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04 - Medical Instruments and Disposables
05 - Agricultural Chemicals including Fertilizers
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68 - Transportation Equipment and Accessories
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72 - Conveyors, Hoists, Cranes, Elevators
73 - Machine Tools, Industrial Process Control & Telemetry
80 - Electrical Components, Motors, Appliances and Illumination
85 - Electric Power Plant, Distribution Systems and Conservation
86 - Communications - Circuits and Apparatus
88 - Electrical and Electronic Test and Measurement
89 - Active and Passive Circuit Components
92 - Computers
99 - Lasers, Plasma, Quantum Mechanicals & Cryogenics

I P H

N E W S B R I E F

INTELLECTUAL PROPERTY HAPPENINGS August, 1987

IPH is a monthly news brief for technology executives, inventors and software creators. News covered includes information, behind the scenes events and insights into the development of intellectual property and its protection through patents, copyrights, trade secrets, trademarks and similar rights.

Japanese Flood Patent Office With Superconductor Inventions

Large Japanese companies have filed more than 1500 patent applications on superconductor inventions within the last year -- Sumitomo Electric alone filed 700 applications and six other companies have filed more than 50 applications. Japanese companies hope to use their patents to help dominate the emerging new technology and to obtain cross-licenses from holders of any basic patents.

The Japanese and everyone else in the field is waiting with interest for the publication of IBM's basic patent application. IPH predicts this could occur as early as October of this year.

Whether or not GOCO Labs are under Federal Technology Transfer Executive Order Still Unresolved

During the draft stage of President Reagan's Executive Order on Federal Technology Transfer (FT^2) (IPH 6/87), one provision, 1(b)(1), linked the GOCOs (government-owned contractor-operated laboratories) with the GOGOs (government-owned government-operated laboratories). This provision related to Executive department and agency heads delegating authority to the Federal laboratories "to license, assign, or waive rights to intellectual property developed by the laboratory." In the course of Executive branch negotiation, the Department of Energy took a firm position that GOCOs, which were under DOE, should not be included and they were omitted.

However, another provision, 1(b)(4), remained intact. This stated that the head of each Executive department and agency shall promote the commercialization of patentable results of federally funded research by "granting to all contractors... title to patents made in whole or in part with Federal funds, in exchange for royalty-free use by... the Government". No distinction was made between a GOCO contractor and other government contractors. The Department of

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Energy is resisting the GOCOs coming under the provision while others in the Executive branch say they do come under the provision. A White House official involved in the preparation of the Executive Order indicates the controversy may eventually have to be resolved by William Graham, the President's Science Adviser.

Meanwhile, it is believed that a new law will be introduced shortly to provide clearly for technology transfer from GOCOs. This may be the best procedure since GOCOs, which include some of the world's leading laboratories, are not the same as ordinary government contractors and yet they are not Federal laboratories in the usual sense and the employees are not under Civil Service.

GE Buys License to British Universities' Invention - Pays Millions

GE has recently entered into an agreement with BTG (British Technology Group) for a license to advanced medical scanning devices and has agreed to pay several million dollars. Three British universities will share in the proceeds. BTG will now seek payments from Toshiba, Diasonics, Siemens and Philips.

IPH continues to be amazed at the success record of BTG which among other things, is set-up to commercialize the technology of British universities and British government labs.

Animal Patents

The halt in legislative efforts to declare a moratorium on patents on animals (IPH 2/86 & 7/87) proved to be short-lived. Congressman Charles Rose (D-NC), with six co-sponsors, introduced legislation this month putting a two-year moratorium on patenting animals modified, altered, or in any way changed through genetic engineering technology and revoking any patents previously granted. A similar bill is expected to be introduced by Senator Mark O. Hatfield (R-Ore) after the August recess.

No patents have been issued, as yet, but pending are 15 relating to such matters as introducing disease resistance; ability to adapt to different geographic locations and climates; higher meat content; more efficient growth; and use in developing new pharmaceuticals. The moratorium is supported by a coalition of a number of major national farm, animal welfare, environmental and religious groups who pledge to launch a national campaign to build further support.

Nearly all the arguments are the same emotional ones that preceded the Supreme Court's Chakrabarty decision in 1980. (This held that live, genetically altered microorganisms were patentble.)

However, agricultural organizations are arguing such patents will result in a new kind of tenant farming. They say farmers will either no longer own the new and better animals they use or will have to pay royalties on them. This situation, they claim, will lead to corporate

consolidation of the livestock industry. Agricultural groups point out that five major companies now control 120 seed companies that were formerly independent before seed patenting started in 1970. The situation brings back memories: Farmers managed to keep yellow margarine from consumers because it competed with butter. In that case, common sense finally prevailed and consumers were able to buy margarine premixed with yellow powder.

Both the emotional arguments and those based on concerns for the farmers are believed to be without merit and stem from unreined imaginations. No proposal has been made to stop research and use of new animals, only that the patent incentive be stopped.

Instead of hurting the farmer, the potential for helping the farmer (as well as improving the lot of mankind) is great. Encouragement should be given to development of animals that will help the food problems of Africa -- such inventions as domestic animals for food and milk that can survive in hostile regions. Tobacco farmers could switch to aquaculture if a fast-growing fish tolerant of temperate zones was developed. Beef raisers, too, might benefit from aquaculture. Fish has passed beef as entree of choice in restaurants. Since such inventions will come from the Department of Agriculture and numerous universities and foundations in addition to private industry, it is hard to see that any corporation will have a lock on these new technologies, and such inventions should be encouraged by a viable patent and not discouraged, as the opponents would prefer.

Instead of declaring a moratorium, why not allow the patents to come out? If an actual trend proves to be negative, address the problem at that time. A moratorium would avoid ever determining if there is indeed a real problem.

Electronic Companies Change Strategies to Emphasize their Intellectual Property -- Take Hard Line on their Rights

IPH has already reported TI's chip war that netted them $268 plus million (IPH 4/87), IBM's multimillion-dollar secret settlements with Japanese infringers (IPH 1/86 & 2/87), Intel's winning fight (so far) with NEC on important chip circuits (IPH 2/87) and Apple Computer's restriction against anyone using the Mac-type of interface with competitor's products (the look-and-feel theory of copyright law) (IPH 2/87).

Other examples of the hardening attitudes: IBM's enforcement of its rights against clones of its new PS/2 computer line; Corning's victory against Southern New England Telephone stopping its optical fiber joint venture with SpecTran; Intel's refusal to second source its 32 bit technology to AMD (now in hot contract dispute); and likewise, Motorola's refusal to second source its 32 bit technology to Thompson-CSF (dispute settled); National's lawsuit against United Microelectronics and also against Toshiba on its universal receiver-

transmitter chips; Unison's settlement with Broderbund by a payment of cash and cessation of infringing production on a "look-and-feel" copyright suit, and Valid Logic's prompt settlement of the patent lawsuit brought against Teradyne for CAD hardware modeling (expected to cost Teradyne millions plus in royalties). These cases are all only the tip of the iceberg.

The new change of attitudes can best be summed up by Larry Tesler, Apple Computer's Vice-President for Advanced Technology who recently said, "In the past Apple had few patents, but our rate of applying for patents is increasing rapidly. The feeling is shifting here, from an emphasis on getting products out fast to an emphasis on inventing things along the way. It's a move toward new and unique developments to give our products more differentiation."

--And the Chemical Industry is Doing the Same Thing

Witness DuPont's so far mostly successful world-wide battle to protect Kevlar from infringement by Akzo. DuPont flatly states that without patent protection there would be no Kevlar -- they would not have spent the $500 plus million dollars in development costs.

Other examples are: (1) Electro-Biology winning $9.8 million dollars in damages from American Medical Electronics (AME) for a bone growth stimulator -- AME says they could not continue as a going business if the judgment is affirmed on appeal; (2) NL Chemical's suit against United Catalysts on printing ink viscosity enhancers; (3) Monsanto's world-wide battle against Stauffer Chemical on herbicides (Roundup versus Touchdown, Monsanto recently won in Japan); (4) Merck's fight against Mylan (indomethocin for arthritis); and (5) GE's battle with Mitsubishi on its modified polyphenylene oxide patent in Japan. These are also only tips of the iceberg.

DuPont's suit to block Allied Signal's Petra line of thermoplastic polyester resins and its victory against Phillips on melt-processable ethylene copolymer resins further indicate DuPont's strong strategic use of the patent laws.

The stronger and more dependable patent system is partly responsible for the increased R&D spending of chemical manufacturers -- 5% increase to $9.3 billion versus only a 2% increase last year. This compares to a mere 1.9% for all businesses (percentages adjusted for inflation).

Research Corporation Reorganizes -- Becomes More Involved in Commercialization

The granddaddy of university invention management organizations has transferred its technology development and licensing activities to a new company, Research Corporation Technologies. The new company has taken over the agreements to evaluate, patent and license the inventions of 300 universities and will expand into new activities. These new activities include investing in and assisting new companies to exploit inventions and joining with state economic development groups and private investors to develop technology.

AUZVILLE JACKSON, JR.

desperately needed—is in external relations. Argonne had a fortress mentality."

There is an extremely unlikely possibility that the Administration could decide that the national labs should follow the AEC into oblivion. Otherwise the omens for Argonne look favorable. A DOE press release on the change in contract says that DOE will extend its contract with Argonne and that its Chicago operations office "will negotiate the expected five year contract."

A DOE veteran knowledgeable about the national labs review says the perception at DOE that Argonne "was quietly going to seed," has changed and that the recent contract action is "tangible evidence of greatly increased confidence in Argonne and Argonne's future" at DOE.

—JOHN WALSH

"Sclerosis" Blamed for Economic Stagnation

Democracies may be choked by the special interest groups they foster, Mancur Olson says

"Economic sclerosis" is the term University of Maryland economist Mancur Olson uses in describing the rigidity that afflicts American enterprise in the latter 20th century. With support from the National Science Foundation (NSF), Olson has written a new book, *The Rise and Decline of Nations*,* that boldly claims to explain how this economic disease grows and why it is likely to attack any democratic society that remains stable and affluent.

His theory, in the words of one NSF staffer familiar with it, is "big-think economics, as opposed to the kind of work we usually sponsor, which is full of equations." The new book has been criticized for its lack of "hard data crunching" or empirical research. Yet it has sparked interest because of its breadth and plausibility.

Olson's theory works as follows. In societies that permit free trade and free organization, coalitions will form around marketable goods and services. Groups of producers, like those who grow wheat or own oil, will organize to protect their assets and, if possible, boost profits by raising prices. Physicians and lawyers do much the same in joining professional societies. Labor unions organize workers to bargain for wages.

In the early stages of this coalition-building process, there are relatively few interest groups, and their memberships are small compared to the society in which they operate. As they develop, they try to impose a variety of specialized rules on the economy that supports them. By law or collusive contract, they make penalties for those who would market the same goods or services outside the group. They also offer selective advantages to those who join and cooperate. Because these groups are small (Olson says they typically include no more than 1 percent of the people in their state), they have no incentive to boost members' welfare by boosting the state's welfare. Instead, they concentrate on promoting their own narrow interests, even at the cost of retarding the general economy. A modest effort at self-aggrandizement may bring great rewards.

As time goes by, tariffs, price supports, monopoly prices, wage guarantees, and business codes grow more numerous. All are intended to channel commerce into areas that benefit the special groups that fought for them. The combined effect is to create obstacles to trade and to prevent innovation. The economy suffers. In the past, nations suffering from this affliction have enjoyed renewed growth after a cataclysm has intervened to wipe out existing trade barriers, or when new territory has been opened for development. Sometimes the power of a domestic group is undercut by low-cost imports, if the imports are not blocked. Rarely has any nation abolished special interest codes voluntarily.



Mancur Olson

Olson's theory has something to say about inflation and business cycles, as well. Inflation may be a common symptom of nations in a sclerotic condition, Olson believes, because it offers a brief measure of relief from economic stagnation. Special interest groups, being run by committee rule, generally maneuver slowly. For this reason, they cannot always adjust their demands upward as rapidly as the nominal value of goods and services increases. This is particularly true if inflation appears suddenly, without warning. Thus inflation may be tolerated because it temporarily devalues the cost of products within the control of special interests. In time, this form of relief fails because the special interests soon catch up and raise their demands in pace with inflation.

In the contrary case, during periods of sudden price decline, the advantage held by interest groups is intensified. Those who operate outside the protection of a group may be forced to lower prices or wages. But the interest groups, again moving slowly, haggle over proposals while the storm rages around them. They may not reduce their demands until a recession has already damaged the economy. After a period of negotiation, they may begin to adjust, but by then investment in new projects will have been cut short, worsening the prospects for recovery. Thus Olson sees a real risk that the inflexibility of special interest groups can lead in bad times to a "vicious downward spiral."

It would be difficult to prove this thesis with numerical data, simply because the volume of information required would be overwhelming. Thus Olson cites several broad historical economic trends as evidence of its validity. His chief example of a democracy that has survived without invasion, revolution, or

**The Rise and Decline of Nations: Economic Growth, Stagflation, and Social Rigidities* (Yale University Press, New Haven, Conn., 1982.)

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dictatorship is Britain. He writes that Britain harbors "precisely the powerful network of special interest organizations that the argument developed here would lead us to expect in a country with its record of military security and democratic stability." Today Britain has one of the lowest economic growth rates among all the democracies, despite the fact that from the middle of the 18th to the middle of the 19th centuries it had one of the fastest rates of growth. This is due, Olson believes, to the gradual accumulation of special interest organizations that inhibit growth. The "British disease," he says, will afflict any democracy that remains stable for a long period.

Looking at the rest of Europe, Olson finds positive evidence that social disruption and reorganization may encourage growth. He reports a colleague's finding that 51 percent of the associations existing in the United Kingdom in 1971 had been founded before 1939. Only 37 percent of the French, 24 percent of the West German, and 19 percent of the Japanese organizations existed before the war. Postwar economic growth in the latter three nations has been described as a "miracle," Olson notes. He argues that it is due to the elimination of long-established privileges held before the war by unions and business groups.

A student of Olson's also made an analysis of growth patterns in the United States. He found that those settled later, primarily western states, had a higher average growth rate than those settled early in U.S. history. In addition, states belonging to the Confederacy, which experienced a social cataclysm during the Civil War, have had a higher growth rate since the war than those on the winning side. Olson attributes this to the destruction of special interest groups in the South.

In a third analysis, Olson looked at towns in England and Europe to see how they fared over two centuries. He found that, except in the case of national capitals, the towns that were the largest and wealthiest in 1600 ceded rank to new towns that rose rapidly to the top by 1800. In England, the third-ranked town, York, fell to 17th place in this period, while Manchester, Liverpool, and Birmingham rose from obscurity to second, third, and fourth rank. Olson believes their success was chiefly due to the relative freedom from the oppressive business codes of the guilds. For the most part, he argues, the guilds retarded the growth of the prosperous towns where they had the greatest influence.

If Olson's theory of economic sclerosis is correct, what does it imply for government policy-makers? Olson says that some readers thought he might be advocating revolution or dictatorship as a means to higher national productivity. This is not the case. Olson's policy recommendations are mild and, by his own description, unoriginal. The most important is that the government should maintain an "open and competitive environment." He writes that "If the government is always intervening on behalf of special interests, there is no macroeconomic policy that can put things right." It would be an accomplishment simply to refrain from adopting new tariffs and subsidies. In an ideal world, existing special interest legislation might be repealed.

Second, Olson makes the commonsense recommendation that countries fighting inflation should apply controls, such as constraints on money supply, in a steady and gradual fashion rather than in sharp bursts. Olson mentions the case of a Danish cartel that waited 10 years to change its prices, even though it was losing profits throughout the period. Government policy must demonstrate resolve if it is to budge slow-moving interest groups.

Third, during times of "unnaturally high" unemployment, Olson suggests the government should offer temporary rewards to companies that raise wages slowly. This might encourage employers to spend available cash on hiring new workers, he says, rather than on raising the pay of those already employed.

Perhaps the most frequent criticism of Olson's work is that there are many other plausible explanations of the trends he cites. Consider the example of the recent boom in the nations defeated in the second world war. A former colleague of Olson's at Maryland, Robin Marris, argued that this spurt of growth actually reflected something he called "catch-up": the rapid rebuilding of industry with the most advanced technology. The absence of interest groups was less important, in Marris' view.

Olson agrees that many factors other than the degree of interest group sclerosis affect economic performance. He concedes that more empirical research is needed if his ideas are to gain acceptance. But he also believes that his thesis has an advantage over most others. "The strongest argument in its favor," he says, "is that it is a simple theory that explains so very much. It is supported not so much by one piece of evidence as by the variety of evidence." Few economists dare to generalize as broadly as Olson, and this boldness is what makes his work intriguing.—ELIOT MARSHALL

Legislation Would Take Program Away from NCI

The House Appropriations Committee has passed a proposal to transfer funding responsibility for an important international program on toxic chemicals from the National Cancer Institute to the office of the director of the National Institutes of Health. Representative David Obey (D–Wisc.) sponsored the measure, citing, in his opinion, inappropriate behavior by the NCI. Institute officials allegedly pressured the international program not to publish controversial data on benzene after they met with industry representatives (*Science*, 3 September, p. 914). Institute and program officials deny any improper actions.

The program is conducted by the World Health Organization's International Agency for Research on Cancer (IARC) and evaluates the carcinogenicity of chemicals. Many governments regulate chemicals based on conclusions reported in IARC monographs. The controversy over benzene arose when IARC for the first time ventured into the area of quantitative risk assessment, estimating how much risk is associated with certain levels of exposure.

The NCI now contributes about $500,000 annually to the monograph program's budget of $700,000. The legislation to shift the program's funding is part of a House appropriations bill that is expected to be voted on when Congress returns from recess.

—Marjorie Sun

Genex Raises $19 Million from Stock Offering

The Genex Corporation took a gamble on the Stock Exchange on 29 September and it came out reasonably well. At a time when new issues in general and biotechnology stocks in particular are supposed to be out of favor, the Rockville, Maryland, company raised $19 million from its first public stock offering. Its offering sold out on the first day, but its share prices have since declined.

One of the largest biotechnology companies to start up in the past few

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Norm LATKER - SOME INFO ON MDL.

Molecular Connection

November 1987

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MOLECULAR DESIGN LIMITED ENTERS MERGER AGREEMENT

Steven Goldby

Last month Molecular Design Limited merged with Pergamon Holding Corporation, part of a multi-billion-dollar, U.K.-based group.

Molecular Design Limited's Corporate Mission remains the same: To be the leading software firm serving the needs of the world's chemical and pharmaceutical industries for management and communication of chemical research information.

Our company will realize several advantages from this merger. For one, Molecular Design Limited will now have the stability and financial resource to achieve its goals faster. For another, because Pergamon is a leader in several aspects of information and communication worldwide, the synergy between the two organizations will enable us to apply our technology to related fields.

Molecular Design Limited will remain the same in all important ways; it will consist of the same people in the same place with the same policies. Our customers will notice no change in our policies as a result of the merger. However, customers can now rest assured that Molecular Design Limited will continue to respond to their information management needs for many years to come.

Following is an article that appeared on the front page of the financial section of London's *The Times* on October 5, 1987.

Pergamon in 37m US buy
By Our City Staff

Mr. Robert Maxwell's privately controlled Pergamon empire is paying £36.8 million for an American computer software business. Molecular Design of San Leandro, California, will form part of Mr. Maxwell's electronic publishing operations which he plans to inject into his quoted flagship, the British Printing and Communication Corporation, later this year.

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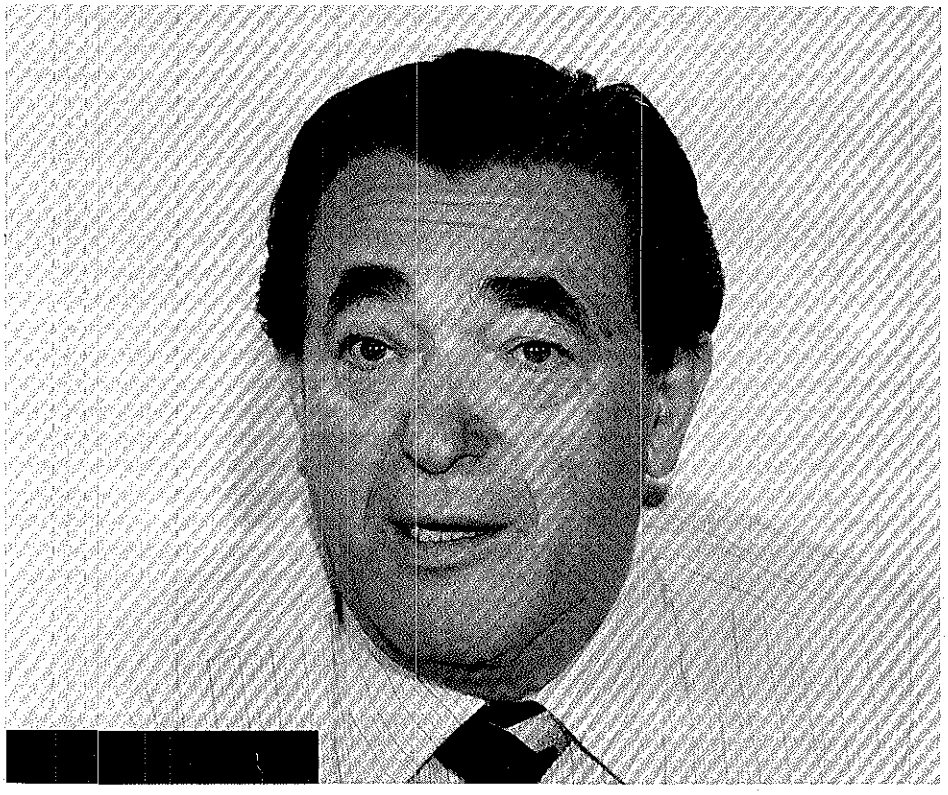

Mr. Robert Maxwell, illustrious head of the international Pergamon printing and communications empire, which now includes Molecular Design Limited.

CPSS AND THE IBM PS/2 SERIES

Peter Cohan

With the release of IBM's new Personal System 2 (PS/2) line of personal computers (PC's), a question arose in the minds of many chemists: Will Molecular Design Limited's Chemist's Personal Software Series™ (CPSS) run on PS/2 computers? The answer is yes.

In line with our commitment to keep our software abreast of hardware technology trends, Molecular Design Limited is currently arranging to have all four computers of the new PS/2 line — models 30, 50, 60 and 80 — in-house; some models have already arrived. Currently, all three of the CPSS version 1.1 PC programs can be used on all four of the new IBM computers.

A big change between the older PC's and the new PS/2's is that the latter uses 3½ inch diskettes rather than the older 5¼ inch diskettes. The PS/2 model 30 computer reads and writes 720 KB 3½ inch diskettes, while the 50, 60 and 80 models will read and write either 720 KB or a 1.44 MB 3½ inch diskettes. The CPSS programs are currently available on 720 KB 3½ inch diskettes for use with all four of the PS/2's.

Another feature of the new PS/2's is a mouse that is an integral part of the system, freeing up one of the I/O ports for other uses. CPSS version 1.1 fully supports this mouse.

As for the graphics, CPSS 1.1 supports EGA in either color or shades of gray (depending on the terminal) for the three models that offer EGA, models 50, 60 and 80. It also supports CGA (in shades of gray only) on all four PS/2 models. CPSS does not currently support VGA; Molecular Design Limited is investigating supporting VGA in future CPSS releases.

Finally, Molecular Design Limited will work on making CPSS compatible with the soon-to-be-released, new IBM operating system, OS/2, as soon as it is available.

So, for those of you with an eye on one of the new IBM computers, do not worry. You will still be able to use your trusty CPSS programs! □

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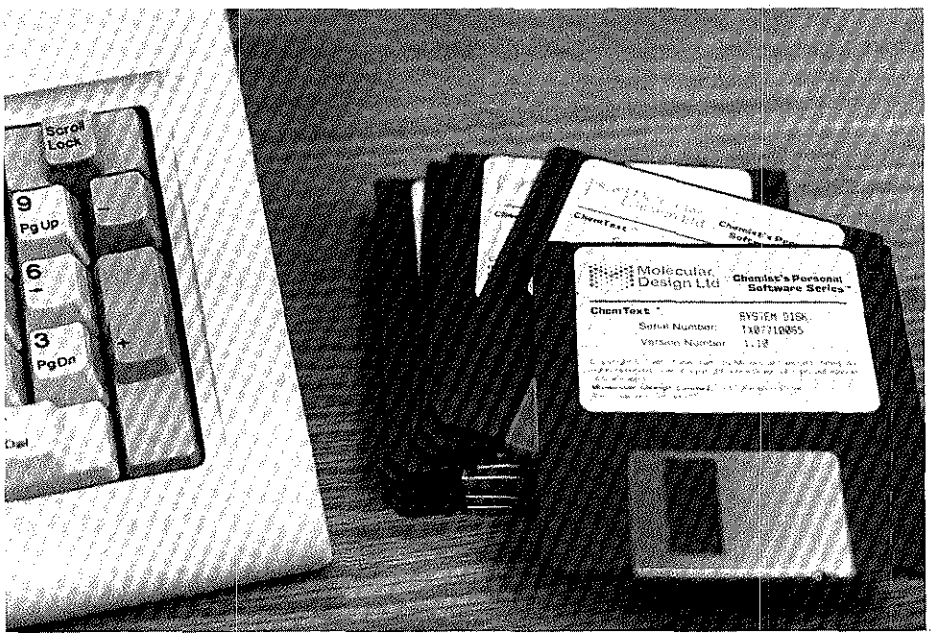

Molecular Design Limited provides CPSS 1.1 programs on 3½ inch diskettes for use with microcomputers that have 3½ inch disk drives.

TWO NEW STRATEGIC RELATIONSHIPS

Steven Goldby

Molecular Design Limited's policy has always been to work closely with suppliers of complementary products to ensure state-of-the-art software capable of integration with a variety of pertinent applications. Two new corporate agreements — one with International Business Machines Corporation (IBM) and one with Chemical Design Limited — are the most recent examples of this strategy.

In July, Molecular Design Limited and IBM announced a strategic relationship to develop jointly an integrated system and application environment for managing and communicating chemical information. Under IBM's Industry Marketing Assistance Program (IMAP), Molecular Design Limited will also assist IBM in marketing and installing the IBM systems and related software.

As provided by the joint development agreement, Molecular Design Limited is enhancing the performance of its software applications on the IBM System/370 line. We at Molecular Design Limited are working towards integrating our applications with IBM applications and system software to support a system environment for chemical information management. IBM is providing us with computer systems, workstations and technical assistance for the joint effort.

IBM's new 9370 super minicomputer and Personal System/2 workstation lines are ideally suited to Molecular Design Limited's marketplace. Our applications software combined with IBM's products will provide a fine-tuned, full-featured solution to our customers.

Under the IMAP program, IBM draws on industry knowledge and application marketing capability of

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NEW FEATURES IN REACCS 7.0

Kevin Cronin

This month, the REACCS product team released a new version of REACCS, REACCS version 7.0, with several new features that simplify and extend the program's reaction searching capabilities. Many of these enhancements had been suggested by the REACCS user community.

The most significant new features of REACCS 7.0 are Atom-to-Atom Mapping and Automatic Reacting Center Perception; these simplify and increase the accuracy of reaction substructure searching by establishing a one-to-one correspondence between atoms in reactants and products. To utilize the new capabilities of this release, all Molecular Design Limited reaction databases have been atom-atom mapped.

Other REACCS 7.0 enhancements include Automatic Searching of Multiple Databases, Menu-driven Data Searching, and a Graphical Form Editor. With the form editor, the chemist can create customized forms for data display on a graphics terminal, allowing different work groups to display specific data relevant to their research in easily interpretable formats (Figure 1).

REACCS 7.0 is compatible with ChemBase™, allowing chemists to exchange easily reactions and data between the two programs.

These new capabilities, and other enhancements not mentioned here, will make REACCS an easier-to-use, more powerful tool for research chemists. For more information, contact Peter Cohan at the San Leandro office. □

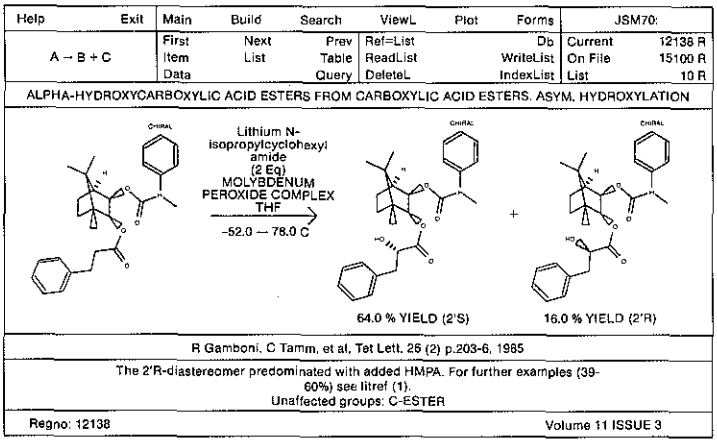


Figure 1: The above "hit" is from a search for the α-hydroxylation of carboxylic acid esters. It displays the results in a user-edited form, built with the form editor, a new feature of REACCS 7.0. Using this feature, users can customize forms to display data according to personal or group preferences. This reaction demonstrates the ability of REACCS to recognize and distinguish absolute stereochemistry.

WELCOME TO NEW CUSTOMERS

Tom Jones

Once again, new customers have joined the growing ranks of Molecular Design Limited software users. Below is a list of just some of our many new customers, all of whom we wish to welcome.

The University of Mississippi: The University's School of Pharmacy has recently licensed MACCS-II, REACCS, and the Fine Chemicals Directory, Current Literature File and Theilheimer databases. The software will be run on a MicroVAX II. REACCS and associated databases will be used by medicinal chemists to establish synthetic routes to potential new drugs or to improve existing syntheses. Pharmacognosists will use REACCS to select reactions for functional group modification in biologically active natural products. All scientists in medicinal chemistry, pharmacology, pharmacognosy, and pharmaceutics will use MACCS-II to catalogue their research. MACCS-II will also be used by the school for inventory of hazardous chemicals used there.

DevTech B.V.: The Dutch material science company, DevTech B.V., has licensed a full line of Molecular Design Limited mini/mainframe software for use in a VAX environment. To aid its research in the properties of materials, it licensed MACCS-II and the Customization Module, REACCS and all of the REACCS databases, and ADAPT with COMPDS.

Sigma Tau: One of the largest research sites in Italy, the pharmaceutical company Sigma Tau is Molecular Design Limited's first Italian customer. Sigma Tau licensed REACCS with several databases, including Theilheimer, JSM, CLF and ORGSYN, for use on a MicroVAX 2000. It also licensed all of the Chemist's Personal Software Series™ (CPSS) products; it plans to use ChemBase™ as a front end to REACCS via ChemTalk™/ ChemHost™, thus reducing interactive time on the host computer.

Glaxo, BASF and Penwalt: See the article, "Three Companies Standardize with Molecular Design Limited Software," on page 9. □

INTEGRATING DATA FROM ANALYTICAL INSTRUMENTS INTO CHEMTEXT™

Joseph F. Donahue

One of the many exciting ChemText™ applications is the incorporation of graphics from a variety of sources into reports and posters, thereby avoiding the "cut-and-paste" technique. ChemText documents can incorporate graphics and/or data from several other programs, such as Chem-X, Lotus 1-2-3, AutoCad, SAS, and RS/1. In addition, ChemText documents can incorporate spectra from analytical instrumentation. There are many different ways that spectra can be transferred from a laboratory instrument to ChemText on a personal computer (PC), and some transfers are easier than others. The method of choice depends upon the laboratory's hardware and software environment. This article examines some situations and gives a few hints on how to accomplish the transfer easily.

The most common scenario is a stand-alone instrument, such as an NMR, IR, or HPLC, that does not use a personal computer as a controller. First, it must be confirmed that the instrument supports Hewlett-Packard Graphics Language (HPGL), *i.e.*, that it can plot to a Hewlett-Packard (HP) pen plotter. If it does, the procedure is fairly straightforward. To get the information to the PC the user should: 1) Connect the cable that would normally go to the plotter from an RS-232 serial port on the instrument to an RS-232 serial port on the PC. 2) Set up the PC so that it is ready to receive data; this is done using a terminal emulator such as ChemTalk™. 3) Once the emulator is started, set up its communication parameters — such as baud rate, stop bits, and parity — to match those of the instrument and place the emulator in the "terminal mode." (The information on the instrument's communication parameters is usually available from the manual or your service representative.) 4) Set up the emulator to do an ASCII file capture. 5) Plot your spectrum from the instrument as normal. Instead of the file being sent to an HP plotter, it will scroll across the PC screen and be saved to a file on the hard disk. (Figure 1)

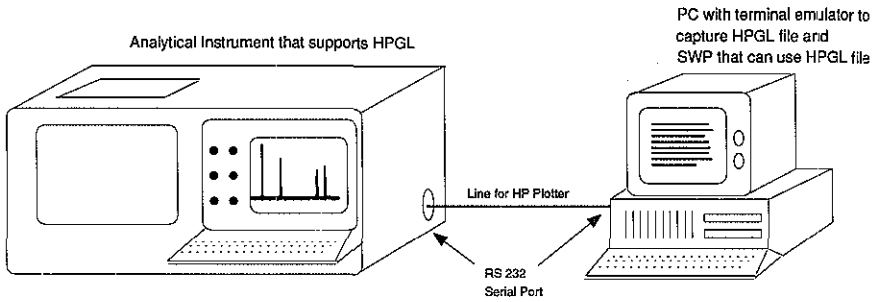


Figure 1. Example configuration to import graphics from instrument to PC.

Before importing graphics into ChemText, you must first convert them into a Molecular Design Limited metafile format, the format understood by ChemText (and other Molecular Design Limited programs). The FROMHPGL utility that comes with ChemText can be used to convert the HPGL file on the PC to this format. Once this is done, it is easy to read the graphic image into ChemText, via the USE METAFILE command in the main menu. Using a mouse, you can then easily resize the image, and/or append to it other information, including structures, arrows, and text.

At American Cyanamid in Princeton, New Jersey, chemists Bob Manfre and Leif Thompson have set up two instruments from which they can retrieve HPGL files. One is a Varian XL-300 NMR and the other is a Spectra Physics 8800 HPLC which stores its data on a Hewlett-Packard HP1000/3357 Laboratory Data System (LDS).

The hard-copy device attached to the Varian is a Nicolet Zeta8 pen plotter, but the Varian also supports the HP7475 pen plotter for output. To get the HPGL file to the PC, Manfre ran a 25-pin straight-through cable from the plotter port on the NMR to a serial port on his PC, started the terminal emulator, set it up to perform an ASCII file capture, and then "plotted" the spectrum from the NMR as he normally would had the HP plotter been connected. He converted the HPGL file, now on the PC, to a metafile, read it into ChemText for inclusion into a report, and modified it by inserting the chemical structure of salicylaldehyde and by indicating the proper chemical shift assignments (Figure 2). He then inserted the spectrum into a report.

To obtain output from the LDS, Thompson used system commands to save the HPGL file to a spooling file. He then transferred the file to the PC by using ChemTalk to capture the released file, or by using Xmodem (public domain software), which was installed on the LDS, to download it. The LDS was connected from a RS232 multiplexer port to a serial port on the PC with a 25-pin straight-through cable.

These examples illustrate how the HPGL files can be transferred from a stand-alone instrument to the PC. Of course, if a Laboratory Information Management System (LIMS), such as RLAB-II from Nelson Analytical, is running on a PC to control one or several instruments, then your HPGL files are already there. Adding ChemText and an Apple LaserWriter to the PC will allow output of analytical reports from the same workstation. If reports or posters are generated from another PC with ChemText, the HPGL file can be transferred via a diskette.

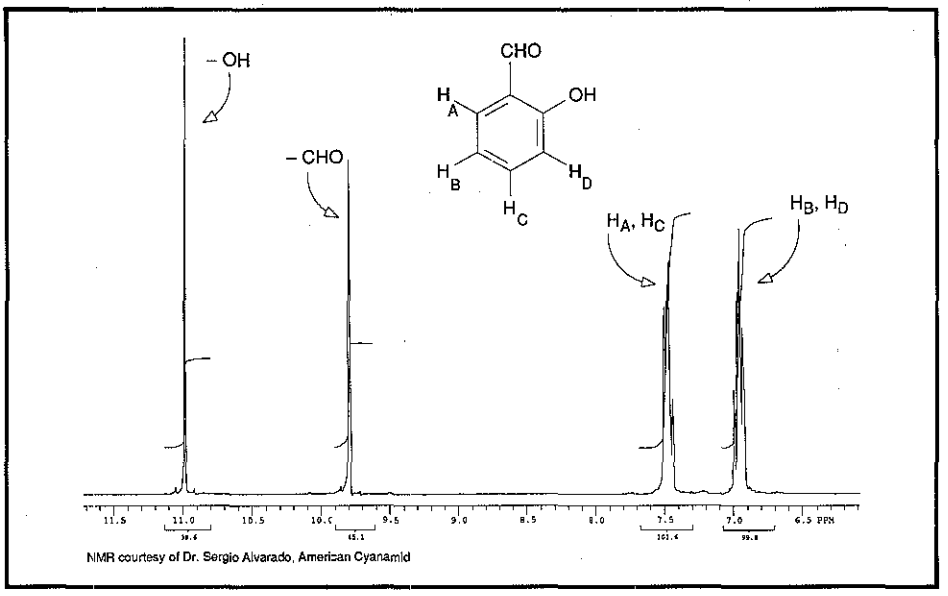
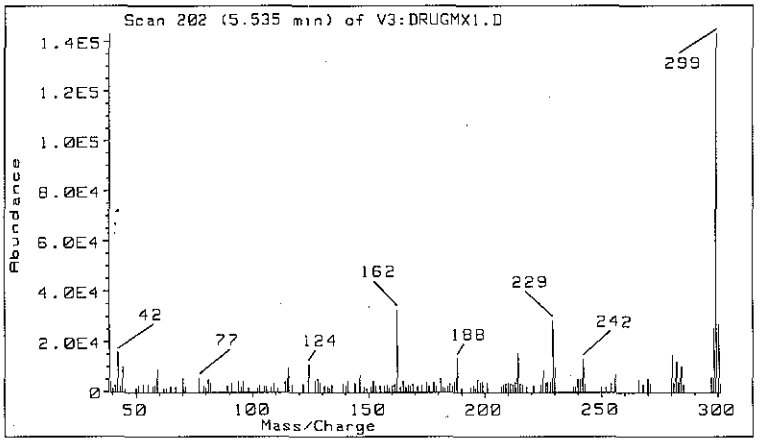


Figure 2. NMR file from Varian XL-300

The output of the spectrum from the analytical instrument...



and after it had been edited in ChemText.

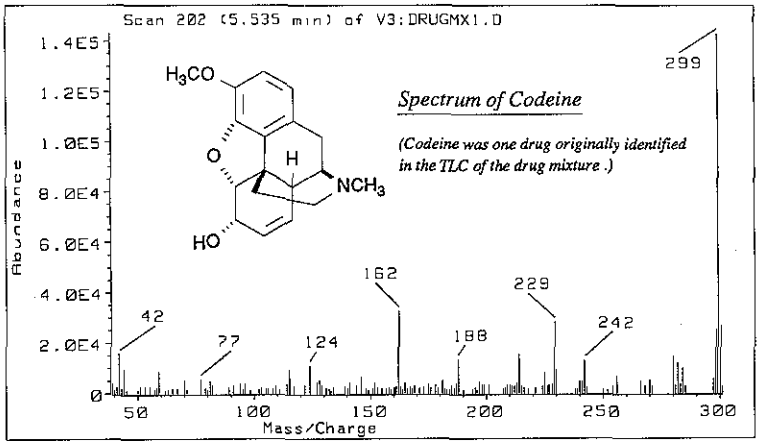


Figure 3.

Some analytical instrument workstations have the ability to output the spectra in a metafile format directly. A contributed program is available from Hewlett-Packard that converts HP ChemStation graphics into the Molecular Design Limited metafile format. The contributed program is a modified version of the MSD Data Editor revision 3.1 and is compatible with the MS, GC and LC (revisions 3.2 and earlier) software. The metafile could then be transferred over Ethernet to a PC, or to a host computer accessible to the PC. Figure 3 shows a scan of codeine from an HP 5890/5970 GC/MS which was linked to an HP9000 ChemStation, both as it appeared on the instrument, and after it was modified for insertion into a report.

In conclusion, ChemText is well suited for including modified analytical spectra into chemical reports, allowing scientists to prepare publication quality graphics easily, and also offering a means of electronic storage of analytical data. The best method of obtaining the data from the instrument depends on many variables, including the type of instrument, whether or not it supports HPGL, if it is controlled by a LIMS system on a personal or super-mini computer, and if it can communicate with a mainframe computer. If you have questions about the specific instruments/LIMS systems in your lab, call your Molecular Design Limited Chemist's Personal Software Series™ (CPSS) customer service representative or your local field support specialist. □

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A SMALL MACCS-II USER WITH A BIG JOB:

Maxima and the Army's Antiviral Drug Development Program

Lise M. Dumont

Because of the diversity of the industry we serve, it would not be easy to define the typical Molecular Design Limited software user. But, if one were to come to mind, it would not look anything like the MAXIMA Corporation.

It is not surprising that the MAXIMA Corporation does not fit the mold — amorphous as it is — of our typical customer; it is in essentially the same business as Molecular Design Limited — computerized information management. And, a division of the MAXIMA Corporation is in precisely the same business — computerized *chemical* information management. The difference is that Molecular Design Limited provides a product, and the MAXIMA Corporation provides a service using that product.

The Maxima Corporation has been managing information of all sorts with appropriate software systems for a variety of clients for ten years. Enter, in 1985, the United States Army Medical Research Institute of Infectious Disease (USAMRIID), a new client with very specific requirements. USAMRIID needed someone to manage all of its chemical and research information for its Cooperative Antiviral Drug Development Program (The Program). The MAXIMA Corporation responded by opening a new branch of its company devoted exclusively to this task. Hereinafter called MAXIMA for convenience, that branch, at its own site, now consists of ten full-time employees, a MicroVAX II, several personal computers (PC's), and a wide range of Molecular Design Limited Software, including MACCS-II, ChemTalk™/ChemHost™ and ChemBase™.

The Program is an interesting one. It fills a vital void in antiviral research by striving to develop effective antiviral agents against exotic RNA viruses that threaten military personnel worldwide. Examples are insect- and rodent-transmitted RNA viruses belonging to toga-, bunya- and arenaviridae. Though these and other viruses threaten the lives and well-being of scores of people in developing countries, commercial research to develop antiviral agents against them is sparse, since most pharmaceutical companies consider such a venture unprofitable. Thus, potentially promising agents against these diseases can be considered orphan drugs — drugs too costly to develop. The Program also seeks to develop antiviral agents against the AIDS virus, as it is a growing threat to the public in general and to military personnel in particular.

To achieve its goals, The Program works as a cooperation between public and private sectors. The public sectors are USAMRIID and other government agencies it collaborates with, such as the National Institute of Allergy and Infectious Disease and the National Cancer Institute The private sectors are contributing companies —which may be any pharmaceutical, biotechnology or chemical company with promising compounds — and extramural contractors who assist in various ways with the research, such as MAXIMA.

For the contributing companies, The Program can be immensely profitable. A participating company sends compounds of its choice to USAMRIID's Department of Antiviral Studies (The Department) for screening. The Department tests compounds *in vitro* for their action against a variety of viral-induced diseases. Promising compounds are then tested *in vivo* in infected mice and hamsters, and then in appropriate large animal species. When appropriate, USAMRIID can perform volunteer clinical studies and global field trials. If the Department identifies a promising compound, it will encourage the submitter to file a patent, to develop the drug, and to file an

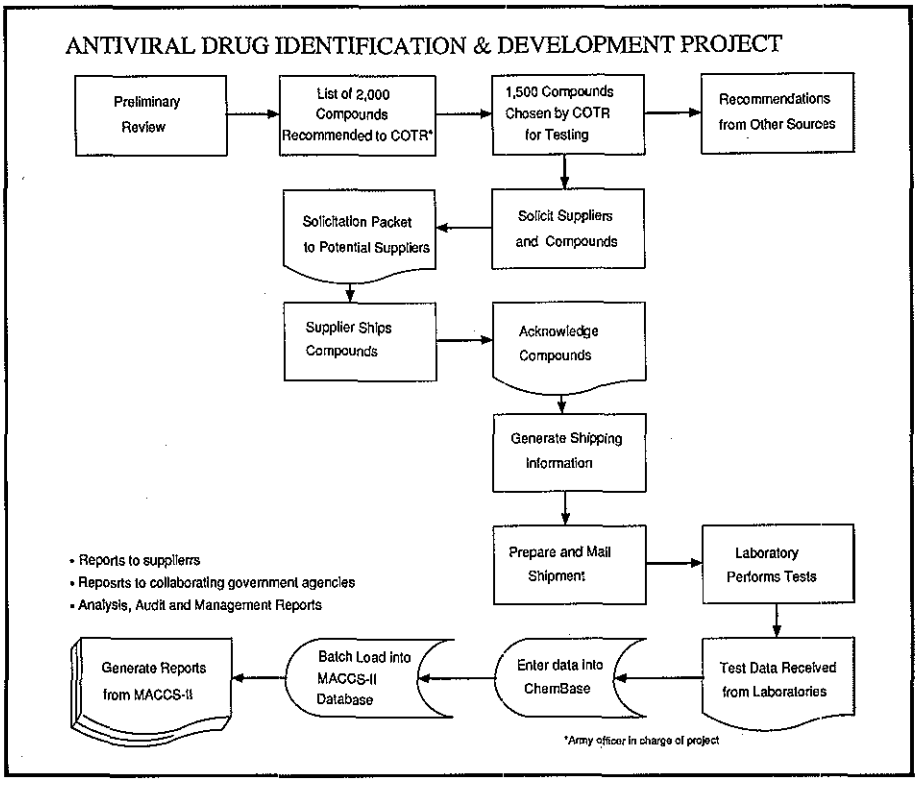

Figure 1.

Investigational New Drug application. The Department is prepared to undertake these tasks if the submitter is unwilling or unable. The whole process may lead to the submission of an FDA New Drug Application. "Thus, for its investment of compounds for screening and testing, the pharmaceutical company may reap the benefits of a fully approved, patented product that is ready to market."[1]

MAXIMA has the job of managing all of the research information for The Program. Considering the fact that USAMRIID each year selects 1500 candidates to study, and that information must flow readily between the many participants in The Program, this is no small task. But with MACCS-II and other Molecular Design Limited software, it is one they are able to handle smoothly and effectively.

Figure 1 presents an overview of how research information flows in The Program. All of the data are stored in MACCS-II, from the preliminary review data — which includes Structure Activity Relationship (SAR) determinations, to shipping information, to laboratory test data, to clinical test data. All reports are generated directly using MACCS-II and printed using a LaserWriter. Figure 2 presents in more detail the database requirements at one of the many different steps in the drug development process. Again, all data are stored in MACCS-II databases on the MicroVAX II, and all of the reports are generated directly from the databases using MACCS-II forms and a LaserWriter.

To minimize interactive time on the MicroVAX II during periods of peak load, all data is entered in ChemBase and then batch loaded to MACCS-II via ChemTalk/ChemHost in the evening. This method saves valuable time for the person doing data entry. Further, it helps MAXIMA to run smoothly the relatively large MACCS-II program on the relatively small CPU of a minicomputer. Also, since individual chemists keep personal databases in ChemBase, after an initial MACCS-II search, further searches are done over personal databases in ChemBase, again off-loading interactive time from the host computer. Another advantage of ChemTalk and ChemHost is that Army personnel, at their separate site, can access the MACCS-II databases with a modem, when necessary.

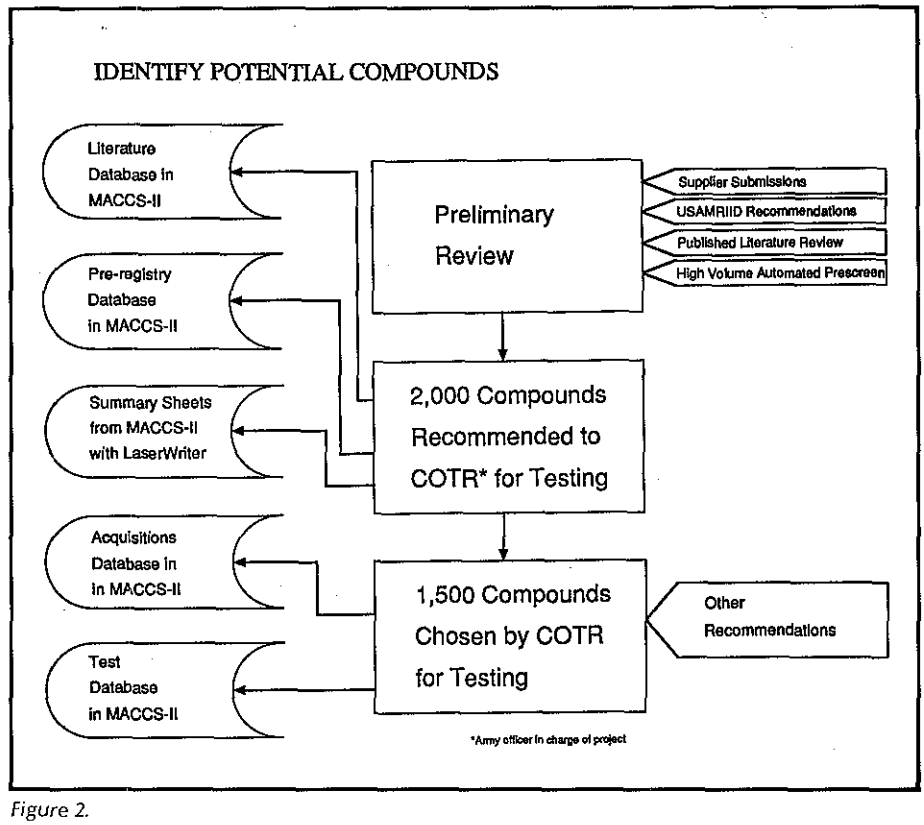

Figure 2.

In the future, MAXIMA plans to offer its services to whomever else may need them. It will provide requirements analyses to suggest optimum hardware/software configuration based on client needs. A client using MAXIMA services would not have to hire the personnel to create and maintain its databases; MAXIMA's experienced staff would do the job for them.

Anyone interested in MAXIMA's services or interested in participating in the Program as a contributing company, should contact:

Dr. Edward L. Stephen
Program Director
Antiviral Testing and Evaluation
The Maxima Corporation
P.O. Box 248
Monrovia, MD 21770. □

[1] From, "The Cooperative Antiviral Drug Development Program: An Interaction between Public and Private Sectors," a brochure distributed by the United States Army Medical Research Institute of Infectious Diseases.

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A CHEMBASE™ DATABASE AS A CHEMICAL CATALOGUE

Donna del Rey

Substructure searching capabilities of ChemBase™ allow a chemist to search a molecular database for a specific class of compound. Because it runs on a Personal Computer (PC), and thus can read and write to floppy diskettes, ChemBase can create and/or read portable databases. At Dr. Theador Schuchardt & Co., a subsidiary of the German company E. MERCK, Darmstadt, product managers recognized that these features of ChemBase make it an ideal means of providing an electronic, searchable catalogue to their customers. And that is just what they did.

The catalogue is called MS-CASS for MERCK-Schuchardt Computer Assisted Substructure Search. The company provides the database, which just fits on one high-density diskette, free to anyone who has ChemBase and wants to do substructure searches to find the needed reagent or group of reagents. Currently, there are 4000 reagents in MS-CASS. Each entry has a molecular structure, designation, catalogue number, molecular formula, molecular weight, package size(s), and price(s) in German marks. A bound catalogue sent with the diskette provides more detailed information (approximately 30 types of information) once the chemist has identified the compound needed. The company first announced MS-CASS in March of this year, and has since distributed more than 200 catalogues in Germany, France, Scandinavia, Belgium, the Netherlands, Switzerland, Italy and Spain.

The product manager of the MERCK-Schuchardt range (or division) that distributes MS-CASS at MERCK-Schuchardt, Dr. Schwoebel, calls the catalogue, "very successful. People really like to work with it." The advantage to chemists, of course, is that they can quickly locate a particular group of reagents without having to use ambiguous names or know exact formulas. ChemBase's substructure searching capabilities give the catalogue this significant advantage over bound catalogues. The advantage to MERCK-Schuchardt may be increased sales. Dr. Schwoebel says that, although the project is too young to provide definitive numbers, he thinks the people who have MS-CASS are ordering more MERCK-Schuchardt reagents than they did without the electronic catalogue.

It took three people, only one of them working on the project full-time, four months to complete the database. Twice a year an updated catalogue will be distributed. Dr. Schwoebel says that in the future he and his colleagues may add more fields to the database so that the catalogue will provide more information, e.g. applications of the reagents. But, for now, they are pleased with the response to the first released version of MS-CASS. □

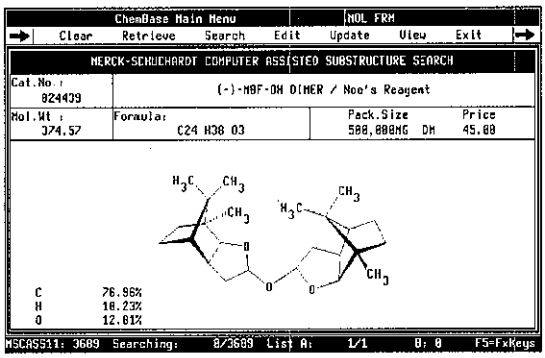

Figure 1: Noe's reagent, as it appears in MS-CASS, with stereo-chemistry indicated. This particular form shows the structure, the catalogue number, the molecular weight, the molecular formula, package size(s) and price(s) in German marks.

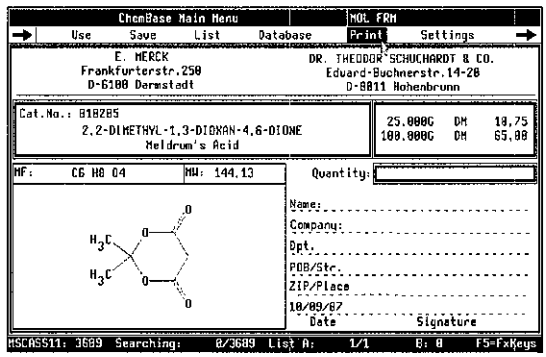

Figure 2: Meldrum's acid displayed using an order form created in ChemBase.

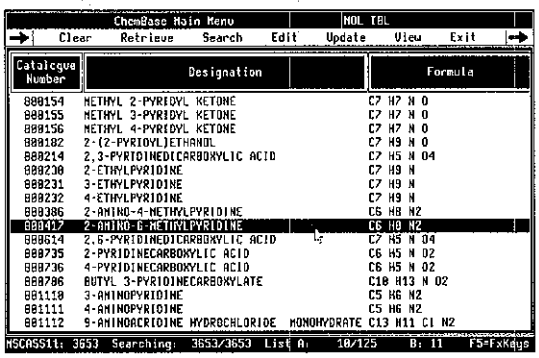

Figure 3: Using "View Table" in ChemBase, the user can view a list of MS-CASS entries in table form. This particular list of 125 pyridine containing compounds was generated by doing a substructure search for pyridine. The arrow is highlighting the tenth compound on the list.

THREE COMPANIES STANDARDIZE WITH MOLECULAR DESIGN LIMITED SOFTWARE

Marie Cornez

A trend is developing in the chemical and pharmaceutical industries. At the vanguard are the large international chemical company, BASF, the pharmaceutical company, Glaxo, and the pharmaceutical division of Pennwalt Corporation. All three are making a plenary effort to standardize — and thereby expedite and economize — the way their companies store, access and communicate their chemical, biological and associated information. At the hub of the movement is Molecular Design Limited's integrated software.

Each began its pursuit from a different foundation. BASF had been handling its chemical information with an in-house database system. The company had licensed some of Molecular Design Limited's software since 1985 at some of their sites for specific applications. Glaxo Holdings PLC in the United Kingdom and its U.S. subsidiary Glaxo, Inc. were handling their chemical information with an in-house information management program called CBIS — Chemical Biological Information System — designed and maintained at the U.K. site. The Rochester-based New York pharmaceutical division of Pennwalt Corporation was handling its biological and chemical information with, "separate computerized and paper systems," according to Dr. Ronald Griffith, who is responsible for implementing the new system there.

Each launched the undertaking by acquiring similar software resources; all three have licensed Molecular Design Limited's REACCS, MACCS-II, the Customization Module, the Database Interface Module (to Oracle), several databases, and all of the Chemist's Personal Software Series™ (CPSS) programs.

Currently being set up by Dr. Griffith and an interdepartmental team, the new system at Pennwalt will be, "an integrated chemical and biological information management system, based on Molecular Design Limited software and Oracle." The new system will consolidate all research data from the organic chemistry, analytical chemistry, and pharmacology departments. Most of the data will be stored in Oracle, with a linkage to the chemical structures in MACCS-II, a linkage made possible by the Database Interface Module. An important feature of the Pennwalt system is that, rather than establishing a separate data entry group, Pennwalt is developing "a sophisticated, automated data-entry system." Appropriate chemists in each laboratory will be able to enter either chemical or pharmacological data directly on specific forms which will be designed with the Customization Module. All laboratories will have "viewports" — *i.e.* Personal Computers (PC's) linked to Pennwalt's VAX 785 cluster via ChemTalk™/ChemHost™ — so that all of the Pennwalt's research scientists can access the data as they need it. Individual chemists will be able to keep personal databases in ChemBase™; these may include data downloaded from REACCS, MACCS-II or Oracle. Both chemists and secretaries will use ChemText™, fully integrated with the system, to generate reports, letters and other documents.

Glaxo is setting up a similar system at two distinct sites on both sides of the Atlantic. Glaxo's North Carolina site and Glaxo Group Research Ltd. in the U.K. have both licensed the Molecular Design Limited software listed above. A number of VAX 8700's will be used at both sites, all of which will be linked together to form an international system. The IBM PC AT with ChemTalk/ ChemHost will be the standard terminal in the U.S., allowing convenient communication between the mainframe and PC programs. In the U.K., a mixture of PC's and high quality graphics terminals will provide the workstation environment. Glaxo's new system will be arranged so that chemists will still use CBIS, now in conjunction with MACCS-II and Oracle.

Finally, BASF is creating a chemical and biological information management system along the same lines, but on an even larger scale. While Pennwalt is standardizing the flow of chemical and biological information among different departments at one site, and while Glaxo is doing the same among three different sites and their individual departments, BASF is standardizing the flow of relevant information at and among many of its sites around the world. The concept consists of combining the existing in-house information systems with Molecular Design Limited's Software. As at Pennwalt and Glaxo, individual chemists will use the PC programs to maintain and search personal databases; access or, where appropriate, enter information from or to REACCS, MACCS-II and/or Oracle; and create documents, which may include directly information from the other programs in the system, or from many other sources.

The advantage of a standardized, integrated system such as this one is that all of BASF's sites will be managing and communicating their chemical information — perhaps their most important corporate resource — in the same effective manner, allowing for the unimpeded flow of information throughout the company (except where the flow should, for proprietary reasons, and can, be impeded). R.P. Iden of BASF summarizes the benefit of its new system: "We realized we had to standardize the flow of chemical information to keep up with our scientists needs; a standardized chemical information management system will provide us a significant competitive advantage." □

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IBM and AT are registered trademarks of International Business Machines Corporation.

CPSS 1.1 ALLOWS FULL INTEGRATION

Andrew Walls

In September, the Chemist's Personal Software Series™ (CPSS) product team released the latest upgraded versions of ChemTalk™ and ChemBase™, completing the release of the fully integrated version 1.1 of CPSS.

With this version of CPSS, the three Personal Computer (PC) programs — ChemTalk, ChemBase and ChemText™ — reside in a single directory, substantially reducing disk space requirements. Further, all user files are stored in the same area, CPSS's "Clipboard," making file manipulation and transfer between applications easy.

Because the three programs are now integrated, a user can, for example, enter a molecule in a ChemBase database; the user can then move directly into ChemTalk (without first exiting to DOS) — where the molecule will already be on the screen — and send the molecule to a mini- or mainframe MACCS-II database; and/or the scientist can directly enter ChemText and include the molecule — again already on the screen — in a document (figure 1). After the user saves the molecule in any one of the programs, the file will appear on the clipboard of all three of the programs.

Other enhancements to the CPSS 1.1 release include easier access to pull-down menus, easier program installation, better organized documentation, and the option to use various mouse drivers for more generic support of mice. There are also several improvements specific to the individual programs. In addition, CPSS users now have the opportunity to access Molecular Design Limited's private network on the electronic bulletin board, The Source℠.

As with earlier CPSS releases, this fully integrated release of CPSS also communicates with MACCS-II and REACCS. Thus, Molecular Design Limited now provides a fully integrated line of software to the chemical and pharmaceutical industries. □

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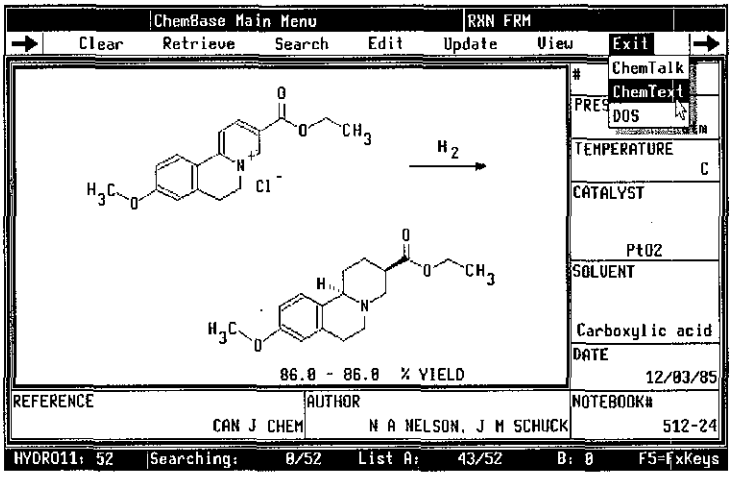
The Source is a registered servicemark of Source Telecomputing Corporation, a subsidiary of Reader's Digest Association, Inc.



This ChemBase screen shot illustrates the integration of the CPSS products. A scientist can exit directly from ChemBase to ChemText without first exiting to DOS. The image on the screeh, in this case a reaction and form, will automatically appear on the screen in ChemText. The image can then be inserted in a document as is or with some ChemText enhancements. The image may also be saved in a directory common to all of the CPSS programs.

MERGER AGREEMENT

Continued

Molecular Design provides computer programmes widely used in chemical research by blue-chip clients such as ICI, Glaxo, Dupont, Kodak and Hoechst.

It supplies up-to-date information about research into a particular area. Pergamon said yesterday: "It enables engineers to study the structure and properties of new compounds without actually having to expensively synthesize them in the laboratory, thereby reducing the time and money spent on synthesizing and testing endless numbers of compounds."

Molecular Design employs 130 people, 35 of whom are PhDs in chemistry or computer sciences.

The acquisition is a natural fit for Mr. Maxwell's US-based Pergamon Orbit Infoline operation which supplies information on patents, chemistry, physics, and engineering.

Pergamon Orbit Infoline and Molecular Design, together with various text and reference book publishing businesses, will be acquired by BPCC later this year. The price to be paid Pergamon will be established by independent valuation and approval by BPCC shareholders.

Mr. Maxwell said last night: "The purchase of Molecular Design reinforces the group's strategy to exploit the new dimension of growth afforded by electronic publishing and worldwide on-line services for its customers". □

TRIVIA QUESTION

During the first nine months of 1987, how many copies of ChemText were sold?

(Answer on page 11).

GOOD PEOPLE, GOOD CHEMISTRY

Lise M. Dumont

Dr. Ronald Griffith, Pennwalt Corporation
Dr. Ronald Griffith, formerly head of central nervous system research at the Pharmaceutical Division of Pennwalt Corporation, has been promoted to director of the organic chemistry department. Dr. Griffith has been with Pennwalt for 13 years. In his former position, among other things, Dr. Griffith oversaw the department's molecular modeling system. Now he is responsible for all of medicinal chemistry and process development research. In addition, Dr. Griffith is leading an inter-departmental team engaged in building an integrated chemical and biological information management system based on Molecular Design Limited software (see, "Three Companies Standardize with Molecular Design Limited Software," p. 9).

Dr. Pat Mize, Becton Dickinson
Dr. Pat Mize has been promoted to project leader of the group studying protein/polymer interactions at Becton Dickinson, where he has been a research scientist since 1984. While a research scientist, Dr. Mize used CHEMLAB-II and REACCS to do QSAR studies to help him make novel inhibitors and substrates for enzymes. Using these new compounds, he and his group were able to design cascade enzyme amplification systems, and then design immunoassays for herpes and adenoviruses that his company claims are the most sensitive to date. His new mission is to understand the interactions between proteins, such as antibodies, and the polymers to which they bind during an immunoassay. Along with a variety of molecular modeling software and REACCS, Dr. Mize will also use the Chemist's Personal Software Series™ (CPSS) programs to aid in his research. He says he has "totally converted to ChemText™ as a word processor"; he likes to use it not only to create documents, but also, "as a sketch pad to sketch out new ideas and concepts."

Molecular Design Limited congratulates Dr. Griffith and Dr. Mize on their new positions. □

TWO NEW STRATEGIC RELATIONSHIPS

Continued

selected firms to assist IBM in the marketing and installation of IBM products. As an IMAP participant, Molecular Design Limited will provide national support to IBM branch offices for complementary marketing of our computer-aided chemistry applications and IBM systems.

In August, Molecular Design Limited announced another important corporate agreement. At the meeting of the American Chemical Society in New Orleans, Molecular Design Limited and Chemical Design Limited, of Oxford, England, announced a new strategic alliance aimed at attaining closer links between our software for chemical information management and Chemical Design's software for molecular modeling.

Chemical Design leads the field of molecular modeling with more than 250 installations of its Chem-X software worldwide. Chem-X is used by both industrial and academic researchers in areas as diverse as pharmaceuticals and petro-chemicals, polymers and proteins Thus, its use is often complementary with the use of Molecular Design Limited's products MACCS-II and REACCS. The collaboration will result in a closer coupling of Chemical Design's modeling and Molecular Design Limited's database products. Cooperation in the area of 3-D databases is also likely.

Keith Davies, chief executive officer of Chemical Design, states, "Many of our customers have shown great interest in using Chem-X in conjunction with MACCS-II and REACCS." As a result of this new agreement, in the near future chemists will indeed be able to combine the power of Molecular Design Limited's and Chemical Design's software systems, thereby using each program to better advantage.

Both of these agreements are significant steps in Molecular Design Limited's continuing strategy of joining together with other important suppliers to the chemical research information community; they complement the company's existing strategic relationships with Digital, ISI and Oracle. □

IBM is a registered trademark of International Business Machines Corporation.
Digital is a trademark of Digital Equipment Corporation.
ISI is a registered trademark of the Institute for Scientific Information.
Oracle is a registered trademark of Oracle Corporation.

ANSWER TO TRIVIA QUESTION (p. 10): 660 copies. ChemText 1.0 was not actually released until March 31, 1987.

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Established in 1978, Molecular Design Limited is the industry leader in chemical information management with more than 200 installations to-date on VAX, IBM, and other super-minicomputers and mainframes. Its new microcomputer software products join a worldwide roster of widely accepted programs designed for chemical research management, design automation and communication.

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