

Two-Stage Deep-Learning Classifier for Diagnostics of Lung Cancer Using Metabolites

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Supplemental Table S1. Metabolites used as lung cancer biomarkers (References numbers are from the main article).

Name of Metabolite	Type	Reference Number
1-Methylxanthine	SQ	8
1,6-Anhydroglucose	SQ	8
10-nonadecenoate	AD	8
12-HETE	SQ	8
17-methylstearate	SQ	8
2-deoxyadenosine 5-monophosphate	SQ	8
2-deoxyguanosine	AD	8
2-Hydroxybutyrate	SC	14
2-hydroxybutyrate	AD	8
2-methylsuccinic acid	AD	8
2-O-methylguanosine	SQ	8
2-piperidinone	SQ	8
3-hydroxybutyrate	SC	14
3-Hydroxydecanoate	AD	8
3-hydroxydecanoate	SC	14
3-Methyl-2-oxobutyrate	NS	8
3-methylhistamine	NS	8
3-phenylpropanoic acid	AD	8
4-acetamido-3-methoxyphenyl beta-D-glucopyranosiduronic acid	SQ	8
4-acetamidophenol	SC	14
4-hydroxyproline	SC	14
5-dodecenoate	NS	8
5-methylthioadenosine	AD	8
7-dehydrocholesterol	AD	8
8-Tocopherol	AD	8
a-glucopyranosiduronic acid	SC	14
a-hydroxybutyric acid	AD	8
acetoacetate	AD	8

acetylcarnitine	AD	8
acisoga	SC	14
adenosine 5-monophosphate	SC	14
adenosine 5'-monophosphate	NS	8
ADpSGEGDFXAEGGGVR	AD	8
adrenate	SC	14
Alanine	AD	8
alanylleucine	SC	14
alanylphenylalanine	NS	8
alanylphenylalanine	AD	8
arachidonate	AD	8
arachidonic acid	SQ	8
arginine	SQ	8
ascorbate	NS	8
aspartic acid	SQ	8
aspartyltryptophan	SC	14
atenolol	SC	14
azelate	SQ	8
bilirubin	AD	8
carnitine	AD	8
cellobiose	AD	8
cholate	SC	14
cis-inositol	NS	8
citric acid	AD	8
cortisol	NS	8
cysteine	SQ	8
dehydromucic acid	NS	8
delta-tocopherol	AD	8
DGLA	SQ	8
dipropylacetic acid	SQ	8
docosadienoate	SQ	8
docosadienoate	AD	8
docosapentaenoate	AD	8
docosatrienoate	SC	14
DSGEGDFXAEGGGVR	NS	8
eicosanoic acid	SQ	8
Eicosenoate	SC	14
eicosenoate	NS	8
eicosenoylglycerol	SC	14
erythritol	SC	14
erythronate	NS	8

galactonate	AD	8
galactose	SQ	8
gamma-glutamylcysteine	SC	14
gamma-tocopherol	SQ	8
glutamine-leucine	NS	8
glutathione	SQ	8
glycerol	SQ	8
glycerol 2-phosphate	SC	14
glycine	NS	8
glycochenodeoxycholate	NS	8
glycocholate	SQ	8
Hexanoylcarnitine	AD	8
hydroxybutyrylcarnitine	NS	8
hypoxanthine	AD	8
hypoxanthine	SQ	8
I-urobilinogen	AD	8
indoleacetylglutamine	AD	8
isoleucine	AD	8
isoleucylglutamine	NS	8
isoleucylserine	SC	14
laurylcarnitine	NS	8
laurylcarnitine	AD	8
leucine	SQ	8
leucylglutamine	SC	14
leucylglycine	SQ	8
linolenate	AD	8
lysine	SC	14
malonic acid	SQ	8
mannose	NS	8
methionine	SC	14
methionine	SQ	8
metoprolol	SQ	8
myo-inositol	SQ	8
N-(2-Furoyl)glycine	SQ	8
N-(2-Furoyl)glycine	AD	8
N-acetylaspartate	NS	8
N-Acetylmethionine	SC	14
N-Acetylneuraminate	NS	8
N-acetylputrescine	NS	8
N-ethylglycinexylidide	SC	14
N(1)-acetylspermine	SQ	8

N1-methyladenosine	AD	8
naproxen	AD	8
nonadecanoate	SC	14
octadecanedioate	SC	14
palmitoleic acid	NS	8
palmitoylcarnitine	SC	14
pelargonate	SQ	8
pelargonate	SQ	8
phenol	NS	8
phenylalanine	SC	14
phenylalanine	SQ	8
phenylalanylleucine	SQ	8
phenylalanylvaline	SC	14
phosphate	AD	8
pyroglutamine	SQ	8
quinat	AD	8
R-hydroxybutyric acid	SQ	8
ribitol	SQ	8
ribofuranose	NS	8
ribose	NS	8
ribose	SQ	8
salicylic acid	AD	8
serine	NS	8
serylleucine	SQ	8
sorbitol	AD	8
spermidine	NS	8
stearoyl sphingomyelin	SC	14
sulfate	SC	14
taurodeoxycholate	SQ	8
theobromine	SQ	8
theobromine	NS	8
theophylline	NS	8
threitol	SC	14
threonine	NS	8
threonylvaline	NS	8
thymine	SC	14
tocopherol	SQ	8
trimethylamine N-oxide	AD	8
trizma acetate	AD	8
tryptophan	NS	8
tryptophan	AD	8

tyrosine	NS	8
tyrosylleucine	NS	8
uridine 5-monophosphate	SQ	8
uridine diphosphate-N-acetylgalactosamine	SC	14
uridine monophosphate	NS	8
valine	AD	8
valylglycine	SQ	8
valylisoleucine	SQ	8
valylphenylalanine	NS	8
valylvaline	NS	8
xanthosine	AD	8
xanthosine 5-monophosphate	AD	8