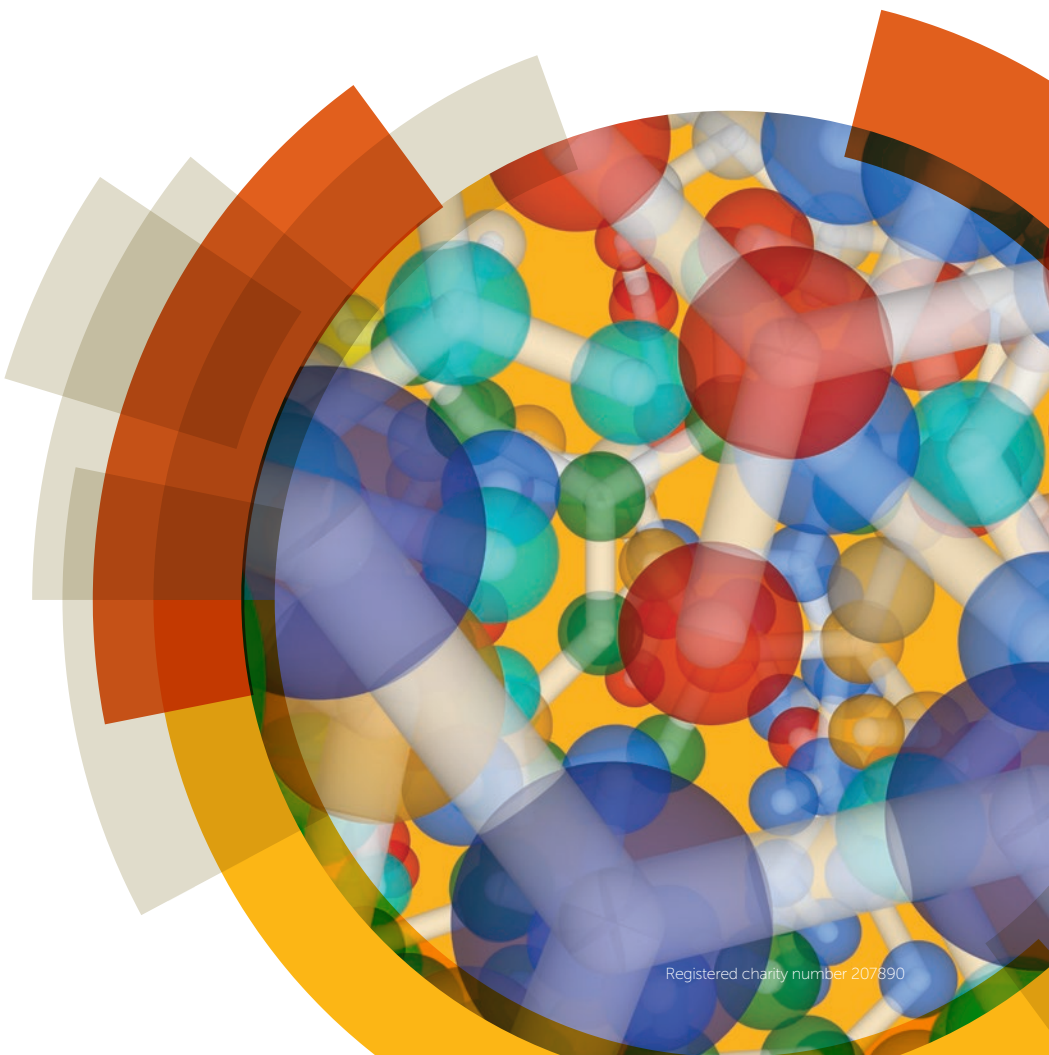
21 April 2015, Zhejiang University, Hangzhou, China

2nd Organic Chemistry Frontiers International Symposium



Book of Abstracts

Welcome address from the Royal Society of Chemistry

Dear Colleagues,

Welcome to the 2nd Organic Chemistry Frontiers International Symposium, co-organized by Royal Society of Chemistry and Department of Chemistry, Zhejiang University.

This meeting belongs to the series of international symposia sponsored the by *Organic Chemistry Frontiers*, a collaborative journal between the Chinese Chemistry Society, the Royal Society of Chemistry and Shanghai Institute of Organic Chemistry.

This symposium will feature a selection of lectures focusing on advancing research in organic chemistry. We hope that these presentations will stimulate the exchange of ideas and experiences between all participants and the symposium will forester new research collaborations for the sake of better chemistry and better world.

Organic Chemistry Frontiers is a high-profile international journal with free access in 2014 and 2015. It reports the leading edge research in the field and ensures that every submission to the journal receives high quality publication service, including rapid publication time, free charge of colour in the text, flexible length and a platform with exceptional high visibility for dissemination of your work.

We do hope that we will have the opportunity to publish some of your work soon and if you would like to be a referee for the journal, please let us know. Further information about the journal can be found on the internet http://rsc.li/frontiers-organic.

Finally, we thank you all for the contribution and hope that everyone enjoys this exciting event!

Sincerely yours,

Professor Shengming Ma
Editor-in-Chief,
Organic Chemistry Frontiers
Zhejiang University

Dr. Daping Zhang
Executive Editor,
Organic Chemistry Frontiers
Royal Society of Chemistry

Welcome address from Zhejiang University

Dear Colleagues,

We are pleased to being co-organizing the 2nd Organic Chemistry Frontiers International Symposium. On behalf of the Department of Chemistry, Zhejiang University, I would like to extend my sincere congratulations on the opening of this symposium and welcome all the delegates.

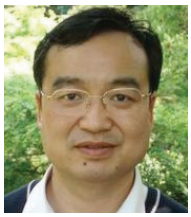
This symposium promises to be a very exciting meeting with a number of lectures given by leading international scientists from the field of organic chemistry. We hope this meeting will provide an ideal forum for all participants to discuss the tremendous progresses in the field, fostering international collaboration between Chinese Scientists and international scientific community.

The Department of Chemistry at Zhejiang University is one of the recognized and leading institutions in China. This department is the home to

- 180 faculty members and staffs including 44 professors and 30 associate professors
- 10 postdoctors
- 523 graduate students
- 230 undergraduates

The Department is devoted to advancing and disseminating knowledge, educating students and providing scientific leadership in the chemical sciences in China. It is a National Basic Research & Teaching Personnel Training Bases and a National Teaching Bases for Basic Engineering Courses. The department has nine institutes and a chemical experimental center, which is the first State Experimental Teaching Demonstration Center of Higher Educational Institutions.

Once more we are very happy to welcome you to the 2nd Organic Chemistry Frontiers International Symposium. We hope you would find the symposium inspiring and rewarding, and we wish you all a pleasant stay in Hangzhou.



Professor Yan-Guang Wang
Dean of Department of Chemistry
Zhejiang University

Programme

Tuesday 21 April
Lecture Room, 5th Floor, Mathematics Center, Yuquan Campus, Zhejiang University

Time	Event	Session chair
08:30	**Opening remarks**	
09:00	**Erik Sorensen, *Princeton University, USA*** Seeking opportunities for C–H functionalization methods in organic synthesis	Shengming Ma *Zhejiang University*
09:25	**Lutz Ackermann, *Georg August-Universität Göttingen, Germany*** Selectivity in metal-catalyzed C–H activation	
09:50	**Zhangjie Shi, *Peking University*** Direct transformation of benzyl alcohols and their ethers	
10:15	**Yonggui Robin Chi, *Singapore Nanyang Technological University, Singapore*** Opportunities with *N*-heterocyclic carbene organocatalysis: New basic activation modes	
10:40	**Coffee & break**	
11:00	**Louis Fensterbank, *UPMC, France*** Some new stories about gold(I) and related catalyses	Stuart Conway *University of Oxford*
11:25	**Zhan Lu, *Zhejiang University, China*** Radical anion on nitrogen compounds	
11:50	**Cristina Nevado, *University of Zurich, Switzerland*** Cyclization cascades via *N*-amidyl radicals: Novel access to complex heterocycles	
12:15	**Lunch**	
13:30	**Masahiro Terada, *Tohoku University, Japan*** Kinetic resolution of racemic amino alcohols through intermolecular acetalization catalyzed by chiral brønsted acid	Erik Sorensen *Princeton University*
13:55	**Chulbom Lee, *Seoul National University, South Korea*** Traceless C–C bond formations using sulfones	
14:20	**Coffee & break**	
14:35	**Ang Li, *Shanghai Institute of Organic Chemistry, China*** Total synthesis of indole terpenoids	Cristina Nevado *University of Zurich*
15:00	**Mei-Xiang Wang, *Tsinghua University, China*** Synthesis and molecular recognition of corona[n]arenes	
15:25	**Stuart Conway, *University of Oxford, UK*** Chemical probes for targeting and imaging hypoxia in tumours	
15:50	**Exchange meeting**	
16:50	**Closing remarks**	

Speaker biographies

Professor Ang Li

Ang Li received his B.Sc. from Peking University (China) in 2004, where he worked with Prof. Zhen Yang. He earned his Ph.D. at The Scripps Research Institute (US) in 2009, under the supervision of Prof. K. C. Nicolaou. After a brief stay as a research fellow at Institute of Chemical and Engineering Sciences in Singapore, he joined Shanghai Institute of Organic Chemistry, Chinese Academy of Sciences, as a professor in 2010. His current research is focused on the total synthesis of structurally and biologically interesting natural products. He has accomplished the total syntheses of a number of natural products, such as fusarisetin A, daphenylline, rubriflordilactone A, dixiamycin C, and taiwaniadduct D. He received Wei-Shan Award for Natural Product Synthesis from Chinese Chemical Society in 2013.

Professor Chulbom Lee

Chulbom Lee obtained his B.S. and M.S. degrees (1988 and 1990) from Seoul National University, where his advisor was Professor Eun Lee. After military service, he came back to SNU as a Research Associate at the Institute of Basic Sciences. In 1992, he was selected as a National Merit Scholar in Chemistry by the Korean Ministry of Education and went to Stanford University for his Ph.D. studies under the guidance of Professor Barry M. Trost. In 1998, he moved to Memorial Sloan-Kettering Cancer Center to work with Professor Samuel J. Danishefsky as a U.S. Army Breast Cancer Research Fellow. Upon completing his postdoctoral studies in 2001, he joined the faculty of the Chemistry Department of Princeton University as Assistant Professor. In 2008, he moved back to his alma mater, SNU. He is currently Associate Chair of the Department while serving as Vice President of the Korean Chemical Society and the Korean Society of Organic Synthesis. He was the recipient of the Roche Award in Organic Chemistry (1998), the U.S. Army Breast Cancer Research Fellowship (1999-2001), the Thieme Journal Award (2001), the Amgen Young Investigator Award (2006), and the SNU Chemistry Teaching Award (2011). His research is focused on the development of novel reactions and strategies for chemical synthesis.

Professor Cristina Nevado

Cristina Nevado was born in 1977 in Madrid, where she graduated in chemistry at the Autónoma University in 2000. In October 2004 she received her PhD in organic chemistry at the same university working with Prof. Antonio M. Echavarren in the cyclization of enynes catalysed by platinum and gold complexes. In December 2006 she joined the group of Prof. Alois Fürstner at the Max-Planck-Institut für Kohlenforschung (Germany) where she was part of the team who conquered the first total synthesis of Iejimalide B, a marine macrolide possessing a very sensitive architecture. In May 2007 she started her independent career as an Assistant Professor at the University of Zürich. In 2011, Cristina was awarded the *Chemical Society Reviews Emerging Investigator Award* and the *Thieme Chemistry Journal Award* in recognition of her contributions in the field of synthetic organic chemistry. In 2012 she received an ERC *Junior Investigator grant* and has been awarded the *Werner Prize* of the Swiss Chemical Society. In 2013 she became Full Professor at the Organic Chemistry Institute of the University of Zürich. Rooted in the wide area of organic chemistry, her research program is focused on complex chemical synthesis and new organometallic reactions.

Professor Erik Sorensen

Erik J. Sorensen is the *Arthur Allan Patchett Professor in Organic Chemistry* in the Department of Chemistry at Princeton University. He received his Ph.D. degree in Chemistry in 1995 from the University of California, San Diego under the direction of Prof. K. C. Nicolaou. From 1995–1997, he was a National Science Foundation postdoctoral fellow in the laboratory of Prof. Samuel Danishefsky at The Memorial Sloan-Kettering Cancer Center in New York. In 1997, he joined the faculty in the Department of Chemistry at The Scripps Research Institute and the Skaggs Institute for Chemical Biology and achieved the rank of Associate Professor with tenure in 2001. In 2003, he moved to Princeton University, where he is a Professor in the Department of Chemistry.

Erik's laboratory pursues concepts and methods that have the potential to advance the field of complex chemical synthesis. They are especially interested in the problem of constructing molecular complexity rapidly from abundant compounds, questions concerning the structural origins of architecturally unique natural products, evaluating hypotheses about the chemical basis of the biological activities of natural products and non-natural molecules, and the design and synthesis of novel anti-bacterial/anti-infective agents.

For his achievements in chemical research and education, Erik received a Beckman Young Investigator Award, a Camille Dreyfus Teacher-Scholar Award, the Pfizer Global Research Award for Excellence in Organic Chemistry, the AstraZeneca Award for Excellence in Chemistry, the Lilly Grantee Award, the Bristol-Myers Squibb Unrestricted Grant in Synthetic Organic Chemistry, and A Focused Giving Award from Johnson & Johnson. In 2001, he was a Woodward Scholar at Harvard University. In 2007, he was the Givaudan/Karrer Distinguished Visiting Professor at the University of Zürich. In 2009, he received the Arthur C. Cope Scholar Award from the American Chemical Society.

Professor Louis Fensterbank

Louis Fensterbank was born in Poitiers in 1967 and raised in Tours. While graduating from the Ecole Superieure de Chimie Industrielle de Lyon (ESCIL) in 1990, he joined the team of Scott Sieburth at SUNY Stony Brook, worked on silicon-tethered reactions and obtained his Ph.D. in 1993. After a temporary lecturer position at the Université Pierre & Marie Curie (UPMC) in 1994, he was appointed by the CNRS in 1995 as a Chargé de Recherche in Max Malacria's team. In 2004, he obtained a professorship position at UPMC and in 2008, he was nominated junior member of the Institut Universitaire de France. In 2009, he was a Visiting Scientist at the Australian National University, Canberra. He was awarded by the French Academy of Science in 2014 the Clavel-Lespiau Prize for his work his organic synthesis.

His research interests concern the discovery of new molecular transformations relying on radical or organometallic processes and their applications to the synthesis of substrates with relevant properties (natural products, probes, ligands…). He has co-authored more than 170 publications.

Professor Lutz Ackermann

Lutz Ackermann studied chemistry at the Christian-Albrechts-Universität Kiel, Germany, and obtained his Ph.D. in 2001 for research under the supervision of Prof. Dr. A. Fürstner at the Max-Planck-Institut für Kohlenforschung in Mülheim/Ruhr, Germany. He was a postdoctoral fellow in the research group of Prof. R. G. Bergman at the University of California at Berkeley, USA, before initiating his independent career in 2003 at the Ludwig-Maximilians-Universität in Munich, supported by the Emmy Noether-programme of the DFG. In 2007, he was promoted to full professor at the Georg August-Universität Göttingen. His research was recognized, among others, with an Astra Zeneca Excellence in Chemistry Award , and an ERC Grant, as well as with visiting professorships at the Università di Milano, Italy (2007), the University of Wisconsin, Madison, USA (2008), and Osaka University (JSPS fellowhship, 2009). The development of novel concepts for sustainable catalysis constitutes one of his major current research interests.

Professor Masahiro Terada

Professor Masahiro Terada was born in Tokyo in 1964. He was graduated from Department of Applied Chemistry, Tokyo Institute of Technology in 1986 and completed his Ph.D. degree in 1993 from Tokyo Institute of Technology under the direction of Professor Koichi Mikami. During his Ph.D. studied, he was appointed as an assistant professor in Professor Mikami's Laboratory at Tokyo Institute of Technology (1989-2001). He worked as a postdoctoral fellow with Professor M. D. Shair at Harvard University in 1999-2000 and moved to Tohoku University as an associate professor in 2001. He has been a Professor of Chemistry at the Graduate School of Science, Tohoku University (Japan) since 2006. He is the recipient of the Incentive Award in Synthetic Organic Chemistry, Japan (2003), The Chemical Society of Japan Award for Creative Work (2008), Mukaiyama Award (2010), Daiichi-Sankyo Award for Medicinal Organic Chemistry (2011), and The Nagoya Silver Medal (2012). His current research interests are focused on the development of new and useful synthetic methodologies based on the design of novel chiral Brønsted acid and base catalysts as well as the utilization of transition metal catalysts.

Professor Mei-Xiang Wang

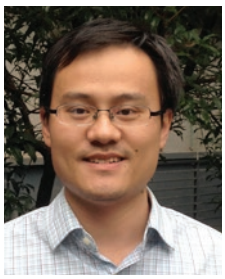
Prof. Dr. Wang received a BS degree in 1983 from the Department of Chemistry, Fudan University. After spending 3 years in General Research Institute of Non-ferrous Metals as a research associate, he joined Institute of Chemistry, Chinese Academy of Sciences (ICCAS) at Beijing as a research student. He obtained his master degree (1989) and PhD (1992) under the supervision of Professor Zhi-Tang Huang. He then worked at ICCAS in the next 17 years, ranking from assistant professor, associate professor and professor. During 2000 to 2004, he served as the Director of ICCAS and the Director of CAS Center for Molecular Sciences. In 2009, he moved to Tsinghua University. His research interests include macrocyclic and supramolecular chemistry, enantioselective biotransformations using whole cell catalysts, selective organic reactions and asymmetric synthesis, anion-pi non-covalent bond interactions and high valent organocopper chemistry.

Professor Stuart J. Conway

Stuart Conway is a Professor of Organic Chemistry at the University of Oxford, and the E. P. Abraham Cephalosporin Fellow in Organic Chemistry at St Hugh's College, Oxford. He studied Chemistry with Medicinal Chemistry at the University of Warwick before undertaking PhD studies with Professor David Jane in the Department of Pharmacology at the University of Bristol. Stuart completed post-doctoral studies with Professor Andrew Holmes FRS at the University of Cambridge working on the synthesis of inositol polyphosphates. In 2003, he was appointed as a Lecturer in Bioorganic Chemistry at the University of St Andrews, in 2008 was appointed as an Associate Professor at Oxford, and in October 2014 he was promoted to Full Professor. Between March and August 2013 Stuart was a Visiting Associate at the California Institute of Technology, hosted by Professor Bob Grubbs and Professor Dianne Newman. Stuart's research focuses on the development of molecular tools to enable the study of biological systems; this work has been recognised by the award of the 2012 Prize for a Young Medicinal Chemist in Academia by the European Federation for Medicinal Chemistry.

Professor Yonggui Robin Chi

Robin Chi received undergraduate trainings from Tsinghua University and Hong Kong Baptist University (2002); Ph.D. from the University of Wisconsin-Madison (2007), and postdoctoral training from University of California-Berkeley (2009). Afterward he joined Singapore Nanyang Technological University as an assistant professor and was then promoted to tenured associate professor. He hold joint-appointments as Singapore National Research Foundation (NRF) fellow, guest professor and distinguished joint professor at the international joint laboratory for chiral synthesis and green pesticides at Guizhou University, China. His group's research concerns fundamental and application advancements of organocatalysis, organic synthesis, functional molecules and materials.



Professor Zhan Lu

Zhan Lu was born in 1981 in the Zhejiang Province. He received a BSc (2003) and a Ph.D. degree (2008) under the supervisor of Professor Shengming Ma in Chemistry from Zhejiang University. After postdoctoral research with Professor Shannon S. Stahl and Professor Tehshik P. Yoon at University of Wisconsin-Madison, he returned to Zhejiang University in 2013 and joined the chemistry faculty. Currently his research interests focus on radical chemistry, first-row transition-metal catalysis, new methodologies for asymmetric synthesis.

Professor Zhang-Jie Shi

Dr. Shi, Professor in Chemistry from Peking University, is now serving as an Editorial Board member of *Organic Chemistry Frontiers*. He received a BS degree in 1996 from the Department of Chemistry, East China Normal University. He further joined Shanghai Institute of Organic Chemistry, Chinese Academy of Sciences (SIOC, CAS) and obtained his PhD degree (2001) under the supervision of Professor Shengming Ma. He then moved to Harvard University as a postdoctoral researcher with Professor Gregory Verdine and later as a research associate with Professor Chuan He at the University of Chicago. In 2004, he joined the faculty of College of Chemistry and Chemical Engineering, Peking University and was promoted to full professor in 2008.

He has received many international awards, including the Mr. and Mrs. Sun Chan Memorial Award in 2014, OMCOS Award in 2013, and Tetrahedron Young Investigator Award in 2011 where he was the inaugural Asian recipient.

Dr. Shi was recognized for his seminal contribution in organometallic chemistry and catalysis, especially in the field of the activation of “inert” bonds and small molecules. So far, he has published more than 100 peer-reviewed papers which have been cited over 7,100 times by others.

Chemical probes for targeting and imaging hypoxia in tumours

Professor Stuart J. Conway

Department of Chemistry, University of Oxford, Oxford, UK; stuart.conway@chem.ox.ac.uk

The increased resistance of hypoxic cells to all forms of cancer therapy presents a major barrier to the successful treatment of most solid tumors. Inhibition of the essential kinase Checkpoint kinase 1 (Chk1) has been described as a promising cancer therapy for tumors with high levels of hypoxia-induced replication stress. However, as inhibition of Chk1 affects normal replication and induces DNA damage, these agents also have the potential to induce genomic instability and contribute to tumourigenesis. To overcome this problem, we have developed a bioreductive prodrug, which functions as a Chk1/Aurora A inhibitor specifically in hypoxic conditions (Figure 1).[1] To achieve this activity, a key functionality on the Chk1 inhibitor (CH-01) is masked by a bioreductive group, rendering the compound inactive as a Chk1/Aurora A inhibitor. Reduction of the bioreductive group nitro moiety, under hypoxic conditions, reveals an electron-donating substituent that leads to fragmentation of the molecule, affording the active inhibitor. Most importantly, we show a significant loss of viability in cancer cell lines exposed to hypoxia in the presence of CH-01. This novel approach targets the most aggressive and therapy-resistant tumor fraction while protecting normal tissue from therapy-induced genomic instability.

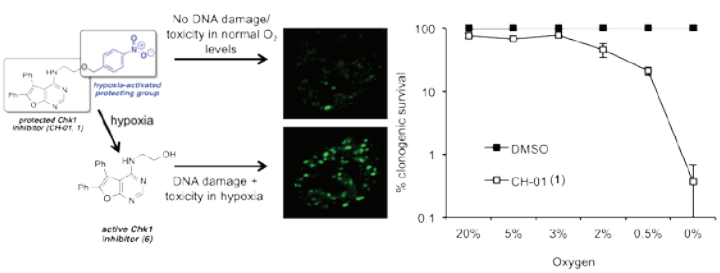


Fig. 1. Addition of a bioreductive group to a kinase inhibitor targets Chk1/ Aurora kinase inhibition to regions of hypoxia.

One of the challenges associated with the clinical use of bioreductive drugs is to understand the biodistribution of these compounds. Therefore, to further the technology that we have developed, we have begun to develop bioreductive groups that *simultaneously deliver a bioactive "cargo" compound and report on the location of compound delivery*. To achieve this aim we first designed a fluorogenic bioreductive group based on the nitroquinoline structure (Figure 2). In proof-of-concept studies we attached the nitroquinoline-based bioreductive group to one of our previously developed BET bromodomain inhibitors as the cargo.[2,3] We demonstrated that the nitroquinoline group was reduced by human cytochrome p450 reductase under hypoxic conditions and fragmented to release the active bromodomain inhibitor. In addition, the fluorescence of the bioreductive group was shown to increase upon reduction. However, despite this compound demonstrating that it is possible to develop a fluorogenic bioreductive group, its emission properties were unsuitable for use in cells. To overcome this shortcoming we have designed second generation compounds based on fluorophores that emit at longer wavelength and which are more suited to applications in a cellular setting and *in vivo*.

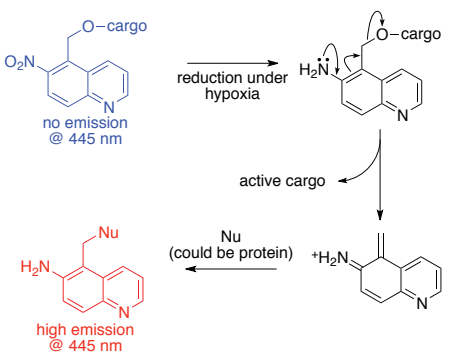


Fig. 2. The principle of a fluorogenic hypoxia-activated group. The group shown in blue is significantly less fluorescent than the products of bioreduction, shown in red.

References

1. Cazares-Korner, C.; Pires, I. M.; Swallow, I. D.; Grayer, S. C.; O'Connor, L. J.; Olcina, M. M.; Christlieb, M.; Conway, S. J.; Hammond, E. M. CH-01 Is a Hypoxia-Activated Prodrug That Sensitizes Cells to Hypoxia/Reoxygenation Through Inhibition of Chk1 and Aurora a. *ACS Chem. Biol*. 2013, **8**, 1451–1459.
2. Hewings, D. S.; Wang, M.; Philpott, M.; Fedorov, O.; Uttarkar, S.; Filippakopoulos, P.; Picaud, S.; Vuppusetty, C.; Marsden, B.; Knapp, S.; Conway, S. J.; Heightman, T. D. 3,5-Dimethylisoxazoles Act as Acetyl-Lysine-Mimetic Bromodomain Ligands. *J. Med. Chem.* 2011, **54**, 6761–6770.
3. Hewings, D. S.; Fedorov, O.; Filippakopoulos, P.; Martin, S.; Picaud, S.; Tumber, A.; Wells, C.; Olcina, M. M.; Freeman, K.; Gill, A.; Ritchie, A. J.; Sheppard, D. W.; Russell, A. J.; Hammond, E. M.; Knapp, S.; Brennan, P. E.; Conway, S. J. Optimization of 3,5-Dimethylisoxazole Derivatives as Potent Bromodomain Ligands. *J. Med. Chem*. 2013, **56**, 3217–3227.

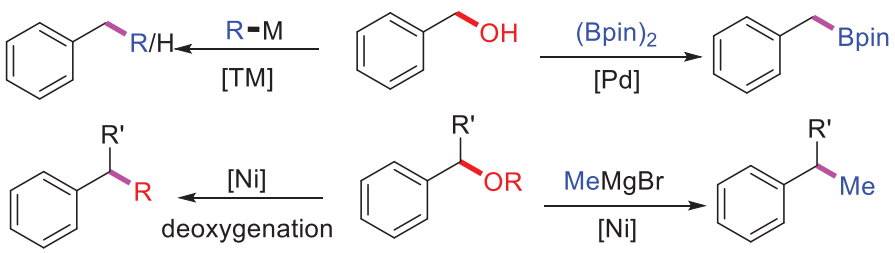
Direct transformation of benzyl alcohols and their ethers

Zhi-Chao Cao, Zhang-Jie Shi

College of Chemistry and Molecular Engineering, Peking University

zshi@pku.edu.cn

Alcohols and their ethers are ubiquitous in nature. Direct transformation of benzyl alcohols via transition metal catalysis present an atom- and step-economic way to construct useful and valuable chemicals. Herein we mostly focused on the direct transformation from benzyl alcohols and their derivatives to furnish important and useful benzylic boronates and other useful chemists.[1-3] Most importantly, with the use of diarylmethyl ether, the extrusion of oxygen of the ether was first reported via Ni catalysis.[4]



References

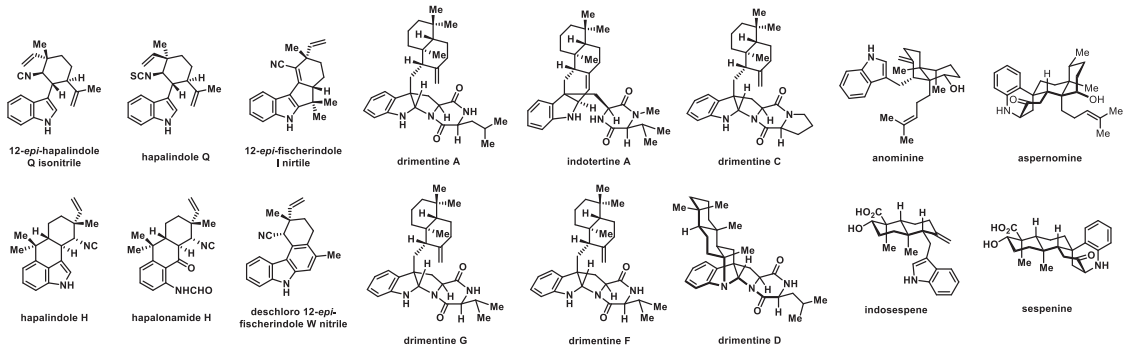
1. Z.-C. Cao, D.-G. Yu, R.-Y. Zhu, J.-B. Wei, and Z. -J. Shi. *Chem. Commun*. 2015, **51**, 2683-2686.
2. D.-G. Yu, X. Wang, R.-Y. Zhu, S. Luo, X.-B. Zhang, B.-Q. Wang, Z.-J. Shi *J. Am. Chem. Soc.* 2012, **134**, 14638–14641.
3. B.-T. Guan, S.-K. Xiang, B.-Q. Wang, Z.-P. Sun, Y. Wang, K.-Q. Zhao, and Z. -J. Shi. *J. Am. Chem. Soc.* 2008, **130**, 3269-3269.
4. Unpublished results.

Total Synthesis of Indole Terpenoids

Ang Li

Shanghai Institute of Organic Chemistry, CAS, Shanghai 200032, China
ali@sioc.ac.cn

The total synthesis of indole terpenoids, such as the xiamycin family, hapalindole family, drimentine family, and anominine family,[1–6] are presented. The reactivities of the indole C2, C3, C4, and benzylic positions are explored. A bioinspired aza-Prins cyclization strategy is exploited in a series of syntheses. The work provides experimental evidences to corroborate the biosynthetic hypotheses of some indole terpenoids.



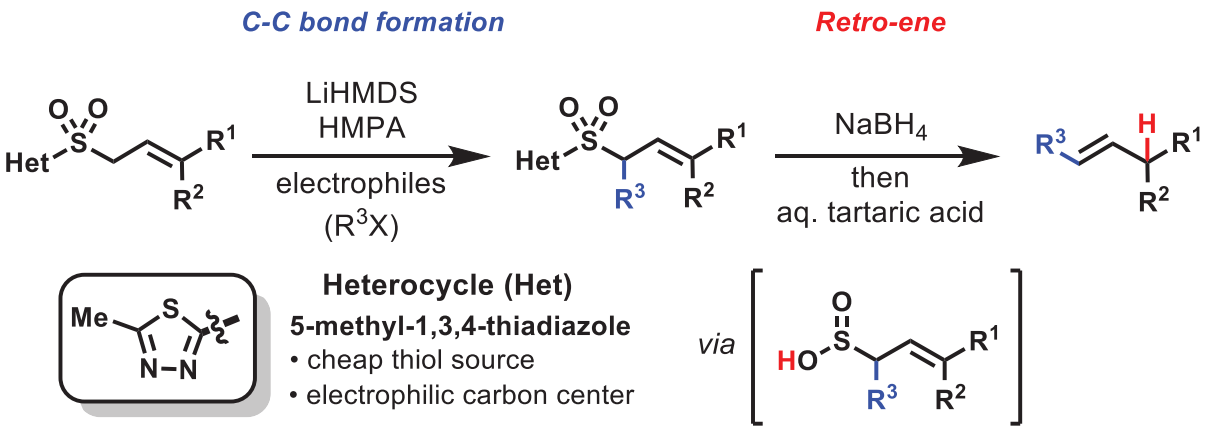
References

1. Z. Meng, H. Yu, L. Li, W. Tao, H. Chen, M. Wan, D.J. Edmonds, J. Zhong, A. Li, *Nat. Commun*. **6** (2015), 6096.
2. Z. Lu, M. Yang, P. Chen, X. Xiong, A. Li, *Angew. Chem. Int. Ed*. **53** (2014), 13840.
3. Y. Sun, P. Chen, D. Zhang, M. Baunach, C. Hertweck, A. Li, *Angew. Chem. Int. Ed*. **53** (2014), 9012.
4. Y. Sun, R. Li, W. Zhang, A. Li, *Angew. Chem. Int. Ed*. **52** (2013), 9201.
5. M. Bian, Z. Wang, X. Xiong, Y. Sun, C. Matera, K.C. Nicolaou, A. Li, *J. Am. Chem. Soc*. **134** (2012), 8078.
6. S. Zhou, H. Chen, Y. Luo, W. Zhang, A. Li, manuscript submitted.

Traceless C–C bond formations using sulfones

Jin Choi, Young Hyun Chae, Hyun Jung Yoo, and Chulbom Lee*
Department of Chemistry, Seoul National University, Seoul 151-747, Korea
chulbom@snu.ac.kr

Our laboratory has been interested in sulfinyl retro-ene reactions that can be performed in tandem with the Diels-Alder reaction.[1] In continuing investigations, we have developed another tandem protocol involving alkylation and retro-ene reactions using heterocyclic sulfones. This methodology has been designed to accomplish C–C bond formations, in a traceless fashion, by taking advantage of the reactivity of sulfone and allylic sulfinic acid functionalities. Similarly to that of carbonyl compounds, the α-position of allylic sulfones can be exploited for diverse C–C bond forming processes (alkylation, aldol-type, and Michael reactions, etc.) using various electrophiles. Subsequently, the sulfone moiety is converted into an allylic sulfinic acid poised for a retro-ene reaction, which gives rise to reductive alkene rearrangement with extrusion of SO_2, under one-pot, mild conditions. From a survey of various sulfones attached to a heterocycle, thiadiazolylsulfones have been identified as an efficient structural unit for the new traceless methodology that can be used for the streoselective synthesis of functionalized alkenes. The details of our studies will be discussed in this presentation.



Reference

1. J. Choi, H. Park, H. Yoo, S. Kim, E. J. Sorensen, C. Lee; *J. Am. Chem. Soc.* 2014, **136**, 9918.

Cyclization cascades via N-amidyl radicals: Novel access to complex heterocycles

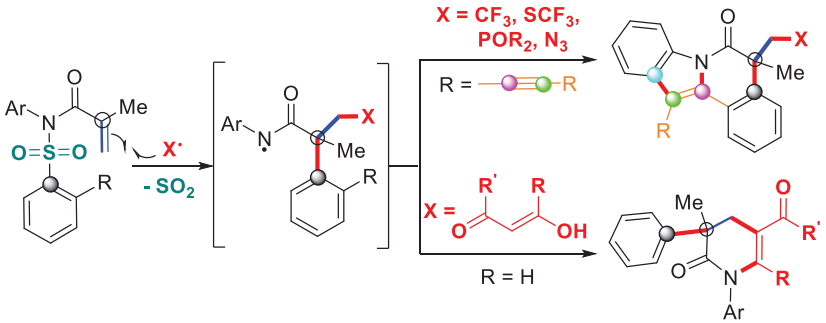
Noelia Fuentes, Wanging Kong, Luis Fernández, Estíbaliz Merino and Cristina Nevado*

Department of Chemistry, University of Zürich, Winterthurerstrasse 190, 8057-Zurich (Switzerland)

cristina.nevado@chem.uzh.ch

Radical reaction cascades represent a valuable tool to access densely functionalized structures.[1] Recently our group reported the addition of a variety of radicals to the double bond of N-(arylsulfonyl)acrylamides where depending on the nature of the substituents at the nitrogen atom, different reaction outcomes were observed.[2]

Herein, we present our results on the chemoselective addition of in-situ generated carbo- and heteroatom-centred radicals to the double bond of N-(arylsulfonyl)-acrylamides. An amidyl radical intermediate is proposed as the key platform for the rapid build-up of molecular complexity by formation of several C-C and C-X bonds in a single synthetic operation yielding highly functionalized isoquinolinones and dihydropyridinones in a highly regioselective manner.[3] The scope and synthetic application of these transformations, together with mechanistic studies, will be presented.



References

1. For example: B. B. Snider, Handbook of C-H Transformations: *Applications in Organic Synthesis*, Ed. G. Dyker, Wiley-VCH:Weinheim, 2005, vol. 2, pp. 371.
2. a) W. Kong, M. Casimiro, E. Merino, C. Nevado, *J. Am. Chem. Soc.* 2013, **135**, 14480;
   b) W. Kong, M. Casimiro, N. Fuentes, E. Merino, C. Nevado, *Angew. Chem. Int. Ed.* 2013, **52**, 13086;
   c) W. Kong, E. Merino, C. Nevado, *Angew. Chem. Int. Ed.* 2014, **53**, 5078;
   d) W. Kong, N. Fuentes, A. García-Dominguez; E. Merino, C. Nevado, *Angew. Chem. Int. Ed.* 2014, **53**, 5078.
3. N. Fuentes, A. García-Dominguez; E. Merino, C. Nevado, *J. Am. Chem. Soc.* 2015, **137**, 964.

Seeking opportunities for C–H functionalization methods in organic synthesis

Erik J. Sorensen

Department of Chemistry, Princeton University, Washington Road, Princeton, New Jersey, 08544, USA,
Email: ejs@princeton.edu

Our laboratory is actively seeking creative opportunities for the expansive collection of methods that are capable of functionalizing unactivated carbon–hydrogen bonds. Our prior tendency to ask, “how might we leverage appropriately placed functional groups to do synthesis?” has given way to a bolder question of “how might we create multifunctional compounds through the execution of direct, site-selective functionalizations of unactivated C–H bonds?” As members of the NSF-sponsored Center for C–H Functionalization, we are actively collaborating with several research laboratories to demonstrate the impact that C–H functionalization methods can have on the planning and execution of syntheses of structurally intricate natural products. This lecture will address some of these efforts.

This lecture will also describe our recent development of a dual-catalytic method to dehydrogenate organic compounds. This method, which is loosely ‘nature-inspired’, converts certain hydrocarbons to alkenes with the cogeneration of hydrogen gas.

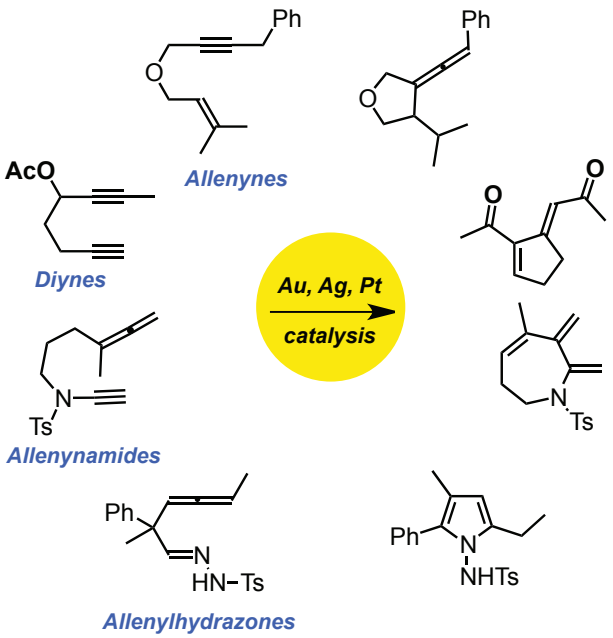
Some new stories about gold(I) and related catalyses

Louis Fensterbank*

UPMC Univ Paris 06, Sorbonne Universités, Institut Parisien de Chimie Moléculaire (UMR CNRS 8232), 4 place Jussieu, C. 229, 75005 Paris (France)

Email: louis.fensterbank@upmc.fr

Our laboratory has been interested over the last ten years in the use of electrophilic complexes (Au, Pt, Ag, Ir) for the access to molecular complexity from readily available precursors.[1] Some of these transformations lend themselves to their asymmetric version notably by using the chiral anion strategy.[2] Interestingly, the electrophilic gold catalysis based on the carbene formation from the rearrangement of propargyl acetates can also lead to a new type of polycyclopropanated polymers.[3] Examples along these lines will be presented and discussed.



References

1. Fensterbank, L.; Malacria, M. *Acc. Chem. Res*. 2014, **47**, 953-965.
2. a) Barbazanges, M. et al. *Chem. Eur. J*. 2011, **17**, 13789-13794.
   b) Augé, M. et al. *Chem. Commun*. 2013, **49**, 7833-7835.
3. Nzulu, F. et al. *Macromolecules* 2014, **47**, 6652-6656.

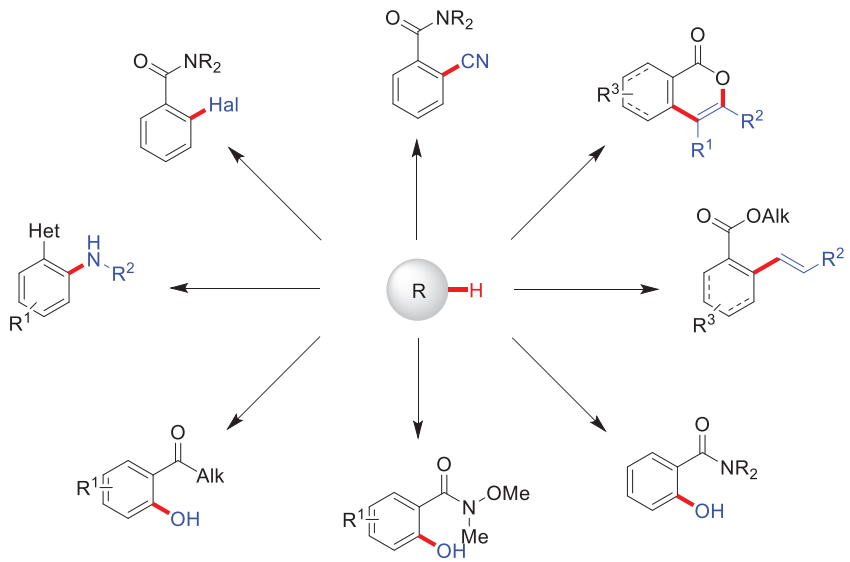
Selectivity in metal-catalyzed C–H activation

Lutz Ackermann*

Georg-August-University Göttingen, Institute for Organic and Biomolecular Chemistry, Tammannstr. 2, 37077 Göttingen, Germany

Lutz.Ackermann@chemie.uni-goettingen.de

Catalytic C–H functionalizations are attractive tools for a streamlining of organic synthesis, avoiding the preparation and use of prefunctionalized starting materials.[1] Recently, we have introduced carboxylates as additives for site-selective direct arylations and alkylations employing versatile ruthenium(II) complexes,[2] which were found to display complementary chemo- and site-selectivities as compared to palladium,[3a] nickel,[3b] cobalt[3c] or iron[3d] catalysts. Detailed mechanistic insight into the working mode of the C–H ruthenation step set the stage for the development of ruthenium(II)-catalyzed twofold C–H bond functionalizations as well as step-economical oxidative annulations of alkynes.[4] The oxidative C–H bond functionalization strategy proved to be broadly applicable,[5] and also enabled among others ruthenium(II)-catalyzed oxygenations, nitrogenations, cyanations and halogenations.



References

1. a) L. Ackermann, *Modern Arylation Methods*, Wiley-VCH, Weinheim, 2009.
   b) D. Alberico, M. Scott, M. E. Lautens, *Chem. Rev*. 2007, **107**, 174–238.
2. Recent examples: a) N. Hofmann, L. Ackermann, *J. Am. Chem*. Soc. 2013,**135**, 5877–5884.
   b) M. Schinkel, I. Marek, L. Ackermann, *Angew. Chem. Int. Ed*. 2013, **52**, 3977–3980.
   A review: c) L. Ackermann. *Chem. Rev*. 2011, **111**, 1315–1345.
3. a) L. Ackermann, A. Althammer, S. Fenner, *Angew. Chem. Int. Ed*. 2009, **48**, 201–204.
   b) W. Song, S. Lackner, L. Ackermann, *Angew. Chem. Int. Ed*. 2014, **53**, 2477–2480.
   c) W. Song, L. Ackermann, *Angew. Chem. Int. Ed*. 2012, **51**, 8251–8254.
   d) Q. Gu, H. H. Al Mamari, K. Graczyk, E. Diers, L. Ackermann, *Angew. Chem. Int. Ed*. 2014, **53**, 3868–3871.
4. a) L. Ackermann, A. V. Lygin, N. Hofmann, *Angew. Chem. Int. Ed*. 2011, **50**, 6379–6382.
   b) L. Ackermann, *Acc. Chem. Res*. 2014, **47**, 281–295.
5. a) L. Ackermann, L. Wang, A. V. Lygin, *Chem. Sci*. 2012, **3**, 177–180.
   b) S. I. Koszushkov, L. Ackermann, *Chem. Sci.* 2013, **4**, 886–896.

Kinetic resolution of racemic amino alcohols through intermolecular acetalization catalyzed by chiral brønsted acid

Masahiro Terada*

Department of Chemistry, Tohoku University, Sendai 980-8578, Japan
mterada@m.tohoku.ac.jp

The conversion of racemic compounds into enantiomerically enriched products via kinetic resolution is one of the most fundamental and powerful methods in asymmetric synthesis. A selective acylation is the most common approach to the kinetic resolution of racemic secondary alcohols to obtain enantiomerically enriched ones and a number of methods have been accomplished by using enzymes and chiral metal catalysts. In contrast, an acetalization of alcohols is one of the most fundamental methods for protection of a hydroxy group and hence is widely utilized in organic synthesis, because acetal is readily formable/removable protective group under catalytic acidic conditions. In this context, selective acetalization of one enantiomer of racemic secondary alcohols potentially provides an efficient alternative to the kinetic resolution through the conventional acylation procedure. However, kinetic resolution of racemic secondary alcohols through acetalization has never been reported so far, despite the fact that the acetalization is the representative method for protection of a hydroxy group. The challenge for developing kinetic resolution of racemic secondary alcohols through acetalization inspired utilization of a chiral phosphoric acid catalyst, which has emerged as an efficient chiral Brønsted acid catalyst for a wide variety of enantioselective transformations.[1] Herein we report the highly efficient kinetic resolution of racemic amino alcohols through acetalization for the first time using chiral phosphoric acid catalyst 1 (Figure 1).[2] The developed kinetic resolution enables efficient access to a range of enantiomerically enriched amino alcohols 2 which are useful as a chiral unit for biologically active and relevant molecules.

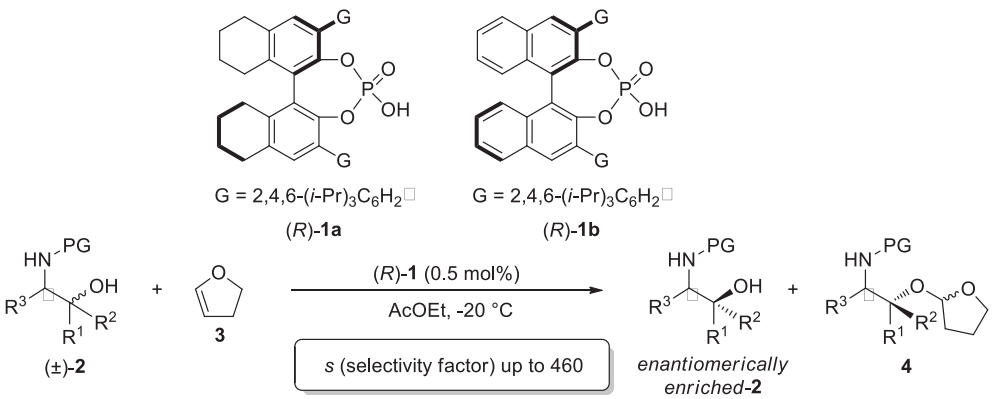


Figure 1 Kinetic resolution of racemic amino alcohols through acetalization catalyzed by a chiral phosphoric acid.

References

1. (a) M. Terada, *Chem. Commun*. 2008, 4097-4112.
   (b) M. Terada, Bull. *Chem. Soc. Jpn*. 2010, **83**, 101-119.
   (c) M. Terada, *Synthesis* 2010, 1929-1982 (Comprehensive Review).
2. T. Yamanaka, A. Kondoh, M. Terada, *J. Am. Chem. Soc*. 2015, **137**, 1048.

Synthesis and molecular recognition of corona[n]arenes

Mei-Xiang Wang

Department of Chemistry, Tsinghua University, Beijing 100084, China
wangmx@mail.tsinghua.edu.cn

For more than a decade, we have established and developed the macrocyclic and supramolecular chemistry of heteracalixaromatics (Figure 1A)[1]. Owing to the self-tunability of a *V-shaped cavity* and electronic property originated from the interplay between the bridging heteroatoms and adjacent aromatic rings, heteracalixaromatics exhibit unique binding properties and have become powerful and versatile synthetic receptors to recognize diverse charged and electron neutral guest species. To seek for novel and functional macrocyclic hosts that have a *cylindroid cavity*, we have very recently proposed corona[n](het)arenes (Figure 1B), a new type of synthetic macrocycles which are composed of heteroatoms and *para*-(het)arylenes in an alternative fashion[2]. In this talk, I will describe a practical and efficient method for the synthesis of various oxygen, sulfur and sulfone-linked corona[*6*](het)arenes. The conformational structures of the macrocycles will be discussed. I will also demonstrate their applications in selective binding towards organic cations in both organic and aqueous solution. The easy availability, molecular diversity and unique molecular recognition property would render corona[*6*](het)arenes attractive macrocyclic receptors in supramolecular chemistry.

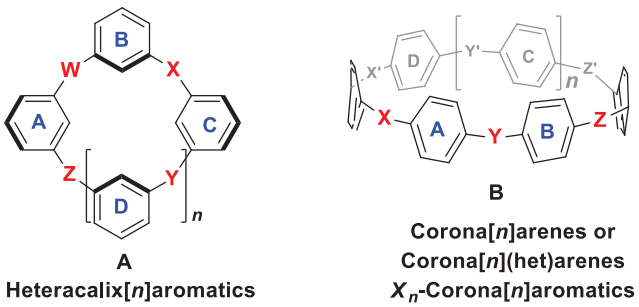


Figure 1. General structures of heteracalix[n]aromatics (A) and corona[n]arenes (B)

References

1. (a) M.-X. Wang, *Acc. Chem. Res*. 2012, **45**, 182.
   (b) H. Zhang, B. Yao, L. Zhao, D.-X. Wang, B.-X. Xu, M.-X. Wang, *J. Am. Chem. Soc*. 2014, **136**, 6326.
   (c) D.-X. Wang, M.-X. Wang, *J. Am. Chem. Soc*. 2013, **135**, 892.
2. (a) Q.-H. Guo, Z.-D. Fu, L. Zhao, M.-X. Wang, *Angew Chem. Int. Ed*. 2014, **53**, 13548.
   (b) Q.-H. Guo, L. Zhao, M.-X. Wang, *unpublished results*.

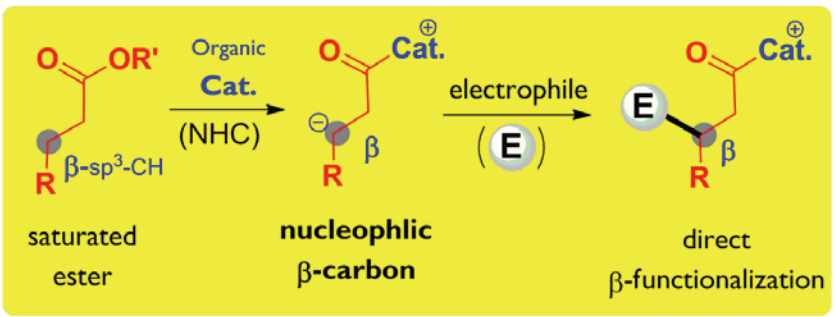
Opportunities with N-heterocyclic carbene organocatalysis: New basic activation modes

Tingshun Zhu, Yonggui Robin Chi*

International Joint Laboratory for Chiral Synthesis and Green Pesticides, Key Laboratory of Green Pesticide and Agricultural Bioengineering, Ministry of Education, Guizhou University, Guiyang 550025, China; and Division of Chemistry and Biological Chemistry, School of Physical and Mathematical Sciences, Nanyang Technological University, Singapore 637313

E-mail: robinchi@ntu.edu.sg; chiyg0098@126.com

The Chi group works on the discovery and development of sustainable organic catalysis and new synthetic strategies for organic synthesis, pharmaceutical manufacturing, and materials assemblies or modifications. One focus is to develop basic new action modes for the functionalization of relatively inert C-H[1], C-C[2], N-S, and other non-reactive chemical bonds by using N-heterocyclic carbene (NHC) organic catalysts or through the combination of multiple catalysts. Recent advancements for new activation mode development include NHC-catalyzed activation of stable saturated esters (for both α, and β sp3-CH)[1], and cooperative organic (NHC) and transition metal catalysis.[3] Very recently, we have realized single electron chemistry (radical chemistry)[4] for unusual activation of organic molecules using carbene catalysis. Applications of these new activation modes for rapid (essentially one step) assembly of functional molecules for biomedical and agriculture uses have also been carried out either in our laboratories or through collaborations.[5]



Reference

1. Z. Fu, J. Xu, T. Zhu, W. W. Y. Leong, Y. R. Chi*, *Nature Chemistry*, 2013, **5**, 835–839.
2. B-S. Li, et. al. and Y. R. Chi*, *Nature Communications*, 2015, **6**, doi:10.1038/ncomms7207
3. K. Namitharan, T. Zhu, J. Cheng, P. Zheng, X. Li, S. Yang, B-A. Song, Y. R. Chi*, *Nature Communications* 2014, **5**, doi: 10.1038/ncomms4982.
4. Y. Zhang et. al. and Y. R. Chi*, *J. Am. Chem. Soc.*, 2015, **137**, 2416–2419
5. T. Zhu, P. Zheng, C. Mo, S. Yang, B-A. Song, Y. R. Chi, *Nature Communications*, 2014, **5**, doi: 10.1038/ncomms6027.

Radical anion on nitrogen compounds

Zhan Lu *

Department of Chemistry, Zhejiang University, Hangzhou 310027, People's Republic of China
**Corresponding author: luzhan@zju.edu.cn*

Nitrogen-based compounds could be found in numerous bioactive natural products and artificial drugs. Nitro group is a potential good protecting group for nitrogen atoms due to be easily reduced to generate free amine, besides over 200 nitro derivatives have been isolated from plants, fungi, bacteria, and mammals to exhibit a wide range of biological activities including antimicrobial, antituberculosis, antiprotozoal, antitumor, anticancer, and cell signaling properties.[1] Our research[2-6] is based on easily reduced nitrogen compounds, such as nitro compounds, imines, pyridines and so on, to develop new organic transformations, especially asymmetric transformations. We also try to design new catalysts based on nitrogen radical anion, discover the relationship between substrates and catalysts, create catalytic models.

References

1. (a) Parry, R.; Nishinob, S.; Spainb, *J. Nat. Prod. Rep*. 2011, **28**, 152;
   (b) Ju, K. S.; Parales, R. E. *Microbiol. Mol. Biol. Rev*. 2010, **74**, 250.
2. Chen, J.-H.; Xi, T.; Lu, Z. *Org. Lett*. 2014, **16**, 6452.
3. Chen, J.-H.; Xi, T.; Ren, X.; Cheng, B.; Guo, J.; Lu, Z. *Org. Chem. Front*. 2014, **1**, 1306.
4. Wang, C.-F.; Lu, Z. *Org. Chem. Front*. 2015, **2**, 179.
5. Chen, J.-H.; Cheng, B.; Cao, M.-Y. Lu, Z. *Angew. Chem. Int. Ed*. 2015, DOI: 10.1002/anie.201411884.
6. Guo, J.; Chen, J.-H.; Lu, Z. *Chem. Commun*.2015, DOI: 10.1039/C5CC01084E.

Notes

Notes

Notes

Index of presenting authors

Join the world's leading chemistry community

Affiliate membership of the Royal Society of Chemistry is offered to full paying non-member delegates of this conference, at no extra cost*.

As a member we can help you:

Get funding –with travel grants and bursaries to attend the right conferences and events

Tap into a global network – that offers opportunities to promote and share your work, ideas and expertise

Plan and manage your career – with specialist advice, events and development opportunities such as Chartered status

Be the first to know – about the latest innovations and research in your field with access to our top quality publications and other major publishers content

To take advantage of this offer look out for the electronic membership invitation, or simply speak to a member of staff at the conference.

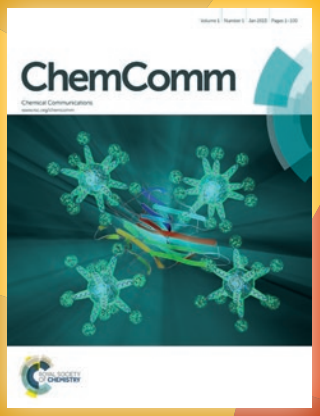
Find out more about membership, go to www.rsc.org/join or contact membership@rsc.org

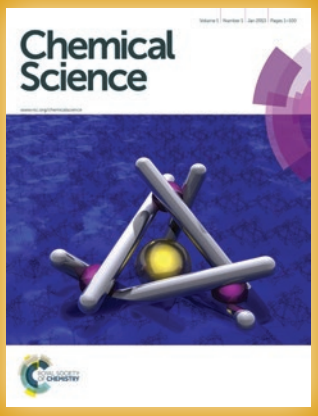
*Duration of membership is until 31 December 2015.
This offer is valid until 31 May 2015.

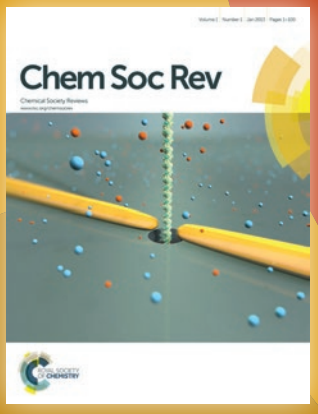
ROYAL SOCIETY OF CHEMISTRY

ROYAL SOCIETY OF CHEMISTRY

Make the most of our publications







As one of the world's leading academic publishers, we produce more than 35 peer-reviewed journals and two magazines, and have over 1,000 books covering everything from medicinal chemistry to nanoscience.

The 2013 Journal Citation Reports® reinforces our exceptional standards*:

- Of the top 20 journals in the multidisciplinary category, six are from the Royal Society of Chemistry. No other publisher has more.
- 83% of our journals now have an IF above 3 – and 33% are above 5.

With content valued by the global scientific community, access is a highlight for our members.

As a member you get free access to:

- One online journal of your choice
- A further 15 free downloads – choose journal article or eBook chapters
- The entire RSC Journals Archive – 260,000 articles across all areas of the chemical science from 1841 – 2007
- Additionally, for just £50 a year (excluding VAT) you can subscribe to any of our other journals online

* Data based on 2013 Journal Citation Reports ®, (Thomson Reuters, July 2014)

Royal Society of Chemistry
www.rsc.org
Registered charity number: 207890

Thomas Graham House
Science Park, Milton Road
Cambridge, CB4 0WF, UK
Tel: +44 (0)1223 420066

Burlington House
Piccadilly, London
W1J 0BA, UK
Tel: +44 (0)20 7437 8656

International Offices
São Paulo, Brazil
Beijing, China
Shanghai, China
Bangalore, India
Tokyo, Japan
Philadelphia, USA

081433