

Supplemental Tables

Excel file

Tab 01

A list of metabolites identified in the metabolomic analysis.

Tab 02

A list of metabolites with the most significant alterations between BPH1 and PC-3 cells.

Tab 03

Data used to generate the volcano plot for the comparison of BPH1 and PC-3 cells.

[IS] d4-succinate [10.462]
[011] Pyruvic acid [6.707]
[012] L-Lactic acid [6.845]
[051] L-Alanine 1 [7.471]
[052] L-Valine 2 [9.154]
[200] Phosphate [9.9]
[053] L-Leucine 2 [9.951]
[190] Glycerol [9.947]
[054] L-Isoleucine 2 [10.232]
[76] L-threonine 1 [10.231]
[050] Glycine [10.464]
[017] Succinic acid [10.517]
[018] Fumaric acid [10.949]
[059] L-Serine 2 [11.184]
[060] L-Threonine 2 [11.475]
[210] Thymine [11.611]
[074] Beta-Alanine 1 [12.058]
[78] Iminodiacetic acid 1 [12.502]
[217] 1-methyl nicotinamide 1 [12.752]
[019] D-Malic acid [12.810]
[118] D-threitol [12.971]
[x] salicylic acid [13.061]
[062] L-Methionine 2 [13.206]
[065] L-Aspartic acid 2 [13.225]
[070] Pyroglutamic acid [13.236]
[056] L-Phenylalanine 1 [13.564]
[221] Creatinine [13.649]
[252] 2-Hydroxyglutaric acid
[301] Hypotaurine [14.134]
[066] L-Glutamic acid 2 [14.421]
[x] ribonic acid-gamma-lactone 1 [15.077]
[x] 1,6-anhydro-glucose [15.352]
[191] glycerol 3-phosphate [16.085]
[194] O-Phosphoethanolamine [16.261]
[008] 3-Phosphoglyceric acid [16.525]
[206] Hypoxanthine 1 [16.472]
[013] Citric acid [16.646]
[015] Isocitric acid [16.614]
[110] alpha-D-glucosamine 1-phosphate [16.662]
[158] Myristic acid [16.919]
[x] methyl-beta-D-galactopyranoside [16.967]
[209] Adenine [17.106]
[100] D-Fructose 1 [17.213]
[x] gluconic acid lactone 1 [17.337]
[057] L-Tyrosine 1 [17.379]
[111] D-Galactosamine 3 [17.557]
[001] D-glucose 2 [17.660]
[223] L-Ascorbic acid [17.975]

Krebs cycle metabolites (8)

[IS] d4-succinate [10.462]
[011] Pyruvic acid [6.707]
[012] L-Lactic acid [6.845]
[013] Citric acid [16.646]
[015] Isocitric acid [16.614]
[017] Succinic acid [10.517]
[018] Fumaric acid [10.949]
[019] D-Malic acid [12.810]

Nucleotides (7)

[206] Hypoxanthine 1 [16.472]
[207] Adenosine [23.883]
[208] Inosine [23.453]
[209] Adenine [17.106]
[210] Thymine [11.611]
[212] Adenosine monophosphate 1 [26.907]
[217] 1-methyl nicotinamide 1 [12.752]

[332] Kynurenic acid [19.159]
[107] Myoinositol [19.395]
[058] L-Tryptophan 2 [20.512]
[109] Inositol phosphate
[208] Inosine [23.453]
[207] Adenosine [23.883]
[113] Cellobiose 2 [24.762]
[x] turanose 1 [24.872]
[179] Glycerol 1-octadecanoate [24.975]
[212] Adenosine monophosphate 1 [26.907]
[180] Cholesterol [27.629]

carbohydrates (8)

[001] D-glucose 2 [17.660]
[008] 3-Phosphoglyceric acid [16.525]
[100] D-Fructose 1 [17.213]
[107] Myoinositol [19.395]
[109] Inositol phosphate
[111] D-Galactosamine 3 [17.557]
[113] Cellobiose 2 [24.762]
[118] D-threitol [12.971]

Lipids (6)

[158] Myristic acid [16.919]
[179] Glycerol 1-octadecanoate [24.975]
[180] Cholesterol [27.629]
[190] Glycerol [9.947]
[191] glycerol 3-phosphate [16.085]
[194] O-Phosphoethanolamine [16.261]

amino acids (17)

[050] Glycine [10.464]
[051] L-Alanine 1 [7.471]
[052] L-Valine 2 [9.154]
[053] L-Leucine 2 [9.951]
[054] L-Isoleucine 2 [10.232]
[056] L-Phenylalanine 1 [13.564]
[057] L-Tyrosine 1 [17.379]
[058] L-Tryptophan 2 [20.512]
[059] L-Serine 2 [11.184]
[060] L-Threonine 2 [11.475]
[062] L-Methionine 2 [13.206]
[065] L-Aspartic acid 2 [13.225]
[066] L-Glutamic acid 2 [14.421]
[070] Pyroglutamic acid [13.236]
[074] Beta-Alanine 1 [12.058]
[76] L-threonine 1 [10.231]
[78] Iminodiacetic acid 1 [12.502]

Other intermediates 7)

- [x] ribonic acid-gamma-lactone 1 [15.077]
- [x] salicylic acid [13.061]
- [x] ribonic acid-gamma-lactone 1 [15.077]
- [x] 1,6-anhydro-glucose [15.352]
- [x] methyl-beta-D-galactopyranoside [16.967]
- [x] gluconic acid lactone 1 [17.337]
- [x] turanose 1 [24.872]

end metabolites (6)

- [200] Phosphate [9.9]
- [221] Creatinine [13.649]
- [223] L-Ascorbic acid [17.975]
- [252] 2-Hydroxyglutaric acid
- [301] Hypotaurine [14.134]
- [332] Kynurenic acid [19.159]

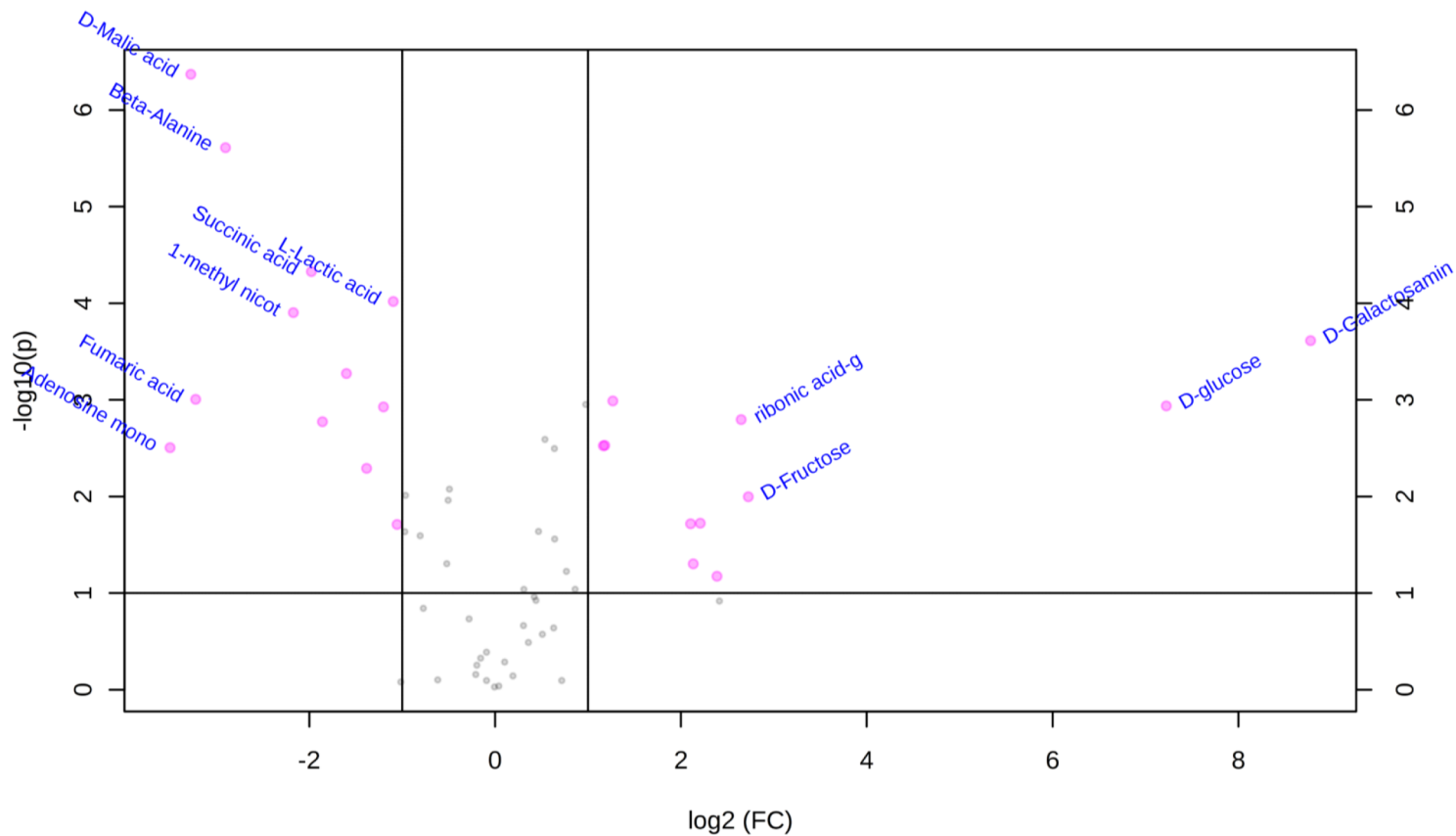
Table S2

	Fold Change	log2(FC)
D-Galactosamine	438.5	8.7764
D-glucose	149.44	7.2235
Adenosine monophosphate	0.088545	-3.4975
D-Malic acid	0.10336	-3.2742
Fumaric acid	0.10716	-3.2221
Beta-Alanine	0.13389	-2.9009
D-Fructose	6.6127	2.7252
ribonic acid-gamma-lactone	6.2682	2.6481
methyl-beta-D-galactopyranoside	5.33	2.4141
gluconic acid lactone	5.2338	2.3879
Cellobiose	4.6205	2.2081
1-methyl nicotinamide	0.22209	-2.1708
turanose	4.3849	2.1326
Kynurenic acid	4.2991	2.104
Succinic acid	0.25405	-1.9768
Creatinine	0.2759	-1.8578
Hypotaurine	0.32995	-1.5997
O-Phosphoethanolamine	0.38355	-1.3825
alpha-D-glucosamine 1-phosphate	2.4068	1.2671
Citric acid	0.43496	-1.201
3-Phosphoglyceric acid	2.2665	1.1805
L-Tryptophan	2.2422	1.1649
L-Lactic acid	0.46798	-1.0955
L-Aspartic acid	0.48145	-1.0545
Adenosine	0.49508	-1.0143

Table S3

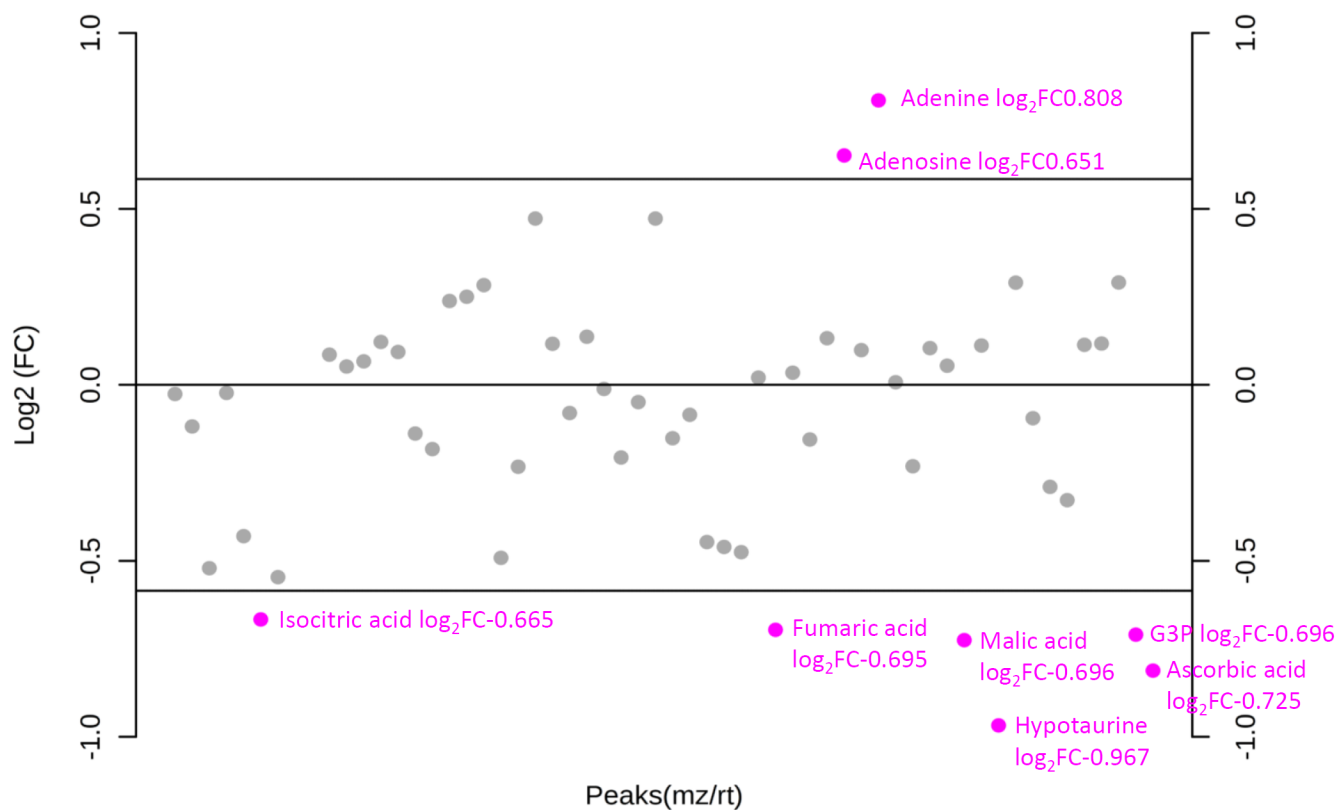
	FC	log2(FC)	raw.p val	log10 P
D-Malic acid	0.10336	-3.2742	4.27E-07	6.3698
Beta-Alanine	0.13389	-2.9009	2.45E-06	5.6103
Succinic acid	0.25405	-1.9768	4.70E-05	4.3278
L-Lactic acid	0.46798	-1.0955	9.58E-05	4.0186
1-methyl nicotinamide	0.22209	-2.1708	0.000125	3.9032
D-Galactosamine	438.5	8.7764	0.0002437	3.6132
Hypotaurine	0.32995	-1.5997	0.0005332	3.2731
Fumaric acid	0.10716	-3.2221	0.0009867	3.0058
alpha-D-glucosamine 1-phosphate	2.4068	1.2671	0.0010258	2.9889
D-glucose	149.44	7.2235	0.0011545	2.9376
Citric acid	0.43496	-1.201	0.0011825	2.9272
ribonic acid-gamma-lactone	6.2682	2.6481	0.0015986	2.7963
Creatinine	0.2759	-1.8578	0.0016823	2.7741
3-Phosphoglyceric acid	2.2665	1.1805	0.0029565	2.5292
L-Tryptophan	2.2422	1.1649	0.0029842	2.5252
Adenosine monophosphate	0.088545	-3.4975	0.0031227	2.5055
O-Phosphoethanolamine	0.38355	-1.3825	0.0051117	2.2914
D-Fructose	6.6127	2.7252	0.010059	1.9975
Cellobiose	4.6205	2.2081	0.018885	1.7239
Kynurenic acid	4.2991	2.104	0.019147	1.7179
L-Aspartic acid	0.48145	-1.0545	0.019465	1.7107
turanose	4.3849	2.1326	0.049755	1.3032
gluconic acid lactone	5.2338	2.3879	0.066873	1.1747

Li, et al. supplemental Fig 1



Li, et al. supplemental Fig 2

PC-3



Li, et al. supplemental Fig 3

