MS29 IMPROVING STRUCTURES USING BIO-INFORMATICS
Chairpersons: Philip Eric Bourne, R. Sowdhamini

MS29.26.1
Acta Cryst. (2005). A**61**, C42
How the RCSB Validates PDB Structures
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The RCSB validates PDB data while considering the evolving nature of data and nomenclature standards. In order to provide the community with high quality data, the RCSB Protein Data Bank (www.pdb.org) has developed a number of tools that support the deposition and processing of X-ray and NMR structures and that are based upon the mmCIF dictionary [1]. A key feature is the Validation Suite [2], which produces a validation report highlighting close contacts, bond and angle deviations, chirality problems, missing and extra atoms and residues, and distant waters. Authors are encouraged to validate their structures before data deposition.

As the number of structures being determined is constantly increasing, the automation of data validation is extremely important. To reach this end, there needs to be consistency in the syntax and representation of incoming structure data. Tools are being developed to aid this process.

The RCSB also collaborates with wwPDB members to validate the entire PDB archive, and to distribute these data in a way that is most useful to members of the community.

The RCSB PDB is funded by NSF, NIGMS, Office of Science DOE, NLM, NCI, NCRR, NIBIB, and NINDS.

[1] Bourne P.E., Berman H.M., Watenpaugh K., Westbrook J.D., Fitzgerald P.M.D., *Meth. Enz.*, **1997**, 277, 571. [2] Westbrook J., Feng Z., Burkhardt K., Berman H.M., *Meth. Enz.* **2003**, 374, 370.
Keywords: structure validation, structure analysis, mmCIF

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A Systematic Study of Flexibility in Protein Structures and its Implications in Protein Structure Prediction
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Despite some level of overall similarity, proteins sharing the same fold usually display a significant structure variation that prohibits effective use of more distantly related proteins in detailed structure prediction, such as done in comparative modeling.

New generation of proteins structure alignments allow describing and classifying differences in structures between related proteins. The broad survey of structure variations within fold groups performed using FATCAT and POSA algorithms shows that proteins sharing a common fold display strong regularities in how their structure changes in response to mutations and/or substrate or inhibitor binding. Most of the structural variation within any given fold can be described by a small number of parameters, usually a position of a pivot point(s) and an angle(s) of rotation around it.

The results of this survey have important implications for comparative modeling and structural genomics. Flexible templates, rearranged according to the rules independently discovered for a given fold can be used for more accurate comparative modeling. At the same time, relatively small number of structures can be used to characterize structural divergence of large protein families. Specific examples for both applications are discussed.
Keywords: protein structures, structure prediction, flexibility

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Bioinformatics Approach to Characterization of SGNH/GDSL-hydrolases
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The present analysis is aimed to recognize structural elements of SGNH/GDSL family of enzymes with a novel folding type using bioinformatics tools on data of primary and secondary structures. Out of 770 proteins sequences deposited, data of seven different structures of GDSL hydrolases are solved, only; those of the best resolution were selected among twenty available in PDB (including mutants): rhamnogalacturonan acetyleserase from *Aspergillus aculeatus*, thioesterase I from *E. coli*, platelet-activating factor acetylhydrolase IBγ from *Bos taurus*, platelet-activating factor human acetylhydrolase IBβ, and esterase from *Streptomyces scabies*. Two novel enzymes of our interest, esterase from *Pseudomonas aeruginosa* and lipase from *Streptomyces rimosus*, were included in the analysis and compared with GDSL hydrolases of known three-dimensional structures. These two enzymes were recognized as the members of the SGNH/GDSL family with a fold being different from the common α/β hydrolase fold. Alignment of amino acid sequences of SGNH/GDSL hydrolases studied reveals similarity about 20%. However, four blocks of conserved sequence, with one conserved residue in each block (S,G,N,H) are common characteristics.
Keywords: databases, bioinformatics, novel hydrolase fold

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Validation and Classification of Protein Structures
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We discuss and summarize several new developments regarding the automated validation of protein structures, the decomposition of protein structures into domains, and the classification of protein domains.. As a specific example we present results on the assignment problem of oxygen and nitrogen atoms in the side chains of Glutamine (GLN) and Asparagine (ASN) in some detail. These atoms are difficult to distinguish in the interpretation of electron densities and it is known [1] that approximately 15% to 20% of the assignments in all known structures are incorrect.

We demonstrate how mean force potentials [2] derived from a set of high resolution PDB [3] protein structures can be used to recognize and correct erroneous N/O assignments. Since the potentials are derived from erroneous data sets this is an interesting and challenging problem for the development of potential functions. We show that within a few cycles of potential compilation and error correction the potentials converge to a stable functional form. The detected erroneous assignments fully agree with expert curated assignments [4]. The ASN/GLN flipper is available as a WEB service at http://services.came.sbg.ac.at/flipper.

[1] Hooft R.W.W et al, *Proteins*, 1996, **26**, 363. [2] Sippl, M.J., *Proteins*, 1993, **17**, 355. [3] Berman, H.M. et al, *Nucleic Acids Res., 2000,* **28**, 235. [4] Word, J.M. et al, *J. Mol. Biol.*, 1999, **285**, 1735.
Keywords: structure validation, domain assignment, structure comparison, potential of mean force

MS29.26.5
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ESPript/ENDscript: Sequence and 3D Information from Protein Structures
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The fortran program ESPript has been created to display on a single PostScript figure, multiple sequence alignments adorned with secondary structure elements [1]. A web server is available at http://espript.ibcp.fr/ESPript/ESPript. It has been linked to three web tools: ProDom which identifies protein domains, PredictProtein which predicts secondary structure elements and NPS@ which runs sequence

alignment programs.

An extension of ESPript named ENDscript has been made available at the same electronic address [2]. It enables the creation from a single Protein Data Bank identifier, of a multiple sequence alignment figure adorned with secondary structures of each sequence of known structure. ENDscript uses programs such as BLAST, CLUSTAL and PHYLODENDRON to work on protein sequences and such as DSSP and CNS to work on protein coordinates. Similar structures are superimposed in turn with the program PROFIT. Final 3D figures are drawn with MOLSCRIPT, BOBSCRIPT and DINO, so as to show sequence conservation as well as structure conservation.

[1] Gouet P., Courcelle E., Stuart D. I., Metoz F., *Bioinformatics*, 1999, **15**, 305. [2] Gouet P., Courcelle E. , *Bioinformatics*, 2002, **18**, 767.

Keywords: bioinformatics, sequence homology, protein structure comparison

MS30 ART AND CRYSTALLOGRAPHY

Chairpersons: Edgar Meyer, Cristina Acidini

MS30.26.1

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Plastic Visions in Art and Science

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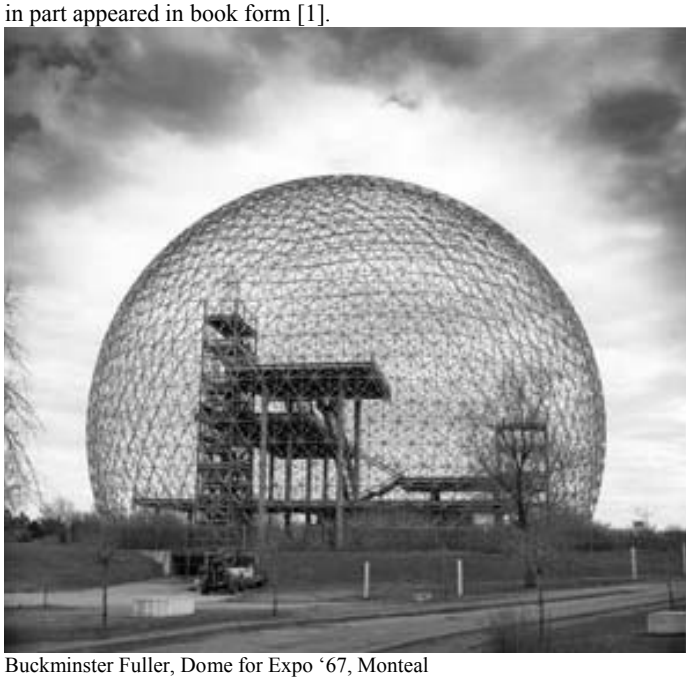
Techniques of instrumental seeing, such as sonar, electron microscopy and X-ray diffraction, pose particular problems in spatial visualisation and representation. However, the basic skills of mental modelling and graphic representation have existed in various guises in art, architecture, technology and science since the Renaissance (at least). The kinds of skills demanded in crystallography will be set in a broader context of visualization through the selective examination of key episodes from the era of Leonardo to the present day. Some of the examples will be drawn from my regular column in *Nature*, which has in part appeared in book form [1].



Buckminster Fuller, Dome for Expo '67, Monteal

[1] Kemp M.K., *Visualisations. The Nature Book of Art and Sceince*, 2000.

Keywords: X-ray diffraction techniques, molecular modelling, computer modelling solids

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M.C. Escher and the Crystallographers

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Forty-five years ago, a relatively unknown Dutch graphic artist, M.C. Escher, gave a standing-room-only lecture to the Fifth International Congress of the IUCr in Cambridge, England. There was an accompanying exhibit of his work that amazed the crystallographers. His pioneering work in exploring colour symmetry was a rare instance of an artist investigating a field before "official crystallography even thought about [it]."[1] Escher's quest to understand periodic tilings (which he called 'regular divisions of the plane') was stimulated in 1935 by two articles in *Zeitschrift für Kristallographie*; roughly 20 years later crystallographers (notably, Caroline MacGillavry and J.D.H. and Gabrielle Donnay) sought him out to learn from his work. In 1960, Escher's book *The Graphic Work of M.C. Escher* contained a crystallographer's explanation of symmetry and symmetry groups. In 1965, the IUCr published [1] for which MacGillavry had collaborated with Escher.

We discuss how Escher's quest to understand the subject of coloured periodic tilings differed from that of the crystallographers', and how even today, some of his original investigations are worthy of further scientific inquiry.

[1] MacGillavry C.H., *Symmetry Aspects of M.C. Escher's Periodic Drawings*, IUCr, Utrecht, 1965. [2] Schattschneider D., *M.C. Escher: Visions of Symmetry*, Freeman W.H., New York, 1990, Harry Abrams, New York, 2004.

Keywords: M.C. Escher, colour symmetry, crystallographic teaching

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Ancient Crystalline Materials for the Arts of Beauty

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Dedicated to the memory of HUBERT CURIEN

Recent progress in the analysis and structural characterisation of materials has had an increasing impact on studies of archaeological specimens. We shall mainly focus on cosmetic chemicals, also used as pigments and medicines. Many crystalline compounds found in Egyptian tombs have been identified. The structural information has ultimately revealed that the Egyptians had developed a *wet chemical synthesis of lead-containing compounds not occurring in nature.* Archaeological data (2000-1200 BC) and Greco-Roman texts (50 AD) have been crucial in tracing back this technology about 1500 years earlier than it has been previously assumed [1].

Greek texts from the 4th century BC describe a remarkable method of synthesis and comment on the widespread use of ceruse (lead white) still continuing until the present day. A marked difference in the historical use of cosmetics by the Egyptian and Greco-Roman societies will be emphasised.

The archaeological materials may suffer alterations over the centuries. Time may be then viewed as a "fourth dimension" for the purpose of approaching the significance of *"molecular messengers"* in *"Molecular and Structural Archaeology"*. Thus we have observed by X-ray diffraction a keratin α-helix, still perfectly preserved, in human hair 2500 years old. In contrast the structure of skin elements has been altered by the mummification process.

[1] Walter P., Martinetto P., Tsoucaris G., Breniaux R., Lefebvre M.A., Richard G., Talabot J., Dooryhée E., *Nature*, 1999, **397**, 483-484.

Keywords: structural analysis, archaeological materials, lead

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Art in Crystallography in Art

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What is our legacy to future generations? Over the last 50 years, crystallography has changed science, society, and the world. When one considers the enormous impact our structural studies have had on the material, chemical, and life sciences, we find ourselves challenged to present to a discerning public the fruits of our research in a form that is appealing to the eye and of lasting value. Posterity will know