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THE NEWSLETTER OF THE DEPARTMENT OF CHEMISTRY & BIOCHEMISTRY

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DEPARTMENT OF CHEMISTRY & BIOCHEMISTRY ENJOYS RECORD-BREAKING SUMMER

By: Glenys Young, Office of Communications & Marketing

The Texas Tech University Department of Chemistry & Biochemistry saw its most lucrative summer on record in 2017, with faculty members bringing in grants and awards worth more than $5 million. "Each one of these awards has its own accolades associated with it and its scientific component, making it very competitive," said Yehia Mechref, a professor and chair of the department since June 1. "In this day and age, receiving federal funds is not trivial. Federal money is very scarce and we as a department, over a three-month period, we successfully brought $5.1 million. "I've been here for seven years. If we go by history, this is the most successful summer by far. If you count the awards numerically – forget about the dollar sign associated with them – this is by far the largest number of awards the department received in a summer. If you count individuals, you're talking about nine awards."

Awards | Assistant professor John D'Auria received a National Science Foundation (NSF) collaborative grant; associate professor Michael Findlater received an NSF and a contract from Chevron-Phillips Chemistry; assistant professor Michael Latham received a Presidents' Collaborative Research Initiative award; W. David Nes, a Paul Whitfield Horn Professor, received a grant from the National Institutes of Health (NIH) ; associate professor Dimitri Pappas received a CH Foundation gift; Professor L. William Poirier received an NSF grant; assistant professor Benjamin Wylie received a Maximizing Investigators' Research Award from the NIH; and professor Mechref received an NIH competing renewal award of his R01, an NIH subcontract and a CH Foundation gift. More information about each award are included elsewhere in this newsletter.

New Leadership | Mechref is quick to point out that although the $5.1 million in funding came through under his tenure as department chair, it's not his doing. "I cannot take the credit for all of this; it's a department that's only successful through the efforts of everybody," he said. "We are successful as a department because of our students, our staff and our faculty. Each of us contributes in his or her own way. We are successful as a department; it's a true group effort." "Our department is like a puzzle – you won't see the beautiful picture until all the pieces of the puzzle are in place."

In leading the department, Mechref said his goals are aligned with those of the university at large. "One of the main goals that this department has contributed to in the past, and should continue to contribute to, is to enhance the research reputation of Texas Tech University," he said. "We need to continue to perform cutting-edge research, and we need to fulfill the strategic research areas being defined by the university.

"The department is successful as a result of the efforts of the students, the staff and the faculty – in that order," he said. "Without our smart, hardworking undergraduate and graduate students, we would not be able to fulfill the research component. Without the critical support of our staff, we would not be able to fulfill the educational or research component. And without our faculty, we could not fulfill any of the three components. We gel together as a unit."

To read the full article, go to: http://today.ttu.edu/posts/2017/09/chemistry-grants

TEXAS TECH UNIVERSITY
Department *of* Chemistry & Biochemistry™

INSIDE THIS ISSUE

New Department Chairman

The department's faculty, staff, and students welcome **Professor Yehia Mechref** as the new Chairman of the Department of Chemistry and Biochemistry, as of June 1, 2017, and sincerely thank Professor Hope-Weeks for her outstanding service as past Chair.

New Faculty Member

In fall 2017, **Dr. Kristin Hutchins** has joined the faculty of the Department of Chemistry and Biochemistry as a tenure-track Assistant Professor. She will teach organic chemistry-related courses and her research projects are in the areas of organic, materials, and supramolecular chemistry.

PROFESSOR AWARDED DISTINGUISHED GUEST SCIENTIST FELLOWSHIP

Prof. Bill Poirier was awarded a Distinguished Guest Scientist Fellowship from the Hungarian Academy of Sciences, to bring "internationally acclaimed foreign researchers as Visiting Fellows to conduct top-level research in Hungary", working to advance the field of rovibrational spectroscopy in various ways.

COMPUTATIONAL CHEMISTRY APPLIED TO PROTON CANCER THERAPY

Prof. Jorge Morales is conducting innovative research in computational chemistry to study proton cancer therapy (PCT) reactions. PCT is a relatively new cancer treatment that obliterates cancer tumors with high-energy proton beams. While clinically approved, many mechanistic details of PCT remain unknown. The Morales group is elucidating details via computer simulations without putting patients at risk and at very low cost. PCT reactions under study include water radiolysis and DNA damage by protons and electrons. This research on PCT and other work by the group has been featured recently in eHealthNews.eu and EurekAlert.org (Targeted, High-Energy Cancer Treatments Get a Supercomputing Boost).

http://www.ehealthnews.eu/research/5246-targeted-high-energy-cancer-treatments-get-a-supercomputing-boost and https://eurekalert.org/pub_releases/2017-05/uota-thc050817.php.

Retirement Congratulations!

Dr. Robert W. Shaw - Retired August 2017

Member of Texas Tech University Faculty Since 1981

Dr. Richard A. Bartsch - Retired January 2011

Member of Texas Tech University Faculty Since 1974

- In Memoriam

Dr. Roy E. Mitchell
(July 2017)

Dr. John A. Anderson
(March 2017)

Dr. David B. Knaff
(January 2016)

David W. Purkiss
(December 2015)

Dr. Clinton M. McPherson
(January 2014)

Dr. John N. Marx
(December 2012)

Dr. Robert A. Holwerda
(August 2011)

Dr. Dennis C. Shelly
(November 2008)

GETTING THE METAL OUT!

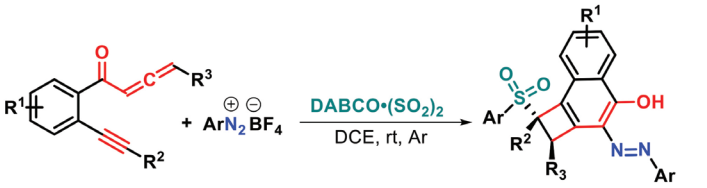
Metal-Free Access to Functionalized Cyclobuta[a]naphthalen-4-ols by Merging [2 + 2] Cycloaddition with Radical 1,4-Addition

Professor Guigen Li, who is managing two highly successful research groups (at TTU and in China at Nanjing U.), and his coworkers have recently reported a "greening" of sulfone chemistry. Sulfones are found in many pharmaceuticals and bioactive natural products, especially in the form of arylsulfones. Typically, these functional groups are introduced by using either an active metal, metal salts, or transition metal complexes. However, due to a little serendipity during previous and ongoing projects, Prof Li's group had speculated that with the right mixture of salts, DABSO, and unsaturated carbon-carbon bonds it would be possible to install sulfonyl and azo functionalities into molecular frameworks in a cascade reaction. To demonstrate this, the group has recently reported a novel one-pot procedure for the synthesis of cyclobuta[a] naphthalen-4-ols by treating benzene-linked allene-ynes with aryldiazonium tetrafluoroborates and DABCO-bis(sulfur dioxide).[1] The proposed mechanism for this reaction involves the following sequence: a [2 + 2] cycloaddition, insertion of SO_2, 1,4-addition, diazotization and finally tautomerization. They have demonstrated that the reaction works well on over 50 substrates with excellent diastereoselectivity and yield. This work was supported by a Texas Tech Presidential Enhancement Program (for visiting associates Prof. Bo Jiang and Dr. Wen-Juan Hao).

[1] Jiang, B., Liu, F., Wang, J.-Y., Zhou, P., Li, G., Hao, W.-J. and Tu, S.-J. (), Merging [2 + 2] Cycloaddition with Radical 1,4-Addition: Metal-Free Access to Functionalized Cyclobuta[a]naphthalen-4-ols. Angew. Chem. Int. Ed.. Accepted online 14 Sept 2017. doi:10.1002/anie.201707615

**If you would like read further about this exciting discovery visit:

http://onlinelibrary.wiley.com/doi/10.1002/anie.201707615/full



55 Examples
Up to 94% yield and >99:1 dr

PROFESSOR'S COLLABORATIVE WORK GIVES EXPLANATION FOR ORGANIC CHEMISTRY REACTIONS

A new study helps to understand the relationship between SN2 & E2 reactions.

By Glenys Young

A Texas Tech University computational and theoretical chemist, along with collaborators around the world, is working to finally answer an old question in organic chemistry.

In a paper published in the journal Nature Communications, a research team of experimentalists at the University of Innsbruck in Austria, computational and theoretical chemists at Harbin University in China, and Texas Tech's own Bill Hase – a Paul Whitfield Horn Professor and the Robert A. Welch Chair in the Department of Chemistry & Biochemistry – showed their study of the competition between two important reactions of organic chemistry, the E2 elimination reaction and the S_N2 substitution reaction.

"We established, at the atomistic level, the manner in which these reaction mechanisms occur," Hase said. "It is important to understand how reactions occur at the atomistic level because these mechanisms are important in biological reactions and organic synthesis."

Many chemical reactions are a sequence of very complex processes which are still not fully understood. With laboratory experiments, Roland Wester from the Institute for Ion Physics and Applied Physics at the University of Innsbruck studies such reactions to better understand their dynamics. Wester has built a unique experiment that allows ions and molecules to react and be observed. The angle and velocity at which the ions impinge on a detector is measured.

In a synergistic collaboration with the Wester research group, a research group at Harbin University led by Li Yang and Jiaxu Zhang and the Hase research group at Texas Tech perform chemical dynamics simulations to assist in providing an atomic-level understanding of the experimental measurements. The simulations are performed at Texas Tech and require a high-performance computing infrastructure, benefiting from the university's High Performance Computing Center (HPCC). The simulations are validated by comparing them with experimental measurements.

In a recent study, a team within the Wester group investigated organic compounds with several methyl groups attached to their central carbon atom and also a chlorine or iodine halogen atom attached to this carbon. In a vacuum chamber, the researchers collided these molecules with fluoride, chloride or iodide anions.

An exciting feature of the experiments, as well as for the simulations, is that it is unpredictable which of two chemical reactions, E2 or S_N2, will take place. Either the ion binds to the molecule and the halogen atom bond breaks (S_N2 reaction) or the ion strikes a hydrogen atom from the methyl group and thereby flies away with it (E2 reaction). The two reactions are in competition.

With the Wester group's apparatus, angles at which the reaction products scatter from the reactive collision, and the products' velocities, are measured. This measurement provides information regarding the relative importance of the E2 and S_N2 reactions. Simulations of the reactive collisions give the relative probabilities of the E2 and S_N2 reactions and atomic-level animations of their mechanisms.

**To continue reading about this exciting study visit: http://today.ttu.edu/posts/2017/06/hase

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- O Department of Chemistry & Biochemistry Endowment
- O Chemistry & Biochemistry Scholarships
- O Unrestricted (To be used at the Chairman's discretion)

For an extended list, please see our website: ***www.depts.ttu.edu/chemistry/departmental/donation.php***

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DEPARTMENT **GRANT AWARDS**

Professor John D'Auria

Prof. D'Auria received an NSF Collaborative grant of $800,000 (3 years) for his proposal entitled Collaborative Research: A systems approach toward understanding the diversification of tropane and granatane alkaloid biosynthesis. Dr. D'Auria is the lead PI on the grant along with Dr. Cornelius Barry from MSU and Dr. Charles Stewart Jr. from ISU. The total award is $800,000 (3 years) while TTU share is $332,348.

Professor Michael Findlater

Prof. Findlater and Prof. Weile Yan (Civil & Env Eng) have been awarded an EAGER grant of $80,000 by the Engineering Division of NSF for their proposal Crown Ether-enhanced Electrodialysis for Selective Removal of Problematic Ions in Feed Water and Waste Fluid of Unconventional Energy Production. Professors Findlater and Yan are developing new technology to remediate wastewater associated with hydraulic fracturing.

Professor Dimitri Pappas

Prof. Pappas received a CH Foundation's gift of $102,126 (1 year) for his grant award entitled A Microchip Sepsis Detection System for Point of Service Healthcare.

Professor Michael Latham

Prof. Latham received a TTU Presidents' Collaborative Research Initiative award for a proposal entitled A Structural Basis for a Form of Mental Retardation. This is a collaborative grant with Drs. Clint Macdonald and Petar Grozdanov from TTUHSC (Lubbock, TX). This award provides seed money for experiments to understand how a single mutation of a protein found in brain cells can cause a severe form of mental retardation. The total award is $50,000 for one year, while Prof. Latham's share is $25,000.

Professor Bill Poirier

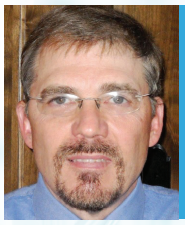
Prof. Poirier has received a grant in the amount of $498,009 from the National Science Foundation (NSF) for a three year project entitled: CDS&E: Massively Parallel Quantum Dynamics: Computing many accurate quantum states for real molecular applications, to develop methods to scale exact quantum dynamical molecular simulations across the next generation of massively parallel supercomputers. Poirier and coworkers are developing the world's first massively parallel exact quantum dynamics code, which may dramatically improve the accuracy, reliability and true predictive power of molecular simulations. Prof. Poirier has also received a grant in the amount of $240,000 from the Robert A. Welch Foundation, for a three year invited renewal on a project entitled: New Methodologies for Accurate Quantum Calculations of the Dynamics of Atomic Nuclei.

Professor Benjamin Wylie

Prof. Wylie received a Maximizing Investigators' Research Award (MIRA) (R35) from the National Institutes of Health (NIH). His proposal was entitled Functional Interplay of Lipid Membrane Components: Activation, Inhibition, and Raft Formation. The Wylie lab will receive $1,745,725 over five years.

Professor Guigen Li

Horn Prof. Guigen Li's Welch grant entitled Group-Assisted Purification (GAP) Chemistry for Asymmetric Synthesis and Catalysis was renewed at $240,000 (direct cost) for three years to continue the study of GAP chemistry and technology invented by Prof. Li at Texas Tech. By using GAP chemistry, the traditional purification via chromatography and recrystallization in organic and medicinal synthesis can be avoided. Two patents have been filed, and a company based on this technology has been established by Dr. Cole Seifert and Carder Brooks (M.S.), both of whom graduated from Texas Tech.



Professor David Nes

Horn Prof. David Nes has received an R33 grant in the amount of $881,354 from the National Institutes of Health (NIH) for a three year study. The title of the funded proposal is Discovery of new anti-amoeba therapeutics. The grant is a continuation award of Prof. Nes' current R21 grant that runs through May 2018. The ongoing research program seeks development of new potent steroidal inhibitors. More specifically, this work is aimed to develop transition state analogs and mechanism-based suicide substrates as anti-amoeba agents that target enzymes (sterol methyltransferases) specific to the amoeba pathogen (Acanthamoeba and Naegleria) not synthesized in the animal host.

Professor and Chair Yehia Mechref

Prof. Mechref has received an NIH R01 competing renewal award for $1,151,179M (4-years) for Sensitive and Quantitative MS-based Glycomic Mapping Platform. Per ORS records, this is the first successful NIH R01 competing renewal that TTU has received since at least 1996. The proposed research will enable the development of tools for the characterization of protein carbohydrate structures at sensitivity, throughput, and level of detail not previously possible. These tools will enable researchers to better understand the attributes and biomedical significance of glycans in the development and progression of a wide array of diseases.

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