The Art of Molecular Graphics

It's a Matter of Scale

Bruce P. Gaber

Center for Bio/Molecular Science and Engineering, Naval Research Laboratory, Washington, DC 20374 USA. bgaber@cbmse.nrl.navy.mil

Ompared to the almost incomprehensibly vast length scales of astronomy, the range over which molecular structures are developed seem rather constrained. Nonetheless, as illustrators of the molecular world, we must remain mindful and true to the spatial dimensions of things molecular.

Molecular structures are small to be sure, but they span no more than about three orders of magnitude. We might think of the range of items we call "molecular" as falling on a continuum of sizes (Figure 1). At the lower end of the scale, we encounter individual atoms and bonds. The length scale here is on the order of a tenth of a nanometer or so. As the atoms combine into small molecules, we extend our scale to around 1 nm. We can refer to the region from 0.1 to 1 nm as "molecular scale." As small molecules combine to form larger polymeric structures, we encounter a length scale around 10 nm. Here we find proteins, nucleic acids, and polysaccharides. As this region falls in the middle of our continuum, I call it (contrary to some usage) "mesomolecular." At the extreme of what we might still consider molecular structures, we encounter high-order aggregates of biomolecules giving rise to viruses and cell membranes. This region, extending to around 100 nm, we can call "supramolecular."

While the range over which we depict things molecular is fairly narrow (at least by astronomical standards), it is still a considerable stretch in terms of illustration. Consider the simple spheres illustrated in Figure 2. The "molecular" sphere at a scale of 1 nm is barely discernible relative to the "supramolecular" sphere at 100 nm. At the lower end of our continuum, an atom at 0.1 nm is not even visible.

The key to handling scales effectively in molecular illustrations is a determination, at the outset, of which single element is most important to the composition. That focal element's scale determines the scale of the balance of the composition. As a rule of thumb, try to span no more than one order of magnitude around the focal image scale. For example, if the focal element is the overall structure of a virus (supramolecular), you may be able to depict a part of the mesomolecular

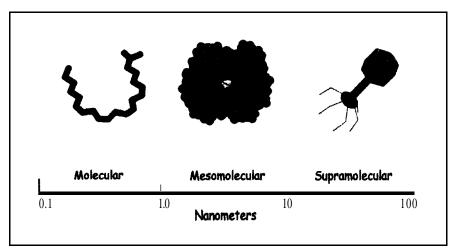


Figure 1. The spatial scale of molecular objects spans approximately three orders of magnitude, ranging from atoms and bonds at 0.1 nm to supramolecular structures, such as virsues, at hundreds of nanometers.

News and Views

INDEX

The Art of Molecular Graphics It's a Matter of Scale	__ 545
Book Reviews Job\$ in the Drug Industry: A Career Guide for Chemists; Modem Computer Algebra; Chemical Applications of Molecular Modelling	546
Website Reviews chemistry.about.com, drugdiscoveryonline.com	548
Meeting Report Eighth International Conference on Intelligent Systems for Molecular Biology	549
Company Profile GeneFormatics Inc.	550
Meeting Abstracts Protein Flexibility and Folding	550
Upconiing Meetings	560

News and Views Editor Shauna Farr-Jones, Ph.D. 915 Cole St. P.M. Box 375 San Francisco, CA 94117-4315 shauna_farrjones@yahoo.com

