

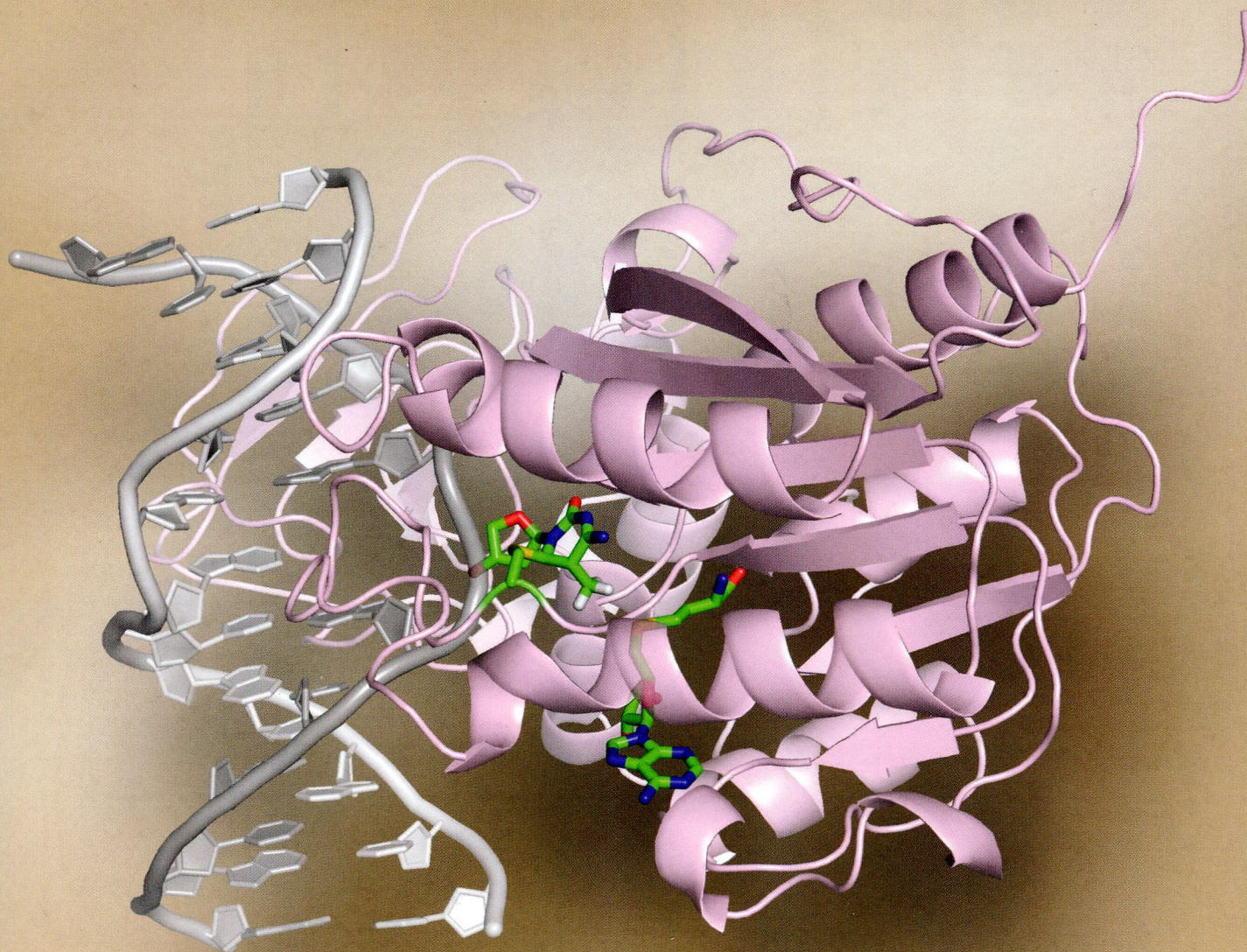
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# BIOCHEMISTRY

including biophysical chemistry & molecular biology

SEPTEMBER 17, 2013 • VOLUME 52 NUMBER 37

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**ON THE COVER:** The detailed atomistic reaction mechanism for the epigenetic methylation of cytosine has been elucidated for the representative prokaryotic DNA methyltransferase *HhaI*, utilizing ab initio quantum mechanical/molecular mechanical-molecular dynamics simulations. Shown here is the intermediate in the reaction pathway. The methyl group has been transferred from *S*-adenosyl-L-methionine to carbon 5 of cytosine, and the covalent Michael adduct between a conserved cysteine residue of the enzyme and carbon 6 of cytosine has formed. The image was produced using PyMOL (Schrödinger, LLC) [Yang, J., et al. (2013) *Biochemistry* 52, 2828–2838].

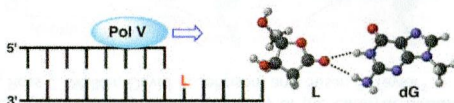
## Rapid Reports

6301 **S**

dx.doi.org/10.1021/bi400997h

**DNA Polymerase V Kinetics Support the Instructive Nature of an Oxidized Abasic Lesion in *Escherichia coli***

John Ernest V. Bajacan and Marc M. Greenberg\*



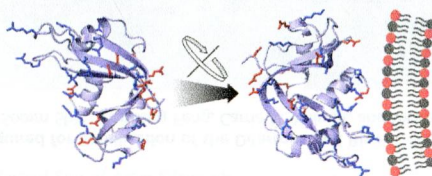
## Articles

6304

dx.doi.org/10.1021/bi400619m

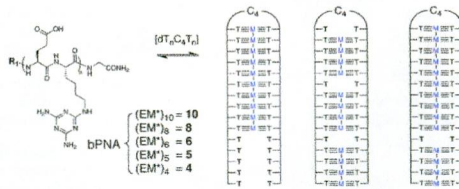
**Contribution of Electrostatics to the Binding of Pancreatic-Type Ribonucleases to Membranes**

Nadia K. Sundlass, Chelcie H. Eller, Qiang Cui, and Ronald T. Raines\*



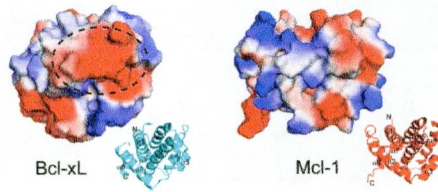
**Bifacial Peptide Nucleic Directs Cooperative Folding and Assembly of Binary, Ternary, and Quaternary DNA Complexes**

Xijun Piao, Xin Xia, and Dennis Bong\*



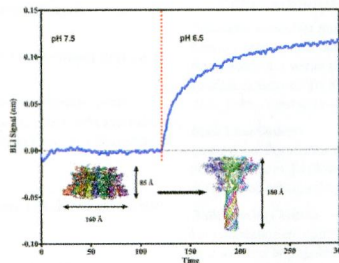
**Anti-apoptosis Proteins Mcl-1 and Bcl-xL Have Different p53-Binding Profiles**

Hongwei Yao, Shufu Mi, Weibin Gong, Jian Lin, Nuo Xu, Sarah Perrett, Bin Xia, Jinfeng Wang,\* and Yingang Feng\*



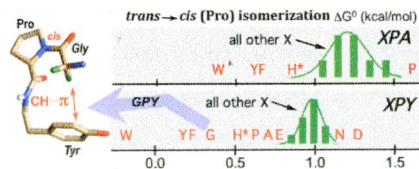
**Monitoring the Kinetics of the pH-Driven Transition of the Anthrax Toxin Prepore to the Pore by Biolayer Interferometry and Surface Plasmon Resonance**

Subhashchandra Naik, Susan Brock, Narahari Akkaladevi, Jon Tally, Wesley McGinn-Straub, Na Zhang, Phillip Gao, E. P. Gogol, B. L. Pentelute, R. John Collier, and Mark T. Fisher\*

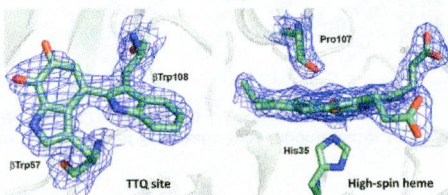


Local Control of *cis*-Peptidyl-Prolyl Bonds Mediated by CH $\cdots\pi$  Interactions: The Xaa-Pro-Tyr Motif

Himal K. Ganguly, Hundeeep Kaur, and Gautam Basu\*

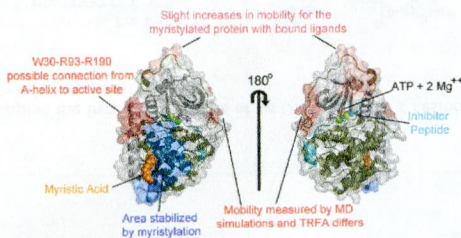
Carboxyl Group of Glu113 Is Required for Stabilization of the Diferrous and Bis-Fe<sup>IV</sup> States of MauG

Nafez Abu Tarboush, Erik T. Yuki, Soomil Shin, Manliang Feng, Carrie M. Wilmot, and Victor L. Davidson\*



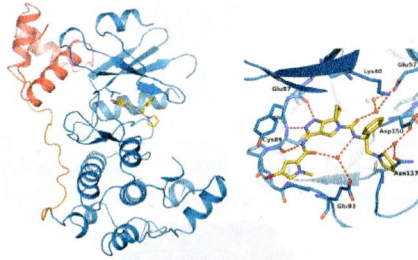
## Influence of N-Myristylation and Ligand Binding on the Flexibility of the Catalytic Subunit of Protein Kinase A

Adam C. Bastidas, Levi C. Pierce, Ross C. Walker, David A. Johnson, and Susan S. Taylor\*



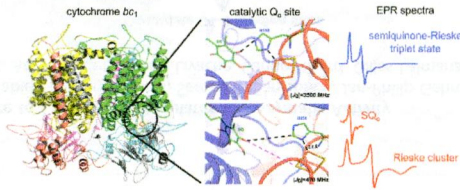
### Structural Insight into Maternal Embryonic Leucine Zipper Kinase (MELK) Conformation and Inhibition toward Structure-Based Drug Design

Giulia Canevari,\* Stefania Re Depaolini, Ulisse Cucchi, Jay A. Bertrand, Elena Casale, Claudia Perrera, Barbara Forte, Patrizia Carpinelli, and Eduard R. Felder



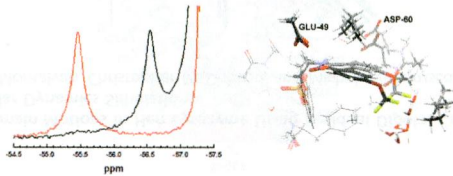
### Triplet State of the Semiquinone–Rieske Cluster as an Intermediate of Electronic Bifurcation Catalyzed by Cytochrome *bc*<sub>1</sub>

Marcin Sarewicz, Malgorzata Dutka, Sebastian Pintscher, and Artur Osyczka\*



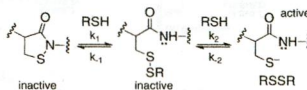
### Allostery and Substrate Channeling in the Tryptophan Synthase Bifunctional Complex: Evidence for Two Subunit Conformations and Four Quaternary States

Dimitri Niks, Eduardo Hilario, Adam Dierkers, Huu Ngo, Dan Borchardt, Thomas J. Neubauer, Li Fan,\* Leonard J. Mueller,\* and Michael F. Dunn\*



### Thiol-Dependent Recovery of Catalytic Activity from Oxidized Protein Tyrosine Phosphatases

Zachary D. Parsons and Kent S. Gates\*

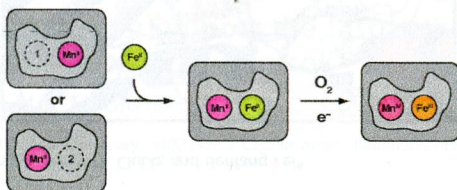


6424 **5**

dx.doi.org/10.1021/bi400819x

### Structural Basis for Assembly of the Mn<sup>IV</sup>/Fe<sup>III</sup> Cofactor in the Class Ic Ribonucleotide Reductase from *Chlamydia trachomatis*

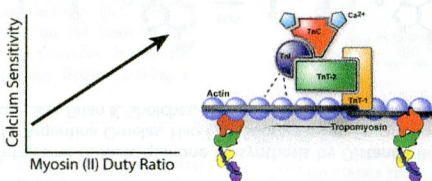
Laura M. K. Dassama, Carsten Krebs, J. Martin Bollinger Jr., Amy C. Rosenzweig, and Amie K. Boal\*

6437 **5**

dx.doi.org/10.1021/bi400262h

### The Myosin Duty Ratio Tunes the Calcium Sensitivity and Cooperative Activation of the Thin Filament

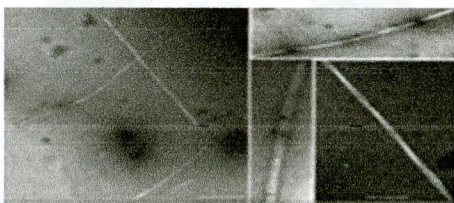
Milad Webb, Del R. Jackson Jr., Travis J. Stewart, Samuel P. Dugan, Michael S. Carter, Christine R. Cremona, and Josh E. Baker\*

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dx.doi.org/10.1021/bi400442d

### Interaction of 14-3-3 $\zeta$ with Microtubule-Associated Protein Tau within Alzheimer's Disease Neurofibrillary Tangles

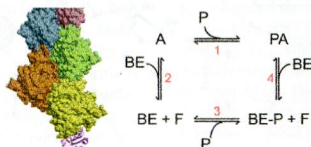
Hamid Y. Qureshi, Tong Li, Ryen MacDonald, Chul Min Cho, Nicole Leclerc, and Hemant K. Paudel\*

6456 **5**

dx.doi.org/10.1021/bi400682n

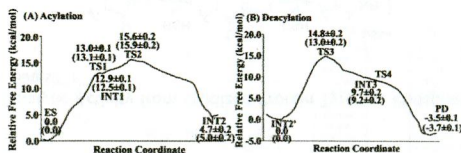
### Interaction of Profilin with the Barbed End of Actin Filaments

Naomi Courtemanche and Thomas D. Pollard\*



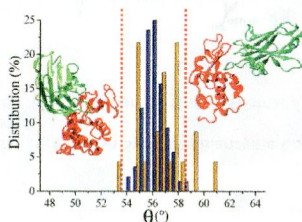
## Fundamental Reaction Pathway and Free Energy Profile for Butyrylcholinesterase-Catalyzed Hydrolysis of Heroin

Yan Qiao, Keli Han,\* and Chang-Guo Zhan\*



## Characterization of the Interdomain Motions in Hen Lysozyme Using Residual Dipolar Couplings as Replica-Averaged Structural Restraints in Molecular Dynamics Simulations

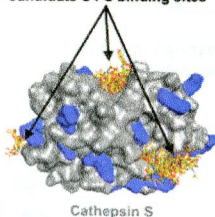
Alfonso De Simone, Rinaldo W. Montalvao, Christopher M. Dobson, and Michele Vendruscolo\*



## Binding of Chondroitin 4-Sulfate to Cathepsin S Regulates Its Enzymatic Activity

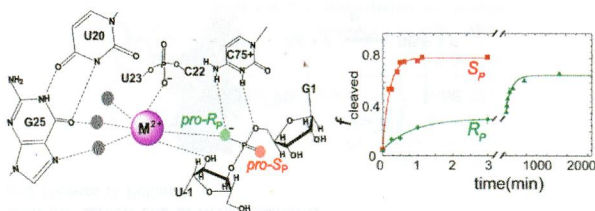
Juliette Sage, Florian Mallèvre, Fabien Barbarin-Costes, Sergey A. Samsonov, Jan-Philipp Gehrcke, Maria Teresa Pisabarro, Eric Perrier, Sylvianne Schnebert, André Roget, Thierry Livache, Carine Nizard, Gilles Lalmanach, and Fabien Lecaille\*

Candidate C4-S binding sites



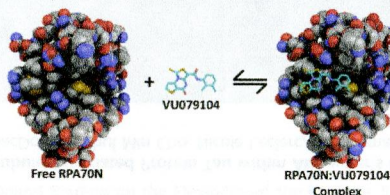
### Thio Effects and an Unconventional Metal Ion Rescue in the Genomic Hepatitis Delta Virus Ribozyme

Pallavi Thaplyal, Abir Ganguly, Barbara L. Golden,\* Sharon Hammes-Schiffer,\* and Philip C. Bevilacqua\*



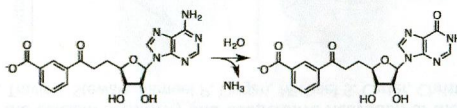
### Surface Engineering of RPA70N Enables Cocrystallization with an Inhibitor of the Replication Protein A Interaction Motif of ATR Interacting Protein

Michael D. Feldkamp, Andreas O. Frank, J. Phillip Kennedy, James D. Patrone, Bhavatarini Vangamudi, Alex G. Waterson, Stephen W. Fesik, and Walter J. Chazin\*



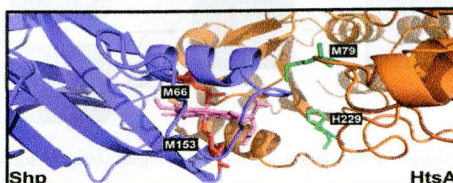
### Deamination of 6-Aminodeoxyfutasoline in Menaquinone Biosynthesis by Distantly Related Enzymes

Alissa M. Goble, Rafael Toro, Xu Li, Argentina Ornelas, Hao Fan, Subramaniam Eswaramoorthy, Yury Patskovsky, Brandon Hillerich, Ron Seidel, Andrej Sali, Brian K. Shoichet, Steven C. Almo, Subramanyam Swaminathan, Martin E. Tanner, and Frank M. Raushel\*



### Axial Ligand Replacement Mechanism in Heme Transfer from Streptococcal Heme-Binding Protein Shp to HtsA of the HtsABC Transporter

Yanchao Ran, G. Reza Malmirchegini, Robert T. Clubb, and Benfang Lei\*



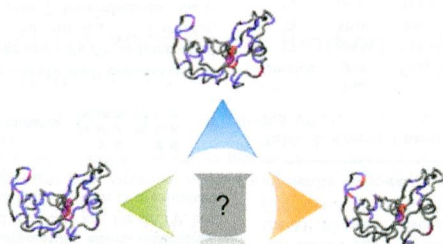


6548 **S**

dx.doi.org/10.1021/bi400973e

### What's in Your Buffer? Solute Altered Millisecond Motions Detected by Solution NMR

Madeline Wong, Gennady Khirich, and J. Patrick Loria\*

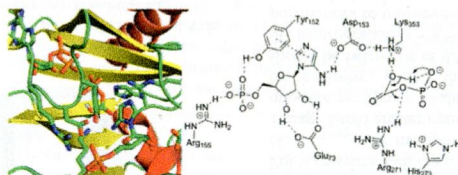


6559 **S**

dx.doi.org/10.1021/bi400444y

### Site-Directed Mutagenesis of Catalytic Residues in *N*<sup>5</sup>-Carboxyaminoimidazole Ribonucleotide Synthetase

Mahender B. Dewal and Steven M. Firestone\*



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dx.doi.org/10.1021/bi401026d

### The Periplasmic Cavity of LacY Mutant Cys154→Gly: How Open Is Open?

Xiaoxu Jiang, Arnold J. M. Driessen, Ben L. Feringa, and H. Ronald Kaback\*

