Accord for Access Version 1.1

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Introduction. Accord for Microsoft Access is an add-in for Microsoft Access that allows a chemist to develop database applications searchable by chemical structure. Once a database is created, the user can store chemical molecules and reactions in relational tables; search for these molecules using exact, substructure, and/or similarity search options; produce publication quality diagrams for forms and reports; calculate chemical properties; cut and paste to and from standard chemical drawing packages; read and write standard chemical formats; import and export chemical datasets; transfer datasets to Accord for Excel; and create links to other databases on a particular desktop or over a network.[1]

System Requirements. System requirements for Accord for Access Version 1.1a are an IBM compatible PC using an Intel 486 or higher processor running in enhanced mode, at least 8 MB free hard disk space, at least 8 MB of memory, Microsoft Windows 3.1 or higher, and Microsoft Access 2.0 or higher. A chemical structure editor is also required to input chemical structures as Accord objects or as structure queries, although this is not listed in the system requirements. This review was based on installation and testing on a Micron Millenium running Windows95 and Microsoft Access in Microsoft Office version 4.3. ChemDraw Pro Version 4.0.1 was used as the structure editor.

Installation, Help, and Documentation. Microsoft Access and Windows 3.1 or higher must be on a computer prior to installation of Accord for Access. The program is easily installed from five disks following the usual Windows procedures.

Accord can be used as a stand-alone application or can be shared by multiple users over a network. A special INSTALL TXT file on the first disk explains how to set up the network version. Further details are in the Microsoft Access user's guide. This reviewer used the stand-alone version. You also must have ODBC Support enabled in Microsoft Access. The default Access setup should have installed this, but if you used a custom setup, you may need to go back and reinstall Access. If you do not, you will not be able to connect to Accord chemical databases.

Accord can be launched by clicking on the Microsoft Access icon. Open an existing Access database or select New database from the File menu and then pull down the File menu to Add-ins and select Accord. This loads Accord and opens the Accord toolbar. You can also prepare a macro to open Accord automatically.

Accord for Access comes with a three part user's guide. Part 1, Getting Started, explains how to install and configure Accord; gives an overview of Accord elements; and steps you through creating a simple chemical database application. Part 2, Tables, Queries, Forms & Reports, explains these elements in more detail. Part 3 describes the database functions. Users are expected to be familiar with the design, implementation, and use of Access Basic modules before attempting to create a database. The accompanying Tutorial guide provides a step-by-step guide to storing, managing, and searching chemical data within Access. There is also a New features guide explaining new capabilities that have been added with the release of version 1.1.

Operating the Software. The examples included with Accord for Access are very easy to use and provide a good demonstration of the functionality of the application. Beyond knowing how to launch a database, a user does not need to have much familiarity with Access or even with the concept of relational databases to make good use of an Accord application.

It is a different story, however, when it comes to creating a database. Knowledge of Access is required. This reviewer has had experience with both dBASE and FoxPro in creating database applications on a Macintosh so the concept of relational databases is not a new one nor is their creation. Still, sessions with the Access manuals were necessary to create a new database.

The User's Guide section on creating an application has eight steps. Under each step there is a brief explanation and a few useful tips. The guide was created for version 1.0 so the screens and dialog boxes displayed in the examples do not always match those you will see using later versions. The New features guide does help some with these problem.

Tables are the heart of an Access application. Native Access tables can store CAS Registry numbers, chemical names and formulas, property and spectral data, test results, bibliographic information, and many other types of information. The special feature of Accord is the Accord Chemistry Table which contains Chemistry Objects, usually structure information. Each record in such a table is a chemical entity, a molecule for example. Although native Access tables can store graphic images, there is no mechanism for searching these images. Using the Chemistry Objects in an Accord table, you can store and index structural information for fast search and retrieval. Use the Create Table button on the Accord Toolbar to create your table. The primary key is the link you will use to connect the Chemistry Table with tables containing other data. You can also attach tables created for some other application, or you can import data from another chemical system using the Import Table tool.

Once the tables are designed, it is easy to create queries using the Access Form Wizard or simply designing your own. This is a good place to put aside the Accord manual and go to the Access User's Guide that has much more detailed procedures with illustrations. These queries are used for providing a display of your data, for asking questions about the information stored in your tables, and for creating forms. Once you understand the Access query process, you can turn to the additional tools provided by Accord. These tools allow you to specify chemical query criteria. For example, you can specify that your query finds all the compounds in the database that have a certain substructure. Because the query criteria are completely compatible with

native Access criteria, you can combine the two in more complex queries, for example, all the compounds with a certain substructure that have a given melting point range. If you want to generate a view of your data that brings together related data from different tables, you can design a query with no criteria specified.

Forms are the primary means of entering chemistry objects and other data into your tables. So, the next step is to design a form based on the query you just developed. The Access Form Wizard makes it easy to create very simple forms. The Accord manual tells you how to add an Accord Chemistry Control to your form using the Unbound Object Frame tool and lists steps for invoking chemistry methods and displaying chemical properties via your form, but the reviewer found these to be a bit cryptic. The Access User's Guide can help you with designing an efficient form, but there is nothing about the Accord features. Although you can design simple forms almost by hit or miss, if you want to develop a complex application, it would be a good idea to get help from the Synoposes support people or another, more experienced user.

Now you are ready to add data using your form. This can be done using a chemical editor. This reviewer used ChemDraw, but ISIS Draw and ChemWindows would work just as well. The manual explains how to import data from a file into a table or a query. Accord supports the MDL SD (SDFMOL) and Standard Molecular Data (SMDMOL) file formats. You can also import from, and export to, Accord for Excel databases. If the data you want to import are not in one of the formats mentioned above, you will first have to convert the data into one of these formats. For a large datafile this could be a time-consuming project. If your form is based on a query that includes fields from more than one table, it can be used to enter data into all of them at once.

Once the data are entered you can display, try out, and refine your database, designing new tables, forms, and queries as you think of more and more things to do with the application. You can develop reports to print out the data for distribution or inclusion in documents you are preparing.

There are more features than those described here. A thorough familiarity with all available tools plus the capabilities of linking to databases in other applications would make it possible for a chemist to create many useful applications for both individual and group use.

Software Distribution. Accord for Access is produced and distributed by Synopses Scientific Systems, 116 Village Boulevard, Suite 200, Princeton Forestal Village, Princeton, NJ 08540-5799 in the U.S. Tel. (609) 734 7431; Fax: (609) 520 1702. In Europe the address is 175 Woodhouse Lane, Leeds LS2 3AR UK. Tel: +44 (0) 113 245 3339 Fax: +44 (0) 113 243 8733. E-mail support is available at support@synopses.co.uk, and they have a web site at URL:http://www.synopsys.co.uk. The price of Accord for Access 2.0 is $995 for commercial, $795 for government, and $595 for academic users. An upgrade to the new Accord for Access95 would be $275. Prices for these and other products can be found on the Synopses Web Site.

New Features. Version 1.1a of Accord for Access includes reaction support along with some other performance improvements. In addition to chemical structures you can load entire reactions into your database that can then be searched for reactant or product. The example reactions database included with the Accord for Access package illustrates these features nicely.

The area of chemical information is one that is moving quickly. During the time this review was in preparation, a new version of Accord for Access was released adding web capabilities and greatly increasing the potential usefulness of the product. In addition other chemical information producers have announced products that could be used in combination with Accord to create and manipulate large amounts of information found in commercial databases like Chemical Abstracts and Beilstein CrossFire.

At the ACS meeting in Orlando, Synopses announced a collaboration between Chemical Abstracts Service and Synopsys to integrate SciFinder with Accord. Scientists who have access to SciFinder can search both their own proprietary and CAS public databases and transfer data easily between SciFinder and Accord for Excel and Access.[3] In addition, the new Excel client for Beilstein CrossFire is a whole new source for data for Accord files and greatly increases the usefulness of the product.

The new version, Accord for Microsoft Access95, is a 32-bit program. I only have Access 2.0, a 16-bit program, so I could not try out the new version with the web links. The Synopses web site states that chemical databases created with Accord for Access95 can be published on the open Internet or on a corporate intranet using the Accord WebDriver, and then, using the Accord Internet Chemistry viewer, users can search and view the chemical objects in these web databases.[4]

Conclusions. Recently on the CHMINF-L e-mail list someone asked if there was a database program that would permit searching by structure. None of the conventional database programs available at the time provided that capability. Accord for Access does. It offers the perfect way to create a database combining structural and property data, reaction information, and other kinds of information useful to researchers, students, and lab workers. With the new Web Accord products, an already useful program will become even more so.

The main problem with Accord, in version 1.1a, is that it takes some time to learn how to create your own applications. If a user knows Access and has all the required programs loaded on his/her computer, it is not hard to get a simple application up and running using the manuals for Access and for Accord. For more complicated things, the manuals are not much help. Fortunately the Synopses staff is helpful and answers questions put to them at meetings or via their e-mail support address or Web site quickly. If you want to do extensive database development, it would be very helpful to attend a basic training session where someone helps you to work through all the steps and explains, with many illustrations, what all the Accord Chemistry Controls do and how to make the best use of them. Alternatively, you might want to invest in the new Software Development Kit that can be used to develop applications in C or Visual Basic or in other environments, such as Notes, Access, Word, FoxPro, Paradox, or Omnis 7.[5]

REFERENCES AND NOTES

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