

Supplementary Text

Metabolic profiles are principally different between cancers of the liver, pancreas and breast.

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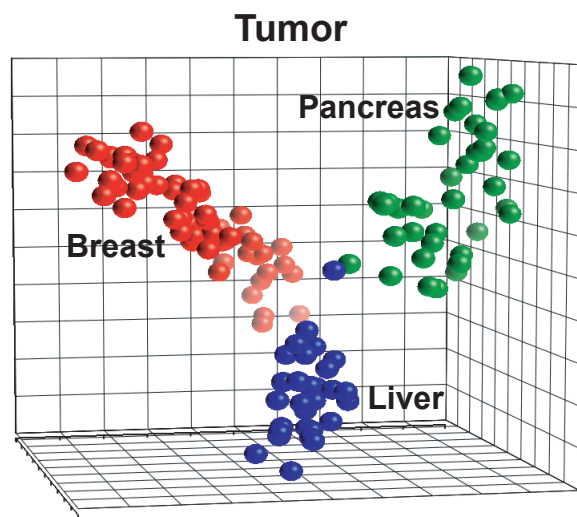
Supplemental Figure legends

Supplemental Figure 1. Metabolites patterns can distinguish tumor or nontumor specimens among cancers. (a) A principal component analysis plot is shown comparing the metabolite status of tumor specimens or (b) nontumor specimens among patients with liver, pancreas and breast cancer.

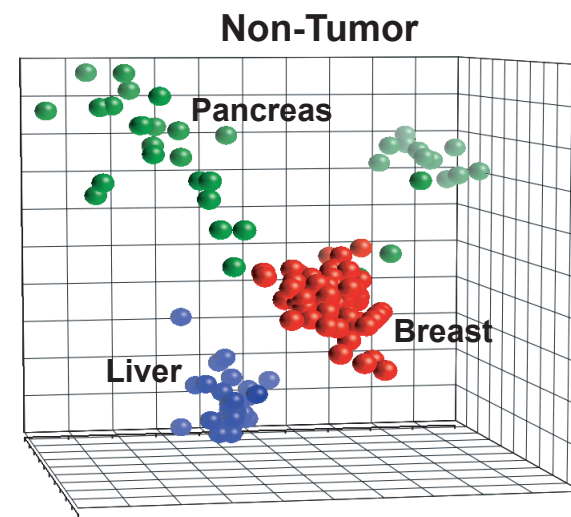
Supplemental Figure 2. Tumor-specific metabolite can distinguish cancer types. (a) A principal component analysis plot is shown comparing the metabolite status of liver, pancreas or breast specimens based on tumor-specific metabolites.

Supplemental Figure 3. Metabolites patterns can distinguish cancer types. (a) A VENN diagram is presented for metabolites that were yielded among liver, pancreas or breast specimens. (b) VENN diagrams are presented comparing tumor-specific metabolite abundance and cancer-specific metabolite yield for each cancer type.

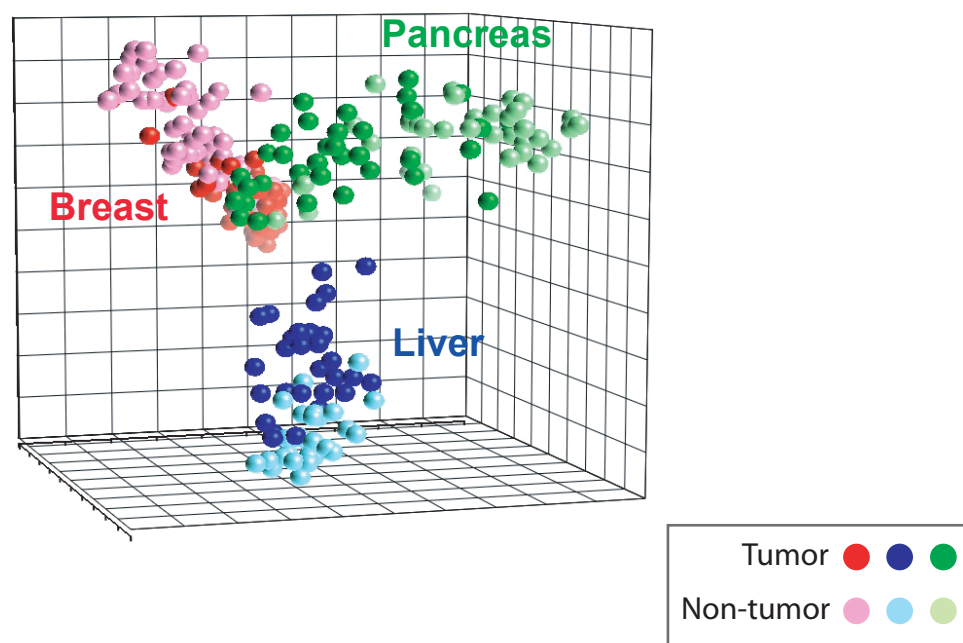
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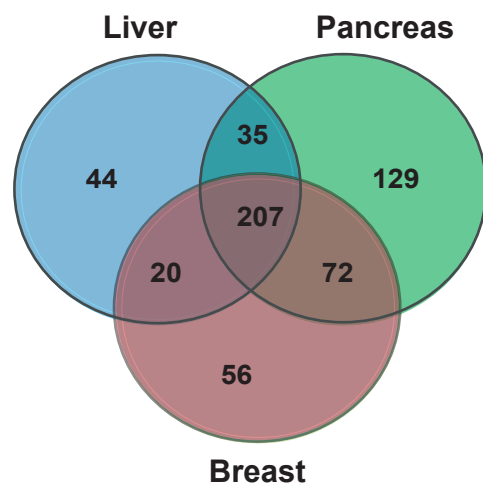
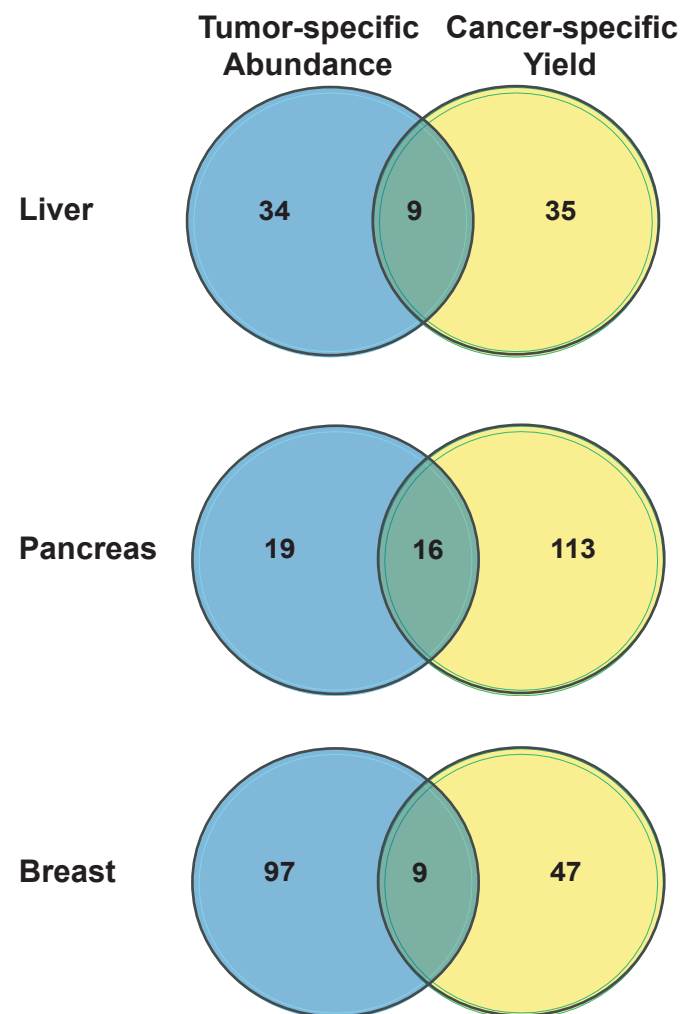


B.



A.



A.**B.**

Supplemental Table 1: Clinical Characteristics of Patients at Diagnosis

	HCC (n=30)	Pancreas (n=38)	Breast (n=65)			
Clinical Variable	Value^a	Value	Value	P-value^b (HCC vs Pancreas)	P-value^b (HCC vs Breast)	P-value^b (Pancreas vs Breast)
<i>Gender</i>						
Male; Female	25 (83); 5	10 (26); 13	0; 65 (100)	0.0035	0.0001	0.0001
<i>Age--yr</i>						
Median (Range)	49 (27-77)	69 (38-82)	51 (30-93)	<0.0001^c	0.1455 ^c	<0.0001^c
<i>TNM Stage</i>						
I	12 (40)	5 (13)	6 (10)	0.0037	0.0005	0.0339
II	8 (27)	27 (71)	44 (73)			
III	10 (33)	3 (8)	15 (25)			
IV	0	3(8)	0			
<i>Survival months</i>						
Median (Range)	53.3 (3.8-64.2)	11 (1.2-70.8)	50 (0-148)			
Events	13	26	30			

^a Each value represents: the number of patients (the % of patients); ^b χ^2 Test; ^c Unpaired Student's T Test;

Supplemental Table 2: Differentially abundant metabolites in liver cancer

Metabolite	Super Pathway	Sub Pathway	Parametric p-value	Permutation p-value	FC TvsNT
2-aminobutyrate	Amino acid	Butanoate metabolism	<0.0001	< 1e-07	0.50
cysteine	Amino acid	Cysteine, methionine, SAM, taurine metabolism	<0.0001	0.000	0.31
cystine	Amino acid	Cysteine, methionine, SAM, taurine metabolism	0.005	0.006	0.33
S-adenosylhomocysteine (SAH)	Amino acid	Cysteine, methionine, SAM, taurine metabolism	<0.0001	< 1e-07	0.44
gamma-aminobutyrate (GABA)	Amino acid	Glutamate metabolism	<0.0001	< 1e-07	0.28
pyroglutamine*	Amino acid	Glutamate metabolism	<0.0001	< 1e-07	0.51
urocanate	Amino acid	Histidine metabolism	0.002	0.001	2.27
methylglutaryl carnitine	Amino acid	Lysine metabolism	0.001	0.001	0.38
5-methylthioadenosine (MTA)	Amino acid	Polyamine metabolism	<0.0001	< 1e-07	3.45
isobutyryl carnitine	Amino acid	Valine, leucine and isoleucine metabolism	<0.0001	< 1e-07	0.28
isovaleryl carnitine	Amino acid	Valine, leucine and isoleucine metabolism	0.005	0.008	0.53
tiglyl carnitine	Amino acid	Valine, leucine and isoleucine metabolism	<0.001	< 1e-07	0.48
valeryl carnitine	Amino acid	Valine, leucine and isoleucine metabolism	<0.0001	< 1e-07	3.13
N-acetylmannosamine	Carbohydrate	Aminosugars metabolism	<0.0001	<0.0001	0.44
mannose	Carbohydrate	Fructose, mannose, galactose, starch, and sucrose metabolism	<0.0001	< 1e-07	0.46
sorbitol	Carbohydrate	Fructose, mannose, galactose, starch, and sucrose metabolism	<0.0001	< 1e-07	0.31
tagatose	Carbohydrate	Fructose, mannose, galactose, starch, and sucrose metabolism	<0.0001	< 1e-07	0.27
glucose	Carbohydrate	Glycolysis, gluconeogenesis, pyruvate metabolism	<0.0001	< 1e-07	0.28
glucuronate	Carbohydrate	Glycolysis, gluconeogenesis, pyruvate metabolism	< 1e-07	< 1e-07	0.37
6-phosphogluconate	Carbohydrate	Nucleotide sugars, pentose metabolism	0.002	0.002	0.54
ribitol	Carbohydrate	Nucleotide sugars, pentose metabolism	<0.0001	< 1e-07	0.37
ribose 5-phosphate	Carbohydrate	Nucleotide sugars, pentose metabolism	<0.0001	<0.0001	0.39
xylitol	Carbohydrate	Nucleotide sugars, pentose metabolism	<0.0001	< 1e-07	0.32
glucarate (saccharate)	Cofactors and vitamins	Ascorbate and aldarate metabolism	<0.0001	< 1e-07	0.48
gulono-1,4-lactone	Cofactors and vitamins	Ascorbate and aldarate metabolism	<0.0001	< 1e-07	0.29
5-methyltetrahydrofolate (5MeTHF)	Cofactors and vitamins	Folate metabolism	<0.0001	<0.0001	0.50
nicotinamide	Cofactors and vitamins	Nicotinate and nicotinamide metabolism	0.001	0.001	0.24
nicotinamide riboside*	Cofactors and vitamins	Nicotinate and nicotinamide metabolism	< 1e-07	<0.0001	0.47
pyridoxal	Cofactors and vitamins	Pyridoxal metabolism	< 1e-07	< 1e-07	0.50
flavin adenine dinucleotide (FAD)	Cofactors and vitamins	Riboflavin metabolism	<0.0001	< 1e-07	0.41
riboflavin (Vitamin B2)	Cofactors and vitamins	Riboflavin metabolism	<0.0001	< 1e-07	0.51
alpha-tocopherol	Cofactors and vitamins	Tocopherol metabolism	<0.0001	<0.0001	0.32
pyridoxate	Cofactors and vitamins	Vitamin B6 metabolism	<0.0001	< 1e-07	0.44
fumarate	Energy	Krebs cycle	< 1e-07	< 1e-07	0.50
malate	Energy	Krebs cycle	< 1e-07	< 1e-07	0.42
glycochenodeoxycholate	Lipid	Bile acid metabolism	0.004	0.004	0.37
glycocholate	Lipid	Bile acid metabolism	0.001	0.001	0.25
glycoursodeoxycholate	Lipid	Bile acid metabolism	<0.0001	<0.0001	0.37
2-methylmalonyl carnitine	Lipid	Carnitine metabolism	<0.0001	<0.0001	1.96
butyryl carnitine	Lipid	Carnitine metabolism	< 1e-07	< 1e-07	13.70
deoxycarnitine	Lipid	Carnitine metabolism	<0.0001	< 1e-07	2.08
glutaroyl carnitine	Lipid	Carnitine metabolism	<0.0001	< 1e-07	0.40
hexanoyl carnitine	Lipid	Carnitine metabolism	<0.0001	< 1e-07	4.35
palmitoyl carnitine	Lipid	Carnitine metabolism	<0.0001	< 1e-07	3.13
stearoyl carnitine	Lipid	Carnitine metabolism	0.003	0.004	3.03
docosapentaenoate (n3 DPA; 22:5n3)	Lipid	Essential fatty acid	<0.0001	0.001	0.52
linolenate [alpha or gamma; (18:3n3 or 6)]	Lipid	Essential fatty acid	<0.0001	< 1e-07	0.36
choline	Lipid	Glycerolipid metabolism	<0.0001	0.001	2.13
glycerol	Lipid	Glycerolipid metabolism	<0.0001	<0.0001	0.44

glycerophosphorylcholine (GPC)	Lipid	Glycerolipid metabolism	<0.0001	< 1e-07	0.38
phosphoethanolamine	Lipid	Glycerolipid metabolism	<0.0001	< 1e-07	2.13
phosphopantetheine	Lipid	Glycerolipid metabolism	0.006	0.003	0.54
docosadienoate (22:2n6)	Lipid	Long chain fatty acid	<0.0001	<0.0001	2.08
docosapentaenoate (n6 DPA, 22:5n6)	Lipid	Long chain fatty acid	<0.0001	<0.0001	2.17
7-beta-hydroxycholesterol	Lipid	Sterol/Steroid	<0.0001	0.000	2.08
xanthosine	Nucleotide	Purine metabolism, (hypo)xanthine/inosine containing	< 1e-07	< 1e-07	0.18
adenine	Nucleotide	Purine metabolism, adenine containing	>0.0001	>0.0001	2.50
adenosine 2'-monophosphate (2'-AMP)	Nucleotide	Purine metabolism, adenine containing	< 1e-07	< 1e-07	0.39
adenosine 3',5'-diphosphate	Nucleotide	Purine metabolism, adenine containing	>0.0001	< 1e-07	0.37
adenosine 3'-monophosphate (3'-AMP)	Nucleotide	Purine metabolism, adenine containing	>0.0001	< 1e-07	0.39
adenosine 5'-monophosphate (AMP)	Nucleotide	Purine metabolism, adenine containing	>0.0001	>0.0001	0.30
urate	Nucleotide	Purine metabolism, urate metabolism	>0.0001	< 1e-07	0.47
5,6-dihydrouracil	Nucleotide	Pyrimidine metabolism, uracil containing	>0.0001	< 1e-07	3.57
beta-alanine	Nucleotide	Pyrimidine metabolism, uracil containing	>0.0001	< 1e-07	0.48
gamma-glutamylglutamate	Peptide	g-glutamyl	>0.0001	>0.0001	0.27
gamma-glutamylglutamine	Peptide	g-glutamyl	0.002	0.003	0.30
gamma-glutamylmethionine*	Peptide	g-glutamyl	>0.0001	< 1e-07	0.42
gamma-glutamyltyrosine	Peptide	g-glutamyl	< 1e-07	< 1e-07	0.53
VGAHAGEYGAELER*	Peptide	Polypeptide	< 1e-07	< 1e-07	0.23
hippurate	Xenobiotics	Benzoate metabolism	>0.0001	>0.0001	0.41
glycerol 2-phosphate	Xenobiotics	Chemical	< 1e-07	< 1e-07	0.25
erythritol	Xenobiotics	Sugar, sugar substitute, starch	>0.0001	< 1e-07	0.47
galacturonate	Xenobiotics	Sugar, sugar substitute, starch	>0.0001	>0.0001	0.49

Abbreviations: FC: Fold Change; T: tumor; NT: nontumor

Red: Abundant in tumor; Blue: Abundant in nontumor

Metabolites in bold are unique to liver cancer

Supplemental Table 3: Differentially abundant metabolites in pancreas cancer

Metabolite	Super Pathway	Sub Pathway	Parametric p-value	Permutation p-value	FC TvsNT
taurine	Amino acid	Cysteine, methionine, SAM, taurine metabolism	<0.0001	< 1e-07	2.63
N-acetyl-aspartyl-glutamate (NAAG)	Amino acid	Glutamate metabolism	0.001	0.001	0.48
cysteine-glutathione disulfide	Amino acid	Glutathione metabolism	<0.0001	0.001	4.76
glutathione, oxidized (GSSG)	Amino acid	Glutathione metabolism	0.001	0.002	3.85
glutathione, reduced (GSH)	Amino acid	Glutathione metabolism	0.004	0.004	3.70
guanidinoacetate	Amino acid	Guanidino and acetamido metabolism	0.003	0.004	0.26
C-glycosyltryptophan*	Amino acid	Tryptophan metabolism	< 1e-07	< 1e-07	2.00
kynurenine	Amino acid	Tryptophan metabolism	<0.0001	0.000	2.17
ornithine	Amino acid	Urea cycle; arginine-, proline-, metabolism	<0.0001	0.001	0.49
isovalerylcarnitine	Amino acid	Valine, leucine and isoleucine metabolism	<0.0001	< 1e-07	2.04
maltotriose	Carbohydrate	Fructose, mannose, galactose, starch, and sucrose metabolism	0.008	0.009	4.00
nicotinamide adenine dinucleotide (NAD+)	Cofactors and vitamins	Nicotinate and nicotinamide metabolism	0.001	0.001	0.22
nicotinamide ribonucleotide (NMN)	Cofactors and vitamins	Nicotinate and nicotinamide metabolism	<0.0001	< 1e-07	0.15
citrate	Energy	Krebs cycle	0.004	0.003	3.13
succinate	Energy	Krebs cycle	<0.0001	<0.0001	0.42
succinylcarnitine	Energy	Krebs cycle	<0.0001	0.000	0.35
taurochenodeoxycholate	Lipid	Bile acid metabolism	0.007	0.007	0.49
decanoylcarnitine	Lipid	Carnitine metabolism	<0.0001	<0.0001	2.08
hexanoylcarnitine	Lipid	Carnitine metabolism	< 1e-07	< 1e-07	2.63
octanoylcarnitine	Lipid	Carnitine metabolism	<0.0001	< 1e-07	2.44
1,2-dipalmitoylglycerol	Lipid	Diacylglycerol	0.007	0.006	0.45
prostaglandin E2	Lipid	Eicosanoid	<0.0001	< 1e-07	2.63
linoleate (18:2n6)	Lipid	Essential fatty acid	<0.0001	< 1e-07	0.51
linolenate [alpha or gamma; (18:3n3 or 6)]	Lipid	Essential fatty acid	<0.0001	< 1e-07	0.36
butyrylcarnitine	Lipid	Fatty acid metabolism (also BCAA metabolism)	< 1e-07	< 1e-07	3.13
17-methylstearate	Lipid	Fatty acid, branched	<0.0001	< 1e-07	0.43
9,10-hydroxyoctadec-12(Z)-enoic acid	Lipid	Fatty acid, dihydroxy	<0.0001	< 1e-07	0.40
palmitate, methyl ester	Lipid	Fatty acid, methyl ester	0.009	0.002	0.51
13-HODE + 9-HODE	Lipid	Fatty acid, monohydroxy	<0.0001	<0.0001	0.49
glycerol	Lipid	Glycerolipid metabolism	<0.0001	< 1e-07	0.39
glycerol 3-phosphate (G3P)	Lipid	Glycerolipid metabolism	0.001	0.001	0.35
glycerophosphorylcholine (GPC)	Lipid	Glycerolipid metabolism	<0.0001	<0.0001	0.35
10-nonadecenoate (19:1n9)	Lipid	Long chain fatty acid	<0.0001	<0.0001	0.46
dihomo-linoleate (20:2n6)	Lipid	Long chain fatty acid	0.002	0.002	0.50
eicosenoate (20:1n9 or 11)	Lipid	Long chain fatty acid	<0.0001	0.001	0.42
margarate (17:0)	Lipid	Long chain fatty acid	<0.0001	< 1e-07	0.48
myristate (14:0)	Lipid	Long chain fatty acid	<0.0001	0.000	0.52
myristoleate (14:1n5)	Lipid	Long chain fatty acid	<0.0001	< 1e-07	0.40
nonadecanoate (19:0)	Lipid	Long chain fatty acid	0.001	0.001	0.53
palmitoleate (16:1n7)	Lipid	Long chain fatty acid	<0.0001	< 1e-07	0.53
1-oleoylglycerophosphoinositol*	Lipid	Lysolipid	<0.0001	<0.0001	0.22
1-palmitoylglycerophosphoinositol*	Lipid	Lysolipid	0.001	0.001	0.22
5-dodecenoate (12:1n7)	Lipid	Medium chain fatty acid	0.010	0.012	0.51
laurate (12:0)	Lipid	Medium chain fatty acid	<0.0001	< 1e-07	0.47
1-docosahexaenoylglycerol (1-monodocosahexaenoin)	Lipid	Monoacylglycerol	0.001	0.000	0.31
1-myristoylglycerol (1-monomyristin)	Lipid	Monoacylglycerol	<0.0001	< 1e-07	0.09
1-oleoylglycerol (1-monoolein)	Lipid	Monoacylglycerol	0.009	0.008	0.33
1-palmitoylglycerol (1-monopalmitin)	Lipid	Monoacylglycerol	0.004	0.003	0.32
1-pentadecanoylglycerol (1-monopentadecanoin)	Lipid	Monoacylglycerol	<0.0001	< 1e-07	0.34

1-stearoylglycerol (1-monostearin)	Lipid	Monoacylglycerol	<0.0001	<0.0001	0.24
2-linoleoylglycerol (2-monolinolein)	Lipid	Monoacylglycerol	<0.0001	<0.0001	0.22
2-myristoylglycerol (2-monomyristin)	Lipid	Monoacylglycerol	<0.0001	< 1e-07	0.18
2-oleoylglycerol (2-monoolein)	Lipid	Monoacylglycerol	0.004	0.003	0.51
2-palmitoylglycerol (2-monopalmitin)	Lipid	Monoacylglycerol	<0.0001	< 1e-07	0.13
stearoyl sphingomyelin	Lipid	Sphingolipid	0.001	0.001	0.50
cytidine	Nucleotide	Pyrimidine metabolism, cytidine containing	<0.0001	<0.0001	0.38
isoleucylisoleucine	Peptide	Dipeptide	0.004	0.004	3.23
pro-hydroxy-pro	Peptide	Dipeptide	<0.0001	< 1e-07	2.22
threonylphenylalanine	Peptide	Dipeptide	0.003	0.003	2.56
N-ethylglycinexylidide*	Xenobiotics	Drug	<0.0001	< 1e-07	0.53

Abbreviations: FC: Fold Change; T: tumor; NT: nontumor

Red: Abundant in tumor; Blue: Abundant in nontumor

Metabolites in bold are unique to pancreatic cancer

Supplemental Table 4: Differentially abundant metabolites in breast cancer

Metabolite	Super Pathway	Sub Pathway	Parametric p-value	Permutation p-value	FC TvsNT
aspartate	Amino acid	Alanine and aspartate metabolism	0.001	0.001	1.47
beta-alanine	Amino acid	Alanine and aspartate metabolism	< 1e-07	< 1e-07	2.63
N-acetylalanine	Amino acid	Alanine and aspartate metabolism	< 1e-07	< 1e-07	2.17
N-acetylaspartate (NAA)	Amino acid	Alanine and aspartate metabolism	< 1e-07	< 1e-07	10.20
N-acetyl-aspartyl-glutamate (NAAG)	Amino acid	Alanine and aspartate metabolism	< 1e-07	< 1e-07	2.63
cystathionine	Amino acid	Cysteine, methionine, SAM, taurine metabolism	< 1e-07	< 1e-07	5.26
cysteine	Amino acid	Cysteine, methionine, SAM, taurine metabolism	< 1e-07	< 1e-07	4.00
cystine	Amino acid	Cysteine, methionine, SAM, taurine metabolism	< 1e-07	< 1e-07	4.00
N-acetylmethionine	Amino acid	Cysteine, methionine, SAM, taurine metabolism	< 1e-07	< 1e-07	3.57
S-adenosylhomocysteine (SAH)	Amino acid	Cysteine, methionine, SAM, taurine metabolism	<0.0001	< 1e-07	2.63
S-adenosylmethionine (SAM)	Amino acid	Cysteine, methionine, SAM, taurine metabolism	<0.0001	< 1e-07	1.96
taurine	Amino acid	Cysteine, methionine, SAM, taurine metabolism	< 1e-07	< 1e-07	3.57
glutamate	Amino acid	Glutamate metabolism	< 1e-07	< 1e-07	5.88
5-oxoproline	Amino acid	Glutathione metabolism	< 1e-07	< 1e-07	2.08
glutathione, reduced (GSH)	Amino acid	Glutathione metabolism	<0.0001	<0.0001	2.56
betaine	Amino acid	Glycine, serine and threonine metabolism	< 1e-07	< 1e-07	2.50
glycine	Amino acid	Glycine, serine and threonine metabolism	< 1e-07	< 1e-07	2.94
N-acetylserine	Amino acid	Glycine, serine and threonine metabolism	< 1e-07	< 1e-07	2.33
N-acetylthreonine	Amino acid	Glycine, serine and threonine metabolism	< 1e-07	< 1e-07	2.22
serine	Amino acid	Glycine, serine and threonine metabolism	< 1e-07	< 1e-07	2.38
threonine	Amino acid	Glycine, serine and threonine metabolism	<0.0001	< 1e-07	1.96
N6-acetyllysine	Amino acid	Lysine metabolism	< 1e-07	< 1e-07	3.13
3-(4-hydroxyphenyl)lactate	Amino acid	Phenylalanine & tyrosine metabolism	< 1e-07	< 1e-07	2.94
putrescine	Amino acid	Polyamine metabolism	< 1e-07	< 1e-07	4.55
C-glycosyltryptophan*	Amino acid	Tryptophan metabolism	< 1e-07	< 1e-07	5.00
kynurenine	Amino acid	Tryptophan metabolism	< 1e-07	< 1e-07	3.57
tryptophan	Amino acid	Tryptophan metabolism	< 1e-07	< 1e-07	2.22
tryptophan betaine	Amino acid	Tryptophan metabolism	< 1e-07	< 1e-07	2.63
dimethylarginine (SDMA + ADMA)	Amino acid	Urea cycle; arginine-, proline-, metabolism	< 1e-07	< 1e-07	4.17
proline	Amino acid	Urea cycle; arginine-, proline-, metabolism	< 1e-07	< 1e-07	3.13
stachydrine	Amino acid	Urea cycle; arginine-, proline-, metabolism	< 1e-07	< 1e-07	2.27
trans-4-hydroxyproline	Amino acid	Urea cycle; arginine-, proline-, metabolism	< 1e-07	< 1e-07	4.35
urea	Amino acid	Urea cycle; arginine-, proline-, metabolism	< 1e-07	< 1e-07	2.70
2-methylbutyrocarnitine	Amino acid	Valine, leucine and isoleucine metabolism	<0.0001	<0.0001	2.13
hydroxyisovaleroyl carnitine	Amino acid	Valine, leucine and isoleucine metabolism	< 1e-07	< 1e-07	2.33
leucine	Amino acid	Valine, leucine and isoleucine metabolism	< 1e-07	< 1e-07	2.04
erythronate*	Carbohydrate	Aminosugars metabolism	< 1e-07	< 1e-07	4.35
fucose	Carbohydrate	Aminosugars metabolism	< 1e-07	< 1e-07	2.70
N-acetylglucosamine	Carbohydrate	Aminosugars metabolism	<0.0001	< 1e-07	2.38
N-acetylglucosamine 6-phosphate	Carbohydrate	Aminosugars metabolism	< 1e-07	< 1e-07	2.56
N-acetylneuraminate	Carbohydrate	Aminosugars metabolism	< 1e-07	< 1e-07	3.03
fructose	Carbohydrate	Fructose, mannose, galactose, starch, and sucrose metabolism	<0.0001	< 1e-07	2.56
maltose	Carbohydrate	Fructose, mannose, galactose, starch, and sucrose metabolism	<0.0001	< 1e-07	3.03
maltotetraose	Carbohydrate	Fructose, mannose, galactose, starch, and sucrose metabolism	<0.0001	< 1e-07	2.27
maltotriose	Carbohydrate	Fructose, mannose, galactose, starch, and sucrose metabolism	<0.0001	< 1e-07	2.63
mannose	Carbohydrate	Fructose, mannose, galactose, starch, and sucrose metabolism	<0.0001	< 1e-07	2.13
mannose-6-phosphate	Carbohydrate	Fructose, mannose, galactose, starch, and sucrose metabolism	< 1e-07	< 1e-07	5.88
sorbitol	Carbohydrate	Fructose, mannose, galactose, starch, and sucrose metabolism	<0.0001	< 1e-07	2.17
3-phosphoglycerate	Carbohydrate	Glycolysis, gluconeogenesis, pyruvate metabolism	<0.0001	< 1e-07	2.13

fructose-6-phosphate	Carbohydrate	Glycolysis, gluconeogenesis, pyruvate metabolism	< 1e-07	< 1e-07	7.14
glucose	Carbohydrate	Glycolysis, gluconeogenesis, pyruvate metabolism	0.001	0.002	2.00
glucose-6-phosphate (G6P)	Carbohydrate	Glycolysis, gluconeogenesis, pyruvate metabolism	< 1e-07	< 1e-07	8.33
lactate	Carbohydrate	Glycolysis, gluconeogenesis, pyruvate metabolism	< 1e-07	< 1e-07	4.00
phosphoenolpyruvate (PEP)	Carbohydrate	Glycolysis, gluconeogenesis, pyruvate metabolism	<0.0001	<0.0001	1.96
gluconate	Carbohydrate	Nucleotide sugars, pentose metabolism	0.000	< 1e-07	3.03
Isobar: ribulose 5-phosphate, xylulose 5-phosphate	Carbohydrate	Nucleotide sugars, pentose metabolism	< 1e-07	< 1e-07	3.13
ribose	Carbohydrate	Nucleotide sugars, pentose metabolism	< 1e-07	< 1e-07	3.33
ribulose	Carbohydrate	Nucleotide sugars, pentose metabolism	<0.0001	< 1e-07	1.96
ascorbate (Vitamin C)	Cofactors and vitamins	Ascorbate and aldarate metabolism	<0.0001	< 1e-07	5.88
threonate	Cofactors and vitamins	Ascorbate and aldarate metabolism	<0.0001	< 1e-07	2.22
1-methylnicotinamide	Cofactors and vitamins	Nicotinate and nicotinamide metabolism	< 1e-07	< 1e-07	2.94
nicotinamide	Cofactors and vitamins	Nicotinate and nicotinamide metabolism	< 1e-07	< 1e-07	2.70
pantothenate	Cofactors and vitamins	Pantothenate and CoA metabolism	< 1e-07	< 1e-07	2.94
riboflavin (Vitamin B2)	Cofactors and vitamins	Riboflavin metabolism	0.000	< 1e-07	2.17
citrate	Energy	Krebs cycle	0.001	0.001	2.17
fumarate	Energy	Krebs cycle	<0.0001	< 1e-07	2.22
malate	Energy	Krebs cycle	< 1e-07	< 1e-07	4.55
succinylcarnitine	Energy	Krebs cycle	0.000	< 1e-07	2.94
phosphate	Energy	Oxidative phosphorylation	< 1e-07	< 1e-07	3.13
pyrophosphate (PPi)	Energy	Oxidative phosphorylation	<0.0001	< 1e-07	2.70
3-dehydrocarnitine*	Lipid	Carnitine metabolism	<0.0001	< 1e-07	2.56
acetylcarnitine	Lipid	Carnitine metabolism	< 1e-07	< 1e-07	2.04
carnitine	Lipid	Carnitine metabolism	<0.0001	< 1e-07	2.44
deoxycarnitine	Lipid	Carnitine metabolism	< 1e-07	< 1e-07	3.57
hexanoylcarnitine	Lipid	Carnitine metabolism	<0.0001	< 1e-07	2.70
oleoylcarnitine	Lipid	Carnitine metabolism	<0.0001	< 1e-07	3.03
palmitoylcarnitine	Lipid	Carnitine metabolism	<0.0001	< 1e-07	3.23
stearoylcarnitine	Lipid	Carnitine metabolism	< 1e-07	< 1e-07	5.56
dihomo-linolenate (20:3n3 or n6)	Lipid	Essential fatty acid	< 1e-07	< 1e-07	4.35
docosahexaenoate (DHA; 22:6n3)	Lipid	Essential fatty acid	< 1e-07	< 1e-07	3.13
docosapentaenoate (n3 DPA; 22:5n3)	Lipid	Essential fatty acid	< 1e-07	< 1e-07	4.17
docosapentaenoate (n6 DPA, 22:5n6)	Lipid	Essential fatty acid	<0.0001	< 1e-07	2.27
eicosapentaenoate (EPA; 20:5n3)	Lipid	Essential fatty acid	< 1e-07	< 1e-07	2.63
linolenate [alpha or gamma; (18:3n3 or 6)]	Lipid	Essential fatty acid	<0.0001	< 1e-07	2.17
butyrylcarnitine	Lipid	Fatty acid metabolism (also BCAA metabolism)	< 1e-07	< 1e-07	4.17
2-hydroxypalmitate	Lipid	Fatty acid, monohydroxy	< 1e-07	< 1e-07	2.78
4-hydroxyphenylpyruvate	Lipid	Fatty acid, monohydroxy	<0.0001	< 1e-07	1.96
choline phosphate	Lipid	Glycerolipid metabolism	< 1e-07	< 1e-07	2.70
cytidine 5'-diphosphocholine	Lipid	Glycerolipid metabolism	< 1e-07	< 1e-07	8.33
ethanolamine	Lipid	Glycerolipid metabolism	< 1e-07	< 1e-07	4.17
glycerol	Lipid	Glycerolipid metabolism	<0.0001	< 1e-07	2.27
glycerol 3-phosphate (G3P)	Lipid	Glycerolipid metabolism	<0.0001	< 1e-07	2.27
phosphoethanolamine	Lipid	Glycerolipid metabolism	< 1e-07	< 1e-07	9.09
inositol 1-phosphate (I1P)	Lipid	Inositol metabolism	< 1e-07	< 1e-07	4.76
myo-inositol	Lipid	Inositol metabolism	<0.0001	< 1e-07	1.96
scyllo-inositol	Lipid	Inositol metabolism	<0.0001	< 1e-07	2.17
10-nonadecenoate (19:1n9)	Lipid	Long chain fatty acid	< 1e-07	< 1e-07	2.70
adrenate (22:4n6)	Lipid	Long chain fatty acid	< 1e-07	< 1e-07	4.35
arachidonate (20:4n6)	Lipid	Long chain fatty acid	< 1e-07	< 1e-07	4.35
cis-vaccenate (18:1n7)	Lipid	Long chain fatty acid	<0.0001	< 1e-07	2.38
dihomo-linoleate (20:2n6)	Lipid	Long chain fatty acid	< 1e-07	< 1e-07	3.57
docosadienoate (22:2n6)	Lipid	Long chain fatty acid	< 1e-07	< 1e-07	4.55

docosatrienoate (22:3n3)	Lipid	Long chain fatty acid	<0.0001	< 1e-07	4.35
eicosenoate (20:1n9 or 11)	Lipid	Long chain fatty acid	< 1e-07	< 1e-07	3.45
linoleate (18:2n6)	Lipid	Long chain fatty acid	< 1e-07	< 1e-07	1.96
margarate (17:0)	Lipid	Long chain fatty acid	< 1e-07	< 1e-07	2.00
myristoleate (14:1n5)	Lipid	Long chain fatty acid	< 1e-07	< 1e-07	1.96
oleate (18:1n9)	Lipid	Long chain fatty acid	< 1e-07	< 1e-07	2.70
palmitate (16:0)	Lipid	Long chain fatty acid	< 1e-07	< 1e-07	1.96
palmitoleate (16:1n7)	Lipid	Long chain fatty acid	< 1e-07	< 1e-07	2.08
stearidonate (18:4n3)	Lipid	Long chain fatty acid	<0.0001	< 1e-07	2.04
1-oleoylglycerophosphocholine	Lipid	Lysolipid	<0.0001	< 1e-07	4.35
1-oleoylglycerophosphoethanolamine	Lipid	Lysolipid	<0.0001	<0.0001	2.13
1-palmitoylglycerophosphocholine	Lipid	Lysolipid	< 1e-07	< 1e-07	7.14
1-stearoylglycerophosphocholine	Lipid	Lysolipid	< 1e-07	< 1e-07	7.14
1-stearoylglycerophosphoethanolamine	Lipid	Lysolipid	< 1e-07	< 1e-07	4.00
1-stearoylglycerophosphoinositol	Lipid	Lysolipid	<0.0001	< 1e-07	2.78
2-arachidonoylglycerophosphocholine*	Lipid	Lysolipid	<0.0001	< 1e-07	5.00
2-arachidonoylglycerophosphoethanolamine*	Lipid	Lysolipid	< 1e-07	< 1e-07	2.86
2-docosahexaenoylglycerophosphoethanolamine*	Lipid	Lysolipid	<0.0001	< 1e-07	3.45
2-docosapentaenoylglycerophosphoethanolamine*	Lipid	Lysolipid	< 1e-07	< 1e-07	4.35
2-linoleoylglycerophosphocholine*	Lipid	Lysolipid	<0.0001	< 1e-07	2.78
2-linoleoylglycerophosphoethanolamine*	Lipid	Lysolipid	<0.0001	< 1e-07	2.22
2-oleoylglycerophosphocholine*	Lipid	Lysolipid	<0.0001	< 1e-07	3.85
2-oleoylglycerophosphoethanolamine*	Lipid	Lysolipid	<0.0001	< 1e-07	4.00
2-palmitoleoylglycerophosphocholine*	Lipid	Lysolipid	<0.0001	< 1e-07	3.13
2-palmitoylglycerophosphocholine*	Lipid	Lysolipid	<0.0001	< 1e-07	4.17
1-palmitoylplasmenyethanolamine	Lipid	Lysolipid	<0.0001	< 1e-07	4.55
1-oleoylglycerol (1-monoollein)	Lipid	Monoacylglycerol	<0.0001	< 1e-07	5.00
1-palmitoylglycerol (1-monopalmitin)	Lipid	Monoacylglycerol	<0.0001	< 1e-07	3.45
1-stearoylglycerol (1-monostearin)	Lipid	Monoacylglycerol	< 1e-07	< 1e-07	4.55
sphinganine	Lipid	Sphingolipid	<0.0001	< 1e-07	6.25
sphingosine	Lipid	Sphingolipid	< 1e-07	< 1e-07	2.56
palmitoyl sphinomyelin	Lipid	Sphingolipid	< 1e-07	< 1e-07	2.44
hypoxanthine	Nucleotide	Purine metabolism, (hypo)xanthine/inosine containing	< 1e-07	< 1e-07	2.33
xanthosine	Nucleotide	Purine metabolism, (hypo)xanthine/inosine containing	< 1e-07	< 1e-07	2.44
adenosine	Nucleotide	Purine metabolism, adenine containing	<0.0001	< 1e-07	2.78
adenosine 3'-monophosphate (3'-AMP)	Nucleotide	Purine metabolism, adenine containing	< 1e-07	< 1e-07	2.27
N1-methyladenosine	Nucleotide	Purine metabolism, adenine containing	< 1e-07	< 1e-07	2.27
guanine	Nucleotide	Purine metabolism, guanine containing	< 1e-07	< 1e-07	3.03
guanosine	Nucleotide	Purine metabolism, guanine containing	< 1e-07	< 1e-07	3.13
urate	Nucleotide	Purine metabolism, urate metabolism	<0.0001	< 1e-07	6.25
cytidine 5'-monophosphate (5'-CMP)	Nucleotide	Pyrimidine metabolism, cytidine containing	<0.0001	< 1e-07	2.38
5,6-dihydrouracil	Nucleotide	Pyrimidine metabolism, uracil containing	< 1e-07	< 1e-07	2.13
pseudouridine	Nucleotide	Pyrimidine metabolism, uracil containing	< 1e-07	< 1e-07	2.17
uracil	Nucleotide	Pyrimidine metabolism, uracil containing	< 1e-07	< 1e-07	4.55
uridine	Nucleotide	Pyrimidine metabolism, uracil containing	< 1e-07	< 1e-07	2.27
aspartylleucine	Peptide	Dipeptide	<0.0001	< 1e-07	9.09
glycylproline	Peptide	Dipeptide	< 1e-07	< 1e-07	2.04
gamma-glutamylglutamate	Peptide	gamma-glutamyl	<0.0001	< 1e-07	2.50
gamma-glutamylleucine	Peptide	gamma-glutamyl	< 1e-07	< 1e-07	2.56
glycerol 2-phosphate	Xenobiotics	Chemical	<0.0001	< 1e-07	2.04
ergothioneine	Xenobiotics	Plant	< 1e-07	< 1e-07	2.27

Abbreviations: FC: Fold Change; T: tumor; NT: nontumor

Red: Abundant in tumor; Blue: Abundant in nontumor
Metabolites in bold are unique to breast cancer

Supplemental Table 5: Comparison of Tumor and Cancer Specific Metabolites

Metabolite	Super Pathway	Sub Pathway	Liver	Pancreas	Breast
			FC TvsNT	FC TvsNT	FC TvsNT
aspartate	Amino acid	Alanine and aspartate metabolism			1.47
beta-alanine	Amino acid	Alanine and aspartate metabolism	0.48		2.63
N-acetylalanine	Amino acid	Alanine and aspartate metabolism			2.17
N-acetylaspartate (NAA)	Amino acid	Alanine and aspartate metabolism			10.20
N-acetyl-aspartyl-glutamate (NAAG)	Amino acid	Alanine and aspartate metabolism		0.48	2.63
2-aminobutyrate	Amino acid	Butanoate metabolism	0.50		
cystathionine	Amino acid	Cysteine, methionine, SAM, taurine metabolism			5.26
cysteine	Amino acid	Cysteine, methionine, SAM, taurine metabolism	0.31		4.00
cystine	Amino acid	Cysteine, methionine, SAM, taurine metabolism	0.33		4.00
N-acetylmethionine	Amino acid	Cysteine, methionine, SAM, taurine metabolism			3.57
S-adenosylhomocysteine (SAH)	Amino acid	Cysteine, methionine, SAM, taurine metabolism	0.44		2.63
S-adenosylmethionine (SAM)	Amino acid	Cysteine, methionine, SAM, taurine metabolism			1.96
taurine	Amino acid	Cysteine, methionine, SAM, taurine metabolism		2.63	3.57
gamma-aminobutyrate (GABA)	Amino acid	Glutamate metabolism	0.28		
glutamate	Amino acid	Glutamate metabolism			5.88
pyroglutamine*	Amino acid	Glutamate metabolism	0.51		
5-oxoproline	Amino acid	Glutathione metabolism			2.08
cysteine-glutathione disulfide	Amino acid	Glutathione metabolism		4.76	
glutathione, oxidized (GSSG)	Amino acid	Glutathione metabolism		3.85	
glutathione, reduced (GSH)	Amino acid	Glutathione metabolism		3.70	2.56
betaine	Amino acid	Glycine, serine and threonine metabolism			2.50
glycine	Amino acid	Glycine, serine and threonine metabolism			2.94
N-acetylserine	Amino acid	Glycine, serine and threonine metabolism			2.33
N-acetylthreonine	Amino acid	Glycine, serine and threonine metabolism			2.22
serine	Amino acid	Glycine, serine and threonine metabolism			2.38
threonine	Amino acid	Glycine, serine and threonine metabolism			1.96
guanidinoacetate	Amino acid	Guanidino and acetamido metabolism		0.26	
urocanate	Amino acid	Histidine metabolism	2.27		
methylglutaryl carnitine	Amino acid	Lysine metabolism	0.38		
N6-acetyllysine	Amino acid	Lysine metabolism			3.13
3-(4-hydroxyphenyl)lactate	Amino acid	Phenylalanine & tyrosine metabolism			2.94
5-methylthioadenosine (MTA)	Amino acid	Polyamine metabolism	3.45		
putrescine	Amino acid	Polyamine metabolism			4.55
C-glycosyltryptophan*	Amino acid	Tryptophan metabolism		2.00	5.00
kynurenine	Amino acid	Tryptophan metabolism		2.17	3.57
tryptophan	Amino acid	Tryptophan metabolism			2.22
tryptophan betaine	Amino acid	Tryptophan metabolism			2.63
dimethylarginine (SDMA + ADMA)	Amino acid	Urea cycle; arginine-, proline-, metabolism			4.17
ornithine	Amino acid	Urea cycle; arginine-, proline-, metabolism		0.49	
proline	Amino acid	Urea cycle; arginine-, proline-, metabolism			3.13
stachydrine	Amino acid	Urea cycle; arginine-, proline-, metabolism			2.27
trans-4-hydroxyproline	Amino acid	Urea cycle; arginine-, proline-, metabolism			4.35
urea	Amino acid	Urea cycle; arginine-, proline-, metabolism			2.70
2-methylbutyrylcarnitine	Amino acid	Valine, leucine and isoleucine metabolism			2.13
hydroxyisovaleryl carnitine	Amino acid	Valine, leucine and isoleucine metabolism			2.33
isobutyrylcarnitine	Amino acid	Valine, leucine and isoleucine metabolism	0.28		
isovalerylcarnitine	Amino acid	Valine, leucine and isoleucine metabolism	0.53	2.04	
leucine	Amino acid	Valine, leucine and isoleucine metabolism			2.04
tiglyl carnitine	Amino acid	Valine, leucine and isoleucine metabolism	0.48		

valerylcarnitine	Amino acid	Valine, leucine and isoleucine metabolism	3.13		
erythronate*	Carbohydrate	Aminosugars metabolism			4.35
fucose	Carbohydrate	Aminosugars metabolism			2.70
N-acetylglucosamine	Carbohydrate	Aminosugars metabolism			2.38
N-acetylglucosamine 6-phosphate	Carbohydrate	Aminosugars metabolism			2.56
N-acetylmannosamine	Carbohydrate	Aminosugars metabolism	0.44		
N-acetylneuraminic acid	Carbohydrate	Aminosugars metabolism			3.03
fructose	Carbohydrate	Fructose, mannose, galactose, starch, and sucrose metabolism			2.56
maltose	Carbohydrate	Fructose, mannose, galactose, starch, and sucrose metabolism			3.03
maltotetraose	Carbohydrate	Fructose, mannose, galactose, starch, and sucrose metabolism			2.27
maltotriose	Carbohydrate	Fructose, mannose, galactose, starch, and sucrose metabolism		4.00	2.63
mannose	Carbohydrate	Fructose, mannose, galactose, starch, and sucrose metabolism	0.46		2.13
mannose-6-phosphate	Carbohydrate	Fructose, mannose, galactose, starch, and sucrose metabolism			5.88
sorbitol	Carbohydrate	Fructose, mannose, galactose, starch, and sucrose metabolism	0.31		2.17
tagatose	Carbohydrate	Fructose, mannose, galactose, starch, and sucrose metabolism	0.27		
3-phosphoglycerate	Carbohydrate	Glycolysis, gluconeogenesis, pyruvate metabolism			2.13
fructose-6-phosphate	Carbohydrate	Glycolysis, gluconeogenesis, pyruvate metabolism			7.14
glucose	Carbohydrate	Glycolysis, gluconeogenesis, pyruvate metabolism	0.28		2.00
glucose-6-phosphate (G6P)	Carbohydrate	Glycolysis, gluconeogenesis, pyruvate metabolism			8.33
glucuronate	Carbohydrate	Glycolysis, gluconeogenesis, pyruvate metabolism	0.37		
lactate	Carbohydrate	Glycolysis, gluconeogenesis, pyruvate metabolism			4.00
phosphoenolpyruvate (PEP)	Carbohydrate	Glycolysis, gluconeogenesis, pyruvate metabolism			1.96
6-phosphogluconate	Carbohydrate	Nucleotide sugars, pentose metabolism	0.54		
gluconate	Carbohydrate	Nucleotide sugars, pentose metabolism			3.03
Isobar: ribulose 5-phosphate, xylulose 5-phosphate	Carbohydrate	Nucleotide sugars, pentose metabolism			3.13
ribitol	Carbohydrate	Nucleotide sugars, pentose metabolism	0.37		
ribose	Carbohydrate	Nucleotide sugars, pentose metabolism			3.33
ribose 5-phosphate	Carbohydrate	Nucleotide sugars, pentose metabolism	0.39		
ribulose	Carbohydrate	Nucleotide sugars, pentose metabolism			1.96
xylitol	Carbohydrate	Nucleotide sugars, pentose metabolism	0.32		
ascorbate (Vitamin C)	Cofactors and vitamins	Ascorbate and aldarate metabolism			5.88
glucarate (saccharate)	Cofactors and vitamins	Ascorbate and aldarate metabolism	0.48		
gulono-1,4-lactone	Cofactors and vitamins	Ascorbate and aldarate metabolism	0.29		
threonate	Cofactors and vitamins	Ascorbate and aldarate metabolism			2.22
5-methyltetrahydrofolate (5MeTHF)	Cofactors and vitamins	Folate metabolism	0.50		
1-methylnicotinamide	Cofactors and vitamins	Nicotinate and nicotinamide metabolism			2.94
nicotinamide	Cofactors and vitamins	Nicotinate and nicotinamide metabolism	0.24		2.70
nicotinamide adenine dinucleotide (NAD+)	Cofactors and vitamins	Nicotinate and nicotinamide metabolism		0.22	
nicotinamide ribonucleotide (NMN)	Cofactors and vitamins	Nicotinate and nicotinamide metabolism		0.15	
nicotinamide riboside*	Cofactors and vitamins	Nicotinate and nicotinamide metabolism	0.47		
pantothenate	Cofactors and vitamins	Pantothenate and CoA metabolism			2.94
pyridoxal	Cofactors and vitamins	Pyridoxal metabolism	0.50		
flavin adenine dinucleotide (FAD)	Cofactors and vitamins	Riboflavin metabolism	0.41		
riboflavin (Vitamin B2)	Cofactors and vitamins	Riboflavin metabolism			2.17
riboflavin (Vitamin B2)	Cofactors and vitamins	Riboflavin metabolism	0.51		
alpha-tocopherol	Cofactors and vitamins	Tocopherol metabolism	0.32		
pyridoxate	Cofactors and vitamins	Vitamin B6 metabolism	0.44		
citrate	Energy	Krebs cycle		3.13	2.17
fumarate	Energy	Krebs cycle	0.50		2.22
malate	Energy	Krebs cycle	0.42		4.55
succinate	Energy	Krebs cycle		0.42	
succinylcarnitine	Energy	Krebs cycle		0.35	2.94
phosphate	Energy	Oxidative phosphorylation			3.13

pyrophosphate (PPi)	Energy	Oxidative phosphorylation			2.70
glycochenodeoxycholate	Lipid	Bile acid metabolism	0.37		
glycocholate	Lipid	Bile acid metabolism	0.25		
glycoursodeoxycholate	Lipid	Bile acid metabolism	0.37		
taurochenodeoxycholate	Lipid	Bile acid metabolism		0.49	
2-methylmalonyl carnitine	Lipid	Carnitine metabolism	1.96		
3-dehydrocarnitine*	Lipid	Carnitine metabolism			2.56
acetylcarnitine	Lipid	Carnitine metabolism			2.04
carnitine	Lipid	Carnitine metabolism			2.44
decanoylcarnitine	Lipid	Carnitine metabolism		2.08	
deoxycarnitine	Lipid	Carnitine metabolism	2.08		3.57
glutaroyl carnitine	Lipid	Carnitine metabolism	0.40		
hexanoylcarnitine	Lipid	Carnitine metabolism	4.35	2.63	2.70
octanoylcarnitine	Lipid	Carnitine metabolism		2.44	
oleoylcarnitine	Lipid	Carnitine metabolism			3.03
palmitoylcarnitine	Lipid	Carnitine metabolism	3.13		3.23
stearoylcarnitine	Lipid	Carnitine metabolism	3.03		5.56
1,2-dipalmitoylglycerol	Lipid	Diacylglycerol		0.45	
prostaglandin E2	Lipid	Eicosanoid		2.63	
dihomo-linolenate (20:3n3 or n6)	Lipid	Essential fatty acid			4.35
docosahexaenoate (DHA; 22:6n3)	Lipid	Essential fatty acid			3.13
docosapentaenoate (n3 DPA; 22:5n3)	Lipid	Essential fatty acid	0.52		4.17
docosapentaenoate (n6 DPA, 22:5n6)	Lipid	Essential fatty acid	2.17		2.27
eicosapentaenoate (EPA; 20:5n3)	Lipid	Essential fatty acid			2.63
linolenate [alpha or gamma; (18:3n3 or 6)]	Lipid	Essential fatty acid	0.36	0.36	2.17
butyrylcarnitine	Lipid	Fatty acid metabolism (also BCAA metabolism)	13.70	3.13	4.17
17-methylstearate	Lipid	Fatty acid, branched		0.43	
9,10-hydroxyoctadec-12(Z)-enoic acid	Lipid	Fatty acid, dihydroxy		0.40	
palmitate, methyl ester	Lipid	Fatty acid, methyl ester		0.51	
13-HODE + 9-HODE	Lipid	Fatty acid, monohydroxy		0.49	
2-hydroxypalmitate	Lipid	Fatty acid, monohydroxy			2.78
4-hydroxyphenylpyruvate	Lipid	Fatty acid, monohydroxy			1.96
choline	Lipid	Glycerolipid metabolism	2.13		
choline phosphate	Lipid	Glycerolipid metabolism			2.70
cytidine 5'-diphosphocholine	Lipid	Glycerolipid metabolism			8.33
ethanolamine	Lipid	Glycerolipid metabolism			4.17
glycerol	Lipid	Glycerolipid metabolism	0.44	0.39	2.27
glycerol 3-phosphate (G3P)	Lipid	Glycerolipid metabolism		0.35	2.27
glycerophosphorylcholine (GPC)	Lipid	Glycerolipid metabolism	0.38	0.35	
phosphoethanolamine	Lipid	Glycerolipid metabolism	2.13		9.09
phosphopantetheine	Lipid	Glycerolipid metabolism	0.54		
inositol 1-phosphate (I1P)	Lipid	Inositol metabolism			4.76
myo-inositol	Lipid	Inositol metabolism			1.96
scyllo-inositol	Lipid	Inositol metabolism			2.17
10-nonadecenoate (19:1n9)	Lipid	Long chain fatty acid		0.46	2.70
adrenate (22:4n6)	Lipid	Long chain fatty acid			4.35
arachidonate (20:4n6)	Lipid	Long chain fatty acid			4.35
cis-vaccenate (18:1n7)	Lipid	Long chain fatty acid			2.38
dihomo-linoleate (20:2n6)	Lipid	Long chain fatty acid		0.50	3.57
docosadienoate (22:2n6)	Lipid	Long chain fatty acid	2.08		4.55
docosatrenoate (22:3n3)	Lipid	Long chain fatty acid			4.35
eicosenoate (20:1n9 or 11)	Lipid	Long chain fatty acid		0.42	3.45
linoleate (18:2n6)	Lipid	Long chain fatty acid		0.51	1.96

margarate (17:0)	Lipid	Long chain fatty acid		0.48	2.00
myristate (14:0)	Lipid	Long chain fatty acid		0.52	
myristoleate (14:1n5)	Lipid	Long chain fatty acid		0.40	1.96
nonadecanoate (19:0)	Lipid	Long chain fatty acid		0.53	
oleate (18:1n9)	Lipid	Long chain fatty acid			2.70
palmitate (16:0)	Lipid	Long chain fatty acid			1.96
palmitoleate (16:1n7)	Lipid	Long chain fatty acid		0.53	2.08
stearidonate (18:4n3)	Lipid	Long chain fatty acid			2.04
1-oleoylglycerophosphocholine	Lipid	Lysolipid			4.35
1-oleoylglycerophosphoethanolamine	Lipid	Lysolipid			2.13
1-oleoylglycerophosphoinositol*	Lipid	Lysolipid		0.22	
1-palmitoylglycerophosphocholine	Lipid	Lysolipid			7.14
1-palmitoylglycerophosphoinositol*	Lipid	Lysolipid		0.22	
1-palmitoylplasmenylethanolamine	Lipid	Lysolipid			4.55
1-stearoylglycerophosphocholine	Lipid	Lysolipid			7.14
1-stearoylglycerophosphoethanolamine	Lipid	Lysolipid			4.00
1-stearoylglycerophosphoinositol	Lipid	Lysolipid			2.78
2-arachidonoylglycerophosphocholine*	Lipid	Lysolipid			5.00
2-arachidonoylglycerophosphoethanolamine*	Lipid	Lysolipid			2.86
2-docosaehaenoylglycerophosphoethanolamine*	Lipid	Lysolipid			3.45
2-docosapentaenoylglycerophosphoethanolamine*	Lipid	Lysolipid			4.35
2-linoleoylglycerophosphocholine*	Lipid	Lysolipid			2.78
2-linoleoylglycerophosphoethanolamine*	Lipid	Lysolipid			2.22
2-oleoylglycerophosphocholine*	Lipid	Lysolipid			3.85
2-oleoylglycerophosphoethanolamine*	Lipid	Lysolipid			4.00
2-palmitoleoylglycerophosphocholine*	Lipid	Lysolipid			3.13
2-palmitoylglycerophosphocholine*	Lipid	Lysolipid			4.17
5-dodecenoate (12:1n7)	Lipid	Medium chain fatty acid		0.51	
laurate (12:0)	Lipid	Medium chain fatty acid		0.47	
1-docosaehaenoylglycerol (1-monodocosaehaenoin)	Lipid	Monoacylglycerol		0.31	
1-myristoylglycerol (1-monomyristin)	Lipid	Monoacylglycerol		0.09	
1-oleoylglycerol (1-monoolein)	Lipid	Monoacylglycerol		0.33	5.00
1-palmitoylglycerol (1-monopalmitin)	Lipid	Monoacylglycerol		0.32	3.45
1-pentadecanoylglycerol (1-monopentadecanoin)	Lipid	Monoacylglycerol		0.34	
1-stearoylglycerol (1-monostearin)	Lipid	Monoacylglycerol		0.24	4.55
2-linoleoylglycerol (2-monolinolein)	Lipid	Monoacylglycerol		0.22	
2-myristoylglycerol (2-monomyristin)	Lipid	Monoacylglycerol		0.18	
2-oleoylglycerol (2-monoolein)	Lipid	Monoacylglycerol		0.51	
2-palmitoylglycerol (2-monopalmitin)	Lipid	Monoacylglycerol		0.13	
palmitoyl sphingomyelin	Lipid	Sphingolipid			2.44
sphinganine	Lipid	Sphingolipid			6.25
sphingosine	Lipid	Sphingolipid			2.56
stearoyl sphingomyelin	Lipid	Sphingolipid		0.50	
7-beta-hydroxycholesterol	Lipid	Sterol/Steroid		2.08	
hypoxanthine	Nucleotide	Purine metabolism, (hypo)xanthine/inosine containing			2.33
xanthosine	Nucleotide	Purine metabolism, (hypo)xanthine/inosine containing		0.18	2.44
adenine	Nucleotide	Purine metabolism, adenine containing		2.50	
adenosine	Nucleotide	Purine metabolism, adenine containing			2.78
adenosine 2'-monophosphate (2'-AMP)	Nucleotide	Purine metabolism, adenine containing		0.39	
adenosine 3',5'-diphosphate	Nucleotide	Purine metabolism, adenine containing		0.37	
adenosine 3'-monophosphate (3'-AMP)	Nucleotide	Purine metabolism, adenine containing		0.39	
adenosine 3'-monophosphate (3'-AMP)	Nucleotide	Purine metabolism, adenine containing			2.27
adenosine 5'-monophosphate (AMP)	Nucleotide	Purine metabolism, adenine containing		0.30	

N1-methyladenosine	Nucleotide	Purine metabolism, adenine containing			2.27
guanine	Nucleotide	Purine metabolism, guanine containing			3.03
guanosine	Nucleotide	Purine metabolism, guanine containing			3.13
urate	Nucleotide	Purine metabolism, urate metabolism	0.47		6.25
cytidine	Nucleotide	Pyrimidine metabolism, cytidine containing		0.38	
cytidine 5'-monophosphate (5'-CMP)	Nucleotide	Pyrimidine metabolism, cytidine containing			2.38
5,6-dihydrouracil	Nucleotide	Pyrimidine metabolism, uracil containing	3.57		2.13
pseudouridine	Nucleotide	Pyrimidine metabolism, uracil containing			2.17
uracil	Nucleotide	Pyrimidine metabolism, uracil containing			4.55
uridine	Nucleotide	Pyrimidine metabolism, uracil containing			2.27
aspartylleucine	Peptide	Dipeptide			9.09
glycylproline	Peptide	Dipeptide			2.04
isoleucylisoleucine	Peptide	Dipeptide		3.23	
pro-hydroxy-pro	Peptide	Dipeptide		2.22	
threonylphenylalanine	Peptide	Dipeptide		2.56	
gamma-glutamylglutamate	Peptide	gamma-glutamyl	0.27		2.50
gamma-glutamylleucine	Peptide	gamma-glutamyl			2.56
gamma-glutamylglutamine	Peptide	g-glutamyl	0.30		
gamma-glutamylmethionine*	Peptide	g-glutamyl	0.42		
gamma-glutamyltyrosine	Peptide	g-glutamyl	0.53		
VGAHAGEYGAEALER*	Peptide	Polypeptide	0.23		
hippurate	Xenobiotics	Benzoate metabolism	0.41		
glycerol 2-phosphate	Xenobiotics	Chemical	0.25		2.04
N-ethylglycinexylidide*	Xenobiotics	Drug		0.53	
ergothioneine	Xenobiotics	Plant			2.27
erythritol	Xenobiotics	Sugar, sugar substitute, starch	0.47		
galacturonate	Xenobiotics	Sugar, sugar substitute, starch	0.49		

Abbreviations: FC: Fold Change; T: tumor; NT: nontumor

Red: Abundant in tumor; Blue: Abundant in nontumor

Metabolites in bold are unique

Supplemental Table 6: Tumor and Cancer Specific Metabolites

LIVER*	TUMOR**	NONTUMOR**	FC***
urocanate	40659.08	18028.14	2.26
phosphopantetheine	31849.95	48295.13	0.66
5-methyltetrahydrofolate (5MeTHF)	7141.31	14246.60	0.50
galacturonate	265826.73	539625.87	0.49
nicotinamide riboside*	3165759.00	6702463.37	0.47
glutaroyl carnitine	64350.48	160229.84	0.40
adenosine 3',5'-diphosphate	26555.38	71919.40	0.37
gulono-1,4-lactone	104870.79	360242.78	0.29
tagatose	104964.12	390381.91	0.27

PANCREAS	TUMOR	NONTUMOR	FC
isoleucylleucine	48932.50	15329.26	3.19
prostaglandin E2	9370.14	3596.63	2.61
pro-hydroxy-pro	324715.29	144824.62	2.24
decanoylcarnitine	48411.18	23244.56	2.08
nonadecanoate (19:0)	231055.77	440188.07	0.52
palmitate, methyl ester	44492.64	88156.48	0.50
13-HODE + 9-HODE	355554.34	725568.67	0.49
taurodeoxycholate	3676.80	7568.63	0.49
17-methylstearate	99147.01	229072.08	0.43
9,10-hydroxyoctadec-12(Z)-enoic acid	15689.83	39399.28	0.40
1-pentadecanoylglycerol (1-monopentadecanoin)	17550.71	51064.91	0.34
1-docosahexaenoylglycerol (1-monodocosahexaenoin)	7733.67	24589.60	0.31
guanidinoacetate	32019.91	124774.01	0.26
2-linoleoylglycerol (2-monolinolein)	10234.91	47673.76	0.21
2-myristoylglycerol (2-monomyristin)	31612.10	174590.85	0.18
1-myristoylglycerol (1-monomyristin)	108955.66	1242653.04	0.09

BREAST	TUMOR	NONTUMOR	FC
2-docosahexaenoylglycerophosphoethanolamine*	145964.86	42545.76	3.43
N6-acetyllysine	87503.55	27750.20	3.15
1-methylnicotinamide	112630.05	38100.52	2.96
pyrophosphate (PPi)	30727.21	11347.00	2.71
1-palmitoylplasmylethanolamine	65251.76	25597.64	2.55
palmitoyl sphinomyelin	1853678.99	756591.68	2.45
hydroxyisovaleroyl carnitine	71642.63	30895.24	2.32
threonate	19053.90	8615.93	2.21
S-adenosylmethionine (SAM)	14091.79	7238.30	1.95

* Metabolites are ordered from most abundant in tumor to least abundant in tumor

** The relative abundance in tumor or nontumor tissue is shown (mean value)

*** FC: Fold Change (Tumor versus Nontumor abundance)

Supplemental Table 7: Differentially abundant metabolites in early stage liver cancer

Metabolite	Super Pathway	Sub Pathway	Parametric p-value	Permutation p-value	FC TvsNT
N-acetylasparagine	Amino acid	Alanine and aspartate metabolism	0.029	0.063	1.89
N-acetylaspartate (NAA)	Amino acid	Alanine and aspartate metabolism	0.031	0.031	1.61
cysteine	Amino acid	Cysteine, methionine, SAM, taurine metabolism	0.009	0.012	0.37
S-adenosylhomocysteine (SAH)	Amino acid	Cysteine, methionine, SAM, taurine metabolism	0.012	0.018	0.47
gamma-aminobutyrate (GABA)	Amino acid	Glutamate metabolism	0.043	0.051	0.43
serine	Amino acid	Glycine, serine and threonine metabolism	0.040	0.031	1.64
urocanate	Amino acid	Histidine metabolism	0.033	0.125	2.04
phenylacetylglutamine	Amino acid	Phenylalanine & tyrosine metabolism	0.006	0.063	0.40
5-methylthioadenosine (MTA)	Amino acid	Polyamine metabolism	0.012	0.016	2.86
kynurenine	Amino acid	Tryptophan metabolism	0.014	0.020	2.27
isobutyrylcarnitine	Amino acid	Valine, leucine and isoleucine metabolism	0.005	0.010	0.32
valerylcarnitine	Amino acid	Valine, leucine and isoleucine metabolism	0.004	0.008	5.56
N-acetylmannosamine	Carbohydrate	Aminosugars metabolism	0.050	0.043	0.55
mannose	Carbohydrate	Fructose, mannose, galactose, starch, and sucrose metabolism	0.013	0.014	0.53
sorbitol	Carbohydrate	Fructose, mannose, galactose, starch, and sucrose metabolism	0.002	0.004	0.44
tagatose	Carbohydrate	Fructose, mannose, galactose, starch, and sucrose metabolism	0.018	0.016	0.27
glucose	Carbohydrate	Glycolysis, gluconeogenesis, pyruvate metabolism	0.002	0.002	0.49
glucuronate	Carbohydrate	Glycolysis, gluconeogenesis, pyruvate metabolism	<0.0001	0.002	0.35
Isobar: fructose 1,6-diphosphate, glucose 1,6-6-phosphogluconate	Carbohydrate	Glycolysis, gluconeogenesis, pyruvate metabolism	0.030	0.035	2.38
ribitol	Carbohydrate	Nucleotide sugars, pentose metabolism	0.011	0.031	0.44
ribose 5-phosphate	Carbohydrate	Nucleotide sugars, pentose metabolism	0.038	0.041	0.42
UDP-glucose	Carbohydrate	Nucleotide sugars, pentose metabolism	0.030	0.063	0.45
xylitol	Carbohydrate	Nucleotide sugars, pentose metabolism	0.013	0.063	0.45
glucarate (saccharate)	Carbohydrate	Nucleotide sugars, pentose metabolism	0.021	0.027	0.38
gulono-1,4-lactone	Cofactors and vitamins	Ascorbate and aldarate metabolism	<0.0001	0.002	0.35
nicotinamide	Cofactors and vitamins	Ascorbate and aldarate metabolism	0.007	0.010	0.29
nicotinamide adenine dinucleotide reduced	Cofactors and vitamins	Nicotinate and nicotinamide metabolism	0.002	0.063	0.22
nicotinamide riboside*	Cofactors and vitamins	Nicotinate and nicotinamide metabolism	0.026	0.125	0.34
phosphopantetheine	Cofactors and vitamins	Nicotinate and nicotinamide metabolism	<0.0001	0.002	0.52
flavin adenine dinucleotide (FAD)	Cofactors and vitamins	Pantothenate and CoA metabolism	0.020	0.063	0.44
alpha-tocopherol	Cofactors and vitamins	Riboflavin metabolism	0.014	0.016	0.49
malate	Cofactors and vitamins	Tocopherol metabolism	0.024	0.094	0.40
2-methylmalonyl carnitine	Energy	Krebs cycle	0.001	0.004	0.51
3-dehydrocarnitine*	Lipid	Carnitine metabolism	0.008	0.020	2.33
butyrylcarnitine	Lipid	Carnitine metabolism	0.007	0.012	1.85
deoxycarnitine	Lipid	Carnitine metabolism	0.001	0.004	12.82
glutaroyl carnitine	Lipid	Carnitine metabolism	0.002	0.004	2.86
hexanoylcarnitine	Lipid	Carnitine metabolism	0.021	0.025	0.46
docosapentaenoate (n3 DPA; 22:5n3)	Lipid	Carnitine metabolism	0.007	0.006	4.76
eicosapentaenoate (EPA; 20:5n3)	Lipid	Essential fatty acid	0.020	0.016	0.53
linolenate [alpha or gamma; (18:3n3 or 6)]	Lipid	Essential fatty acid	0.026	0.016	0.53
sedoheptulose-7-phosphate	Lipid	Essential fatty acid	0.049	0.039	0.42
choline	Lipid	Fatty acid, dicarboxylate	0.004	0.063	0.35
glycerol	Lipid	Glycerolipid metabolism	0.030	0.031	2.27
glycerophosphorylcholine (GPC)	Lipid	Glycerolipid metabolism	0.022	0.029	0.43
phosphoethanolamine	Lipid	Glycerolipid metabolism	0.011	0.010	0.31
scyllo-inositol	Lipid	Glycerolipid metabolism	<0.0001	0.002	2.63
adrenate (22:4n6)	Lipid	Inositol metabolism	<0.0001	0.004	0.51
	Lipid	Long chain fatty acid	0.010	0.031	1.96

dihomo-linoleate (20:2n6)	Lipid	Long chain fatty acid	0.020	0.094	2.08
docosadienoate (22:2n6)	Lipid	Long chain fatty acid	0.003	0.031	3.33
docosapentaenoate (n6 DPA, 22:5n6)	Lipid	Long chain fatty acid	0.004	0.008	2.63
docosatrienoate (22:3n3)	Lipid	Long chain fatty acid	0.016	0.094	3.45
eicosenoate (20:1n9 or 11)	Lipid	Long chain fatty acid	0.008	0.063	2.94
1-oleoylglycerophosphoinositol*	Lipid	Lysolipid	0.025	0.063	2.17
2-arachidonoylglycerophosphocholine*	Lipid	Lysolipid	0.016	0.031	0.42
2-linoleoylglycerophosphocholine*	Lipid	Lysolipid	0.042	0.125	0.43
caproate (6:0)	Lipid	Medium chain fatty acid	0.028	0.033	1.69
phytosphingosine	Lipid	Sphingolipid	0.027	0.125	0.38
sphingosine	Lipid	Sphingolipid	0.028	0.031	0.53
7-beta-hydroxycholesterol	Lipid	Sterol/Steroid	0.032	0.033	2.22
squalene	Lipid	Sterol/Steroid	0.012	0.031	0.44
xanthosine	Nucleotide	Purine metabolism, (hypo)xanthine/inosine containing	0.001	0.006	0.23
adenine	Nucleotide	Purine metabolism, adenine containing	0.019	0.023	2.00
adenosine	Nucleotide	Purine metabolism, adenine containing	0.045	0.047	0.51
adenosine 2'-monophosphate (2'-AMP)	Nucleotide	Purine metabolism, adenine containing	0.010	0.014	0.43
adenosine 3',5'-diphosphate	Nucleotide	Purine metabolism, adenine containing	0.003	0.063	0.27
adenosine 5'-monophosphate (AMP)	Nucleotide	Purine metabolism, adenine containing	0.032	0.033	0.31
3-aminoisobutyrate	Nucleotide	Pyrimidine metabolism, thymine containing; Valine, leucine and isoleucine metabolism/	0.013	0.094	3.33
5,6-dihydrouracil	Nucleotide	Pyrimidine metabolism, uracil containing	0.004	0.006	3.85
beta-alanine	Nucleotide	Pyrimidine metabolism, uracil containing	0.009	0.014	0.47
aspartylleucine	Peptide	Dipeptide	0.024	0.023	0.38
glycylleucine	Peptide	Dipeptide	0.012	0.016	0.50
lysylleucine	Peptide	Dipeptide	0.031	0.063	0.52
prolylleucine	Peptide	Dipeptide	0.001	0.004	0.51
gamma-glutamylglutamate	Peptide	g-glutamyl	0.005	0.010	0.22
gamma-glutamylglutamine	Peptide	g-glutamyl	0.031	0.039	0.18
gamma-glutamylmethionine*	Peptide	g-glutamyl	0.001	0.004	0.29
gamma-glutamyltyrosine	Peptide	g-glutamyl	<0.0001	0.002	0.54
cysteine-glutathione disulfide	Peptide	Glutathione metabolism	0.026	0.035	0.20
glutathione, oxidized (GSSG)	Peptide	Glutathione metabolism	0.011	0.063	0.18
glutathione, reduced (GSH)	Peptide	Glutathione metabolism	<0.0001	0.031	0.03
ophthalmate*	Peptide	Glutathione metabolism	0.001	0.031	0.04
S-methylglutathione	Peptide	Glutathione metabolism	0.002	0.063	0.16
VGAHAGEYGAEALER*	Peptide	Polypeptide	0.012	0.006	0.31
hippurate	Xenobiotics	Benzoate metabolism	0.009	0.063	0.26
glycerol 2-phosphate	Xenobiotics	Chemical	0.001	0.004	0.26
erythritol	Xenobiotics	Sugar, sugar substitute, starch	<0.0001	0.002	0.39
galacturonate	Xenobiotics	Sugar, sugar substitute, starch	<0.0001	0.002	0.38

Abbreviations: FC: Fold Change; T: tumor; NT: nontumor

Red: Abundant in tumor; Blue: Abundant in nontumor

Metabolites in bold are unique to liver cancer

Supplemental Table 8: Differentially abundant metabolites in early stage pancreas cancer

Metabolite	Super Pathway	Sub Pathway	Parametric p-value	Permutation p-value	FC TvsNT
aspartate	Amino acid	Alanine and aspartate metabolism	0.004	0.016	0.42
2-aminobutyrate	Amino acid	Butanoate metabolism	0.041	0.047	0.53
cystine	Amino acid	Cysteine, methionine, SAM, taurine metabolism	0.007	0.016	0.48
N-acetyl-aspartyl-glutamate (NAAG)	Amino acid	Glutamate metabolism	0.033	0.047	0.41
kynurenine	Amino acid	Tryptophan metabolism	0.007	0.016	2.78
isovalerylcarnitine	Amino acid	Valine, leucine and isoleucine metabolism	0.022	0.016	3.03
nicotinamide ribonucleotide (NMN)	Cofactors and vitamins	Nicotinate and nicotinamide metabolism	0.011	0.031	0.05
pantothenate	Cofactors and vitamins	Pantothenate and CoA metabolism	0.009	0.016	0.51
alpha-ketoglutarate	Energy	Krebs cycle	0.035	0.031	2.13
fumarate	Energy	Krebs cycle	0.048	0.047	0.51
hexanoylcarnitine	Lipid	Carnitine metabolism	0.009	0.031	2.70
octanoylcarnitine	Lipid	Carnitine metabolism	0.015	0.016	2.13
decanoylcarnitine	Lipid	Carnitine metabolism	0.028	0.063	1.96
succinylcarnitine	Lipid	Carnitine metabolism	0.037	0.063	0.28
butyrylcarnitine	Lipid	Fatty acid metabolism (also BCAA metabolism)	0.022	0.047	2.63
glycerol 3-phosphate (G3P)	Lipid	Glycerolipid metabolism	0.021	0.016	0.30
docosatrienoate (22:3n3)	Lipid	Long chain fatty acid	0.045	0.016	0.39
1-palmitoylglycerophosphoethanolamine	Lipid	Lysolipid	0.001	0.016	0.52
1-oleoylglycerophosphoethanolamine	Lipid	Lysolipid	0.011	0.016	0.48
1-oleoylglycerophosphoinositol*	Lipid	Lysolipid	0.010	0.016	0.38
stearoyl sphingomyelin	Lipid	Sphingolipid	0.034	0.047	0.45
cytidine	Nucleotide	Pyrimidine metabolism, cytidine containing	0.020	0.031	0.24
phenol red	Xenobiotics	Chemical	0.047	0.031	2.04

Abbreviations: FC: Fold Change; T: tumor; NT: nontumor

Red: Abundant in tumor; Blue: Abundant in nontumor

Metabolites in bold are unique to pancreatic cancer

Supplemental Table 9: Differentially abundant metabolites in early stage breast cancer

Metabolite	Super Pathway	Sub Pathway	Parametric p-value	Permutation p-value	FC TvsNT
beta-alanine	Amino acid	Alanine and aspartate metabolism	0.046	0.063	2.17
N-acetylaspartate (NAA)	Amino acid	Alanine and aspartate metabolism	0.036	0.125	6.67
N-acetylmethionine	Amino acid	Cysteine, methionine, SAM, taurine metabolism	0.019	0.031	2.63
S-adenosylhomocysteine (SAH)	Amino acid	Cysteine, methionine, SAM, taurine metabolism	0.021	0.063	1.96
taurine	Amino acid	Cysteine, methionine, SAM, taurine metabolism	0.042	0.063	2.70
betaine	Amino acid	Glycine, serine and threonine metabolism	0.034	0.031	2.38
N-acetylthreonine	Amino acid	Glycine, serine and threonine metabolism	0.041	0.063	2.08
tryptophan betaine	Amino acid	Tryptophan metabolism	0.032	0.063	2.04
pyrophosphate (PPi)	Energy	Oxidative phosphorylation	0.040	0.063	10.00
3-hydroxybutyrate (BHBA)	Lipid	Ketone bodies	0.019	0.031	2.17
ergothioneine	Xenobiotics	Plant	0.049	0.125	1.85

Abbreviations: FC: Fold Change; T: tumor; NT: nontumor

Red: Abundant in tumor; Blue: Abundant in nontumor

Metabolites in bold are unique to breast cancer

Supplemental Table 10: Comparison of Tumor and Cancer Specific Metabolites at Early-Stage

Metabolite	Super Pathway	Sub Pathway	Liver	Pancreas	Breast
			FC TvsNT	FC TvsNT	FC TvsNT
aspartate	Amino acid	Alanine and aspartate metabolism		0.42	
N-acetylasparagine	Amino acid	Alanine and aspartate metabolism	1.89		
N-acetylaspartate (NAA)	Amino acid	Alanine and aspartate metabolism	1.61		6.67
2-aminobutyrate	Amino acid	Butanoate metabolism		0.53	
cysteine	Amino acid	Cysteine, methionine, SAM, taurine metabolism	0.37		
cystine	Amino acid	Cysteine, methionine, SAM, taurine metabolism		0.48	
N-acetylmethionine	Amino acid	Cysteine, methionine, SAM, taurine metabolism			2.63
S-adenosylhomocysteine (SAH)	Amino acid	Cysteine, methionine, SAM, taurine metabolism	0.47		1.96
taurine	Amino acid	Cysteine, methionine, SAM, taurine metabolism			2.70
gamma-aminobutyrate (GABA)	Amino acid	Glutamate metabolism	0.43		
N-acetyl-aspartyl-glutamate (NAAG)	Amino acid	Glutamate metabolism		0.41	
betaine	Amino acid	Glycine, serine and threonine metabolism			2.38
N-acetylthreonine	Amino acid	Glycine, serine and threonine metabolism			2.08
serine	Amino acid	Glycine, serine and threonine metabolism	1.64		
urocanate	Amino acid	Histidine metabolism	2.04		
phenylacetylglutamine	Amino acid	Phenylalanine & tyrosine metabolism	0.40		
5-methylthioadenosine (MTA)	Amino acid	Polyamine metabolism	2.86		
kynurenine	Amino acid	Tryptophan metabolism	2.27	2.78	
tryptophan betaine	Amino acid	Tryptophan metabolism			2.04
isobutyrylcarnitine	Amino acid	Valine, leucine and isoleucine metabolism	0.32		
isovalerylcarnitine	Amino acid	Valine, leucine and isoleucine metabolism		3.03	
valerylcarnitine	Amino acid	Valine, leucine and isoleucine metabolism	5.56		
N-acetylmannosamine	Carbohydrate	Aminosugars metabolism	0.55		
mannose	Carbohydrate	Fructose, mannose, galactose, starch, and sucrose metabolism	0.53		
sorbitol	Carbohydrate	Fructose, mannose, galactose, starch, and sucrose metabolism	0.44		
tagatose	Carbohydrate	Fructose, mannose, galactose, starch, and sucrose metabolism	0.27		
glucose	Carbohydrate	Glycolysis, gluconeogenesis, pyruvate metabolism	0.49		
glucuronate	Carbohydrate	Glycolysis, gluconeogenesis, pyruvate metabolism	0.35		
Isobar: fructose 1,6-diphosphate, glucose 1,6-	Carbohydrate	Glycolysis, gluconeogenesis, pyruvate metabolism	2.38		
6-phosphogluconate	Carbohydrate	Nucleotide sugars, pentose metabolism	0.44		
ribitol	Carbohydrate	Nucleotide sugars, pentose metabolism	0.42		
ribose 5-phosphate	Carbohydrate	Nucleotide sugars, pentose metabolism	0.45		
UDP-glucose	Carbohydrate	Nucleotide sugars, pentose metabolism	0.45		
xylitol	Carbohydrate	Nucleotide sugars, pentose metabolism	0.38		
glucarate (saccharate)	Cofactors and vitamins	Ascorbate and aldarate metabolism	0.35		
gulono-1,4-lactone	Cofactors and vitamins	Ascorbate and aldarate metabolism	0.29		
nicotinamide	Cofactors and vitamins	Nicotinate and nicotinamide metabolism	0.22		
nicotinamide adenine dinucleotide reduced (NADH)	Cofactors and vitamins	Nicotinate and nicotinamide metabolism	0.34		
nicotinamide ribonucleotide (NMN)	Cofactors and vitamins	Nicotinate and nicotinamide metabolism		0.05	
nicotinamide riboside*	Cofactors and vitamins	Nicotinate and nicotinamide metabolism	0.52		
pantothenate	Cofactors and vitamins	Pantothenate and CoA metabolism		0.51	
phosphopantetheine	Cofactors and vitamins	Pantothenate and CoA metabolism	0.44		
flavin adenine dinucleotide (FAD)	Cofactors and vitamins	Riboflavin metabolism	0.49		
alpha-tocopherol	Cofactors and vitamins	Tocopherol metabolism	0.40		
alpha-ketoglutarate	Energy	Krebs cycle		2.13	
fumarate	Energy	Krebs cycle		0.51	
malate	Energy	Krebs cycle	0.51		
pyrophosphate (PPi)	Energy	Oxidative phosphorylation			10.00
2-methylmalonyl carnitine	Lipid	Carnitine metabolism	2.33		
3-dehydrocarnitine*	Lipid	Carnitine metabolism	1.85		

butyrylcarnitine	Lipid	Carnitine metabolism	12.82	2.63	
decanoylcarnitine	Lipid	Carnitine metabolism		1.96	
deoxycarnitine	Lipid	Carnitine metabolism	2.86		
glutaroyl carnitine	Lipid	Carnitine metabolism	0.46		
hexanoylcarnitine	Lipid	Carnitine metabolism	4.76	2.70	
octanoylcarnitine	Lipid	Carnitine metabolism		2.13	
succinylcarnitine	Lipid	Carnitine metabolism		0.28	
docosapentaenoate (n3 DPA; 22:5n3)	Lipid	Essential fatty acid	0.53		
eicosapentaenoate (EPA; 20:5n3)	Lipid	Essential fatty acid	0.53		
linolenate [alpha or gamma; (18:3n3 or 6)]	Lipid	Essential fatty acid	0.42		
sedoheptulose-7-phosphate	Lipid	Fatty acid, dicarboxylate	0.35		
choline	Lipid	Glycerolipid metabolism	2.27		
glycerol	Lipid	Glycerolipid metabolism	0.43		
glycerol 3-phosphate (G3P)	Lipid	Glycerolipid metabolism		0.30	
glycerophosphorylcholine (GPC)	Lipid	Glycerolipid metabolism	0.31		
phosphoethanolamine	Lipid	Glycerolipid metabolism	2.63		
scyllo-inositol	Lipid	Inositol metabolism	0.51		
3-hydroxybutyrate (BHBA)	Lipid	Ketone bodies			2.17
adrenate (22:4n6)	Lipid	Long chain fatty acid	1.96		
dihomo-linoleate (20:2n6)	Lipid	Long chain fatty acid	2.08		
docosadienoate (22:2n6)	Lipid	Long chain fatty acid	3.33		
docosapentaenoate (n6 DPA, 22:5n6)	Lipid	Long chain fatty acid	2.63		
docosatrienoate (22:3n3)	Lipid	Long chain fatty acid	3.45	0.39	
eicosenoate (20:1n9 or 11)	Lipid	Long chain fatty acid	2.94		
1-oleoylglycerophosphoethanolamine	Lipid	Lysolipid		0.48	
1-oleoylglycerophosphoinositol*	Lipid	Lysolipid	2.17	0.38	
1-palmitoylglycerophosphoethanolamine	Lipid	Lysolipid		0.52	
2-arachidonoylglycerophosphocholine*	Lipid	Lysolipid	0.42		
2-linoleoylglycerophosphocholine*	Lipid	Lysolipid	0.43		
caproate (6:0)	Lipid	Medium chain fatty acid	1.69		
phytosphingosine	Lipid	Sphingolipid	0.38		
sphingosine	Lipid	Sphingolipid	0.53		
stearoyl sphingomyelin	Lipid	Sphingolipid		0.45	
7-beta-hydroxycholesterol	Lipid	Sterol/Steroid	2.22		
squalene	Lipid	Sterol/Steroid	0.44		
xanthosine	Nucleotide	Purine metabolism, (hypo)xanthine/inosine containing	0.23		
adenine	Nucleotide	Purine metabolism, adenine containing	2.00		
adenosine	Nucleotide	Purine metabolism, adenine containing	0.51		
adenosine 2'-monophosphate (2'-AMP)	Nucleotide	Purine metabolism, adenine containing	0.43		
adenosine 3',5'-diphosphate	Nucleotide	Purine metabolism, adenine containing	0.27		
adenosine 5'-monophosphate (AMP)	Nucleotide	Purine metabolism, adenine containing	0.31		
cytidine	Nucleotide	Pyrimidine metabolism, cytidine containing		0.24	
3-aminoisobutyrate	Nucleotide	Pyrimidine metabolism, thymine containing; Valine, leucine and isoleucine metabolism/	3.33		
5,6-dihydrouracil	Nucleotide	Pyrimidine metabolism, uracil containing	3.85		
beta-alanine	Nucleotide	Pyrimidine metabolism, uracil containing	0.47		
aspartylleucine	Peptide	Dipeptide	0.38		2.17
glycylleucine	Peptide	Dipeptide	0.50		
lysylleucine	Peptide	Dipeptide	0.52		
prolylleucine	Peptide	Dipeptide	0.51		
gamma-glutamylglutamate	Peptide	g-glutamyl	0.22		
gamma-glutamylglutamine	Peptide	g-glutamyl	0.18		
gamma-glutamylmethionine*	Peptide	g-glutamyl	0.29		
gamma-glutamyltyrosine	Peptide	g-glutamyl	0.54		

cysteine-glutathione disulfide	Peptide	Glutathione metabolism	0.20		
glutathione, oxidized (GSSG)	Peptide	Glutathione metabolism	0.18		
glutathione, reduced (GSH)	Peptide	Glutathione metabolism	0.03		
ophthalmate*	Peptide	Glutathione metabolism	0.04		
S-methylglutathione	Peptide	Glutathione metabolism	0.16		
VGAHAGEYGAEALER*	Peptide	Polypeptide	0.31		
hippurate	Xenobiotics	Benzoate metabolism	0.26		
glycerol 2-phosphate	Xenobiotics	Chemical	0.26		
phenol red	Xenobiotics	Chemical		2.04	
ergothioneine	Xenobiotics	Plant			1.85
erythritol	Xenobiotics	Sugar, sugar substitute, starch	0.39		
galacturonate	Xenobiotics	Sugar, sugar substitute, starch	0.38		

Abbreviations: FC: Fold Change; T: tumor; NT: nontumor

Red: Abundant in tumor; Blue: Abundant in nontumor

Metabolites in bold are unique