



Prescription for Maryland Progress  
in Biotechnology

**Rx: UMBI**



University of Maryland  
Biotechnology Institute

## UMBI Spin-Out Company Creates and Launches New Scientific Software to Aid in Drug Design

Using UMBI licensed intellectual property, VeraChem, LLC has created scientific software to provide expert users with tools for computer-aided drug discovery and molecular design. VeraChem's recent first sale, a pre-release version of Vconf, was followed by the September 8th launch of Vcharge, a new software product designed to compute molecular properties important in drug design.

Vcharge combines speed and accuracy in a unique software package available for use with Linux and Windows operating systems, and is the first in a series to bring advanced computational methods in an afford-

able and user-friendly format to experts in the pharmaceutical and biotechnology industries.

Dr. Mike Gilson, Chief Scientific Officer of VeraChem, LLC and Professor at UMBI's Center for Advanced Research in Biotechnology says, "Vcharge allows the designer to compute the atomic charges of a candidate drug molecule as a step in determining whether it will effectively bind a targeted protein. Most drugs work by binding tightly to a targeted protein molecule. For example, HIV protease inhibitors help patients by binding and blocking the function of a protein that the AIDS virus needs to survive

and reproduce. Each atom of a protein carries a small electrical charge and, since opposite charges attract while like charges repel, it is important that the atoms of a drug molecule have charges which complement the targeted protein."

In addition to Vcharge, the entrepreneurs at VeraChem have developed a proprietary software toolkit with a range of functionalities, including ligand-protein docking and scoring, powerful conformational search of candidate drug molecules, and the computation of atomic energy forces.

The official launch of another new product, Vconf is expected in late fall 2004.

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### Points of Interest:

- IHV hosted Dr. Richard Klausner, the Executive Director of the Bill and Melinda Gates Foundation on September 21, 2004 in Baltimore. IHV and COMB have submitted a joint research proposal to the Gates Foundation focusing on AIDS vaccine delivery and stability.
- COMB faculty gave a keynote address, and staff earned best poster at the International Symposium on Fish Endocrinology in Spain.

## Chefs, Food Distributors, R&D, Sales and Marketing Executives Tour COMB To Learn of New Technologies in Aquaculture

More than 70 members of the Research Chefs Association (RCA) toured UMBI's Center of Marine Biotechnology (COMB) to learn more about scientific efforts to spawn and breed Maryland blue crabs, Mediterranean gilthead seabream, and other highly valued, marketable fish and shellfish. Attendees

learned of the latest research related to fish and crab hormones, oyster diseases, and aquaculture biofiltration. The food scientists saw technologies developed at COMB that allow fish and crabs to reproduce in a fully contained, recirculating, disease-free, environmentally-friendly system. This unique system facilitates

the spawning of fish year-round by precisely regulating light and water temperature to emulate different seasons. Captive-born fish grown in these tanks, often at extremely high densities, and using UMBI's patented technology, can reach market size in nearly one-half the time as those living in the wild.