



DIRECTOR'S CORNER

It gives me great pleasure to announce that Dr. Teru Nakagawa accepted our offer to join us here at the Center for Structural Biology! Teru will be moving from UCSD, where he has been an Assistant Professor of Chemistry and Biochemistry. He will be appointed as an Associate Professor in the Department of Molecular Physiology & Biophysics and will serve along with Melanie Ohi as scientific co-director of the CSB Cryo-EM Facility.

The recruitment of new faculty member with a high level of expertise represents the first key step in the reorganization of cryo-EM in the CSB. We are now in a position to begin the search for a Director of Operations for the CSB cryo-EM Facility. Filling this position will in turn enable the implementation of an operations and training plan, which will open up the potential for much broader use of cryo-EM resources than has been available in the past. Current expectation is to be fully operational by the end of 2012.

The new BCL::Juf09D server developed in the **Meiler lab** combines secondary structure prediction and trans-membrane span prediction from the protein sequence. It has been optimized for both membrane proteins as well as soluble proteins and prediction accuracies are comparable to highest-quality predictors. The server is available at:

http://www.meilerlab.org/index.php/servers/show?s_id=5



IN THE SPOTLIGHT

Kate Mittendorf, of the Sanders Lab, passed her PhD qualifying exam in Biochemistry.

The **Sanders Lab** clarified the relationship of cholesterol to Alzheimer's disease and had an article published in the journal Science.

Sabuj Pattanayek welcomed a baby boy, Eshan, on Saturday July 7, 2012. Congratulations Sabuj!

Jens Meiler welcomed a baby girl, Sarah, on Sunday, June 24, 2012. Congratulations Jens!

Tina Iverson welcomed a baby boy, Taylor, on Tuesday, April 24, 2012. Congratulations Tina!

AWARDS

Aaron Mason, of the Eichman Lab, received a 3-year American Cancer Society postdoctoral fellowship.

Michael Waterman was presented with John H. Exton Award for Research Leading to Innovative Biological Concepts at the spring faculty meeting on May 17, 2012.

Richard Armstrong has been named a fellow of the American Chemical Society. This is truly a significant honor that recognizes sustained contribution to the discipline of chemistry, an award that is richly deserved.

Stephen Fesik, Professor of Biochemistry, has been awarded the 2012 American Association for Cancer Research Award for Outstanding Achievement in Chemistry in Cancer Research.

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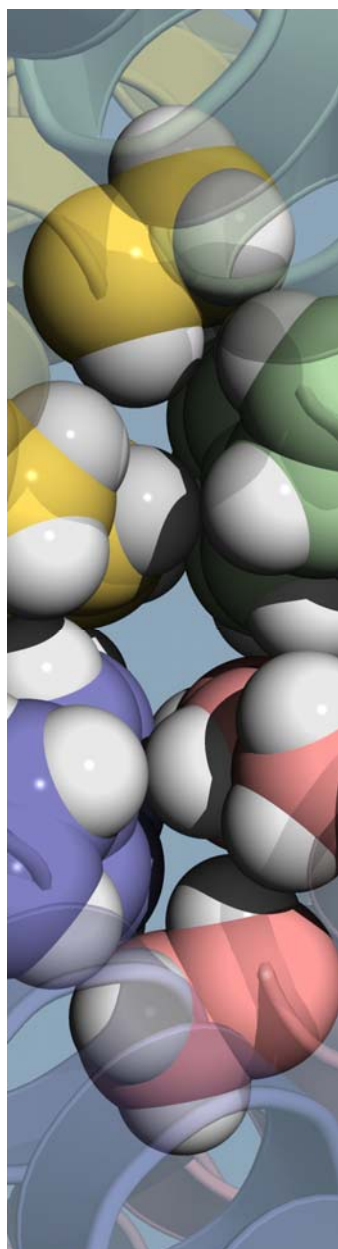
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COMINGS AND GOINGS

Andreas Frank, of the Fesik lab, received a job offer from Novartis. He will join the Novartis scientific staff on October 1, 2012.

Feng Wang joined the Fesik Lab on July 2, 2012 from the Medical Biophysics Department at the University of Toronto.

Elaine Maria de Souza-Fagundes, of the Fesik Lab, finished her postdoc fellowship and returned to Brazil in April 2012.

Hai-Young Kim, of the Fesik Lab, received a job offer from Merck and joined its scientific staff on June 1, 2012.

Julia Koehler, of the Meiler Lab, accepted a postdoc position at John Hopkins.

Rachel Crowder, of the Chazin Lab, completed her MSc in Biochemistry on June 1st and will be starting her work as an independent scientific illustrator.

Steffan Lindert, of the Meiler Lab, accepted a postdoctoral fellowship with the American Heart Association.

Teru Nakagawa, will be joining the CSB from UCSB where he was an Assistant Professor of Chemistry and Biochemistry. He will now be the Associate Professor in the Department of Molecular Physiology & Biophysics and will serve along with Melanie Ohi as scientific co-director of the CSB Cryo-EM Facility.

GRANTS

The **Iverson Lab** received a American Heart Association Grant.

Jens Meiler and **Laura Mizoue** (co-PI) were awarded a new R01 grant from NIGMS entitled "Computational Design of Protein-Ligand interfaces—a Therapeutic Strategy."

Michael Feldkamp of the Chazin Lab received an NIH F32 postdoctoral fellowship starting on July 1st.

RECENT PUBLICATIONS

- P. J. Barrett, Y. Song, W. D. Van Horn, E. J. Hustedt, J. M. Schafer, A. Hadziselimovic, A. J. Beel and C. R. Sanders. "The amyloid precursor protein has a flexible transmembrane domain and binds cholesterol." *Science* **336**(6085): 1168-1171 (2012).
- S. Brandon, A. H. Beth and E. J. Hustedt. "The global analysis of DEER data." *J Magn Reson* **218**: 93-104 (2012).
- C. A. Brosey, B. Chagot and W. J. Chazin. "Preparation of the modular multi-domain protein RPA for study by NMR spectroscopy." *Methods Mol Biol* **831**: 181-195 (2012).
- S. H. Cho and F. P. Guengerich. "Mutation Spectra of S-(2-Hydroxy-3,4-epoxybutyl) glutathione: Comparison with 1,3-Butadiene and Its Metabolites in the Escherichia coli rpoB Gene." *Chem Res Toxicol* (2012).
- S. Damo, W. J. Chazin, E. P. Skaar and T. E. Kehl-Fie. "Inhibition of bacterial superoxide defense: A new front in the struggle between host and pathogen." *Virulence* **3**(3) (2012).
- C. L. Deatherage, A. Hadziselimovic and C. R. Sanders. "Purification and Characterization of the Human gamma-Secretase Activating Protein." *Biochemistry* **51**(25): 5153-5159 (2012).

RECENT PUBLICATIONS (CONTINUED)

- M. Egli. "The Steric Hypothesis for DNA Replication and Fluorine Hydrogen Bonding Revisited in Light of Structural Data." *Acc Chem Res* (2012).
- G. D. Guler, H. Liu, S. Vaithiyalingam, D. R. Arnett, E. Kremmer, W. J. Chazin and E. Fanning. "Human DNA helicase B (HDHB) binds to replication protein A and facilitates cellular recovery from replication stress." *J Biol Chem* **287**(9): 6469-6481 (2012).
- A. Hermann, R. Donato, T. Weiger and W. J. Chazin. "S100 calcium binding proteins and ion channels." *Front Pharmacology* Retrieved 4, 20 (2012).
- A. E. Johnson, S. E. Collier, M. D. Ohi and K. L. Gould. "Fission yeast Dma1 requires RING domain dimerization for its ubiquitin ligase activity and mitotic checkpoint function." *J Biol Chem* (2012).
- A. Ketkar, M. K. Zafar, S. Banerjee, V. E. Marquez, M. Egli and R. L. Eoff. "Conformationally Restrained North-Methanocarpa-2'-deoxyadenosine Corrects the Error-Prone Nature of Human DNA Polymerase Iota." *J. Am. Chem. Soc.* **134**, 10698-10705 (2012).
- J. Z. Liu, S. Jellbauer, A. J. Poe, V. Ton, M. Pesciaroli, T. E. Kehl-Fie, N. Restrepo, M. P. Hosking, R. A. Edwards, A. Battistoni, P. Pasquali, T. E. Lane, W. J. Chazin, T. Vogl, J. Roth, E. P. Skaar and M. Raffatellu. "Zinc sequestration by the neutrophil protein calprotectin enhances Salmonella growth in the inflamed gut." *Cell Host Microbe* **11**(3): 227-239 (2012).
- H. S. McHaourab, Y. L. Lin and B. W. Spiller. "Crystal structure of an activated variant of small heat shock protein hsp16.5." *Biochemistry* **51**(25): 5105-5112 (2012).
- R. Mueller, E. S. Dawson, C. M. Niswender, M. Butkiewicz, C. R. Hopkins, C. D. Weaver, C. W. Lindsley, P. J. Conn and J. Meiler. "Iterative experimental and virtual high-throughput screening identifies metabotropic glutamate receptor subtype 4 positive allosteric modulators." *J Mol Model* (2012).
- P. S. Pallan, V. E. Marquez and M. Egli. "The conformationally constrained N-methanocarpa-dT analogue adopts an unexpected C4'-exo sugar pucker in the structure of a DNA hairpin." *Biochemistry* **51**(13): 2639-2641 (2012).
- P. S. Pallan, C. R. Allerson, A. Berdeja, P. P. Seth, E. E. Swayze, T. P. Prakash and M. Egli. "Structure and nuclease resistance of 2',4'-constrained 2'-O-methoxyethyl (cMOE) and 2'-O-ethyl (cEt) modified DNAs." *Chem Commun (Camb)* (2012).
- S. M. Shell and W. J. Chazin. "XPF-ERCC1: on the bubble." *Structure* **20**(4): 566-568(2012).
- Q. Sun, J. P. Burke, J. Phan, M. C. Burns, E. T. Olejniczak, A. G. Waterson, T. Lee, O. W. Rossanese and S. W. Fesik. "Discovery of Small Molecules that Bind to K-Ras and Inhibit Sos-Mediated Activation." *Angew Chem Int Ed Engl* **51** (25): 6140-6143 (2012).
- W. D. Van Horn and C. R. Sanders. "Prokaryotic diacylglycerol kinase and undecaprenol kinase." *Annu Rev Biophys* **41**: 81-101 (2012).
- W. Wan, H. Wille, J. Stohr, U. Baxa, S. B. Prusiner and G. Stubbs. "Degradation of Fungal Prion HET-s(218-289) Induces Formation of a Generic Amyloid Fold." *Biophys J* **102**(10): 2339-2344 (2012).
- G. R. Watkins, N. Wang, M. D. Mazalouskas, R. J. Gomez, C. R. Guthrie, B. C. Kraemer, S. Schweiger, B. W. Spiller and B. E. Wadzinski. "Monoubiquitination promotes calpain cleavage of the protein phosphatase 2A (PP2A) regulatory subunit alpha4, altering PP2A stability and microtubule-associated protein phosphorylation." *J Biol Chem* (2012).
- C. K. Williams, S. Vaithiyalingam, M. Hammel, J. Pipas and W. J. Chazin. "Binding to retinoblastoma pocket domain does not alter the inter-domain flexibility of the J domain of SV40 large T antigen." *Arch Biochem Biophys* **518**(2): 111-118 (2012).
- Y. Xiao and F. P. Guengerich. "Metabolomic analysis and identification of a role for the orphan human cytochrome P450 2W1 in selective oxidation of lysophospholipids." *J Lipid Res* (2012).
- R. Yang, J. Shi, I. J. Byeon, J. Ahn, J. H. Sheehan, J. Meiler, A. M. Gronenborn and C. Aiken. "Second-site suppressors of HIV-1 capsid mutations: restoration of intracellular activities without correction of intrinsic capsid stability defects." *Retrovirology* **9**: 30 (2012).
- L. Zhao, P. P. Christov, I. D. Kozekov, M. G. Pence, P. S. Pallan, C. J. Rizzo, M. Egli and F. P. Guengerich. "Replication of n(2),3-ethenoguanine by DNA polymerases." *Angew Chem Int Ed Engl* **51**(22): 5466-5469 (2012).