# Molecular Inventor: Discovering Novel Compounds In A Collaborative Environment

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The motivation to develop tools for scientific collaboration is reflected in the nature of the research procedure typical for academic and industrial environments. During the search for a new lead compound or a mechanistic explanation for a biological activity, many scientists within a research institution together with their external collaborators are involved in communicating information assembled in the course of a project. Collaborative computing techniques allow each member of this ad–hoc team or workgroup to review the tremendous amount of information that is easily accumulated, and to manage this information in a straightforward manner.

More and more research is being carried out by interdisciplinary teams of scientists, often requiring to work on–line simultaneously. They may be at one geographic location within an organization, or be distributed around the world and eventually separated by time zones. With the emerging new technologies for electronic conferences, electronic bulletin boards and electronic publishing, there are new ways for scientists to share their results.

The need for collaboration is often overlooked because it is easily taken for granted that people are already involved in sharing information. This premise is flawed as it confuses the term communication with collaboration. While the implementation of better communication tools facilitates collaboration, true collaboration is a much higher level of interaction.

Information sharing in chemical and biological research relies on a suitable mechanism for communicating 3D structural information. Traditional information transfer mechanisms between independent applications, such as cut–and–paste or drag–and–drop, have been implemented for years on personal computers, but up to now, this functionality was limited to text– and image–based data types.

The Open Inventor graphics toolkit [1] implements an elegant mechanism for 3D information transfer through its definition of a 3D interchange file format that describes 3D models of arbitrary complexity as simple ASCII text. Therefore, standard information transfer mechanisms such as the clipboard provided as part of common windowing environments may be employed without modification.

With respect to 3D molecular information, however, Open Inventor has two major shortcomings: (1) the general–purpose architecture of Open Inventor does not provide the level of performance optimization required for specific molecular graphics rendering tasks, and (2) the information being managed by the Open Inventor object database lacks data structures to include non–graphical chemistry related information.

Therefore, we extended Open Inventor to define molecular graphics rendering primitives. These extensions will include mechanisms for fast construction of molecular surfaces, solid contours, volume rendering, slice planes, and property analysis based on texture mapping [2], in addition to a variety of standard molecular representations, such as space–filling, ball–and–stick, wire models and ribbons. Collectively, these extensions are called Molecular Inventor.

As an extension to Open Inventor, Molecular Inventor inherits all benefits of the standard toolkit, in particular the 3D information transfer mechanisms that are an enabling technology for collaborative computing. In this way, the molecular graphics extensions allow for the implementation of chemistry specific collabo–rative tools that may trigger vital communication on the desktop.

Within this framework, any molecular visualization application build on top of Molecular Inventor can automatically import and export 3D structural infor–mation and share it with any other tool adopting this mechanism. As the Open Inventor file format is simple text, 3D structural information may be transfered to a variety of productivity tools, such as a spreadsheet application used for statis–tical analysis and data management.

Of particular importance is annotation in 3D. Other than providing a descrip–tion of a molecular scenario in form of text and images, 3D annotation permits to document structural features and properties as part of the molecular model, to store these annotations and to communicate the annotated information via a mechanism called store–and–forward. With this mechanism, annotated molecules may be communicated by electronic mail and reviewed later by the recipient.

Molecular Inventor also permits 3D structural information to be shared on a virtual whiteboard, as part of an electronic conferencing tool for live discussion between two or more active conference participants. To prevent massive network traffic, structural information is kept local. The information actually transmitted is limited to changes of the object orientation or updates in the 3D structure. This information may be combined with any other type of information, such as images, sound, videos and other media.

Publication often concludes an entire project or a phase of research activity, permitting a broader audience to benefit from the assembled information. With the recent introduction of the virtual reality modeling language (VRML) [3], which is based on Open Inventor, electronic publication may now include complete 3D scenarios as part of HTML documents. In this way, structural information stored as a Molecular Inventor model may be directly published on the world–wide web.

In summary, Molecular Inventor provides a flexible framework for trans–fering 3D molecular information among a variety of applications. By interfacing with tools for collaborative computing, this framework defines a powerful infrastructure for collaboration in chemistry.


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