Full list of publications

(March 09, 2020)

Of the 155 publications, 115 are found in the web of knowledge. *h*-index = 40

Theses (3)
Original Publications (98)
Reviews (42)
Miscellaneous (12)

Theses (3)

Shima, S. (1983) Effect of ammonium ion on the nitrogenase activity of *Azolla*, Bachelor thesis, Osaka Prefecture University, Osaka, Japan.

Shima, S. (1985) Microbial ecology of *Bradyrhizobium japonicum* strains, Master thesis, Osaka Prefecture University, Osaka, Japan.

Shima, S. (1991) Genetical and biochemical study on cellulases from mesophilic Clostridia, Ph.D. thesis, University of Tokyo, Tokyo, Japan.

Original Publications (98) (*corresponding author)

1. Huang, G., Wagner, T., Demmer, U., Warkentin, E., Ermler, U., & Shima, S.* (2020) The hydride transfer process in NADP dependent methylene-tetrahydromethanopterin dehydrogenase. ***J. Mol. Biol.*** doi: 10.1016/j.jmb.2020.01.042.

2. Hemmann, J.L., Wagner, T., Shima, S., & Vorholt, J.A.* (2019) Methylofuran is a prosthetic group of the formyltransferase/hydrolase complex and shuttles one-carbon units between two active sites. ***Proc. Natl. Acad. Sci. USA*** 116, 25583-25590.

3. Ilina, Y., Lorent, C., Katz, S., Jeoung, J.H., Shima, S., Horch, M.*, Zebger, I.* & Dobbek, H.* (2019) X-ray crystallography and vibrational spectroscopy reveal key determinants of biocatalytic dihydrogen cycling by [NiFe] hydrogenases. ***Angew. Chem. Int. Edit.*** 58,

18710-18714.

4. Huang, G., Wagner, T., Wodrich, M.D., Ataka, K., Bill, E., Ermler, U., Hu, X. & Shima, S.* (2019) The atomic-resolution crystal structure of activated [Fe]-hydrogenase. ***Nat. Catal.*** 2, 537-543.

5. Pan, H-J, Huang, G., Wodrich, M.D. Tirani, F.F. Ataka, K., Shima, S.* & Hu, X.* (2019) A catalytically active [Mn]-hydrogenase incorporating a non-native metal cofactor. ***Nat. Chem.*** 11, 669–675.

6. Engilberge, S., Wagner, T., Santoni, G., Breyton, C., Shima, S., Franzetti, B., Riobé, F., Mauryd, O. & Girard, E.* (2019) Protein crystal structure determination with the crystallophore, a nucleating and phasing agent. ***J. Appl. Crystalogr.*** 52: 722-731.

7. Vögeli, B., Shima, S., Erb, T.* & Wagner, T.* (2019) Crystal structure of archaeal HMG-CoA reductase: insights into structural changes of the C-terminal helix of the class-I enzyme. ***FEBS Lett.*** 593, 543–553.

8. Watanabe, T., Wagner, T., Huang, G., Kahnt, J., Ataka, K., Ermler, U. & Shima, S.* (2019) The bacterial [Fe]-hydrogenase paralog HmdII uses tetrahydrofolate derivatives as substrates. ***Angew. Chem. Int. Ed.*** 58, 3506 –3510.

9. Bernhardsgrütter, I., Vögeli, B., Wagner, T., Peter, D.M., Cortina, N.S., Kahnt, J., Bange, G., Engilberge, S., Girard, E., Riobé, F., Maury, O., Shima, S., Zarzycki, J. & Erb, T.J.* (2018) The multicatalytic compartment of propionyl-CoA synthase sequesters a toxic metabolite. ***Nat. Chem. Biol.*** 14, 1127–1132.

10. Wagner, T., Huang. G., Ermler, U. & Shima, S.* (2018) How [Fe]-hydrogenase from *Methanothermobacter* is protected against light and oxidative stress. ***Angew. Chem. Int. Ed.*** 57, 15056-15059.

11. Vögeli, B., Rosenthal, R.G., Stoffel, G.M.M., Wagner, T., Kiefer, P., Cortina, N.S., Shima, S. and Erb, T.J.* (2018) InhA, the enoyl-thioester reductase from *Mycobacterium tuberculosis* forms a covalent adduct during catalysis. ***J. Biol. Chem.*** 293, 17200-17207.

12. Engilberge. S., Riobé, F.*, Wagner, T., Di Pietro, S., Breyton, C., Franzetti, B., Shima, S., Girard, E.*, Dumont, E. & Maury, O.* (2018) Unveiling the binding modes of the crystallophore, a terbium-based nucleating and phasing molecular agent for protein crystallography. ***Chem. Eur. J.*** 24, 9739-9746.

13. Vögeli, B., Engilberge, S., Girard, E., Riobé, F., Maury, O., Erb, T. J., Shima, S. & Wagner, T.* (2018) The archaeal acetoacetyl-CoA-thiolase/HMG-CoA-synthase complex channels the intermediate via a fused CoA-binding site. ***Pros. Natl. Acad. Sci. USA*** 115, 3380-3385.

14. Huang, G., Wagner, T., Ermler, U. Bill, E., Ataka, K. & Shima, S.* (2018) Dioxygen sensitivity of [Fe]-hydrogenase in the presence of reducing substrates. ***Angew. Chem. Int. Ed.***

57, 4917-4920.

15. Wagner, T., Koch, J., Ermler, U. & Shima, S.* (2017) Methanogenic heterodisulfide reductase (HdrABC-MvhAGD) uses two noncubane [4Fe-4S] clusters for reduction. ***Science*** 357, 699–703.

16. Bai, L., Wagner, T., Xu, T., Hu, X., Ermler, U. & Shima, S.* (2017) Water-bridged H-bonding network contributes to the catalysis of a SAM-dependent C-methyltransferase HcgC. ***Angew. Chem, Int. Ed.***, 56, 10806–0809.

17. Wagner, T., Wegner, C.-E., Kahnt, J., Ermler, U. & Shima, S.* (2017) Phylogenetic and structural comparisons of the three types of methyl- coenzyme M reductase from *Methanococcales* and *Methanobacteriales*. ***J. Bacteriol.*** 357, 699–703.

18. Rosenthal, R.G., Vögeli, B., Wagner, T., Shima, S. & Erb, T.J.* (2017) 'Negative catalysis' by a conserved threonine prevents self-intoxication of enoyl-thioester reductases. ***Nat. Chem. Biol.*** 13, 745-749.

19. Bai, L., Fujishiro, T., Huang, G., Koch, J., Takabayashi, A., Yokono, M., Tanaka, A., Xu, T., Hu, X., Ermler, U. & Shima, S.* (2017) Towards artificial methanogenesis: biosynthesis of the [Fe]-hydrogenase cofactor and characterization of the semisynthetic hydrogenase. ***Faraday Discussion***, 198, 37-58.

20. Wagner, T., Ermler, U. & Shima, S.* (2016) The methanogenic CO_2 reducing-and-fixing enzyme is bifunctional and contains 46 [4Fe-4S] clusters. ***Science*** 354: 114-117.

21. Wagner, T., Kahnt, J., Ermler, U. & Shima, S.* (2016) Didehydroaspartate modification in methyl-coenzyme M reductase catalyzing methane formation. ***Angew. Chem. Int. Ed.*** 55: 10630-10633.

22. Upadhyay, V., Ceh, K., Tumulka, F., Abele, R., Hoffmann, J., Langer, J., Shima, S.* & Ermler, U.* (2016) Molecular characterization of methanogenic N^5-methyl-tetrahydromethanopterin: coenzyme M methyltransferase. ***Biochim. Biophys. Acta.***1858: 2140-2144.

23. Fujishiro, T., Bai, L., Xu, T., Xie, X., Schick, M. Kahnt, J., Rother, M., Hu, X., Ermler, U. & Shima, S.* (2016) Identification of HcgC as SAM-dependent pyridinol methyltransferase in [Fe]-hydrogenase cofactor biosynthesis. ***Angew. Chem. Int. Ed.*** 55: 9648-9651.

24. Wagner, T., Ermler, U. & Shima, S.* (2016) MtrA of the sodium ion pumping methyltransferase binds cobalamin in a unique mode. ***Sci. Rep.*** 6, 28226. doi: 10.1038/srep28226.

25. Duin, E.C., Wagner, T., Shima, S., Prakash, D., Cronin, B., Yáñez-Ruiz, D.R., Duval, S., Ruembeli, R., Stemmler, R.T., Thauer, R.K.* & Kindermann, M.* (2016) Mode of action uncovered for the specific reduction of methane emissions from ruminants by the small

molecule 3-nitrooxypropanol. ***Proc. Natl. Acad. Sci. USA***, 113, 6172-6177.

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28. Fujishiro, T., Ataka, K., Ermler, U. & Shima, S.* (2015) Towards a functional identification of catalytically inactive [Fe]-hydrogenase paralogs. ***FEBS J.*** 282, 3412–3423.

29. Fujishiro, T., Kahnt, J., Ermler, U. & Shima, S.* (2015) Protein-pyridinol thioester precursor for biosynthesis of the organometallic acyl-iron ligand in [Fe]-hydrogenase cofactor, ***Nat. Commun.*** 6: 6895, doi:10.1038/ncomms7895.

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31. Fujishiro, T., Ermler U. & Shima, S.* (2014) A possible iron delivery function of the dinuclear iron center of HcgD in [Fe]-hydrogenase cofactor biosynthesis. ***FEBS Lett.*** 588: 2789-2793.

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of coenzyme F_{430} in deep-sea sediments, a key molecule for biological methanogenesis. ***Organic Geochemistry***, 58, 137−140.

38. Mills, D.J., Vitt, S., Strauss, M., Shima, S. & Vonck, J.* (2013) De novo modeling of the F_{420}-reducing [NiFe]-hydrogenase from a methanogenic archaeon by cryo-electron microscopy. ***eLife***, 2, e00218.

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