

Absolute Concentration of 116 Compounds (pmol/10⁶ cells)

Compound name	Pathway Label	PubChem CID	Fresh			Bead			Beadless		
			Donor 1	Donor 2	Donor 3	Donor 1	Donor 2	Donor 3	Donor 1	Donor 2	Donor 3
A_0001	NAD ⁺	NAD ⁺ 5893	7.1	6.7	6.4	160	141	215	421	227	327
A_0002	cAMP	cAMP 6076	0.2	0.3	0.3	0.5	0.5	0.4	1.4	0.7	0.7
A_0003	cGMP	cGMP 24316	N.D.	N.D.	N.D.	N.D.	N.D.	N.D.	N.D.	N.D.	N.D.
A_0004	NADH	NADH 439153	8.3	5.0	3.9	14	20	14	38	20	32
A_0005	Xanthine	Xanthine 1188	1.1	N.D.	0.4	1.6	N.D.	0.6	0.5	N.D.	0.8
A_0006	ADP-ribose	ADP-Rib 445794	0.05	0.04	0.03	0.6	0.4	1.0	1.5	0.6	1.5
A_0007	Mevalonic acid	Mevalonic acid 134965	N.D.	N.D.	N.D.	N.D.	N.D.	N.D.	N.D.	N.D.	N.D.
A_0008	UDP-glucose	UDP-Glc 8629	4.7	7.7	8.1	71	52	98	273	152	255
A_0009	Uric acid	Uric acid 1175	3.3	6.2	1.4	1.6	1.1	N.D.	2.1	0.3	N.D.
A_0010	NADP ⁺	NADP ⁺ 5886	2.0	0.9	0.8	3.1	4.1	4.4	5.9	4.3	5.3
A_0011	IMP	IMP 8582	77	10	7.4	2.1	2.8	16	83	23	51
A_0012	Sedoheptulose 7-phosphate	S7P 165007	N.D.	N.D.	N.D.	N.D.	N.D.	N.D.	N.D.	N.D.	N.D.
A_0013	Glucose 6-phosphate	G6P 5958	3.8	8.1	4.3	8.6	7.9	2.9	13	14	17
A_0014	Fructose 6-phosphate	F6P 603	1.4	2.8	1.5	3.5	3.0	1.8	5.3	6.3	7.6
A_0015	Fructose 1-phosphate	D-F1P 439394	N.D.	N.D.	N.D.	N.D.	N.D.	N.D.	14	7.9	N.D.
A_0016	Galactose 1-phosphate	Gal1P 123912	N.D.	N.D.	N.D.	N.D.	N.D.	N.D.	1.4	1.0	3.1
A_0017	Glucose 1-phosphate	G1P 65533	1.7	1.2	1.0	3.2	3.7	1.8	3.2	2.4	4.9
A_0018	Acetoacetyl CoA	AAcCoA 92153	N.D.	N.D.	N.D.	N.D.	N.D.	N.D.	N.D.	N.D.	N.D.
A_0019	Acetyl CoA	AcCoA 444493	0.2	0.2	0.13	1.0	1.3	1.6	2.0	0.09	3.6
A_0020	Folic acid	Folic acid 6037	0.3	0.3	0.3	1.2	1.5	0.7	0.4	0.2	0.6
A_0021	Ribose 5-phosphate	R5P 439167	3.3	3.8	2.1	1.9	2.7	4.2	5.6	1.8	6.7
A_0022	CoA	CoA 87642	0.8	0.6	0.4	1.7	1.8	3.2	2.6	2.4	2.9
A_0023	Ribose 1-phosphate	R1P 439236	1.4	0.9	0.9	2.1	N.D.	1.6	7.0	3.4	4.8
A_0024	Ribulose 5-phosphate	Ru5P 439184	0.4	0.8	N.D.	0.09	N.D.	0.3	1.0	0.5	1.4
A_0025	Xylulose 5-phosphate	X5P 439190	N.D.	N.D.	N.D.	N.D.	N.D.	N.D.	N.D.	N.D.	N.D.
A_0026	Erythrose 4-phosphate	E4P 122357	N.D.	N.D.	N.D.	N.D.	N.D.	N.D.	N.D.	N.D.	N.D.
A_0027	HMG CoA	HMG-CoA 445127	0.3	0.2	0.2	0.5	0.8	0.4	1.5	0.7	1.3
A_0028	Glyceraldehyde 3-phosphate	Glyceraldehyde 3-phosphate 729	0.8	1.2	0.9	N.D.	N.D.	1.6	1.6	0.2	4.2
A_0029	NADPH	NADPH 5884	6.5	4.0	3.3	10	14	8.2	12	7.8	11
A_0030	Malonyl CoA	Malonyl-CoA 644066	N.D.	N.D.	N.D.	0.4	0.7	0.2	0.3	0.12	0.4
A_0031	Phosphocreatine	Phosphocreatine 9548602	0.011	0.3	0.3	3.0	N.D.	0.05	2.8	0.12	N.D.
A_0032	XMP	XMP 73323	4.2	0.2	0.14	0.3	0.3	0.2	0.9	0.3	0.6
A_0033	Dihydroxyacetone phosphate	DHAP 668	3.9	3.1	0.7	N.D.	N.D.	1.8	1.4	2.0	4.6
A_0034	Adenylosuccinic acid	Succinyl AMP 447145	1.7	0.7	0.4	1.0	1.5	1.2	6.5	3.3	5.7
A_0035	Fructose 1,6-diphosphate	F1,6P 172313	7.3	30	18	27	26	18	43	59	34
A_0036	6-Phosphogluconic acid	6-PG 91493	1.5	11	7.9	21	9.7	4.8	6.7	3.6	5.3
A_0037	N-Carbamoylaspartic acid	Carbamoyl-Asp 93072	N.D.	0.2	2.2	1.4	0.6	2.0	21	26	24
A_0038	PRPP	PRPP 7339	8.8	34	48	4.7	6.3	21	72	53	52
A_0039	2-Phosphoglyceric acid	2-PG 439278	0.4	0.5	0.5	1.2	0.7	1.0	1.0	1.0	1.1
A_0040	2,3-Diphosphoglyceric acid	Diphosphoglycerate 186004	1.3	5.9	6.8	9.6	6.3	17	16	26	16
A_0041	3-Phosphoglyceric acid	3-PG 439183	3.5	3.7	4.1	8.5	4.3	8.4	8.5	8.2	8.3
A_0042	Phosphoenolpyruvic acid	PEP 1005	N.D.	0.6	0.9	1.6	N.D.	2.3	1.9	0.9	1.3
A_0043	GMP	GMP 6804	15	4.7	2.3	3.8	4.9	18	37	14	29
A_0044	AMP	AMP 6083	38	8.6	5.1	7.8	7.5	105	177	58	145
A_0045	2-Oxoisovaleric acid	2-KIV 49	N.D.	N.D.	N.D.	N.D.	N.D.	N.D.	5.5	4.0	6.6
A_0046	GDP	GDP 8977	13	8.4	6.3	22	19	53	103	50	88
A_0047	Lactic acid	Lactic acid 612	112	114	218	1,959	1,618	1,307	15,714	7,418	14,009
A_0048	ADP	ADP 6022	56	30	27	100	88	335	489	254	449
A_0049	GTP	GTP 6830	34	61	54	273	177	348	440	287	387
A_0050	Glyoxylic acid	Glyoxylic acid 760	N.D.	N.D.	N.D.	N.D.	N.D.	N.D.	N.D.	N.D.	N.D.
A_0051	ATP	ATP 5957	157	290	274	1,586	1,078	1,838	1,619	1,198	1,677
A_0052	Glycerol 3-phosphate	Glycerol 3-phosphate 439162	4.1	4.3	8.9	126	103	219	310	134	178
A_0053	Glycolic acid	Glycolic acid 757	50	23	19	51	115	24	23	14	N.D.
A_0054	Pyruvic acid	Pyruvic acid 1060	36	22	32	83	75	55	140	76	230
A_0055	N-Acetylglutamic acid	N-AcGlu 70914	N.D.	1.0	0.9	2.1	N.D.	2.9	1.8	2.0	3.1
A_0056	2-Hydroxyglutaric acid	2-Hydroxyglutaric acid 43	1.3	N.D.	0.4	2.2	2.7	1.2	5.2	3.6	7.1
A_0057	Carbamoylphosphate	Carbamoyl-P 278	N.D.	N.D.	N.D.	N.D.	N.D.	0.13	N.D.	N.D.	N.D.
A_0058	Succinic acid	Succinic acid 1110	15	7.3	8.6	22	33	26	94	52	93
A_0059	Malic acid	Malic acid 525	56	26	20	N.D.	N.D.	35	325	241	292
A_0060	2-Oxoglutaric acid	2-OG 51	N.D.	N.D.	N.D.	N.D.	N.D.	N.D.	63	22	30
A_0061	Fumaric acid	Fumaric acid 444972	1.6	N.D.	0.4	N.D.	N.D.	4.9	65	41	56
A_0062	Citric acid	Citric acid 311	8.4	50	63	116	124	82	425	286	243
A_0063	cis-Aconitic acid	cis-Aconitic acid 643757	N.D.	1.0	1.5	1.3	0.4	1.1	11	6.3	4.9
A_0064	Isocitric acid	Isocitric acid 1198	N.D.	N.D.	0.06	N.D.	N.D.	N.D.	16	8.8	3.3
C_0001	Urea	Urea 1176	N.D.	N.D.	N.D.	N.D.	N.D.	N.D.	N.D.	N.D.	N.D.
C_0002	Gly	Gly 750	145	222	212	1,697	1,410	2,199	1,507	1,041	2,141
C_0003	Putrescine	Putrescine 1045	N.D.	N.D.	N.D.	N.D.	N.D.	N.D.	N.D.	N.D.	N.D.
C_0004	Ala	Ala 602	25	116	136	766	315	430	800	330	1,098
C_0005	β-Ala	b-Ala 239	5.6	7.9	3.0	142	33	54	427	65	86
C_0006	Sarcosine	Sarcosine 1088	N.D.	N.D.	N.D.	N.D.	N.D.	N.D.	N.D.	N.D.	N.D.
C_0007	γ-Aminobutyric acid	g-Aminobutyric acid 119	15	8.4	3.1	12	N.D.	3.9	21	4.7	9.3
C_0008	N,N-Dimethylglycine	DMG 673	N.D.	N.D.	N.D.	N.D.	N.D.	N.D.	N.D.	N.D.	N.D.
C_0009	Choline	Choline 305	50	34	67	343	183	445	275	251	383
C_0010	Ser	Ser 617	30	60	82	138	138	159	108	134	607
C_0011	Carnosine	Carnosine 439224	1.1	2.7	1.4	0.3	N.D.	1.7	0.4	N.D.	N.D.
C_0012	Creatinine	Creatinine 588	1.3	2.6	1.5	3.2	N.D.	N.D.	4.2	N.D.	0.7
C_0013	Pro	Pro 614	42	129	138	358	144	842	1,783	956	1,904

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			Donor 1	Donor 2	Donor 3	Donor 1	Donor 2	Donor 3	Donor 1	Donor 2	Donor 3
C_0014 Betaine	Betaine	247	N.D.	N.D.	N.D.	N.D.	N.D.	N.D.	N.D.	N.D.	N.D.
C_0015 Val	Val	1182	N.D.	37	52	219	229	351	314	286	637
C_0016 Thr	Thr	6288	56	82	83	369	391	632	466	512	1,111
C_0017 Homoserine	Homoserine	12647	N.D.	N.D.	N.D.	N.D.	N.D.	N.D.	N.D.	N.D.	N.D.
C_0018 Betaine aldehyde	BTL	249	N.D.	N.D.	N.D.	N.D.	N.D.	N.D.	N.D.	N.D.	N.D.
C_0019 Cys	Cys	594	N.D.	N.D.	N.D.	N.D.	N.D.	N.D.	N.D.	2.3	5.1
C_0020 Hydroxyproline	Hydroxyproline	5810	N.D.	7.4	6.2	46	21	N.D.	35	N.D.	8.4
C_0021 Creatine	Creatine	586	23	11	15	34	2.0	4.1	61	3.3	3.9
C_0022 Ile	Ile	791	11	40	56	218	225	290	315	265	602
C_0023 Leu	Leu	857	14	42	59	207	213	262	293	248	574
C_0024 Asn	Asn	236	5.4	36	48	185	104	189	173	112	525
C_0025 Ornithine	Ornithine	389	1.4	1.3	N.D.	22	15	14	29	15	40
C_0026 Asp	Asp	424	783	978	436	1,977	1,975	2,289	358	518	1,437
C_0027 Homocysteine	Homocysteine	778	N.D.	N.D.	N.D.	N.D.	N.D.	N.D.	N.D.	N.D.	N.D.
C_0028 Adenine	Adenine	190	1.0	1.0	N.D.	N.D.	N.D.	N.D.	0.7	N.D.	N.D.
C_0029 Hypoxanthine	Hypoxanthine	790	N.D.	N.D.	N.D.	N.D.	N.D.	N.D.	2.6	N.D.	4.7
C_0030 Spermidine	Spermidine	1102	N.D.	N.D.	N.D.	N.D.	N.D.	4.0	2.4	1.5	2.2
C_0031 Gln	Gln	738	52	63	67	1,275	1,203	1,906	576	792	1,892
C_0032 Lys	Lys	866	55	62	45	175	181	171	145	127	376
C_0033 Glu	Glu	611	122	713	617	3,875	3,388	5,976	3,273	2,947	6,057
C_0034 Met	Met	876	5.0	14	18	39	48	55	53	38	94
C_0035 Guanine	Guanine	764	N.D.	N.D.	N.D.	N.D.	N.D.	N.D.	N.D.	N.D.	N.D.
C_0036 His	His	773	11	18	19	66	63	78	66	61	137
C_0037 Carnitine	Carnitine	85	17	11	17	N.D.	N.D.	N.D.	N.D.	N.D.	N.D.
C_0038 Phe	Phe	994	10	22	26	82	97	107	135	122	280
C_0039 Arg	Arg	6322	31	31	34	143	113	88	92	49	161
C_0040 Citrulline	Citrulline	9750	4.0	3.0	2.8	4.9	N.D.	N.D.	2.3	N.D.	N.D.
C_0041 Tyr	Tyr	1153	12	21	26	73	80	88	129	112	252
C_0042 S-Adenosylhomocysteine	SAH	439155	N.D.	N.D.	N.D.	N.D.	N.D.	N.D.	1.3	N.D.	N.D.
C_0043 Spermine	Spermine	1103	N.D.	N.D.	N.D.	N.D.	N.D.	13	9.3	5.5	6.2
C_0044 Trp	Trp	1148	N.D.	5.8	5.7	19	19	18	29	24	57
C_0045 Cystathionine	Cystathionine	834	N.D.	N.D.	N.D.	N.D.	N.D.	N.D.	N.D.	N.D.	3.4
C_0046 Adenosine	Adenosine	60961	N.D.	N.D.	N.D.	N.D.	N.D.	3.0	1.5	N.D.	N.D.
C_0047 Inosine	Inosine	6021	N.D.	N.D.	N.D.	N.D.	N.D.	N.D.	N.D.	N.D.	N.D.
C_0048 Guanosine	Guanosine	6802	N.D.	N.D.	N.D.	N.D.	N.D.	N.D.	N.D.	N.D.	N.D.
C_0049 Argininosuccinic acid	ArgSuccinate	16950	N.D.	N.D.	N.D.	N.D.	N.D.	N.D.	5.7	3.3	8.5
C_0050 Glutathione (GSSG)	GSSG	65359	115	132	80	189	377	151	424	774	694
C_0051 Glutathione (GSH)	GSH	124886	101	108	122	216	83	1,118	968	970	2,237
C_0052 S-Adenosylmethionine	SAM	34755	8.2	4.9	3.9	12	N.D.	8.9	9.8	9.3	27
- Adenylate Energy Charge	No Label		0.7	0.9	0.9	1.0	1.0	0.9	0.8	0.9	0.8
- Total Adenylate	No Label		251	328	307	1,694	1,173	2,277	2,285	1,510	2,271
- Guanylate Energy Charge	No Label		0.7	0.9	0.9	1.0	0.9	0.9	0.8	0.9	0.9
- Total Guanylate	No Label		62	74	62	298	201	419	580	352	504
- GSH/GSSG	No Label		0.9	0.8	1.5	1.1	0.2	7.4	2.3	1.3	3.2
- Total Glutathione	No Label		332	372	282	593	838	1,420	1,815	2,519	3,624
- NADPH/NADP+	No Label		3.3	4.5	4.4	3.2	3.4	1.9	2.0	1.8	2.0
- NADH/NAD+	No Label		1.2	0.7	0.6	0.09	0.14	0.06	0.09	0.09	0.10
- NAD+/NADH	No Label		0.9	1.3	1.7	11.3	7.0	15.7	11.1	11.6	10.2
- Lactate/Pyruvate	No Label		3.1	5.1	6.7	24	22	24	112	98	61
- Glycerol 3-phosphate/DHAP	No Label		1.0	1.4	13	N.A.	N.A.	122	217	67	39
- Total Amino Acids	No Label		1,409	2,691	2,160	11,878	10,337	16,132	10,614	8,678	19,946
- Total Essential Amino Acids	No Label		162	324	364	1,393	1,466	1,964	1,814	1,684	3,866
- Total Non-essential Amino Acids	No Label		1,247	2,368	1,796	10,486	8,871	14,168	8,800	6,994	16,080
- Total Glucogenic Amino Acids	No Label		1,340	2,587	2,056	11,496	9,943	15,698	10,177	8,303	18,997
- Total Ketogenic Amino Acids	No Label		157	275	301	1,141	1,206	1,568	1,510	1,411	3,252
- Total BCAA	No Label		25	120	167	643	667	903	921	798	1,812
- Total Aromatic Amino Acids	No Label		22	48	58	173	196	213	293	259	590
- Fischer's Ratio	No Label		1.2	2.5	2.9	3.7	3.4	4.2	3.1	3.1	3.1
- Total Glu-related Amino Acids	No Label		258	954	875	5,716	4,911	8,891	5,790	4,806	10,151
- Total Pyr-related Amino Acids	No Label		256	486	519	2,989	2,274	3,438	2,911	2,045	5,019
- Total Acetyl CoA-related Amino Acids	No Label		80	150	166	618	639	741	781	664	1,609
- Total Fumarate-related Amino Acids	No Label		22	42	52	154	176	196	263	235	532
- Total Succinyl CoA-related Amino Acids	No Label		16	91	126	475	503	696	681	588	1,333
- Total Oxaloacetate-related Amino Acids	No Label		788	1,013	483	2,161	2,079	2,478	532	630	1,962
- Malate/Asp	No Label		0.07	0.03	0.05	N.A.	N.A.	0.02	0.9	0.5	0.2
- Citrulline/Ornithine	No Label		2.9	2.4	N.A.	0.2	N.A.	N.A.	0.08	N.A.	N.A.
- Glu/2-Oxoglutarate	No Label		N.A.	N.A.	N.A.	N.A.	N.A.	N.A.	52	132	205
- G6P/R5P	No Label		1.2	2.2	2.1	4.6	3.0	0.7	2.2	7.9	2.5
- SAM/SAH	No Label		N.A.	N.A.	N.A.	N.A.	N.A.	N.A.	7.4	N.A.	N.A.
- Putrescine/Spermidine	No Label		N.A.	N.A.	N.A.	N.A.	N.A.	N.A.	N.A.	N.A.	N.A.

ID consists of analysis mode and number. 'C' and 'A' showed cation and anion modes, respectively.

N.D. (Not Detected): The target peak or metabolite was below detection limits.

N.A. (Not Available): The calculation was impossible because of insufficiency of the data.

The data are sorted by ID in ascending order.