SUPPLEMENTAL MATERIALS

Supplementary Table 1 List of differential metabolites in lung tissue.

Metabolites	Class	HMDB ID	Adducts	Formula	Mass Error (ppm)
2-amino-4-oxo-pentanoic acid	Amino acids	LMFA01060171	2M+H	C5H9NO3	0.2
5-Aminolevulinic acid	Amino acids	HMDB0001149	M-H	C5H9NO3	4.1
Arginyl-Methionine	Amino acids	HMDB0028715	M+Na	C11H23N5O3S	-7.8
Ergothioneine	Amino acids	HMDB0003045	M+H	C9H15N3O2S	-0.6
Histidinyl-Leucine	Amino acids	HMDB0028889	M+H	C12H20N4O3	-6.2
Histidylaspartic acid	Amino acids	HMDB0028881	M+FA-H	C10H14N4O5	5.9
L-Alanine	Amino acids	HMDB0000161	M-H	C3H7NO2	2.3
L-Histidine	Amino acids	HMDB0000177	M-H	C6H9N3O2	1.9
L-Threonine	Amino acids	HMDB0000167	M-H	C4H9NO3	2.1
L-Tryptophan	Amino acids	HMDB0000929	2M+H	C11H12N2O2	0.0
N-Acetylvanilalanine	Amino acids	HMDB0011716	M-H	C12H15NO5	1.3
Phenylalanyltyrosine	Amino acids	HMDB0029007	M-H	C18H20N2O4	0.4
Proline betaine	Amino acids	HMDB0004827	M+FA-H	C7H13NO2	3.7
Prolyl-Arginine	Amino acids	HMDB0029011	M+Na	C11H21N5O3	4.7
Threoninyl-Leucine	Amino acids	HMDB0029065	M+H	C10H20N2O4	1.1
Tryptophyl-Tryptophan	Amino acids	HMDB0029094	M+H	C22H22N4O3	-3.3
Valyl-Lysine	Amino acids	HMDB0029132	M+H	C11H23N3O3	0.9
2-Methylhippuric acid	Benzenoids	HMDB0011723	M+FA-H	C10H11NO3	1.2
4-Methylbenzoic acid	Benzenoids	HMDB0029635	M+FA-H	C8H8O2	1.5
anacardic acid	Benzenoids	HMDB0033896	M-H	C22H36O3	-1.7
1,3-Benzenediol	Benzenoids	HMDB0032037	M+H	C6H6O2	-4.5
3-Oxo-4,6-choladienoic acid	Bile acids	HMDB0000476	M+FA-H	C24H34O3	-9.0
Bisnorcholic acid	Bile acids	HMDB0002082	M+NH4, M+Na	C22H36O5	0.0
D-Glucopyranose 6-phosphate	Carbohydrates	HMDB0001401	M-H	C6H13O9P	-0.1
D-Sedoheptulose 7-phosphate	Carbohydrates	HMDB0001068	M-H	C7H15O10P	-0.2
Galactose 1-phosphate	Carbohydrates	HMDB0000645	M+K	C6H13O9P	0.0
Gluconic acid	Carbohydrates	HMDB0000625	M-H	C6H12O7	2.8
N-Acetyl-glucosamine 1-phosphate	Carbohydrates	HMDB0001367	M-H	C8H16NO9P	-1.1
N-Acetylglucosamine 6-phosphate	Carbohydrates	HMDB0002817	M+FA-H	C8H16NO9P	2.8
NeuNGc	Carbohydrates	HMDB0062502	M+K	C11H19NO10	3.4
Vanilloside	Carbohydrates	HMDB0029664	M-H	C14H18O8	-7.6
3-hydroxyhexadecanoyl carnitine	Carnitine	HMDB0061642	M+H	C23H45NO5	0.6
11-Dehydrothromboxane B2	Eicosanoids	HMDB0004242	M-H	C20H32O6	-1.9
12,20-dioxoleukotriene B4	Eicosanoids	HMDB0060094	M-H	C20H28O5	-7.9
12-HETE	Eicosanoids	HMDB0006111	M+H	C20H32O3	0.5
12-Keto-leukotriene B4	Eicosanoids	HMDB0004234	M-H	C20H30O4	-0.5
6-trans-12-epi-Leukotriene B4	Eicosanoids	HMDB0005088	M+H	C20H32O4	1.8
Leukotriene B5	Eicosanoids	HMDB0005073	M+H	C20H30O4	-0.6
Misoprostol	Eicosanoids	HMDB0015064	M-H	C22H38O5	-2.1
Prostaglandin B2	Eicosanoids	HMDB0004236	M+Na	C20H30O4	0.1
Prostaglandin D2	Eicosanoids	HMDB0001403	M+FA-H	C20H32O5	-5.5
Thromboxane	Eicosanoids	HMDB0003208	M-H, 2M-H	C20H32O5	-1.6
10-oxo-Nonadecanoic acid	Fatty Acids	LMFA01060128	M+H	C19H36O3	3.6

Continued

Supplementary Table 1 Continued

Metabolites	Class	HMDB ID	Adducts	Formula	Mass Error (ppm)
16-HDoHE	Fatty acids	HMDB0060047	M+H	C22H32O3	-0.2
17-HDoHE	Fatty acids	HMDB0010213	M+Na	C22H32O3	0.2
19,20-DiHDPA	Fatty acids	HMDB0010214	M+H	C22H34O4	-0.2
3-Methyl-5-pentyl-2-furanheptanoic acid	Fatty acids	HMDB0112095	M-H	C17H28O3	2.3
5-Hexyl-2-furanoctanoic acid	Fatty acids	HMDB0112099	M+H, M+Na	C18H30O3	1.6
5-Pentyl-2-furanoctanoic acid	Fatty acids	HMDB0112098	M+H	C17H28O3	0.3
8-Hydroxyoctadecanoic acid	Fatty acids	HMDB0112182	M-H	C18H36O3	0.5
9,10,13-Trihydroxy-11-octadecenoic acid	Fatty acids	HMDB0004710	M-H	C18H34O5	-0.6
9,12,13-TriHOME	Fatty acids	HMDB0004708	M-H	C18H34O5	-0.8
Adipic acid	Fatty acids	HMDB0000448	M+Na	C6H10O4	-3.3
Adrenic acid	Fatty acids	HMDB0002226	M+FA-H	C22H36O2	6.6
Leukotriene A4	Fatty acids	HMDB0001337	M+H, M+Na	C20H30O3	0.6
Valeric acid	Fatty acids	HMDB0000892	M-H	C5H10O2	-0.5
LysoPA(21:0/0:0)	Glycerophospholipids	HMDB0114741	M+NH4	C24H49O7P	-1.7
LysoPC(O-18:0)	Glycerophospholipids	HMDB0011149	M+H	C26H56NO6P	0.0
LysoPC(P-18:0)	Glycerophospholipids	HMDB0013122	M+FA-H	C26H54NO6P	-2.7
LysoPC(P-18:1)	Glycerophospholipids	HMDB0010408	M+H	C26H52NO6P	-0.8
PC(14:1/18:0)	Glycerophospholipids	HMDB0007904	M+FA-H	C40H78NO8P	-0.2
PC(15:0/20:2)	Glycerophospholipids	HMDB0007946	M+H	C43H82NO8P	-1.9
PC(16:0/22:4)	Glycerophospholipids	HMDB0007988	M+FA-H	C46H84NO8P	-2.0
PC(18:0/20:4)	Glycerophospholipids	HMDB0008049	M+FA-H	C46H84NO8P	-2.0
PC(18:2/P-18:1)	Glycerophospholipids	HMDB0008161	M+FA-H	C44H82NO7P	-7.6
PC(20:2/15:0)	Glycerophospholipids	HMDB0008330	M+H	C43H82NO8P	-6.6
PC(22:5/P-18:1)	Glycerophospholipids	HMDB0008721	M+H	C48H84NO7P	-2.8
PC(22:6/18:0)	Glycerophospholipids	LMGP01012107	M+FA-H	C48H84NO8P	-3.8
PC(O-14:0/16:0)	Glycerophospholipids	HMDB0013341	M+H	C38H78NO7P	0.5
PC(O-16:0/0:0)	Glycerophospholipids	LMGP01060010	M+FA-H	C24H52NO6P	-3.7
PC(P-18:1/22:6)	Glycerophospholipids	HMDB0011295	M+H	C48H82NO7P	-7.1
PE(16:0/20:4)	Glycerophospholipids	HMDB0008937	M-H	C41H74NO8P	-0.9
PE(20:0/18:2)	Glycerophospholipids	HMDB0009225	M+H	C43H82NO8P	-1.5
PS(16:1/0:0)	Glycerophospholipids	LMGP03050010	M-H	C22H42NO9P	-9.1
PS(18:3/19:0)	Glycerophospholipids	LMGP03010411	M+FA-H	C43H78NO10P	-1.9
PS(20:0/18:2)	Glycerophospholipids	HMDB0112519	M+H	C44H82NO10P	7.8
PS(20:4/21:0)	Glycerophospholipids	LMGP03010643	M+FA-H	C47H84NO10P	-8.6
PS(22:0/0:0)	Glycerophospholipids	LMGP03050025	M-H	C28H56NO9P	-3.4
PS(22:6/18:2)	Glycerophospholipids	LMGP03010829	M-H	C46H74NO10P	-1.3
PS(22:6/21:0)	Glycerophospholipids	LMGP03010841	M+FA-H	C49H84NO10P	-4.9
SM(d18:1/18:1)	Glycerophospholipids	HMDB0012100	M+H	C41H81N2O6P	-2.1
17-Hydroxylinolenic acid	Lineolic acids	HMDB0011108	M-H	C18H30O3	1.3
MG(18:3/0:0/0:0)	Lineolic acids	HMDB0011570	M+FA-H	C21H36O4	-3.4
Phenethyl decanoate	Lineolic acids	HMDB0032464	M+Na	C18H28O2	8.3
Stearidonic acid	Lineolic acids	HMDB0006547	M+H	C18H28O2	0.7
2-Hydroxylinolenic acid	Lineolic acids	HMDB0031103	M+Na	C18H30O3	8.6
13-cis-Retinoic acid	Lipids	HMDB0006219	M+H	C20H28O2	0.6
18-Hydroxyretinoic acid	Lipids	HMDB0061095	M+H	C20H28O3	0.4
19-Noretiocholanolone	Lipids	HMDB0005886	M+Na	C18H28O2	9.0

Continued

Supplementary Table 1 Continued

Metabolites	Class	HMDB ID	Adducts	Formula	Mass Error (ppm)
3,21-Dihydroxypregn-5-en-20-one	Lipids	HMDB0004026	M+FA-H	C21H32O3	-1.7
4-Hydroxyretinoic acid	Lipids	HMDB0006254	M-H	C20H28O3	-0.3
4-oxo-Retinoic acid	Lipids	HMDB0006285	M+H	C20H26O3	0.8
Adrenosterone	Lipids	HMDB0006772	M+FA-H	C19H24O3	-9.4
Dehydroepiandrosterone	Lipids	HMDB0000077	M+FA-H	C19H28O2	-0.7
Guggulsterone	Lipids	HMDB0002726	M+H	C22H30O3	-0.9
Leukotriene B4 dimethylamide	Lipids	HMDB0005085	M-H	C22H37NO3	-8.9
Propylene glycol stearate	Lipids	HMDB0029764	M+H	C21H42O3	0.4
1,7-Dimethylguanosine	Nucleosides	HMDB0001961	M+H, M+Na	C12H17N5O5	0.7
5'-Phosphoribosyl-N-formylglycinamide	Nucleosides	HMDB0001308	2M-H	C8H15N2O9P	4.7
Adenosine monophosphate	Nucleosides	HMDB0000045	M+H, M+Na	C10H14N5O7P	-0.4
Cytidine	Nucleosides	HMDB0000089	2M+H	C9H13N3O5	-1.1
Guanosine monophosphate	Nucleosides	HMDB0001397	M+Na	C10H14N5O8P	-0.4
N2-Dimethylguanosine	Nucleosides	HMDB0004824	M-H	C12H17N5O5	0.4
N6-Methyladenosine	Nucleosides	HMDB0004044	M+H	C11H15N5O4	-0.1
Thymidine	Nucleosides	HMDB0000273	M-H, M+FA-H	C10H14N2O5	0.8
Uridine 5'-monophosphate	Nucleosides	HMDB0000288	M-H	C9H13N2O9P	-0.8
2-Deoxyribonic acid	Organic acids	HMDB0000366	M+Na	C5H10O5	-1.0
2-Ethyl-2-hydroxy-3-oxobutanoic acid	Organic acids	HMDB0006900	M-H	C6H10O4	1.4
Acetamide	Organic acids	HMDB0031645	M+FA-H	C2H5NO	1.3
2-Heptanone	Organic oxygen	HMDB0003671	M+FA-H	C7H14O	1.4
1,3,7-Trimethyluric acid	Organoheterocyclic	HMDB0002123	M+Na	C8H10N4O3	-6.7
11-beta-Hydroxyandrosterone-3-glucuronide	Organoheterocyclic	HMDB0010351	M-H	C25H38O9	-7.3
7-Methylxanthine	Organoheterocyclic	HMDB0001991	M-H	C6H6N4O2	-7.2
Calycanthidine	Organoheterocyclic	HMDB0030281	M-H	C23H28N4	-4.8
Dehydroascorbic acid	Organoheterocyclic	HMDB0001264	M-H	C6H6O6	1.1
Levoglucosan	Organoheterocyclic	HMDB0000640	M-H	C6H10O5	1.8
Dihydrothymine	Organoheterocyclic	HMDB0000079	M-H	C5H8N2O2	2.1
Galactosylsphingosine	Sphingolipids	HMDB0000648	M-H	C24H47NO7	-1.6
SM(d18:0/16:1)	Sphingolipids	HMDB0013464	M+FA-H	C39H79N2O6P	-9.2

Supplementary Table 2 List of differential metabolites obtained from serum.

Metabolites	Class	HMDB ID	Adducts	Formula	Mass Error (ppm)
L-2-Amino-3-methylenehexanoic acid	Amino acids	HMDB0030410	M+H	C7H13NO2	-3.2
N-Acetyl-L-histidine	Amino acids	HMDB0032055	M+FA-H	C8H11N3O3	8.6
Oleoyl glycine	Amino acids	HMDB0013631	M+H	C20H37NO3	-0.5
Isoleucyl-Hydroxyproline	Amino acids	HMDB0028908	M+K	C11H20N2O4	9.6
Taurolithocholic acid 3-glucuronide	Bile acids	HMDB0002429	M+FA-H	C32H53NO11S	3.9
3beta-Hydroxy-5-cholestenal	Bile acids	HMDB0060131	M+H	C27H44O2	-0.2
Chenodeoxycholic acid	Bile acids	HMDB0000518	M+NH4	C24H40O4	0.6
Muricholic acid	Bile acids	HMDB0000865	M+NH4, M+Na	C24H40O5	-1.3
Taurochenodesoxycholic acid	Bile acids	HMDB0000951	M+H, M+Na	C26H45NO6S	-1.2
20-HEDE	Eicosanoids	LMFA03000010	2M-H	C20H36O3	5.0
PGE2	Eicosanoids	HMDB0001220	M-H	C20H32O5	-1.5
Prostaglandin H3	Eicosanoids	HMDB0013040	M+H	C20H30O5	-0.3

Continued

Supplementary Table 2 Continued

Metabolites	Class	HMDB ID	Adducts	Formula	Mass Error (ppm)
12(R)-HPETE	Eicosanoids	HMDB0004692	M+NH4, M+Na	C20H32O4	0.9
12(S)-HETrE	Eicosanoids	HMDB0062747	M-H	C20H34O3	-1.8
12(S)-HPETE	Eicosanoids	HMDB0004243	M-H	C20H32O4	-2.3
11R-HEPE	Eicosanoids	HMDB0012534	M+H	C20H30O3	0.2
Prostaglandin E1	Eicosanoids	HMDB0001442	M+NH4, M+Na	C20H34O5	0.2
PGB1	Eicosanoids	HMDB0002982	M-H	C20H32O4	0.6
Prostaglandin F2beta	Eicosanoids	HMDB0001483	M-H	C20H34O5	-1.6
2-Propyl-2,4-pentadienoic acid	Fatty acids	HMDB0060682	M+NH4	C8H12O2	-2.7
Stearic acid	Fatty acids	HMDB0000827	M+NH4	C18H36O2	0.5
12-hydroxyicosanoic acid	Fatty acids	HMDB0061664	M+NH4	C20H40O3	-0.2
Octadecanedioic acid	Fatty acids	HMDB0000782	M+H	C18H34O4	0.3
9-Heptadecenoic acid	Fatty acids	HMDB0031046	M+FA-H	C17H32O2	-0.6
3-hydroxyhexadecanoyl carnitine	Fatty acids	HMDB0061642	M+H	C23H45NO5	1.6
2(R)-hydroxydocosanoic acid	Fatty acids	HMDB0061660	M+NH4	C22H44O3	-0.5
2-Hydroxypalmitic Acid	Fatty acids	HMDB0031057	M-H	C16H32O3	1.6
Stearoylcarnitine	Fatty acids	HMDB0000848	M+K	C25H49NO4	-0.6
6-Hydroxyoctadecanoic acid	Fatty acids	HMDB0112193	M-H	C18H36O3	-0.7
9,10-DHOME	Fatty acids	HMDB0004704	M+Na	C18H34O4	6.8
Glycerophosphocholine	Glycerophospholipids	HMDB0000086	M+H	C8H20NO6P	0.1
LysoPE(0:0/22:6)	Glycerophospholipids	HMDB0011496	M+H	C27H44NO7P	-2.4
PC(2:0/18:1)	Glycerophospholipids	NA	M+Na	C28H54NO8P	1.9
PC(18:1/2:0)	Glycerophospholipids	NA	M+Na	C28H54NO8P	3.0
PI(20:5/0:0)	Glycerophospholipids	LMGP06050026	M+H	C29H47O12P	-0.9
LysoPC(15:0)	Glycerophospholipids	HMDB0010381	M+H	C23H48NO7P	0.3
LysoPA(22:6/0:0)	Glycerophospholipids	HMDB0114755	M+NH4	C25H39O7P	-0.8
PE(20:5/0:0)	Glycerophospholipids	NA	M-H	C25H42NO7P	-1.9
LysoPE(0:0/20:1)	Glycerophospholipids	HMDB0011482	M+H	C25H50NO7P	-1.8
LysoPE(0:0/18:2)	Glycerophospholipids	HMDB0011477	M+Na, M+K	C23H44NO7P	-0.5
PC(17:2/18:1)	Glycerophospholipids	NA	M+FA-H	C43H80NO8P	3.6
LysoPE(0:0/22:5)	Glycerophospholipids	HMDB0011494	M+H	C27H46NO7P	5.9
PE(0:0/22:5)	Glycerophospholipids	NA	M-H	C27H46NO7P	-2.4
PE(17:1/19:0)	Glycerophospholipids	NA	M+FA-H	C41H80NO8P	0.6
PA(P-16:0/15:1)	Glycerophospholipids	NA	M+FA-H	C34H65O7P	0.6
PS(20:0/0:0)	Glycerophospholipids	NA	M+H	C26H52NO9P	-2.2
LysoPC(14:0/0:0)	Glycerophospholipids	HMDB0010379	M+H	C22H46NO7P	0.5
PC(P-16:0/18:0)	Glycerophospholipids	HMDB0011208	M+H	C42H84NO7P	-4.0
PE(22:1/18:1)	Glycerophospholipids	HMDB0009521	M+H	C45H86NO8P	-1.4
LysoPC(20:1)	Glycerophospholipids	HMDB0010391	M+FA-H	C28H56NO7P	0.1
PE(0:0/20:3)	Glycerophospholipids	NA	M+FA-H	C25H46NO7P	-6.7
PE(10:0/10:0)	Glycerophospholipids	NA	M+H	C25H50NO8P	8.2
PA(P-16:0/14:1)	Glycerophospholipids	NA	M-H	C33H63O7P	-0.8
PE(O-20:0/18:3)	Glycerophospholipids	NA	M+FA-H	C43H82NO7P	-0.7
PA(O-16:0/12:0)	Glycerophospholipids	NA	M-H	C31H63O7P	-0.7
PS(O-16:0/22:2)	Glycerophospholipids	NA	M+FA-H	C44H84NO9P	-5.2
LysoPC(22:2)	Glycerophospholipids	HMDB0010400	M+H	C30H58NO7P	0.4
LysoPC(O-18:0)	Glycerophospholipids	HMDB0011149	M+Na	C26H56NO6P	-0.4

Continued

Supplementary Table 2 Continued

Metabolites	Class	HMDB ID	Adducts	Formula	Mass Error (ppm)
PA(O-18:0/12:0)	Glycerophospholipids	NA	M-H	C33H67O7P	7.8
PC(20:0/0:0)	Glycerophospholipids	NA	M+H	C28H58NO7P	0.7
LysoPC(0:0/18:0)	Glycerophospholipids	HMDB0011128	M+H	C26H54NO7P	-0.6
LysoPC(20:3)	Glycerophospholipids	HMDB0010394	M+H, M+Na	C28H52NO7P	-4.8
PI(18:2/0:0)	Glycerophospholipids	LMGP06050010	M-H	C27H49O12P	-1.1
PI(18:0/0:0)	Glycerophospholipids	LMGP06050004	M-H	C27H53O12P	-1.4
PA(8:0/i-12:0)	Glycerophospholipids	HMDB0115685	M+Na	C23H45O8P	-0.1
LysoPE(0:0/20:4)	Glycerophospholipids	HMDB0011487	M+Na	C25H44NO7P	3.9
LysoPE(20:5/0:0)	Glycerophospholipids	HMDB0011519	M+H	C25H42NO7P	-0.6
LysoPC(18:2)	Glycerophospholipids	HMDB0010386	M+Na	C26H50NO7P	1.4
Alpha-Linolenic acid	Lineolic acids	HMDB0001388	M+H	C18H30O2	0.9
4,8,12,15-Octadecatetraenoic acid	Lineolic acids	HMDB0032672	M+H	C18H28O2	-0.2
13-HOTE	Lineolic acids	HMDB0010203	M+H	C18H30O3	1.1
3-hydroxylinoleoylcarnitine	Lipids	NA	M+H	C25H45NO5	-0.8
12(S)-Leukotriene B4	Lipids	HMDB0005089	M+NH4	C20H32O4	0.0
N-palmitoyl proline	Lipids	NA	M+K	C21H39NO3	-5.4
13-cis-Retinoic acid	Lipids	HMDB0006219	M+H	C20H28O2	1.7
Lithocholate 3-O-glucuronide	Lipids	HMDB0002513	M+H	C30H48O9	-0.4
Pipericine	Lipids	HMDB0031678	M+H	C22H41NO	3.2
Dihydrocortisol	Lipids	HMDB0003259	M+H	C21H32O5	-0.2
Cortisol	Lipids	HMDB0000063	M+H	C21H30O5	0.0
Cortexolone	Lipids	HMDB0000015	M+H, M+Na	C21H30O4	-0.1
11-deoxycortisol	Lipids	HMDB0000015	M+FA-H	C21H30O4	-1.4
MG(0:0/i-15:0/0:0)	Lipids	HMDB0072849	M+NH4	C18H36O4	0.6
Uridine	Nucleosides	HMDB0000296	M-H	C9H12N2O6	-0.9
Inosine	Nucleosides	HMDB0000195	M+H	C10H12N4O5	-2.6
Hypoxanthine	Nucleosides	HMDB0000157	M+H	C5H4N4O	1.0
2-Deoxypentonic acid	Organic acids	HMDB0059753	M+Na	C5H10O5	-2.3
N-palmitoyl isoleucine	Others	NA	M-H	C22H43NO3	-2.7
Sphingosine 1-phosphate	Sphingolipids	HMDB0000277	M+Na	C18H38NO5P	-1.2
Sphinganine 1-phosphate	Sphingolipids	HMDB0001383	M+H	C18H40NO5P	-1.1