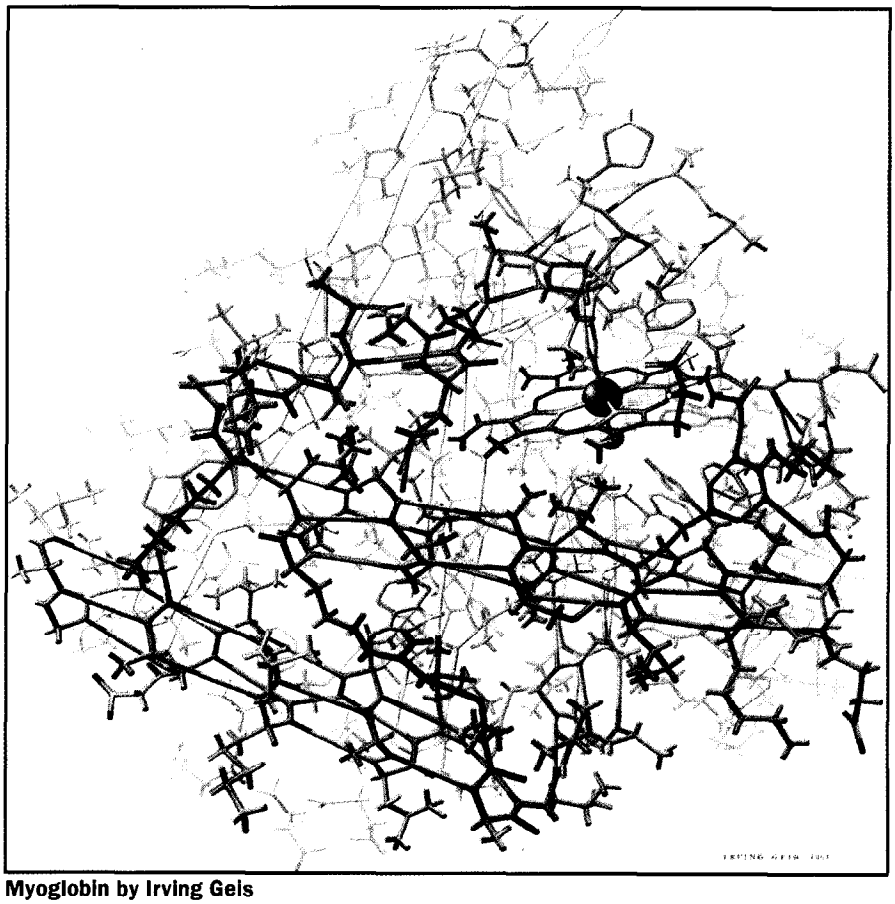
The Art of Molecular Graphics

Irving Geis: Dean of Molecular Illustration

By Bruce Paul Gaber, Ph.D. and David S. Goodsell, Ph.D.

Molecular graphics without computers? Hardly imaginable. But for more than 35 years Irving Geis' meticulously-rendered watercolors and oils have put the art in molecular graphics and defined the way we think about proteins and nucleic acids. We recently spoke with Irving Geis and discovered some of the unique influences that have shaped his singular vision of the molecular world.

Formally trained in architecture, and self-trained in cartooning, Geis began his career in scientific illustration with a painting in *Fortune*, showing the heart and circulatory system. In 1948, he began work with a new magazine created to present science to a popular audience: *Scientific American*. He soon got a reputation for tackling the difficult projects that the other illustrators didn't want, such as complex astronomical illustrations for Fred Whipple. So naturally, when John Kendrew wrote an article on the structure of myoglobin in 1961, Geis was given the project. Typically, *Scientific American* illustrators were given a paper to read and then allowed about two weeks to work through concept sketches to final illustrations. The complex myoglobin painting, however, took six months to complete. According to Geis, editor-in-chief Dennis Flannagan "threw a fit" over his style ("It looks like a mass of crumpled chicken wire"), the delay, and the cost. Time, money, and artistic judgment



Myoglobin by Irving Geis

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notwithstanding, the illustration was seminal as a clear and readable representation of the newly discovered complexity of a protein molecule. Flannagan must have felt this too, for when David Phillips, in 1966, produced an article on the first enzyme structure, lysozyme, Geis was again chosen to do the artwork. These illustrations, representing for the first time the complexity of protein-substrate interaction, took even longer to create, and marked the end of Geis's work with *Scientific American*. Since then, his career has been "a continuous stream of biological molecules."

Irving Geis became known to an entire generation of young biochemists with the 1969 publication of *The Structure and Action of Proteins*. His deceptively simple illustrations perfectly complemented Richard Dickerson's insightful text. The book changed invisible proteins into familiar objects.

A Biochemical Society meeting at the Hilton Hotel in New York brought the two together in the mid sixties. By coincidence, Geis was sponsoring an exhibit of prints by cartoonist, John Held, Jr. at the same hotel. Dickerson, a collector of American art, eventually traveled to Geis' uptown studio to arrange a purchase. On the wall of the studio was a photograph of the myoglobin model recently solved by John Kendrew.

"Have you ever heard of myoglobin?" asked Geis, to which Dickerson wryly answered "Yes," having recently generated the actual myoglobin electron density maps in postdoctoral work with Kendrew.

Several years later, an agent from W. A. Benjamin Publishing contacted Geis, sending regards from a friend on the west coast, thus marking the beginning of a long and fruitful collaboration. Together, they also produced other large-scale works: *Chemistry, Matter, and the Universe*, an introductory chemistry textbook, and *Hemoglobin*, a detailed presentation of this fascinating molecule, and a host of popular and technical articles. Geis credits Dickerson as his mentor in science. Dickerson would provide the biochemical expertise and abundant sketches of the structures involved, from which Geis would create his paintings. But Geis adds: "More and more they became my own creations."

Irving Geis' creations are visual metaphors. Geis asserts, "It's wrong to say 'What does this molecule look like?' Nobody knows what myoglobin looks like. After all, molecules are smaller than light waves! We can only say 'It's something like that' — only create a visual metaphor."

The three illustrations included with this article show the progression of his style, and how his metaphors for molecular subjects have matured along with the field of macromolecular structure.

The first (page 57) is his portrait of myoglobin, created for *Scientific American*. This illustration fully conveys the excitement of the scientific world at finally seeing these complex molecules in all of their atomic detail. It is a "photographic transcription" of the Kendrew models used to interpret the electron density maps. Geis worked directly from photographs of the original model, using shading, color and perspective to add the third dimension to this complex structure. Geis says that creating this drawing was like "drawing a herd of elephants." The use of small distortions and exaggerations — "creative lying" — resolves overlaps to create an understandable image, in spite of the complexity.

The other paintings — *Myoglobin Fold* and *Lac Repressor* — exhibit two themes that pervade Geis's later work:

1. the need to give an overall view of the molecular structure, and
2. the need to represent the molecule's function.

Geis is emphatic when he says "Many published [protein] images give no clue as to how the molecule works!"

Rather than represent molecules atom by atom, Geis has created in these images an "understandable metaphor for molecules," with thick tubes representing the gross molecular structure, and finer details highlighting the function. Myoglobin is seen as a V-shaped protein designed to hold the planar heme molecule, highlighted through clever use of light. In his most recent painting, the lac repressor is seen as a "nutcracker" with an inducer-shaped maw.

During his work with Dickerson, Geis developed a number of methods to address the challenge of depiction of molecular motion, in particular, the celebrated allosteric motions of hemoglobin. Perhaps the most successful of his methods is an illustration showing a series of overlapped snapshots, as used in the lac repressor painting.

What does this master of the brush think of computer graphics? Geis is outspokenly critical of the computer graphics imagery that permeates our journals and scientific presentations. He finds that they are of great use when a scientist wants to focus on the details of individual residues, but that computer graphics images rarely give an interpretable overall picture of the molecule and its function: computer graphics is a "laboratory aid rather than a teaching aid." He attributes the widespread use of computer graphics for publication to its convenience, not to its intrinsic suitability for creating comprehensible images. He finds that most researchers are a "slave to the program and to the coordinates," limited to what the program is able to do, and unable to simplify and organize the presentation. The result is "pictures that are more computer than molecular." He doesn't discount the idea that one could do with a computer what he does with brush and canvas, but insists that the computer illustrator must cease being a slave and begin to be a creative artist.

Lac repressor by Irving Geis

The myoglobin fold by Irving Geis

A Guggenheim fellowship recently allowed Geis to organize, catalogue and photograph 35 years of molecular illustration, including 50 original paintings and 900 sketches and studies, and he is now looking for a site to house the "Geis Archives." These paintings span the history of macromolecular structure, from the first illustration of the atomic structure of a protein, through popular accounts of protein structure as the field gained breadth, to his recent conceptual illustrations of molecules on the cutting edge of the depiction of protein function and assembly.

Dr. Bruce Paul Gaber heads the Laboratory for Molecular Interfacial Interactions at the Naval Research Laboratory in Washington, DC. He is a founding member of the Molecular Graphics Society of the Americas and a member of the International Editorial Board of this Journal. He holds Affiliate Professorships in the Center for Computational Science and Informatics at George Mason University and in the Center for Bioengineering of the University of Washington. Dr. Gaber is Senior Partner of BodhiGraphics, a scientific illustration studio specializing in molecular graphics and modeling. Contact him at either gaber@ nrl.navy.mil or bodhi@his.com. Dr. David S. Goodsell is an Assistant Professor at the Scripps Research Institute in La Jolla, CA. His research combines computer graphics and rational drug design. He is the author of two books on macromolecular and cellular structure: "The Machinery of Life" and "Our Molecular Nature: The Body's Motors, Machines and Messages." More information and examples of his scientific and artistic work can be found at http://www.scripps.edu/ pub/goodsell.

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