J|A|C|S
COMPUTER SOFTWARE
REVIEWS

**Arthur Suite V. 3.0**. Symyx Technologies, Inc., 3100 Central Expressway, Santa Clara, CA 95051. www.symyx.com. See Web site for pricing information.

In a world of ever-increasing automation and computerization, the primary method of recording experimental data remains the traditional laboratory notebook. Arthur Suite is an easy-to-use, intuitive entry into the electronic notebook market. Its key feature is the Reaction Planner, which is an icon-driven interface for designing reactions and entering data into the database. This interface combines familiar tools, including a chemical drawing program, a spreadsheet, and word processing into a package that is designed to emulate the functionality and the overall layout of a typical laboratory notebook. The chemist enters the starting materials, reagents, and expected products into a reaction window using Chemdraw (Cambridge Soft), ISIS/DRAW (Elsevier MDL), or ACD/ChemSketch (ACD). Many commonly used reagents, solvents, and building blocks are accessible through a drop-down menu. In addition, once entered, structures can be accessed through search functions in the program. It is necessary to name chemical compounds as well, and one can use either systematic or idiosyncratic titles, according to one's wishes.

As each structure is entered, a data table is constructed for each of the various reaction components. The scale of a reaction can be entered by manually adjusting either molar or mass amounts. Stoichiometry is modified similarly. Once entered, reactions can be scaled by changing the amounts of a given reagent or substrate; the other quantities are modified accordingly.

Experimental protocols are entered with the aid of a list of icons that indicate common laboratory tools and operations. For example, a chemist writing the phrase "Butyl azide (0.50 g) was added dropwise by syringe into tetrahydrofuran (30 mL) in a 50 mL three-necked flask fitted with a nitrogen inlet, a rubber septum, and a reflux condenser" into a paper notebook would here drag and drop the reagent and solvent from the reaction scheme, which would automatically include the amount of each from the data table. In addition, the operation of "adding dropwise" and the experimental setup would be incorporated using icons; there is a separate table for equipment used in a given procotol. The icons themselves can be modified by the end user, but many were incorporated into the version of the program that we used. Some of the icons are very intuitive—a three-neck flask looks like a three-neck flask—but some take time to get used to: for example, the "degassed" icon is a picture of Edgar Degas! Changes in quantity fields in the experimental section are reflected as those fields also appear in the experimental write-ups.

The results of experiments can be entered into the system in several ways, beginning with the obvious ability to make notations into the database. One can also attach any sort of digital data to the experimental file, which is very useful. This can include, but is not limited to, pdf files of NMR spectra or other data. There are other built-in features such as a TLC-drawing tool and areas for manual entry of tabulated data. Finally, fields for literature references are provided.

Experiments can be stored at any stage in the process and can include the designation that they were not attempted. Once experiments are stored, the database can be searched for compounds by nearly any parameter involved, including name, structure, or substructure, reaction types, particular reaction titles, or more advanced options that include delimitations on yield. As reactions accumulate, this feature becomes more valuable. For example, it becomes a trivial matter to find and identify all instances when a particular reaction or set of reactions was run—a feature that comes in very handy when preparing manuscripts or theses. One very practical feature is that it is possible to print individual worksheets or notebook pages as pdf files using Adobe Acrobat as a file converter; this will find the most use when taking pages for planned experiments into the lab.

Arthur Suite claims to support calculations of physical properties such as log D, solubility, and p$K_a$ using ACD/labs software. Compound naming is also supported using ACD/lab software and AutoNom TT. However, since the reviewers did not own licenses for this third-party software, we were unable to evaluate this functionality first-hand.

Author Suite is also adaptable to parallel synthesis using the Library Builder feature. A similar interface to the Reaction Planner allows for the construction of Markush structures and their elaboration in tabular format. The permutations of compounds are encoded in a compound table represented as a plate-map. First, the user selects the plate dimensions and titles the library. "Substance Bags" are created to list/store library starting materials that are grouped either by substructure commonalities or by a single functional group. For example, Substance Bags might be created for sets of boronic acids and aryl bromides for a library involving the Suzuki-coupling as a key diversifying step. The library building blocks are then dragged onto a plate representation of the Markush reaction, and the Enumerate function is used to populate the specific combinations of building blocks for the library. The Library Builder supports a variety of export options including export to the Reaction Planner, where the tools described previously are used to compose synthetic protocols for the library, compute chemical properties, and record observations. A weighing-table generator provides a summary of the quantity of each reagent required for the complete library and associates the reagent requirements with specific plate wells in a manner that is easy to recognize visually.

The strength of Arthur Suite arises from the assimilation of familiar computer tools such as structure-drawing programs and spreadsheets into a format that very closely resembles the traditional laboratory notebook. The generous use of iconography for common operations is another very attractive feature, as it permits the entering of data quickly and accurately. Overall, we found the program easy to learn and use, despite the time required to learn the identity of the various icons for operations.


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The Suite came with a set of manuals, and the vendor provided a very useful on-line tutorial. The manuals were reasonably informative, especially the illustrated tutorial for beginners, although there was little on-screen help available.

The Suite performed well using both PC and Macintosh formats. There is not a direct cut-and-paste connection possible with CambridgeSoft's Chemdraw on the Macintosh, however, making it necessary to copy and insert structures using SMILES designations. This was inconvenient and deprived the user of the ability to orient the structure in Arthur Suite. This issue does not arise with other drawing programs on the Macintosh and not at all with the PC version.

Further benefits accrue by incorporating the system onto a network. It is possible to share procedures and protocols both internally to an organization or with the public, including publication of protocols on the Internet; for an excellent example of this, see the Web site for the Boston University Center for Chemical Methodologies and Library Development, currently on-line at http://cmldprotocols.bu.edu/cmld/index.jsp. The sharing feature is very important as the nature of Arthur Suite is such that due to the cost and complexity of the system, it is very unlikely to be adopted by individual users. In this regard, it is probably essential to have the services of an experienced administrator in information technology systems for high-level networking applications and project administration. In addition, users from different walks of life will have different needs vis-á-vis security. The vendors state that it is possible to control access to particular experiments as needed. These reviewers were unable to address this point with the single-user version of the Suite made available, but organizations adopting this or, for that matter, any electronic notebook system will need to evaluate security issues carefully within and without their units.

As for many programs, the advantages of using Arthur Suite accrue from the benefits of scale. For an individual user, it is not particularly faster to input data or to plan reactions for a small number of experiments. On the other hand, the ability to copy, paste, and modify larger chemical structures or entire reactions constitutes a very real advantage over paper notebooks when repeating experiments or making analogous compounds over a time scale of years. The ease of searching and networking can greatly facilitate both the collection of relevant data and the sharing of information between colleagues. At its best, the adoption of Arthur Suite by a group or organization can lead to enhanced productivity and collaboration. Another potential value arises from the ability to use the large-scale adoption of this program as a way of codifying the institutional memory of a research group or larger entity through multiple users and across time.

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