Kendrew constructs; Geis gazes

Today we need computers to create images of the complex structures of protein molecules. Irving Geis, nearly 40 years ago, painted a portrait of myoglobin using only his astounding observational skills.

Martin Kemp

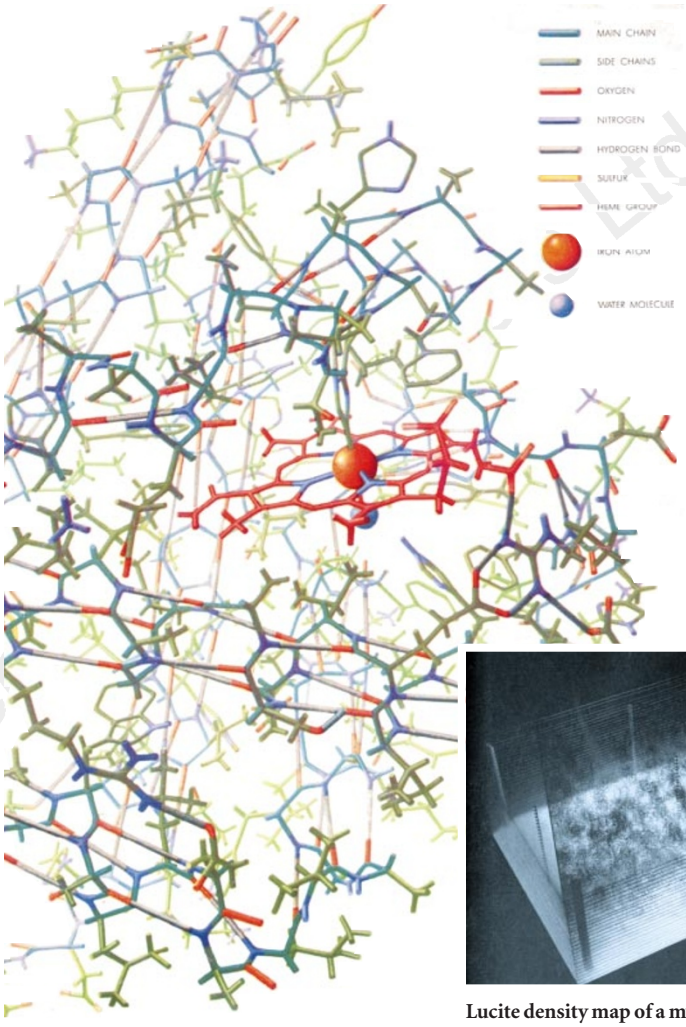
Anyone with even a passing interest in the big molecules that lie at the heart of life knows what they look like on computer screens. Standard imaging packages, such as MolScript, introduced by Per Kraulis in 1991, have made us familiar with the colourful and gently shining tangles of linked atoms, seductively spot-lit and floating weightlessly in space behind the windows of VDUs. What is all too easy to forget is that the basic visual choices in the design of the programs relied on the perceptual and aesthetic visions of the pioneer illustrators during the 1950s and 1960s. Of the illustrators, none was greater than Irving Geis of New York, who died in 1997 at the age of 88.

Having studied architecture, art and design, Geis found his true *métier* as a leading illustrator and artist of science working for *Scientific American* from 1948 onwards. It was in this capacity that he created his first masterpiece of protein portraiture for John Kendrew's article "The Three-dimensional Structure of a Protein Molecule", published in December 1961 (Vol. 205, pages 96–110), which remains a classic of visual and verbal exposition. In the bound annual volume I consulted, Kendrew's article was immediately identifiable by its thumbed pages, dog-eared corners and torn edges reinforced by tape.

Visual and verbal excitement go perfectly hand in hand. Kendrew begins, "When the early explorers of America made their first landfall", and concludes that "students of the living organism do indeed stand on the threshold of a new world". Kendrew and Geis avail themselves of virtually every kind of available technique to portray their new world.

There are flat diagrams of molecular skeletons, linear maps of electron density, line drawings of ball-and-rod structures, X-ray photographs and photo-micrographs, together with photographs of equipment and of various kinds of models composed of clips and rods, Lucite sheets and a lumpy sculpture. And, above all, there is Geis's remarkable painting.

The subject was the 2,600-atom molecule of sperm whale myoglobin, of which Kendrew had caught his first sight on a Sunday in May 1957. At first he worked to a resolution of six angstroms, but determined that a higher resolution was needed — "as in the case of a musical note, the greater the number of higher harmonics that are included, the sharper and more precise is the resulting picture". The two-angstrom scale he finally used involved two sets of 10,000 X-ray reflections. The refined data were used to build the astonishing three-dimensional contour map of electron density on 50 layered sheets of Lucite — at the cost of six man-months of work.



Detail of the model of the sperm whale myoglobin molecule, painted by Irving Geis.

Lucite density map of a myoglobin crystal, constructed by Kendrew *et al.*

"At first sight" the density map "seemed completely irregular", but just as "driving past an orchard" will disclose different orders from different perspectives, so Kendrew found that if he "looked through the stack of Lucite sheets in a direction corresponding to the axis of one of the rods" (the concentrations of higher density already observed at lower resolution), the rods could be seen as hollow and spiral in configuration.

The next step was the construction of a model composed of a forest of uprights with coloured clips which represented the whole molecule with every side chain in place. It was through this forest that Geis gazed with remorseless concentration when painting his portrait of the molecule, using his unrivalled command of perspective, light and shade, and colour recession to reveal the intricate sculptural web of linkages. Looking at it 37 years later, it is difficult to credit that it was not done by computer.

Indeed, there is a case for saying that our current computer graphics, for all their novel features such as animation and stereoscopy, are basically providing a series of powerful, dynamic and convenient glosses on the graphic modes invented by Geis and his fellow pioneers of hand-made representation. □

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