SysChem Technical Overview (For non-chemists)

The software products that SysChem provides are created for the computational chemistry field. They represent revolutionary new tools to aid the organic chemist with the synthesis planning process.

Organic Synthesis

Synthesis means putting together. Organic synthesis is the construction of organic compounds, which are any of a large class of natural and man-made substances that contain the element carbon among others as well. Organic compounds are the basis of biochemistry and organic chemistry. Industries utilizing organic chemistry include:

- Pharmaceuticals (medicines, vitamins)
- Foods (flavoring compounds, food additives, preservatives)
- Perfumes (fragrances)
- Agricultural chemistry (pesticides, growth regulators, herbicides)
- Basic Organic Chemicals (used as building blocks for larger molecules in syntheses)
- There are a variety of other industries who manufacture organic chemical compounds as well.

Products such as pharmaceuticals, pesticides, herbicides and many others have become available through the development of better organic synthesis methods.

Every year an organic chemist can synthesize a handful of organic compounds, or up to a hundred or more in a busy laboratory. Most syntheses of organic molecules require many steps to complete starting with the basic commercially available building blocks. Organic chemists normally will use a published synthesis route if an economical one exists that is not protected by any patent. Occasionally they must come up with their own starting from scratch. Importantly, there is no guarantee that a published synthesis route is the most economical or most efficient at an industrial scale, also if a chemist develops his/her own synthesis route there are still no guarantees of theirs being the most economical.

Organic chemists are always on the lookout for attractive, previously undiscovered synthesis routes. Such novel solutions can be worth thousands or more commonly millions of dollars.

Retrosynthesis

Developing a synthesis route or plan for a desired compound is referred to as "retrosynthesis". Using complex and time-consuming techniques, the organic chemist works backwards from the desired target compound using known reactions until they arrive at available starting materials. Unfortunately, retrosynthesis almost always results in an exponential explosion in possible routes to consider.

The retrosynthetic analysis process is far more difficult for a chemist to perform than it is to analyze a proposed synthesis route. This is where the SysChem products come in.

SysChem Tools

Our software uses many thousands of known chemical reactions and hundreds of thousands of available starting materials to generate a set of proposed solutions for the organic chemist. The program's operation is entirely automated. Upon its completion the organic chemist has a list of possible solution candidates to review for viability.

Every solution candidate consists of documented reactions that lead to compounds from our list of available materials.

The Technology

The key to our software's unique ability is its revolutionary mathematical representation of compounds and reactions.

Currently there are many ways in which organic compounds and reactions are represented. Some use symbols like "$CH_3CH=CHCH_3$". Others use naming techniques like "2-butene". Many use visual displays to portray the compound. Some use a combination of these techniques.

But these models are oriented towards the needs of the chemist, not the computer. For many purposes a computer program has difficulty working directly with data in this form.

A number of data models for compounds and reactions have been developed for the computer. Some of these have even been published and are generally available. Although these representations can be stored and manipulated within the computer, they are still not ideal for processing efficiency.

The SysChem software utilizes a break-through data modeling technique for compounds and reactions. This new data structure is specifically designed to address the unique processing requirements of performing automated retrosynthesis on a computer.

The result is a software system that can process the mind-boggling number of computations associated with retrosynthetic analysis *on a standard desktop computer*.

The Future

There are many exciting plans for the future of SysChem's product line. As revolutionary as our tools are today, their future potential is far greater. We have under development a next-generation leap in our data modeling architecture. This new processing model will be an integral part of our product line's advanced line due out later this year.

Our future also includes options for employing multi-processor machines and/or distributed processing technologies that will enable the software to tackle increasingly sophisticated compounds with even greater speed.

Common Definitions:

Computational Chemistry – Using computers in the field of chemistry to solve difficult chemistry problems.

Synthesis – Step-wise building a more complex molecule from simpler building blocks.

Organic Chemistry – The branch of chemistry devoted to molecules found in nature or molecules that contain the element carbon as well.

Biochemistry – Chemistry of organic molecules as they apply only to living things.

Syntheses – This is plural for synthesis.

Retrosynthesis – A commonly used method to develop a new synthesis for a compound, which works by starting at the desired compound and working backwards until simple building blocks are found. The simple building blocks now become the beginning of the actual synthesis proceeding towards the more complex molecule which is called the target molecule.

Chemical Reaction – Performing some action(s) on a container with a mixture of chemicals, this action causes a change in the chemicals inside leading to some new desired compound. This new compound then may either be the product the chemist desires, or he performs another chemical reaction on it leading him closer to the product he is ultimately trying to make in his synthesis.