



AMERICAN CHEMICAL SOCIETY KENTUCKY LAKE SECTION

KLS-ACS 2012 Officers

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KLS-ACS Web Page

<http://kentuckylake.sites.acs.org/>

September 2012 Kentucky Lake Section Meeting @

Union University

1050 Union University Drive
Jackson, TN 38305

Tuesday, September 18, 2012

Social @ 5:30, Dinner @ 6:00, Presentation @ 7:00

All events will be held in the Carl Grant Events Center on campus

Directions and maps: <http://www.uu.edu/about/map/index.htm#Directions>
From U. S. Highway 45 Bypass, take Union University Drive west to Walker Road. Turn left on Walker Road. The Grant Center is on your left after passing the Welcome House gate and student housing on the left.

The price is \$10 (Students \$5)

Menu Options:

Athenian Chicken, Roasted Pork Loin, Roasted Garlic Mashed Potatoes, Sauteed Green Beans with Bacon, and Chocolate Pie or Peach Cobbler.

Presentation:

Structure-Based De Novo Design and Synthesis of Small Molecule Inhibitors of Protective Antigen (PA): A Novel Anti-Toxin Approach for Combating Anthrax.

Dr. Ashok Philip

Union University School of Pharmacy
Assistant Professor

Comments from the Chair

We are continuing the tradition started last year for honoring an outstanding undergraduate and faculty member for their contribution to research. We are also seeking nominations for an Outstanding High School Chemistry teacher. Nominations are due Friday, October 5th and the form is attached to this email and also available on the KLS website (under the Awards Committee tab on the left). ~Kate Stumpo



Structure-Based De Novo Design and Synthesis of Small Molecule Inhibitors of Protective Antigen (PA): A Novel Anti-Toxin Approach for Combating Anthrax.

Abstract: The significant threat to human health posed by anthrax highlights the need for identifying effective ways to combat this fatal disease. Since proteolytic activation of Protective Antigen (PA) by cellular proteases is a vital step in anthrax poisoning, we accomplished structure-based *de novo* ligand design and synthesis of small molecules with the potential to bind PA and block its proteolytic activation. Structure-based *De novo* design was accomplished with a suite of molecular modeling tools that include Biopolymer module and Docking suite of Sybyl X 2.0 on a ThinkCenter

M Series desktop. A simple, yet highly efficient solution-phase parallel synthesis methodology was then employed to synthesize the “virtual lead” and a library of its structural analogues. This novel approach offers the advantage of selectively targeting and inactivating the bacterial toxin and effectively combat the threat posed by anthrax.

BioSketch:

Ashok Philip, Ph.D.

Assistant Professor of Pharmaceutical Sciences

Union University School of Pharmacy

Dr. Philip received his B.S. (1999) and M.S. (2001) degrees in Pharmacy and his Ph.D. in Medicinal Chemistry from The University of Mississippi in 2006. His Doctoral research involved working on the design, synthesis, molecular modeling and biological evaluation of novel NOP receptor ligands. As a Postdoctoral fellow at Center for Drug Design, University of Minnesota and at St. Jude Children’s Research Hospital, Memphis, TN, Dr. Philip worked on development of novel small molecule inhibitors for potential treatment of pancreatic cancer and glioma respectively. His research interests include the area of Drug Design and Discovery engaging the principles of Organic synthesis, Chemical biology and Molecular Modeling for development of Antianthrax and Antitubercular agents.