

제18회
유기화학분과회 하계워크샵
제4회
유기화학 튜토리얼 강좌



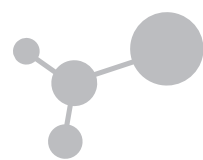
2018년 8월 20 - 21
오크밸리 리조트, 원주



Korean Chemical Society
Division of Organic Chemistry

PROGRAM BOOKLET

<http://kcsorganic.org>



환영합니다



유기분과 하계워크샵 참석 회원님들께,

유기분과 운영진을 대표해서 유기화학분과회 제 18 회 하계워크샵에 참석하신 모든 회원님들을 환영합니다. 유기분과 하계워크샵은 유기분과회의 행사 중 가장 크고 의미 있는 모임입니다. 올해는 강원도 원주시 근처에 있는 오크밸리 리조트에서 진행됩니다. 분과 회원 여러분의 도움과 참여 덕분에 올해에도 성황리에 열릴 수 있게 되어 분과 운영진 모두와 더불어 매우 기쁘게 생각합니다. 월요일 오전에 진행될 하계워크샵의 튜토리얼은 Flow Chemistry와 NMR 구조분석법에 대해 두 분의 전문가께서 각각 맡아서 진행해주시기로 했습니다 (이화여자대학교 김원석, 한국화학연구원 이석근). 강연을 해 주실 두 분 박사님께 이 자리를 빌어 감사드립니다. 또한 다른 일정 때문에 아쉽게도 강연은 할 수 없지만 제7회 젊은 유기화학자 상을 수상하신 부산대학교 주정민 회원께도 축하 드립니다. 올해에는 연구년 때문에 미루어 졌던 제6회 수상자인 중앙대학교 조은진 회원의 강연이 준비되어 있습니다.

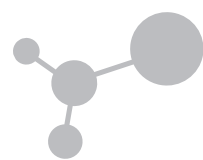
작년에 워크샵의 학술적 의의 고취를 위해 장기자랑 대신 학생 구두발표를 진행하였습니다. 올해에도 작년에 이어 대학원생들로 하여금 그 동안의 연구결과를 소개하는 장소와 기회를 제공하는데 중점을 두었습니다. 또한 우수한 구두 및 포스터 발표자를 선정하고, 선정된 대학원생들에 싱가포르에서 개최될 Junior ACP 학회 참가비를 지원하고자 합니다.

본 행사가 원활히 진행될 수 있도록 어려운 여건에도 기꺼이 여러 형태로 재정 지원을 해 주신 업체 관계자님과 연구책임자님께 유기분과회를 대표해서 감사의 말씀을 드립니다. 또한 본 하계 워크샵 진행을 위해 수고하신 이영호 총무부회장을 비롯한 이선우 학술부회장, 윤창수 홍보부회장, 김학중, 유은정, 김민 운영위원, 도우미 학생들과 한솔오크밸리 리조트 관계자들께도 감사의 말씀을 전합니다. 많은 노력에도 불구하고, 미진한 부분들이 있을 것으로 생각합니다. 향후 개선을 위해, 주저 없이 지적해 주시고 또한 너그러운 마음으로 양해해 주시기를 아울러 부탁드립니다. 본 행사가 분과회원님과 대학원생에게 새롭게 도약할 수 있는 재충전의 기회가 되기를 바랍니다.

환영합니다.

2018년 8월 20일

대한화학회 유기화학분과회 회장 **조 천 규**



PROGRAM SCHEDULE

■ 2018년 8월 20일 (월)

Tutorial Session

09:00 – 09:50 등록

진행 : 김학중 (고려대학교)

09:50 – 10:00 개회사 : 조천규 (한양대학교)

10:00 – 10:50 튜토리얼 강연 I (NMR 강좌) : 이석근 (한국화학연구원)

10:50 – 11:10 Coffee Break

11:10 – 12:00 튜토리얼 강연 II (Flow Chemistry) : 김원석 (이화여자대학교)

12:00 – 13:00 점심식사

Session I

13:00 – 14:00 등록 및 포스터 게시

진행 : 이영호 (POSTECH)

14:00 – 14:30 젊은 유기화학자상 시상 및 기념 강연

(제6회 수상자: 중앙대학교 조은진 시상 및 강연)

(제7회 수상자: 부산대학교 주정민)

Session II

진행 : 이선우 (전남대학교)

14:30 – 15:30 대학원생 발표 – I (10분 발표 + 2분 Q&A; OL001 – OL005)
성명1, 2, 3, 4, 5

15:30 – 15:50 Coffee Break 및 기념촬영

15:50 – 17:40 대학원생 발표 – II (10분 발표 + 2분 Q&A; OL006 – OL014)

17:40 – 18:30 숙소 체크인

18:30 – 19:20 만찬

Poster Session

19:20 – 21:00 포스터 발표

진행 : 유은정 (경희대학교), 김민 (충북대학교)

21:00 – 21:30 감사패 증정, 구두 및 포스터 우수발표자 시상

■ 2018년 8월 21일 (화)

09:30 – 11:00 그룹별 자유토론

11:00 폐회식 및 귀가

What type of research can we do in Organic Chemistry with Modern NMR Techniques now?

Seug-Geun Lee

Department of Chemistry, Hanyang University, Seoul 04763, Republic of Korea

E-mail: leesg@krikt.re.kr

Since NMR technique's first introduction in 1946 by Purcell and Bloch (who received the Nobel Prize in 1952 for their work), NMR spectroscopy has evolved into the key method for the analysis of structure, dynamics, and reactions of molecules. This technique has developed through the introduction of two-dimensional methods (Ernst, 1991 Nobel Prize) and biomolecular research (Wuthrich, 2002 Nobel Prize).

Despite NMR technique's usage in diverse areas of chemistry, its merit does not seem to be acknowledged greatly due to many inferior intrinsic aspects, particularly its sensitivity. However, new NMR techniques, high-field NMR, and demands for cutting edge techniques of analysis seem to change the role of NMR spectroscopy in chemistry. Modern NMR techniques can especially offer unique opportunities to ease the process of performing organic research.

Through this lecture, we will cover the brief history of NMR development as well as various successful applications done in my lab. At the end of this lecture, you will see how practical and accurate this method is.

- 1) Pulsed Field Gradient Experiments
DOSY (Diffusion Ordered Spectroscopy)
- 2) Exchange Spectroscopy(EXSY)
*Activation energy(E_a) *Enthalpy(ΔH^\ddagger) *Entropy(ΔS^\ddagger)
- 3) Double quantum spectroscopy
1D-INADEQUATE (selective excitation)
(Incredible Natural Abundance Double QUAntum Transfer Experiment)
- 4) Quantitative Analysis by NMR Spectroscopy

In the first subject, I will discuss about so-called "NMR-chromatography" which is determined by Pulsed Field Gradient method. Then I will show you how to use EXSY to get physical constants from the equilibrium state and how beneficial selective excitation is. The fourth subject will show you recent new quantitative analysis methods which are either comparable or superior to the conventional methods.

이 석 근 (Sueg-geun Lee)



Address

대전광역시 유성구 원촌동
E-mail: leesg@kRICT.re.kr

Education

Ph.D. (1985) Department of Chemistry, Brown University
M.S. (1978) Department of Chemistry, Yonsei University
B.S. (1976) Department of Chemistry, Yonsei University

Position

2015-Present Visiting Professor, Hanyang University
2012-2015 Visiting Professor, Korea Advanced Institute of Science and Technology (KAIST)
2012-Present Consultant, Korea Research Institute of Chemical Technology (KRICT)
1987-2012 Senior Researcher, Korea Research Institute of Chemical Technology (KRICT)
1985-1987 Post-doc., University of Utah

Representative Publications

1. "CIDNP Evidence for a Hot Carbocation Formed by Electron Transfer Between Two Radicals," S. G. Lee, *J. Chem. Soc., Chem. Commun.*, 1115 (1987).
2. "Triplet-Sensitized Photorearrangements of 2-Phenylallyl Phosphites," W. G. Bentrude, S. G. Lee and et al., *J. Am. Chem. Soc.*, **118**, 6192 (1996).
3. "NMR Study of Intramolecular Exchange in the La(III) Complex of Triethylenetetraaminehexaacetic Acid in Aqueous Solution," S. G. Lee, *Magn. Reson. Chem.*, **38**, 820 (2000).
4. "Complete ^1H and ^{13}C assignments of some epipodophyllotoxin derivatives," Zaesung No and Sueg-Geun Lee, *Magn. Reson. Chem.*, **41**, 283 (2003).
5. "Heteronuclear electronic reference NMR method for the measurement of concentration." S. G. Lee, *Bull. Korean Chem. Soc.*, **28**, 1635 (2007).

Books

1. S.-G. Lee, *Nuclear Magnetic Spectroscopy*, Jayu- Academi Press: Seoul, 2016.
2. S.-G. Lee, *The Analysis of NMR Spectrum*, Hanrimwon Press: Seoul, 2014.

Applications of Flow Chemistry in Organic Synthesis

Wonsuk Kim

Department of Chemistry and Nanoscience, Ewha Womans University, Seoul 03760

E-mail: wonsukk@ewha.ac.kr

In recent years, continuous flow microreactor has been recognized as powerful tools for chemical synthesis from the viewpoint of both academia and industry due to the advantages, such as (1) controlled heat transfer, (2) controlled mixing (both fast and slow) (3) increased solution-solid phase interactions (4) controlled use of high reactive materials, and (5) tailor-made reactor to run serial reactions.¹

Herein, I introduce the concept and applications of flow chemistry in organic synthesis. For examples, a new synthetic method for the synthesis of ketones employing flow microreactor in the presence of acyl chlorides and in situ generated lithium species will be demonstrated. In contrast to standard batch chemistry, over-addition of the organolithium to the ketone for the formation of the undesired tertiary alcohol has been minimized representing a direct approach toward ketones.² In addition, an efficient method for the synthesis of 1-sulfonyl- and sulfamoyl-1,2,3-triazoles which can be serve as a precursor of reactive azavinyl carbenes will be reported using continuous flow microreactor in a short residence time.³ Furthermore, one-flow, multi-step synthesis of *cis*-Diamino Enone from the corresponding alkyne and sulfonyl azide will be demonstrated.

References

¹ (a) Plutschack, M. B.; Pieber, B.; Gilmore, K. *Chem. Rev.* **2017**, *117*, 11796-11893. (b) Porto, R.; Benaglia, M.; Puglisi, A. *Org. Process Res. Dev.* **2016**, *20*, 2-25. (c) Wegner, J.; Ceylan, S.; Kirschning, A. *Adv. Synth. Catal.* **2012**, *354*, 17-57. (d) Wegner, J.; Ceylan, S.; Kirschning, A. *Chem. Commun.* **2011**, *47*, 4583-4592.

² Moon, S.-Y.; Jung, S.-H.; Kim, U. B.; Kim, W.-S. *RSC Adv.* **2015**, *5*, 79385-79390.

³ Kwon, Y.-J.; Won, S.-Y.; Jeon, Y.-K.; Shin, I.; Jeon, H. J.; Lee, S.-g.; Kim, W.-S. *Manuscript in preparation.*

김 원 석 (Wonsuk Kim)

Address

서울특별시 서대문구 이화여대길 52
TEL : 02-3277-2346
E-mail: wonsukk@ewha.ac.kr



Education

Ph.D. (2010) Department of Chemistry, University of Pennsylvania (Prof. Amos B. Smith III)
M.S. (2004) Department of Chemistry, Hanyang University (Prof. Cheon-Gyu Cho)
B.S. (2002) Department of Chemistry, Hanyang University

Position

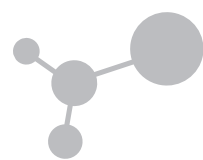
2012-present Assistant/Associate Professor, Ewha Womans University
2011-2012 Post-doc., Massachusetts Institute of Technology (Prof. Timothy F. Jamison)

Representative Publications

1. Kwon, Y.-J.; Jeon, Y.-K.; Sim, H.-B.; Oh, I.-Y.; Shin, I.; Kim, W.-S. "3-Hydroxy-2-(trialkylsilyl)phenyl Triflate: A Benzyne Precursor Triggered via 1,3-C-sp²-O Silyl Migration. *Org. Lett.* **2017**, *19*, 6224-6227.
2. Park, C.-H.; Kwon, Y.-J.; Oh, I.-Y.; Kim, W.-S. "Synthesis of Trisubstituted Pyridines via Chemoselective Suzuki-Miyaura Coupling of 3,5- and 4,6-Dibromo-2-tosyloxypyridines. *Adv. Synth. Catal.* **2017**, *359*, 107-119.
3. Jung, S.-H.; Sung, D.-B.; Park, C.-H.; Kim, W.-S. "Copper-Catalyzed N-Arylation of 2-Pyridones Employing Diaryliodonium Salts at Room Temperature. *J. Org. Chem.* **2016**, *81*, 7717-7724.
4. Moon, S.-Y.; Jung, S.-H.; Kim, U. B.; Kim, W.-S. "Synthesis of Ketones via Organolithium Addition to Acid Chlorides using Continuous Flow Chemistry. *RSC Adv.* **2015**, *5*, 79385-79390.
5. Moon, S.-Y.; Kim, U. B.; Sung, D.-B.; Kim, W.-S. "A Synthetic Approach to N-Aryl Carbamates via Copper-Catalyzed Chan-Lam Coupling at Room Temperature. *J. Org. Chem.* **2015**, *80*, 1856-1865.
6. Moon, S.-Y.; Koh, M.; Rathwell, K.; Jung, S.-H.; Kim, W.-S. "Copper-Catalyzed N-Arylation of tert-butyl N-Sulfonylcarbamates with Diaryliodonium Salts at Room Temperature. *Tetrahedron* **2015**, *71*, 1566-1573.

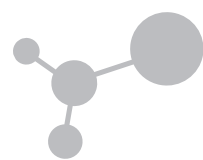


- [OL001] **Yeosan Lee, Jinyoung Park, Seung Hwan Cho***, Generation and Application of (Diborylmethyl) zinc(II) Species: Access to Enantioenriched gem-Diborylalkanes by an Asymmetric Allylic Substitution, *Department of Chemistry, Pohang University of Science and Technology (POSTECH)*
- [OL002] **Yong-Ju Kwon, Wonsuk Kim***, Continuous Flow Synthesis of 1-Sulfonyl and 1-Sulfamoyl-1,2,3-Triazoles, *Department of Chemistry and Nano Science Ewha Womans University*
- [OL003] **Jun-Hyeok Park, Un-Young Kim, Byung-Man Kim, Wang-Hyo Kim, Deok-Ho Roh, Jeong Soo Kim, Tae-Hyuk Kwon***, Molecular Engineering for Enhancement of Photo-, Thermal, and Water Stability of Organic Dyes for Dye-Sensitized Solar Cells, *Department of Chemistry, School of Natural Science, Ulsan National Institute of Science and Technology (UNIST)*
- [OL004] **Hosoowi Lee, Woo-Dong Jang***, Supramolecular Assembly Formed from Bisporphyrin Derivative, *Department of Chemistry, Yonsei University*
- [OL005] **Jaeyeon Lee, Hee-Yoon Lee***, Total Syntheses of Alotaketals A and Phorbaketals, *Department of Chemistry, Korea Advanced Institute of Science and Technology*
- [OL006] **Yuna Kim, Hanseul Lee, Yunmi Lee***, Copper-Catalyzed S_N2' Reduction of Propargylic Chlorides with Diisobutylaluminum Hydride, *Department of Chemistry, Kwangwoon University*
- [OL007] **Da Sol Chung, Jae Sung Lee, U Bin Kim, Sang-gi Lee***, Palladium-Catalyzed Tandem Heck/Divergent Cyclopropanation via Solvent-Driven Regioselective $C(sp^3)$ -H Bond Activation, *Department of Chemistry and Nano Science (BK21 PLUS), Ewha Womans University*
- [OL008] **Yonghyeon Baek, Phil Ho Lee***, Regioselective Synthesis of Indolopyrazines through Sequential Rh-Catalyzed Formal [3+3] Cycloaddition and Aromatization Reaction of Diazoindolinimines with Azirines, *Department of Science, Kangwon National University*
- [OL009] **Sumin Jang, Hyunwoo Kim***, 1H NMR Chiral Analysis of Alcohols at Room Temperature by Chiral Octahedral Gallium Complex, *Department of Chemistry, Korea Advanced Institute of Science and Technology (KAIST)*
- [OL010] **Hanbyul Kim, Su Yeon Choi, Seunghoon Shin***, Asymmetric Synthesis of Dihydropyranones via Au(I)-Catalyzed Intermolecular [4+2] Annulation of Propiolates and Alkenes, *Department of Chemistry and Center for New Directions in Organic Synthesis (CNOS), Hanyang University, 222 Wangsimni-ro, Seongdong-gu, Seoul, 04763 (Korea)*
- [OL011] **Won Jun Jang, Jaesook Yun***, Asymmetric Synthesis of Organoboron Compounds via Copper Catalysis, *Department of Chemistry, Sungkyunkwan University*
- [OL012] **Sourav Sarkar, Mithun Santra, Kyo Han Ahn***, A Two-Photon Active Environment Insensitive Dye with Giant Stokes Shift: An Ideal Platform for Probe Designing and Bio-imaging, *Department of Chemistry, Pohang University of Science and Technology (POSTECH)*
- [OL013] **Donguk Ko, Eun Jeong Yoo***, Pyridinium Zwitterion as a Site-Switchable Dipole, *Department of Applied Chemistry, Kyung Hee University*
- [OL014] **Sikwang Seong, Hyeonggeun Lim, Sunkyu Han***, Biosynthetically Inspired Transformation of (+)-Catharanthine to Post-Iboga Alkaloids, *Department of Chemistry, Korea Advanced Institute of Science & Technology (KAIST); Center for Catalytic Hydrocarbon Functionalizations, Institute for Basic Science (IBS)*



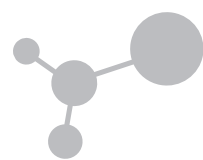
Poster Program

- [PO001] **유현지, 윤소원***, One-Pot Three-Component Synthesis of (Tetrahydro)Quinolines, *Department of Chemistry, Center for New Directions in Organic Synthesis, Hanyang University*
- [PO002] **고태윤, 윤소원***, Pd-Catalyzed Synthesis of (E)-3-Arylmethyleneisoindolin-1-ones, *Department of Chemistry, Center for New Directions in Organic Synthesis, Hanyang University*
- [PO003] **Min Jung Chang, Jung Won Yoon, Shin A Yoon, Chulhun Kang,* Min Hee Lee***, A FRET based ratiometric two-photon mitochondrial pH fluorescent probe, *Department of Chemistry, Sookmyung Women's University*
- [PO004] **Jinhui Joo, Sun Young Park, Jinju Lee, Min Hee Lee***, A development of red-emitting fluorescent probe for imaging of mitochondrial NADH in live cell, *Department of Chemistry, Sookmyung Women's University*
- [PO005] **HyeonOh Shin, Byung-Man Kim, Tae-Hyuk Kwon***, Surface State-mediated Charge Transfer of Cs₂SnI₆ and Its Application in Dye-sensitized Solar Cells, *Department of Chemistry, School of Natural Science, Ulsan National Institute of Science and Technology (UNIST)*
- [PO006] **문다솜, 김성곤***, Stereoselective Palladium-Catalyzed Decarboxylative [4+2] Cycloaddition Reaction of Vinyl Benzoxazinones with Cyclic N-Sulfinamines, *Department of Chemistry, College of Natural Science, Kyonggi University*
- [PO007] **최선영, 김성곤***, Enantioselective organocatalytic Friedel-Crafts reaction of cyclic N-sulfinamines with pyrroles, *Department of Chemistry, College of Natural Science, Kyonggi University*
- [PO008] **김승연, 김성곤***, Stereoselective synthesis of highly functionalized tetrahydroisoquinolines using Lewis acid-catalyzed Friedel-Crafts/Michael cascade reaction, *Department of Chemistry, College of Natural Science, Kyonggi University*
- [PO009] **Hyun-Seok Seo, Hea-jo Kim***, Two Photon-Active Probe for Photodynamic Therapy. *Department of Chemistry, Hankuk University of Foreign Studies*
- [PO010] **Won Joo Lee, Hae-Jo Kim***, A Ratiometric NIR Probe for Mitochondrial Nitroreductase. *Department of Chemistry, Hankuk University of Foreign Studies*
- [PO011] **Sonhwan Kim, Hyeonsu Jeong, Nagendra Nath Yadav, Hyun-Joon Ha***, Synthesis of Lacosamide (Vimpat) and Its Derivatives from Aziridine-(2R)-carboxylate, *Department of Chemistry, Hankuk University of Foreign Studies*
- [PO012] **Youg-Gun Lee, Hyeonsu Jeong, Hyun-Joon Ha,* Jung Woon Yang***, Organocatalyzed asymmetric epoxidation of aziridine-2-ylacrylaldehyde: Synthetic application of chiral vicinal epoxyaziridine, *Department of Chemistry, Hankuk University of Foreign Studies*
- [PO013] **Lingamurthy Macha, Hyun-Joon Ha***, Asymmetric synthesis of piperidine alkaloids microcosamine A and microgrewiapine A from chiral aziridines, *Department of Chemistry, Hankuk University of Foreign Studies*
- [PO014] **Jeongho Kim, Youngmin Kim, Seung Hwan Cho***, Copper-Catalyzed Diastereo- and Enantioselective Addition of 1,1-Diborylalkanes to N,N-Dimethylsulfamonyl Protected Acyclic Aryladimines, *Department of Chemistry, Pohang University of Science and Technology (POSTECH)*
- [PO015] **Chiwon Hwang, Woohyun Jo, Seung Hwan Cho***, Transition-Metal-Free Regioselective Alkylation of Pyridine N-Oxide Using 1,1-Diborylalkanes as Alkylating Reagents, *Department of Chemistry, Pohang University of Science and Technology (POSTECH)*
- [PO016] **Deepak Singh, Hyun-Joon Ha***, Morita-Baylis-Hilman Reaction of Chiral Aziridine Aldehyde and Distereoselective Synthesis of 2,3,4-Trisubstituted Pyrrolidine, *Department of Chemistry, Hankuk University of Foreign Studies*
- [PO017] **Sang-Yun Na, Won Koo Lee, Hyun-Joon Ha***, N-methylative aziridine ring opening and the synthesis of (S)-3-methylamino-3-[(R)-pyrrolidin-3-yl]propanenitrile, *Department of Chemistry, Hankuk University of Foreign Studies*



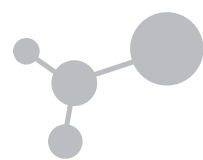
Poster Program

- [PO018] **Jinyoung Park, Seoyoung Choi, Yeosan Lee, Seung Hwan Cho***, Chemo- and Stereoselective Allylboration of Aldehydes and Cyclic Aldimines with Allylic-gem-diboronate Ester, *Department of Chemistry, Pohang University of Science and Technology (POSTECH)*
- [PO019] **Geun Seok Lee, Soon Hyeok Hong***, Visible Light Mediated Ni Catalysis of Triplet Enone Diradicals for Formal Giese Addition of C(sp³)-H Nucleophiles, *Department of Chemistry, College of Natural Sciences, Seoul National University*
- [PO020] **Yeonwoo Jeong, Jeong Woo Hong, Sung Min Kang***, Multipurpose Antifouling Coating of Solid Surfaces with the Sulfated Polysaccharide Fucoidan, *Department of Chemistry, Chungbuk National University*
- [PO021] **Ji-geun Gim, Jeong Tae Lee***, Syntheses of Resveratrol Analogues Containing Heteroatoms, *Department of Chemistry and Institute of Applied Chemistry, Hallym University*
- [PO022] **Ju Mi Lee, Jeong Tae Lee***, Concise Synthesis of Guanidine Containing NSAID Conjugates, *Department of Chemistry and Institute of Applied Chemistry, Hallym University*
- [PO023] **Lee Seul Park, Jeong Tae Lee***, Efficient Syntheses and Antioxidant Activities of Nitrogen Containing Heterocyclic Resveratrol Analogs, *Department of Chemistry and Institute of Applied Chemistry, Hallym University*
- [PO024] **Jong-Gab Jun, Jeong Tae Lee***, Synthesis and Antiinflammatory Activity of Homoisoflavonoids. Kongara Damodar, *Department of Chemistry and Institute of Applied Chemistry, Hallym University*
- [PO025] **민경욱, 서정섭, 고혜민***, Three-Component Reactions of Arynes, Amines, and Nucleophiles via a One-Pot Process, *Department of Bio-Nano Chemistry, Wonkwang University*
- [PO026] **서정훈, 황동욱, 고혜민***, Transition-metal-free synthesis of Aromatic amines via the reaction of benzyne with isocyanates, *Department of Bio-Nano Chemistry, Wonkwang University*
- [PO027] **Kitaek Song, Kunsoon Kim, Daeun Hong, Soon Hyeok Hong***, Development of Highly Versatile and Controllable Ruthenium Based Olefin Metathesis Catalyst, *Department of Chemistry, College of Natural Sciences, Seoul National University*
- [PO028] **정아름, 민선준***, Synthesis of Fused Azacycles via Oxidative C-H Activation, *Department of Applied Chemistry, Hanyang University (ERICA)*
- [PO029] **김지현, 구세영, 정효성, 심인섭, 손수빈, 김수빈, 김형석, 김종승***, Enhancing the Effect of Photodynamic Therapy in Hypoxic Condition by Targeting a Carbonic Anhydrase IX, *Department of Chemistry, Korea University*
- [PO030] **Daeun Hong, Kitaek Song, Kunsoon Kim, Soon Hyeok Hong***, Ring Opening Metathesis Polymerization of Low-Strained Cyclopentene Derivatives Enabled by Highly Active Ruthenium Olefin Metathesis Catalysts, *Department of Chemistry, College of Natural Sciences, Seoul National University*
- [PO031] **Geon Kim, Myungjo J. Kim, Garam Chung, Hee-Yoon Lee,* Sunkyu Han***, (+)-Dimericbiscognienyne A: Total Synthesis and Mechanistic Investigations of the Key Heterodimerization, *Department of Chemistry, Korea Advanced Institute of Science and Technology*
- [PO032] **Sushovan Paladhi, Amol P. Jadhav, In-Soo Hwang, Si-Joon Park, Sang Yeon Park, Choong Eui Song***, The Mimic of Type II Retro-Aldolase Chemistry: Kinetic Resolution of β -Hydroxy Carbonyl Compounds via Enantioselective Retro-Aldol Reaction, *Department of Chemistry, Sungkyunkwan University*
- [PO033] **Jae Hun Sim, Jin Hyun Park, Pintu Maity, Somlee Park, Young Jun Chang, Veeramanocharan Ashokkumar, Choong Eui Song***, Water-Enabled Catalytic Asymmetric Michael Reactions of Unreactive Nitroalkenes: Synthesis of Chiral GABA-Analogs with All-Carbon Quaternary Stereogenic Centers, *Department of Chemistry, Sungkyunkwan University*



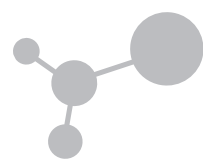
Poster Program

- [PO034] **Yuseop Lee, Mu-Hyun Baik,* Yunho Lee,* Hyunwoo Kim***, Fe(III)-Complexes for the Selective Formation of Cyclic Carbonates from CO₂ and Internal Epoxides, *Department of Chemistry, Korea Advanced Institute of Science and Technology*
- [PO035] **Geunho Choi, Soon Hyeok Hong***, Selective Monomethylation of Amines Using Methanol as a Sustainable C1 Reagent, *Department of Chemistry, College of Natural Sciences, Seoul National University*
- [PO036] **Eunhye Hwang, Hyun-Tak Kim, Wonjoo Jin, Kangmin Lee, Kwanyong Seo,* Tae-Hyuk Kwon***, Pt(II) Complexes with High Emission Quantum Efficiency for Effective Photon Down-shifting on Silicon Solar Cells, *Department of Chemistry, Ulsan National Institute of Science and Technology (UNIST)*
- [PO037] **Kwangho Yoo, Hyojin Park, Byunghyuck Jung,* Min Kim***, Development of an Amino Acid Based Transient Directing Group for Pd-Catalyzed C-H Arylation and Their Synthetic Application, *Department of Chemistry, Chungbuk National University*
- [PO038] **Kwangho Yoo, Narae Han, Min Jae Shin,* Jae Sup Shin,* Min Kim.***, Fine Tuning of Polydiacetylene in Molecular Level for PDA Sensors, *Department of Chemistry, Chungbuk National University*
- [PO039] **Dopil Kim, Jooyeon Lee, Sangdon Choi, Min Kim***, Introducing Phenylacetylene Moiety into Metal-Organic Hybrid Materials, *Department of Chemistry, Chungbuk National University*
- [PO040] **Hyojin Park, Jooyeon Lee, Chinnadurai Satheeshkumar, Myungeun Seo,* Min Kim***, Synthesis of Vinyl-Functionalized Metal-Organic Frameworks and Their Applications, *Department of Chemistry, Chungbuk National University*
- [PO041] **Seongwoo Kim, Hyojin Park, Min Kim***, Practical Postsynthetic Ligand Exchange using Defective Metal-Organic Frameworks, *Department of Chemistry, Chungbuk National University*
- [PO042] **Jung Tae Han, Jaesook Yun***, Enantioselective Boryllation of Vinyl Arenes and its Application to Direct Stereoconvergent Transformation, *Department of Chemistry, Sungkyunkwan University*
- [PO043] **Jiseon Kim, Amit Sharma, Won Young Kim, Jihyeon Kim, Taeho Jeong, Inseob Shim, Kyoung Sunwoo, Geun Young Park, Jong Seung Kim***, A new indomethacin conjugated fluorescent probe for selective imaging of cancer-specific COX-2, *Department of Chemistry, Korea University*
- [PO044] **Myung Sun Ji, Amit Sharma, Kyoung Sunwoo, Hyeong Seok Kim, Jinwoo Shin, Geun Young Park, Soobin Kim, Jong Seung Kim***, A ratiometric fluorescence sensor for detection of bio-thiol in solid tumors, *Department of Chemistry, Korea University*
- [PO045] **Taecheon Kim, Stefan J. McCarver, Chulbom Lee, David W. C. MacMillan***, Sulfonamidation of Aryl and Heteroaryl Halides through Photosensitized Nickel Catalysis, *Department of Chemistry, Seoul National University & Princeton University*
- [PO046] **온누리, 김정곤***, Mechanochemical Post-Polymerization Modification : Solvent Free Solid-State Synthesis of Functional polymer, *Department of Chemistry and Institute of Physical Science, Chonbuk National University*
- [PO047] **Sikwang Seong, Hyeonggeun Lim, Sunkyu Han***, Biosynthetically Inspired Transformation of (+)-Catharanthine to Post-Iboga Alkaloids, *Department of Chemistry, Korea Advanced Institute of Science & Technology (KAIST)*
- [PO048] **Chae Gyu Lee, Byeong-Su Kim,* Tae-Hyuk Kwon***, Iridium Complexes Encapsulated in Redox-Sensitive Self-Cross-Linked Nanogels for Efficient Photodynamic Therapy, *Department of Chemistry, Ulsan National Institute of Science and Technology (UNIST)*
- [PO049] **Sang Weon Roh, Chulbom Lee***, Synthetic Studies toward (+)-Fendleridine Using a Metal-Catalyzed Cascade Cyclization Approach, *Department of Chemistry, Seoul National University*



Poster Program

- [PO050] **Subin Park, Yunmi Lee***, Cu-Catalyzed (Hetero)aryl Amine Addition to Disubstituted Olefins, *Department of Chemistry, Kwangwoon University*
- [PO051] **TaeWoo Kim, Eun Jung Choi, Hwi Hyun Moon, Eun Ho Choi, Chang Suk Oh, Jang Whan Seok, Changsik Song***, Aggregation-Induced Emission and Ion Detection Properties of Hydrazone-based Materials, *Department of Chemistry, Sungkyunkwan University*
- [PO052] **Hye Jin Cho, Kyung-su Kim, Seonggyun Ha, Sun Gu Song, Juhyen Lee, Changsik Song***, Supramolecular Polymerization with Hydrazone-based Molecular Building Blocks: Control of Chirality with Alkyl Substituent, *Department of Chemistry, Sungkyunkwan University*
- [PO053] **Dingxi Li, Jaesook Yun***, Construct Borylated Benzannulated Nitrogen Heterocycles (cis-Indolines or cis-1-Benzo[b]azepines) via Copper-Catalyzed Intramolecular Cyclization, *Department of Chemistry, Sungkyunkwan University*
- [PO054] **Hyun-Tak Kim, Tae-Hyuk Kwon***, Carbon-Heteroatom Bond Formation by Ultrasonic Chemical Reaction for Energy Storage System, *Department of Chemistry, Ulsan National Institute of Science and Technology (UNIST)*
- [PO055] **전태홍, 김장엽, 조천규***, Total Syntheses of Aristotelia Alkaloids, *Department of Chemistry, Hanyang University*
- [PO056] **김영석, 이은성***, A remarkably stable radical zwitterion derived from N-heterocyclic carbene nitric oxide, *Department of Chemistry, Pohang University of Science and Technology*
- [PO057] **Woo-Hyung Kim, Jang-yeop Kim, Cheon-Gyu Cho***, Total synthesis of Ningalin C, Center for New Directions in Organic Synthesis, *Department of Chemistry, Hanyang University*
- [PO058] **왕성동, 조천규***, Total synthesis of (±)-clivonine, Center for New Directions in Organic Synthesis, *Department of Chemistry, Hanyang University*
- [PO059] **이준호, 김호미, 조천규***, Internal H-bonding mediated asymmetric intramolecular Diels-Alder reaction of dienophile-tethered-2-pyrone and formal synthesis of (+)-aplykurodinone-1, *Department of Chemistry, Hanyang University*
- [PO060] **Jeong-Hwa Kim, Dong-Hyun Kim, Cheon-Gyu Cho***, Total Syntheses of (-)-tubifolidine and Uleine, *Department of Chemistry, Hanyang University*
- [PO061] **이지인, 박하현, 정병혁***, 구리 촉매와 phosphino-oxazoline 리간드를 이용한 입체선택적 1,4-알킬 첨가 반응, *School of Basic Science, Daegu Gyeongbuk institute of Science and Technology*
- [PO062] **Ek Raj Baral, Jeung Gon Kim***, Diphenyl Carbonate: A Highly Reactive, Practical, and Safe Carbonyl Source for the Synthesis of Cyclic Carbonates, *Department of Chemistry and Research Institute of Physics and Chemistry, Chonbuk National University*
- [PO063] **Youngnam Lee, Jong-In Hong***, Development of Thermally Activated Delayed Fluorescence Emitters Using Intrinsically Distorted N-Heterocyclic Electron Acceptor, *Department of Chemistry, Seoul National University*
- [PO064] **이정현, 장우동***, Control of Ion Bindings in Oligo Ethylene glycol Strapped Porphyrin Receptors, *Department of Chemistry, Yonsei University*
- [PO065] **Jung Ho Joe, Woo Dong Jang***, Self-Assembled Structure of Dendritic-linear Block Copolymer, *Department of Chemistry, Yonsei University*
- [PO066] **Yon Namkoong, Jong-in Hong***, BODIPY-based Fluorescence Turn-On Probe for Electrochemiluminescent Detection of Hydrogen Peroxide, *Department of Chemistry, Seoul National University*
- [PO067] **Dae Kyum Kim, Chanyoung Maeng, Phil Ho Lee***, One-Pot Synthesis of Indolizines through Sequential Rh-Catalyzed [2+1]-Cyclopropanation, Pd-Catalyzed Ring Expansion, and Oxidation Reactions from Pyridotriazoles and 1,3-Dienes, *Department of Chemistry, Kangwon National University*



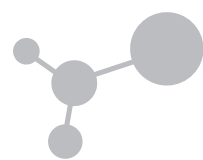
Poster Program

- [PO068] **Dahee Park, Kyusik Um, Phil Ho Lee***, Synthesis of Bicyclic Isothiazoles through an Intramolecular Rh-Catalyzed Transannulation of Cyanothiadiazoles, *Department of Chemistry, Kangwon National University*
- [PO069] **Hyung Jin Seo, Gi Uk Han, Phil Ho Lee***, Synthesis of Imidazopyridines from Cu-Catalyzed, Formal Aza-[3+2] Cycloaddition Reaction of Pyridine Derivatives with α -Diazo Oxime Ethers, *Department of Chemistry, Kangwon National University*
- [PO070] **Kyungsup Lee, Gi Hoon Ko, Phil Ho Lee***, Synthesis of Indolo-1,2-Benzothiazines via Sulfoximines and 3-Diazoindolin-2-imines, *Department of Chemistry, Kangwon National University*
- [PO071] **Seungcheol Lee, Gi Hoon Ko, Phil Ho Lee***, Synthesis of Dihydrophosphaisocoumarins via a Pd-Catalyzed Oxidative Cyclization of Arylphosphonic Acids with 1,3-Dienes, *Department of Chemistry, Kangwon National University*
- [PO072] **Jeong Yun Lee, Sang Hoon Han, Phil Ho Lee***, Synthesis of 5,n-Fused Thiophenes via Rhodium-Catalyzed Intramolecular Transannulation Reaction of Alkynyl Thiadiazole, *Department of Chemistry, Kangwon National University*
- [PO073] **Sejin Jang, Chanyoung Maeng, Phil Ho Lee***, Synthesis of Multisubstituted Allenes, Furans, and Pyrroles through Palladium-Catalyzed Substitution and Cycloisomerization in one pot, *Department of Chemistry, Kangwon National University*
- [PO074] **Juhee Hahm, Gi Uk Han, Phil Ho Lee***, Synthesis of Benzofulvene Derivatives using Rh-Catalyzed Transannulation of Enynyl Triazoles, *Department of Chemistry, Kangwon National University*
- [PO075] **Juyoung Heo, Kyusik Um, Phil Ho Lee***, Rh-Catalyzed Transannulation of 1,2,3-Thiadiazoles via Alkenes for the Synthesis of Dihydrothiophenes and Thiophenes, *Department of Chemistry, Kangwon National University*
- [PO076] **Yong Joo Yun, Sang Hoon Han, Phil Ho Lee***, Synthesis of Isothiazole Derivatives through Rh-Catalyzed Transannulation of 1,2,3-Thiadiazoles with Nitriles, *Department of Chemistry, Kangwon National University*
- [PO077] **조수정, Lee Thi Thuy, 정연우, 강성민, 고상원, 최준식, 조우경***, Spray Coating of Brown Algae-Derived Fucoidan for Antibacterial Applications, *Department of Chemistry, Chungnam National University*
- [PO078] **Joonho Park, Jong-In Hong***, Electrochemiluminescent chemodosimeter for H₂S based on an iridium(III) complex, *Department of Chemistry, Seoul National University*
- [PO079] **조명기, 조재형, 김환명***, A Two-photon Ratiometric Probe for Quantitative Monitoring of hNQO1 in Colon Tissues, *Department of Energy System Research, Ajou University*
- [PO080] **최현진, 김원태, 김환명***, Two-Photon Ratiometric Probe for Monitoring Hydrogen Polysulfides and Its Application in Parkinson's Disease Model, *Department of Energy System Research, Ajou University*
- [PO081] **이동준, 김환명***, Ratiometric two-photon probe for Ca²⁺ and its application in spinal cord injury model, *Department of Energy System Research, Ajou University*
- [PO082] **김윤지, 김환명***, A two-photon fluorescent probe for γ -glutamyltranspeptidase, *Department of Energy System Research, Ajou University*
- [PO083] **박상준, 강지수, 김환명***, A Two-Photon Ratiometric Probe for Carboxylesterase-2, *Department of Energy System Research, Ajou University*
- [PO084] **Kyeong-Im Hong, Sung-Hyun Park, Sung Min Lee, Injae Shin* Woo-Dong Jang***, ES IPT based pH-Sensitive Fluorescent Probe and Its applications, *Department of chemistry, Yonsei University*
- [PO085] **Eunjeong Cho, Aravindan Jayaraman, Sunwoo Lee***, Selective synthesis of α,α -dibromoketones and 1,2-diketone from the reaction with alkyne and dibromoisocyanuric acid, *Department of Chemistry, Chonnam National University*



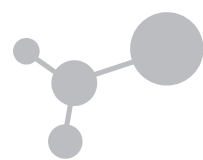
Poster Program

- [PO086] **Subeen Yu, Jeongah Lim, Sunwoo Lee***, Synthesis of Methylthiomethyl Esters from Carboxylic acid, *Department of Chemistry, Chonnam National University*
- [PO087] **Myungjin Kim, Han-Sung Kim, Sunwoo Lee***, One-Pot Synthesis of S-Aryl thioester via Pd-Catalyzed Carbonylation and C-S Coupling, *Department of Chemistry, Chonnam National University*
- [PO088] **SeHyeon Han, Jieun Lee, Sunwoo Lee***, Decarboxylative Coupling of Alkynoic Acids for the Selective Synthesis of Homoisoflavonoids and Flavones, *Department of Chemistry, Chonnam National University*
- [PO089] **Eunhye Lee, Xingshu Li, Juyoung Yoon***, Supramolecular Approach to Overcome the Limitations of Photodynamic Cancer Therapy Using Nanotheranostics, *Department of Chemistry and Nano Science, Ewha Womans University*
- [PO090] **Myungjun Park, Kayoung Jeon, Myeonghwa Jeong, Jaejun Hwang, Youngchan Bang, Bongjin Moon***, Synthesis of new lithium-ion battery electrolyte additives, *Department of Chemistry, Sogang University*
- [PO091] **Joonoh Park, Seongmin Jeon, Sunkyu Han***, Toward the Total Synthesis of Flueggeine A and C, *Department of Chemistry, Korea Advanced Institute of Science and Technology (KAIST)*
- [PO092] **Geonji Kim, Kyungchan Min, Bongjin Moon***, Visible Light Mediated ATRC/ATRP by Phenothiazine Dyes, *Department of Chemistry, Sogang University*
- [PO093] **Jiho Park, Jae-ung Lee, Han Bin Oh,* Bongjin Moon***, Synthesis of p-(Benzenesulfonylmethyl)-benzoate-based Mass Tag for Free Radical-Initiated Peptide Sequencing Mass spectrometry (FRIPS-MS), *Department of Chemistry, Sogang University*
- [PO094] **정다정, 김지원, 이상기***, Transition-Metal-Free Chemo- and Regioselective C(sp²)-H Bond Insertion of 2-Naphthol with Diazoacetate, *Department of Chemistry and Nano Science (BK 21 Plus), Catalysis Research Laboratory, Ewha Womans University*
- [PO095] **Sangbin Jeon, Jinwoo Lee, Sunkyu Han***, Recent Progress toward the Total Synthesis of (-)-Flueggeine D, *Department of Chemistry, Korea Advanced Institute of Science and Technology (KAIST), Center for Catalytic Hydrocarbon Functionalization, Institute of Basic Science (IBS)*
- [PO096] **Deokhee Jo, Sunkyu Han***, Total Syntheses of Spirocyclic PKS-NRPS-based fungal metabolites, *Department of Chemistry, Korea Advanced Institute of Science and Technology (KAIST), Center for Catalytic Hydrocarbon Functionalization, Institute of Basic Science (IBS)*
- [PO097] **김연수, 봉수지, 조용선, 정영훈***, Total Synthesis of (+)-DMDP and (+)-Hyacinthacine A2, *School of Pharmacy, Sungkyunkwan University*
- [PO098] **정준민, 김다은, 고수연, 남기범, 박현주, 정영훈***, Synthesis and Biological Evaluation of Hydroxamates as Selective HDAC6 inhibitors, *School of Pharmacy, Sungkyunkwan University*
- [PO099] **김경목, 정규성***, Carbohydrate recognition through an Aromatic Hybrid foldamer With Extended cavity and sensor of chiral molecules, *Department of Chemistry, Yonsei University*
- [PO100] **채우정, 정규성***, An On-off Fluorescence Sensor for Detecting Trace Water using Aromatic Hybrid Foldamers, *Department of Chemistry, Yonsei University*
- [PO101] **Chai-heon Lee, Tae-Hyuk Kwon***, Enhancing ROS Generation via Photon Energy Transfer of Ir(III) Complex for Low Energy Photodynamic Therapy, *Department of Chemistry, Ulsan National Institute of Science and Technology (UNIST)*
- [PO102] **Le Minh Hoang, Do Tien Dung, Chang Ho Oh***, Synthesis of Lophirone F Hexamethyl Ether, *Department of Chemistry, Research Institute of Natural Sciences, Hanyang University*
- [PO103] **Dong Hwan Oh, Raveendra jillella, Chang Ho Oh***, Au-catalyzed tandem reaction of 2-bisalkynylanilines with aldehyde: an efficient access to 2,2'-disubstituted bisindolylmethanes, *Department of chemistry, Center for New Directions in Organic Synthesis, Hanyang University*



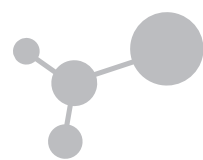
Poster Program

- [PO104] **Juyeon Kang, Chang Ho Oh***, Mechanistic study of gold-catalyzed Synchronized cyclization of Bispropargylic carboxylates, *Department of Chemistry and Research Institute of Natural Science, Hanyang University*
- [PO105] **Yong Woong Jun, Kyeong Hwan Kim, Kyo Han Ahn***, Ratiometric Two-Photon Fluorescent Probe for Tracking Lysosomal ATP, *Department of Chemistry, Pohang University of Science and Technology (POSTECH)*
- [PO106] **정록암, 엄재훈, 공진택, 이희승***, 3D Molecular Architectures with Concave-Faced Cuboid Shape by the Self-Assembly of Chimeric Foldamer, *Department of Chemistry, Korea Advanced Institute of Science and Technology*
- [PO107] **Tamima Umme, Subhankar Singha, Kyo Han Ahn***, Two-photon Ratiometric Fluorescent Probe for Bisulfite Detection, *Department of Chemistry, Pohang University of Science and Technology (POSTECH)*
- [PO108] **Zi Xuan, Yu Lim Lee, Sang-gi Lee***, Dual Rh(II)/Pd(0) Relay Catalysis for One-pot Construction of Heterocycles having Quaternary Carbon Center, *Department of Chemistry and Nanoscience (BK21 Plus), Catalysis Research Laboratory, Ewha Womans University*
- [PO109] **Le Thuy Quynh, Seon Mi Lee, Oh Chang Ho***, Synthesis of Taxamairin B: Use of Au, Pt-Catalyzed Cyclization Reaction, *Department of Chemistry, Center for New Directions in Organic Synthesis, Hanyang University*
- [PO110] **Hyun Ji Jeon, Su Min Park, Sang-gi Lee***, Ligand-Controlled Stereodivergent Palladium Catalysis for the Synthesis of Stereoisomeric Spiro-Furanindolines, *Department of Chemistry and Nanoscience (BK21 Plus), Ewha Womans University*
- [PO111] **Ji Hwan Eom, Yeonwoo Jeong, Sung Min Kang, Woo Kyung Cho***, Antiplaetlet coating with poly ((3-methacryloylamino)propyl-dimethyl(3-sulfopropyl)ammonium hydroxide) on titanium dioxide and stainless steel, *Department of Chemistry, Chungnam National University; Department of Chemistry, Chungbuk National University*
- [PO112] **Mithun Santra, Mingchong Dai, Kyo Han Ahn***, ESIPT Based Organic Dye Nanoparticles and Their Shape-Dependent Luminescence Behavior, *Department of Chemistry, Pohang University of Science and Technology (POSTECH)*
- [PO113] **Hong Ju Yang, Jeong Hun Sohn***, Oxidative dehydrosulfurative azolation of 3,4-dihydropyrimidine-1H-2-thions, *Department of Chemistry, Chungnam National University*
- [PO114] **Jungwook Kim, Youngkyoung Cho, Yeseul Park, Tae Hoon Lee, Hakwon Kim***, Synthesis of Epimeric Isomers of Spinasterol, Dihydroergosterol, Ergosterol and Their Glycosides and Anti-inflammatory Activities, *Department of Applied Chemistry and Global Center for Pharmaceutical Ingredient Materials, Kyung Hee University*
- [PO115] **Seunghyun Choi, Inseok Ko, Jisue Lee, Taehoon Lee, Hakwon Kim***, Synthesis of heterocycle-fused 1,4-naphthoquinone and its toxicity to HeLa cells, *Department of Applied Chemistry and Global Center for Pharmaceutical Ingredient Materials, Kyung Hee University*
- [PO116] **Heejae Choi, Hyunjin Lee, Taehoon Lee, Hakwon Kim***, Pyrazole- and pyrazolone-fused naphthol derivatives and Antioxidant Acitivity, *Department of Applied Chemistry and Global Center for Pharmaceutical Ingredient Materials, Kyung Hee University*
- [PO117] **Lucy Ping, JungHwa Han, JungMin Bak, Suin Park, Jean Bouffard***, N-Heterocyclic Carbene-Mediated Ring Contractions of p- and o-Quinones, *Department of Chemistry and Nano Science, Ewha Womans University*
- [PO118] **Deok-Ho Roh, HyeonOh Shin, Hyun-Tak Kim, Tae-Hyuk Kwon***, Ultrasonic Spray Chemistry: Synthesis of Film-like Microporous Materials and Their Energy Storage Application, *Department of Chemistry, School of Natural Science, Ulsan National Institute of Science and Technology (UNIST)*



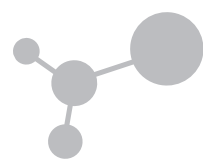
Poster Program

- [PO119] **Ji Hye Kang, Choon Woo Lim***, Synthesis of selenophene-based hydrophobic fluorescent sensor probe for reactive oxygen species (ROS), *Department of Chemistry, College of Life Science and Nano technology, Hannam University*
- [PO120] **Ji Yeon Heo, Choon Woo Lim***, Development of benzoquinone based fluorescent probe for detection of reactive oxygen species, *Department of Chemistry, College of Life Science and Nano technology, Hannam University*
- [PO121] **Seo Ra Kim, Choon Woo Lim***, microwave-assisted efficient H/D exchange methods of 9H-carbazole, 2-phenylpyridine as organic light emitting materials, *Department of Chemistry, College of Life Science and Nano technology, Hannam University*
- [PO122] **Nguyen Huong Quynh, Seunghoon Shin***, Redox Neutral Access to α^4 , α^6 -Synthons via Sulfoxide-Mediated Oxidation of (Di)enynamides, *Department of Chemistry and Center for New Directions in Organic Synthesis, Hanyang University*
- [PO123] **Nguyen Hoang Nguyen, Seunghoon Shin***, An unexpected oxidation of ynamides with m-CPBA followed by asymmetric trans-acetalization catalyzed by chiral phosphoric acid, *Department of Chemistry and Center for New Directions in Organic Synthesis, Hanyang University*
- [PO124] **Seung Woo Kim, Tae-woong Um, Seunghoon Shin***, Metal-Free Iodine-Catalyzed Oxidation of Ynamides and Diaryl Acetylenes into 1,2-Diketo Compounds, *Department of Chemistry, Centre for new Directions in Organic Synthesis (CNOS), Hanyang University*
- [PO125] **권예랑, 이영호*, 박재욱***, Synthesis of N-Acylimines from N-H imines and Acyl Alkyl Carbonates, *Department of Chemistry, POSTECH*
- [PO126] **Jin Yong Park, Young Ho Rhee*, Jaiwook Park***, Synthesis of Half-Sandwich Ruthenium Complexes Containing a Sterically Demanding Cyclopentadienyl Ligand, *Department of Chemistry, POSTECH (Pohang University of Science and Technology)*
- [PO127] **이우형, 김은민, 강은수, 박수은, 주정민***, Synthesis of C2-Alkenylated Pyrroles by Electronically Complementing Ligand Systems, *Department of Chemistry and Chemistry Institute of Functional Materials, Pusan National University*
- [PO128] **Ju Young Lee, Hyunju Park, Eun Jung Yoo***, Palladium-Catalyzed [4+2] Cycloadditions of N-aromatic Zwitterions for the Construction of Fused Heterocyclic Compounds, *Department of Applied Chemistry, Kyung Hee University*
- [PO129] **Dong Guk Nam, Do Hyun Ryu***, Total synthesis of cytotoxic active natural product from Cinnamomum subavenium via MBH ester, *Department of Chemistry, Sungkyunkwan University*
- [PO130] **Su Yong Shim, Yuna Choi, Do Hyun Ryu***, Chiral Lewis Acid Catalyzed Enantioselective Synthesis of Cyclobutanones via Tandem Cyclopropanation/Semi-Pinacol Rearrangement, *Department of Chemistry, Sungkyunkwan University*
- [PO131] **Taehyeong Kim, Anipireddy Venkateswarlu, Do Hyun Ryu***, Highly Enantioselective Allylation of Aldehydes Catalyzed by a Chiral Oxazaborolidinium Ion, *Department of Chemistry, Sungkyunkwan University*
- [PO132] **Ki-Tae Kang, Sang Hyun Park, Do Hyun Ryu***, Enantioselective Strecker reaction of Aldimines with Chiral Oxazaborolidinium Ion Activated Trimethylsilyl Cyanide, *Department of Chemistry, Sungkyunkwan University*
- [PO133] **이주열, 김휘, 류도현***, One-Pot Synthesis of 4,6-Substituted α -Pyrone and α -Pyridones via Mercury(II)-Mediated Decarboxylative Dehydrogenation Reactions, *Department of Chemistry, Sungkyunkwan University*
- [PO134] **Eun Hye Kang, Choon Woo Lim***, pH-controlled pseudo-rotaxane formation of α -cyclodextrin with bis(hydroxymethyl triazolium)octane iodide, *Department of Chemistry, College of Life Science and Nano-technology, Hannam University*



Poster Program

- [PO135] **Danim Lim, Hee-Seung Lee***, Unusual Hexagonal semi-tubular structure derived by self-assembly of β -helical foldamer, *Department of Chemistry, Center for Multiscale Chiral Architectures (CMCA), Korea Advanced Institute of Science and Technology (KAIST)*
- [PO136] **이지윤, 김혜지, De Nirupam, 유은정***, Unprecedented cycloadditions to contract N-heterocycles; Beyond Corey-Chaykovsky Reactions, *Department of Applied Chemistry, Kyung Hee University*
- [PO137] **Jin Hee Cho, Sangmoon Byun, Ahra Cho, B. Moon Kim***, Chemoselective synthesis of unsymmetrical secondary amines from benzonitrile and nitroalkanes using bimetallic PdPt-Fe₃O₄ NPs, *Department of Chemistry, College of Natural Science, The Research Institute of Basic Sciences, Seoul National University*
- [PO138] **이영준¹, 신민철², 김은하^{2*}, 박승범^{1,3*}**, Development of hypoxia detecting fluorescent probe based on conjugating hypoxia-sensitive moiety with Seoul-Fluor, ¹*Department of Chemistry, Seoul National University*; ²*Department of Molecular Science and Technology, Ajou University*; ³*Department of Biophysics and Chemical Biology, Seoul national University*
- [PO139] **Hyungi Kim, Sang-kee choi, Eunha Kim***, Photophysical property study of C-1, C-3 and C-7 modified Indolizine for versatile fluorescent material application, *Department of molecular science and technology, Ajou University*
- [PO140] **Ahra Cho, Sangmoon Byun, Jin Hee Cho, B. Moon Kim***, Alloy AuPd-Fe₃O₄ nanoparticles towards oxidative esterification of 5-hydroxymethylfurfural under mild conditions, *Department of Chemistry, College of Natural Science, The Research Institute of Basic Sciences, Seoul National University*
- [PO141] **Dong Yun Kang, Khyarul Alam, Jin Kyoong Park***, Platinum Catalyzed 1,3-aryl migratory reaction of 2,3-Diaryl indole from ortho-Alkynyl-N-Aryl-N-sulfonylanilines, *Department of Chemistry, Pusan National University*
- [PO142] **Khyarul Alam, Jin Gyeong Kim, Jin Kyoong Park***, TfOH-Promoted Regiodivergent Intramolecular Cycloisomerizations of Ynenamines to Diversified Fused Indoles, *Department of Chemistry, Pusan National University*
- [PO143] **최상기, 김현기, 김은하***, The Aggregation-Induced Emissive Fluorophore Kaleidolizine, *Department of Molecular Science and Technology, School of Engineering, Ajou University*
- [PO144] **Bhawna Barpuzary, Mijin Kim, Young Ho Rhee***, A Synthetic Study Towards Saccharomicin: Asymmetric Synthesis of Saccharosamine-Rhamnose Fragment, *Department of Chemistry, Pohang University of Science and Technology (POSTECH)*
- [PO145] **Sungbeom Seo, Kyu-Sung Jeong***, Anion Encapsulation and Transport with Aromatic Oligomers that containing Hydrogen- and Halogen- bond Donor groups, *Department of Chemistry, Yonsei University*
- [PO146] **Changmuk Kang¹, Ji Yeon Ryu², Junseong Lee², Sukwon Hong^{1,3*}**, Bifunctional N-heterocyclic carbene complexes with Pd-arene interaction for Pd-catalyzed amination, ¹*Department of Chemistry, GIST*; ²*Department of Chemistry, Chonnam National University*; ³*School of Materials Science and Engineering, GIST*
- [PO147] **Wooyong Seong, Sukwon Hong***, Urea Effects in Salen Aluminum Complex for Cyclic Carbonates Synthesis, *Department of Chemistry, Gwangju Institute of Science and Technology (GIST)*
- [PO148] **이상현, 이흥수, 이희윤***, Asymmetric Total Synthesis of (+)-Waihoensene, *Department of Chemistry, Korea Advanced Institute of Science and Technology (KAIST)*
- [PO149] **Yuna Jung¹, Dokyoung Kim^{1,2,3,*}**, Protein Labeling Using Blue-Fluorescent Emitting BODIPY derivatives, ¹*Department of Biomedical Science, Graduate School, Kyung Hee University*; ²*Department of Anatomy and Neurobiology, College of Medicine, Kyung Hee University*; ³*Center for Converging Humanities, Kyung Hee University*



Poster Program

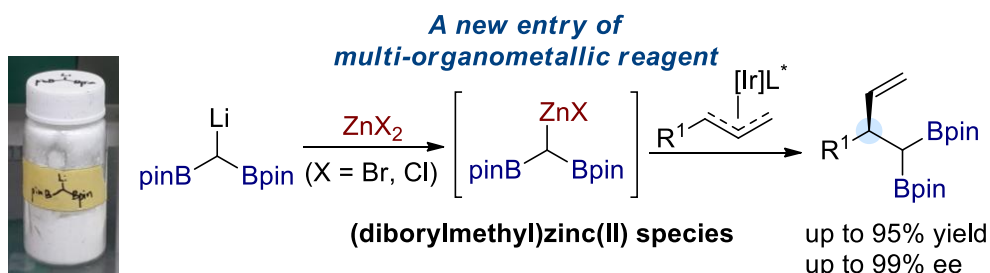
- [PO150] **Minsoo Lee, Hyun-Tak Kim, Ji Hoon Seo, Kwanyong Seo, Tae-Hyuk Kwon***, Toward Efficient Formation of Electrical Double Layer in Optoelectronic Devices by Controlling the Ionic Mobility, *Department of Chemistry, UNIST; Department of Energy Engineering, UNIST*
- [PO151] **Na Hee Kim, Dokyoung Kim***, A fluorescent probe for detection of Gold(III) ions based on the AlEgen disaggregation, *Department of Biomedical Science, Graduate School, Kyung Hee University; Department of Anatomy and Neurobiology, College of Medicine, Kyung Hee University; Center for Converging Humanities, Kyung Hee University*
- [PO152] **Thomas Taehyung Kim, Sunkyu Han***, Towards the Total Synthesis of Herquiline A & B, *Department of Chemistry, KAIST; Center for Catalytic Hydrocarbon Functionalizations, IBS*
- [PO153] **Jung Seung Nam¹, Juhye Kang^{1,2}, Myeong-Gyun Kang^{1,3}, Hyun-Woo Rhee^{3,*}, Mi Hee Lim^{2,*}, Tae-Hyuk Kwon^{1,*}**, Photo-Therapeutics with Ir(III) Complexes toward Two Diseases: Cancer & Alzheimer, *¹Department of Chemistry, UNIST; ²Department of Chemistry, KAIST; ³Department of Chemistry, Seoul National University*
- [PO154] **Jungmin Kwon, B. Moon Kim***, Synthesis of 2-dialkyl-, 2-alkylaryl- or 2-diarylaminoarenesulfonyl fluorides via sulfuranyl fluoride incorporation into arynes, *Department of Chemistry, College of Natural Sciences, Seoul National University*
- [PO155] **Yeolib Jeong, Minjoong Shin, Myungeun Seo, Hyunwoo Kim***, Triaryloxyimino Titanium(IV) Complexes and Application to Stereoselective Lactide Polymerization with Computational Study of Stereoselective Ring-Opening Mechanism, *Department of Chemistry, KAIST; Graduate School of Nanoscience and Technology and Department of Chemistry, KAIST*
- [PO156] **Hye Sung Yang¹, Hyun-Joon Ha^{2,*}, Jung Woon Yang^{1,*}**, New Synthetic Method of Mixed Monosilyl Acetals and Mukaiyama Aldol Reactions: Control Chemoselectivity using Lewis Acid Catalyst, *¹Department of Energy Science, Sungkyunkwan University; ²Department of Chemistry, Hankuk University of Foreign Studies*
- [PO157] **Yubin Yim¹, Ying Hu¹, Liyan Chen¹, Xin Zhou^{3,*}, Jong-Man Kim^{2,*}, Juyoung Yoon^{1,*}**, Discrimination of phosgene using colorimetric and fluorescent probes in solutions and the gas phase, *¹Department of Chemistry and Nano Science, Ewha Womans University; ²Department of Chemical Engineering, Hanyang University; ³College of Chemistry and Chemical Engineering, Qingdao University*
- [PO158] **Tapas R. Pradhan, Hong Won Kim, Jin Kyoong Park***, Regiodivergent Synthesis of 1,3- and 1,4-Enynes via Kinetically Favored Hydropalladation and Ligand-Enforced Carbopalladation, *Department of Chemistry and Chemistry Institute of Functional Materials, Pusan National University*
- [PO159] **Hyunseong Kang, Chang-Hee Lee***, Synthesis and ion-pair recognition property of thiophene- or furan-fused calix[4]pyrroles, *Department of Chemistry, Kangwon National University*

Generation and Application of (Diborylmethyl)zinc(II) Species: Access to Enantioenriched *gem*-Diborylalkanes by an Asymmetric Allylic Substitution

Yeosan Lee^a, Jinyoung Park^a, and Seung Hwan Cho^{a*}

^aDepartment of Chemistry, Pohang University of Science and Technology (POSTECH),
Pohang, 37673 Republic of Korea
E-mail: seunghwan@postech.ac.kr

We report the successful generation of (diborylmethyl)zinc(II) species by transmetalation between isolable (diborylmethyl)lithium and zinc(II) halide (X = Br, Cl) and their application in the synthesis of enantioenriched *gem*-diborylalkanes bearing a stereogenic center at the β -position of the diboryl groups by an asymmetric allylic substitution reaction. The reaction has a broad substrate scope, and various enantioenriched *gem*-diborylalkanes can be obtained in good yields with excellent enantioselectivity. Further elaboration of the enantioenriched *gem*-diborylalkanes provides access to a diverse set of valuable chiral building blocks.¹



References

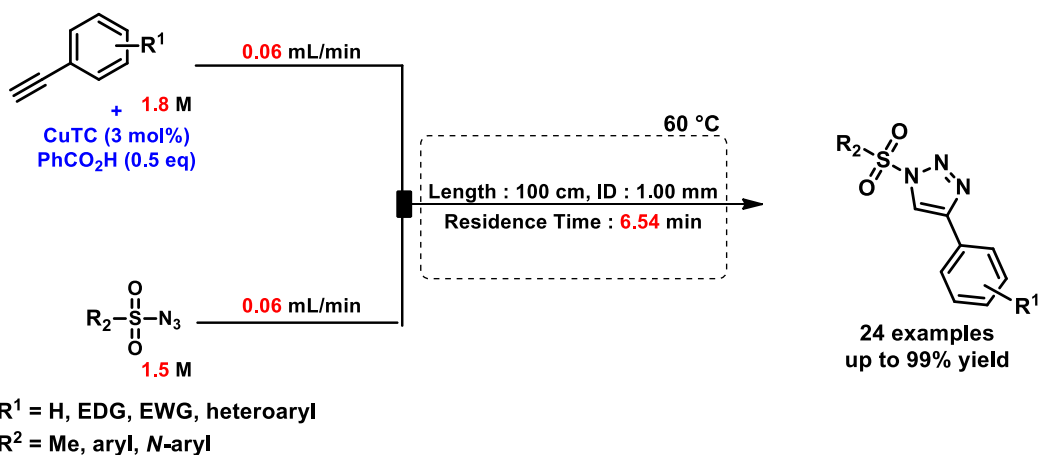
¹ Lee, Y.; Park, J.; Cho, S. H. *Angew. Chem., Int. Ed.* **2018**, *in press*.

Continuous Flow Synthesis of 1-Sulfonyl and 1-Sulfamoyl-1,2,3-Triazoles

권용주,^a 김원석*

Department of Chemistry and Nano Science Ewha Womans University, Seoul 120-750 Korea.
E-mail: wonsukk@ewha.ac.kr

1-Sulfonyl-1,2,3-triazoles are useful compounds which can serve as a precursor of reactive azavinyl carbenes. Because of their weak N1-N2 bond, they can easily transform to diazoimines through ring-chain tautomerization and it leads to subsequent conversion to the transition metal-carbene complexes.¹ Thus, many different batch-type methods for the preparation of 1-sulfonyl-1,2,3-triazoles have been developed. However, most batch-type conditions require long reaction time. Herein, we report an efficient method for the synthesis of 1-sulfonyl- and 1-sulfamoyl-1,2,3-triazoles employing continuous flow microreactor in short residence time. In addition, we generated *cis*-diamino enones with rhodium(II) azavinyl carbenes derived from triazoles by using one flow synthesis system.



References

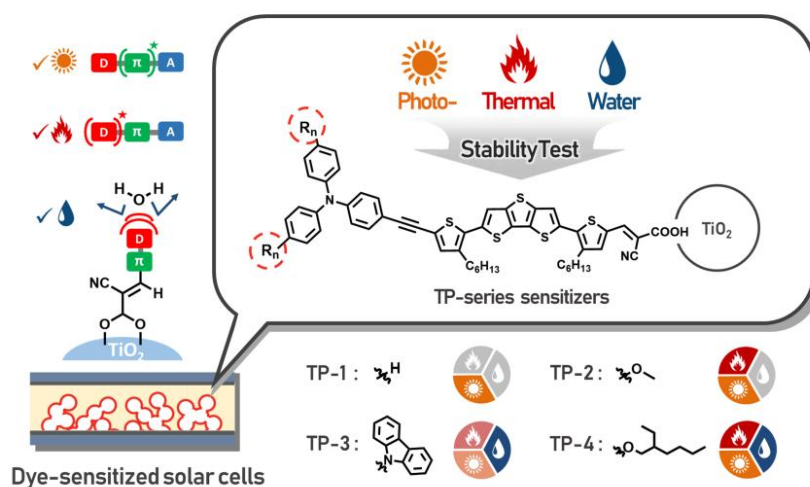
¹ Raushel, J.; Fokin, V. V. *Org. Lett.* **2010**, *12*, 4952-4955.

Molecular Engineering for Enhancement of Photo-, Thermal, and Water Stability of Organic Dyes for Dye-Sensitized Solar Cells

Jun-Hyeok Park, Un-Young Kim, Byung-Man Kim, Wang-Hyo Kim, Deok-Ho Roh, Jeong Soo Kim, and Tae-Hyuk Kwon*

Department of Chemistry, School of Natural Science, Ulsan National Institute of Science and Technology (UNIST), Ulsan 44919, Republic of Korea
E-mail: kwon90@unist.ac.kr

Dye-sensitized solar cells (DSSCs) have attracted attentions because of application to building integrated photo voltaic (BIPV) system. It has several advantages, especially very high efficiency at low illumination. However, there have been still stability issues and molecular strategy for rigid stability have not been systemically suggested. In this work, we suggested functional groups on the donor moiety and reveal relationship between molecular structure and degradation pathways divided into photo/thermal/water environmental factors. In this work, we introduced **TP-series** sensitizers which have basically π -conjugated bridge unit as dithieno[3,2-b:2',3'-d]thiophene(DTT) which planarity and strong stability. In detailed, four sensitizers have different functional groups on donors and we found that functional groups in donor moiety affect PCE and alkoxy functional groups (**TP-2** and **4**) is more effective to obtain high performance, because of increasing donating ability and rapid Intermolecular Charge Transfer (ICT). Furthermore, they show good thermal and light stability because of stabilization excited or oxidized state by donating effect. However, in case of **TP-3**, it exhibited weak thermal and light stability because 3,6-position of carbazole were easily oxidized by external energy, but achieved the highest water stability presumably by the strong hydrophobicity of carbazole group. In contrast, **TP-2** showed the lowest water stability because of high hydrophilicity. Therefore, **TP-4** with a 2-ethylhexyloxy group was designed and synthesized for protecting oxygen on alkoxy group. As a result, **TP-4** achieved high stabilities in terms of thermal, light and water stability and a PCE as high as 8.86% due to the strong electron donating ability as shown in the methoxy group of **TP-2**.



Supramolecular Assembly Formed from Bisporphyrin Derivative

Hosoowi Lee,^a Woo-Dong Jang^{a*}

^a Department of Chemistry, Yonsei University, 03722 Seoul, South Korea
E-mail: wdjang@yonsei.ac.kr

Recently, the control of supramolecular polymerization process has attracted attention to many researchers. We designed bisporphyrin derivative, **C2-TPP**, which composed of two zinc porphyrin units bridged by amide groups and diacetylene moiety. **C2-TPP** exhibited distinct different aggregation mode upon condition of self-assembly process. When the bisporphyrin was dissolved in hot methylcyclohexane (MCH), it showed sharp absorption band indicating molecularly dissolved monomeric state. Depending on the cooling rate of the hot solution, **C2-TPP** resulted in two different types of aggregation state. As the hot solution experienced slow cooling process, absorption spectrum of **C2-TPP** was obtained as blue-shifted absorption band indicating the formation of thermodynamically stable H-aggregates (**H_{agg}**). Meanwhile, when the hot MCH was cooled rapidly, red-shifted absorption band was monitored in absorption spectrum, indicating the formation of J-aggregates (**J_{agg}**) as kinetic product. The kinetic **J_{agg}** was transformed to thermodynamically stable **H_{agg}** and this transformation process was monitored through the change of UV/Vis absorption spectra. **J_{agg}** and **H_{agg}** were visualized by atomic force microscopy; **J_{agg}** and **H_{agg}** were obtained as nanoparticles and nanofiber, respectively. The freshly transformed **H_{agg}** from **J_{agg}** was CD-silent, which is reasonable considering achiral property of the bisporphyrin monomer. After storing fresh **H_{agg}** at room temperature without any disturbance, unexpected CD-activity was detected from aged **H_{agg}** solution. A further study to find out the origin of this unexpected CD-signal from achiral bisporphyrin is still in progress.

Total Syntheses of Alotaketal A and Phorbaketals

Jaeyeon Lee,^a Hee-Yoon Lee^{a*}

^a Department of Chemistry, Korea Advanced Institute of Science and Technology, Yuseong-gu, Daejeon 34141, Korea.

E-mail: leejaeyeon@kaist.ac.kr

Alotaketal A isolated from marine sponge *Hamigera* sp.^[1] and Phorbaketal A from Marine sponge *Phorbas* sp.^[2] in 2009 have almost identical new structural features including unsaturated spiroketals. (Fig.1) Especially These natural products have received attention because of their interesting biological activities such as activation of the cAMP cell signaling pathway which means they could be used as important tools for cell biology research and potential lead compounds for drug development.

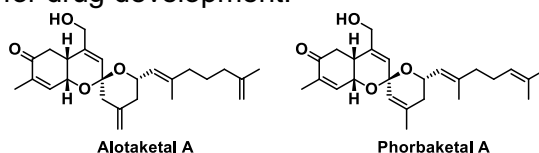


Fig. 1

In 2017, We reported the total synthesis of Phorbaketal A^[3], through Au catalyzed acetal formation of alkyne diols and epoxide rearrangement into the corresponding allylic alcohol as the final step. (Fig.2) The final epoxide rearrangement was quite troublesome as the transformation was not realized by other group despite investigation of a wide range of conditions.^[4]

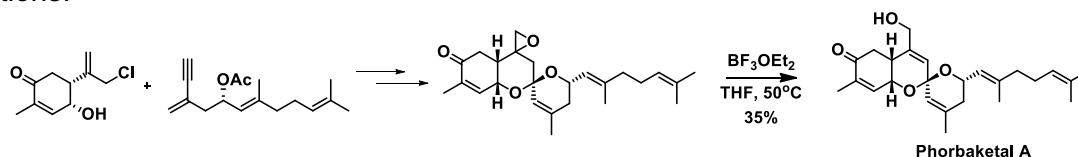


Fig. 2

In this work, we accomplished total synthesis of Alotaketal A and Phorbaketal A utilizing the epoxide next to an alkyne based on the mechanistic insight from our previous total synthesis of Phorbaketal A.^[3] (Fig.3)

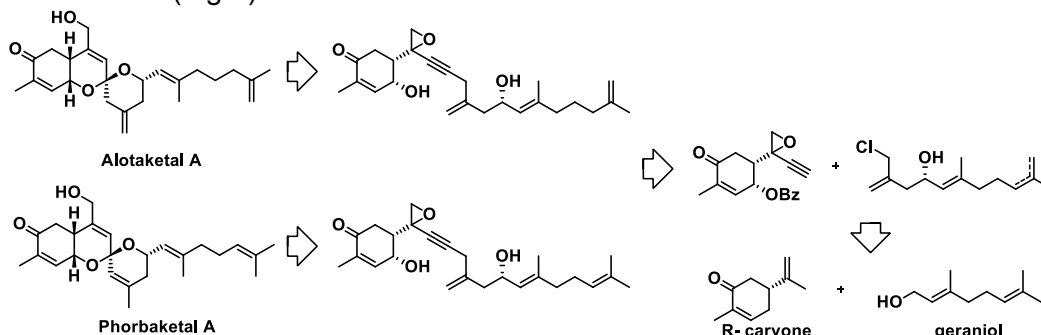


Fig.3

References

- Forestieri, R.; Merchant, C. E.; Voogd, N. J.; Matainaho, T.; Kieffer, T. J.; Andersen, R. J. *Org. Lett.* **2009**, *11*, 5166-5169
- Rho, J.-R.; Hwang, B. S.; Sim, C. J.; Jung, S.; Lee, H.-Y.; Kim, H.-J. *Org. Lett.* **2009**, *11*, 5590-5593
- Joung, S.; Kim, R.; Lee, H.-Y. *Org. Lett.* **2017**, *19*, 3903-3906
- Hubert, J. G.; Furkert, D. P.; Brimble, M. A. *J. Org. Chem.* **2015**, *80*, 2715-2723

Copper-Catalyzed S_N2' Reduction of Propargylic Chlorides with Diisobutylaluminum Hydride

Yuna Kim, Hanseul Lee, Yunmi Lee*

Department of Chemistry, Kwangwoon University, Seoul 01897, Republic of Korea

Email: ymlee@kw.ac.kr

Allenes are very important structures in natural products, pharmaceuticals, and molecular materials.¹ Because of their usefulness for further chemical transformations, allenes are valuable building blocks in organic synthesis.² Conventionally, various methods for the synthesis of allenes have been developed, but there have rarely been known for catalytic S_N2' reduction reactions using aluminum hydrides.³⁻⁴ In this study, we have found a way to prepare allenes through the reaction of propargylic chlorides with inexpensive diisobutylaluminum hydride (DIBAL-H) promoted by copper catalysts. The S_N2' reductions of various propargylic chlorides were carried out in the presence of 1-5 mol % NHC-Cu catalysts under mild reaction conditions. Various mono- and disubstituted allenes were obtained in high yields with excellent regioselectivities. This reaction was also highly stereoselective, proceeding with complete center-to-axis chirality transfer to synthesize chiral allenes.

References

¹Hoffmann, R. A.; Krause, N. *Angew. Chem., Int. Ed.* **2004**, *43*, 1196-1216.

²Rivera, F. P.; Diederich, F. *Angew. Chem., Int. Ed.* **2012**, *51*, 2818-2828.

³Brunner, H.; Miehl, W. *J. Organomet. Chem.* **1984**, *275*, C17-C21.

⁴Krause, N.; Hoffmann-Röder, A. *Tetrahedron* **2004**, *60*, 11671-11694.

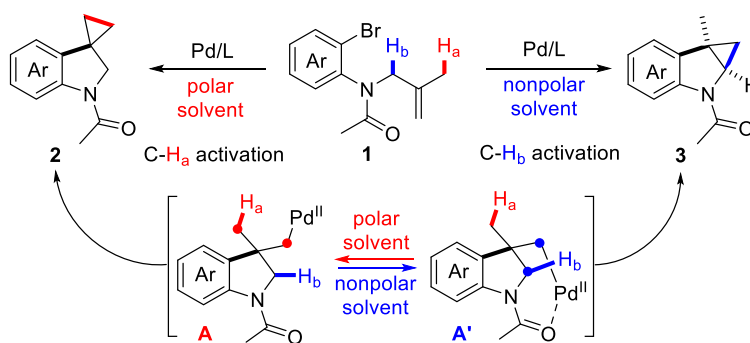
Palladium-Catalyzed Tandem Heck/Divergent Cyclopropanation via Solvent-Driven Regioselective C(sp³)-H Bond Activation

Da Sol Chung, Jae Sung Lee, U Bin Kim, and Sang-gi Lee*

^a Department of Chemistry and Nano Science (BK21 PLUS), Ewha Womans University, 03760, Seoul, Korea.

E-mail: sanggi@ewha.ac.kr

It has been developed a novel palladium-catalyzed tandem Heck/regiodivergent C(sp³)-H bond activation^[1] for selective formation of spiro- and fused-cyclopropanated indolines from the same N-allylated 2-bromoanilines. Solvent could greatly influence to the regioselectivity in C-H activation of σ -alkylPd(II)-intermediate. For example, in a non-polar and non-coordinating solvent, the intramolecular coordination between Pd(II) and the amide carbonyl may favor formation of intermediate **A'**, where close spatial proximity between Pd(II) and C-H_b bond will promote selective formation of fused-cyclopropanated indoline **3**. However, in a polar and highly coordinating solvent such as DMSO, the solvent molecules may displace Pd(II) from interacting intramolecularly with the amide carbonyl to afford an intermediate complex with spatial conformation better represented by **A**, where due to close proximity between Pd(II) and C-H_a bond, will lead to selective formation of spiro-cyclopropanated indoline **2**. Kinetic studies with deuterium-labelled substrate indicated that the cleavage of C-H bonds is turnover limiting step in both catalytic reactions. Time-resolved IR studies suggested coordination of amide carbonyl with Pd(II) plays key role for the regioselectivity.^[2]



References

¹Ping, L.; Chung, D. S.; Bouffard, J.; Lee, S.-g. *Chem. Soc. Rev.* **2017**, *46*, 4299-4328.

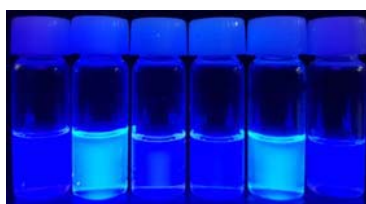
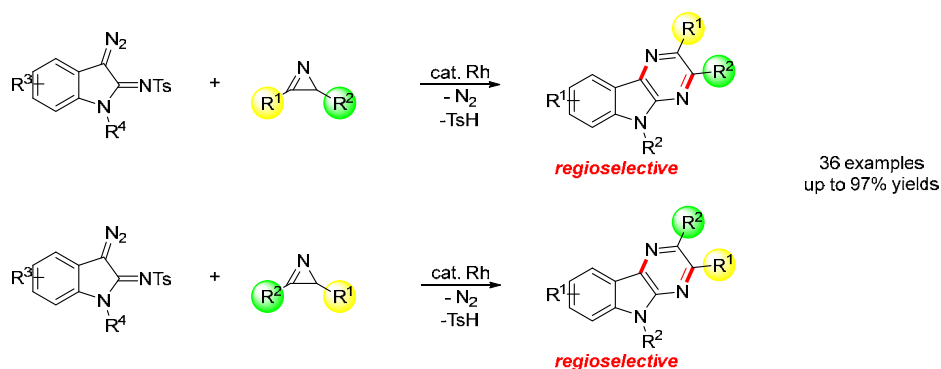
²Chung, D. S.; Lee, J. S.; Lee, J. H.; Kim, U. B.; Lee, W. K.; Lee, S.-g. **2018**, *manuscript in preparation*

Regioselective Synthesis of Indolopyrazines through Sequential Rh-Catalyzed Formal [3 + 3] Cycloaddition and Aromatization Reaction of Diazoindolinimines with Azirines

Yonghyeon Baek,^a Phil Ho Lee^{a*}

^a Department of Science, Kangwon National University, Chuncheon 24341, Republic of Korea,
E-mail: phlee@kangwon.ac.kr

Indolopyrazines possessing both indole and pyrazine moieties are significant structural motifs in a number of naturally occurring products, show a wide range of biological activities, including antitumor and antiviral activities, and function as fluorescent and host materials. In this regard, the indolopyrazine motif has continuously received the attention of synthetic chemists. Thus, establishing synthetic approaches for preparing regioselective indolopyrazines from simply attainable starting materials is highly demanded. We developed a regioselective synthetic method to prepare indolopyrazines through a sequential Rh-catalyzed formal [3 + 3] cycloaddition and aromatization reaction of a wide range of diazoindolinimines with azirines. Because the previously reported synthetic methods afforded mixtures of indolopyrazines, the present method using unsymmetrical azirines has the an excellent merit from a regioselectivity standpoint. Because indolopyrazines are fluorescent, their optical properties in CH₂Cl₂ solution were studied. The extinction coefficients were variable from 107,298 to 585,478 M⁻¹cm⁻¹. The indolopyrazine affords high quantum yields and extinction coefficients, which are an attractive property for biological probes.



Reference

¹ Baek, Y.; Maeng, C.; Kim, H.; Lee, P. H. *J. Org. Chem.* **2018**, *83*, 2349

^1H NMR Chiral Analysis of Alcohols at Room Temperature by Chiral Octahedral Gallium Complex

Sumin Jang, Hyunwoo Kim *

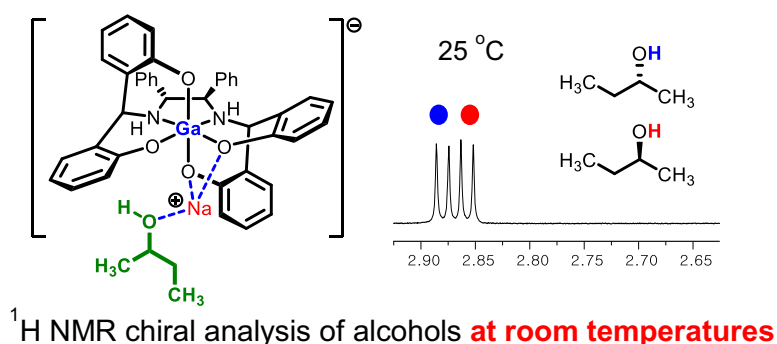
Department of Chemistry, Korea Advanced Institute of Science and Technology (KAIST), Daejeon 34141, Korea.

E-mail: hwkim@kaist.edu

NMR spectroscopy is one of the most convenient and widely used analytical techniques for the determination of chemical structures. The use of chiral solvating agents (CSA) using non-covalent interactions is operationally simple and convenient. However, the analytes are mainly limited to amines or carboxylic acids because they can form relatively strong charged hydrogen bonding. It is still quite challenging to use CSAs for other polar compounds. Indeed, chiral alcohols are common structural motifs synthesized by many stereoselective reactions. For direct chiral analysis of alcohols by ^1H NMR spectroscopy, only a few cases of chiral solvating agents have been reported. Moreover, they tend to exhibit insufficient peak separation and narrow analyte scope. Therefore, a highly efficient chiral solvating agent for chiral alcohols is highly desirable.

In 2015, our lab have demonstrated a chiral octahedral aluminum-ate complex with newly designed hexa-dentate N_2O_4 ligands as an efficient ^1H NMR chiral solvating agent for both positively and negatively charged chiral molecules.¹ Furthermore, in 2018, we have elaborated the use of aluminum complex as a chiral solvating agent to alcohols.² However, due to the weak intermolecular interaction, peak separation was achieved at low temperature.

In this work, we have newly developed a sodium salt of negatively charged octahedral gallium complex to demonstrate a general and efficient chiral solvation of chiral alcohols at room temperature. Previously, for aluminium complex, low temperature measurement was necessary due to the small binding constants with chiral alcohols. However, gallium complex gave clear peak separation at room temperature due to its more basic property. Because our gallium complex provides well resolved and sharp signals of various chiral alcohols including aryl- and alkyl-substituted primary, secondary, and tertiary alcohols, it can be a general method for the determination of the % ee of chiral alcohols under operationally more simple and practical condition.



References

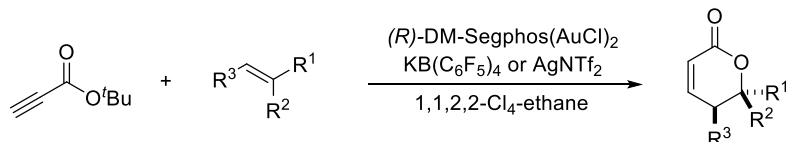
1. Seo, M.; Kim, H. *J. Am. Chem. Soc.* **2015**, *137*, 14190.
2. Seo, M.; Jang, S.; Kim, H. *Chem. Commun.* **2018**, *54*, 6804.

Asymmetric Synthesis of Dihydropyranones via Au(I)-Catalyzed Intermolecular [4+2] Annulation of Propiolates and Alkenes

Hanbyul Kim,^a Su Yeon Choi,^a and Seunghoon Shin^{*a}

^a Department of Chemistry and Center for New Directions in Organic Synthesis (CNOS), Hanyang University, 222 Wangsimni-ro, Seongdong-gu, Seoul, 04763 (Korea)
E-mail: sshin@hanyang.ac.kr

α,β -Unsaturated δ -lactone scaffolds are found in a number of medicinal compounds displaying an array of significant biological activities.¹ Based on the powerful alkynophilic activation of homogeneous Au(I)-catalysis, we recently demonstrated that the dihydropyranones could be assembled in a single step from the intermolecular reaction of propiolates with alkenes.² However, achieving high level of enantiocontrol has remained elusive in this class of intermolecular gold(I)-catalyzed coupling³. Herein, we report a highly enantioselective synthesis of α,β -unsaturated δ -lactones from [4+2] annulation of propiolates and alkenes in upto 95% ee. Notably, for the desired chiral recognition, the choice of 1,1,2,2-tetrachloroethane as solvent was found to be crucial. Furthermore, an anionic surfactant (SDS) improved the product selectivity in the divergence of the cyclopropyl gold carbene intermediate (Scheme 1).⁴



- intermolecular asymmetric Au(I) catalysis
- control of prochiral face of olefins by (L*)Au-alkyne complex
- use of SDS in organic solvents to control selectivity
- 38 examples (63-95 %ee)
- tri-substituted and 1,2-disubstituted olefins & 1,3-dienes

Scheme 1. Enantioselective intermolecular [4+2] annulation

References

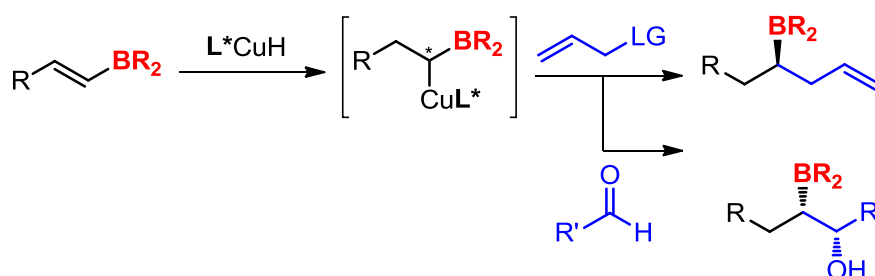
- ¹ B. M. Trost, J. D. Knopf, C. S. Brindle, *Chem. Rev.* **2016**, *116*, 15035-15088.
- ² H.-S. Yeom, J. Koo, H.-S. Park, Y. Wang, Y. Liang, Z.-X. Yu, S. Shin, *J. Am. Chem. Soc.* **2012**, *134*, 208-211.
- ³ For recent reviews on enantioselective Au(I)-catalysis : a) W. Zi, F. D. Toste, *Chem. Soc. Rev.* **2016**, *45*, 4567-4589; b) Y. Li, W. Li, J. Zhang, *Chem. Eur. J.* **2017**, *23*, 467-512; For a single intermolecular example : c) C. García-Morales, B. Ranieri, I. Escofet, L. López-Suarez, C. Obradors, A. I. Konovalov, A. M. Echavarren, *J. Am. Chem. Soc.* **2017**, *139*, 13628-13631.
- ⁴ H. Kim, S. Y. Choi, S. Shin, manuscript submitted.

Asymmetric Synthesis of Organoboron Compounds via Copper Catalysis

Won Jun Jang,^a Jaesook Yun^{a*}

^a Department of Chemistry, Sungkyunkwan University, Suwon 16419, Korea.
E-mail: jwj1027@naver.com

Tandem and multicomponent reaction of alkenylboronates with allylic electrophiles and aldehydes has been developed by Cu–H catalysis.¹ This reaction provides an efficient synthetic method of enantioenriched organoboron compounds in good yield with high enantio- and diastereoselectivity (up to a ratio of >98:2). In Particular, α,β -unsaturated aldehydes as electrophiles were successfully used without significant reduction, affording homoallylic boronates containing an allylic alcohol. In this presentation, we report asymmetric synthesis of chiral organoboron compounds by copper catalyst.



References

¹ (a) Han, J. T.[†]; Jang, W. J.[†]; Kim, N.; Yun, J. *J. Am. Chem. Soc.* **2016**, *138*, 15146. (b) Jang, W. J.; Han, J. T.; Yun, J. *Synthesis* **2017**, *49*, 4753 (c) Jang, W. J.; Yun, J. *Angew. Chem., Int. Ed.* **2018**, *Early View* (DOI:10.1002/anie.201806937)

A Two-Photon Active Environment Insensitive Dye with Giant Stokes Shift: An Ideal Platform for Probe Designing and Bio-imaging

Sourav Sarkar, Mithun Santra & Kyo Han Ahn

*Department of Chemistry, Pohang University of Science and Technology (POSTECH)
77 Cheongam-Ro, Nam-Gu, Pohang, Gyungbuk 37673, Republic of Korea
E-mail: ahn@postech.ac.kr*

Fluorescence emission property of a dye molecule inside cell, such as intensity or spectral position, can be affected by many cellular factors, particularly by viscosity and polarity.¹ Most of commercially available dyes suffer from these problems and that is why it is usually difficult to predict emission property of a dye inside cell during bio-imaging process. As dyes' emission property may dependent on both polarity and viscosity of media, usually we observe cellular imaging results different from that of measured in cuvette, and such discrepancy can cause reliability concern on the bio-imaging data.² Therefore, an ideal fluorescent probe should be least affected by such factors.

Herein we address an 8-hydroxybenzo[g]coumarin based dye 5h, which shows almost non-solvatochromic behavior in a broad polarity zone from dioxane to PBS 7.4, and it's emission intensity is barely influenced by viscosity.³ Furthermore, it shows polarity-insensitive optical brightness property as observed in case of non-polar dioxane to polar ethanol. Unlike other solvatochromic dyes, 5h shows very similar emission spectrum in cuvette and cellular environment. This medium-insensitive optical behavior of dye 5h is expected to remove the complications involved in bio-imaging process.

Moreover, 5h has an easy functionalizable arm for attaching reactive moiety, significant two-photon property and shows giant Stokes shift of ~190 nm. Being cationic in nature, 5h has good aqueous solubility and furthermore, enhanced photostability, which all together makes it an ideal platform for probe designing and bio-imaging.

References

- ¹A. S. Klymchenko, *Acc. Chem. Res.*, **2017**, 50, 366.
- ²A. Bullen and P. Saggau, *Biophysical Journal*, **1999**, 76, 2272.
- ³S. Sarkar et. al. *J. Mater. Chem. B*, **2018**, 6, 4446

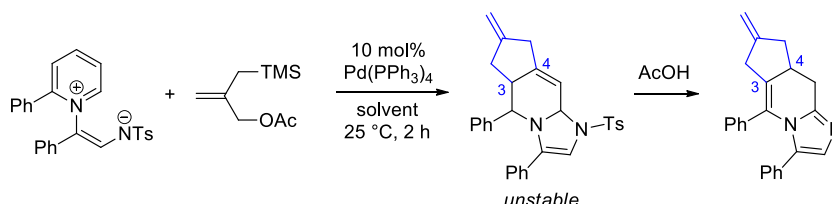
Pyridinium Zwitterion as a Regioselectivity-Switchable Dipole

Donguk Ko, Eun Jeong Yoo*

Department of Applied Chemistry, Kyung Hee University, Yongin 17104, Republic of Korea.
E-mail: ejoyoo@khu.ac.kr

Cycloadditions constitute one of the most important classes of organic reaction giving access to complex cyclic constructs that play a key role in the preparation of natural products, pharmaceutical agents or synthetic materials. Recently, our group discovered that the pyridinium zwitterion could serve as a 1,5-dipole for the construction of medium-sized heterocycles via [5+n]-cycloadditions with electrophilic partners.^[ref] A remarkable feature of pyridinium zwitterions is their stability, where the aromaticity of pyridinium core may stabilize these compounds sufficiently to allow isolation.

In this symposium, we will discuss about the regioselective cycloaddition of pyridinium zwitterions, which are the first example of site-switchable dipole, and palladium-TMM species to provide fused N-heterocycles with excellent selectivity. The cycloaddition of pyridinium zwitterion and palladium-TMM, which was readily generated from 3-acetoxy-2-trimethylsilylmethyl-1-propene, efficiently provided the cycloadduct product where new bonds were formed on C3- and C4-positions of pyridinium zwitterion at room temperature. We also carried out a detailed mechanistic investigation based on DFT computational results for the regio-divergent cycloaddition of pyridinium zwitterion and palladium-TMM.



References

- Lee, D. J.; Han, H. S.; Shin, J.; Yoo, E. J. *J. Am. Chem. Soc.* **2014**, *136*, 11606-11609.
- De, N.; Yoo, E. J. *ACS Catal.* **2018**, *8*, 48.
- Baek, S.-y.; Lee, J. Y.; Ko, D.; Baik, M.-H.; Yoo, E. J. *ACS Catal.* **2018**, *8*, 6353-6361.

Biosynthetically Inspired Transformation of (+)-Catharanthine to Post-Iboga Alkaloids

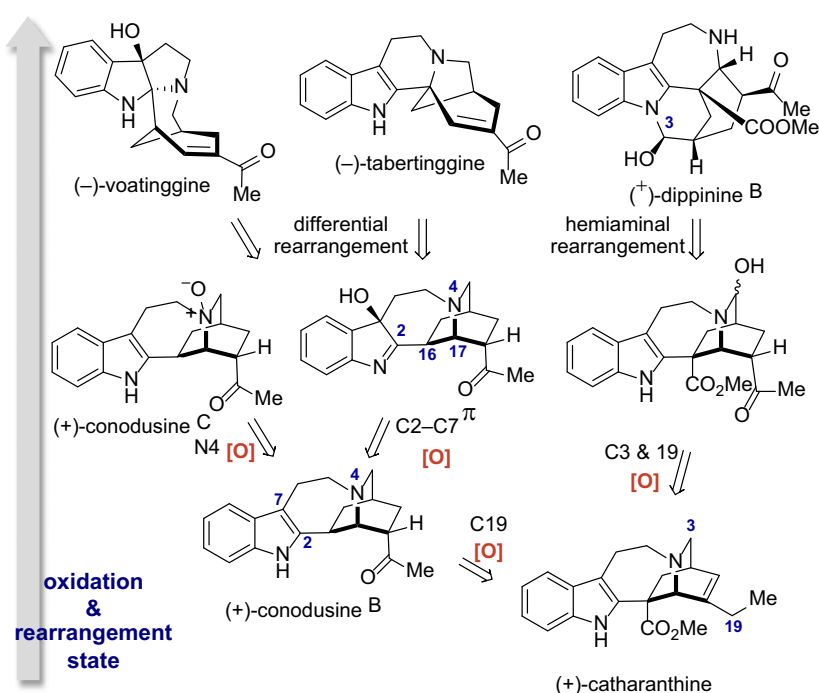
Sikwang Seong,^{ab} Hyeonggeun Lim,^{ab} and Sunkyu Han^{ab*}

^a Department of Chemistry, Korea Advanced Institute of Science & Technology (KAIST), Daejeon 305-701, South Korea.

^b Center for Catalytic Hydrocarbon Functionalizations, Institute for Basic Science (IBS), Daejeon 305-701, South Korea.
E-mail: ssg9547@kaist.ac.kr

Iboga-type alkaloids that have undergone rearrangements to exclude isoquinuclidine moieties can be classified as post-iboga alkaloids. Upto date, various synthetic studies have been undertaken on iboga-type alkaloids, but only a few examples exist on the synthesis of post-iboga alkaloids.

We synthesized various post-iboga alkaloids including conodusine A, B, C, voatinggine, tabertinggine and dippinine B from catharanthine through oxidative conversions and rearrangements.



References

- ¹ Nge, C.-E.; Gan, C.-Y.; Low, Y.-Y.; Thomas, N. F.; Kam, T.-S. *Org. Lett.* **2013**, *15*, 4774–4777.
- ² Kam, T.-S.; Sim, K.-M. *Heterocycles*, **2001**, *55*, 2405–2412.

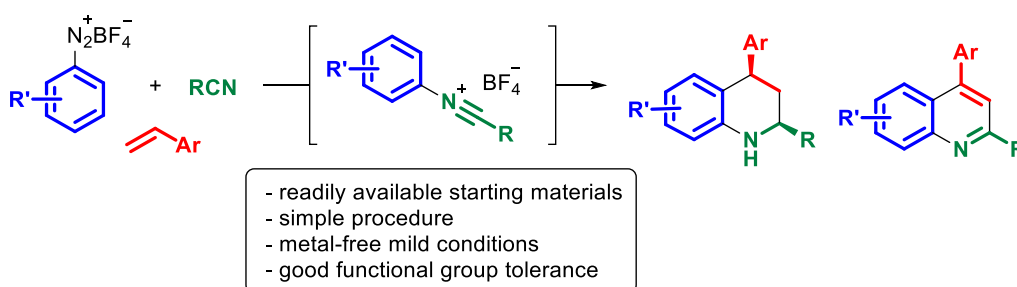
One-Pot Three-Component Synthesis of (Tetrahydro)Quinolines

Huen Ji Yoo and So Won Youn*

Department of Chemistry, Center for New Directions in Organic Synthesis,
Hanyang University, Seoul 04763, Korea.

E-mail: sowony73@hanyang.ac.kr

Recently, we have developed a new highly effective one-pot, three-component reaction of arenediazonium salts, nitriles, and styrenes for the synthesis of quinolines and tetrahydroquinolines.¹ In sharp contrast to the prior works with the same reagent blend, the formation of *N*-arylnitrilium intermediates² from arenediazonium salts and nitriles was followed by reaction with styrenes, leading to 3,4-dihydroquinolinium salts³ as a common intermediate. These could be further selectively transformed to quinolines and tetrahydroquinolines depending on the reaction conditions.⁴ This is the first example of the synthesis of both quinolines and tetrahydroquinolines using arenediazonium salts as a C2 building block for a benzene ring fused to a pyridine/piperidine ring. The advantages of this protocol include its simplicity, metal-free and mild conditions, readily available starting materials, and good functional group tolerance.



References

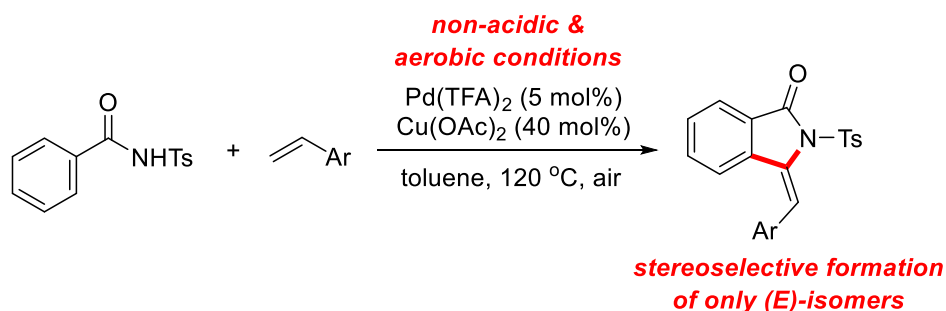
- ¹ Youn, S. W.; Yoo, H. J.; Lee, E. M.; Lee, S. Y. *Adv. Synth. Catal.* **2018**, *360*, 278.
- ² a) Klages, F.; Grill, W.; *Liebigs Ann. Chem.* **1955**, *594*, 21; b) Meerwein, H. *Angew. Chem.* **1955**, *67*, 374; c) Meerwein, H.; Laasch, P.; Mersch, R.; Spille, J.; *Chem. Ber.* **1956**, *89*, 209; d) Petterson, R. C.; Bennett, J. T.; Lankin, D. C.; Lin, G. W.; Mykytka, J. P.; Troendle, T. G.; *J. Org. Chem.* **1974**, *39*, 1841; e) Kikukawa, K.; Kono, K.; Wada, F.; Matsuda, T. *Bull. Chem. Soc. Jpn.* **1982**, *55*, 3671; f) Cano-Yelo, H.; Deronzier, A. *J. Chem. Soc., Perkin Trans. 2* **1984**, 1093; g) Milanese, S.; Fagnoni, M.; Albin, A. *Chem. Commun.* **2003**, 216; h) Milanese, S.; Fagnoni, M.; Albin, A. *J. Org. Chem.* **2005**, *70*, 603; i) Saez, R.; Otero, M. D.; Batanero, B.; Barba, F. *J. Chem. Res.* **2008**, 492; j) Ramanathan, M.; Liu, S. -T. *J. Org. Chem.* **2015**, *80*, 5329.
- ³ Moustafa, A. H.; Hitzler, M. G.; Lutz, M.; Jochims, J. C. *Tetrahedron* **1997**, *53*, 625; b) Wang, H.; Xu, Q.; Shen, S.; Yu, S. *J. Org. Chem.* **2017**, *82*, 770; c) Wang, Y.; Chen, C.; Peng, J.; Li, M. *Angew. Chem.* **2013**, *125*, 5431; *Angew. Chem. Int. Ed.* **2013**, *52*, 5323; d) Sheng, J.; Wang, Y.; Su, X.; He, R.; Chen, C. *Angew. Chem.* **2017**, *129*, 4902; *Angew. Chem. Int. Ed.* **2017**, *56*, 4824.

Pd-Catalyzed Synthesis of (*E*)-3-Arylmethyleneisoindolin-1-ones

Tae Yun Ko and So Won Youn*

Department of Chemistry, Center for New Directions in Organic Synthesis
Hanyang University, Seoul 04763, Korea
E-mail: sowony73@hanyang.ac.kr

Due to their various biological properties and wide application in pharmaceutical research, isoindolinones are one of the most important heterocycle compounds.¹ Especially, 3-arylmethyleneisoindolin-1-ones have been utilized for the synthesis of numerous natural products and pharmacologically important compounds. Among the various synthetic strategies, the majority of synthetic routes relies on the use of acrylates and benzamides.² Even if various methods for the synthesis of isoindolinone derivatives have been reported for decades, more efficient synthetic methods using styrenes are still in great demand. Recently, our group developed a highly efficient one-pot synthesis of (*E*)-3-arylmethyleneisoindolin-1-ones from *N*-Ts-benzamides and styrenes under Pd catalysis, forming new C-C and C-N bonds with high efficiency and stereoselectivity.



References

- ¹ (a) Buttinoni, A.; Ferrari, M.; Colombo, M.; Ceserani, R. *J. Pharm. Pharmacol.* **1983**, *35*, 603–604. (b) Matsumoto, N.; Tsuchida, T.; Maruyama, M.; Sawa, R.; Kinoshita, N.; Homma, Y.; Takahashi, Y.; Iinuma, H.; Naganawa, H.; Sawa, T.; Hamada, M.; Takeuchi, T. *J. Antibiot.* **1996**, *49*, 953–954. (c) Miller, B.; Mao, S.; Rosenker, K. M.; Pierce, J. G.; Wipf, P. *Beilstein J. Org. Chem.* **2012**, *8*, 1091–1907. (d) Speck, K.; Magauer, T.; *Beilstein J. Org. Chem.* **2013**, *9*, 2048–2078. (e) Karmakar, R.; Pahari, P.; Mal, D. *Chem. Rev.* **2014**, *114*, 6213–6284.
- ² (a) Patureau, F. W.; Besset, T.; Glorius, F. *Angew. Chem. Int. Ed.* **2011**, *50*, 1064–1067. (b) Li, D., -D.; Yuan, T. -T.; Wang, G. -W. *Chem. Commun.* **2011**, *47*, 12789–12791. (c) Wrigglesworth, J. W.; Cox, B.; Lloyd-Jones, G. C.; Booker-Milburn, K. I. *Org. Lett.* **2011**, *13*, 5326–5329. (d) Xia, C.; White, A. J. P.; Hii, K. K. M. *J. Org. Chem.* **2016**, *81*, 7931–7938. (e) Laha, J. K.; Hunjan, M. K.; Bhimpuria, R. A.; Kathuria, D.; Bharatam, P. V. *J. Org. Chem.* **2017**, *82*, 7346–7352

A FRET based ratiometric two-photon mitochondrial pH fluorescent probe

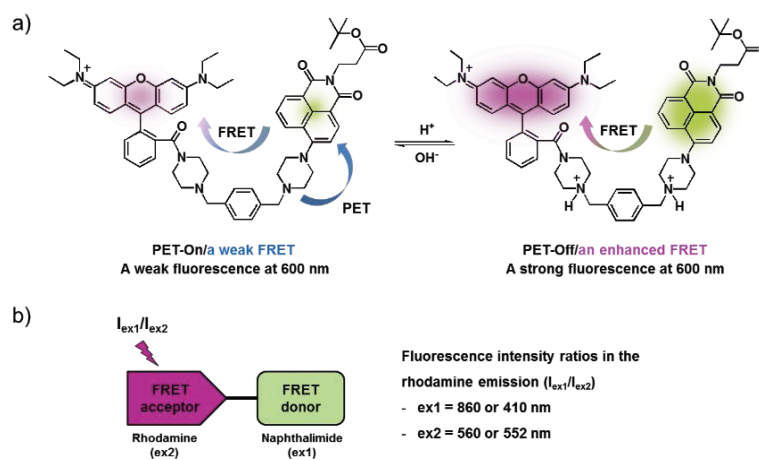
Min Jung Chang,^a Jung Won Yoon,^a Shin A Yoon,^a Chulhun Kang,^{b*} Min Hee Lee^{a*}

^a Department of Chemistry, Sookmyung Women's University, Seoul, 04310, Korea

^b The School of East-West Medical Science, Kyung Hee University, Yongin, 17104, Korea

E-mail: minminkong@sookmyung.ac.kr

We developed a noble two-photon excitable far-visible-emitting FRET system (**1**) composed of naphthalimide-piperazine-rhodamine for the ratiometric imaging of the cellular pH. Probe **1** showed a pH-dependent ratiometric change which was reversible and rapidly responsive to varying pH without interfering from other biological species such as metal ions, anions, and redox species. In addition, **1** can localize to the mitochondria of the live HeLa cells and provide a ratiometric fluorescent change upon acidification of mitochondria induced by the CCCP treatment and nutrient starvation. Moreover, the pH-responsive fluorescence change of **1** in the deep-tissue imaging was identified by the CCCP treatment. Thus, this FRET system could be utilized as an efficient two-photon probe for the imaging of mitochondrial pH in both cells and tissues.

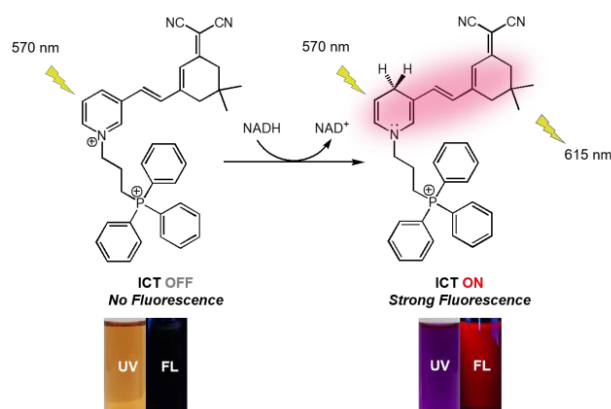


A development of red-emitting fluorescent probe for imaging of mitochondrial NADH in live cell

Jinhui Joo, Sun Young Park, Jinju Lee, Min Hee Lee*

Department of Chemistry, Sookmyung Women's University, Seoul 04310, Korea
E-mail: wnwlsqml2313@gmail.com

Nicotinamide adenine dinucleotide (NADH) is a coenzyme involving in many redox reactions in living cells. In particular, the NADH plays a crucial role in the production of energy in the mitochondria. In this regard, we developed a NIR fluorescent probe (**1**) that can image mitochondrial NADH. This probe consists of NIR fluorophore as signaling unit, electron-deficient moiety as a reactive site to NADH, and triphenylphosphonium salt as mitochondria targeting group. The **1** is almost none-fluorescent, however, upon reacting with NADH a significant fluorescence increase is monitored in both solution and live human cells.



Surface State-mediated Charge Transfer of Cs₂Snl₆ and Its Application in Dye-sensitized Solar Cells

HyeonOh Shin,^a Byung-Man Kim,^b Tae-Hyuk Kwon^{a*}

^a Department of Chemistry, School of Natural Science, Ulsan National Institute of Science and Technology (UNIST), Ulsan 44919, Republic of Korea. ^b School of Energy and Chemical Engineering, Ulsan National Institute of Science and Technology (UNIST), Ulsan 44919, Republic of Korea.

E-mail: kwon90@unist.ac.kr

A vacancy-ordered double perovskite, Cs₂Snl₆, has emerged as a promising lead-free perovskite in the field of optoelectronics. However, its charge transfer kinetics mediated by its surface state remain unclear. Here, we report the charge transfer mechanism of Cs₂Snl₆ and clarify the role of its surface state in the presence of a redox mediator. Specifically, charge transfer through the surface state of Cs₂Snl₆ and its subsequent surface state charging are demonstrated by cyclic voltammetry and Mott–Schottky measurements, respectively. Because it is expected that the charge transfer state of Cs₂Snl₆ is capable of regenerating oxidized organic dyes, a Cs₂Snl₆-based regenerator is developed for a dye-sensitized solar cell (DSSC) structure composed of FTO/dyed mesoporous TiO₂/regenerator/PEDOT/FTO. As expected, the performance of the Cs₂Snl₆-regenerator system is strongly dependent on the highest occupied molecular orbital of the organic dyes. Consequently, Cs₂Snl₆ shows efficient charge transfer with a thermodynamically favorable charge acceptor level, achieving a 79% enhancement in the photocurrent density (14.1 mA cm⁻²) compared with that of a conventional liquid electrolyte (7.9 mA cm⁻²). Our results suggest that the surface state of Cs₂Snl₆ is the main charge transfer pathway in the presence of a redox mediator and should be considered in future designs of Cs₂Snl₆-based devices.

Stereoselective Palladium-Catalyzed Decarboxylative [4+2] Cycloaddition Reaction of Vinyl Benzoxazinones with Cyclic *N*-Sulfinines

Dasom Mun,^a Sung-Gon Kim^{a*}

^a Department of Chemistry, College of Natural Science, Kyonggi University,
154-42 Gwanggyosan-ro, Yeongtong-gu, Suwon 443-760, Republic of Korea
E-mail: sgkim123@kyonggi.ac.kr

Cyclic aminals, although possibly considered metabolically unstable, are the key units or building blocks of diverse commercially available pharmaceuticals and biologically active compounds.¹ The development of generally applicable synthetic tools for cyclic aminals is highly desirable and recently has attracted much attention. A palladium-catalyzed decarboxylative [4+2] cycloaddition of vinyl benzoxazinones with cyclic *N*-sulfinines has been developed for the stereoselective synthesis of tetrahydroquinazolines. The reaction of using Pd(PPh₃)₄ as a catalyst was tolerant to both the variety of substrates and provided access to highly functionalized tetrahydroquinazoline derivatives in typically high yields with excellent diastereoselectivities.

A highly asymmetric decarboxylative [4+2] cycloaddition of vinyl benzoxazinones with cyclic *N*-sulfinines has also been developed. The complex of Pd₂(dba)₃ and chiral phosphoramidate ligand is enantioselective catalyst for decarboxylative [4+2] cycloaddition affording the corresponding enantioenriched benzosulfamidate-fused tetrahydroquinazoline derivatives in good yields and with high enantioselectivities (up to 99% ee).

References

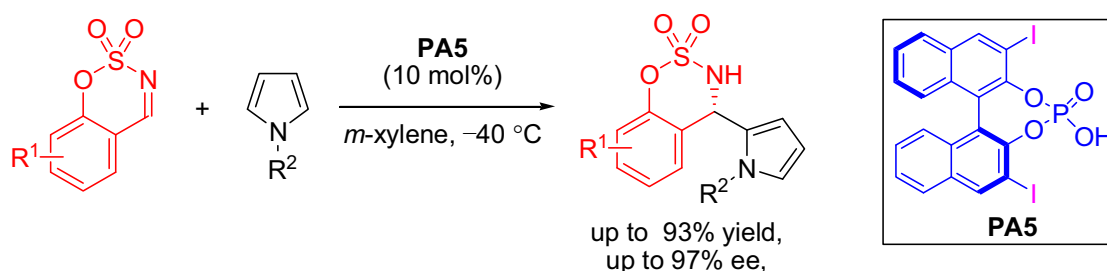
¹ (a) Baumann, M.; Baxendale, I. R. *Beilstein J. Org. Chem.* **2013**, *9*, 2265. (b) *Heterocycles in Natural Product Synthesis*, Majumdar, K. C., Chattopadhyay, S. K., Eds.; Wiley-VCH: Weinheim, **2011**.

Enantioselective organocatalytic Friedel-Crafts reaction of cyclic *N*-sulfimines with pyrroles

Sunyoung Choi,^a Sung-Gon Kim^{a*}

^a Department of Chemistry, College of Natural Science, Kyonggi University,
154-42 Gwanggyosan-ro, Yeongtong-gu, Suwon 443-760, Republic of Korea
E-mail: sgkim123@kyonggi.ac.kr

Pyrroles are widespread in biologically active natural products and pharmaceutical agents.¹ They serve as valuable synthons in organic synthesis and are widely used as pharmacophores in drug discovery.² An enantioselective Friedel-Crafts reaction of cyclic *N*-sulfimines with pyrroles has been developed. Chiral BINOL-derived phosphoric acids are enantioselective catalysts for Friedel-Crafts reaction affording the corresponding pyrrol-2-yl sulfamidate derivatives in good yields and with high enantioselectivities (up to 97% ee) for a broad range of functional groups and substitution patterns.



References

- ¹ (a) J. T. Gupton, *Top. Heterocycl. Chem.* **2006**, 2, 53. (b) C. T. Walsh, S. Gameau-Tsodikova, A. R. Howard-Jones, *Nat. Prod. Rep.* **2006**, 23, 517.
² (a) B. Joicoeur, E. E. Chapman, A. Thompson, W. D. Lubell, *Tetrahedron* **2006**, 62, 11531. (b) I. S. Young, P. D. Thornton, A. Thompson, *Nat. Prod. Rep.* **2010**, 27, 1801.

Stereoselective synthesis of highly functionalized tetrahydroisoquinolines using Lewis acid-catalyzed Friedel–Crafts/Michael cascade reaction

Seungyeon Kim,^a Sung-Gon Kim^{a*}

^a Department of Chemistry, College of Natural Science, Kyonggi University,
154-42 Gwanggyosan-ro, Yeongtong-gu, Suwon 443-760, Republic of Korea
E-mail: sgkim123@kyonggi.ac.kr

Tetrahydroisoquinoline (THIQ) is a well-known privileged scaffold that is commonly encountered in many biologically active natural products and synthetic pharmaceutical compounds.¹ A Lewis acid-catalyzed Friedel–Crafts/Michael cascade reaction between *N*-dialkyl-3-vinylanilines of *N*-tosylaziridines has been developed for the stereoselective synthesis of tetrahydroisoquinolines. The reaction of using Gd(OTf)₃ as a Lewis acid catalyst was tolerant to both the variety of *N*-dialkyl-3-vinylaniline and *N*-tosylaziridine substrates and provided access to highly functionalized tetrahydroisoquinolines in typically high yields with moderate-to-excellent diastereoselectivities.²

A highly enantioselective BOX/Mg(II)-catalyzed Friedel–Crafts/Michael cascade reaction between *N*-dialkyl-3-vinylanilines of *N*-tosylaziridines has also been developed for the synthesis of chiral benzosulfamidate-fused pyrrolidines, which generated in good yields and with high diastereo- and enantioselectivities.

References

¹ O'Hagan, D. *Nat. Pro. Rep.* **2000**, *17*, 435.

² (a) Lee, S. G.; Sin, S.; Kim, S.; Kim, S.-G. *Tetrahedron Lett.* **2018**, *59*, 1480. (b) Lee, S. G.; Kim, S.-G. *Tetrahedron* **2018**, *74*, 3671.

Two Photon-Active Probe for Photodynamic Therapy

Hyun Seok Seo and Hae-Jo Kim*

^a Department of Chemistry, Hankuk University of Foreign Studies, Yongin 17035, Republic of Korea.

*Corresponding author: Tel.: +82 31 330 4703; fax: +82 31 330 4566.

E-mail address: haejkim@hufs.ac.kr

Background: Development of a method to control the function of compounds in a spatiotemporal manner is indispensable in the field of biological chemistry and drug delivery. Ultraviolet (UV) irradiation-induced bond cleavage reaction or conformational change of backbone has been applied in order to control function. However, due to its low short wavelength, UV light exhibits limited penetration depth in biological tissues and can possibly cause tissue damage, which hampers the application of UV light for the treatment of internal tumors.^{1,2}

Near-infrared (NIR) two-photon photolysis can overcome these problems because NIR causes minimal tissue damaging compared with UV. Over the past few decades, NIR light-triggered photodynamic therapy (PDT) has emerged as an alternative treatment approach to chemotherapy and radiotherapy to treat cancer in the clinic.^{3,4}

With the focus of view, we design a probe for tumor therapy that is induced in specific irradiation of NIR wavelength region and release anticancer drug by photolysis of two-photon absorption moiety. Furthermore, for a suitable drug delivery system, a glucose unit is introduced as a biomarker targeting tumor.⁵

Materials and Method: Chemical probe was prepared according to the standard method in the lab and all reagents purchased from the chemical suppliers.

Conclusion: The probe shows increase of fluorescent intensity about 10-fold which is exposed NIR irradiation. This probe is expected to exhibit an effective spatiotemporal tumor therapy in a mouse model of cancer.

References

- ¹ Akira, S.; Jun, Y.; Yoshitake, S.; Toshiaki, F.; Akira O. *Tetrahedron Lett.*, **2010**, *51*, 2868-2871
- ² Yang, Y.; Yang, Y.; Xie Xie.; Wang, Z.; Gong, W.; Zhang, H.; Li, Y.; Yu, F.; Li, Z.; Mei, X. *Biomat.*, **2015**, *48*, 84.
- ³ R. Weissleder, *Nat Biotechnol.*, **2001**, *19*, 316.
- ⁴ Hambley, T.W. *Cancer Res.*, **2009**, *69*, 1259-1262.
- ⁵ Vander Heiden, M.G.; Cantley, L.C.; Thompson, C. B. *science.*, **2009**, *324*, 1029-1033.

A Ratiometric NIR Probe for Mitochondrial Nitroreductase

Won Joo Lee and Hae-Jo Kim*

Department of Chemistry, Hankuk University of Foreign Studies, Yongin 17035, Republic of Korea.

*Corresponding author: Tel.: +82 31 330 4703; fax: +82 31 330 4566.

E-mail address: haejkim@hufs.ac.kr

Background: Nitroreductase (NTR) is activated in such a hypoxic condition as cancer. Therefore, the detection of hypoxic NTR is a feasible tool for the diagnosis of tumor cells, warranting robust detection for a variety of biological studies.^{1,2}

Materials and Method: Chemical probes were prepared according to the standard organic synthetic method and NTR enzyme together with NADH was purchased from the chemical suppliers.

Result: A heptamethinylcyanine-based dual optical probe was developed for selective and sensitive detection of NTR in a NIR fluorescence region.³ The probe exhibited dramatic optical changes with large ratiometric fluorescence as well as intense blue color by the nitro-to-amine functional group transformation and displayed a very low limit of detection of NTR in PBS buffer. Further application of the probe to endogenous NTR was successfully applied in HeLa cells as well as a mouse model of breast cancer, exhibiting its preferential localization in the cellular mitochondria and heavy accumulation in the tumor tissues of living mice enough to obtain brighter tumor imaging through *i.v.* injection

Conclusion: Latent chromogenic and fluorogenic probe was successfully applied for the detection of mitochondrial NTR in vivo as well as in vitro.

References

¹ Xu, K.; Wang, F.; Pan, X.; Liu, R.; Ma, J.; Kong, F.; Tang, B. *Chem. Commun.*, **2013**, 49, 2554.

² Li, Y.; Sun, Y.; Li, J.; Su, Q.; Yuan, W.; Dai, Y.; Han, C.; Wang, Q.; Feng, W.; Li, F. *J. Am. Chem. Soc.*, **2015**, 137, 6407.

³ Chin, J.; Kim, H.-J. *Coord. Chem. Rev.*, **2018**, 354, 169.

Synthesis of Lacosamide (Vimpat) and Its Derivatives from Aziridine-(2*R*)-carboxylate

Sonhwan Kim^a, Hyeonsu Jeong^a, Nagendra Nath Yadav^b and Hyun-Joon Ha^{*}

^aDepartment of Chemistry, Hankuk University of Foreign Studies, Yongin, Kyunggi-Do, 17035, Korea.

^bDepartment of Chemistry, North Eastern Regional Institute of Science and Technology, Nirjuli, Arunachal Pradesh 791109, India

* indicates the main/corresponding author.

E-mail: hjha@hufs.ac.kr; Tel: +82-31-330-4659

An efficient and scalable synthesis of the antiepileptic drug (*R*) - lacosamide and its derivatives was successfully achieved from commercially available aziridine - (2*R*) - carboxylate in three simple sequential steps, including regioselective aziridine ring opening, debenzoylation followed by acetylation in one pot, and amide formation

References

- (1) (a) Choi, D.; Stables, J. P.; Kohn, H. *J. Med. Chem.* **1996**, *39*, 1907. (b) Morieux, P.; Stables, J. P.; Kohn, H. *Bioorg. Med. Chem.* **2008**, *16*, 8968. (c) Wang, Y.; Park, K. D.; Salome, C.; Wilson, S. M.; Stables, J. P.; Liu, R.; Khanna, R.; Kohn, H. *ACS Chem. Neurosci.* **2011**, *2*, 90.
- (2) (a) Krauss, G.; Ben-Menachem, E.; Mameniskiene, R.; Vaiciene-Magistris, N.; Brock, M.; Whitesides, J. G.; Johnson, M. E. *Epilepsia* **2010**, *51*, 951. (b) Brandt, C.; Heile, A.; Potschka, H.; Stoehr, T.; Loscher, W. *Epilepsia* **2006**, *47*, 1803. (c) Simoens, S. *Curr. Med. Res. Opin.* **2011**, *27*, 1329. (d) McCleane, G. *Expert Opin. Invest. Drugs* **2010**, *19*, 1129.
- (3) (a) Cross, S. A.; Curran, M. P. *Drugs* **2009**, *69*, 449. (b) Sridharan, R.; Murthy, B. N. *Epilepsia* **1999**, *40*, 631. (c) Duncan, J. S.; Sander, J. W.; Sisodia, S. M.; Walker, M. C. *Lancet* **2006**, *367*, 1087.
- (4) (a) Andurkar, S. V.; Stables, J. P.; Kohn, H. *Tetrahedron: Asymmetry* **1998**, *9*, 3841. (b) Park, K. D.; Stables, J. P.; Liu, R.; Kohn, H. *Org. Biomol. Chem.* **2010**, *8*, 2803.
- (5) (a) Stecko, S. *J. Org. Chem.* **2014**, *79*, 6342. (b) Wadavrao, S. B.; Narikimalli, A.; Narsaiah, A. V. *Synthesis* **2013**, *45*, 3383. (c) Garg, Y.; Pandey, S. K. *J. Org. Chem.* **2015**, *80*, 4201. (d) Muthukrishnan, M.; Mujahid, M.; Sasikumar, M.; Mujumdar, P. *Tetrahedron: Asymmetry* **2011**, *22*, 1353. (e) Wehlan, H.; Oehme, J.; Schäfer, A.; Rossen, K. *Org. Process Res. Dev.* **2015**, *19*, 1980.

Organocatalyzed asymmetric epoxidation of aziridine-2-ylacrylaldehyde : Synthetic application of chiral vicinal epoxyaziridine

Young-Gun Lee, Hyeonsu Jeong, Hyun - Joon Ha,* and Jung Woon Yang*¹

Department of Chemistry, Hankuk University of Foreign Studies, Yongin, 449-719, Republic of Korea.
hjha@hufs.ac.kr

¹Department of Energy Science, Sungkyunkwan University, Suwon, 440-746, Republic of Korea.
jwyang@skku.edu

(*R*)-phenylethyl aziridine-2-ylloxiran-2-carbaldehyde bearing both of aziridine and oxirane functional group in a single molecule was prepared from aziridine-2-yl-acrylaldehyde through stereoselective epoxidation with organocatalyst. Chemical and regiospecific ring-opening either at aziridine or at oxirane were successfully achieved. In the presence of NHC catalyst and alcohol, oxirane was converted to alkyl 3-(aziridin-2-yl)-3-hydroxypropionate in high yields which allowed us to determine the stereochemistry of epoxy aziridine. On the basis of this reaction, β -hydroxy- α -amino acid derivative was also achieved in 70% overall yield.

References

- ¹ (a) A. Yudin, Ed, Aziridines and Epoxides in Organic Synthesis., Wiley-VCH Verlag GmbH & Co. KGaA, **2006**. (b) M. D'hooghe and H.-J. Ha, Eds. Synthesis of 4-to 7-membered Heterocycles by Ring Expansion: Aza-, oxa- and thiaheterocyclic small-ring systems, Topics in Heterocyclic Chemistry 41, Springer, **2016**. (c) G. Callebaut, T. Meiresonne, N. De Kimpe, S. Mangelinckx, *Chem. Rev.* **2014**, *114*, 7954–8015. (d) Padwa, A.; Murphree, S. S. *ARKIVOC* **2006** (iii) 6-33.
- ² (a) J. M. Concellon, E. Riego, I. A. Rivero, and A. Ochoa *J. Org. Chem.* **2004**, *69*, 6244-6248. (b) J. Collins, M. Drouin, X. Sun, U. Rinner, and T. Hudlicky *2008 Org. Lett.* **2008**, *10*, 361-364.
- ³ Lee, W. K.; Ha, H. J. *Aldrichimica Acta*, **2003**, *36*, 57
- ⁴ Ha, H. J.; Jung, J. H.; Lee, W. K. *Asian J. Org. Chem.* **2014**, *3*, 1020
- ⁵ G. S. Singh, M. D'hooghe and N. De Kimpe, *Chem. Rev.*, **2007**, *107*, 2080-2135 and references cited therein.
- ⁶ (a) F. J. S. Duarte and A. G. Santos *Org. Biomol. Chem.*, **2013**, *11*, 7179-7191. (b) M. Marigo, J. Franzen, T. B. Poulsen, W. Zhuang, and K. A. Jørgensen *J. Am. Chem. Soc.* **2005**, *127*, 6964-6965.
- ⁷ (a) Johnson, R. A.; Sharpless, K. B. In *Comprehensive Organic Synthesis*, Trost, B. M.; Fleming, I., Eds., Pergamon Press: New York, **1991**, Vol. 7, pp. 389-436; (b) Roush, W. R.; Hoong, L. K.; Palmer, M. A. J.; Straub, J. A.; Palkowitz, A. D. *J. Org. Chem.*, **1990**, *55*, 4117-4126; (c) Brown, H. C.; Bhat, K. S.; Randad, R. S. *J. Org. Chem.*, **1989**, *54*, 1570-1576.
- ⁸ (a) Han, S. M.; Ma, S. H.; Ha, H. J.; Lee, W. K. *Tetrahedron* **2008**, *64*, 11110. (b) Jeong, H.; Yadav, N. N.; Ha, H.-J. *Synthesis*, **2017**, *49*, 1264-1272.
- ⁹ K. Y.-K. Chow and J. W. Bode, *J. Am. Chem. Soc.* **2004**, *126*, 8128-8127.
- ¹⁰ Park, C. S.; Choi, H. G.; Lee, H.; Lee, W. K.; Ha, H.-J., *Tetrahedron: Asymmetry* **2000**, *11*, 3283-3292.
- ¹¹ (a) Fumitaka Kudo, Akimasa Miyanaga and Tadashi Eguchi *Nat. Prod. Rep.*, **2014**, *31*, 1056-1073. (b) Gaetano Roncari, Zofia Kurylo-Borowska, and Lyman C. Craig, *Biochemistry*, **1966**, *5* (7), pp 2153–2159

Asymmetric synthesis of piperidine alkaloids microcosamine A and microgrewiapine A from chiral aziridines

Lingamurthy Macha, Hyun-Joon Ha*

Department of Chemistry, Hankuk University of Foreign Studies, Yongin, 449-719, Republic of Korea.
E-mail: hiha@hufs.ac.kr

2-Methyl-3-hydroxy-6-alkylated piperidines constitute an important class of natural alkaloids due to their interesting biological and pharmacological properties (anaesthetic, analgesic, antitumor, antibiotic, CNS stimulating biological properties, antihypertensive and antifungal activities etc.).¹

A divergent, new, and highly stereoselective synthesis of 2-methyl-3-hydroxy-6-alkylated piperidine natural products including microgrewiapine A², microcosamine A³ has been accomplished from aziridine-2(S)-carboxylate as chiral pool starting material. Key features of the strategy include the utility of N-methylative aziridine ring opening reaction, intramolecular reductive amination reaction to form the piperidine framework in high yields and Julia–Kocienski olefination to install the triene side-chain.

References

1. For selected reviews of piperidine alkaloids, see : (a) H. Makabe, *Stud. Nat. Prod. Chem.*, 2014, **42**, 353–371; (b) I. Ojima and D. M. Iula, *Alkaloids: Chemical and Biological Perspectives*, Elsevier, Oxford, UK, **1999**, 13, 371–412.
2. Representative references, for isolation, see: (a) P. C. Still, B. Yi, T. F. G. Cestari, L. Pan, R. E. Pavlovicz, H. B. Chai, T. N. Ninh, C. Li, D. D. Soejarto, D. B. McKay and A. D. Kinghorn, *J. Nat. Prod.*, 2013, **76**, 243–249. (b) C. Viegas Jr., V. da S. Bolzani, M. Furlan, E. J. Barreiro, M. C. M. Young, D. Tomazela and M. N. Eberlin, *J. Nat. Prod.*, 2004, **67**, 908–910
3. C. Rajireddy, B. Latha, K. Warudikar, K.K. Singarapu, *Org. Biomol. Chem.*, 2016, **14**, 251–258.

Copper-Catalyzed Diastereo- and Enantioselective Addition of 1,1-Diborylalkanes to *N,N*-Dimethylsulfamonyl Protected Acyclic Aryladimines

Jeongho Kim^a, Youngmin Kim^a, Seung Hwan Cho^a

^a Department of Chemistry and Division of Advanced Nuclear Engineering, Pohang University of Science and Technology (POSTECH), Pohang, 37673, Republic of Korea.
E-mail: kjh0704@postech.ac.kr

The preparation of chiral β -aminoboron is important in synthetic chemistry because it constitutes a core structure in many biologically active compounds. Previously, we developed an efficient copper(I)-catalytic system for diastereo- and enantioselective addition of 1,1-diborylalkanes to protected aldimines to afford synthetically valuable chiral β -aminoboron compounds.^[1] However, the developed protocol was only restricted to cyclic aldimines as a substrates, whereas general acyclic imines provided inferior stereoselectivity in our previous work. Herein, we describe an improved procedure for the diastereo- and enantioselective copper-catalyzed 1,2-addition of 1,1-diborylalkanes to *N*-protected acyclic aldimines to afford enantioenriched β -aminoboronate esters. The reaction indicates that the diastereoselectivity is quite sensitive to the protecting group, which installation of *N,N*-dimethyl sulfamoyl group to imine give the desired β -aminoboronate esters with good to excellent diastereo- and enantioselectivity. The synthetic utility of the obtained β -aminoboronate esters is provided as well.

References

[1]. Kim, J.; Ko, K.; Cho, S. H. *Angew. Chem., Int. Ed.* **2017**, *56*, 11584-11588

Transition-Metal-Free Regioselective Alkylation of Pyridine *N*-Oxide Using 1,1-Diborylalkanes as Alkylating Reagents

Chiwon Hwang,^a Woohyun Jo,^a Seung Hwan Cho^{a*}

^a Department of Chemistry, Pohang University of Science and Technology (POSTECH), Pohang, 790-784, Republic of Korea

E-mail: cwhwang@postech.ac.kr

The direct alkylation of pyridines has emerged as an expedient and atom-economical strategy for the preparation of alkylated pyridines which form the core structures of many biologically active compounds, pharmaceuticals, and agrochemicals. Consequently, a range of metal-mediated C-H alkylation reactions of pyridines have been successfully developed using late-transition metals as catalysts.¹ The radical C-H alkylation of pyridines in the presence of photocatalysts, metal catalysts, or stoichiometric amounts of oxidants has also been extensively studied in this area of research.² However, concerns regarding high costs and the presence of residual metal impurities often make these approaches unsuitable for industrial and pharmaceutical applications. Moreover, the radical approach has often resulted in the formation of an inseparable mixture of regioisomers. Thus, the development of an efficient and selective method for the alkylation, especially for the methylation, of pyridines under transition-metal-free conditions is still desirable.³

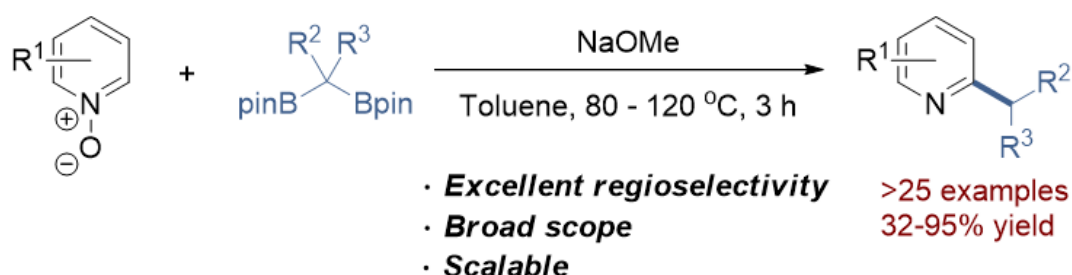


Figure 1. Transition-metal-free regioselective alkylation in pyridine *N*-oxides

In this poster presentation, we will describe an unprecedented base-promoted deborylative alkylation of pyridine *N*-oxides using 1,1-diborylalkanes as alkyl sources.^{4,5} The reaction proceeds efficiently for a wide range of pyridine *N*-oxides and 1,1-diborylalkanes with excellent regioselectivity. The utility of the developed method is demonstrated by the sequential secondary alkylation and methylation of 2,2'-bipyridine *N*-oxides. The reaction also can be applied for the direct introduction of a methyl group to 9-*O*-methylquinine *N*-oxide, thus it can serve as a powerful method for late-stage functionalization.

References

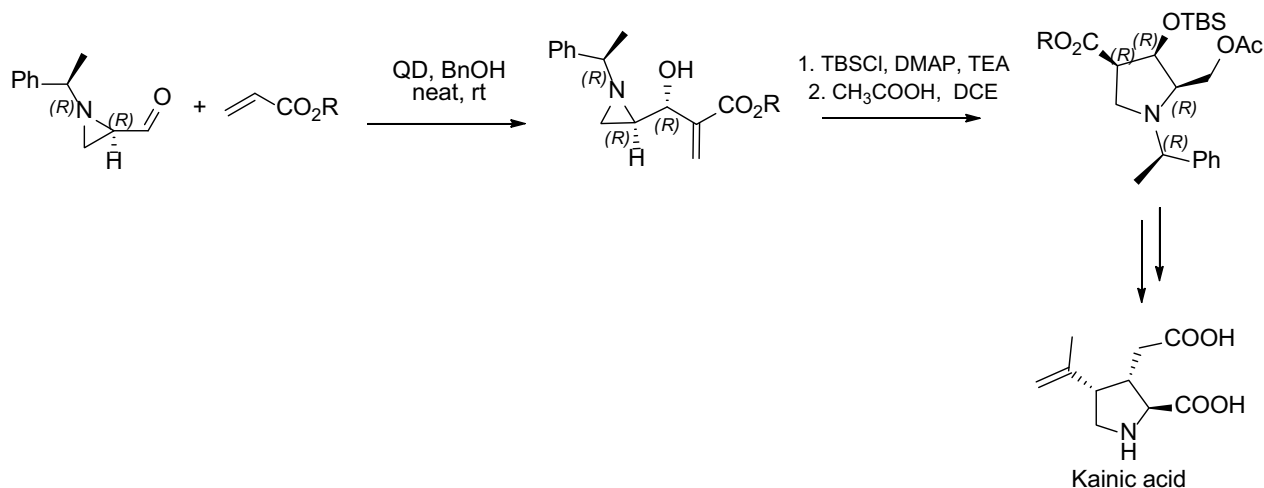
- Y. Nakao, *Synthesis* 2011, 3209
- J. Jin, D. W. C. MacMillan, *Nature*, 2015, 525, 87
- J. Kim, S. H. Cho, *Synlett*, 2016, 27, 2525
- W. Jo, J. Kim, S. Choi, S. H. Cho, *Angew. Chem. Int. Ed.* 2016, 55, 9690
- C. Hwang, W. Jo, S. H. Cho, *Chem. Commun.* 2017, 53, 7573

Morita-Baylis-Hilman Reaction of Chiral Aziridine Aldehyde and Distereoselective Synthesis of 2,3,4-Trisubstituted Pyrrolidine

Deepak Singh, Hyun-Joon Ha*

Department of Chemistry, Hankuk University of Foreign Studies, Yongin, 449-719, Republic of Korea.
E-mail: hjha@hufs.ac.kr

The distereoselective MBH reaction of (R)-1-((R)-1-phenylethyl)aziridine-2-carbaldehyde with alkyl acrylate was achieved in stereo selective manner under various reaction conditions by changing the solvents, bases and alcohol additives. The regiospecific aziridine ring opening of MBH product by acetic acid yielded 2,3,4-trisubstituted pyrrolidine *via* aza Michael reaction, which may have utility for the synthesis of various biologically active compounds including Kainic acid.



References

1. Drewes, S. E.; Emslie, N. D.; Field, S. F.; Khan, A. A.; Ramesar; *N Tetrahedron Asymmetry*, **1992**, 3, 255-260.
2. Stathakis, C. I.; Yioti, E. G.; Gallos, J. K. *Eur. J. Org. Chem.*, **2012**, 4661-4673.

***N*-methylative aziridine ring opening and the synthesis of (S)-3-methylamino-3-[(R)-pyrrolidin-3-yl]propanenitrile**

Sang-Yun Na,^a Won Koo Lee,^b and Hyun-Joon Ha,^{a,*}

^aDepartment of Chemistry, Hankuk University of Foreign Studies, Yongin, Kyunggi-Do, 17035, Korea.

^b Department of Chemistry, Sogang University, Seoul 121-742, Korea

E-mail: hjha@hufs.ac.kr; Tel: +82-31-330-4659

The preparation of (S)-3-methylamino-3-[(R)-pyrrolidin-3-yl]propanenitrile (**1**), a key fragment of fluoroquinolone antibiotic PF-00951966 and others was achieved by *N*-methylative aziridine ring opening, addition of methyl group at the ring nitrogen, and ring-opening via a cyanide nucleophile in a single operation starting from bicyclic (R)-2-[(R)-pyrrolidine-3-yl]aziridine. The starting compound was elaborated from stereoselective conjugate addition of nitromethane to (R)-aziridine-2-yl acrylate followed by selective reduction without breaking the aziridine ring.

References

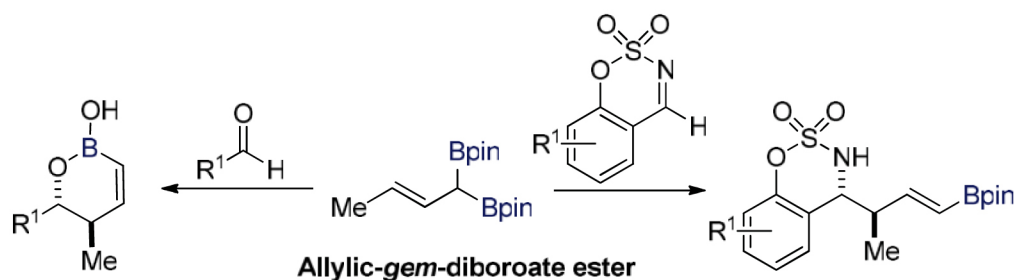
- (1) Lee, J.; Lee, J. E.; Ha, H. J.; Son, S. I.; Lee, W. K. *Tetrahedron Lett.* **2015**, *56*, 856-858.
- (2) Yoon, D. H.; Kang, P.; Lee, W. K.; Kim, Y.; Ha, H. J. *Org Lett.* **2012**, *14*, 429-431.
- (3) Lall, M. S.; Hoge, G.; Tran, T. P.; Kissel, W.; Murphy, S. T.; Taylor, C.; Showalter, H. H. et al. *J Org Chem.* **2012**, *77*, 4732-4739.
- (4) Jung, J. H.; Kim, S.; Eum, H.; Lee, W. K.; Ha, H. J. *Tetrahedron.* **2017**, *73*(41), 5993-5999.

Chemo- and Stereoselective Allylboration of Aldehydes and Cyclic Aldimines with Allylic-gem-diboronate Ester

Jinyoung Park, Seoyoung Choi, Yeosan Lee, Seung Hwan Cho*

^a Department of Chemistry, Pohang University of Science and Technology (POSTECH), Pohang 37673, Republic of Korea
jinyoung@postech.ac.kr

The preparation of new types of organoboron compounds is especially important owing to their stability and ability to undergo a wide range of organic transformations^[1] In recent years, gem-diborylalkanes have emerged as attractive synthetic intermediates for synthesizing organoborons via transitionmetal-catalyzed or transition-metal-free chemo- and stereoselective transformations with suitable electrophiles^[2] Although considerable advances have been made in recent years, most of the methods developed employed alkyl-substituted gem-diboron reagents, the use of which necessitates strong base (MOH or MO-t-Bu, M= Li, Na, K) to activate one of the pinacolato boron(Bpin) units of the gem-diborylalkane chemoselectively through the formation of an α -boryl alkyl metal species or α -borylcarbanion.^[3]



- A new type of *gem*-diboron compound
- Excellent stereoselectivity
- Base-free chemoselective C-B activation
- Excellent functional group tolerance

Herein we report a highly chemo- and stereo selective crotylation of aldehydes and cyclic aldimines with allylic-gem diboronate ester as a new type of organoboron reagent. The allylic-gem-diboronate ester undergoes the crotylation with aldehydes and cyclic aldimines in excellent stereoselectivity, forming anti-5,6-disubstituted oxaborinin-2-ols or (E)- δ -boryl-anti-homoallylic amines in high efficiency. The reaction shows a wide range of substrate scope and excellent functional group tolerance. The synthetic applications of the obtained products, including stereospecific C-C, C-O, and C-Cl bond formation, are also demonstrated.

References

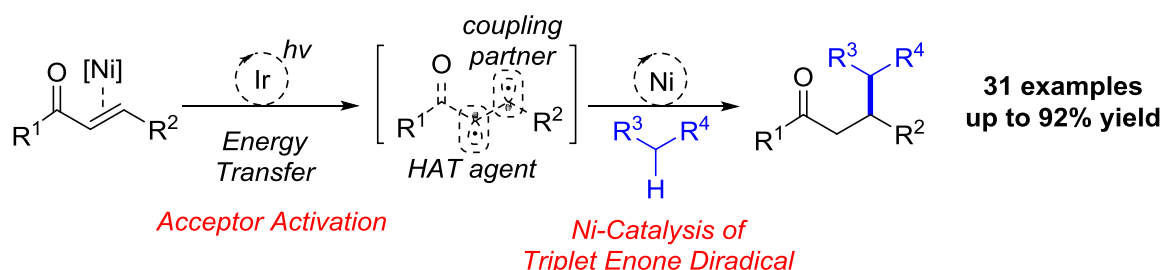
1. (a) Crudden, C. M.; Edwards, D. *Eur. J. Org. Chem.* **2003**, 2003, 4695. (b) Scott, H. K.; Aggarwal, V. K. *Chem. - Eur. J.* **2011**, *17*, 13124. 2. (a) Endo, K.; Ohkubo, T.; Hirokami, M.; Shibata, T. *J. Am. Chem. Soc.* **2010**, *132*, 11033 (b) Li, H.; Zhang, Z.; Shangguan, X.; Huang, S.; Chen, J.; Zhang, Y.; Wang, J. *Angew. Chem., Int. Ed.* **2014**, *53*, 11921, (c) Sun, C.; Potter, B.; Morcken, J. P. *J. Am. Chem. Soc.* **2014**, *136*, 6534. 3. (a) Joannou, M. V.; Moyer, B. S.; Goldfogel, M. J.; Meek, S. J. *Angew. Chem., Int. Ed.* **2015**, *54*, 14141 (b) Hong, K.; Liu, X.; Morcken, J. P. *J. Am. Chem. Soc.* **2014**, *136*, 10581.

Visible Light Mediated Ni Catalysis of Triplet Enone Diradicals for Formal Giese Addition of C(sp³)-H Nucleophiles

Geun Seok Lee and Soon Hyeok Hong*

Department of Chemistry, College of Natural Sciences, Seoul National University, 1 Gwanak-ro, Gwanak-gu, Seoul 08826, Republic of Korea
E-mail: soonhong@snu.ac.kr

An unprecedented utilization of triplet excited enones in Ni-catalysis enabled a formal Giese addition of C(sp³)-H nucleophiles. This mechanism-based approach has greatly widened the reaction scope, allowing the synthesis of previously inaccessible structures. In this process, the enone diradical acts as two distinct reaction centers, participating in both metalation and hydrogen atom transfer through a pseudo-[2+2] metalation-HAT process, which ultimately enables net C-H bond addition across activated olefins for a broad range of substrates in the presence of various functional groups. The developed reaction not only serves as an efficient method for the preparation of functionalized ketones, but can also be considered as an innovative platform for the elusive application of excited enone triplets in transition metal catalysis.



References

¹ Lee, G. S.; Hong, S. H. *Chem. Sci.* **2018**, *9*, 5810-5815.

Multipurpose Antifouling Coating of Solid Surfaces with the Sulfated Polysaccharide Fucoidan

Yeonwoo Jeong, Jeong Woo Hong, Sung Min Kang*

Department of Chemistry, Chungbuk National University, Chungbuk 28644, Republic of Korea.

E-mail: smk16@cbnu.ac.kr

The control of biofouling, which is the unwanted adsorption of biomolecules and organisms on solid surfaces, is a prerequisite for wider applicability of the functional materials that are currently being used in biomedical industries¹. One of the frequently used methods for controlling biofouling is the use of surface coatings with antifouling materials^{2,3}. Herein, fucoidan, which is a marine-derived polysaccharide, is reported as a new type of antifouling material that is safe and broadly applicable⁴. Fucoidan is conjugated with catechols, which are known to act as adhesives for grafting functional molecules onto solid substrates⁵. Fucoidan catechol (FD-C) is subsequently utilized for robust fucoidan coatings of solid substrates, and the FD-C coated platelets and bacteria. The FD-C coating is also confirmed to be nonirritating upon skin contact, demonstrating its potential use in public places for inhibiting contagions.

References

¹Kenawy, E. R.; Worley, S. D.; Broughton, R. *Biomacromolecules*. **2007**, *8*, 1359-1384.

²Callow, J. A.; Callow, M. E. *Nat. Commun.* **2011**, *2*, 244.

³Yebra, D. M.; Kiil, S.; Dam-Johansen, K. *Prog. Org. Coat.* **2004**, *50*, 75-104.

⁴Ale, M. T.; Mikkelsen, J. D.; Meyer, A. S. *Mar. Drugs*. **2011**, *9*, 2106-2130.

⁵Lee, B. P.; Messersmith, P. B.; Israelachvili, J. N.; Waite J. H. *Annu. Rev. Mater. Res.* **2011**, *41*, 99-132.

Syntheses of Resveratrol Analogues Containing Heteroatoms

Ji-geun Gim,^a Jeong Tae Lee^{a,*}

^a *Department of Chemistry and Institute of Applied Chemistry, Hallym University, Chuncheon 24252, Republic of Korea.*

E-mail: jtshl@hallym.ac.kr

Resveratrol(3,5,4'-*trans*-trihydroxystilbene) is a well-known natural product because of its antioxidant activity. A variety of resveratrol analogues have been synthesized to enhance the antioxidant activity. Our research group has synthesized π -system extended resveratrol analogues containing heteroatoms such as nitrogen and chalcogens and measured the antioxidant activity of these compounds. To understand the effect of incorporated heteroatoms in the extended resveratrols on the antioxidant activity in detail, we prepared a set of resveratrol analogues containing heteroatoms and their regioisomers.

Concise Synthesis of Guanidine Containing NSAID Conjugates

Ju Mi Lee,^a Jeong Tae Lee^{a,*}

^a *Department of Chemistry and Institute of Applied Chemistry, Hallym University, Chuncheon 24252, Republic of Korea.*

E-mail: leo900516@gmail.com

The guanidine analog (9,13*b*-dihydro-1*H*-dibenzo[*c,f*]imidazo[1,5-*a*]azepin-3-amine hydrochloride) (**1**) is a mast cell stabilizer commonly used in eye drops for the treatment of allergic conjunctivitis. It is a selective H1-receptor antagonist and is well known not to cross the blood-brain barrier. To enhance its analgesic efficacy herein, we report the synthesis of novel conjugates generated by coupling of **1** with nonsteroidal anti-inflammatory drugs (NSAIDs) such as aspirin and salicylic acid. Furthermore, synthetic approach to other conjugates containing γ -aminobutyric acid (GABA) (neurotransmitter) and gabapentin (anticonvulsant agent) moieties are also in progress. In addition, future studies we will also be directed towards the investigation on the linker moiety between **1** and NSAID.

Efficient Syntheses and Antioxidant Activities of Nitrogen Containing Heterocyclic Resveratrol Analogs

Lee Seul Park,^a Jeong Tae Lee^{a,*}

^a *Department of Chemistry and Institute of Applied Chemistry, Hallym University, Chuncheon 24252, Republic of Korea.*

E-mail: leo900516@gmail.com

Nitrogen containing heterocyclic moieties are important components of various biologically active compounds. Resveratrol (3,5,4'-*trans*-trihydroxystilbene) is a natural product known to have antioxidant activity. To improve its antioxidant efficacy, we have synthesized nitrogen containing π -extended resveratrol analogs using Wittig-Horner and metal-catalyzed reactions as key synthetic features. Antioxidant activities of these compounds were measured by ABTS assay and IC₅₀ values of these compounds were also calculated.

Synthesis and Antiinflammatory Activity of Homoisoflavonoids¹

Kongara Damodar, Jong-Gab Jun*, Jeong Tae Lee*

Department of Chemistry and Institute of Applied Chemistry, Hallym University, Chuncheon 24252,
Republic of Korea

.E-mail: leo900516@gmail.com (J. T. Lee); jgjun@hallym.ac.kr (J. -G. Jun)

We report the first syntheses of natural homoisoflavonoids, (\pm)-portulacanonones A-C (**4**, **8** and **9**), portulacanone D (**6**) isolated from *Portulaca oleracea* L (POL) and their derivatives (**3**, **5** and **7**) along with the synthesis of known derivatives (**1** and **2**) and their *in vitro* inhibitory effect against nitric oxide (NO) production in LPS-induced RAW-264.7 macrophages was also evaluated as an indicator of anti-inflammatory activity. The results showed that all the compounds tested had a concentration-dependent inhibitory effect and had no significant cytotoxicity to the macrophages at their effective concentration for the inhibition of NO production. Of these compounds, compound **3** (97.2% at 10 μ M; IC₅₀ = 1.26 μ M) followed by **6** (portulacanone D) (92.5% at 10 μ M; IC₅₀ = 2.09 μ M), **1** (91.4% at 10 μ M; IC₅₀ = 1.75 μ M) and **7** (83.0% at 10 μ M; IC₅₀ = 2.91 μ M) were the most potent from the series. The findings were further correlated with the suppressed expression of iNOS induced by LPS. Taken together, compound **3** may serve as a lead structure that merits further investigation for a NO production-targeted anti-inflammatory drug development and also could support the usefulness of POL as a folklore medicinal plant in the treatment of inflammatory diseases where NO is involved.

References

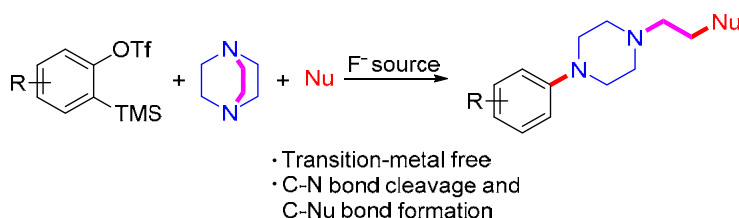
¹ Damodar, K.; Lee, J. T.; Kim, J. -K.; Jun, J. -G. *Bioorg. med. chem. lett.* **2018**, *28*, 2098-2102.

Three-Component Reactions of Arynes, Amines, and Nucleophiles via a One-Pot Process

Gyoungwook Min, Jeongseob Seo, and Haye Min Ko*

Department of Bio-Nano Chemistry, Wonkwang University, 460 Iksandae-ro, Iksan, Jeonbuk 54538, Republic of Korea
E-mail: hayeminko@wku.ac.kr

An unprecedented three-component reaction of arynes, tertiary amines, and nucleophiles has been demonstrated through ammonium salt intermediates. This protocol allows access to tertiary aniline derivatives containing the piperazine motif in good-to-excellent yields. Expansively, this reaction can produce biologically important 2-(4-phenylpiperazin-1-yl)ethyl-containing molecules using arynes, 1,4-diazabicyclo(2.2.2)octane (DABCO), and nucleophiles via a one-pot process.¹



References

- 1) G. Min, J. Seo, and H. M. Ko, *J. Org. Chem.* **2018**, *83*, 8417–8425

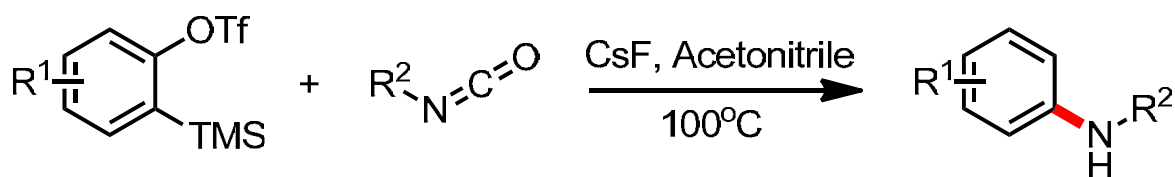
Transition-metal-free synthesis of Aromatic amines *via* the reaction of benzyne with isocyanates

Dong Wook Hwang, Jeong Hoon Seo, Haye Min Ko*

Department of Bio-Nano Chemistry, Wonkwang University, 460 Iksandae-ro, Iksan, Jeonbuk 54538, Republic of Korea

E-mail: hayeminko@wku.ac.kr

An unexpected reaction between benzyne and isocyanates to generate aromatic amines has been developed under transition-metal-free conditions. The *in situ* prepared anions formed through cleavage of the N-C bond in isocyanates, reacted with aryne precursors to afford various aniline derivatives in moderate to excellent yield and tolerated various substituents on the *o*-silyl aryl triflate and the isocyanate.¹



References

¹ J. H. Seo, H. M. Ko, *Tetrahedron Lett.* **2018**, *59*, 671-674

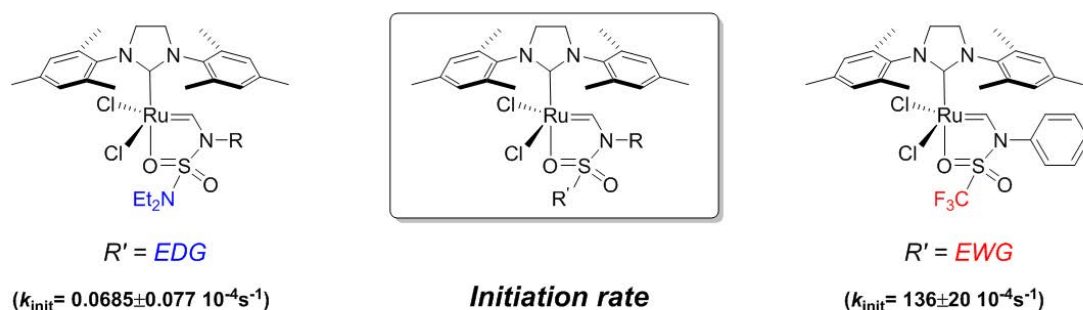
Development of Highly Versatile and Controllable Ruthenium Based Olefin Metathesis Catalyst

*Kitaek Song, Kunsoon Kim, Daeun Hong and Soon Hyeok Hong**

Department of Chemistry, College of Natural Sciences, Seoul National University, 1 Gwanak-ro, Gwanak-gu, Seoul 08826, Republic of Korea

Construction of carbon-carbon double bond via olefin metathesis has received a lot of attention over several decades.¹ Due to its moisture- and air-stability, and tolerance toward many functional groups, well-defined ruthenium based olefin metathesis catalysts, originally developed by the Grubbs group, have been widely used in organic synthesis. Among several modified Ru catalysts, the Hoveyda-type catalysts, based on a chelated *o*-isopropoxy benzylidene ligand scaffold, have good stability and high activity.² Initiation rates of the Hoveyda-type catalysts are directly related to electronic and steric nature of the chelating ligands. Tremendous efforts have been made to control the initiation by modification of the ligands.³ However, a versatile ligand system which is easily tunable by simple synthetic variation is still required for various applications of olefin metathesis.

To address the issue, novel ruthenium-based metathesis catalysts were developed based on a versatile N-vinylsulfonamide ligand scaffold. The developed catalysts exhibit highly controllable initiation behavior by simple modification of the readily available and structurally diverse N-vinylsulfonamide ligands, allowing high degree of tunability of catalyst activity.



References

- ¹Trnka, T. M.; Grubbs, R. H. *Acc. Chem. Res.* **2001**, *34*, 18-29.
- ²Kingsbury, J. S.; Hoveyda, A. H. *J. Am. Chem. Soc.* **1999**, *121*, 791-799.
- ³Engle, K. M.; Grubbs, R. H. *J. Am. Chem. Soc.* **2015**, *137*, 5782-5792.

Synthesis of Fused Azacycles *via* Oxidative C-H Activation

정아름,^a 민선준^{a, b *}

^a Department of Applied Chemistry, Hanyang University (ERICA), Ansan, 15588, South Korea.

^b Department of Chemical & Molecular Engineering, Hanyang University (ERICA), Ansan, 15588, South Korea.

Email: sjmin@hanyang.ac.kr

Tetrahydroisoquinoline derivatives (THIQs) are heterocyclic compounds which consist of hydrogenated form of isoquinolines and they are often found as building blocks in organic synthesis or pharmaceuticals with a wide variety of biological activities. For example, THIQ and its derivatives have been reported as antagonists of dopamine D2 receptors, which would be applicable to development of therapeutic candidates for treatment of Parkinson's diseases. The oxidative C-C bond formation of amines with nucleophiles has received considerable attention in organic synthetic community. While many examples of the intermolecular reactions have been reported, the intramolecular reactions are somewhat limited. Several cyclization reactions of amines with nucleophiles using transition metals such as Fe, Pd, Cu and Ru as oxidants have been reported, but intramolecular oxidative Mannich type cyclizations of ketones are still rare.¹ Thus, the synthesis of fused azacycles *via* direct C-H activation of cyclic amines under mild metal-free conditions is challenging.

In this poster, our synthetic approaches towards fused azacyclic systems such as tetrahydroisoquinolines *via* oxidative C-H activation are described. Our synthetic plan includes a conjugate addition reaction of cyclic amines followed by an intramolecular Mannich cyclization to afford *N*-containing tricyclic system. A novel 'one-pot' process for synthesis of those ring systems using consecutive Michael and Mannich reactions will be also presented.

References

- ¹ Yang, Q.; Zhang, L.; Ye, C.; Luo, S.; Wu, L.-Z.; Tung, C.-H. *Angew. Chem. Int. Ed.* **2017**, *56*, 3694–3698.

Enhancing the Effect of Photodynamic Therapy in Hypoxic Condition by Targeting a Carbonic Anhydrase IX

김지현,^a 구세영,^a 정효성,^b 심인섭,^a 손수빈,^a 김수빈,^a 김형석,^a 김종승,^{a*}

^aDepartment of Chemistry, Korea University, Seoul 02841, Korea

^bDepartment of Biological Sciences, Hyupsung University, Hwasung-si 18330, Korea.

E-mail: jshyeon1@naver.com

A major challenge in photodynamic cancer therapy (PDT) is avoiding PDT-induced hypoxia, which can lead to cancer recurrence and progression through activation of various angiogenic factors and significantly reduce treatment outcomes. Reported here is an acetazolamide (AZ)-conjugated BODIPY photosensitizer (AZ-BPS) designed to mitigate the effects of PDT-based hypoxia by combining the benefits of anti-angiogenesis therapy with PDT. AZ-BPS showed specific affinity to aggressive cancer cells (MDA-MB-231 cells) that overexpress carbonic anhydrase IX (CAIX). It displayed enhanced photocytotoxicity compared to a reference compound, BPS, which is an analogous PDT agent that lacks an acetazolamide unit. AZ-BPS also displayed an enhanced in vivo efficacy in a xenograft mouse tumor regrowth model relative to BPS, an effect attributed to inhibition of tumor angiogenesis by both PDT-induced ROS generation and CAIX knockdown. AZ-BPS was evaluated successfully in clinical samples collected from breast cancer patients. We thus believe that the combined approach described here represents an attractive therapeutic approach to targeting CAIX-overexpressing tumors.

References

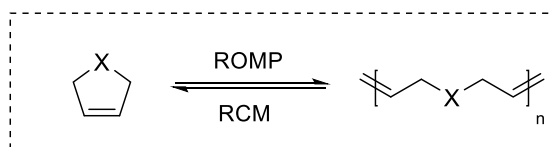
H. S. Jung, J. Han, H. Shi, S. Koo, H. Singh, H.-J. Kim, J. L. Sessler, J. Y. Lee, J.-H. Kim, J. S. Kim, *J. Am. Chem. Soc.* **2017**, 139, 7595-7602.

Ring Opening Metathesis Polymerization of Low-Strained Cyclopentene Derivatives Enabled by Highly Active Ruthenium Olefin Metathesis Catalysts

Daeun Hong, Kitaek Song, Kunsoo Kim, and Soon Hyeok Hong*

Department of Chemistry, College of Natural Sciences, Seoul National University, 1 Gwanak-ro, Gwanak-gu, Seoul 08826, Republic of Korea
E-mail: soonhong@snu.ac.kr

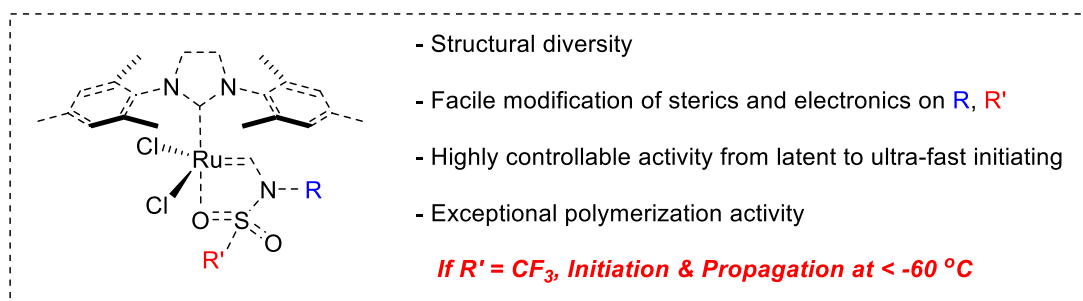
Ring opening metathesis polymerization (ROMP) has been studied for several decades since it is a highly efficient way to obtain variously functionalized linear and controlled polymers. The basic driving force for ROMP is release of strain energy of constrained monomers such as norbornene and its derivatives (>20 kcal/mol). However, cyclopentenes have significantly lower ring strains (4.45-6.84 kcal/mol) than those of norbornene derivatives so that only a few examples of the ROMP of cyclopentenes have been reported. Because the polymerization reaction is an entropically disfavored reaction, low temperature conditions are preferred to drive the reaction thermodynamically toward the polymerization. However, the low temperature conditions have kinetically deleterious effect to initiate the precatalyst which usually requires external energy to dissociate a ligand. Therefore, a fast initiating catalyst which can be initiated at low temperatures will be ideal to perform the polymerization of challenging low strained monomers. Herein, we developed novel ruthenium-based olefin metathesis catalysts which are active even at -60 °C and initiate very fast. With the catalysts, the polymerization of low-strained cyclopentene derivatives was successfully achieved. Especially, cyclopentenes almost unreactive with the previously reported catalysts reacted well delivering the ROMP products in high yields, providing novel polymeric structures.¹



$$\Delta G = \Delta H - T\Delta S$$

($\Delta H = -4.45 \sim -6.84$, $\Delta S < 0$)

Low temperature conditions are favored for ROMP



References

¹ Heji, A.; Scherman, O. A.; Grubbs, R. H., *Macromolecules*, **2005**, *38*, 7214-7218.

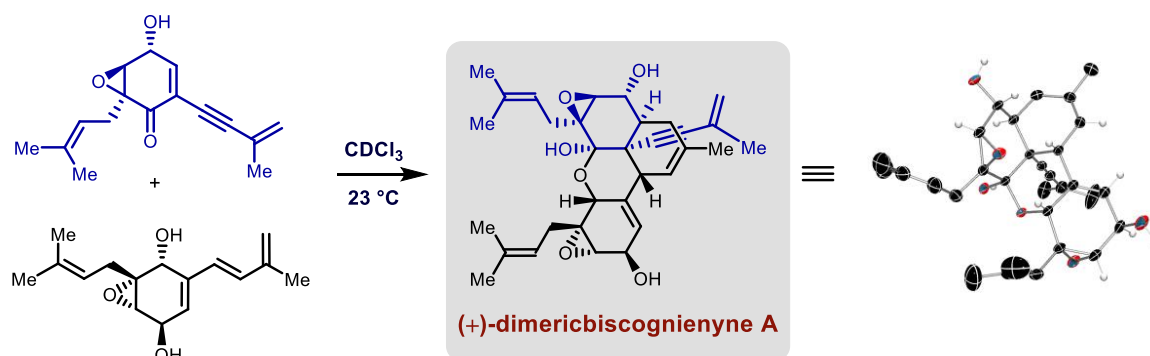
(+)-Dimericbiscognienyne A: Total Synthesis and Mechanistic Investigations of the Key Heterodimerization

Geon Kim,^a Myungjo J. Kim,^a Garam Chung,^{a,b} Hee-Yoon Lee,^{*,a} and Sunkyu Han^{*,a,b}

^a Department of Chemistry, Korea Advanced Institute of Science and Technology, 291 Daehak-ro, Yuseong-gu, Daejeon 34141 (Republic of Korea)
E-mail: sunkyu.han@kaist.ac.kr, leehy@kaist.ac.kr

^b Center for Catalytic Hydrocarbon Functionalizations, Institute for Basic Science, 291 Daehak-ro, Yuseong-gu, Daejeon 34141 (Republic of Korea)
E-mail: sunkyu.han@kaist.ac.kr

The first total synthesis of (+)-dimericbiscognienyne A¹ is described. Key to the successful access to (+)-dimericbiscognienyne A was the biosynthetically inspired Diels–Alder reaction between two differential epoxyquinoid monomers and the subsequent intramolecular hemiacetal formation. The selective formation of the natural product among other potential diastereomers during the late stage [4+2] cycloaddition reaction was investigated by DFT calculations and experimental control studies.



References

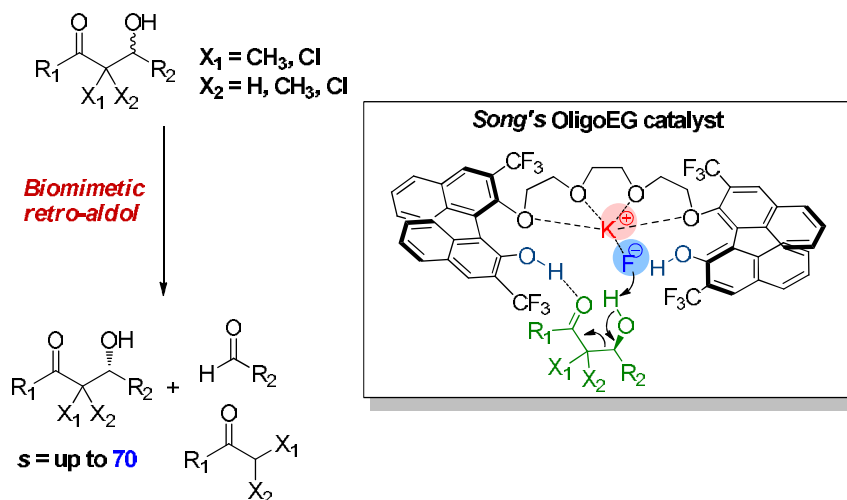
¹ Zhao, H.; Chen, G.-D.; Zou, J.; He, R.-R.; Qin, S.-Y.; Hu, D.; Li, G.-Q.; Guo, L.-D.; Yao, X.-S.; Gao, H. *Org. Lett.* **2017**, *19*, 38–41.

The Mimic of Type II Retro-Aldolase Chemistry: Kinetic Resolution of β -Hydroxy Carbonyl Compounds via Enantioselective Retro-Aldol Reaction

Sushovan Paladhi,^a Amol P. Jadhav,^a In-Soo Hwang,^a Si-Joon Park,^a S. Y. Park,^a Choong Eui Song^{a*}

^a Department of Chemistry, Sungkyunkwan University, Suwon 16419, Korea.
E-mail: s1673@skku.edu

In nature, retro-aldolases degrade aldol adducts to their starting ketones and aldehydes. For instance, fructose-1,6-bisphosphate aldolase can cleave a sugar fructose-1,6-bisphosphate into glyceraldehyde 3-phosphate (GAP, an aldehyde) and dihydroxyacetone phosphate (DHAP, a ketone). Inspired by this nature's retro-aldol strategy, we successfully developed a highly enantioselective biomimetic kinetic resolution of racemic β -hydroxy carbonyl (aldol) compounds through enantioselective retro-aldol process using a Song's oligoEG catalyst as an artificial type-II retro-aldolase. Study of a variety of aldol substrates demonstrated that our biomimetic retro aldol protocol provides rapid entry to highly enantiomerically enriched aldols. In this workshop, the utility of this approach to the synthesis of chiral aldehydes will be also presented.



References

¹ Paladhi, S.; Hwang, I.-S.; Song, C. E. *Org. Lett.* **2018**, *20*, 2003-2006.

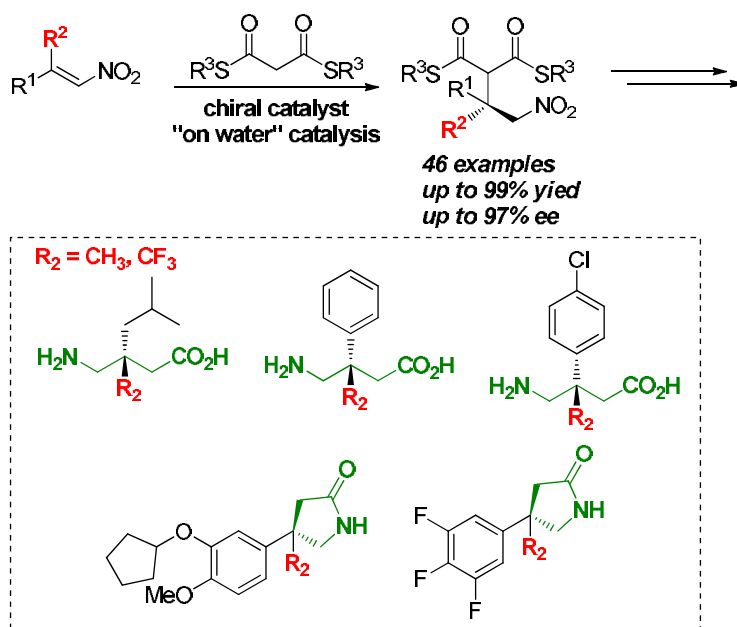
Water-Enabled Catalytic Asymmetric Michael Reactions of Unreactive Nitroalkenes: Synthesis of Chiral GABA-Analogs with All-Carbon Quaternary Stereogenic Centers

J. H. Sim,^a J. H. Park,^a P. Maity,^a S. Park,^a Y. J. Chang,^a V. Ashokkumar,^a C. E. Song^{a*}

^a Department of Chemistry, Sungkyunkwan University, Suwon, 16419, Korea
E-mail: s1673@skku.edu

In nature, water is used not only as a reaction medium but also as a reaction enforcer in enzymatic processes for biosynthetic reactions to sustain life, by inducing hydrophobic interactions between enzymes and substrates.

In this workshop, we will present our recent discovery that water enables new catalytic reactions for otherwise unreactive substrate systems. Under the “on water” reaction conditions, extremely unreactive β,β -disubstituted nitroalkenes smoothly underwent enantioselective Michael addition reactions with dithiomalonates using a chiral organocatalyst, affording both enantiomers of highly enantio-enriched Michael adducts with all-carbon quaternary stereogenic centers. The developed “on water” protocol was successfully applied for the scalable one-pot synthesis of chiral GABA analogs with all-carbon quaternary stereogenic centers at the β -position, which might show highly interesting pharmaceutical properties. This successful catalysis can be ascribed to enforced hydrophobic interactions between catalysts and substrates due to the hydrophobic hydration effects.



References

- ¹ Bae, H. Y.; Song, C. E. *ACS Catal.* **2015**, *5*, 3613-3619.
- ² Sim, J. H.; Song, C. E. *Angew. Chem. Int. Ed.* **2017**, *56*, 1835-1839.

Fe(III)-Complexes for the Selective Formation of Cyclic Carbonates from CO₂ and Internal Epoxides

Yuseop Lee, Indranil Sinha, Choongman Bae, Samat Tussupbayev, Yujin Lee, Min-Seob Seo, Jin Kim, Mu-Hyun Baik*, Yunho Lee*, and Hyunwoo Kim*

주소 Department of Chemistry, Korea Advanced Institute of Science and Technology, Yuseong-gu, Daejeon 34141, Korea

CO₂ is an attractive C1 building block because it is abundant and renewable. Also, it is considered as a phosgene replacement due to its nontoxic nature.¹ Therefore, various kinds of CO₂ utilization methods have been developed² not only because of these prominent features but also concerns of global warming, since CO₂ is one of green house gases. One of the promising CO₂ utilization methods is to make cyclic carbonates from epoxides. Cyclic carbonates are used as polar aprotic solvent, electrolytes or intermediates for organic synthesis. Several catalysts for cyclic carbonates have been reported, including organocatalysts and transition metal complexes. Among them, the properties of salen-based catalysts are quite remarkable, which can switch the selectivity between cyclic carbonates and polycarbonates depending on metal center and ligand structure³.

Recently, Kleij have reported⁴ highly active and selective catalysts for cyclic carbonates with mononuclear Al and dinuclear Fe complexes based on amino tris(phenolate) ligands. According to the DFT computation, authors proposed a transition state where two oxygen atoms each from epoxide and CO₂ bind to the metal center in a cis fashion, thereby greatly lowering the activation barrier.⁵ Thus, highly active and selective catalysts for cyclic carbonate synthesis can be developed on the basis of three fold symmetric amino tris(phenolate) ligand scaffolds. We have designed a new class of NO₃ ligand for selective synthesis of cyclic carbonates resulting from available cis-binding site of the metal center. Here we introduce highly efficient and selective Fe catalysts based on our C_s symmetric NO₃ ligands for coupling of CO₂ and epoxides.

References

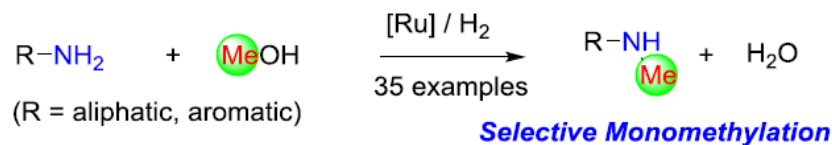
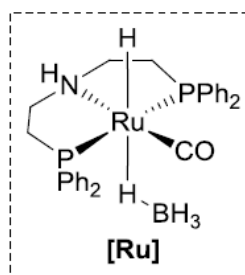
1. McGhee, W.; Riley, D.; Christ, K.; Pan, Y.; Parnas, B. *J. Org. Chem.* **1995**, *60*, 2820.
2. Liu, Q.; Wu, L.; Jackstell, R.; Beller, M. *Nature Communications* **2015**, *6*, 5933.
3. (a) Paddock, R. L.; Nguyen, S. T. *J. Am. Chem. Soc.* **2001**, *123*, 11498. (b) Meléndez, J. North, M.; Pasquale, R. *Eur. J. Inorg. Chem.* **2007**, 3323. (c) Sujith, S.; Min, J. K.; Seong, J. E.; Na, S. J.; Lee, B. Y. *Angew. Chem., Int. Ed.* **2008**, *47*, 7306.
4. Whiteoak, C. J.; Kielland, N.; Laserna, V.; Escudero-Adán, E. C.; Martin, E.; Kleij, A. W. *J. Am. Chem. Soc.* **2013**, *135*, 1228.
5. Whiteoak, C. J.; Kielland, N.; Laserna, V.; Castro-Gómez, F.; Martin, E.; Escudero-Adán, E. C.; Bo, C.; Kleij, A. W. *Chem. Eur. J.* **2014**, *20*, 2264.

Selective Monomethylation of Amines Using Methanol as a Sustainable C1 Reagent

Geunho Choi and Soon Hyeok Hong*

Department of Chemistry, College of Natural Sciences, Seoul National University, 1 Gwanak-ro, Gwanak-gu, Seoul 08826, Republic of Korea
E-mail: soonhong@snu.ac.kr

The N-monomethyl functionality is a common motif in a variety of synthetic and natural compounds. However, facile access to such compounds remains a fundamental challenge in organic synthesis owing to selectivity issues caused by overmethylation. To address this issue, the selective, catalytic monomethylation of various structurally and functionally diverse amines including typically problematic aliphatic primary amines was developed using methanol as the methylating agent, which is a sustainable chemical feedstock.¹ Control experiments indicated that the presence of hydrogen was essential to control dehydration over dehydrogenation of the hemiaminal intermediate. In addition to this work, selective N-formylation and N-methylation reactions of amines using methanol is currently under development.



- Methanol as the C1 source
- Kinetically controlled selectivity
- Selective monomethylation of both aromatic & challenging aliphatic amines

References

¹ Choi, G.; Hong, S. H. *Angew. Chem. Int. Ed.* **2018**, *57*, 6166-6170.

Pt(II) Complexes with High Emission Quantum Efficiency for Effective Photon Down-shifting on Silicon Solar Cells

Eunhye Hwang^a, Hyun-Tak Kim^a, Wonjoo Jin^b, Kangmin Lee^b, Kwanyong Seo^{*,b} and Tae-Hyuk Kwon^{*,a}

^a Department of Chemistry and ^bDepartment of Energy Engineering,
Ulsan National Institute of Science and Technology (UNIST), Ulsan 44919,
Republic of Korea.
E-mail: ehhwang@unist.ac.kr

Silicon solar cell is one of the most developed and commercialized types of photovoltaics. In terms of the overall performance, however, it shows quite low external quantum efficiency (EQE) with the high-energy region light (< 500 nm), which is caused by the severe surface recombination. To enhance the EQE of silicon solar cells in the ultraviolet region, quantum dots which absorb high-energy photons and emit low-energy ones have been reported.¹⁻² However, the quantum dots usually have a limitation in controlling the range of absorbed light and there is also a long-term stability issue.

Here, we present stable Pt(II) complexes with high emission quantum efficiency and easily tunable ligands. We have designed and synthesized four kinds of Pt(II) complexes and applied them as photon down-shifting layers in silicon solar cells. The optical properties and solubility of these compounds were successfully adjusted by ligand tuning. The photon down-shifting layers consisting of the complexes were fabricated by using the ultrasonic spray deposition (USD) method to reduce the aggregation. For the silicon solar cells coated with the thin layers of the Pt(II) complexes, the enhancement in J_{sc} has been observed and the EQE in the ultraviolet region has also been improved. Among them, the case of the compound having the most suitable absorption / emission range and the strong emission property shows the greatest increase in the device performance.

References

1. Tsai, M.-L.; Tu, W.-C.; Tang, L.; Wei, T.-C.; Wei, W.-R.; Lau, S. P.; Chen, L.-J.; He, J.-H. *Nano Lett.* 2016, 16, 1, 309-313
2. Lopez-Delgado, R.; Zhou, Y.; Zazueta-Raynaud, A.; Zhao, H.; Pelayo, J. E.; Vomeiro, A.; Alvarez-Ramos, M. E.; Rosei, F.; Ayon, A. *Sci. Rep.* 2017, 7, 14104

Development of a Amino Acid Based Transient Directing Group for Pd-Catalyzed C-H Arylation and Their Synthetic Application

Kwangho Yoo^a, Hyojin Park^a, Byunghyuck Jung^{b*}, Min Kim^{a*},

^aDepartment of Chemistry, Chungbuk National University, Cheongju, 28644, Korea. ^bSchool of Basic Science, Daegu Gyeongbuk Institute of Science & Technology, Daegu, 42988, Korea.

E-mail: minkim@chungbuk.ac.kr

Recently transition metal-catalyzed C–H bond activation reaction using directing group is one of the interest in organic chemistry. In the past decade, significant progress has been made in terms of the transition metal-catalyzed C-H activation by using directing group such as nitrogen containing structure. However, directing group approaches typically require additional steps for the installation and removal of the chelating component, and diminishes the efficiency and compatibility of the reactions in the practical concept. Recently, C-H bond activation reactions using temporary, transient directing groups that can be reversibly linked to the substrate have developed to overcome these disadvantages.¹

In this presentation, first of all, novel amino acid-based transient ligand development for the first step, palladium-catalyzed C-H bond arylation reaction will be discussed. The new transient directing group reversibly reacts with the aldehydes to imine formation. And the palladium could be positioned and activate the inert C–H bonds by this temporary directing group.^[1-3] The preparation of new ligands and their catalytic activities will be presented along with substrate scopes for *sp*³ C-H bond arylation reactions. And the direct synthesis of anthracenes will also be discussed. From the reaction between *o*-tolualdehydes and aryl iodides, the anthracene derivatives were obtained. The selectivity from silver oxidant, and the substrate scope for anthracenes will be presented.²

References

¹Zhang, F. L.; Hong, K.; Li, T. J., Park; H., Yu, J. Q. *Science* **2016**, 351, 252.

²H. Park, K. Yoo, B. Jung, M. Kim, *Tetrahedron* **2018**, 74, 2048-2055.

Fine Tuning of Polydiacetylene in Molecular Level for PDA Sensors

Kwangho Yoo^a, Narae Han^a, Min Jae Shin,^{b*} Jae Sup Shin,^{a*} Min Kim^{a*}

^aDepartment of Chemistry, Chungbuk National University, Cheongju, 28644, Korea. ^bDepartment of Oriental Cosmetic Science, Semyung University, Jecheon, Chungbuk 27136, Korea
E-mail: minkim@chungbuk.ac.kr

Polydiacetylenes(PDAs) are polymeric systems of diacetylene monomers that have been applied to various sensing applications.¹ Micelle type PDA vesicle is synthesized by UV-mediated photopolymerization, and PDA-liposomes are formed in aqueous solution by following sonication. The color of PDA-liposomes is changed under various external stimuli such as temperature, pH, surfactants and detection of metal ion.

Recently, we have controlled diacetylene molecules in organic chemistry level with several functional groups, and reported interesting color changing phenomena of alkyl chain length controlled PDAs without external stimuli. And it is also revealed that the molecular interaction between PDA-liposomes and external stimuli is directly related with color-changing temperature.²

In this presentation, the synthesis of functionalized PCDA molecules along with supporting characterizations, further studies for stepwise color change of PDA vesicle will be discussed. Although general PDA shows blue-red color transitions, the alkyl chain length-controlled (*e.g.*, methyl and octyl) showed interesting and reversible red-yellow color transition by temperature increase. And unique sensing ability of amine-functionalized PDA vesicles will be presented.

References

¹R. Jelinek, M. Ritenberg, *RSC Adv.* **2013**, 3, 21192.

²N. Han, H. J. Woo, S. E. Kim, S. Jung, M. J. Shin, M. Kim, J. S. Shin, *J. Appl. Poly. Sci.* **2017**, 134, 45011.

³K. Yoo, S. Kim, N. Han, G. E. Kim, M. J. Shin, J. S. Shin, M. Kim, *Dye. Pig.* **2018**, 149, 242.

Introducing Phenylacetylene Moiety into Metal-Organic Hybrid Materials

Dopil Kim,^a Jooyeon Lee,^a Sangdon Choi,^a Min Kim^{a*}

^aDepartment of Chemistry, Chungbuk National University, Cheongju, 28644, Korea.
E-mail: minkim@chungbuk.ac.kr

Metal-organic framework (MOF) and metal-organic polyhedra (MOP) are a porous hybrid material consisted of metal clusters or metal ions and multivalent organic linker molecules.¹ The major differences between MOF and MOP is the repeating units for framework and isolate cage. Since both MOF and MOP has metal clusters or ions as vertex in their structure, catalytic applications using metal parts have been developed for various organic transformations. Moreover, the tunability of organic linker molecule is the major advantage of MOFs and MOPs than other porous materials, and various organic functional groups such as alcohols, amines, azides, amides, etc have been successfully incorporated into MOF pores.² In this presentation, the synthesis of an alkyne-containing dicarboxylic acid ligand for MOF and MOP preparation will be discussed. The phenylacetylene moiety was successfully installed in benzene-1,4-dicarboxylic acid (*p*-BDC) and benzene-1,3-dicarboxylic acid (*m*-BDC) through Sonogashira cross-coupling, and directly applied to MOF and MOP synthesis. Detail ligand preparation and synthetic condition screening will be presented with supporting data.

Reference

¹ Yaghi, O. M.; Li, H.; Davis, C.; Richardson, D.; Groy, T. L. *Acc. Chem. Res.* **1998**, *31*, 474.

² Kim, M.; Cohen, S. M. *CrystEngComm*. **2012**, *14*, 4096.

Synthesis of Vinyl-Functionalized Metal-Organic Frameworks and Their Applications

Hyojin Park,^a Jooyeon Lee,^a Chinnadurai Satheeshkumar,^b Myungeun Seo^{b*}, Min Kim^{a*}

^aDepartment of Chemistry, Chungbuk National University, Cheongju, 28644, Korea. ^bGraduate School of Nanoscience and Technology, KAIST, Daejeon, 34141, Korea
E-mail: minkim@chungbuk.ac.kr

Metal-organic frameworks (MOFs) are 3D porous organic/inorganic hybrid materials. Compare to other porous inorganic materials such as zeolite and mesoporous silica, the organic functional groups could be installed into MOF relatively easily via organic transformation on the linkers. It allows a variety of organic functionalities such as amines, alcohols, halogens, amides, and etc in their ligand on frameworks. And these organic functional groups are aimed for fine-tuning of MOFs to various applications with physical and chemical property changes and further synthesis.¹ Recently, we have introduced carbon-carbon double bond containing (i.e., vinyl-functionalized) BDC (benzene-1,4-dicarboxylate) into MOF. The ligand preparation and detail characterization of vinyl-functionalized MOF will be discussed in this presentation. In addition, we have successfully developed a facile methodology for fabricating a free-standing mixed-matrix membrane (MMM) containing covalently incorporated MOF particles up to 60 wt% by utilizing thiol-ene photopolymerization with MOF consisting of vinyl functionality. Assorted analyses combining FT-IR, TGA (thermogravimetric analysis), SEM (scanning electron microscopy), EDX (energy dispersive X-ray spectroscopy), and PXRD (powder X-ray diffraction) strongly supported that the desired MMM containing well-dispersed MOF particles was successfully produced by C-S bond formation between the MOF surface and the polymer matrix, which provided strong union without interfacial voids. The detail characterization data will be presented and discussed.

Reference

¹ Kim, M.; Cohen, S. M. *CrystEngComm*. **2012**, *14*, 4096-4101.

Practical Postsynthetic Ligand Exchange using Defective Metal-Organic Frameworks

Seongwoo Kim, Hyojin Park, Min Kim*

Department of Chemistry and BK21Plus Research Team, Chungbuk National University, Cheongju, 28644, Republic of Korea
E-mail: minkim@chungbuk.ac.kr

MOFs are of great promise materials for a variety of applications such as gas storage, separation, catalysis, etc, because of the near infinite possibilities regarding their structure, porosity, and chemical functionality.¹ To introduce functional group to MOFs, pre-synthetic method and postsynthetic modification (PSM) are known, and post-synthetic exchange (PSE) method has been reported.

Recently, structural defects were revealed in MOF crystal structures have many interests in coordination material research fields. Since MOFs are constructed by repeating coordination bonds between metal ions (or clusters) and organic ligands, the disappearance of metal clusters or organic linker molecules generate structural defects on the frameworks.² The structural defects could give physically unstable frameworks, however, at the same time, allow more accessible channel or porosity to the guest molecules. Very recently, the defect engineering in MOFs pores are receiving much attention from this point of view.

In this presentation, the practical PSE (postsynthetic ligand exchange) process through defective MOF will be discussed. The existence of defect and increase of defect amount in the framework could accelerate the incorporation of target ligands. And large size or polar functional group substituents are also successfully installed into UiO-66 frameworks through ligand exchange process. The scope of functionalizations and the detail kinetics along with application will be presented.³

References

¹ Zhou, H.-C.; Long, J.-R.; Yaghi, O.-R. *Chem. Rev.* **2012**, *112*, 673.

² Fang, Z.; Bueken, B.; De Vos, D.-E.; Fischer, R.-A. *Angew. Chem. Int. Ed.* **2015**, *54*, 7234.

³ Park, H.; Kim, S.; Jung, B.; Park, M. H.; Kim, Y.; Kim, M. *Inorg. Chem.* **2018**, *57*, 1040.

Enantioselective Boryllallylation of Vinyl Arenes and its Application to Direct Stereoconvergent Transformation

Jung Tae Han^a, Jaesook Yun^{*a}

^a Department of Chemistry, Sungkyunkwan University, Suwon, Korea.
E-mail: jaesook@skku.edu

Cascade reaction of C–B bond and C–C bond formation in a single vessel is an efficient method for preparation of organoboron molecules. Recently, our research group reported a copper-catalyzed enantioselective boryllallylation of vinyl arenes with simple allylphosphates. In this protocol, a variety of vinyl arenes afforded the corresponding coupled product in up to 96% ee.¹ As continuing study, a direct stereoconvergent boryllallylation of vinyl arenes with racemic allylphosphates was established. In this process, both enantiomers of starting allylphosphates were converted into single enantiomer product through two distinct reaction pathways.

References

¹ Kim, N.; Han, J. T.; Ryu, D. H.; Yun, J. *Org. Lett.* **2017**, *19*, 6144-6147.

A new indomethacin conjugated fluorescent probe for selective imaging of cancer-specific COX-2

Jiseon Kim,^a Amit Sharma, Won Young Kim, Jihyeon Kim, Taeho Jeong, Inseob Shim, Kyoung Sunwoo, Geun Young Park, and Jong Seung Kim^{a*}

Supramolecular Nano-organic Material Laboratory, Department of Science, Korea University, Seoul, 02841, Korea.

E-mail: aliceks@korea.ac.kr

For the selective bioimaging of cancer cells, we synthesized and designed an IQ-1, indomethacin-conjugated fluorescence probe. The probe IQ-1 was non-cytotoxic in various human cells. Besides, using confocal fluorescence microscopy we observed that its fluorescence intensity depended on the COX-2 levels. Compared with normal cell lines (RAW 246.7 and fibroblast cells), the probe demonstrated an increased fluorescence in cancer cells (OVCAR 3, HepG2, and HeLa cells) with overexpressed COX-2. LPS-treated inflamed cell lines (RAW 264.7 cells and fibroblast cells) with high COX-2 levels also showed enhanced fluorescence. On the other hand, upon co-treatment with a COX-2 inhibitor such as indomethacin or aceclofenac, the fluorescence intensity of IQ-1 in HeLa cells was decreased. Through these results, we confirm that the newly synthesized IQ-1 has a remarkable targetability towards cancer cells over normal cells with respect to the COX-2 levels, and can be used as a selective bioimaging agent for cancer cells. Therefore, IQ-1 could be structurally transformed for use as a cancer-labelling tool with improved cellular uptake, which is crucial for efficient diagnosis and therapeutic monitoring in precision medicine as part of standard patient care.

References

A ratiometric fluorescence sensor for detection of bio-thiol in solid tumors

Myung Sun Ji,^a Amit Sharma,^a Kyoung Sunwoo,^a Hyeong Seok kim,^a Jinwoo Shin,^a Geun Young Park,^a Soobin Kim,^a Jong Seung kim^{a*}

^a *Department of Chemistry, Korea University, Seoul 02841, Korea.*
E-mail: jongskim@korea.ac.kr

Abstract

To provide proper treatment and improve survival of patients, early detecting of cancer is critical. Here, we reported a highly sensitive ratiometric (yellow emission (550 nm) to blue emission (496 nm)) fluorescent probe **1** developed for detection of thiol-containing amino acids. This probe successfully eliminates interference from background auto-fluorescence, and discriminates between human carcinoma and normal cells by detecting intracellular thiol levels in living cells ($P < 0.05$). Furthermore, probe **1** could identify growing tumors by measuring GSH in the tissues as well as in the fresh blood of tumor xenograft mice. Additionally, the ratio of the emission intensity at two different wavelengths can provide quantitative analysis of glutathione (GSH) in the living systems. It suggests that it represents a promising prognostic and diagnostic marker, with extensive and simple potential clinical applications.

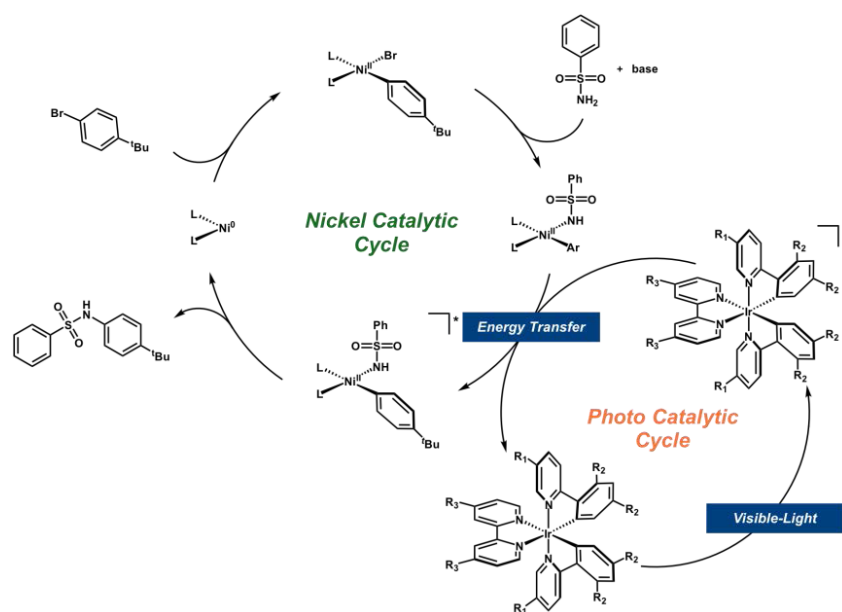
Sulfonamidation of Aryl and Heteroaryl Halides through Photosensitized Nickel Catalysis

Taeheon Kim,^a Stefan J. McCarver,^b Chulbom Lee,^a David W. C. MacMillan^{b*}

^a Department of Chemistry, Seoul National University, Seoul 08826, South Korea. ^b Merck Center for Catalysis at Princeton University, Princeton, New Jersey 08544, United States.

E-mail: myhomen@snu.ac.kr

The cross-coupling of amines with aryl halides is a powerful strategy for constructing valuable aryl amines. Synthesis of aryl sulfonamides is particularly important due to their presence in a broad range of pharmaceuticals and agrochemicals. In this poster, we present a protocol, which uses photocatalyst in combination with a catalytic nickel to couple various sulfonamides with aryl halides under mild reaction conditions. The reaction mechanism involves the energy transfer from an activated photocatalyst to organometallic nickel that forms an electronically destabilized Ni(II) intermediate. The reactive intermediate can undergo otherwise unfavorable C–N bond reductive elimination. The new method offers a mild and useful alternative for palladium or copper-catalyzed strategies, which often require high reaction temperatures.



References

- 1, Kim, T.; McCarver, S. J.; Lee, C.; MacMillan, D. W. C. *Angew. Chem. Int. Ed.* **2018**, *57*, 3488.

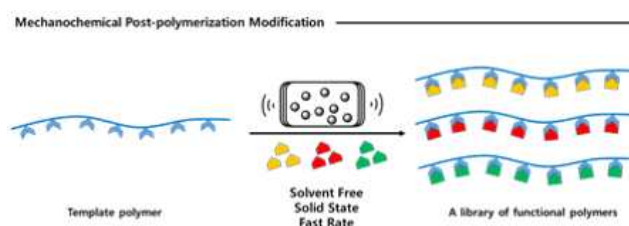
Mechanochemical Post-Polymerization Modification : Solvent Free Solid-State Synthesis of Functional polymer

온누리, 김정곤*

Department of Chemistry and Institute of Physical Science, Chonbuk National University, 567
Baekje-daero, Deokjin-gu, Jeonju-si, Jeollabuk-do 54896 Republic of Korea.
E-mail: jeunggonkim@jbnu.ac.kr

The post-polymerization was successfully accomplished using the mechanochemical method.¹ Mechanochemical synthesis is the chemical transformation induced by means of mechanical force. The fast and efficient synthesis of a library of macromolecules with functional diversity and structural uniformity was realized without a solvent by means of high speed ball-milling technique.²⁻⁴

A series of polymers from 4-vinylbenzaldehyde(4-VBA) underwent solid-state Schiff base formations with a series of amines and derivatives. The efficient mixing and energy delivery by the collisions between balls not only promoted prompt imine formation but also eliminated the need of chemical solvent, which is highly desirable for green chemical synthesis. A series of polymers from 4-vinylbenzaldehyde(4-VBA) reacted with a series of amines and derivatives to form solid-state Schiff base.



Reference

- ¹Klimakow, M.; Klobes, P.; Thunemann, A. F.; Rademann, K.; Emmerling, F. *Chem. Mater.* **2010**, *22*, 5216–5221.
- ²Ravnsbæk, J. B.; Swager, T. M. *ACS Macro Lett.* **2014**, *3*, 305–309.
- ³Gratz, S.; Borchardt, L. *RSC Adv.* **2016**, *6*, 64799–64802.
- ⁴Ohn, N.; Shin, J.; Kim, S. S.; Kim, J. G. *ChemSusChem.* **2017**, *10*, 3529–3533.

Biosynthetically Inspired Transformation of (+)-Catharanthine to Post-Iboga Alkaloids

Sikwang Seong,^{ab} Hyeonggeun Lim,^{ab} and Sunkyu Han^{ab*}

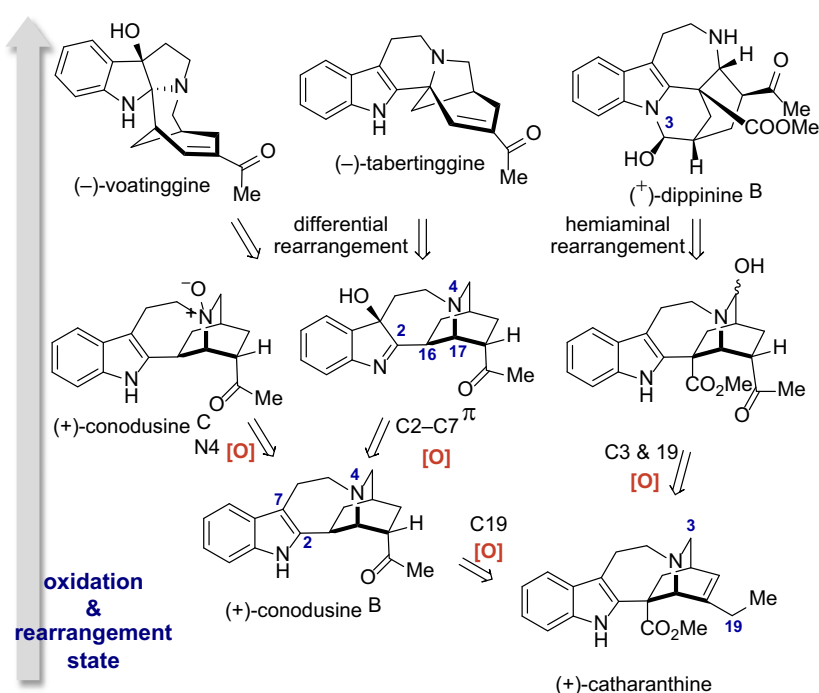
^a Department of Chemistry, Korea Advanced Institute of Science & Technology (KAIST), Daejeon 305-701, South Korea.

^b Center for Catalytic Hydrocarbon Functionalizations, Institute for Basic Science (IBS), Daejeon 305-701, South Korea.

E-mail: rahzell@kaist.ac.kr

Iboga-type alkaloids that have undergone rearrangements to exclude isoquinuclidine moieties can be classified as post-iboga alkaloids. Upto date, various synthetic studies have been undertaken on iboga-type alkaloids, but only a few examples exist on the synthesis of post-iboga alkaloids.

We synthesized various post-iboga alkaloids including conodusine A, B, C, voatinggine, tabertinggine and dippinine B from catharanthine through oxidative conversions and rearrangements.



References

¹ Nge, C.-E.; Gan, C.-Y.; Low, Y.-Y.; Thomas, N. F.; Kam, T.-S. *Org. Lett.* **2013**, *15*, 4774–4777.

² Kam, T.-S.; Sim, K.-M. *Heterocycles*, **2001**, *55*, 2405–2412.

Iridium Complexes Encapsulated in Redox-Sensitive Self-Cross-Linked Nanogels for Efficient Photodynamic Therapy

Chae Gyu Lee,^a Byeong-Su Kim,^{a*} and Tae-Hyuk Kwon^{a*}

^a Department of Chemistry,
Ulsan National Institute of Science and Technology (UNIST), Ulsan 44919,
Republic of Korea.

E-mail: chaeqlee@unist.ac.kr

Ir(III) complexes have attracted much attentions in bio-imaging and targeted therapies due to their outstanding advantages such as large Stokes shift, short incubation time, long luminescence lifetime, enhanced photo-stability and simple color tuning method. Furthermore, Ir(III) complexes showed remarkable efficiency of reactive oxygen species (ROS) generation as photosensitizers via electron (type I) and energy transfer (type II).¹ Despite these great characteristics, the use of Ir(III) complexes as therapeutic agents has been limited because of their poor biocompatibility and water solubility.

Herein, we provide reduction-triggered self-cross-linked polymer based Ir(III) complexes for enhancing the cell viability, **TIr3PSSG**. We synthesized iridium complexes (TIr3) encapsulated in self-cross-linked hyperbranched polyglycerol nanogels (PSSG nanogels) by using the thiol-disulfide intermolecular exchanges.² This Ir(III) complex involved nanogel was much soluble in physiological environments compared to the Ir(III) complex. With these formed nanoparticles, we expect enhancement of cell viability and photo-toxicity index for cancer cells due to better biocompatibility and enhanced permeability and retention (EPR) effect of nanoparticles.

References

¹ Nam, J. S.; Kang, M. G.; Kang, J.; Park, S. Y.; Lee, S. J.; Kim, H. T.; Seo, J. K.; Kwon, O. H.; Lim, M. H.; Rhee, H. W.; Kwon, T. H., Endoplasmic Reticulum-Localized Iridium(III) Complexes as Efficient Photodynamic Therapy Agents via Protein Modifications. *J. Am. Chem. Soc.* **2016**, 138 (34), 10968-77.

² Son, S.; Shin, E.; Kim, B.-S., Redox-Degradable Biocompatible Hyperbranched Polyglycerols: Synthesis, Copolymerization Kinetics, Degradation, and Biocompatibility. *Macromolecules* **2015**, 48 (3), 600-609.

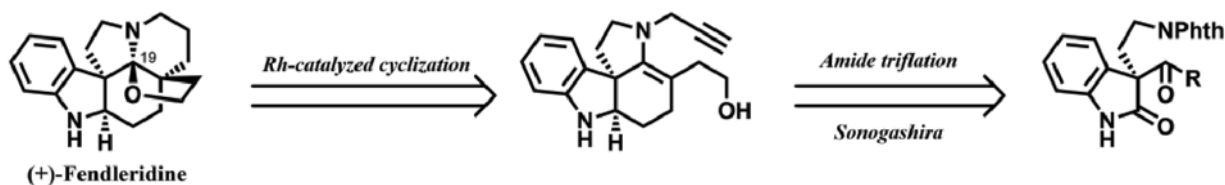
Synthetic Studies toward (+)-Fendleridine: Using Metal Catalysis Cascade Cyclization Approach

Sang Weon Roh, Chulbom Lee*

Department of Chemistry Seoul National University, Seoul, 08826, Korea
E-mail: chulbom@snu.ac.kr

(+)-Fendleridine is a botanic alkaloid natural product possessing a hexacyclic skeleton that consists of 5/6-membered carba-, aza- and oxacycles with an N,O-acetal at C19. Owing to the novel structure that constitutes the common core of a variety of the aspidosperma alkaloid congeners, fendleridine has received much attention from the synthetic community.

Herein, we present our synthetic efforts toward the enantioselective total synthesis of (+)-fendleridine. Main features of our strategy include the asymmetric acyl-migration,¹ Pd-catalyzed cross-coupling of an imido-yl-triflate to form the 2-alkynylindoline core, and Rh-vinylidene mediated cascade cyclization² to concomitantly construct two non-aromatic six-membered rings with the N,O-acetal functionality. Details of our synthetic studies will be described in this poster.



References

- ¹Duffey, T. A.; Shaw, S. A.; Vedejs, E. J. Am. Chem. Soc. 2009, 131, 14.
- ²Kim, H.; Lee, C. J. Am. Chem. Soc. 2006, 128, 6336.

Cu-Catalyzed (Hetero)aryl Amine Addition to Disubstituted Olefins

Subin Park, Yunmi Lee*

Department of Chemistry, Kwangwoon University, Seoul 01897, Republic of Korea

Email: ymlee@kw.ac.kr

The importance of nitrogen-containing structures in medicinal chemistry and agrochemical research continues to inspire efforts toward the development of metal catalyzed amination to alkenes.¹ The addition of an N-H bond to a carbon-carbon double bond, called hydroamination, provides an atom-economical route to nitrogen-containing compounds.² Numerous protocols regarding to hydroamination using various catalysts such as alkali metals,³ transition metals,⁴ organic acids,⁵ and organo-f-element metals (actinides⁶ and lanthanides⁷) have been studied. In this study, we developed a new catalytic system for hydroamination using an NHC-Cu catalyst, that is readily accessible, environmentally benign and easy to handle. The direct addition of (hetero)aryl amines to disubstituted olefins was promoted by the presence of NHC-CuCl and KO^t-Bu and proceeded efficiently in toluene at 80 °C. This copper-catalyzed amination provided new versatile amine compounds with high yields.

References

- ¹ (a) Müller, T. E.; Beller, M. *Chem. Rev.* **1998**, *98*, 675. (b) Müller, T. E.; Hultzsch, K. C.; Yus, M.; Foubelo, F.; Tada, M. *Chem. Rev.* **2008**, *108*, 3795.
- ² Munro-Leighton, C.; Delp, S.A.; Blue, E.D.; Gunnoe, T. B. *Organometallics* **2007**, *26*, 1483.
- ³ Hartung, C. G.; Breindl, C.; Tillack, A.; Beller, M. *Tetrahedron* **2000**, *56*, 5157.
- ⁴ Jimenez, O.; Müller, T. E.; Sievers, C.; Spirkl, A.; Lercher, J. A. *Chem. Commun.* **2006**, 2974.
- ⁵ Schlummer, B.; Hartwig, J. F. *Org. Lett.* **2002**, *4*, 1471.
- ⁶ Stubbert, B. D.; Stern, C. L.; Marks, T. J. *Organometallics* **2003**, *22*, 4836.
- ⁷ Hong, S.; Mark, T. J. *Acc. Chem. Res.* **2004**, *37*, 673.

Aggregation-Induced Emission and Ion Detection

Properties of Hydrazone-based Materials

TaeWoo Kim, Eun Jung Choi, HwiHyun Moon, Eun Ho Choi, ChangSuk Oh, JangWhan Seok

*and Changsik Song**

Department of Chemistry, Sungkyunkwan University, 2066 Seobu-ro, Jangan-gu, Suwon-si,

Gyeonggi-do 16419 Republic of Korea

E-mail: songcs@skku.edu

Aggregation-induced emission (AIE) is an abnormal phenomenon observed in certain organic luminophores where a remarkable fluorescence emerges due to the restricted rotation or vibration in the solid state. Such "AIEgen" molecules can be applied to various applications such as bio sensor or imaging. In this study, we synthesized various bis-hydrazone derivatives, and found that some of them resulted in the AIE properties. The structural effect showing the AIE property was confirmed by the different substitution patterns (para-, meta-) and the number of substitutions (mono-, bis-, and tris-). These AIEgenic bis-hydrazones was applied to sensors with polymer films to detect various metal ions.

Supramolecular Polymerization with Hydrazone-based Molecular Building Blocks: Control of Chirality with Alkyl Substituent

HyeJin Cho,^a Kyung-su Kim,^a Seonggyun Ha,^a Sun Gu Song,^a Juhyen Lee,^a and Changsik Song^{a*}

^a Department of Chemistry, Sungkyunkwan University, 2066 Seobu-ro, Jangan-gu, Suwon-si, Gyeonggi-do 16419 Republic of Korea.

E-mail: songcs@skku.edu

Chirality is one of the most important properties which can be found in nature. For example, biological processes occur in a chiral manner, which the chirality depends on that of the reactors, like proteins. Considering that those chiral reactors are supramolecules in most cases, supramolecular assembly plays a key role to investigate our chiral nature. In this study, novel benzoyl hydrazone para-pyridinium conjugates were synthesized and assembled by direct intermolecular interactions. The formation of the polymers could be controlled reversibly according to the pH environment. It is found that the assembly of **BH1** is helical, thus several alkyl substituents were employed to control the chirality. The effect of alkyl groups was investigated with UV-Vis spectroscopy, circular dichroism (CD) spectroscopy, and scanning electron microscopy (SEM).

Construct Borylated Benzannulated Nitrogen Heterocycles (*cis*-Indolines or *cis*-1-Benzo[*b*]azepines) via Copper-Catalyzed Intramolecular Cyclization

DingXi Li^a, Jaesook Yun^{*a}

^a Department of Chemistry, Sungkyunkwan University, Suwon, Korea.
E-mail: jaesook@skku.edu

An efficient synthetic method of borylated benzannulated nitrogen heterocycles, 2,3-substituted *cis*-indolines¹ or *cis*-1-benzo[*b*]azepines² via copper-catalyzed intramolecular cyclization has been developed. The tandem, intramolecular reaction is applicable to various vinyl arenes or *E/Z*-dienyl arenes with a tethered imine group. This protocol involves borylcupration of C–C unsaturated bond, followed by capture of the generated nucleophilic copper with an imine in an intramolecular process.

References

¹ Invited by Chemistry-An Asian Journal Issue press.

² Manuscript in preparation.

Carbon-Heteroatom Bond Formation by Ultrasonic Chemical Reaction for Energy Storage System

김현탁,^a 권태혁 a*

^a Department of Chemistry, Ulsan National Institute of Science and Technology (UNIST), Ulsan 44919, Republic of Korea.

*E-mail: kwon90@unist.ac.kr

The direct formation of C–N and C–O bonds from inert gases is essential for chemical/biological processes and energy storage systems.^{1,2} However, its application to carbon nanomaterials for improved energy storage remains technologically challenging.³ We describe a simple and very fast method to form C–N and C–O bonds in reduced graphene oxide (RGO) and carbon nanotubes (CNTs) by ultrasonic chemical reaction. Electrodes of nitrogen- or oxygen-doped RGO (N-RGO or O-RGO, respectively) are fabricated via the fixation between N₂ or O₂ carrier gas molecules and ultrasonically activated RGO.⁴⁻⁶ The materials exhibited much higher capacitance after doping (133, 284, and 74 F g⁻¹ for O-RGO, N-RGO, and RGO, respectively). The simplicity and controllability of structural parameters in this approach can open many opportunities in the design and fabrication of electrochemical energy storage devices, as well as other energy conversion applications.

References

¹ Canfield, D. E. ; Glazer, A. N.; Falkowski, P. G. *Science* **2010**, 330, 192.

² Ludwig, E. M.; Hosie, A. H. F.; Bourdès, A.; Findlay, K.; Allaway, D.; Karunakaran, R.; Downie, J. A.; Poole, P. S. *Nature* **2003**, 422, 722.

³ Jeon, I. Y.; Choi, H. J.; Jung, S. M.; Seo, J. M.; Kim, M. J.; Dai, L.; Baek, J. B. *J. Am. Chem. Soc.* **2013**, 135, 1386

⁴ Bang, J. H.; Suslick, K. S. *Adv. Mater.* **2010**, 22, 1039.

⁵ Xu, H. X.; Suslick, K. S. *J. Am. Chem. Soc.* **2011**, 133, 9148.

⁶ Suslick, K. S. *Science* **1990**, 247, 1439.

Total Syntheses of Aristotelia Alkaloids

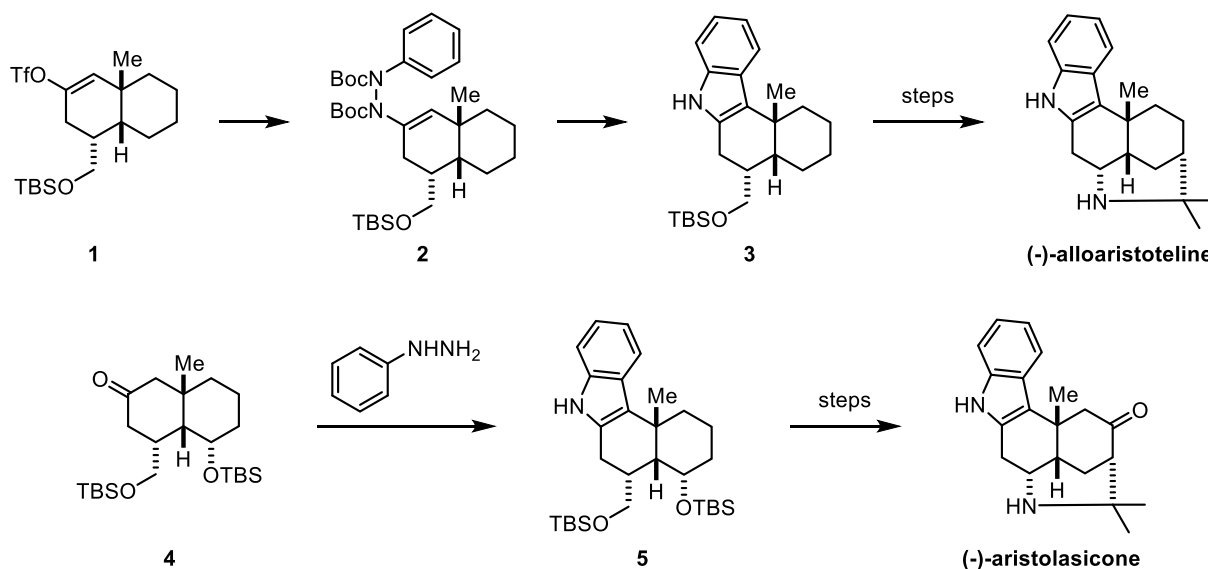
Tae-Hong Jeon, Jang-Yeop Kim and Cheon-Gyu Cho*

Department of Chemistry, Hanyang University, Seoul 133-791, Korea
E-mail: ccho@hanyang.ac.kr

Abstract

In our recent report, we have demonstrated that ene-hydrazide prepared from enol triflate in regiochemically defined form may undergo Fischer indolization with no regiochemical scrambling.¹ Applying to this method, we recently reported total syntheses of (+)-aspidospermidine and (-)-tabersonine.² As a part of our ongoing study for application of this method to the synthesis of natural products, we designed synthetic routes toward the total syntheses of aristotelia alkaloids, (-)-alloaristoteline and (-)-aristolasicone.

We began the synthetic exploration by preparing enol triflate **1** from the corresponding enone via a Michael addition using Me_2CuLi followed by in-situ triflation. Subsequent C-N coupling with phenyl hydrazide afforded the key ene-hydrazide **2**. Regioselective Fischer indolization under Lewis acidic conditions furnished indole **3** pertaining a cis-fused decalin core of (-)-alloaristoteline. During the study, we observed an unexpected regiochemical control when cis-2-decalone **4** was subjected to the classical Fischer indolization. The origin of the regioselectivity as well as our progress in the total syntheses of (-)-alloaristoteline and (-)-aristolasicone will be discussed.



References

- ¹ Lim, B.-Y.; Jung, B.-E.; Cho, C.-G. *Org. Lett.* 2014, 16, 4492.
- ² Kim, J.-Y.; Suhl, C.-H.; Lee, J.-H.; Cho, C.-G. *Org. Lett.* 2017, 19, 6168-6171

A remarkably stable radical zwitterion derived from *N*-heterocyclic carbene nitric oxide

김영석,^a 이은성^{a*}

^a Department of Chemistry, Pohang University of Science and Technology, Pohang, Korea.
E-mail: twoyoung93@postech.ac.kr

For the past few years, *N*-heterocyclic carbene (NHC) have been introduced to stabilize various organic radicals and radical ions, as a variety of previously inaccessible organic radicals have been successfully prepared and characterized with an aid of NHCs.^[1] These radicals were successfully stabilized due to the π -accepting properties of NHCs that delocalize the spin density, as well as the steric protection of the bulky NHC substituents. Here we report the synthesis and characterization of a remarkably stable radical zwitterion **A**.^[2] It is notable that **A** shows remarkable stability toward air and moisture. For example, solution of **A** in wet technical-grade benzene showed no detectable decomposition over 12 days. In addition, **A** is stable even under chromatographic condition as shown in the clean TLC spot in **Figure 1**. Also, benzene solution of **2** was still EPR active even after the filtration through silica gel under air. With the help from the novel properties of NHCs, this work clearly shows a successful example of designing a stable radical. Possible applications of the stable radical **A** is currently under investigation.

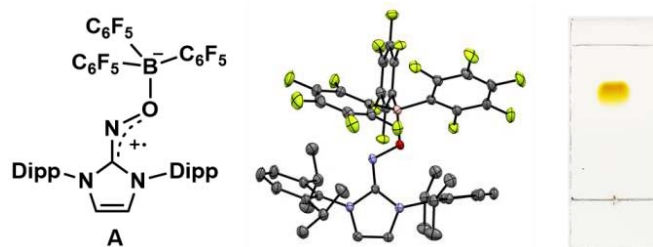


Figure 1. A remarkably stable radical zwitterion **A**.

References

- ¹ Kim, Y.; Kim, K.; Lee, E., *Angew. Chem. Int. Ed.* **2018**, *57*, 262-265.
- ² Kim, Y.; Lee, E., *Chem. Commun.* **2018**, *54*, 6824-6827.

Total synthesis of Ningalin C

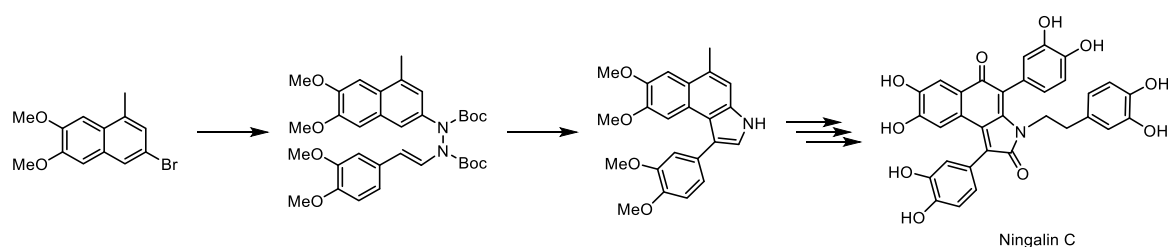
Woo-Hyung Kim, Jang-Yeop Kim and Cheon-Gyu Cho*

Center for New Directions in Organic Synthesis, Department of Chemistry, Hanyang University, 222 Wangshimni-ro, Seongdong-gu, Seoul 04763, Korea

Abstract

Dark-red amorphous powder ningalin C comes from dark purple *Didemnum* sp in Ningaloo Reef region at the northwest cape of Western Australia. This compound is polar, highly-colored alkaloid and possess highly unsaturated, carbon skeletons.¹

Reaction between 5-bromo-3-methyl-2-pyrone and dimethoxy benzyne gave us synthetically useful naphthalene for natural product synthesis. With this naphthalene, we were able to synthesize key intermediates effectively. From those key intermediates, we recently had successfully synthesized ningalin D and G.² Recently, we have further extended the above strategy and completed the synthesis of ningalin C. The key to the success was the assembly of the indole through the successive C-N coupling reactions. Functional group transformations, oxidations and necessary substituents allowed the synthesis of the title natural product, ningalin C.



References

- 1) Heonjoong Kang and William Fenical*, *J. Org. Chem.* **1997**, *62*, 3254-3262
- 2) Jang-Yeop Kim, Dong-Hyun Kim, Tae-Hong Jeon, Woo-Hyung Kim, and Cheon-Gyu Cho*, *Org. Lett.* **2017**, *19*, 4688-4691

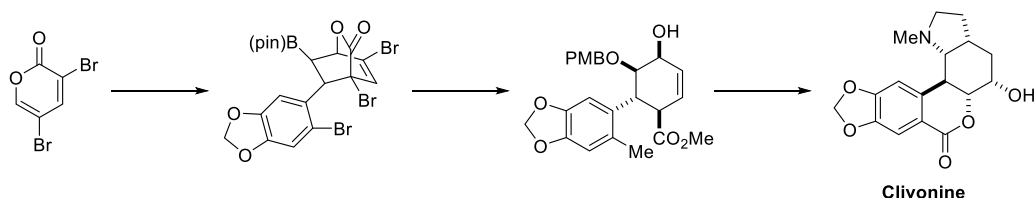
Total synthesis of (±)-clivonine

Cheng-Dong Wang and Cheon-Gyu Cho*

Center for New Directions in Organic Synthesis, Department of Chemistry, Hanyang University, 222 Wangsimni-ro, Seongdong-gu, Seoul 04763, Korea
E-mail: ccho@hanyang.ac.kr

Abstract

Diels-Alder reaction of 2-pyrone can be exceptionally powerful for the synthesis of structurally complex natural products, constructing multiple carbon-carbon bonds in a single operation¹. As a part of our ongoing study exploring the utility of 3,5-dibromo-2-pyrone in target-oriented synthesis², we have further envisioned that the aforementioned synthetic strategy could be also effective for clivonine. Our efforts toward this natural product will be presented.



References

- ¹ (a) Chung, S. I.; Seo, J. B.; Cho, C.-G. *J. Org. Chem.* 2006, 71, 6701. b) Shin, J. T.; Hong, S. H.; Shin, S. H.; Cho, C.-G. *Org. Lett.* 2006, 8, 3339.
- ² (a) Chang, J. H.; Kang, H.-U.; Jung, I.-H.; Cho, C.-G. *Org. Lett.* 2010, 12, 2016. (b) Tam, N. T.; Jung, E.-J.; Cho, C.-G. *Org. Lett.* 2010, 12, 2012. (c) Tam, N. T.; Cho, C.-G. *Org. Lett.* 2008, 10, 601. (d) Tam, N. T.; Chang, J.; Jung, E.-J.; Cho, C.-G. *J. Org. Chem.* 2008, 73, 6258. (e) Shin, I.-J.; Choi, E.-S.; Cho, C.-G. *Angew. Chem., Int. Ed.* 2007, 46, 2303. (f) Tam, N. T.; Cho, C.-G. *Org. Lett.* 2007, 9, 3319. (g) Kim, H.-Y.; Cho, C.-G. *Prog. Heterocycl. Chem.* 2007, 18, 1. (h) Ryu, K.; Cho, Y.-S.; Cho, C.-G. *Org. Lett.* 2006, 8, 3343.

Internal H-bonding mediated asymmetric intramolecular Diels-Alder reaction of dienophile-tethered-2-pyrone and formal synthesis of (+)-aplykurodinone-1

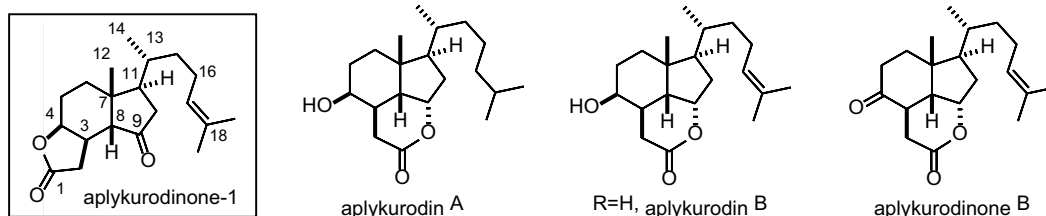
Joon-Ho Lee, Hyo-Mi Kim and Cheon-Gyu Cho*

Department of Chemistry, Hanyang University, Seoul 133-791, Korea

Abstract

Aplykurodines are steroids natural products which have tricyclic ring core with various biological activities including cytotoxicity against a range of human cancer cells. Aplykurodinone-1 whose structure is shown below has gained much interest for the unusual cis-fused hydrindane core decorated with six contiguous stereocenters, also found in other aplykurodines, and C11 side chain presenting C20 issue in steroid synthesis.¹

As a part of our ongoing study on 3,5-dibromo-2-pyrone toward target oriented synthesis,² we have devised a new synthetic route to (+)-aplykurodinone-1 by way of internal hydrogen bonding mediated asymmetric intramolecular Diels-Alder reaction. This elaborated 2-pyrone IMDA reaction turned out to proceed in perfect π -facial and endo selectivity, providing the cis-hydrindane core as well as all substituents with right stereochemistry necessary for the synthesis of aplykurodinone-1. Transformations including hydrogenation, lactone ring formation and elimination gave the Danishefsky's intermediate as a formal synthesis of (+)-aplykurodinone-1.



References

- ¹ (a) Ortega, M. J.; Zubia, E.; Salva, J. *J. Nat. Prod.* **1997**, *60*, 488–489. (b) Spinella, A.; Gavagnin, M.; Crispino, A.; Cimino, G.; Martinez, E.; Ortea, J.; Sodano, G. *J. Nat. Prod.* **1992**, *55*, 989–993. (c) Miyamoto, T.; Higuchi, R.; Komori, T. *Tetrahedron Lett.* **1986**, *27*, 1153–1156. (d) Gavagnin, M.; Carbone, M.; Nappo, M.; Mollo, E.; Roussis, V.; Cimino, G. *Tetrahedron.* **2005**, *61*, 617–621.
- ² (a) Kim, W.-S.; Kim, H.-J.; Cho, C.-G. *J. Am. Chem. Soc.* **2003**, *125*, 14288. (b) Tam, N. T.; Cho, C.-G. *Org. Lett.* **2007**, *9*, 3391. (c) Shin, I.-J.; Choi, E.-S.; Cho, C.-G. *Angew. Chem. Int. Ed.* **2007**, *46*, 2303. (d) Chang, J. H.; Kang, H.-U.; Jung, I.-H.; Cho, C.-G. *Org. Lett.* **2010**, *12*, 2016. (e) Jung, Y.-G.; Kang, H.-U.; Cho, H.-K.; Cho, C.-G. *Org. Lett.* **2011**, *13*, 5890. (f) Jung, Y.-G.; Lee, S.-C.; Cho, H.-K.; Nitin, B. D.; Song, J.-Y.; Cho, C.-G. *Org. Lett.* **2013**, *15*, 132. (g) Cho, H.-K.; Lim, H.-Y.; Cho, C.-G. *Org. Lett.* **2013**, *15*, 5806. (h) Shin, H.-S.; Jung, Y.-G.; Cho, H.-K.; Park, Y.-G.; Cho, C.-G. *Org. Lett.* **2014**, *16*, 5718.

Total Syntheses of (-)-tubifolidine and Uleine

Jeong-Hwa Kim, Dong-Hyun Kim and Cheon-Gyu Cho*

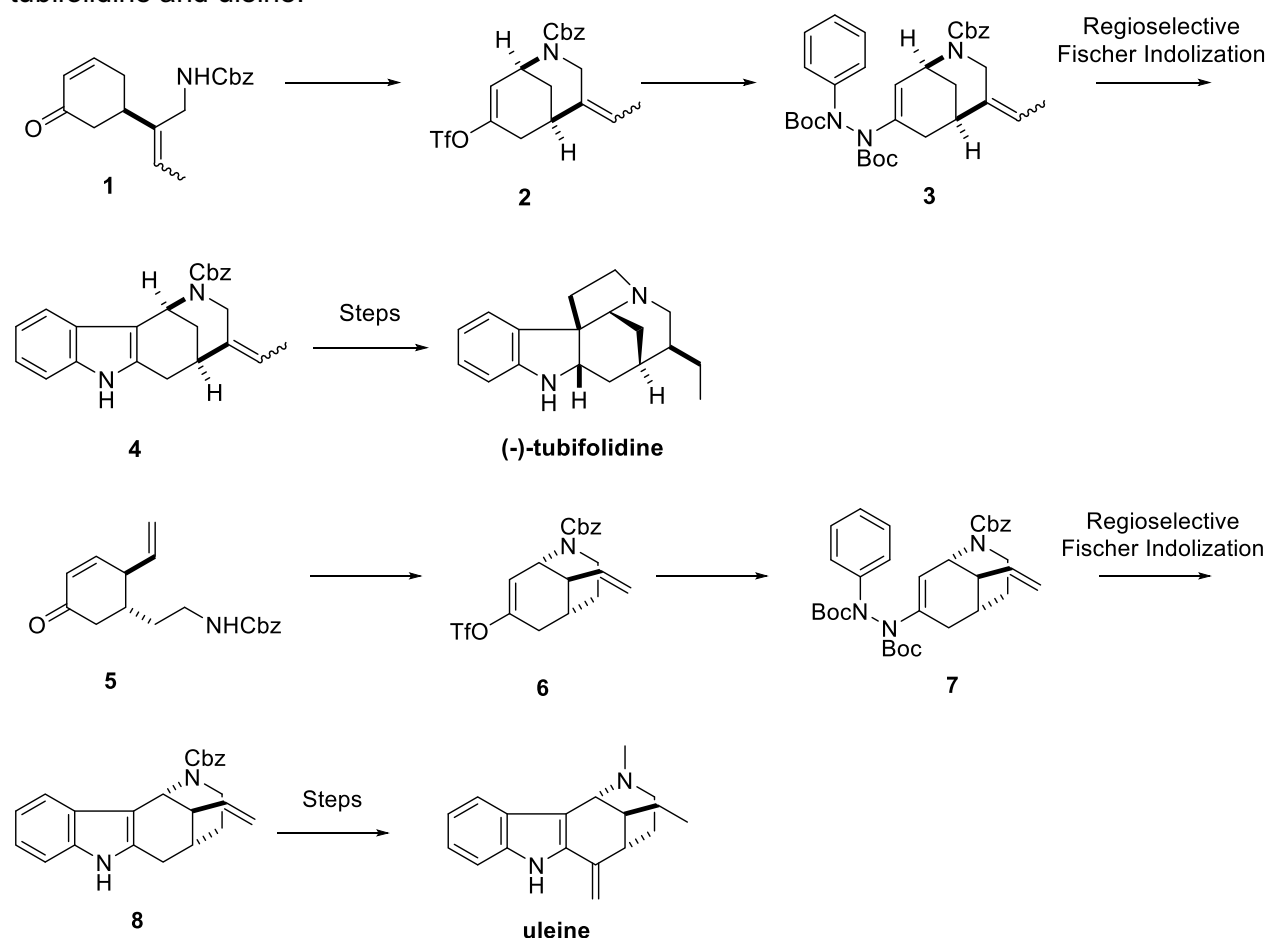
Department of Chemistry, Hanyang University, Seoul 133-791, Korea

E-mail: jeonghwa5527@hanyang.ac.kr

Abstract

We have previously reported a synthesis of ene-hydrazide from enol triflate and a subsequent indolization reaction as a new entry to the regioselective Fischer indole synthesis.¹ In this process, a base-catalyzed intramolecular aza-Michael reaction, in situ trapping of the resulting enolate, and subsequent C-N coupling with phenyl hydrazide afforded the key ene-hydrazides. This new synthetic strategy has been successfully applied to the total synthesis of (+)-aspidospermidine and (-)-tabersonine.²

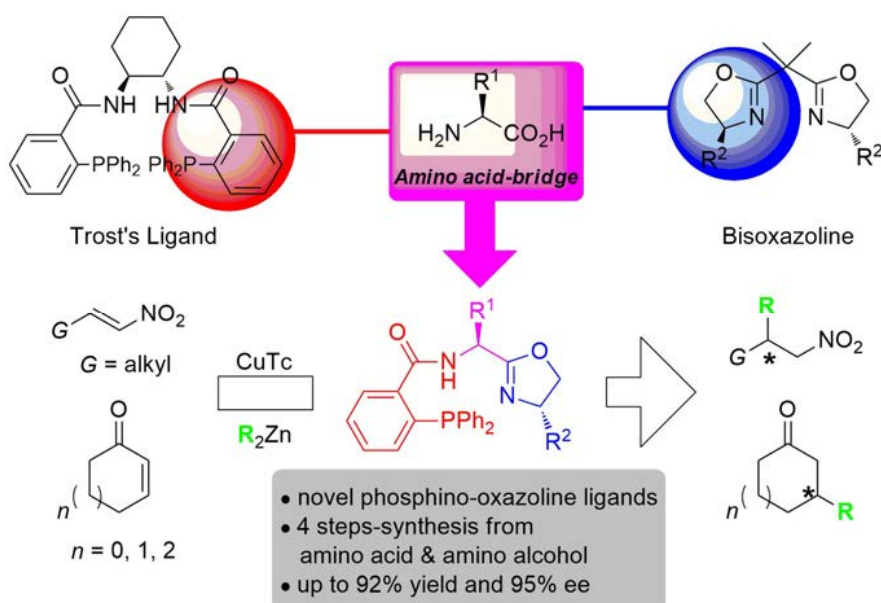
Toward further development of our strategy, we have envisaged a new synthetic route to (-)-tubifolidine and uleine. With carbamate **1** and **5**, the carbamic anion mediated Michael addition followed by triflation will give bicyclic compound **2** and **6**. Buchwald-Hartwig type amination and regioselective Fischer indolization under Lewis acidic conditions would selectively afford desired indole **4** and **8**. Presented herein are the progress toward the syntheses of (-)-tubifolidine and uleine.



구리 촉매와 phosphino-oxazoline 리간드를 이용한 입체선택적 1,4-알킬 첨가 반응

이지인,^a 박하현,^a 신민경,^a 김민재,^a 이주형,^a 진형규,^a 정병혁^{a*}

^a School of Basic Science, Daegu Gyeongbuk Institute of Science and Technology,
Daegu 42988, Republic of Korea.
E-mail: byunghyuck.jung@dgist.ac.kr



Amine 을 포함한 다양한 생리활성을 갖는 화합물들의 효율적인 입체 선택적 반응 개발의 중요성은 계속 강조되어 왔다. 기존에 알려진 방법 중 하나인 nitroalkene 에 1,4-첨가 반응의 경우 Hoveyda group, Mikami group, Charette group 이 보고한 예들이 알려져 있지만 친핵체로 알킬기를 첨가하는 반응은 예가 드물다. 따라서 이를 개선하기 위해 새로운 카이랄 리간드-구리 촉매를 이용한 입체선택적인 첨가 반응을 연구하였다. 새로운 카이랄 리간드는 Trost's ligand 의 phosphinobenzoic acid 부분과 Bisoxazoline 의 mono-oxazoline 부분을 amino acid bridge 를 통해 연결하여 합성하였고, 이 새로운 리간드와 구리 촉매를 이용해 nitroalkene 과 cyclic enone 에 알킬기를 입체선택적으로 첨가하는 반응을 성공적으로 진행할 수 있습니다. 리간드와 alkene 기의 작용기를 바꿔서 반응을 보낸 결과로 수득률은 92%, ee 는 95%까지 얻을 수 있었다.

References

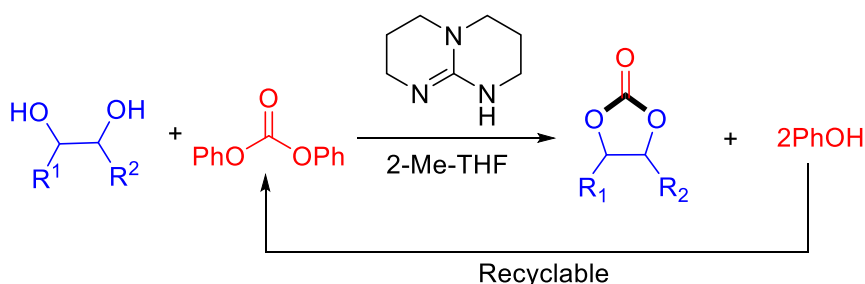
¹ Shin, M.; Gu, M.; Lim, S.S.; Kim, M.-J.; Lee, J.-H.; Jin, H.-G.; Jang, Y. H.; Jung, B. *Eur. J. Org. Chem.* **2018**, 3122-3130.

Diphenyl Carbonate: A Highly Reactive, Practical, and Safe Carbonyl Source for the Synthesis of Cyclic Carbonates

Ek Raj Baral, Jeung Gon Kim*

Department of Chemistry and Research Institute of Physics and Chemistry, Chonbuk National University, Jeonju 54896, Republic of Korea.
E-mail: jeunggonkim@jbnu.ac.kr

Phosgene gas has been extensively used as carbonyl source for the synthesis of the carbonates and related compounds.¹ Because of high toxicity of phosgene, other reagents like alkyl chloroformates, urea, and 1,1'-carbonyldiimidazole (CDI) have been practiced in its replacement.² Carbonmonoxide also became an alternative for carbonyl source but it is also toxic, and it requires expensive high-pressure resist reactor.³ Due to all of these, organic carbonates like dimethyl carbonate (DMC) and diphenyl carbonate (DPC) attracted attention as carbonyl source.⁴ The inexpensive, solid, stable, and more reactive DPC is more practicable than DMC for the carbonylation. Here, we present the DPC as an effective and practical carbonyl source for the synthesis of important carbonates with the combination of an efficient catalyst 1,5,7-triazobicyclo[4.4.0]dec-5-ene (TBD) from 1,2-diols under mild and operationally simple conditions (Scheme 1). This synthetic strategy can be used for the synthesis of sterically demanding cyclic carbonates such as tetra substituted pinacol carbonates, which are not accessible *via* other conventional methods.



Scheme 1. Synthetic strategy for cyclic carbonates using DPC as carbonyl source

References

- ¹ Cotarca, L.; Eckert, H. *Phosgenations – A Handbook*; Wiley-VCH: Weinheim, 2003; pp. 9–16.
- ² Jerris, P. J.; Wovkulich, P. M.; Smith III, A. B. *Tetrahedron Lett.* **1979**, *20*, 4517–4520.
- ³ Barnard, C. F. J. *Organometallics* **2008**, *27*, 5402–5422
- ⁴ Shaike, A. G.; Sivaram, S. *Chem. Rev.* **1996**, *96*, 951–976.

Development of Thermally Activated Delayed Fluorescence Emitters Using Intrinsically Distorted *N*-Heterocyclic Electron Acceptor

Youngnam Lee and Jong-In Hong*

Department of Chemistry, Seoul National University, Seoul 151-747, Korea

E-mail: jihong@snu.ac.kr

The development of organic light emitting diodes (OLEDs) for display devices has attracted significant attention over the past decade. In recent years, thermally activated delayed fluorescence (TADF) has attracted a lot of interest because TADF enables ultimate internal quantum efficiency (IQE) through reverse intersystem crossing (RISC) from the triplet state (T1) to the singlet state (S1). Herein, we report new donor-acceptor-donor TADF emitters using Intrinsically distorted *N*-heterocyclic electron acceptors with differently positioned electron donors. These four emitters are synthesized and characterized. The transient photoluminescence (PL) clearly showed both prompt PL and delayed PL, confirming that the emitters are able to harvest both singlet and triplet states. Also, OLED devices show the high external quantum efficiency beyond the traditional fluorescence emitters. Details of photophysical properties and device data will be presented.

Control of Ion Bindings in Oligo Ethylene glycol Strapped Porphyrin Receptors

Jeong Heon Lee and Woo Dong Jang*

Department of Chemistry, Yonsei University, Seoul 03722, Korea
wdjang@yonsei.ac.kr

In this research, porphyrin-based receptors, containing tetra and penta ethylene glycol chain and triazole groups (4EG-P_{Zn}, 5EG-P_{Zn}), have designed for halide and alkali metal ion recognition. 4EG-P_{Zn} and 5EG-P_{Zn} show ion recognitions by color change of solutions. To confirm ion recognitions, UV-Vis absorption spectra were monitored. 4EG-P_{Zn} and 5EG-P_{Zn} showed different binding affinities to various ions according to the variation of solvent systems. In THF, when 4EG-P_{Zn} and 5EG-P_{Zn} were treated with excess TBAX (X=Cl⁻, Br⁻, F⁻), the two molecules exhibited red-shifted absorption spectra. However, when the same procedure was repeated in 10% ACN/CHCl₃, there was no appreciable spectral change. For alkali metal ion recognition, 4EG-P_{Zn} and 5EG-P_{Zn} were treated with LiPF₆, NaBPh₄, and KBPh₄. Both molecules showed no change on absorption spectra in THF. In contrast, 4EG-P_{Zn}'s absorption spectra were red shifted when the solution was treated with excess LiPF₆ in 10% ACN/CHCl₃ system; no spectral change was observed for adding NaBPh₄, and KBPh₄. 5EG-P_{Zn} showed similar spectral change in 10% ACN/CHCl₃ system with LiPF₆ addition, but its absorption spectra were also red shifted by addition of NaBPh₄, and KBPh₄. This result means that 4EG-P_{Zn} has selectivity of lithium ion because of smaller binding site than 5EG-P_{Zn}. A rough liquid-liquid extraction of lithium ion was performed in H₂O/CHCl₃ system. Both 4EG-P_{Zn} and 5EG-P_{Zn} captured lithium ion successfully and showed visible color change of CHCl₃ layer. Comparing with other ion receptors, 4EG-P_{Zn} and 5EG-P_{Zn} have the advantage that color change through ion binding is easily observed with naked eyes.

Self-Assembled Structure of Dendritic-linear Block Copolymer

Jung Ho Joe, Woo Dong Jang*

Department of Chemistry, Yonsei University, Seoul 03722, Korea
E-mail: wdjang@yonsei.ac.kr

Well-ordered nanoscale structures can be produced through self-assembly process from block copolymers (BCPs) having immiscible fragment. In this research, we studied self-assembled structure of BCP which is consist of dendrimer and linear poly(2-oxazoline) was studied (**D-b-PiPrOx**). This janus structure was contains hydrophobic long alkyl chain and amphiphilic poly(2-isopropyl-2-oxazoline). Atomic Force Microscopy (AFM) and Small-Wide Angle X-ray Scattering (SWAXS) were used to characterize the self-assembled structure. In bulk state, self-assembled **D-b-PiPrOx** formed different structures depending on temperature. In AFM study, **D-b-PiPrOx** showed nanofiber shapes above its glass transition temperature (T_g). The molecular weight of each polymer block also affected the size of the self-assembled structure. As the molecular weight of each block increased, the diameter of the nanofiber was increased. In SWAXS data, the *d*-spacing of the self-assembled **D-b-PiPrOx** was affected by not only molecular weight but also molecular shape. The density of the dendrimer end group is so high that the size of dendrimer block had a greater effect on the diameter of nanofiber.

BODIPY-based Fluorescence Turn-On Probe for Electrochemiluminescent Detection of Hydrogen Peroxide

Yon Namkoong, Jong-in Hong*

Department of Chemistry, Seoul National University, Seoul 08826, Korea

E-mail: jihong@snu.ac.kr

Hydrogen peroxide (H_2O_2), generated through various metabolic pathways in biological systems, acts as a signaling molecule. As one of reactive oxygen species, H_2O_2 is well known for its cytotoxicity at its abnormal concentration, which causes oxidative stress in cells and results in cellular damages. Here we report an efficient probe (Probe **1**) for H_2O_2 . With its high turn-on ratio and adequate reactivity, probe **1** showed remarkable sensitivity and selectivity. Bright red fluorescence was observed after 30 min incubation of probe **1** with H_2O_2 . The fluorophore of probe **1** is fully substituted with alkyl groups to enhance stability of radical species generated during the electrochemiluminescence (ECL) process. As a result, probe **1** provided ECL turn-on in response to H_2O_2 with tripropylamine as a reductive co-reactant in aqueous organic cosolvent. Although numerous ECL luminophores were reported based on BODIPY, there are only a few cases of BODIPY-based ECL sensors. Our study demonstrates the possibility of BODIPY dyes for detection of meaningful biotargets such as H_2O_2 utilizing ECL.

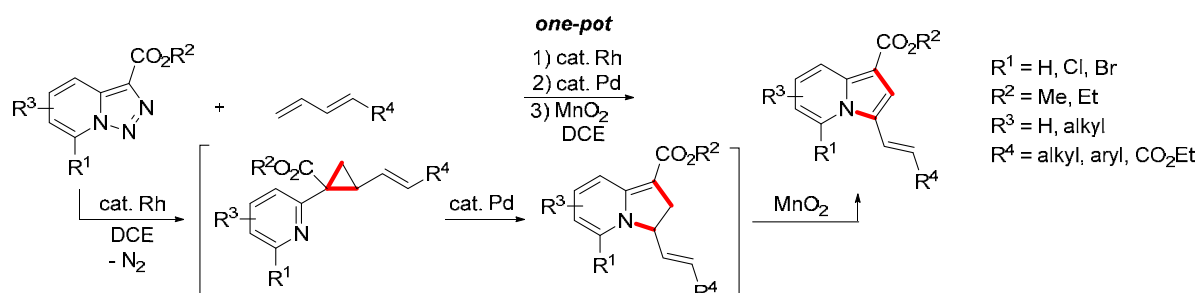
One-Pot Synthesis of Indolizines through Sequential Rh-Catalyzed [2 + 1]-Cyclopropanation, Pd-Catalyzed Ring Expansion, and Oxidation Reactions from Pyridotriazoles and 1,3-Dienes

Dae Kyum Kim,^a Chanyoung Maeng,^a Phil Ho Lee^{a*}

^a Department of Science, Kangwon National University, Chuncheon 24341, Republic of Korea,
E-mail: phlee@kangwon.ac.kr

Development of synthetic methods for accessing a variety of functionalized *N*-heterocyclic compounds is a significant objective in the fields of organic and medicinal chemistry. Because indolizine derivatives containing nitrogens at their ring junction have been found in a number of natural products, pharmaceuticals, and bioactive compounds, the development of expeditious approaches for the construction and functionalization of indolizine derivatives has gained much attention. However, 3-(alkenyl)indolizine derivatives, a vital skeleton for building phosphoinositide 3-kinase inhibitors, have rarely been reported.

For this reason, we developed a one-pot synthetic route to 3-(alkenyl)indolizine derivatives via sequential Rh-catalyzed [2 + 1]-cyclopropanation, Pd-catalyzed ring expansion, and oxidation reactions from pyridotriazoles and 1,3-dienes.



References

¹Kim, H.; Kim, S.; Kim, J.; Son, J.-Y.; Baek, Y.; Um, K.; Lee, P. H. *Org. Lett.* **2017**, *19*, 5677

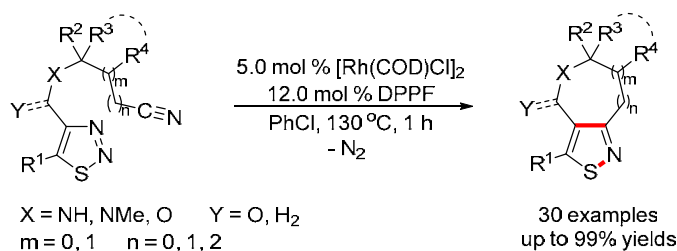
Synthesis of Bicyclic Isothiazoles through an Intramolecular Rh-Catalyzed Transannulation of Cyanothiadiazoles

Dahee Park,^a Kyusik Um,^a Phil Ho Lee^{a*}

^a Department of Science, Kangwon National University, Chuncheon 24341, Republic of Korea,
E-mail: phlee@kangwon.ac.kr

Bicyclic isothiazole ring systems are privileged structural motifs found in many pharmaceutical compounds and functional materials. They have been widely used as significant privileged scaffolds in a myriad of areas such as organic electroluminescent materials, semiconductors, pesticides, anticancer drugs, and ligands. Thus, development of an efficient synthetic method for functionalized bicyclic isothiazoles is highly desired.

Therefore we developed an intramolecular Rh(I)-catalyzed transannulation of readily available cyanothiadiazoles containing an ester, amide, or ether as a linker, serving as an efficient platform for the construction of a wide range of bi-, tri-, and tetracyclic isothiazoles in good to excellent yields together with the release of molecular nitrogen. These results suggest that the carbon atom in the α -thiavinyl carbene is nucleophilic and that the sulfur atom is electrophilic.



Reference

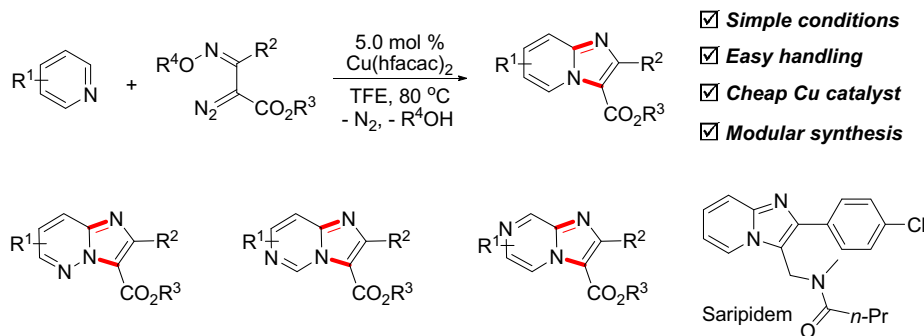
¹ Seo, B.; Kim, S.; Kim, Y. G.; Beak, Y.; Um, K.; Lee, P. H. *J. Org. Chem.* **2017**, *82*, 10574

Synthesis of Imidazopyridines from Cu-Catalyzed, Formal Aza-[3 + 2] Cycloaddition Reaction of Pyridine Derivatives with α -Diazo Oxime Ethers

Hyung Jin Seo,^a Gi Uk Han,^a Phil Ho Lee^{a*}

^a Department of Science, Kangwon National University, Chuncheon 24341, Republic of Korea,
E-mail: phlee@kangwon.ac.kr

N-Containing heterocyclic compounds are extremely important in the study of biological activity and for pharmaceutical utilization. Especially, imidazopyridines with both pyridine and imidazole moieties, which comprise a typical, privileged scaffold, exhibit gastroprotective properties and function as sedative, anxiolytic, and insomnia medicine. For this reason, the development of a synthetic method for imidazopyridine and its derivatives from easily accessible compounds is needed. So we developed a Cu-catalyzed, formal aza-[3 + 2] cycloaddition reaction with pyridine derivatives and α -diazo oxime ethers in trifluoroethanol to synthesize imidazopyridines with the release of molecular nitrogen and elimination of alcohol. This method enabled modular synthesis of a wide range of *N*-heterobicyclic compounds such as imidazopyridazines, imidazopyrimidines, and imidazopyrazines.



Reference

¹Park, S.; Kim, H.; Son, J.-Y.; Um, K.; Lee, S.; Baek, Y.; Seo, B.; Lee, P. H. *J. Org. Chem.* **2017**, *82*, 10209

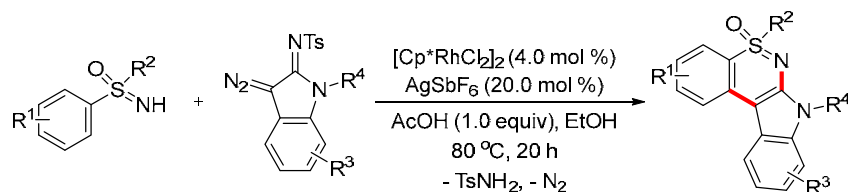
Synthesis of Indolo-1,2-Benzothiazines via Sulfoximines and 3-Diazoindolin-2-imines

Kyungsup Lee,^a Gi Hoon Ko,^a Phil Ho Lee^{a*}

^a Department of Science, Kangwon National University, Chuncheon 24341, Republic of Korea,
E-mail: phlee@kangwon.ac.kr

Sulfoximines are significant compounds that are found in pharmaceuticals, bioactive compounds, and agrochemicals. Accordingly, the development of novel synthetic methods for sulfoximines and their modifications have become highly attractive. To date, many synthetic methods using these tools have been reported in the literature. These methods have focused mainly on the preparation of linear sulfoximines and their derivatives. However, synthetic approaches for the construction of cyclic sulfoximines have been relatively limited.

We developed a novel synthetic method for indolo-1,2-benzothiazines via the Rh-catalyzed cyclization of *S*-aryl sulfoximines with 3-diazoindolin-2-imines together with the release of molecular nitrogen and *p*-toluenesulfonamide. The present method involved the N-H/C-H activation of *S*-aryl sulfoximines. A wide-ranging scope of both *S*-aryl sulfoximines and 3-diazoindolin-2-imines was demonstrated.



Reference

¹Ko, G. H.; Son, J.-Y.; Kim, H.; Maeng, C.; Baek, Y.; Seo, B.; Um, K.; Lee, P. H. *Adv. Synth. Catal.* **2017**, *359*, 3362

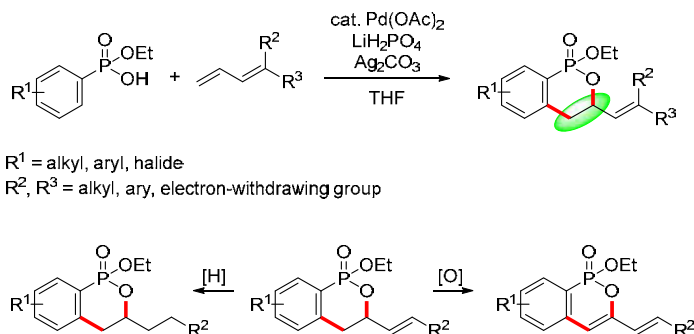
Synthesis of Dihydrophosphaisocoumarins via a Pd-Catalyzed Oxidative Cyclization of Arylphosphonic Acids with 1,3-Dienes

Seungcheol Lee,^a Gi Hoon Ko,^a Phil Ho Lee^{a*}

^a Department of Science, Kangwon National University, Chuncheon 24341, Republic of Korea,
E-mail: phlee@kangwon.ac.kr

Organophosphorus compounds are an omnipresent structural motif found in living organisms and biologically active compounds, and their facile synthesis is important in the preparation of synthetic intermediates, agrochemicals, and pharmaceuticals. Additionally, these compounds have continuously attracted great interest due to their role as bioisosteres of carbonyl and carboxylate groups. Accordingly, much effort has been devoted not only to construct skeletons of phosphorus compounds but also to introduce new functional groups onto these compounds. However, in contrast their acyclic analogs, the synthesis and application of phosphaheterocyclic compounds have been rarely investigated.

We developed an efficient synthetic method for the selective preparation of dihydrophosphaisocoumarins and their derivatives through a Pd-catalyzed oxidative cyclization reaction of a wide range of arylphosphonic acid monoethyl esters with activated and unactivated 1,3-dienes, including 1-aryl-substituted 1,3-dienes and 1-alkyl-substituted 1,3-dienes, thus opening a new avenue for the synthesis of phosphaheterocyclic compounds.



Reference

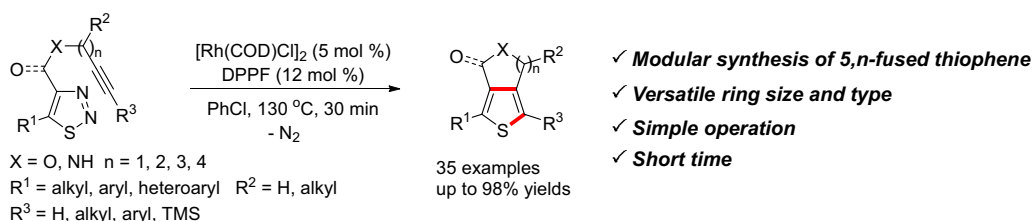
¹ Son, J.-Y.; Kim, H.; Jeon, W. H.; Baek, Y.; Seo, B.; Um, K.; Lee, K.; Lee, P. H. *Adv. Synth. Catal.* **2017**, *359*, 3194

Synthesis of 5,*n*-Fused Thiophenes via Rhodium-Catalyzed Intramolecular Transannulation Reaction of Alkynyl Thiadiazole

Jeong Yun Lee,^a Sang Hoon Han,^a Phil Ho Lee^{a*}

^a Department of Science, Kangwon National University, Chuncheon 24341, Republic of Korea,
E-mail: phlee@kangwon.ac.kr

Fused thiophenes have been recognized as very important scaffolds in the field of pharmaceutical and functional materials sciences. For this reason, the development of an efficient synthetic method for functionalized fused thiophenes is highly attractive and poses a significant challenge. However, because some of the previously reported synthetic methods demand a strong base, long reaction times, and vigorous reaction conditions, the development of efficient synthetic approaches to overcome these shortcomings has been continuously required. Herein, we developed a method for the synthesis of a wide range of fused thiophenes, including those fused with lactams, lactones, or cyclic ethers, from a rhodium-catalyzed intramolecular transannulation reaction of alkynyl thiadiazoles. This transannulation reaction provides an efficient platform for the construction of a variety of 5, *n*-fused thiophenes from readily available starting materials together with the release of molecular nitrogen.



Reference

¹Kim, J. E.; Lee, J.; Yun, H.; Baek, Y.; Lee, P. H. *J. Org. Chem.* **2017**, *82*, 1437

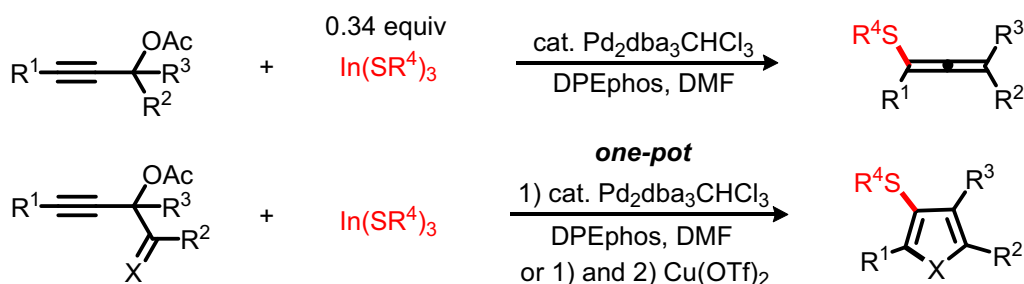
Synthesis of Multisubstituted Allenes, Furans, and Pyrroles through Palladium-Catalyzed Substitution and Cycloisomerization in one pot

Sejin Jang,^a Chanyoung Maeng,^a Phil Ho Lee^{a*}

^a Department of Science, Kangwon National University, Chuncheon 24341, Republic of Korea,
E-mail: phlee@kangwon.ac.kr

Recently, an efficient synthetic method towards multisubstituted furans and pyrroles bearing hetero-substituents was reported through metal-catalyzed 1,2-shifts of diverse migrating groups in allenyl systems. However, the introduction of a wide variety of substituents at the 4-position of furans and pyrroles is impossible due to requirement of [1,3]-H shift in these methods. Therefore, the development of an efficient synthetic method for multisubstituted furans and pyrroles bearing 3-heteroatom substituents as well as substituents at the 4-position has been a continuing challenge.

Herein, we report Pd-catalyzed propargyl substitution reactions of propargyl acetates with indium organothiolates for the synthesis of multisubstituted allenyl sulfides. This procedure employed tandem Pd-catalyzed propargyl substitution and cycloisomerization reactions from indium organothiolates and propargyl acetates bearing acyl and imidoyl groups for the synthesis of multisubstituted furans and pyrroles in one-pot.



$\text{R}^1, \text{R}^2, \text{R}^3 = \text{H}, \text{alkyl}, \text{aryl}$ $\text{R}^4 = \text{alkyl}, \text{aryl}$
 $\text{X} = \text{O}, \text{NOR}^5$ $\text{R}^5 = \text{Me}, \text{Bn}$

Reference

¹ Ryu, T; Eom, D; Shin, S; Son, J.-Y.; Lee, P. H. *Org. Lett.* **2017**, *19*, 452

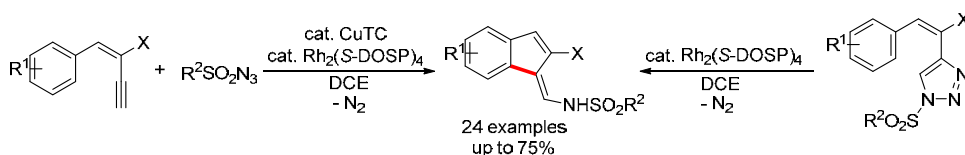
Synthesis of Benzofulvene Derivatives using Rh-Catalyzed Transannulation of Enynyl Triazoles

Juhee Hahm,^a Gi Uk Han,^a Phil Ho Lee^{a*}

^a Department of Science, Kangwon National University, Chuncheon 24341, Republic of Korea,
E-mail: phlee@kangwon.ac.kr

Benzofulvenes are key privileged scaffolds present in natural products, biologically and pharmacologically active molecules, functional materials, and metallocene catalysts. Due to its significance, it is still of considerable interest and necessity to develop efficient synthetic methods for functionalized benzofulvenes. Recently, *N*-sulfonyl-1,2,3-triazoles, easily obtained from click reactions, have been used for the preparation of a large number of heterocyclic and carbocyclic compounds through Rh-catalyzed denitrogenative cyclization.

On the basis of these results, Rh-catalyzed denitrogenative cyclization of (*E*)-ethyl 2-(1-alkyl and arylsulfonyl-1*H*-1,2,3-triazol-4-yl)-3-aryl acrylate generated from (*E*)-ethyl 2-benzylidenebut-3-ynoates and *N*-sulfonyl azides in the presence of a copper catalyst was demonstrated for the synthesis of a wide range of functionalized benzofulvenes. Additionally, we have developed straightforward synthetic procedures for three benzofulvenes through tandem Cu-catalyzed [3 + 2] cycloaddition and Rh-catalyzed denitrogenative cyclization from (*E*)-ethyl 2-benzylidenebut-3-ynoates and *N*-sulfonyl azides in a one-pot.



R¹ = H, 2-Me, 3-Me, 4-Me, 4-MeO, 3,5-(MeO)₂, 4-Cl, 3-Br, 4-AcO, 2-F-4-MeO
 R¹-C₆H₄ = 2-naphthyl, 2-furyl R² = Me, *i*-Pr, 4-Me-C₆H₄, 4-MeO-C₆H₄
 X = CO₂Et, CH₂OMe, Ac

Reference

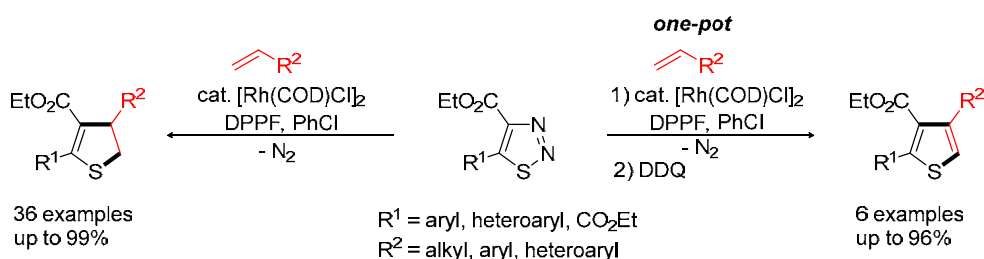
¹ Shin, S.; Son, J.-Y.; Chio, C.; Kim, S.; Lee, P. H.. *J. Org. Chem.* **2016**, *81*, 11706

Rh-Catalyzed Transannulation of 1,2,3-Thiadiazoles via Alkenes for the Synthesis of Dihydrothiophenes and Thiophenes

Juyoung Heo,^a Kyusik Um,^a Phil Ho Lee^{a*}

^a Department of Science, Kangwon National University, Chuncheon 24341, Republic of Korea,
E-mail: phlee@kangwon.ac.kr

Sulfur-containing five-membered heterocyclic compounds such as dihydrothiophenes and thiophenes represent key structural motifs due to their biological activities in natural products and pharmaceuticals. In addition, thiophene derivatives are very attractive compounds in the field of material science due to their peculiar structural rigidity and useful electronic properties. Thus, the development of synthetic methods for these core scaffolds has received considerable attention in contemporary chemistry. The regioselective introduction of a wide range of substituents onto dihydrothiophene and thiophene rings from readily available starting materials is required. In this study, the regioselective synthesis of a wide range of dihydrothiophenes was developed from the rhodium-catalyzed transannulation of 1,2,3-thiadiazoles with aliphatic, aromatic, and heteroaromatic alkenes. Tandem rhodium-catalyzed transannulation of 1,2,3-thiadiazoles with alkenes followed by 2,3-dichloro-5,6-dicyano-1,4-benzoquinone (DDQ) oxidation was also demonstrated for the one-pot regioselective synthesis of various thiophenes. This method was employed to efficiently synthesize pentaoligomeric compounds consisting of three benzene and two dihydrothiophene rings. Advantages of the present method include a broad substrate scope, wide functional group compatibility, and high regioselectivity.



Reference

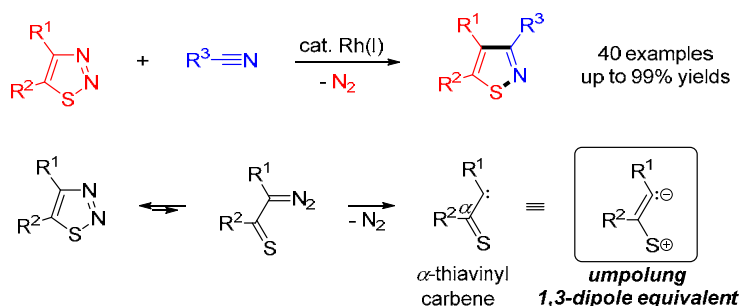
¹ Son, J. Y.; Kim, J.; Han, S. H.; Kim, S. H.; Lee, P. H. *Org.Lett.* **2016**, *18*, 5408

Synthesis of Isothiazole Derivatives through Rh-Catalyzed Transannulation of 1,2,3-Thiadiazoles with Nitriles

Yong Joo Yun,^a Sang Hoon Han,^a Phil Ho Lee^{a*}^a Department of Science, Kangwon National University, Chuncheon 24341, Republic of Korea
E-mail: phlee@kangwon.ac.kr

Isothiazoles are valuable structural motifs found in many natural products, pharmaceutical compounds, and functional materials. For this reason, streamlined methods for their synthesis from readily available compounds must be developed.

Herein, we developed a synthetic method for obtaining a wide variety of isothiazoles by the Rh-catalyzed transannulation of 1,2,3-thiadiazoles with alkyl, aryl, and heteroaryl nitriles, which proceeds via an α -thiavinyl Rh-carbenoid intermediate. The results suggest that during its reaction with nitriles, the α -thiavinyl carbene acts as an umpolung 1,3-dipole equivalent, in contrast to its behavior during its reaction with alkynes. The developed method was successfully employed to synthesize pentaoligomeric arylene compounds consisting of three benzene and two isothiazole rings.



Reference

¹ Seo, B.; Kim, Y. G.; Lee, P. H. *Org. Lett.* **2016**, *18*, 5050

Spray Coating of Brown Algae-Derived Fucoidan for Antibacterial Applications

Soojeong Cho,¹ Le Thi Thuy,² Yeonwoo Jeong,³ Sung Min Kang,³ Sangwon Ko,⁴ Joon Sig Choi,² Woo Kyung Cho^{1,*}

¹Department of Chemistry, Chungnam National University, Daejeon 34134, Republic of Korea

²Department of Biochemistry, Chungnam National University, Daejeon 34134, Republic of Korea

³Department of Chemistry, Chungbuk National University, Cheongju 28644, Republic of Korea

⁴Transportation Environmental Research Team, Korea Railroad Research Institute, Uiwang 16105, Republic of Korea

E-mail: wkcho@cnu.ac.kr

Abstract

Bacteria can adhere to various surfaces and rapidly proliferate, forming biofilm. Biofilm can serve as a reservoir of spreading the bacterial cells and can be crucial problems for public health. To prevent bacterial contamination on surfaces, antibacterial materials and their coating methods have been extensively studied. ¹ Herein, we synthesized an antibacterial material by introducing catechol group into brown algae (*Fucus vesiculosus*)-derived fucoidan via amide coupling. Spray coating method was devised with the use of the crosslinking between iron(III) and catechol-conjugated fucoidan (FD-C). ^{2,3} The FD-C was applied to stainless steel and titanium dioxide by spray coating, and the FD-C-coated substrates were characterized by using ellipsometer, contact angle goniometer, Fourier-transform infrared spectroscopy, X-ray photoelectron spectroscopy and Atomic Force Microscopy. We demonstrated that the FD-C-coated substrates showed excellent antibacterial property, compared to bare substrates. The antibacterial effect was more effective with thicker FD-C coating. We also applied the FD-C coating to straps of train and confirmed the antibacterial effect of the spray coating. We think our approach can be utilized antibacterial coatings for equipment in public transportation to prevent infectious harmful substances from spreading.

References

- ¹ Lichter, J.A; Van Vliet, K.J.; Rubner, M. F. *Macromolecules* **2009**, 42, 8573-8586.
- ² Harrington, M.J.; Masic, A.; Holten-Andersen, N.; Waite, J.H.; Fratzi, P. *Science*, **2010**, 328, 216-220.
- ³ Kim, S.D; Kang, S. M. *Chem. Asian J.* **2014**, 9, 63-66.

Electrochemiluminescent chemodosimeter for H₂S based on an iridium(III) complex

Joon Ho Park and Jong-In Hong*

Department of Chemistry, Seoul National University, 1 Gwanak-ro, Gwanak-gu, Seoul 08826, Korea
E-mail: jihong@snu.ac.kr

Hydrogen sulfide (H₂S) has been known as a toxic gas with unpleasant rotten egg smell. However, it is now recognized as an important biological regulator and a signaling molecule in many physiological processes and diseases. It is important, therefore, to understand the role of H₂S in biological samples, which has remained challenging due to limited methods for detecting endogenous H₂S.

Electrogenerated chemiluminescence (ECL) is the generation of light through electron transfer reactions of electrochemically generated radical species at the surface of working electrode. Recently, the use of ECL has drawn a lot of interests due to their advantages such as high sensitivity, wide linear response range, good reproducibility and simple analytical process. Accordingly, ECL based chemosensors are powerful candidates for point-of-care-testing (POCT). Herein, we introduce a new ECL chemodosimetric probe for H₂S based on cyclometalated Ir(III) complexes. Probe **1** has an azido methyl benzoyl moiety as a reaction site on the main ligand. We took advantage of the reduction of azide to the corresponding amine by H₂S, which leads to a cascade reaction of intramolecular cyclization and cleavage. Our system showed a good “turn-off” ECL sensing property. Details of synthesis and photophysical studies will be presented.

A Two-photon Ratiometric Probe for Quantitative Monitoring of hNQO1 in Colon Tissues

조재형,^a 조명기,^a 김환명 a*

^a Department of Energy System Research, Ajou University, Suwon, 16499, Korea
E-mail: kimhm@ajou.ac.kr

Human NAD(P)H:quinone oxidoreductase 1 (hNQO1) is a flavoenzyme catalyzes two- or four-electron reduction of endogenous and exogenous quinones to their hydroquinone forms ¹. Specially, hNQO1 is over-expressed in tumor cells compared with normal cells of the same origin ². Over-expression of hNQO1 activity have been measured in human breast, lung, liver and colon cancer. Human colonic carcinomas also show a markedly increase activity of hNQO1 ³. In this work, ratiometric two-photon fluorescence probe was designed for quantitative analysis of hNQO1 activity related to human cancer and normal tissues. Using two-photon fluorescence microscopy, the hNQO1 activity can be measured from deep tissue without homogenates of the tissue. Furthermore, the ratiometric system that change emission wavelength activated with enzyme produces precise quantitative analysis of hNQO1 activity in different samples through dual channel monitoring unlike the turn-on system ⁴. This ratiometric two-photon fluorescent probe shows perceptible blue-to-yellow emission wavelength change activated with hNQO1, high stability and selectivity. This probe can monitor hNQO1 quantitatively in living cells and human colon tissue.

References

- ¹ Nebert, D. W.; Roe, A. L.; Vandale, S. E.; Bingham, E.; Oakley, G. G. *Genet. Med.* **2002**, *4*, 62.
- ² Belinsky, M.; Jaiswal, A. K. *Cancer Metastasis Rev.* **1993**, *12*, 103.
- ³ Schor, N. A.; Cornelisse, C. J. *Cancer Res.* **1983**, *43*, 4850.
- ⁴ Lee, H. W.; Heo, C. H.; Sen, D.; Byun, H. O.; Kwak, I. H.; Yoon, G.; Kim, H. M. *Anal. Chem.* **2014**, *86*, 10001.

Two-Photon Ratiometric Probe for Monitoring Hydrogen Polysulfides and Its Application in Parkinson's Disease Model

김원태,^a 최현진,^a 김환명^{a*}

^a Department of Energy System Research, Ajou University, Suwon, 16499, Korea
E-mail: kimhm@ajou.ac.kr

Hydrogen polysulfides (H_2S_n , $n>1$) are Hydrogen sulfide (H_2S) derived signaling molecules that are produced primary during the cross talk between H_2S and reactive oxygen species (ROS)/ reactive nitrogen species (RNS). Earlier, it was believed that H_2S is the main signaling molecule in the family of reactive Sulphur species (RSS); however, Evidences suggest that H_2S_n might be the actual signaling molecules that activate ion channels, transcription factors, and tumor suppressors with higher potency than H_2S ^{1,2}. One example is S-sulfhydration³. A number of H_2S_n molecular markers have been reported using fluorescence spectroscopy to observe H_2S_n in living systems in recent decades. However, most of them have limitations imposed by fluorescence turn-on responses and the short excitation wavelengths. An alternative approach for the detection of H_2S_n is ratiometric imaging with two-photon microscopy (TPM). In this study, we developed a ratiometric TP probe for mitochondrial H_2S_n . especially, using thioester carbamate as a H_2S_n receptor moiety is greatly selective to H_2S_n . using this sensitive selective probe, we observed mitochondrial H_2S_n is generated more in PD neuron than in normal neuron.

References

- ¹ Kimura, Y.; Mikami, Y.; Osumi, K.; Tsugane, M.; Oka, J. I. and Kimura, H. *FASEB J.* **2013**, *27*, 2451.
- ² Mishanina, T. V.; Libiad, M.; Banerjee, R.; *Nat. Chem. Biol.* **2015**, *11*, 457.
- ³ Kimura, H. *Molecules.* **2014**, *19*, 16146.

Ratiometric two-photon probe for Ca^{2+} and its application in spinal cord injury model

이동준,^a 김환명 a*

^a Department of Energy System Research, Ajou University, Suwon, 16499, Korea
E-mail: kimhm@ajou.ac.kr

Intracellular Ca^{2+} ($[\text{Ca}^{2+}]_i$) play a role in regulation various cellular functions.¹ Abnormal $[\text{Ca}^{2+}]_i$ is related to human disease such as neurodegeneration, heart disease, and skeletal muscle defects.² Most small molecule probes for Ca^{2+} also limit their applications in live cell imaging owing to the turn-on response process with single detection window, rapid photobleaching, shallow penetration depth and short wavelength excitation light, which can cause photodamage. A suitable approach is the use to ratiometric probe with two-photon microscopy (TPM), which employs two near-infrared photons as the excitation source.³ The TPM has become one of the most powerful technique for imaging studies in living systems, owing to its advantages including greater tissue penetration depth, localization of excitation, low photo-damage, and longer observation times.⁴ We developed a ratiometric two-photon probe for $[\text{Ca}^{2+}]_i$ two-photon brightness. Using ratiometric TPM imaging, we observed the quantitative analysis of $[\text{Ca}^{2+}]_i$ in live neurons and several tissues. This probe derived from dual dyes with different Stokes shifts and probe had dual channel, Ca^{2+} sensing window and internal reference window, without FRET interference. This ratiometric probe can analyze quantitative $[\text{Ca}^{2+}]_i$ in live cells and tissues including rat spinal cord tissue.

References

- ¹ Emerit, J.; Edeas, M.; Bricaire, F. *Biomed. Pharmacother.* **2004**, *58*, 39-46.
- ² Berchtold, M.W.; Brinkmeier, H.; Münterner, M. *Physiol. Rev.* **2000**, *80*, 1215-1265.
- ³ Helmchen, F.; Denk, W. *Nat. Methods*, **2005**, *2*, 932-940.
- ⁴ Kim, H.M.; Cho, B. R. *Chem. Rev.* **2015**, *115*, 5014-5055.

A two-photon fluorescent probe for γ -glutamyltranspeptidase

김윤지,^a 김환명 a*

^a Department of Energy System Research, Ajou University, Suwon, 16499, Korea

E-mail: kimhm@ajou.ac.kr

γ -Glutamyltranspeptidase (GGT) is a cell-surface-bound enzyme, which selectively catalyzes the cleavage of the γ -glutamyl bond in glutathione (GSH)¹. It is found that GGT plays important role in cellular GSH and cysteine homeostasis, involving in various physiological and pathological processes². Indeed, it has been discovered that overexpressed levels of GGT are associated with tumorigenesis in several human cancer cell, including ovarian and colon cancer³. Therefore, GGT has been recognized as a potential biomarker of malignant tumors. From this point of view, there is growing interest in fluorescent probes for GGT and several GGT activatable fluorescent probes have been developed for the detection and imaging of GGT both in tumor cells and living animals⁴. However, only a few one-photon ratiometric fluorescent probe is known that is favorable for biological imaging. In this work, we developed a new ratiometric two-photon fluorescent probe for GGT by incorporating the γ -glu-substrate and indocyanine fluorophore. This probe showed both one- and two-photon excited fluorescence and large Stokes shift as well as high cell loading ability and also it was readily activated by GGT and successfully applied for one- and two-photon microscopy imaging in live samples.

References

1. Yao, D.; Jiang, D.; Huang, Z.; Lu, J.; Tao, Q.; Yu, Z. and Meng, X. *Cancer*. **2000**, *88*, 761.
2. Fraser, A.; Ebrahim, S.; Smith, G. D.; Lawlor, D. A. *Pathology*. **2007**, *46*, 158.
3. Hanigan, M. H.; Frierson Jr, H. F.; Brown, J. E.; Lovell, M. A.; Taylor, P. T. *Cancer Res*, **1994**, *54*, 286.
4. Urano, Y.; Sakabe, M.; Kosaka, N.; Ogawa, M.; Mitsunaga, M.; Asanuma, D.; Kamiya, M.; Young, M. R.; Nagano, T.; Choyke, P. L.; Kobayashi, H. *Sci. Transl. Med.* **2011**, *3*, 110.

A Two-Photon Ratiometric Probe for Carboxylesterase-2

강지수,^a 박상준,^a 김환명 a*

^a Department of Energy System Research, Ajou University, Suwon, 16499, Korea
E-mail: kimhm@ajou.ac.kr

Carboxylesterases are widely distributed throughout the body and catalyze the hydrolysis of esters, amides, thioesters, and carbamates.¹ The abnormal activity of CE1 and CE2 is closely related to human diseases. Especially CE2 has become increasingly interested because the level of CE2 expression is altered when cancer develops.²

Previously, a lot of fluorescent probes have been developed to detect CE2 activity such as fluorescein diacetate (FDA).³ However, these probes have some limitations of imposed by fluorescence turn-on responses using a single detection window, short excitation wavelength, pH-sensitivity and instability in biological environment. An alternative approach for the detection of CE2 in live cell is a two-photon microscopy (TPM) with a ratiometric two-photon probe.

In this work, we have developed a new emission ratiometric TP probes that selectively detect CE2 activity in living sample. These probes show that the activity of CE2 in breast cancer cells is very low compared to that in normal cells.

References

- ¹ Laizure, S.C.; Herring, V.; Hu, Z.; Witbrodt, K.; Parker, R. B. *Pharmacotherapy*. **2013**, *33*, 210–222.
- ² Xu, G.; Zhang, W. M.; Ma, K and McLeod, H. L. *Clin. Cancer Res.* **2002**, *8*, 2605-2611.
- ³ Wang, J.; Williams, E. T.; Bourgea, J. Y.; Wong, N and Patten, C. J. *Drug Metab. Dispos.* **2011**, *39*, 1329-1333.

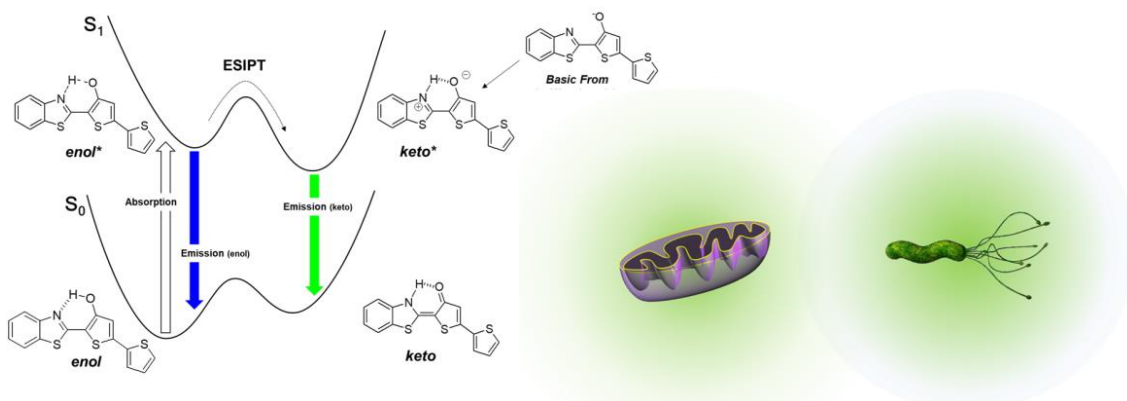
ESIPT based pH-Sensitive Fluorescent Probe and Its applications

Kyeong-Im Hong,^a Sung-Hyun Park,^a Sung Min Lee,^a Injae Shin,^{a,*} and Woo-Dong Jang^{a,*}

Department of chemistry, Yonsei University, Seoul 03722, Korea

E-mail: wjjang@yonsei.ac.kr

Because it shows a remarkably large Stokes shift to solve the problems caused by self-absorption, excited-state intramolecular proton transfer (ESIPT) is attracting the attention of scientists¹⁻². We have synthesized a new type of ESIPT-based pH-sensitive fluorescent probes. The ESIPT probes clearly showed dual emission behavior in response to solvent polarity. Moreover, it showed pH responsive absorption and fluorescence emission changes in aqueous phase. Among them, dithiophene-bearing ESIPT probe (**2**) exhibited turn-on fluorescence emission as increasing pH above physiological condition. We have demonstrated response of the application of dithiophene-bearing ESIPT probe (**2**) on biological specimen. As a result, we have successfully visualized the mitochondrial compartment and *H. pylori*. Detailed aspect of this system will be discussed in this symposium.



References

- Zang, J, Ji, S, Chen, Y, Guo, H, Yang, P, *Phys. Chem. Chem. Phys.* **2012**, *14*, 8803-8817.
- Furukawa, S, Shono, H, Mutai, T, Araki, K, *ACS Appl. Mater. Interfaces.* 2014, *6*, 13184-13187.

Selective synthesis of α,α -dibromoketones and 1,2-diketone from the reaction with alkyne and dibromoisocyanuric acid.

Eunjeong Cho, Aravindan Jayaraman, Sunwoo Lee*

Department of Chemistry, Chonnam National University, Gwangju 61186, Republic of Korea

Dibromoketone and 1,2-Diketone can be transformed for the synthesis of biologically active heterocyclic compounds and good building block candidate. Classical methods using bromine sources such as Br₂, NBS, 1,3-dibromo-5,5-dimethylhydantoin showed limited examples of the formation of 2,2-dibromo-1,2-diarylethanones.

Previously, we reported the synthesis of 2,2-dichloro-1,2-diarylethanones from the reaction of diaryl alkyne and trichloroisocyanuric acid (TCCA).

To expand our studies, we tried to employ dibromoisocyanuric acid (DBCA) as brominating reagent. We found that 1,2-Diketone is synthesized at the same time. We treated reaction under something different way and found condition that 1,2-diketone is predominantly formed. Mostly, Synthesis of 1,2-Diketone is performed in the presence of Metal. In the light of metal free, our studies have some advantages and we hope to contribute new process.

Synthesis of Methylthiomethyl Esters from Carboxylic acid

Subeen Yu, Jeongah Lim, Sunwoo Lee*

Department of Chemistry, Chonnam National University, Gwangju, 61186, Republic of Korea.

E-mail: sunwoo@chonnam.ac.kr

Methylthiomethyl (MTM) esters are frequently used as protecting groups for carboxylic acids and as activating groups for the amidation of acids. In addition, they exhibit a unique chemical property of electron transfer under photochemical conditions. Furthermore, they are often used in bio-active reagents due to their good absorbability and as flavor additives in some dairy and oil products. Therefore, the synthesis of MTM esters has received much attention in the organic synthesis, materials, and pharmaceutical domains. Many preparation methodologies have been reported for MTM esters.

Herein, we report the synthesis of MTM esters by the reaction between carboxylic acid derivatives (cinnamic acid and benzoic acid) and DMSO in the presence of a base. Carboxylic acids, such as cinnamic acid derivatives and benzoic acid derivatives, reacted with DMSO in the presence of Et³N to result in the corresponding MTM esters; further, the yields were found to be good. It was found that benzoic acid was slightly more reactive than cinnamic acid in this reaction.

One-Pot Synthesis of S-Aryl thioester via Pd-Catalyzed Carbonylation and C-S Coupling

Myungjin Kim, Han-Sung Kim, Sunwoo Lee*

Department of Chemistry, Chonnam National University, Gwangju 61186, Republic of Korea.

E-mail: sunwoo@chonnam.ac.kr

Thioesters were synthesized via palladium-catalyzed carbonylation of thioacetates and aryl iodides. S-Aryl thioacetates coupled with carbon monoxide and aryl iodides to afford the desired S-aryl thioesters in good yields. The reaction showed good functional group tolerance toward fluoro, chloro, ketone, ester, aldehyde, cyano, and nitro groups. The tandem reaction of the direct S-arylation of aryl iodides from potassium thioacetate (KSAc) and subsequent carbonylation of the intermediates S-aryl thioacetates provided S-aryl thioesters in moderate-to-good yields.

Decarboxylative Coupling of Alkynoic Acids for the Selective Synthesis of Homoisoflavonoids and Flavones

Sehyeon Han,^a Jieun Lee,^a and Sunwoo Lee^{a*}

^a Department of Chemistry, Chonnam National University, Gwangju 61186, Republic of Korea

sunwoo@chonnam.ac.kr

The development of simple and convenient method for the preparation of aryl alkynoic acids made it easy accessible tool for the introduction of alkynyl group in organic synthesis.¹ In this presentation, we would like to discuss some of our recent research progress towards the decarboxylative coupling reactions of alkynoic acids. Homoisoflavonoid and flavone were selectively obtained from the reaction with salicylaldehydes and arylpropionic acid in the presence of ruthenium catalyst and base. When the reaction was conducted in DMSO, a variety of homoisoflavonoids were exclusively obtained in good yields. While, several flavones were dominantly formed under *t*-AmOH solvent.²

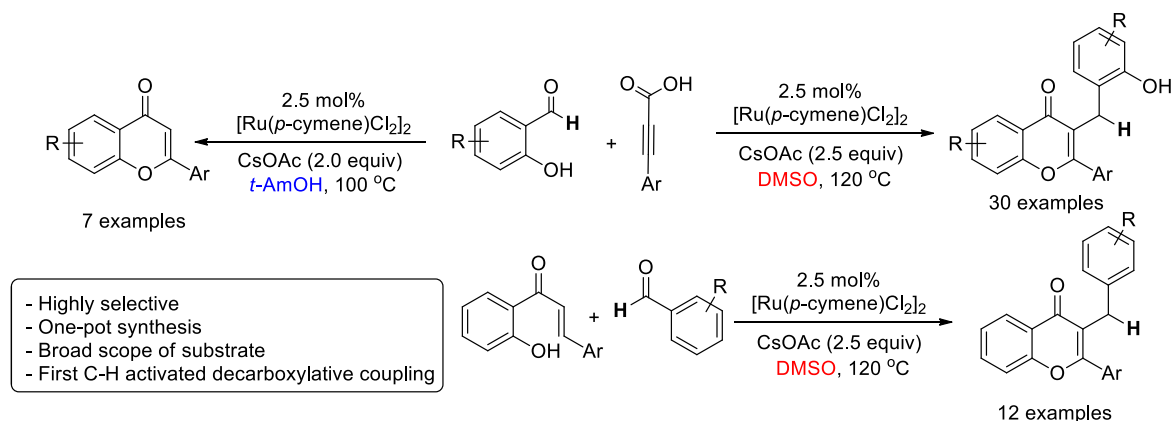


Figure 1. Synthesis of Homoisoflavonoids & Flavones

Acknowledgements

The authors thank the National Research Foundation of Korea (NRF-2015R1A4A1041036, NRF-2017R1A2B2002929) for generous financial support.

References

- (a) Moon, J.; Jeong, M.; Nam, H.; Ju, J.; Moon, J. M.; Jung, H. M.; Lee, S. *Org. Lett.* **2008**, *10*, 945.
(b) Park, K.; Lee, S. *RSC Adv.* **2013**, *3*, 1416. (c) Irudayanathan, F. M.; Lee, S. *Org. Lett.* **2017**, *19*, 2318.
- Raja, G. C. E.; Ryu, J. Y.; Lee, J.; Lee, S. *Org. Lett.* **2017**, *19*, 6606.

Supramolecular Approach to Overcome the Limitations of Photodynamic Cancer Therapy using Nanotheranostics

Eunhye Lee,¹ Xingshu Li,¹ and Juyoung Yoon^{1*}

¹ Department of Chemistry and Nano Science, Ewha Womans University,
Seoul 03760, South Korea

E-mail address: ljbona@gmail.com

Recently, many strategies have been developed to overcome the limitations of PDT such as oxygen self-enriching, fractional PDT and combination with other therapeutic modalities. Despite these efforts, strategies that lead to improved effects by overcoming all three problems of traditional PDT have not been reported thus far.

Inspired by the well-known prodrug concept and the successful use of concomitant drugs in clinical medicine, we embarked on a study aimed at developing an alternative approach to PDT. The effort focused on the design of a stimuli-responsive supramolecular nanostructure, comprising a PS and an anticancer agent. This strategy is reported to directly assemble a phthalocyanine photosensitizer with an anticancer drug mitoxantrone to form uniform nanostructures. This display nanoscale optical properties and have the capability of undergoing nucleic-acid driven disassembly.

This co-assembly was also designed to display nanoscale optical properties as well as activatable singlet oxygen generation and chemotherapeutic abilities. In vivo, it is believed that this supramolecular approach with a high level of accumulation of PcS-MA in tumor can be used for cancer imaging and have significantly improved anticancer effect compared to that of PcS.

References

1. Zhou, Z.; Song, J.; Nie, L.; Chen, X. Reactive Oxygen Species Generating Systems Meeting Challenges of Photodynamic Cancer Therapy *Chem. Soc. Rev.* **2016**, *45*, 6597– 6626
2. Castano, A. P.; Mroz, P.; Hamblin, M. R. Photodynamic Therapy and Anti-Tumor Immunity *Nat. Rev. Cancer* **2006**, *6*, 535– 545
3. X. Li, S. Lee and J. Yoon, *Chem. Soc. Rev.* **2018**, *47*, 1174
4. X. Li, C.Y. Kim, S. Lee, D. Lee, H. M. Chung, G. Kim, S. H. Heo, C. Kim, K. S. Hong and J.Yoon, *J. Am. Chem. Soc.* **2017**, *139*, 10880

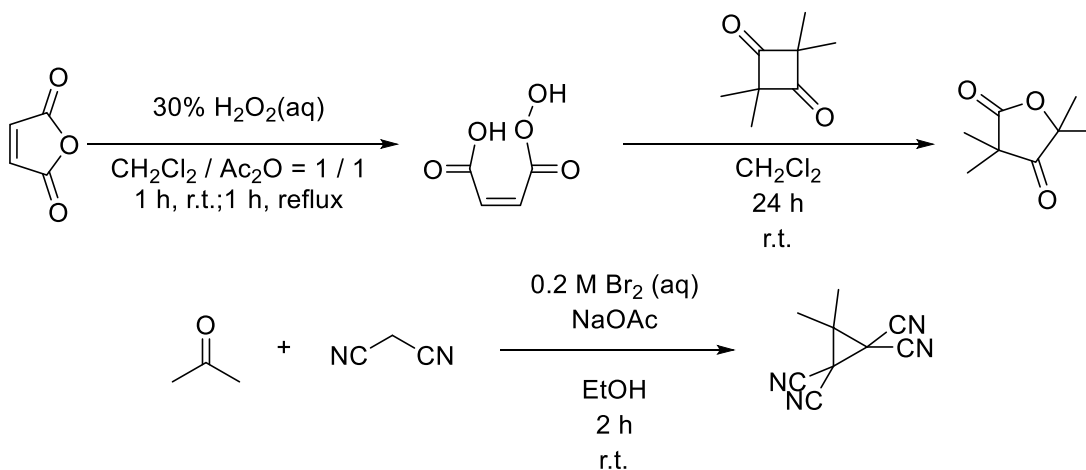
Synthesis of new lithium-ion battery electrolyte additives

Myungjun Park, Kayoung Jeon, Myeonghwa Jeong, Jaejun Hwang, Youngchan Bang, and Bongjin Moon*

Department of Chemistry, Sogang University, 35 Baekbeom-ro, Mapo-gu, Seoul 04107, Korea.
E-mail: bjmoon@sogang.ac.kr

Lithium-ion battery is one of the most popular types of rechargeable batteries. Due to the increasing need of portable electronics, development of more stable and efficient lithium-ion battery is very important. Lithium-ion battery consists of positive electrode (metal oxide cathode), negative electrode (graphite anode), and organic electrolytes. The electrolyte is a mixture of organic carbonates such as ethylene carbonate or diethyl carbonate containing various types of lithium salts (LiPF_6 , LiBF_4). However, the organic carbonate solvent decomposes on the electrode surface during charging-discharging cycles and the decomposed materials cause undesirable side reactions, thereby destroying the structure of negative electrode. It is known that this can be prevented by solid electrolyte interface (SEI) formed on the negative electrode surface by electrochemical reduction of an organic carbonate solvent for the first charge. As a result of electrode decomposition, gas and heat generation is one of the major issues. To circumvent this problem, various additives are employed. Performance of organic electrolytes plays an important role in cell life, stability, and high energy density.

In this study, we have designed and synthesized two new electrolyte additives of lithium-ion battery. 3,3,5,5-tetramethyl 2,4(3*H*,5*H*)-furanone was synthesized in 2 steps and in 49% yields starting from commercially available starting materials. The high oxidation state compound such as lactone is reduced in preference to lithium-ion battery electrolyte, and consequently helps forming stable SEI. 3,3-dimethyl-1,1,2,2-tetracyanocyclopropane was synthesized in 1 step and in 40% yields. The compound that contains the cyano groups protects the battery from the over-charge and extends the cell life.



References

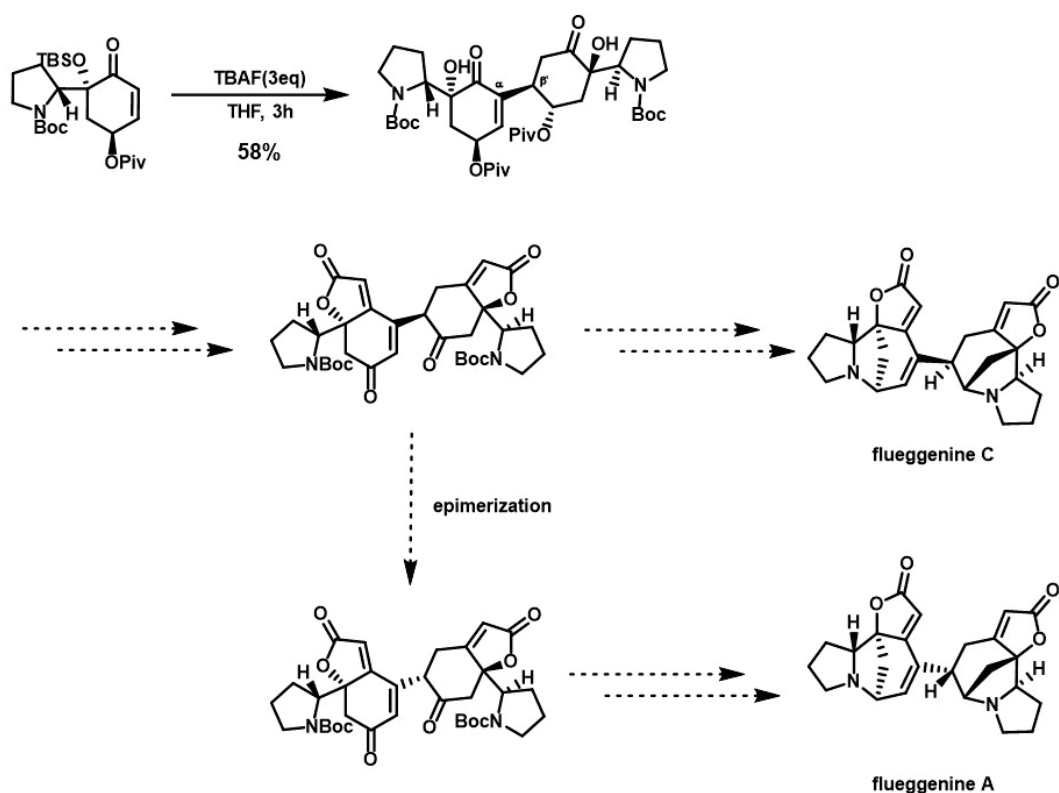
- ¹ Peter, Y. J.; Jerry, Y. *J. Org. Chem.* **1972**, *37*, 1058-1059.
- ² Douglass, F. T.; Jack, Q. *J. Chem. Educ.* **2013**, *90*, 1103-1104.
- ³ Vereshchagin, A.; Elinson, M.; Stepanov, N.; Nikishin, G. *ISRN.Org. Chem.* **2011**, 469453, 1-5.

Toward the Total Synthesis of Flueggenine A and C

Joonoh Park,^a Seongmin Jeon,^a Sunkyu Han^{a*}

^a Department of Chemistry, Korea Advanced Institute of Science and Technology (KAIST)
E-mail: sunkyu.han@kaist.ac.kr

A key step for the first total synthesis of flueggenine C was dimerization between the two γ -hydroxyl enone monomer via Rauhut-Currier reaction.¹ Directing effect of γ -hydroxyl group was considered as a significant factor for determining stereochemistry at C β' . However, inversion of the γ -hydroxyl group to change the stereogenic center resulted in [3+2] compound instead of the desired dimer, being an obstacle toward flueggenine A. Notably, monomers with electron-withdrawing groups on γ -position dimerized at TBAF condition. It seemed that mild basic fluoride anion abstracted the highly acidic γ -proton, making a dienolate intermediate, which acted as a nucleophile for 1,4-Michael addition. The stereochemistry of the resulting dimer was expected to match with flueggenine A due to its favorable chair-like transition state. However, contrary to the expectation, the product was revealed as a precursor of flueggenine C. The modified strategy to get flueggenine A is epimerization introducing ketone at γ -position.



References

¹ Jeon, S.; Han, S. J. Am. Chem. Soc. 2017, 139, 6302-6305.

Visible Light Mediated ATRC/ATRP by Phenothiazine Dyes

Geonji Kim, Kyungchan Min, and Bongjin Moon*

Department of Chemistry, Sogang University, 35 Baekbeom-ro, Mapo-gu, Seoul 04107, Korea.
E-mail: bjmoon@sogang.ac.kr

Atom transfer radical cyclization (ATRC) is a useful method for formation of ring systems. This reaction can be catalyzed by transition metals such as copper, ruthenium, and nickel. Recently, it has been discovered that such reactions can be also catalyzed by a photo-catalyst under visible-light irradiation at room temperature. Atom transfer radical polymerization (ATRP) is one of the most widely used methods among the reversible deactivation radical polymerization (RDRP) techniques. This method typically employs a redox-sensitive transition metal catalyst to form carbon-carbon bonds transferring halogen atoms.

In this study, we have synthesized an organic photo-catalyst based on phenothiazine. We expected strong absorption in the visible light region, reversible single electron transfer and high stability of the radical cation. We then executed visible light-mediated atom transfer radical cyclization (ATRC) of *N*-allyl-*N*-4-tosyl-2-bromo-2,2-dimethylacetamide and visible light-mediated metal free atom transfer radical polymerization (ATRP) of methyl methacrylate using the phenothiazine dye. The ATRP was carried out with methyl-2-bromo methyl propionate as a radical initiator that can be activated by phenothiazine dyes under illumination of blue LED at room temperature.

In order to make progress in this polymerization, we suggested that release of free bromide anion disturbed the polymerization and stabilization of the released bromide anion may help the polymerization control. So for this reason, we synthesized cyanostar that might enable to bind bromide anion enhancing its stability.

References

- ¹ Lee, S. M.; Chene, C. S.; Flood, A. H. *Nature Chemistry*. **2013**, *10*, 1038.

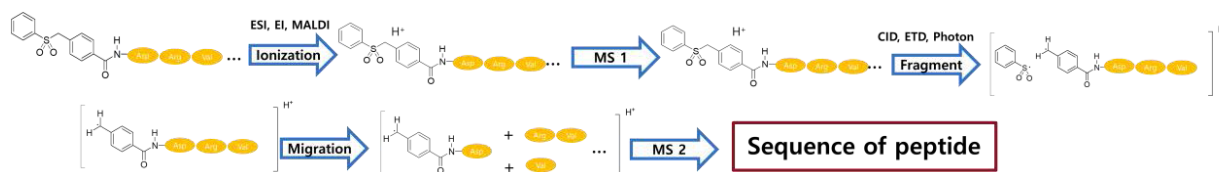
Synthesis of *p*-(Benzenesulfonylmethyl)benzoate-based Mass Tag for Free Radical-Initiated Peptide Sequencing Mass spectrometry (FRIPS-MS)

Jiho Park^a, Jae-ung Lee^b, Han Bin Oh, and Bongjin Moon*

Department of Chemistry, Sogang University, 35 Baekbeom-ro, Mapo-gu, Seoul 04107, Korea.
E-mail: bjmoon@sogang.ac.kr

Free radical-initiated peptide sequencing mass spectrometry (FRIPS-MS) is one of the powerful tools for peptide sequencing by mass spectrometry. This technique requires a chemical mass tag bearing a special functional group which can be cleaved to generate a high energy radical species under the collision induced ionization (CID) conditions in gas phase. When biomolecules such as peptide are tagged by the FRIPS mass tag and subjected to tandem mass spectroscopy, the specific and homolytic bond cleavage occurs in the mass tag. The resulting radical site in the mass tag can then migrate into the peptide backbone resulting in electron captured dissociation (CID)-like backbone fragmentation, which provides more information of the peptide sequence.

In this study, we envisioned that $\text{RCH}_2\text{-SO}_2\text{R}'$ would be suitable functional group that can be homolytically cleaved under CID ionization conditions at low energy. Actually, bond energy of $\text{C}_6\text{H}_5\text{CH}_2\text{-SO}_2\text{CH}_3$ is known to be as low as 222 kJ/mol ($\text{CH}_3\text{-SO}_2\text{CH}_3 = 280$ kJ/mol, $(\text{CH}_3)_2\text{C-CH}_3 = 335$ kJ/mol). So, we have designed and synthesized a new mass tag reagent based on *p*-(benzenesulfonylmethyl) benzoate moiety. Although we reacted sodium benzenethiolate with *p*-chloromethylbenzoate methyl ester to obtain the corresponding thioether as a precursor for *p*-(benzenesulfonylmethyl) benzoate, surprisingly the product was already *p*-(benzenesulfonylmethyl) benzoate. After careful investigation, we found that the thiolate salt reagent had already been oxidized to sulfonate after long time storage on the benchtop.¹ Then we used DCC coupling to introduce NHS group to the tag for conjugation with *N*-terminal amine of peptides.



References

¹ Kim, Y. H.; Yoon, D. C. *Tetrahedron Lett*, **1988**, 29, 6453-6456.

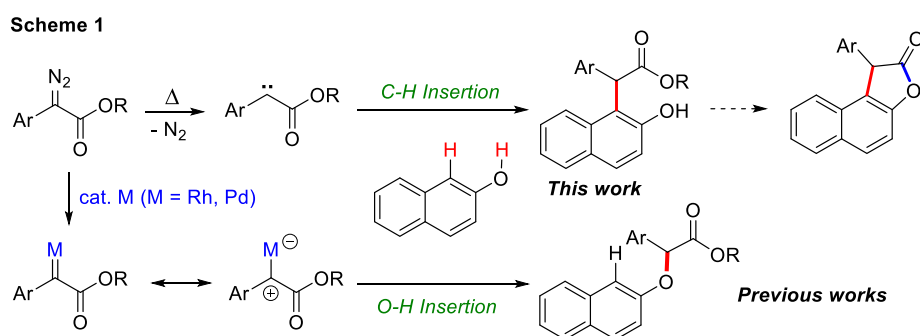
Transition-Metal-Free Chemo- and Regioselective C(sp²)-H Bond Insertion of 2-Naphthol with Diazoacetate

Da Jung Jung, Ji Won Kim, Sang-gi Lee*

Department of Chemistry and Nano Science (BK 21 Plus), Catalysis Research Laboratory, Ewha Womans University, Seoul 03760, Republic of Korea.

E-mail: sanggi@ewha.ac.kr

Diazo compounds, as precursors of reactive metal carbenoids, have been overwhelmingly utilized for the development of versatile synthetic methods in modern organic synthesis. For examples, donor/acceptor metal-carbenoids possessing tractable electrophilic reactivity have been used in various transformations including cyclopropanations, X-H bond (X= O, N, C, S) insertions, and ylide formations.¹ Meanwhile, controlling reactivity of donor/acceptor carbenes toward O-H or C-H bond insertions of phenol derivatives has been considered as one of the challenging issues. In recent studies, it has been demonstrated that in the presence of Au² and boron³ catalysts, the α -diazoesters could undergo the chemoselective and sitespecific C-H bond substitution into the phenols. In present work, to our surprise, we found that thermally induced less controllable metal-free carbenes are introduced into β -naphthol exclusively via α -C(sp²)-H bond insertion to afford 2-naphthol-substituted carboxylates, which can be readily transformed into naphtho[2,1-*b*]furan-2(1H)-ones, pharmaceutically useful bioactive frameworks.



References

¹ (a) Ford, A.; Miel, H.; Ring, A.; Slattery, C. N.; Maguire, A. R.; McKervey, M. A. *Chem. Rev.* **2015**, *115*, 9981-10080. (b) Davies, H. M. L.; Morton, D. *Chem. Soc. Rev.* **2011**, *40*, 1857-1869 (c) Davies, H. M. L.; Beckwith, E. J. *Chem. Rev.* **2003**, *103*, 2861-2903.

² (a) Yu, Z.; Ma, B.; Chem, M.; Wu, H. -H.; Liu, L.; Zhang, J. *J. Am. Chem. Soc.* **2014**, *136*, 6904-6907. (b) Xi, Y.; Su, Y. Yu, Z.; Dong, B.; McClain, E. J.; Lan, Y.; Shi, X. *Angew. Chem. Int. Ed.* **2014**, *53*, 9817-9821.

³ Yu, Z.; Li, Y.; Shi, J.; Ma, B.; Liu, L. Zhang, J. *Angew. Chem. Int. Ed.* **2016**, *55*, 14807-14811.

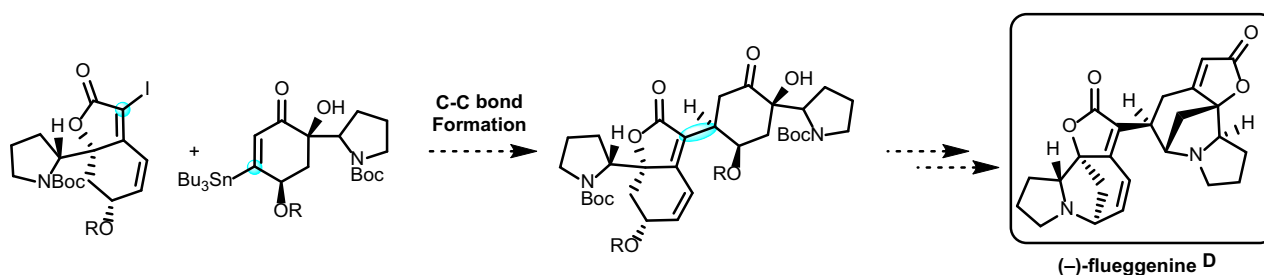
Recent Progress toward the Total Synthesis of (–)-Flueggenine D

Sangbin Jeon^{1,2}, Jinwoo Lee^{1,2} and Sunkyu Han^{1,2*}

¹Department of Chemistry, Korea Advanced Institute of Science and Technology (KAIST)

²Center for Catalytic Hydrocarbon Functionalization, Institute of Basic Science (IBS)

Securinega alkaloids have served as an arena for the discovery of new reactivities and the development of innovative synthetic strategies. The development of novel chemical methods that enables connections of either monomeric or oligomeric securinega units has emerged as a compelling field of study. Flueggenine D is a dimeric securinega alkaloid including α - δ' linkage between two monomeric units.¹ For the construction of this carbon-carbon bond, we set two strategies: Pd-catalyzed Stille reaction and Rh-catalyzed conjugate addition. Herein, we present our recent progress toward total synthesis of (–)-flueggenine D based on these strategies.



References

¹ Zhang, H.; Wei, W.; Yue, J. –M. *Tetrahedron* **2013**, 69, 3942-3946.

Total Syntheses of Spirocyclic PKS-NRPS-based fungal metabolites

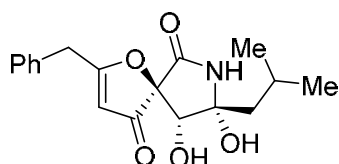
Deekhee Jo^{ab} and Sunkyu Han^{ab*}

^a Department of Chemistry, Korea Advanced Institute of Science and Technology (KAIST), Daejeon 34141, Korea.

^b Center for Catalytic Hydrocarbon Functionalizations, Institute for Basic Science (IBS), Daejeon 34141, Korea.

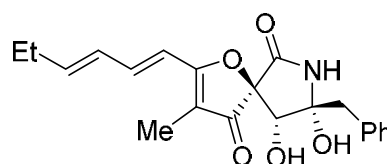
E-mail: sunkyu.han@kaist.ac.kr

Total syntheses of spirocyclic fungal metabolites (\pm)-berkeleyamide D and (\pm)-azaspirene were achieved. Structural analysis and reported biosynthetic studies of γ -hydroxy/methoxy- γ -lactam-based natural products prompted us to devise biomimetic synthetic solutions to these natural products. We constructed the key spirocyclic structure via a series of oxidations and cyclizations of biosynthetically relevant linear precursors. While our streamlined syntheses of berkeleyamide D and azaspirene sought inspiration from its biogenetic hypothesis, experimentally observed chemical reactivities of biosynthetically relevant precursors conversely provide insights to the biosynthesis of natural products of this family.



(\pm)-berkeleyamide D

total steps: 10



(\pm)-azaspirene

total steps: 6

References

- ¹ Jo, D.; Han, S. *Org. Chem. Front.* **2017**, 4, 506.
- ² Kang, T.; Jo, D.; Han, S. *J. Org. Chem.* **2017**, 82, 9335.
- ³ Jo, D.; Han, S. *Chem. Commun.* **2018**, 54, 6750.

Total Synthesis of (+)-DMDP and (+)-Hyacinthacine A2

김연수,^a 봉수지,^a 조용선,^a 정영훈^{a*}

^a School of Pharmacy, Sungkyunkwan University, Suwon 440-746, Republic of Korea

E-mail: ols37@naver.com

Polyhydroxylated pyrrolizidine alkaloids and their synthetic analogues have attracted a great deal of attention in recent years due to their ability to mimic sugars, and competitively and selectively inhibit glycosidases¹ and glycosyltransferase. Consequently, polyhydroxylated piperidine alkaloids have been subjects of intensive research, and various synthetic approaches to produce them have been reported.

Among these, (+)-Hyacinthacine A2 (i.e. 7-deoxyaustraline), isolated from the bulbs of hyacinths (*Hyacinthus orientalis*) and *Scilla campanulata* (Hyacinthaceae)², exhibit antihyperglycemic effect in streptozotocin-induced diabetic mice and also show antiviral and anti-HIV activity.

Due to the unique structural feature and interesting biological property², a number of efforts have been devoted to the development of various approaches for the efficient synthesis of (+)-Hyacinthacine A2.

Recently, regioselectivity and diastereoselective amination of various 1,2-anti-dibenzyl ether using chlorosulfonyl isocyanate(CSI)³ and its application to the synthesis of various biologically active alkaloids have been reported from our laboratory.

In this presentation, we describe a concise and efficient asymmetric of (+)-Hyacinthacine A2. The total synthesis of (+)-Hyacinthacine A2 has been accomplished in 13 steps from readily available methyl- α -D-mannopyranoside, and the key steps in this route involve Wittig reaction, CSI-mediated amination, intramolecular ring cyclizing metathesis and amine cyclization.

References

¹Barret, J. E.; Flockerzi, V *In Handbook of Experimental Pharmacology*. **1996**, 119, 411–482.

²Asano, N; Kurori, H *Tetrahedron Asymmetry*. **2000**, 11, 1.

³Kim, J. D.; Lee, M. H. *Tetrahedron Lett*. **2000**, 41, 5073

Synthesis and Biological Evaluation of Hydroxamates as Selective HDAC6 inhibitors

정준민^a, 김다은^a, 고수연^a, 남기범^a, 박현주^a, 정영훈^{a*}

^a*School of Pharmacy, Sungkyunkwan University, Suwon 440-746, Republic of Korea*
E-mail: yhjung@skku.edu

In epigenetic pathways, histone deacetylase plays a key role in regulation of gene expression. The role of HDAC is the removal of acetyl group of lysine residue on the gene which decrease expression of tumor suppress genes. Thereupon, HDAC inhibition has emerged as an attractive target for the development of new anti-tumor agents. Consequently, the identification of potential HDAC inhibitor is an important therapeutic strategy for treatment of cancers.

In our previous study, we have introduced hydroxamate group as a zinc binding group and various phenyl and cinnamyl substituents as a cap group. We have also changed the chain length and linker moiety (thiazole, oxazole, oxadiazole). Evaluation of these compounds for their HDAC6/1 inhibitory activity by enzymatic assay afforded BKS-112 as a promising lead compound.

In this study, the derivatives of BKS-112 have been designed and synthesized. Synthesis has been carried out by introduction of naphthalene, biphenyl, biphenyl ether substituents as a cap group for the formation of hydrophobic interaction and increased rigidity. Benzamide moiety has also been introduced as a cap group for the formation of hydrogen bond. From the evaluation of these compounds for their HDAC6/1 inhibitory activity, compound with naphthalene substituent showed the best activity and selectivity so far. Nowadays, syntheses of compounds with various naphthalene substituents are in progress.

References

¹ Yoo, J. K.; Kim, S. J. *Eur. J. Med. Chem.* **2016**, *116*, 126-135

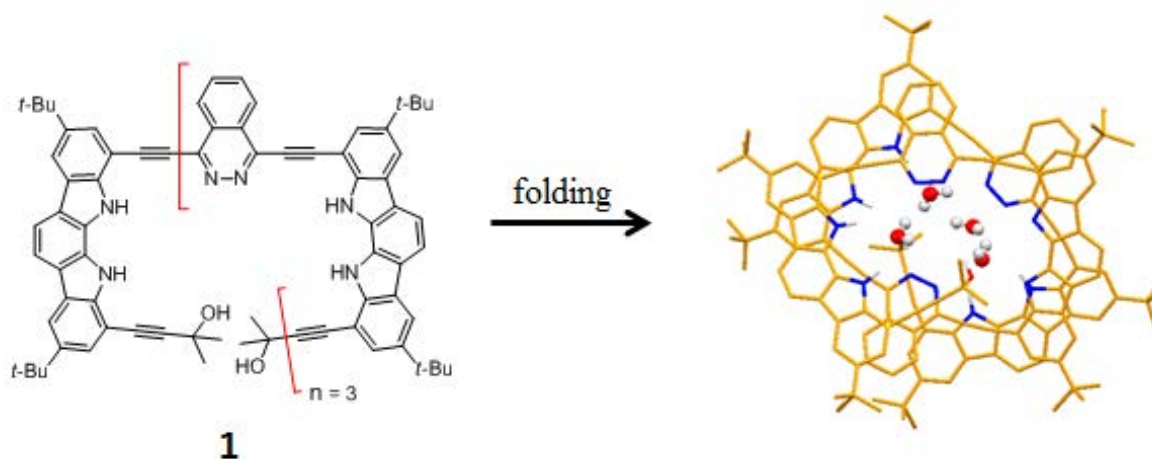
² 대한민국 특허, 출원번호: 10-2018-0045283

Carbohydrate recognition through an Aromatic Hybrid foldamer With Extended cavity and sensor of chiral molecules

Kyung-Mog Kim, and Kyu-Sung Jeong *

Department of Chemistry, Yonsei University, Seoul 03722, Korea
kkmog90@yonsei.ac.kr

An aromatic hybrid foldamer **1** was prepared by alternatively connecting indolocabazoles and phthalazines through ethynyl bonds. The foldamer folded into a stable helical conformation with an internal helical cavity which was wrapped by hydrophilic functional groups; indolic NHs and phthalazine nitrogens. Helical folding of **1** is induced by dipole interaction through the ethynyl bond and π - π stacking between two repeating units. Folding into helical conformation in the solid state was unambiguously proven by single-crystal X-ray structure of **1**. It resembles an empty cylinder. The artificial helix tube can be used in various applications like anion sensor, molecular container, and water channel. However, there was a difficulty in biologically important molecular recognition due to the limitation of the size of the inner cavity. The size of the internal cavity can be controlled by changing the type of oligomers subunit, the linking position, and the length of the oligomer. Among them, studies have been actively carried out to control internal cavity by changing the kinds of the oligomers subunits and the length of the oligomers. So we controlled the internal cavity by changing the linking position of the oligomer. In this way, we intend to use biologically important molecules having chirality as recognition and separation or molecular filters and sensors, by using foldamer with large internal cavity size. Details will be described in the poster presentation.

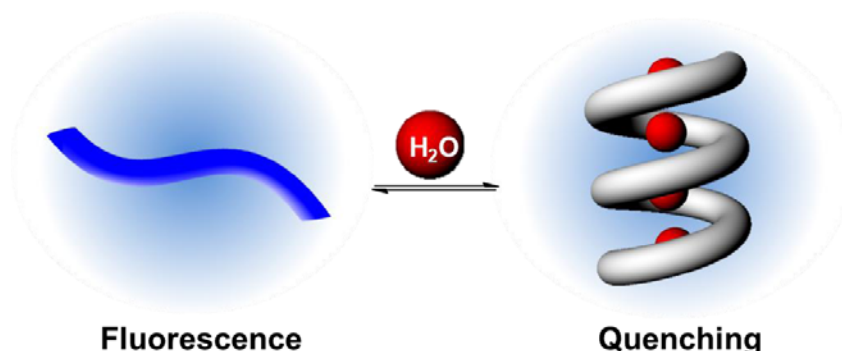
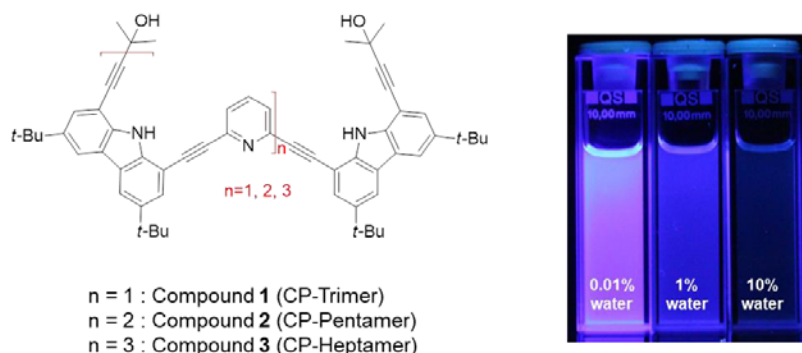


An On-off Fluorescence Sensor for Detecting Trace Water using Aromatic Hybrid Foldamers

Woojeong Chae^a and Kyu-Sung Jeong*

^a Department of Chemistry, Yonsei University, Seoul, Korea
E-mail: cwj7235@gmail.com

The most widely used technique to determine water content on the laboratory scale is Karl-Fisher titration, which has limitations to monitor in real-time and move.¹ Herein, we have been prepared carbazole-pyridine foldamers **1–3** which fold into helical conformations with an internal cavity to detect trace amounts of water. Two repeating units, carbazole and pyridine, linked alternatively through ethynyl bonds prefer to adopt a syn-coplanar conformation due to dipole-dipole interactions, and this conformational propensity leads to helical folding. The folding features of **1–3** were studied by ¹H NMR, 2D-ROESY NMR, UV-visible, and fluorescence spectroscopy. When folded into a helical conformation, the aromatic foldamers display considerable fluorescence changes due to the π -stacking of the backbone aromatic planes. More specifically, foldamers are strongly fluorescent in unfolded conformation but its fluorescence is nearly quenched in folded conformation. Fluorescence spectra also showed that the longer foldamer has the greater the sensitivity to water. The foldamers can be used as a fluorescence sensor that detects a very small amount of water by changing the folding and unfolding mode of the foldamer. Details will be discussed in the poster presentation.



References

¹ J. Mitchell Jr. and D. M. Smith, *Aquametry: A Treatise on Methods for the Determination of Water*, Wiley, New York, pt. 1, 2nd edn, 1977.

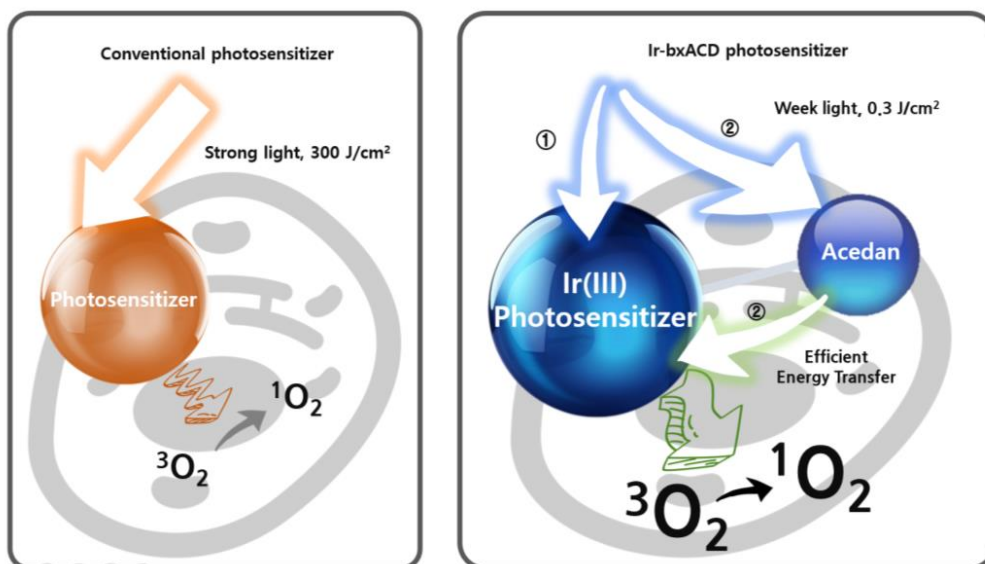
Enhancing ROS Generation via Photon Energy Transfer of Ir(III) Complex for Low Energy Photodynamic Therapy

Chai-heon Lee^a and Tae-Hyuk Kwon^a

^a Department of Chemistry, Ulsan National Institute of Science and Technology (UNIST), Ulsan 44919, Republic of Korea.

E-mail: ki8364@gmail.com

Ir(III) complexes with great reactive oxygen species (ROS) generation efficiency have attracted attention as photosensitizer for photodynamic therapy (PDT) because ROS such as singlet oxygen and superoxide radical induce protein inactivation and trigger cancer cell death.¹ However, the Ir(III) complexes produce not enough amount of ROS to kill cancer cells due to low absorption coefficient despite their great ROS generation efficiency. Therefore, high-energy irradiation ($>35 \text{ J/cm}^2$) is necessary for PDT, which causes normal tissue damage in clinical application.² Herein, we report novel Ir(III) complex, Ir-bxACD, incorporating acedan dye which has strong absorption coefficient, high quantum yield, and great two-photon activation property. As the Ir-bxACD is irradiated, the highly efficient intra-molecular energy transfer ($\geq 98\%$) occur because the emission energy of acedan dye is well-matched to absorption region of Ir(III) complex. Thereby, the enhanced amount of exciton of Ir-bxACD by energy transfer improves absolute amount of singlet oxygen. As a result, the Ir-bxACD with low-energy irradiation ($\leq 0.3 \text{ J/cm}^2$) triggers effective apoptosis on mitochondria of living cancer cells, even with two-photon activation. Consequently, we present rationally designed Ir(III) photosensitizer for PDT incorporating acedan dye, and propose the possibility of PDT using non-invasive irradiation.



References

- Nam, J. S.; Kang, M.-G.; Kang, J.; Park, S.-Y.; Kim, H.-T.; Lee, S. J. C.; Seo, J. K.; Kwon, O.-H.; Lim, M. H.; Rhee, H.-W.; Kwon, T.-H. *J. Am. Chem. Soc.* **2016**, 138, 10968.
- Wu, N.; Cao, J.-J.; Wu, X.-W.; Tan, C.-P.; Ji, L.-N.; Mao, Z.-W. *Dalton Trans.*, **2017**, 46, 13482

Synthesis of Lophirone F Hexamethyl Ether

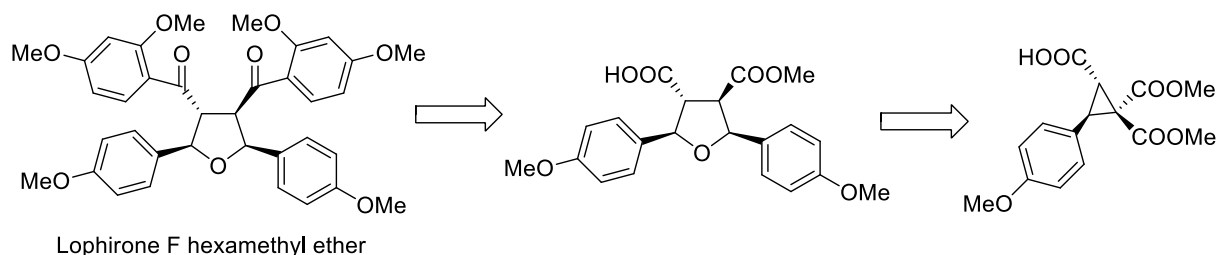
Le Minh Hoang, Do Tien Dung, and Chang Ho Oh*

Department of Chemistry, Research Institute of Natural Sciences, Hanyang University,
Seongdong-gu Seoul, 04763, Korea

E-mail: changho@hanyang.ac.kr

Lophirone F has been isolated from the stem bark of *Lophira Lanceolata* growing in the tropical forests of Africa. We have successfully synthesized its hexamethyl ether with reasonable yield by taking advantage of the [3+2] cyclization between a substituted cyclopropane and *p*-methoxybenzaldehyde.

This work launches an approach towards the syntheses of THF-based natural products that we are currently engaged with.



References

- ¹ Hossay Abas, Sean M. Linsdall, Mathias Mamboury, Henry S. Rzepa and Alan C. Spivey*, *Org. Lett.*, **2017**, 19(10), 2486-2489.
- ² Shanina D. Sanders, Andrea Ruiz-Olalla and Jeffrey S. Johnson*, *Chem. Commun.*, **2009**, 5135-5157
- ³ A. Murakami, S. Tanaka, H. Hirota ^a, R. Irie ^a, N. Takeda, A. Tatematsu, K. Koshimizu, *Phytochemistry*, **31**, **1992**, 2689-2693

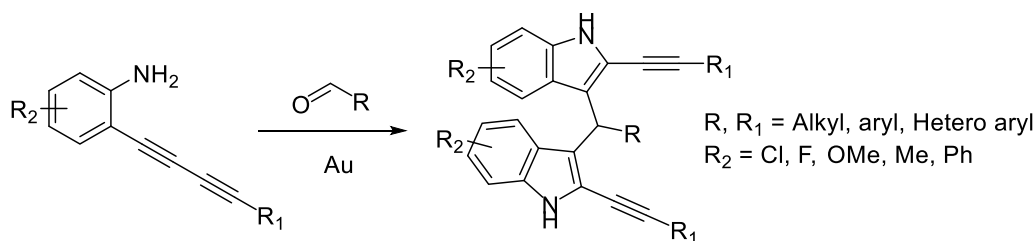
Au-catalyzed tandem reaction of 2-bisalkynylanilines with aldehyde: an efficient access to 2,2'-disubstituted bisindolymethanes

Dong Hwan Oh, Raveendra Jillella, and Chang Ho Oh*

Department of chemistry, Center for New Directions in Organic Synthesis, Hanyang University, Seoul 04763, Korea

E-mail: Changho@hanyang.ac.kr

Indole scaffolds are represented as one of the privileged structural motifs in biologically active natural products and drug molecules which have vital medicinal values.¹ Bis-indolymethanes (BIMs) are good intermediates for the synthesis of numerous bioactive molecules.² The existing methods for the synthesis of BIMs mostly involve the electrophilic substitution reaction of indoles with carbonyl compounds employing various Lewis acid catalysis. Recently, transition metal-catalyzed tandem one-pot annulation of o-alkynylanilines followed by in-situ trapping with suitable electrophiles has become an extremely useful protocol for the construction of 2,3-difunctionalized indoles. Based on this concept, our on-going efforts on tandem cyclization reactions for the development of 3-substituted indoles were stimulated by the metal catalysts.³ In this Poster, we wish to disclose an efficient Au-catalyzed tandem cyclization of O-bisalkynylanilines followed by trapping with various aldehydes to access an efficient bis(2-alkynyl phenyl) indolymethanes.



References

1. A. J. Ochanowska-Karamyan, M. T. Hamann, *Chem. Rev.*, 2010, **110**, 4489; (b) M. Bandini and A. Eichholzer, *Angew. Chem., Int. Ed.*, 2009, **48**, 9608; (c) G. R. Humphrey, J. T. Kuethe, *Chem. Rev.*, 2006, **106**, 2875.
2. (a) B. R. De Miranda, J. A. Miller, R. J. Hansen, P. J. Lunghofer, S. Safe, D. L. Gustafson, D. Colagiovanni and R. B. Tjalkens, *J. Pharmacol. Exp. Ther.*, 2013, **345**, 125; (b) X. Li, S. O. Lee and S. Stephen, *Biochem. Pharmacol.*, 2012, **83**, 1445; (c) S. Chintharlapalli, R. Burghardt, S. Papineni, S. Ramaiah, K. Yoon and S. Safe, *J. Biol. Chem.*, 2005, **280**, 24903.
3. (a) C. H. Oh, S. Karmakar, H. Park, Y. Ahn and J. W. Kim, *J. Am. Chem. Soc.*, 2010, **132**, 1792. (b) R. Jillella, C. H. Oh, *RSC Adv.*, 2018, **8**, 22122 (c) C. H. Oh, H. S. Park, N. Park, S. Y. Kim and L. Piao, *Synlett*, 2014, 0579.

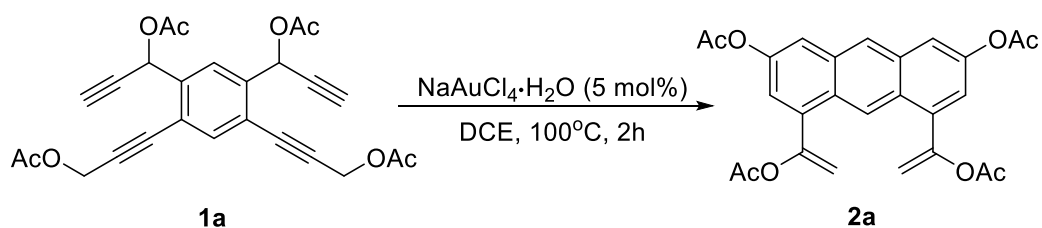
Mechanistic study of gold-catalyzed Synchronized cyclization of Bispropargylic carboxylates

Juyeon Kang and Chang Ho Oh*

Department of Chemistry and Research Institute of Natural Science
Hanyang University, Seongdong-gu Seoul, 04763, Korea
Email: changho@hanyang.ac.kr

Gold catalysis has emerged as an efficient methodology to activate π -systems of carbon-carbon double and triple bonds. The electrophilic π -system activation with alkenes, alkynes, and allenes toward for subsequent nucleophilic attack relies on electron deficiency of gold catalysts.

We have applied gold-catalyzed reaction to the substrates which have two set of two different propargylic carboxylates. In case of the benzene type substrates, the reaction has been extended successfully to syntheses of anthracene derivatives. We extended the range of molecules with two pairs of propargylic carboxylates at two different positions in benzene to confirm the gold catalysis for the fourth substrate.



Scheme 1

References

- ¹ Hashimi, A. S. K. *Adv. Synth. Catal.* 2013, 355, 2481 – 2487.
- ² Zhao, J.; Hughes, C. O.; Toste, F. D. *J. Am Chem Soc.* 2006, 128, 7436.

A Ratiometric Two-Photon Fluorescent Probe for Tracking Lysosomal ATP

Yong Woong Jun,^a **Kyeong Hwan Kim**, and Kyo Han Ahn^{a*}

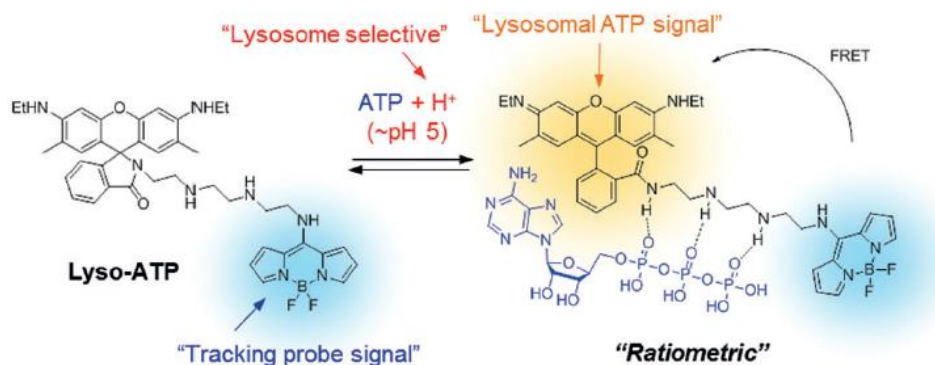
^a Department of Chemistry, Pohang University of Science and Technology (POSTECH) 77 Cheongam-Ro, Nam-Gu, Pohang 37673 (Rep. of Korea).

ahn@postech.ac.kr

Vesicles exchange cellular substances through membrane fusion processes, kiss-and-run and full-collapse fusion process.¹ Direct observation of the processes in living cells, however, remains as a challenge owing to many technical obstacles. Herein, we disclose an in cellulo assay that enables direct monitoring of the membrane fusion processes between vesicles (lysosomes).

We focused on lysosomes that release endogenous signaling through the membrane fusion processes.² Specifically, we targeted the lysosomal ATP, a ubiquitous cellular element, since it not only is energy source in living organisms but also plays distinct roles as a signaling unit for such as immunogenic cell death, apoptosis, and neuro-transmission.³

We report a ratiometric two-photon probe which can track lysosomal ATP in real-time. The lysosomal membrane fusion processes in cells were directly observed and the concentration of lysosomal ATP was measured by applying the probe to two-photon live-cell imaging.



References

- ¹ S. Martens, H. T. McMahon, *Nat. Rev. Mol. Cell. Biol.* **2008**, 9, 543 – 565.
- ² J. P. Luzio, P. R. Pryor, N. A. Bright, *Nat. Rev. Mol. Cell. Biol.* **2007**, 8, 622 – 632.
- ³ J. M. Zhang, H. K. Wang, C. Q. Ye, W. Ge, Y. Chen, Z. L. Jiang, C. P. Wu, M. M. Poo, S. Duan, *Neuron* **2003**, 40, 971 – 982

3D Molecular Architectures with Concave-Faced Cuboid Shape by the Self-Assembly of Chimeric Foldamer

정록암,^a 엄재훈,^a 공진택,^a 이희승^{a*}

^a Department of Chemistry, Korea Advanced Institute of Science and Technology,
291 Daehak-ro, Yuseong-gu, Daejeon 305-701, Korea
E-mail: hee-seung_lee@kaist.ac.kr

Nature systems create complicated complex structures by using self-assembly. The design of the building block is very important to understand the formation principle of the complex structure. We used an octameric foldamer composed of 2-aminoisobutyric acid (Aib) and a cyclic β -amino acid (*trans*-2-aminocyclopentane carboxylic acid, ACPC) in a 1:1-alternating α/β -peptide foldamer. These foldamers are reported to display two helical conformations, the 11-helix and the 14/15-helix.¹ This phenomenon is similar to structural changes with the 3_{10} -helix and the α -helix in natural proteins. The intermediate of structural changes can be understood through self-assembly.

Our group recently reported various foldectures which have highly homogeneous and unique 3D morphologies derived from the self-assembly of foldamers.²⁻⁵ To understand the correlation between the helical type and the 3-dimensional structure, it is necessary to study the foldamers with chimeric helical types. Herein we report a new foldecture which has a concave-faced cuboid shape by the self-assembly of chimeric foldamer of 11- and 14/15-helix. Foldamer packing structure was resolved by powder X-ray diffraction (PXRD) analysis and provides important structure information for the unusual 3D architecture. This study will play an important role in designing complex 3D architecture analogous to proteins.

References

- ¹ S. H. Choi, I. A. Guzej, L. C. Spencer and S. H. Gellman, *J. Am. Chem. Soc.*, **2008**, 130, 6544–6550.
- ² Kwon, S.; Jeon, A.; Yoo, S. H.; Chung, I. S.; Lee, H.-S. *Angew. Chem. Int. Ed.* **2010**, 49, 8232–8236.
- ³ Kwon, S.; Shin, H. S.; Gong, J.; Eom, J.-H.; Jeon, A.; Yoo, S. H.; Chung, I. S.; Cho, S. J.; Lee, H.-S. *J. Am. Chem. Soc.* **2011**, 133, 17618–17621.
- ⁴ Yoo, S. H.; Eom, T.; Kwon, S.; Gong, J.; Kim, J.; Cho, S. J.; Driver, R. W.; Lee, Y.; Kim, H.; Lee, H.-S. *J. Am. Chem. Soc.* **2015**, 137, 2159–2162.
- ⁵ J.-H. Eom, J. Gong, S. Kwon, A. Jeon, R. Jeong, R.W. Driver, H.-S. Lee, *Angew. Chem. Int. Ed.* **2015**, 54, 13204–13207.

Two-photon Ratiometric Fluorescent Probe for Bisulfite Detection

Tamima Umme, Subhankar Singha and Kyo Han Ahn*

Department of Chemistry, Pohang University of Science and Technology (POSTECH), Republic of Korea.

E-mail: ahn@postech.ac.kr

Abstract:

Biothiols such as Cysteine (Cys) and hydrogen sulfide (H_2S) undergo metabolism to generate sulfur dioxide (SO_2) as the end-product, which spontaneously forms bisulfite (HSO_3^-) in physiological systems.¹ In contrary, sulfur dioxide derivatives are health hazards and act as environmental pollutant. Excessive intake of SO_2 , which ultimately produces bisulfite, may cause several critical health complications including respiratory diseases and even lung cancer.² Accordingly, it is utmost necessary to develop an effective detection method for bisulfite to investigate the biothiol metabolism pathway as well as $\text{SO}_2/\text{HSO}_3^-$ induced health disorders. In our continuous efforts to develop fluorescent probe for redox related species,³ this time we developed a two-photon (TP) active fluorescent probe developed for the selective detection of bisulfite ions. The probe is based on a benzocoumarin (BC) dye containing an aldehyde moiety, which shows ratiometric fluorescence response (emission shift = 63 nm) in presence of bisulfite. Furthermore, this probe is also effective for ratiometric imaging of endogenous bisulfite ions in HeLa cells under two-photon excitation.

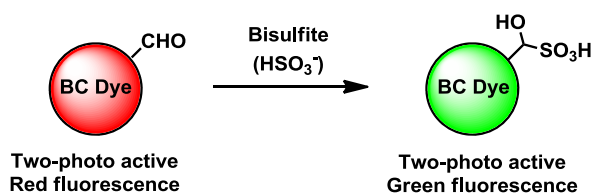


Fig. 1. Schematic illustration of two-photon **BC-Dye** reacting with bisulfite.

References

- ¹Ubuka, T.; Ohta, J.; Yao, W. B.; Abe, T.; Teraoka, T.; Kurozumi, Y. *Amino Acids*, **1992**, 2 (1–2), 143–155.
- ²Sang, N.; Yun, Y.; Yao, G.; Li, H.; Guo, L.; Li, G. *Toxicol. Sci.* **2011**, 124, 400–413.
- ³Hridesh A.; Suman P.; Anirban P.; Yong W. J.; Juryang B.; Kyo H. A.; Divesh N. S.; Amitava D. *J. Mater. Chem. B*, **2016**, 4, 7888–7894.

Dual Rh(II)/Pd(0) Relay Catalysis for One-pot Construction of Heterocycles having Quaternary Carbon Center

Zi Xuan, Yu Lim Lee, and Sang-gi Lee*

Department of Chemistry and Nanoscience (BK21 Plus), Catalysis Research Laboratory,
Ewha Womans University, Seoul 03760, Republic of Korea
E-mail : sanggi@ewha.ac.kr

Heterocyclic compounds having a quaternary carbon center are frequently found in a range of natural products and bioactive molecules (Figure 1). Accordingly, the development of an efficient and environmentally benign synthetic methods is highly desirable. In this regards, dual relay catalysis is considered as one of the most promising sustainable strategies. However, the success of dual relay catalysis could largely be determined by the catalysts' compatibility and balanced kinetics. Previously, we have demonstrated the compatibility between Rh(II) and Pd(0) catalysts.¹ More recently, we also reported an asymmetric dual Rh(II)/Pd(0) relay catalysis, *i.e.*, Rh(II)-catalyzed enantioselective C(sp³)-H insertion/Pd(0)-catalyzed diastereoselective allylation of diazoamides.² Herein, we present a Rh(II)/Pd(0) dual relay catalysis for one-pot synthesis of 3,3-disubstituted benzofuran-2-one and indolin-2-one moieties through sequential C(sp²)-H insertion/ allylic alkylation of aryl α -diazo compounds.

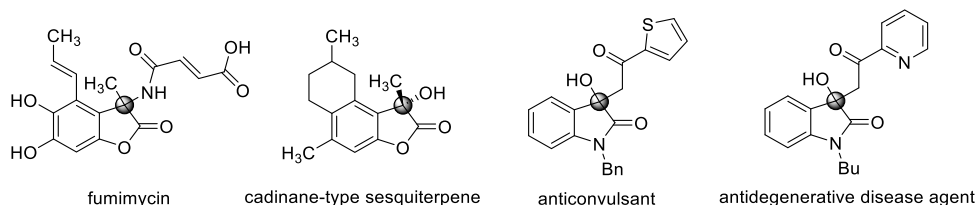
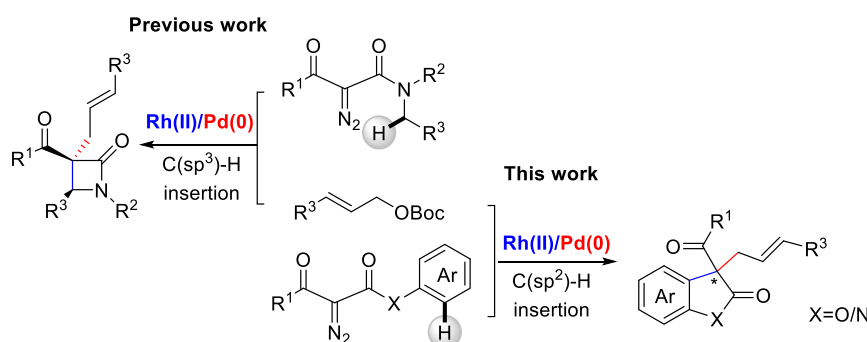


Figure 1. Heterocyclic compounds having a quaternary carbon center.



References

- Chen, Z-S.; Huang, L-Z.; Jeon, H. J.; Xuan, Z.; Lee, S.-g. *ACS Catal.* **2016**, *6*, 4914.
- Huang, L-Z.; Xuan, Z.; Jeon, H. J.; Du, Z-T.; Kim, J. H.; Lee, S.-g. *ACS Catal.* **2018**, *8*, 7340.

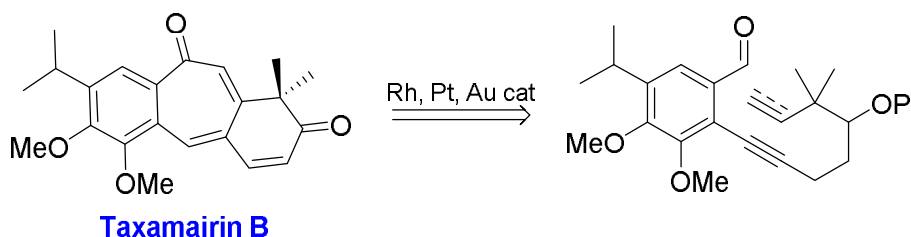
Synthesis of Taxamairin B : Use of Au, Pt-Catalyzed Cyclization Reaction

Le Thuy Quynh,^a Seonmi Lee,^a Chang Ho Oh^{a*}

^a Department of Chemistry, Center for New Directions in Organic Synthesis, Hanyang University, Seoul 04763, Korea

E-mail: Changho@hanyang.ac.kr

During the last three decades the variety of icetexane natural products have been used as tools to study biological properties of significant interests such as anti cancer, anti-HIV agents, antioxidant^[1,2a]... The subclass of highly unsaturated icetexanes are Taxamairin A and B which were isolated in 1987 from *Taxus mairei*. An initial survey of Taxamairin A and B identified inhibitory activity against hepatoma (liver tumor) cells^[2]. Since that time, this natural product attracted the interest of both chemists and our group. We have studied cycloisomerization reaction of enynal and diynal by utilizing rhodium, platinum and gold catalyst to construct the 6-7-6 tricyclic-key skeleton of Taxamairin and a variety of natural product.



References

- [1] a) E. A. Berger, P. M. Murphy and J. M. Farber, *Annu. Rev. Immunol.*, **1999**, *17*, 657–700. b) A. Kelecom, *Tetrahedron*, **1983**, *39*, 3603–3608.
 [2] a) J. Liang, Z. Min, M. Inuma, T. Tanaka and M. Mizuno, *Chem. Pharm. Bull.*, **1987**, *35*, 2613–2614. 42. BJ. b) Liang, Z. Min, T. Tanaka, M. Mizuno and M. Inuma, *Huaxue Xuebao*, **1988**, *46*, 21–25

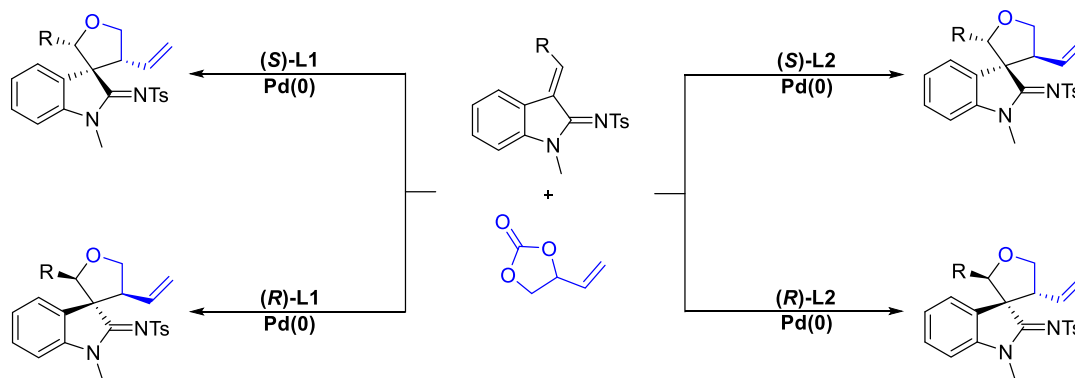
Ligand-Controlled Stereodivergent Palladium Catalysis for the Synthesis of Stereoisomeric Spiro-Furanindolines

Hyun Ji Jeon, Su Min Park, and Sang-gi Lee

Department of Chemistry and Nanoscience (BK21 Plus), Ewha Womans University, 03760, Seoul, Republic of Korea.

E-mail: sanggi@ewha.ac.kr

Stereodivergent (enantiodivergent and diastereodivergent) catalysis is one of the most fascinating yet challenging strategies, because it can allow access to the possible stereoisomers having two or more stereogenic centers.^[1] Although the use of different catalysts has been extensively studied for the stereodivergent catalytic reactions,^[2] switching solvents or additives often achieved controlling the stereochemical outcomes.^[3] Nevertheless, it has not been developed the efficient stereodivergent catalytic reactions, in which both the enantio- and diastereoselectivities can be controlled simply by changing the ligands. In present work, we have investigated the transition-metal-catalyzed ligand-controlled stereodivergent dipolar cycloaddition reactions. The zwitterionic alkoxy p-allyl Pd complex, generated in situ from the vinyl ethylene carbonate, could act as a 1,3-dipole, which may undergo dipolar cycloadditions with stable indolinylidene dipolarophiles. The enantio- and diastereoselectivities of the reactions could be controlled mainly by choice of chiral ligand affording one of the possible stereoisomeric spiro-furanindolines selectively.



References

- [1] (a) I. P. Beletskaya, C. Najera, M. Yus, *Chem. Rev.*, **2018**, *118*, 5080–5200. (b) S. Krautwald, E. M. Carreira, *J. Am. Chem. Soc.* **2017**, *139*, 5627–5639.
- [2] M. Bihania, J. C-g. Zhaoa, *Adv. Synth. Catal.* **2017**, *359*, 534-575
- [3] Q. Cheng, F. Zhang, Y. Cai, Y-l. Guo, S-l. You, *Angew. Chem. Int. Ed.* **2018**, *57*, 2134–2138.
astname, F. A.; Lastname, S. A. *J. Import. Res.* **2008**, *8*, 50-57.

Antiplaetlet coating with poly ((3-methacryloylamino)propyl-dimethyl(3-sulfopropyl)ammonium hydroxide) on titanium dioxide and stainless steel

Ji Hwan Eom,^a Yeonwoo Jeong,^b Sung Min Kang^b, Woo Kyung Cho^{a*}

^a Department of Chemistry, ChungNam National University, Daejeon 34134, Republic of Korea

^b Department of Chemistry, Chungbuk National University, Cheongju, 28644, Republic of Korea

*E-mail: wkcho@cnu.ac.kr

When medical devices such as stent and catheter are inserted in blood vessel, platelet adhesion can cause a serious problem like blood coagulation, resulting in vascular clogging.¹ To inhibit platelet adhesion on medical devices, in this work, we employed zwitterionic material, (3-methacryloylamino)propyl-dimethyl(3-sulfopropyl)ammonium hydroxide (MPDSAH)² by considering that zwitterionic polymers have antifouling effects by strongly stabilizing the hydration layer formed by aqueous solution³. Titanium dioxide (TiO₂) and stainless steel (SS), which are mainly used in medical devices, were chemically modified by surface-initiated atom transfer radical polymerization of MPDSAH. The surface-grafted polymeric films were characterized with ellipsometer, contact angle goniometer, X-ray photoelectron spectroscopy, and atomic force microscopy. Compared with bare substrates, the poly(MPDSAH)-coated substrates effectively reduced both fibrinogen and platelet adhesions. The platelet adhesion was reduced by 86% and 92% for the polymer-coated TiO₂ and SS substrates, respectively.

References

¹ Chiumiento, A.; Lamponi, S.; Barbucci, R. *Biomacromolecules* **2007**, *8*, 523-531.

² Cho, W. K.; Kong, B.; Choi, I. S. *Langmuir* **2007**, *23*, 5678-5682

³ He, M.; Gao, K.; Zhou, L.; Jiao, Z.; Wu, M.; Cao, J.; You, X.; Cai, Z.; Su, Y.; Jiang, Z. *Acta Biomaterialia* **2016** *40*, 142-152

ESIPT Based Organic Dye Nanoparticles and Their Shape-Dependent Luminescence Behavior

Mithun Santra, Mingchong Dai, and Kyo Han Ahn*

Department of Chemistry, POSTECH, 77 Cheongam-Ro, Nam-Gu, Pohang, Gyungbuk, 37673, Republic of Korea

Fluorophores which can emit both in solution and in solid states have potential application to medical and biochemical sensing. Addressing the very issue herein we disclose several bent shaped 1-(benzo[d]thiazol-2-yl)-6-substituted-naphthalen-2-ol dyes, which also have an excited-state intramolecular proton-transfer (ESIPT) feature modulating their optical properties. All the compounds and their 2-methoxy derivatives showed luminescence both in solution as well as in solid states, plausibly because of unfavorable orbital interactions between stacked molecules nearby.

The ESIPT dyes also possess large Stokes shifts, along with good optical brightness. Emission property of the dyes can be significantly tuned by changing the 6-substituent. Moreover using these dyes organic nanoparticles were synthesized by sonication method and characterized with DLS measurements. The new organic nanoparticles were used in cellular imaging in both one-photon and two-photon microscopic modes. The approach of molecular shape control demonstrated here thus opens a door toward solid-state luminescent organic materials, organic nanoparticles and their potential application.

References

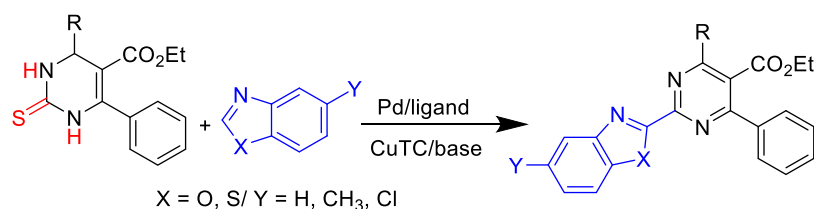
1. *ACS Appl. Bio Mater.* **2018**, 1, 136-145

Oxidative dehydrosulfurative azolation of 3,4-dihydropyrimidine-1H-2-thions.

Hong-Ju Yang and Jeong-Hun Sohn*

Department of Chemistry, Chungnam National University, Deajeon 305-764, Korea

We present dehydrosulfurative C-C cross-coupling reaction of 3,4-dihydropyrimidine-1H-2-thiones (DHPMs) with azoles and concomitant oxidative dehydrogenation under a Pd/Cu catalytic system to provide diverse 2-azolylpyrimide in a single step.¹ The reaction proceeded efficiently with a wide range of DHPM substrates and azoles as coupling partners.



References

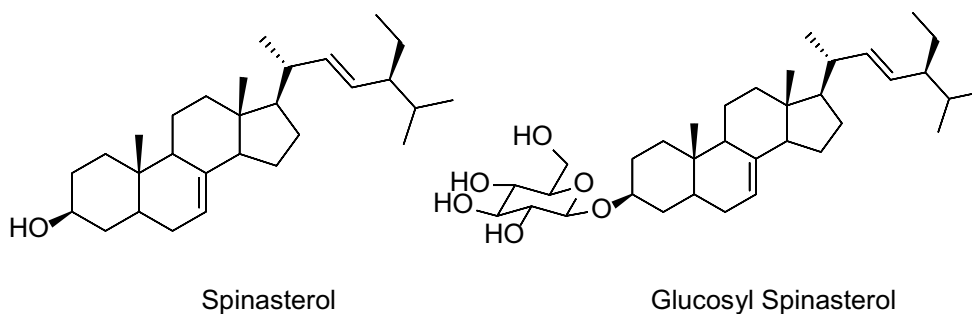
1. (a) Phna, N. H. T.; Kim, H.; Shin, H.; Lee, H. -S.; Sohn, J. -H. *Org. Lett.* **2016**, *18*, 5154-5157 (b) Kim, H.; Phan, N. H. T.; Shin, H. Lee, H. -S.; Sohn, J. -H. *Tetrahedron* **2017**, *73*, 6604-6613. (c) Kim, H.; Lee, H.; Shin, H.; Sohn, J. -H. *Org. Lett.* **2018**, *20*, 1961-1965.

Synthesis of Epimeric Isomers of Spinasterol, Dihydroergosterol, Ergosterol and Their Glycosides and Anti-inflammatory Activities

Jungwook Kim, Youngkyoung Cho, Yeseul Park, Tae Hoon Lee, Hakwon Kim*
Department of Applied Chemistry and Global Center for Pharmaceutical Ingredient Materials,
Kyung Hee University, Yongin-si, Gyeonggi-do 17104, Korea
E-mail:hwkim@khu.ac.kr

Natural spinasterol-glucose (3-O- β -D-glucopyanosylspinasterol), isolated from *Stewartia koreana* leaves, has been identified as a compound to exhibit a potent anti-inflammatory activity. In previous studies, we have involved in the development of new sterols structurally similar to spinasterol, such as stellasterol (5,6-dihydroergosterol) and ergosterol ((3 β , 5 α)-ergost-8(14)-en-3-ol). We found that stellasterol, ergosterol and their glycosides showed anti-inflammatory activity similar to spinasterol and its glycosides.

In present study, we synthesized epimers of stellasterol and its glycosides, ergosterol and its glycosides with the inversed stereochemistry of C3 position in steroidal backbone. We also investigated their anti-inflammatory activities and compared the expression levels on pro-inflammatory cytokines in human keratinocyte by TNF- α /IFN- γ .



Synthesis of heterocycle-fused 1,4-naphthoquinone and its toxicity to HeLa cells

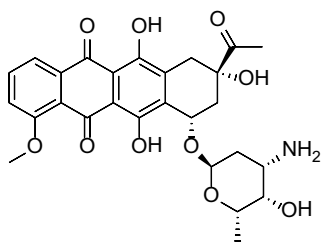
Seunghyun Choi, Inseok Ko, Jisue Lee, Tae Hoon Lee, Hakwon Kim*

*Department of Applied Chemistry and Global Center for
Pharmaceutical Ingredient Materials, Kyung Hee University,
Yongin-si, Gyeonggi-do 17104, Korea
E-mail:hwkim@khu.ac.kr*

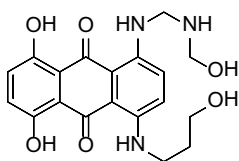
1,4-Naphthoquinones are widely distributed in nature and many pharmaceutically important compounds containing a quinone moiety, such as anthracycline, mitoxantron and saintopin, show an excellent anticancer activity. There are main reasons why quinone moieties have cytotoxic effects.

They form semiquinone radical that can transfer an electron to oxygen to produce superoxide. Both semiquinone radical and superoxide can generate hydroxyl radical, which is the cause of DNA strand breaks. Due to the cytotoxicity they can inhibit proliferation of cancer cells. Among various quinones, 1,4-naphthoquinone derivatives have shown important biological activities, and especially heterocycle-fused 1,4-naphthoquinones exhibited significant cytotoxicity against to human cancer cells.

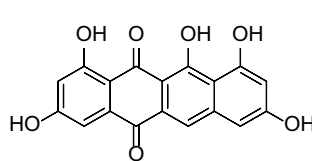
Recently, we have been confirmed in the synthesis of physiologically active 1,4-naphthoquinone derivatives which would be cytotoxic to HeLa cells. In this report, a synthesis of novel heterocyclic 1,4-naphthoquinone derivatives, such as pyrazole or pyrazolone derivatives, from alkoxy-naphthalene and the cytotoxicity on HeLa cells will be described.



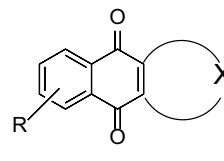
Daunorubicin



Mitoxantrone



Saintopin



2,3-heterocycle-fused
1,4-naphthoquinone

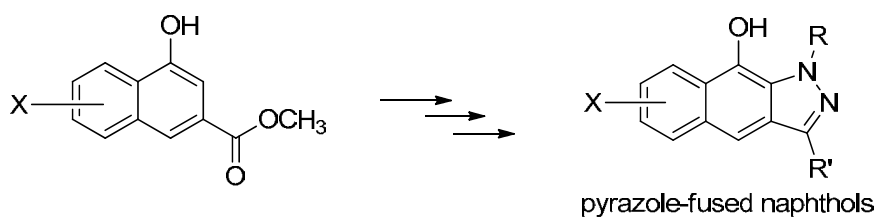
Pyrazole- and pyrazolone-fused naphthol derivatives and Antioxidant Acitivity

Heejae Choi, Hyunjin Lee, Taehoon Lee, Hakwon Kim*

*Department of Applied Chemistry and Global Center for
Pharmaceutical Ingredient Materials, Kyung Hee University,
Yongin-si, Gyeonggi-do 17104, Korea
E-mail: hwkim@khu.ac.kr*

Phenol moieties present various biological activities, such as antitumor and antioxidant. We have already synthesized various 1,4-naphthoquinone derivatives and tested its biological activity. Based on this result, we have continued to develop the synthesis of new naphthol derivatives containing heterocyclic ring.

This present study is concerned with the synthesis of novel 2,3-pyrazole and pyrazolone-fused 1-naphthol derivatives from methyl 4-hydroxy-2-naphthoic acid by the intramolecular Ulmann-type reaction to form pyrazolone ring. Pyrazolone-fused 1-naphthol (9-Hydroxy-1-phenyl-1*H*-benzo[*f*]indazol-3(2*H*)-one) and pyrazole-fused 1-naphthol (3-methoxy-1-phenyl-1*H*-benzo[*f*]indol-9-ol) were synthesized and the chemical structures were characterized using spectral and analytical techniques. Their antioxidant activities were tested using DPPH method compared with ascorbic acid as a control substance.

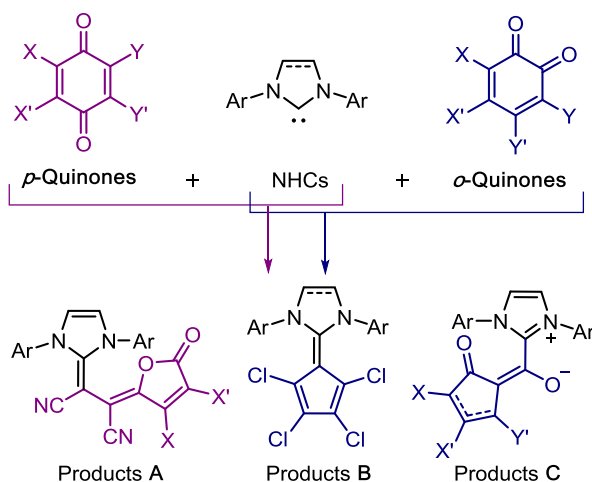


N-Heterocyclic Carbene-Mediated Ring Contractions of *p*- and *o*-Quinones

Lucy Ping,^a JungHwa Han,^a Suin Park,^a JungMin Bak,^a Jean Bouffard^{a*}

^a Department of Chemistry and Nano Science, Ewha Womans University,
52 Ewhayeodae-gil, Seodaemun-gu, Seoul 03760 Korea
E-mail: bouffard@ewha.ac.kr

The reactivity of N-heterocyclic carbenes (NHCs) and quinones has not been previously reported. In our study, we found that nucleophilic NHCs induce the ring contraction of electrophilic quinones to give products¹ that are distinct from those arising from the nucleophilic attack of quinones by other P- or N-centered nucleophiles, such as phosphines and pyridines.² In the case of dicyano-*p*-quinones, furanone-based push-pull chromophores were isolated. *o*-Chloranil resulted in charge-separated NHC fulvalenes, whereas non-halogenated *o*-quinones resulted in α -acylimidazolium cyclopentenone derivatives. We propose the electrocyclic ring opening of initial NHC-quinone adducts as a common mechanistic pathway to give the eventual ring-contracted products.



References

- ¹ Ping, L.; Bak, J.; Kim, Y.; Bouffard, J. *J. Org. Chem.*, **2018**, ASAP, DOI: 10.1021/acs.joc.8b01236
² (a) Ramirez, F.; Rhum, D.; Smith, C. P. *Tetrahedron*, **1965**, *21*, 1941–1959.; (b) Loskutov, V. A.; Mamatyuk, V. I.; Beregovaya, I. V. *Russ. Chem. Bull.*, **1999**, *48*, 371–374.; (c) Koch, A. S.; Harbison, W. G.; Hubbard, J. M.; de Kort, M.; Roe, B. A. *J. Org. Chem.*, **1996**, *61*, 5959–5963.; (d) Katritzky, A. R.; Fan, W.-Q.; Li, Q.-L.; Bayyuk, S. *J. Heterocyclic Chem.*, **1989**, *26*, 885–892.

Ultrasonic Spray Chemistry: Synthesis of Film-like Microporous Materials and Their Energy Storage Application

Deok-Ho Roh,^a HyeonOh Shin,^a Hyun-Tak Kim,^a Tae-Hyuk Kwon,^{a*}

^a Department of Chemistry, School of Natural Science, Ulsan National Institute of Science and Technology (UNIST), Ulsan 44919, Republic of Korea
E-mail: Kwon90@unist.ac.kr

Conjugated microporous polymers (CMPs)¹ are potentials material for energy storage application owing to their rigid and cross-linked microporous structures. However, it is still challenge to form film-like CMPs and integrate the CMPs into devices for further application because of its poor solubility and processability issues. Herein, we present a simple and very fast methods to synthesize film-like CMPs by ultrasonic spray chemistry (USC), which allows *in situ* polymerization and thin-film fabrication process simultaneously. By using USC, the homo coupling of triphenylamine (TPA) based monomers are easily achieved to produce the three different types of CMP-films that have different core unit between TPA group, **CMP-TPA**, **CMP-DTT**, and **CMP-BT**. Compared with standard batch chemistry method of oxidative coupling reaction, USC delivers enhancement of synthetic yield of CMP-films because of releasing of enormous energy by collapsing of vacuum bubble that is formed during cavitation. As the increase of ultrasound frequency from 120 kHz to 180 kHz, the synthetic yield and porosity of CMP-films were also enhanced and their confirmation and characterization were carried out by UV-vis, infra-red spectroscopy, transmission electron microscopy, and methylene blue adsorption method. We applied CMP-films to supercapacitor owing to their thin-film and microporosity. **CMP-BT (180 kHz)** exhibited much higher capacitance 153 F/g than 22 F/g for **CMP-DTT (180 kHz)**, and 27 F/g for **CMP-TPA (180 kHz)** due to its polarized structures. Furthermore, layer-by-layer (LBL) **CMP-BT (180 kHz)**/single-wall carbon nanotube (**SWCNT**) electrode was prepared by USC for increasing conductivity and porosity of electrodes. This electrode demonstrated very high specific capacitances (583 F/g), working in very fast scan rate of 50 V/s, and high cycling stability (95% retention of the specific capacitances after 20,000 cycles). This results suggested that ultrasonic spray chemistry offer a new way for overcoming the present processability issues of microporous materials

References

¹ Xu, Y.; Jin, S.; Xu, H.; Nagai, A.; Jiang, D. *Chem. Soc. Rev.* **2013**, *42*, 8012-8031.

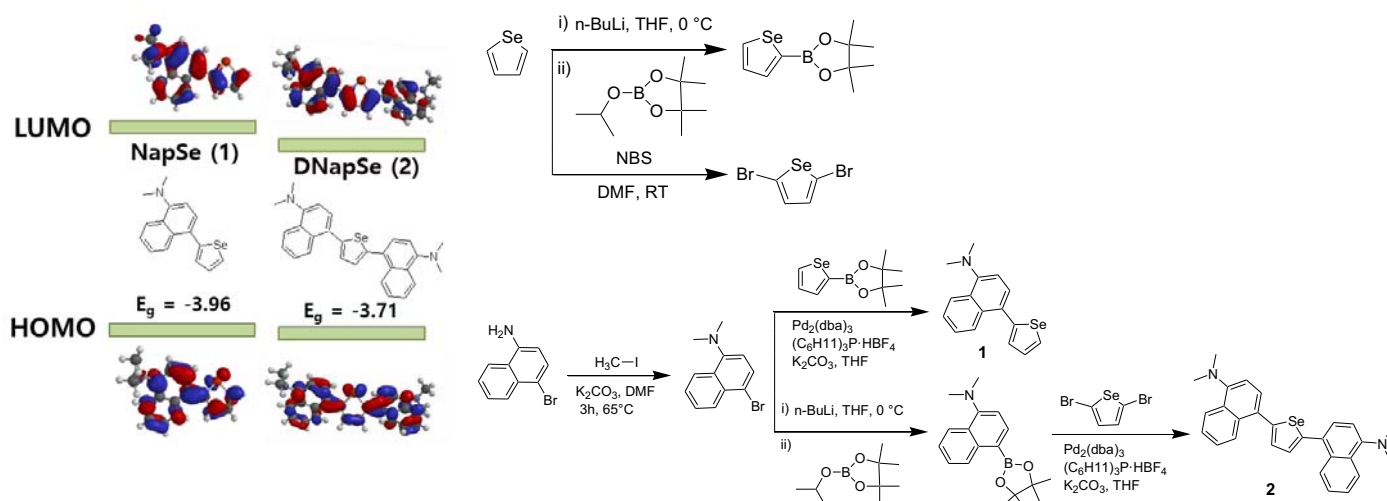
Synthesis of selenophene-based hydrophobic fluorescent sensor probe for reactive oxygen species (ROS)

Ji Hye Kang and Choon Woo Lim*

Department of Chemistry, College of Life Science and Nano technology, Hannam University, Daejeon 305-811, Republic of Korea
E-mail: cwlim@hnu.kr

Many activities in the development of selenofluoroprobes are related to the detection of reactive oxygen species (ROS). The biological activities and peculiar reactivity of organoselenium compounds toward ROS make them prospective candidates for developing probes for ROS.¹

We designed and synthesized new fluorescent probe (NapSe (1) and DNapSe (2)) for reactive oxygen species (ROS) using Suzuki-Miyaura reaction with derivatized selenophene² and naptalene³. Their chemical structures were characterized by ¹H-NMR, ¹³C-NMR and FAB-Mass spectrometry. Their photophysical properties were examined through UV-vis / fluorescence spectroscopy. And we compared the properties of (1) and (2). Quantum chemical calculations on 1 and 2 were employed at the B3LYP/6-31G* (d) theoretical level to understand the structure-property relationship of the compounds at the molecular level. The calculated energy bandgap (E_g) of (1) and (2) is 3.96 and 3.71 eV respectively. We investigated properties as fluorescent probes potential for reactive oxygen species (ROS).



References

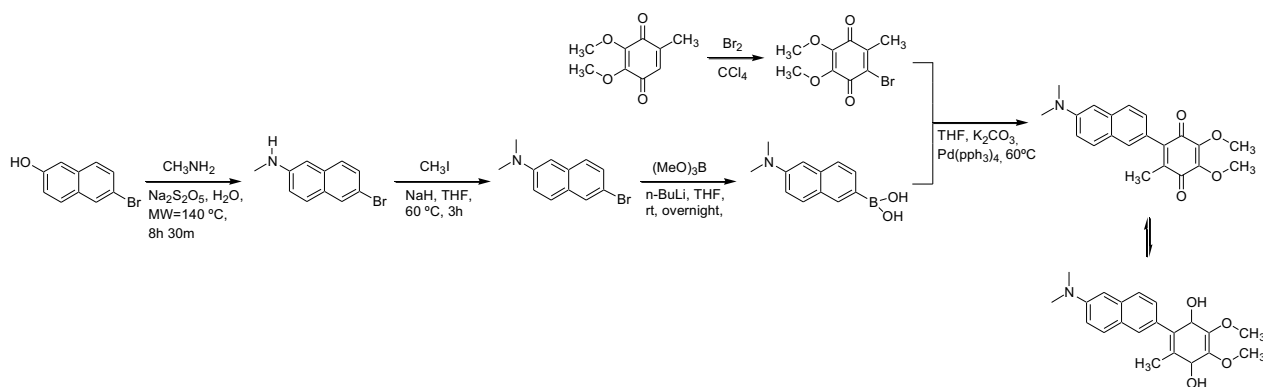
- ¹ *Coordination Chemistry Reviews* **2015**, 300, 86-100
- ² *Chem. Mater.* **2011**, 23, 4435-4444
- ³ *J. Org. Chem* **1996**, 60, 4051-4066

Development of benzoquinone based fluorescent probe for detection of reactive oxygen species

Ji Yeon Heo and Choon Woo Lim *

Department of Chemistry, College of Life Science and Nano-technology, Hannam University, Daejeon 305-811, Republic of Korea
E-mail: cwlim@hnu.kr

Reactive oxygen species (ROS) have emerged as prevalent and important components of both physiological and pathological processes.¹ The involvement of Coenzyme Q10 (CoQ) is appeared in biochemical clinical studies as an antioxidant in vivo and in vitro oxidation processes.² We synthesized fluorescent probe using Suzuki-Miyaura coupling reaction with 6-(Dimethylamino)-naphthalene-2-boronic acid and 6-bromo-2,3-dimethoxy-5-methyl-1,4-benzoquinone. The synthesized products were fully characterized by ¹H NMR, ¹³C NMR, UV-vis spectroscopy and mass spectrometry.



References

- (a) J. R. Stone and S. Yang, *Antioxid. Redox Signaling*, 2006, 8, 243; (b) B. DAutrEaux and M. B. Toledano, *Nat. Rev. Mol. Cell Biol.*, 2007, 8, 813; (c) C. C. Winterbourn, *Nat. Chem. Biol.*, 2008, 4, 278.
- E. Ferri et al, *Molec. Aspects Med.*, 1994, 15, 83-88.

Microwave-assisted efficient H/D exchange methods of 9H-carbazole, 2-phenylpyridine as organic light emitting materials

Seo Ra Kim and Choon Woo Lim*

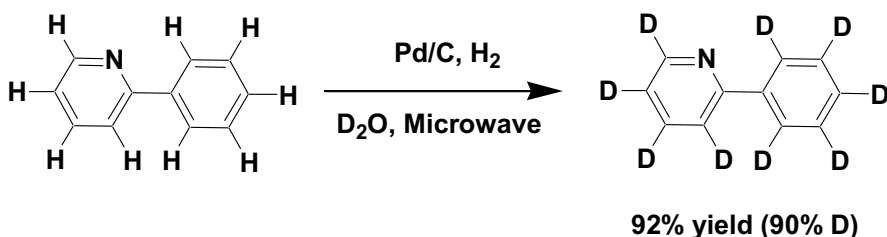
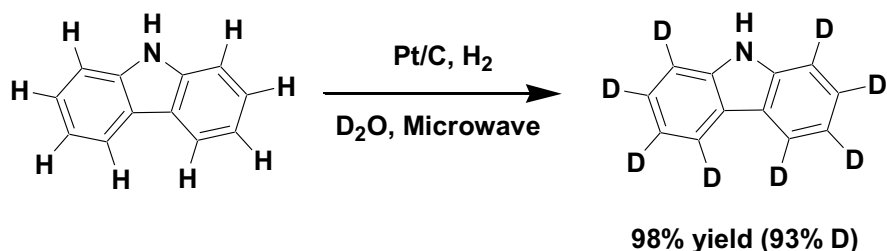
Department of chemistry, College of Life Science and Nano technology, Hannam University, Daejeon 305-811, Republic of Korea

E-mail: cwlim@hnu.kr

It has been reported that the deuteration of Ir(ppy)₃ has a significant effect on the stability and lifetime of OLED devices.¹ Effective and applicable deuteration methods were developed using D₂O as a deuterium source under hydrogen atmosphere.²

We report microwave-assisted efficient H/D exchange methods, which were catalyzed by Pt/C or Pd/C under hydrogen atmosphere. Microwave irradiation provides advantages over conventional heating in chemical transformation; these advantages include accelerated reaction rates, significant energy savings, high chemical yields, and cleaner reactions.³

9H-Carbazole and 2-phenylpyridine are widely used in organic light-emitting materials and are chosen as candidate materials for H/D exchange experiment. Their optimized experimental conditions were established, based on temperature, amount of catalyst and reaction time.⁴ Deuterated 9H-carbazole and 2-phenylpyridine were confirmed by high resolution FAB-Mass spectroscopy. The overall quantity of D atoms was determined, using 1, 4-dioxane as an internal standard by ¹H NMR experiments. H/D exchange yields of deuterated 9H-carbazole (93%) and 2-phenylpyridine (90%) are obtained.



References

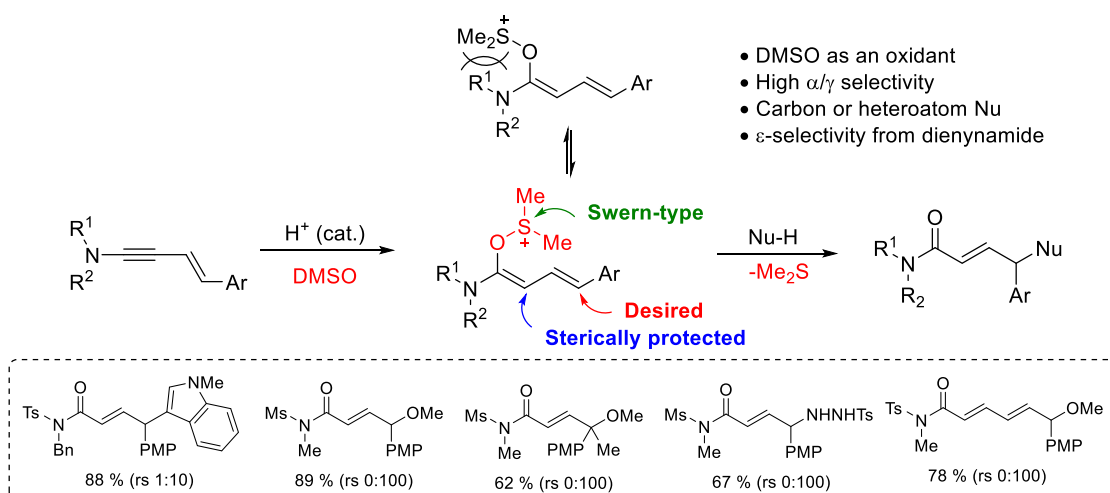
- ¹ Ping Wang, Fei-Fei Wang, *J. Mater. Chem. C*. **2013**, 1, 4821-4825.
- ² Hironao Sajiki, Nobuhiro Ito, *Tetrahedron Letters*. **2005**, 46, 6995-6998.
- ³ Kappe C. O., *Chem. Soc. Rev.* **2008**, 37, 1127-1139.
- ⁴ Tamim A. Darwish, Arthur R.G. Smith, *Tetrahedron Letters*. **2012**, 53, 931-935.

Redox Neutral Access to α^4 , α^6 -Synthons via Sulfoxide-Mediated Oxidation of (Di)enynamides

Quynh H. Nguyen and Seunghoon Shin^{a,*}

^aDepartment of Chemistry and Center for New Directions in Organic Synthesis, Hanyang University, 222 Wangsimni-ro, Seoul 04763, Korea

Recently we have developed a robust activation of ynamides by HNTf₂ catalyst enabling oxidative coupling of diverse C-nucleophiles.¹ These umpolung enolate discovery allows for outstanding opportunity for redox-efficient processes and enables novel disconnection approaches through non-traditional methods.² We envisioned that oxidation of enynamide would provide dienolium synthon (α^4), allowing addition of nucleophilic partners at the γ -position, where the steric hindrance between amide nitrogen (NR¹R²) and oxidant (OSMe₂) moiety may direct the regio-selectivity. Meanwhile, one inherent limitation in the gold- or Brønsted acid-catalyzed oxidation of alkynes is the necessity to use pyridine-derived *N*-oxides as terminal oxidant which liberates pyridine that undermine atom-economy and potentially inhibits the acid-catalyzed cycle. Employing dimethyl sulfoxide (DMSO) as terminal oxidant led to an efficient γ -selective couplings without intervention of side pathways. In addition to carbon nucleophiles, 1°, 2°-alcohols and tosyl hydrazide could be employed as nucleophiles. Using dienynamides as substrates, ϵ -addition (α^6) could be realized with excellent selectivity.³



References

1. a) D. V. Patil, S. W. Kim, Q. H. Nguyen, H. Kim, S. Wang, T. Huang, S. Shin, *Angew. Chem. Int. Ed.* **2017**, *56*, 3670; b). S.W. Kim, T.W. Um, S. Shin, *Chem. Commun.* **2017**, *53*, 2733.
2. a) D. Seebach, *Angew. Chem. Int. Ed.* **1979**, *18*, 239; for notable examples: b) S. Arava, J. N. Kumar, S. Maksymenko, M. A. Iron, K. N. Parida, P. Fristrup, A. M. Szpilman, *Angew. Chem. Int. Ed.* **2017**, *56*, 2599.
3. Q. H. Nguyen, Shin, S. *manuscript in preparation.*

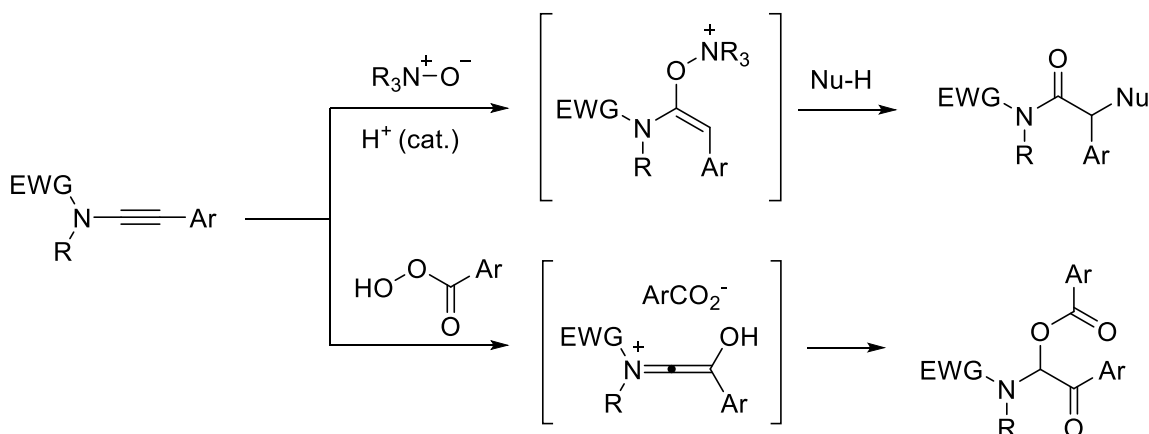
An unexpected oxidation of ynamides with *m*-CPBA followed by asymmetric trans-acetalization catalyzed by chiral phosphoric acid

Nguyen H. Nguyen,^a Seunghoon Shin,^{*a}

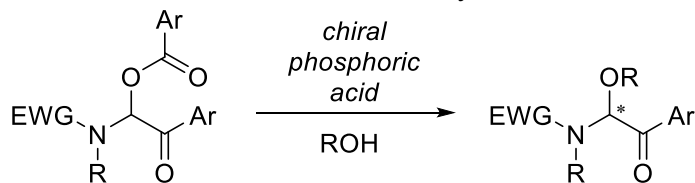
^a Department of Chemistry and Center for New Directions in Organic Synthesis (CNOS), Hanyang University, 222 Wangsimni-ro, Seongdong-gu, Seoul, 04763 (Korea)

E-mail: sshin@hanyang.ac.kr

Ynamides are one of the most versatile building blocks in organic synthesis.¹ Recently, our group reported that pyridine-*N*-oxides or sulfoxides can oxidize ynamides at the α -position in the presence of Brønsted acid.² Inspired by the success of this work, we further investigated the effects of stronger oxidants for ynamide oxidation. Interestingly, with *m*-CPBA as an oxidant, we observed the formation of α,α -N,O-acetals, which is thought to form via β -oxidation of ynamides (Scheme 1). From further investigations we found that the initial N,O-acetal underwent an enantioselective trans-acetalization in the presence of chiral phosphoric acid (Scheme 2). The products N,O-acetals were configurationally stable, and can be potentially useful synthetic intermediates.



Scheme 1. Oxidation of ynamide



Scheme 2. Enantioselective trans-acetalization

References

¹ K. A. DeKorver, H. Li, A. G. Lohse, R. Hayashi, Z. Lu, Y. Zhang, R. P. Hsung, *Chem. Rev.*, **2010**, *110*, 5064–5106.

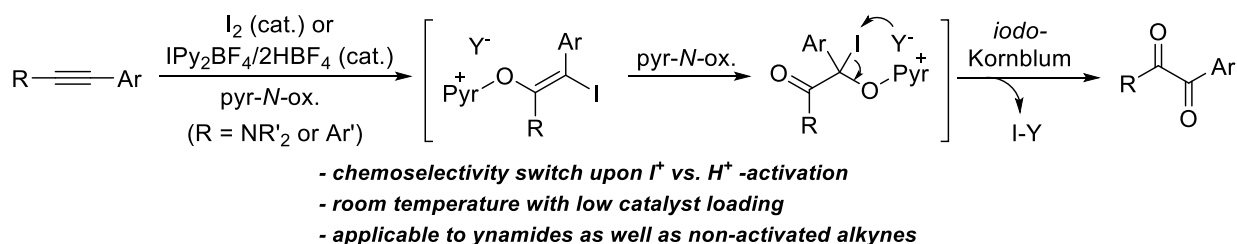
² (a) D. V. Patil, S. W. Kim, Q. H. Nguyen, H. Kim, S. Wang, T. Hoang, S. Shin, *Angew. Chem. Int. Ed.* **2017**, *56*, 3670–3674; (b) S. W. Kim, T-W. Um, S. Shin, *Chem. Commun.*, **2017**, *53*, 2733–2736; (c) Q. H. Nguyen, Nguyen H. Nguyen, S. Shin, *manuscript in preparation*.

Metal-Free Iodine-Catalyzed Oxidation of Ynamides and Diaryl Acetylenes into 1,2-Diketo Compounds

Seung Woo Kim, Tae-wong Um and Seunghoon Shin*

Department of Chemistry, Centre for new Directions in Organic Synthesis (CNOS), Hanyang University, 222 Wangsimni-ro, Seongdong-gu, Seoul Korea, 04763
sshin@hanyang.ac.kr

Molecular iodine has been widely used in organic synthesis, due to its easy handling and inexpensive price. Besides the stoichiometric iodofunctionalizations that incorporate iodine atom in the product, various of iodine-based catalysis have been developed, including dehydration, condensation, conjugate addition, esterification, acetalization and glycosylation. Some of these processes are suspected to be mediated by HI generated in-situ from the hydrolysis of I₂ and few reports propose a I-I regeneration for a catalyst turnover, due to the unfavorable enthalpy. Herein, we demonstrate that molecular iodine can catalyze selective oxidation of ynamide into ketoamide compounds. Ynamides as well as diaryl acetylenes are appropriate substrates for this transformation.



References

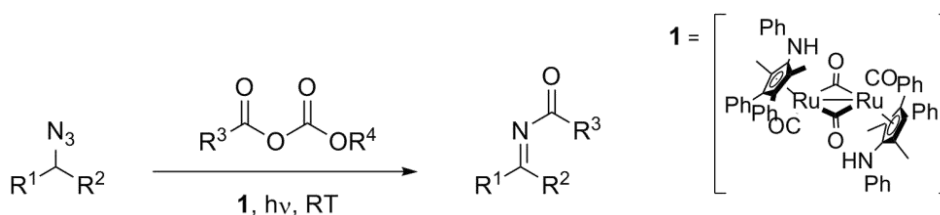
¹ Kim, S. W.; Um, T. W.; Shin, S. H. *J. Org. Chem.* **2018**, *83*, 4703-4711.

Synthesis of N-Acylimines from N-H imines and Acyl Alkyl Carbonates

권예람,^a 이영호,^{a*} 박재욱,^{a*}

^a Department of Chemistry, POSTECH, 77 Cheongam-Ro, Nam-Gu, Pohang, Gyeongbuk, Korea 37673
E-mail: yhrhee@postech.ac.kr, pjw@postech.ac.kr

N-Acylketimines have been recognized as important intermediates in organic synthesis. N-Acylimines have electron-withdrawing acyl moiety to increase the low electrophilicity of imine. Synthesis of N-acylketimines continuously attracts considerable attention from chemists, the general method for N-acylketimines is rarely reported due to the instability of N-acylketimines. N-acylketimines are known to be too unstable to be stored and easily tautomerized to corresponding enamide. Therefore, they are generally prepared in situ for the reaction with nucleophiles. We successfully synthesized various N-acylketimines including enolizable aliphatic ones from the alkyl azides in a one-pot procedure. We demonstrated the stability of N-Acylketimines and the applicability of cyclic N-acylketimine in nucleophilic addition of Grignard reagent to afford acetamide with high diastereoselectivity.



References

¹ Kwon, Y.; Rhee, Y. H.; Park, J. *Adv. Synth. Catal.* **2017**, 359, 1503-1507.

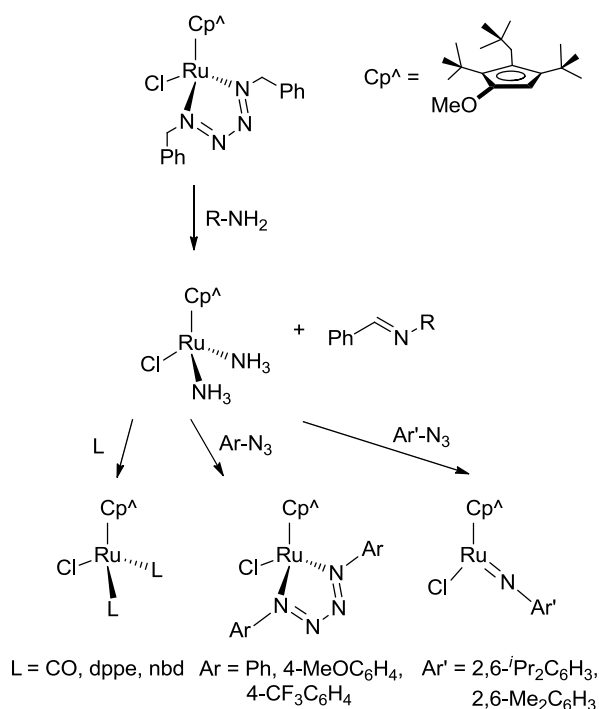
Synthesis of Half-Sandwich Ruthenium Complexes Containing a Sterically Demanding Cyclopentadienyl Ligand

Jin Yong Park, Young Ho Rhee,* Jaiwook Park*

Department of Chemistry, POSTECH (Pohang University of Science and Technology), Pohang, 37673, Republic of Korea.

E-mail: yhrhee@postech.ac.kr
pjw@postech.ac.kr

A dimeric ruthenium half-sandwich complex $[\text{Cp}^{\wedge}\text{RuCl}_2]_2$ ($\text{Cp}^{\wedge} = \eta^5\text{-1-methoxy-2,4-di-tert-butyl-3-neopentylcyclopentadienyl}$) containing sterically demanding cyclopentadienyl ligand. They show interesting catalytic activities such as a reaction of alkynes, synthesis of enamides. Interestingly, a ruthenium bisammine complex was observed in the reaction of a ruthenium tetraazadiene complex with primary amines. The ruthenium complex was confirmed as an efficient precursor for the synthesis of various Ru(II) complexes containing a sterically demanding cyclopentadienyl ligand. In the reaction with aryl azide, ruthenium imido complexes were formed. The ruthenium complexes were applied in the synthesis of N-substituted imines.



Scheme 1. Ligand Exchange Reaction of Ruthenium Bisammine Complex

References

- ¹ Park, J. Y.; Kim, Y.; Bae, D. Y.; Rhee, Y. H.; Park, J. *Organometallics* **2017**, *36*, 3471-3476.

Synthesis of C2-Alkenylated Pyrroles by Electronically Complementing Ligand Systems

Woohyeong Lee, Eunmin Kim, Eun Su Kang, Soo Eun Park and Jung Min Joo*

*Department of Chemistry and Chemistry Institute of Functional Materials, Pusan National University, Busan 46241, Republic of Korea.
E-mail : dngud1204@gmail.com*

C-H functionalization of the parent pyrroles presents challenges in achieving regioselectivity and preventing polymerization of the pyrroles under acidic and oxidative conditions. These issues have been tackled via dehydrogenative C-H alkenylation with alkenes, also known as the Fujiwara-Moritani reaction.¹ We have developed complementing ligands systems. For C2-alkenylation of electron-rich *N*-alkylpyrroles, an electrophilic palladium catalyst derived from Pd(OAc)₂ and 4,5-diazafluoren-9-one (DAF) was used. Alternatively, a combination of Pd(OAc)₂ and a mono-protected amino acid ligand, Ac-Val-OH, was useful for C5-alkenylation of *N*-alkylpyrroles possessing electron-withdrawing groups at the C2 position.

References

¹ C. Liu, J. Yuan, M. Gao, S. Tang, W. Li, R. Shi, A. Lei, *Chem. Rev.* **2015**, *115*, 12138

Palladium-Catalyzed [4+2] Cycloadditions of N-aromatic Zwitterions for the Construction of Fused Heterocyclic Compounds

Ju Young Lee, Hyunju Park and Eun Jung Yoo*

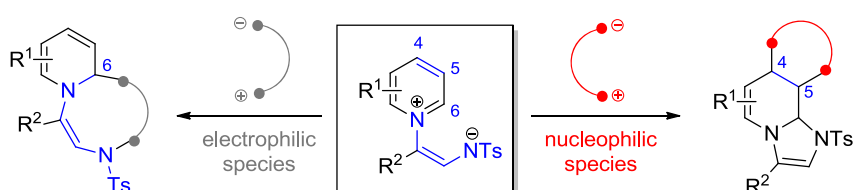
Department of Applied Chemistry, Kyung Hee University, Yongin 17104, Republic of Korea

* Email: ejyoo@khu.ac.kr

Cycloadditions constitute one of the most important classes of organic reactions giving access to complex organic skeleton in a single step operation which play a key role in the synthesis of natural products, pharmaceutical agents or synthetic materials. Recently, our group discovered that the pyridinium zwitterion could serve as a 1,5-dipole for the construction of medium-sized heterocycles via [5+n]-cycloadditions with electrophilic partners.¹

It has multiple reaction sites which can be tuned by the electronic demand of the catalyst-substrate complex. The origin of the site selectivity and the mechanism of this reaction are investigated in this combined experimental and computational methods. We found that mode of Pd(0)-catalyzed [4+2] cycloaddition with nucleophilic partner is totally different from Rh(II)-catalyzed [5+3] cycloadditions with electrophilic partner.²

In this symposium, we will show that the frontier molecular orbitals of the pyridinium substrate and activated catalyst complex reveal that the pyridinium zwitterion can act as both a nucleophile and an electrophile depending on the reaction partner in a manner much more defined than that of conventional substrates, leading to the observed regiodivergent chemical reactivity.



References

¹D. J. Lee, J. H. Shin and E.J. Yoo, *J. Am. Chem. Soc.* **2014**, 136, 11606-11609.

²Lee, D. J.; Ko, D.; Yoo, E. J. *Angew. Chem., Int. Ed.* **2015**, 54, 13715-13718.

Total synthesis of cytotoxic active natural product from Cinnamomum subavenium via MBH ester

Dong Guk Nam, Do Hyun Ryu*

Department of Chemistry, Sungkyunkwan University, 2066, Seobu-ro, Jangan-gu,
Suwon-si, Gyeonggi-do, 16419, Republic of Korea.
E-mail: dhryu@skku.edu.

Secobutanolide and Subamolide series has been reported with their excellent biological cytotoxicity. These material has excellent activities on Hep G2 cell line, A2780 cell, P-388 and etc. And Morita-Baylis-Hillman (MBH) ester carbon frameworks can be precursors for these structures. Our group reported asymmetric synthesis of (z)- β -iodo Morita-Baylis-Hillman ester with oxazaborolidinium catalyst (COBI). With MBH ester precursors, secobutanolide and subamolide series are successfully synthesized in several steps include geometry selective iodo-isomerization. This synthesis was first chiral example of these materials with good yield and excellent enantioselectivity.

References

- ¹ Ryu, D. H. et al, *Org. Lett.* **2007**, 24, 5087.
² Ryu, D. H et al, *Angew. Chem. Int. Ed.* **2009**, 48, 4398.

Palladium-Catalyzed [4+2] Cycloadditions of N-aromatic Zwitterions for the Construction of Fused Heterocyclic Compounds

Ju Young Lee, Hyunju Park and Eun Jung Yoo*

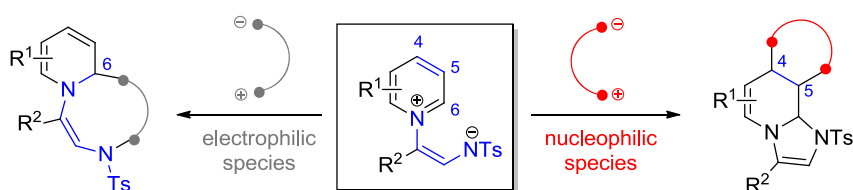
Department of Applied Chemistry, Kyung Hee University, Yongin 17104, Republic of Korea

* Email: ejyoo@khu.ac.kr

Cycloadditions constitute one of the most important classes of organic reactions giving access to complex organic skeleton in a single step operation which play a key role in the synthesis of natural products, pharmaceutical agents or synthetic materials. Recently, our group discovered that the pyridinium zwitterion could serve as a 1,5-dipole for the construction of medium-sized heterocycles via [5+n]-cycloadditions with electrophilic partners.¹

It has multiple reaction sites which can be tuned by the electronic demand of the catalyst-substrate complex. The origin of the site selectivity and the mechanism of this reaction are investigated in this combined experimental and computational methods. We found that mode of Pd(0)-catalyzed [4+2] cycloaddition with nucleophilic partner is totally different from Rh(II)-catalyzed [5+3] cycloadditions with electrophilic partner.²

In this symposium, we will show that the frontier molecular orbitals of the pyridinium substrate and activated catalyst complex reveal that the pyridinium zwitterion can act as both a nucleophile and an electrophile depending on the reaction partner in a manner much more defined than that of conventional substrates, leading to the observed regiodivergent chemical reactivity.



References

¹D. J. Lee, J. H. Shin and E.J. Yoo, *J. Am. Chem. Soc.* **2014**, 136, 11606-11609.

²Lee, D. J.; Ko, D.; Yoo, E. J. *Angew. Chem., Int. Ed.* **2015**, 54, 13715-13718.

Palladium-Catalyzed [4+2] Cycloadditions of N-aromatic Zwitterions for the Construction of Fused Heterocyclic Compounds

Ju Young Lee, Hyunju Park and Eun Jung Yoo*

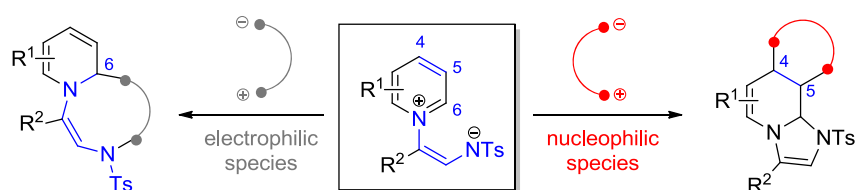
Department of Applied Chemistry, Kyung Hee University, Yongin 17104, Republic of Korea

* Email: ejyoo@khu.ac.kr

Cycloadditions constitute one of the most important classes of organic reactions giving access to complex organic skeleton in a single step operation which play a key role in the synthesis of natural products, pharmaceutical agents or synthetic materials. Recently, our group discovered that the pyridinium zwitterion could serve as a 1,5-dipole for the construction of medium-sized heterocycles via [5+n]-cycloadditions with electrophilic partners.¹

It has multiple reaction sites which can be tuned by the electronic demand of the catalyst-substrate complex. The origin of the site selectivity and the mechanism of this reaction are investigated in this combined experimental and computational methods. We found that mode of Pd(0)-catalyzed [4+2] cycloaddition with nucleophilic partner is totally different from Rh(II)-catalyzed [5+3] cycloadditions with electrophilic partner.²

In this symposium, we will show that the frontier molecular orbitals of the pyridinium substrate and activated catalyst complex reveal that the pyridinium zwitterion can act as both a nucleophile and an electrophile depending on the reaction partner in a manner much more defined than that of conventional substrates, leading to the observed regiodivergent chemical reactivity.



References

¹D. J. Lee, J. H. Shin and E. J. Yoo, *J. Am. Chem. Soc.* **2014**, 136, 11606-11609.

²Lee, D. J.; Ko, D.; Yoo, E. J. *Angew. Chem., Int. Ed.* **2015**, 54, 13715-13718.

Chiral Lewis Acid Catalyzed Enantioselective Synthesis of Cyclobutanones via Tandem Cyclopropanation/Semi-Pinacol Rearrangement

심수용, 최유나, 류도현*

Department of Chemistry, Sungkyunkwan University, Suwon 16419, Korea
E-mail: dhryu@skku.edu

Cyclobutane derivatives are found in a wide range of natural products and important building blocks in organic synthesis because they can be converted to various organic compounds through ring opening or ring expansion reactions. Especially, cyclobutanone is one of the most versatile chemical candidates for the functionalized cyclobutanes through various chemical transformations. But, [2+2] cycloaddition for the preparation of cyclobutanone was rarely been reported and there are limited examples to synthesize chiral cyclobutanones. In this research, we report enantioselective synthesis of cyclobutanone catalyzed by chiral oxazaborolidinium ion (COBI) from α -silyloxyacroleins and α -alkyl or α -aryl diazoesters via tandem cyclopropanation/semi-pinacol rearrangement. Various cyclobutanones possessing β -quaternary chiral carbon were obtained in high yield (up to 91%) with excellent enantio- and diastereoselectivity (up to 98% ee and up to > 20 : 1 dr). In addition, support for the proposed mechanism of this reaction was provided by isolating the intermediate 1-formyl-1-silyloxycyclopropane and confirming its stereoselective *trans*-formation to cyclobutanone.

References

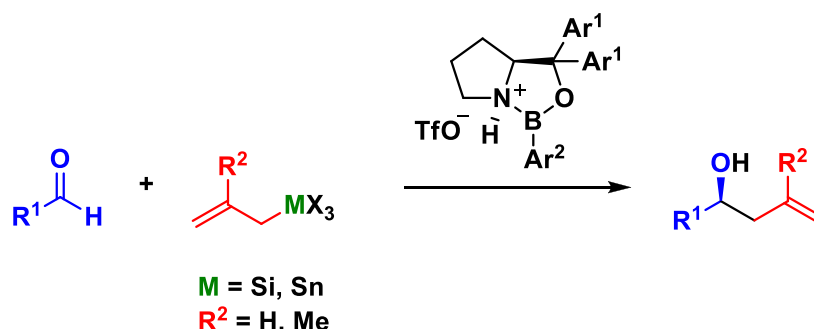
- ¹ Gao, L.; Hwang, G.-S.; Ryu, D. H. *J. Am. Chem. Soc.* **2011**, *133*, 20708-20711.
- ² Shim, S. Y.; Kim, J. Y.; Hwang, G.-S.; Ryu, D. H. *Org. Lett.* **2016**, *18*, 160-163.
- ³ Shim, S. Y.; Cho, S. M.; Venkateswarlu, A.; Ryu, D. H. *Angew. Chem. Int. Ed.* **2017**, *56*, 8663-8666.
- ⁴ Shim, S. Y.; Choi, Y.; Ryu, D. H. *J. Am. Chem. Soc.* **2018**, *Accepted*.

Highly Enantioselective Allylation of Aldehydes Catalyzed by a Chiral Oxazaborolidinium Ion

Taehyeong Kim, Anipireddy Venkateswarlu, Do Hyun Ryu*

Department of Chemistry, Sungkyunkwan University, Suwon, 16419, Korea.
E-mail: dhryu@skku.edu

The enantioselective allylation of aldehydes to form homoallylic alcohols is one of the most frequently used carbon–carbon bond-forming reaction in chemical synthesis and for several decades, has been a testing ground for new asymmetric methodology. Enantiomerically pure homoallylic alcohols are common synthetic intermediates, and are typically generated by allylmetal-aldehyde addition reactions. A novel strategy has been developed for an enantioselective allylation reaction of various aldehydes with aromatic and aliphatic groups catalyzed by a chiral oxazaborolidinium ion. The reaction with allylsilane and allylstannane reagents provides homoallylic alcohols in good yields and with high enantioselectivity. Therefore, this reaction will show promising utility in various other challenging chemical reactions and conspicuous biological activity.



References

- ¹ Kaib, P. S. J.; Schreyer, L.; Lee, S.; Properzi, R.; List, B. *Angew. Chem. Int. Ed.* **2016**, *55*, 13200-13203.
- ² Mahlau, M.; Garcia-Garcia, P.; List, B. *Chem. Eur. J.* **2012**, *18*, 16283-16287.
- ³ Belekon, Y. N.; Chusov, D.; Borkin, D. A.; Yashkina, L. V.; Bolotov, P.; Skrupskaya, T.; North, M. *Tetrahedron: Asymmetry* **2008**, *19*, 459-466.

Enantioselective Strecker reaction of Aldimines with Chiral Oxazaborolidinium Ion Activated Trimethylsilyl Cyanide

Ki-Tae Kang,^a Sang Hyun Park,^a Do Hyun Ryu^{a*}

^a Department of Chemistry, Sungkyunkwan University, 300, Cheoncheon, Jangan, Suwon, 16419, Republic of Korea
E-mail: dhryu@skku.edu

In the presence of a catalytic amount of chiral oxazaborolidinium ion (COBI), aldimine reacted with trimethylsilyl cyanide (TMSCN) to afford α -aminonitriles in excellent yields and enantioselectivities. The three-component asymmetric process studied here significantly improves upon the original Strecker reaction, and has advantages over previous reactions using unstable imines. High levels of enantioselectivities in the synthesis of α -aminonitrile derivatives with wide substrate generality were obtained via these reactions. The reaction proceeded in good yields (up to 98%) with excellent enantioselectivities (up to 97% ee).

References

- ¹ Ishitani, H.; Komiyama, S.; Kobayashi, S.; *Angew. Chem. Int. Ed.* **1998**, *37*, 3186-3188.
- ² Ishitani, H.; Komiyama, S.; Hasegawa, Y.; Kobayashi, S.; *J. Am. Chem. Soc.* **2000**, *122*, 762-766.

One-Pot Synthesis of 4,6-Substituted α -Pyrone and α -Pyridones via Mercury(II)-Mediated Decarboxylative Dehydrogenation Reactions

이주열, 김휘, 류도현*

Department of Chemistry, Sungkyunkwan University, Suwon 16419, Korea.

E-mail: dhryu@skku.edu

α -Pyrone and α -Pyridone derivatives exist abundantly in nature including animals, plants and microorganisms, and take part in many different types of biological processes. Therefore, efficient synthesis of multi-substituted α -pyrones and α -pyridones have attracted much attention of many chemists. In this research, 6-ester-substituted α -pyrones and α -pyridones are successfully synthesized through organocatalytic Michael addition-lactonization of β,γ -unsaturated α -keto ester or β,γ -unsaturated α -imino ester with dithiomalonate followed by mercury(II) acetate-induced hydrolysis-decarboxylation-dehydrogenation reaction cascade.

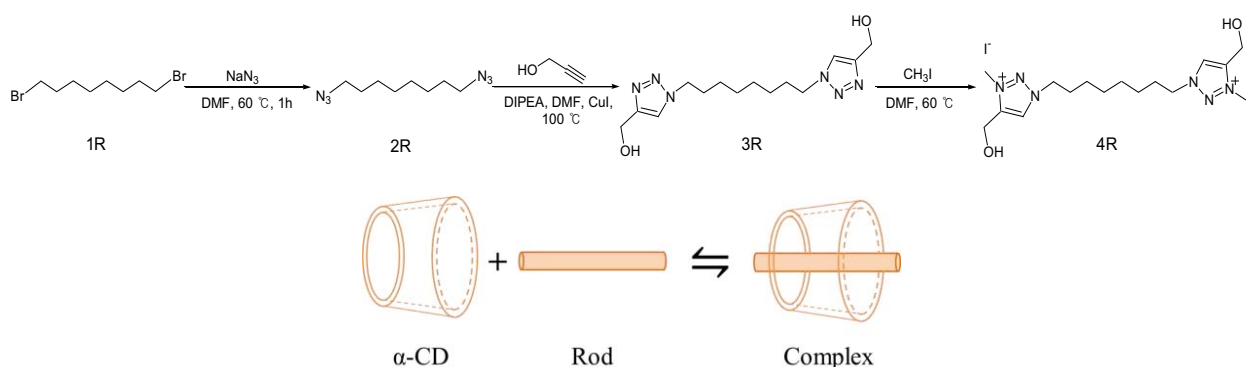
References

1. Jin, H.; Lee, J.; Shi, H.; Lee, J. Y.; Yoo, E. J.; Song, C. E.; Ryu, D. H. *Org. Lett.* **2018**, *20*, 1584.
2. Lee, J.; Jin, H.; Ryu, D. H. manuscript in preparation

pH-controlled pseudo-rotaxane formation of α -cyclodextrin with bis(hydroxymethyl triazolium)octane iodide

Eun Hye Kang and Choon Woo Lim*

Department of Chemistry, College of Life Science and Nano-technology, Hannam University, Daejeon 305-811, Republic of Korea
Email: cwlim@hnu.kr



Cyclodextrin is one of the most important host materials these days of supramolecular chemistry. The well-documented ability of the parent CDs to form inclusion complexes with a wide range of guest species in aqueous solutions has been exploited by many academic researchers

We synthesized cationic rod molecule to study pseudo-rotaxane formation of cyclodextrin. Bis(hydroxymethyl triazolium)octane iodide(4R), rod molecule was prepared by click reaction of 1,8-diazido-octane(2R) with propargyl alcohol, followed by methylation. Their chemical structures were characterized by ^1H NMR spectroscopy.

We studied concentration- and pH-dependent complexation between alpha-cyclodextrin and 4R acting as a threading molecule. And the complexes called pseudo-rotaxane were confirmed by ^1H NMR spectroscopy and 2D Nuclear Overhauser Effect(NOE) experiment. The value of the binding constant is around $5.5 \times 10^1 \text{ M}^{-1}$ at pH 6 and $2.11 \times 10^2 \text{ M}^{-1}$ at pH 13. Activation energy barrier of pseudo-rotaxane formation was examined by temperature-dependent ^1H NMR experiment in different pH conditions.

References

¹.*Chem. Rev.* 1998, 98, 1959-1976

Unusual Hexagonal semi-tubular structure derived by self-assembly of β -helical foldamer

Danim Lim^a and Hee-Seung Lee^{a*}

^a Department of Chemistry, Center for Multiscale Chiral Architectures (CMCA), Korea Advanced Institute of Science and Technology (KAIST), Daejeon 34141, Republic of Korea.
E-mail: hee-seung_lee@kaist.ac.kr

An area of microstructures derived from self-assembly natural as well as unnatural peptide have been shown various applications in diverse fields ranging from nanotechnology to medicinal chemistry.¹ Particularly, self-assembled structures derived from unnatural peptide sequences – ‘foldamer’, have been exhibited intriguing physical properties which is otherwise difficult to achieve with natural sequences. In addition, synthetic amino acid contained enhanced physical and chemical stability of oligomeric sequence.

We envisioned that a simple modification at the terminus of oligomer could be an effective strategy to enhance the physical and chemical stability. In this reason, we have appended bis(benzyloxy)benzyl moiety at the C-terminus of short helical β -peptide. The peptide was prepared by coupling bis(benzyloxy)benzyl amine with the carboxylic acid part of trans-ACPC (trans-2-aminocyclopentanecarboxylic acid) hexamer building block. The self-assembled morphological analysis of designed oligomer was carried out by using SEM, TEM and AFM. TEM image showed that the edge of the tube is hollow compare to the middle of the tube is filled up so that showing the unique semi-tubular structure. TGA analysis showed that this semi-microtube has thermal stability up to 300 °C. In addition, the structure was remained stable under the acid treatment even for 15 hours. Showing the increase of both physical and chemical stability compare to the foldamer comparison. This simple terminal modification strategy of foldamer will pave the way to enhance both physical and chemical stability of self-assembled structure of peptide.

References

¹ Gazit, E. *Chem. Soc. Rev.* **2007**, 36, 1263-1269.

Unprecedented cycloadditions to contract *N*-heterocycles ; Beyond Corey-Chaykovsky Reactions

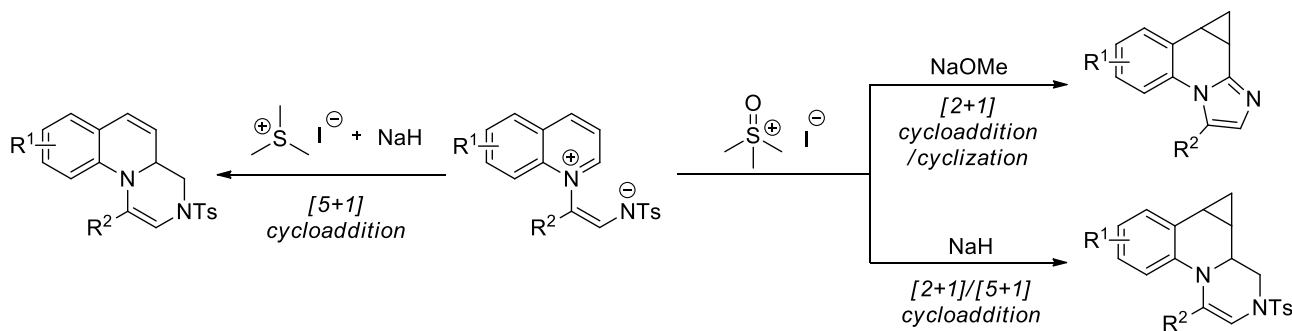
Jiyoun Lee, Hyeji Kim, Nirupam De and Eun Jeong Yoo*

Department of Applied Chemistry, Kyung Hee University, Yongin 17104, Republic of Korea.

E-mail: ejyoo@khu.ac.kr

Cyclopropane ring is one of the unique structural units present in wide range of natural and synthetic compounds exhibiting biological and pharmaceutical activity, such as natural products Trovafloxacin, Duocarmycin A and (-)-Cycloclavine possess fused cyclopropane skeleton. Due to high angle strain (28 Kcal/mol) the synthesis of cyclopropane containing compounds, specially cyclopropane-fused heterocycles useds are challenging task.

Recently, our group discovered that the pyridinium-zwitterion could serve as a 1,5-dipole for the construction of medium-sized heterocycles via [5+n]-cycloadditions with electrophilic partners. In this symposium we will disclose a new metal-free cycloaddition reaction of analogous quinolinium-zwitterion with 1C coupling partners to form cyclopropane fused heterocyclic compounds.



References

1. Lee, D. J.; Han, H. S.; Shin, J.; Yoo, E. J. *J. Am. Chem. Soc.* **2014**, *136*, 11606.
2. Lee, D. J.; Ko, D.; Yoo, E. J. *Angew. Chem., Int. Ed.* **2015**, *54*, 13715.
3. Shin, J.; Lee, J.; Ko, D.; De, N.; Yoo, E. J. *Org. Lett.* **2017**, *19*, 2901.

Chemoselective synthesis of unsymmetrical secondary amines from benzonitrile and nitroalkanes using bimetallic PdPt-Fe₃O₄ NPs

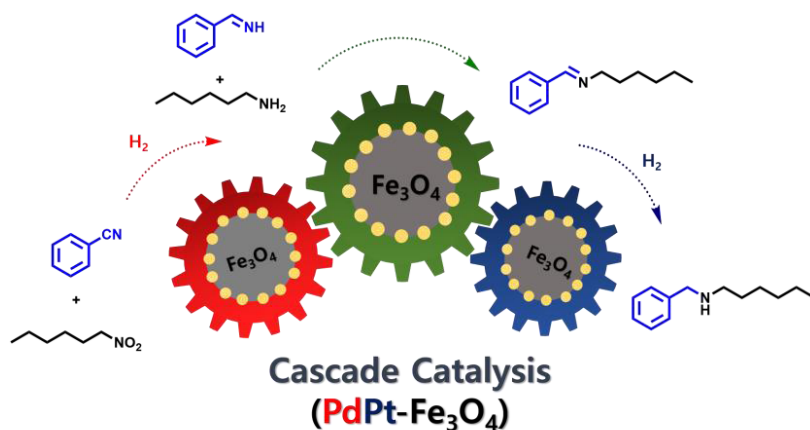
Jin Hee Cho,^a Sangmoon Byun,^b Ahra Cho,^a B. Moon Kim*

^a Department of Chemistry, College of Natural Science, Seoul National University, Seoul 151-747, Republic of Korea. ^b The Research Institute of Basic Sciences, Seoul National University, 1 Gwanak-ro, Gwanak-gu, Seoul, 08826, Republic of Korea
E-mail:kimbm@snu.ac.kr

We have reported successful catalytic nitro-reduction¹ and arylsilylation² using PdPt-Fe₃O₄ heterodimeric nanocrystals as novel magnetically recyclable catalysts.

Herein, we report the development of a new one-pot method for the selective synthesis of secondary amines via reductive amination of nitriles with nitroalkanes using the PdPt-Fe₃O₄ catalysts. This catalysts are very efficient for one-pot cascade hydrogenation of a nitroalkanes and the reductive alkylation of the resulting amines with an imine generated in situ from benzonitrile from the same catalysts. This method allows for the highly chemoselective synthesis of unsymmetrical secondary amines with the advantage of avoiding the use of alkyl halides and/or carbonyl compounds. Also, the direct use of benzonitrile and nitroalkanes offer an efficient, green strategy for the preparation of amines, which are important building block for pharmaceutical, agrochemical and biotechnology applications.

This bimetallic catalysts show a great potential to become an innovative and promising tool for the industrial synthesis of secondary amines, providing advantages such as high efficiency, sustainability and environment-friendliness.



References

- ¹ S. Byun, Y. Song, B. M. Kim, *ACS Appl. Mater. Interfaces*, **2016**, *8*, 14637.
- ² J. Jang, S. Byun, B. M. Kim, S. W. Lee, *Chemical Communication*, **2018**, *54*, 3492–3495

Development of hypoxia detecting fluorescent probe based on conjugating hypoxia-sensitive moiety with Seoul-Fluor

이영준¹, 신민철², 김은하^{2*}, 박승범^{1,3*}

¹Department of Chemistry, Seoul national University, Seoul, 08826, Korea. ²Department of Molecular Science and Technology, Ajou University, Suwon 16499, Korea. ³Department of Biophysics and Chemical Biology, Seoul national University, Seoul, 08826, Korea
E-mail: p20509p@ajou.ac.kr

Hypoxia, oxygen insufficient condition, is important indicator of diseases. In case of tumor tissue, rapid growing of tissue leads to lack of oxygen supply and that induces hypoxia condition. Therefore, design of molecular indicator of hypoxia will be useful for tumor study. Because fluorescent bioprobes have attractive features, such as high sensitivity, non-invasive imaging in live cell condition, high selectivity, we decided to develop fluorescent bioprobes for monitoring hypoxic condition. we apply azo group that is reducible under hypoxic condition in Seoul-Fluor system. fluorophore conjugated with azo group is non-fluorescence. But, under hypoxic condition, reduction of azo group leads fluorescence increase.

Photophysical property study of C-1, C-3 and C-7 modified Indolizine for versatile fluorescent material application.

Hyungi Kim,^a Sang-kee Choi,^a Eunha Kim^{a*}

^a Department of molecular science and technology, Ajou University, Suwon 16499, Korea
E-mail: newworld@ajou.ac.kr

Indolizine is an N-bridgehead bicyclic heterocycle aromatic compound having 10 electrons satisfying the Huckel's rule. We applied the density functional theory (DFT) calculation to obtain the electron density in the indolizine structure. As a result, it was found that C-1, C-3 and C-6 had a large difference in electron density. In order to synthesize color-full 75 Kaleidoscopic indolizine, were synthesized by combining 3 positions of electron withdrawing group and electron donating group. The photophysical property was excitation from short wavelength and found fluorescent material with various wavelength. It was confirmed that the solvatochromic effect of the fluorescent substance occurs in the solution state and in the solid state. We are developing paper based sensors using 75 kaleidoscopic indolizine material.

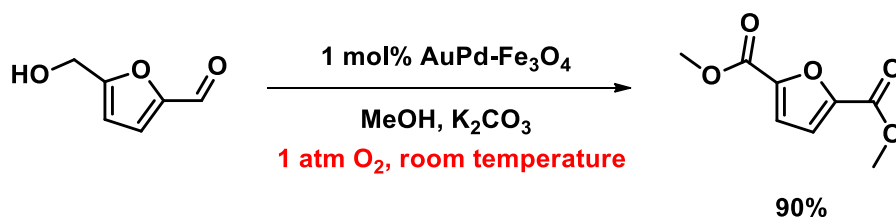
Alloy AuPd-Fe₃O₄ nanoparticles towards oxidative esterification of 5-hydroxymethylfurfural under mild conditions

Ahra Cho,^a Sangmoon Byun,^b Jin Hee Cho,^a B. Moon Kim^{a*}

^a Department of Chemistry, College of Natural Science, Seoul National University, Seoul 151-747, Republic of Korea. ^b The Research Institute of Basic Sciences, Seoul National University, 1 Gwanak-ro, Gwanak-gu, Seoul, 08826, Republic of Korea
E-mail: kimbm@snu.ac.kr

Developing heterogeneous catalysis for transforming sustainable biomass into high value-added intermediates or chemicals is of extreme importance.¹ A number of catalysts have been developed for the conversion of 5-hydroxymethylfurfural (HMF) into high value-added 2,5-furandicarboxylic acid (FDCA) that can form polyethylene furanoate (PEF).² However, furan-2,5-dimethylcarboxylate (FDMC) has attracted more attention as a monomer because of its higher solubility than FDCA, which has poor solubility in most solvents.³ In addition, it is important to be able to show catalytic activity at mild conditions to recycle expensive noble metals in manufacturing.

To our best knowledge, a catalyst capable of converting HMF to FDCA or FDMC at room temperature and 1 atm O₂ has not been reported. Herein, we report high-performance bimetallic alloy AuPd-Fe₃O₄ catalyst, which exhibits high efficiency in the synthesis of furan-2,5-dimethylcarboxylate (FDMC) through one-pot oxidative esterification from 5-hydroxymethylfurfural (HMF) at atmospheric pressure of O₂ at room temperature. Compared with each reactions employing either of the monometallic catalyst, the alloy AuPd-Fe₃O₄ nanoparticles (NPs) exhibited synergy effect, showing unprecedented, high catalytic activity. Also, 1:1 Au/Pd ratio was found to be the best combination for the highest FDMC yield. Interestingly, monometallic Au-Fe₃O₄ catalyst showed high yield and selectivity for the synthesis of 5-hydroxymethyl furoic acid methyl ester (HMFE). The magnetically recyclable AuPd-Fe₃O₄ NPs were readily recycled and reused three times using an external magnet, and the particles showed no significant change after recycle.



References

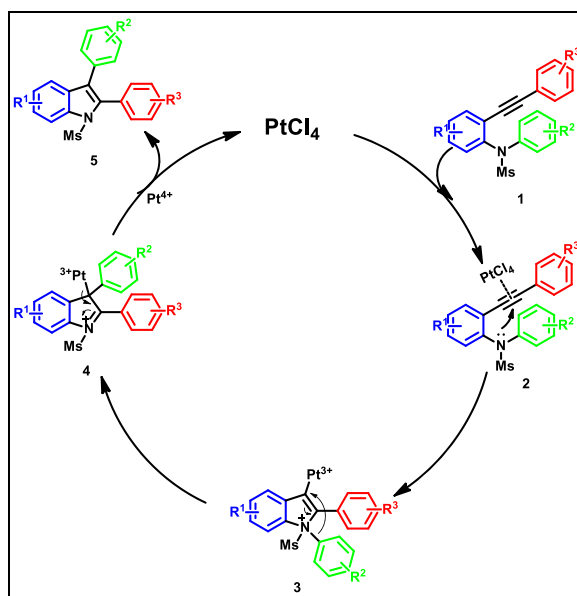
- ¹ Gallezot, P. *Chem. Soc. Rev.* **2012**, *41*, 1538-1558.
- ² Eerhart, A. J. J. E.; Faaij, A. P. C.; Patel, M. K. *Energy & Environmental Science* **2012**, *5*, 6407.
- ³ Taarning, E.; Nielsen, I. S.; Egeblad, K.; Madsen, R.; Christensen, C. H. *ChemSusChem* **2008**, *1*, 75-78.

Platinum Catalyzed 1,3-aryl migratory reaction of 2,3-Diaryl indole from *ortho*-Alkynyl-N-Aryl-N-sulfonylanilines

Dong Yun Kang, Khyarul Alam, and Jin Kyoong Park*

Department of Chemistry, Pusan National University, 2 Busandaehak-Ro 63Beon-Gil, Geumjeong-Gu, Busan 46241, Republic of Korea
E-mail: dkdk1634@gmail.com

Indole is an aromatic two-ring heterocyclic compound and has a biological activity. Particularly 2,3-diaryl indoles have been reported to have anti-cancer activity in several studies^[1]. Synthesizing 2,3-disubstituted indoles directly from *ortho*-alkynyl-N,N-disubstituted anilines are already known. Most of case synthesized 2,3-disubstituted indoles using transition metal through metal catalyzed 1,3-migratory reaction. Although sulfonyl, acyl, allyl group have been proposed but aryl migration is not known yet.^[2] Herein, we describe a PtCl₄-catalyzed 1,3- aryl migratory reaction of *ortho*-alkynyl-N-aryl-N-methylsulfonyl aniline derivatives affords 1-(methylsulfonyl)-2,3-diphenyl-1H-indole in reasonable yields.



References

- (1) Bernard L. Flynn, Ernest Hamel, and M. Katherine Jung *J. Med. Chem.*, 2002, 45, 2670–2673. (2) T. Rukkijakan et al., *Bioorg. Med. Chem. Lett.*, 2016, 26, 2119–2123.
- ²Itaru Nakamura et al., *Angew. Chem.*, 2007, 119, 2334–2337

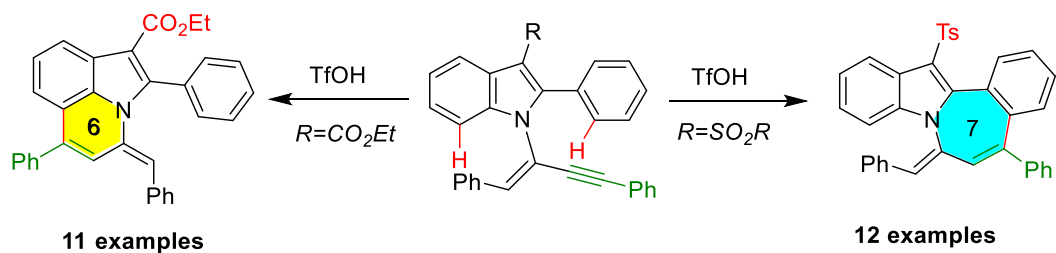
TfOH-Promoted Regiodivergent Intramolecular Cycloisomerizations of Ynenamines to Diversified Fused Indoles

Khyarul Alam, Jin Gyeong Kim, and Jin Kyoon Park

The Department of Chemistry and Chemistry Institute of Functional Materials,
Pusan National University, Busan 46241, Korea.
E-mail: meowwww@naver.com

Polyfused N-heterocycles, in particular polyfused indoles, are privileged structure found in many natural products and synthetic compounds with a broad spectrum of biological functions and medicinal applications. In our previous report¹, we have presented a highly regioselective and stereospecific cycloisomerization of ynamide derived from N-alkynyl indole to isoindolo[2,1-a]indoles and indolo[2,1-a]isoquinolines *via* transition metal catalyzed 5-*exo-dig* and 6-*endo-dig* cyclization respectively.

In this study, we have Expanded to the case of ynenamine derivatives², obtained from simple hydoralkynylation of *N*-alkynyl indoles, with TfOH resulting in pyrrolo[3,2,1-*ij*]quinoline *via* 6-*endo-dig* cyclization at indole C-7 position along with the trace formation of benzo[3,4]azepino[1,2-*a*]indole *via* 7-*endo-dig* cyclization to indole C-2 phenyl ring. The nature of 6-*endo-dig* and 7-*endo-dig* cyclization can be controlled by tuning the electronic influences of indole C-3 substituents. Substrates with carbonyl group (-CO₂Et, -COME etc.) gave 6-*endo-dig* cyclized products while substrate with sulfonyl group (-Ts, -Ms etc.) gave 7-*endo-dig* cyclized products in good to excellent yield.



References

- ¹ K. Alam, S. W. Hong, K. H. Oh, J. K. Park, *Angew. Chem. Int. Ed.* **2017**, *56*, 13387-13391.
- ² V. Dwivedi, M. Hari Babu, R. Kant, M. Sridhar Reddy, *Chem. Commun.* **2015**, *51*, 14996-14999.

The Aggregation-Induced Emissive Fluorophore Kaleidolizine

Sang-Kee Choi, Hyungi Kim and Eunha Kim*

Department of Molecular Science and Technology, School of Engineering, Ajou University, Suwon, 206 World cup-ro, Yeongtong-gu, Korea

E-mail : ehkim01@ajou.ac.kr

The fluorescence was used in various field because of its sensitive property. But the sensitivity cannot be improved in condensed phases such as aggregates of solid-state film. Conventional dyes have the property of quenching when it aggregates. Only a limited number of organic fluorescent dyes have been reported as representing Aggregation-Induced Emission(AIE) characteristics. Many of Kaleidolizine(KIz) fluorescent compound exhibit fluorescence emission both in diverse organic solvent and in solid state due to its unique chemical structure. However, several Kaleidolizine derivatives have low fluorescent intensity in solution state but have high fluorescent intensity in their solid state. AIE probes have ultrahigh imaging contrast, good photostability, and increased intensity with low concentration¹). Here in, we are introducing the new AIE fluorophore Kaleidolizine with its analysis and its properties to prove its mechanism and it can be applied on solution polarity sensor, OLED and chemical sensor such as VOC detector.

References

¹ Xuesong Li et al, J. Am. Chem. Soc., 2017, 139, 17022-17030

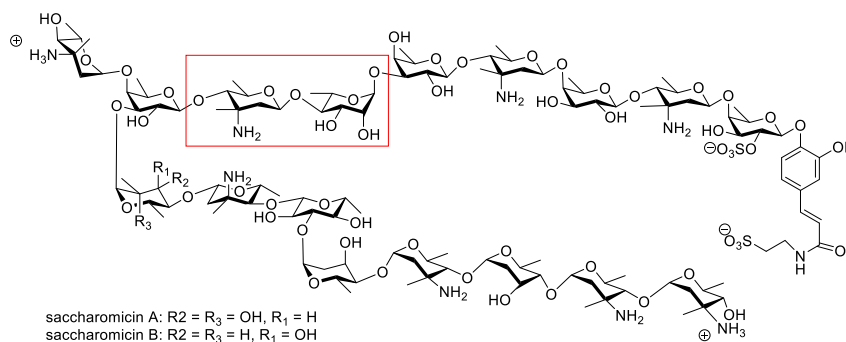
A Synthetic Study Towards Saccharomicin: Asymmetric Synthesis of Saccharosamine-Rhamnose Fragment

Bhawna Barpuzary, Mijin Kim, Young Ho Rhee*

Department of Chemistry, Pohang University of Science and Technology (POSTECH), Pohang, Republic of Korea 37673.

E-mail: yhrhee@postech.ac.kr

A concise stereoselective synthesis of branched disaccharide, β -D-Sac-(1 \rightarrow 4)- α -L-Rha of Saccharomicin, a heptadecasaccharide antibiotic, has been developed.¹ The foremost and stereoselectivity predicting step is the synthesis of branched disaccharide fragment *via* Pd-catalyzed asymmetric hydroalkoxylation followed by Ru-catalyzed ring closing metathesis.² The nitrogen insertion on C-3 carbon of the sensitive branched disaccharide is successfully achieved by its carbamate cyclization to produce the saccharosamine-rhamnose fragment derivative in the absolute configuration.



References

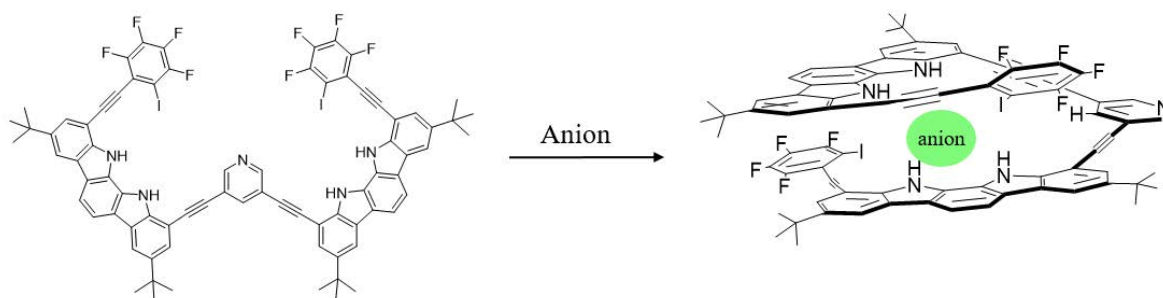
- ¹ Kong, F.; Zhao, N.; Siegel, M. M.; Janota, K. J.; Ashcroft, S.; Koehn, F. E.; Borders, D. B.; Carter, G. T. *J. Am. Chem. Soc.* **1998**, *120*, 13301-13311.
- ² Lim, W.; Kim, J.; Rhee, Y. H. *J. Am. Chem. Soc.* **2014**, *136*, 13618-13621.

Anion Encapsulation and Transport with Aromatic Oligomers that containing Hydrogen- and Halogen- bond Donor groups

Sungbeom Seo and Kyu-Sung Jeong*

Department of Chemistry, Yonsei University, Seoul 03722, Korea.
ssb12@yonsei.ac.kr

Halogen bonding gains lots of attractions. This is because their properties are fundamentally different from that of hydrogen bonding. For examples, halogen bonding prefers halide anion to oxoanion and they are not highly dependent on solvent polarity. However, lots of studies were delocalized to solid state study and they only use halogen bond interactions, so the study about combinations of halogen bond with other noncovalent interactions in solution phase are still at the beginning state. Herein, we have synthesized helical aromatic oligomers containing indolic NHs, pyridine CH and tetrafluorobenzenes as a halogen bond donor group. Each units was linked by ethynyl bonds by Sonogashira reactions so that they can encapsulate halide anions. To confirm anion binding and complexed conformations, we will proceed 1D-, 2D-proton- and fluorine- NMR studies. Biding constant will be measured by Uv-vis titration and additional ITC titration. The results will be supported by crystal structure. Furthermore, the anion transport possibility will be confirmed by Fluorescence and ISE methods. Details will be discussed in the presentation.



Bifunctional *N*-heterocyclic carbene complexes with Pd-arene interaction for Pd-catalyzed amination

Changmuk Kang,^a Ji Yeon Ryu,^b Junseong Lee^b and Sukwon Hong^{a,c*}

^a Department of Chemistry, Gwangju Institute of Science and Technology, 123 Cheomdan-gwagi-ro, Buk-gu, Gwangju 61005, Republic of Korea. ^b Department of Chemistry, Chonnam National University, 77 Yongbong-ro, Buk-gu, Gwangju 61186, Republic of Korea. ^c School of Materials Science and Engineering, Gwangju Institute of Science and Technology, 123 Cheomdan-gwagi-ro, Buk-gu, Gwangju 61005, Republic of Korea
E-mail: shong@gist.ac.kr

Buchwald-Hartwig amination has been developed as an important method of making C-N bond formation.¹ Buchwald biarylphosphine ligands were mainly used for the amination, and a key feature of these phosphine ligands is an interaction between the 'lower' ring of phosphine ligands and metals bound to phosphine.² Pd-catalyzed amination with *N*-heterocyclic carbene (NHC) ligands has also been developed as an alternative to phosphine ligands because NHC-metal complexes have high thermal and air stability. Imidazo[1,5-*a*]pyridine(ImPy)-derived *N*-heterocyclic carbene ligands, first reported in 2005,^{3,4} have been synthesized and characterized. These ImPy ligands can be equipped with a biaryl moiety in an analogous manner to the Buchwald biaryl phosphine ligands and also be equipped with the diethylene glycol group to activate a cation of a base. To evaluate the biaryl-ImPy carbene ligands, palladium was introduced to the biaryl ImPy ligands.⁵ It turns out that the biaryl-ImPy Pd complexes are efficient catalysts for the Buchwald-Hartwig aminations. In the presence of sodium tert-butoxide, various aryl, alkyl amines can react with aryl chlorides to make a new carbon-nitrogen bond in high yields within a short period of time.

References

- 1 Surry, D. S.; Buchwald, S. L. *Angew. Chem. Int. Ed.* **2008**, *47*, 6338-6361.
- 2 Barder, T. E.; Biscoe, M. R.; Buchwald, S. L. *Organometallics* **2007**, *26*, 2183-2192.
- 3 Burstein, C.; Lehmann, C. W.; Glorius, F. *Tetrahedron* **2005**, *61*, 6207-6217.
- 4 Alcarazo, M.; Roseblade, S. J.; Cowley, A. R.; Ferna'ndez, R.; Brown, J. M.; Lassaletta, J. M. *J. Am. Chem. Soc.* **2005**, *127*, 3290-3291.
- 5 Calimsiz, S.; Sayah, M.; Hoi, K. H.; Lough, A. J.; Organ, M. G. *Angew. Chem. Int. Ed.* **2009**, *48*, 2383-2387.

Urea Effects in Salen Aluminum Complex for Cyclic Carbonates Synthesis

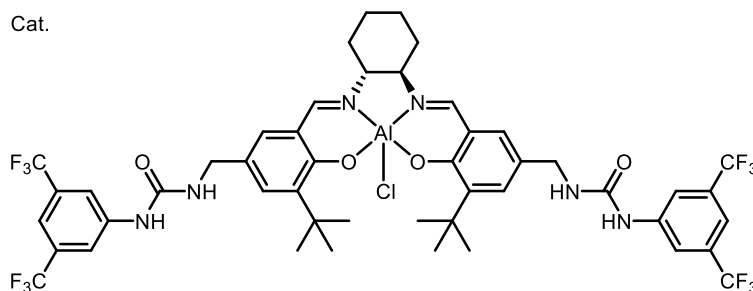
Wooyong Seong,^a Sukwon Hong^{a*}

^a Department of Chemistry, Gwangju Institute of Science and Technology, Gwangju Institute of Science and Technology, Cheomdan-Gwagiro 123, Buk-gu, Gwangju, 61005, Korea.
E-mail: shong@gist.ac.kr

A urea containing salen aluminum complex as catalysts for the synthesis of cyclic carbonates has been developed. It took 6 steps to prepare the designed self-assembly bimetallic salen aluminum complex. The total yield of catalyst synthesis was 44%¹.

Bimetallic Al (III) Salen Cl complex activated by urea catalyst for cyclic carbonate synthesis reaction has been developed. The urea moiety gives bimetallic scaffold to the complex in solution system. It determined by urea additive studies and kinetic studies. Also, urea activated salen ligand was bimetallic catalyst. It determined by urea salen Ni catalyst's crystallography by DMF evaporation. The Turn over frequency (TOF) was increased 3 times better with Bimetallic Al (III) Salen Cl complex than with Al(III) Jacobsen salen Cl complex in 10 bar of CO₂ and 90 °C condition.

we applied our previous bis-urea-functionalized salen ligand that designed to self- assemble through urea-urea hydrogen bonding to cyclic carbonates synthesis reaction with Al metal. Bimetallic urea salen Al complex improved reaction rate (up to 13 times, in mild condition (40 °C, 1 bar closed CO₂)) in cyclic carbonate synthesis of epoxide with CO₂. Additive studies with urea and kinetic studies through catalysts concentration was occurred to evidence bimetallic pathway. And crystal structure of Ni complex shows direct evidence for forming bimetallic complex between urea ligands or it's metalated complexes. Modifications of ligand structures to further improve the catalyst are currently in progress.²



References

¹ Catalyst synthesis scheme from : J. Park, K. Lang, K. A. Abboud and S. Hong, Chem. Eur. J. 2011,17,2236-2245

² (a) C. Maeda, Y. Miyazaki and T. Ema, Catal. Sci. Technol., 2014,4,1482-1497. (b) X. Wu and M. North. ChemSusChem. 2017,10,74-78.

Asymmetric Total Synthesis of (+)-Waihoensene

Sanghyeon Lee,^a Hongsoo Lee,^a Hee-yoon Lee^{a*}

^a Department of Chemistry, Korea Advanced Institute of Science and Technology (KAIST), Daejeon, Korea.

E-mail: brory2000@kaist.ac.kr

Tandem cycloaddition reaction of allenyl diazo compound mediated by trimethylenemethane(TMM) diyl provides an rapid excess to the linear triquinane and angular triquinane structures.¹ Our group reported several total syntheses of terpene compounds containing triquinane scaffold utilizing this strategic reaction, and it enabled the successful total synthesis of especially challenging tetracyclic diterpenoid compounds, such as (-)-crinipellin A and (rac)-waihoensene.^{2,3}

Waihoensene is a diterpene compound having highly congested 6/5/5/5 tetracyclic structure with four contiguous quaternary carbon centers. Together with these complex structural factors, its biogenetic relationship with laurenene, which is the only isolated natural product with all-carbon fanestrane scaffold, made it a meaningful target compound in synthetic organic chemistry.

In extension to our reported racemic total synthesis of waihoensene utilizing TMM diyl mediated tandem cycloaddition reaction, we completed the asymmetric total synthesis of (+)-waihoensene, and so we could unambiguously confirm the absolute configuration of (+)-waihoensene. This is the first asymmetric total synthesis of laurenene related natural products. Additionally, the key TMM diyl cycloaddition reaction was further studied, and competitive reaction pathways were described in detail.

References

¹ Kang, T.; Kim, W.-Y.; Yoon, Y.; Kim, B. G.; Lee, H.-Y. *J. Am. Chem. Soc.* **2011**, *133*, 18050-18053.

² Kang, T.; Song, S. B.; Kim, W.-Y.; Yoon, Y.; Kim, B. G.; Lee, H.-Y. *J. Am. Chem. Soc.* **2014**, *136*, 10274-10276.

³ Lee, H.; Kang, T.; Lee, H.-Y. *Angew. Chem. Int. Ed.* **2017**, *56*, 8254-8257.

Protein Labeling Using Blue-Fluorescent Emitting BODIPY derivatives

Yuna Jung,^a Dokyong Kim^{*a, b, c}

^a Department of Biomedical Science, Graduate School, Kyung Hee University, 26 Kyungheedaero, Dongdaemun-Gu, Seoul 02447, Republic of Korea;

^b Department of Anatomy and Neurobiology, College of Medicine, Kyung Hee University, 26 Kyungheedaero, Dongdaemun-Gu, Seoul 02447, Republic of Korea;

^c Center for Converging Humanities, Kyung Hee University, 26 Kyungheedaero, Dongdaemun-Gu, Seoul 02447, Republic of Korea.

E-mail: jungpeng159@gmail.com, dkim@khu.ac.kr

Labeling of intrinsic biomolecules using signaling units has been widely known as an effective method for monitoring molecular interactions and bio-imaging. Among those application, fluorescence-based protein labeling has become into spotlight in basic science; chemistry, biology because of its simplicity and reliability with high sensitivity. Visualization of protein activities has a great possibility to study protein functions, dynamics, and behaviors. Up to this point, various protein labeling technics and materials have been developed. In this study, we introduced a new protein labeling material, which has bright blue fluorescence. It is important to study biological system, on the other hand, the development of blue-fluorescent emitting dye for protein labeling have been scarcely explored.

A new blue-emitting dye, 8-amino-BODIPY (boron-dipyrrromethane), has valuable properties such as (i) sharp and intense absorption and fluorescence emission peaks, (ii) solvent-insensitive emission wavelengths, (iii) compact structure, (iv) high photo-stability, (v) labeling selectivity of specific amino acid such as cysteine or lysine, and (vi) mild condition of labeling. We proved the new protein labeling method using 8-amino-BODIPY derivatives for lysozyme and bovine serum albumin (BSA). The labeling result of protein is verified via chromatography (HPLC) and Matrix-assisted laser desorption/ionization mass spectroscopy (MALDI-TOF) analysis. We believe that our new dyes would be capable for application in order to study the protein dynamics in living cells and tissues, and fluorescence resonance research with intrinsic fluorescent biomolecules.

Keywords: BODIPY dye, Protein labeling, Fluorescence labeling, Blue-emitting BODIPY

References

¹ D. Kim* et al., *Bull. Korean Chem. Soc.* **2017**, 38, 995–996.

Toward Efficient Formation of Electrical Double Layer in Optoelectronic Devices by Controlling the Ionic Mobility

Minsoo Lee,^{a,†} Hyun-Tak Kim,^{a,†} Ji Hoon Seo,^{b,†} Kwanyong Seo,^{*,b} and Tae-Hyuk Kwon^{*,a}

^aDepartment of Chemistry, Ulsan National Institute of Science and Technology, Ulsan, 44919, Republic of Korea

^bDepartment of Energy Engineering, Ulsan National Institute of Science and Technology, Ulsan, 44919, Republic of Korea

Ionic material-based electrical double layers (EDLs) have emerged to enhance the performance of optoelectronic devices, such as light-emitting electrochemical cells (LECs) and polymer solar cells (PSCs), because they permit facile control of charge injection/extraction barriers by controlling the electrode conduction band (CB). Nevertheless, the correlation between mobile ion kinetics and EDLs formation in PSCs currently remains unclear. Here, a simple and effective method for accomplishing precise interfacial energy level adjustment is presented using iridium (Ir) (III) complexes with different cations (Ir-Li⁺, Ir-Na⁺, Ir-K⁺). The effects of the ionic kinetics of Ir(III) complexes and the EDLs formation on the energy level tuning are investigated by measuring the turn-on-voltage in LECs, and current density, CB shifting, and electron mobility in PSCs as a function of the cation type. The turn-on voltage in LECs and current density in PSCs improve remarkably owing to precise interfacial energy level matching with the optimum Ir-K⁺ complex in the PEO channel. The mobility of the mobile ions affects the CB directly, resulting in enhanced PSCs device performance by efficient EDLs formation. Furthermore, the PSCs containing the Ir(III) complexes exhibit great enhancement in ultraviolet (UV) light stability owing to the strong UV light absorption capacity of the Ir (III) complexes.

References

1. Lee, S.; Nguyen, T. L.; Lee, S. Y.; Jang, C. H.; Lee, B. R.; Jung, E. D.; Park, S. Y.; Yoon, Y. J.; Kim, J. Y.; Woo, H. Y.; Song, M. H. *Adv. Mater.* **2018**, 30 (14), 1706034.
2. Liu, C.; Tan, Y.; Li, C.; Wu, F.; Chen, L.; Chen, Y. *Appl. Mat. Int.* **2015**, 7 (34), 19024-33.

A fluorescent probe for detection of Gold(III) ions based on the AIEgen disaggregation

Na Hee Kim^a, Dokyoung Kim^{b,c}

^a Department of Biomedical Science, Graduate School, Kyung Hee University, Seoul 02447, Republic of Korea. ^b Department of Anatomy and Neurobiology, College of Medicine, Kyung Hee University, Seoul 02447, Republic of Korea. ^c Center for Converging Humanities, Kyung Hee University, Seoul 02447, Republic of Korea

E-mail: pionaheek@gmail.com, dkim@khu.ac.kr

Gold has been widely used in the world as a high-value material. Recently, the unique chemical-/photophysical- properties of gold and gold ions have been making a big issue of their use for various purpose across the basic science and advanced system.

In biological environments, metallic gold presented oxidized form such as gold ion (Au(I) and Au(III)) because of the presence of hydrogen peroxide (H₂O₂). The ionic forms can cause adverse effects due to the high reactivity and potential toxicity.

Recently reported probes for gold ion sensing have some limitations such as complex mechanism, slow response time, and sophisticated synthetic procedure.

In this study, a new fluorescence probe for the detection of gold ions was developed based on the disaggregation of AIE(aggregation-induced emission) molecules. This probe is based on the propeller shaped tetraphenylethylene (TPE) which is non-emissive in dilute solutions by free rotation-induced non-radiative decay of fluorescence, and emissive in aggregated form. A TPE-based fluorescent probe for Au(III), **AuP-1**, shows excellent sensing properties including: (i) high sensitivity, (ii) fast response time, (iii) high selectivity, (iv) biocompatible (low cellular toxicity, fluorescent imaging), and (v) broad applicability (paper-based strip). We expect the advantageous properties of the present fluorescent probe could be applied for the gold ion-related chemical and biological studies.

References

¹ N.H. Kim., D. Kim; *Dyes Pigm*, **2018**, In press

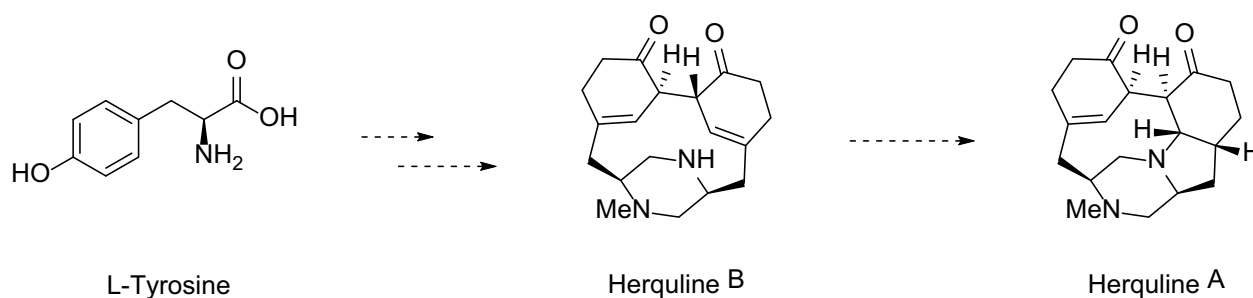
Towards the Total Synthesis of Herquline A & B

Thomas Taehyung Kim,^{ab} and Sunkyu Han^{ab*}

^a Department of Chemistry, Korea Advanced Institute of Science & Technology (KAIST), Daejeon 305-701, South Korea.

^b Center for Catalytic Hydrocarbon Functionalizations, Institute for Basic Science (IBS), Daejeon 305-701, South Korea.
E-mail: thomasth.kim@kaist.ac.kr

In 2016, Houk and Tang have proposed a very detailed and persuasive biosynthesis of Herquline A (**2**) and Herquline B (**1**)¹. Herquline A (**2**) and B (**1**) were first isolated in 1979 by Omura and showed promising platelet inhibition and replication of the influenza virus. These strained diketopiperazine natural products however, have not yet been synthesized to date, most likely due to its strained pentacyclic core and the difficulty in controlling the stereochemistry of the C2-C2' bond. Inspired by Tang's biosynthetic studies on Herquline A and Herquline B, we have begun the total synthesis of Herquline A and B.



References

1. Yu, X.; Liu, F.; Zou, Y.; Tang, M-C.; Hang, L.; Houk, K.N; Tang, Yi. *J. Am. Chem. Soc.* **2016**, *138*,13529-13532.

Photo-Therapeutics with Ir(III) Complexes toward Two Diseases: Cancer & Alzheimer

Jung Seung Nam,^a Juhye Kang,^{a,b} Myeong-Gyun Kang,^{a,c} Hyun-Woo Rhee,^{c*} Mi Hee Lim,^{b*} and
Tae-Hyuk Kwon^{a*}

^a *Department of Chemistry, Ulsan National Institute of Science and Technology (UNIST), Ulsan 44919, Republic of Korea.*

^b *Department of Chemistry, Korea Advanced Institute of Science and Technology (KAIST), Daejeon 34141, Republic of Korea.*

^c *Department of Chemistry, Seoul National University, Seoul 08826, Republic of Korea.*
E-mail: j.s.nam@unist.ac.kr

The reactive oxygen species (ROS) has been intimately involved in lots of chemical reaction in cellular compartments. Thereby various kinds of reactions with ROS have been elucidated as the connected rings between cause and phenomena of some diseases like cancer, Alzheimer's disease or others.¹ Therefore, the most of researchers have understood that innately over-produced ROS deteriorate normal cycle for the cell in biological aspects. However, continuous researches reversed previous common sense.² It means that the amount of ROS over specific threshold can have potential to application for some treatment of cancer or others. In this perspective, Ir(III) complexes as photo-activatable tool (**TIr1-4** & **Ir-1**) were utilized for ROS generation. Exogenous ROS produced by Ir(III) complexes could oxidize protein or peptide, which induce prompt cancer cell death as well as modulation of amyloidogenic peptides that are the cause for neurodegenerative diseases.³⁻⁴ As a result, this research extended the utilization of Ir(III) complexes as photo-activatable tool for not only cancer but also Alzheimer's disease.

References

- ¹ Holmstrom, K. M. and Finkel, T. *Nat. Rev. Mol. Cell Biol.* **2014**, *15*, 411-421
- ² Galandari, S. *et al. Free Rad. Biol. and Med.* **2017**, *104*, 144-164
- ³ Nam, J. S. *et al. J. Am. Chem. Soc.* **2016**, *138*, 10968-10977.
- ⁴ Kang, J. *et al. Chem. Eur. J.* **2017**, *23*, 1645-1653

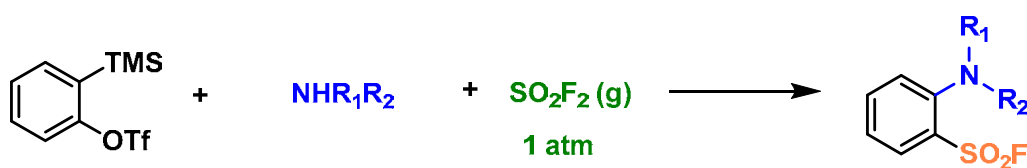
Synthesis of 2-dialkyl-, 2-alkylaryl- or 2-diarylaminoarenesulfonyl fluorides via sulfonyl fluoride incorporation into arynes

Jungmin Kwon and B. Moon Kim*

Department of Chemistry, College of Natural Sciences, Seoul National University, 1 Gwanak-ro, Gwanak-gu, Seoul 08826, Republic of Korea
E-mail: kimbm@snu.ac.kr

Sulfonyl fluorides have found significant utility in chemistry and chemical biology.¹ They have attracted much attention due to their unique balance between stability and chemoselectivity.²

Despite the significance of sulfonyl fluorides, however, direct synthetic approaches toward arenesulfonyl fluorides have been limited. Recently, Willis group reported a transition-metal catalyzed one-pot synthesis of arenesulfonyl fluorides from aryl bromides.³ This process involves palladium-catalyzed sulfonylation of aryl bromides using DABSO as a SO₂ source, followed by one-pot treatment of the resultant sulfinate with an electrophilic fluorine source. The reactions' tolerance is noteworthy, nevertheless, an alternative, metal-free synthetic protocol would be more desirable than the two-step reactions involving sulfonylation followed by fluorination. We herein report the development of an efficient protocol providing 2-dialkyl-, 2-alkylaryl- or 2-diarylamino-substituted arenesulfonyl fluorides without using metal-based reagents. This new transition-metal-free multicomponent coupling reaction involves arynes, secondary amines, and sulfonyl fluoride gas. Nucleophilic attack of a secondary amine on *in situ* generated arynes followed by reaction with sulfonyl fluoride proceeds efficiently under mild conditions, affording diverse 2-aminoarenesulfonyl fluoride derivatives in good to excellent yields. We have demonstrated that zwitterionic intermediate formed from the reaction of arynes with amines can capture electrophile SO₂F₂, offering a novel and practical protocol for the synthesis of 2-amino substituted arenesulfonyl fluorides.



References

- ¹ Narayanan, A.; Jones, L. H. *Chem. Sci.* **2015**, *6*, 2650.
- ² Dong, J.; Krasnova, L.; Finn, M. G.; Sharpless, K. B. *Angew. Chem., Int. Ed.* **2014**, *53*, 9430.
- ³ Davies, A. T.; Curto, J. M.; Bagley, S. W.; Willis, M. C. *Chem. Sci.* **2017**, *8*, 1233.

Triaryloxyimino Titanium(IV) Complexes and Application to Stereoselective Lactide Polymerization with Computational Study of Stereoccontrolled Ring-Opening Mechanism

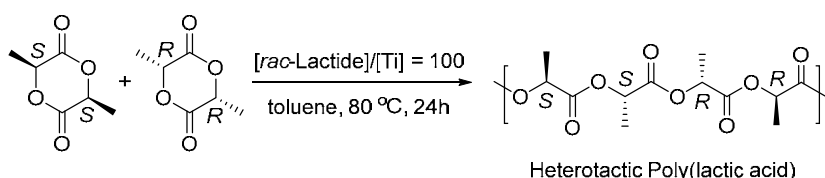
Yeolib Jeong,^a Minjoong Shin,^b Myungeun Seo,^b Hyunwoo Kim^{*a}

^a Department of Chemistry, KAIST, Yuseong-gu, Daejeon 34141, Korea. ^b Graduate School of Nanoscience and Technology and Department of Chemistry, KAIST, Yuseong-gu, Daejeon 34141, Korea.

E-mail: plus0700@kaist.ac.kr

For the past decade, polylactic acid or polylactide has been one of the most promising ecofriendly, biodegradable products and alternative to petrochemical-based polymers. At the same time, various methods for ring-opening lactide polymerization have been developed with organic, organometallic catalysts¹⁻⁵. Especially metal complexes attract attention as effective method to control to get good polymer dispersity(PDI) and selectivity with high reaction speed. In early days, complex with alkali and alkali-earth metals such as Al, Zn, Mg were combined with bidentate ketiminate or schiff base ligands. Group(IV) metal alkoxides like Ti, Zr and Hf increased reactivity and distinct metal effects occurred, connected to much heavier lanthanide and yttrium. For instance, using Hf or Lanthanide under same ligand system usually increased stereoselectivity compared with smaller metal atoms like Al, Ti, etc.

We here report a new type of Ti(IV) based catalyst system with iminotris(phenolate) tripodal ligand which is able to control stereoselectivity by simple structure modification. And the origin of stereocontrol by ligand modification was demonstrated through DFT calculation of mechanistic pathway.



References

- ¹ Cheng, M.; Attygalle, A. B.; Lobkovsky, E. B.; Coates, G. W. *J. Am. Chem. Soc.* **1999**, *121*, 11583-11584.
- ² Kim, Y. J.; Jnaneshwara, G. K.; Verkade, J. G. *Inorg. Chem.* **2003**, *42*, 1437-1447.
- ³ Chmura, A. J.; Davidson, M. G.; Frankis, C. J.; Jones, M. D.; Lunn, M. D.; *Chem. Commun.* **2008**, 1293-1295.
- ⁴ Vieira, I.S.; Whitelaw, E. L.; Jones, M. D.; Heres-Pawlis, S. *Chem. Eur. J.* **2013**, *19*, 4712-4716.
- ⁵ Marshall, E. L.; Gibson V. C.; Rzepa, H. S.; *J. Am. Chem. Soc.* **2005**, *127*, 6048-6051.

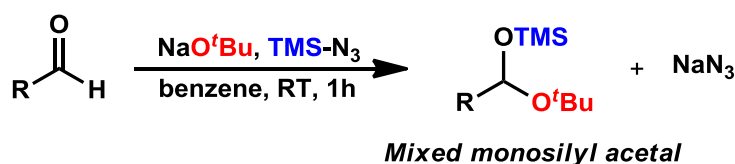
New Synthetic Method of Mixed Monosilyl Acetals and Mukaiyama Aldol Reactions: Control Chemoselectivity using Lewis Acid Catalyst

Hye Sung Yang,^a Hyun-Joon Ha,^{b*} and Jung Woon Yang^{a*}

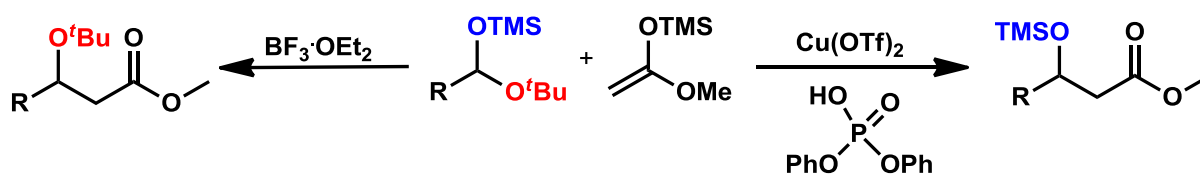
^a Department of Energy Science, Sungkyunkwan University, Suwon 16419, South Korea. ^b Department of Chemistry, Hankuk University of Foreign Studies, Yongin 17035, South Korea.

E-mail: hsjy221@hanmail.net

O,O-Mixed acetals are well known as synthetic equivalents of aldehydes or esters and are widely used in diverse synthetic organic reactions, such as the Mukaiyama aldol, Diels-Alder, and radical cyclization reactions. So we developed a highly selective, direct, and simple synthetic method for the synthesis of monosilyl acetals from aldehydes. In particular, we succeeded in chemoselective Mukaiyama aldol reactions with mixed monosilyl acetals, relying on the discriminative activation of the alkoxy group on the acetal by different oxophilic catalysts. Furthermore, this study provided the existence of an oxonium ion intermediate and of its kinetically controlled reaction with the pre-equilibrated silyl enol ether obtained from (*E*)- and (*Z*)- isomerization.



Chemoselective Mukaiyama aldol reaction



References

- ¹ S. M. Kim, H. S. Yang, H. Eum, H. -J. Ha, J. W. Yang, *Chem. Eur. J.* **2017**, *23*, 16432-16437

Discrimination of phosgene using colorimetric and fluorescent probes in solutions and the gas phase

Yubin Yim,^a Ying Hu,^a Liyan Chen^a, Xin Zhou^c, Jong-Man Kim^{b*} and Juyoung Yoon^{a*}

^a Department of Chemistry and Nano Science, Ewha Womans University, Seoul 120-750, Korea

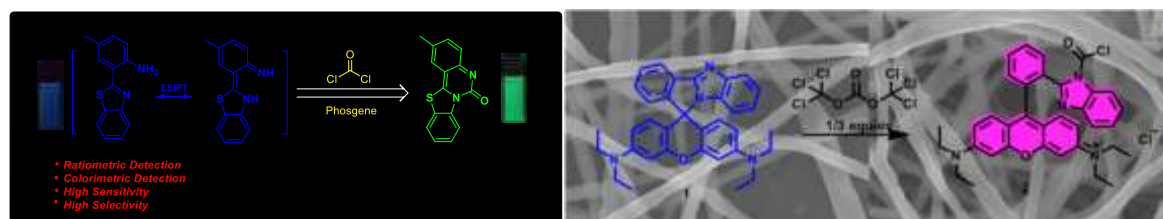
^b Department of Chemical Engineering, Hanyang University, 04763, Korea

^c College of Chemistry and Chemical Engineering, Qingdao University, Shandong 266071, People's Republic of China

E-mail: yubin1171@gmail.com

Phosgene is a highly toxic substance that has become a serious potential threat to public health safety. Therefore, the ability to quickly and accurately analyze highly toxic chemical weapons (CWAs) and related chemicals is essential to mitigate serious threats to human beings and public security due to unexpected terrorist attacks and occupational accidents.

In this study we designed 2-(2-aminophenyl)benzothiazole binding dye and o-phenylenediamine moiety dye capable of both fluorescence and colorimetric discrimination with phosgene and protic nerve agent mimics, solution or gas phase of diethyl chlorophosphate(DCP). In addition, these dyes are expected to be used for constructing a portable a kit that can be used for rea-time monitoring of DCP and phosgene in the field in a discriminative and simple and safe manner.



References

¹ Wu, D.; Chen, L.; Kwon, N.; Yoon, J., *Chem*, **2016**, 1, 674-698

² Zhou, X.; Zeng, Y.; Chen, L.; Wu, X.; Yoon, J. *Angew. Chem. Int. Ed.* **2016**, 55, 4729-4733

³ Hu, Y.; Chen, L.; Jung, H.; Zeng, Y.; Lee, S.; Swamy, K.M.; Zhou, X.; Kim, M. H.; Yoon, J. *ACS Appl. Mater. Interfaces*, **2016**, 8, 22246-22252

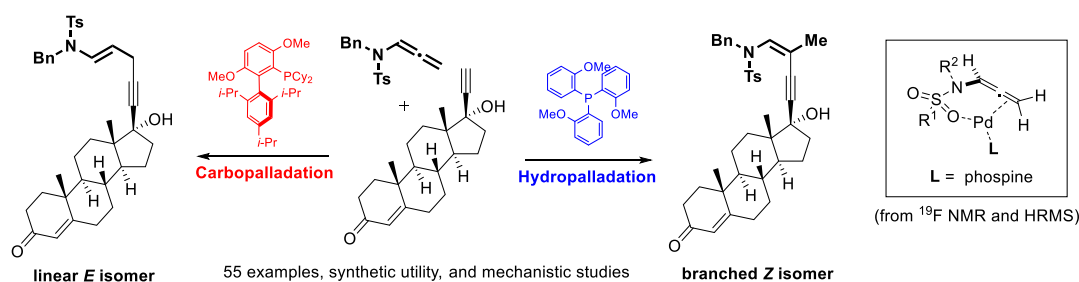
Regiodivergent Synthesis of 1,3- and 1,4-Enynes via Kinetically Favored Hydropalladation and Ligand-Enforced Carbopalladation

Tapas R. Pradhan,^a Hong Won Kim,^b Jin Kyoong Park^{a*}

^a Department of Chemistry and Chemistry Institute of Functional Materials, Pusan National University, Busan 46241, Korea.

E-mail: jkyoon@pusan.ac.kr

Abstract: In continuation of our recent research on ynamides,¹ we reported herein, a regio- and stereoselective hydroalkynylations of a readily available allenic skeleton, N-sulfonylallenamide. Although, hydroalkynylations were successfully applied to electron-neutral/electron-deficient cumulene (allenoates and allenylphosphine oxides),² regiodivergent and stereoselective alkynylation is a significant challenge, since the two contiguous reactive π -systems are prone to isomerization and may afford a mixture of regio- and very often, stereoisomers. In order to address the aforementioned challenges, we attempted to take advantage of the potential chelating amide group of the substrate for control of the stereoselectivity and to screen sterically and electronically differentiated phosphine ligands for the desired regiocontrol. Moreover, the present transformation represents a complementary, highly regiodivergent, and stereospecific cross-coupling approach for the syntheses of conjugated and skipped ynenamides promoted by two different ligands, using a single metal catalyst.³ Neighboring group chelation and phosphine-ligand selection were found to be crucial to develop a reaction that takes place under such mild conditions to allow easy modification of complex substrates such as steroids, carbohydrates, alkaloids, chiral ligands, and vitamins with a broad scope and excellent chemoselectivity. We also proposed reasonable mechanisms in which the ligand-controlled hydro- and carbopalladation processes in the current divergent reaction operate separately by the formation of σ -vinyl-Pd intermediate, based upon experimental results.



References

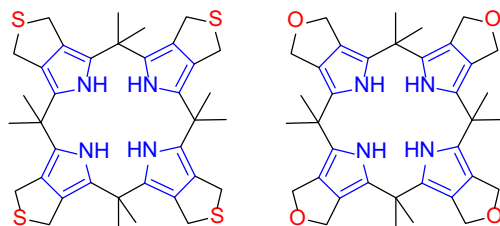
- (a) Oh, K. H.; Kim, J. G.; Park, J. K. *Org. Lett.* **2017**, *19*, 3994; (b) Alam, K.; Hong, S. W.; Oh, K. H.; Park, J. K. *Angew. Chem. int. Ed.* **2017**, *56*, 13387.
- (a) Trost, B. M.; Kottirsch, G. *J. Am. Chem. Soc.* **1990**, *112*, 2816; (b) Yamaguchi, M.; Omata, K.; Hirama, M. *Tetrahedron Lett.* **1994**, *35*, 5689; (c) Yamaguchi, M.; Kido, Y.; Omata, K.; Hirama, M. *Synlett* **1995**, 1181; (d) Bruyere, D.; Grigg, R.; Hinsley, J.; Hussain, R. K.; Korn, S.; De La Cierva, C. O.; Sridharan, V.; J. Wang, J.; *Tetrahedron Lett.* **2003**, *44*, 8669; (e) Rubin, M.; Markov, J.; Chuprakov, S.; Wink, D. J.; Gevorgyan, V. *J. Org. Chem.* **2003**, *68*, 6251; (f) T. Nishimura, X. Guo, T. Hayashi, *Chem. Asian J.* **2008**, *3*, 1505; (g) Sawano, T.; Ou, K.; Nishimura, T.; Hayashi, T. *J. Org. Chem.* **2013**, *78*, 8986.
- Pradhan, T. R.; Kim, H. W.; Park, J. K. *Angew. Chem. Int. Ed.* DOI: 10.1002/anie.201805408.

Synthesis and ion-pair recognition property of thiophene- or furan-fused calix[4]pyrroles

Hyunseong Kang and Chang-Hee Lee*

*Department of Chemistry, Kangwon National University, Chun Cheon 24341, Korea.
chhlee@kangwon.ac.kr.*

Selective recognition of ion-pair has drawn great attentions due to their applications in medicinal and environmental chemistry. The designing and synthesizing ion-pair receptors possessing high selectivity is highly desirable in conjunction with the development of real chemosensors. Among those receptors, calix[4]pyrroles are well known to be efficient receptors for various anionic species and ion-pair in some cases. Variety of modification of the parent macrocycle have been developed for the last ten years. Those modifications are generally focused on either the β -pyrrolic positions or the *meso*-positions. Usually introduction of electron donating substituents at β -pyrrolic positions decreases the anion binding affinity because weakened hydrogen bonding and destabilizing steric interactions incurred upon anion binding. Here, we report novel ion-pair receptors bearing functionalities that can recognize both cations and anions with high affinity and selectivity. The ion-pair binding properties of the synthesized receptors will be presented in detail.



Sugar binding control of Dual stimuli-responsive poly(2-isopropyl-2-oxazoline) containing phenylboronic acids

Ji Young Lee and Woo Dong Jang*

Department of Chemistry, Yonsei University, Seoul 03722, Korea
wdjang@yonsei.ac.kr

Boronic acid has been researched a lot because of its sensing sugar ability. In this research, phenylboronic acid pinacol esters were introduced to both ends of poly(2-isopropyl-2-oxazoline) to make chemo and thermo-responsive polymer (**PBAE-POx**). To observe the thermo-responsive property of the polymer, the cloud point temperature (T_{CP}) was measured by the transmittance change using UV-Vis spectroscopy. The T_{CP} of the polymer can be varied by adding sugars because the diol moiety of the boronic acid bonds with cis diol of the sugar. Among various sugars, **PBAE-POx** showed the largest T_{CP} change (6 °C) immediately when fructose was added. This result means that **PBAE-POx** has stronger binding affinity with fructose by forming cyclic boronate ester and its reaction time was very short.

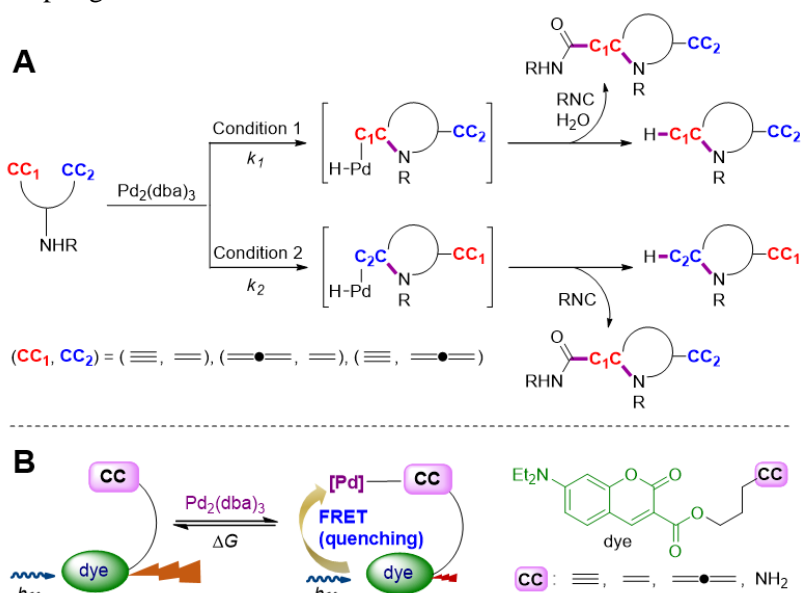
Unravelling Origin of Selectivity toward Carbon-Carbon Multiple Bonds in Palladium-Catalyzed Hydroamination

이지홍, 손정훈*

Department of Chemistry, Chungnam National University, Daejeon 305-764, Korea

Email: sohnjh@cnu.ac.kr

Carbon-carbon multiple bonds of alkene, alkyne and allene are versatile functional groups for transition metal catalyzed carbon-carbon and carbon-heteroatom coupling reactions. Among these reactions, hydroamination reactions, in which an H-N unit of amines is added across a C-C π bond of alkene, alkyne and allene, is in principle one of the most atom-economical methods. Despite their versatile utility in synthetic chemistry with significant advances for regio- and stereoselectivity,¹ there have been still unresolved substantial issues such as quantitative reactivity of these three functionalities toward a metal catalyst, which enables for the chemoselective reaction when these functionalities coexist in a substrate. We studied Pd-catalyzed hydroamination of aminoenyne, aminoallenene, and aminoallenyne and established the selectivity toward either allene or alkyne group. To understand the origin of the selectivity and the activation mode of the reaction, we determined the preference of the Pd toward the three functionalities by using time-dependent fluorescence quenching, which provides kinetic and thermodynamic parameters in the complexation between Pd and the three functionalities.² The preference was well correlated with the chemoselectivity and kinetics of the hydroamination reactions and these results led to design of tandem reaction combining selective hydroamination to either alkyne or allene and C-C coupling with isonitrile.



References

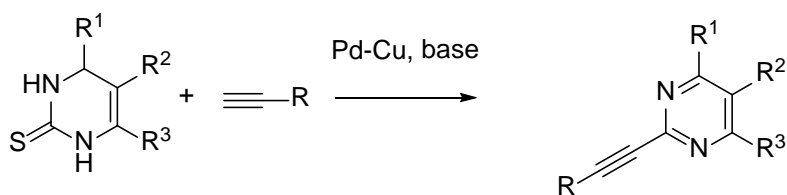
- (a) Müller, T. E.; Hultsch, K. C.; Yus, M.; Foubelo, F.; Tada, M. *Chem. Rev.* **2008**, *108*, 3795-3892. (b) Huang, L.; Arndt, M.; Gooßen, K.; Heydt, H.; Gooßen, L. J. *Chem. Rev.* **2015**, *115*, 2596-2697.
- (a) Sohn, J.-H.; Kim, K. H.; Lee, H.-Y.; No, Z. S.; Ihee, H. *J. Am. Chem. Soc.* **2008**, *130*, 16506-16507. (b) Kim, K. H.; Ok, T.; Lee, K.; Lee, H.-S.; Chang, K. T.; Ihee, H.; Sohn, J.-H. *J. Am. Chem. Soc.* **2010**, *132*, 12027-12033. (c) Lee, O. S.; Kim, K. H.; Kim, J.; Kwon, K.; Ok, T.; Ihee, H.; Lee, H.-Y.; Sohn, J.-H. *J. Org. Chem.* **2013**, *78*, 8242-8249. (d) Lee, J.; Kim, K. H.; Lee, O. S.; Choi, T. -L. Lee, H. -S.; Ihee, H.; Sohn, J. -H. *J. Org. Chem.* **2016**, *81*, 7591-7596.

Oxidative dehydrosulfurative cross-coupling of 3,4-dihydropyrimidin-1*H*-2-thiones with alkynes

Ngoc Son Le Pham and Jeong-Hun Sohn*

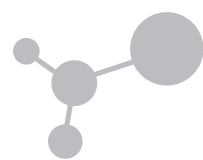
^a Department of Chemistry, Chungnam National University, Yuseong-gu, Deajeon 305-764, Korea.
E-mail: sohnjh@cnu.ac.kr

A method for the synthesis of 2-alkynylpyrimidines from the readily available 3,4-dihydropyrimidin-1*H*-2-thiones (DHPMs) via dehydrosulfurative C-C cross-coupling with alkynes and concomitant oxidative dehydrogenation under a Pd/Cu catalytic system is described.¹ This reaction protocol provides unprecedented diversity of fully substituted 2-alkynylpyrimidines in a single step from a wide range of DHPM and alkyne coupling partners.



References

¹ (a) For oxidative dehydrosulfurative C-N cross-coupling reaction of DHPMs with amines, see: Phan, N. H. T.; Kim, H.; Shin, H.; Lee, H. S.; Sohn, J. H. *Org. Lett.* **2016**, *18*, 5154-5157. (b) For oxidative dehydrosulfurative arylation reaction of DHPMs, see: Kim, H.; Phan, N. H. T.; Shin, H.; Lee, H.; Sohn, J. H. *Tetrahedron*. **2017**, *73*, 6604-6613. (c) For oxidative dehydrosulfurative C-O cross-coupling reaction of DHPMs with boronic esters, see: Kim, H.; Lee, H.; Shin, H.; Sohn, J. H. *Org. Lett.* **2016**, *18*, 5154-5157



Exhibitors and Sponsors

 TCI · 세진시아이	
	
	
	
	



 자유아카데미	 LG화학
 IDC ASIA iGroup Korea	 ISU 이수화학
	 IWOO Scientific Corporation
	 Biotage ®
 LCB LegoChemBio	 TORAY 한국도레이과학진흥재단



제6회 젊은 유기화학자 수상자



조은진 (Cho, Eun Jin)

학력 및 경력

1997 - 2002 서울대학교 화학과, 이학사
 2002 - 2004 서울대학교 화학과, 이학석사 (지도교수: 이은)
 2005 - 2008 Univ. of Wisconsin 화학과, 이학박사 (지도교수: Daesung Lee)
 2009 - 2011 MIT, Postdoc (지도교수: Stephen L. Buchwald)
 2011 - 2015 한양대학교 ERICA 응용화학 및 바이오테크놀로지학과, 조교수
 2015 - 현재 중앙대학교 화학과, 부교수

수상 내역

2016 Asian Core Program Lectureship Award
 2015 The Distinguished Lectureship Award (일본화학회)
 2014 젊은과학자상 (한국유기합성학회)
 2014 Asian Core Program Lectureship Award
 2013 청암 사이언스펠로 (포스코 청암재단)

제7회 젊은 유기화학자 수상자



주정민 (Joo, Jung Min)

학력 및 경력

1997 - 2001 서울대학교 화학과, 이학사
 2001 - 2003 서울대학교 화학과, 이학석사 (지도교수: 이은)
 2003 - 2008 Princeton Univ. 화학과, 이학박사 (지도교수: Chulbom Lee)
 2009 - 2011 Columbia University, Postdoc (지도교수: Dalibor Sames)
 2011 - 2013 Eli Lilly and Company, Research Scientist
 2013 - 현재 부산대학교 화학과, 조교수, 부교수

수상 내역

2018 ACS Catalysis Early Career Advisory Board
 2017 Asian Core Program Lectureship Award
 2016 청암 사이언스펠로 (포스코 청암재단)
 2015 Asian Core Program Lectureship Award



Visible-Light-Induced Fluoroalkylations

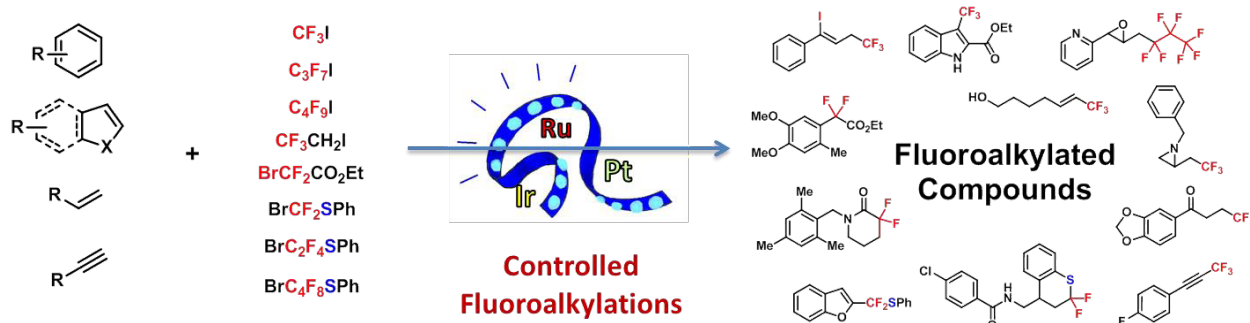
Eun Jin Cho

Department of Chemistry, Chung-Ang University, Seoul 06974, Korea

E-mail: ejcho@cau.ac.kr

Recently, visible light photocatalysis has attracted substantial attention due to its environmental compatibility and mechanistic versatility in promoting a large number of synthetically important reactions. We have developed a variety of radical transformations using Ru-, Ir-, Pt-based photocatalysts and organophotocatalysts under visible light irradiation.

Fluoroalkylated organic compounds play significant roles in the pharmaceutical, agrochemical, and material sciences owing to the substantial influence that fluorine substitution has on the physical and chemical properties of substances. Visible light-induced methods allowed access to fluoroalkyl group-containing molecules, such as $-CF_3$, $-CF_2R$, $-CF_2SPh$, and $-CF_2OPh$ groups. In the studies, electron deficient carbon-centered fluoroalkyl radicals were successfully generated by the appropriate choice of fluoroalkyl source, photocatalyst, additives, and solvent. Notably, we have observed that additives significantly affect the efficiencies and selectivities of these reactions and can even change the outcome of the reaction by playing additional roles during its course. By understanding the roles of additives, we developed several controlled fluoroalkylation reactions where different products were formed selectively from the same starting substrates.



In addition, we designed a strategy for the synthesis of new class of synthetic building blocks, differential di-halo functionalized quinolines, utilizing photocatalytic activation of halogen bond donor-acceptor complex formed in situ between CBR_3F and *N*-methyl morpholine (NMM). In the process, a fluorinated reagent, CBR_3F was used as a one-carbon synthon and also as source of Br and F to provide 4-bromo-2-fluoroquinolines reacting with easily available 2-alkynyl anilines. The critical role of fluorine atom in CBR_3F for this transformation was realized by theoretical and experimental studies.



다차원 유기소재 연구단

Multidimensional Organic Materials Research Center

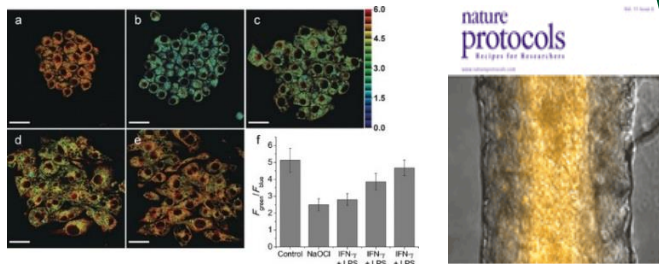
윤주영

Office : 82-2-3277-2400, E-mail : jyoony@ewha.ac.kr
 Homepage : home.ewha.ac.kr/~jyoony

이화여대 다차원 유기소재 연구단(단장 윤주영)은 분자인식 연구를 기반으로 하여 지능형 형광화학센서를 개발하고 있다. 특정 표적을 인식하는 물질과 형광체를 결합하여 생체내 이미징, 표적지향 약물전달 및 광열·광역학 치료가 가능한 물질을 개발하고 새로운 다차원 의약 전달 및 광열·광역학 치료 시스템 연구를 활발히 진행하고 있다.

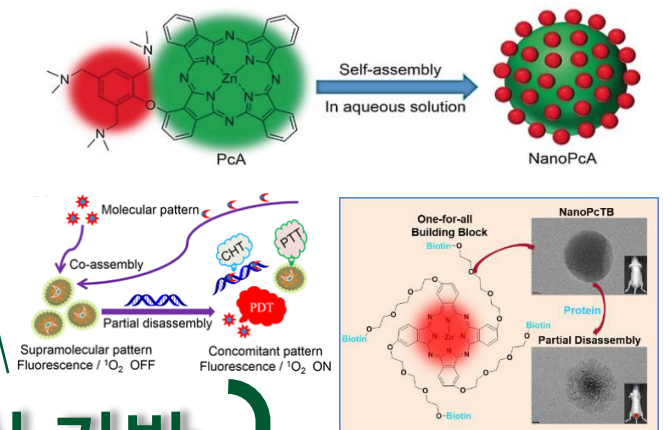
생체 내 주요물질 감지

활성산소종 (reactive oxygen species), biothiols 및 금속 이온 등에 선택적인 형광 프로브 연구



Angew. Chem. Int. Ed. 2018, 57, 1567.
 Nat. Protoc. 2016, 11, 1219.

광열/ 광역학 치료제 개발

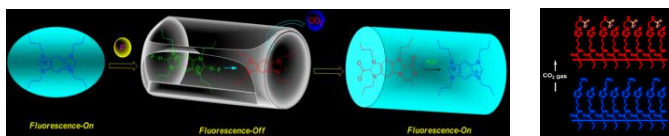


Angew. Chem. Int. Ed. 2018.
 ACS Nano 2018, 12, 681.
 J. Am. Chem. Soc. 2017, 139, 10880.

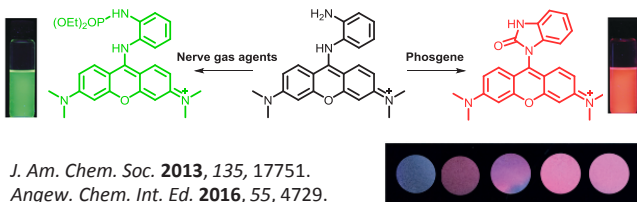
분자인식 기반 지능형 센서 연구

다양한 가스 검출

음이온과의 수소 결합 메커니즘 또는 고분자를 이용한 이산화탄소 형광 검출



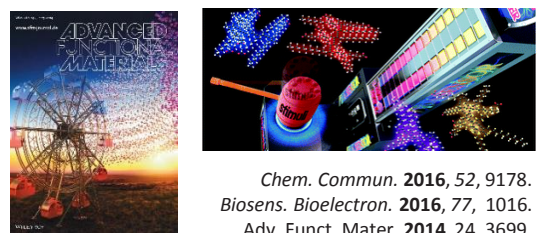
포스젠 가스를 색 또는 형광 변화로 검출할 수 있는 새로운 방법 제시



J. Am. Chem. Soc. 2013, 135, 17751.
 Angew. Chem. Int. Ed. 2016, 55, 4729.

Polydiacetylene (PDAs)

폴리디아세틸렌(PDA) 센서는 공액고분자 중의 하나로, 외부 자극에 의해 확연한 색 변화를 보이게 되어 다양한 센서 연구에 응용되고 있다.



Chem. Commun. 2016, 52, 9178.
 Biosens. Bioelectron. 2016, 77, 1016.
 Adv. Funct. Mater. 2014, 24, 3699.



전남대학교 화학과 기초연구실 (이선우교수)



한국연구재단
National Research Foundation of Korea

단일단계 합성법 개발 연구실

Single Step Synthesis Methodology Laboratory

광주광역시 북구 용봉로 77 전남대 화학과
Tel) 062-530-3385; E-mail) sunwoo@chonnam.ac.kr

연구단 소개

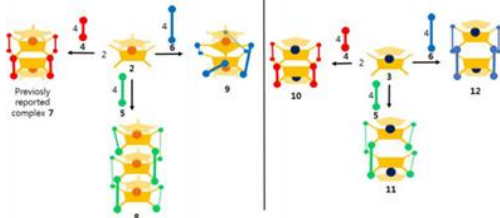
전남대 화학과 기초연구실이 수행하는 연구 과제는 유기물 합성, 리간드 디자인 및 합성, 그리고 촉매 제조 및 물성 조절에 대한 연구가 유기적으로 상호 작용하면서 복합적으로 진행되어야 하므로 단독 연구보다는 유기화학, 무기화학 및 촉매전문가들로 구성된 소규모 팀으로 진행한다. 따라서 본 연구실은 전이 금속 촉매를 이용한 합성법 개발에 대한 경험과 전문 지식이 있는 연구책임자를 중심으로 유기화학 분야 2인(유기반응법 개발 전문가, 유기촉매를 이용한 합성법 전문가)과 촉매반응 분야 2인(무기화학 분야 1인, 촉매화학 분야 1인)으로 구성하였다. 4명의 공동 연구진들의 전공 분야는 연구주제의 핵심 기술인 유기 합성(단일단계 다성분계합성법, 리간드 합성, 생리활성물질 합성)과 촉매(금속촉매, 유기촉매, 균일계촉매, 불균일계 촉매)이며, 이들은 과제의 성공적 수행을 위해 해당 분야의 전문 지식 및 연구력을 개별 과제 수행의 형태가 아닌 연구 책임자를 중심으로 한 상호 유기적인 관계를 바탕으로 연구를 진행하고자 한다.

대표성과목록

저널명	IF	JCR %	논문수	공동논문수
J. Am. Chem. Soc.	13.858	6.0	1	
Org. Lett.	6.579	5.1	3	1
Chem. Commun.	6.319	13.8	1	
Adv. Synth. Catal.	5.646	2.8	1	1
Chem. Eur. J.	5.317	17.4	1	
Inorg. Chem.	4.859	8.7	2	2
J. Org. Chem.	4.849	13.6	3	3
Mol. Catal.	4.211	24.6	1	
합계			13	7

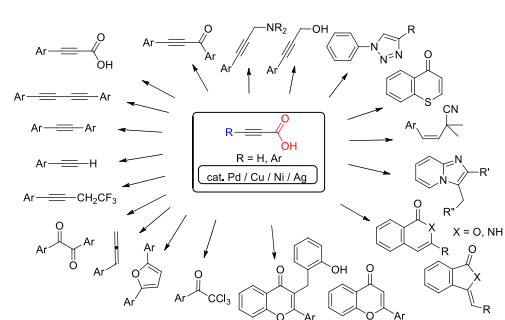
대표적 연구 내용 및 업적

선택적 반응 촉매 개발

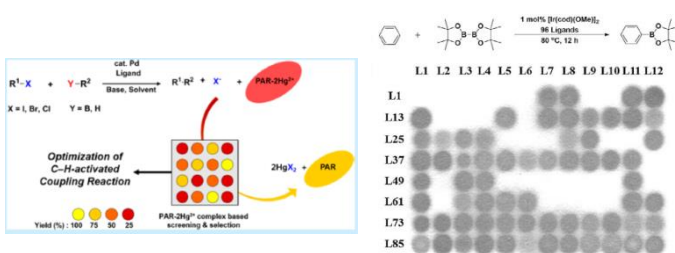


J. Am. Chem. Soc. **2015**, *137*, 13018–13023,
Inorg. Chem. **2017**, *56*, 5471–5477

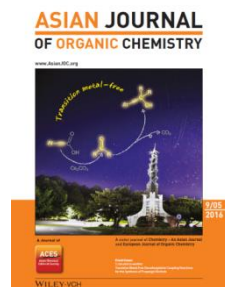
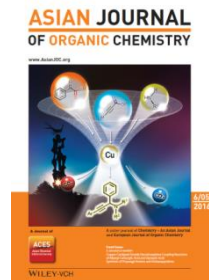
효율적 단일단계 합성법 개발



초고속 탐색법 개발



Org. Lett. **2016**, *18*, 1720-1723
Chem. Eur. J. **2017**, *23*, 6282-6285





한양대학교 화학과

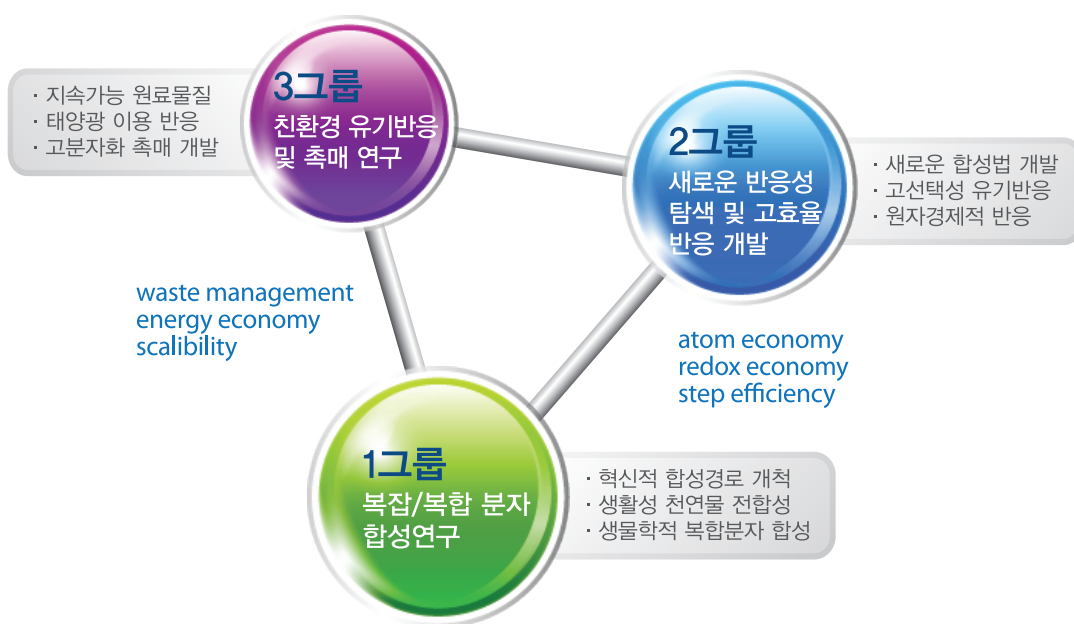
차세대유기합성연구센터

Center for New Directions in Organic Synthesis

2014년 5월 한국연구재단 선도연구센터(SRC)로 선정되어 새로운 효율성, 선택성, 환경친화성 유기반응의 개발과 이를 복잡/복합 유기분자 합성에 적용하는 새로운 형태의 통합적 협력연구를 수행하고 있습니다. 주요 연구내용은 새로운 반응성의 탐색을 통한 고효율, 고선택적 유기반응 개발, 친환경 유기반응과 촉매 시스템 개발, 그리고 합성전략과 경로의 개척을 통한 복잡/복합 유기분자 합성입니다.



- 제1그룹 : 조천규 (한양대학교), 하현준 (한국외국어대학교), David Y.-K. Chen (서울대학교), 신승훈 (한양대학교)
 제2그룹 : 윤소원 (한양대학교), 오창호 (한양대학교), 박철민 (울산과학기술대학교), 천철홍 (고려대학교),
 제3그룹 : 홍순혁 (서울대학교), 조은진 (중앙대학교), 정영근 (서울대학교)



멀티스케일 카이랄 구조체 연구센터

http://cmca.kaist.ac.kr

Center for Multiscale Chiral Architectures (CMCA)

2018년 6월 한국연구재단이 지원하는 선도연구센터로 선정된 멀티스케일 카이랄 구조체 연구센터(Center for Multiscale Chiral Architectures, CMCA; 센터장: 이희승)는 분자 수준 - 나노미터 수준 - 거시적 수준을 포괄하는 멀티스케일 카이랄 구조체의 구현 및 응용에 대한 통합적 집단연구를 목표로 하고 있습니다. 우리 연구센터는 향후 7년간 다양한 빌딩블록을 활용한 분자/나노미터/거시적 수준의 계층적 자기조직을 통해서 각 단계의 카이랄성이 제어된 멀티스케일 카이랄 구조체를 구현하는 예측가능하고 신뢰성 높은 합성 방법론을 개발하고자 합니다. 동시에, 멀티스케일 카이랄성에 관한 도전적 집단연구를 통해 기존의 한계를 극복하고 특정 스케일에 국한되지 않는 화학의 새로운 연구영역을 개척할 수 있을 것입니다. 카이랄 초분자화학을 공통분모로 갖되 이론, 물리, 유기, 무기, 나노, 고분자 등 화학의 모든 세부연구 분야를 대표하는 핵심 연구원들로 이루어진 CMCA 연구센터는 긴밀하고 유기적인 집단연구를 수행함으로써 제시한 목표를 달성하고 국가과학기술의 수준을 제고하는 데 크게 기여할 수 있는 선도 연구센터로 발돋움할 것입니다.



제1그룹

멀티스케일 카이랄성의 발현 및 상호전이원리 연구



제2그룹

외부자극 기반 멀티스케일 카이랄성 유도



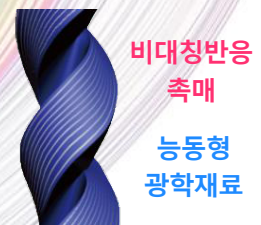
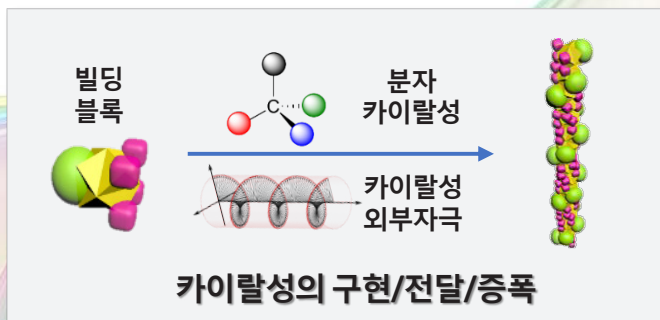
제3그룹

멀티스케일 카이랄성을 이용한 입체선택성 전이 및 증폭



기존 방법론의 한계를 뛰어넘는 멀티스케일 카이랄 구조체의 구현과 응용

- 카이랄성 전달 메커니즘의 이해에 기반한 멀티스케일 카이랄 구조체의 디자인 원리 확립
- 카이랄 상호작용의 제어를 통한 카이랄성의 전사 및 증폭



멀티스케일 카이랄 구조체의 응용

멀티스케일 카이랄 구조체 연구센터
Center for Multiscale Chiral Architectures (CMCA)

센터장 : 이희승 교수 (KAIST 화학과)
전화 : 042)350-2846
이메일 : hee-seung_lee@kaist.ac.kr

- 거대분자합성 연구단 @ 서울대학교 화학부 -

: 유기화학을 바탕으로 복잡하지만 규칙적이고 정교한 다양한 거대분자/고분자를 창의적/선택적/고효율적 방법으로 합성 및 응용을 추구합니다.

TLC's Lab

J. Am. Chem. Soc. **2011**, 133, 11904
J. Am. Chem. Soc. **2012**, 134, 14291
J. Am. Chem. Soc. **2013**, 135, 17695
J. Am. Chem. Soc. **2017**, 139, 3082
J. Am. Chem. Soc. **2018**, 140, 475
J. Am. Chem. Soc. **2018**, 140, 6088
J. Am. Chem. Soc. **2018**, 140, 8599

J. Am. Chem. Soc. **2012**, 134, 7270
J. Am. Chem. Soc. **2013**, 135, 3760
J. Am. Chem. Soc. **2013**, 135, 10769
J. Am. Chem. Soc. **2014**, 136, 10508
J. Am. Chem. Soc. **2015**, 137, 9262
J. Am. Chem. Soc. **2016**, 138, 2244
J. Am. Chem. Soc. **2016**, 138, 8612
J. Am. Chem. Soc. **2016**, 138, 11227
J. Am. Chem. Soc. **2017**, 139, 11309
Angew. Chem. Int. Ed. **2017**, 56, 14474
J. Am. Chem. Soc. **2018**, 140, 834
J. Am. Chem. Soc. **2018**, 140, 4335
J. Am. Chem. Soc. **2018**, 140, ASAP

Controlling Nanostructure

- Single molecules using dendrimers
- Self-Assembly via INCP & CDSA

Methodology


- TM Catalysis
- Living polymerization
- Cascade/tandem polym.
- Conjugated polymers

organic & polymer synthesis

Functional Materials

- OPV & OTFT
- Polymer sensors
- Organic memory

J. Am. Chem. Soc. **2007**, 129, 9842
ChemSusChem, **2014**, 8, 337
Polym. Comm., **2017**, 8, 7507
Adv. Fun. Mat. **2017**, 1606294



[연구원 모집]

본 창의연구단에서 세계 선도적 연구를 주도적으로 수행할 수 있는 창의적이고 역동적인 인재를 모집합니다. 열정적인 연구원들의 많은 관심과 지원 부탁드립니다.

1. 모집분야: 유기화학 전분야, 유기금속, 고분자화학
2. 지원자격: 상기 분야의 박사학위 소지자
3. 지원자 제출서류: CV와 학위 요약문 (최태림 교수: tlc@snu.ac.kr)

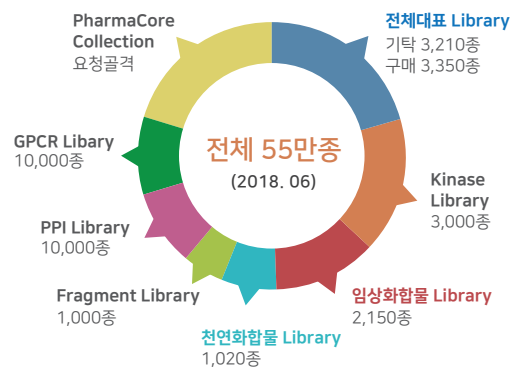


We take care of your compounds and create new value for you!

▶ 화합물 기탁의 장점

- 기탁 화합물에 대한 활용실적을 정기적으로 통보 받을 수 있음
- 기탁 화합물의 활용결과로 유효화합물(Hit)이 도출된 경우
 - 활용자와 협의하여 후속연구에 공동연구자로 참여 가능
- 기탁 화합물의 활용결과를 논문/특허 출판할 경우
 - 기탁자의 기여도에 따라 공동저자 및 공동출원인으로 참여 가능
- 기탁 화합물의 활용결과로 수익(기술료 등)이 발생할 경우
 - 기탁자의 기여도에 따라 수익의 일부를 분배 받을 수 있음

제공 라이브러리 종류



▶ 한국화학물은행의 역할

화합물 수집 및 관리



- 국내외 산·학·연에서 기탁된 55만종의 신약소재 화합물 보유
- 유기합성, 조합화학 합성화합물 및 천연물 라이브러리 보유
- 중요골격 화합물은 전문가 위탁합성 및 외국구매를 통하여 확보
- 다양성, 약물성 검비한 고수준 신약소재 화합물 75만종 확보 예정

화합물 약효시험(HTS) 활용지원



- 신약개발 및 BT 연구를 위한 고효율약효시험(HTS)에 화합물제공
- 800여개 신약개발 타겟 및 BT 프로젝트 연구에 활용
- 활용편의를 위한 목적별 라이브러리 구축 (천연물, 임상화합물 등)
- 신약개발 후속연구 지원(한국화학연구원 의약바이오연구본부 연계)

데이터베이스 구축 및 정보 제공



- 화합물 구조-물성-약효 통합정보시스템 구축
- 신약소재 화합물 정보 DB 구축 및 신약개발 관련정보 제공
- 국내 화합물 정보의 통합관리 및 효율적 공동활용 시스템 구축
- 기탁 화합물 및 약효시험결과를 매개로한 산·학·연 공동연구 중개

▶ 관리·유통 전담기관제도 및 의무기탁 규정

한국화학물은행은 국가연구개발사업 수행을 통해 창출된 연구성과물 중 화합물 및 관련 정보의 관리·유통 전담기관으로 지정되어 있습니다. (과학기술정보통신부고시 제2017-7호)



「공동관리규정」 제25조13항 : 국가연구개발사업을 통하여 창출된 성과물(화합물)은 전담기관에 의무적으로 기탁하여야 한다.

국가연구개발 우수성과 선정시 전담기관(한국화학물은행)에 기탁된 성과만 인정하도록 「국가연구개발 과제평가 표준지침」에 명시. (2016.12.09 개정)

▶ 화합물 기탁 및 활용에 관한 문의

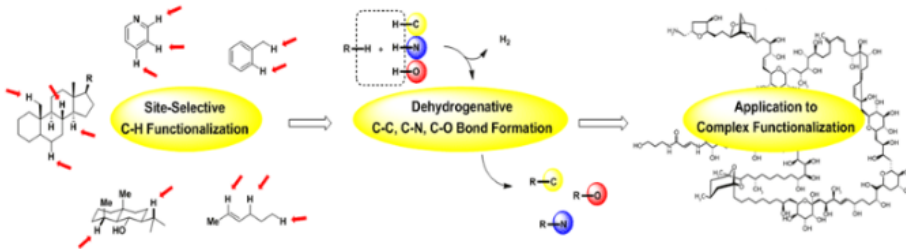


(우.34114) 대전광역시 유성구 가정로 141
한국화학연구원 한국화학물은행
Tel. 042-860-7190 Fax. 042-860-7096
E-mail : chembank@kRICT.re.kr
http://www.chembank.org

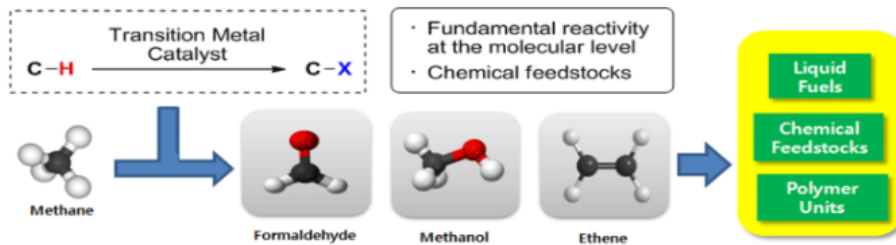
CCHF

CENTER FOR CATALYTIC HYDROCARBON FUNCTIONALIZATIONS

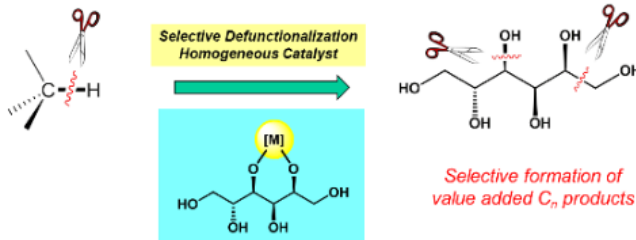
- Catalytic C-H bond Activation for Direct C-C, C-O and C-N bond Formation



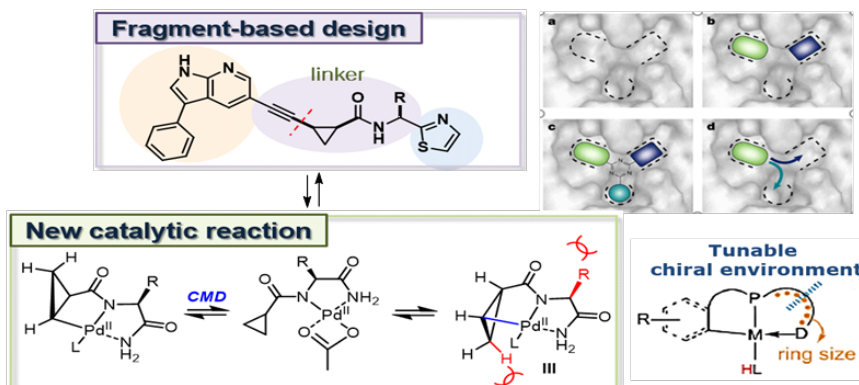
- Methane (CH₄) Functionalization



- Catalytic Selective Defunctionalization



- New paradigm in fragment-based approach to override drug resistance



CCHF에서는 세계적 수준의 연구를 수행할 창의적이고 역동적인 인재를 모십니다. 역량 있는 연구원들의 많은 관심 바랍니다.

모집분야

유기(금속)화학
계산화학
의약화학

Prof. Sukbok Chang

Office

042-350-2841

E-mail

sbchang@kaist.ac.kr

Web Site

sbchang.kaist.ac.kr

Prof. Sungwoo Hong

Office

042-350-2811

E-mail

hongorg@kaist.ac.kr

Web Site

ddnpslab.kaist.ac.kr

cchf.ibs.re.kr



Precious metal compounds and catalysts

20% 특별 할인!

담당자를 통한 주문에 한하여 할인가가 적용됩니다.

담당자 하순봉 책임 : 011-568-3100 (ayden.ha@thermofisher.com)

박찬진 선임 : 010-4489-7781 (cj.park@thermofisher.com)

* 기간 2018년 7월 1일 ~ 9월 30일

고순도 특수 금속 및 특수 애플리케이션용 원소 제조는 Alfa Aesar의 핵심 사업분야입니다. 당사는 순도가 매우 높은 제품을 전문적으로 개발하고 있습니다. Alfa Aesar는 고순도 귀금속 제품(금, 이리듐, 오스뮴, 팔라듐, 백금, 로듐, 루테튬 및 은) 및 귀금속 화합물, 귀금속 촉매제 등을 다양하게 공급하고 있습니다.

Precious Metal Compounds & Catalysts

Alfa Aesar는 350여 가지 이상의 광범위한 귀금속 화합물 및 촉매제를 공급하고 있습니다. 대부분의 재료는 생산 수량에 맞춰 재고로 확보하고 있기 때문에 즉시 배송이 가능합니다. 엄격한 품질 관리 기준과 종합적인 성분 분석표(Certificates of Analysis, CoA)를 통하여 제품의 품질에 중점을 두고 있습니다. 맞춤형 제조, 특수 포장 및 신속한 배송은 당사가 고객님께 약속 드리는 중요한 서비스입니다.

Precious Metal Compounds and Homogenous Catalysts

Alfa Aesar는 다양한 귀금속염 및 용액제를 엄격한 사양에 따라 제조하여 공급하고 있습니다. 균일 촉매제는 키타 치환을 비롯하여 고도의 특이 반응이 필요한 경우에 적합한 제품군입니다. 당사의 균일 촉매제는 여러 가지 화학변환에 사용될 수 있습니다.

Catalysts in Varying Purities and Concentrations

귀금속 화학 물질은 선택도가 높아 수소화, 수소화구소 첨가, 이성질체화, 카르보닐화 등 다양한 반응에서 불균일 촉매제로 가장 먼저 손꼽힙니다. Alfa Aesar는 제약 산업의 유기 합성을 비롯하여 다양한 연구에 맞는 순도와 농도를 제공합니다. 또한, Sponge Nickel™ 촉매제는 물론 비대칭 수소화 반응, 노벨 팔라듐 커플링 촉매제, 백금족 금속(PGM) 기반의 불균일 촉매제를 위한 일련의 키타 리간드를 제공합니다. 당사의 촉매 최적화 서비스에는 다단계 합성에서의 촉매 공정 개발, 지식-기반형 촉매제 선택, 제품 정제 기술(Smopex®) 및 공정 확장 등이 있습니다.

Fuel Cell Catalysts for Anodes, Cathodes, Electrodes

Alfa Aesar는 연료 전지의 연구 및 개발을 위한 촉매제와 관련 제품군을 벌크 또는 세미-벌크 수량의 재고로 독점 공급하고 있습니다. 귀금속 촉매제 HiSPEC® 계열은 연료 전지 연구를 위한 양성자 교환막(PEM) 및 직접 메탄올 연료 전지에서 뛰어난 성능을 갖고 있습니다. HiFUEL® 연료 개질 촉매제와 가스 처리 제품군은 연료 전지 및 기타 분산형 수소 처리 실험에 사용되는 비금속 촉매제입니다. Alfa Aesar는 Nafion® 교환막, Toray™ 카본지, 음극, 양극 및 막 전극 접합체(MEA) 제품을 비롯하여 다양한 연료 전지 구성 요소를 제공하고 있습니다.

Smopex® Scavenger Systems

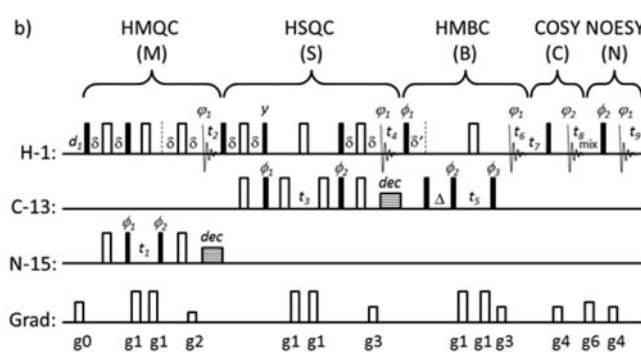
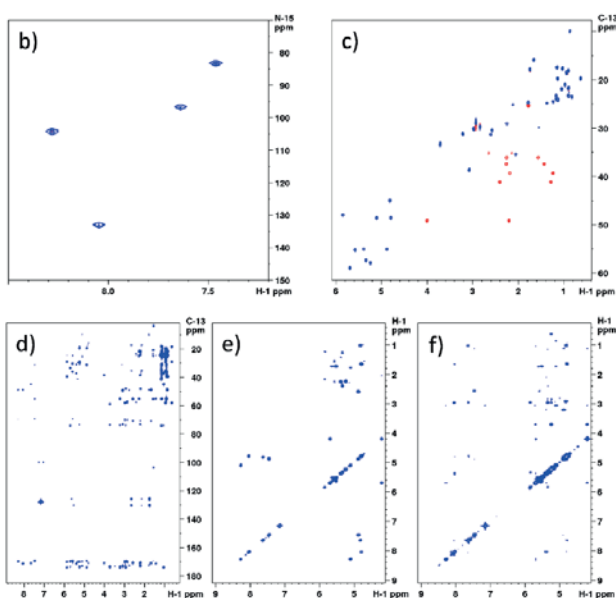
금속 촉매제는 제약산업에서 미립자를 효율적으로 치환 또는 결합할 수 있도록 쓰이고 있습니다. 이는 금속 촉매제가 아니면 불가능한 일입니다. 하지만, 이런 금속은 최종 제품에서 불순물로 남습니다. Smopex 금속 스캐빈저는 이러한 금속 불순물들을 제거하는 가장 효율적인 옵션 중 하나입니다.

Specialty Silver Compounds

Alfa Aesar는 고순도 은 제품에 특화된 선도 기업으로 잘 알려져 있습니다. 또한, 여러 가지 출발 물질을 채택하여, 특정 불순물을 지속적으로 제어해 나갈 수 있습니다. 당사는 한번 생산에 25 ~ 200kg까지 생산할 수 있는 능력도 보유하고 있습니다. 대다수의 은 화합물은 감광성이 있습니다. 당사의 모든 특수 은 화합물은 차광 기능의 용기에 포장됩니다. 또한, Alfa Aesar는 여타의 은 화합물도 맞춤형으로 개발하거나 제조하고 있습니다.



- Always multi-receive
- Further Enhanced dynamic range
- NMR Thermometer™
- Big performance in a small package



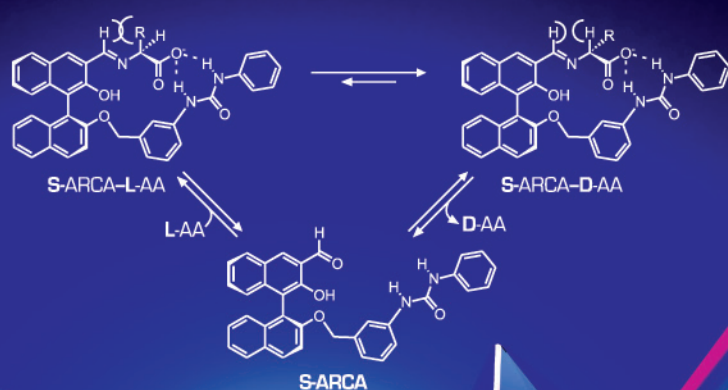
NOAH*: NMR Supersequences for Small Molecule Analysis and Structure Elucidation. Five conventional NMR pulse sequences combined into one supersequence: HMQC (¹⁵N), HSQC (¹³C), HMBC (¹³C), COSY, NOESY

think forward

NMR Solutions

A SIMPLE SOLUTION, A FULL SPECTRUM OF POSSIBILITIES

Our award-winning ARCA(Alanine Racemase Chiral Analogue) technology has the ability to produce almost any kind of unnatural amino acid through chiral resolution or chiral conversion. A unique technology with a competitive edge, AminoLogics is the solution.



- Unnatural amino acids
- Protected amino acids
- Amine compounds
- Chiral separation

AMINOLOGICS

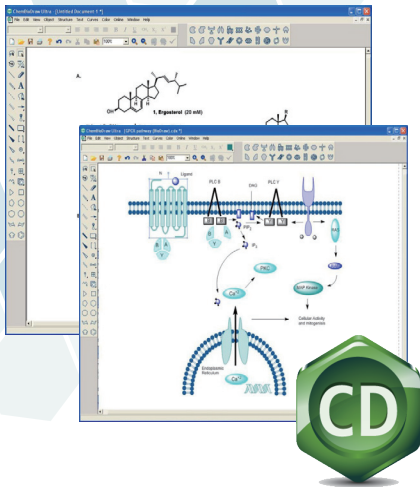
3F., Samoh B/D, 151 Yeoksam-ro, Gangnam-gu, Seoul, Republic of Korea

Tel: +82 2 761 4570 Fax: +82 2 553 4573 Email: aminoacid@aminologics.com www.aminologics.com

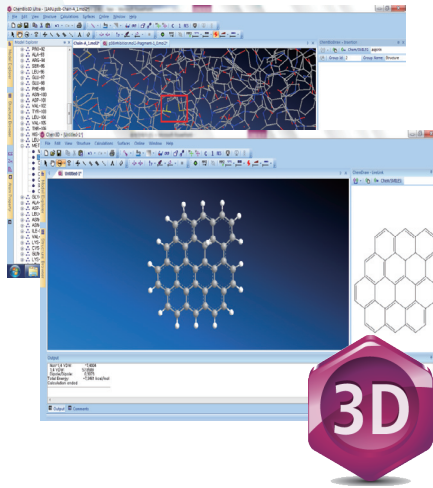
Site Subscription은 ChemDraw Professional과 ChemOffice Professional 두 가지 형태의 서비스를 제공합니다.

ChemDraw / ChemOffice Professional Application

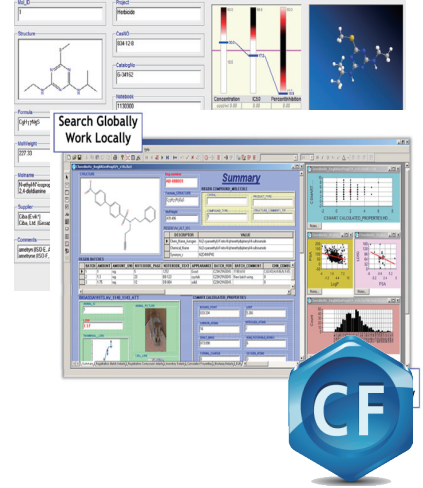
ChemDraw



Chem3D



ChemFinder



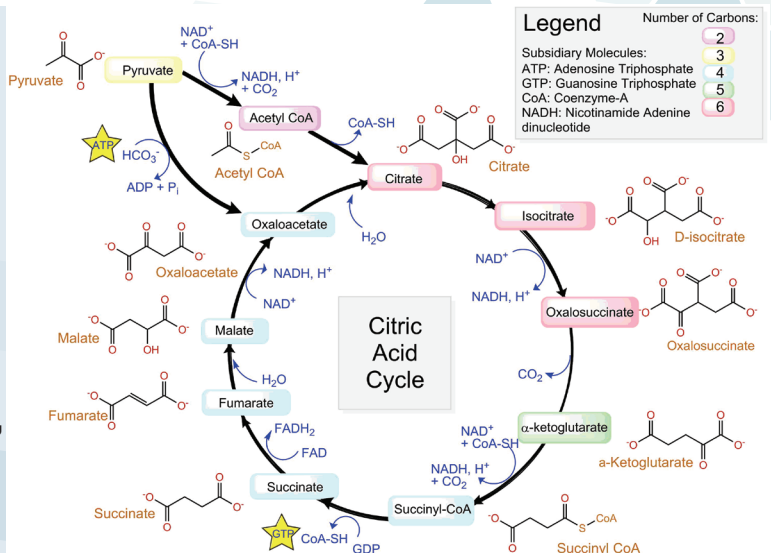
About Site Subscription

Site Subscription Service는 해당 기관의 도메인이 포함된 메일주소(@domain.xxx) 사용자에게 한해 인원 수 제한 없이 자유롭게 사용할 수 있는 연간 서비스입니다.

Site Subscription User에 한해 매년 1회 ChemDraw 제품군에 대한 사용자 방문 교육을 제공합니다.

ChemDraw 주요특징

- > 화학구조의 각종 physicochemical properties 예측, 1H/13C NMR 예측
- > 정확한 Stereochemistry 분석
- > 다양한 형태의 Biological drawing templates 지원(amino acids, peptides, DNA 및 RNA sequences 등 포함)



최적의 농축 시스템

Yamato 회전 증발 농축기 & Vacuubrand 진공 펌프



SINCE 1889



회전 증발 농축기

RE-301BW

- ◆ 원터치 전동 리프트
- ◆ 디지털 세팅 & 디스플레이
- ◆ 용매 고임 및 역류 방지 콘덴서
- ◆ 내구성과 진공도가 우수한 진공 seal

990만원
(부가세 별도)

vacuubrand

VACUUBRAND만의
지능형 'Adaptive' 진공조절 펌프

PC3001 VARIO

- ◆ 시료의 변화를 실시간 모니터링하여 최적의 진공조건을 제공
- ◆ 혼합물 각각의 끓는점을 감지하여 적응
- ◆ 고점도 물질 및 혼합물의 분리 농축에 최적
- ◆ 고속 증발 실현으로 30%이상 농축 시간 단축
- ◆ No Bumping
- ◆ 1.5 Torr, 33 L/min



(주)수림교역

www.sulim.com Tel. 031) 420-8670, Fax. 420-8673, E-mail. slc@chol.com

ChroZen* UHPLC, 생산성과 효율성을 위한 최고의 선택

* ChroZen은 Chromatograph와 정점, 절정을 뜻하는 Zenith의 합성어로
“최고의 분석기기를 약속하는” 영린기기의 의지가 담긴 새로운 브랜드 명입니다.



생산성 및 효율성의 극대화

ChroZen UHPLC는 동일 시료 분석 시 기존 HPLC 대비 4배~10배 빠른 분석 결과를 신뢰성 있는 데이터로 제공하며, 낮은 유속과 적은 시료 주입량 설정으로 이동상과 시료의 소모량을 최소화 하여 비용을 절감 함으로써 높은 생산성과 효율성을 보장합니다.

우수한 분리능과 감도

광량의 손실을 줄이면서 광학적 명확성(Optical Clarity)을 확보해 주는 Liquid Core Waveguide 기술이 적용된 Flow Cell을 장착하여 Path Length를 줄이지 않고도 시스템 확산(System Dispersion)을 감소시켰으며, 빠른 데이터 수집 속도로(125 Hz) 분석 결과를 정확하게 처리하여 감도와 분리능이 향상 되었습니다.

최고의 펌프 성능

직렬로 연결된 독립 구동 방식의 펌프 헤드를 통해 정확하고 정밀한 유속을 제공함으로써 데이터 재현성을 확보하고, 빠른 기울기 용리 적용을 통해 정밀한 용매 조성비를 구현해 냅니다.

견고한 내구성

ChroZen UHPLC는 실제 최대 내압 18,800 psi까지 수용이 가능한 견고한 시스템 내구성을 갖추었습니다. Column의 장기간 사용으로 인한 시스템 내압이 증가하더라도 ChroZen UHPLC의 높은 압력 범위는 Column의 최대 압력까지 사용할 수 있는 환경을 제공합니다.



LaboACE
Recycling Preparative HPLC



New Generation Recycling Preparative HPLC

Advanced Separation Efficiency

LaboACE LC-5060



JAI Japan Analytical Industry Co., Ltd.

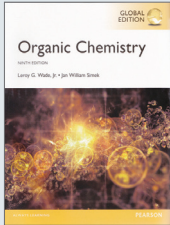
서울지사 : 02-553-1190

대전지사 : 042-638-1050

홈페이지 : www.jaikorea.co.kr

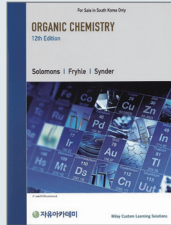


Organic Chemistry 9/e



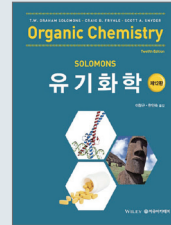
저 자: Wade 외
출 판 사: Pearson
출판년도: 2017년
쪽 수: 1400쪽
ISBN: 97811292151106

Organic Chemistry 12/e



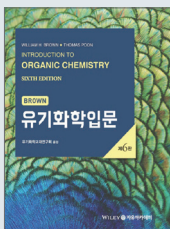
저 자: Solomons 외
출 판 사: Wiley
출판년도: 2016년
쪽 수: 1124쪽
ISBN: 9781118875766

유기화학 제12판



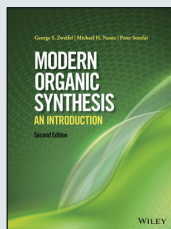
저 자: Solomons 외
역 자: 이창규 외
출판년도: 2017년
쪽 수: 1240쪽
ISBN: 9791158081263

유기화학입문 제6판



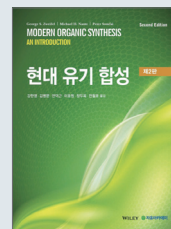
저 자: Brown 외
역 자: 유기화학교재연구회
출판년도: 2017년
쪽 수: 720쪽
ISBN: 9791158081195

Modern Organic Synthesis : An Introduction 2/e



저 자: Zweifel 외
출 판 사: Wiley
출판년도: 2017
쪽 수: 416쪽
ISBN: 9781119086536

현대 유기 합성 제2판



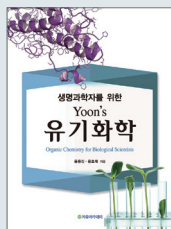
저 자: Zweifel 외
역 자: 강한영·김병문·안덕근
이효원·장두욱·전철호
출판년도: 2018년
쪽 수: 400쪽
ISBN: 9791158081645

이공학도를 위한 Yoon's 핵심유기화학



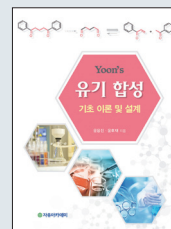
저 자: 윤용진
출판년도: 2015년
쪽 수: 592쪽
ISBN: 9791158080396

생명과학자를 위한 Yoon's 유기화학



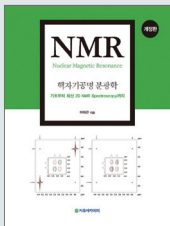
저 자: 윤용진·윤효재
출판년도: 2016년
쪽 수: 476쪽
ISBN: 9791158081133

Yoon's 유기 합성 기초 이론 및 설계



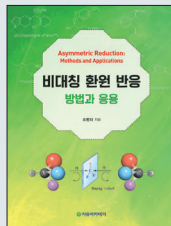
저 자: 윤용진·윤효재
출판년도: 2017년
쪽 수: 352쪽
ISBN: 9791158081485

NMR: 핵자기공명분광학 개정판



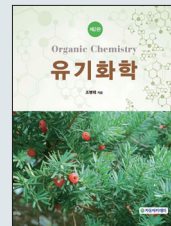
저 자: 이석근
출판년도: 2016년
쪽 수: 464쪽
ISBN: 9791158080952

비대칭 환원 반응 방법과 응용



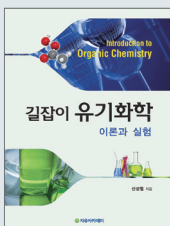
저 자: 조병태
출판년도: 2016년
쪽 수: 432쪽
ISBN: 9791158081065

유기화학 제2판



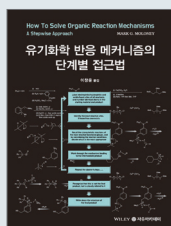
저 자: 조병태
출판년도: 2017년
쪽 수: 656쪽
ISBN: 9791158081355

길잡이 유기화학 이론과 실험



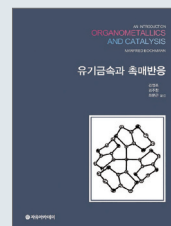
저 자: 신성철
출판년도: 2016년
쪽 수: 416쪽
ISBN: 9791158080464

유기화학 반응 메커니즘의 단계별 접근법



저 자: Moloney
역 자: 이창윤
출판년도: 2017년
쪽 수: 256쪽
ISBN: 9791158081188

유기금속과 촉매반응



저 자: Bochmann
역 자: 김영조·김주창·최문근
출판년도: 2018년
쪽 수: 424쪽
ISBN: 9791158081676

내일을 만드는 화학

خم집도 안 날만큼 강하게
하지만 깃털처럼 가볍게
모두 담는 것은 욕심일까
꿈에서만 가능한 이야기일까
가능해질 때까지 꿈을 꾸자
꿈의 소재를 만들자
모든 것의 기초가 될
내일의 바탕을 만들자



기술을 더욱 안전하고 스마트하게 진화시키는 **소재 솔루션**

LG화학은 금속을 대체할 만큼 강하면서도 가벼운 친환경적인 꿈의 플라스틱과 최적화된 스마트 솔루션을 제공하여 인류의 미래를 위한 소재를 만듭니다



유기합성 세계 최고의 전문가들이 검증한 Full-text resource 단독 제공!

Science of Synthesis

Full-text resource for methods in
synthetic organic chemistry

관련 문의: IDC ASIA(iGroup Korea)
김태형 팀장
Email: josephkim@igroupkorea.com
Tel: 02-6968-1708

Best methods. Best results.



Request
a free trial:
www.thieme.com/sos



보급형 MPLC system & Cartridge

www.isuind.co.kr



Tel : (02)576-3941 Fax : (02)576-1631

Keep It Simple, Smart



Interchim® Software ver. 5.1
User-friendly
Click & Drag Gradient
AGO

Unit Control
15" touch screen
Remote Control
USB x4

Fraction Collector
2 long racks
112 tubes 18x150mm
Drainage system of free collector

Modular & Easy to Maintain
Built to last

14" - 35.5cm width
Smallest footprint on the market

Solvent tray w/drainage system

Injection
Liquid or solid injection
Dry-Load w/column equilibration.

PF-XS 420 Ultra:
Load & Go™ technology: an automated
4 port electric valve manage solid injection
(Dry-load)

Pump
PF-XS420: Binary Gradient

PF-XS420+ & PF-XS 420 Ultra:
Quaternary Gradient + Air purge

| Accurate, Linear & Repeatable |

Detection
PF-XS420 & PF-XS420+: UV: 200-400nm
PF-XS420 Ultra: UV: 200-800nm
Multi wavelength & Scan collection
Spectral view & Purity confirmation
Flow Cell - optical length: 0.3mm

Flash columns up to F0800

Integrated flash cols holder

**When you see it first you'll wonder how we ever put so much technology and knowledge in such a small machine!
Don't question anymore yourself, now it's time to take pleasure in trying it.**

Though to follow you everywhere, the system fits into all fume hoods, nevertheless it can be installed on side safely with its fume enclosure option

PF-XS420* (220v)
P/N: 1R1070

PF-XS420* (110v)
P/N: 1R1071

PF-XS420 Ultra (220v)
P/N: 1R5880

PF-XS420 Ultra (110v)
P/N: 1R5881



Multiple Preparative HPLC LC-forte/R Series

Prep-HPLC, MPLC, CHIRAL, GPC All in One System!!

Chiral 분리를 위한
CHIRAL ART

Polymer, Olygomer 분리를 위한
YMC-GPC

천연물 분리를 위한
YMC-Actus Triart

추출물 분획을 위한
YMC-DispoPackAT



Prep-HPLC Mode

- 일반적인 분리 정제를 위한 Gradient Prep Mode
- 분석 HPLC의 Method를 그대로 Scale-up하여 분리 정제



Recycling Prep Mode

- Sample 순환을 이용하여 Column 길이의 한계 초월
- 유사한 구조, 유사한 물성, 유사한 분자량을 가진 화합물의 분리 정제

Prep GPC Mode

- 고분자 화합물을 분자량 크기별로 분리 정제
- Recycling 기법을 이용하여 분리 정제 효과 극대화

Prep Chiral Mode

- 분리 정제 중간에 Sample을 연속 주입 "Stacking Injection"
- 단일 용매 조건에서 단위 시간당 최대의 Chiral 분리 정제 가능

Prep MPLC Mode

- 천연물 추출물 분획에 최적화한 분리 정제 가능
- 효과적인 구간 분리 정제로 유효 물질 발굴 가속화
- 유기 합성물의 고순도/고수율 분리 정제



Free Demo in your site!!

YMC Co., Ltd.
<http://www.ymckorea.com>
 TEL. 031. 716. 1631

MPLC REVOLUTION



CombiFlash NextGen Family



< CombiFlash® NextGen 300+ >
Effective and easy Industry Leader
기능성과 편리성을 갖춘 최고사양 모델



- ◀ Faster
- ◀ Compact
- ◀ Convenient

지금 새로운
Teledyne ISCO MPLC
를 만나보세요!



< CombiFlash® NextGen 300 >
Needs Customizing
사용자의 요구사항으로 제작가능한 모델



< CombiFlash® NextGen >
Economical and Essential
필수적 기능을 갖춘 경제적 모델



(주)이우과학교역 <http://www.iwoo.co.kr/>
TEL:02)3473-2332 FAX:02)579-8873



Focus on Rotary Evaporation!

KJF Roti package!

#1. RC900/600 + SC920/950 + C900

#2. RC900/600 + N820 + VC900 + C900

*Option : N820 / 840 / 842 / 860 선택 가능.

Vacuum system



SC950



SC920

Roti package



C900



SC920



RC900

What's more?

- *High Tech – Remote Control
- *Compact – Inner Mount
- *Efficiency – Inverse Rotation



RC900

Vacuum controller



VC900

What's difference?

- *Safety – Condenser
- *Simple – Angle / Flask
- *Smart – Memory function



RC600

Gas pump



N810/ N820/ N840/ N842/ N860



Tel : 02-959-0257
www.knfkorea.com





Supporting the Whole Organic Workflow

Organic Synthesis



Biotage® Initiator+
Microwave Synthesizer

Purification



Isolera™ Flash Purification Systems

Evaporation



Biotage® V-10 Touch Evaporator

Biotage first pioneered microwave heating in chemical synthesis and pre-packed flash chromatography cartridges. Today, we are a trusted supplier of these technologies to chemistry professionals worldwide. Now open in Korea, we are ready to support every step of your drug discovery journey.

Contact Us today for a Free Demo.

QUICK FACT

회사명	(주)레고켐 바이오사이언스
설립일	2006. 5. 2
상장일	2013. 5. 10 (코스닥)
업종	의학 및 약학연구개발업
대표이사	김용주
자본금	52.9 억원
임직원수	115 명
본사	대전대덕구문평서로8-26
홈페이지	www.legochembio.com

THERAPEUTIC AREAS

- ADC/PDC
- 항생제
- 항응혈제
- 항염증제

CORE CAPACITIES

- 후보물질 발굴 및 사업화 경험과 능력
 - 30년 이상 선도물질 발굴 ~ 미 FDA 승인 전 과정 경험
 - 글로벌제약사들과 기술이전/공동연구 경험
- 핵심기술의 우수성
 - LegoChemistry 를 통한 후보물질 발굴 역량
 - ConjuAll 을 통한 차세대 ADC 원천기술 확보

RECENT CORPORATE HIGHLIGHTS

- 2018
 - LCB02-0133 항응혈제 중국판권 기술이전(Lee's pharm)
 - Takeda 와 신규 ADC 후보물질 발굴 위한 리서치 라이선스 계약 체결
 - ADC 플랫폼 미국 특허 등록
 - LCB17-0877 기술이전 (브릿지바이오)

CONTACT

김우식 IR, PR / 팀장
Tel: (042) 861-0688
Email: jdy@legochembio.com

세계적 신약개발의 꿈과 열정을 가진 사람들이 만든 회사

(주)레고켐 바이오사이언스는 대기업의 신약연구소장을 포함, 30 여년 넘게 신약이란 외길을 걸어오며, 우리나라 글로벌 신약연구개발의 길을 개척해 온 CEO 와 함께 역량 있는 연구진들이 힘을 합쳐 만든 신약연구개발 전문회사입니다.

그 동안의 신약개발 노하우를 집약한 "**LegoChemistry**" 란 합성신약 기반기술과 차세대 항암치료제인 ADC(Antibody-Drug Conjugate: 항체-약물 복합체) 원천기술을 획기적으로 개선한 "**ConjuAll**" 기반기술을 통해 글로벌 신약을 개발하고 있습니다.

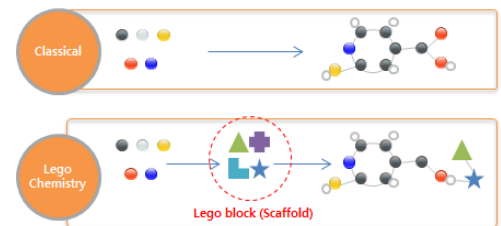
중장기적으로 임상개발 후보 5 개와 글로벌 기술이전 5 건 이상 보유라는 비전을 설정,

"오직 신약만이 살 길"이라고 믿는 꿈과 열정으로 가득 찬 사람들과 함께 세계적 경쟁력을 가진 대한민국의 대표적 신약개발 회사로 만들어 나갈 것입니다.

핵심기술

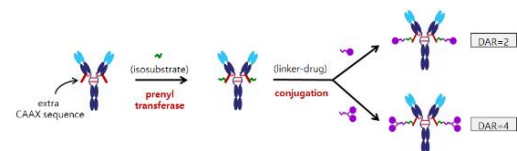
LegoChemistry™

의약화학 합성 기반기술을 바탕으로 한 효율적인 후보물질 발굴, 20 여개 이상의 고유 모핵구조(scaffold)를 기반으로 다양한 타겟에 맞는 맞춤형 신약후보를 신속하고 지속적으로 발굴할 수 있는 노하우 보유



차세대 ADC 링커기술 ConjuAll™

고유 기술 ConjuAll™ 을 통한 안전한 링커 및 단일물질의 차세대 항체-약물 결합체 (Antibody-Drug Conjugate, ADC) 개발로 기존 1 세대 ADC 기술의 한계를 극복한 차세대 원천기술 확보



신약 파이프라인

	Product	LCB / Partner	Target / Indication	Discovery	Preclinic	Phase 1	Phase 2
Antibiotics	LCB01-0371 (PO)	LCB	Gram+ (MRSA, VRE, S. pneumonia), M. tuberculosis		RMX		
	LCB01-0371 (IV)	LCB	Gram+ (MRSA, VRE, S. pneumonia), M. tuberculosis		RMX		
	LCB10-0200	LCB	Gram-negative bacteria (MDR-PA, A. baumannii, K. pneumoniae)		GEOM		
	β-lactamase inhibitor (BLI)	LCB	Gram-negative bacteria (MDR-PA, A. baumannii, K. pneumoniae)				
Anti-coagulants	Nokxaban (GCC-4401C/LCB02-0133)	Green Cross	Anti-coagulants				
Anti-inflammation	LCB17-0877	Bridge Bio	Novel ATX inhibitor		bridgebio		
ADC	LCB14-0110	Fosun Pharma	HER2		FOSUN PHARMA 复星医药		
	ADC14-1XXX	Green Cross	Mesothelin				
	ADC14-15XX	Takeda	Undisclosed		Takeda		



어디, 새로운 소재 없을까?

소재의 차이가 미래의 차이다

도레이첨단소재는 믿습니다. 소재, 그 무한한 가능성이 활짝 피어난다면,
미래는 지금보다 훨씬 즐겁고, 아름답고, 살기좋은 곳이 될 것입니다.

소재, 그 무한한 가능성

'TORAY' 도레이첨단소재

필름 광학용 필름 및 차세대 고기능 필름
섬유 위생용 및 산업용 부직포, 고기능 원사

IT 디스플레이 소재, 반도체 및 전자정보재료 등
친환경 수처리용 필터(RO, UF, MBR)

탄소섬유 산업용 탄소섬유, 탄소섬유 복합재료(CFRP) 등
PPS PPS수지, 컴파운드

LabNetwork Product

WuXi Catalog

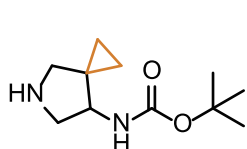
> 5,000 BBs in stock

> 3,000 Templates developed

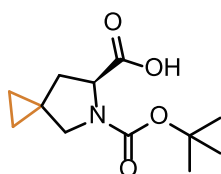
104K screening compounds



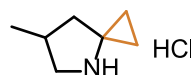
Cyclopropane Templates



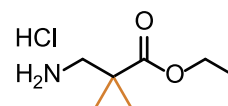
WXCD00100627



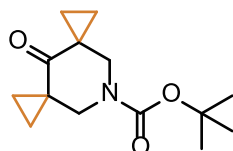
WXCD00102217



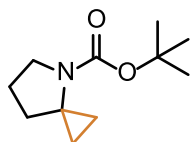
WXCD00300782



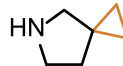
WXCD00192557



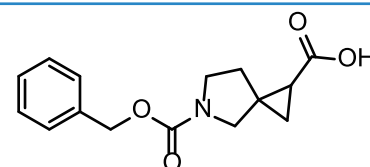
WXCD00102935



WXCD00100225

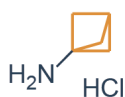


WXCD00100224

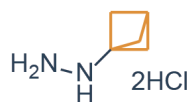


WXCD00100109

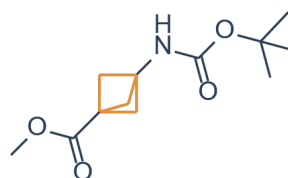
Bicyclo[1.1.1]pentane Building Blocks



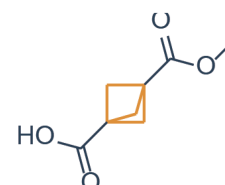
WXCD00601023



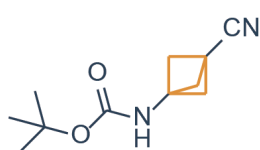
WXCD00304472



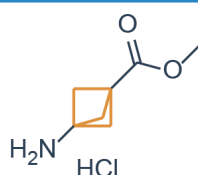
WXCD00120630



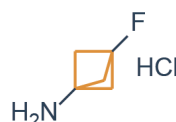
WXCD00120556



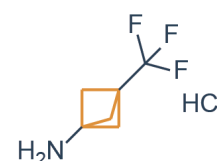
WXCD00120788



WXCD00120657



WXCD00120783



WXCD00601033

제 18회 유기화학분과회 하계워크숍 사은 이벤트



TOKYO CHEMICAL INDUSTRY CO., LTD.

행사기간 : 2018.8.20(MON)~22(WED)

(재고 소진시 이벤트가 사전종료 될 수 있습니다.)

100개
한정



P 플러스친구



10000²mAh

보조배터리

고정밀 배터리셀 사용

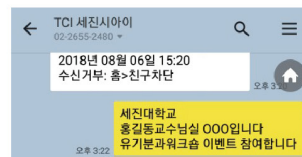
양방향 콕차지 지원

14.1mm의 초슬림 디자인

[참여방법]

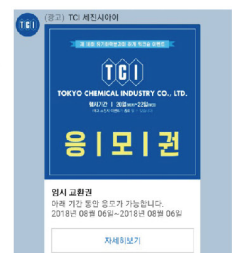
Step1. TCI 시약 구매하기 (웹, 플친, 전화, 현장 등 모든 주문 가능!)

Step2. 플친 구매 인증 후 교환권 받기



Step3. 사은품 교환하기

(20일 : 현장 교환, 21일~22일 : 택배발송)



<https://www.sejinci.co.kr>

<https://www.TCIchemicals.com/ko/kr>