

Abstracts, Division of Biological Chemistry, 199th National Meeting of the American Chemical Society, April 22-27, 1990

R. David Cole, Chair; Perry A. Frey, Chair Elect;
David S. Sigman, Program Chair; Vern Schramm, Program Chair Elect

MONDAY MORNING—1990 PFIZER AWARD IN ENZYME CHEMISTRY SYMPOSIUM IN HONOR OF JAMES WELLS—R. YOUNT, PRESIDING

1. Site-Directed Mutagenesis: Probes of Mechanism and Structure of Aspartate Aminotransferase. *J. Kiracki*, Department of Biochemistry, University of California, Berkeley, CA 94720.

No abstract available.

2. Engineering Proteins with Enhanced Thermal and Proteolytic Stability. *R. Sauer*, Department of Chemistry, Massachusetts Institute of Technology, Cambridge, MA 02139.

No abstract available.

3. Deducing and Manipulating Structural Motifs in Proteins with Unsolved Structures. *Paul Schimmel*, Department of Biology, Massachusetts Institute of Technology, Cambridge, MA 02139.

Structural motifs in proteins with unsolved structures can be suggested by sequence comparisons with and functional relationships to proteins with known three-dimensional structures. Structural models based on such analyses lack credibility, particularly when sequence similarities to proteins with solved structures are limited. However, specific deletions and mutations can be introduced into a protein of unknown structure to test specific features of any structural model. These approaches have been used to develop models of structural units within some of the members of the aminoacyl tRNA synthetase class of enzymes. For a synthetase of unsolved structure, experimental evidence has been obtained for a large insertion into a predicted functional domain and for the location of an important segment of a substrate binding domain. Further applications have led to constructs which allow study of interdomain packing interactions and of chimeric proteins which have substituted a domain of one enzyme for that of another.

4. Engineering Specificity in Proteins. *J. Wells*.

No abstract available.

MONDAY AFTERNOON—ACS AWARD IN PURE CHEMISTRY SYMPOSIUM IN HONOR OF PETER SCHULTZ—W. DeGRADO, PRESIDING

5. De Novo Design of Helical Proteins. *William F. DeGrado*, E. I. du Pont de Nemours and Company, Central Research and Development Department, Experimental Station, Wilmington, DE 19880-0328.

Our group has recently adopted a synthetic approach to understanding the structural basis for protein function. To test some of the rules and concepts which are believed to be important for protein folding and stability, we are attempting to design some simple proteins which should fold into pre-

termined three-dimensional structures. Two types of helical proteins have been designed: the first is an idealized version of a four-helix bundle, a folding pattern found in the structures of a variety of natural water-soluble proteins including myohemerythrin, cytochrome *c*, and apoferitin, while the other class of design proteins is meant to mimic the structures of proteins which form ion channels such as the acetylcholine receptor. Although these two classes of proteins differ in their properties and function, they both are composed of bundles of α -helices. The synthesis and characterization of these proteins are currently underway and will be the focus of the talk.

6. Antibody Catalysis: Perspectives and Prospects. *D. Hilvert*, Departments of Chemistry and Molecular Biology, Research Institute of Scripps Clinic, 10666 North Torrey Pines Road, La Jolla, CA 92037.

The selectivity and diversity of the mammalian immune system can be exploited to generate antibody molecules with tailored catalytic activities. For example, we have used rationally designed transition-state analogs to prepare immunoglobulins that promote two concerted chemical reactions, a sigmatropic Claisen rearrangement and a Diels-Alder cycloaddition. These antibodies are proving to be valuable tools for evaluating how enzymes exploit binding energy to achieve large rate accelerations and exacting regio- and stereoselectivities. Related catalysts are likely to have significant practical utility, as Claisen rearrangements and Diels-Alder cycloadditions are among the most important transformations available to synthetic organic chemists for the construction of complex natural products, therapeutic agents, and synthetic materials of all kinds. Additional, ongoing studies directed toward the improvement of the generation of catalytic antibodies using molecular biology and genetics will also be discussed.

7. Protein Dissection Using Peptide Models. *Peter S. Kim*, Whitehead Institute and Department of Biology, Massachusetts Institute of Technology, Cambridge, MA 02142.

There is now experimental evidence indicating that some proteins can be broken into modules. These modules correspond to autonomous folding units and often are substantially smaller than a domain. Studies of subdomains allow one to dissect structure/function relationships in proteins and to begin understanding protein folding in structural terms. We have been studying two types of modules: (1) disulfide-bonded peptide pairs corresponding to protein folding intermediates of bovine pancreatic trypsin inhibitor (BPTI); (2) peptide dimers formed by the isolated "leucine zipper" motif, which corresponds to a coiled-coil structure found in several DNA binding proteins. In both cases, it is possible to obtain modules of proteins that show substantial folded structure in aqueous solution.

8. Interplay between Chemistry and Biology: Catalyst Design. *P. G. Schultz*, Department of Chemistry, University of

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