

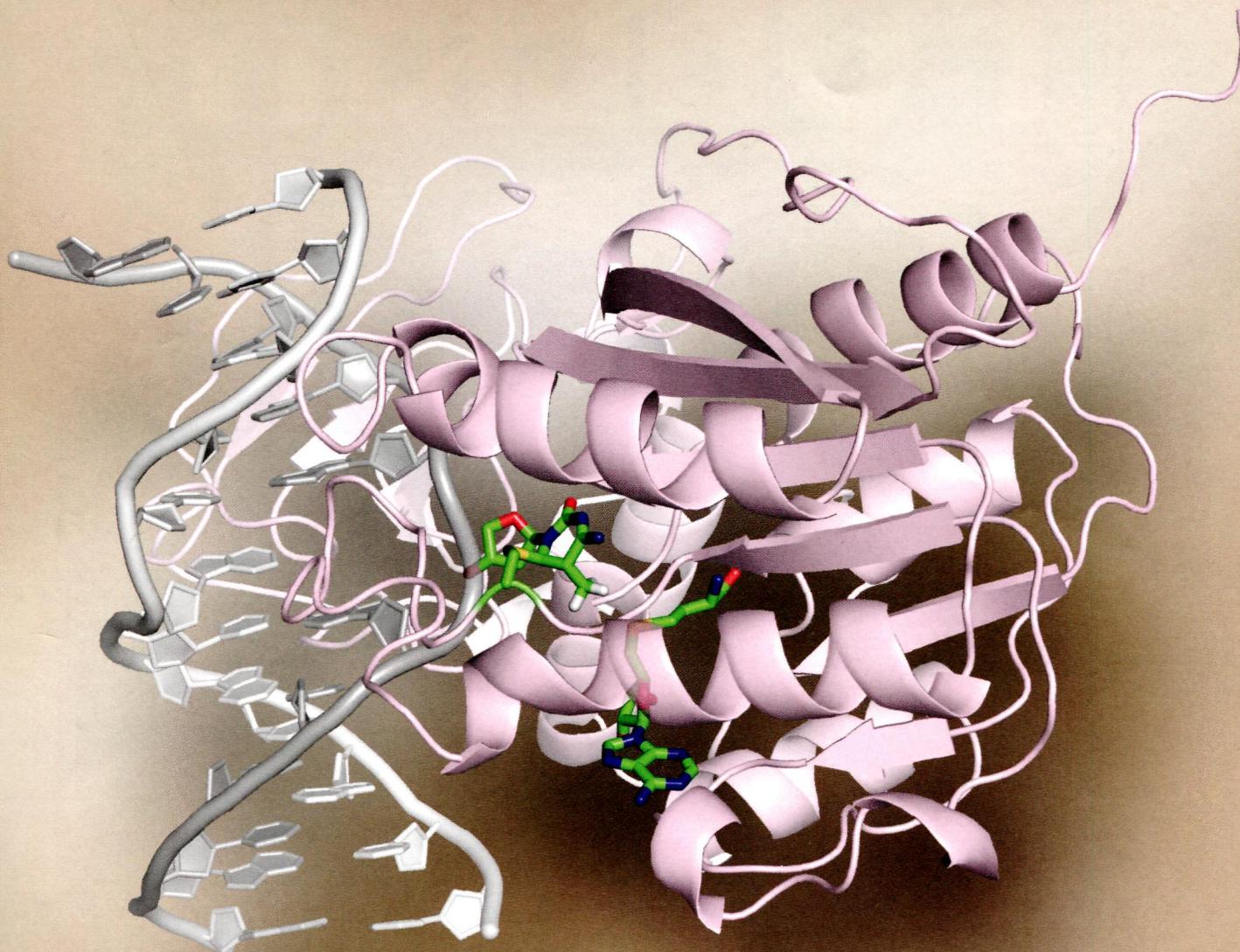
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# BIOCHEMISTRY

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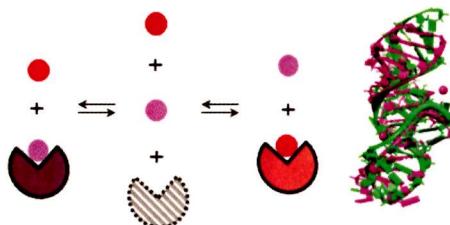
**ON THE COVER:** The detailed atomistic reaction mechanism for the epigenetic methylation of cytosine has been elucidated for the representative prokaryotic DNA methyltransferase *HhaI*, utilizing ab initio quantum mechanical/molecular mechanical-molecular dynamics simulations. Shown here is the intermediate 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].

## Articles

6575 

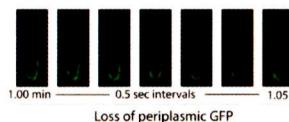
### Thermodynamics and Kinetics of Adaptive Binding in the Malachite Green RNA Aptamer

Jason B. Da Costa, Aurelia I. Andreiev, and Thorsten Dieckmann\*

[dx.doi.org/10.1021/bi400549s](https://doi.org/10.1021/bi400549s)6584 

### Localized Permeabilization of *E. coli* Membranes by the Antimicrobial Peptide Cecropin A

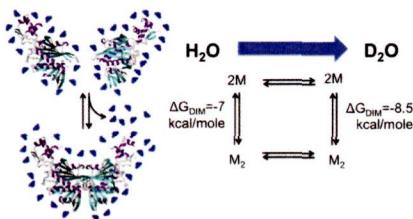
Nambirajan Rangarajan, Somenath Bakshi, and James C. Weisshaar\*

[dx.doi.org/10.1021/bi400785j](https://doi.org/10.1021/bi400785j)

6595

**A Large Solvent Isotope Effect on Protein Association Thermodynamics**  
Christopher Eginton and Dorothy Beckett\*

dx.doi.org/10.1021/bi400952m



6601

**Topology of the Yeast Ras Converting Enzyme As Inferred from Cysteine Accessibility Studies**

Emily R. Hildebrandt, Dillon M. Davis, John Deaton, Ranjith K. Krishnankutty, Edward Lilla, and Walter K. Schmidt\*

PEG-Maleimide 5000  
(R - PEG 5000)

O=C1C=CC(=O)N1R + HS-C(=O)NH-R -> O=C1C=CC(=O)N1SC(=O)NH-R

free thiol (cysteine)      covalent adduct

dx.doi.org/10.1021/bi400647c

dx.doi.org/10.1021/bi400450q

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**Loss of Electrostatic Interactions Causes Increase of Dynamics within the Plastocyanin–Cytochrome f Complex**  
Sandra Scanu, Johannes M. Foerster, Monika Timmer, G. Matthias Ullmann, and Marcellus Ubbink\*

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**DEER EPR Measurements for Membrane Protein Structures via Bifunctional Spin Labels and Lipodisq Nanoparticles**  
Indra D. Sahu, Robert M. McCarrick, Kaylee R. Troxel, Rongfu Zhang, Hubbell J. Smith, Megan M. Dunagan, Max S. Swartz, Prashant V. Rajan, Brett M. Kroncke, Charles R. Sanders, and Gary A. Lorigan\*

dx.doi.org/10.1021/bi4007622

6633

**Arabidopsis thaliana Nfu2 Accommodates [2Fe-2S] or [4Fe-4S] Clusters and Is Competent for *in Vitro* Maturation of Chloroplast [2Fe-2S] and [4Fe-4S] Cluster-Containing Proteins**  
Huanyao Gao, Sowmya Subramanian, Jérémie Couturier, Sunil G. Naik, Sung-Kun Kim, Thomas Leustek, David B. Knaff, Hui-Chen Wu, Florence Vignols, Boi Hanh Huynh, Nicolas Rouhier, and Michael K. Johnson\*

dx.doi.org/10.1021/bi400770d

6646

**Crystal Structure of Psb31, a Novel Extrinsic Protein of Photosystem II from a Marine Centric Diatom and Implications for Its Binding and Function**  
Ryo Nagao, Michihiro Suga, Ayako Niikura, Akinori Okumura, Faisal Hammad Mekky Koua, Takehiro Suzuki, Tatsuya Tomo, Isao Enami, and Jian-Ren Shen\*

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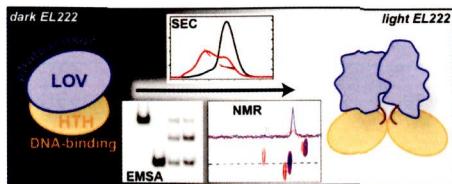
Biochemistry, Volume 52, Issue 38

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Biochemistry, Volume 52, Issue 38

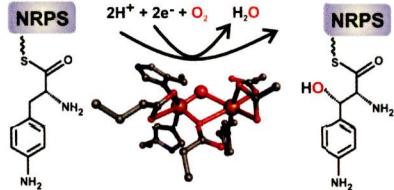
Blue Light-Induced Dimerization of a Bacterial LOV-HTH DNA-Binding Protein

Brian D. Zoltowski, Laura B. Motta-Mena, and Kevin H. Gardner\*



**Structure of a Dinuclear Iron Cluster-Containing  $\beta$ -Hydroxylase Active in Antibiotic Biosynthesis**  
Thomas M. Makris, Cory J. Knot, Carrie M. Wilmet,\* and John D. Lipscomb\*

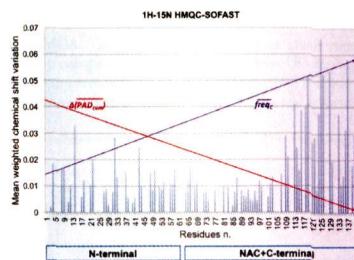
Thomas M. Makris, Cory J. Knott, Carrie M. Willmot,<sup>†</sup> and John D. Lipscomb<sup>†</sup>



A Molecular Dynamics Simulation-Based Interpretation of Nuclear Magnetic Resonance Multidimensional Heteronuclear Spectra of  $\alpha$ -Synuclein-Dopamine Adducts

## Spectra of $\alpha$ -Synuclein Dopamine Adducts

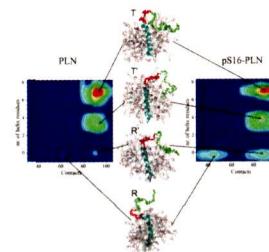
Domenica Dibenedetto, Giulia Bossetti,\* Rocco Caliandro, and Paolo Carloni



## **Structures of the Excited States of Phospholamban and Shifts in Their Populations upon Phosphorylation**

Alfonso De Simone, Martin Gustavsson, Rinaldo W. Montalvao, Lei Shi, Gianluigi Veglia, and Michele Vendruscolo\*

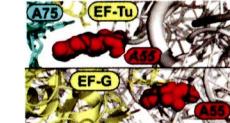
Alfonso De Simone, Martin Gustavsson, Rinaldo W. Montalvao, Lei Shi, Gianluigi Vigna, and Michele Verdarsolo



## Highly Conserved Base A55 of 16S Ribosomal RNA Is Important for the Elongation Cycle of Protein Synthesis

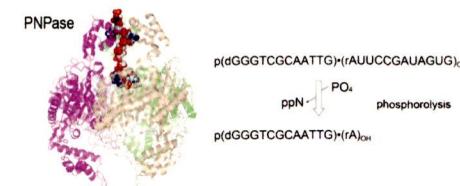
Rhubananda Sahu, Prashant K. Khade, and Simpson Joseph\*

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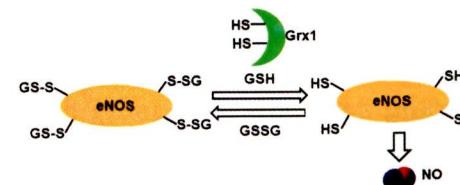
## Discrimination of RNA from DNA by Polynucleotide Phosphorylase

Dissemination of HIV from DMSO, Polymers Mihaela-Carmen Unciuleac and Stewart Shuman\*



## Redox Modulation of Endothelial Nitric Oxide Synthase by Glutaredoxin-1 through Reversible Oxidative Post-Translational Modification

Chun-An Chen,\* Francesco De Pascali, Ariel Basye, Craig Hemann, and Jay L. Zweier\*



**Characterizing the Promiscuity of LigAB, a Lignin Catabolite Degrading Extradiol Dioxygenase from *Sphingomonas paucimobilis* SYK-6**

Kevin P. Barry and Erika A. Taylor\*

