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Frodo and the ribosome: how to display low resolution structural models with Frodo

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The molecular graphics display program Frodo implemented for the Evans & Sutherland PS300, has recently been extended with a new display object, which is called Bones². The Bones object consists of a set of points and a link list describing how the points are connected. In addition, each point is assigned a level on the basis of which it is possible to select parts for displaying and to differentiate the points by colouring. Although Bones was introduced to display skeletonized electron density, it was clear to us that it could be used to display almost anything. The ribosome interacts with a large number of macromolecules, both proteins and nucleic acids, during the protein synthesis. Locations of functional sites, binding sites and locations of the ribosomal constituents have been suggested. To be able to get a view of the spatial implications of these hypotheses, we have made a Bones file containing these structures. Each of the two subunits of the ribosome were made as contours obtained from a replica of a plaster model based on data from electron microscopy. The backbones of the known structures of elongation factor Tu, C-terminal fragment of L7/L12, tRNAPhe and a mRNA in helical conformation were made as Bones objects as well. The full structures may be obtained by using the 3D structure recognition options when using the atomic coordinates of the proteins in question as a database. Positions of ribosomal proteins determined by neutron scattering and immuno electron microscopy are defined in the Frodo coordinate file. They can be displayed as dotted spheres generated by the Mol option Surf. The location of functional sites and binding sites can be visualized in the same way.

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A liquid crystal stereo viewer for use with computer display systems and television transmissions

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In a recent publication we described a new high speed liquid crystal shutter which could be used with computer display systems to provide a 3D image. In essence, left and right eye views of a molecule or other object are displayed alternately and in rapid succession; the shutters, which are worn as spectacles, are synchronized with the displayed images so that the left eye only sees the left image and the right eye only sees the right image, the observer perceiving a fully-coloured 3D picture. We have now developed the system further so that real objects can be televised and the televised picture (as a video recording, closed-circuit television picture, or broadcast picture) can be viewed in 3D. For example, it is possible to make a television recording of a lecture or demonstration in which CPK, Labquip, or other molecular models are being used and to show this in 3D. Video recordings taken from a computer display system can be edited into the television recording and also viewed in 3D. The system involves two synchronized, but otherwise, standard television cameras which are mounted side-by-side. The output signals are combined so that successive interlaced frames show the views seen by the two cameras alternately. The television picture is viewed with the liquid crystal shutters in the same way as for computer display systems.

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Conformational analysis and an NMR study of a trisaccharide, constituting a model for branching points in polysaccharides

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NMR-spectroscopy has become one of the most versatile techniques for structural studies of bacterial polysaccharides which are built of oligosaccharide repeating units. Information on residues, substituents and mode of linkages is obtained without destruction of the material. In order to understand all provided by NMR-spectra a comprehensive chemical shift database, and a set substitution rules for all types of linkages are required. Our present database, including disaccharides, is now extended to comprise also information on sterically hindered trisaccharides. Such oligosaccharides can be found in branched polysaccharides. To study this phenomenon several trisaccharides, *inter alia* 1, were synthesized together with the disaccharides B-C and A-C.

