FACULTY OF ENGINEERING AND TECHNOLOGY

Department of Biotechnology

Use of molecular graphics packages

The term molecular graphics first occurred in the seventies when molecular scientists adapted a new method from researchers in the field of structural investigation [1-3]. In the latter field computer graphical representations of electron densities (obtained from x-ray diffraction measurements) as isosurfaces have lead to an enormous step forward in the determination of protein structures: molecular structures (represented as “chicken wire” line graphs [4]) could be fitted interactively to the experimentally determined electron densities represented as nets of lines. The computer graphically supplied technique replaced a standard method based on complicated models made out of sticks and modeling clay. Computer graphical tools in the early stage of molecular graphics were dominated by vector graphical representations on special graphics computer hardware based on calligraphic technology [5,6]: Only lines and dots could be represented and almost all manipulation of the molecular scenarios had to be performed on a main frame computer and then submitted to the graphics hardware.

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The aims of research in these early days of molecular graphics were not so far away from the aims of chemists in this field today: One was interested in the quantitative treatment of intraand intermolecular arrangements controlled by distance criteria which could be applied interactively. Distance vectors between selected atomic increments could be recorded and displayed during interactive manipulations of the molecular scenario and a possible overlap of molecular surfaces (represented as a collection of dots (dotted surfaces) based on a hard sphere model - the so-called CPK-model) could hardly be recognized. Almost all of early molecular graphics applications came from the field of pharmaceutical chemistry and many of the applicants were from chemical companies. The new field grew fast.

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The Molecular Graphics Society (today Molecular Graphics and Modelling Society) Molecular Graphics - Trends and Perspectives Jürgen Brickmann, Thomas E. Exner, Matthias Keil, and Richard J. Marhöfer Physikalische Chemie I and Darmstädter Zentrum für Wissenschaftliches Rechnen (DZWR), Technische Universität Darmstadt, Petersenstraße 20, D-64287 Darmstadt, Germany. Tel: +49-6151-162198; Fax: +49-6151-164298. E-mail: brick@pc.chemie.tu-darmstadt.de Received: 2 November 1999/ Accepted: 15 December 1999/ Published: 28 February 2000 Abstract

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The principles of molecular graphics are discussed in context with the optimization of manmachine communication in molecular sciences. The state of the art in this field is demonstrated with several examples. The paper is focussed on the discussion of a strategic basis of the information transfer between human activities and computational processes. It is demonstrated that enhancement of interactivity in the visualization process may lead to the generation of new insight on one side and the development of new computational algorithms based on the human visual pattern recognition strategy. Keywords Molecular graphics, Man-machine communication, Information transfer, Graphical excellence Correspondence to: J. Brickmann Dedicated to Professor Paul von Ragué Schleyer on the occasion of his 70th birthday was founded in 1983 and the Journal of Molecular Graphics was set up shortly thereafter.

Many of the papers in this journal and others were related to new graphic techniques (see for example Brickmann et al. [7-9]), in particular also as a consequence of the dramatic increase of raster graphics technologies pioneered by the new hardware devices of the Silicon Graphics company and others. While in the beginning of the eighties nearly nobody believed that this technology could ever be fast enough to allow interactivity on the basis of space filling molecular models, the new technique replaced the old one within a few years. New hardware developments and the generation of graphical software standards made it easy to generate images of very high complexity with interactive refresh rate without extensive graphics programming [10-15]. Today the question in the field is no longer “how to represent (technically) a certain molecular scenario” but “what should be represented” [16-19] in order to obtain a maximum of information from the underlying data and to get an optimal insight from the image

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This paper is not focussed on the description of new algorithms or new programs in the field of molecular graphics. We are dealing here with more general aspects, namely the strategic basis of molecular graphics for the optimization of the information transfer between human activity and computational processes and vice versa. If not indicated otherwise, we use the term molecular graphics representation (MGR) synonymously for the representation of molecular scenarios as screen images, as slides or hardcopies, as video sequences, and also as virtual scenarios which can be inspected and manipulated interactively (locally or over the net).

Molecular objects are essentially three-dimensional, molecular information may be adequately represented even in a space which has much more dimensions. Molecular graphics representations (MGRs) must take this multi-dimensionality into account. Since molecules and molecular data are not objects of our everyday life, there is much room for the creation of MGRs. There are technical possibilities to generate quasi three dimensional representations of model scenarios by placing the human inspector in a large cubic box – the CAVE [22] – wherein images of a scenario are projected to the walls and an interactive device (data glove etc.) can be used in order to interfere with the 3D-world but in this paper this new approach is not in the focus of our consideration. Independently from this new technical

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Excellence in statistical graphics consists of complex ideas communicated with clarity, precision, and efficiency. Graphical displays should (i) show the data (ii) induce the viewer to think about the substance rather than about methodology, graphic design, the technology of graphic production, or something else (iii) avoid distorting what the data have to say (iv) present many numbers in a small space (v) make large data sets coherent (vi) encourage the eye to compare different pieces of data (vii) reveal the data at several levels of detail, from a broad overview to the fine structure (viii) serve a reasonably clear purpose: description, exploration, tabulation, or decoration (ix) be closely integrated with the statistical and verbal descriptions of a data set

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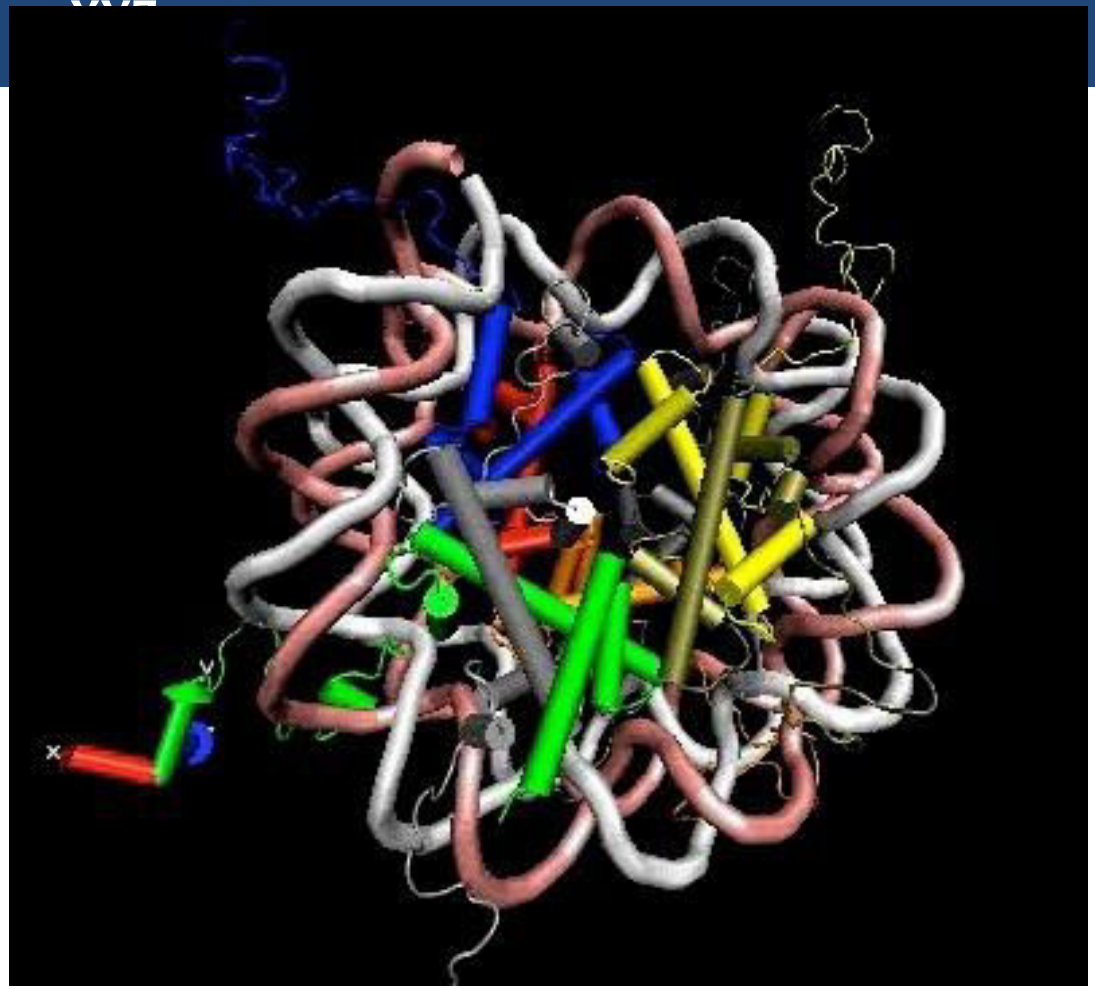
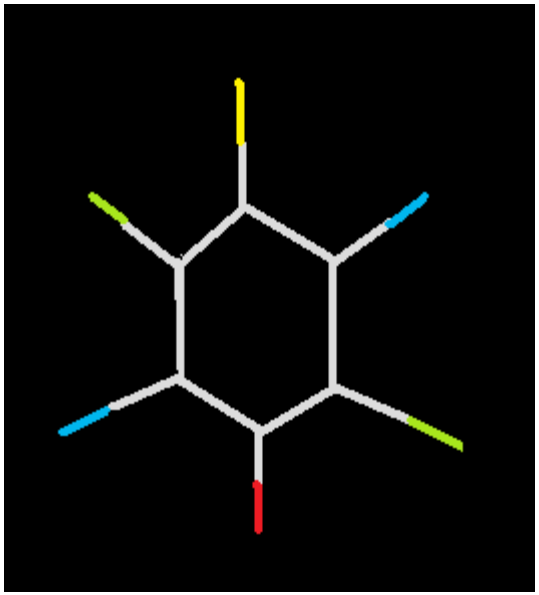


MOLECULAR GRAPHICS: The discipline and philosophy of **studying molecules** and their properties through **graphical representations**



Vector Graphics

- No 3-D renderings used
- Hence, Geometrical attributes like bond length, torsional angle cannot be used
- a.k.a 1-D Diagram

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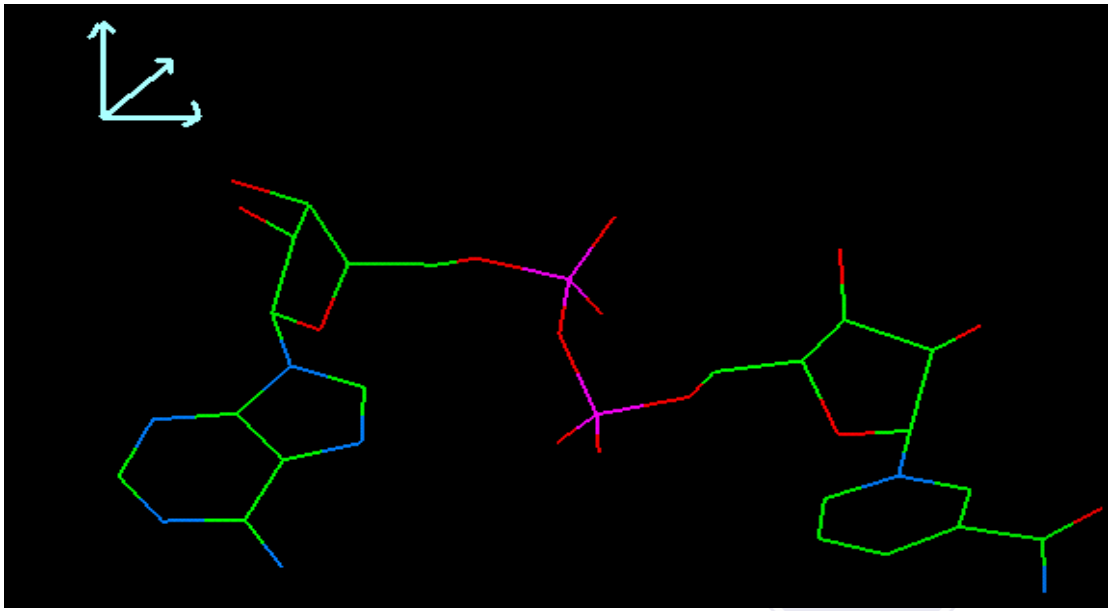

3-D Rendered Image

x,y,z coordinates should be known

All geometric transformations (rotation, scaling, etc) can be done

Reference frames

Drawing molecules requires a transformation between molecular coordinates and the screen

Molecular transformations requires:

- **Scaling of the display (but not the molecule).**
- **Translations of the molecule and objects on the screen.**
- **Rotations about points and lines**

DIFFERENT ATTRRIBUTES

TRANSLATION :A translation moves an object into a different position in a scene

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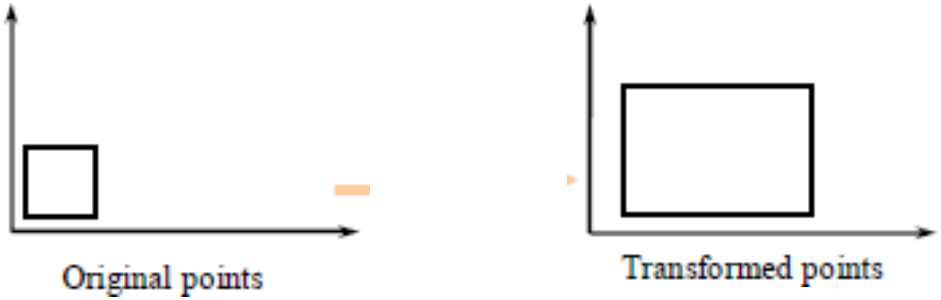
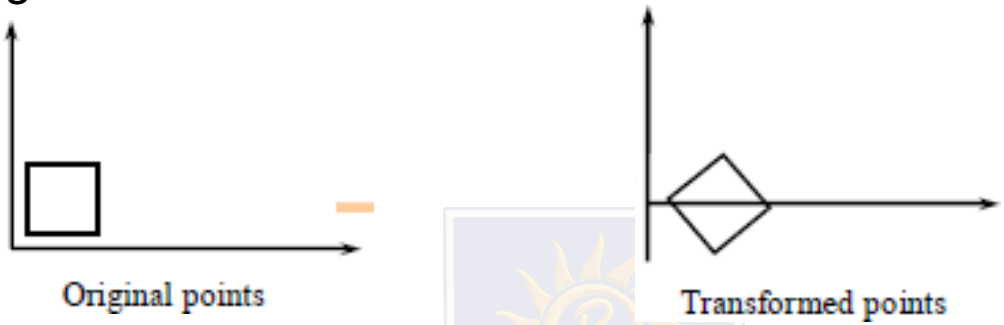
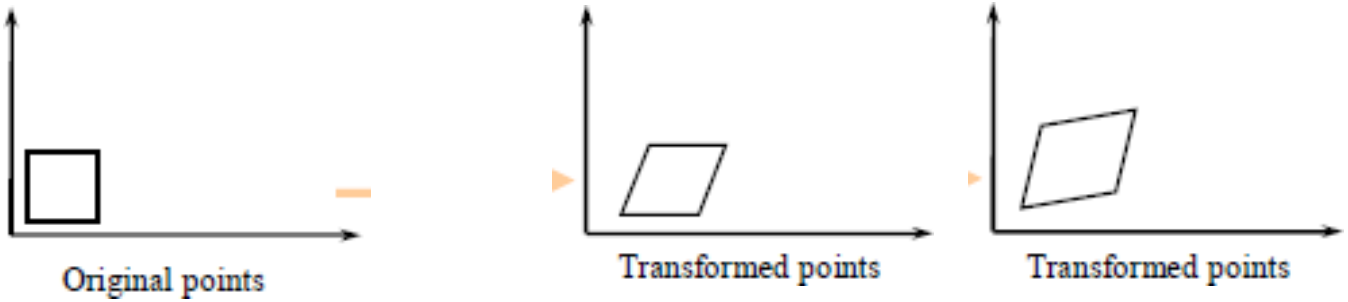
SCALING : A scaling changes the size of an object with two scale factors, Sx and Sy



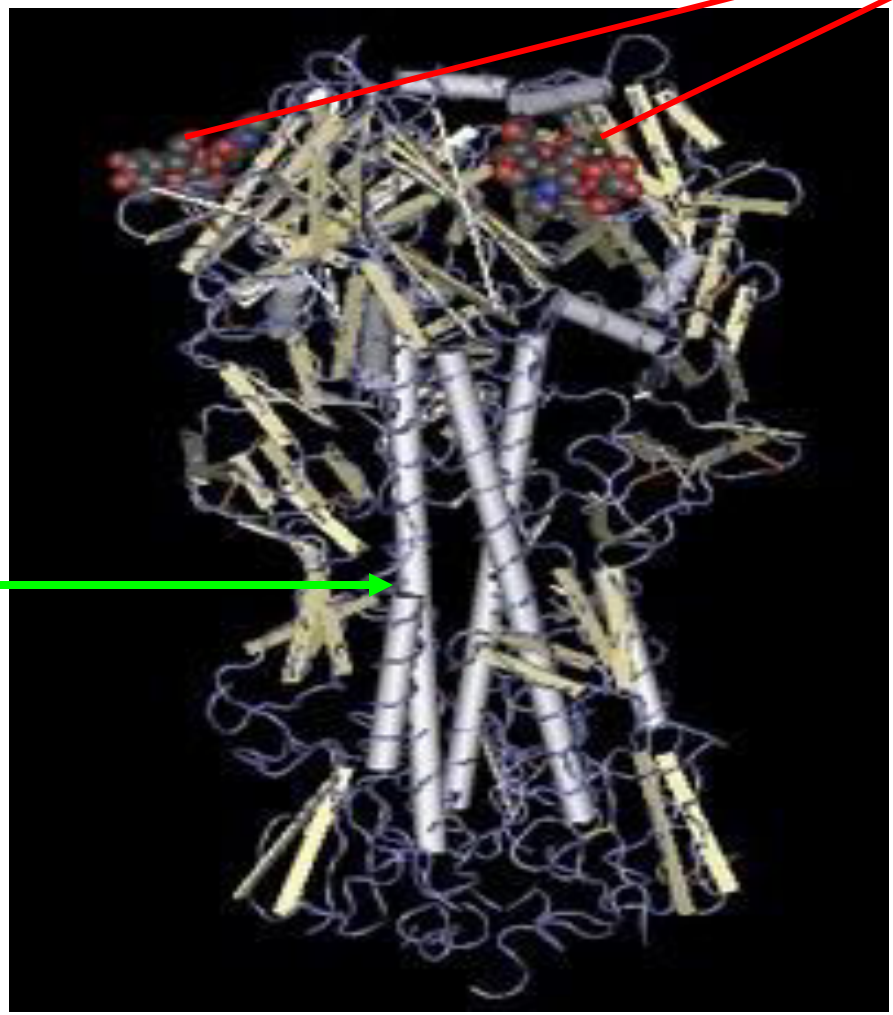
ROTATION : Using the trigonometric relations, a point rotated by an angle about the origin



SHEARING : A shearing affects an object in a particular direction (in 2D, it's either in the x or in the y direction)

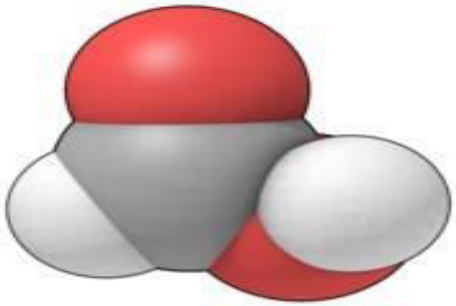


Ribbon Model



Structure of Hemagglutinin

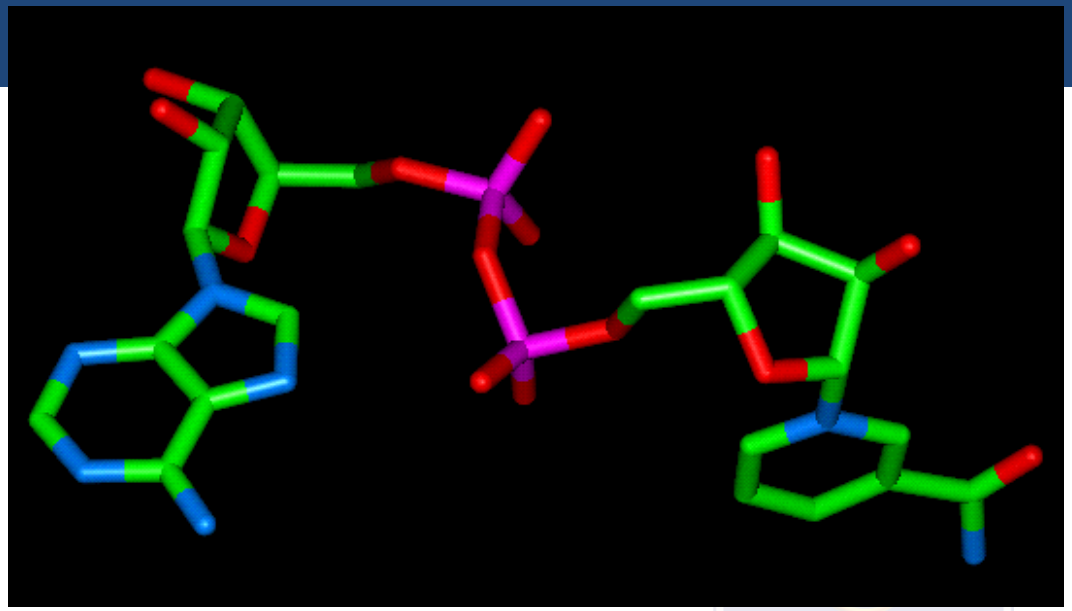
Space-Fill Models



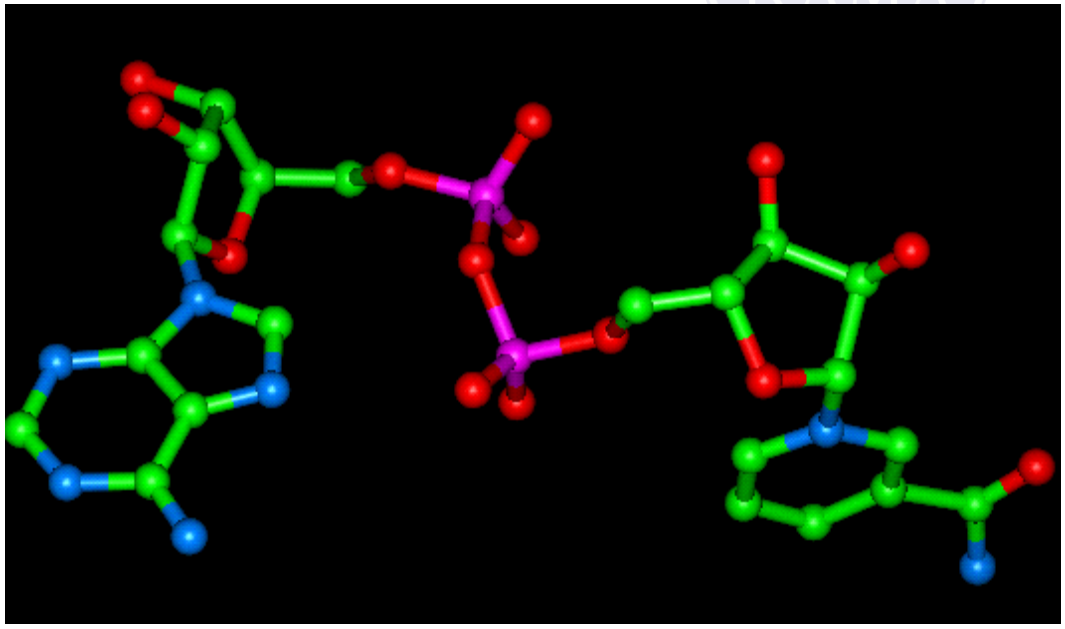
Structure of Formic Acid

Atoms are drawn to suggest the amount of space they occupy
CPK Model = Corey, Pauling, Koltan

The quantum mechanical representation of molecules, there are only (positively charged) nuclei and a "cloud" of negative electrons. The electron cloud defines an approximate size for the molecule



Cylindrical or
"Licorice" modes



Cylindrical-Med

Structure Visualization & Manipulation Softwares

RasMol

Swiss PDB viewer

Molscript

Ribbons

Grasp

VMD

WebMol

Chime

Cn3D

PyMol

QMol

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MCQs

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