Supplemental Table 1. All metabolites detected in discovery metabolomics and their relationship to neutrophilic airway inflammation

Metabolite	**Pathway**	**Correlation***	**Ratio***	**Q-value**
alanine	Amino acid	0.68	36.89	0.009
asparagine	Amino acid	0.52	3.51	0.023
aspartate	Amino acid	0.75	11.90	0.011
creatine	Amino acid	0.43	1.97	0.025
cysteine	Amino acid	0.68	20.14	0.014
methionine	Amino acid	0.60	2.70	0.023
N-acetylmethionine	Amino acid	0.45	2.48	0.034
taurine	Amino acid	0.69	8.59	0.012
glutamate	Amino acid	0.76	6.06	0.011
glutamine	Amino acid	0.66	2.97	0.019
pyroglutamine*	Amino acid	0.42	2.09	0.035
5-oxoproline	Amino acid	0.62	4.00	0.016
cysteine-glutathione disulfide	Amino acid	0.69	9.04	0.015
glutathione, oxidized (GSSG)	Amino acid	0.34	2.52	0.032
glycine	Amino acid	0.63	6.95	0.016
N-acetylserine	Amino acid	0.59	2.52	0.025
serine	Amino acid	0.76	19.97	0.009
threonine	Amino acid	0.80	14.71	0.008
histidine	Amino acid	0.64	3.64	0.019
trans-urocanate	Amino acid	0.34	2.13	0.039
lysine	Amino acid	0.75	141.81	0.007
N6-acetyllysine	Amino acid	0.76	12.00	0.010

phenylalanine	Amino acid	0.74	36.15	0.005
tyrosine	Amino acid	0.75	44.10	0.006
putrescine	Amino acid	0.35	6.53	0.046
C-glycosyltryptophan*	Amino acid	0.62	8.58	0.017
kynurenine	Amino acid	0.65	2.46	0.030
tryptophan	Amino acid	0.73	32.66	0.010
5-aminovalerate	Amino acid	0.45	6.87	0.025
arginine	Amino acid	0.63	29.21	0.014
citrulline	Amino acid	0.79	24.29	0.004
dimethylarginine (SDMA + ADMA)	Amino acid	0.65	2.98	0.015
ornithine	Amino acid	0.75	71.71	0.009
proline	Amino acid	0.79	13.50	0.007
urea	Amino acid	0.55	3.56	0.024
4-methyl-2-oxopentanoate	Amino acid	0.50	2.34	0.037
isoleucine	Amino acid	0.61	6.63	0.018
leucine	Amino acid	0.37	5.42	0.040
valine	Amino acid	0.76	43.61	0.004
erythronate*	Carbohydrate	0.67	9.10	0.014
1,5-anhydroglucitol (1,5-AG)	Carbohydrate	0.81	6.98	0.013
glucose	Carbohydrate	0.65	9.23	0.018
glucose-6-phosphate (G6P)	Carbohydrate	0.54	4.39	0.028
lactate	Carbohydrate	0.71	4.14	0.012
ascorbate (Vitamin C)	Cofactors and vitamins	0.43	6.48	0.030
adenosine 5'diphosphoribose	Cofactors and vitamins	0.37	1.72	0.039
nicotinamide	Cofactors and vitamins	0.45	3.16	0.024
nicotinamide adenine dinucleotide (NAD+)	Cofactors and vitamins	0.63	3.53	0.031
pantothenate	Cofactors and vitamins	0.37	1.69	0.036
citrate	Energy	0.66	4.09	0.026
fumarate	Energy	0.43	2.23	0.027
malate	Energy	0.66	2.89	0.022

phosphate	Energy	0.55	4.17	0.019
acetylcarnitine	Lipid	0.50	3.64	0.021
carnitine	Lipid	0.43	3.21	0.028
linoleate (18:2n6)	Lipid	0.52	3.24	0.030
octadecanedioate	Lipid	0.55	1.99	0.035
ethanolamine	Lipid	0.65	7.78	0.016
glycerol	Lipid	0.57	14.37	0.037
phosphoethanolamine	Lipid	0.52	4.40	0.021
myo-inositol	Lipid	0.43	2.29	0.032
scyllo-inositol	Lipid	0.53	4.50	0.032
arachidonate (20:4n6)	Lipid	0.64	9.16	0.021
dihomo-linoleate (20:2n6)	Lipid	0.76	12.55	0.013
eicosenoate (20:1n9 or 11)	Lipid	0.70	5.96	0.017
1-stearoylglycerophosphoethanolamine	Lipid	0.68	2.48	0.034
2-arachidonoylglycerophosphoethanolamine*	Lipid	0.65	4.10	0.031
2-docosahexaenoylglycerophosphoethanolamine*	Lipid	0.66	2.71	0.026
2-oleoylglycerophosphoethanolamine*	Lipid	0.73	5.43	0.023
caprate (10:0)	Lipid	0.38	1.50	0.029
sphingosine	Lipid	0.59	2.55	0.046
cholesterol	Lipid	0.67	2.10	0.027
2'-deoxyinosine	Nucleotide	0.62	3.59	0.012
hypoxanthine	Nucleotide	0.54	4.81	0.020
xanthine	Nucleotide	0.76	15.06	0.005
adenine	Nucleotide	0.40	2.95	0.029
adenosine	Nucleotide	-0.69	0.22	0.018
adenosine 5'-monophosphate (AMP)	Nucleotide	0.60	4.72	0.036
urate	Nucleotide	0.34	2.40	0.035
alanylalanine	Peptide	0.40	1.26	0.033
alanylleucine	Peptide	0.82	4.36	0.003
alanylvaline	Peptide	0.81	5.79	0.000

alpha-glutamyltyrosine	Peptide	0.61	2.37	0.028
alpha-glutamylvaline	Peptide	0.77	48.79	0.002
aspartylleucine	Peptide	0.78	29.57	0.002
aspartylphenylalanine	Peptide	0.73	15.02	0.011
glycylisoleucine	Peptide	0.78	8.61	0.001
glycylleucine	Peptide	0.73	33.94	0.005
glycylproline	Peptide	0.60	3.16	0.020
glycylvaline	Peptide	0.76	11.96	0.001
isoleucylvaline	Peptide	0.74	4.28	0.008
leucylleucine	Peptide	0.50	1.93	0.022
lysylleucine	Peptide	0.79	5.39	0.003
pyroglutamylvaline	Peptide	0.82	10.26	0.007
serylleucine	Peptide	0.76	6.00	0.004
threonylleucine	Peptide	0.78	3.31	0.006
threonylphenylalanine	Peptide	0.79	10.36	0.002

*Correlation = Pearson correlation to BALF % neutrophils; Ratio = ratio of metabolite concentrations in samples with bronchitis to those with no/mild bronchitis