

GTP	C00044	0	0	0	0	1	1	4.87E-03
Lysine	C00047	0	0	0	0	0	0	4.05E-04
Aspartate	C00049	0	1	0	0	0	1	4.23E-03
Glutathione	C00051	0	0	0	0	0	0	1.66E-02
CMP	C00055	0	0	0	0	0	0	3.60E-04
Flavin mononucleotide	C00061	0	0	0	0	0	0	5.37E-05
Arginine	C00062	0	0	0	0	0	0	5.69E-04
CTP	C00063	0	0	0	0	0	0	2.73E-03
Glutamine	C00064	0	0	1	0	0	1	3.81E-03
Serine	C00065	0	0	0	0	0	0	6.80E-05
Methionine	C00073	0	0	0	0	0	0	1.45E-04
Phosphoenolpyruvate	C00074	0	0	0	0	0	0	1.84E-04
UTP	C00075	0	0	0	0	0	0	8.29E-03
Ornithine	C00077	0	0	0	0	0	0	1.01E-05
Tryptophan	C00078	0	0	0	0	0	0	1.21E-05
Phenylalanine	C00079	0	0	0	0	0	0	1.82E-05
Inosine-triphosphate	C00081	0	0	0	0	0	0	2.05E-04
Tyrosine	C00082	0	0	0	0	0	0	2.89E-05
Malonyl-CoA	C00083	0	0	0	0	0	0	3.54E-05
Succinyl-CoA	C00091	0	1	0	0	0	1	2.33E-04
Propionyl-CoA	C00100	0	0	0	0	0	0	5.32E-06
Inosine-diphosphate	C00104	0	0	0	0	0	0	2.38E-05
Anthranilate	C00108	0	0	0	0	0	0	3.48E-06
Dihydroxyacetonephosphate	C00111	0	0	0	0	0	0	3.74E-04
PRPP	C00119	0	0	0	0	0	0	2.58E-04
Fumarate	C00122	0	0	1	0	0	1	1.15E-04
Glutathione disulfide	C00127	0	0	0	0	0	0	2.37E-03
Inosine-monophosphate	C00130	0	0	0	0	0	0	2.72E-04
dATP	C00131	0	0	0	0	0	0	1.55E-05
Histidine	C00135	0	0	0	0	0	0	6.76E-05
Myo-inositol	C00137	0	0	0	0	0	0	5.72E-06
GMP	C00144	0	0	0	0	0	0	2.37E-05
Adenine	C00147	0	0	0	0	0	0	1.47E-06
Proline	C00148	0	0	0	0	0	0	3.85E-04
Malate	C00149	0	0	1	0	0	1	1.68E-03
Asparagine	C00152	0	0	0	0	0	0	5.11E-04
Homocysteine	C00155	0	0	0	0	0	0	3.70E-04
4-Hydroxybenzoate	C00156	0	0	0	0	0	0	5.22E-05
Citrate	C00158	0	0	1	0	0	1	1.96E-03

NADH	C00004	0	0	0	0	0	0	4.50E-04
ADP	C00008	0	0	0	0	0	0	6.30E-04
AMP	C00020	0	0	0	0	0	0	1.60E-04
Pyruvate	C00022	0	0	0	0	0	0	1.24E-03
L-Glutamate	C00025	0	0	1	0	0	1	8.18E-02
2-Oxoglutarate	C00026	0	0	0	0	0	0	1.11E-03
GDP	C00035	0	0	0	0	0	0	2.20E-04
L-Alanine	C00041	0	0	0	0	1	1	2.47E-02
Succinate	C00042	1	0	0	0	0	1	3.40E-04
GTP	C00044	0	0	0	0	1	1	5.90E-04
L-Aspartate	C00049	0	1	0	0	0	1	1.57E-02
L-Arginine	C00062	0	0	0	0	0	0	3.58E-02
L-Glutamine	C00064	0	0	1	0	0	1	8.04E-02
Phosphoenolpyruvate	C00074	0	0	0	0	0	0	1.90E-04
L-Tryptophan	C00078	0	0	0	0	0	0	3.00E-05
L-Phenylalanine	C00079	0	0	0	0	0	0	3.50E-04
L-Tyrosine	C00082	0	0	0	0	0	0	1.60E-04
D-Fructose 6-phosphate	C00085	0	0	0	0	0	0	3.20E-04
D-Glucose 6-phosphate	C00092	0	0	1	0	0	1	3.70E-03
sn-Glycerol 3-phosphate	C00093	0	0	0	0	0	0	5.00E-04
D-Glucose 1-phosphate	C00103	0	0	0	0	0	0	9.00E-05
Glycerone phosphate	C00111	0	0	0	0	0	0	7.20E-04
D-Ribose 5-phosphate	C00117	0	0	0	0	0	0	4.10E-04
Fumarate	C00122	0	0	1	0	0	1	1.65E-03
GMP	C00144	0	0	0	0	0	0	6.00E-05
Adenine	C00147	0	0	0	0	0	0	5.00E-05
Malate	C00149	0	0	1	0	0	1	1.68E-03
L-Asparagine	C00152	0	0	0	0	0	0	4.66E-03
Citrate	C00158	0	0	1	0	0	1	1.47E-03
3-Phospho-D-glycerate	C00197	0	0	0	0	0	0	8.90E-04
D-Ribulose 5-phosphate	C00199	0	0	0	0	0	0	2.00E-05
Isocitrate	C00311	0	0	0	0	0	0	1.90E-04
6-Phospho-D-gluconate	C00345	0	0	0	0	0	0	8.70E-04
D-Fructose 1,6-bisphosphate	C00354	0	0	0	0	0	0	8.76E-03
Pantothenate	C00864	0	0	0	0	0	0	2.10E-04

Table S2. Information of selected pathways in training set and test set.

	Organism	Metabolite	KEGG ID	Map 00625	Map 00626	Map 02020	Map 03070	Map 04122	MPF
Training Set	E.coli	ATP	C00002	0	0	0	1	0	1
		NAD	C00003	0	0	0	0	0	0
		NADH	C00004	0	0	0	0	0	0
		ADP	C00008	0	0	0	0	0	0
		Coenzyme-A	C00010	0	0	0	0	0	0
		UDP	C00015	0	0	0	0	0	0
		FAD	C00016	0	0	0	0	0	0
		AMP	C00020	0	0	0	0	0	0
		Acetyl-CoA	C00024	1	0	0	0	0	1
		Glutamate	C00025	0	0	1	0	0	1
		α -Ketoglutarate	C00026	0	0	0	0	0	0
		UDP-glucose	C00029	0	0	0	0	0	0
		Alanine	C00041	0	0	0	0	1	1
		UDP-N-acetyl-glucosamine	C00043	0	0	0	0	0	0
		GTP	C00044	0	0	0	0	1	1
		lysine	C00047	0	0	0	0	0	0
		Aspartate	C00049	0	1	0	0	0	1
		Glutathione	C00051	0	0	0	0	0	0
		CMP	C00055	0	0	0	0	0	0
		Flavin mononucleotide	C00061	0	0	0	0	0	0
		Arginine	C00062	0	0	0	0	0	0
		CTP	C00063	0	0	0	0	0	0
		Methionine	C00073	0	0	0	0	0	0
		Phosphoenol- pyruvate	C00074	0	0	0	0	0	0
		UTP	C00075	0	0	0	0	0	0
		Ornithine	C00077	0	0	0	0	0	0
		Inosine-triphosphate	C00081	0	0	0	0	0	0
		Tyrosine	C00082	0	0	0	0	0	0
		Malonyl-CoA	C00083	0	0	0	0	0	0
		Succinyl-CoA	C00091	0	1	0	0	0	1
		Propionyl-CoA	C00100	0	0	0	0	0	0
		Inosine-diphosphate	C00104	0	0	0	0	0	0
		Anthranilate	C00108	0	0	0	0	0	0
Fumarate	C00122	0	0	1	0	0	1		
Inosine-monophosphate	C00130	0	0	0	0	0	0		

		GMP	C00144	0	0	0	0	0	0
		Adenine	C00147	0	0	0	0	0	0
		Proline	C00148	0	0	0	0	0	0
		Malate	C00149	0	0	1	0	0	1
		Asparagine	C00152	0	0	0	0	0	0
		Homocysteine	C00155	0	0	0	0	0	0
		Citrate	C00158	0	0	1	0	0	1
		Phenylpyruvate	C00166	0	0	0	0	0	0
		UDP-glucuronate	C00167	0	0	0	0	0	0
		2,3-Dihydroxybenzoic acid	C00196	0	0	0	0	0	0
		Adenosine	C00212	0	0	0	0	0	0
		Acetyl phosphate	C00227	0	0	0	0	0	0
		Gluconate	C00257	0	0	0	0	0	0
		Glycerate	C00258	0	0	0	0	0	0
		Uridine	C00299	0	0	0	0	0	0
		Citrulline	C00327	0	0	0	0	0	0
		Acetoacetyl-CoA	C00332	0	0	0	0	0	0
		Dihydroorotate	C00337	0	0	0	0	0	0
		6-phospho-D-gluconate	C00345	0	0	0	0	0	0
		Glucosamine-6 phosphate	C00352	0	0	0	0	0	0
		Fructose-1,6-bisphosphate	C00354	0	0	0	0	0	0
		dAMP	C00360	0	0	0	0	0	0
		dGMP	C00362	0	0	0	0	0	0
		Cytosine	C00380	0	0	0	0	0	0
		Guanosine	C00387	0	0	0	0	0	0
		Aconitate	C00417	0	0	0	0	0	0
		N-acetyl-ornithine	C00437	0	0	0	0	0	0
		Carbamyl-aspartate	C00438	0	0	0	0	0	0
		Cytidine	C00475	0	0	0	0	0	0
		Shikimate	C00493	0	0	0	0	0	0
		ADP-glucose	C00498	0	0	0	0	0	0
		Cyclic-AMP	C00575	0	0	0	0	0	0
		Histidinol	C00860	0	0	0	0	0	0
		Quinolate	C03722	0	0	0	0	0	0
	S.cerevisiae	NADH	C00004	0	0	0	0	0	0
		ADP	C00008	0	0	0	0	0	0
		AMP	C00020	0	0	0	0	0	0
		Pyruvate	C00022	0	0	0	0	0	0
		Succinate	C00042	1	0	0	0	0	1

		L-Arginine	C00062	0	0	0	0	0	0		
		L-Glutamine	C00064	0	0	1	0	0	1		
		Phosphoenolpyruvate	C00074	0	0	0	0	0	0		
		L-Tryptophan	C00078	0	0	0	0	0	0		
		L-Phenylalanine	C00079	0	0	0	0	0	0		
		L-Tyrosine	C00082	0	0	0	0	0	0		
		D-Fructose 6-phosphate	C00085	0	0	0	0	0	0		
		D-Glucose 6-phosphate	C00092	0	0	1	0	0	1		
		sn-Glycerol-3-phosphate	C00093	0	0	0	0	0	0		
		Glycerone phosphate	C00111	0	0	0	0	0	0		
		Fumarate	C00122	0	0	1	0	0	1		
		GMP	C00144	0	0	0	0	0	0		
		Adenine	C00147	0	0	0	0	0	0		
		Malate	C00149	0	0	1	0	0	1		
		Citrate	C00158	0	0	1	0	0	1		
		6-Phospho-D-gluconate	C00345	0	0	0	0	0	0		
		D-Fructose-1,6-bisphosphate	C00354	0	0	0	0	0	0		
		Test Set	E.coli	S-adenosyl-L-methionine	C00019	0	0	0	0	1	1
				GDP	C00035	0	0	0	0	0	0
				Succinate	C00042	1	0	0	0	0	1
Glutamine	C00064			0	0	1	0	0	1		
Serine	C00065			0	0	0	0	0	0		
Tryptophan	C00078			0	0	0	0	0	0		
Phenylalanine	C00079			0	0	0	0	0	0		
Dihydroxy-acetonephosphate	C00111			0	0	0	0	0	0		
PRPP	C00119			0	0	0	0	0	0		
Glutathione disulfide	C00127			0	0	0	0	0	0		
dATP	C00131			0	0	0	0	0	0		
Histidine	C00135			0	0	0	0	0	0		
Myo-inositol	C00137			0	0	0	0	0	0		
4-Hydroxybenzoate	C00156			0	0	0	0	0	0		
Valine	C00183			0	0	0	0	0	0		
Threonine	C00188			0	0	0	0	0	0		
3-Phosphoglycerate	C00197			0	0	0	0	0	0		
Adenosine-phosphosulfate	C00224			0	0	0	0	0	0		
Guanine	C00242			0	0	0	0	0	0		
Deoxyguanosine	C00330			0	0	0	0	0	0		
dTDP	C00363	0	0	0	0	0	0				
dCTP	C00458	0	0	0	0	0	0				

S.cerevisiae	dTTP	C00459	0	0	0	0	0	0
	Deoxyadenosine	C00559	0	0	0	0	0	0
	ATP	C00002	0	0	0	1	0	1
	NAD+	C00003	0	0	0	0	0	0
	L-Glutamate	C00025	0	0	1	0	0	1
	2-Oxoglutarate	C00026	0	0	0	0	0	0
	GDP	C00035	0	0	0	0	0	0
	L-Alanine	C00041	0	0	0	0	1	1
	GTP	C00044	0	0	0	0	1	1
	L-Aspartate	C00049	0	1	0	0	0	1
	D-Glucose 1-phosphate	C00103	0	0	0	0	0	0
	D-Ribose 5-phosphate	C00117	0	0	0	0	0	0
	L-Asparagine	C00152	0	0	0	0	0	0
	3-Phospho-D-glycerate	C00197	0	0	0	0	0	0
	D-Ribulose 5-phosphate	C00199	0	0	0	0	0	0
	Isocitrate	C00311	0	0	0	0	0	0
	Pantothenate	C00864	0	0	0	0	0	0

Table S3. Information of predicted and measured concentrations in training set and test set.

	Organism	Metabolite	KEGG ID	Ce	Cp	Error
Training Set	E.coli	ATP	C00002	2.02	2.31	-0.29
		NAD	C00003	2.59	2.82	-0.22
		NADH	C00004	4.08	3.86	0.22
		ADP	C00008	3.26	3.92	-0.67
		Coenzyme-A	C00010	2.86	2.64	0.22
		UDP	C00015	2.75	2.53	0.22
		FAD	C00016	3.76	3.98	-0.22
		AMP	C00020	3.55	3.75	-0.20
		Acetyl-CoA	C00024	3.22	3.44	-0.22
		Glutamate	C00025	1.02	1.27	-0.26
		α -Ketoglutarate	C00026	3.35	3.47	-0.12
		UDP-glucose	C00029	2.60	3.02	-0.41
		Alanine	C00041	2.59	2.37	0.22
		UDP-N-acetyl-glucosamine	C00043	2.03	3.10	-1.06
		GTP	C00044	2.31	2.09	0.22
		lysine	C00047	3.39	3.62	-0.22
		Aspartate	C00049	2.37	2.15	0.22
		Glutathione	C00051	1.78	2.00	-0.22
		CMP	C00055	3.44	3.52	-0.07
		Flavin mononucleotide	C00061	4.27	4.05	0.22
		Arginine	C00062	3.24	3.02	0.22
		CTP	C00063	2.56	2.57	-0.01
		Methionine	C00073	3.84	3.62	0.22
		Phosphoenolpyruvate	C00074	3.74	3.62	0.12
		UTP	C00075	2.08	2.36	-0.27
		Ornithine	C00077	5.00	3.43	1.56
		Inosine-triphosphate	C00081	3.69	3.47	0.22
		Tyrosine	C00082	4.54	4.27	0.27
		Malonyl-CoA	C00083	4.45	4.23	0.22
		Succinyl-CoA	C00091	3.63	3.45	0.18
		Propionyl-CoA	C00100	5.27	4.67	0.60
		Inosine-diphosphate	C00104	4.62	3.78	0.85
		Anthranilate	C00108	5.46	4.85	0.61
Fumarate	C00122	3.94	3.72	0.22		
Inosine-monophosphate	C00130	3.57	3.81	-0.25		

		GMP	C00144	4.63	3.82	0.80
		Adenine	C00147	5.83	5.47	0.37
		Proline	C00148	3.41	3.64	-0.22
		Malate	C00149	2.77	2.77	0.01
		Asparagine	C00152	3.29	3.51	-0.22
		Homocysteine	C00155	3.43	3.63	-0.20
		Citrate	C00158	2.71	2.54	0.17
		Phenylpyruvate	C00166	4.05	4.27	-0.22
		UDP-glucuronate	C00167	3.25	3.23	0.02
		2,3-Dihydroxybenzoic acid	C00196	3.86	5.18	-1.32
		Adenosine	C00212	6.88	5.73	1.16
		Acetyl phosphate	C00227	2.97	3.24	-0.27
		Gluconate	C00257	4.38	3.99	0.39
		Glycerate	C00258	2.85	3.75	-0.89
		Uridine	C00299	2.68	4.16	-1.48
		Citrulline	C00327	2.87	3.32	-0.45
		Acetoacetyl-CoA	C00332	4.66	4.44	0.22
		Dihydroorotate	C00337	4.92	4.74	0.19
		6-phospho-D-gluconate	C00345	2.42	2.77	-0.35
		Glucosamine-6 phosphate	C00352	2.94	3.64	-0.70
		Fructose-1,6-bisphosphate	C00354	1.82	2.04	-0.22
		dAMP	C00360	5.05	4.75	0.30
		dGMP	C00362	4.29	4.30	-0.01
		Cytosine	C00380	4.85	4.26	0.59
		Guanosine	C00387	5.79	5.18	0.61
		Aconitate	C00417	4.79	4.46	0.33
		N-acetyl-ornithine	C00437	4.36	3.21	1.16
		Carbamyl-aspartate	C00438	3.23	3.71	-0.48
		Cytidine	C00475	5.59	4.84	0.75
		Shikimate	C00493	4.85	4.63	0.22
		ADP-glucose	C00498	5.37	4.61	0.76
		Cyclic-AMP	C00575	4.45	4.68	-0.22
		Histidinol	C00860	4.89	4.63	0.26
		Quinolate	C03722	4.94	4.72	0.22
	S.cerevisiae	NADH	C00004	3.35	4.09	-0.75
		ADP	C00008	3.20	3.42	-0.22
		AMP	C00020	3.80	3.57	0.22
		Pyruvate	C00022	2.91	2.68	0.22
		Succinate	C00042	3.47	3.25	0.22

		L-Arginine	C00062	1.45	3.02	-1.58		
		L-Glutamine	C00064	1.09	2.41	-1.32		
		Phosphoenolpyruvate	C00074	3.72	3.62	0.11		
		L-Tryptophan	C00078	4.52	4.63	-0.11		
		L-Phenylalanine	C00079	3.46	4.41	-0.95		
		L-Tyrosine	C00082	3.80	4.33	-0.54		
		D-Fructose 6-phosphate	C00085	3.49	3.45	0.04		
		D-Glucose 6-phosphate	C00092	2.43	2.48	-0.05		
		sn-Glycerol 3-phosphate	C00093	3.30	3.08	0.22		
		Glycerone phosphate	C00111	3.14	3.24	-0.10		
		Fumarate	C00122	2.78	3.73	-0.95		
		GMP	C00144	4.22	3.78	0.44		
		Adenine	C00147	4.30	5.59	-1.29		
		Malate	C00149	2.77	2.77	0.01		
		Citrate	C00158	2.83	2.61	0.22		
		6-Phospho-D-gluconate	C00345	3.06	2.84	0.22		
		D-Fructose 1,6-bisphosphate	C00354	2.06	2.04	0.02		
		Test Set	E.coli	S-adenosyl-L-methionine	C00019	3.74	3.68	0.06
				GDP	C00035	3.17	3.21	-0.04
				Succinate	C00042	3.24	3.05	0.20
Glutamine	C00064			2.42	2.36	0.06		
Serine	C00065			4.17	3.64	0.53		
Tryptophan	C00078			4.92	4.69	0.23		
Phenylalanine	C00079			4.74	4.35	0.39		
Dihydroxyacetonephosphate	C00111			3.43	2.89	0.53		
PRPP	C00119			3.59	3.23	0.36		
Glutathione disulfide	C00127			2.63	2.87	-0.25		
dATP	C00131			4.81	4.19	0.62		
Histidine	C00135			4.17	3.79	0.38		
Myo-inositol	C00137			5.24	4.94	0.30		
4-Hydroxybenzoate	C00156			4.28	4.66	-0.38		
Valine	C00183			2.40	3.59	-1.19		
Threonine	C00188			3.75	3.52	0.23		
3-Phosphoglycerate	C00197			2.81	3.45	-0.63		
Adenosine-phosphosulfate	C00224			5.18	4.66	0.52		
Guanine	C00242			3.73	4.97	-1.24		
Deoxyguanosine	C00330			6.28	5.28	1.00		
dTDP	C00363	3.42	3.29	0.13				
dCTP	C00458	4.46	2.55	1.91				

		dTTP	C00459	2.34	3.33	-1.00
		Deoxyadenosine	C00559	5.55	6.04	-0.49
	S.cerevisiae	ATP	C00002	2.47	2.08	0.39
		NAD+	C00003	3.33	2.86	0.46
		L-Glutamate	C00025	1.09	1.52	-0.44
		2-Oxoglutarate	C00026	2.95	3.36	-0.40
		GDP	C00035	3.66	3.21	0.45
		L-Alanine	C00041	1.61	2.42	-0.81
		GTP	C00044	3.23	2.02	1.21
		L-Aspartate	C00049	1.80	2.41	-0.60
		D-Glucose 1-phosphate	C00103	4.05	3.49	0.56
		D-Ribose 5-phosphate	C00117	3.39	3.20	0.18
		L-Asparagine	C00152	2.33	3.80	-1.47
		3-Phospho-D-glycerate	C00197	3.05	3.45	-0.39
		D-Ribulose 5-phosphate	C00199	4.70	3.14	1.56
		Isocitrate	C00311	3.72	3.22	0.50
		Pantothenate	C00864	3.68	3.63	0.05

L-Asparagine	C00152	4.66E-03	0	2	0.33203515	2.7589712	-0.45936516	8.5307722	0	0	22.50805	0	0	-3.544	0.152	0
Citrate	C00158	1.47E-03	0.33333333	3	0.28641728	2.8216975	-0.70779455	63.881168	0	0	31.61699	0	0	-1.998	0.126	1
3-Phospho-D-glycerate	C00197	8.90E-04	0	3	0.22090781	2.7090659	-0.68446761	8.5307722	0	0	30.51699	15.676527	0	-2.337	0.186	0
D-Ribulose 5-phosphate	C00199	2.00E-05	0	5	0.42681855	2.8199623	-0.57482624	8.5307722	0	0	61.03399	15.676527	0	-3.058	0.152	0
Isocitrate	C00311	1.90E-04	0.0952381	7	0.4389635	2.8126755	-0.70789599	42.213158	0	0	26.47555	0	0	-2.072	0.112	0
6-Phospho-D-gluconate	C00345	8.70E-04	0	2	0.45794708	2.8827114	-0.67311466	8.5307722	0	0	55.89255	15.676527	0	-4.157	0.122	0
D-Fructose 1,6-bisphosphate	C00354	8.76E-03	1	2	0.35713339	2.9941537	-0.67311382	32.012836	0	1	69.49251	31.353054	0	-4.186	0.107	0
Pantothenate	C00864	2.10E-04	0	2	0.34613365	2.923965	-0.43633202	79.255997	12.949531	0	125.4419	66.652031	0	-1.494	0.115	0
L-Serine	C00065	0.00077	0	6	0.39069223	2.7133796	-0.44136977	0	0	0	28.75803	0	0	-2.811	0.187	0
D-Glucose 1-phosphate	C00103	0.00023	0	7	0.50497961	2.9663177	-0.55763352	39.541901	0	1	55.89255	15.676527	1	-2.677	0.136	0
D-Ribose 5-phosphate	C00117	0.00024	0	5	0.49509793	2.9520912	-0.629421	8.5307722	0	1	47.43403	15.676527	0	-3.131	0.154	0
D-Glyceraldehyde 3-phosphate	C00118	0.00012	0.04444444	10	0.2391061	2.7103465	-0.63274568	8.5307722	0	0	30.51699	15.676527	0	-2.131	0.213	0
L-Leucine	C00123	0.00123	0	1	0.2142	2.8748624	-0.33988363	47.089787	0	0	83.53349	66.652031	0	-1.667	0.22	1
L-Valine	C00183	0.00601	0	1	0.2142	2.8494208	-0.31706995	29.857702	0	0	67.72499	66.652031	0	-2.286	0.231	0
(S)-Lactate	C00186	0.00369	0	1	0.31986156	2.6253042	-0.57461077	12.796158	0	0	37.86697	33.326015	0	-0.734	0.248	0
L-Threonine	C00188	0.00081	0	3	0.36300907	2.7927809	-0.3988986	12.796158	0	0	44.56652	33.326015	0	-2.502	0.183	0
D-Ribulose 5-phosphate	C00199	0.00043	0	5	0.42681855	2.8199623	-0.57482624	8.5307722	0	0	61.03399	15.676527	0	-3.058	0.152	0
Isocitrate	C00311	0.00026	0.2	5	0.4389635	2.8126755	-0.70789599	42.213158	0	0	26.47555	0	0	-2.072	0.112	0
L-Isoleucine	C00407	0.00037	0	1	0.2142	2.8866551	-0.31279653	38.388474	0	0	83.53349	66.652031	0	-1.757	0.22	0

Bacillus subtilis

Figure S1. Distribution of predictive errors in both training set (a) and test set (b).

