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Supplementary material:

Table 1: Compound identification in *E. coli* metabolome analysis

Structural formula	PubChemID	Predicted retention time	Database
CC(O)(C(=O)OCCO)n1cnc2c(N)ncnc12	5745135	1.109	PubChem
CC(=O)Nc1nc(=O)n2cnc(CC(O)CO)c2[nH]1	5273998	1.087	PubChem
CC1NC(C(O)C1O)c2[nH]nc3c(=O)[nH]c(=O)[nH]c23	9881807	1.187	PubChem
Nc1ncnc2n(cnc12)C3OC(CO)C(O)C3O	191	1.229	PubChem, ChEBI, MetaCyc, EcoCyc
CC1OC(C(O)C1O)n2cnc3c(=O)nc(N)[nH]c23	101255	1.241	PubChem
CC(=O)OCCCOn1cnc2c(=O)nc(N)[nH]c12	6320052	0.807	PubChem
CC(=O)OCCOCn1cnc2[nH]c(N)nc(=O)c12	11346170	0.807	PubChem
CC(=O)OCCOCn1cnc2c(=O)nc(N)[nH]c12	3011667	0.807	PubChem
CC(=O)Nc1nc(=O)c2n(COCCO)cnc2[nH]1	11471131	0.79	PubChem
CC(=O)Nc1nc(=O)c2ncn(COCCO)c2[nH]1	3109164	0.79	PubChem
CC(=NNC(=O)C(=O)N)CCn1[nH]c(=O)ccc1=O	365874	0.758	PubChem
CC(O)C(O)C(O)c1cnc2[nH]c(N)nc(=O)c2n1	5007917	0.747	PubChem
CC(=C1C(=O)NC(=O)N(CC=C)C1=O)NNC(=O)N	6807374	0.689	PubChem
NC1=C2N=CN(C3OC(CO)C(O)C3=O)C2N=CN1	443235	0.673	ChEBI, MetaCyc
NC(COC1OC(CO)C(O)C(O)C1O)C(=O)O	132873	0.662	ChEBI
NC(C(O)CC(=O)C(=O)O)C(O)C(O)C(O)CO	349961	0.654	ChEBI
NC(C(O)CC(=O)C(=O)O)C(O)C(O)C(O)CO	5460034	0.654	ChEBI
CC1NC(C(O)C1O)C2NN=C3C2=NC(=O)NC3=O	9881806	0.654	PubChem
CC1OC(C(O)C1O)n2ccn3c(=O)nc(N)nc23	11300122	0.654	PubChem

This table shows the results for candidate compounds obtained by mass-based database search. These compounds are sorted by the difference between the measured retention time (1.1338) and the predicted retention time. The fourth compound colored gray is the only one registered in the *E. coli* compound database EcoCyc and was successfully identified as the target compound.