

THE NUCLEUS

January 2007

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Monthly Meeting

Joint Meeting with BAGIM

A First-Time Mentor

NEBHE Science Network by Jin Ji

Chair's Statement

By Mukund Chorghade

Summer Research Scholar

Design and Synthesis of Novel Inhibitors of Dihydroorotase

2007 Chair's Statement

By Mukund Chorghade

It is a singular honor and privilege to assume the office of Chair for the Northeastern Section. The breadth, depth and sophistication of the talent and creativity of the individuals in the section are truly outstanding. We have eminent researchers and professionals representing the strategic triad of academia, government and industry from all sub-disciplines of chemistry. We enjoy a cherished and hallowed tradition of excellence. The warmth and gracious hospitality with which we welcome participation by our members, collaborators and distinguished guests has been the hallmark of our tradition and the well-spring of our progress

It will be my endeavor to (1) Foster greater interactions between the ACS and the other professional bodies catering to the cause of chemistry - The American Institute of Chemists and the International Union of Pure and Applied Chemistry come readily to mind. A one-day joint meeting featur-

ing several prominent scientists has been arranged on March 30. This could be the forerunner of an annual Life Sciences Symposium and could provide a useful forum for productive exchange of ideas. (2) Encourage a vitalized speakers bureau to provide guest lectures to schools, universities and civic and community groups. The topics can encompass issues of topical interest, e.g., chemical safety, environmental and the contributions made by chemists/chemistry to the benefit of society at large. (3) Expand the activities of the Professional Training/Education and Career Services committees. Regular workshops will be used to educate students at local colleges/universities and mid-career professionals about the diverse opportunities in chemistry, current trends in globalization, resume writing, interviewing skills/techniques and related topics. Such workshops will also benefit mid-career and chemists undergoing a career transition. (4) Build a much-needed bridge

between the medicinal and process chemistry groups and facilitate via symposia and discussion groups new perspectives on the progress of a drug from conception to commercialization. (5) Organize a few lunch time lectures to attract researchers who, because of their busy schedules, are not able to attend the evening lectures. The ACS has novel programs like the science café's that will be of great interest to our members. (6) Increase participation of members in the section activities and increase the membership of the ACS and the section. This will also allow greater opportunities for networking among chemists. Greater emphasis will be placed on attracting chemists in the biotechnology / biopharmaceutical industries and participation of their employers via corporate sponsorships (7) Stimulate additional participation of the section in the international activities of the ACS. Our members are involved in a wide array

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Two Day Training Course in Heterocyclic Chemistry

April 9th and 10th, 2007 at the MIT Endicott House, Dedham

The 2-day training course in heterocyclic chemistry includes:

Twelve hours of lectures by Professors

Albert Padwa (Emory Univ.) and Will Pearson (Univ. of Michigan)

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FOR MORE INFORMATION, PRICING and COURSE CATALOG

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Cover: *From L-R: Evan Heyn, Mary Mahaney, Chair of the NESACS Board of Publications, Vincent Gale, Advertising Manager of the Nucleus and recipient of the second Arno Heyn Memorial Book Award, Michael P. Filosa, Editor of the Nucleus, Vivian Walworth, Board of Publications, Robert Heyn and Janice Heyn.*

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Grants-in-Aid Awarded to Under-graduates

NESACS Career Services at Monthly Meetings

The Education Committee has awarded Grants-in-Aid of \$250 each to four undergraduates at colleges and universities within the Northeastern Section to enable them to attend the ACS National Meeting in Chicago, Illinois to present a paper at the Undergraduate Research Poster Session in the Division of Chemical Education on Monday, March 27, 2007. Matching funds have been committed by the institutions to support the students' travel. The recipients are also required to participate in the Northeast Student Chemistry Research Conference (NSCRC) in April 2007.

The awardees, their research supervisors, and the titles of the papers are as follows:

Richard Hughes, Jr., Boston College, (Prof. Lawrence Scott) *Towards the Synthesis of Arm-Chair Carbon Nanotubes*

Pareesh Agarwal, Massachusetts Institute of Technology (Prof. Christopher Cummins) *An Isolable and Monomeric Phosphorous Radical that is Resonance-Stabilized by the Vanadium (IV/V) Redox Couple*

Taryn Palluccio, Bridgewater State College (Prof. Stephen Waratuke) *Hydroaminations of Alkynes, Enynes and Dienes Using Titanium Catalysts*

Chaoyuan Kuang, Massachusetts Institute of Technology (Prof. Graham Walker) *Regulation of Activity of E.coli Proteins UmuC and UmuD*

Applications for the travel stipend are accepted from students majoring in chemistry, biochemistry, chemical engineering, or molecular biology who are in good standing with at least junior status, and are currently engaged in undergraduate research. ◇

The NESACS Career Services Committee is dedicated to providing ACS Members with the best tools to manage careers. We offer career guidance and focus on the components needed for targeting the job market: personal assessment, identifying market trends, credentials, research and networking. We have a comprehensive (lecture, demo and review) program that provides assistance in writing winning resumes and cover letters as well as various techniques and skills needed for a successful interview.

In collaboration with the Speaker's Bureau, we will organize a program of resume reviews and short lectures focusing on current topics at Section Meetings. Two distinguished recruiters in our area, Megan Driscoll and Jennifer Sass of PharmaLogics Recruiting, will join me in offering valuable perspectives and 1:1 career counseling to members. These sessions will typically be held between 2:30 pm and 4:30 pm. Members will be able to benefit from such networking: this will be a regular feature of Section Meetings in 2007.

In general our members have provided positive feedback. Reproduced below are comments from one member who benefited from our programs:

"My career counseling session with Dr. Chorghade began with some basic questions designed to engage me and focus me on clearly stating my objectives. The process of reviewing my CV began with an examination of its overall structure and an assessment of the impression of prospective screeners. This overview was followed by a detailed review focused on content, wording and vocabulary. I have read several books on resume writing and

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Dishman Pharmaceuticals
And Chemicals Limited
Houghton Chemical Company
Organix, Inc.
Vertex

Wallace J. Gleekman

The Editor of the Nucleus is saddened to report the death of long-time NESACS stalwart and retired Brookline High School teacher, Wally Gleekman on November 23, 2006. A more complete remembrance will be published in a future issue. MPF ◇

attended many workshops. The assistance that I received through ACS career services has been the most knowledgeable and helpful that I have experienced. While the improvements to my CV are significant, the feedback I received on my qualifications and search strategies was profound. The best part of the process is the quality of assistance and sincere caring of the counselor." ◇

Monthly Meeting

The 875th Meeting of the Northeastern Section of the American Chemical Society

Jointly with the Boston Area Group for Informatics and Modeling (BAGIM)

Thursday – January 18, 2007

Harvard Faculty Club,
20 Quincy St., Cambridge, MA.

2:30 pm Career Services Presentations and Resume Reviews, Mukund Chorghade, Chair, NESACS; Megan Driscoll and Jennifer Sass of PharmaLogics Recruiting.

4:30 pm Board Meeting

5:30 pm Social Hour

6:30 pm Dinner

8:00 pm Evening Meeting, Dr. Mukund Chorghade, Chair, presiding
Dr. Yvonne Connolly Martin, Senior Research Fellow (retired),
Volwiler Society, Abbott Laboratories.
Lessons from 41 Years as a Computational Chemist

Dinner reservations should be made no later than noon, Thursday, January 11, 2007. Please call or fax Marilou Cashman at 800-872-2054 or e-mail at Mcash0953(at)aol.com. Please specify vegetarian. Reservations not cancelled at least 24 hours in advance must be paid. Members, \$28; Non-members, \$30; Retirees, \$15; Students, \$10.

THE PUBLIC IS INVITED

Anyone who needs special services or transportation, please call Marilou Cashman a few days in advance so that suitable arrangements can be made. Free parking in the Broadway St. Garage (3rd level or higher). Enter from Cambridge Street via Felton Street.

Biography



Yvonne Martin retired at the end of October from her position as Senior Research Fellow, Volwiler Society, Abbott Laboratories. Her research interests include strategies for increasing the molecular diversity of compound collections; to triage hits from HTS; to predict the potency, binding affinity, or absorption, distribution, metabolism, and excretion (ADME) properties of small molecules from their molecular structures; and for the computer design of novel compounds including 3D database searching, *de novo* design, and pharmacophore mapping. Dr. Martin did her undergraduate work in chemistry and biology at Carleton College, Northfield, Minnesota and her PhD work in chemistry at Northwestern University focusing on physical biochemistry. Her entire career (40+ years), except for a stay with Corwin Hansch, has been at Abbott Laboratories; the past 35 years involving various aspects of computer-assisted drug design. She is a member of the Advisory Board for the QSAR and Modeling Society, an editor for the publication "*Perspectives in Drug Design and Discovery*" and a section editor for "*QSAR: Annual Reports in Computational Chemistry*". Dr. Martin is on the editorial boards for "*The Journal of Computer Aided Molecular Design*" and "*QSAR & Combinatorial Science*" and is a former member of the NIH Biodata Management and Analysis Study Section. Honors received include Phi Beta Kappa; NIH pre-doctoral fellow; AAAS fellow; IUPAC fellow; life-time member of the Molecular Graphics and Modeling Society; and the Accomplishment Award, The Society for Biomolecular Sciences (2005). ◇

Career Services

Are you interested in changing jobs? Do you wonder whether your interviewing abilities could be enhanced? Could your resume use some work? If yes, please join us at the January meeting, where you can receive advice from industry professionals.

Topics and services which we will cover: how to put together an eye-catching resume, best interviewing strategies, and how to find the most appropriate opportunities ◇

Abstract

Lessons from 41 Years as a Computational Chemist

This talk will address the following questions: how many ways can a computational chemist impact the efficiency of drug discovery? Do models always have to be accurate to be useful? Are there other ways that a computational chemist can impact drug discovery than by developing or using quantitative or 3D molecular modeling? ◇

2nd Heyn Book Award Prize to Vincent Gale

The second Arno Heyn Memorial Book Prize Award was made to long-time *Nucleus* Advertising Manager, Vincent Gale. Vince has served *the Nucleus* for sixteen years. He was recruited by former *Nucleus* Editor, Arno Heyn when Arno recreated *the Nucleus* in the form it has today. Vince is also the advertising manager for a number of other newsletters published by ACS Sections including *The Indicator*, *The Vortex*, *The Catalyst*, *The Crucible*, *The Del-Chem Bulletin* and *The Capital Chemist*. Vince also maintains a website to manage and promote advertising in the aforementioned ACS sectional newsletters: www.mboservices.net.

The prize was presented at the November meeting held at UMASS Boston by Board of Publications member and long-time friend of Arno Heyn, Vivian Walworth. In attendance from the Heyn family were Arno's sons Evan and Bob, also present was Bob's wife, Janice Heyn. Last year's recipients of the first Arno Heyn Prize were former *Nucleus* editor, Mark Spittler and former NESACS Webmaster, Sam Kounaves. MPF ◇

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A First-Time Mentor

By Jin Ji, PhD
Chairperson, Speakers Bureau of NESACS

Our story begins at the Annual Long-Range Planning Meeting of the Northeast Section of American Chemical Society (NESACS) back in June of 2006. As the new chairperson of the Speakers Bureau of NESACS and a new board member of NESACS, I was attending my first Long-Range Planning meeting. The purpose of the meeting was twofold: to encourage communications among many committees within NESACS, and to stimulate dialogue between NESACS and other organizations in the New England area. I wondered to myself, "How will this meeting impact the Speakers Bureau's activities?"

NESACS wanted to establish an active outreach committee whose goal was to bridge the chasm between chemistry and the public. The outcome: a Speakers Bureau was created and the NESACS Chair, Dr. Pam Mabrouk, appointed me its chairperson starting in January 2006. The idea was to organize volunteer speakers, who as experts and professionals in chemistry fields could speak to schools, industries and different communities and organizations about the benefits of our profession. The events would be free to the audience. Six months into building the bureau, the bureau had attracted twelve passionate professionals and willing speakers. We had even planned a series of career counseling events at monthly NESACS meetings starting in September. But what else?

At the Long-Range Planning meeting, besides the board members that I often saw at regular monthly board meetings, I noticed a few new faces. One of them was Emorcia Hill from New England Board of Higher Education (NEBHE). She discussed an annual event that NEBHE was organizing – the Science Network at MIT on November 18th, 2006 which is an event to introduce college and high school students who are interested in sciences and technologies to peers and to inspiring mentors in these fields.

Emorcia described how much impact and guidance the events in the past had offered to the students. She also stressed that with more and more students attending the event each year, NEBHE was constantly looking for qualified experts and professionals in these fields to be inspiring mentors.

"That's interesting!" I thought to myself, "Introducing students to the possibilities of a career in chemistry or chemistry-related sciences is exactly what our Speakers Bureau should be doing! That's something we definitely should take part in." After Emorcia spoke, I introduced myself and we decided to discuss further the collaborations between our two organizations.

The planning went smoothly. I sent out a solicitation within the bureau and three speakers, Mukund Chorghade, Robert Litman and Michael Filosa, responded with positive feedback. They were all enthusiastic about becoming advisors for the event. Susan Bryant, the coordinator of the event, was very appreciative of Speakers Bureau's participation and mentioned that NEBHE hoped "to continue working with the Speakers Bureau in the future."

Saturday, November 18th, 2006, would be an interesting day for the many students and mentors who participated in the Science Network at MIT – and a delightful day for Robert Litman, Michael Filosa and myself who had the honor of representing the bureau. The event was full of young curious minds, lots of energy and an abundance of excitement when it came to learning about careers in science, technology and engineering. They had endless questions.

All the mentors and advisors were divided into different groups and matched with students who have specific interests in their fields. Having been working in biochemical fields and developing medical devices, I was assigned to be a mentor for a group of

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REPORT FROM SEOUL

Morton Z. Hoffman, Boston University
<hoffman@bu.edu>

U.S. National Representative to the IUPAC Committee on Chemistry Education and ACS Division of Chemical Education Liaison to IUPAC

The 19th International Conference on Chemical Education (ICCE) was held on August 12-17, 2006, at Sookmyung Women's University in Seoul, Korea. Attracting almost 400 participants from 36 nations around the world, including more than 20 from the United States, the conference, which had as its theme, *Chemistry and Chemistry Education for Humanity*, was organized by a committee headed by Conference Chairman Jung-II Jin and Organizing Committee Chairman Choon Do. Welcoming remarks were made by Eun Lee, President of the Korean Chemical Society, which co-sponsored (with IUPAC) the conference as part of its 60th anniversary celebration and recognition of 2006 as the "Year of Chemistry" as declared by the government of the Republic of Korea.

The conference featured a number of very distinguished chemists and educators as plenary lecturers: Bassam Shakhshiri (USA), *Enlightenment, The Responsibilities of the Enlightened, and Exhortations for Good Teaching*; Nobel Laureate Aaron Ciechanover (Israel), *The Ubiquitin Proteolytic System: From Basic Mechanisms Through Human Diseases and onto Drug Targeting*; Su-Moon Park (Korea), *Chemistry Education for More Chemistry Majors*; ACS President Ann Nalley (USA), *Applications of Computer Molecular Modeling in Teaching Organic Chemistry*; Onno De Jong (The Netherlands), *Making Chemistry Meaningful: Conditions for Improving Context-Based Chemistry Education*; Viktor Obendrauf (Austria), *More Small-Scale Hands-on Experiments for Easier Teaching and Learning*; Peter Atkins (UK), *The Challenge of Education*. A chemistry demonstration presentation by David Katz (USA), *Chemical Principles Visualized*, and a forum on *Young*

Ambassadors for Chemistry (YAC): Past and Future led by Lida Schoen (Netherlands) were also part of the highlighted program.

After the welcoming reception on Saturday evening, the sessions began on Sunday morning with symposia on the public understanding of chemistry, the role of chemists, inorganic chemistry, multimedia and visualization, how students learn, and teacher education. During the next days, other symposia were presented on women and chemistry; green chemistry; general, analytical, organic, polymer, environmental, computational, forensic, and physical chemistry and material science; networking and accreditation of chemistry and chemical engineering education; microscale laboratory techniques; web-based teaching and learning arts in chemical education future of

textbooks; instructional strategies; experiments and demonstrations; gifted learners. In total, more than 300 presentations were made, including 120 posters, many of which were offered by elementary, middle, and high school teachers. Details of the program are available on the ICCE 2006 website: <http://www.19icce.org/>.

One outstanding part of the meeting program was the exhibit of posters by school children on the theme, *Chemistry for Humanity*, which was organized by "Science Across the World," the IUPAC Committee on Chemistry Education (CCE), and the Korean Chemical Society. An initial group of 945 entries from 32 countries had been winnowed down to 13 posters (age 10-13) and 41 posters (age 14-16) for presentation at ICCE. A jury, consisting Lida Schoen (Netherlands), Eva

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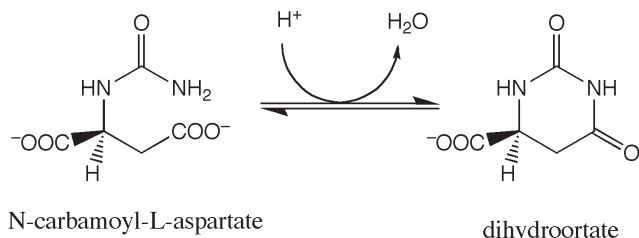


Summer Scholar

Design and Synthesis of Novel Inhibitors of Dihydroorotase

by Kerry Heinzelmann, Advisor: Evan Kantrowitz, Boston College
Department of Chemistry, Merkert Chemistry Center, Chestnut Hill, MA 02467

Dihydroorotase (DHOase) is the second enzyme in pyrimidine nucleotide metabolism; it catalyzes the reversible ring closure of *N*-carbamoyl-*L*-aspartate (CA) to form dihydroorotate (DHO).



DHOase is a member of the amidohydrolase superfamily of enzymes. The mechanism of the enzymes in this superfamily involve Zn^{2+} ions.¹ In mammals, DHOase is part of the multifunctional enzyme CAD along with aspartate transcarbamoylase and carbamoyl phosphate synthetase, but in bacteria DHOase is an independent enzyme.² The structure of homodimeric *E. coli* DHOase has been determined, and the active site was shown to contain two Zn^{2+} ions.³ In the determined structure one active site contains CA and the other contains DHO (see Figure 1).

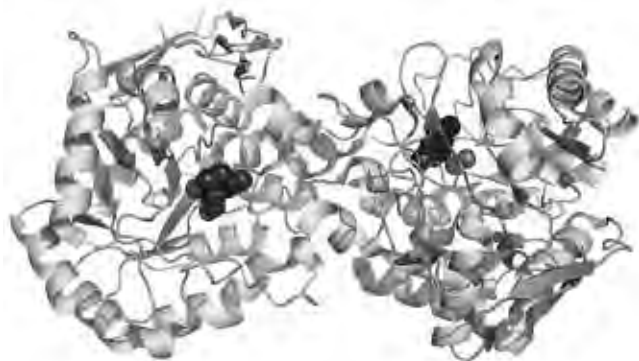


Figure 1. Structure of homodimeric *E. coli* DHOase (PDB entry 1J79). The structure of each monomer is organized as a “TIM” barrel. The product DHO is shown in the right active site, while the substrate CA is shown in the left active site. The two Zn^{2+} ions in each active site are also shown.

The DHO from the malaria parasite (*P. falciparum*) and *E. coli* DHOase have 27.5% conserved residues, including all residues involved in catalysis and metal binding. This suggests that the active site structure of *P. falciparum* DHOase is similar to the structure of *E. coli* DHOase, and that their catalytic mechanisms are the same. Seymour *et al.*⁴ have shown that an inhibitor of DHOase results in the accumulation of carbamoyl aspartate and an overall decrease in the formation of pyrimidine nucleotides. There-

fore, since *P. falciparum* does not have a salvage pathway for pyrimidine nucleotides, inhibitors of *P. falciparum* DHOase have the potential to have anti-malarial activity.

The active site of DHOase was found to be a pocket within a pocket. When DHO binds to the enzyme, it binds to the lower pocket, adjacent to the Zn^{2+} ions, leaving the hydrophobic upper pocket empty. Because the upper pocket remains empty, a potential inhibitor of DHOase may bind to this upper pocket, or it may expand off of the substrate to fill the upper pocket. A virtual screening system developed in the Kantrowitz lab was used to identify potential inhibitors of DHOase by docking a library of compounds to the active site with and without DHO bound. Identified compounds were evaluated kinetically and used to design second generation inhibitors.

Results

Identification of possible DHOase inhibitors

As a means to identify an entirely new classes of inhibitors we used a virtual screening that allows for the rapid evaluation of interactions between an enzyme active site and small molecule compounds. This was accomplished computationally using available docking programs.

Optimization of virtual screening for DHOase

Because of the different algorithms used, a specific docking program may be better suited for a particular target active site. Therefore, we tested three programs to see which would be the best for DHOase. The three programs tested were AUTODOCK3,⁵ DOCK5⁶ and SURFLEX.⁷

Program optimization was performed on DHOase with the substrate carbamoyl aspartate bound in one active site and the product DHO bound in the other (PDB entry 1J79³). The molecule in the active site was removed and its coordinates changed so that it was in a different spatial position, unrelated to the actual binding site. The DHO or CA was then docked into the active site using AUTODOCK3, DOCK5 and SURFLEX. The RMS deviation between the DHO from the X-ray structure and the best conformer from AUTODOCK3 was 0.36 Å, 0.49 Å for DOCK5 and 3.5 Å for SURFLEX. The large RMS deviation with SURFLEX was due to its inability to position the carboxylate in the proper orientation. Therefore AUTODOCK3 was selected to be used to identify new inhibitors (see below)

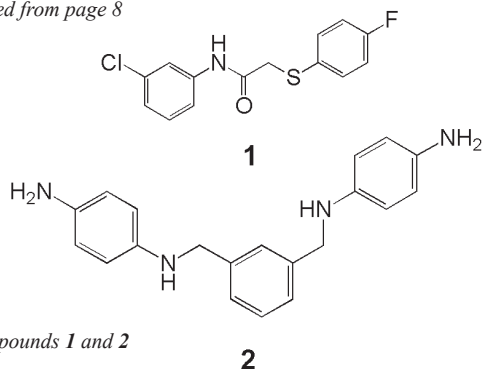
Identification of new inhibitors of DHOase by vHTS

All of the compounds in the Sigma-Aldrich catalog were docked to the DHO site in DHOase using AUTODOCK3. The two compounds that gave the best results from the docking were **1** and **2**.

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Summer Scholar

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Compounds 1 and 2

Ability of 1 and 2 to inhibit DHOase

1 and **2** were tested for their ability to inhibit DHOase. Reactions were setup at sub-saturating concentrations of DHO, and in the absence and presence of increasing concentrations of either **1** or **2**. As seen in Figure 2, **1** was not able to inhibit DHOase over the concentration range tested, while **2** exhibited significant inhibition.

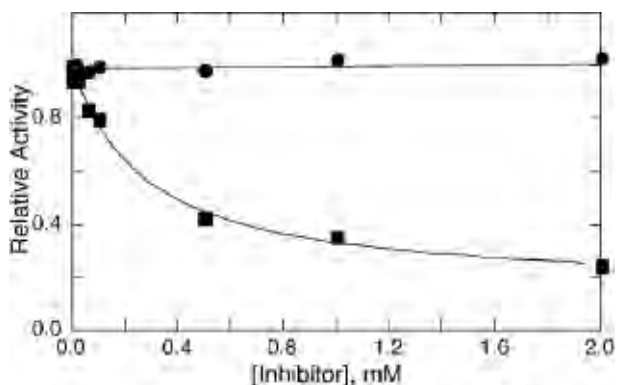
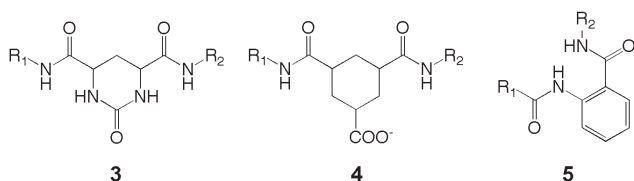


Figure 2. Inhibition of DHOase by inhibitors 1 (circles) and 2 (squares).

Modifications to the structure of 2



Compounds 3, 4 and 5

Modifications of **2** were docked in order to optimize the inhibitory effects on DHOase. Molecules with different base units (**3**, **4**, **5**) were examined, with the R groups representing different cyclic amines and then docked to check their respective affinity for the active site. The base unit most like the substrate, 2-oxohexahydropyrimidine-4,6-dicarboxylic acid, **3**, was selected for the synthesis of the first set of compounds. Compound **3** was not commercially available, however its synthesis had been previously reported.⁸ Problems occurred during the synthesis of **3**

including consistently low yields of the desired oxidation product, and formation of undesirable side products. Because of the problems with the synthesis of **3**, structurally similar compounds that were commercially available and showed binding affinity for the enzyme were considered as base units instead. We are currently using one such compound, 1,3,5-cyclohexanetricarboxylic acid **4**, as a base unit for synthesis of potential inhibitors. As seen in Figure 3, two of the carboxylic acids of **4** are initially benzyl protected using 2 equivalents of benzyl alcohol. An amine is then coupled to the unprotected carboxylic acid in the presence of DCC, HOBt, and Et₃N. Finally, after the two acid groups are deprotected by catalytic hydrogenation, another amine can be coupled to one acid group by using the same coupling conditions.

(e) Future directions

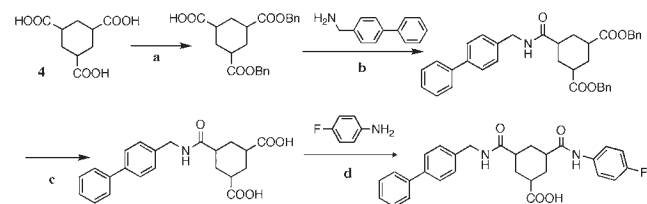


Figure 3. Synthesis using the 1,3,5-cyclohexanetricarboxylic acid, **4**, base unit. (a) CDI, Benzyl alcohol, rt 24 h; (b, d) DCC, HOBt and Et₃N; (c) 10% Pd/C, CH₃OH, 18 h.

This project is being continued during the current academic year as part of an undergraduate research project. Currently, a series of molecules with compound **4** as their base unit are being synthesized. AUTODOCK was used to help select the R groups that would enhance binding to DHOase. Once these syntheses are complete, the compounds will be assayed to determine their ability to inhibit DHOase. In the future, we plan on synthesizing compounds with 1,3,5-benzenetricarboxylic acid **5** as the base unit, and comparing the inhibition of these compounds to those containing **4**.

Experimental Procedure

Enzyme purification

The plasmid that contained the gene for *E. coli* DHOase (obtain from Frank Raushel, Texas A&M University) was transformed into a special *E. coli* strain that can be induced to produce T7 polymerase. The strain/plasmid combination was grown in YT media at 37°C until the A₆₀₀ reached 0.6, at which time 0.4 mM IPTG was added to induce the production of the enzyme. After overnight growth, the cells were harvested by centrifugation followed by sonication to break open the cells. Ammonium sulfate was added to the clarified lysate to 60% saturation. The precipitate, containing the protein, was dissolved in buffer (50 mM Tris-phosphate, 100 μM ZnCl₂), then dialyzed against the same buffer. Anion-exchange chromatography was then used to purify the DHOase using Source Q resin (GE Health-

continued on page 10

Summer Scholar

Continued from page 9

Care). The column was eluted with a gradient of NaCl in the above buffer. Fractions containing enzyme were combined and checked for purity by SDS-gel electrophoresis.

Enzyme activity determination

The activity of the DHOase in the absence and presence of inhibitors was determined by measuring the initial rate of the reaction in the reverse direction. The amount of *N*-carbamoyl-*L*-aspartate formed was determined colorimetrically as previously reported.⁹

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National Chemistry Week Report

By Christine Jaworek-Lopes

Approximately 3000 individuals learned about NCW through the events held this year. The breakdown was as follows: ~450 individuals attended the kick-off event at Wellesley College, ~1500 individuals visited the Children's Museum and ~1000 individuals visited the MOS on October 28, 2006. Over 100 volunteers from 12 different organizations (ACS members, Phyllis A. Brauner Memorial Committee, Emmanuel College, Gordon College, Malden High School, Mass General Hospital, Merck Chemical Company, Northeastern University, Simmons College, Suffolk University, Tufts University, Wellesley College) contributed to the successful week.

The NCW committee would like to offer **Salutes to Excellence Awards** to the following: **Merck Chemical Company** for financial support of the events as well as providing all the materials for the chromatography demonstration performed at the MOS-Boston, **Boston Children's Museum**, **Museum of Science-Boston**, and **Wellesley College**.

As of November 14, 2006, only two puzzle solutions and no posters were submitted as part of the contest.

NCW 2007 will be from October 21 – October 27, 2007. The theme is “*The Many Faces of Chemistry*.” The kick-off event on October 21 will be held at the Museum of Science as well as an outreach event on October 22. A third event will be held at the Children's Museum on October 27. ◇

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Report from Seoul

Continued from page 7

Åkesson (Sweden), Margaret-Ann Armour (Canada), Peter Atkins (U.K.), Karl Brachtl (Austria), Marianne Cutler (UK), Morton Hoffman (USA), Onno De Jong (Netherlands), Mordechai Livneh (Israel), Jim McQuillan (New Zealand), Mauro Mocerino (Australia), and Kay Stephenson (UK), chose the winning posters in the two age categories. The winners received certificates of recognition and small electronic devices as gifts.

Social activities associated with the conference included a visit to the Korean Folk Village, preceded by lunch in a traditional Korean family roadside restaurant (leaving shoes at the door, seating on mats on the floor, following the colorimetric rule for spiciness [the redder the food, the hotter it is]); Participants' Night with national songs and performances; and a banquet in a high-rise building with a striking view along the Hangang River with entertainment by an ensemble of singers and instrumentalists performing Korean classical-modern "fusion" music on traditional instruments.

The ICCE was the occasion of the annual meeting of the CCE. Chaired by Peter Mahaffy (Canada), the committee consists of eight titular members, eight divisional representatives, and 19 national representatives. The Committee approved the minutes of its meeting in Beijing in August 2005, received the minutes of the CCE strategy meeting in Puerto Rico earlier in 2006, and reports from the following subcommittees: Development of Materials for Raising Awareness about the Chemical Weapons Convention; Public Understanding of Chemistry; Chemistry for Development; Microscale Group; DIDAC (development of didactic tools). CCE received an update on the Bologna process in Europe and the development of the EuroBachelor degree in chemistry. CCE will meet next in Torino, Italy, on the occasion of the IUPAC General Assembly and Congress, August 4-12, 2007, *Chemistry Protecting Health, Natural Environment and Cultural*

Connections to Chemistry

By Ruth Tanner

The *Connections to Chemistry* program took place at Burlington High School (Burlington, MA) on Wednesday, October 18th, 2006, 3:30–8:00 PM. Each registrant participated in two of the five different workshops that were scheduled including a workshop on engineering in chemistry, a National Chemistry Week workshop on paints and coatings, and a workshop on starting a high school chemistry club, one of the new initiatives of the Education Division of the ACS. Terri Taylor, the Manager of the ACS Office of High School Chemistry in Washington welcome the participants on behalf of the American Chemical Society at the opening meeting and also gave the workshop on high school chemistry

clubs. (Her office donated 150 of the canvas CHED bags for the program from the BCCE program held at Purdue University this past summer.) Dr. Daniel Nocera, Professor of Chemistry and W. M. Keck Professor of Energy at the Massachusetts Institute of Technology gave a very spirited evening address: *The Energy Future of Our Planet* which was followed by a raffle of American Chemical Society items (mugs and laser pen pointers), subscriptions to the Journal of Chemical Education (2 of which, were donated by the Journal) memberships in CHED (donated by CHED), and memberships in CTC (Chemistry Teacher Connection). ◇

Heritage <www.iupac2007.org>.

The 20th ICCE will be held on August 3-8, 2008, in Pointe aux Piments, Mauritius. The theme of the conference will be *Chemistry in the Information and Communications*

Technologies;

see <http://www.uom.ac.mu/20icce.htm> for more information.

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Brauner Memorial Lecture *October 22, 2006*



Professor Bassam Z. Shakhshiri, candidate for ACS President, during his presentation of the Phyllis A. Brauner Memorial Lecture at Wellesley College on October 22, 2006.



(l-r) Doris Lewis (Suffolk University), Bassam, Susan Brauner, Hyacinth Brauner.

Photos by Morton Z. Hoffman

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Calendar

Please check NESACS website and university websites for late breaking changes.

Jan 17

Milton R. Smith, III (Michigan State Univ.)
"TBA."
(Woodward Lecture Series, Harvard-MIT Inorganic Chemistry Seminar.)
MIT, Room 6-120, 4:00 p.m.

Jan 22

Jeffery Kelly (The Scripps Research Institute)
"TBA"
(Woodward Lecture Series, Organic Chemistry Seminar)
Harvard Univer, Pfizer Lecture Hall 4:15 p.m.

Jan 23

Prof. Anne Gershenson (Brandeis Univ.)
"Single Molecule Studies of Molecular Mousetraps: Serpin Folding & Protease Inhibition"
Boston College, Merkert 130 4:00 PM

Jan 24


Dr. William Reiff, (Northeastern Univ.)
"TBA"
Northeastern Univ. Hurtig Hall Rm 129 12 Noon

Jan 30

Prof Gregory Petsko (Brandeis Univ.)
"Structural Neurology: A New Approach to the Understanding, Treatment and Prevention of Neurodegenerative Diseases"
Boston College, Merkert 130 4:00 PM

Jan. 31

Dr. Elena Rybak-Akimova (Tufts Univ.)
"TBA"
UMass Dartmouth; Building Group II, Room 115
4:00 PM




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Chair's Statement

Continued from page 2

of activities here-the collaboration with the German Chemical Society has been outstanding! Plans are well under way for extensive collaboration with the Indian and the Chinese Chemical Societies. One of ACS's most successful mechanisms for delivering highly focused technical content in the United States has been through the ProSpec-tives series of conferences. The prestigious "ProSpectives" conference will be organized at various locations in India and China.

So, dear members, please join us in what promises to be an outstanding year of progress and additional programs. Volunteers like you are a tremendous source of ideas that constitute the lifeblood of an organization. Join a committee of your choice, provide creative inputs into the programs and join us in increasing the public's awareness and enjoyment of Chemistry. ◇

A First-Time Mentor

Continued from page 6

students who had interests in medical fields. This was an utterly new experience for me as I have always considered myself a learner and constantly identified people in my professional careers as my own mentors.

Many of the students in my group only knew how to get into medical fields through premedical studies and Medical school. Once they found out that I majored in chemistry and was working at Harvard Medical School developing medical devices, they began probing for details: "How did you get to where you are today?", "Were there any obstacles?", "How did you know this was what you wanted to do?"...

It made me think. I must have asked similar questions when searching for a path for my life. I must still be asking these questions in my heart, or out loud, but not realizing it. The answers to these questions are helpful to the people who asked the questions, also those who through their hearts answered the questions. It was a day reflecting as well as advising. It was a day in which so many promising students learned about us, our work and, their future. ◇

All notices for the Calendar should be sent to

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