

Publications

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Books

Bergfors, T., Editor. **Protein Crystallization: Third Edition.** 2022. International University Line, La Jolla, California, 670 pp.

Bergfors, T., Editor. **Protein Crystallization: Second Edition.** 2009. International University Line, La Jolla, California, 500 pp.

Bergfors, T., Editor. **Protein Crystallization: Techniques, Strategies, and Tips.** 1999. International University Line, La Jolla, California, 300 pp.

Journal articles or book chapters

2025 (in press)

Newman, J. and Bergfors, T. The starting point for biomolecular crystallisation. In: **Biomacromolecular crystallization across experimentation and modeling.** Springer Nature Switzerland.

2024

Huseby, D.L., Cao, S., Zamaratski, E., Sooriyaarachchi, S., Ahmad, S., Bergfors, T., etc. Antibiotic class with potent in vivo activity targeting lipopolysaccharide synthesis in Gram-negative bacteria. **PNAS** 121, e2317274121.

2020

Bergfors, T., Majumdar, S. Commentary: Screening cells for crystals: a synergistic approach. **J. Appl. Crystallography** 53, 1414-1415.

2016

Sooriyaarachchi, S., Chofor, R. Risseeuw, M, Bergfors, T., et al. Targeting an aromatic hotspot in *Plasmodium falciparum* 1-deoxy-D-xylulose-5-phosphate reductoisomerase with beta-arylpropyl analogues of fosmidomycin. **ChemMedChem** 11, 1-14.

2015

Chofor, R., Sooriyaarachchi, S., Risseeuw, M, Bergfors, T., et al. Synthesis and bioactivity of beta-substituted fosmidomycin analogies targeting 1-deoxy-D-xylulose-5-phosphate reductoisomerase. **J Med. Chem.** 58, 2988-3001.

2014

D'Arcy, A., Bergfors, T., Cowan-Jacob, S.W., Marsh, M. Microseed matrix screening for optimization in protein crystallization: what have we learned? **Acta Cryst.** F70, 1117-1126.

2013

Jansson, A., Bergfors, T., et al., DXR inhibition by potent mono- and disubstituted fosmidomycin analogues. **J. Med. Chem.** 56, 6190-6199.

Björkelid, C., Bergfors, T., Raichurkar, A.K.V., Mukherjee, K., Malolanarasimhan, K., Bhandodkar, B., Jones, T.A. Structural and biochemical characterization of

compounds inhibiting *Mycobacterium tuberculosis* patothenate kinase. **J. Biol. Chem.** 288, 18260-18270.

2012

Björkelid, C., Bergfors, T., Unge, T., Mowbray, S.L., Jones, T.A. Structural studies on *Mycobacterium tuberculosis* DXR in complex with the antibiotic FR-900098. **Acta Cryst.** D68, 134-143.

Fullam, E., Pojer, F., Bergfors, T., Jones, T.A., Cole, S.T. Structure and function of the transketolase from *Mycobacterium tuberculosis* and comparison with the human enzyme. **Open Biology** 2, 1-8.

2011

Björkelid, C., Bergfors, T., Henriksson, L.M., Stern, A.L., Unge, T., Mowbray, S.L., Jones, T.A. Structural and functional studies of mycobacterial IspD enzymes. **Acta Cryst.** D67, 403-414.

Andaloussi, M., Henriksson, L., Wieckowska, A., Lindh, M., Björkelid, C., Larsson, A., Surisetti, S., Iyer, H., Bachally, S., Bergfors, T., et al. . Design, synthesis and x-ray crystallographic studies of alpha-aryl substituted fosmidomycin analogues as inhibitors of *Mycobacterium tuberculosis* 1-deoxy-D-xylulose-5-phosphate reductoisomerase. **J. Med.Chem.** 54, 4964-4976.

Stojanoff, V., Jakoncic, J., Oren, D.A., Nagarajan, V., Navarro Poulsen, J-C., Adams, Cioaba, M.A., Bergfors, T., Sommer, M.O.A. From screen to structure with a harvestable microfluidic device. **Acta Cryst.** F67, 971-975.

2009

Bergfors, T. The RAPID crystallization strategy for structure-based inhibitor design. **From Molecules to Medicines.** Editors: Sussman, J. and Spadon, P. Springer Press, 11-19

2008

Ericsson, D., Kasrayan, A., Johansson, P., Bergfors, T., Sandström, A, Bäckvall, J-E, Mowbray, S. X-ray structure of *Candida antarctica* lipase A shows a novel lid structure and a likely mode of interfacial activation. **J. Mol. Biol.** 376, 109-119.

Covarrubias, A. S., Högbom, M., Bergfors, T., Carroll, P., Mannerstedt, K., Oscarson, S., Parish, T., Jones, T.A., Mowbray, S. Structural, biochemical, and *in vivo* investigations of the threonine synthase from *Mycobacterium tuberculosis*. **J. Mol. Biol.** 381, 622-633.

2007

Ubhayasekera, W., Tang, C.M., Ho, S., Berglund, G., Bergfors, T., Chye, M-L, and Mowbray, S. Crystal structures of a family 19 chitinase from *Brassica juncea* show flexibility of binding cleft loops. **FEBS Letters.** 274, 3695-3703.

Bergfors, T. Automated liquid-handling systems for submicroliter crystallization. **Protein Crystallization for Structural Genomics.** Ed. Chayen, N. International University Line, La Jolla, California.

Bergfors, T. Succeeding with seeding: some practical advice. **Evolving Methods for Macromolecular Crystallography**. Editors: Read, R. & Sussman, J. Springer Press, 1-10.

2006

Bergfors, T. Crystallization strategy at the Uppsala University RAPID Center. **Synchrotron Radiation Science & Technology** 13, 5-9.

Bergfors, T. Screening and optimization methods for non-automated crystallization laboratories. **Methods Mol. Biol.** 363, 131-151.

2005

Covarrubias, A., Larsson, A., Högbom, M., Lindberg, J., Bergfors, T., Björkelid, C., Mowbray, S., Unge, T. and Jones, T.A. Structure and function of carbonic anhydrases from *Mycobacterium tuberculosis*. **J. Biol. Chem.** 280, 18782-18789.

Johansson, P., Unge, T., Cronin, A., Arand, M., Bergfors, T., Jones, T.A. and Mowbray, S. Structure of an atypical epoxide hydrolase from *Mycobacterium tuberculosis* gives insights into its function. **J. Mol. Biol.** 351, 1048-1056.

Larsson, A., Bergfors, T., Dultz, E., Irwin, D., Roos, A., Driguez, H., Wilson, D. and Jones, T.A. Crystal structure of *Thermobifida fusca* endoglucanase Cel6A in complex with substrate and inhibitor: the role of tyrosine Y73 in substrate ring distortion. **Biochemistry** 44, 12915-12922.

2004

Roos, A., Anderson, C.E., Bergfors, T., Jacobsson, M, Karlen, A, Unge, T., Jones, T.A., and Mowbray, S. *Mycobacterium tuberculosis* ribose-5-phosphate isomerase has a known fold, but a novel active site. **J. Mol. Biol.** 335, 799-809.

2003

Bergfors, T. Seeds to Crystals. **J. Struct. Biol.** 142, 66-76.

Johansson, P. Denman, S., Brumer, H., Kallas, Å., Henriksson, H., Bergfors, T., Teeri, T., and Jones, T.A. Crystallization and preliminary X-ray analysis of a xyloglucan endotransglycosylase from *Populus tremula x tremuloides*. **Acta Cryst.** D59, 535-537.

Jakobsson, E., Alvite, G., Bergfors, T., Esteves, A., and Kleywegt, G. The crystal structure of *Echinococcus granulosus* fatty-acid-binding protein 1. **BBA-Proteins and Proteomics** 49, 40-50.

Arand, M., Hallberg, B., Zou, J., Bergfors, T., Oesch, F., van der Werf, M., de Bont, J., Jones, T. & Mowbray, S. 1.2 Å structure of *Rhodococcus erythropolis* limonene-1,2-epoxide hydrolase reveals a novel mechanism. **EMBO J.** 22, 2583-2592.

Arand, M., Cronin, A., Oesch, F., Hallberg, M., Zou, JY, Bergfors, T., Mowbray, S., and Jones, T.A. The tell-tale structures of epoxide hydrolases. **Drug Metabolism Reviews** 35:7 Suppl. 1.

2002-1984

Van Aalten, D.M.F., Milne, K.G., Zou, J.Y., Kleijwegt, G., Bergfors, T., Ferguson, M.A.J., Knudsen, J. and Jones, T.A. Binding site differences revealed by crystal structures of *Plasmodium falciparum* and bovine Acyl-CoA binding protein. **J. Mol. Biol.** (2001) 309, 181-192.

Zou, J., Hallberg, B.M., Bergfors, T., Oesch, F., Arand, M., Mowbray, S. and Jones, T.A. Structure of *Aspergillus niger* epoxide hydrolase at 1.8Å resolution: implications for the structure and function of the mammalian microsomal class of epoxide hydrolases. **Structure** (2000) 8, 111-122.

Hallberg, B.M., Bergfors, T., Backbro, K., Pettersson, G., Henriksson, G., and Divne, C. A new scaffold for binding haem in the cytochrome domain of the extracellular flavocytochrome cellobiose dehydrogenase. **Structure** (2000) 8, 79-88.

Chaudhuri, B.N., Kleywegt, G.J., Broutin-L'Hermite, I., Bergfors, T., Senn, H., Le Motte, P., Partouche, O., and Jones, T.A. Structures of cellular retinoic acid binding proteins I and II in complex with synthetic retinoids. **Acta Cryst.** (1999) D55, 1850-1857.

Kleywegt, G.J., Bergfors, T., Senn, H., Le Motte, P., Gsell, B., Shudo, K., and Jones, T.A. Crystal structures of cellular retinoid acid binding proteins I and II in complex with all-trans retinoic acid and a synthetic retinoid. **Structure** (1994) 2:1241-1258.

Bergfors, T., Kleywegt, G.J., and Jones, T.A. Crystallization and X-ray analysis of recombinant bovine cellular retinoic acid binding protein. **Acta Cryst.** (1994) D50, 370-374.

Uppenberg, J., Patkar, S., Bergfors, T., and Jones, T.A. Crystallization and preliminary studies of lipase B from *Candida antarctica*. **J. Mol. Biol.** (1994) 235, 790-792.

Kuehn, M.J., Ogg, D.J., Kihlberg, J., Slonim, L., Flemmer, K., Bergfors, T., and Hultgren, S. Structural basis of pilus subunit recognition by the PapD chaperone. **Science** (1993) 272, 1234-1241.

Rouvinen, J., Bergfors, T., Teeri, T. and Jones, A. The three dimensional structure of the core protein of cellobiohydrolase II. **Science** (1990) 249, 380-386.

Jones, T.A., Cowan, S., Newcomer, M. and Bergfors, T. Crystallographic studies on two families of retinoid binding proteins. **Frontiers in Drug Research**, Alfred Benzon Symposium 28, Munksgaard, Copenhagen. (1990).

Cowan, S., Bergfors, T., Jones, T.A., Tibbelin, G., Olin, B., Board, P., and Mannervik, B. Crystallization of GST2, a human class alpha glutathione transferase. **J. Mol. Biol.** (1989) 208, 369-370.

Bergfors, T., Rouvinen, J., Lehtovaara, P., Caldentey, X., Tomme, P., Claeysens, M., Pettersson, G., Teeri, T., Knowles, J. and Jones, T.A. Crystallization of the core protein of cellobiohydrolase II from *Trichoderma reesei*. **J. Mol. Biol.** (1989) 209, 167-169.

Jones, T.A., Bergfors, T., Sedzik, J. and Unge, T. The three dimensional structure of P2 myelin protein. **EMBO J.** (1988) 7, 1597-1604.

Sedzik, J., Bergfors, T., Jones, T.A. and Weise, M. Bovine P2 myelin basic protein crystallizes in three different forms. **J. Neurochem.** (1988) 50, 1908-1913.

Bergfors, T., Sedzik, J., Unge, T., Fridborg, K., Weise, M. and Jones, T.A. Crystallization of P2 myelin protein. **J. Mol. Biol.** (1987) 198, 357-358.

Hultcrantz, R., Ericsson, J. and **Hirth, T.** Levels of malondialdehyde production in rat liver following loading and unloading with iron. **Virchows Arch (Cell Pathol)** (1984) 45, 135-146.

Abok, K., **Hirth, T.**, Ericsson, J., and Brunk, U. Effect of iron on the stability of macrophage lysosomes. **Virchows Arch (Cell Pathol)** (1983) 43, 85-101.