David A. C. Beck

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Education

Ph.D. University of Washington, Medicinal Chemistry, Biomolecular Structure & Design (2006).
in lucem Molecular Mechanics: Design, Validation, and Applications of a Scalable-Parallel Software Environment for Molecular Dynamics

B.S. Drexel University, Computer Science (2000).

Experience

- Research Assistant Professor, Department of Chemical Engineering, U. of Washington — 2011-current
- Directory of Research – Life Sciences, eScience Institute, U. of Washington — 2009-current
- Post-Doctoral Fellow, Bioengineering, U. of Washington — 2007-2009
- Post-Doctoral Fellow, Medicinal Chemistry, U. of Washington — 2006-2007

Research Interests

- Systems & synthetic biology of microbial cultures and communities
  - Pathway reconstruction and analysis of *omics datasets with relevance to biofuels production, biogeochemical cycling, the microbiome of built environments, and human health
  - Development of techniques for analysis, comparison, and unification of transcriptomics and proteomics datasets
- Biophysical chemistry software, methods and applications
  - Author of *in lucem* Molecular Mechanics (*il*mm, **Beck, D.A.C.**, Alonso, D.O.V., & Daggett, V)
  - Methods and software development for *in silico* drug and protein design in high-performance computing (HPC) environments
  - Dynameomics: mass annotation of protein dynamics and unfolding in water by high-throughput atomistic molecular dynamics simulations
- eScience
  - Workflow design and engineering for data-intensive analytics in biology and chemistry
  - Data mining, management and sharing strategies for large biological datasets

Software

- *in lucem* Molecular Mechanics (*il*mm)
  - Scalable-parallel software environment for molecular mechanics simulation and analysis
- Engines for Biology (E4B)
  - SQL database engines for native access to common file formats for biology and chemistry including sequence files (FASTA, FASTQ), structural data (PDBML), proteomics (mzXML, protXML)
- Parallel-distributed-query BLAST (pdqBLAST)
  - Scalable-parallel toolkit for extremely large query and search database BLAST with SQL backend, suitable for deployment on cloud resources

Professional Committees, Societies, and Service

- Computers in Biology and Medicine (Elsevier Journal) Editorial Board Member — 2010-2013
- National Energy Research Scientific Computer Center (NERSC) — 2007-2012

User's Group Executive Committee (NUGEX) representative for Office of Biology and Environmental Research

Awards

- Molecular Biophysics Training Grant — 2002-2005
  NIH Molecular Biophysics Training Grant
  National Research Service Award, 5 T32 GM 08268
  University of Washington

Invited Panels / Presentations

- Data Intensive Science Workshop — May 16-17, 2011, Washington, DC
- National Science Foundation: Data-Intensive Sciences Workshop — September 19-20, 2010, Seattle, WA
- Department of Energy: Opportunities in Biology at the Extreme Scale of Computing — August 17-19, 2009, Chicago, IL
- Department of Energy: Large Scale Computing and Storage Requirements for Biological and Environmental Research — May 7-9, 2009, Washington, DC
- Microsoft Technical Computing All Hands Meeting — March 5, 2007, Redmond, WA
  Dynameomics: Mass Annotation of Protein Dynamics through Molecular Dynamics Simulations, lecture
- Microsoft eScience Workshop — October 14, 2006, Baltimore, MD
  Exploring Protein Folding Dynamics Using Analysis Tools against a Simulation Database, lecture
- European Molecular Biology Organization: Course on Biomolecular Simulation — June 28 - July 4, 2006, Paris, France
  Molecular Dynamics, lecture
  Protein Folding / Unfolding, lecture
- Supercomputing 2005, Department of Energy, National Energy Research Scientific Computing — November 15, 2005, Seattle, WA
  Dynameomics: Protein Mechanics, Folding and Unfolding through Large Scale All-Atom Molecular Dynamics Simulations, lecture

Publications

- Kalyuzhnaya, M.G., Yang, S., Rozova, O.N., Smalley, N.E., Clubb, J., Lamb A., Nagana Gowda G.A., Raftery, D., Fu, Y., Bringel F., Vuilleumier, S., **Beck, D.A.C.**, Trotsenko, Y.A., Khmelenina, V.N., and Lidstrom, M.E. (2013) Highly Efficient Methane Biocatalysis Revealed in a Methanotrophic Bacterium. **Nature Comm.** *In press.*
- **Beck D.A.C.**, Kalyuzhnaya M.G., Malfatti S., Tringe S., Glavina del Rio T., Ivanova N., Lidstrom M. E., Chistoserdova L. (2013) A metagenomic insight into freshwater methane-utilizing communities and evidence for cooperation between the Methylococcaceae and the Methylophilaceae. **PeerJ** 1:e23.
- Khmelenina V. N., **Beck D.A.C.**, Munk C., *et al.* (2013) Draft Genome Sequence of Methylomicrobium buryatense Strain 5G, a Haloalkaline-Tolerant Methanotrophic Bacterium. **Genome Announc.** Jul-Aug; 1(4): e00053-13.

- Vorobev A., **Beck D.A.C.**, Kalyuzhnaya M.G., Lidstrom M. E., Chistoserdova L. (2013) Comparative transcriptomics in three Methylophilaceae species uncover different strategies for environmental adaptation. **PeerJ** 1:e115.
- Krumholz LR, Wang L, **Beck D.A.C.**, Wang T, Hackett M, Mooney B, Juba TR, McInerney MJ, Meyer B, Wall JD, Stahl DA. Membrane protein complex of APS reductase and Qmo is present in Desulfovibrio vulgaris and Desulfovibrio alaskensis. **Microbiology.** 2013 Oct;159(Pt 10):2162-8. doi: 10.1099/mic.0.063818-0.
- Yang S., Matsen J.B., Konopka M., Green-Saxena A., Clubb J., Sadilek M., Orphan V.J., **Beck, D.A.C.**, and M.G. Kalyuzhnaya. Global molecular analyses of methane metabolism in methanotrophic Alphaproteobacterium, *Methylosinus trichosporium* OB3b. Part II. metabolomics and 13C-labeling study. **Front. Microbiol.**, 03 April 2013.
- Matsen J.B., Yang S., Stein L.Y., **Beck, D.A.C.**, and M.G. Kalyuzhnaya. Global molecular analyses of methane metabolism in methanotrophic alphaproteobacterium, *Methylosinus trichosporium* OB3b. Part I: transcriptomic study. **Front. Microbiol.**, 03 April 2013.
- Hirano T.*, **Beck D.A.C.***, Wright C., Demuth D.R., Hackett M., Lamont R.J. Regulon Controlled by the GppX Hybrid Two Component system in *Porphyromonas gingivalis*. **Mol. Oral Microbiology.** 28(1):70-81 2013. *Contributed equally
- McCully M.E., **Beck D.A.C.**, Daggett V. Multimolecule simulations of protein unfolding and aggregation. **Proceedings of the National Academy of Sciences USA.** 109(44):17851-6 2012.
- McCully M.E., **Beck D.A.C.**, Daggett V. Promiscuous contacts and heightened dynamics increase thermostability in an engineered variant of the engrailed homeodomain. **Protein Engineering & Selection**. 26(1):35-45 2012.
- Hirano T.*, **Beck D.A.C.***, Demuth D.R., Hackett M., Lamont R.J. Deep Sequencing of Porphyromonas gingivalis and Comparative Transcriptome Analysis of a LuxS Mutant. **Front Cell Infect Microbiol.** 2:79 2012. *Contributed equally
- Toofanny, R.D., Simms, A., **Beck, D.A.C.**, and V. Daggett. Implementation of 3D spatial hashing in a large-scale molecular dynamics simulation database for rapid atomic contact detection. **BMC Bioinformatics.** 12:334, 2011.
- **Beck D.A.C.**, Hendrickson E.L., Vorobev A., Wang T., Lim S., Kalyuzhnaya M.G., Lidstrom M.E., Hackett M., Chistoserdova L. An integrated proteomics/transcriptomics approach points to oxygen as the main electron sink for methanol metabolism in Methylotenera mobilis. **J Bacteriol.** 2011, Jul 15.
- Lapidus A., Clum A., Labutti K., Kaluzhnaya M.G., Lim S., **Beck D.A.C.**, Glavina Del Rio T., Nolan M., Mavromatis K., Huntemann M., Lucas S., Lidstrom M.E., Ivanova N., Chistoserdova L. Genomes of three methylotrophs from a single niche reveal the genetic and metabolic divergence of the methylophilaceae. **J Bacteriol**. 193(15):3757-64, 2011.
- Kalyuzhnaya M.G., **Beck D.A.C.**, Vorobev A., Smalley N., Kunkel D.D., Lidstrom M.E., Chistoserdova L. Novel methylotrophic isolates from lake sediment, description of Methylotenera versatilis sp. nov. and emended description of the genus Methylotenera. **Int J Syst Evol Microbiol**, 2011, Feb 18.
- Kalyuzhnaya, M.G., **Beck, D.A.C.**, and L. Chistoserdova. Functional metagenomics of methylotrophs. **Methods in Enzymology**, 495:81-98, 2011.
- Ojala, D.S., **Beck, D.A.C.**, and M.G. Kalyuzhnaya. Genetic systems for moderately halo(alkali)philic bacteria of the genus *Methylomicrobium*. **Methods in Enzymology**, 495:99-118, 2011.
- Barga, R., Howe, B., **Beck, D.A.C.**, Bowers, S., Dobyns, W., Haynes, W., Higdon, R., Howard, C., Roth, C., Stewart, E., Welch, D., and Kolker, E. Bioinformatics and Data-Intensive Scientific Discovery. **OMICS**, 15(4), 2011.

- Hendrickson E.L., **Beck D.A.C.**, Wang T., Lidstrom M. E., Hackett. M., and L. Chistoserdova. The expressed genome of *Methylobacillus flagellatus* defined through proteogenomics and new insights into methylotrophy. **Journal of Bacteriology**, 192: 4859-4867, 2010. [DOI]
- McCully, M.E., **Beck, D.A.C.**, Fersht, A.R., and V. Daggett. Refolding of the Engrailed Homeodomain: Structural basis for the accumulation of a folding intermediate. **Biophysical Journal**, 99: 1628-1636, 2010. [DOI]
- van der Kamp, M.W., Schaeffer, R.D., Jonsson, A.L., Scouras, A.D., Simms ,A., Toofanny, R.D., Benson, N.C., Anderson, P.C., Merkley, E.D., Rysavy, S., Bromley, D., **Beck, D.A.C.** and V. Daggett. Dynameomics: A comprehensive database of protein dynamics. **Structure**, 18: 423-435, 2010. [DOI]
- Kalyuzhnaya, M.G., **Beck, D.A.C.**, Suciu, D., Pozhitkov, A., Lidstrom M.E., and L. Chistoserdova. Functioning in situ: gene expression in *Methylotenera mobilis* in its native environment as assessed via transcriptomics. **ISME Journal**, 4: 388-398, 2009. [DOI]
- **Beck D.A.C.**, Alonso D.O.V., Inoyama D., and V. Daggett. The intrinsic conformational propensities of the 20 naturally occurring amino acids and reflection of these propensities in proteins. **Proceedings of the National Academy of Sciences USA** 105: 12259-12264, 2008. [DOI]
- McCully, M.E., **Beck, D.A.C.**, and V. Daggett. Microscopic Reversibility of Protein Folding in Molecular Dynamics Simulations of the Engrailed Homeodomain. **Biochemistry** 47: 7079-7089, 2008. [DOI]
- Smolin, N., Li B., **Beck, D.A.C.**, and V. Daggett. Side-chain dynamics are critical for water permeation through aquaporin-1. **Biophysical Journal** 95:1089-1098, 2008. [DOI]
- **Beck, D.A.C.**, Jonsson, A.L., Schaeffer, R.D., Scott, K.A., Day, R., Toofanny, R.D., Alonso, D.O.V., and V. Daggett. Dynameomics: mass annotation of protein dynamics and unfolding in water by high-throughput atomistic molecular dynamics simulations. **Protein Engineering Design & Selection**, 21, 353-368, 2008. [DOI]
- **Beck, D.A.C.** and V. Daggett. A One-Dimensional Reaction Coordinate for Identification of Transition States from Explicit Solvent Pfold-Like Calculations. **Biophysical Journal**, 93, 8832-3391, 2007. [HTML] [PDF]
- **Beck, D.A.C.**, Bennion, B.J., Alonso, D.O.V and V. Daggett. Simulations of macromolecules in protective and denaturing osmolytes: properties of mixed solvent systems and their effects on water and protein structure and dynamics. **Methods in Enzymology**, 428, 373-396, 2007. [DOI]
- **Beck, D.A.C.**, White, G.W.N., and V. Daggett, Exploring the energy landscape of protein folding using replica-exchange and conventional molecular dynamics simulations. **Journal of Structural Biology**, 157, 514-523, 2007. [DOI]
- **Beck, D.A.C.**, Armen, R.S. and V. Daggett, Cutoff size need not strongly influence molecular dynamics results on solvated polypeptides. **Biochemistry**, 44, 609-616, 2005. [DOI] *(#12 most cited paper for Biochemistry in 2005)*
- **Beck, D.A.C.** and V. Daggett, Methods for Molecular Dynamics Simulations of Protein Folding/Unfolding in Solution, **Methods**, 34, 112-120, 2004. [DOI]
- Day, R., **Beck, D.A.C.**, Armen, R. and V. Daggett, A Consensus View of Fold Space: Combining SCOP, CATH, and the Dali Domain Dictionary, **Protein Science**, 12, 2150-2160, 2003. [DOI]
- **Beck, D.A.C.**, Alonso, D.O.V. and V. Daggett. A microscopic view of peptide and protein solvation. **Biophysical Chemistry** 100, 221-237, 2003. [DOI]