
157	Gln-Gly	Benzenoids	derivatives	1.70	0.00	0.47	-1.08	down
158	Rolipram	--	--	1.32	0.03	0.27	-1.91	down
159	Cys Phe Lys	Organoheterocyclic compounds	Pyrrolidines	1.65	0.00	0.46	-1.12	down
160	Alloxydim	--	--	1.48	0.01	0.47	-1.10	down
161	Cucurbitacin I	Organic oxygen compounds	Organooxygen compounds	1.52	0.01	0.33	-1.60	down
162	Simetryn	Lipids and lipid-like molecules	Steroids and steroid derivatives	1.68	0.00	0.46	-1.11	down
163	L-Homocystine	Organoheterocyclic compounds	Triazines	1.56	0.00	0.43	-1.23	down
164	Epoxiconazole	Amino acid and Its metabolomics	Amino acids	1.64	0.00	0.21	-2.24	down
165	(2Z)-((4R,5S,6S)-6-(β-D-Gluco pyranosyloxy)-4,5-dihydroxy clohex-2-en-1-ylidene)acetonitr	Phenylpropanoids and polyketides	Stilbenes	1.61	0.00	0.28	-1.85	down
166	ile	Organic oxygen compounds	Organooxygen compounds	1.57	0.00	0.49	-1.02	down
167	6-Furfurylaminopurine riboside	Nucleosides, nucleotides, and analogues	Purine nucleosides	1.46	0.01	0.35	-1.51	down

	(3S,7R)-11-methoxy-3,7-dimethyl-6,8,16,20-tetraoxapentacyclo[10.8.0.0.0.2,9.0.3,7.0.13,18]icosa-1,4,9,11,13(18)-pentaene-17,1								
168	9-dione	Phenylpropanoids and polyketides	Coumarins and derivatives	1.54	0.00	0.26	-1.93	down	
169	Avicularin	Phenylpropanoids and polyketides	Flavonoids	1.47	0.01	0.33	-1.58	down	
			Benzene and substituted						
170	2-Aminoethyl diphenylborinate	Benzenoids	derivatives	1.08	0.05	0.44	-1.18	down	
171	Byakangelicol	Phenylpropanoids and polyketides	Coumarins and derivatives	1.49	0.01	0.43	-1.23	down	
172	Val Trp Ile	--	--	1.57	0.00	0.25	-1.97	down	
173	7-Chloro-6-[4-(diethylamino)phenyl]quinoline-5,8-dione	Organoheterocyclic compounds	Quinolines and derivatives	1.62	0.00	0.40	-1.32	down	
174	2-Amino-3-(3-methylbut-2-enylthio)propionic acid	Organic acids and derivatives	Carboxylic acids and derivatives	1.77	0.00	0.37	-1.43	down	
175	Thiodicarb	Organic acids and derivatives	Organic carbonic acids and derivatives	1.35	0.01	0.49	-1.04	down	
176	Triphenyl phosphate	Aldehyde,Ketones,Esters	Esters	1.59	0.00	0.28	-1.82	down	
177	Thr-His	Organic acids and derivatives	Carboxylic acids and derivatives	1.69	0.00	0.48	-1.06	down	
178	Coumafuryl	Phenylpropanoids and polyketides	Coumarins and derivatives	1.62	0.00	0.28	-1.84	down	
179	Lupinine	Alkaloids and derivatives	Lupin alkaloids	1.58	0.00	0.29	-1.78	down	
180	3,4-Dimethoxycinnamic acid	Phenolic acids	Phenolic acids	1.71	0.00	0.44	-1.17	down	
181	Nitrazepam	Organoheterocyclic compounds	Benzodiazepines	1.62	0.00	0.19	-2.37	down	
182	[4,5,7-trihydroxy-2-(3,4,5-trihydroxyphenyl)-3,4-dihydro-2H-1-benzopyran-3-yl]oxidanesulfonic acid	Phenylpropanoids and polyketides	Flavonoids	1.50	0.01	0.29	-1.79	down	

183	Thifensulfuron-methyl 1-(2,4-Dichlorophenyl)-2-(1-im	Organoheterocyclic compounds	Thiophenes	1.47	0.00	0.48	-1.06	down
184	idazolyl)ethanol	Benzenoids	Benzene and substituted derivatives	1.51	0.01	0.30	-1.75	down
185	Reticulataxanthin	Lipids and lipid-like molecules	Prenol lipids	1.40	0.02	0.24	-2.05	down
186	Metixene	Organoheterocyclic compounds	Benzothiopyrans	1.73	0.00	0.33	-1.62	down
187	(+)-Isocorydine	Alkaloids and derivatives	Aporphines	1.47	0.01	0.26	-1.94	down
188	Iridin	Phenylpropanoids and polyketides	Isoflavonoids	1.62	0.00	0.42	-1.24	down
189	Velcorin	Organic acids and derivatives	Organic carbonic acids and derivatives	1.69	0.00	0.42	-1.27	down
190	α -Carboxybenzylpenicillin	Organic acids and derivatives	Carboxylic acids and derivatives	1.62	0.00	0.49	-1.02	down
191	Tyr Gly Gly	--	--	1.68	0.00	0.39	-1.36	down
192	Methoxyphenamine {[4-(5,7-dihydroxy-4-oxo-3,4-d ihydro-2H-1-benzopyran-2-yl)- 5-hydroxy-13,13-dimethyl-8-o xatetracyclo[7.4.1.0(2),0(1)(2), (1)]tetradeca-2(7),3,5-trien-9-yl]methoxy}sulfonic acid	Benzenoids	Benzene and substituted derivatives	1.61	0.00	0.46	-1.11	down
193	2-Isopropoxyphenyl	--	--	1.22	0.03	0.04	-4.66	down
194	N-methylcarbamate	Benzenoids	Phenol ethers	1.63	0.00	0.31	-1.71	down
195	Hydroferulic acid	Phenylpropanoids and polyketides	Phenylpropanoic acids	1.62	0.00	0.42	-1.25	down
196	Ala Tyr Asp	--	--	1.63	0.00	0.46	-1.12	down
197	His Ile Ser	--	--	1.51	0.00	0.32	-1.66	down
198	Cevadine	Lipids and lipid-like molecules	Steroids and steroid derivatives	1.73	0.00	0.49	-1.04	down
199	Val Leu Lys Asp Ser	--	--	1.66	0.00	0.42	-1.26	down

			Benzene and substituted					
216	Tolterodine	Benzenoids	derivatives	1.71	0.00	0.49	-1.04	down
217	NBD-FTY720 phenoxy	--	--	1.69	0.00	0.27	-1.89	down
218	Methyl diacetox-8-gingerdiol	--	--	1.28	0.01	0.32	-1.65	down
219	Tyr Val Met	--	--	1.68	0.00	0.44	-1.19	down
220	Azocyclotin	--	--	1.65	0.00	0.43	-1.23	down
221	Tolmetin	Organic oxygen compounds	Organooxygen compounds	1.65	0.00	0.30	-1.75	down
222	isofraxidin	--	--	1.33	0.01	0.42	-1.27	down
			Benzene and substituted					
223	Letrozole	Benzenoids	derivatives	1.39	0.02	0.32	-1.66	down
224	Palustrine	Phenylpropanoids and polyketides	Macrolactams	1.74	0.00	0.36	-1.48	down
225	Met Lys Asn His Leu	--	--	1.45	0.00	0.50	-1.00	down
226	Methylprednisolone succinate	Lipids and lipid-like molecules	Steroids and steroid derivatives	1.74	0.00	0.28	-1.84	down
	2-Pyridinecarboxamide, 4-[4-[[[4-chloro-3-(trifluoromethyl)phenyl]amino]carbonyl]amino]phenoxy]-N-methyl- Medroxyprogesterone							
227		Organic oxygen compounds	Organooxygen compounds	1.34	0.01	0.46	-1.12	down
228	17-acetate	Lipids and lipid-like molecules	Steroids and steroid derivatives	1.74	0.00	0.42	-1.25	down
229	Val-Ser	--	--	1.66	0.00	0.46	-1.13	down
Negative ion (ESI-)								
		Hormones and hormone related	Hormones and hormone related					
1	cholic acid	compunds	compunds	1.39	0.01	0.11	-3.14	down
2	2,3-Dihydroxybenzoic acid	Organic acids	Organic acids	1.62	0.00	0.45	-1.15	down
3	Shikimic Acid	Organic acid And Its derivatives	Organicacid and Its derivatives	1.32	0.02	0.49	-1.02	down
4	Methylmalonic Acid	Organic acid And Its derivatives	Organicacid and Its derivatives	1.64	0.00	0.36	-1.46	down

5	3-(Methylthio)propionic acid	Organic acid And Its derivatives	Organicacid and Its derivatives	1.64	0.00	0.48	-1.06	down
6	Pregnenolone sulfate	Lipids and lipid-like molecules	Steroids and steroid derivatives	1.60	0.00	0.48	-1.05	down
7	1-Oleoyl-sn-glycero-3-phosphocholine	-	-	1.69	0.00	0.19	-2.37	down
8	alpha-Muricholic acid	Bile acids	Bile acids	1.33	0.02	0.09	-3.46	down
9	Dattelic acid	Phenylpropanoids and polyketides	Cinnamic acids and derivatives	1.68	0.00	0.41	-1.28	down
10	Artomunoxanthentrione	Organoheterocyclic compounds	Benzopyrans	1.71	0.00	0.40	-1.32	down
11	Nilutamide	Organoheterocyclic compounds	Azolidines	1.64	0.00	0.47	-1.10	down
12	Myricetin	Flavonoids	Flavonols	1.65	0.00	0.45	-1.16	down
13	1-Aminocyclohexanoic acid	Organic acid And Its derivatives	Organicacid and Its derivatives	1.68	0.00	0.48	-1.06	down
14	Raltitrexed	Organic acids and derivatives	Carboxylic acids and derivatives	1.72	0.00	0.36	-1.46	down
15	Pantetheine 4'-phosphate;4'-Phosphopantetheine;Phosphopantetheine;D-Pantetheine 4'-phosphate	Organic acids and derivatives	Carboxylic acids and derivatives Organic sulfonic acids and derivatives	1.17	0.04	0.25	-2.03	down
16	Sulfoacetic acid	Organic acids and derivatives	derivatives	1.61	0.00	0.36	-1.48	down
17	Thr Arg Lys Glu	--	--	1.68	0.00	0.43	-1.21	down
18	His Gln Val Lys	--	--	1.34	0.01	0.36	-1.49	down
19	11-deoxy-PGF1	Lipids and lipid-like molecules	Fatty Acyls	1.68	0.00	0.47	-1.10	down
20	Adenosine 2'-Phosphate 6-(2,4-dihydroxyphenoxy)-3,4,5-trihydroxyoxane-2-carboxylic acid	Nucleotide And Its metabolomics	Nucleotide and Its metabolomics	1.39	0.01	0.39	-1.36	down
21	c acid	Organic oxygen compounds	Organooxygen compounds	1.65	0.00	0.44	-1.17	down
22	Isobavachalcone	Phenylpropanoids and polyketides	Linear 1,3-diarylpropanoids	1.66	0.00	0.44	-1.19	down
23	Psoralen	Lignans and Coumarins	Coumarins	1.71	0.00	0.42	-1.26	down

	Sodium methallylsulfonate:Sodium		Organic sulfonic acids and derivatives					
24	methallyl sulfonate	Organic acids and derivatives	derivatives	1.57	0.00	0.49	-1.02	down
25	L-Pipecolic acid	--	--	1.72	0.00	0.39	-1.34	down
26	4-Methylbenzamide oxime	--	--	1.63	0.00	0.44	-1.20	down
27	3,3'-Bisjuglone	Benzenoids	Naphthalenes	1.74	0.00	0.40	-1.31	down
28	Estradiol-17 3-sulfate	--	--	1.69	0.00	0.40	-1.33	down
29	5-Fluorouracil	Organoheterocyclic compounds	Diazines	1.66	0.00	0.46	-1.11	down
	5-Amino-2-p-toluidinobenzene sulfonic acid	Benzenoids	Benzene and substituted derivatives					
30	sulfonic acid	Benzenoids	derivatives	1.49	0.00	0.41	-1.29	down
31	Decarboxy-Norlobaric Acid	Phenylpropanoids and polyketides	Depsidones and depsidones	1.71	0.00	0.41	-1.29	down
	N-γ-Acetyl-N-2-Formyl-5-Met							
32	hoxykynurenamine	Amino acid and Its metabolomics	Amino acid derivatives	1.65	0.00	0.46	-1.11	down
			Benzene and substituted derivatives					
33	Chlorobenzene	Benzenoids	derivatives	1.70	0.00	0.44	-1.19	down
			Benzene and substituted derivatives					
34	Boscalid	Benzenoids	derivatives	1.61	0.00	0.35	-1.49	down
35	Trietazine	Organoheterocyclic compounds	Triazines	1.19	0.02	0.39	-1.36	down
36	Oleoylglycerone phosphate	Organic oxygen compounds	Organooxygen compounds	1.53	0.00	0.40	-1.34	down
	(1S)-1,5-Anhydro-1-(1,3,6-trihydroxy-5-methoxy-9-oxo-9H-xanthen-2-yl)-D-glucitol	Organoheterocyclic compounds	Benzopyrans	1.66	0.00	0.40	-1.32	down
37	anthen-2-yl)-D-glucitol	Organoheterocyclic compounds	Benzopyrans	1.66	0.00	0.40	-1.32	down
38	Prunasin	Alkaloids	Alkaloids	1.74	0.00	0.40	-1.33	down
	Pyrimidine-4-Carboxylic Acid(sodium salt)	Organoheterocyclic compounds	Diazines	1.64	0.00	0.48	-1.05	down
39	Acid(sodium salt)	Organoheterocyclic compounds	Diazines	1.64	0.00	0.48	-1.05	down
40	Picloram	Organoheterocyclic compounds	Pyridines and derivatives	1.05	0.03	0.46	-1.12	down

41	2-Arachidonyl Glycerol ether	Lipids and lipid-like molecules	Endocannabinoids	1.71	0.00	0.36	-1.47	down
42	Lolitre K	Organoheterocyclic compounds	Naphthopyrans	1.22	0.02	0.46	-1.13	down
43	Ziprasidone	Organoheterocyclic compounds	Diazinanes	1.71	0.00	0.44	-1.17	down
44	Aspartyl adenylate	Nucleosides, nucleotides, and analogues	Purine nucleotides	1.61	0.00	0.30	-1.73	down
45	5'-Methoxyhydnoctocarpin-D	Lignans, neolignans and related compounds	Flavonolignans	1.67	0.00	0.44	-1.20	down

Supplemental Table 4. Upregulated differential metabolites between the *Pneumocystis*-infected WT mice and BAFF-R^{-/-} *Pneumocystis*-infected mice under ESI- and ESI+ modes.

No.	Compounds	Class.I	Class.II	VIP	p_value	Fold_Change	Log2FC	Type
Positive ion (ESI+)								
1	MG(0:0/18:1(9Z)/0:0)	Lipids and lipid-like molecules	Glycerolipids	1.89	0.01	2.68	1.42	up
2	15-Dehydro-prostaglandin D2	Lipids and lipid-like molecules	Fatty Acyls	1.63	0.02	2.51	1.33	up
3	Caffeine	Alkaloids	Alkaloids	1.66	0.03	2.54	1.34	up
4	2-Ethyl-4-hydroxy-5-methyl-3(2H)-furanone	Organoheterocyclic compounds	Dihydrofurans	1.38	0.04	2.56	1.36	up
5	L-Kynurenine	--	--	1.82	0.01	2.34	1.23	up
6	(2S)-4-(2-aminophenyl)-2-azaniumyl-4-oxobutanoate	Organic oxygen compounds	Organooxygen compounds	1.85	0.01	3.12	1.64	up
7	Norspermine;N,N'-Bis(3-aminopropyl)-1,3-propanediamine	Organic nitrogen compounds	Organonitrogen compounds	1.43	0.04	2.32	1.21	up
8	7-Deoxyloganetate	Lipids and lipid-like molecules	Prenol lipids	1.82	0.01	2.61	1.39	up
9	Pro Arg Trp	--	--	1.66	0.03	2.23	1.16	up
10	Oxaloglutarate	Organic acids and derivatives	Carboxylic acids and derivatives	1.81	0.02	2.22	1.15	up
11	DL-2-Aminocaprylic acid	--	--	2.24	0.00	2.34	1.22	up

12	Neamine;Neomycin A 3-Methylsalicylaldehyde;2-Hyd	Organic oxygen compounds	Organooxygen compounds	1.74	0.02	2.79	1.48	up
13	roxy-3-methylbenzaldehyde	Organic oxygen compounds	Organooxygen compounds	1.61	0.02	2.06	1.04	up
14	Phe Asn Thr Lys	--	--	1.62	0.04	2.22	1.15	up
15	1,24-Dihydroxyvitamin D3	Lipids and lipid-like molecules	Steroids and steroid derivatives	2.06	0.01	7.52	2.91	up
16	Normeperidine	Organoheterocyclic compounds	Piperidines	1.64	0.02	7.19	2.85	up
17	N-Acetyl-5-Hydroxytryptamine	Tryptamines,Cholines,Pigments	Tryptamines	1.71	0.03	2.40	1.26	up
18	Dimethyl trisulfide	Organosulfur compounds	Organic trisulfides	1.55	0.05	3.30	1.72	up
19	Flufenacet	Benzenoids	Benzene and substituted derivatives	1.55	0.03	2.62	1.39	up
20	2-Aminobenzimidazole 16,16-Dimethyl-6-ketoprostagl	Organoheterocyclic compounds	Benzimidazoles	1.62	0.04	2.38	1.25	up
21	andin E1	Lipids and lipid-like molecules	Fatty Acyls	1.65	0.02	3.11	1.64	up
22	Bispyribac	Organic oxygen compounds	Organooxygen compounds	1.45	0.05	2.52	1.34	up
23	TyrMe-Asp-OH	--	--	1.61	0.02	2.34	1.22	up
24	2-Phenylbutyramide	Benzenoids	Benzene and substituted derivatives	1.82	0.02	2.03	1.03	up
25	Picoxystrobin	Benzenoids	derivatives	1.46	0.04	2.62	1.39	up
26	Nocodazole	Organoheterocyclic compounds	Benzimidazoles	1.75	0.02	2.79	1.48	up
27	Treprostinil	Benzenoids	Benzene and substituted derivatives	1.90	0.00	2.05	1.04	up
28	Ala Pro Met 1H-1,4-Diazepine,	--	--	1.59	0.04	2.52	1.34	up
29	4-(aminoacetyl)hexahydro-2-m ethyl-1-[(4-methyl-5-isoquinoli	Organic acids and derivatives	Carboxylic acids and derivatives	1.61	0.02	2.44	1.29	up

	nyl)sulfonyl]-, (2S)-							
30	Alloxydim	Organic oxygen compounds	Organooxygen compounds	1.63	0.04	2.09	1.07	up
31	L-Homocystine	Amino acid and Its metabolomics	Amino acids	1.62	0.03	2.55	1.35	up
	(3S,7R)-11-methoxy-3,7-dimethyl-6,8,16,20-tetraoxapentacyclo[10.8.0.0.2,9.0.3,7.0.13,18]icosa-1,4,9,11,13(18)-pentaene-17,19-dione	Phenylpropanoids and polyketides	Coumarins and derivatives	1.50	0.04	2.19	1.13	up
32			Amino acid and Its metabolomics					
33	Ala-Glu	Amino acid and Its metabolomics	metabolomics	1.80	0.01	2.22	1.15	up
			Benzene and substituted derivatives					
34	2-Aminoethyl diphenylborinate	Benzenoids	derivatives	1.63	0.03	3.02	1.60	up
35	Nitrazepam	Organoheterocyclic compounds	Benzodiazepines	1.45	0.04	2.69	1.43	up
		Lignans, neolignans and related compounds						
36	(-)-Secoisolariciresinol		Dibenzylbutane lignans	1.70	0.02	2.61	1.38	up
	1-(2,4-Dichlorophenyl)-2-(1-imidazolyl)ethanol	Benzenoids	Benzene and substituted derivatives	1.44	0.05	2.18	1.13	up
37								
38	Dibenz[a,h]acridine	Organoheterocyclic compounds	Quinolines and derivatives	1.77	0.02	2.14	1.10	up
39	(+)-Isocorydine	Alkaloids and derivatives	Aporphines	1.52	0.04	2.69	1.43	up
40	His Ile Ser	--	--	1.70	0.02	2.66	1.41	up
41	5'-Methoxybilobetin	Phenylpropanoids and polyketides	Flavonoids	1.55	0.04	2.40	1.26	up
			Benzene and substituted derivatives					
42	Sotalol	Benzenoids	derivatives	1.52	0.02	2.30	1.20	up
			Benzene and substituted derivatives					
43	Penfluridol	Benzenoids	derivatives	1.50	0.04	2.47	1.30	up
44	N-Butyryl-L-homocysteine	Organic acids and derivatives	Carboxylic acids and derivatives	1.87	0.02	2.32	1.22	up

thiolactone

Negative ion (ESI-)

No.	Compounds	Class.I	Class.II	VIP	p_value	Fold_Change	Log2FC	Type
1	cholic acid	Hormones and hormone related compounds	Hormones and hormone related compounds	1.23	0.04	2.12	1.08	up
2	4-Chloro-2-methylphenol	Benzenoids	Phenols	1.59	0.02	2.39	1.26	up
3	1-Oleoyl-sn-glycero-3-phosphocholine	-	-	1.59	0.03	4.14	2.05	up
4	Adenosine 2'-Phosphate	Nucleotide And Its metabolomics	Nucleotide and Its metabolomics	1.60	0.02	2.14	1.10	up
5	17 α -Ethinylestradiol	Hormones and hormone related compounds	Hormones and hormone related compounds	1.67	0.02	2.05	1.03	up
6	Ergothioneine	Organic acid And Its derivatives	Organic acid and Its derivatives	1.48	0.02	2.22	1.15	up
7	Oleoylglycerone phosphate	Organic oxygen compounds	Organooxygen compounds	1.80	0.02	2.33	1.22	up

Supplemental Table 5. Downregulated differential metabolites between the *Pneumocystis*-infected WT mice and BAFF-R^{-/-} *Pneumocystis*-infected mice under ESI- and ESI+ modes.

No.	Compounds	Class.I	Class.II	VIP	p_value	Fold_Change	Log2FC	Type
Positive ion (ESI+)								
1	PA(15:0/22:2(13Z,16Z)) TG(16:0/14:1(9Z)/20:3(5Z,8Z, 11Z))	Lipids and lipid-like molecules	Glycerophospholipids	1.50	0.03	0.44	-1.18	down
2	PE-NMe(14:0/20:1(11Z))	Lipids and lipid-like molecules	Glycerolipids	2.01	0.01	0.34	-1.54	down
3	PE-NMe(14:0/18:1(11Z))	Lipids and lipid-like molecules	Glycerophospholipids	1.45	0.04	0.45	-1.14	down
4	PE-NMe(14:0/18:1(11Z))	Lipids and lipid-like molecules	Glycerophospholipids	2.05	0.00	0.44	-1.19	down
5	PC(16:1(9Z)/18:1(11Z))	Lipids and lipid-like molecules	Glycerophospholipids	1.39	0.04	0.49	-1.03	down
6	PE-NMe2(15:0/16:0)	Lipids and lipid-like molecules	Glycerophospholipids	1.98	0.00	0.34	-1.55	down

7	D-erythro-3-Methylmalate;(2R,3S)-3-Methylmalate	Lipids and lipid-like molecules	Fatty Acyls	1.44	0.03	0.41	-1.27	down
8	Alitretinoin	Lipids and lipid-like molecules	Prenol lipids	2.02	0.00	0.49	-1.03	down
9	PA(22:1(13Z)/19:2(10Z,13Z))	Lipids and lipid-like molecules	Glycerophospholipids	2.10	0.00	0.44	-1.20	down
10	TG(20:0/18:4(6Z,9Z,12Z,15Z)/18:1(9Z))	Lipids and lipid-like molecules	Glycerolipids	1.76	0.05	0.46	-1.13	down
11	PC(20:5(5Z,8Z,11Z,14Z,17Z)/18:1(9Z))	Lipids and lipid-like molecules	Glycerophospholipids	1.79	0.02	0.27	-1.87	down
12	PC(18:1(9Z)/22:2(13Z,16Z))	Lipids and lipid-like molecules	Glycerophospholipids	2.03	0.01	0.47	-1.10	down
13	Hexadecanoic Acid(C16:0)	Lipids and lipid-like molecules	Fatty Acyls	1.62	0.01	0.46	-1.11	down
14	Isopropyl alcohol	Organic oxygen compounds	Organooxygen compounds	1.69	0.01	0.47	-1.10	down
15	DG(20:4(5Z,8Z,11Z,14Z)/22:5(4Z,7Z,10Z,13Z,16Z)/0:0)	Lipids and lipid-like molecules	Glycerolipids	1.52	0.01	0.34	-1.55	down
16	Taurodeoxycholate;Taurodeoxycholic acid (±)5-HETE [(±)5-hydroxy-6E,8Z,11Z,14Z-eicosatetraenoic acid]	Lipids and lipid-like molecules	Steroids and steroid derivatives	2.15	0.00	0.44	-1.18	down
17	Aldehydo-D-galactose	Organic oxygen compounds	Organooxygen compounds	2.26	0.00	0.45	-1.15	down
18	3-Hydroxybutyrylcarnitine	Lipids and lipid-like molecules	Fatty Acyls	1.66	0.02	0.50	-1.00	down
19	Carnitine C13:0	FA	CAR	2.03	0.00	0.38	-1.40	down
20	D-PANTOTHENIC ACID	--	--	1.35	0.04	0.41	-1.28	down
21	5-Hydroxytryptophol	Alkaloids	Plumerane	2.01	0.00	0.38	-1.39	down
22	PA(21:0/12:0)	Lipids and lipid-like molecules	Glycerophospholipids	2.16	0.00	0.46	-1.11	down
23	2-Amino-4-hydroxy-6-hydroxymethyl-7,8-dihydropteridine	--	--	1.50	0.03	0.40	-1.32	down

25	Cytidine	Nucleotide And Its metabolomics	Nucleotide and Its metabolomics	1.77	0.01	0.50	-1.01	down	
26	TG(14:0/18:1(11Z)/18:1(11Z))	Lipids and lipid-like molecules	Glycerolipids	2.12	0.01	0.37	-1.45	down	
27	Eicosapentaenoyl PAF C-16 11-nor-9-carboxy-Delta(9)-tetr	Lipids and lipid-like molecules	Glycerophospholipids	2.06	0.00	0.47	-1.10	down	
28	ahydrocannabinol	Organoheterocyclic compounds	Benzopyrans	1.46	0.04	0.50	-1.01	down	
29	Pro Pro Ile	--	--	1.94	0.00	0.41	-1.29	down	
30	Jasmone	Others	Others	1.68	0.02	0.50	-1.01	down	
31	22-Angeloyltheasapogenol A	Lipids and lipid-like molecules	Prenol lipids	1.72	0.05	0.41	-1.27	down	
32	Isopropamide 5-Geranoxy-7-methoxycoumar	Benzenoids	Benzene and substituted derivatives	2.18	0.00	0.44	-1.19	down	
33	in	Lipids and lipid-like molecules	Prenol lipids	1.72	0.01	0.39	-1.37	down	
34	Farnesylthiosalicylic acid	Lipids and lipid-like molecules	Prenol lipids	2.24	0.00	0.29	-1.77	down	
35	Minocycline N-3-Oxododecanoyl-L-homose	Phenylpropanoids and polyketides	Tetracyclines	1.92	0.01	0.47	-1.08	down	
36	rine lactone	Organic acids and derivatives	Carboxylic acids and derivatives	2.17	0.00	0.23	-2.11	down	
37	Lys Lys Gly	--	--	1.66	0.03	0.44	-1.20	down	
38	Lobaric acid	Phenylpropanoids and polyketides	Depsidones and depsidones	2.32	0.00	0.24	-2.08	down	
39	Azelaic acid (3beta,22R,23R,24S)-3,22,23-	--	--	2.10	0.00	0.13	-2.95	down	
40	Trihydroxystigmastan-6-one	Lipids and lipid-like molecules	Steroids and steroid derivatives	1.82	0.01	0.43	-1.23	down	
41	3-hexanoyl-NBD Cholesterol	Lipids and lipid-like molecules	Steroids and steroid derivatives	1.62	0.02	0.33	-1.62	down	
Negative ion (ESI-)									
	cis-7,10,13,16,19-Docosapenta								
1	enoic acid	Lipids and lipid-like molecules	Fatty Acyls	1.97	0.01	0.42	-1.24	down	
2	Oleandolide	Phenylpropanoids and polyketides	Macrolides and analogues	1.51	0.02	0.50	-1.01	down	

3	4-hydroxybenzenesulfonic acid	Organic acid And Its derivatives	Sulfonic acids	2.02	0.00	0.33	-1.61	down
4	FFA(20:3)	Lipids	Free fatty acids	2.21	0.00	0.49	-1.02	down
5	3-Sulfocatechol	Benzene and substituted derivatives	Phenolics	1.99	0.00	0.39	-1.34	down
6	Hexanoyl Glycine	Amino acid and Its metabolomics	Amino acid derivatives	2.25	0.00	0.20	-2.33	down
7	alpha-Bisabolol oxide C	Organoheterocyclic compounds	Oxanes	2.11	0.00	0.14	-2.84	down
8	Hydrocortisone acetate	Lipids and lipid-like molecules	Steroids and steroid derivatives	1.63	0.01	0.43	-1.21	down
9	Fast green FCF	--	--	1.44	0.02	0.39	-1.34	down
10	2-Hydroxy-2-methylbutyric acid	Organic acids	Organic acids	1.81	0.00	0.32	-1.65	down
11	Altanserin	Organic oxygen compounds	Organooxygen compounds	2.05	0.00	0.40	-1.34	down
12	4-Hydroxybenzoic Acid	Phenolic acids	Phenolic acids	2.04	0.00	0.34	-1.56	down
13	Phenol	Phenolic acids	Phenolic acids	1.99	0.00	0.37	-1.44	down
14	Lys Thr Gln Lys	--	--	2.17	0.00	0.33	-1.60	down
15	Phenethyl rutinoside	Organic oxygen compounds	Organooxygen compounds	2.10	0.00	0.39	-1.36	down
16	Sericetin	Phenylpropanoids and polyketides	Flavonoids	2.20	0.00	0.41	-1.27	down

Figure legends of the Supplemental Figures

Supplemental Figure 1. Heatmaps presented a different pattern of metabolites between the control group and *Pneumocystis*-infected WT mice in positive ion modes.

Supplemental Figure 2. Heatmaps presented a different pattern of metabolites between the control group and *Pneumocystis*-infected WT mice in negative ion modes.

Supplemental Figure 3. Heatmaps showed differential metabolic profiling of lung samples between *Pneumocystis*-infected WT mice and *Pneumocystis*-infected BAFF-R^{-/-} mice in positive ion modes.

Supplemental Figure 4. Heatmaps showed differential metabolic profiling of lung samples between the *Pneumocystis*-infected WT mice and *Pneumocystis*-infected BAFF-R^{-/-} mice in negative ion modes.

Supplemental Figure 5. Violin plot of the top 20 differential metabolites between the control group and *Pneumocystis*-infected WT mice.

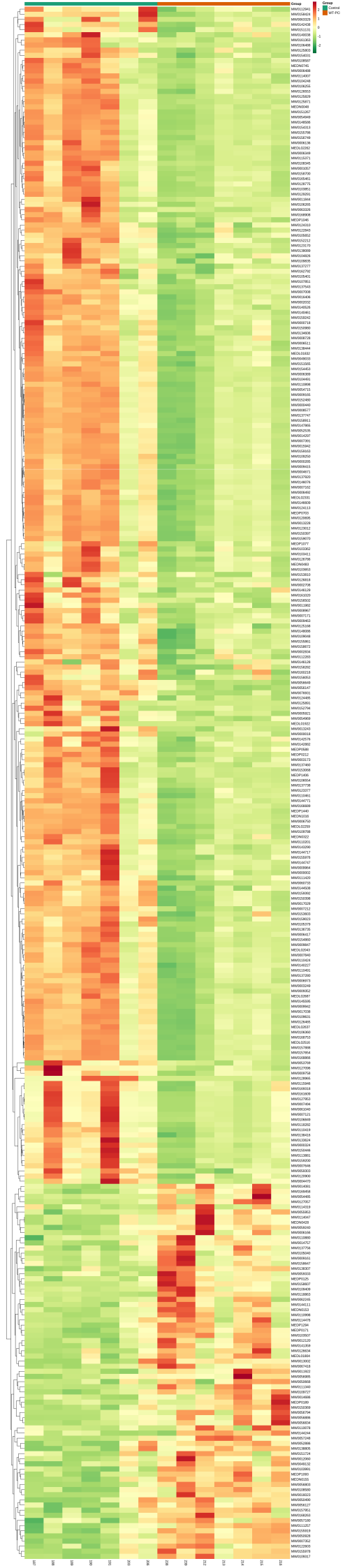
Supplemental Figure 6. The pathway map of tryptophan metabolism in the comparison between the control group and *Pneumocystis*-infected WT mice.

Supplemental Figure 7. Violin plot of the top 20 differential metabolites between the *Pneumocystis*-infected WT mice and *Pneumocystis*-infected BAFF-R^{-/-} mice.

Supplemental Figure 8. The pathway map of adipocytokine signaling pathway in the comparison between the *Pneumocystis*-infected WT mice and *Pneumocystis*-infected BAFF-R^{-/-} mice.

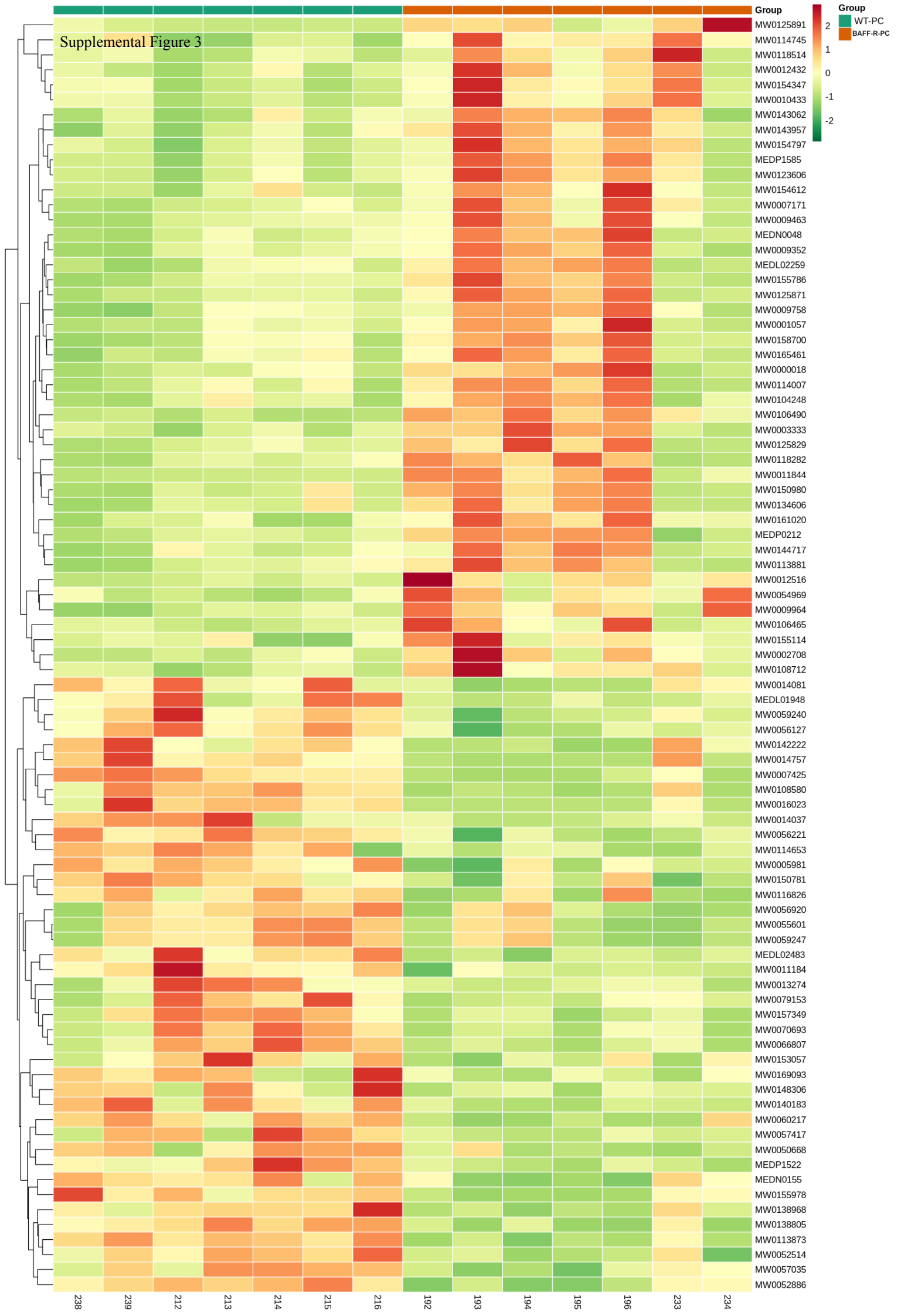
Supplemental Figure 9. The pathway map of fatty acid elongation in the comparison between the *Pneumocystis*-infected WT mice and *Pneumocystis*-infected BAFF-R^{-/-} mice.

Supplemental Figure 1



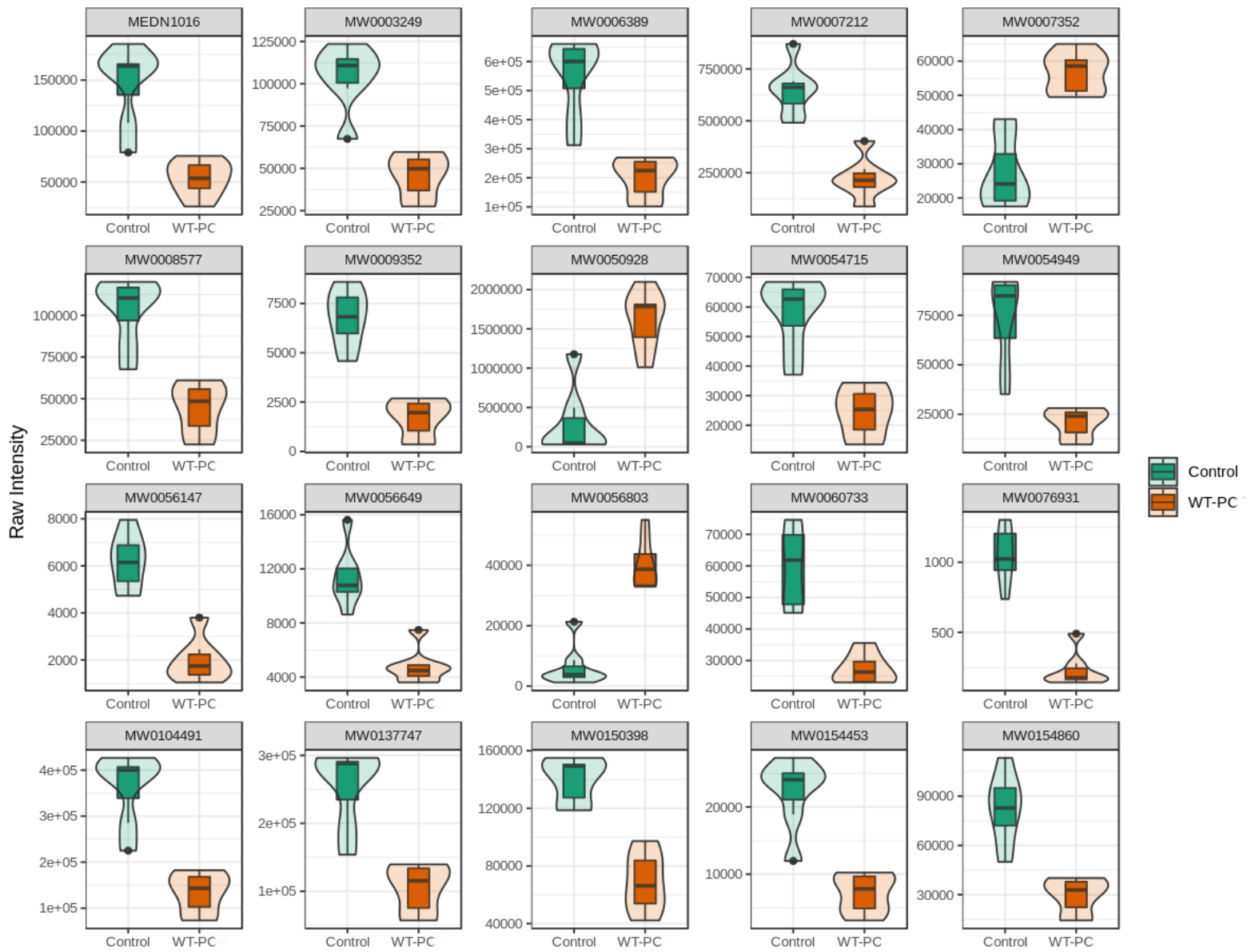
Supplemental Figure 2





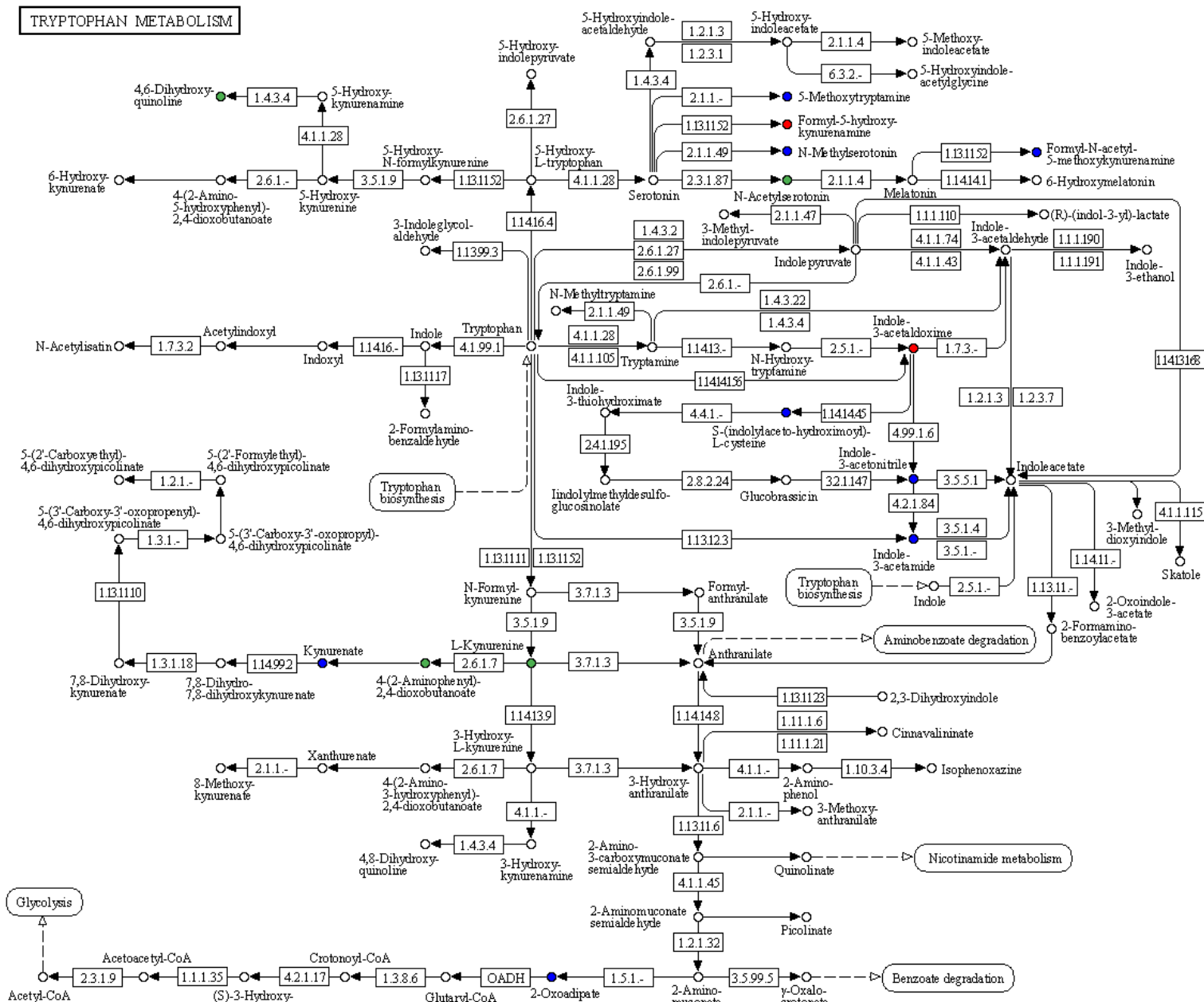
Supplemental Figure 5

Violin Plot of Raw Values



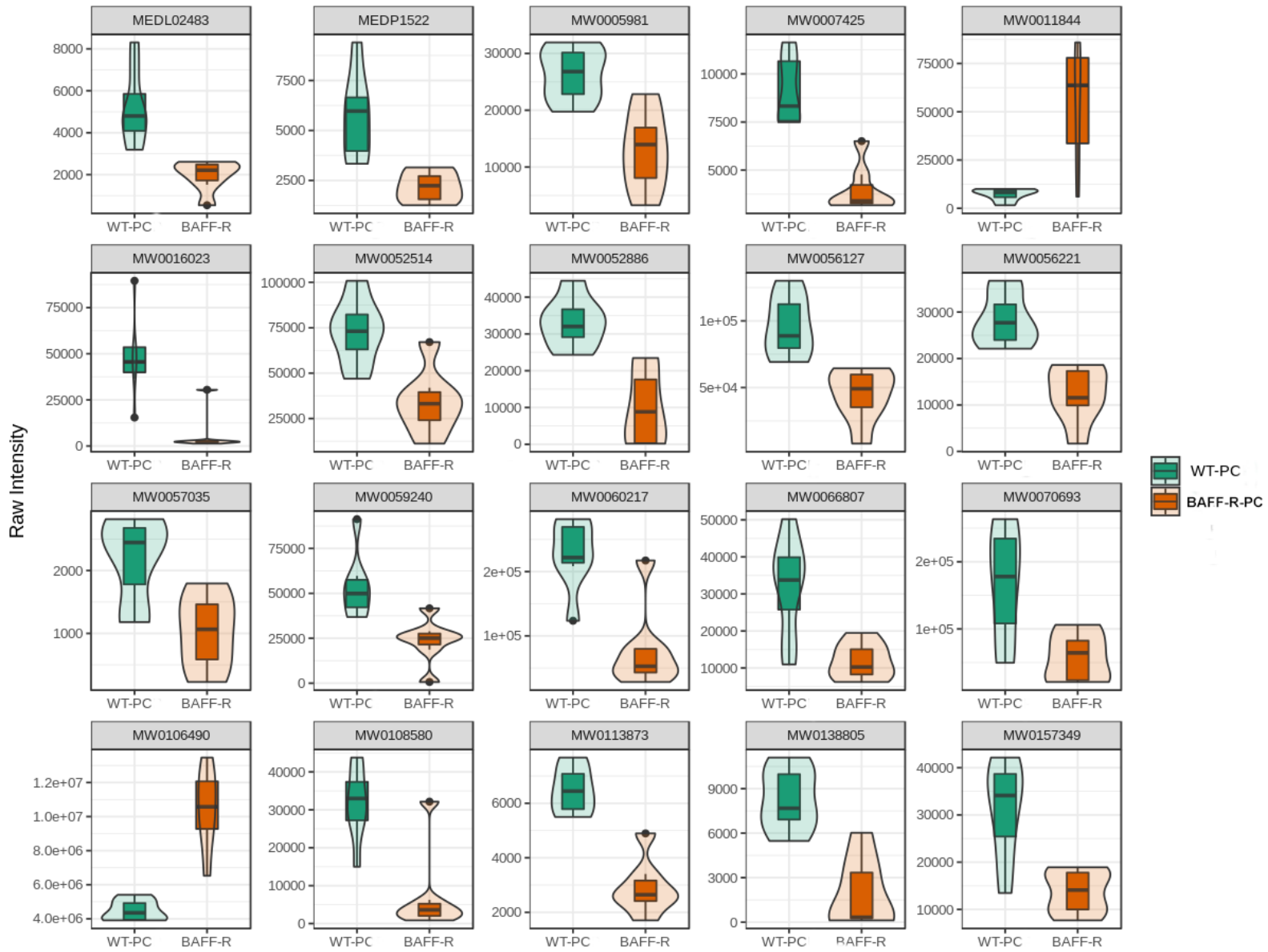
Supplemental Figure 6

TRYPTOPHAN METABOLISM

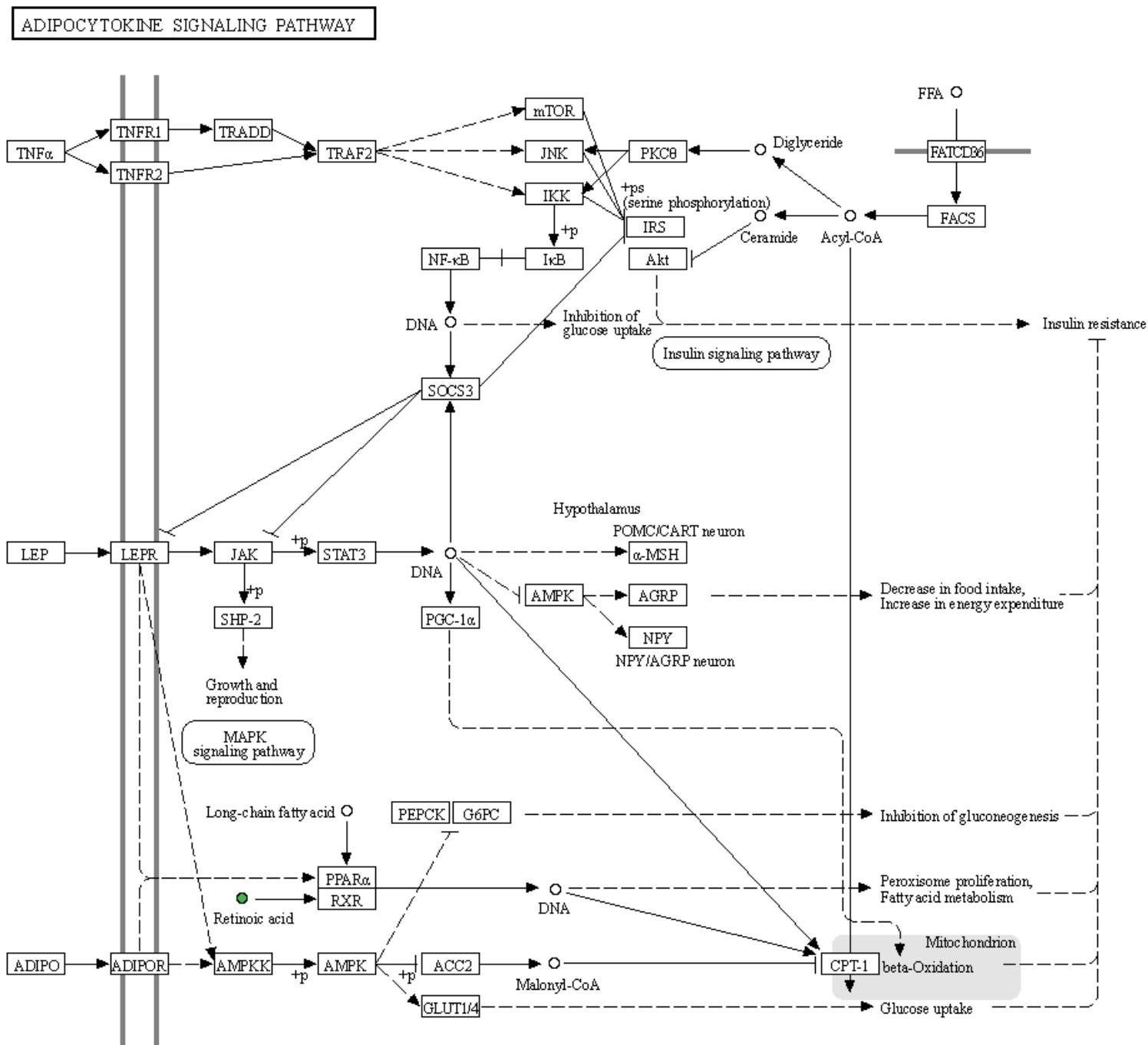


Supplemental Figure 7

Violin Plot of Raw Values



Supplemental Figure 8



FATTY ACID ELONGATION

