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July 23, 2013
Volume 52, Issue 29
Pages 4871-5028

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About 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]. View the article.

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ARTICLES

Photoconversion Mechanism of the Second GAF Domain of Cyanobacteriochrome AnPixJ and the Cofactor Structure of Its Green-Absorbing State

Francisco Velazquez Escobar, Tillmann Utesch, Rei Narikawa, Masahiko Ikeuchi, Maria Andrea Mroginski, Wolfgang Gärtner, and Peter Hildebrandt

pp 4871-4880
Publication Date (Web): June 28, 2013 (Article)
DOI: 10.1021/bi400506a

ACS Section: General Biochemistry

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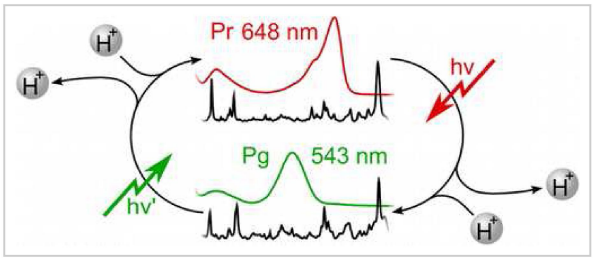

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Following DNA Chain Extension and Protein Conformational Changes in Crystals of a Y-Family DNA Polymerase via Raman Crystallography

Shirly J. Espinoza-Herrera, Vineet Gaur, Zucai Suo, and Paul R. Carey

pp 4881-4890
Publication Date (Web): July 3, 2013 (Article)
DOI: 10.1021/bi400524h

Section: Enzymes

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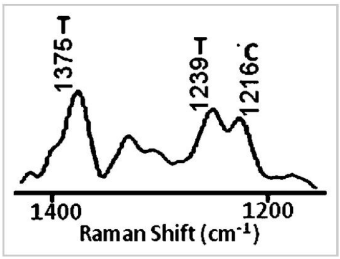

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Enthalpy–Entropy Compensation in Biomolecular Halogen Bonds Measured in DNA Junctions

Megan Carter, Andrea Regier Voth, Matthew R. Scholfield, Brittany Rummel, Lawrence C. Sowers, and P. Shing Ho

pp 4891-4903
Publication Date (Web): June 24, 2013 (Article)
DOI: 10.1021/bi400590h

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Thermodynamic and Structural Analysis of Human NFU Conformational Chemistry

Jingwei Li, Shu Ding, and J. A. Cowan

pp 4904-4913
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Effects of Asparagine Mutagenesis of Conserved Aspartic Acids in Helix 2 (D2.50) and 3 (D3.32) of M_1–M_4 Muscarinic Receptors on the Irreversible Binding of Nitrogen Mustard Analogs of Acetylcholine and McN-A-343

Hinako Suga and Frederick J. Ehlert

pp 4914-4928
Publication Date (Web): July 5, 2013 (Article)
DOI: 10.1021/bi4003698

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A Sensitive Assay Using a Native Protein Substrate for Screening HIV-1 Maturation Inhibitors Targeting the Protease Cleavage Site between the Matrix and Capsid

Sook-Kyung Lee, Nancy Cheng, Emily Hull-Ryde, Marc Potempa, Celia A. Schiffer, William Janzen, and Ronald Swanstrom

pp 4929-4940
Publication Date (Web): June 13, 2013 (Article)
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Examination of the Polypeptide Substrate Specificity for *Escherichia coli* ClpA

Tao Li and Aaron L. Lucius

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Organization of F-Actin by Fesselin (avian smooth muscle synaptopodin 2)

Mechthild M. Schroeter, Albina Orlova, Edward H. Egelman, Brent Beall, and Joseph M. Chalovich

pp 4955-4961
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Relative Free Enthalpies for Point Mutations in Two Proteins with Highly Similar Sequences but Different Folds

Niels Hansen, Jane R. Allison, Florian H. Hodel, and Wilfred F. van Gunsteren

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Publication Date (Web): June 26, 2013 (Article)
DOI: 10.1021/bi400272q

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Aggregation of Alzheimer's Amyloid β-Peptide in Biological Membranes: A Molecular Dynamics Study

Justin A. Lemkul and David R. Bevan

pp 4971-4980
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DOI: 10.1021/bi400562x

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Efavirenz Stimulates HIV-1 Reverse Transcriptase RNase H Activity by a Mechanism Involving Increased Substrate Binding and Secondary Cleavage Activity

John M. Muchiri, Dongge Li, Carrie Dykes, and Robert A. Bambara

pp 4981-4990
Publication Date (Web): June 27, 2013 (Article)
DOI: 10.1021/bi400618q

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Pan T. X. Li

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Dependence of the Product Chain-Length on Detergents for Long-Chain *E*-Polyprenyl Diphosphate Synthases

Jian-Jung Pan, Gurusankar Ramamoorthy, and C. Dale Poulter

pp 5002-5008
Publication Date (Web): June 26, 2013 (Article)
DOI: 10.1021/bi400681d

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Kinetic and Isotopic Characterization of L-Proline Dehydrogenase from *Mycobacterium tuberculosis*

Hector Serrano and John S. Blanchard

pp 5009-5015
Publication Date (Web): June 19, 2013 (Article)
DOI: 10.1021/bi400338f

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Active-Site Inhibitors Modulate the Dynamic Properties of Human Monoacylglycerol Lipase: A Hydrogen Exchange Mass Spectrometry Study

Ioannis Karageorgos, Thomas E. Wales, David R. Janero, Nikolai Zvonok, V. Kiran Vemuri, John R. Engen, and Alexandros Makriyannis

pp 5016-5026
Publication Date (Web): June 24, 2013 (Article)
DOI: 10.1021/bi400430k

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ADDITIONS AND CORRECTIONS

Correction to A Yeast Telomerase Complex Containing the Est1 Recruitment Protein Is Assembled Early in the Cell Cycle

Timothy M. Tucey and Victoria Lundblad

pp 5027-5027
Publication Date (Web): July 11, 2013 (Addition/Correction)
DOI: 10.1021/bi4006804

CAS Section: Microbial, Algal, and Fungal Biochemistry

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