

BOGUSLAW P. NOCEK, Ph.D.

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RESEARCH INTERESTS

I am interested in using X-ray crystallography to understand biological processes in atomic detail. I would like to direct my structural biology skills toward challenging projects to address questions central to biological systems and understanding their functions.

A. RESEARCH EXPERIENCE

- 2008-Present **Assistant scientist/X-ray Crystallographer**
Center for Structural Genomics of Infectious Diseases, Argonne National Laboratory/University of Chicago, IL.
- 2004 – 2008 **Postdoctoral scientist/Investigator**, Midwest Center for Structural Genomics/Structural Biology Center, Argonne National Laboratory, IL.
- 2003 – 2004 **Postdoctoral fellow**, Department of Chemistry, Montana State University, Bozeman, MT
- 1999 – 2003 **Graduate assistant**, Department of Biochemistry, Utah State University, UT.

EDUCATION

- 2003 **Ph. D., Biochemistry**, Utah State University, Logan, UT
- 1999 **M. S., Chemical Engineering**, Silesian Technical University, Gliwice, Poland
- 1997 **A. A., Organization and Management**, Katowice School of Management, Poland

B. PROFESIONAL ACTIVITIES

Reviewer: Reviewer for LDRD grants in Argonne National Laboratory.
Journal reviewer of Acta Crystallographica D Biological Crystallography and Journal of Structural and Functional Genomics.

Administration and Committee:

Mentor-Mentee Program Coordinator in Biosciences Division, Argonne National Laboratory.
Chaired the chemistry and biochemistry session for the 4th Annual Postdoctoral Research Symposium, Argonne National Laboratory, 27th October 2011
Organized and guided tours of MCSG/CSGID (BIO) and SBC (APS) facilities.
Invited and hosted several seminar speakers for the Biosciences Division.

C. PUBLICATIONS

REFEREED JOURNAL ARTICLES

1. Weglarz-Tomczak A., Poreba M., Gajda A., Berlicki L., **Nocek B.**, Mulligan R., Joachimiak A., Drag M., Mucha A., *An integrated approach to the ligand binding specificity of Neisseria meningitidis M1 alanine aminopeptidase by fluorogenic substrate profiling, inhibitory studies and molecular modeling.* Biochimie accepted
2. **Nocek B.**, Tikhonov A., Babnigg G., Gu M., Zhou M., Makarova K.S., Vondenhoff G., Van Aerschot A., Kwon K., Anderson W.F., Severinov K., Joachimiak A., *Structural and functional characterization of microcin C resistance peptidase MccF from Bacillus anthracis.* J Mol Biol. 2012 Jul 20;420(4-5):366-83.
3. Forlani G., Petrollino D., Fusetti M., Romanini L., **Nocek B.**, Joachimiak A., Berlicki L., Kafarski P. *□(1)Pyrroline-5-carboxylate reductase as anew target for therapeutics:*

- inhibitor of the enzyme from Streptococcus pyogenes and effects in vivo.* Amino Acids. 2012 Jun;42(6):2283-91.
4. Babu, M., Beloglazova, N., Flick, R., Graham, C., Skarina, T., **Nocek, B.**, Gagarinova, A., Pogoutse, O., Brown, G., Binkowski, A., Phanse, S., Joachimiak, A., Koonin, E.V., Savchenko, A., Emili, A., Greenblatt, J., Edwards, A.M., Yakunin, A.F. *A dual function of the CRISPR-Cas system in bacterial antiviral immunity and DNA repair.* Mol Microbiol. 2011 Jan;79(2):484-502.
 5. **Nocek, B.**, Stein A.J., Jedrzejczak, R., Cuff, ME., Li, H., Volkart, L., Joachimiak A. *Structural studies of ROK fructokinase YdhR from Bacillus subtilis: insights into substrate binding and fructose specificity.* J Mol Biol. 2011 Feb 18;406(2):325-42.
 6. Eschenfeldt, W.H., Maltseva, N., Stols, L., Donnelly, M.I., Gu, M., **Nocek, B.**, Tan, K., Kim, Y., Joachimiak A. *Cleavable C-terminal His-tag vectors for structure determination.* J Struct Funct Genomics. 2010 Mar;11(1):31-9.
 7. **Nocek, B.**, Gillner, D., Fan, Y., Holz, R., and Joachimiak, A. (2010). *Structural Basis for Catalysis by the Mono and Dimetalated forms of the dapE-encoded N-succinyl-L,L-Diaminopimelic Acid Desuccinylase* J Mol Biol. 2010 Apr 2;397(3):617-62.
 8. Binkowski, T.A., Cuff, M., **Nocek, B.**, Chang, C., Joachimiak, A. (2010). *Assisted assignment of unknown ligand electron-density.* J Struct Funct Genomics. 2010 Mar;11(1):21-30.
 9. **Nocek, B.**, Kochinyan, S., Proudfoot, M., Brown, G., Evdokimova, E., Osipiuk, J., Edwards, A. M., Savchenko, A., Joachimiak, A. & Yakunin, A. F. (2008). *Polyphosphate-dependent synthesis of ATP and ADP by the family-2 polyphosphate kinases in bacteria.* Proc Natl Acad Sci U S A **105**, 17730-5.
 10. Kim, Y., Quartey, P., Li, H., Volkart, L., Hatzos, C., Chang, C., **Nocek, B.**, Cuff, M., Osipiuk, J., Tan, K., Fan, Y., Bigelow, L., Maltseva, N., Wu, R., Borovilos, M., Duggan, E., Zhou, M., Binkowski, T. A., Zhang, R. G. & Joachimiak, A. (2008). *Large-scale evaluation of protein reductive methylation for improving protein crystallization.* Nat Methods **5**, 853-854.
 11. Gillner, D. M., Bienvenue, D. L., **Nocek, B. P.**, Joachimiak, A., Zachary, V., Bennett, B. & Holz, R. C. (2009). *The dapE-encoded N-succinyl-L,L-diaminopimelic acid desuccinylase from Haemophilus influenzae contains two active-site histidine residues.* J Biol Inorg Chem **14**, 1-10.
 12. **Nocek, B.**, Bigelow, L., Abdullah, J. & Joachimiak, A. (2008). *Structure of SO2946 orphan from Shewanella oneidensis shows "jelly-roll" fold with carbohydrate-binding module.* J Struct Funct Genomics **9**, 1-6.
 13. **Nocek, B.**, Mulligan, R., Bargassa, M., Collart, F. & Joachimiak, A. (2008). *Crystal structure of aminopeptidase N from human pathogen Neisseria meningitidis.* Proteins **70**, 273-9.
 14. **Nocek, B.**, Evdokimova, E., Proudfoot, M., Kudritska, M., Grochowski, L. L., White, R. H., Savchenko, A., Yakunin, A. F., Edwards, A. & Joachimiak, A. (2007). *Structure of an amide bond forming F(420):gamma-glutamyl ligase from Archaeoglobus fulgidus -- a member of a new family of non-ribosomal peptide synthases.* J Mol Biol **372**, 456-69.
 15. Krishnakumar, A. M., **Nocek, B. P.**, Clark, D. D., Ensign, S. A. & Peters, J. W. (2006). *Structural basis for stereoselectivity in the (R)- and (S)-hydroxypropylthioethanesulfonate dehydrogenases.* Biochemistry **45**, 8831-40.
 16. **Nocek, B.**, Cuff, M., Evdokimova, E., Edwards, A., Joachimiak, A. & Savchenko, A. (2006). *1.6 Å crystal structure of a PA2721 protein from pseudomonas aeruginosa--a potential drug-resistance protein.* Proteins **63**, 1102-5.
 17. Pandey, A. S., **Nocek, B.**, Clark, D. D., Ensign, S. A. & Peters, J. W. (2006). *Mechanistic implications of the structure of the mixed-disulfide intermediate of the disulfide oxidoreductase, 2-ketopropyl-coenzyme M oxidoreductase/carboxylase.* Biochemistry **45**, 113-20.
 18. **Nocek, B.**, Chang, C., Li, H., Lezondra, L., Holzle, D., Collart, F. & Joachimiak, A. (2005). *Crystal structures of delta1-pyrroline-5-carboxylate reductase from human pathogens Neisseria meningitidis and Streptococcus pyogenes.* J Mol Biol **354**, 91-106.
 19. Copik, A. J., **Nocek, B. P.**, Swierczek, S. I., Ruebush, S., Jang, S. B., Meng, L., D'Souza V, M., Peters, J. W., Bennett, B. & Holz, R. C. (2005). *EPR and X-ray crystallographic*

- characterization of the product-bound form of the MnlI-loaded methionyl aminopeptidase from Pyrococcus furiosus. Biochemistry* **44**, 121-9.
20. **Nocek, B.**, Boyd, J., Ensign, S. A. & Peters, J. W. (2004). *Crystallization and preliminary X-ray analysis of an acetone carboxylase from Xanthobacter autotrophicus strain Py2. Acta Crystallogr D Biol Crystallogr* **60**, 385-7.
 21. **Nocek, B.**, Jang, S. B., Jeong, M. S., Clark, D. D., Ensign, S. A. & Peters, J. W. (2002). *Structural basis for CO₂ fixation by a novel member of the disulfide oxidoreductase family of enzymes, 2-ketopropyl-coenzyme M oxidoreductase/carboxylase. Biochemistry* **41**, 12907-13.
 22. **Nocek, B.**, Clark, D. D., Ensign, S. A. & Peters, J. W. (2002). *Crystallization and preliminary X-ray analysis of an R-2-hydroxypropyl-coenzyme M dehydrogenase. Acta Crystallogr D Biol Crystallogr* **58**, 1470-3.

TALKS (Invited talks)

1. Bacterial strategies of resistance to antibiotic MicrocinC, 5th CSGID Annual Meeting, Northwestern University, April 3rd, 2012 Chicago, IL
2. Polyphosphate Kinases 2-High energy storage systems. Bio-Nano Technology Conference, University of Bialystok, Poland, March 9th, 2011.
3. Structure of the HK97-like Bacteriophage DNA Packaging Portal. Breckenridge, Colorado, Keystone Symposia, Structural Genomics. January 8-13, 2010.
4. From structure to function: Studies of amide bond forming F420-0:gamma-glutamyl ligase non-ribosomal peptide synthases. Loyola University Chicago, Department of Chemistry, January 31st, 2008.
5. High-resolution structural studies of 2-ketopropyl coenzyme M oxidoreductase/carboxylase. Insights into the mechanism of 2KPCC. Structural Genomics for Pathogenic Protozoa, Department of Biochemistry, University of Washington, Seattle, February 10th, 2004.

TALKS (Symposia, colloquia)

1. Structural Studies of the HK97-like Bacteriophage DNA Packaging Portal, Argonne National Lab. June 30th 2010, 10th Annual MCSG meeting.
2. Polyphosphate Kinases 2-High energy storage systems Bio-division seminars, Argonne National Lab May 6th, 2010.
3. Structure and function of polyphosphate kinase 2. 9th Annual MCSG Meeting, Argonne, IL, April 16, 2009.
4. Fructokinase - the gateway to fructose metabolism. Structural insights into metabolism of fructose in *B. subtilis*. 8th Annual MCSG Meeting, Argonne, IL, March 8, 2008.
5. Structural studies of amide bond forming. F420-0:gamma-glutamyl ligase non-ribosomal peptide synthases from *Archaeoglobus fulgidus*. Bioscience Division, Argonne National Laboratory, IL, December 6th, 2007.
6. Structural characterization of delta1-pyrroline-5-carboxylate reductase from human pathogens. University of Chicago, Department of Microbiology, October 20, 2006.
7. Structural insights into the mechanism of proline biosynthesis. Bioscience Division, Argonne National Laboratory, IL, November 6th, 2005.

POSTER PRESENTATIONS (The first author is a primary presenter)

1. **B. Nocek**, C. Hatzos-Skintges, R. Jedrzejczak, G. Babnigg, A. Joachimiak
A tale of two redesigned proteins, Diffraction Methods in Structural Biology, Gordon Conference, Lewiston, ME, 15-20 July 2012.
2. **B. Nocek**, C. Tesar, C. Hatzos-Skintges, B. Feldmann, A. Joachimiak
Structural insights into mechanism of ADP synthesis by Polyphosphate Kinase 2 High-Throughput Structural Biology, Keystone Symposia, Keystone, Co. 22-27 January 2012.

3. **B. Nocek**, M. Zhou, K. Kwon, W. Anderson, A. Joachimiak. Structural characterization of microcin immunity protein MccF from *Bacillus anthracis*. International Conference on Structural Genomics, Toronto, Canada 10-14 May 2011.
4. N. Beloglazova, P. Petit, R. Flick, G. Brown, T. Skarina, **B. Nocek**, M. Kudritska, M. D. Zimmerman, A. Binkowski, M. Chruszcz, S. Wang, J. Osipiuk, W. Minor, A. Joachimiak, A. Savchenko, and A. F. Yakunin Cas1, Cas2, Cas3...: structure and activity of the core CRISPR nucleases. International Conference on Structural Genomics, Toronto, Canada 10-14 May 2011.
5. A. Starus, **B. Nocek**, A. Joachimiak, R. Holz. DapE-encoded N-succinyl-L,L-diaminopimelic acid desuccinylase (DapE) from *Haemophilus influenzae* as a Prospective Target for the Development of a Novel Class of Antibiotics. 15th International Conference on Biological Inorganic Chemistry (ICBIC 15), Vancouver, Canada. 7-12 August 2011.
6. **B. Nocek**, A. Stein, R. Mulligan, E. Duggan, J. Abdullah and A. Joachimiak, Structure of the HK97-like Bacteriophage DNA Packaging Portal, Structural Genomics: Expanding the Horizons of Structural Biology, Keystone Symposia, Breckenridge, Co. 8-13 January 2010.
7. N. Maltseva, W.H. Eschenfeldt, L. Stols, M.I. Donnelly, M. Gu, **B. Nocek**, K.Tan , Y. Kim and A. Joachimiak. Application of the C-terminal His-tag vectors for salvaging approach. Structural Genomics: Expanding the Horizons of Structural Biology, Keystone Symposia, Breckenridge, Co., 8-13 January 2010.
8. Babnigg, R. Jedrzejczak, **B. Nocek**, A. Stein, W. Eschenfeldt, N. Marshall, A. Weger, L. Stols, K. Buck, and A. Joachimiak Comparison of high-throughput techniques for the expression of protein complexes G Structural Genomics: Expanding the Horizons of Structural Biology, Keystone Symposia, Breckenridge, Co. 8-13 January 2010.
9. **B. Nocek**, D. Gillner, R. Holz, and A. Joachimiak. Structural Studies of the Mono- and Di-metalated Forms of the N-succinyl-L,L-Diaminopimelic Acid Desuccinylase NIGMS workshop, Enabling Technologies in Structure and Function, April 19-21, Bethesda, MD
10. N. Marshall, A. Stein, **B. Nocek**, R. Jedrzejczak, G. Babnigg, A. Joachimiak High-throughput Structure Determination of Molybdopterin Converting Factor from *Helicobacter pylori* NIGMS workshop, Enabling Technologies in Structure and Function, Bethesda, Md, 19-21 April 2010.
11. G. Babnigg, R. Jedrzejczak, **B. Nocek**, A. Stein, W. Eschenfeldt, N. Marshall, A. Wagner, R. Wu, L. Stols, K. Buck, A. Joachimiak. A high-throughput pipeline for the production of protein-protein complexes. NIGMS workshop, Enabling Technologies in Structure and Function, Bethesda, Md. 19-21 April 2010.
12. **B. Nocek**, D-H Chen, A. Stein, R. Mulligan, J. Abdullah, R. Jedrzejczak, W. Chiu, A. Joachimiak, Crystallographic and Cryo-EM studies of the HK97-like bacteriophage DNA packaging portal American Crystallographic Association, Annual meeting, Chicago, Il. 24-29 July 2010.
13. S.L. Ginell, R. Alkire, C. Chang, M.E. Cuff, N. Duke, G. Kazimierz, Y. Kim, K. Lazarski, J. Lazarz, M. Molitsky, **B. Nocek**, J. Osipiuk, S. Park, G. Rosenbaum, Frank J. Rotella, K.Tan, Rg Zhang, A. Joachimiak. The Structural Biology Center User Program at the Advanced Photon Source, Argonne National Laboratory. American Crystallographic Association, Annual meeting, Chicago, Il. Annual meeting 24-29 July 2010.
14. G. Babnigg, R. Jedrzejczak, **B. Nocek**, A. Stein, W. Eschenfeld, L. Bigelow, C.-S. Chang, G. Chhor, M. Cuff, Y. Fan, G. Joachimiak, Y.-C. Kim, H. Li, J. Osipiuk, E. Rakowski, K. Tan, C. Tesar, A.Weger, R. Wu, A. Joachimiak. The Production of Protein-protein Complexes for Structural Characterization. American Crystallographic Association, Annual meeting, Chicago, Il. 24-29 July 2010.
15. **B. Nocek**, E. Kuznetsova, E. Evdokimova, A. Savchenko, A. Edwards, A. Yakunin, A. Joachimiak. ACA 2009. Structural and enzymatic characterization of mitochondrial HAD-like phosphatase from *Saccharomyces cerevisiae*. Toronto, Ontario, Canada, 25-30 July 2009.
16. Sather, C. Hatzos, C. Tesar, G. Joachimiak, M. Zhou, Y. Kim, K. Tan, C. Chang, R. Zhang, **B. Nocek** and A. Joachimiak. Protein Crystallization by in situ Proteolysis. 2009

- NIGMS Workshop: Enabling Technologies for Structural Biology Bethesda, NIH, Bethesda, Md. 4-6 March 2009.
17. **B. Nocek**, J. Osipiuk, E. Evdokimova, A. Savchenko, A. Edwards, A. Yakunin, A. Joachimiak. The first structural studies of bacterial Polyphosphate Kinase. Users Meeting, Argonne National Laboratory, Argonne, Il, 4-6 May 2009.
 18. J. Osipiuk, **B. Nocek**, E. Evdokimova, A. Savchenko, A. Yakunin, A. Edwards, A. Joachimiak. X-ray crystal structures of Polyphosphate Kinases from *Pseudomonas aeruginosa* and *Sinorhizobium meliloti*. 22nd Annual Symposium of the Protein Society. San Diego, Ca. 19-23 July 2008.
 19. **B. Nocek**, R. Mulligan, S. Clancy, and A. Joachimiak. Crystal structure of the ATP-binding domain of the regulatory protein KdpD from *Pseudomonas syringae*. Structural Genomics, Keystone symposia, Steamboat springs, Co. 6-11 Jan 2008.
 20. Joachimiak, J. Abdullah, G. Babnigg, L. Bigelow, A. Binkowski, C. Chang, S. Clancy, G. Cobb, M. Cuff, M. Donnelly, W. Eschendorf, Hatzos, R. Hendricks, G. Joachimiak, L. Keigher, Y. Kim, H. Li, N. Maltseva, E. Marland, S. Moy, R. Mulligan, **B. Nocek**, J. Osipiuk, A. Sather, M. Schiffer, G. Shackelford, L. Stols, K. Tan, C. Tesar, R. Wu, L. Volkart, R. Zhang, M. Zhou, J. Thornton, R. Laskowski, J. Watson, W. Anderson, O. Kiryukhima, D. Miller, G. Minasov, L. Shuvalova, Y. Tang, X. Yang, C. Orengo, D. Lee, R. Marsden, Z. Otwinowski, D. Borek, A. Kudlicki, A. Q. Mei, M. Rowicka, A. Edwards, E. Evdokimova, J. Guthrie, A. Khachatryan, M. Kudrytska, A. Savchenko, T. Skarina, X. Xu, W. Minor, M. Chruszcz, M. Cymborowski, M. Grabowski, P. Lasota, P. Miles, M. Zimmerman, H. Zheng, D. Fremont, T. Brett, C. Nelson. Midwest Center for Structure Genomics-Expanding protein fold space and discovering function. Structural Genomics, Keystone symposia, Steamboat springs, Co. 6-11 January 2008.
 21. **B. Nocek**, R. Mulligan, M. Bargassa, F. Collart, and A. Joachimiak. Crystal Structure of Aminopeptidase N from Human Pathogen *Neisseria meningitides*. Proteins from birth to death -21st annual symposium of the protein society, Boston, Massachusetts, July 21–25, 2007.
 22. M. E. Cuff, **B. Nocek**, L. Volkart, P. Quartey A. Joachimiak. NagC from *Bacillus subtilis*: The Structural and Functional Characterization of a Fructokinase. Proteins from birth to death -21st annual symposium of the protein society, Boston, Massachusetts, July 21–25, 2007.
 23. R-g Zhang, A. Binkowski, C-s Chang, M. Cuff, M. Cymborowski, N. Duke, Y-c Kim, **B. Nocek**, J. Osipiuk, F. Rotella, K. Tan, Z. Otwinowski, W. Minor and A. Joachimiak. Expanding Structural Genomics High-throughput Protein Structure Determination Pipeline to Challenging Targets. American Crystallographic Association 2007 Annual Meeting, Salt Lake City, Utah, 21-27 July 2007.
 24. E. Evdokimova, **B. Nocek**, M. Kudrytska, A. Joachimiak, A. Yakunin and A. Savchenko. Crystal Structure and Catalytic Mechanism of an Amide Bond Forming Enzyme: F420 gamma-Glutamyl Ligase from *Archaeoglobus fulgidus*. International Conference Biocatalysis-2007: Fundamentals and Applications, Moscow-St. Petersburg, Russian Federation, 17-22 June 2007.
 25. **B. Nocek**, R. Mulligan, M. Bargassa, F. Collart, and A. Joachimiak. Structural studies of Aminopeptidase N from Human Pathogen *Neisseria meningitides*. 2007 Users Meetings for DOE/BES User Facilities, Argonne National Laboratory, Argonne, Il, 7-12 May 2007.
 26. A.S. Pandey, **B. Nocek**, and J.W. Peters. High resolution and analog bound structures towards the mechanism of 2-Ketopropyl Coenzyme M Oxidoreductase/ Carboxylase. West Coast Protein Crystallography Workshop, Pacific Grove, Ca. 11-14 March 2007.
 27. R. Wilton, R. Wu, A. Binkowski, **B. Nocek**, R-g. Zhang, A. Joachimiak. Characterization of *Bacillus anthracis* IMPDH kinetics and identification of small molecule inhibitors. Great Lakes Regional Center of Excellence for Biodefense and Emerging Infectious Diseases. Fourth Annual Meeting, Sc. Nov-2 Dec 06 2007.
 28. R-g. Zhang, A. Binkowski, C. Chang, M. Cuff, M. Cymborowski, N. Duke, Y. Kim, **B. Nocek**, J. Osipiuk, F. Rotella, K. Tan, Z. Otwinowski, W. Minor and A. Joachimiak. Structural Genomics High-throughput Protein Structure Determination Pipeline to Challenging Targets. ICSG, Beijing, China 22-26 Oct 2006.

29. **B. Nocek**, E. Evdokimova, M. Kudritska, A. Yakunin, A. Savchenko, A. Edwards, and A. Joachimiak. Structure of F420-0:γ-Glutamyl Ligase from *Archaeoglobus fulgidus*: Insights into the last step of Coenzyme F420 biosynthesis. American Crystallographic Association, Annual Meeting, Honolulu, Hi. 22-27 July 2006.
30. **B. Nocek**, C. Chang, L. Volkart, H. Li, D. Holzle, F. Collart and A. Joachimiak. Structural insights into the mechanism of proline biosynthesis. Structural Genomics, Keystone symposia, Keystone, Co. 29 Jan- 3 Feb 2006.
31. M. Cymborowski, M. Chruszcz, M. Cuff, Z. Dauter, K. Lazarski, Y. Kim, W. Minor, **B. Nocek**, J. Osipiuk, R. Zhang. The integration of data reduction and structure solution- from diffraction images to an initial model in minutes. Keystone Symposia, Joint Meeting of Structural Genomics and Frontiers of Structural Biology, Keystone, Co. 29 Jan-3 Feb 2006.
32. **B. Nocek**, A. Binkowski, H. Li, F. Collart, A. Joachimiak. Crystal Structure of a Novel Tetrahedral-Shaped Protease from *Shigella Flexneri*. American Crystallographic Association, Annual Meeting, Orlando, Fl. May 2005.
33. **B. Nocek**, A. Binkowski, M. Zhou, D. Holzle, A. Joachimiak. Crystal structure of The TeTR-like transcriptional regulator from an opportunistic pathogen *Bacillus cereus*. ICSG Washington, D.C. 17-21 November 2004.
34. **B. Nocek**, A.S. Pandey, S. McGlynn and J.W. Peters. X-ray crystal structure of 2-ketopropyl coenzyme m oxidoreductase / carboxylase a unique member of the fad-dependent NAD(P)H disulfide oxidoreductase family. Northwestern Crystallographic Meeting, Seattle, 24-27 June 2004.
35. **B. Nocek**, S-B. Jang, MS. Jeong, D.D. Clark, S.A. Ensign, J.W. Peters. Structure of 2-Ketopropyl Coenzyme M Oxidoreductase / Carboxylase. American Chemical Society- 58th Northwest Regional Meeting, Bozeman, Mo. 12-14 June 2004.

PDB PUBLICATIONS (166 overall)

1mo9, 1mok, 1u69, 1y0k, 1y9k, 1yqg, 1wkm, 1ylo, 1yvo, 1z6m, 1zk8, 2a5z, 2ag8, 2ahr, 2amf, 2arz, 2b1y, 2c3d, 2esh, 2c3c, 2ewc, 2fa1, 2fb0, 2fdr, 2fkb, 2fyw, 2g7z, 2g9i, 2gfn, 2gtq, 2h5n, 2cfc, 2i1s, 2hqy, 2iaf, 2idl, 2nnp, 2nr5, 2ocd, 2p06, 2p3p, 2phn, 2pli, 2qh8, 2qnt, 2qsi, 2qyb, 2r48, 2r4q, 2r5r, 2r8r, 3b49, 3bio, 3c7j, 3can, 3ck2, 3czp, 3czq, 3d1p, 3e0r, 3e7n, 3dns, 3e9a, 3e3x, 3ehd, 3eer, 3f0c, 3eur, 3exn, 3f0c, 3fdi, 3epq, 3fh3, 3fgg, 3fsg, 3fm5, 3g0m, 3g48, 3gem, 3gbx, 3g5j, 3gjz, 3h1s, 3h07, 3gse, 3gyg, 3hf7, 3hhh, 3hqx, 3i07, 3ieb, 3iou, 3iq1, 3jsa, 3ic1, 3k0b, 3jr2, 3iuk, 3isz, 3kc2, 3kd3, 3kdr, 3knw, 3l0z, 3l84, 3lkv, 3lkl, 3lm9, 3lv9, 3lxy, 3lv9, 3lm9, 3lkl, 3lzh, 3lqk, 3m7i, 3lus, 3m6l, 3m34, 3nav, 3n2a, 3n9i, 3nrs, 3nke, 3ndk, 3o1k, 3nzs, 3ohr, 3ogh, 3opk, 3oug, 3p9z, 3pfm, 3pam, 3pes, 3pu9, 3pzj, 3pyz, 3qbo, 3qqz, 3qoc, 3rf6, 3rhf, 3rpf, 3rrl, 3s52, 3s9x, 3sr3, 3t5m, 3t68, 3t6m, 3u1b, 3ugs, 3ulw, 3uzr, 3tyx, 3v4z, 4dbx, 4dca, 4de4, 4dib, 4e16, 4e5s, 4e94, 4fce, 4eys, 4exk, 4gj1, 4f3u, 4h2k, 4h1h.

WEB PUBLICATIONS AND COMMENTARIES

1. Lemon BJ, **Nocek B**, Peters JW. *Condensation and Commentary on Crystal Structure of a Carbon Monoxide Dehydrogenase Reveals a [Ni-4Fe-5S] Cluster*. ChemTracts–Inorganic Chemistry 2002; 15(1): 1-7.
2. **Nocek B**, Peters JW. *Condensation and Commentary on Crystal Structure of a Novel Red Copper Protein from Nitrosomonas europaea*. ChemTracts–Inorganic Chemistry 2001; 14 (12): 11-16.
3. Coenzyme F420 synthesis. PSI/NATURE structural biology webpage 2008
4. High-energy storage system. PSI/NATURE structural biology webpage 2009

D. MAJOR ACCOMPLISHMENTS

Major contributions to Midwest Center of Structural genomics (MCSG) program.

I joined MCSG in 2004 as an investigator to study structures of proteins using X-ray crystallography with a focus on novel enzymes and their function in the biological processes. I have successfully led studies on many highly competitive and challenging projects and have determined and deposited over 100 structures of MCSG targets in the Protein Data Bank. This achievement made me one of the **major contributors** to the 1,000-structure deposit milestone from a single group in the world (the final number reached was 1350 protein structures)

More importantly, 35 of the structures that I have determined provided **the first structural characterization** of these protein targets. These are extremely important results, as the first structures are incredibly important to the scientific community. They provide invaluable insights to understanding a protein and its function, allowing further studies. Selected examples of the proteins that I have structurally characterized for the first time are: two representatives of Polyphosphate Kinases 2 (**PPK2**), two representatives of Pyrroline-5-Carboxylase (**P5CR**), Aminopeptidase N (**APN**), DapE enzymes in the presence of metal (**DapE**).

I have published the results of these studies in high-profile peer-reviewed journals, including PNAS, JMB and Protein Science. Additionally, a Nature Knowledgebase highlighted my work on PPK2 enzymes as a feature article. Also, the studies of P5CR were featured as an APS scientific research highlight in the 2005 annual APS report.

I have also significantly contributed (determined structures and analyzed data) to the development of new approaches for improving methods of protein crystallization, an important step in structure determination. We have developed a new approach to the **reductive methylation** of proteins in order to improve their crystallization. These studies were published in the prestigious journal **Nature Methods** in 2008, and have already been cited over 40 times. This approach reduces the costs of crystallization and increases the chance of obtaining high quality protein crystals. The Nature Knowledgebase selected our publication describing this method as a feature article. Other significant contributions are the development of new methods for high-throughput protein-protein complex production/crystallization and determination of MBP-fusion target protein complexes as a rescue strategy to enhance solubility, improve folding and facilitate crystallization leading to structure determination.

I have established many collaborations with scientists around the world. These efforts are directed towards broadening understanding of many protein targets that I have characterized structurally. The long-term goal is to find the inhibitors that could be used as leads for drug design against bacterial pathogens. Toward this goal, I am designing, coordinating and pursuing

structural studies of new inhibitors of PPK2 enzymes with Dr. Alexander Yakunin's group from University of Toronto, Canada and Dr. Lukasz Berlicki's group from Wroclaw University of Technology, Poland (WUT). I also started collaboration on the characterization of bacterial pyrroline-carboxylases with Dr. Giuseppe Forlani from University of Ferrara, Italy and Dr. Berlicki from WUT. Together with Dr. Rick Holz from Loyola University, Chicago, we are studying M20 metalloenzymes involved in lysine biosynthesis.

Major contributions to Center for Structural Genomics of infectious Diseases (CSGID) program

In June 2008, I joined the Center for Structural Genomics of Infectious Diseases at Argonne, to study the structure and function of enzymes from major human pathogens. Recently, the CSGID announced the achievement of a significant milestone as it determined over **500** structures from organisms that cause infectious diseases. I have contributed more than **50** structures toward this goal. I have determined many important structures but the most important and unexpected discovery was of microcin immunity protein from *Bacillus anthracis* (MccF). Microcins are small antibiotic-like compounds produced by *E. coli* and its close relatives. Bacteria produce these compounds and deploy them to get rid of related, competing species. Microcin-producing bacteria are immune to their own microcins as they produce MccF protein, which hydrolyses this compound. In collaboration with Dr. Konstantin Severinov's group, we have discovered that MccF proteins are more widespread than previously thought, and they are present in many pathogens. We have shown that various representatives of the MccF can specifically detoxify non-hydrolyzable aminoacyl adenylates differing in their aminoacyl moieties. We proposed that bacterial MccF serve as a source of bacterial antibiotic resistance. This study was recently published in the Journal of Molecular Biology.