3-hydroxypropionyl-CoA synthase 6.2.1.36

1 Nomenclature

EC number
6.2.1.36

Systematic name
hydroxypropionate:CoA ligase (AMP-forming)

Recommended name
3-hydroxypropionyl-CoA synthase

Synonyms
3-hydroxypropionyl-CoA synthetase (AMP-forming) <1> [2]

2 Source Organism

<1> *Metallosphaera sedula* (UNIPROT accession number: A4YGR1) [1,2]
<2> *Sulfolobus tokodaii* (UNIPROT accession number: Q973W5) [1]

3 Reaction and Specificity

Catalyzed reaction
3-hydroxypropionate + ATP + coenzyme A = 3-hydroxypropionyl-CoA + AMP + diphosphate

Natural substrates and products
- **S** 3-hydroxypropionate + ATP + coenzyme A <1,2> (<1,2> the enzyme is involved in autotrophic CO_2 fixation [1]; <1> the enzyme is involved in the autotrophic 3-hydroxypropionate/4-hydroxybutyrate cycle (autotrophic carbon dioxide assimilation pathway in archaea) [2]) (Reversibility: ?) [1,2]
- **P** 3-hydroxypropionyl-CoA + AMP + diphosphate

Substrates and products
- **S** 3-chloropropionate + ATP + coenzyme A <2> (<2> 64% of the activity with 3-hydroxypropionate [1]) (Reversibility: ?) [1]
- **P** 3-chloropropionyl-CoA + AMP + diphosphate
- **S** 3-hydroxypropionate + ATP + coenzyme A <1,2> (<1,2> the enzyme is involved in autotrophic CO_2 fixation [1]; <1> the enzyme is involved in the autotrophic 3-hydroxypropionate/4-hydroxybutyrate cycle (autotrophic carbon dioxide assimilation pathway in archaea) [2]; <1> the en-

D. Schomburg and I. Schomburg (eds.), *Class 3.4–6 Hydrolases, Lyases, Isomerases, Ligases: EC 3.4–6*, Springer Handbook of Enzymes S10, DOI 10.1007/978-3-642-36260-6_86,

zyme is specific for 3-hydroxypropionate and propionate [1]) (Reversibility: ?) [1,2]
P 3-hydroxypropionyl-CoA + AMP + diphosphate
S 3-hydroxypropionate + CTP + coenzyme A <1> (<1> 13% of the activity with ATP [1]) (Reversibility: ?) [1]
P 3-hydroxypropionyl-CoA + CMP + diphosphate
S 3-hydroxypropionate + UTP + coenzyme A <1> (<1> 32% of the activity with ATP [1]) (Reversibility: ?) [1]
P 3-hydroxypropionyl-CoA + UMP + diphosphate
S 3-mercaptopropionate + ATP + coenzyme A <2> (<2> 36% of the activity with 3-hydroxypropionate [1]) (Reversibility: ?) [1]
P 3-mercaptopropionyl-CoA + AMP + diphosphate
S acetate + ATP + coenzyme A <1,2> (<1> 42% of the activity with 3-hydroxypropionate [1]; <2> 65% of the activity with 3-hydroxypropionate [1]) (Reversibility: ?) [1]
P acetyl-CoA + AMP + diphosphate
S acrylate + ATP + coenzyme A <1,2> (<1> 77% of the activity with 3-hydroxypropionate [1]; <2> 96% of the activity with 3-hydroxypropionate [1]) (Reversibility: ?) [1]
P acryloyl-CoA + AMP + diphosphate
S butyrate + ATP + coenzyme A <1,2> (<1> 20% of the activity with 3-hydroxypropionate [1]; <2> 27% of the activity with 3-hydroxypropionate [1]) (Reversibility: ?) [1]
P butyryl-CoA + AMP + diphosphate
S propionate + ATP + coenzyme A <1,2> (<2> 98% of the activity with 3-hydroxypropionate [1]; <1> the enzyme is specific for 3-hydroxypropionate and propionate [1]) (Reversibility: ?) [1]
P propionyl-CoA + AMP + diphosphate
S Additional information <1,2> (<1,2> less than 1% of the activity with 3-hydroxypropionate: 3-hydroxybutyrate, crotonate, glycerate, malonate [1]) (Reversibility: ?) [1]
P ?

Turnover number (s^{-1})

5.4 <1> (acrylate, <1> pH 8.5, 45°C [1]) [1]
5.6 <1> (aropionate, <1> pH 8.5, 45°C [1]) [1]
5.7 <1> (3-hydroxypropionate, <1> pH 8.5, 45°C [1]) [1]

Specific activity (U/mg)

6.7 <2> (<2> pH 8,5, 65°C [1]) [1]
18 <1> (<1> pH 8,5, 45°C, autotrophically grown cells [1]) [1]

K_m-Value (mM)

0.045 <1> (ATP, <1> pH 8.5, 45°C [1]) [1]
0.12 <1> (propionate, <1> pH 8.5, 45°C [1]) [1]
0.18 <1> (3-hydroxypropionate, <1> pH 8.5, 45°C [1]) [1]
1.42 <1> (acrylate, <1> pH 8.5, 45°C [1]) [1]

pH-Optimum

8.5 <1,2> (<1,2> assay at [1]) [1]

Temperature optimum (°C)

45 <1> (<1> assay at [1]) [1]
55 <1> (<1> assay at [2]) [2]
65 <2> (<2> assay at [1]) [1]

4 Enzyme Structure

Molecular weight

140000 <2> (<2> gel filtration [1]) [1]
340000 <1> (<1> gel filtration [1]) [1]

Subunits

dimer <2> (<2> 2 * 74000, SDS-PAGE [1]) [1]
homotetramer <1> (<1> 4 * 78000, SDS-PAGE [1]) [1]

5 Isolation/Preparation/Mutation/Application

Purification

<1> [1]
<2> (recombinant enzyme) [1]

Cloning

<2> (expression in Escherichia coli) [1]

6 Stability

Temperature stability

80 <1> (<1> 15 min, stable up to 80°C [1]) [1]
100 <1> (<1> 15 min, 50% loss of activity [1]) [1]

References

[1] Alber, B.E.; Kung, J.W.; Fuchs, G.: 3-Hydroxypropionyl-coenzyme A synthetase from Metallosphaera sedula, an enzyme involved in autotrophic CO_2 fixation. J. Bacteriol., **190**, 1383-1389 (2008)
[2] Berg, I.A.; Kockelkorn, D.; Buckel, W.; Fuchs, G.: A 3-hydroxypropionate/4-hydroxybutyrate autotrophic carbon dioxide assimilation pathway in Archaea. Science, **318**, 1782-1786 (2007)