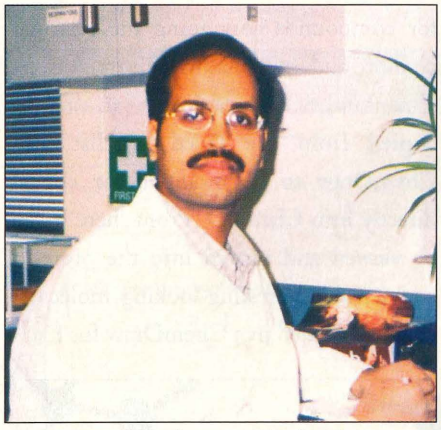
ChemOffice Ultra 2002

ChemDraw, ChemFinder,



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I HAVE WITNESSED THE REVOLUTION in structure drawing—a transition from the use of plastic stencils to computer software. Since my graduate days at the University of Delhi, I have been using ChemDraw and I have witnessed the growth in its scope and capabilities first-hand. With all the add-ons now available, ChemOffice is truly a virtual office that satisfies the documentation and database management needs of chemists. I thank the minds working at CambridgeSoft for creating such a valuable companion for the chemistry community.

Satisfying the Needs of a Chemist

For the medicinal chemists, ChemOffice plays a major role in the entire drug discovery process from conception to creation. ChemOffice is also relied upon heavily when managing and organizing results that are generated. As the drug discovery industry becomes more and more competitive, any amount of time saved could result in a companies fortune. ChemOffice helps in this race to succeed by making structure drawing and database management easy and fast.

ChemDraw

ChemDraw is an outstanding package for chemical structure drawing and editing. The *Document Settings* feature gives this package an edge when preparing chemical schemes for manuscripts that will be published. To my knowledge, almost all publishers recommend using graphics prepared in ChemDraw. This insures a professional and neat appearence.

Chemically intelligent features like *Analyze Structure, Show Stereochemistry* and *Convert Name to Structure* save time and decrease the chance of error.

Chem3D

Chem3D, another important part of the suite, serves the computational chemistry and molecular modeling needs of bench chemists and organic chemists alike. In addition, Chem3D can also be integrated with GAMESS for increased modeling capabilities.

ChemFinder

ChemFinder is a must-have for laboratories with high volume chemistry work. Custom databases, designed with ChemFinder, can be used for various purposes concerning chemical intelligence. See *Figure 2* for an example.

Once a structure is inputed, the molecular formula and molecular weight can be automatically generated. This

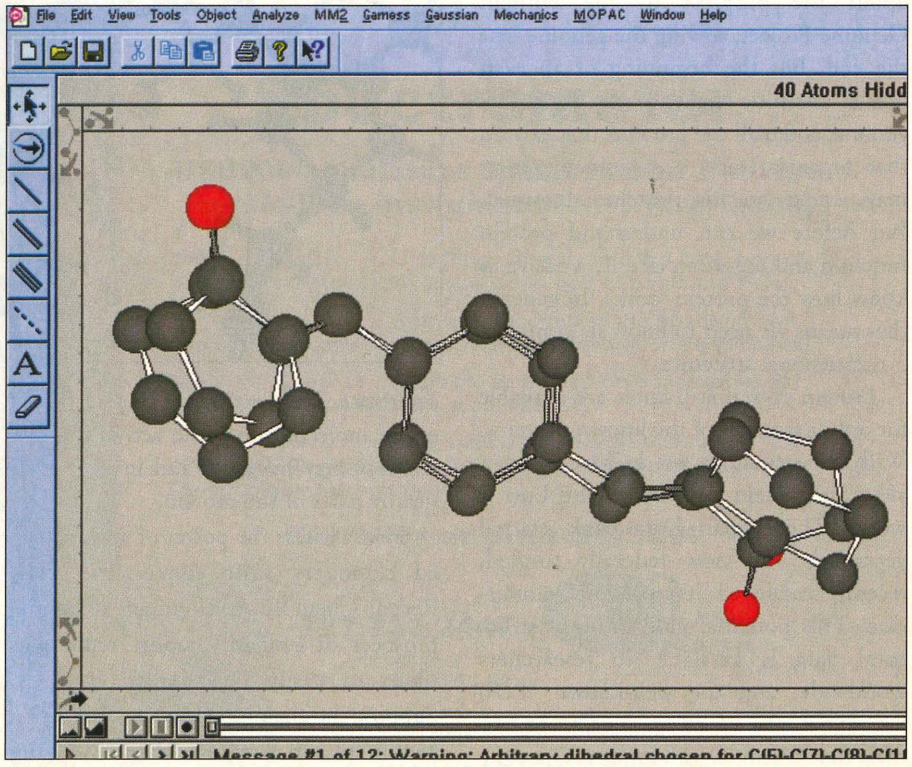

Figure 1. *Structural similarity comparison of 1,4-bis(2-oxo-1- cyclohexylmethylene)benzene and 1,4-bis(2-oxo-1-cyclopentylmethylene)benzene by "overlay" feature of Chem3D.*

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BioAssay, E-Notebook

makes ChemFinder superior and different from other database management systems involving chemical structures.

The most powerful feature of ChemFinder, in my opinion, is its ability to perform structure and substructure searches. The databases included in ChemOffice also provide chemists with a wealth of information. ChemMSDX, for example, provides the material safety information on most commercially available chemicals with a click of the mouse.

ChemRXN offers a variety of synthetic reactions found in chemical literature. Thanks to the ability to add more reactions, this database can also serve as an in-house library for synthetic chemists that can be easily generated from the strong foundation provided by CambridgeSoft.

ChemACX and ChemACX-SC provide information about suppliers of commercially available chemicals.

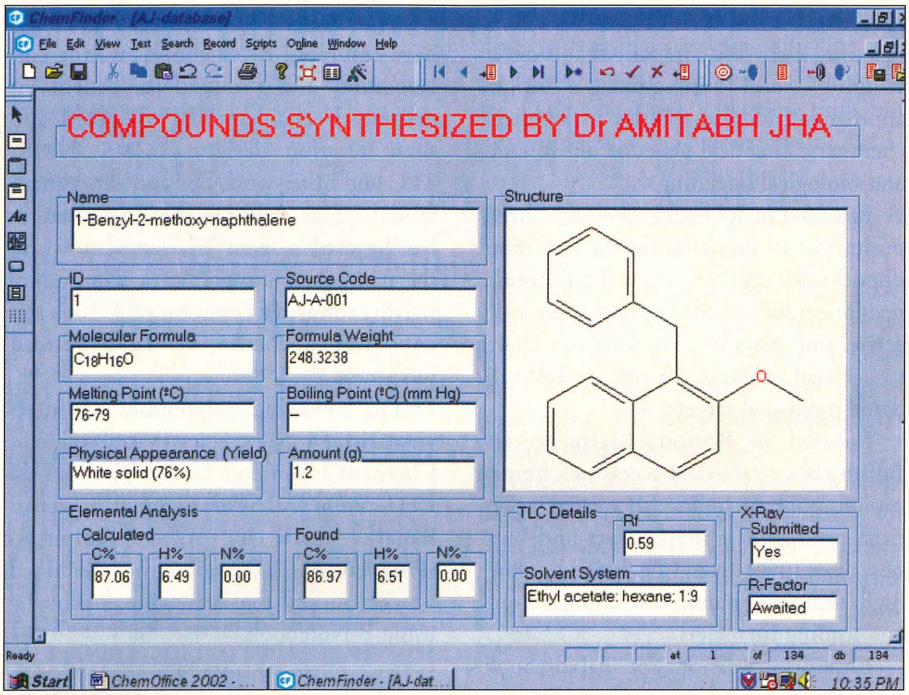

Figure 2. *A page of a custom designed database on ChemFinder.*

E-Notebook

E-Notebook takes laboratory record keeping to a new dimension. The conventional way of recording data in paper laboratory notebooks may not be very time consuming for chemists, but it is generally very inconsistent due to a lack of universal format. E-Notebook makes reports more uniform and ensures that all the proper data is recorded. The conventional method also brings up issues concerning the legibility of handwriting. Results can often be misinterpreted when data is read incorrectly. Data retreival and sharing is also a problem when dealing with paper notebooks. All of these challenges to the conventional paper notebook have been addressed by E-Notebook.

Where huge amounts of data were involved, a need has always existed for a solution that could deliver faster results with more focused searching. E-Notebook has filled this void. It streamlines the data storage process and makes the retrieval very easy. Another noteworthy aspect of E-Notebook is stoichiometry calculations. One just has to draw the reaction scheme and enter the crucial information such as mass, volume and density of the limiting reagent and E-Notebook will do the rest.

BioAssay Manager

Under a drug discovery setup, molecules synthesized by chemists find their way to biology laboratories where they undergo a battery of biological assays (in-vitro or in-vivo). As a result, huge amounts of data are generated on efficacy and toxicity of these compounds. These data need to be managed and presented efficiently to decipher which information is useful.

BioAssay Manager aims to make this part easy. Depending on the assay used, the BioAssay Manager template can be modified and data can be uploaded. BioAssay Manager uses either MS Access or Oracle as the database host, depending on the scale of the project. Once the parameters are set and the corresponding data uploaded, the BioAssay Manager makes presentation of the data simple. For example, a graph of percent inhibition versus concentration can be obtained with a single mouse click.

Conclusion

ChemOffice, with all its add-ons, is a superb package and should be a requirement of any organic chemistry or medicinal chemistry laboratory. In my opinion, there is always room for improvement, but I still rate this software suite a 5 out of 5 based on its present capabilities.