

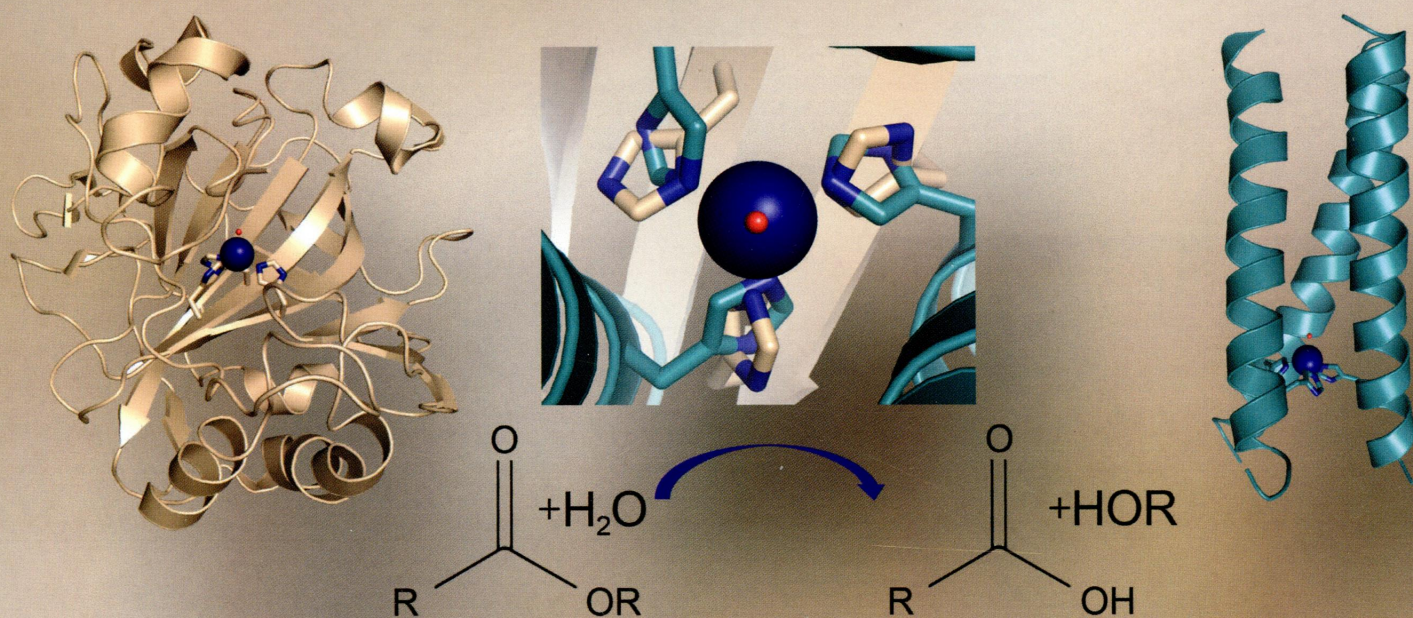
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**ON THE COVER:** Using de novo and redesign approaches toward the preparation of structural and functional models of hydrolytic zinc metalloenzymes. [Zastrow, M. L., and Pecoraro, V. L. (2014) *Biochemistry* 53, 957–978]

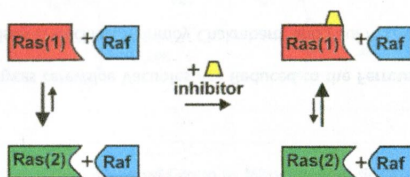
## Articles

3867

[dx.doi.org/10.1021/bi401689w](https://doi.org/10.1021/bi401689w)

### Elucidating the Mode of Action of a Typical Ras State 1(T) Inhibitor

Ina C. Rosnizeck, Daniel Filchtinski, Rui Pedro Lopes, Bärbel Kieninger, Christian Hermann, Hans Robert Kalbitzer, and Michael Spoerner\*

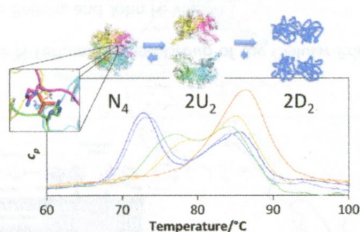


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[dx.doi.org/10.1021/bi500137b](https://doi.org/10.1021/bi500137b)

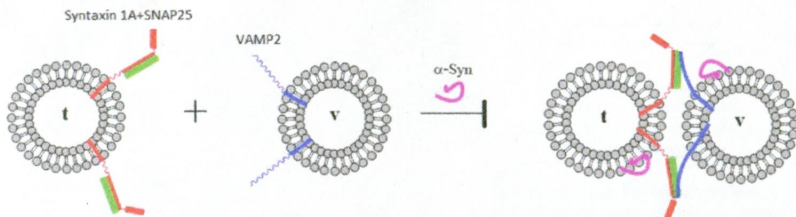
### Intersubunit Salt Bridges with a Sulfate Anion Control Subunit Dissociation and Thermal Stabilization of *Bacillus* sp. TB-90 Urate Oxidase

Takao Hibi,\* Yuta Hayashi, Harumi Fukada, Takafumi Itoh, Tomohiro Nago, and Yoshiaki Nishiya



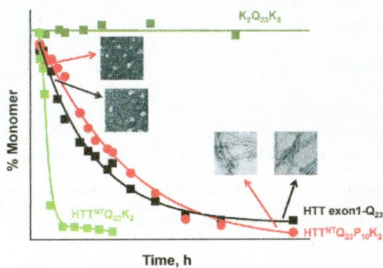
### Nonaggregated $\alpha$ -Synuclein Influences SNARE-Dependent Vesicle Docking via Membrane Binding

Ying Lai, Sunae Kim, Jobin Varkey, Xiaochu Lou, Jae-Kyun Song, Jiajie Diao, Ralf Langen, and Yeon-Kyun Shin\*



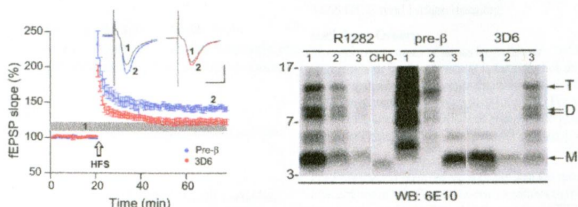
### Aggregation Behavior of Chemically Synthesized, Full-Length Huntingtin Exon1

Bankanidhi Sahoo, David Singer, Ravindra Kodali, Thole Zuchner, and Ronald Wetzel\*



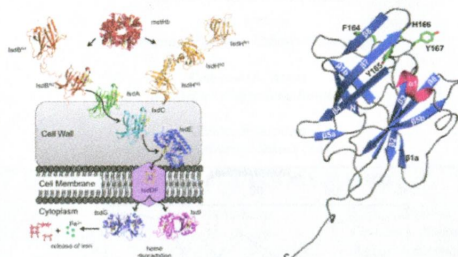
### Secreted Amyloid $\beta$ -Proteins in a Cell Culture Model Include N-Terminally Extended Peptides That Impair Synaptic Plasticity

Alfred T. Welzel, John E. Maggio, Ganesh M. Shankar, Donald E. Walker, Beth L. Ostaszewski, Shaomin Li, Igor Klyubin, Michael J. Rowan, Peter Seubert, Dominic M. Walsh,\* and Dennis J. Selkoe\*



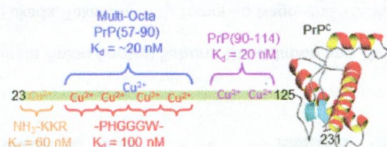
### Solution Structure and Molecular Determinants of Hemoglobin Binding of the First NEAT Domain of IsdB in *Staphylococcus aureus*

Brittany A. Fonner, Brian P. Tripet, Brian J. Eilers, Jessica Stanisich, Rose K. Sullivan-Springhetti, Rebecca Moore, Mengyao Liu, Benfang Lei, and Valérie Copié\*



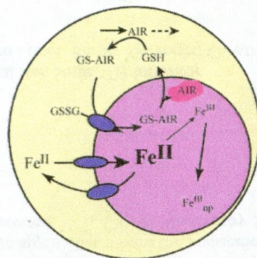
### Copper(II) Sequentially Loads onto the N-Terminal Amino Group of the Cellular Prion Protein before the Individual Octarepeats

Helen F. Stanyon, Khushbu Patel, Nadia Begum, and John H. Viles\*



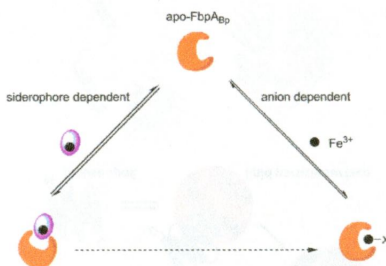
### High-Spin Ferric Ions in *Saccharomyces cerevisiae* Vacuoles Are Reduced to the Ferrous State during Adenine-Precursor Detoxification

Jinkyu Park, Sean P. McCormick, Allison L. Cockrell, Mrinmoy Chakrabarti, and Paul A. Lindahl\*

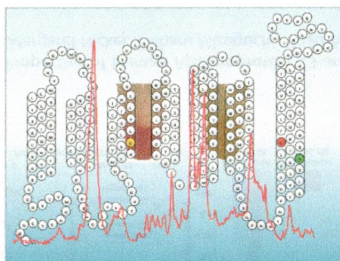


***Bordetella pertussis* FbpA Binds Both Unchelated Iron and Iron Siderophore Complexes**

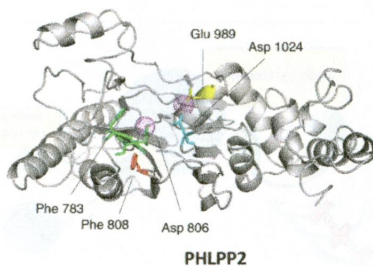
Sambuddha Banerjee, Aruna J. Weerasinghe, Claire J. Parker Siburt, R. Timothy Kreulen, Sandra K. Armstrong, Timothy J. Brickman, Lisa A. Lambert, and Alvin L. Crumbliss\*

**Retinal Chromophore Structure and Schiff Base Interactions in Red-Shifted Channelrhodopsin-1 from *Chlamydomonas augustae***

John I. Ogren, Sergey Mamaev, Daniel Russano, Hai Li, John L. Spudich, and Kenneth J. Rothschild\*

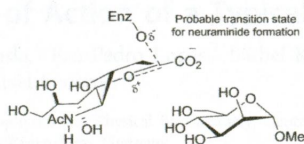
**Biochemical Characterization of the Phosphatase Domain of the Tumor Suppressor PH Domain Leucine-Rich Repeat Protein Phosphatase**

Emma Sierecki and Alexandra C. Newton\*



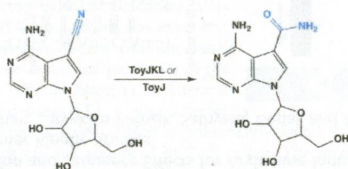
### Neuraminidase Substrate Promiscuity Permits a Mutant *Micromonospora viridifaciens* Enzyme To Synthesize Artificial Carbohydrates

Lydia L. Cheng, Fahimeh S. Shidmoosavee, and Andrew J. Bennet\*



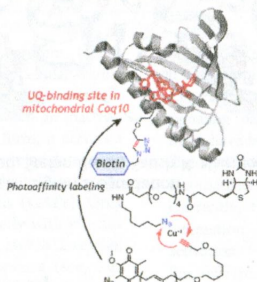
### The Alpha Subunit of Nitrile Hydratase Is Sufficient for Catalytic Activity and Post-Translational Modification

Micah T. Nelp, Andrei V. Astashkin, Linda A. Breci, Reid M. McCarty, and Vahe Bandarian\*



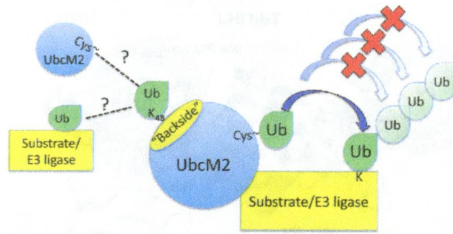
### Identification of the Binding Site of the Quinone-Head Group in Mitochondrial Coq10 by Photoaffinity Labeling

Masatoshi Murai, Kohei Matsunobu, Sawako Kudo, Kentaro Ifuku, Makoto Kawamukai, and Hideto Miyoshi\*



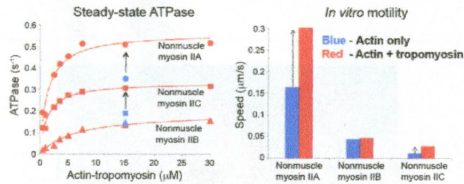
### The Ubiquitin-Conjugating Enzyme, UbcM2, Is Restricted to Monoubiquitylation by a Two-Fold Mechanism That Involves Backside Residues of E2 and Lys48 of Ubiquitin

Linda Nguyen, Kendra S. Plafker, Andrew Starnes, Matt Cook, Rachel E. Klevit, and Scott M. Plafker\*



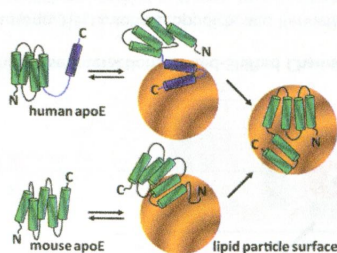
### Regulation of Nonmuscle Myosin II by Tropomyosin

Bipasha Barua,\* Attila Nagy, James R. Sellers, and Sarah E. Hitchcock-DeGregori



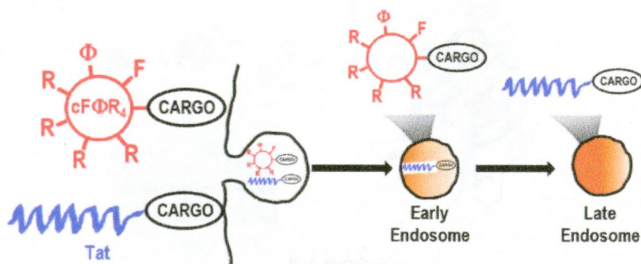
### Influence of Domain Stability on the Properties of Human Apolipoprotein E3 and E4 and Mouse Apolipoprotein E

David Nguyen, Padmaja Dhanasekaran, Margaret Nickel, Chiharu Mizuguchi, Mayu Watanabe, Hiroyuki Saito, Michael C. Phillips, and Sissel Lund-Katz\*

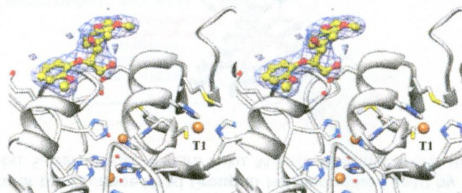


**Early Endosomal Escape of a Cyclic Cell-Penetrating Peptide Allows Effective Cytosolic Cargo Delivery**

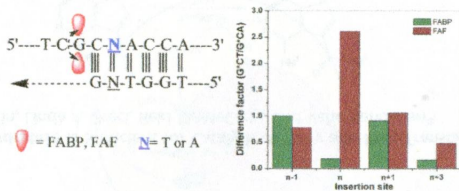
Ziqing Qian, Jonathan R. LaRochelle, Bisheng Jiang, Wenlong Lian, Ryan L. Hard, Nicholas G. Selner, Rindrada Luechapanichkul, Amy M. Barrios, and Dehua Pei\*

**Roles of Small Laccases from *Streptomyces* in Lignin Degradation**

Sudipta Majumdar,\* Tiit Lukk, Jose O. Solbiati, Stefan Bauer, Satish K. Nair, John E. Cronan, and John A. Gerlt

**Conformational Insights into the Lesion and Sequence Effects for Arylamine-Induced Translesion DNA Synthesis: <sup>19</sup>F NMR, Surface Plasmon Resonance, and Primer Kinetic Studies**

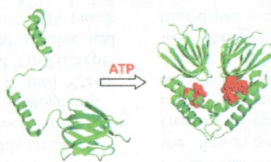
Vipin Jain, Vaidyanathan G. Vaidyanathan, Satyakam Patnaik, Sathyaraj Gopal, and Bongsup P. Cho\*





ATP-Induced Dimerization of the F<sub>0</sub>F<sub>1</sub> ε Subunit from *Bacillus* PS3: A Hydrogen Exchange–Mass Spectrometry Study

Antony D. Rodriguez, Stanley D. Dunn,\* and Lars Konnermann\*



## EXPERIMENTAL PROCEDURES

Protein purification and hydrogen exchange were performed as described previously (17). Briefly, the ε subunit was purified from *Bacillus* PS3 cells expressing a recombinant ε subunit under the control of the *lac* operon. The cells were grown in the presence of 1% lactose, and the ε subunit was purified from the culture supernatant by ion exchange chromatography. The purified ε subunit was then subjected to hydrogen exchange in the presence of 100 μM ATP. The exchange was stopped by the addition of 10% trichloroacetic acid, and the resulting peptides were analyzed by liquid chromatography–mass spectrometry (LC–MS/MS). The mass spectrometry data were analyzed using the MaxQuant software package (18). The resulting mass spectrometry data were then analyzed using the HydroX software package (19) to determine the hydrogen exchange rates of the peptides. The hydrogen exchange rates were then used to calculate the solvent accessibility of the peptides, which was used to determine the structure of the ε subunit dimer.

Supporting Information available via online article

The ε subunit of the F<sub>0</sub>F<sub>1</sub> ATP synthase is a peripheral membrane protein that is located in the cytoplasmic face of the membrane. It is a dimeric protein, and its dimerization is regulated by ATP. The ε subunit is composed of two subunits, each of which is approximately 30 kDa in size. The two subunits are connected to each other by a disulfide bond. The ε subunit is a highly flexible protein, and its structure is not well understood. However, it is believed that the ε subunit dimer is involved in the regulation of the ATP synthase activity. The ε subunit dimer is thought to act as a switch that can turn the ATP synthase on or off. When the ε subunit dimer is in the "open" state, the ATP synthase is active. When the ε subunit dimer is in the "closed" state, the ATP synthase is inactive. The transition between the open and closed states is regulated by ATP. When ATP is bound to the ε subunit dimer, it causes the dimer to close, which in turn inactivates the ATP synthase. When ATP is released from the ε subunit dimer, it causes the dimer to open, which activates the ATP synthase.

The structure of the ε subunit dimer is shown in Figure 1. The two subunits are connected to each other by a disulfide bond. The ε subunit dimer is a highly flexible protein, and its structure is not well understood. However, it is believed that the ε subunit dimer is involved in the regulation of the ATP synthase activity. The ε subunit dimer is thought to act as a switch that can turn the ATP synthase on or off. When the ε subunit dimer is in the "open" state, the ATP synthase is active. When the ε subunit dimer is in the "closed" state, the ATP synthase is inactive. The transition between the open and closed states is regulated by ATP. When ATP is bound to the ε subunit dimer, it causes the dimer to close, which in turn inactivates the ATP synthase. When ATP is released from the ε subunit dimer, it causes the dimer to open, which activates the ATP synthase.