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AUGUST 6, 2013 • VOLUME 52 NUMBER 31

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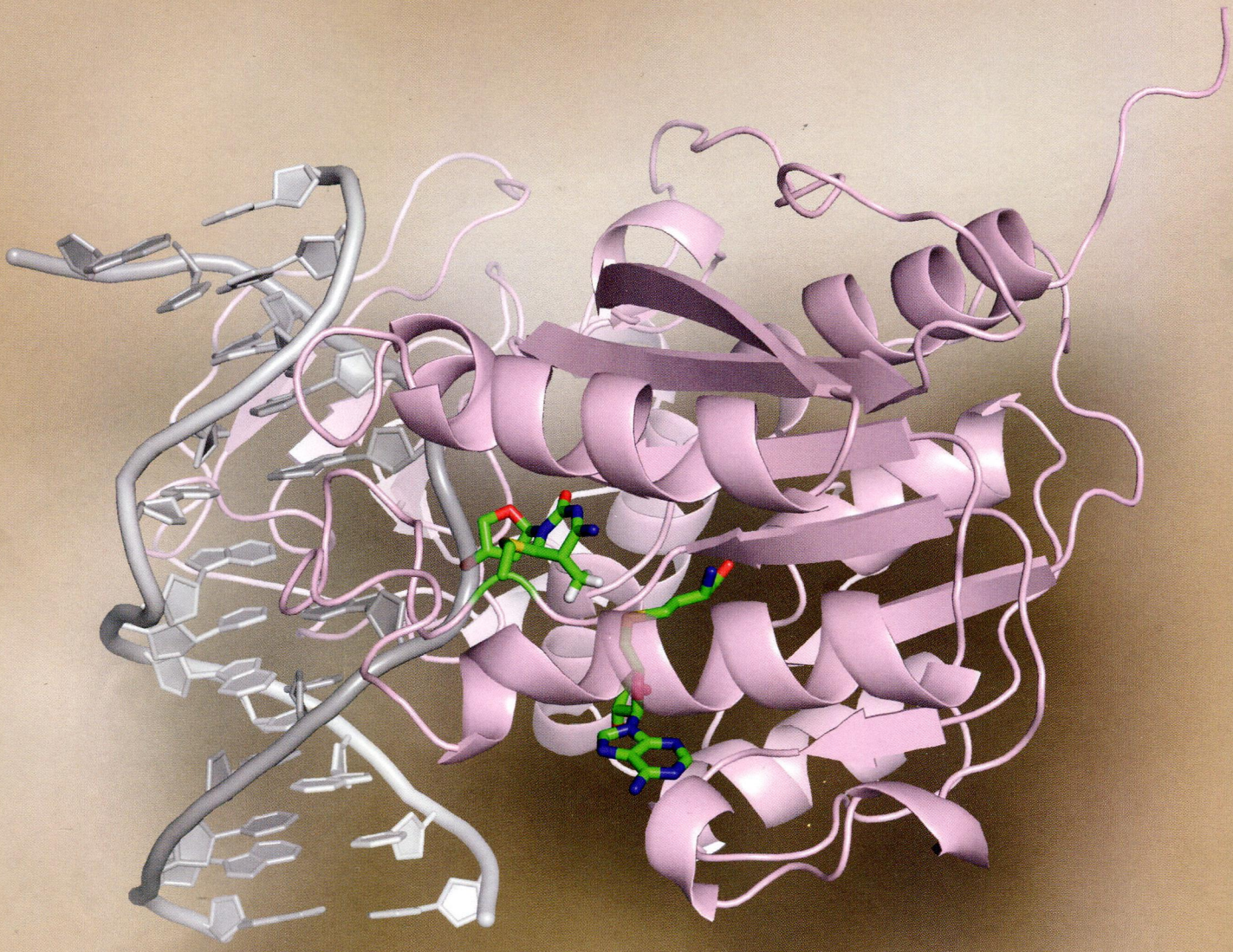

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AUGUST 6, 2013
VOLUME 52 ISSUE 31

BICHAW 52(31) 5155−5328 (2013)
ISSN 0006-2960
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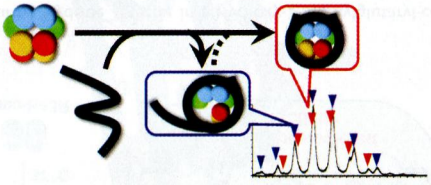
ON THE COVER: The detailed atomistic reaction mechanism for the epigenetic methylation of cytosine has been elucidated for the representative prokaryotic DNA methyltransferase *HhaI*, utilizing ab initio quantum mechanical/molecular mechanical-molecular dynamics simulations. Shown here is the intermediate 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

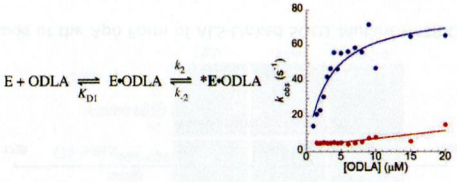
5155 Ⓢ dx.doi.org/10.1021/bi4005655

Conclusive Evidence of the Reconstituted Hexasome Proven by Native Mass Spectrometry
Nanako Azegami, Kazumi Saikusa, Yasuto Todokoro, Aritaka Nagadoi, Hitoshi Kurumizaka, Yoshifumi Nishimura,* and Satoko Akashi*



5158 Ⓢ dx.doi.org/10.1021/bi400807r

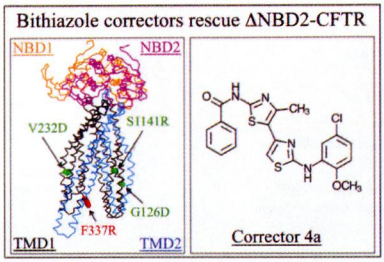
***Escherichia coli* Heptosyltransferase I: Investigation of Protein Dynamics of a GT-B Structural Enzyme**
Daniel J. Czyzyk, Shreya S. Sawant, Carlos A. Ramirez-Mondragon, Manju M. Hingorani, and Erika A. Taylor*



5161 dx.doi.org/10.1021/bi4008758

Bithiazole Correctors Rescue CFTR Mutants by Two Different Mechanisms

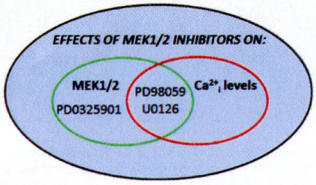
Tip W. Loo, M. Claire Bartlett, and David M. Clarke*



5164 dx.doi.org/10.1021/bi4007644

Off-Target Effects of MEK Inhibitors

Eric M. Wauson,* Marcy L. Guerra, Barbara Barylko, Joseph P. Albanesi, and Melanie H. Cobb*



Articles

5167 dx.doi.org/10.1021/bi400502c

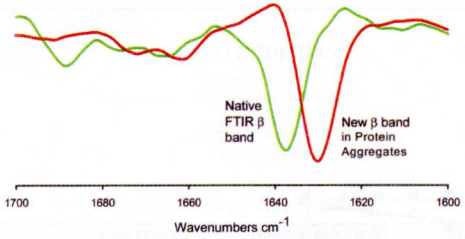
Cooperative Unfolding of Compact Conformations of the Intrinsically Disordered Protein Osteopontin

Dennis Kurzbach, Gerald Platzer, Thomas C. Schwarz, Morkos A. Henen, Robert Konrat,* and Dariush Hinderberger*

5176 dx.doi.org/10.1021/bi400625v

Distinct β-Sheet Structure in Protein Aggregates Determined by ATR–FTIR Spectroscopy

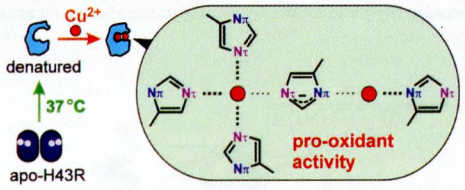
Bhavana Shivu,* Sangita Seshadri, Jie Li, Keith A. Oberg, Vladimir N. Uversky, and Anthony L. Fink



5184 dx.doi.org/10.1021/bi400370w

Pro-Oxidant Copper-Binding Mode of the Apo Form of ALS-Linked SOD1 Mutant H43R Denatured at Physiological Temperature

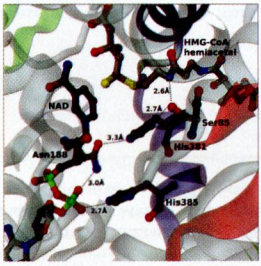
Nobuhiro Fujimaki, Furi Kitamura, and Hideo Takeuchi*



5195 dx.doi.org/10.1021/bi400335g

A Novel Role for Coenzyme A during Hydride Transfer in 3-Hydroxy-3-methylglutaryl-coenzyme A Reductase

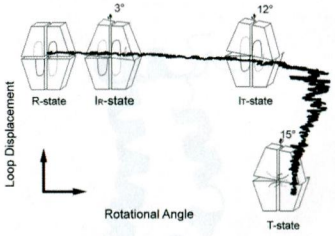
C. Nicklaus Steussy, Chandra J. Critchelow, Tim Schmidt, Jung-Ki Min, Louise V. Wrensford, John W. Burgner II, Victor W. Rodwell, and Cynthia V. Stauffacher*



5206 dx.doi.org/10.1021/bi400532n

Mechanism of Displacement of a Catalytically Essential Loop from the Active Site of Mammalian Fructose-1,6-bisphosphatase

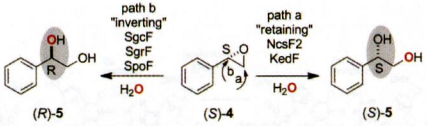
Yang Gao, Cristina V. Iancu, Susmith Mukind, Jun-Yong Choe, and Richard B. Honzatko*



5217 dx.doi.org/10.1021/bi400572a

Predictive Model for Epoxide Hydrolase-Generated Stereochemistry in the Biosynthesis of Nine-Membered Enediyne Antitumor Antibiotics

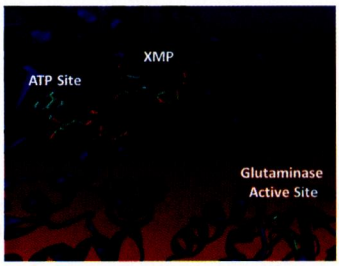
Geoffrey P. Horsman, Anna Lechner, Yasuo Ohnishi, Bradley S. Moore, and Ben Shen*



5225 dx.doi.org/10.1021/bi3017075

Substrate Activation and Conformational Dynamics of Guanosine 5′-Monophosphate Synthetase

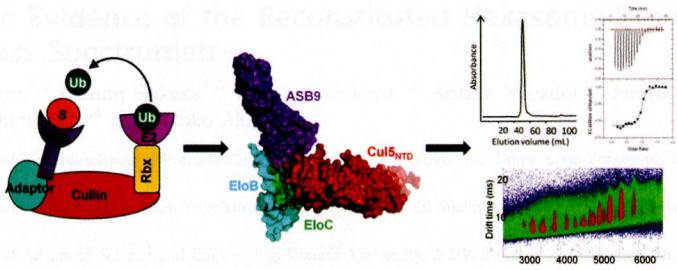
Justin C. Oliver, Rebecca S. Linger, Sridar V. Chittur, and V. Jo Davisson*



5236 dx.doi.org/10.1021/bi400758h

Multimeric Complexes among Ankyrin-Repeat and SOCS-box Protein 9 (ASB9), ElonginBC, and Cullin 5: Insights into the Structure and Assembly of ECS-type Cullin-RING E3 Ubiquitin Ligases

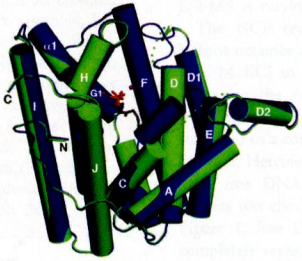
Jemima C. Thomas, Dijana Matak-Vinkovic, Inge Van Molle, and Alessio Ciulli*



5247 dx.doi.org/10.1021/bi400797c

Unexpected Reactivity of 2-Fluorolinalyl Diphosphate in the Active Site of Crystalline 2-Methylisoborneol Synthase

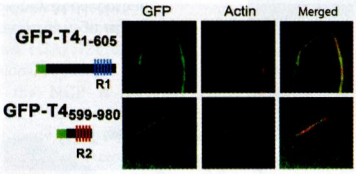
Mustafa Köksal, Wayne K. W. Chou, David E. Cane,* and David W. Christianson*



5256 dx.doi.org/10.1021/bi400585h

R1 Motif Is the Major Actin-Binding Domain of TRIOBP-4

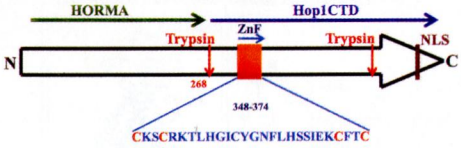
Jianjun Bao, Elizabeth Bielski, Ankita Bachhawat, Doaa Taha, Laura K. Gunther, Kavitha Thirumurugan, Shin-ichiro Kitajiri,* and Takeshi Sakamoto*



5265 S dx.doi.org/10.1021/bi4005528

N-Terminal Disordered Domain of *Saccharomyces cerevisiae* Hop1 Protein Is Dispensable for DNA Binding, Bridging, and Synapsis of Double-Stranded DNA Molecules But Is Necessary for Spore Formation

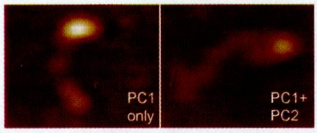
Krishnendu Khan, T. P. Vipin Madhavan, Rucha Kshirsagar, Kannan N. Boosi, Parag Sadhale, and K. Muniyappa*



5280 dx.doi.org/10.1021/bi400233e

Polycystin-2 Induces a Conformational Change in Polycystin-1

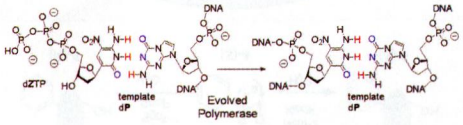
Peter Oatley, Md. Mesbah Uddin Talukder, Andrew P. Stewart, Richard Sandford, and J. Michael Edwardson*



5288 S dx.doi.org/10.1021/bi400558c

Directed Evolution of Polymerases To Accept Nucleotides with Nonstandard Hydrogen Bond Patterns

Roberto Laos, Ryan Shaw, Nicole A. Leal, Eric Gaucher, and Steven Benner*



5295 dx.doi.org/10.1021/bi4006623

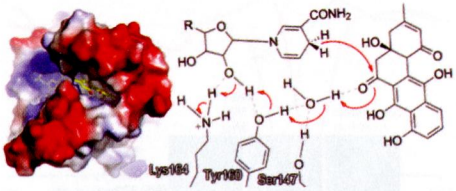
Three-Dimensional Structure and Interaction Studies of Hepatitis C Virus p7 in 1,2-Dihexanoyl-*sn*-glycero-3-phosphocholine by Solution Nuclear Magnetic Resonance

Gabriel A. Cook, Lindsay A. Dawson, Ye Tian, and Stanley J. Opella*

5304 dx.doi.org/10.1021/bi400712q

Structural and Functional Analysis of Angucycline C-6 Ketoreductase LanV Involved in Landomycin Biosynthesis

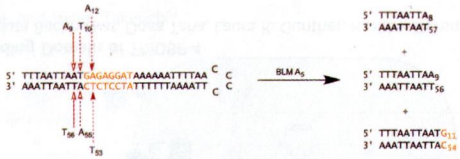
Pasi Paananen, Pekka Patrikainen, Pauli Kallio, Pekka Mäntsälä, Jarmo Niemi, Laila Niiranen, and Mikko Metsä-Ketelä*



5315 dx.doi.org/10.1021/bi400779r

Characterization of Bleomycin-Mediated Cleavage of a Hairpin DNA Library

Zachary J. Segerman, Basab Roy, and Sidney M. Hecht*



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