

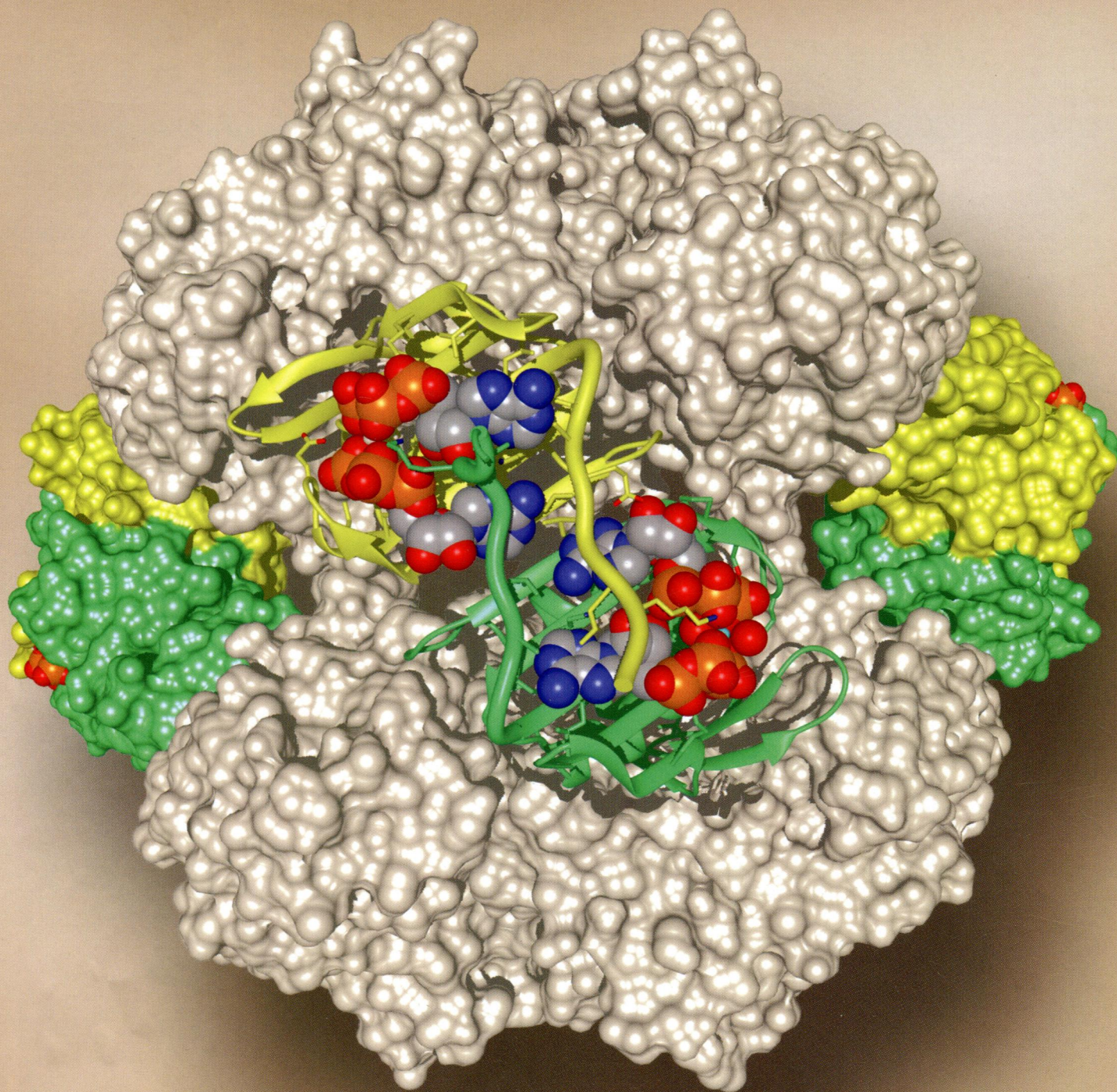
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# BIOCHEMISTRY

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**ON THE COVER:** Three-dimensional structure of the *Escherichia coli* aspartate transcarbamoylase holoenzyme in the R state with two ATP molecules and a  $Mg^{2+}$  cation bound to each regulatory chain. The two catalytic trimers are shown as surface representations (tan). One chain of each of the three regulatory dimers is colored yellow, while the other is colored green. The two regulatory dimers on the sides are shown as surface representations, while the third, in front, is shown as a ribbon trace. The binding of the two ATP molecules and one  $Mg^{2+}$  molecule induces an alteration of the N-termini of the regulatory chains (thick lines), displacing them into the adjacent regulatory chain and thereby strengthening the dimer interface and further stabilizing the R state of the enzyme. This figure was generated using UCSF Chimera. [Cockrell, G. M., et al. (2013) *Biochemistry* 52, 8036–8047]

## Editorial

1723

[dx.doi.org/10.1021/bi500258s](https://doi.org/10.1021/bi500258s)

**Call for Papers! A Special Thematic Compilation/Special Issue Crossover with ACS Chemical Biology, ACS Medicinal Chemistry Letters, and the Journal of Medicinal Chemistry Focused on New Frontiers in Kinases**

Jeffrey L. Benovic\* and Richard N. Armstrong\*

## Articles

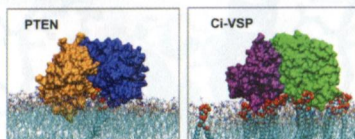
1724



[dx.doi.org/10.1021/bi5000299](https://doi.org/10.1021/bi5000299)

**Interactions of Phosphatase and Tensin Homologue (PTEN) Proteins with Phosphatidylinositol Phosphates: Insights from Molecular Dynamics Simulations of PTEN and Voltage Sensitive Phosphatase**

Antreas C. Kalli, Isabel Devaney, and Mark S. P. Sansom\*



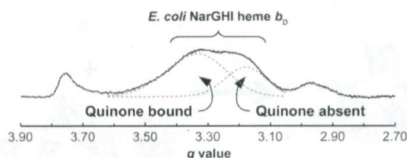
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[dx.doi.org/10.1021/bi500121x](https://doi.org/10.1021/bi500121x)

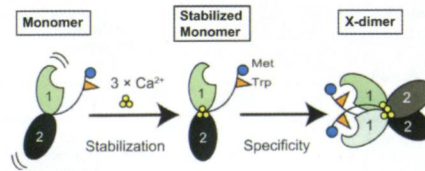
**Q-Site Occupancy Defines Heme Heterogeneity in *Escherichia coli* Nitrate Reductase A (NarGHI)**

Justin G. Fedor, Richard A. Rothery, Karissa S. Giraldi, and Joel H. Weiner\*



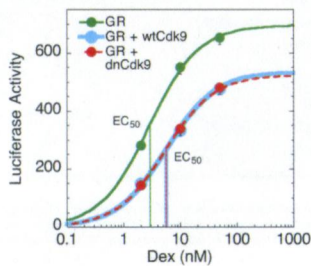
### Identification and Characterization of the X-Dimer of Human P-Cadherin: Implications for Homophilic Cell Adhesion

Shota Kudo, Jose M. M. Caaveiro, Shuichiro Goda, Satoru Nagatoishi, Keisuke Ishii, Tadashi Matsuura, Yukio Sudou, Tatsuhiko Kodama, Takao Hamakubo, and Kouhei Tsumoto\*



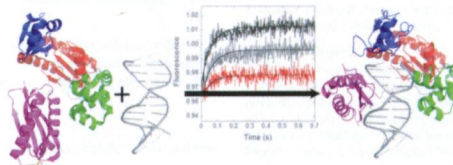
### A Kinase-Independent Activity of Cdk9 Modulates Glucocorticoid Receptor-Mediated Gene Induction

Rong Zhu, Xinping Lu, Madhumita Pradhan, Stephen P. Armstrong, Geoffrey B. Storch, Carson C. Chow, and S. Stoney Simons Jr.\*



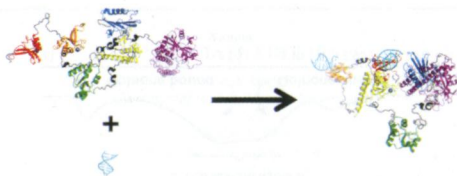
### Conformational Dynamics of a Y-Family DNA Polymerase during Substrate Binding and Catalysis As Revealed by Interdomain Förster Resonance Energy Transfer

Brian A. Maxwell, Cuiling Xu, and Zucai Suo\*



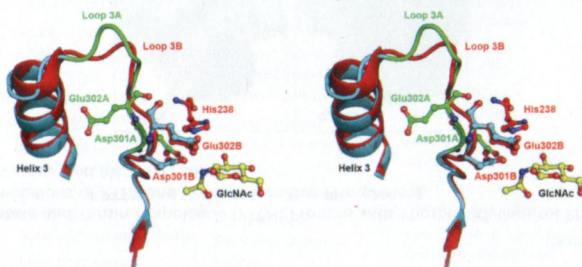
**Conformational Activation of Poly(ADP-ribose) Polymerase-1 upon DNA Binding Revealed by Small-Angle X-ray Scattering**

Steven O. Mansoorabadi, Meilan Wu, Zhihua Tao, Peng Gao, Sai Venkatesh Pingali, Liang Guo, and Hung-wen Liu\*



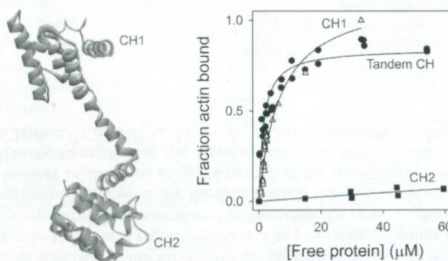
**Structure and Activity of the *Streptomyces coelicolor* A3(2)  $\beta$ -N-Acetylhexosaminidase Provides Further Insight into GH20 Family Catalysis and Inhibition**

Nhung Nguyen Thi, Wendy A. Offen, François Shareck, Gideon J. Davies, and Nicolas Doucet\*



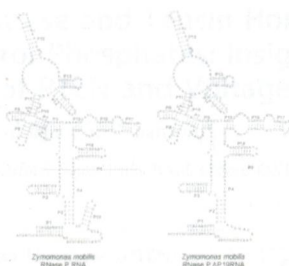
**The Actin Binding Affinity of the Utrophin Tandem Calponin-Homology Domain Is Primarily Determined by Its N-Terminal Domain**

Surinder M. Singh, Swati Bandi, Steve J. Winder, and Krishna M. G. Mallela\*

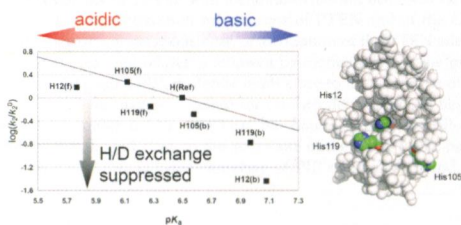


**On the Role of the Appended P19 Element in Type A RNAs of Bacterial RNase P**

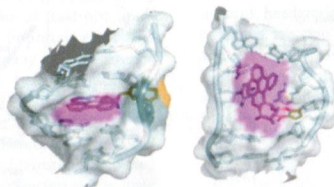
Vassiliki Stamatopoulou, Chrisavgi Toumpeki, Anastassios Vourekas, Maria Bikou, Marianthi Tsitilaidou, Andreas G. Tzakos, Amalia Afendra,\* Constantin Drinas, and Denis Drinas\*

**Imidazole C-2 Hydrogen/Deuterium Exchange Reaction at Histidine for Probing Protein Structure and Function with Matrix-Assisted Laser Desorption Ionization Mass Spectrometry**

Naoka Hayashi, Hiroki Kuyama, Chihiro Nakajima, Kazuki Kawahara, Masaru Miyagi, Osamu Nishimura, Hisayuki Matsuo, and Takashi Nakazawa\*

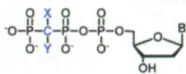
**Nuclear Magnetic Resonance Studies of an *N*<sup>2</sup>-Guanine Adduct Derived from the Tumorigen Dibenzo[*a,h*]pyrene in DNA: Impact of Adduct Stereochemistry, Size, and Local DNA Sequence on Solution Conformations**

Fabián A. Rodríguez, Zhi Liu, Chin H. Lin, Shuang Ding, Yuqin Cai, Alexander Kolbanovskiy, Marina Kolbanovskiy, Shantu Amin, Suse Brojde, and Nicholas E. Geacintov\*



**Transition State in DNA Polymerase  $\beta$  Catalysis: Rate-Limiting Chemistry Altered by Base-Pair Configuration**

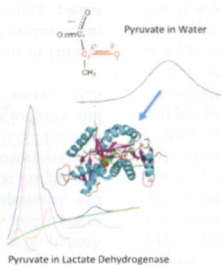
Kerriann Oertel, Brian T. Chamberlain, Yue Wu, Elena Ferri, Boris A. Kashemirov, William A. Beard, Samuel H. Wilson, Charles E. McKenna,\* and Myron F. Goodman\*



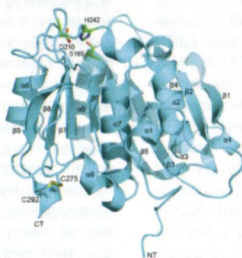
B = G or T  
 CXY = CH<sub>2</sub>, CHF, CF<sub>2</sub>, CHCl, CCl<sub>2</sub>, CHBr, CBr<sub>2</sub>, CCl, CHCH<sub>3</sub>, C(CH<sub>3</sub>)<sub>2</sub>, CFCH<sub>3</sub>, CHN<sub>3</sub>, CN<sub>2</sub>CH<sub>3</sub>.

**Energy Landscape of the Michaelis Complex of Lactate Dehydrogenase: Relationship to Catalytic Mechanism**

Huo-Lei Peng, Hua Deng, R. Brian Dyer, and Robert Callender\*

**Crystal Structure and Thermodynamic and Kinetic Stability of Metagenome-Derived LC-Cutinase**

Sintawee Sulaiman, Dong-Ju You, Eiko Kanaya, Yuichi Koga, and Shigenori Kanaya\*



**Structural and Mechanistic Insights into the PAPS-Independent Sulfotransfer Catalyzed by Bacterial Aryl Sulfotransferase and the Role of the DsbL/Dsbl System in Its Folding**

Goran Malojčić,\* Robin L. Owen, and Rudi Glockshuber

