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**Supplementary Table.** Absolute (non-normalized) concentrations of 59 metabolites profiled by NMR in each urine sample for acute pancreatitis patients, chronic pancreatitis patients, and healthy controls. Values are reported as mean±SD with units of µmol/L. Boxplots of each metabolite (non-normalized concentrations) are shown the Supplementary Figure.

Metabolite	Acute pancreatitis	Chronic pancreatitis	Healthy controls	Metabolite	Acute pancreatitis	Chronic pancreatitis	Healthy controls
1,6-Anhydro β D glucose	70±86	65±37	170±220	Kynurenine	84±141	89±37	24±4.7
1-Methylnicotinamide	7.1±2.9	230±230	20±21	Lactate	32±15	69±39	66±54
2-Amino adipate	150±120	450±340	140±47	Lactose	66±59	130±72	70±46
2-Methylglutarate	13±9.6	18±7.4	24±13	Malonate	68±38	290±360	89±41
2-Oxoglutarate	34±24	95±70	58±49	Mannose	31±32	23±17	8.9±7.9
3-Hydroxyisovalerate	8.1±4.1	21±10	17±9.0	Methylguanidine	11±12	47±78	18±16
3-Indoxylsulfate	32±30	162±110	100±59	N,N Dimethylglycine	8.7±3.3	42±45	11±5.0
4-Aminohippurate	16±5.3	110±140	52±55	N-Methylhydantoin	11±2.8	40±27	20±8.8
ADP	3.1±1.9	10±8.3	5.4±5.7	N-Phenylacetyl glycine	100±49	330±240	140±69
Acetate	16±7.9	45±24	29±15	O-Acetylcholine	23±22	42±50	24±16
Acetoacetate	24±24	130±109	35±12	O-Phosphocholine	32±24	43±37	15±6.9
Acetone	84±100	32±22	9.5±4.1	Phenylacetyl glycine	83±80	400±330	98±82
Adenosine	7.3±4.5	28±19	4.8±3.6	Pyruvate	11±6.4	34±25	14±3.4
Alanine	35±7.7	86±68	68±46	Quinolate	15±11	28±24	27±25
Allantoin	39±26	67±31	30±11	Ribose	230±220	440±290	82±80
Betaine	30±30	420±650	26±18	Succinate	10±11	41±21	35±26
Caffeine	31±18	67±25	43±25	Taurine	230±200	380±260	120±57
Choline	24±22	45±33	11±5.9	Threonine	33±14	98±100	63±30
Citrate	180±110	430±630	910±620	Trigonelline	28±26	83±84	89±60
Creatine	51±39	170±88	89±69	Trimethylamine	2.5±1.7	12±8.7	4.6±2.4
Creatinine	2,200±1,260	6,100±3,800	3,500±1,600	Trimethylamine N-oxide	110±100	520±690	140±110
Dimethylamine	100±75	220±74	120±48	Tryptophan	15±7.1	41±34	22±19
Ethanolamine	76±40	200±140	180±130	Tyramine	21±15	72±33	36±20
Formate	52±31	57±39	96±67	Tyrosine	14±6.9	40±21	27±18
Fumarate	2.9±1.7	3.9±2.2	2.7±1.3	Valine	7.3±1.8	19±12	13±6.8
Glucose	8,200±16,820 <sup>a</sup>	420±430	110±190	Xanthine	49±14	97±88	38±22
Glycine	130±63	370±500	300±191	cis-Aconitate	80±58	200±120	130±59
Hippurate	340±290	530±480	410±270	pi.Methylhistidine	84±36	440±590	100±60
Hypoxanthine	9.2±6.8	97±181	14±5.2	tau.Methylhistidine	56±43	120±91	48±18
Inosine	10±7.5	25±33	5.2±4.9				

<sup>a</sup> One acute pancreatitis patient had a raw glucose of 38 mM. Without this value, mean glucose values for acute pancreatitis patients are 650±110 µmol/L.

**Supplementary Figure.** Boxplots of absolute (non-normalized) concentrations of 59 profiled urinary metabolites. The box covers the first (Q1) and third (Q3) quartile of the data. The line in the box represents the median value. The whiskers extend to  $\pm 1.5$  interquartile range (IQR), where  $IQR=Q3-Q1$ . Outliers are shown as points. Concentration units are expressed in  $\mu\text{mol/L}$ .





