BUTTERWORTH HEINEMANN

1994 Molecular Graphics Art Show and Video Show

David S. Goodsell,* Teresa A. Larsen,* and T.J. O'Donnell†

**The Scripps Research Institute, La Jolla, California USA, †O'Donnell Associates, Chicago, IL*

The 1994 Molecular Graphics Art Show and Video Show were presented at the 13th annual international meeting of the Molecular Graphics and Modelling Society. The art show—shown in the Mary & Leigh Block Gallery on the campus of Northwestern University, Evanston, Illinois—included original artworks by eighteen artists and the video show included nine original animated works. All were chosen for their ability to present the complexity, diversity, and beauty of the molecular world in visual form. Works from a wide range of disciplines were represented, including work by scientists actively involved in structural research, by commercial illustrators presenting these results to students and physicians, and by fine artists exploring the meanings and implications of these molecules in our lives. Included in this issue of the Journal of Molecular Graphics *are comments by the juror of the show, T.J. O'Donnell, a catalogue of the art show, and a catalogue of the video show.*

JUROR'S COMMENTS

T.J. O'Donnell

Science is a creative endeavor. Scientists create by connecting theories and data and bringing that understanding into clearer focus. We may delight in reading observations of newly discovered sea creatures feeding near the sulfurous heat of deep ocean fissures. We might feel excitement at reports of direct observations of enzyme activity by atomic force microscopy. When the relationship of helical geometry and hydrogen bonding to the profound biological process of DNA replication was first revealed by X-ray crystallography and molecular models, we surely realized that the creation of the double helix was marvelous and beautiful.

Address reprint requests to: David S. Goodsell, Dept. of Molecular Biology, The Scripps Research Institute, 10666 N. Torrey Pines Road, La Jolla, CA 92037 USA

Artists create by connecting emotional, intellectual, spiritual, and physical things, thereby revealing something about our world or ourselves that may have eluded us before. The individual experience of a great work of art is so much like the experience of a great work of science that the similarity of these human endeavours cannot be doubted.

The works presented in the Molecular Graphics Art Show must not be seen as just scientific figures. In fact, if viewed as such, they would surely be judged as failures. Creating figures for a scientific publication requires objective editing, the highlighting of important aspects, and the removal of extraneous bits. In my opinion, many scientific figures may be justifiably viewed as works of art. The works presented in the Molecular Graphics Art Show were constructed with just as much care and thought as those created for a scientific publication, but perhaps with fewer restrictions and a more personal, rather than objective, basis. When a work of molecular graphics art is successful, it will have engaged our emotional, intellectual, spiritual, and physical understandings of its subject.

In two works on the subject of AIDS—my phscologram *HIV Protease Active Site* (#1, 2) and Simon Friedman's photograph *Know the Enemy* (#10)—menacing images, full of fire and darkness, spy on the inner haunts of the mortal enemy HIV. Science has relayed to us images and data of incredible detail and precision about the structure of the HIV protease enzyme and the molecules capable of rendering it harmless. We want to believe that the results of this intelligence operation will give us the key to destroying the enemy, but we remember that the battlefield is the delicate human body and its intricate immune system. These fiery images can incite us to action or terrorize us into retreat.

Many of the works in this show are portraits of individual molecules: proteins, nucleic acids, and viruses. Mike Hahn's ink-jet on paper *Ceci n'est pas une molecule* (#14) and Art Olson's photograph *Molecular Transit* (#20) are humorous; Jane Richardson's protein ribbon drawings (#24, 25) and Mike Carson's *DNurbs: DNA modeled with NURBS* (#5) strive to show structure without detail as in an

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architectural drawing; Teresa Larsen's photograph *Replication Fork Model* (#16) and Junko Suzuki's sculpture *incidence–coincidence · GENOME–GENDER XX/XY* (#29) investigate molecular shape in a large context, resulting in images/objects resembling jewelry.

We incorporate the results of molecular exploration into our daily lives. We take vitamins in the form of purified molecules. We shun cholesterol and nicotine and choose between aspirin and ibuprofen. Providing a framework for the understanding of the relative size and function of molecules, proteins, cells, and organs is seen in the watercolor of David Goodsell (#30), Bettina Brendel's lithograph (#4), and the illustrations of Marie Dauenheimer (#8, 9) Betsy Palay (#21, 22), and Lisa Shoemaker (#27, 28).

The works in the Molecular Graphics Art Show are not items plucked from the pages of scientific journals, chosen for their beauty or design or concept. The works shown are all intentional works of art, the work of explorers returning from their expeditions, anxious to show the results of their discoveries. Whether an artist tries to describe discoveries made about the light in the South of France, the emotions of the human soul, the revealing mysteries of dreams, or the workings of the molecular world, their common goal is to illuminate the position of ourselves in the universe.

CATALOGUE OF THE ART SHOW

Curated by David S. Goodsell

1. HIV Protease Active Site with Inhibitor (phscologram, light box)
2. HIV Ion Channel (phscologram, light box)

T.J. O'Donnell, Juror
O'Donnell Associates, Chicago, IL, USA

T.J. O'Donnell's works were created while producing traditional scientific illustrations of HIV Protease. He writes: "Such illustrations are typically constructed to visually reflect and clarify scientific data and arguments in any accompanying text, but often obscure other aspects of the material under study. In the images presented here I use accurate scientific data in an attempt to free my viewpoint from scientific constraints. As the scientific method strives to distill an essence from the rich mixture of reality, I am striving to reveal the richness that remains within the distilled data." The images were created using Gramps, rendering using RayT, and presented as a barrier strip autostereograms, or "phscolograms," in collaboration with Ellen Sandor and Stephan Meyers.

3. Migration of Molecules (acrylic on canvas)
4. Micro-layers (lithograph on paper)

Bettina Brendel
Los Angeles, CA, USA

Migration of Molecules and Micro-layers are part of a series exploring molecules and cells. Describing the works, Bettina Brendel writes: "*Migration of Molecules* suggests a slow motion or change in the structure of a molecular substance as visualized by the magnifying, inner eye of the artist. Ovular shapes emerge and recede in random pattern on a white background . . . *Micro-layers* envisions a cross-section of living tissue in its variety of textures and graininess in magnification."

5. DNurbs: DNA Modeled with NURBS (photographic print)
6. PNP: Target for Drug Design (photographic print)

Mike Carson
University of Alabama, Birmingham, AL, USA

The two images by Mike Carson utilize the novel molecular graphics techniques he has developed in the Inventor environment. *DNurbs: DNA Modeled with NURBS* is a DNA model rendered with a small number of bicubic patches defining each base pair. *PNP: Target for Drug Design* shows a potential target for anticancer drug design along with an imported dart to hit the target.

7. Molecular Cardiology: Unlocking the Secrets of the Heart (dye sublimation print)
8. Structure of Very-Low-Density-Lipoprotein (VLDL) (illustration on board)

Marie Dauenheimer
Reston, VA, USA

Marie Dauenheimer uses a combination of hand drawn illustration and computer animation to present molecular information in a colorful and interesting manner. *Molecular Cardiology* is a still image taken from an educational videotape for physicians. The image was created using Softimage and is presented as a 3M dye sublimation print. Artery texture maps were hand painted in watercolor. *Structure of VLDL* appeared as a journal cover and was drawn in airbrushed watercolor and colored pencils.

9. Untitled (xerographic print on paper)

Markus Eng
Seattle, WA, USA

Markus Eng prefers to think of his work as "studies, instead of drawings, because they really aren't images of anything specific." He writes: "The studies are never finished drawings. Rather, they illustrate relationships and connections between forms. Chaos is hidden in stable patterns." An initial ink drawing on graph paper serves as a template; xerographic copies of the template are used as tiles to build the final image.

10. Know the Enemy (photographic print)

Simon H. Friedman
University of California, San Francisco, CA, USA

Simon Friedman's *Know the Enemy* is a literal personification of HIV protease. He writes: "In a sense, it is a 'call to arms' to those involved in drug design against this therapeutic target." The image was rendered using Conic in MIDAS-Plus, manipulated in Adobe Photoshop, and finished on Showcase.

11. Myoglobin Fold (photographic print)
12. ATCase T and R States (photographic print)
13. TATA Box Binding Protein (photographic print)

Irving Geis
New York, NY, USA

Irving Geis is a pioneer in the field of molecular illustration. His paintings of myoglobin, hemoglobin, and lysozyme and his illustrations for *Structure and Actions of Proteins* set the standard for subsequent work in the field. *Myoglobin Fold, ATCase T and R States* and *TATA Box Binding Protein* present various aspects of his unique style.

14. Ceci n'est pas une molecule (photographic print)
15. Sense or Antisense? (builder's block, plaster, and paint

Mike Hann
Glaxo Research & Development Greenford, Middlesex, UK

"*Ceci n'est pas une molecule,*" writes Mike Hann, "serves to remind us that all of the graphics images presented here are not molecules, not even pictures of molecules, but pictures of icons which we believe represent some aspects of the molecule's properties." The image was generated in Insight II; the background and text were added using Photoshop. *Sense or Antisense?* takes a more whimsical look at molecules, likening the curve of the DNA helix to human forms.

16. Replication Fork Model (photographic print)
17. Solenoid Model (photographic print)

Teresa A. Larsen
The Scripps Research Institute, La Jolla, CA, USA

Teresa Larsen uses computer graphics and animation to explore and present the complexities of macromolecular interaction. *Solenoid Model* and *Replication Fork Model* explore aspects of DNA packing and replication. The images were rendered using Gramps, with custom DNA and spherical harmonic models.

18. Tiger, Tiger Burning Bright (photographic print)

Garrett M. Morris
The Scripps Research Institute, La Jolla, CA, USA

Garrett Morris uses texture mapping to convey the complex surface properties of molecules. About *Tiger, Tiger Burning Bright,* he writes: "The texture resembles tiger skin, but this belies the hidden information within." The image was rendered with AVS.

19. Through the Looking Glass (photographic print)
20. Molecular Transit (photographic print)

Arthur J. Olson
The Scripps Research Institute, La Jolla, CA, USA

Arthur Olson's two images explore molecular subjects with a whimsical twist. *Through the Looking Glass* was created as a journal cover describing the synthesis of a "mirror image" protein—using all D-amino acids. Thus the "real world" side of the mirror shows the unnatural enantiomer of the protein and a reversed schematic of its action. Apparently, it was difficult to get the printers to realize the correct sense of this image! *Molecular Transit* ties together the theme of the 1994 MGMS meeting with its venue. The images were created using texture mapping in AVS.

21. Pain Transmission (acrylic on paper)
22. Gilead Sciences Nucleotide-based Pharmaceuticals (acrylic on paper)

Betsy Palay
Artemis, Palo Alto, CA, USA

Betsy Palay is a scientific illustrator of molecular and medical subjects: "Clear communication through illustration and design." *Pain Transmission* and *Gilead Sciences Nucleotide-based Pharmaceuticals* were produced to accompany reports of pharmaceutical research. They were created in airbrushed acrylic.

23. Crystal View (photographic print)

Michael E. Pique
The Scripps Research Institute, La Jolla, CA, USA

Mike Pique's computer imagery continues to combine diverse elements from crystallography, computational chemistry, and macromolecular studies. *Crystal View* is an allegory on the process of crystal structure solution. The images were rendered with AVS with custom modules and produced with a Solitaire Film Recorder.

24. Triose Phosphate Isomerase (α/β barrel) (ink and watercolor on paper)
25. γ Crystallin (greek keys) (ink and watercolor on paper)

Jane Richardson
Duke University Medical Center, Durham, NC, USA

Jane Richardson revolutionized the analysis of protein architecture with her *Anatomy and Taxonomy of Protein*

Structure. The ribbon diagram has since become one of the indispensable tools of the structural scientist. *Triose P Isomerase* and γ *Crystallin* are two hand colored examples of her ribbon diagrams.

26. S1-Pocket Backdoor (photographic print)

Kenneth A. Satyshur
University of Wisconsin, Madison, WI, USA

Kenneth Satyshur produced *S1-Pocket Backdoor* during analysis of pepstatin binding to pepsin. The image is rendered in SYBYL.

27. Translocation of Eukaryotic Secretory Proteins (illustration on board)
***28. Attenuation of the trp Operon in* E. coli** (illustration on board)

Lisa A. Shoemaker
Illuminations, Roseville, MN, USA

The three-dimensional and colorful technique of Lisa Shoemaker is designed to "capture the attention of the student and emphasize the real substance of molecular processes and structures." *Translocation of Eukaryotic Secretory Proteins* and *Attenuation of the trp Operon in* E. coli were rendered in airbrush and hand painting with color intense dyes, acrylics, and pencils.

29. incidence–coincidence · GENOME–GENDER XX/XY (stainless steel and glass)

Junko Suzuki
Tokyo, Japan

Since 1987, the work of Junko Suzuki has included images of genes and chromosomes. About the present work, Junko Suzuki writes: "The last pair in the 46 chromosomes, XX–XY, gives the judgement of sex and can be interpreted to be a form of alphabet. *X* and *Y* mean the first and second unknown. This aspect reminds one of the chromosomes' ability in changing."

30. Picturing Biochemistry (ink and watercolor on paper)

David S. Goodsell, Curator
University of California, Los Angeles, CA, USA

David Goodsell combines hand drawn and computer graphic illustration to explore macromolecular size, shape, and distribution. In *Picturing Biochemistry,* he uses simple outlines and subdued colors to keep the complex scene from becoming mired in detail.

CATALOG OF THE VIDEO SHOW

Produced by Teresa A. Larsen

1. Rhinovirus Meets Receptor (0:59)

Jean-Yves Sgro
University of Wisconsin, Madison, WI, USA
Producer: Jean-Yves Sgro

Rhinovirus 16, represented as a radially depth-cued molecular surface, turns, rolls and eventually meets a model receptor on a model cell.

2. Myoglobin Hydration by Molecular Dynamics and Other Simulations (4:46)

Bernard R. Brooks
National Institutes of Health, Bethesda, MD, USA
Producers: Peter J. Steinbach, Satnam Mathur, Milan Hodoscek

This movie depicts the behavior of surface water molecules in a study of protein hydration (see PNAS 90 (1993): 9135–9139). Other sequences include a rendering of B-DNA and a lipid bilayer of DPPC (see Venable et al., Science 262 (1993): 223–226), and modeling chemically altered myoglobins (see JBC 268, #4 (1993): 2953–2959).

3. Telomerase & DNA Replication (3:49)

Thomas Macke
The Scripps Research Institute, La Jolla, CA, USA
Producer: Teresa Larsen
Collaborators: Mike Pique, Teresa Larsen

This video illustrates telomere replication schematically. DNA polymerase cannot replicate the extreme 3′ end of linear DNA; replication is shown with the loss of the 3′ end. To get around this problem, cells use telomerase to extend the 3′ end before replication; the video shows how telomerase prevents the loss of the 3′ end. Telomerase is thought to play role in cellular aging and cancer.

4. Molecular Biology AVS Sampler 1993–1994 (2:48)

Michael Pique
The Scripps Research Institute, La Jolla, CA, USA
Producer: Michael Pique
Collaborators: many scientists at The Scripps Research Institute.

This video presents a collage of projects: studies at the The Scripps Research Institute, aided by AVS software, include the effect of mutations in enzymes, protein folding simulations, X-ray diffraction of metalloprotein structures, electron microscopy of viruses, DNA replication, fractal geometry of protein surfaces, and production of dozens of illustrations for scientific journals and textbooks.

5. Acetylcholinesterase (3:46)

Richard Gillilan
Robert Rosenberg
Cornell Theory Center, Ithaca, NY, USA
Producers: Richard Gillilan, Robert Rosenberg
Collaborators: Daniel Ripoll, Joel Sussman, Israel Silman

An artistic and scientifically loaded presentation, this video shows a study of the electrostatic potential of acetylcholinesterase, culminating with a flight into the active site.

6. Molecular Surfaces: The True Story (2:59)

Michel F. Sanner
The Scripps Research Institute, La Jolla, CA, USA
Producers: Michel F. Sanner, Teresa Larsen
Collaborators: Arthur J. Olson, Bruce Duncan

This video illustrates the construction of the solvent excluded surface defined by a probe sphere rolling over a set of atoms. It also shows the relation between the solvent excluded surface and the solvent accessible surface. As an application, the surface is computed for crambin undergoing normal mode motion.

7. Visualizing DNA Crystal Packing Interactions (3:21)

Teresa Larsen
The Scripps Research Institute, La Jolla, CA, USA
Producer: Teresa Larsen
Collaborators: Richard E. Dickerson, Jordi R. Quintana, Arthur J. Olson, David S. Goodsell

Extended crystal structures prove difficult to study for packing interactions because the presence of many molecules obscures contacts. To get around this, volume rendering and texture mapping are used to represent the molecular surface of crytalline DNA, and to show the location and proximity of crystal packing interactions. In this way, contacts and their influences on the DNA structure can be readily interpreted.

8. Normal Modes of G-actin (4:38)

Richard Gillilan
Peter Maxfield
Cornell Theory Center, Ithaca, NY, USA
Producers: Richard Gillilan, Peter Maxfield
Collaborator: Monique Tirion

In this educational piece, normal mode motions of G-actin are discussed along with introductory material on proteins and ribbon representations.

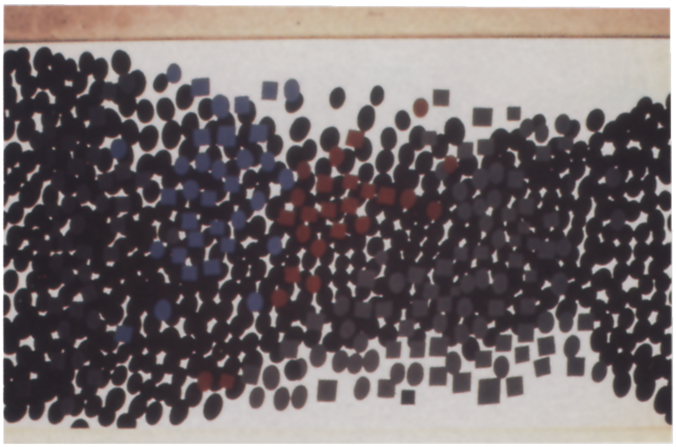
9. Echoes of the Sun (excerpt) (11:02)

Nelson Max
Lawrence Livermore National Laboratory, Livermore, CA, USA

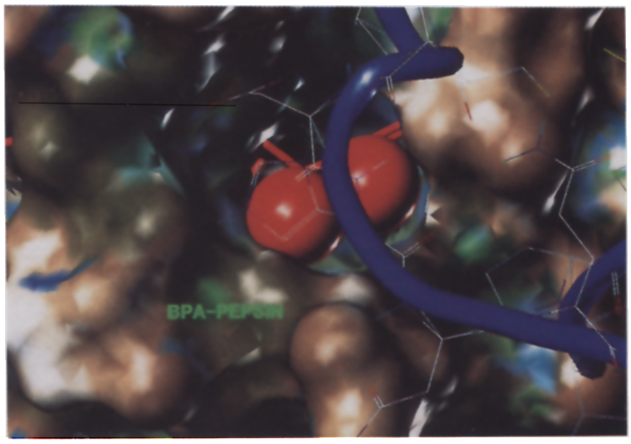
This outstanding computer graphics segment shows reactions of photosynthesis and glycolysis using enzyme structures solved by X-ray crystallography. Computer models of cells, cellular organelles and other intracellular structures make for a spectacular visual experience. This undistributed video comes to us again courtesy of Nelson Max and Fujitsu, Limited of Japan.

INDEX OF ART WORKS

Video show

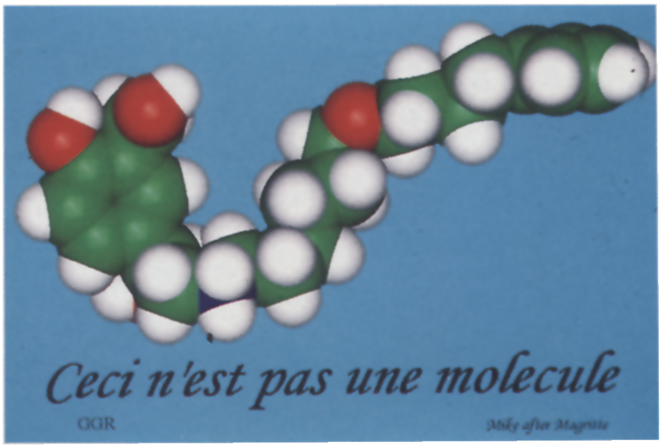


3 *Migration of Molecules*, B. Brendel



26 *SI-Pocket Backdoor*, K.A. Satyshur

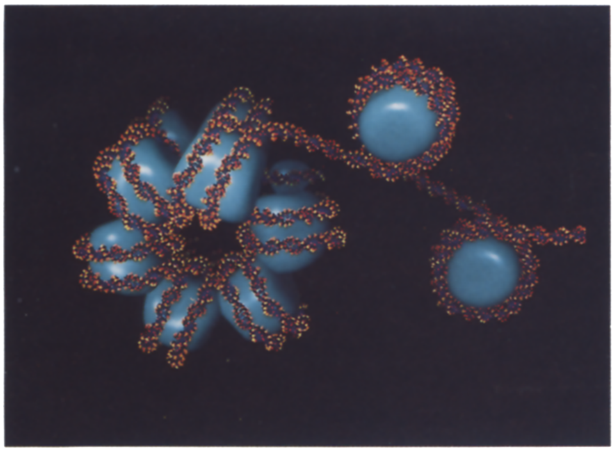
29 *incidence-coincidence* ● *GENOME–GENDER XX/XY*, J. Suzuki



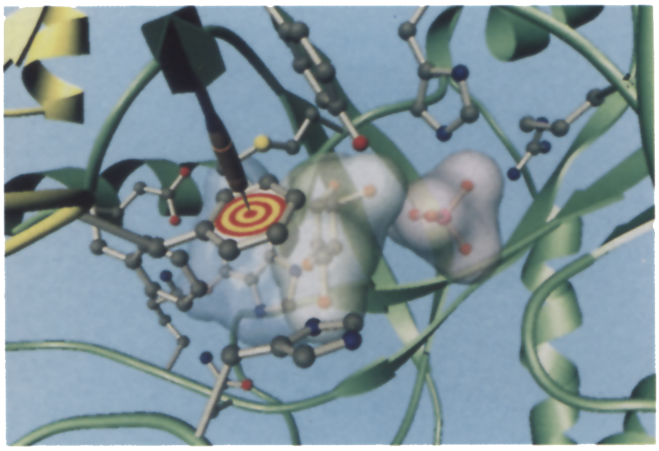
14 *Ceci n'est pas une molecule*, M. Hann

5 *DNurbs: DNA Modeled with NURBS*, M. Carson

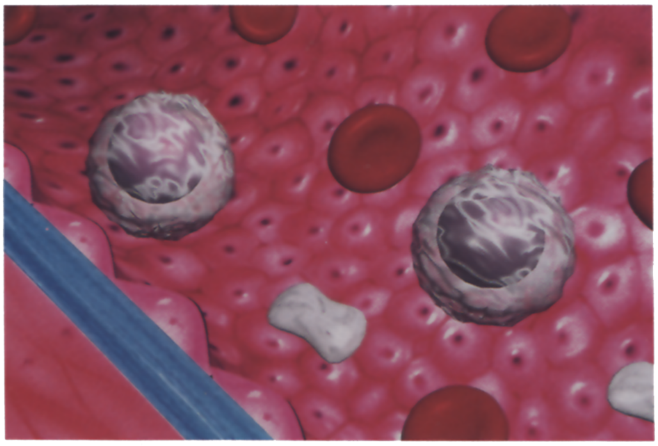
1 *HIV Protease Active Site with Inhibitor*, T.J. O'Donnell



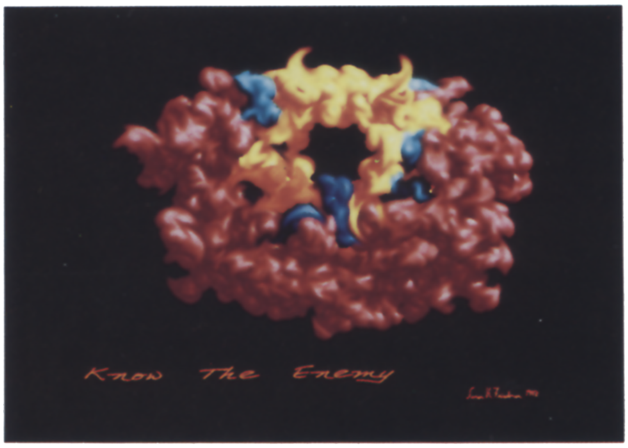
17 *Solenoid Model*, T.A. Larsen



6 *PNP: Target for Drug Design*, M. Carson

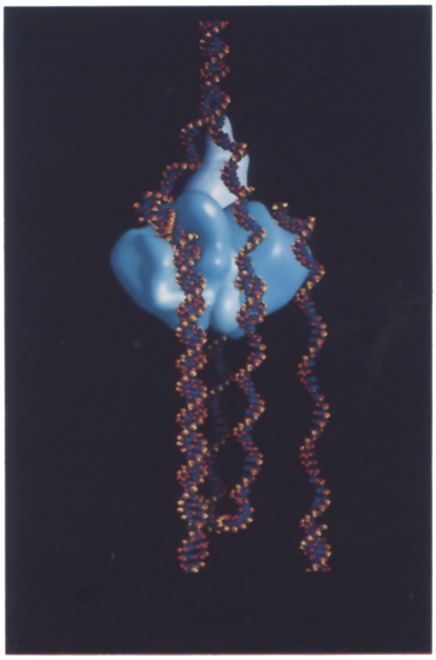


7 *Molecular Cardiology: Unlocking the Secrets of the Heart*, M. Dauenheimer

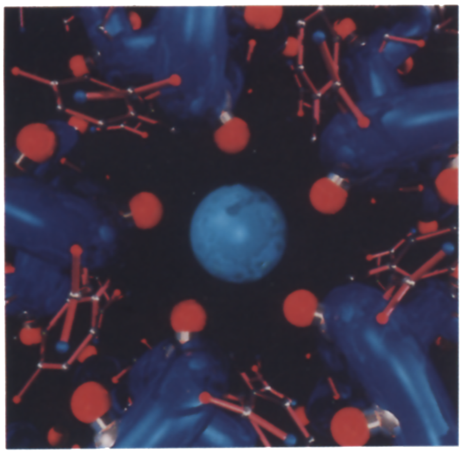


10 *Know the Enemy*, S.H. Friedman

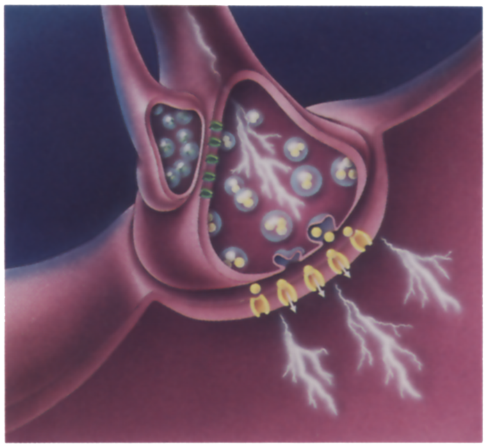
15 *Sense or Antisense?*, M. Hann



16 *Replication Fork Model*, T.A. Larsen

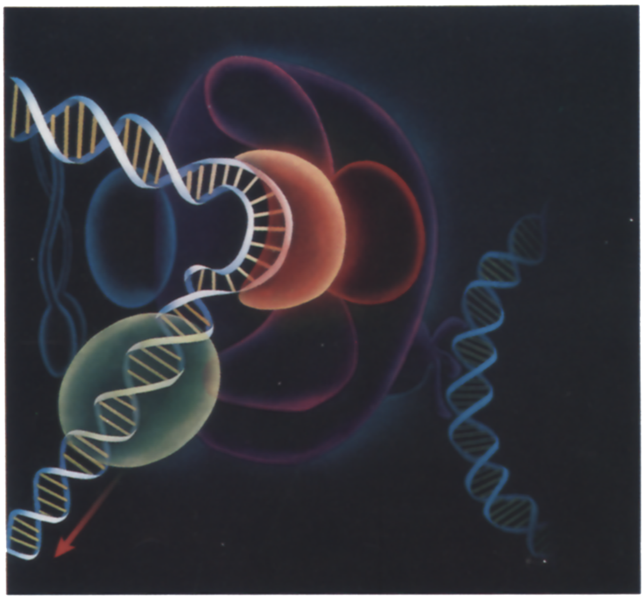


2 *HIV Ion Channel*, T.J. O'Donnell



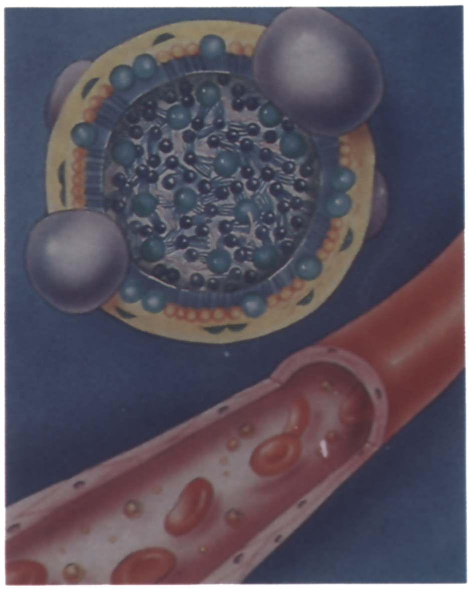
21 *Pain Transmission*, B. Palay

12 *ATCase T and R States*, I. Geis

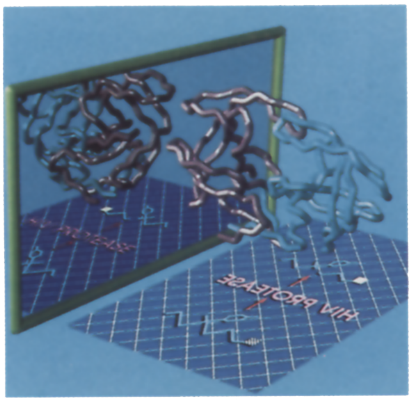


13 *TATA Box Binding Protein*, I. Geis

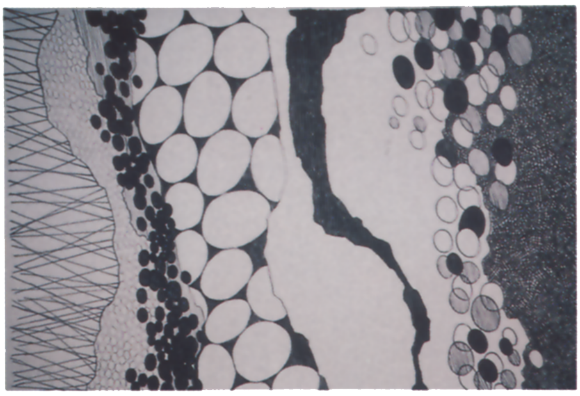
11 *Myoglobin Fold*, I. Geis



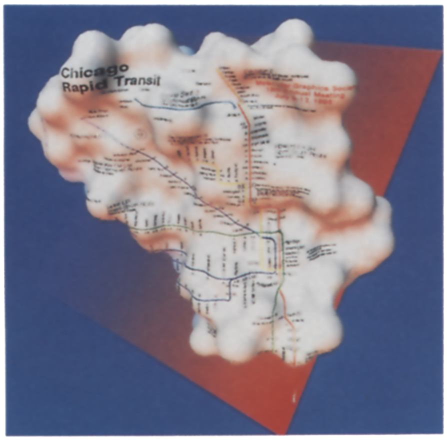
8 *Structure of Very-Low-Density-Lipoprotein (VLDL)*, M. Dauenheimer



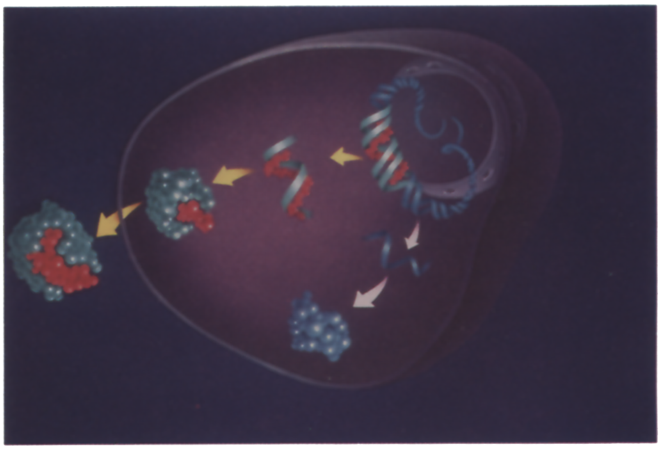
19 *Through the Looking Glass,* A.J. Olson



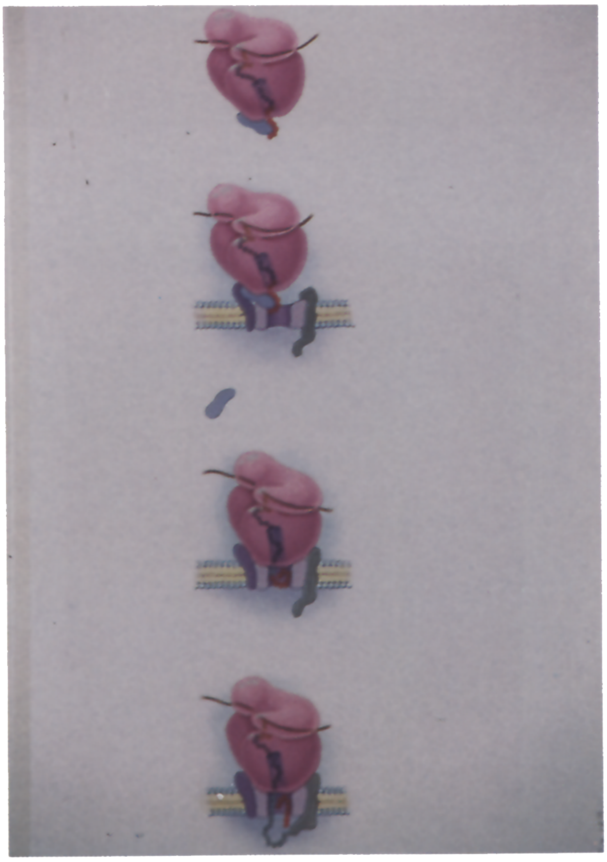
4 *Micro-layers,* B. Brendel



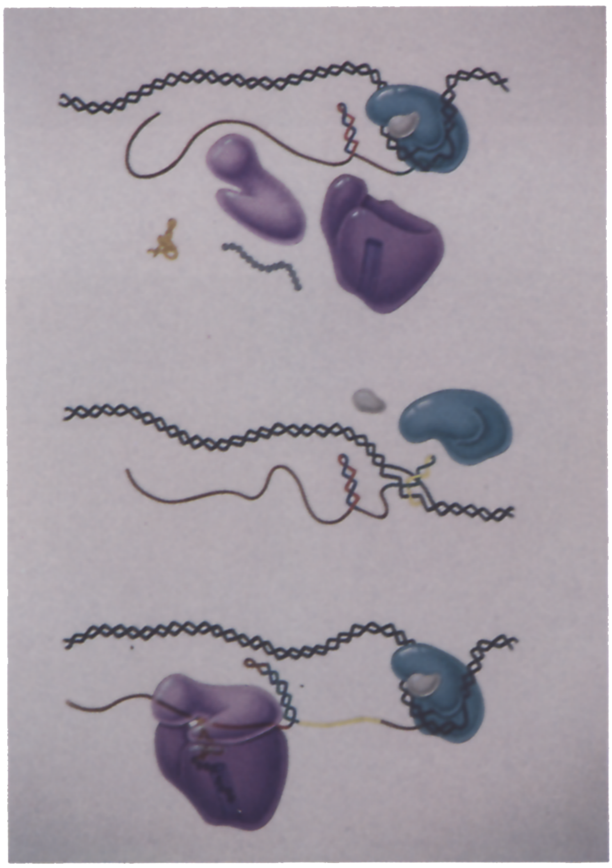
20 *Molecular Transit,* A.J. Olson



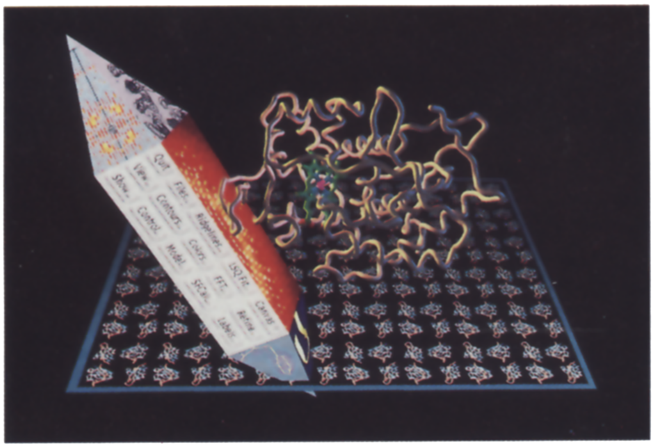
22 *Gilead Sciences Nucleotide-based Pharmaceuticals,* B. Palay



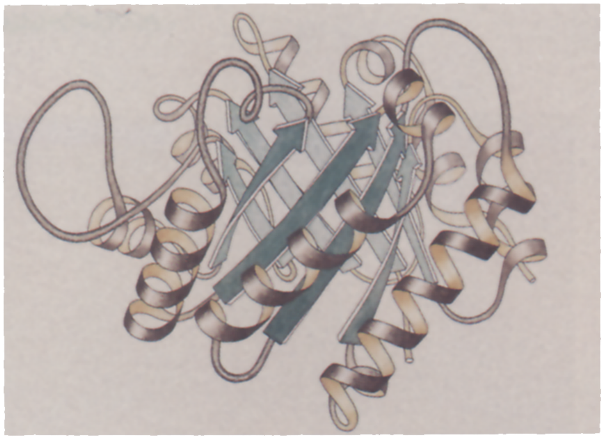
27 *Translocation of Eukaryotic Secretory Proteins,* L.A. Shoemaker



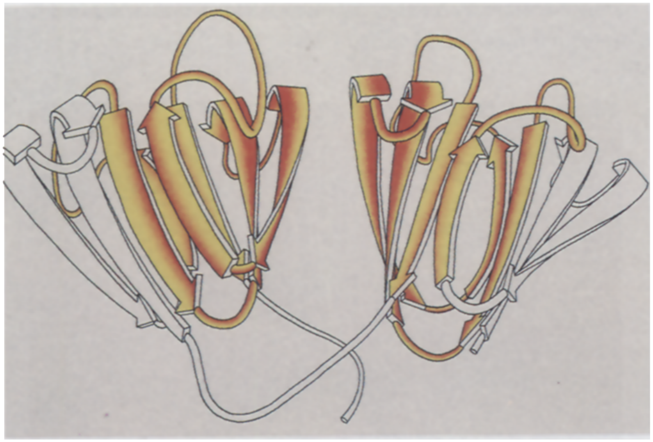
28 *Attenuation of the trp Operon in* E. Coli, L.A. Shoemaker



23 *Crystal View,* M.E. Pique

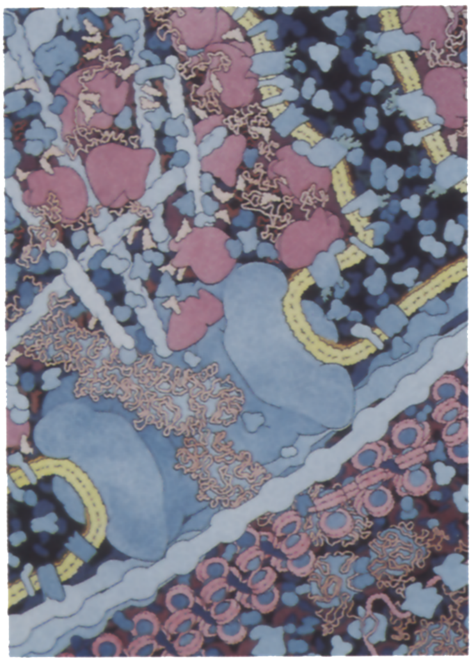


24 *Triose Phosphate Isomerase (α/β barrel),* J. Richardson



25 γ *Crystallin (Greek keys),* J. Richardson

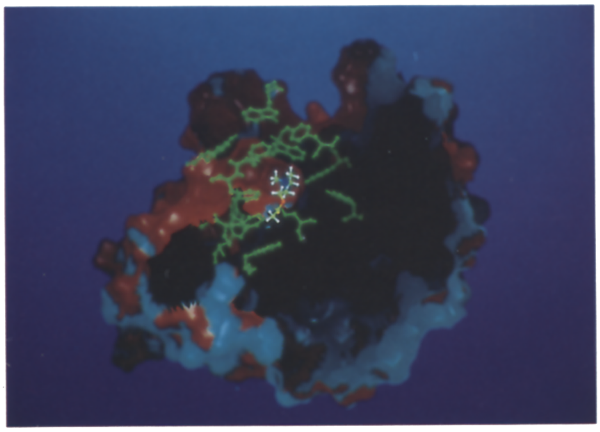
9 *Untitled,* M. Eng



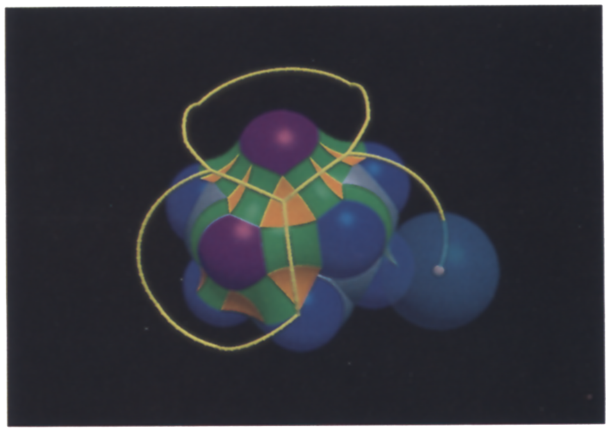
30 *Picturing Biochemistry,* D.S. Goodsell

18 *Tiger, Tiger Burning Bright,* G.M. Morris

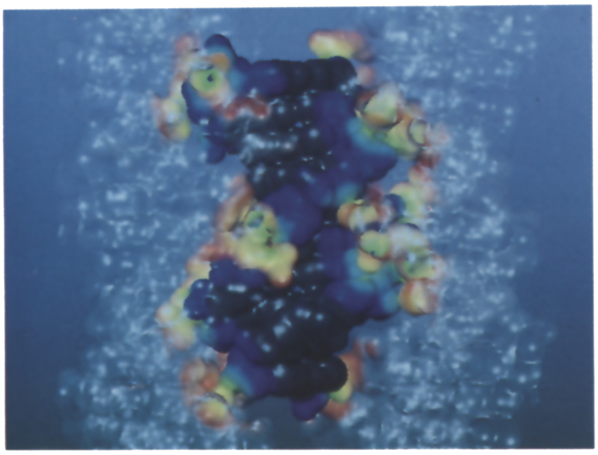
Selected Images from the Video Show



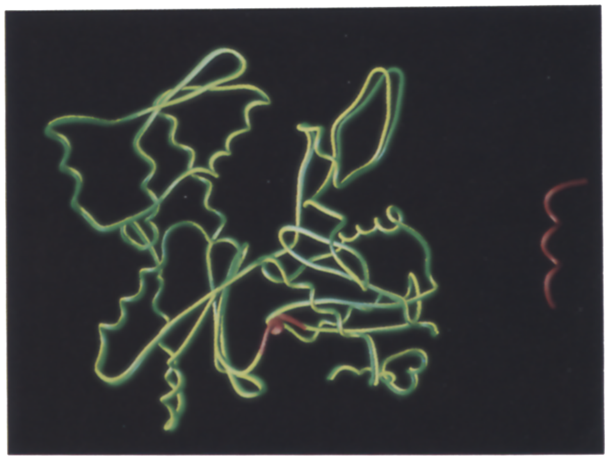
5 *Acetylcholinesterase*, R. Gillilan and R. Rosenberg



6 *Molecular Surfaces: The True Story*, M.F. Sanner



7 *Visualizing DNA Crystal Packing Interactions*, T. Larsen



8 *Normal Modes of G-actin*, R. Gillilan and P. Maxfield