# The Blue Ridge Chemist

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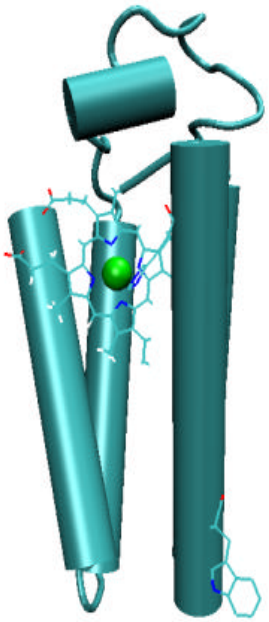

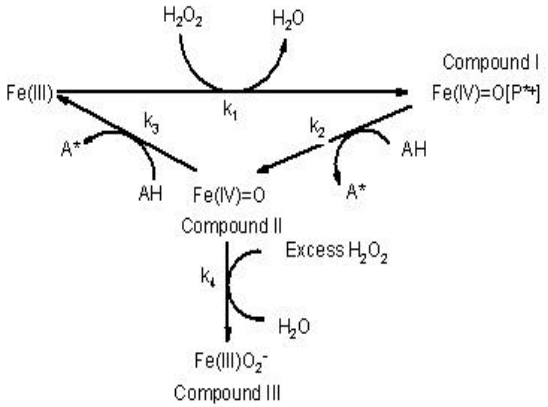


**"Tinker Toys for Big Boys:**
**The Design of Novel Catalytic Activities into Proteins"**

**Virginia Tech Hosts March Meeting**

**http:/membership.acs.org/v/vbr**

## VIRGINIA BLUE RIDGE SECTION
## AMERICAN CHEMICAL SOCIETY

### 591th SECTION MEETING

### Hosted by Virginia Tech

### Wednesday, March 23, 2005

### PROGRAM:

| | |
|---|---|
| 5:30-6:30 | Social Time, Owens Hall |
| 6:30-7:30 | Dinner, Ballroom, Owens Hall |
| 7:30-9:00 | Talk, Ballroom, Owens Hall |

The social time, dinner, and talk will take place in Owens Hall at Virginia Tech. Dr. Joel Gillespie will be speaking on "Tinker Toys for Big Boys: The Design of Novel Catalytic Activities into Proteins".

Dinner will be a served plate dinner consisting of mixed, tossed salad with choice of three dressings; entree (choose one -- need count in advance): chicken marsala *OR* fettucine primavera alfredo (vegetarian); glazed baby carrots; duchess potatoes, dinner rolls with butter, carrot cake; iced tea and hot tea; regular and decaf coffee; and water Cost for the dinner is $12.00, with students and retired ACS members half price.

Reservations WITH MEAL CHOICE for the dinner must be made by CLOSE OF BUSINESS TUESDAY, MARCH 16, EIGHT DAYS before the meeting, by contacting Paul Deck at pdeck@vt.edu or by phone (voice mail) 540-231-3493, or regular mail to 107 Davidson Hall, Blacksburg VA 24061

**Joel R. Gillespie**
**Virginia Bioinformatics Institute/ Virginia Tech**


Joel Gillespie received a bachelor's degree as a double major in Chemistry and Biology from Roanoke College in 1992. He subsequently obtained his Ph.D. in Biological Chemistry from the Johns Hopkins University School of Medicine in 1997 under the tutelage of David Shortle where he developed novel heteronuclear NMR techniques for examining the structure of denatured proteins. He performed postdoctoral research on the role of protein misfolding in primary amyloidosis while in the Department of Chemistry and Biochemistry at the University of California, Santa Cruz with Anthony Fink. In addition, Dr. Gillespie researched the mechanisms of ATP-induced allosteric control in eukaryotic chaperonins complexes using small angle X-ray scattering while a NIH fellow in the Department of Biological Sciences and the Geballe Laboratory for Advanced Materials (GLAM) at Stanford University. He joined the Virginia Bioinformatics Institute (VBI) as a Research Assistant Professor in 2002. Dr. Gillespie's research interests are in the areas of molecular recognition and biological self-assembly, with an emphasis on protein folding, protein design, and the role of protein misfolding in disease.



**"Tinker Toys for Big Boys:**
**The Design of Novel Catalytic Activities into Proteins"**

Most of the chemical reactions that take place in living organisms do not occur quickly enough under physiological conditions to sustain life. The architecture of enzymes has evolved over time to properly position and orient chemically reactive amino acid side chains or other reactive species in space, resulting in the enhancement of chemical reaction rates by many orders of magnitude while simultaneously incorporating extremely high regio- and stereo-specificity. To orient these groups proteins must adopt complex three-dimensional structures consisting of thousands or even tens of thousands of atoms. Amazingly, these collections of atoms can form complex protein structures within a matter of milliseconds without the expenditure of external energy! How these folding reactions occur remains one of the must fundamental of unanswered questions in modern molecular biology.

Here we will focus on how recent advances in computational and genetic engineering technology have made it possible to approach the protein folding problem from a different direction- by designing and engineering relatively simple protein sequences capable of folding into stable, well-defined three-dimensional structures. In addition to defining the structure of such proteins, it is now becoming possible to engineer specific catalytic activity into the protein chains, opening a broad and fascinating frontier for the rational design of enzymes to effect interesting chemistry in a variety of environments and with unique substrate specificities. Particular attention will be paid to the design of novel heme-peroxidase enzymes "tailor-made" to have use in industrial, environmental bioremediation, and nanotechnology applications. In addition, we will discuss how relatively weak inter- and intra-molecule forces can be indirectly manipulated to enhance the thermodynamic stability and catalytic activity of designed proteins using both computational and directed evolution techniques.

## Undergraduate/High School Poster Session

The Virginia Blue Ridge Section of the American Chemical Society is sponsoring the thirteenth Annual Undergraduate/High School Poster Session as a part of the April 20, 2005 meeting at Radford University. The posters will consist of an 8'(high) by 4'(wide) board.

If you have a student or students, who will be participating, submit the following information to Chris Hermann by April 1, 2005 via e-mail [chermann@radford.edu], by fax [540-831-6615], or by mail [Box 6949, Department of Chemistry and Physics, Radford University, Radford, VA 24142]. If you have any questions, call Chris Hermann at 540-831-5413 (office), 540-639-6705 (home), or 540-818-2431 (cell). All students and faculty will get e-mail confirmation.

Name of Project: _____

_____

_____

Name(s) of Student(s): _____

_____

Affiliation (name of high school, college, or university)

_____

Class of Student(s) (freshman, sophomore, junior, senior) (circle)

Student(s) e-mail address: _____

Advisor's Name, Address, Telephone Number, and e-mail address:

_____

_____

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## Directions for Virginia Tech

Follow I-81 to Exit 118. There is one exit ramp for all three of the exits (118 A, B, and C). Take Exit 118B onto U.S. 460 West. If you have not been to Blacksburg for a few years, note that there is a new limited-access bypass that runs directly from I-81 to the campus entrance at Southgate Drive. At the south end of Blacksburg, stay on U.S. 460 West, signed for "Virginia Tech, Bluefield." (Do NOT take "Business" US 460 which is also called South Main Street in Blacksburg.) Your first traffic light will be VA 314, Southgate Drive. Turn right onto Southgate (speed limit 35). (*) Drive about one mile on Southgate, and turn left onto Spring Road. You will see Lane Stadium. Drive past the Stadium, and turn right onto Washington Street. Cassell Coliseum will be on your right. Drive past the tennis courts, about a quarter mile, to Kent Street. (See detail map). Turn left onto Kent Street and head down the hill (speed limit 15). Just after the road curves toward the left, Owens Hall will be on your left.

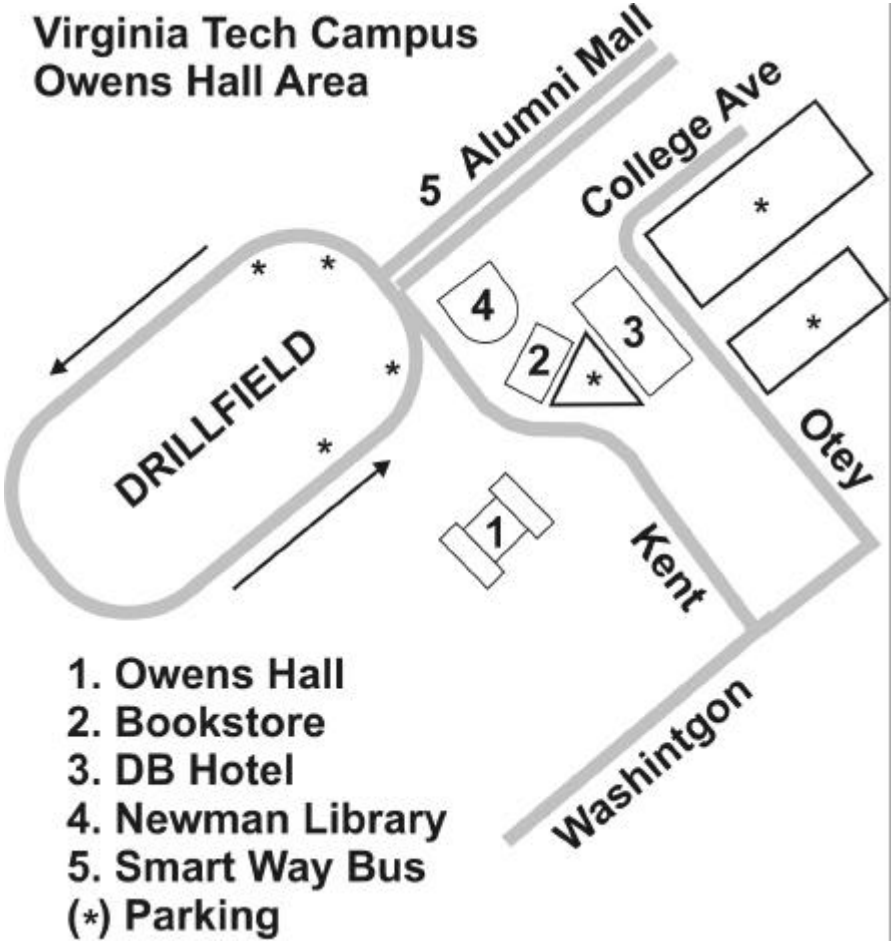
(*) If you are coming from the North, follow US 460 East all the way to Southgate Drive and turn left. Pick up the above directions at (*).

If you are especially lucky you will find parking in the small lot across from Owens and next to the bookstore. More parking can be found around the Drillfield just ahead. Traffic on Drillfield Drive is one-way (counter-clockwise as viewed from above). Alternatively, there are two Faculty/Staff lots (see map) on Otey Street and College Avenue which become "open" public parking after 5 PM. To access these lots you must drive back out to Washington Street, turn left, and then left again onto Otey Street. If you park in the larger lot on College Avenue, be careful to park in the area marked "F/S" (Faculty/Staff), and NOT in the area set aside for Donaldson Brown Hotel guests. The lot on Otey Street is a gated lot, but the gate raises automatically after 5 PM.

Additional maps and directions can be found on the web at http://www.unirel.vt.edu/directions/

The SmartWay Bus travels from Roanoke and Salem to Blacksburg and back. Schedules and other information can be found at http://www.smartwaybus.com. The bus stop nearest Owens Hall is at Squires Student Center, about a ten minute walk. Please be advised, however, that the last eastbound bus leaves Blacksburg at 8:20 PM.

**Map of Virginia Tech**



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The April Virginia Blue Ridge Section meeting is scheduled for Wednesday, April 20 at Radford University. The speaker will be Dr. Eugene Stevens speaking on "Green Plastics". The contact person is Chris Hermann.