



# Molecular Illustration in Chemistry and Biology: examples, state-of-art and outlook

Marc Baaden

## ► To cite this version:

Marc Baaden. Molecular Illustration in Chemistry and Biology: examples, state-of-art and outlook. Reality Through Image, AEIMS Congress, Nov 2011, Strasbourg, France. pp.74-78. hal-03948350

**HAL Id: hal-03948350**

**<https://hal.science/hal-03948350>**

Submitted on 20 Jan 2023

**HAL** is a multi-disciplinary open access archive for the deposit and dissemination of scientific research documents, whether they are published or not. The documents may come from teaching and research institutions in France or abroad, or from public or private research centers.

L'archive ouverte pluridisciplinaire **HAL**, est destinée au dépôt et à la diffusion de documents scientifiques de niveau recherche, publiés ou non, émanant des établissements d'enseignement et de recherche français ou étrangers, des laboratoires publics ou privés.

# Molecular Illustration in Chemistry and Biology: examples, state-of-art and outlook

Marc  
Baaden

Since the works of Leonardo da Vinci, scientific illustration has made much progress: going from simple drawings towards more and more refined and complex representations as knowledge progressed. The transition from the macroscopic to the microscopic level is, in reality, a continuous one. In practice, disciplines such as medical and molecular illustration do still represent separate universes. This may be explained by the great diversity of the objects that are represented. Nevertheless many techniques employed in both domains are similar. Furthermore, until very recently, the molecular world was totally invisible to us. Quoting Richard Feynman describing the nanoworld that had just about been discovered at the end of the 50s: “there is plenty of room at the bottom”. One may add that there are also plenty of things to see at the bottom! Here, we explore this universe at the heart of everyone to discover how scientists try to depict it.

In the molecular world, the visual representation of the structure of a molecule and its properties is key: “tell me about your assembly, and I tell you who you are”. Yet, this is only possible since a relatively short span of time: molecular modelling of biological macromolecules originated in the early 60s, when Sir John Kendrew created physical wire models or models in plastic rubber. Several years later, Cyrus Levinthal and his colleagues at MIT used an oscilloscope to visualize molecular models, also using a “wire frame” representation – described by simple lines. Since this era, technical progress

Researcher at CNRS  
studying the chemistry-  
biology-computer  
science interface

Marc Baaden is  
a computational  
chemist at CNRS  
in Paris, focusing on  
interactive approaches  
to molecular modelling  
of complex biological  
systems.

Molecular visualization  
is an essential part  
of this work combining  
high-performance  
computing and virtual  
reality, with particularly  
exciting perspectives  
offered by the latest  
graphics processors.

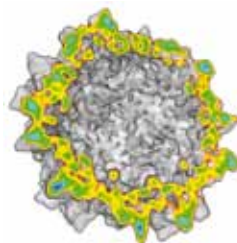
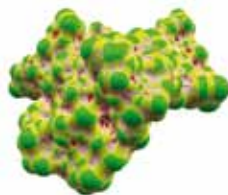
considerably improved molecular visualisation. Illustrations of molecules in scientific articles became commonplace. A transition from hand-drawn models to the current computer generated images occurred.

Recent years have shown a turn in the possibilities offered for scientific visualization, in particular concerning the realism of the representations and performance. It is possible to interactively visualise molecular assemblies of increasing size. Often, this requires combining different types of representations and of data to better understand such molecular systems. Concerning performance, the computing power at our disposal has continually grown and has greatly helped researchers to better approach the objects of their studies. Another important point is to try and render the *invisible* with easily comprehensible metaphors. In this context, analogies with macroscopic objects are very useful. This is why it is important to employ different lighting techniques to properly “highlight” molecules and their complex shapes. Technical progress enabled us to re-think the molecular world.

Given the technological and scientific progress, data is no longer purely static, but dynamic: thanks to computer simulations and molecular modelling it is possible to generate actual movies depicting the evolution of molecular systems. Such simulations generate huge amounts of data that have to be treated and simplified in order to analyse them. The analysis of this data is vital to separate random oscillatory motions from important molecular mechanisms. The simplification of such data may be achieved by abstraction, only representing the elements that are of immediate concern for the study to be carried out. It is also possible to use tools that are traditionally dedicated to other fields such as the video game industry or the film industry, in order to enhance the realism of such animations. Huge amounts of data obtained by computer simulations require artistic and educational approaches in order to render them comprehensible.

Sometimes there is only a little step from science to art. Illustrations of molecular systems often decorate the covers of specialized journals where an artistic character is also considered. Molecules may comprise intriguing shapes that provide a source of inspiration for artists. Some researchers even generated illustrations for their research that ended up in museums or galleries.

The evolution of scientific illustration of molecular systems in chemistry and biology opens up perspectives that would benefit from the expertise of scientific illustrators.





b.

BPTI  
(bovine pancreatic trypsin  
inhibitor), Matthieu Chavent  
& Marc Baaden, 2011