From 3D Structure to Rational Drug Design
Shaping Biomedicine as an Information Science
Timothy Lenoir, Stanford University

Abstract
Sometime in the mid-1960s biology became an information science. While work in the genetic code by Watson and Crick, Jacob and Monod, Gamow, and others is usually credited with propelling biology into the Information Age, I intend to explore the transformation of biology by what have become essential tools to the practicing biochemist and molecular biologist: namely, the contributions of information technology. About the same time as Jacob and Monod work, developments in computer architectures and algorithms for generating models of chemical structure and simulations of chemical interactions were created that allowed computational experiments to interact with and draw together theory and laboratory experiment. Developments of computer graphics and computer-generated visualizations of numerical computations began to suggest a new form of scientific practice in which computer experiments would occupy equal status with...continued on next page

Chairman’s Message
Happy New Year! I trust the end of the millennium finds you happy and well. My name is Ean Warren and I am the new Chair for the Santa Clara Valley Section. We have a busy year ahead of us. In this first Chair’s Message, I would like to highlight some of the events occurring in the first half of the new year. By the time you receive this newsletter, the first event, the George Washington Carver Science Fair, will have been held on January 5th. On January 20th, we will have our first dinner meeting of the new year. After dinner, Dr. Timothy Lenoir will talk on Shaping Biology as an Information Science. As with all of our dinner meetings, you don’t have to attend the dinner to hear the lecture. In addition, you don’t need to be an ACS member; feel free to invite any of your family, friends, or colleagues to any of our events. February 17th’s dinner meeting will feature Dr. Sam Luoma of the U.S. Geological Survey and he will speak on the state of the San Francisco Bay. Be sure to look for the announcement on our web page or in our February newsletter.

Mark your calendar for March 26 to 30. The National meeting will be held in San Francisco, with the Carter KIDVENTION on March 25 and a...continued on next page
From 3D Structure to Rational Drug Design, continued from front page

both analysis and laboratory experiments—in which a separation between computer simulation and laboratory experiment would be increasingly difficult to draw. This paper will explore early developments associated with computational chemistry, including the introduction of computer modeling, applications of artificial intelligence, and visualization techniques in organic chemistry in the 1960s and ‘70s. Foci of interest will be the work of Cyrus Levinthal, Joshua Lederberg, EJ Corey and Todd Wipke. Alongside the heterogeneous and hybrid form of computer-based experimentation and theorizing evident in their work, I explore the notion that they were suggesting a different conception of theorizing itself, based on models of information-processing and best captured by the phrase “knowledge engineering.” I extrapolate a line of thinking from this early work which I argue is intensifying in the late 1990s, instanced in recent work in genomics through application of techniques from robotics, computational geometry and other fields to determining protein structure via experimentation “in silico.”

Biography

Timothy Lenoir is professor of history and chair of the Program in History and Philosophy of Science. Lenoir is the author of The Strategy of Life: Teleology and Mechanics in Nineteenth Century German Biology, Dordrecht and Boston: D. Reidel, 1982. Paperback edition by the University of Chicago Press, 1989, which examines the development of non-Darwinian theories of evolution, particularly in the German context during the nineteenth century. His other books include: Politik im Tempel der Wissenschaft: Forschung und Machtausübung im deutschen Kaiserreich, Frankfurt/Main: Campus Verlag, 1992; Instituting Science: The Cultural Production of Scientific Disciplines, Stanford: Stanford University Press, 1997, a volume which examines the formation of disciplines and the role of public institutions in the construction of scientific knowledge; an edited volume, Inscribing Science: Scientific Texts and the Materiality of Communication, Stanford: Stanford University Press, 1998. Lenoir is currently engaged in an investigation of the introduction of computers into biomedical research from the early 1960s through the 1990s, particularly the development of computer graphics, medical visualization technology, the development of virtual reality and its application in surgery. With funding from the Alfred P. Sloan Foundation, Lenoir is currently completing a web project on the history of human computer interaction. He will follow this project with a related effort to create a web-based archive for the history of genomics and bioinformatics. Lenoir has been a Fellow of the John Simon Guggenheim Foundation and twice a Fellow of the Institute for Advanced Studies in Berlin. He was named Peter Bing Fellow for Excellence in Teaching in 1998.

URGENT!

Scientists are needed on Capitol Hill. Things may be nutty up there, but it would be a lot worse if it were not for a dedicated group of Congressional Science Fellows. I promise you that a year on the Hill is an education. The application deadline is January 15, 2000. For details, go to:

http://www.aps.org

Happy Year 2000!
Editor’s Corner

Welcome, everyone, to the year 2000! During the next few months we will be starting an e-mail distribution of this newsletter. The e-mail version will be sent out about 3 weeks before you would normally get the hardcopy.

Come See Autumn Stanley on “Three Who Made a Difference: Women Inventors”

Sponsored: Women Chemists Committee
Speaker: Autumn Stanley, author of the book “Mothers and Daughters of Invention” (Rutgers University Press, 1993)

Stanley has published the definitive work on women inventors. Having researched this book for ten years, she terms her efforts “the ultimate in detective work.” She will discuss the inventions of Diane Pennica of Genentech Corp and other women inventors who have made major technical and scientific contributions.

In the introduction to her book she notes “...including women’s contributions will not merely revise but transform the history, and especially the prehistory, of technology. When technology is no longer just what men do, but what people do, both the definition of technology and the definition of significant technology must inevitably change.”

Date: Saturday, January 29, 2000
Time: 11:30 AM to 2:30 PM
Place: College of Notre Dame
1500 Ralston Avenue, Belmont, CA
Cost: Buffet Lunch $16 (Students or unemployed $8)
Reservations: Tracey Dunit (510) 848-0512
   e-mail calacs@sirius.com by January 24
Directions from the East Bay: West on Highway 92 (from San Mateo Bridge cross over Highway 101), take Ralston Avenue exit, turning left onto Ralston Avenue. Drive east about 2 miles to the College of Notre Dame entrance at 1500 Ralston Ave. Follow the WCC signs to the Dining Hall. Ralston Avenue is currently closed for construction at El Camino, so Highway 101 is not a good alternative. (www.cnd.edu)

Employment Help in Other Areas of California

The following are names and addresses of contacts in other California Sections. You may write to them or call to find out how to receive their job listings or how to place a job listing with them. Do not send self-addresses envelopes unless requested to do so.

California Section
Ms. Holly Kreuter
American Chemical Society, California Section
2140 Shattuck Avenue, Rm 1101
Berkeley, CA 94704
510-848-0512

California Los Padrmas Section
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Santa Barbara, CA 93106-9510
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Mojave Desert Section
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Naval Air Warfare Center, Code 4T42200D
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Orange County Section
Geoff Anderson, Hycor Biomedical
78272 Chapman Avenue
Garden Grove, CA 92641
714-895-9558
Ron Denedour
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Sacramento Section
John R. Bingham
809 W. Stadium Lane, Sacramento, CA 95209
916-927-7088
916-927-7006 FAX

San Diego Section
Renate Valois
619-260-4513
619-260-2211 FAX
email: pascal@acusd.edu

San Gorgonio Section
Valerie Barrett, Sunkist Growers
email: vbarrett@sunkistgrowers.com

Southern California Section
Send a self-addressed, 55 cent stamped business envelope to:
ACS job listing
14934 South Figueroa Street, Gardena, CA 90248
310-327-1216
email: office@scalacs.com

Welcome, everyone, to the year 2000! During the next few months we will be starting an e-mail distribution of this newsletter. The e-mail version will be sent out about 3 weeks before you would normally get the hardcopy.

Hopefully, this will make it easier for people to plan for our dinner meetings and other events. In addition, people who live outside of our territory will be able to get the announcements. Note that, since the Chemployment abstracts are a special service for our section members they will only be included in the hardcopy version of the Silicon Valley Chemist.
This year the National Chemistry Week was special. It was part of the International Chemistry Celebration. Our activities reflected our theme of colors and polymers. We presented posters that were colored by elementary school student and were placed on the SamTrans and CalTrain vehicles. Our thanks and appreciation goes to the schools and teachers listed on this page.

In Los Altos, we had the “Chemistry on the Soccer Field” program. The young players enjoyed making slime. The Santa Clara University and Stanford University student affiliates handled this activity in a wonderful manner, with their advisors Dr. Linda Brunauer and Dr. Jon Touster respectively. The event was so successful that our volunteers were approached by parents and teachers asking how they can do such activity in schools or at birthday parties. Dr. Bonnie Charpentier was also a major contributor to the success of this event.

Another activity took place at the Millbrae Library. This activity was a week long. Colored posters made by the elementary school student about chemistry were displayed in three poster windows in the library. Dr. George Fohlen and the high school students Science Club performed this event. The magazines, “Wonder of Science” and “ChemMatters” were distributed.

At the Tech Museum in San Jose, the San Jose State University Student Affiliate chapter and their advisors, Dr. Elaine Collins and Dr. Roger Terril put on a wonderful performance doing demonstrations. This event attracted many people both young and old.

The event took place over the span of two days.

We also received proclamations from the cities of Los Altos, Millbrae and Sunnyvale commemorating the occasion. Below, are the elementary schools and the teachers whose students participated in the posters coloring:

Cherry Chase Elementary School: Alice Pounds, Principal
Encinal School: Sharon Cottle, Charlene Mattos and Sheila Warren, Teachers
Laurel School: Carrie Bacci, Jerian Hirsch and Cathleen O’Conner, Teachers
Ms. Linda Brezinski also provided us with posters colored by Ms. Carla Eaton’s class at Hayman’s School in Santa Clara.

We are very happy with all the National Chemistry Week’s events for this year. As you read above, we could not have been able to do all these activities without the dedication and assistance of all the volunteers mentioned above. I think this should be an inspiration for all the 3,300 members to volunteer their efforts to be able to raise the level of the Santa Clara Valley Section’s activity to the next level.

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LITERATURE SEARCHES
JANUARY 2000 NEWSLETTER TOPICS:

From 3D Structure to Rational Drug Design Shaping Biomedicine as an Information Science
Chairman’s Message
National Chemistry Week International Chemistry Celebration
Come See Autumn Stanley on “Three Who Made a Difference: Women Inventors”

Editor’s Corner
CHEMPSLOYMENT ABSTRACTS

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FUTURE MEETINGS

Feb 17 SCV Dinner Meeting  
Dr. Sam Luoma
Mar 29 Mosher Award Luncheon
Mar 26-31 National ACS Meeting
May 20 Art and Wine Festival and Exhibit

For the latest information, please visit the SCVACS Web Site: http://www.scvacs.org

CHEMPSLOYMENT ABSTRACTS

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