



High Performance Discovery Software

Strategic Framework

October 2006

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I. Introduction

SysChem springs from the visionary amalgamation of innovative organic chemistry and sophisticated software development. Founded by experts in both fields, SysChem brings to market a revolutionary means to accomplish retrosynthesis, guaranteeing more efficient manufacturing processes and significant savings to any customer engaged in the production and sale of organic molecules.

SysChem has, in effect, found the Rosetta Stone for chemical retrosynthesis.

Company Mission

SysChem's mission is to be the leading supplier of novel synthetic routes, providing organic chemists with the most cost-effective synthetic solutions.

By reducing the costs of producing pharmaceuticals and other organic products, SysChem will make it possible for producers to increase profits while maintaining or reducing prices for purchasers of the end product.

Organic Synthesis

Organic synthesis is the construction of organic compounds, which are any of a large class of natural and man-made substances that contain carbon. Organic compounds are the basis of biochemistry and organic chemistry. Industries utilizing organic chemistry include:

- Pharmaceuticals and Neutraceuticals
- Agricultural chemistry (pesticides, herbicides)
- Foods (flavor compounds, food additives, preservatives)
- Perfumes (technology for manufacturing fragrances)
- Research and Development on new products for these industries.

Products such as pharmaceuticals, pesticides, herbicides, pigments, and many others have become available through organic synthesis.

Organic chemists regularly attempt to synthesize organic compounds. Many of these compounds are complex and require multiple steps. Confronted by such challenges, organic chemists typically rely on published organic synthesis routes. Published routes to synthesizing a compound are tried and true, guaranteeing results. However, there is no guarantee that published synthesis routes are the least expensive or most efficient.

For this reason, organic chemists are always on the lookout for attractive, previously undiscovered synthesis routes. Such novel solutions can be worth thousands, and even millions of dollars.

Retrosynthesis

One means to develop a synthesis route – a plan for manufacturing a desired organic compound – is “retrosynthesis.” Using complex and time-consuming techniques, organic chemists work backwards from the desired target compound using known reactions until they arrive at available starting materials.

Working backwards results in an “exponential explosion” in possible syntheses to consider.

To understand the daunting nature of this “*exponential explosion*” one need only consider that the average pharmaceutical compound run through SystematicChem© will be analyzed by the software hundreds of millions of times to explore all the possibilities.

Obviously, it would not be possible for a chemist to come close to what the software does. Therefore, the optimal arrangement would be for the software to generate large numbers of reasonable syntheses. A company’s chemists can then evaluate the results to reveal the very best manufacturing method(s).

A Revolutionary Answer to a Nagging Problem

Many naturally occurring chemical compounds are essential for modern medicines and many other products. Unfortunately, many of these compounds are in short supply in nature. Researchers may spend hundreds of man-years manually trying to come up with synthetic alternatives.

The software products that SysChem provides represent revolutionary new tools to assist the organic chemist with the synthesis planning process. Scientists worldwide agree there is a need for improved organic synthesis. One of the most important pathways is retrosynthesis – working backwards from the end point to find better starting points.

Chemical reactions can be viewed in two directions: the *synthetic* direction, corresponding to how it would actually be produced in a laboratory or a factory, and the *retrosynthetic* (or *antithetic*) direction, going backwards from a target molecule to starting materials by way of retro-reactions or *transforms*.

Retrosynthesis is often applied when a synthetic route to a target molecule has to be developed. The term *retrosynthetic analysis*, a synonym for retrosynthesis, expresses more clearly its ‘imaginary’ character.¹

One of the leading Internet databases of information for organic chemistry resides at www.organicworldwide.net, a Web site formed in 1996 to independently serve organic chemists by providing access to information critical to their profession.

According to this site, the need for computers in retrosynthesis is critical.

Retrosynthetic analysis in itself is already a powerful tool for the chemist. However, the enormous amount of chemical knowledge available nowadays makes it difficult to use RA efficiently and thoroughly. Most of the information is relatively inaccessible, especially the newer reactions and developments in scope of older ones. In practice, the synthetic chemist is limited by the information that is most readily available to her/him. Furthermore, there is a tendency to accept the first reasonable solution and to focus attention to that direction, whereas a more thorough analysis may result in a much better solution saving weeks or even months work in the laboratory. The required extra effort is almost always a worthwhile investment. The application of a computer program which can assist in retrosynthetic analysis is then of great value. A computer program has no bias and, of course, has total recall.²

SystematiChem© is an innovative organic chemistry software system that redefines the process of organic chemical synthesis planning. SystematiChem's© groundbreaking new approach to the problems faced during organic synthesis planning and retrosynthesis is the revolutionary next step in pharmaceutical and chemical research and development. SystematiChem© allows companies to find more cost-effective ways to produce pharmaceutical drugs and chemical compounds.

¹ Definition of retrosynthesis from <http://www.cmbi.kun.nl/cheminf/ira/>

² Source: www.organicworldwide.net

II. SysChem's Product

SysChem's products are large numbers of advanced syntheses that show the organic chemist almost every single possible synthetic method possible. The company's current system, SystematiChem©, is fully operational today. Additional products are in development.

SysChem software uses tens of 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. On average, the chemist will have many thousands of syntheses to pick from. This wide variety of choices gives SysChem's customers an opportunity to find the one synthesis that is perfectly attuned with their goals for production.

Companies can set any priorities they like for a good synthesis. Since they will have so many choices, a perfect match should not be hard to find.

Every solution candidate consists of documented reactions that lead to the desired compound, drawn from SystematiChem's© extensive list of commercially available materials.

Even an advanced chemist will find these syntheses useful to quickly determine viable synthesis routes or to identify a desired novel solution that might otherwise have been missed.

III. The Technology

What makes SystematiChem© unique is its revolutionary mathematical representation of compounds and reactions.

Currently there are many ways in which organic compounds and reactions are represented. Compounds and reactions may be represented by symbols like "CH₃CH=CHCH₃." Or they may be represented through naming techniques, such as "2-butene." Often, visual displays will be used to portray a compound. In many cases, a combination of these techniques will be employed.

All these models are oriented to the needs of the chemist, not the computer. A computer program has difficulty working directly with data in this form.

A number of data models for organic compounds and reactions have been developed for the computer. Some of these have 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, simply because they impose limiting theories and strategies on the transaction.

Instead of applying strategic-bond theories or disconnection strategies, the SysChem model allows SystematiChem© software to directly consider every reaction in its database against the target and intermediate compounds. It directly applies every reaction that qualifies. SysChem's software does not have any preset rules (such as the various strategies used by other software like LHASA) which is why SystematiChem© can find the very best syntheses out of all the possibilities. SysChem's software does not make any assumptions whatsoever. All solutions are presented to the chemist to decide for him/herself if a particular method is practical or valuable. Chemists should prefer more choices than fewer, so they can be more confident they are presenting the very best option when a decision needs to be made about implementing a new method of manufacture.

IV. Future Tech Developments

SysChem currently has under development the next generation of SystematiChem© technology – methods for constructing much larger "biomolecules." This breakthrough utilizes the next-generation of SysChem's proprietary mathematical model.

As revolutionary as the current SystematiChem© product is now, the company anticipates this new product will make yet another quantum leap in the synthesis planning tools market. It will run even faster and will be capable of generating more sophisticated solution pathways for ordinary synthetic molecules, as well as much larger biological molecules.

SysChem is developing many important new features to take both of these products to the next level. They include:

- Improvements to the content and comprehensiveness of current reaction and compound databases:
 - Detail data such as reaction yield and process information
 - Protective group chemistry
 - Corey's published reactions
 - Organic Syntheses (a publication) integration
- Improvements in the handling of reaction selectivity.

In addition, SysChem is evaluating a SystematiChem© product designed for multi-processor and/or distributed processing systems.

V. Market Analysis

At present, the annual worldwide market for synthetic organic compounds is approximately **\$500 billion**.³

Worldwide, approximately **10,000 companies** are producing organic synthetic molecules.⁴

There are approximately **120,000 marketed synthetic organic compounds**. Using SystematiChem©, **SysChem can cut manufacturing costs by an average of 50%** for an average of 75% (90,000) of these compounds.

The worldwide opportunity for SystematiChem© is exceptional. SystematiChem© provides an automated solution to large companies – primarily, but not exclusively, pharmaceutical – which generate billions of dollars in annual revenue through the manufacture and distribution of prescription and over-the-counter products.

Consider, for example, the value to a major pharmaceutical house of identifying a less expensive way to produce a name-brand, patent-protected drug. A company holding this advantage could conceivably lower its prices – to public acclaim – while increasing its profitability. Only SysChem can offer that edge to an original manufacturer.

Now imagine the value of holding the patent on the least expensive manufacturing route after a drug is on the open market. For the drug's inventor, this guarantees continued legal market domination into the foreseeable future. And if the inventor isn't a SysChem customer, an aggressive generic competitor can contract with SysChem and corner the market.

SystematiChem© also provides solutions for manufacturers of basic building-block chemicals, as well as manufacturers of nutraceuticals, agricultural chemicals, and fragrances. These companies are always seeking a competitive edge and ways to enhance profits. SysChem offers both.

Because orders are received and fulfilled via the Internet, SysChem can offer its product to any company worldwide that uses organic chemistry to manufacture a compound.

As SystematiChem© is the only product of its type – addressing retrosynthesis with a completely automated solution, the opportunities to define and exploit profitable market niches are significant.

³ Source: US Department of Commerce, 2003 data

⁴ Source: Web search of organic chemical producers, 2006

VI. Sales and Marketing

SystematiChem© is marketed and sold through a combination of strategies designed to introduce SysChem's product to key players in the marketplace. Sales and promotion focuses on two primary groups:

1. Corporations with incomes directly resulting from the synthesis of organic compounds. These industries include: Pharmaceuticals, herbicides, pesticides, and general organic compounds for various industries.
2. Corporations serving as sub-contractors in synthesis development for the corporations listed in item #1.

SysChem expects the bulk of its sales to result from relationships with primary synthetic compound manufacturers.

SysChem's approach to sales is collaborative. SysChem does not need to capture the entire market to be highly successful and so chooses to negotiate fair terms with ethical players. While SysChem stands prepared to fill one-time orders, it actively seeks out long-term relationships with the right kinds of companies.

VII. The Competition

Most large chemical companies have been struggling to develop technology similar to SystematiChem© since 1980. For a number of very good reasons, none have been successful to date. Nor are they likely to be successful in the future.

Currently, there are no real competitors to SystematiChem©.

Most of the existing software products in the synthesis-planning tools market are interactive tools that have little or no automated synthesis route generation capabilities. Others are essentially educational assistants that have little or no useful commercial value.

Current retrosynthetic software tools are necessarily biased, as they employ a predisposed pathway to find a solution. Nonetheless, interactive synthesis planning tools like WODCA⁵ and LHASA⁶ can be helpful to someone with an advanced knowledge of organic chemistry. The downside is that the expert user must implement complex strategies in attempting to solve a problem. Because these programs require highly-trained users – and can be time-consuming to operate – they are generally unpopular among bench chemists.

Even expert chemists, once locked into the bias of typical retrosynthetic software tools, cannot help but add their personal biases toward certain solution pathways. The resulting solutions may not be close to providing the most cost-effective and shortest pathway to a compound's synthetic creation.

The approaches offered by would-be competitors ignore a multitude of viable options, whereas SystematiChem© is able to effectively find every potential solution and present them to the chemist for review. The differences between these methodologies are extraordinary. The results of SystematiChem© vs. traditional software tools can mean savings of millions of dollars in the production of a single drug by a pharmaceutical company.

It is almost always easier and faster (and requires far less expertise) to select solutions from a set of valid candidates (i.e. those presented by SystematiChem©) than to construct independent synthesis paths, even with the guidance of a would-be competitor's interactive synthesis planning software.

⁵ WODCA is an acronym for **W**orkbench for the **O**rganization of **D**ata for **C**hemical **A**pplications.

⁶ LHASA is an acronym for **L**ogic and **H**euristics **A**ppplied to **S**ynthetic **A**nalysis.

VIII. Competitive Advantage

SysChem has developed a proprietary software solution to retrosynthesis and holds all data, system design, and programming internally. SysChem has not published any data on system design publicly. Further, SysChem has not – and never will – disclose critical details of its software design to any third party. Copies of any SysChem software will not be transferred to any third party, ever. The security of our proprietary technology is of the greatest importance at SysChem Inc.

SysChem has utilized a unique system design and has adapted countless modifications to the process. Each of these modifications and adaptations are unique and specific to this development process.

While it is theoretically possible that a competitor may arise, the software industry has been attempting a solution similar to SystematiChem© for over twenty years. SysChem has created a product unlike any other software system on the market. Since the development of SystematiChem©, significant modifications and enhancements have been made to the product. SystematiChem© is now so unique that it would be virtually impossible to duplicate anytime in the foreseeable future.

SysChem will continue to aggressively develop improvements to the SystematiChem© product. As the chemistry world adopts SystematiChem© syntheses as their primary methods of manufacture, word of the breakthrough will spread. Knowledge that future versions are always under development will reassure current customers and attract others.

To ensure customer buy-in and satisfaction, SysChem will actively solicit feedback through creation of a SysChem Client Council. As members of the SysChem Client Council, customers will be able to ask questions, exchange ideas and posit suggestions for future versions of SystematiChem©. By employing proactive measures such as

these, SysChem will encourage a higher level of support for SysChem and SystematiChem© products.

SysChem believes it has at least a 2-3 year head start on any potential competitor. The combination of aggressive marketing, continued product enhancement and active customer engagement in the development of future versions of SysChem products will help the company maintain its standing as the only real alternative for cost-effective retrosynthesis.

IX. Management

At the core of SysChem is a dedicated team of innovators, well versed in successful software development and organic chemistry. The Company has spent several years researching, developing, and recently introducing the SystematiChem© product to the market.

SysChem has deliberately followed a three-step process in building the company:

STEP 1:

Transform the idea of computerizing retrosynthesis into a marketable product.

STEP 2:

Build on the talents of the three key players in the development of SystematiChem©. The three principals have invested more than 10,000 hours into the development of SystematiChem©. They continue to work on the next refinements of what is already a revolutionary breakthrough. The three core members of SysChem are committed to the long-term success of both their product and their company.

STEP 3:

Add the business expertise needed to develop minimalist administrative structures that support the product, without adding layers of bureaucracy.

Following this model, SysChem is able to simultaneously pursue three options for corporate development:

1. Partnership with a venture capitalist or group interested in investing in a sustainable enterprise with high growth potential.
2. Standing alone, growing through continued investment of sweat equity by the principals and strategic market development.
3. Growing a hybrid, utilizing outside cash and in-kind investment, government grants and loans, small business loans and reinvestment of income from sales to augment sweat equity.

X. SysChem's Operational Model

Utilizing current computing capacity, SysChem can process up to ten (10) molecules each day.

Following the upgrade of computational hardware, SysChem anticipates an increase in processing capacity to 120 molecules per day.

The Company uses a "Service Bureau" approach, whereby clients submit their chemical compound problems to SysChem for the generation of potential synthetic solutions. Employing this business model, SysChem will be able to receive orders from across the globe, via the Internet, and distribute solutions the same way.

By special arrangement, SysChem will assist commercial research labs in development of new compounds.

SysChem also analyzes promising compounds and tests patentable routes in its own lab. SysChem offers pre-tested patentable manufacturing routes for these compounds to its customers.

In addition to the advantage of speed, the model guarantees that only SysChem has access to its source code, protecting its proprietary process from pirating.

XI. Looking Ahead

Extensive research has been conducted on the industry, the need for retrosynthetic software tools, and the competition. The SystematiChem© product is designed to fill an unsatisfied need for automated retrosynthetic analysis in the organic chemical marketplace.

The opportunity for profit through the sale of novel synthetic routes is extraordinary. The annual gross financial potential for a product such as SystematiChem© conservatively falls into the \$100M+ range. The impact to pharmaceutical companies, as well as other manufacturers, could easily exceed several billion dollars.

The SystematiChem© product has already been significantly upgraded. Version 1B provides effective solutions to customers with a wide variety of needs. The Company will continue to refine and develop further versions of the SystematiChem© technology, enhancing and expanding its market niche.