

Full list of publications

(September 15, 2020)

Of the 157 publications, 119 are found in the web of knowledge. *h*-index = 41

Theses (3)
Original Publications (100)
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 (100) (*corresponding author)

1. Huang, G., Arriaza-Gallardo, F.J., Wagner, T., Shima S.* (2020) Crystal structures of [Fe]-hydrogenase from *Methanobacillus paynteri* suggest a path of the FeGP-cofactor incorporation process. *Inorganics*, in press.
2. Engilberge, S., Wagner, T., Carpentier, P., Girarde, E.* and Shima, S.* (2020) Krypton-derivatization highlights O₂-channeling in a four-electron reducing oxidase. *Chem. Comm.* doi: 10.1039/D0CC04557H.
3. 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.* 432, 2042-2054.

4. Hemmann, J.L., Wagner, T., Shima, S., & Vorholt, J.A.* (2019) Methylfuran 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.
5. 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.
6. 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.
7. 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.
8. 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. Crystallogr.* 52: 722-731.
9. 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.
10. 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.
11. 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.
12. 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.
13. 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.
14. 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.

15. 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.
16. 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.
17. 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.
18. 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.
19. 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.
20. 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.
21. 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.
22. Wagner, T., Ermler, U. & Shima, S.* (2016) The methanogenic CO₂ reducing-and-fixing enzyme is bifunctional and contains 46 [4Fe-4S] clusters. *Science* 354: 114-117.
23. 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.
24. Upadhyay, V., Ceh, K., Tumulka, F., Abele, R., Hoffmann, J., Langer, J., Shima, S.* & Ermler, U.* (2016) Molecular characterization of methanogenic N⁵-methyl-tetrahydromethanopterin: coenzyme M methyltransferase. *Biochim. Biophys. Acta.* 1858: 2140-2144.
25. 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.

26. 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.
27. 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.
28. Shima, S.*, Chen, D., Xu, X., Wodrich, M.D., Fujishiro, T., Schultz, K.M., Kahnt, J., Ataka, K. & Hu, X.* (2015) Reconstitution of [Fe]-hydrogenase using model complexes. *Nat. Chem.* 7, 995-1002.
29. Hidese, R., Ataka, K., Bill. E. & Shima, S.* (2015) Cu^I and H₂O₂ inactivate and Fe^{II} inhibits [Fe]-hydrogenase at very low concentrations. *ChemBioChem* 16, 1861–1865.
30. Fujishiro, T., Ataka, K., Ermler, U. & Shima, S.* (2015) Towards a functional identification of catalytically inactive [Fe]-hydrogenase paralogs. *FEBS J.* 282, 3412–3423.
31. 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.
32. Kojima, H., Moll, J., Kahnt, J., Fukui, M. & Shima, S.* (2014) A reversed genetic approach reveals the coenzyme specificity and other catalytic properties of three enzymes putatively involved in anaerobic oxidation of methane with sulfate. *Environ. Microbiol.* 16: 3431–3442.
33. 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.
34. Vitt, S., Ma, K., Warkentin, E., Moll, J., Pierik, A.J., Shima, S.* & Ermler, U.* (2014) The F₄₂₀-reducing [NiFe]-hydrogenase complex from *Methanothermobacter marburgensis*, the first X-ray structure of a group 3 family member. *J. Mol. Biol.* 426: 2813-2826.
35. Kaneko, M.*, Takano, Y., Chikaraishi, Y., Ogawa, N.O., Asakawa S., Watanabe, T., Shima, S., Krüger, M., Matsushita, M., Kimura, H. & Ohkouchi, N. (2014) Quantitative analysis of coenzyme F430 in environmental samples: a new diagnostic tool for methanogenesis and anaerobic methane oxidation. *Anal Chem.* 86: 3633-3638.
36. Fujishiro, T., Tamura, H., Schick, M., Kahnt, J., Xie, X., Ermler, U. & Shima, S.* (2013) Identification of the HcgB enzyme in [Fe]-hydrogenase-cofactor biosynthesis. *Angew. Chem. Int. Ed.* 52, 12555 –12558.

37. Tamura, H., Salomone-Stagni, M., Fujishiro, T., Warkentin, E., Meyer-Klaucke, W., Ermler, U. & Shima, S.* (2013) Crystal structures of [Fe]-hydrogenase in complex with inhibitory isocyanides: implications for H₂-activation site. *Angew. Chem. Int. Ed.* 52, 9656–9659.
38. Milucka, J.* , Widdel, F. & Shima, S. (2013) Immunological detection of enzymes for sulfate reduction in anaerobic methane-oxidizing consortia. *Environ. Microbiol.* 15, 1561–1571.
39. Takano, Y.* , Kaneko, M., Kahnt, J., Imachi, H., Shima, S. & Ohkouchi, M. (2013) Detection of coenzyme F₄₃₀ in deep-sea sediments, a key molecule for biological methanogenesis. *Organic Geochemistry*, 58, 137–140.
40. Mills, D.J., Vitt, S., Strauss, M., Shima, S. & Vonck, J.* (2013) De novo modeling of the F₄₂₀-reducing [NiFe]-hydrogenase from a methanogenic archaeon by cryo-electron microscopy. *eLife*, 2, e00218.
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42. Schick, M., Xie, X., Ataka, K., Kahnt, J., Linne, U. & Shima, S.* (2012) Biosynthesis of the iron-guanylylpyridinol cofactor of [Fe]-hydrogenase in methanogenic archaea as elucidated by stable-isotope labeling. *J. Am. Chem. Soc.* 134, 3271–3280.
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44. Shima, S.*, Schick, M., Kahnt, J., Ataka, K., Steinbach, K. & Linne, U. (2012) Evidence for acyl-iron ligation in the active site of [Fe]-hydrogenase provided by mass spectrometry and infrared spectroscopy. *Dalton Trans.* 41, 767–771.
45. Basen, M., Krüger, M., Milucka, J., Kuever, J., Kahnt, J., Grundmann, O., Meyerdierks, A., Widdel, F. & Shima, S.* (2011) Bacterial enzymes for dissimilatory sulfate reduction in a marine microbial mat (Black Sea) mediating anaerobic oxidation of methane. *Environ. Microbiol.* 13, 1370–1379.
46. Shima, S.* & Ataka, K. (2011) Isocyanides inhibit [Fe]-hydrogenase with very high affinity. *FEBS Lett.* 585, 353–356.
47. Shima, S.*, Vogt, S., Göbels, A. & Bill E. (2010) Iron-chromophore circular dichroism of [Fe]-hydrogenase: the conformational change required for H₂ activation. *Angew. Chem. Int. Ed.* 49, 9917–9921.
48. Salomone-Stagni, M., Stellato, F., C. Matthew Whaley, M., Vogt, S., Morante, S., Shima, S., Rauchfuss, T.B. & Meyer-Klaucke, W.* (2010) The iron-site structure of [Fe]-hydrogenase

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49. Ceh, K., Demmer, U., Warkentin, E., Moll, J., Thauer, R.K., Shima, S. & Ermler, U.* (2009) Structural basis of the hydride transfer mechanism in F₄₂₀ dependent methylene-tetrahydromethanopterin dehydrogenase. *Biochemistry* 48, 10098–10105.
 50. Hiromoto, T., Warkentin, E., Moll, J., Ermler, U. & Shima, S.* (2009) The crystal structure of an [Fe]-hydrogenase substrate complex reveals the framework for H₂-activation. *Angew. Chem. Int. Ed.* 48, 6457–6460.
 51. Hiromoto, T., Ataka, K., Pilak, O., Vogt, S., Stagni, M.S., Meyer-Klaucke, W., Warkentin, E., Thauer, R.K., Shima, S.* & Ermler, U.* (2009) The crystal structure of C176A mutated [Fe]-hydrogenase suggests an acyl-iron ligation in the active site iron complex. *FEBS Lett.* 583, 585–590.
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