DNA is the blueprint for life, but proteins and RNAs are the macromolecules that make life happen. One of the grand challenges for 21st century research is to develop a molecular-level understanding of the function of these molecular nanomachines. This knowledge will help us better understand how protein or RNA dysfunction can lead to disease, and can provide a framework for molecular-based treatment of diseases. This symposium features application of various experimental and modeling approaches to understand the interrelationships between structure, dynamics, and biological function of proteins and RNAs.
STRUCTURE AND DYNAMICS OF BIOMACROMOLECULES

Maryland Biophysics Program Symposium
Wednesday, January 22, 2014, 9 am - 5:20 pm
Kay Boardroom - 1111 Kim Engineering Bldg

PROGRAM

8:30 am    Registration
9:00 am    Welcome and Introductory remarks

MORNING SESSION CHAIR: T KWAKU DAYIE

9:10 am    Ad Bax (National Institutes of Health): What can NMR tell us about how a virus enters its host cell?
9:50 am    David Case (Rutgers University): Chemical shift dispersion in proteins and nucleic acids
10:30 am   Coffee Break

10:50 am   Juli Feigon (University of California, Los Angeles) The architecture of Tetrahymena telomerase holoenzyme
11:30 am   T. Kwaku Dayie (University of Maryland): Recoding cellular messages: developing tools for probing the role of RNA conformational switching
12:00 pm   Donna Baldisseri (Bruker BioSpin): Bruker advancements for biomolecular NMR

12:20 pm   Lunch Break/Poster Session/Tour of the Biomolecular NMR Facility

AFTERNOON SESSION CHAIR: DAVID FUSHMAN

2:00 pm    Lewis Kay (University of Toronto): Seeing the invisible by solution NMR
2:40 pm    Philip Anfinrud (National Institutes of Health): Watching a signaling protein function in real time with X-rays
3:20 pm    Coffee Break
3:40 pm    David Fushman (University of Maryland): Deciphering the “ubiquitin code”: understanding the linkage-signal relationships in polyubiquitin
4:10 pm    George Lorimer (University of Maryland): Dissecting the inner workings of a nanomachine with multiple spectroscopic probes
4:40 pm    Angela M. Gronenborn (University of Pittsburgh): Synergy between NMR, cryo-EM and large-scale MD simulations – Novel findings for HIV capsid function
5:20 pm    Closing Remarks
5:25 pm    Reception

Supported by IPST, Maryland Biophysics Program, Department of Chemistry and Biochemistry, and Bruker BioSpin Corp.

Organizers: David Fushman, T. Kwaku Dayie
For more information: Star Jackson (starj@umd.edu)
SPEAKER BIOSKETCHES

Dr. Ad Bax received his undergraduate and Ph.D. degrees in applied physics from Delft University of Technology in the Netherlands. After working as a post-doctoral fellow at Colorado State University, he joined the Laboratory of Chemical Physics at NIDDK (NIH) where he is currently the Chief of the Section on Biophysical NMR Spectroscopy. Dr. Bax is a member of the US National Academy of Sciences, the Corresponding Member of the Royal Netherlands Academy of Sciences, a Fellow of the American Academy of Arts and Sciences, and a Fellow of the American Association for the Advancement of Science. His research interest is in NMR and its application in chemistry, biochemistry, and biology.

Dr. David Case is a Professor of Chemistry at Rutgers University. He received a B.S. in chemistry from Michigan State (working with Tom Pinnavaia and Jim Harrison) and AM in physics and Ph.D. in chemical physics from Harvard working with Nobel laureates Dudley Herschbach and Martin Karplus. He was on the faculty of the University of California, Davis, and then The Scripps Research Institute before moving to Rutgers University in 2008. His research efforts are in the area of theoretical and computational chemistry, with emphases on computational aspects of biomolecular NMR, electronic structures of active sites of metalloproteins, molecular dynamics simulations of proteins and nucleic acids, and oversees development of the AMBER suite of programs for biomolecular simulation.

Dr. Juli Feigon received her B.A. from Occidental College and her M.S. and Ph.D. from the University of California, San Diego where she studied with Dr. David Kearns. Her postdoctoral work at the Massachusetts Institute of Technology, as a Damon Runyon-Walter Winchell Cancer Fund Postdoctoral Fellow, was with Dr. Alex Rich. Dr. Feigon joined the UCLA faculty in 1985 and has received numerous honors and awards that include the NSF Presidential Young Investigator award, and election to the US National Academy of Sciences. As a structural biophysicist, her lab has pioneered the application of solution macromolecular NMR spectroscopy to the study of DNA and RNA and their interactions with proteins and various ligands. In addition to NMR, her group uses various approaches such as X-ray crystallography, SAXS, and electron microscopy, and various biochemical and molecular biology tools to ascertain biological function.

Dr. T. Kwaku Dayie is an Associate Professor in the Department of Chemistry and Biochemistry at the University of Maryland. After receiving his BA in physics from Hamilton College and Ph.D. in biophysics from Harvard where he studied with Gerhard Wagner, he did postdoctoral training at the Massachusetts Institute of Technology and then at The Scripps Research Institute with Jamie Williamson as a Jane Coffin Childs Memorial Fund Fellow. Before joining the University of Maryland in 2008, he was a Research Scientist at the Cleveland Clinic. Research Interests: development and application of labeling and NMR methods for the study of RNA structure, dynamics, and function; and understanding structural mechanisms underlying RNA dependent signaling and recoding.

Dr. Donna Baldisseri is Senior Applications Scientist at Bruker BioSpin Corporation. She obtained her BA in chemistry from Boston University and a Ph.D. in chemistry from Wesleyan University. After a post-doctoral fellowship at the NIH with Dennis Torchia, she has worked in the field of Biomolecular NMR at Bruker Instruments, at the NCI in Frederick, and as a Research Professor at the University of Maryland School of Medicine in Baltimore, and subsequently joined Bruker BioSpin in 2002.
**Dr. Lewis E. Kay** is a University Professor in the Departments of Chemistry, Biochemistry and Molecular Genetics at the University of Toronto, and holds a Canada Research Chair in Proteomics, Bioinformatics and Functional Genomics. He received an undergraduate degree in biochemistry from the University of Alberta and a PhD in biophysics from Yale (with Jim Prestegard). Dr. Kay was a post-doctoral fellow at the NIH with Ad Bax, and joined the faculty at the University of Toronto in 1992, where he has been a Full Professor since 1995. Dr. Kay’s work has been recognized by numerous awards and honors, including the Royal Society of Chemistry Khorana Prize, and the election as a Fellow of the Royal Society of London and of the Royal Society of Canada. Research interests: development and application of NMR methods for the study of protein structure and dynamics, understanding the functional dynamics.

**Dr. Philip Anfinrud** received his undergraduate degree in chemistry from North Dakota State University and a PhD in physical chemistry from Iowa State University. After working as a post-doctoral fellow at University of Pennsylvania, in 1990 he joined Harvard University where he was an Assistant Professor and then Associate Professor of Chemistry. In 1998 Dr. Anfinrud joined the Laboratory of Chemical Physics at NIDDK (NIH) where he is currently the Chief of the Laboratory of Ultrafast Biophysical Chemistry. He was awarded Beckman Young Investigator Award and NSF Young Investigator award, and in 2006 was elected a fellow of the American Association for the Advancement of Science. His research is focused on development and application of ultrafast time-resolved laser spectroscopy and x-ray diffraction in order to investigate the relationships between protein structure, dynamics, and function.

**Dr. David Fushman** is a Professor at the Department of Chemistry and Biochemistry, University of Maryland. After receiving his Master’s and Ph.D. degrees in theoretical physics from Kazan State University (USSR), he did postdoctoral training at Kazan Institute of Biology, USSR Academy of Sciences. Before joining the University of Maryland in 2000, he was an Alexander von Humboldt fellow at University of Frankfurt (Germany) and a Research Associate at Rockefeller University (New York). Research Interests: structure – dynamics – function relationships in biological macromolecules, and the structural mechanisms underlying intracellular signaling, especially, ubiquitin-mediated signaling pathways.

**Dr. George H. Lorimer** is a Distinguished University Professor at University of Maryland. He received his undergraduate education from University of St. Andrews (Scotland), a M.S. degree from University of Illinois, and a Ph.D. from Michigan State University. Dr. Lorimer was a post-doctoral fellow at Max-Planck Gesellschaft in Berlin (Germany), a research fellow at Australian National University in Canberra, and a scientist at the Institute of Biochemistry in Munich (Germany), before joining DuPont Co (Delaware), where he served as a Principal Investigator, later Research Leader, and then DuPont Fellow. In 1998 he joined the Department of Chemistry and Biochemistry at the University of Maryland. Dr. Lorimer is a member of the US National Academy of Sciences, a Fellow of the Royal Society of London, and a recipient of the Alexander von Humboldt Research Prize. Research interests: protein folding, allostery, molecular chaperones, mechanistic enzymology.

**Dr. Angela M. Gronenborn** is a Rosalind Franklin Professor and Chair of the Department of Structural Biology at University of Pittsburgh. She received her undergraduate and doctoral degrees from the University of Cologne, Germany. After postdoctoral training and subsequent scientific work at the National Institute for Medical Research in London, Dr. Gronenborn was a Head of the Biological NMR Group at the Max-Planck Institute in Munich. She then joined the Laboratory of Chemical Physics at NIDDK (NIH) where she served as a Chief of the Structural Biology Section before moving to University of Pittsburgh in 2005. Dr. Gronenborn is a member of the US National Academy of Sciences and a Fellow of the American Association for the Advancement of Science and of the Royal Society of Chemistry, U.K. Dr. Gronenborn’s research interest is in structure and dynamics of biological macromolecules.