

Metabolites	Benign Disease			Pancreatic Adenocarcinoma		
	Mean	Median	SD	Mean	Median	SD
X2.Aminobutyrate	8.812195	8.5	4.234099	8.111628	8.5	3.772785
X2.Hydroxybutyrate	26.41707	24.3	11.34456	28.9814	25.7	15.76242
X2.Hydroxyisobutyrate	1.363415	0.6	2.608904	1.455814	0.7	3.010561
X2.Hydroxyisovalerate	2.143902	1.8	1.181958	2.465116	1.8	1.707391
X2.Oxoisocaproate	1.631707	1.7	1.017212	1.923256	1.4	1.614051
X3.Hydroxybutyrate	293.2366	185	343.0797	500.2	322.2	713.7162
X3.Hydroxyisovalerate	0.6926829	0.5	0.3601321	0.8046512	0.5	0.6520858
X3.Methyl.2.oxovalerate	2.243902	2	1.039723	2.611628	2.2	1.51755
X4.Pyridoxate	1.563415	1.7	0.5660195	1.281395	1.3	0.6238345
Acetate	35.74878	35.7	11.73887	36.95349	36.1	15.65403
Acetone	56.00244	41.4	52.07044	85.83488	68.5	83.07633
Adipate	2.853659	2.5	1.970038	2.860465	2.2	1.625121
Alanine	152.1122	145.6	40.02675	137.4651	131.4	39.89244
Arginine	29.07805	33.3	7.708	29.92791	33.3	9.204045
Asparagine	11.16585	10.3	4.171607	9.444186	8.8	3.326109
Aspartate	10.32439	8.4	5.120292	10.6093	9.4	4.762943
Betaine	16.59756	14.6	7.649428	15.2	14.4	5.789605
Carnitine	15.16098	13.5	6.650634	13.43488	12.4	4.716783
Choline	5.665854	4.5	3.817827	5.846512	3.6	5.304461
Citrate	50.49268	48.6	14.86138	52.59535	46.3	22.34376
Creatine	12.87317	11.7	7.313687	8.418605	6.6	5.814401
Creatinine	22.99756	21.9	9.329911	23.15116	20.4	8.731835
Dimethylamine	0.9243902	0.7	0.5228673	0.9186047	0.9	0.3041427
Ethanol	6.234146	4	8.861592	3.630233	2.9	3.241291
Formate	10.14634	10.2	2.966993	10.95581	10.1	3.36171
Glucose	2263.134	2195.9	620.6144	2628.214	2417.2	940.8767
Glutamate	106.3171	92.3	61.25102	154.5372	141.6	71.58267
Glutamine	63.60244	33.2	53.60643	46.2814	19.8	57.91539
Glycerol	299.7512	286.4	159.6791	250.7419	198.3	219.6803
Glycine	112.2683	111	27.00311	109.3581	105.7	28.7368
Histidine	24.86098	24.7	5.36488	23.85349	24	4.945048
Hypoxanthine	2.595122	2.4	1.497657	2.713953	2.4	1.771411
Isobutyrate	5.692683	6	1.856124	5.137209	4.7	2.045439
Isoleucine	29.05122	28.2	7.428396	29.52558	29.8	9.33626
Isovalerate	2.62439	2.3	2.342304	2.148837	1.5	1.862458
Lactate	920.2805	821.3	390.0682	867.8512	764	370.0508
Leucine	50.37317	48.3	14.81052	49.42791	48.3	15.2883
Lysine	60.39756	59.2	15.49388	54.17209	53	12.57604
Malonate	14.71463	8.8	33.25021	18.51628	8.6	55.31793
Mannose	23.77073	23.8	9.31843	28.13721	22.9	16.69039
Methanol	20.78537	12.7	37.45351	15.64651	8.2	21.82151
Methionine	7.35122	7.6	2.753009	7.453488	7.2	3.201291
Methylsuccinate	5.7	5.2	2.189406	5.562791	5.4	2.52502
O.Acetylcarnitine	4.104878	3.5	2.305532	4.24186	4.1	2.276299
Ornithine	21.55854	20	7.114386	19.47209	18.4	6.687562
Phenylalanine	24.16341	23.4	6.950027	26.21395	24.2	8.355967
Proline	53.8122	52.6	13.66532	45.72791	44.5	13.22768
Propylene.glycol	57.81951	56.9	20.14149	53.51163	54.3	20.3684
Pyroglutamate	12.02195	10.4	5.917242	11.5814	9.1	6.642441
Pyruvate	4.378049	1.5	6.580673	5.044186	1.9	7.442711
Serine	56.22195	56.4	14.00072	55.98605	56.2	14.40786
Suberate	9.278049	9.2	5.123647	8.160465	6.8	5.983793
Succinate	3.963415	2.6	4.177963	4.197674	2.6	4.508483
Threonine	48.09024	47.4	11.72179	43.00698	41.6	10.05704
Tryptophan	4.107317	3.1	3.359344	3.646512	2.8	3.073493
Tyrosine	21.72683	20.3	6.751408	21.3093	20.4	5.287578
Urea	245.461	208.3	149.4185	195.2791	173.5	93.42391
Valine	90.48537	90.9	20.79402	83.71163	84.2	23.73509