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For further information contact:
Frank Koch
Syntex Corporation
Palo Alto, California 94304
415 327-0110
or
E. F. Rodgers
IBM Data Processing Division
White Plains, New York 10601
914 WHite Plains 9-1900

SYNTEX SCIENTISTS PROBE MEDICAL MYSTERY; USE COMPUTERS IN ADVANCED RESEARCH

PALO ALTO, Calif., May 26 . . . . Two computer systems at the Syntex Research Center here are helping to solve one of nature's toughest medical mysteries.

For more than 20 years, doctors have used chemical substances called steroids to treat conditions ranging from poison ivy to pregnancy problems. They know the way steroids affect the human body, but no one has yet fully discovered how steroids work.

Using an IBM 1800 data acquisition and control system, coupled with an IBM System/360, Syntex scientists are trying to find some of the answers.

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"Since 1944 Syntex chemists have synthesized more than 14, 000 steroids, each having its own complex molecular structure," said Dr. Robert A. Sparks, director of research information and data processing for Syntex. "A steroid's benefits and side effects are related to its structure. A computer can aid in correlating the structure of steroids with their biological activity. We believe that this correlation will help us synthesize new and better compounds.

"By combining the data acquisition capabilities of the 1800 with the processing power of a System/360 Model 50, we are attacking this problem with a greater chance of success than ever before possible," Dr. Sparks said.

Steroid compounds are necessary in many essential life processes. The body produces them naturally. They also are created synthetically in the laboratory. Examples of steroids include progesterone, which is necessary to maintain pregnancy, and cortisone, which can alleviate painful inflammation.

Syntex uses a variety of complex scientific instruments to determine the structure of steroid compounds. One of these, for example, measures X-rays diffracted through a single steroid crystal. The device -- called an X-ray diffractometer -- measures from 3, 000 to 4, 000 diffractions over a period of several days. Other instruments measure the wavelength and intensity of light absorbed by the compounds.

The 1800 system is capable of receiving signals simultaneously from these instruments, translating the data into computer code and transmitting it automatically to the System/360 for processing and storage on magnetic disks. This data will then be instantly available to researchers at typewriter-like IBM 2741 terminals in six laboratories at the Research Center.

The processed data will aid the researchers in the determination of the structure of new chemical compounds. A two-dimensional diagram of the structure can then be drawn on an electronic drawing board. The drawing board transmits the diagram directly to the 1800, where it is translated into computer code and relayed to the System/360 for future retrieval.

When a scientist wishes to identify a steroid structure which produces a specific effect in laboratory animals, he can ask the System/360 -- via his terminal -- for descriptions of all similar compounds previously analyzed. He also can ask the system to reject compounds showing additional undesired affects. In that way, it is possible to choose those structures for further investigation that show a maximum of desirable activity and a minimum of undesired affects.

This research could point the way to the development of more effective steroids than any available today. Syntex may find that a specific structural characteristic in a group of compounds is beneficial in treating a certain condition, while other characteristics cause undesirable side effects and should be eliminated.

"In the synthesis of new and more complex compounds, Syntex chemists rely on sophisticated analytical instrumentation," Dr. Sparks said. "I believe that within the next few years, computers such as the 1800 system will be more important than any single instrument now in use, primarily because they increase the usefulness of all other instruments.

"Syntex is one of the first pharmaceutical companies to tie such a wide variety of instruments to computers. But I feel that in the near future, most pharmaceutical firms, chemical companies, and university laboratories will adopt similar research techniques."

The System/360 Model 50 installed at Syntex is leased from IBM by Allen-Babcock Computing, Inc., a computer time-sharing firm headquartered in Los Angeles. Syntex currently uses six terminals. Other firms, some as far away as Los Angeles, Houston, and Boston, rent approximately 40 more terminals.

Syntex products include Synalar, used to treat inflammatory diseases of the skin, and Norinyl, an oral contraceptive.

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