

Software Reviews

Molecular Conceptor Version 1.0.

Synergix Ltd.
www.molecular-conceptor.com

Molecular Conceptor is in its essence a discovery program, designed to teach students in the field of pharmaceutical drug design the rationale, process, and mental rigor involved in the development of modern drugs. Focusing on a wide variety of disciplines, the program gives a brilliant overview of the continuous integration of skills and techniques to develop what in the future might bring forth medicines that cure specifically and efficiently. For all this, it also achieves something that I consider very important; to quote Clay P. Bedford, "You can teach a student a lesson for a day; but if you can teach him to learn by creating curiosity, he will continue the learning process as long as he lives."

Installation of the program is very easy with plug-and-play that allows for automatic menu driven installation. The requirement of the USB HASP key acts as copy protection, but it's installation is also not difficult—at least for me it was not; using Windows 2000 to test the program, after insertion of the HASP key, Windows automatically detected it and finished the required installation. Whether or not the attached manual is sufficient for the truly unexperienced, I'm not sure of, but I can foresee some possible difficulties with older Windows operating systems, which might make installation slightly more troublesome, but the average Windows user should be able to circumvent these by simply doing a usual driver installation.

The program itself is divided into four subsections: drug discovery, molecular basis in drug design, strategies and principles in drug design, and topics in drug design. The first section gives an overview of drugs and drug development in the past, as well as some of the difficulties that modern pharmaceutical companies experience. Because I am a computational chemist myself, the second subsection was of great interest. It highlights the importance of molecular geometry in modern drug design and gives an excellent overview of concepts such as conformation and chirality and develops pragmatically to include all of the major areas of computational technique and its use in determining such molecular features such as conformation energy, potential surfaces, and a variety of other physicochemical properties.

The third subsection is the crux of the program. It divides drug design into the well-known pharmacophore-based design and possibly less appreciated receptor-based design approaches to modern drug development. The use of three-dimensional images (which the user can rotate in real-time) of all of the structures discussed is what truly makes this a creative discovery process. The bottom-up approach followed during the teaching process would make it easy for any student with a decent understanding of the basic principles of chemistry to learn and understand the challenges of drug design. The last subsection gives a quick overview of the use of modern graphics in molecule visualization

and manipulation and addresses the developing area in pharmaceutical design, peptidomimeticism.

Even though I am not a pharmaceutical chemist myself, I found the program exceedingly enjoyable and afterward even cornered a fellow colleague (he is into pharmaceutical chemistry) to discuss a few interesting things that I discovered. Sitting here now, I can look back and say that the program allowed me to discover the intricacies of drug development and gave me a new appreciation of the complex nature of enzymes and proteins and their interaction.

To facilitate the learning process, a search engine is included in the package and that also acts as a cross-reference mechanism. If a student quickly needs to find a certain topic or subtopic, as they say, it is available at the touch of a button. In the upcoming version of *Molecular Conceptor* (version 1.02, August 2002), the developers have decided to include a "references" button, which will allow the user to immediately find the references from which each page in the program was derived. With all this information available, avid students will be able to do further studies as they prefer.

There were a few minor difficulties that the developers of *Molecular Conceptor* will have to address. The odd spelling mistake, the strange color schemes, and the use of unsuitable fonts did not go unnoticed. The program is not suitable to run along other programs without slowing them down appreciably, especially if there are graphics that can be manipulated involved. Personally, I will never advocate a voice reading all the text for me, but that is just an opinion, and the user is offered the choice to have it switched off (while listening to Bach's 48 Preludes and Fugues...).

An important question that would come to mind for any company or academic institution is that of price concerned. The implementation of the program is such that it can be accessed via intranet; thus, licenses are sold for multiple copies, 10 or more people would be able to access it at once, the license is therefore a site license rather than a single-user license, and the licenses do not expire over time—upgrade versions of the software will be made available over time at roughly 18–24 month intervals. With this in mind, the software is still expensive and I would probably only buy it if I was sure that some of the mistakes I noticed above were in the pipeline to be fixed—you would not expect spelling mistakes in academic software! However, bear in mind that the development of any software package is an ongoing saga between users and maintenance staff, and ultimately, the corroboration of both parties defines the development and final application of the later versions.

Furthermore, one has to marvel at how much information is made available (and future versions promise to be even more comprehensive). It is in a certain sense an information database that can act as a learning tool for beginners or as a lookup for more advanced students.

To give an overall opinion, I would say that the program was enjoyable and, using their own creative insight, will give students the opportunity to learn something as well. The discussion is thought-provoking and well-presented. To finish with another quote from

William Archer, "One of the first and most important things for a critic to learn is how to sleep undetected at the theater." Well, I can promise that there was never any sleeping involved for me, and I think the writers of the program have unwittingly created a "monster", because every medicinal compound I will ever get the opportunity to model will undoubtedly produce ques-

tions of conformation, mimicry, and molecular recognition.

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10.1021/cg0200457