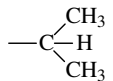
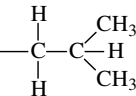
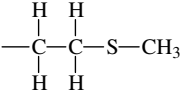
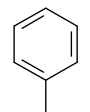
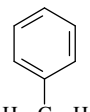
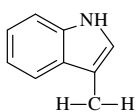
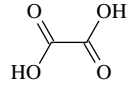
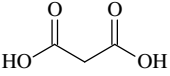
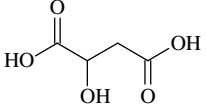
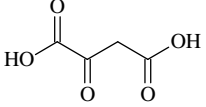
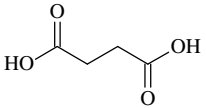
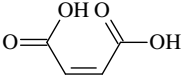
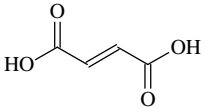
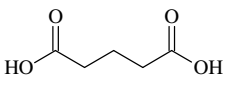
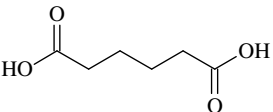


Supplementary Table S1. C2-substituted monocarboxylate substrates X-CHR-COO⁻.

Substrate	X	R	X=NH ₃ ⁺ aa analog	Hydrophobicity of R (7)	Size of R	pK
glycolate	OH					3.82
glyoxylate	O	—H	glycine	0.48	-1.90	3.32
acetate	H					4.76
lactate	OH					3.86
pyruvate	O	—CH ₃	alanine	0.62	-1.46	2.50
propionate	H					4.87
α-hydroxyisovalerate	OH		valine	1.08	-0.59	
α-ketoisovalerate	O					4.77
isovalerate	H					
α-hydroxyisocaproate	OH		leucine	1.06	-1.16	
α-ketoisocaproate	O					4.84
isocaproate	H					
2-hydroxy-4-methylthiobutyrate	OH		methionine	0.64	-1.16	
2-keto-4-methylthiobutyrate	O					
4-methylthiobutyrate	H					
phenylglycolate	OH		phenylglycine			3.41
phenylglyoxylate	O					2.15
phenylacetate	H					4.31
phenyllactate	OH		phenylalanine	1.19	1.15	
phenylpyruvate	O					4.66
phenylpropionate	H					
indole-3-lactate	OH		tryptophan	0.81	2.45	
indole-3-pyruvate	O					4.77
indole-3-propionate	H					

Supplementary Table S2. Dicarboxylate substrates of CitP.

Common name	Number of C atoms	OH substituent	Structural formula	pK
Oxalate	2	-		(1) 1.23
			(2) 4.19	
Malonate	3	H		(1) 2.83
			(2) 5.69	
Malate	4	OH		(1) 3.40
			(2) 5.11	
Oxaloacetate	4	O		(1) 2.22
			(2) 3.89	
Succinate	4	H		(1) 4.16
			(2) 5.61	
Maleate (cis)	4	H		(1) 1.83
			(2) 6.07	
Fumarate (trans)	4	H		(1) 3.03
			(2) 4.44	
Glutarate	5	H		(1) 4.31
			(2) 5.41	
Adipate	6	H		(1) 4.43
			(2) 5.41	