PROGRAM BOOKLET

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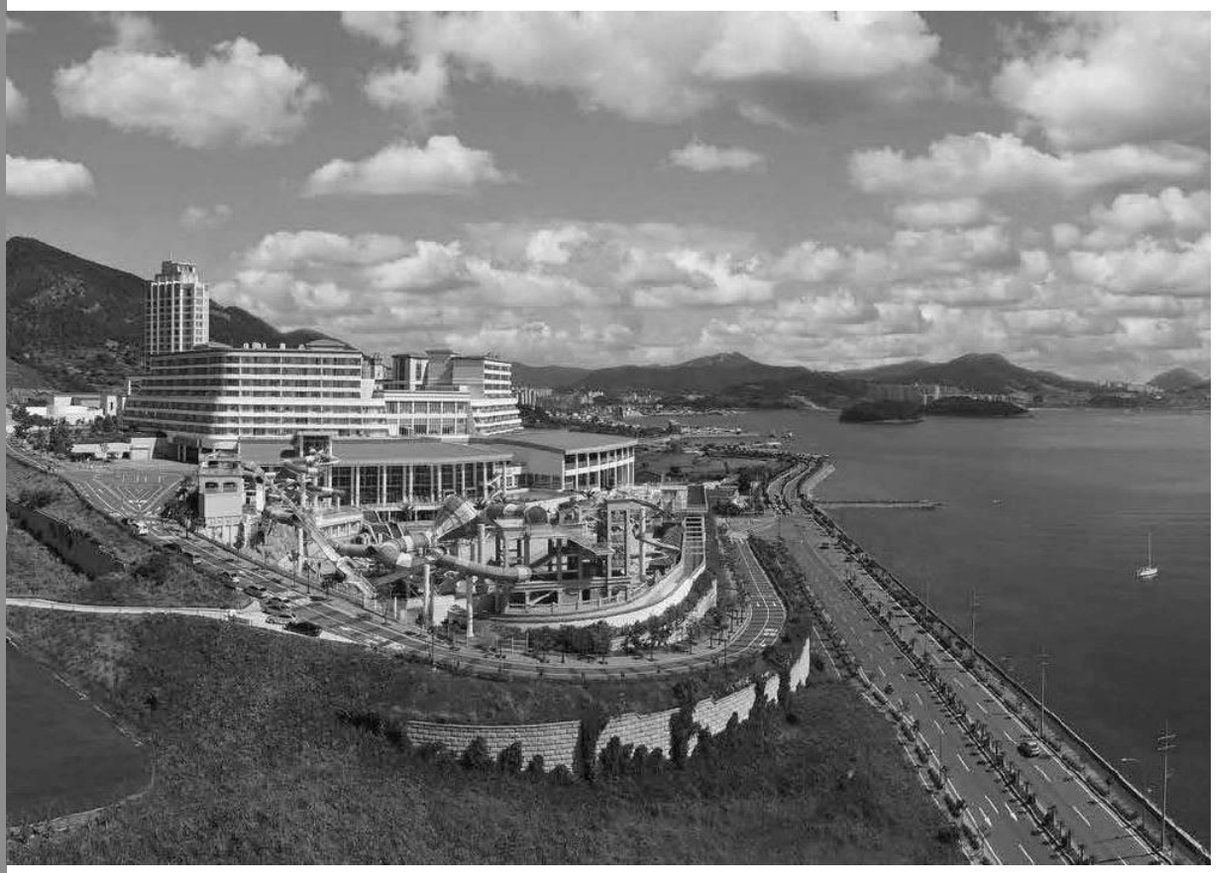
제19회 유기화학분과회 하계워크샵
제5회 유기화학 튜토리얼 강좌



2019년 8월 18일 – 20일

디오션 리조트, 여수

| 공식후원사 | TCI · 세진시아이

| 후원 | 여수시 전라남도 전라남도 문화관광재단

Korean Chemical Society
Division of Organic Chemistry

환영합니다

유기분과 하계 워크샵 참석 회원님들께,

제 19회 유기분과 하계 워크샵에 참석하신 모든 회원님들을 환영합니다. 올해는 여수에 위치한 디오션 리조트에서 많은 회원님들과 학생들을 모시고 성황리에 워크샵을 개최하게 되었습니다. 유기분과 운영진을 대표하여 감사의 말씀을 드립니다.

올해에는 회원님들의 다양한 의견을 참고하여 프로그램 운영에 있어서 약간의 변화를 주었습니다. 워크샵은 일요일(18일) 오후에 진행되는 튜토리얼로 시작합니다. 튜토리얼은 윤창수 (한국화학연구원), 고휘원 (한국써모피셔), 김현우 (카이스트), 정세희 (CAS한국지부) 강연자께서 실험실 안전, 질량분석법, 계산유기화학, SciFinder 활용법 등에 대하여 강연을 하십니다.

월요일(19일) 오전에는 젊은 유기화학자 상 시상 및 기념 강연이 예정되어 있습니다. 제 7회 수상자 주정민 부산대학교, 2018년 수상) 회원과 제 8회 수상자 유은정 경희대학교) 회원께 축하를 드립니다.

월요일(19일) 오후에는 포스터와 학생 구두 발표를 진행합니다. 학생들에게 연구 결과를 발표하고 토론하는 기회를 제공하고, 우수 포스터 및 우수 구두 결과 발표자를 선정하여 포상하며, 부산에서 개최되는 Junior ACP 학회의 참가 자격을 부여하는 자리입니다. 늘 그렇듯이 회원님들의 기대를 넘어서는 포스터와 구두 발표, 그리고 토론을 기대합니다.

제 19회 유기분과 하계 워크샵을 준비하는데 다양한 형태의 도움이 있었습니다. 재정적으로 도움을 주신 업체 관계자님 및 회원님, 워크샵에 참여하신 회원님, 또한 마음으로 응원해 주시는 회원님들께 감사를 드립니다. 문봉진 총무부회장을 비롯하여 양정운 학술부회장, 한수봉 홍보부회장, 조은진 운영위원, 김 민 운영위원, 조승환 운영위원께서도 많은 수고를 하셨습니다. 행정 업무를 총괄하신 김은경 실장님, 도우미 학생, 리조트 관계자 분들께도 깊은 감사를 드립니다.

하계 워크샵은 궁극적으로 학생들을 위한 자리입니다. 이 자리가 학생들에게 있어 연구 결과를 공유하고, 타 학교 학생들과 교류하며, 실험실에서 벗어나 재충전하는 시간이 되기를 바랍니다.

다시 한번 환영합니다.

2019년 8월 18일

대한화학회 유기화학분과회 회장 **이 덕 형**

■ 2019년 8월 18일 (일)

Tutorial Session

14:00 – 15:00 튜토리얼 세션등록

15:00 – 15:05 튜토리얼 세션 개회사 및 인사말씀

진행: 한수봉 (한국화학연구원)

15:05 – 15:45 튜토리얼 강연 I (윤창수, 한국화학연구원)

- 유기화학 실험실 안전

15:45 – 16:25 튜토리얼 강연 II (고휘원, 써모피셔)

- 유기화학자가 꼭 알아야 할 질량분석법 원리

16:25 – 16:40 Coffee Break

16:40 – 17:20 튜토리얼 강연 III (김현우, KAIST)

- 초심자를 위한 계산유기화학 교육

17:20 – 17:50 튜토리얼 강연 IV (정세희, CAS)

- 유기화학자들을 위한 전략적 SciFinder 활용법

■ 2019년 8월 19일 (월)

Session I

10:00 – 10:55 등록 (포스터 부착)

진행: 문봉진 (서강대학교)

10:55 – 11:00 개회사 및 인사말씀

11:00 – 12:00 젊은 유기화학자상 시상 및 기념강연

- 제7회 수상자: 부산대학교 화학과 주정민
- 제8회 수상자: 경희대학교 응용화학과 유은정

12:00 – 13:30 점심 식사 (포스터 부착)

Session II

진행: 이준희 (동국대학교)

13:30 – 15:00 포스터 발표

15:00 – 16:00 학생발표 (10분 발표 + 2분 질의응답; OL01 – OL05)

16:00 – 16:20 Coffee Break 및 기념촬영

16:20 – 17:30 학생발표 (10분 발표 + 2분 질의응답; OL06 – OL11)

17:30 – 17:50 Coffee Break

17:50 – 18:20 학생 구두 및 포스터 우수발표자 시상

■ 2019년 8월 20일 (화)

09:30 – 11:00 그룹별 자유토론

11:00 – 11:30 폐회식

유기화학 실험실 안전 (Chemical Lab Safety)

윤 창 수
한국화학연구원 의약바이오연구본부
E-mail: csyun@krict.re.kr

유기화학실험실에서 직접 연구활동에 참여하고 있는 대학원생들에게 실험실 안전의식을 향상시키고 안전 사고 예방을 위하여 아래와 같은 내용의 주제를 가지고 실험실 안전 교육을 다루고자 한다.
또한, 실험실내 사소한 부주의로 인하여 발생할 수 있는 실제 화학실험실 사고사례 등을 살펴보며 안전한 실험 및 안전한 연구환경 유지를 위한 방안을 제시하여 유기화학 실험실 안전 확보에 도움을 주고자 한다.

1) 개인보호장구 (Personal Protective Equipments, PPEs)

2) 응급 상황 시 대처 요령 (Emergency Situation)

3) 유해 화학물질 사용 및 보관 (Chemical Hazards)

4) 화학실험실 사고 사례 (Chemical Accidents)

윤 창 수 (Chang-Soo Yun)

Address

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Education

Ph.D. (2000)	Department of Chemistry, Korea University (Prof. Deok-Chan Ha)
M.S. (1996)	Department of Chemistry, Korea University (Prof. Deok-Chan Ha)
B.S. (1994)	Department of Chemistry, Chungnam National University

Position

2017-Present	Principal Researcher, Korea Research Institute of Chemical Technology (KRICT)
2003-2017	Senior Researcher, Korea Research Institute of Chemical Technology (KRICT)
2002-2003	Post-doc, Johns Hopkins University (Prof. Michael S. Yu)
2000-2002	Post-doc, University of Pennsylvania (Prof. Gary A. Molander)

Representative Publications

1. “A natural compound, aristoyagonine, is identified as a potent bromodomain inhibitor by mid-throughput screening”, Y. H. Kim, M. Kim, M. Yoo, J. E. Kim, H. K. Lee, J-N. Heo, C. O. Lee, M. Yoo, K-Y. Jung, C-S. Yun, S. W. Moon, H. K. Chang, C-W. Chung, S. Pyo, S. U. Choi, C. H. Park, *Biochem. Biophys. Res. Commun.* **2018**, *503*, 882.

2. “Zebrafish as a screening model for testing the permeability of blood-brain barrier to small molecules”, C. Woo, H. R. Kim, B. H. Lee, J. S. Song, C-S. Yun, M. Bae, P. Kim, S. Ahn, J. Y. Yang, D. S. Shin, G. R. Kim, S. S. Kim, J. Che, S. H. Lim, K. Lee, J. Ahn, Y. Lee, *Zebrafish*, **2017**, *14*, 322.

3. “Novel 2,4-diaminopyrimidines bearing fused tricyclic ring moiety for anaplastic lymphoma kinase (ALK) inhibitor”, R. Achary, G. R. Mathi, D. H. Lee, C-S. Yun, C. O. Lee, H. R. Kim, C. H. Park, P. Kim, J. Y. Hwang, *Bioorg. Med. Chem. Lett*. **2017**, *27*, 2185.

What is LC-MS? : 유기화학자가 꼭 알아야 할 질량분석법 원리

Hwee-Won Koh
Thermo Fisher Scientific, Seoul 06349, Republic of Korea
E-mail: hweewon.koh@thermofisher.com

A wide range of studies on organic chemistry using mass spectrometry is drawing attention to the need due to its high resolution and accurate mass. Therefore, analyses of organic chemistry combined with state-of-art mass spectrometry are increasing along with improvement of both instrumentation and software.
We will present first-hand a short but eventful history of Orbitrap mass spectrometry, from laying down the first principles to its current status as the leading mass spectrometric technique for high-resolution, high accuracy quantitative analysis.
In this presentation, introduce basic LC-MS theory and the newest Orbitrap MS Spectrometer for an organic chemist.

고 휘 원 (Hwee-Won Koh)

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Education

M.S. (2002) Department of Chemistry, Yonsei University

Position

2015- Present Thermo Fisher Scientific / Chromatography & Mass Spec Division
Manager, Application Scientists

2002-2015 SCINCO CO. LTD. (Thermo Fisher Scientific Exclusive Distributor)
Application & Marketing Manager

초심자를 위한 계산유기화학
Beginner's Guide to Computational Organic Chemistry

Hyunwoo Kim
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최근 계산화학 특히 양자화학이 각광을 받고 있습니다. 계산화학의 발전으로 인해 분자의 평형상태 구조, 반응 에너지와 같은 중요한 값들을 상당히 정확하게 얻을 수 있게 되었습니다. 지난 수십 년간 발전해온 컴퓨터의 발전과 더불어 "괜찮은 수준의 이론"을 "실제 시스템"에 적용시킬 수 있는 여건이 마련되었습니다. 또한 컴퓨터 소프트웨어의 발전으로 인해 특별한 교육과 이론적 이해가 없어도 계산화학을 수행할 수 있게 되었습니다. 그래서 지금은 계산화학이 화학 전 분야에 있어 필수적인 요소가 되었으며, 유기화학 분야에서도 계산화학의 중요성은 계속 강조되고 있습니다.

하지만 유기화학 분야 연구자는 실험에 대한 이론과 통찰력을 바탕으로 연구를 수행하고 있으며, 논문에 포함될 추가적인 논의 자료로 계산화학을 주로 활용하고 있습니다. 본 강의에서는 계산화학 프로그램을 전혀 사용해 보지 않은 유기화학자들을 대상으로, 계산화학을 수행하는 방법을 간단히 소개하고, 앞으로 유기화학 연구에 있어 계산화학을 활용하는 몇 가지 개인적인 팁을 공유하고자 합니다.

Reference

"A Guide to Molecular Mechanics and Quantum Chemical Calculations" Warren J. Hehre, 2003. Available at www.wavefun.com

김 현 우 (Hyunwoo Kim)

Address

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Education

Ph.D. (2009) Department of Chemistry, University of Toronto (Prof. Jik Chin)
M.S. (2004) Department of Chemistry, Seoul National University (Prof. B. Moon Kim)
B.S. (2000) Department of Chemistry, Seoul National University

Position

2011-present Assistant/Associate Professor, KAIST
2010 Post-doc., Columbia University (Prof. James L. Leighton)

Representative Publications

1. “A Gallium-based Chiral Solvating Agent Enables the Use of ^{1}H NMR Spectroscopy to Differentiate Chiral Alcohols”, S. Jang, H. Kim, *iScience* **2019**, *accepted*.
2. “Ligand-Controlled Direct Hydroformylation of Trisubstituted Olefins”, T. Shin, H. Kim, S. Kim, A. Lee, M.-S. Seo, J. Choi, H. Kim, H. Kim, *Org*. *Lett*. **2019**, 21, 5789 [**Featured as a Cover**].
3. “Hydrogen-Bonding Assisted Ketimine Formation of Benzophenone Derivatives”, M.-S. Seo, S. Jang, H. Jung, H. Kim, *J. Org. Chem.* **2018**, 83, 14300 [**Featured as a Cover**].
4. “Chiral Aluminum Solvating Agent (CASA) for ^{1}H NMR Chiral Analysis of Alcohols at Low Temperature”, M.-S. Seo, S. Jang, H. Kim, *Chem*. *Commun*. **2018**, 54, 6804 [**Featured in Emerging Investigators Issue 2018**].
5. “^{1}H NMR Chiral Analysis of Charged Molecules via Ion Pairing with Aluminum Complexes”, M.-S. Seo, H. Kim, *J*. *Am*. *Chem*. Soc. **2015**, *137*, 14190.
6. “Rhodium-Catalyzed Asymmetric 1,4-Addition of ,-Unsaturated Imino Esters Using Chiral Bicyclic Bridgehead Phosphoramite”, S. Lee, H. Kim, *J*. *Am*. *Chem*. Soc. **2015**, 137, 11250.

Strategic SciFinder Search for Organic Chemists
유기화학자들을 위한 전략적 SciFinder 활용법

SeHee Jung
Customer Success Specialist, ACS International
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CAS, a division of the American Chemical Society, is a global organization of expert scientists, technologists and business leaders with a successful and long history of over 110 years delivering scientific information. Everyday, CAS collects and analyzes the world's disclosed science to help advance discovery and accelerate innovation.

Through analytical studies of the last two decades worth chemical information gathered by CAS, 3 significant information trends were observed. The volume of information available in scientific journals and patents has grown exponentially over time. The complexity of the data indexed in patents has increased. It is now common to see patents with numerous notable chemical compounds of concepts that need to be made discoverable. Boundaries are blurring between different research areas and scientific disciplines. The interconnected data means your next idea could come from someplace unexpected.

Therefore, time is critical in obtaining the latest and most accurate information as you are balancing multiple projects and needing to get back to the lab to complete your current studies. Herein, I will introduce the most efficient way to search chemistry information in SciFinder and how to manage the results to quickly transfer to your journal publication.

1) Reaction search using Structure drawing editor
2) Analyzing and refining reaction results
3) Simplifying chemical structure for broader reaction searches
4) How to use SciPlanner
5) Transferring the saved answers to citation manager software

At the end of this lecture, you will be a step forward to being a SciFinder expert.

정 세 희 (SeHee Jung)

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Education

M.Chem (2013) Department of Chemistry, University of Oxford (Prof. Mark Moloney)
B.A. (2012) Department of Chemistry, University of Oxford

Position

2018-Present Customer Success Specialist, ACS International
2013-2016 Research Scientist, LG Chem

Representative Patents

1. “Polymerization composition, polymer using polymerization composition, and polymer electrolyte membrane therefrom”, S. Jung, J. J. Han, H. W. Ryu, Y. J. Jang, Y. Kim, E. Kang, WO2016068606 (2016).
2. “Ion exchange membrane, electrochemical cell, flow battery and fuel cell comprising thereof, and its manufacturing method”, S. H. Jung, M. E. Seo, J. J. Han, C. S. Jeon, Y. J. Jang, KR2017092321 (2017).
3. “Compound comprising aromatic ring and polymer electrolyte membrane using same”, Y. J. Jang, J. J. Han, Y. Kim, E. Kang, S. Jung, H. W. Ryu, WO2016122287 (2016).
4. “Fluorine-based compound for brancher, polymer therefrom, and polymer electrolyte membrane therewith”, H. W. Ryu, S. Jung, J. J. Han, Y. J. Jang, Y. Kim, E. Kang, WO2016068605 (2016), KR2016050005 (2016), CN107074706 (2017), KR1771323 (2017), EP3214070 (2017), JP2017538661 (2017), JP6447850 (2019), US20170226054 (2017).
5. “An aromatic ring-containing compound, a polymer polymerized from the same, a polymer electrolyte membrane, an electrolyte type fuel cell, and a redox flow battery”, Y. J. Jang, J. J. Han, Y. Kim, E. Kang, S. Jung, H. W. Ryu, Y. Yu, WO2016122195 (2016), KR2016091842 (2016), CN107207427 (2017), EP3252034 (2017), KR1821479 (2018), JP2018509488 (2018), JP6460243 (2019), CN107207427 (2019), EP3252034 (2019), US20180006320 (2018).

제7회 젊은 유기화학자 수상자

주정민 (Joo, Jung Min): 부산대학교 화학과

학력 및 경력

2001	서울대학교 화학과, 이학사
2003	서울대학교 화학과, 이학석사 (지도교수: 이은)
2008	Princeton Univ. 화학과, 이학박사 (지도교수: Chulbom Lee)
2009 – 2011	Columbia Univ. 박사 후 연구원 (지도교수: Dalibor Sames)
2011 – 2013	Eli Lilly and Company, 연구원
2013 – 현재	부산대학교 화학과, 조교수/부교수

연구분야: 헤테로고리 합성방법론 연구와 기능성 물질로의 응용

C−H Functionalization of Five-membered Heteroarenes with Alkenes and Alkynes

Jung Min Joo

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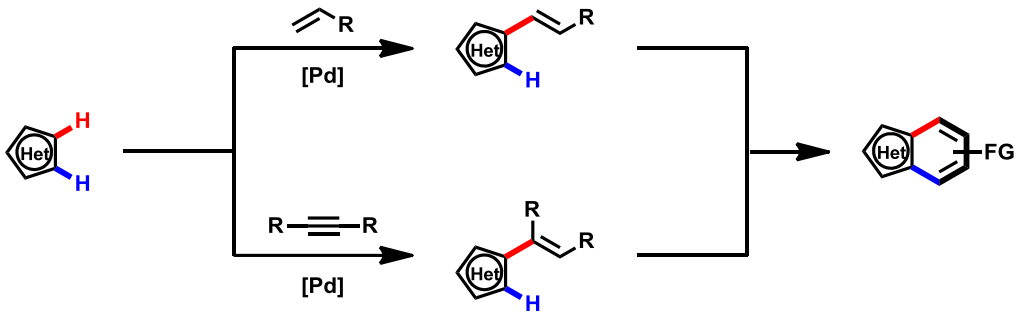
Heteroarenes are a ubiquitous structural motif of new pharmaceuticals, agrochemicals, and functional materials. Thus, the development of methods for the synthesis of structurally diverse heteroarenes represents an important objective in organic synthesis. We have developed Pd-catalyzed C−H functionalization reactions of five-membered heteroarenes using alkenes and alkynes. Electronic characters of palladium catalytic systems were manipulated to achieve regioselective C−H functionalization of nitrogen-containing five-membered heteroarenes, such as pyrazoles, imidazoles, and pyrroles. Readily available acrylates, acryl amides, and styrene derivatives as well as terminal and internal alkynes were employed as alkenyl group donors in these C−C bond forming reactions to provide alkenyl heteroarenes with desired substitution patterns. Furthermore, a benzannulation strategy involving subsequent C−H functionalization followed by oxidative cyclization was developed to afford benzo-fused heteroaromatic rings. This approach allows the systematic preparation of new, highly functionalized heterocyclic compounds and their applications to ligands for transition-metal-catalyzed reactions and redox active materials.



제8회 젊은 유기화학자 수상자

유은정 (Yoo, Eun Jeong): 경희대학교 응용화학과

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연구분야: 금속 촉매 반응의 방법론 연구 및 헤테로 고리 합성법 개발

Synthesis of N-Heterocycles via Cycloadditions of N-Aromatic Zwitterions

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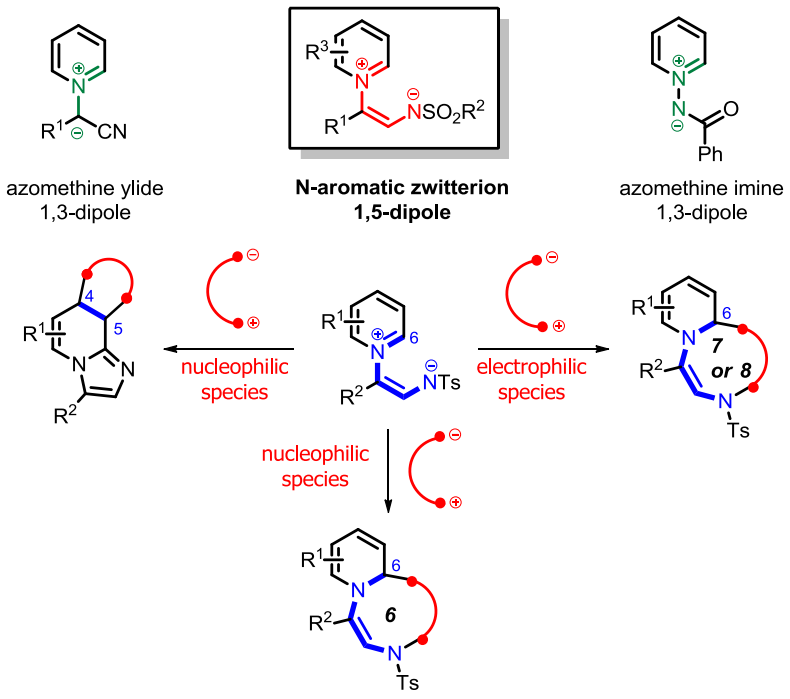
[*m*+*n*]-Dipolar cycloaddition is a powerful and widely used strategy for synthesizing heterocyclic compounds in a single operation without giving rise to byproducts. Most studies have mainly focused on [3+2]-dipolar cycloaddition using well-known 1,3-dipoles and 2π-dipolarophiles, while scarce attention has been focused on the development of new types of dipoles, such as 1,2-dipole, 1,4-dipole, and 1,5-dipole, for the formation of non-five-memberted heterocycles. An air-stable N-aromatic zwitterion is efficiently prepared via the rhodium-catalyzed reaction between heteroarenes and 1-sulfonyl-1,2,3-triazoles. This unprecedented N-aromatic zwitterion is quite stable and exhibits different pattern of charge distribution in comparison with that of typical azomethine ylides. In this presentation, 1,5-dipolar cycloaddition of N-aromatic zwitterions, which is an extraordinary tool for formation of medium-sized N-heterocyclic compound, will be present.

In addition, the site-selective cycloaddition between N-aromatic zwitterions and dipolar species, which could provide fused N-heterocyclic compounds, will be discussed. The successful development of the various straightforward routes for biologically relevant N-heterocycles demonstrates the potential utilities of N-aromatic zwitterions in organic syntheses.



[OL01] **Seung Youn Hong, Yoonsu Park, Yeongyu Hwang, Yeong Bum Kim, Mu-Hyun Baik,* Sukbok Chang***, Selective Formation of γ-Lactams via C−H Amidation Enabled by Tailored Iridium Catalysts, *Department of Chemistry, Korea Advanced Institute of Science and Technology (KAIST).*

[OL02] **Kyu Ree Lee, Da Jung Jung, Sang-gi Lee***, Catalyst-controlled divergent intramolecular cyclization of *N*-sulfonyl-1,2,3-triazoles with allyl alcohol, *Department of Chemistry and Nanoscience (BK 21 Plus), Ewha Womans University*.

[OL03] **황준영, 지아영, 이상혁, 강은주***, Redox-selective Iron Catalysis for α-Amino C-H Bond Functionalization via Aerobic Oxidation, *Department of Applied Chemistry, Kyung Hee University.*

[OL04] **Woohyeong Lee, Changhoon Shin, Soo Eun Park, Jung Min Joo***, Pd-Catalyzed Hydroarylation of Diaryl Alkynes with Azoles, *Department of Chemistry and Chemistry Institute of Functional Materials, Pusan National University.*

[OL05] **Kyeong-Im Hong, Hyeongcheol Kim, Woo-Dong Jang***, Triazole-bearing Calix[4]pyrrole as an Ion-pair Receptor for Lithium Chloride, *Department of Chemistry, Yonsei University.*

[OL06] **Jiyun Kim, Hyungwoo Hahm, Ji Yeon Ryu, Junseong Lee, Sukwon Hong***, Pyridine chelated Imidazo[1,5-a]pyridine N-Heterocyclic Carbene Nickel(II) Complexes for Acrylate Synthesis from Ethylene and CO_2, *Department of Chemistry, Gwangju Institute of Science and Technology (GIST).*

[OL07] **Hyungmo Koo, Hunyoung Kim,* Kyungsoo Oh***, Modularized Troubleshooting Continuous-Flow for Organic Reactions: Synthesis of Isoxazoles Using Acyl Chlorides and Alkynes, *Center for Metareceptome Research, College of Pharmacy, Chung-Ang University*.

[OL08] **Jiye Jeon, Cheol-Hong Cheon***, Development of A Novel Synthetic Route for Hinckdentine A, *Department of Chemistry, Korea University.*

[OL09] **Han-Sung Kim, Sunwoo Lee***, ElectroChemical Reaction of β-Amidovinyl Sulfones from Arylsulfonyl hydrazides and Tertiary Aliphatic Amines, *Department of Chemistry, Chonnam National University.*

[OL10] **Da Seul Lee, Ho Seong Hwang, Eun Jin Cho***, Visible-Light-promoted Synthesis of Fluoroalkylated Oximes, *Department of Chemistry, Chung-Ang University.*

[OL11] **Yonghoon Moon, Sungwoo Hong***, Photocatalytic Aminopyridylation of Alkene Using *N*-Aminopyridinium Salts as Bifunctional Reagents, *Department of Chemistry, Korea Advanced Institute of Science and Technology (KAIST)*.

[PO001] **Deepak Singh, Hyun-Joon Ha***, Metal-Free Aza-Claisen Type Ring Expansion of Vinyl Aziridines: An Expeditious Synthesis of Seven Membered N-Heterocycles, *Department of Chemistry, Hankuk University of Foreign Studies.*

[PO002] **Seongwoo Kim, Min Kim***, Europium Catalysis: Redox Cycle for Aerobic Oxidation of Alcohol, *Department of Chemistry, Chungbuk National University.*

[PO003] **김승태, 류도현*,** Asymmetric Synthesis of Enantioenriched 2-Aryl-2,3-Dihydrobenzofuran *via* Tandem Cyclopropanation/Intramolecular Rearrangement, *Department of Chemistry, Sungkyunkwan University.*

[PO004] **Yonghyeon Baek, Sang Hoon Han, Mu-Hyun Baik*, Phil Ho Lee*,** Selective C–C bond formation from Rh-catalyzed C–H activation reaction of 2-arylpyridines with 3-aryl-2H-azirines, *Department of Chemistry, Kangwon National University.*

[PO005] **Kyusik Um, Kyungsup Lee, Phil Ho Lee*,** Tosyl Hydrazine Promoted Tandem Condensation and Cyclization of Acyl Azobenzenes Enabling Access to 2H-Indazoles under Metal-Free Aerobic Conditions, *Department of Chemistry, Kangwon National University.*

[PO006] **Gi Uk Han, Kyungsup Lee, Phil Ho Lee*,** Synthesis of Diaryl Ketones *via* Oxidative Cleavage reaction of the C–C Double Bonds in N-Sulfonyl Enamides, *Department of Chemistry, Kangwon National University.*

[PO007] **Sang Hoon Han, Chanyoung Maeng, Phil Ho Lee*,** Rhodium-Catalyzed Regioselective C3-Alkylation of 2-Arylimidazo[1,2-a]pyridines with Aryl Diazoesters, *Department of Chemistry, Kangwon National University.*

[PO008] **Chanyoung Maeng, Gi Hoon Ko, Kang Mun Lee*, Phil Ho Lee*,** Pyrazinoindole-Based Lewis-Acid/Base Assembly: Intriguing Intramolecular Charge-Transfer Switching from the Dual-Sensing of Fluoride and Acid, *Department of Chemistry, Kangwon National University.*

[PO009] **Gi Hoon Ko, Chanyoung Maeng, Phil Ho Lee***, Regioselective Synthesis of Indolopyrazines : Sequential Rh-Catalyzed Formal [3 + 3] Cycloaddition and Aromatization Reaction using Diazoindolinimines with Azirines, *Department of Chemistry, Kangwon National University.*

[PO010] **Da Sol Chung, Jiwon Hwang, Sang-gi Lee*,** Alkyl to Alkyl Palladium Migration *via* C(sp^3)-H Bond Activation: An Efficient Synthesis of 3-Vinylindolin-2-ones, D*epartment of Chemistry and Nanoscience (BK21 PLUS), Ewha Womans University.*

[PO011] **Dong-Hyun Kim, Ji-Su Lim, Cheon-Gyu Cho*,** Total Syntheses of (+)-Uleine and (-)-Tubifolidine *via* Regioselective Fischer Indole Synthesis, *Department of Chemistry, Hanyang University.*

[PO012] **박윤지, 이태우, 양정운*,** Glycerol conversion to high-value chemicals: the implication of unnatural α-amino acid syntheses using natural resources, *Department of Chemistry, Sungkyunkwan University.*

[PO013] **Taehyun Lim, B.Moon Kim***, Synthesis of α-aminophosphonates through phosphonylation of benzyne-imine adducts, *Department of Chemistry, Seoul National University.*

[PO014] **Ahra Cho, Jin Hee Cho, B. Moon Kim*,** A high-performance AuPd-Fe_3O_4 catalyst approach for the synthesis of furan-2,5-dimethylcarboxylate under mild conditions, *Department of Chemistry, Seoul National University.*

[PO015] **최경민, 박호윤, 이철범*,** Rhodium-Catalyzed Tandem Addition-Cyclization-Rearrangement of Alkynylhydrazones, *Department of Chemistry, Seoul National University.*

[PO016] **Sangbin Jeon, Jinwoo Lee, Sunkyu Han***, Total Syntheses of Dimeric Securinega Alkaloids, *Department of Chemistry, Korea Advanced Institute of Science and Technology (KAIST).*

[PO017] **Eunkyeong Seo, Dahyeon Yang, Jieun Lee, Sunwoo Lee*,** Metal-free transamidation of primary amides using TMSCl, *Department of Chemistry, Chonnam National University.*

[PO018] **Sunghyun Hwang, Wookyong Eo, Chulbom Lee*,** Synthetic Studies toward Madeirolide A, *Department of Chemistry, Seoul National University.*

[PO019] **김재형, 성은영, 강은주*,** Multifunctional Fe-Iminopyridine Complexes for the Synthesis of Cyclic Carbonates, *Department of Applied Chemistry, Kyung Hee University*.

[PO020] **Taeil Shin, Hyunwoo Kim*,** Catalyst Development for Direct Hydroformylation of Trisubstituted Olefins *via* Ligand Design, *Department of Chemistry, Korea Advanced Institute of Science and Technology (KAIST).*

[PO021] **Junghoon Kim, Seung Hwan Cho*,** Access to Enantioenriched Benzylic 1,1-Silylboronate Esters by Palladium-Catalyzed Enantiotopic-Group Selective Suzuki-Miyaura Coupling of (Diborylmethyl)silanes with Aryl Iodides, *Department of Chemistry, Pohang University of Science and Technology (POSTECH).*

[PO022] **Jin Hee Cho, Sangmoon Byun, Ahra Cho, B. Moon Kim*,** Mild and selective synthesis of unsymmetrical secondary amines from arylnitriles and nitroalkanes catalyzed by bimetallic PdPt–Fe_3O_4 nanoparticles, *Department of Chemistry, Seoul National University.*

[PO023] **Hoimin Jung, Malte Schrader, Dongwook Kim, Mu-Hyun Baik*, Yoonsu Park*, Sukbok Chang*,** Harnessing Secondary Coordination Sphere Interactions Enables the Selective Amidation of Benzylic C−H Bonds, *Department of Chemistry, Korea Advanced Institute of Science and Technology (KAIST).*

[PO024] **Eunchan Jeong, Joon Heo, Sehoon Park*, Sukbok Chang*,** Alkoxide-Promoted Selective Hydroboration of N-Heteroarenes: Pivotal Roles of in situ Generated BH_3 in the Dearomatization Process, *Department of Chemistry, Korea Advanced Institute of Science and Technology (KAIST).*

[PO025] **Hyojae Lee, Yeosan Lee, Seung Hwan Cho*,** Palladium-Catalyzed Chemoselective Negishi Cross-Coupling of Bis[(pinacolato)boryl]methylzinc Halides with Aryl (Pseudo)Halides, *Department of Chemistry, Pohang University of Science and Technology (POSTECH).*

[PO026] **Hae Eun Lee, Khyarul Alam, Ha Joon Kim, Jin Kyoon Park*,** Design and Synthesis of Sterically Demanding Palladium-PEPPSI Precatalyst of *a*NHC based on Imidazo[1,2-a]pyridine, *Department of Chemistry and Chemistry Institute of Functional Materials, Pusan National University.*

[PO027] **Tapas R. Pradhan, Hong Won Kim, Jin Kyoon Park*,** Regiodivergent Hydroalkynylation for the Synthesis of 1,3- and 1,4-Ynenamides *via* Kinetically Favored Hydropalladation and Ligand-Enforced Carbopalladation, *Department of Chemistry and Chemistry Institute of Functional Materials, Pusan National University.*

[PO028] **Changseok Lee, Sungwoo Hong*,** 1,1-Difunctionalization of Unactivated Alkenes *via* Cationic Palladium Catalysis, *Department of Chemistry, Korea Advanced Institute of Science and Technology (KAIST).*

[PO029] **Kangjae Lee, Sungwoo Hong***, Alkoxy Radical Generation and Functionalization of Pyridinium Derivatives *via* Quinolinone Photocatalysis, *Department of Chemistry, Korea Advanced Institute of Science and Technology (KAIST).*

[PO030] **이안수, 김현우*,** Bicyclic Bridgehead Phosphoramidites (Briphos): Tunable π-Acceptor Phosphine Ligands, *Department of Chemistry, Korea Advanced Institute of Science and Technology (KAIST).*

[PO031] **Khyarul Alam, Jin Gyeong Kim, Dong Yun Kang, Jin Kyoon Park*,** Electronically Controlled Regiodivergent Cycloisomerizations of Ynenamines to Fused Indoles Promoted by

Trifluoromethanesulfonic Acid, *Department of Chemistry and Chemistry Institute of Functional Materials, Pusan National University.*

[PO032] **Jung Tae Han, Jaesook Yun*,** Enantioselective Synthesis of *α*-Chiral *β*-Hydroxy Allenes *via* Copper-Catalyzed Allenylboration of Vinyl Arenes, *Department of Chemistry, Sungkyunkwan University.*

[PO033] **Yeong Bum Kim, Jung-Woo Park*, Sukbok Chang*,** Ruthenium(II)-catalyzed Divergent Transformation of Acyl Azides, *Department of Chemistry, Korea Advanced Institute of Science and Technology (KAIST).*

[PO034] **Hangyeol Choi, Sungwoo Hong*,** Visible-Light Excitation of Quinolinone-Containing Substrate Enables Divergent Radical Cyclization, *Department of Chemistry, Korea Advanced Institute of Science and Technology (KAIST).*

[PO035] **Hanbyul Kim, Jiwon Jang, Seunghoon Shin*,** Asymmetric [3,3]-Sigmatropic Rearrangement *via* Au(I)-Catalyzed Intermolecular Reaction of Propiolates and Allyl Sulfides, *Department of Chemistry and Center for New Directions in Organic Synthesis (CNOS), Hanyang University.*

[PO036] **Jia Lee, Juhyeon Park, Sukbok Chang*,** Co–Catalyzed Intramolecular C–H Amidation Using Azidoformate, *Department of Chemistry, Korea Advanced Institute of Science and Technology (KAIST).*

[PO037] **Sikwang Seong, Hyeonggeun Lim, Sunkyu Han*,** Biosynthetically Inspired Transformation of Iboga to Monomeric Post-iboga Alkaloids, *Department of Chemistry, Korea Advanced Institute of Science and Technology (KAIST).*

[PO038] **Jinwoo Lee, Sangbin Jeon, Sunkyu Han*,** Towards the Total Synthesis of (-)-Flueggenine A and C, *Department of Chemistry, Korea Advanced Institute of Science and Technology (KAIST).*

[PO039] **Taehwan Kim, Sungwoo Hong*,** Regiodivergent Ring-Opening Cross-Coupling of Vinyl Aziridines with Phosphorus Nucleophiles, *Department of Chemistry, Korea Advanced Institute of Science and Technology (KAIST).*

[PO040] **Donguk Ko, Jiyoung Kim, Ju Young Lee, Eun Jeong Yoo*,** Stereoselective Cu-Catalyzed [5 + 1] Cycloaddition: A Surrogate of Hetero Diels-Alder Reaction, *Department of Applied Chemistry, Kyung Hee University.*

[PO041] **Jihyeon Kim, Gangadhararao Golime, Hun Young Kim*, Kyungsoo Oh*,** Copper(II)-Catalyzed Aerobic Oxidation of Amines: Divergent Reaction Pathways by Solvent Control to Imines and Nitriles, *Center for Metareceptome Research, Chung-Ang University.*

[PO042] **Tengda Si, Hun Young Kim*, Kyungsoo Oh*,** Substrate Promiscuity of *ortho*-Naphthoquinone Catalyst: Catalytic Aerobic Amine Oxidation Protocols to Cross Deaminative Coupling and *N*-Nitrosation, *Center for Metareceptome Research, Chung-Ang University.*

[PO043] **Changmuk Kang, Ji Yeon Ryu, Junseong Lee*, Sukwon Hong*,** N-heterocyclic carbene ligands of biaryl structure for Pd-catalyzed amination, *Department of Chemistry, Gwangju Institute of Science and Technology (GIST).*

[PO044] **Dilip V. Patil, Ganganna Bogonda, Hun Young Kim*, Kyungsoo Oh*,** Visible Light-Promoted Thiyl Radical Generation from Sodium Sulfinates: A Radical-Radical Coupling to Thioesters, *Center for Metareceptome Research, Chung-Ang University.*

[PO045] **Quynh H. Nguyen, Seunghoon Shin*,** Visible Light Photoredox Catalysis: Robust Access to α-Carbonyl Radicals from Enoxybenzotriazoles, *Department of Chemistry, Hanyang University.*

[PO046] **Youyoung Kim, Yoonsu Park, Sukbok Chang*,** Delineating Physical Organic Parameters in Site-Selective C–H Functionalization of Indoles, *Department of Chemistry, Korea Advanced Institute of Science and Technology (KAIST).*

[PO047] **Jinwoo Kim, Kwangmin Shin, Seongho Jin, Dongwook Kim, Sukbok Chang*,** Oxidatively Induced Reductive Elimination: Expanding the Scope, Catalyst Systems, and Oxidation Tools, *Department of Chemistry, Korea Advanced Institute of Science and Technology (KAIST).*

[PO048] **Joon Heo, Hyunwoo Kim, Junho Kim, Mu-Hyun Baik*, Sukbok Chang*,** Copper-Mediated Amination of Aryl C–H Bonds with the Direct Use of Aqueous Ammonia *via* a Disproportionation Pathway, *Department of Chemistry, Korea Advanced Institute of Science and Technology (KAIST).*

[PO049] **Eunjoon Park, Cheol-Hong Cheon*,** Total syntheses of (*rac*)- and (+)-Goniomitine *via* intramolecular imino-Stetter reaction, *Department of Chemistry, Korea University.*

[PO050] **조영인, 천철홍*,** Concise Total Synthesis of Phenanthroindolizidine and Phenanthroquinolizidine Alkaloids Using the Building Block Strategy, *Department of Chemistry, Korea University.*

[PO051] **Minhan Lee, Jung-Woo Park*, Sukbok Chang*,** Diverted Approach to Access Site-Selctive Amidation of Carbonyl Compounds: Umpolung Reactivity of Iridium Nitrenoid, *Department of Chemistry, Korea Advanced Institute of Science and Technology (KAIST).*

[PO052] **Jinwoo Shin, Jiseon Kim, Jusung Ahn, Hyeong Seok Kim, Ji Hyeon Kim, Subin Son, Myung Sun Ji, Wonseok Choi, Jong Seung Kim*,** Dual-functional Fluorescent Molecular Rotor toward Microviscosity Imaging during Reticulophagy, *Department of Chemistry, Korea University.*

[PO053] **Kwangho Yoo, Narae Han, Min Jin Shin*, Jae Sup Shin*, Min Kim***, Organic Functionalization on Polydiacetylenes System for Sensing Applications, *Department of Chemistry, Chungbuk National University.*

[PO054] **Eunhye Hwang, Ji Hoon Seo, Kwanyong Seo, Tae-Hyuk Kwon*,** Enhancing the Performance and Stability of Perovskite Solar Cells by Applying Multifunctional Pt(II) Complex, *Department of Chemistry, Ulsan National Institute of Science and Technology (UNIST).*

[PO055] **Heejo Moon, Yuna Jung, Youngseo Kim, Byeong Wook Kim, Jin Kyu Choi, Na Hee Kim, Myung Sook Oh, Sungnam Park*, B. Moon Kim*, Dokyoung Kim*,** A Highly Stable Donor-Accptor Type Oxazepine-Containing Fluorophore and Its Applications in Bio-imaging, *Department of Chemistry, Seoul National University.*

[PO056] **HyeonOh Shin, Deok-Ho Roh, Hyun-Tak Kim, Tae-Hyuk Kwon*,** Ultrasonic Spray Chemistry: In-situ Synthesis of Thin-Film Conjugated Microporous Polymers and Their Energy Storage Applications, *Department of Chemistry, Ulsan National Institute of Science and Technology (UNIST).*

[PO057] **Jun-Hyeok Park, Un-Young Kim, Byung-Man Kim, Wang-Hyo Kim, Deok-Ho Roh, Jeong Soo Kim, Tae-Hyuk Kwon***, Molecular Design Strategy toward Robust Organic Dyes in Thin-Film Photoanodes, *Department of Chemistry, Ulsan National Institute of Science and Technology (UNIST).*

[PO058] **노덕호, 권태혁*,** Control of Electronic Coupling for Retarding Back Electron Transfer in Molecular Solar Cells, *Department of Chemistry, Ulsan National Institute of Science and Technology (UNIST).*

[PO059] **Subin Son, Hyeong Seok Kim, Kyoung Sunwoo, Jinwoo Shin, Jiseon Kim, Jusung Ahn, Wonseok Choi, Jong Seung Kim*,** Chemiluminescent Probe for the In Vitro and In Vivo Imaging of Cancers Over-Expressing NQO1, *Department of Chemistry, Korea University.*

[PO060] **Youngmu Kim, Yuna Song, Varun Kumar Singh, Minsang Kwon*,** Function and oxygen tolerance of initiator-transfer agent-terminator (iniferter) in photomediated reversible addition-fragmentation chain transfer (photo-RAFT), *Department of Materials Science and Engineering, Ulsan National Institute of Science and Technology (UNIST).*

[PO061] **조명기, 김환명***, A Two-Photon Fluorescence Probe for Monitoring hNQO1 Enzyme Activity in Human Colon Tissues, *Department of Energy Systems Research, Ajou University.*

[PO062] **Chang Wook Song, Umme Tamima, Ye Jin Reo, Mingchong Dai, Sourav Sarkar, Kyo Han Ahn*,** Polarity- and Viscosity-Sensitive, Deep-Red Emissive Probe for Lipid Droplets, *Department of Chemistry, Pohang University of Science and Technology (POSTECH).*

[PO063] **Byeong Wook Kim, Hua Li, Gyochang Keum*, B. Moon Kim***, Evaluation of the mutagenicity of 2,7-diaminofluorene and 2,7-diaminocarbazole derivatives in the AMES test, *Department of Chemistry, Seoul National University.*

[PO064] **김현탁, 권태혁***, Carbon-Heteroatom Bond Formation by Ultrasonic Chemical Reaction for Energy Storage System, *Department of Chemistry, Ulsan National Institute of Science and Technology (UNIST).*

[PO065] **김태일, 김영미***, Selective Monitoring and Imaging of Eosinophil Peroxidase Activity with a J-Aggregating Probe, *Department of Chemistry, Kyung Hee University.*

[PO066] **Si Joon Park, In-Soo Hwang, Min Jung Jung, So Young Shim, Han Yong Bae, Ji Yoon Jung, Choong Eui Song***, Water-Induced Hydrophobic Chiral Amplification, *Department of Chemistry, Sungkyunkwan University.*

[PO067] **박상준, 김환명***, Quantitative Detection of Intracellular Polarity Distribution, *Department of Energy Systems Research, Ajou University.*

[PO068] **장수민, 김현우***, A Gallium-Based Chiral Solvating Agent Enables the Use of ^{1}H NMR Spectroscopy to Differentiate Chiral Alcohols, *Department of Chemistry, Korea Advanced Institute of Science and Technology (KAIST).*

[PO069] **Subin Son, Hyeong Seok Kim, Kyoung Sunwoo, Jinwoo Shin, Jiseon Kim, Jusung Ahn, Wonseok Choi, Jong Seung Kim***, NQO1 Probe Using Chemiluminescence for Cancer Cells and Mouse Model Imaging, *Department of Chemistry, Korea University.*

[PO070] **Minkyu Kyeong, Sukwon Hong***, BODIPY-Containing Polymers for Use as Dopant-Free Hole Transporting Materials for Durable Perovskite Solar Cells, *Department of Chemistry, Gwangju Institute of Science and Technology.*

[PO071] **Hosoowi Lee, Woo-Dong Jang***, Helical Living Supramolecular Polymerization from Achiral Bisporphyrin Derivative, *Department of Chemistry, Yonsei University.*

[PO072] **이주연, 황길태***, Synthesis and photophysical property of pH-sensitive fluorescein derivatives, *Department of Chemistry, Kyungpook National University.*

[PO073] **Jintaek Gong, Aram Jeon, Jun Kyun Oh, Sunbum Kwon, Wonchul Lee, Sang Ouk Kim, Sung June Cho, Hee-Seung Lee*,** γ-Aminobutyric acid Nanobelt Formation *via* Spontaneous Self-Assembly, *Department of Chemistry, Korea Advanced Institute of Science and Technology (KAIST).*

[PO074] **Jaewook Kim, Jintaek Gong, Hee-Seung Lee***, Synthesizing Square-plate Foldecture Without Macrodipole, *Department of Chemistry, Korea Advanced Institute of Science and Technology (KAIST).*

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[PO076] **Chaiheon Lee, Jung Seung Nam, Chae Gyu Lee, Jeong Kon Seo, Tae-Hyuk Kwon***, Monitoring Mitochondrial Response to Oxidative Stress *via* An Intramolecular Energy Transfer

based Iridium(III) photosensitizer, *Department of Chemistry, Ulsan National Institute of Science and Technology (UNIST).*

[PO077] **Hyeonbin Ha, Dopil Kim, Min Kim***, Flexibility Controls of Metal-Organic Frameworks by Metal Cation Exchanges and Regioisomerisms, *Department of Chemistry, Chungbuk National University.*

[PO078] **Yonghwan Kwon, Doyon Kim, Yeonjin Noh, Min Sang Kwon***, Improvement for dehalogenation via organic photoredox catalyst: Approaching ppm-level visible-light-driven reductive dehalogenation, *Department of Materials Science and Engineering, Ulsan National Institute of Science and Technology (UNIST).*

[PO079] **Minsoo Lee, Hyun-Tak Kim, Ji Hoon Seo, Kwanyong Seo*, Tae-Hyuk Kwon***, Elevated Stability and Efficiency of Organic Solar Cells *via* Electric Double Layer Formation usin Ir(III) Complex, *Department of Chemistry, Ulsan National Institute of Science and Technology (UNIST).*

[PO080] **Danim Lim, Wonchul Lee, Jonghoon Choi, Jintaek Gong, Hee-Seung Lee***, Study of *β*-Peptide Foldamers containing Tetrahydrothiophene : Fine Tuning of the Secondary Structure Derived by Single Atom Change, *Department of Chemistry, Korea Advanced Institute of Science and Technology (KAIST).*

[PO081] **Jung Seung Nam, Juhye Kang, Mi Hee Lim*, Tae-Hyuk Kwon***, Chemical strategies to modify amyloidogenic peptides by iridium(III) complexes: Coordination and photo-induced oxidation, *Department of Chemistry, Ulsan National Institute of Science and Technology (UNIST).*

[PO082] **Chae Gyu Lee, Chaiheon Lee, Byeong-Su Kim*, Tae-Hyuk Kwon***, Combination of Ir(III) Complex and Cancer-Environment-Customized Nanogel for Efficient Photodynamic Therapy, *Department of Chemistry, Ulsan National Institute of Science and Technology (UNIST).*

[PO083] **Seung Woo Hong, Gil Tae Hwang***, 2-Fluorenyl-1,2,3-triazole-labeled 2'-deoxynucleosides for potential SNP probes, *Department of Chemistry, Kyungpook National University.*

[PO084] **Seungwon Lee, Kyung-Mog Kim, Kyu-Sung Jeong***, A molecularly imprinted synthetic foldamer as a stereospecific and selective receptor for tartaric acid, *Department of Chemistry, Yonsei University.*

[PO085] **Byung-Chang Oh, Eunyoung Yoon, Jintaek Gonh, Russell W. Driver, Jaewook Kim, Hee-Seung Lee***, THF-containing amino acid revisited: Effects of ATFC as an alternative of ACPC in foldamer, *Department of Chemistry, Korea Advanced Institute of Science and Technology (KAIST).*

[PO086] **Umme Tamima, Mithun Santra, Chang Wook Song, Ye Jin Reo, Kyo Han Ahn***, A Benzopyronin-based Two-photon Ratiometric Fluorescent Probe with Complete Spectral Separation for Imaging of Lysosomal Bisulfite, *Department of Chemistry, Pohang University of Science and Technology (POSTECH).*

[PO087] **Rokam Jeong, Jae-Hoon Eom, Jintaek Gong, Hee-Seung Lee***, Foldectures from the Self-Assembly of *α/β*-Foldamers with Conformational change from 11-helix to 14/15-helix, *Department of Chemistry, Korea Advanced Institute of Science and Technology (KAIST).*

[PO088] **Ji Su Park, Kyungjin Min, Doo Ri An, Hye-Jin Yoon, B. Moon Kim*, Se Won Suh*, Hyung Ho Lee***, Substrate synthesis and structural analysis of peptidoglycan peptidase3, a bacterial cell-shape determining protein, *Department of Chemistry, Seoul National University.*

[PO089] **이수빈, 임현석***, A p27 Activator Identified *via* Forward Chemical Genetics Selectively Kills Leukemia Cells, *Department of Chemistry, Pohang University of Science and Technology (POSTECH).*

[PO090] **Hyungi Kim, Jun-Sik Min, Eunha Kim***, Development of a fluorescent sensor array for pH sensing, *Department of Molecular Science and Technology, Ajou University.*

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Selective Formation of γ-Lactams via C−H Amidation Enabled by Tailored Iridium Catalysts

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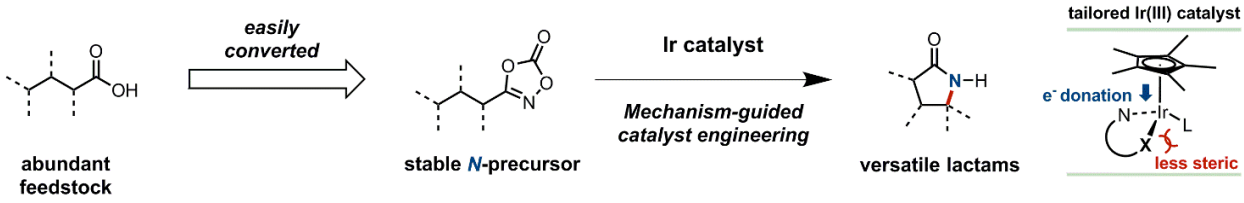
The direct amidation of C–H bonds to obtain nitrogen-containing heterocycles is a highly desirable reaction, because it will open the door to many new applications in chemical synthesis. Although tremendous progress has been made, our current ability to prepare heterocycles via such direct C–H functionalization is limited. Here we present a novel methodology that employs Ir-based catalysts and dioxazolone substrates to access short-lived Ir-nitrenoid complexes, which are key intermediates in the efficient construction of γ-lactams through direct C−H bond amidation. Stoichiometric studies with robust carbonylnitrene precursor, 1,4,2-dioxazol-5-ones, suggest that the insertion of C−H into metal-nitrenoid moiety is possible and mechanistic clues from the initial proof-of-concept studies further enabled the rational design of efficient and versatile catalysts that allows for the straightforward amidations of various sp^3- and sp^2 C−H bonds with exceptional selectivity leading to γ-lactam products. The power of this new method is demonstrated in the successful late-stage functionalization of bio-active molecules with amino acid derivatives to produce molecules that are highly sought after for pharmaceutical and other applications in synthesis.



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Catalyst-controlled divergent intramolecular cyclization of *N*-sulfonyl-1,2,3-triazoles with allyl alcohol

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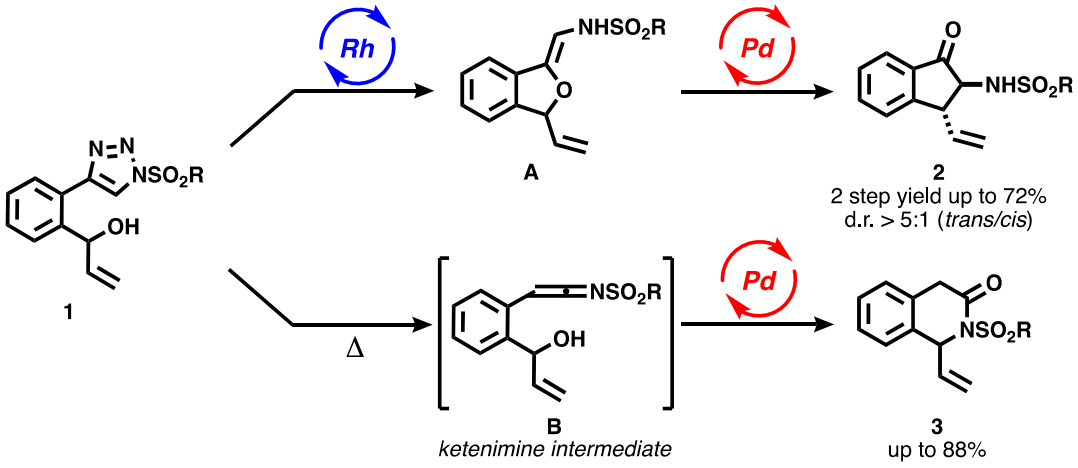
Divergent catalysis could provide structurally diverse compounds from the same precursor through controlling the catalytic reaction pathways and has been considered as a powerful strategy for the discovery of novel functional materials and drugs. During our ongoing researches in this area,[1] catalyst-controlled intramolecular divergent catalytic transformations of *N*-sulfonyl-1,2,3-triazoles **1** have been developed to afford 2-aminoindanone **2** and dihydroisoquinolinone **3** derivatives.

In Rh(II)/Pd(0) dual catalytic system, the *in situ* generated α-imino Rh(II)-carbenoid undergoes O–H insertion to afford benzofuran product **A** for the first step, which then undergo allylic rearrangement in the presence of Pd(0) catalyst. Whereas, in Pd(0) catalytic conditions, the thermally induced *N*-sulfonyl ketenimine **B** was generated as reactive intermediate,[2] which subsequently undergoes nucleophilic addition and allylic rearrangement to obtain the products.



Catalyst-controlled Divergent Transformations

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Redox-selective Iron Catalysis for α-Amino C-H Bond Functionalization via Aerobic Oxidation

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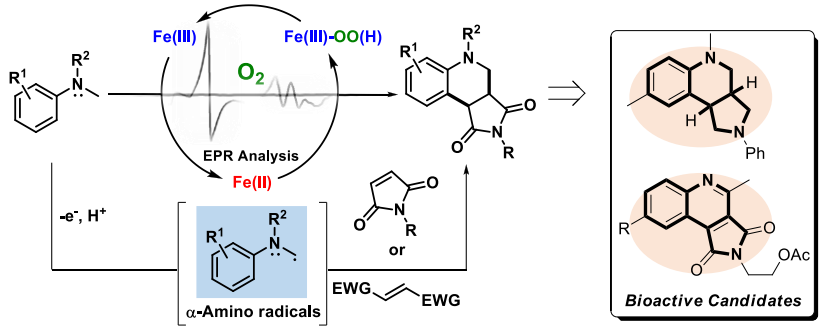
Tertiary amine could be oxidized to a nucleophilic α-aminoalkyl radical species or electrophilic iminium ion under the various transition metal catalysis (Ru, Co, and Cu etc.). However, oxidative transformation of amines by iron salts have been limited in the iminium ion formation due to the uncontrollable oxidative property.[2] Herein, redox-selective iron catalysis for the radical functionalization of the α-amino C-H bond in tertiary anilines is presented. In this strategy, single-electron oxidation and α-deprotonation of tertiary anilines (E_{ox}=0.7 V) using catalytic $Fe(phen)_3(PF_6)_2$ ($E_{1/2}$=1.10 V) affords α-aminoalkyl radicals (rather than iminium ions) which can be coupled with electrophilic partners to afford various tetrahydroquinoline derivatives.[2] Mechanistically, the $Fe(phen)_3^{2+/3+}$ catalytic cycle is maintained by O_2 or a TBHP oxidant, and the presence of the oxygen bound iron complex, $[Fe(phen)_2\text{-}O_2]^+$, was elucidated by UV-vis spectroscopy, electron paramagnetic resonance (EPR), and electrospray ionization mass spectrometry. Enabled through the oxygen bound iron species, this non-heme iron catalyst behaves similarly to bioinspired heme iron catalysts and is important for inducing this selective and mild reaction.



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Pd-Catalyzed Hydroarylation of Diaryl Alkynes with Azoles

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Thiazole-containing π-conjugated moieties are important structural units in the development of new electronic and photo-chromic materials. We have developed a palladium-catalyzed *syn*-hydroarylation reaction of diaryl alkynes with thiazoles, which provides access to thiazole-containing triarylethylenes. Pd(II) complexes derived from Pd(0) species and carboxylic acids facilitated C–H functionalization of the unsubstituted thiazole with high C5 selectivity. The catalytic system was also compatible with other azoles, allowing the stereoselective syntheses of various trisubstituted olefins.

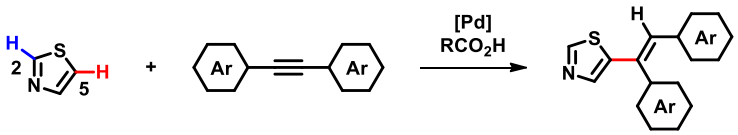

Figure 1. Hydroarylation of diaryl alkynes with thiazole

Triazole-bearing Calix[4]pyrrole as an Ion-pair Receptor for Lithium Chloride

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The importance of lithium extraction is being increased owing to expand of lithium markets and the limited lithium deposit. Many researchers have explored a new method for lithium extraction from seawater. In this regards, ion-pair receptors able to extract Li^+ salts were developed. Most of ion-pair receptors could extract lithium salts such as $Li(NO_2)_2$.[1] To extract the lithium salts from seawater, the development of new ion-pair that can extract lithium salts such as LiCl and LiBr is needed.

Calix[4]pyrroles have been investigated for ion-pair receptors by many researches.[2] Recently, we developed triazole-bearing calix[4]pyrroles that showed strong affinities toward halide anions.[3] We designed a new type triazole bearing calix[4]pyrrole (**1**) for ion-pair receptor having oligoethylene glycol strap to facilitate the binding LiCl or LiBr. Through ^{1}H NMR spectral studies, we successfully confirmed the formation of **1**•LiCl and **1**•LiBr complexes in organic solvent. Furthermore, LiCl and LiBr was extracted to organic solvent using **1** through liquid-liquid (L/L-) extraction or Solid-liquid (S/L-) extraction. Detailed aspect of this system will be discussed in this symposium.

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Pyridine chelated Imidazo[1,5-a]pyridine N-Heterocyclic Carbene Nickel(II) Complexes for Acrylate Synthesis from Ethylene and CO_2.

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A series of novel pyridine chelated imidazo[1,5-a]pyridine-3-ylidene (py-ImPy) ligands were developed for the catalytic synthesis of acrylate using ethylene and carbon dioxide (CO_2), a highly promising reaction for carbon dioxide capture and utilization (CCU). Their Ni(II) complexes py-ImPy Ni(II) complexes were prepared via silver transmetalation and the molecular structures were characterized by X-ray crystallography. The bidentate py-ImPy nickel(II) complexes exhibit catalytic activities in the ethylene-CO_2 coupling reaction (turnover number up to ***). Considering bisphosphine ligands have been typically used in this transformation, the current results with bidentate NHC-Ni(II) catalysts could deserve attention.

Modularized Troubleshooting Continuous-Flow for Organic Reactions: Synthesis of Isoxazoles Using Acyl Chlorides and Alkynes

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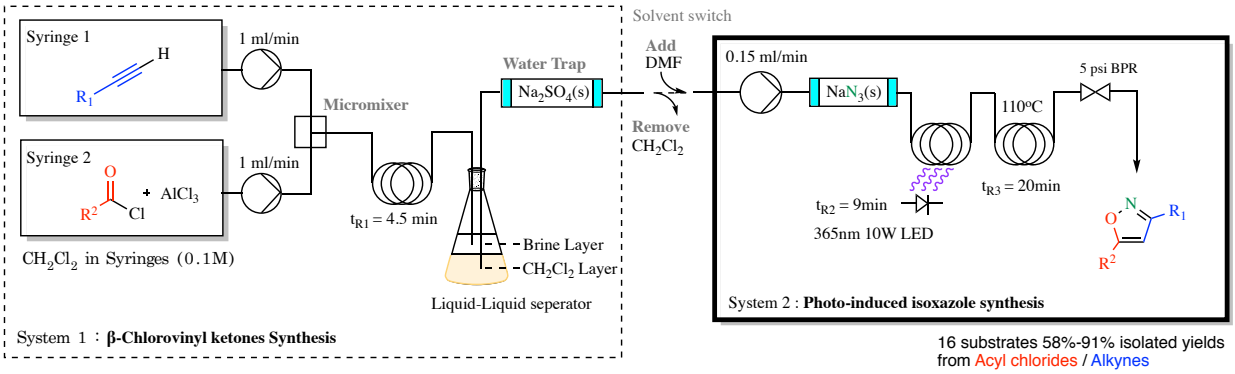
In the previous study, we developed a selective synthesis of (*E*)-β-chlorovinyl ketones applying flow system.[1] Using this system, we effectively synthesized isoxazole containing well-known drugs such as Valdecoxib, Oxacillin, and Cloxacillin as well as biologically active isoxazole substrates. To solve the side reaction occurring in each reaction step about isoxazole synthesis, we discovered modularized flow systems. The multi-step continuous-flow system, unlike the batch reaction, can be adjusted easily so that the reagents can only react on the appropriate points.



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Development of A Novel Synthetic Route for Hinckdentine A

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Hinckdentine A was isolated from the bryozoan *Hincksinoflustra denticulate* by Blackman, Taylor and co-workers in 1987. It has a unique architecture consisting of seven-membered lactam ring fused to tribromoindolo[1,2-c]quinazoline. Since its extremely low bioavailability (0.0005%), its bioactivity has not been explored yet. Because of its interesting structure and the demand for exploring biological activities, there have been considerable effects on the development of an efficient synthetic route to this natural product, and three total syntheses, including two asymmetric total syntheses, of this natural product have been reported.

We recently developed an efficient method for the synthesis of 2-substituted indole-3-acetic acid derivatives from aldimine derived from 2-aminocinnamic acids and aldehydes via the cyanide-catalyzed imino-Stetter reaction. We envisioned that hinckdentine A could be synthesized from 2,2-disubstituted indol-2-one, which could be synthesized by oxidative rearrangement of 2-arylindole-3-acetic acid derivative. The indole compound could be prepared from an aldimine derived from 4,6-bromo-2-nitrocinnamic acid and 5-bromo-2-nitrobenzaldehyde via the cyanide-catalyzed imino-Stetter reaction. The corresponding indole compound already has three bromines and an amine functional group for the D-ring formation, which could allow us to complete the total synthesis of the natural product via completely different strategy from the previous syntheses. In this poster presentation, we will disclose the total synthesis of Hinckdentine A using 2-arylindole derivatives as a key intermediate prepared from readily available starting materials via the cyanide-catalyzed imino-Stetter reaction.

ElectroChemical Reaction of β-Amidovinyl Sulfones from Arylsulfonyl hydrazides and Tertiary Aliphatic Amines

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The synthesis of vinyl sulfones has attracted much attention due to their biological activities, antithyroid drugs, or hypoglycemia.[1] Vinyl sulfones are important intermediates and reagents for the synthesis of organic compounds.[2] Given the importance of vinyl sulfones, we need to develop more synthetic methods to meet the needs of such compounds. Herein, we introduce the aerobic oxidative reaction of arylsulfonyl hydrazides with tertiary aliphatic amines to give the corresponding vinyl sulfones in the presence of electrochemical conditions. This method provides a practical, mild, and environmentally friendly procedure to synthesize vinyl sulfones in good to moderate yields.

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Visible-Light-promoted Synthesis of Fluoroalkylated Oximes

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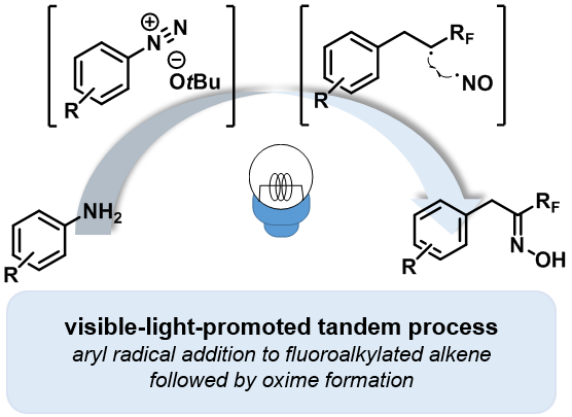

A method has been developed for the synthesis of fluoroalkylated oximes, potential fluoroalkyl building blocks for the synthesis of various organofluorine compounds, from easily available amino substrates and fluoroalkylated alkenes.[1] *t*BuONO was utilized both as a diazotizing agent and as a NO radical source for the oxime synthesis in the process, and the use of a photocatalyst under visible-light irradiation increased the efficiency of the reaction. Various fluoroalkylated oximes were prepared by a tandem process of aryl radical addition to fluoroalkylated alkene and consecutive oxime generation process, albeit in moderate yields. This differentiated approach, transferring an aromatic system into an electron-deficient fluoroalkylated alkene, expands the scope of substrates where electron-poor aromatic systems could be utilized.[2]

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Photocatalytic Aminopyridylation of Alkene Using N-Aminopyridinium Salts as Bifunctional Reagents

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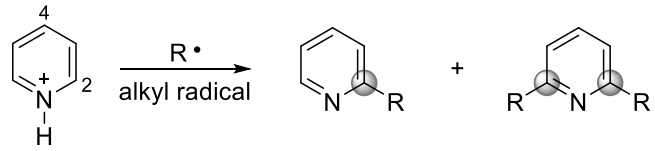
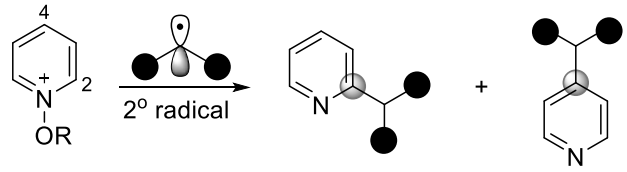
We developed a new photocatalytic strategy for alkene aminopyridylation using N-aminopyridinium salts as both aminating and pyridylating reagents. In this study, amino and pyridyl groups are simultaneously incorporated into alkenes with complete regioselectivity, affording a variety of aminoethyl pyridine derivatives. Notably, we discovered that radical trapping with N-aminopyridinium salts occurs exclusively at the C4-position, and the capacity for controlling C-4 regioselectivity could be rationalized by extensive DFT based analysis. This transformation is characterized by a broad substrate scope, good functional group compatibility, and metal-free mild conditions. The utility of this transformation was further demonstrated by late-stage functionalization of complex biorelevant molecules.

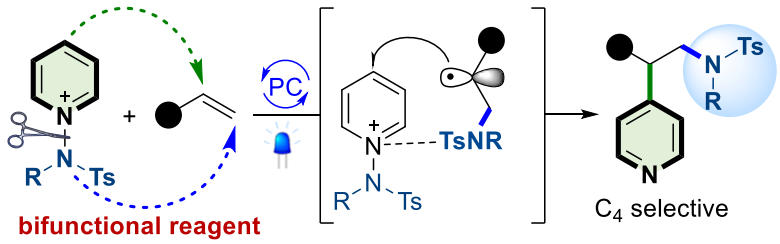
a) acid-promoted Minisci-type alkylation of pyridine



b) radical-mediated pyridylation using N-alkoxypyridinium salts



c) **This work**: alkene aminopyridylation using N-aminopyridinium salts



Metal-Free Aza-Claisen Type Ring Expansion of Vinyl Aziridines: An Expeditious Synthesis of Seven Membered N-Heterocycles

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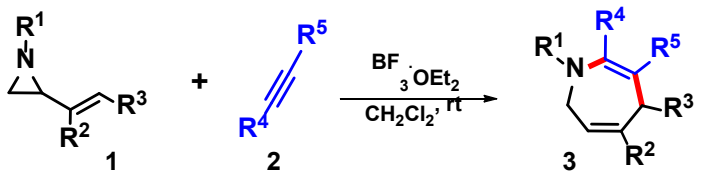
A metal free, Lewis acid catalyzed approach for the intermolecular [5+2] cycloadditon of vinyl aziridines with alkynes has been reported for the synthesis of highly functionalized seven membered N-heterocycles. The method has broad substrate scope and applicable for both terminal and internal alkynes as well as vinyl aziridines under mild reaction conditions which delivers a variety of structurally different azepines ring systems in high yield up to 92%.



Transition Metal Free
23 Examples, 64-92% Yield
Mild Reaction Conditions

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Europium Catalysis: Redox Cycle for Aerobic Oxidation of Alcohol

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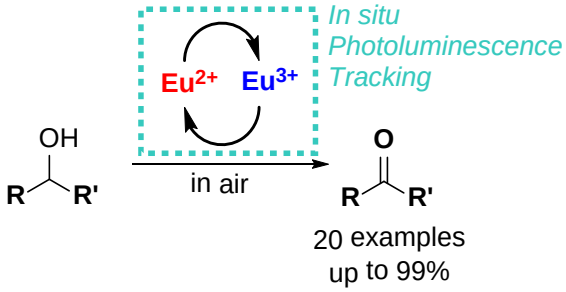
Herein, the redox cycle of europium for aerobic oxidation of alcohols to corresponding aldehydes will be presented. Lanthanide chemistry is a versatile and useful tool for various, traditional organic synthesis. Several important lanthanide reagents such as SmI_2 and CAN (ceric ammonium nitrate) are widely used to the oxidation-reduction during organic synthesis with stoichiometric manners. In the catalytic manner, a variety of Lewis acid catalysis has been developed using lanthanide salts such as $La(NO_3)$, $Sc(OTf)_3$, and etc. However, there are very limited studied for the catalytic applications of lanthanide with redox changes of metal in the literatures since lanthanide metals normally have a single, +3 stable oxidation state.[1] Europium (Eu, atomic number 63), can have relatively stable two oxidation states (Eu(II) and Eu(III)) due to the half-filled $4f^7$ electronic configuration. We have utilized the redox cycle between Eu(II) to Eu(III) to organic transformation, especially the aerobic oxidation of alcohols to corresponding aldehydes. The redox cycle of europium was activated by the external oxidants (TEMPO, O_2, and NO_3^-) in the acidic condition, and their cycle was working for alcohol oxidation to corresponding aldehyde and not for carboxylic acid (i.e., no over-oxidation). The europium-catalyzed aerobic oxidation has a variety of substrate scopes including secondary alcohols and aliphatic alcohols in the optimized condition.[2] The detail mechanistic proposal with condition screening will be discussed during the presentation. We believe that the present europium-catalyzed aerobic oxidation brings new possibility and interest of lanthanide metals to develop redox-cycle based organic transformations in the future.



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Asymmetric Synthesis of Enantioenriched 2-Aryl-2,3-Dihydrobenzofuran *via* Tandem Cyclopropanation/Intramolecular Rearrangement

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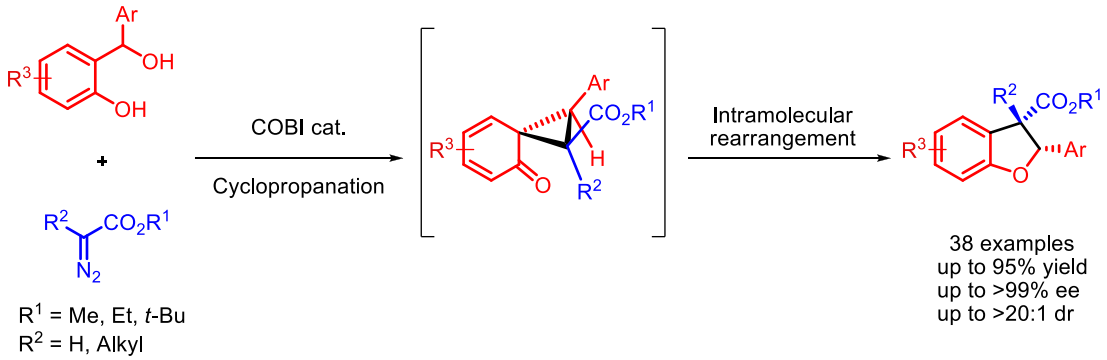
Chiral 2-Aryl-2,3-dihydrobenzofuran derivatives are basic structure of numerous naturally occurring biological active compounds. Although various catalytic methods have been developed, access to chiral 2-aryl-2,3-dihydrobenzofuran with broad applicability was not fully studied. In this research, we developed the enantioselective synthesis of 2-aryl-2,3-dihydrobenzofuran catalyzed by chiral oxazaborolidinium ion(COBI) from *ortho*-Quinone methides and *α*-diazoester *via* tandem Michael-initiated cyclopropanation/intramolecular rearrangement. Various 2,3-dihydrobenzofuran possessing quaternary carbon center were obtained in high yield (up to 94%) with excellent enantio- and diastereoselectivity (up to >99% *ee* and up to > 20:1 *dr*).[1)]



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(DOI: 10.1002/anie.201906954R1 and 10.1002/ange.201906954R1)

Selective C–C bond formation from Rh-catalyzed C–H activation reaction of 2-arylpyridines with 3-aryl-2H-azirines

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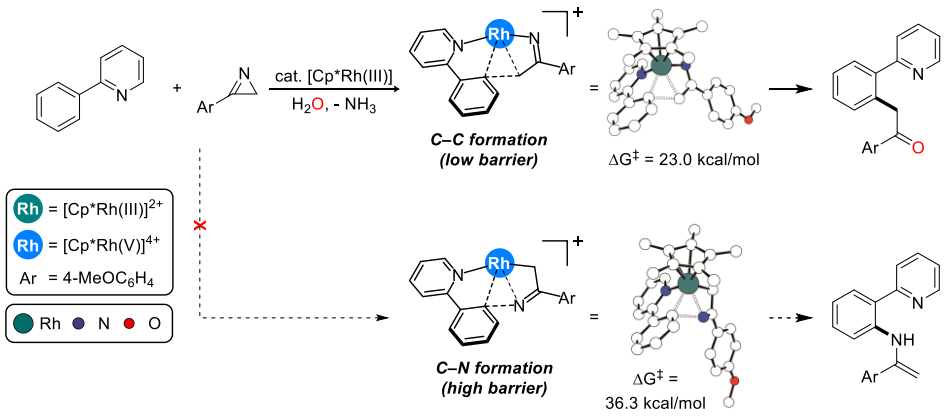
A novel method for the synthesis of acylmethyl-substituted 2-arylpyridine derivatives using 3-aryl-2*H*-azirines was developed by exploring a prototype reaction using DFT-calculations and carrying out targeted experiments guided by the calculated mechanism. 2*H*-Azirine was initially hypothesized to ring-open at the metal center to furnish familiar metal nitrene complexes that may undergo C–N coupling. Computational studies quickly revealed and prototype experimental work confirmed that neither the formation of the expected metal nitrene complexes nor the C–N coupling were viable. Instead, azirine ring-opening followed by C–C coupling was found to be much more favorable to give imines that readily underwent hydrolysis in aqueous conditions to form acylmethyl-substituted products. This new method was highly versatile and selective toward a wide range of substrates with high functional group tolerance. The utility of the new method is demonstrated by a convenient one-pot synthesis of biologically relevant heterocycles such as pyridoisoindole and pyridoisoqunolinone.



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Tosyl Hydrazine Promoted Tandem Condensation and Cyclization of Acyl Azobenzenes Enabling Access to 2H-Indazoles under Metal-Free Aerobic Conditions

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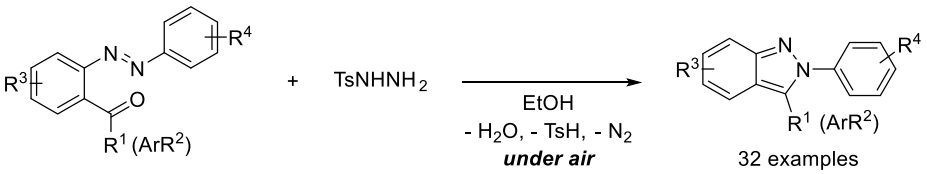
We envisioned that the treatment of 2-acyl azobenzenes with tosyl hydrazine would produce the corresponding tosyl hydrazones along with the release of water, and then, the hydrozones would be easily transformed to 2-aryl-2*H*-indazoles having 3-alkyl- or 3-aryl groups through intramolecular cyclization with concomitant release of molecular nitrogen and sulfinic acid under metal-free conditions. Herein, we describe an efficient synthetic method for 2-aryl-2*H*-indazoles having alkyl- or aryl groups at the 3-position through intramolecular cyclization of tosyl hydrazone having an azobenzene moiety, which is generated in situ from the condensation of 2-acyl azobenzene with tosyl hydrazine together with the release of water, molecular nitrogen, and sulfinic acid under metal-free aerobic conditions. All of the examples produced the corresponding 2*H*-indazoles in quantitative yields. The present reaction was determined to have a wide substrate scope and good functional group tolerance.



R^1 = Me, *n*-Pr, Cy ArR^2 = Ph

R^2 (in the case of Ar = Ph) = Me, MeO, F, Cl, Br, CO_2Me, NO_2, thiophen-2-yl

R^3, R^4 = H, Me, MeO, Cl, Br, 4-CO_2Et

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Synthesis of Diaryl Ketones *via* Oxidative Cleavage reaction of the C–C Double Bonds in *N*-Sulfonyl Enamides

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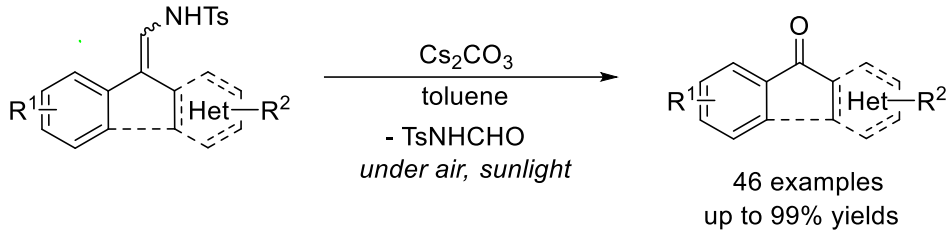
An oxidative cleavage of a C−C double bond is developed from the photochemical [2+2]-cycloaddition of diaryl *N*-tosyl enamides, aryl heteroaryl *N*-tosyl enamides, and *N*-tosyl cyclic enamides with singlet molecular oxygen, followed by a ring-opening reaction mediated by Cs_2CO_3 under air and sunlight without the use of photosensitizer, producing symmetrical and unsymmetrical diaryl, heterodiaryl, and cyclic ketones in good to excellent yields. Moreover, the oxidative cleavage of C−C triple bonds from 1-alkynes is demonstrated for the synthesis of symmetrical and unsymmetrical ketones from the Cu-catalyzed [3+2]-cycloaddition, Rh-catalyzed alkoxyarylation, photooxygenation, and ring-opening reaction in one-pot. Because the synthesis of the symmetrical and unsymmetrical diaryl and/or heterodiaryl ketones bearing an electron-donating group is not easy, the present method is notable.



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Rhodium-Catalyzed Regioselective C3-Alkylation of 2-Arylimidazo[1,2-a]pyridines with Aryl Diazoesters

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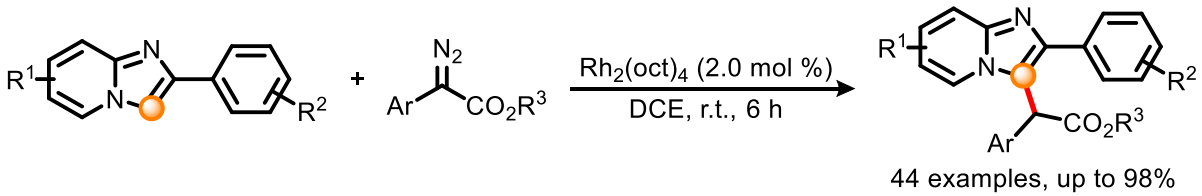
Imidazo[1,2-a]pyridines are significant privileged scaf-folds in azaheterocycle chemistry,[1] and they are commonly found in natural products, pharmaceuticals, and biologically active compounds. Among azaheterocycles, imidazopyridines and espe-cially 3-alkyl-2-arylimidazo[1,2-a]pyridines are not only essential pharmacophores but also practical synthetic intermediates that can be easily converted into valuable molecules.

A regioselective C3-alkylation based on the reaction of 2-arylimidazo[1,2-a]pyridines with a wide range of aryl α-diazoesters in the presence of a Rh(II) catalyst in dichloroethane at room temperature was developed. This method could be applied in the synthesis of benzoimidazoquinolizinone and cyclo-heptaimidazopyridinone, which are novel heterocyclic scaffolds.



44 examples, up to 98%

References

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Pyrazinoindole-Based Lewis-Acid/Base Assembly: Intriguing Intramolecular Charge-Transfer Switching from the Dual-Sensing of Fluoride and Acid

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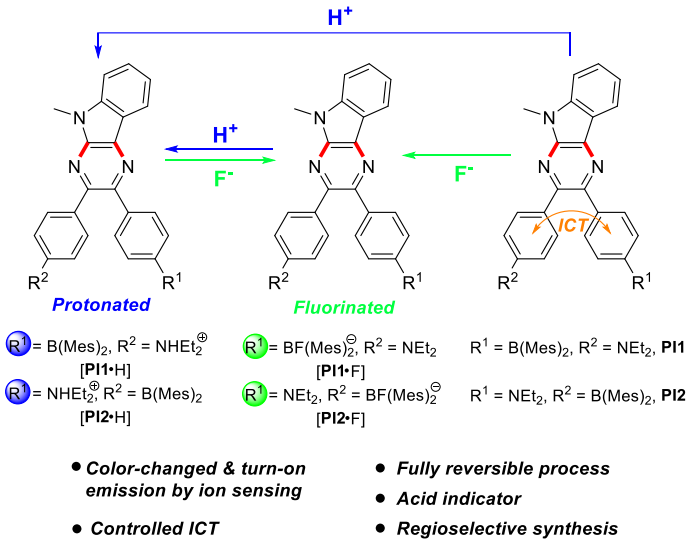
Pyrazinoindole-based Lewis-acid/base assemblies are prepared through the use of regioselective formal [3 + 3] cycloaddition reactions and their intriguing photophysical properties are described. The assemblies exhibit strong emissions in THF solution, which are attributed to through-space intramolecular charge-transfer (ICT) transitions between the branched Lewisacid/ base moieties. Furthermore, these show ratiometrically color-change responses in PL titration experiments, which give rise to new colors through turn-on emissions ascribable to ICT transitions that alternate between the pyrazinoindole units and each triarylboryl or amino moiety, a consequence of the binding of the fluoride or acid. Pieces of filter paper covered by these assemblies demonstrated exhibited blue-shifted color changes when immersed in aqueous acidic solutions, suggesting that these are promising candidate indicators that detect acid through emissive color. Computational data for these assemblies and their corresponding adducts verify the existence of ICT transitions that alternate through fluoride or acid binding.



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

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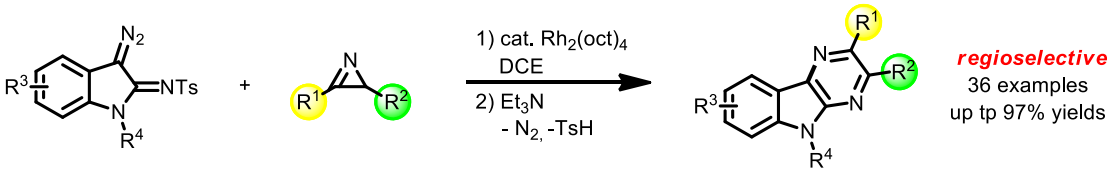
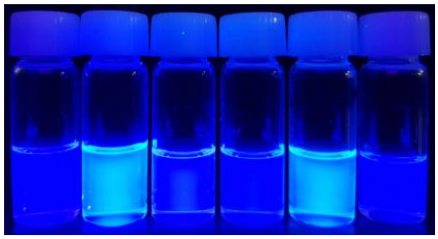
Indolopyrazines possessing both indole and pyrazine moieties are significant structural motifs in a number of naturally occurring products, show a wide range of biological activities, including antitumor and antiviral activities, and function as fluorescent and host materials. In this regard, the indolopyrazine 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 CH_2Cl_2 solution were studied. The extinction coefficients were variable from 107,298 to 585,478 $M^{-1}cm^{-1}$. The indolopyrazine affords high quantum yields and extinction coefficients, which are an attractive property for biological probes.





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Alkyl to Alkyl Palladium Migration *via* C(sp^3)-H Bond Activation: An Efficient Synthesis of 3-Vinylindolin-2-ones

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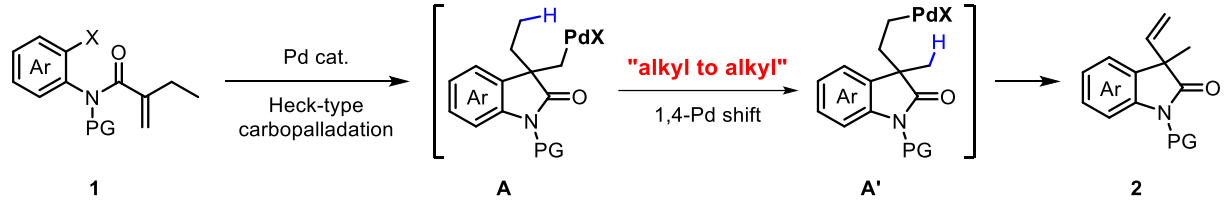
Transition metal-catalyzed C–H bond functionalization is widely developed due to its powerful and atom-economic advantage. To enable through-space interaction of a metal center with a neighboring C–H bond, metal migration strategy, including a C–H activation for forming a five membered palladacycle intermediate, has been frequently utilized.[1] However, most reported 1,4-Pd migrations were limited to alkyl C(sp^3)-Pd to aryl C(sp^2)-Pd or aryl C(sp^2)-Pd to aryl C(sp^2)-Pd migrations. No research on alkyl C(sp^3)-Pd to alkyl C(sp^3)-Pd migration was reported.

During our recent study on regiodivergent cyclopropanation of σ-alkylPd(II)-intermediate **A** generated by Heck-type carbopalladation,[2] unprecedented alkyl C(sp^3)-Pd to alkyl C(sp^3)-Pd migration was observed, from intermediate **A** to **A'**, and it underwent β-hydride elimination to afford the quaternary vinylated oxindoles **2**. To the best of our knowledge, this is the first example of an alkyl to alkyl 1,4-Pd migration.



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Total Syntheses of (+)-Uleine and (-)-Tubifolidine via Regioselective Fischer Indole Synthesis

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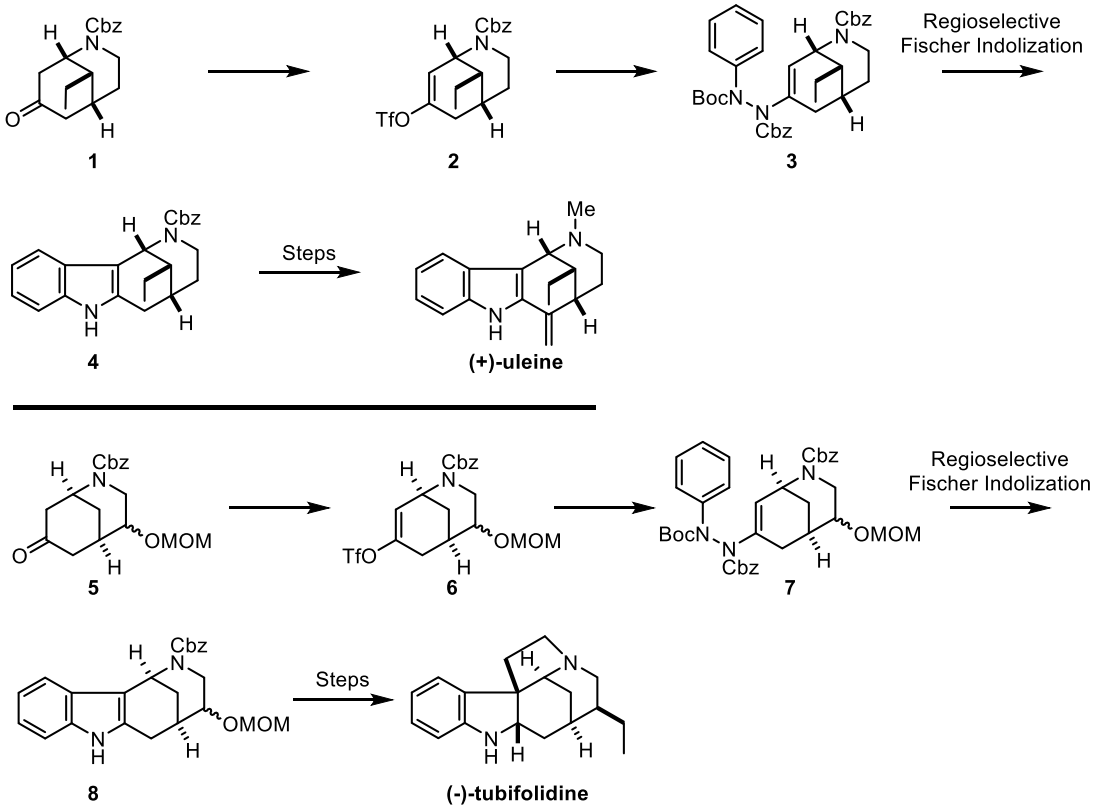
Abstract

We have previously reported the synthesis of ene-hydrazide from enol triflate and subsequent indolization reaction as a new entry to a 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-hydrazide. 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 (+)-uleine and (-)-tubifolidine by ways of bicyclic carbamates **1** and **5**. Formation of enol triflates **2** and **6** followed by C-N coupling reactions with phenyl hydrazide and regioselective Fischer indolization under Lewis acidic conditions would selectively give desired indole **4** and **8**, respectively. Our recent progress on the total syntheses of (+)-uleine and (-)-tubifolidine will be presented.



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Glycerol conversion to high-value chemicals: the implication of unnatural α-amino acid syntheses using natural resources

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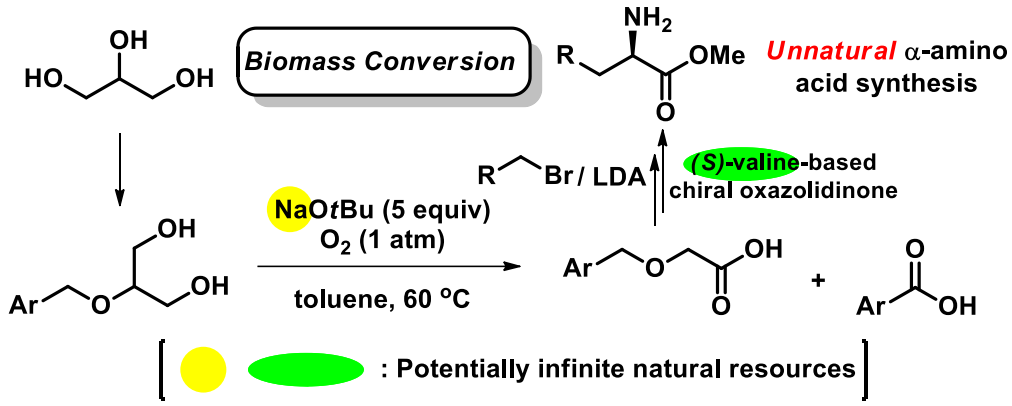
Glycerol, known as glycerine, is a triol that can be generated as a by-product during the synthesis of biodiesel from vegetable oils, such as soybean and sunflower oils.[1] Nowadays, efforts are being made to synthesize renewable materials utilizing biomass derivatives containing overproduced glycerol in industrial research.[2] Glycerol is recognized as a privileged scaffold due to its potential as a high-value carbon and oxygen source and an alternative to our gradually depleting existing natural resources.[3]

Herein, *O*-benzylglycerol derivatives have been synthesized from glycerol, which can act as a promising carbon source from a myriad of biomass materials obtained from nature. These derivatives were subjected to a transition-metal free oxidative dehomologation reaction using a NaO*t*Bu-O_2 system, leading to two different carboxylic acid products. The use of *O*-benzylglycerol enables the construction of unnaturalα-amino acids utilising potentially infinite natural resources, such as sodium and (S)-α-amino acid, thereby contributing to a new type of glycerol valorization.[4]



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Synthesis of α-aminophosphonates through phosphonylation of benzyne-imine adducts

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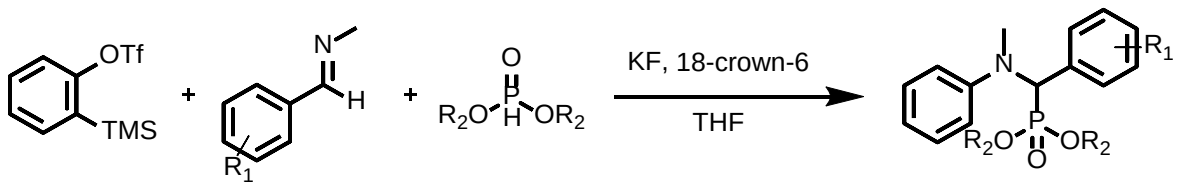
Organophosphorus compounds are becoming increasingly useful in many applications such as industrial, agricultural and medicinal chemistry. In particular α-aminophosphonates and α-aminophosphonic acids are structurally analogous to many enzyme inhibitors and antitumor agents and therefore expected to possess diverse biological activities. Therefore development of efficient synthetic methods for the α-aminophosphonates has become increasingly important.

A number of methods have been developed for the synthesis of α-aminophosphonates and methods employing transition metal catalysts containing [Ni], [Rh][1], [Co][2] and others have recently attracted much attention. However, these methods require harsh reaction conditions and use of toxic metal catalysts.

To develop a more efficient and mild procedure, we have developed multicomponent phosponylation reaction involving arynes, imines and dialkyl phosphites. This method obviates the use of transition metal-based reagents. Reactions of a wide range of imines, arynes and phosphites can efficiently be carried out under optimized conditions. A plausible reaction mechanism is suggested, where an iminium zwitterion, generated from a nucleophilic addition of an imine to an aryne, abstracts a proton from dialkyl phosphite, causing the phosphite anion to add into the iminium carbon, which results in the formation of the desired α-aminophosphonate. Also, by a deuterium isotope study, we have found an evidence that deprotonated phosphites undergoes nucleophilic addition to iminium intermediate to provide α-aminophosphonates.



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A high-performance AuPd-Fe_3O_4 catalyst approach for the synthesis of furan-2,5-dimethylcarboxylate under mild conditions

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Heterogeneous catalysis has been explored as an important tool for the production of high value-added chemicals from sustainable biomass.[1] Among these chemicals, 5-hydroxymethylfurfural (HMF) has attracted significant interest since it can be transformed into a highly versatile industrial intermediate, 2,5-furandicarboxylic acid (FDCA),[2] which can be utilized as a monomer for the production of polyethylene furanoate (PEF). However, because FDCA exhibits poor solubility in most solvents, furan-2,5-dimethylcarboxylate (FDMC) has been considered more advantageous as a monomer.[3] Much effort has been concentrated toward the development of efficient catalysts for the oxidation of HMF to FDCA, high-performance catalysts for the direct oxidative esterification of HMF to FDMC under extremely mild conditions have been rare.

Herein, we report one-pot oxidative esterification of 5-hydroxymethylfurfural (HMF) to furan-2,5-dimethylcarboxylate (FDMC) at r.t. under atmospheric pressure of O_2 using high-performance bimetallic AuPd-Fe_3O_4 catalyst.[4] The alloy AuPd-Fe_3O_4 nanoparticles (NPs) exhibited high selectivity toward FDMC with unprecedented catalytic activity, compared with those of monometallic catalysts (Au-Fe_3O_4 and Pd-Fe_3O_4). Interestingly, monometallic Au-Fe_3O_4 nanoparticles showed high selectivity to the synthesis of 5-hydroxymethyl furoic acid methyl ester (HMFE). We also found that the ratio of the two metals in the bimetallic catalyst influenced the reaction outcome and the best Au/Pd metal ratio for the highest activity and selectivity of FDMC synthesis was 1.00:1.18. The AuPd-Fe_3O_4 catalyst was readily reusable for three times and the used nanoparticles showed no significant change in morphology.

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Rhodium-Catalyzed Tandem Addition–Cyclization–Rearrangement of Alkynylhydrazones

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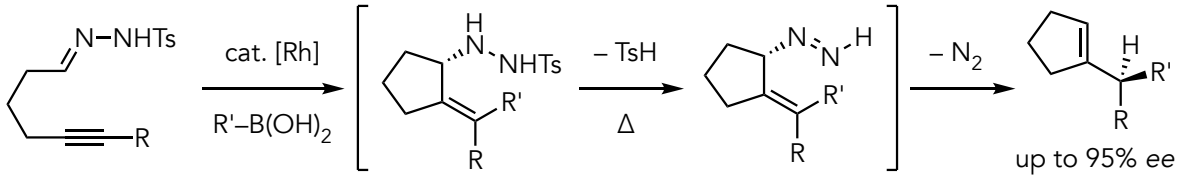
Presented in this poster will be our recent progress on the development a tandem protocol based on the merger of rhodium catalysis and a retro-ene process.[1] In this strategy employing a single rhodium catalyst, alkyne-tethered hydrazones and organoboronic acids undergo a cascade of addition–cyclization–rearrangement reactions to afford cycloalkene products. Mechanistic studies suggest that the process is commenced by the rhodium-catalyzed addition–cyclization and completed with the allylic diazene rearrangement. This reaction can be rendered asymmetric by using chiral diene ligands for the rhodium catalyst, whereby enantioselective addition to the C=N bond establishes the C–N stereocenter whose chirality is transferred to its allylic position via suprafacial rearrangement.



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Total Syntheses of Dimeric Securinega Alkaloids

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Securinega alkaloids have served as an arena for the discovery of new chemical reactivities and the development of innovative synthetic strategies. Recently, there has been an outburst of isolation reports of dimeric, trimeric, and other high-order securinega alkaloids which draw the attention of the synthetic community. Constructing carbon-carbon bonds between either monomeric or oligomeric securinega subunits is the key challenge in the synthesis of high-order securinega alkaloids. Previously, we completed the total synthesis flueggenine C via accerated Rauhut–Currer reaction as a key step. Flueggenine D is a dimeric securinega alkaloid including α–δ′ linkage between two monomeric units.[1] We envisioned that a palladium-catalyzed Stille cross-coupling reaction would enable the construction of this carbon-carbon bond. The key dimeric precursor with a α–δ′ linkage between two subunits was successfully prepared from coupling partners. We sought to complete the first total synthesis of flueggenine D by utilizing this key dimer precursor.

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Metal-free Transamidation of Primary Amides using TMSCl

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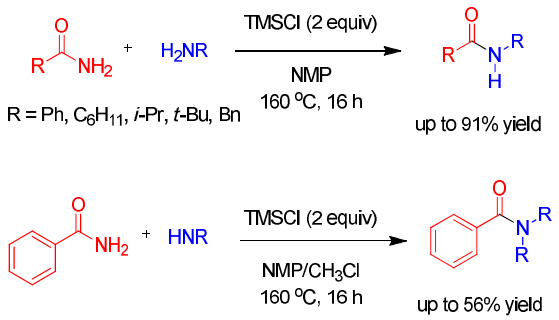
The amide functional group is one of the most important moieties in nature because it is the backbone of proteins and peptides. Amide-containing compounds have received much attention because they are widely used for the synthesis of bioactive molecules in pharmaceutical and agricultural chemistry, and are also of great relevance to material science. Therefore, synthesis methods for the preparation of the amide functional group have been widely developed. Transamidation of amides with amines has recently gained considerable momentum, although the activation of the C-N bonds of amides is hardly achieved, because of the ready availability of amines and straightforward tools. A number of efficient methods for this modern strategy have been intensively developed for decades. Although it is known that the transamidation of secondary amides is a challenging project, and that the transamidation of primary amides is relatively more studied, the latter still has some hurdles to overcome. Recently, we found that TMSCl activated secondary amides in nickel-catalyzed transamidation reactions, and we reported the direct transamidation of secondary amides with primary and secondary amine.[1] Based on these results, we envisioned that TMSCl might activate primary amides in transamidation reactions without any metal catalyst. To the best of our knowledge, TMSCl-mediated transamidations have not been reported. Herein, we report metal-free transamidation of primary amides using TMSCl.

We developed metal-free transamidation of primary amides. TMSCl acted as the activator in transamidation. In the presence of TMSCl, primary amides reacted with primary amines to yield transamidated secondary amides in NMP solvent. The transamidation of benzamide with secondary amines for the formation of tertiary amides succeeds in NMP/CH3Cl solvent.



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Synthetic Studies toward Madeirolide A

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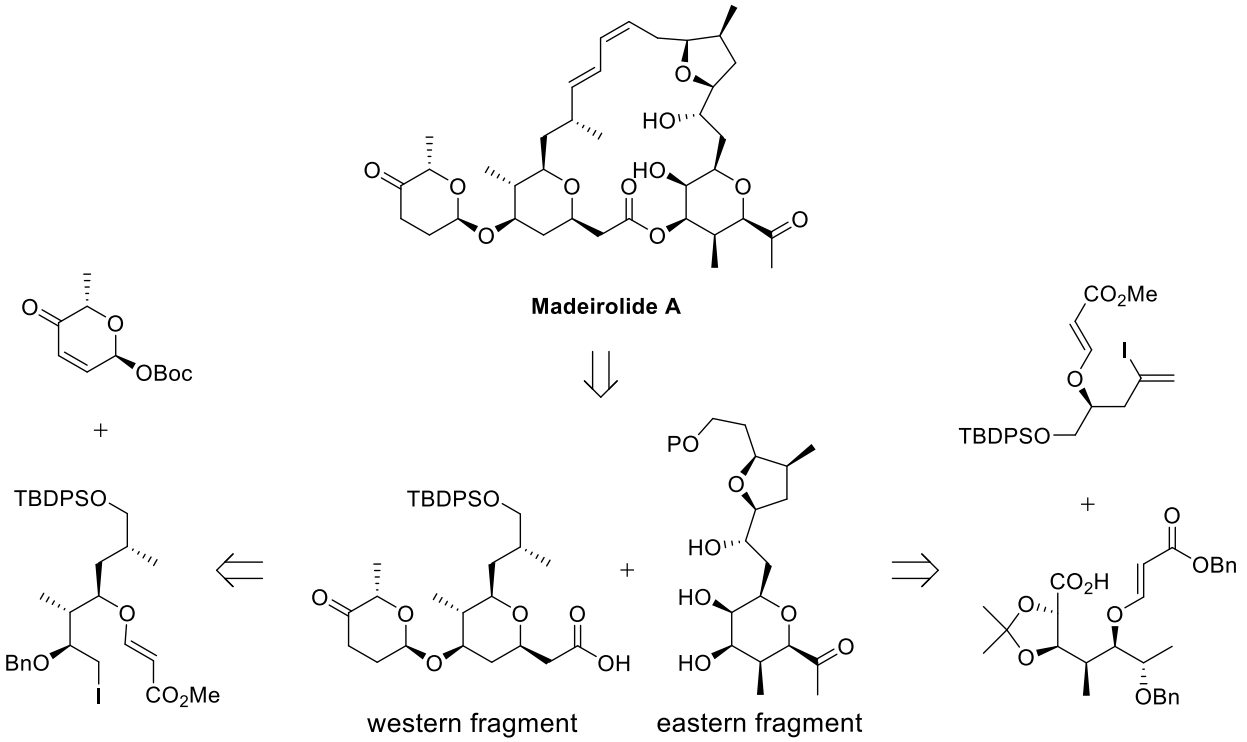
Madeirolide A is a novel polyketide natural product isolated from the marine sponge *Leiodermatium* sp. harvested from the southwestern sea of Porto Santo, Portugal, by Wright and Winder in 2009.[1] Madeirolide A exhibits modest inhibitory activity against the fungal pathogen *Candida albicans* (MIC = 12.5 μg/mL) but no appreciable cytotoxicity against tumor cell lines, in contrast to the structurally similar mandelalides that show high antitumor activity. Madeirolide A contains three oxacycle moieties within a 24-membered macrolactone backbone adorned with 16 stereogenic centers. However, there is uncertainty over the stereostructure of this natural product, which, together with the unusual bioactivity profile, renders madeirolide A a compelling target for total synthesis studies.[2-4]
Presented in this poster are our efforts towards a convergent and enantioselective synthesis of madeirolide A, which have led to the syntheses of three oxacyclic subunits based on visible-light-induced photocatalytic radical cyclization.



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Multifunctional Fe-Iminopyridine Complexes for the Synthesis of Cyclic Carbonates

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In the catalytic system for a typical cyclic carbonate synthesis, Lewis-acidic compounds, such as metal–organic complexes or hydrogen bond donors, commonly activate the epoxide ring opening with a remarkable acceleration of the reaction rate.[1] And Lewis-basic compounds, such as amine and nitrogen heterocycle or NHC and ylides, activate the CO_2 to convert zwitteric CO_2 product which can also accelerate a cyclic-carbonate synthesis.[2] Many metal complexes of Al, Cr, Mn, Co, Zn or Fe have attracted much attention presumably owing to the significant features of ligands. Above all, Fe(II)-iminopyridine complexes are easy to modify structure in tuning their steric and electronic properties by modification the framework of the ligand.[3]

Functionally designed Fe(II)-iminopyridine complexes have dissociable imino groups to form empty site of Fe center acting as Lewis acid for epoxide activation.[4] Additionally, iminopyridine units in ligand can be modified to introduce the functional groups to activate epoxide or CO_2. The hydroxyl group was found to effect the epoxide activation by hydrogen bonding, and the imidazole group can activate CO_2 by nucleophilic attachment. With several Fe-ligand complexes, we will report the catalytic system for the cyclic carbonate synthesis under mild reaction conditions (reaction temperature and CO_2 pressure), which are capable of dual activation of epoxide and CO_2.

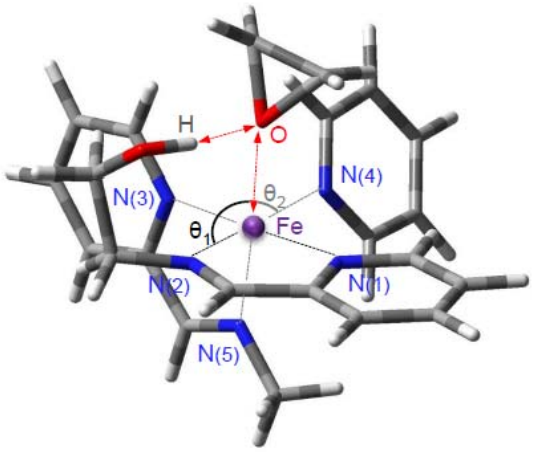

Figure 1. Mimetic diagram of epoxide activation with Fe(II)-iminopyridine complex.

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Catalyst Development for Direct Hydroformylation of Trisubstituted Olefins via Ligand Design

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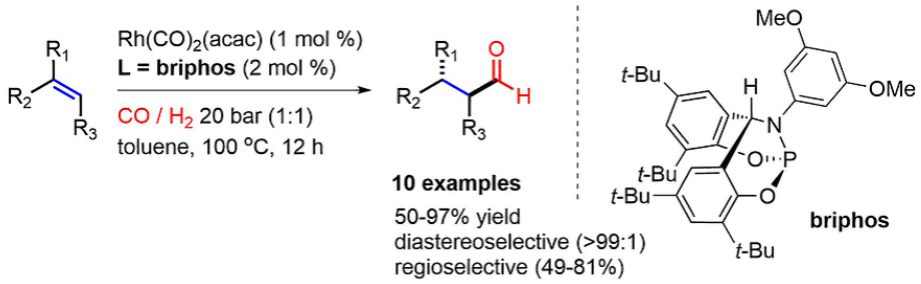
Hydroformylation is a highly atom-economical synthetic reaction to prepare aldehyde by addition of CO and H_2 to olefins. It is an industrially utilizing homogeneous catalytic reaction as the resulting aldehyde products are used to further preduce oxo-alcohols more than 10 milion tons annually.[1] For the direct hydroformylation of internal olefins without involving the isomerization process, the substrate scope was only extended to 1,1- or 1,2-disubstitued olefins, whereas more substituted olefins such as tri- or tetra-substituted olefins were rarely used.[2] It is thus highly desirable to improve the reactivity in order to expand utility of the hydroformylation.

Here we describe the Rh-catalyzed direct hydroformylation of tri-substituted olefins by ligand moodifiaction of bicyclic bridgehead phosphoramidite(Briphos) ligands. Due to the geometrical constraints, the briphos ligands exhibit enhanced π-accepting properties that can be further modulated by substituents.[3] When we prepared briphos ligands with *tert*-butyl groups at the *ortho* and *para* positions of the phenol rings in order to enhance steric bulkiness, the briphos ligands showed remarkable reactivity and good selectivity in hydroformylation of tri-substituted olefins.



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Access to Enantioenriched Benzylic 1,1-Silylboronate Esters by Palladium-Catalyzed Enantiotopic-Group Selective Suzuki-Miyaura Coupling of (Diborylmethyl)silanes with Aryl Iodides

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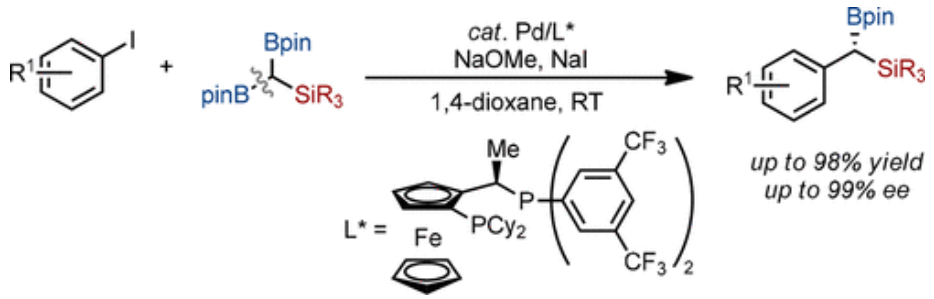
Chiral molecules that contain two different main group elements at the same sp^3 carbon center are highly versatile intermediates in organic synthesis. Such reagents provide significant advantages for increasing molecular diversity and complexity through stereospecific and/or iterative carbon–carbon and carbon–heteroatom bond-forming reactions. Among them, chiral 1,1-silylboronate esters are particularly appealing because of their stability, low toxicity, and ease of handling. Nevertheless, despite their potential usefulness, only a limited success for the preparation of chiral 1,1-silylboronate esters have been reported.[1]

In this poster, I will describe a new synthetic method for the preparation of enantioenriched benzyilic 1,1-silylboronate esters by Pd-catalyzed system for the enantiotopic-group selective cross-coupling of (diborylmethyl)silanes with aryl iodides. The reaction shows broad scope and a range of enantioenriched benzylic 1,1-silylboronate esters are obtained in good to excellent yields with excellent enantioselectivity. The obtained enantioenriched benzylic 1,1-silylboronate esters can be transformed to other synthetically useful compounds through C–O, C–N, and C–C bond forming reactions, highlighting the usefulness of the obtained boronate esters.[2]



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Mild and selective synthesis of unsymmetrical secondary amines from arylnitriles and nitroalkanes catalyzed by bimetallic PdPt–Fe_3O_4 nanoparticles

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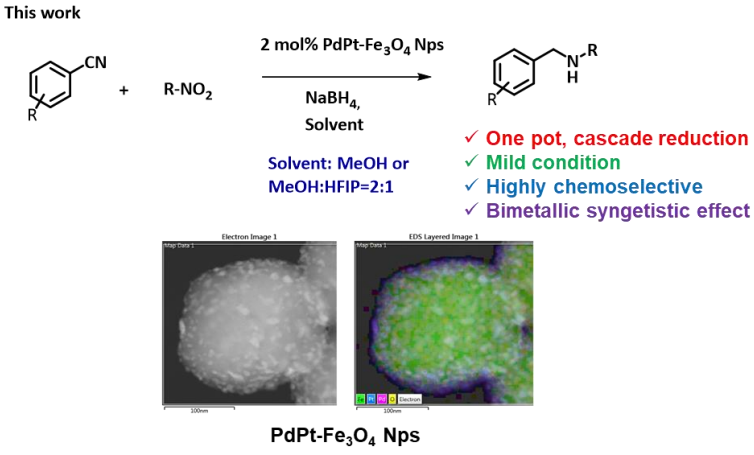
Bimetallic nanoparticles (NPs) have shown outstanding achievement as a catalyst in organic chemistry. In many cases, it has been proven that the bimetallic alloy NPs exhibit enhanced catalytic activity compared to their mono metal counterparts due to the strong synergy between the two metals. In this connection, we have developed successful catalytic reduction of nitro compounds[1] and silylation of aryl halides[2] using PdPt–Fe_3O_4 NP catalyst.
Herein, we report selective synthesis of unsymmetrical secondary amines via one-pot cascade hydrogenation of arylnitriles with nitroalkanes or alkylamines using PdPt–Fe_3O_4 NPs as a catalyst. This catalytic system gives a straightforward route to secondary amines obviating the use of alkyl halides or carbonyl compounds. With the use of PdPt-Fe_3O_4, benzonitrile was converted to symmetrical dibenzylamine in excellent (98%) yield with $NaBH_4$ in MeOH. In addition, the PdPt bimetallic catalyst was proven to be superior to either Pd or Pt monometallic one in both reactivity and selectivity. Synthesizing various unsymmetrical secondary amines under mild conditions was possible with this bimetallic catalytic system. Arylnitriles containing an electron-donating substituent were rather resistant to the reductive amination, however, when HFIP was used as a co-solvent, the reaction selectivity and yield for unsymmetrical secondary amines increased. Due to the magnetic property of Fe_3O_4 support, the bimetallic catalyst could easily be recycled through the use of an external magnet at least four times.



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Harnessing Secondary Coordination Sphere Interactions Enables the Selective Amidation of Benzylic C−H Bonds

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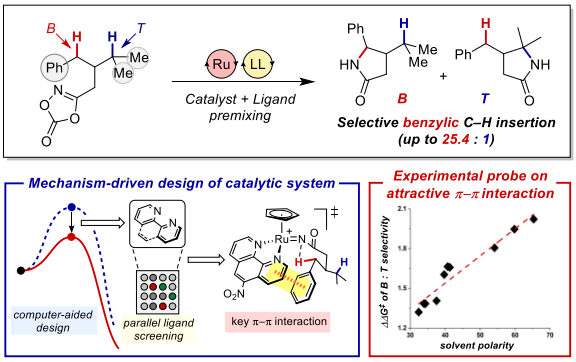
Engineering site-selectivity is highly desirable especially in C−H functionalization reactions.[1] We report a new catalyst platform that is highly selective for the amidation of benzylic C−H bonds controlled by π-π interactions in the secondary coordination sphere. Mechanistic understanding of the previously developed iridium catalysts[2] that showed poor regioselectivity gave rise to the recognition that the π-cloud of an aromatic fragment on the substrate can act as a formal directing group through an attractive non-covalent interaction with the bidentating ligand of the catalyst. Based on this mechanism-driven strategy, we developed a cationic (η^5-C_5H_5)Ru(II) catalyst with a neutral polypyridyl ligand to obtain a record-setting benzylic selectivity in an intramolecular C−H lactamization in the presence of tertiary C−H bonds at the same distance. Experimental and computational techniques were integrated to identify the origin of this unprecedented benzylic selectivity, and robust linear free energy relationship between solvent polarity index and the measured site-selectivity was found to clearly corroborate that the solvophobic effect drives the selectivity under Curtin-Hammett control. Generality of the reaction scope and applicability towards versatile γ-lactam synthesis were demonstrated.



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Alkoxide-Promoted Selective Hydroboration of *N*-Heteroarenes: Pivotal Roles of *in situ* Generated BH_3 in the Dearomatization Process

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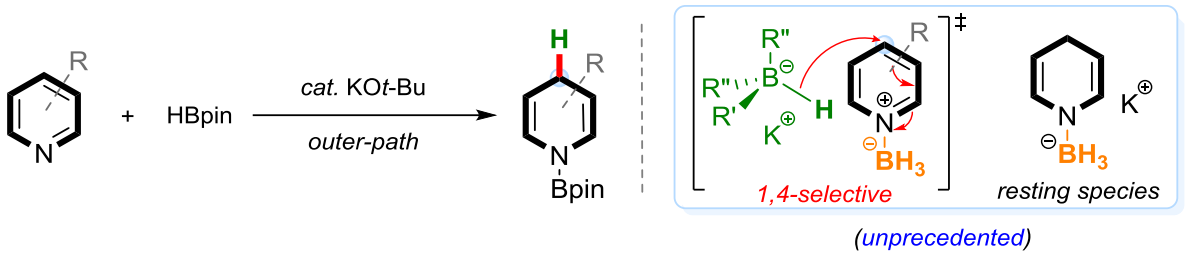
While numerous organo(metallic)catalyst systems were documented for dearomative hydroboration of *N*-aromatics,[1] alkoxide base catalysts have not been disclosed thus far. Described herein is the first example of alkoxide-catalyzed hydroboration of *N*-heteroaromatics including pyridines, providing a broad range of reduced *N*-heterocycles with high efficiency and selectivity.[2] Mechanistic studies revealed an unprecedented counterintuitive dearomatization pathway, in which (i) pyridine-BH_3 adducts undergo a hydride attack by alkoxyborohydrides, (ii) *in situ* generated BH_3 serves as a catalytic promoter, and (iii) 1,4-dihydropyridyl borohydride is in a predominant resting state.



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Palladium-Catalyzed Chemoselective Negishi Cross-Coupling of Bis[(pinacolato)boryl]methylzinc Halides with Aryl (Pseudo)Halides

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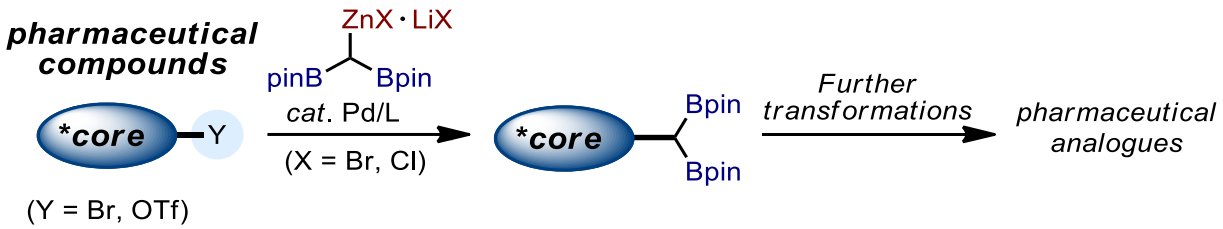
We describe a palladium-catalyzed chemoselective Negishi cross-coupling of a bis[(pinacolato)boryl]methylzinc halide with aryl (pseudo)halides. This reaction affords an array of benzylic 1,1-diboronate esters, which can serve as useful synthetic handles for further transformations. The developed coupling reaction is compatible with various functional groups and can be easily scaled up. The coupling of bis[(pinacolato)boryl]methylzinc halides with pharmaceuticals and the subsequent late-stage manipulations demonstrate the power of the developed protocol.[1]



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Design and Synthesis of Sterically Demanding Palladium-PEPPSI Precatalyst of *a*NHC based on Imidazo[1,2-a]pyridine

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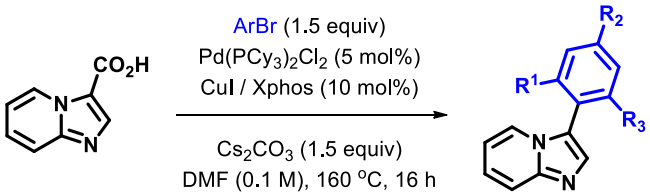
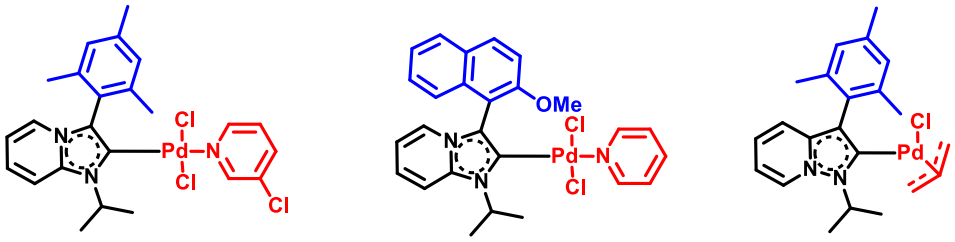
Phosphine ligands have been chosen for a long time in the field of organic chemistry especially in C-C cross coupling reactions. However, N-heterocyclic carbenes (NHCs) are widely being replaced as valid alternatives due to their strong σ-donating capability and higher stability towards air and moisture.[1,2] Although various modifications of N-substituents on NHC backbone are accessible, very few with the sterically bulky C-substituents have been reported due to their synthetic limitations.

As a result of our continuous research on the development of novel abnormal NHC ligands, we found good reaction conditions for C-3 arylation of imidazo[1,2-*a*]pyridine backbone especially with sterically bulky substituent. Pd/Cu-catalyzed decarboxylative arylation was suitable to install a wide range of sterically bulky substituents. And stable Pd and Rh complexes of imidazo[1,2-*a*]pyridines were synthesized through the transmetalation of their Ag complex. And the measurement of the CO stretching frequency of dicarbonyl Rh-imidazo [1,2-*a*]pyridine turned out that our abnormal NHC has lower TEP value (TEP: 2035.7 cm^{-1}) than other known normal NHCs. Many of Pd complexes have been prepared and are being tested in C-C coupling reactions. Furthermore, the complexations with other transition metals, such as, Rh, Ru and Ir are being under investigation.





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Regiodivergent Hydroalkynylation for the Synthesis of 1,3- and 1,4-Ynenamides via Kinetically Favored Hydropalladation and Ligand-Enforced Carbopalladation

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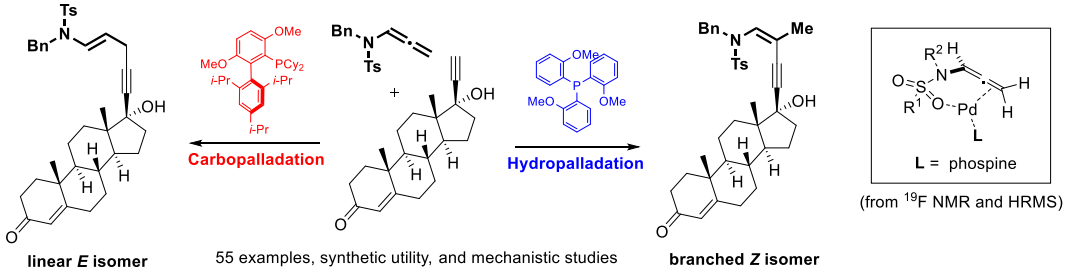
Abstract: In continuation of our recent research on ynamides,[1] we reported herein, a regio- and stereoselective hydroalkynylations of a readily available allenic skeleton, N-sulfonylallenamide. Although, hydroalkynylations were successfully applied to electron-neutral/electron-deficient cumulene (allenoates 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 chemo-selectivity. 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.



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1,1-Difunctionalization of Unactivated Alkenes via Cationic Palladium Catalysis

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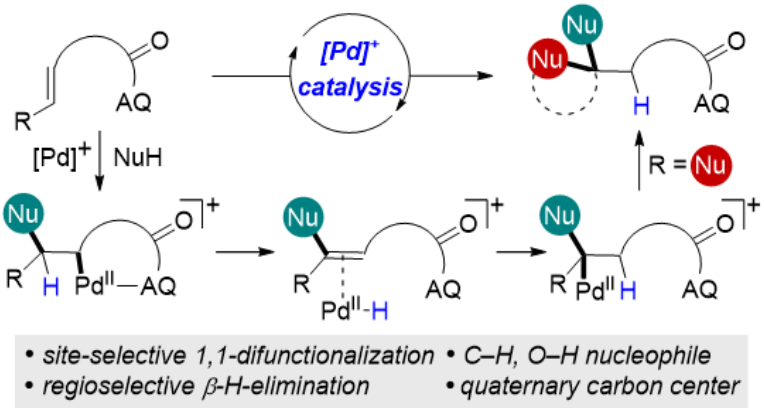
Palladium-catalyzed difunctionalization of alkenes has received much attention as a powerful synthetic method for rapidly constructing valuable building blocks of pharmaceuticals and natural products. Unlike the considerable development of 1,2-vicinal difunctionalization, however, 1,1-geminal difunctionalization of unactivated alkenes remains a difficult research area. We reported a new synthetic strategy using a cationic palladium species to facilitate the 1,1-geminal difunctionalization of unactivated alkenes at either the γ- or δ- position, which can be applied to internal alkenes as well as terminal alknenes. Our strategy is also applicable to unsymmetric 1,1-difunctionalization of alkenes having tethered hydroxyl or carboxylic acid groups, which enables constructing complex molecules with oxo quaternary carbon centers under mild reaction conditions.



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Alkoxy Radical Generation and Functionalization of Pyridinium Derivatives *via* Quinolinone Photocatalysis

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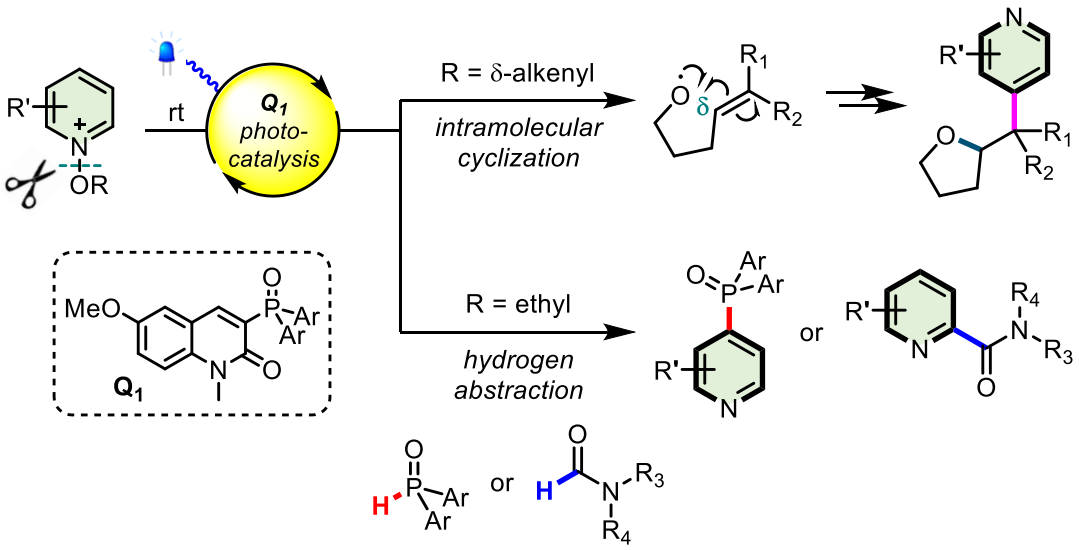
We developed a novel visible-light-enabled alkoxy radical ring-closure and pyridylation from *N*-alkenyloxypyridinium salts. This straightforward approach features a photoredox tandem radical strategy involving a sequential fragmentation of an *N*-alkoxypyridinium salt, a radical cyclization process, and a pyridylation process. The transformation exhibited broad substrate scope, good functional group compatibility, and metal-free mild conditions with quinolinone organophotocatalyst, offering a powerful synthetic tool for assembling various pyridine-tethered tetrahydrofuran products and late-stage functionalization of complex biorelevant molecules. Moreover, radical cascade cyclization could be successfully achieved for accessing the synthetically important bicyclic oxaspiro ring systems.

Also, a new approach to site-divergent functionalization of pyridine derivatives was accomplished. The site-selectivity is switchable between ortho and para position of heteroaryl core by coupling radical sources generated *via* hydrogen abstraction by ethoxy radical. Under optimized conditions, phosphinoyl radical favors para position, while carbamoyl radical shows the preference to ortho position. Furthermore, we carried out the late-stage modification of medicinally relevant molecules and could obtain corresponding products with good functional group tolerance.



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Bicyclic Bridgehead Phosphoramidites (Briphos): Tunable π-Acceptor Phosphine Ligands

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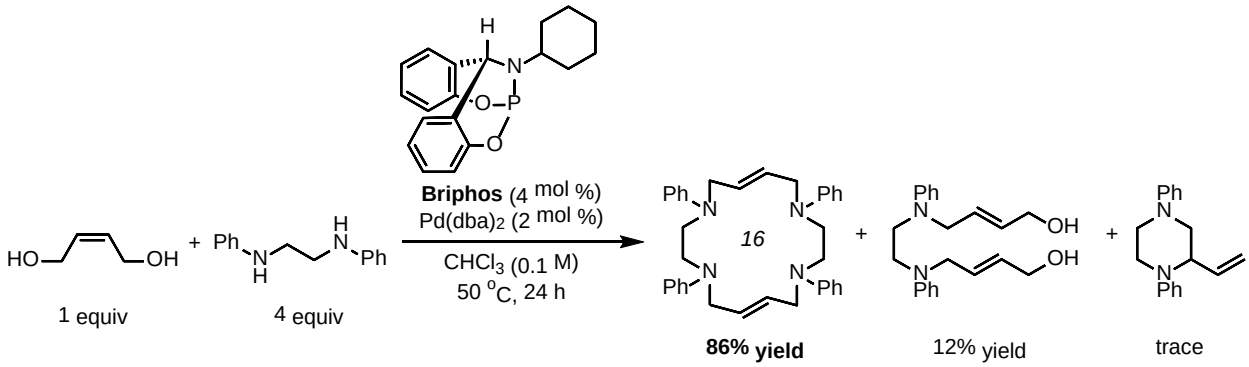
Chemical reaction is a crucial component of our everyday lives. The most powerful and efficient chemical reactions commonly use catalysis to control reactivity and selectivity. Thus, the discovery of new catalyst and catalysis concepts with broad utility beyond established reactivity will give a great impact on academic and industrial organic synthesis.

We have developed a new class of bicyclic bridgehead phosphoramidite (briphos) ligands based on the bicyclo[3.3.1]nonane structure.[1] The geometrical constraints in briphos with respect to its monocyclic analogs enhance π-acceptor ability. The enhanced π-acceptor ability of briphos gives dramatic ligand acceleration effect (LAE) in low-valent transition metal-catalyzed reactions. Furthermore, facile tuning of briphos leads to new catalytic reactivity[2] in Pd(0)-catalyzed allylic substitutions as well as asymmetric induction[3,4] and control of regioselectivity[5] in Rh(I)-catalyzed conjugate additions.

I will discuss our recent findings on unprecedented access to aza-macrocycles. We discovered that allylic diols react with diamines to give tetraaza macrocycles instead of one to one diaza products. The briphos ligands together with Pd(0) catalyst was highly efficient for activation of allyl diols. The coupling reaction provided a variety of tetraaza macrocycles and proceeded under mild reaction conditions with high yields.



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Electronically Controlled Regiodivergent Cycloisomerizations of Ynenamines to Fused Indoles Promoted by Trifluoromethanesulfonic Acid

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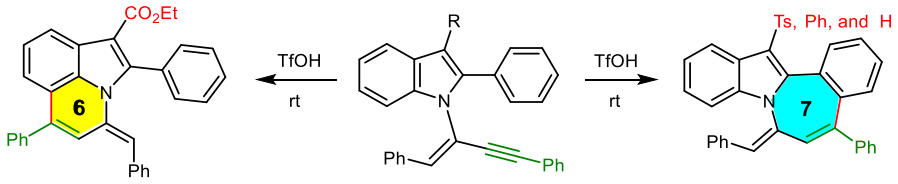
Polyfused N-heterocycles, particularly polyfused indoles, are privileged structures found in many natural products and synthetic compounds with a broad spectrum of biological functions and medicinal applications. In particular, pyrrolo[3,2,1-*ij*]quinolines and benzo[3,4]azepino[1,2-*a*]indoles have become topics of intense research for synthetic organic chemists because of their significant bioactivities. The exploration of novel synthetic pathways for polyfused N-heterocycles based on cycloisomerization reactions of alkyne derivatives is considerably attractive because these reactions permit the prompt synthesis of a small library of compounds through a very simple one-pot process. Trifluoromethanesulfonic acid (TfOH)-mediated cycloisomerizations of ynenamines derived from N-alkynyl indoles, were controlled through the choice of the electron-withdrawing functional group at C-3 of indoles to provide pyrrolo[3,2,1-*ij*]quinolines and benzo[3,4]azepino[1,2-*a*]indoles via *6-endo-dig* and *7-endo-dig* cyclizations, respectively. The natures of the different cyclizations could be controlled by tuning the electronic influences; indole substrates with carbonyl groups (such as -CO_2Et and -COMe) gave products with six-membered rings, while substrates with sulfonyl groups (such as Ts and -Ms) gave products with seven-membered rings in moderate to good yields.



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Enantioselective Synthesis of *α*-Chiral *β*-Hydroxy Allenes via Copper-Catalyzed Allenylboration of Vinyl Arenes

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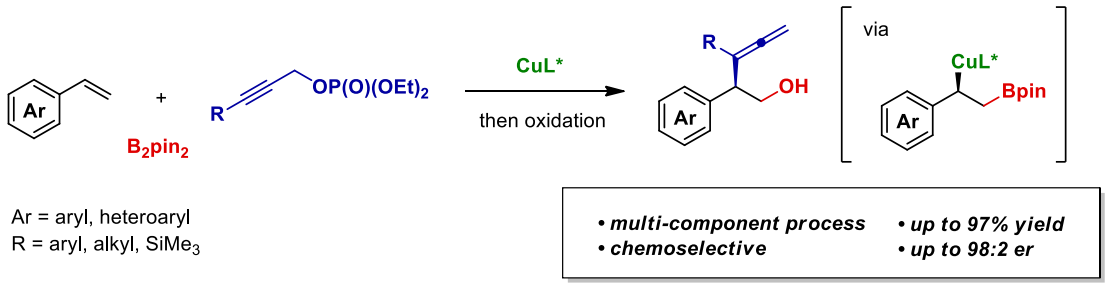
Copper-catalyzed enantioselective allenylboration of vinyl arenes with bis(pinacolato)diboron (B_2pin_2) and propargylic phosphates is reported. This method facilitates a concise access to chiral *α*-branched allenes containing a synthetically useful boronyl group at the *β*-position with high enantioselectivity up to 98:2 er. In the presence of CuCl/chiral Josiphos catalyst, the synthesis of *α*-chiral *β*-hydroxy allenes was achieved through highly S_N2'-selective substitution of a borylalkyl copper species to propargyl electrophiles, followed by oxidation. Catalyst-controlled divergent cyclization with the resulting allenols enabled the construction of chiral *O*-heterocycles.



Ruthenium(II)-catalyzed Divergent Transformation of Acyl Azides

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Iron-based enzymes (*e.g.*, cytochrome P450, oxygenase, etc) display intriguing examples of diversifying catalytic activities from remote C–H activation. Synthetic efforts have been made to design metal-ligand complexes to imitate these transformations. While promising, there is a lack of catalyst systems for the chemo-control towards such reactivity in single catalyst platform. Given these challenges, we designed the strategy in which both C–H oxidation and remote desaturation are driven by piano-stool Ru complexes with quinolin-8-amine-based bidendate ligands. This Ru complex platform enabled the formation of Ru-nitrenoids by reacting cationic ruthenium precursor with acyl azides, which would lead to both C–H amidation and desaturation events through C–H abstraction. More importantly, we found that the electronic control on the ligand of ruthenium complex lead to promising selectivity of each pathway. we have developed ruthenium-catalyzed selective transformations, intramolecular C–H amidation and desaturation of alkane using acyl azides.

References

[1] Yeong Bum, Kim.; Jung-Woo, Park.; and Sukbok Chang;, manuscript in preparation

Visible-Light Excitation of Quinolinone-Containing Substrate Enables Divergent Radical Cyclization

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Photocatalytic reactions have been intensively investigated as powerful tools due to its straightforward and eco-friendly advantages. Despite of the merits of photocatalytic reactions, visible-light mediated synthesis has primarily relied on the use of photocatalysts which absorb visible-light region and drive the chemical reaction through either electron or energy transfer. Ideally, photocatalytic reaction which does not use any external photocatalyst is highly desirable in terms of green chemistry and atom-economy.

In this work, we have demonstrated the ability of quinolinone-containing substrate to serve as effective photoreductant to trigger radical-based bond-forming processes without the need for an external photocatalyst. Utilizing this feature, we developed a novel visible-light mediated cascade reactions. This divergent radical cyclizations controlled by radical sources provided synthetically and biologically valuable tetrahydro- or dihydro-phenanthridin-6(*5H*)-one derivatives under mild and metal-free reaction condition. [1,2]

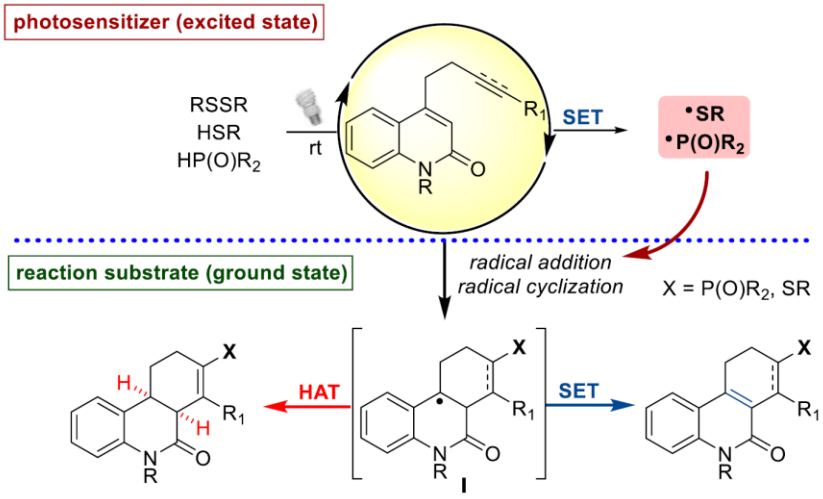

Figure 1 Direct excitation of quinolinone-containing substrates for divergent radical cascade cyclization

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Asymmetric [3,3]-Sigmatropic Rearrangement via Au(I)-Catalyzed Intermolecular Reaction of Propiolates and Allyl Sulfides

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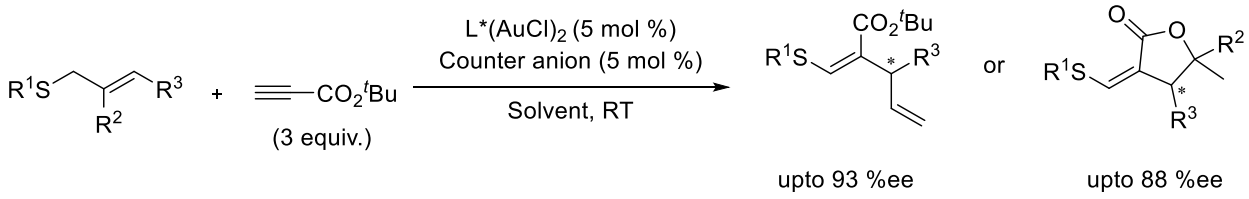
Enantioselective gold-catalyzed catalysis is challenging, especially in an intermolecular mode, because of the linear coordination geometry of the alkyne-gold(I) complex where the chiral ligand lies away from the reaction site. Promoted by our recent success in promoting intermolecular enantioselective coupling of propiolates and alkenes[1], we embarked on the enantioselective reaction between allyl ethers and propiolates[2], where the reaction proceed through O-attack of allyl ether, followed by a [3,3]-sigmatropic rearrangement. In this reaction, allyl sulfides displayed a complementary scope of the migrating allyl moiety and gave upto 93 %ee of the rearranged products.



Scheme 1. Enantioselective intermolecular [3,3]-sigmatropic rearrangement

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Co–Catalyzed Intramolecular C–H Amidation Using Azidoformate

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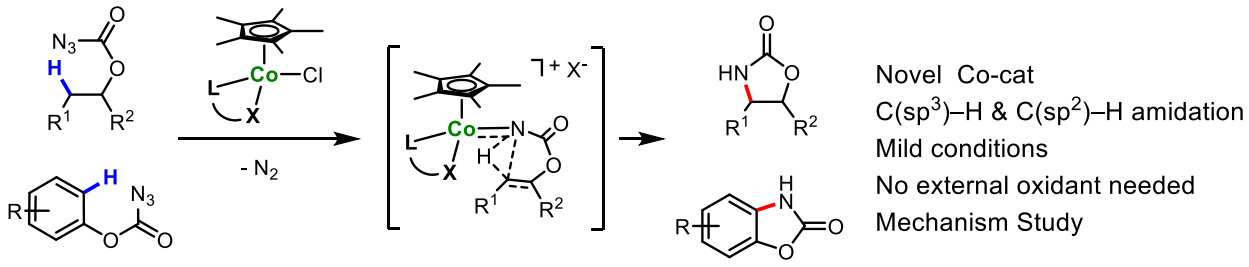
The demand for the facile intramolecular C–H amidation has increased due to versatile utility of product moieties in synthetic and medicinal chemistry. Recently, Singh group developed C(sp^2)–H amidation using Fe and Lebel group employed Rh_2 developing diastereoselective intramolecular amidation.[1,2] Here in, we adopt the tailored Cobalt catalyst with LX type ligand for the intramolecular C–H amidation. The reaction is implemented by formation of Co-imido species from azidoformate as internal oxidant. It showcases for the first time that the unique cobalt catalyst system is applied for both C(sp^3)–H and C(sp^2)–H amidation under mild and external oxidant-free conditions. Detailed mechanistic study will be discussed further.



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Biosynthetically Inspired Transformation of Iboga to Monomeric Post-iboga Alkaloids

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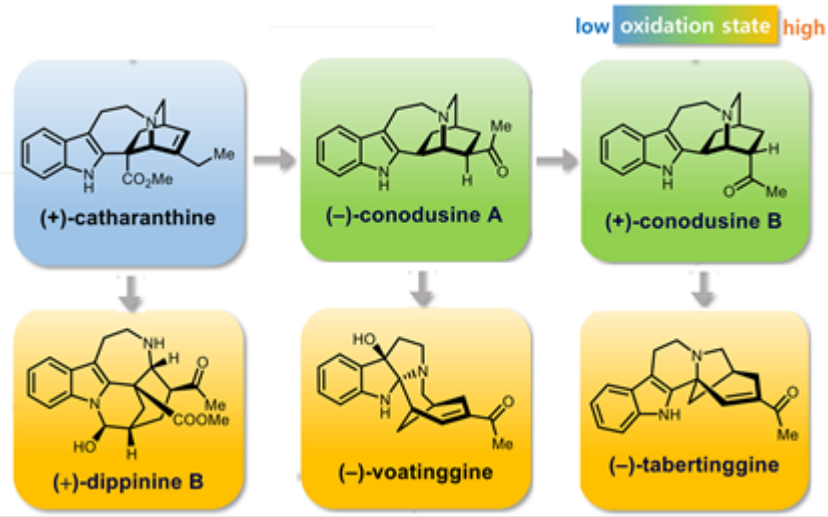
Iboga alkaloids have attracted significant attention from chemists due to their intriguing polycyclic structures and potential therapeutic utilities.[1] We coined the term “post-iboga” alkaloids to describe the types of natural products that are biosynthetically downstream of the iboga-type alkaloids which include rearranged indole and/or isoquinuclidine scaffolds or dimeric iboga alkaloids.

We reported transformation of (+)-catharanthine to different iboga and post-iboga natural products.[2] We developed a streamlined synthetic sequence that transformed (+)-catharanthine to conodusines A and B. We discovered that hydroxyindolenine derivate of (–)-conodusines A and (+)-B underwent distinct structural reorganizations under different acidic conditions to yield (–)-voatinggine and (–)-tabertinggine, respectively. Finally, we showed that a well-orchestrated gradual net oxidations of (+)-catharanthine led to (+)-dippinine B.



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Towards the Total Synthesis of (–)-Flueggenine A and C

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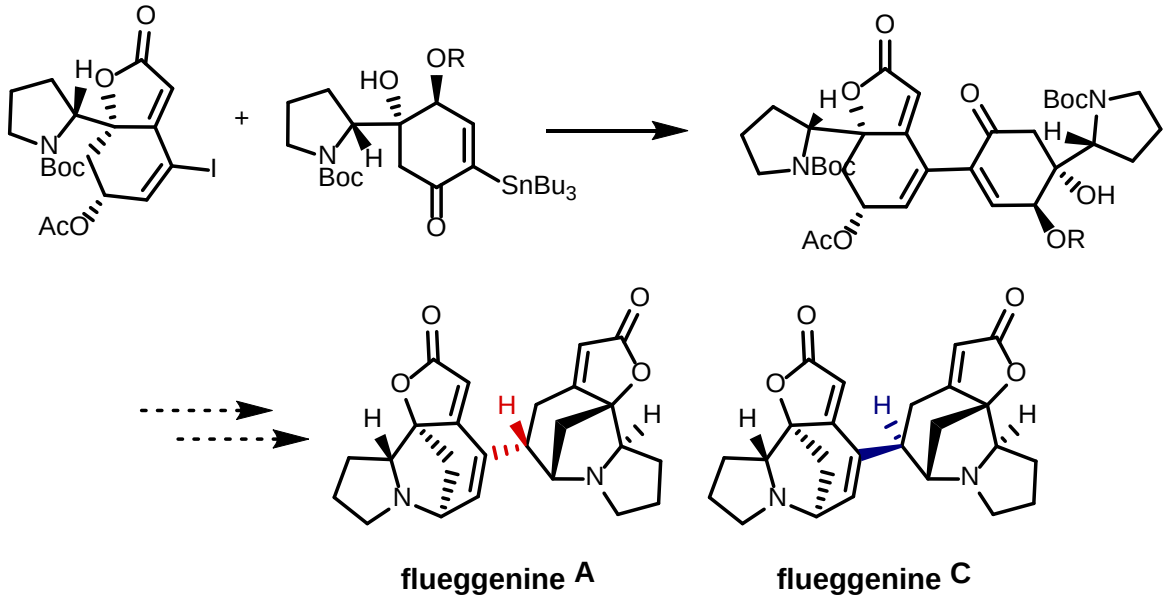
Flueggenine A and C is a dimeric securinega alkaloid with including γ –δ′ linkage between two monomeric units with different stereo chemistry on δ′. Recently, our group have completed total synthesis of flueggenine C via accelerated Rauhut-Currier (RC) reaction[1] and also shown that flueggenine A was not possible to synthesize by RC reaction[2]. We envisioned that a palladium coupled Stille cross-coupling reaction would give carbon-carbon bond formation between two monomeric subunits. Here in we will show progress towards the total synthesis of flueggenine A and C



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Regiodivergent Ring-Opening Cross-Coupling of Vinyl Aziridines with Phosphorus Nucleophiles

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Phosphorus containing organocompounds are frequently used in a wide range of applications in organic chemistry. In this research, catalytic cross-coupling of vinyl aziridines and phosphorus reactants have been developed under mild condition with copper and silver. At room temperature, phosphoryl radicals generated by copper enable S_N2'-type ring opening reactions of vinyl aziridine to afford amino alkylphosphorus products. On the other hand, in-situ generated phosphate anions via the Ag-catalyzed aerobic oxidation of phosphoryl reactants underwent S_N2 reaction to provide phosphorus containing amine products. To understand the stereochemical fate of the stereogenic center, enantiopure vinyl aziridine ester were subjected to the reactions, stereochemistry was retained. There is difference of regioselectivity between phosphoryl radicals and phosphate anions. In addition, only anti-vinyl aziridine ester can react with in-situ generated phosphate anion. We present NBO charge analysis to elucidate the reaction mechanism. Furthermore, this divergent methodology serves as a powerful tool for the stereospecific synthesis of phosphorus-containing amino acid derivatives.

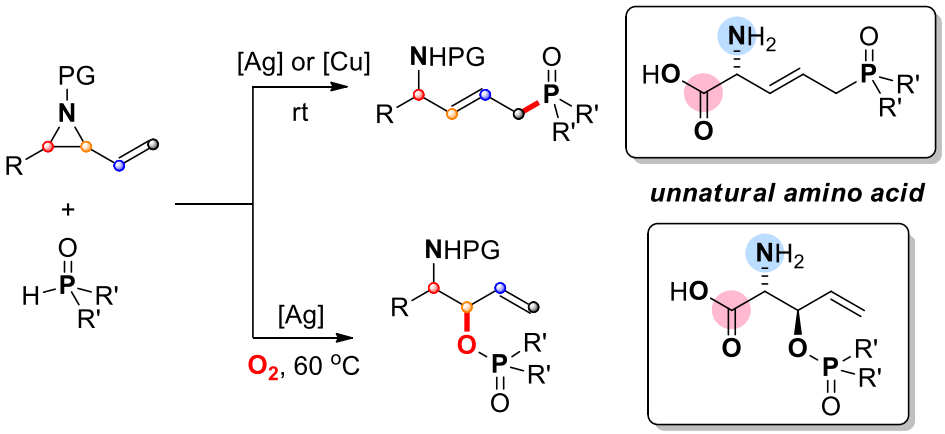

Figure 1. Regioselective and Divergent Catalytic Ring-Opening of Vinyl Aziridines.

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Stereoselective Cu-Catalyzed [5 + 1] Cycloaddition: A Surrogate of Hetero Diels-Alder Reaction

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[m + n] Cycloadditions are one of the most powerful methods for the construction of polycyclic N-heterocycles which are the core skeletons in enormous number of natural products and biologically active compounds. Especially, the asymmetric hetero Diels-Alder reaction, representative [4 + 2] cycloaddition, is one of the most powerful strategy for optically active six-membered heterocyclic compounds in a single operation. Our group has disclosed that an N-aromatic zwitterion with unusual charge distribution could serve as a five-atom donor, leading to the development of many [5 + n] cycloadditions for medium-sized heterocycles. In this symposium, we will discuss the asymmetric copper-catalyzed [5 + 1] cycloaddition of quinolinium zwitterions and terminal alkynes, resulting in the formation of optically pure six-membered ring systems. The developed cycloaddition to six-membered adducts is characterized by high stereoselectivity and good functional group tolerance, and thus has sufficient potential as a surrogate of asymmetric hetero Diels-Alder reaction.

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Copper(II)-Catalyzed Aerobic Oxidation of Amines: Divergent Reaction Pathways by Solvent Control to Imines and Nitriles

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The dehydrogenative coupling of amines by copper catalysts was investigated in the presence of molecular oxygen. By modulating the aerobic oxidation pathways of $Cu(OAc)_2$ catalyst in different reaction solvents, the selective formations of homo-coupled imines, cross-coupled imines, and nitriles have been achieved from amine derivatives. The discovery of the multiple catalytic pathways of $Cu(OAc)_2$ signifies the oxidation potential control of the catalytically active copper species by the reaction solvents under aerobic oxidation conditions. The key to successful implementation of such divergent catalytic pathways has been the different reaction kinetics to intermediate species, where the specific reaction solvents stabilize the respective intermediate species for on demand reaction pathways to imines and nitriles. Without significant change of the reaction conditions, the $Cu(OAc)_2$-catalyzed aerobic oxidations provide the divergent amine oxidation pathways, the feature important for understanding the aerobic oxidation catalyst system.

Given that the aerobic oxidation protocols are of significant interest to chemical industry from the point of green chemistry, the copper-catalyzed aerobic oxidation reactions should attract the continued research efforts in the development of green chemical processes.

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Substrate Promiscuity of *ortho*-Naphthoquinone Catalyst: Catalytic Aerobic Amine Oxidation Protocols to Cross Deaminative Coupling and *N*-Nitrosation

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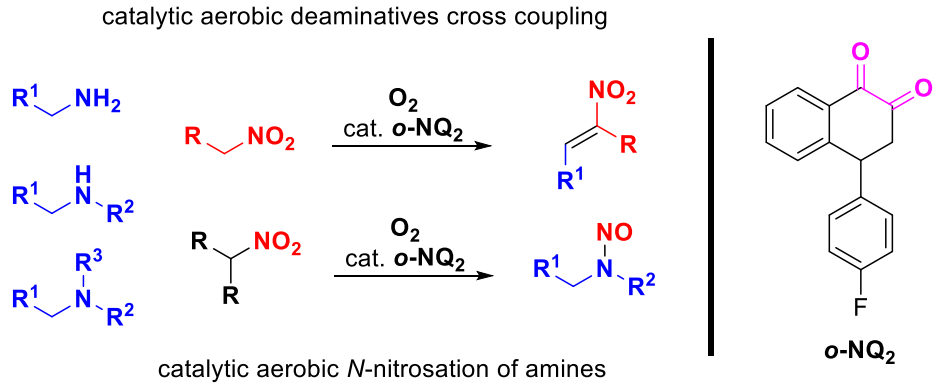
Abstract: *ortho*-Naphthoquinone-based organocatalysts[1] have been identified as versatile amine oxidation catalysts in the presence of aerobic oxygen. Primary aryl amines are readily coupled with primary nitroalkanes via deaminative pathway to give nitroalkene derivatives in excellent yields. Secondary and tertiary amines are inert to *ortho*-naphthoquinone catalysts, however secondary nitroalkanes are readily converted by *ortho*-naphthoquinone catalysts to the corresponding nitrite species that in situ oxidizes the amines to the *N*-nitroso compounds[2]. Without using harsh oxidants in a stoichiometric amount, the current aerobic catalytic oxidation protocol utilizes the substrate promiscuity feature to provide a facile access to amine oxidation products under mild reaction conditions.



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N-heterocyclic carbene ligands of biaryl structure for Pd-catalyzed amination

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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. Theses 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 increase the reactivity. To evaluate the biaryl-ImPy carbene ligands, palladium was introduced to the biaryl ImPy ligands to form Pd complexes.[5] The ligands, which were not made into a complex form, were used to generate a catalyst in-situ in the reaction. 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.

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Visible Light-Promoted Thiyl Radical Generation from Sodium Sulfinates: A Radical-Radical Coupling to Thioesters

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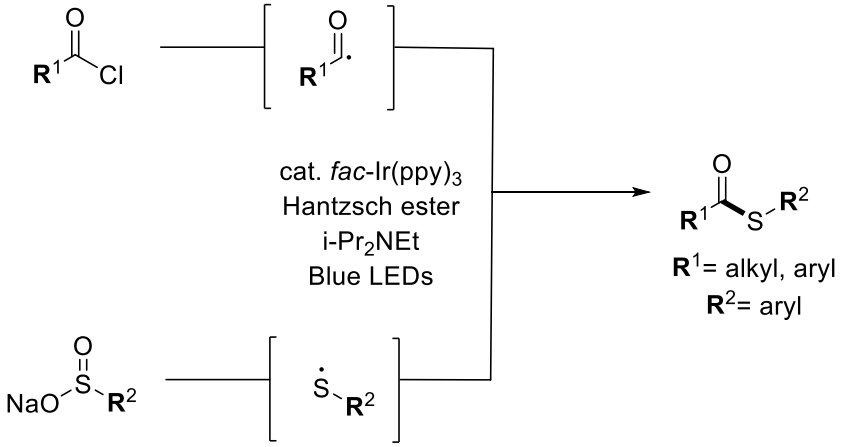
Acyl radicals can be readily generated under various reaction conditions including the photoredox catalysis conditions.[1] However, the synthetic utilization of acyl radicals in the radical−radical cross-coupling reactions has been limited to few radical species such as molecular oxygen and peroxides. There has been an increasing demand of organosulfur compounds in the development of drugs and materials, and the recent advances in the C−S bond formations by transition metal catalysis and Brønsted acid catalysis amply demonstrate the full potential of organosulfur compounds.[2] Recently, in our laboratory we have developed a new radical−radical cross-coupling reactions of thiyl radicals from the parasitic photoredox reaction pathway of sodium sulfinates with acyl radical (Scheme 1).[3] The current radical−radical cross-coupling strategy allows a direct synthetic access to thioesters, a useful building block in the Fukuyama coupling and Liebeskind−Srogl coupling reactions.



Scheme 1. Acyl Radical-thio radical coupling to thioesters

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Visible Light Photoredox Catalysis: Robust Access to α-Carbonyl Radicals from Enoxybenzotriazoles

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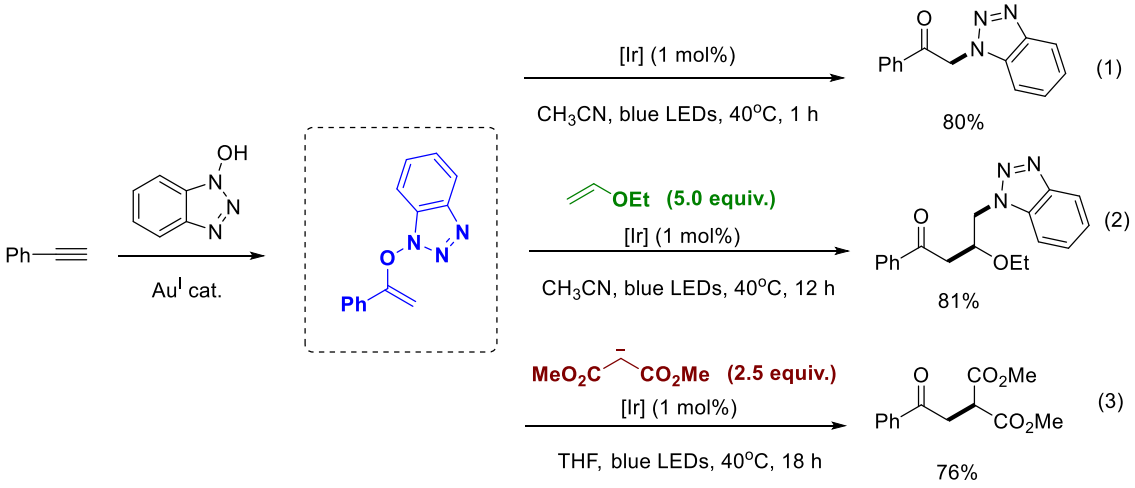
Over the past few decades, visible light photoredox catalysis has emerged as an appealing tool to access radical intermediates, enabling C-C and C-Heteroatom bond formations.[1] In continuation of our interest in the N-O bond-mediated oxidative transformations,[2] we introduce herein enoxybenzotriazoles as substrates for the photoredox catalysis. We envisioned that the cleavage of N-O bond would produce α-carbonyl radicals.[3] In contrast to conventional reactivity of carbonyl compounds, such as those of enolates and α-ketyl radicals, these α-carbonyl radical may mediate novel transformations with unprecedented selectivity. We present herein three novel reactions: (Eq. 1) *O*- to *C*- transposition of benzotriazolyl group, leading to α-triazolyl carbonyl compounds; (Eq. 2) Group transfer radical addition (GTRA) via reactions with alkenes; and (Eq. 3) Coupling with malonates, leading to 1,4-dicarbonyl compounds.



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Delineating Physical Organic Parameters in Site-Selective C–H Functionalization of Indoles

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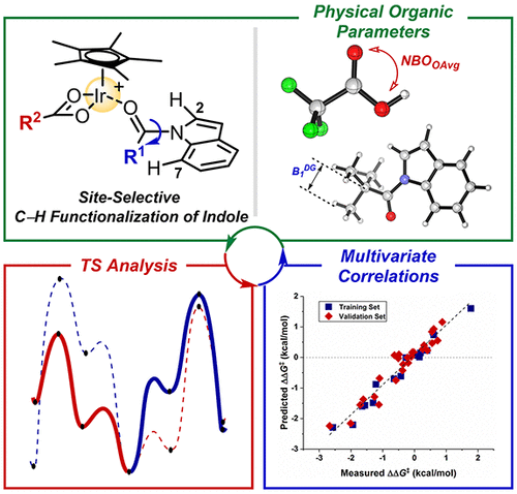
Site-selective C–H functionalization is a great challenge in homogeneous transition-metal catalysis. Herein, we present a physical organic approach to delineate the origin of regioselective amidation of *N*-acylindoles through Ir(III) catalysis. Bulkiness of *N*-directing groups of indole substrates and electronics of carboxylate additives were identified as two major factors in controlling C2 and C7 selectivity,[1] and their microscopic mechanisms were studied with DFT-based transition state analysis. Computational insights led us to interrogate a linear free energy relationship, and parametrization of molecular determinants enabled the establishment of an intuitive yet robust statistical model that correlates an extensive number of validation data points in high accuracy. This mechanistic investigation eventually allowed the development of a new C2 amidation and alkenylation protocol of indoles, which affords the exclusive functionalization at the C2 position with up to >70:1 selectivity.[2]



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Oxidatively Induced Reductive Elimination: Expanding the Scope, Catalyst Systems, and Oxidation Tools

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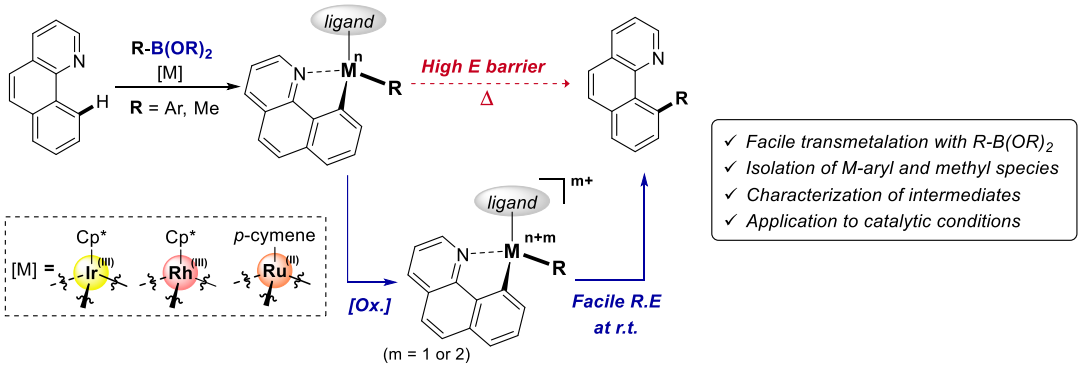
The introduction of carbon-carbon bonds on C–H in direct manner has been widely utilized for the preparation of synthetic or natural products. For conduction of successful catalytic cycle, the key reductive elimination should be analyzed. However, presumably due to the difficulties in the intermediate preparation, the study on the reductive elimination has been concentrated on only several species such as Pd, Ni, or Pt catalysts, although direct C–H aryl/alkylation using different metal catalysts also has been actively reported.

In this study, using boronic esters nucleophiles as aryl/alkylation partners, we prepared and characterized half-sandwich Ir^{III}, Rh^{III}, and Ru^{II} aryl and methyl species with cyclometalated benzo[*h*]quinoline ligand as intermediates for the reductive elimination. Combining cyclic voltammetry analysis and stoichiometric oxidation, we revealed that oxidation of the metalacycle intermediates can facilitate their reductive elimination, which is not easily achieved in thermal conditions. DFT calculation suggested that the oxidation of the metal center significantly mitigates energy barrier for the reductive elimination. Based on the stoichiometric reactivity and calculation results, we adopted the concept of this 'oxidatively induced reductive elimination' into the catalytic conditions. Finally, as an unreported example, we disclosed Ir-catalyzed direct C–H arylation using aryl boroic ester nucleophiles under mild conditions.



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Copper-Mediated Amination of Aryl C–H Bonds with the Direct Use of Aqueous Ammonia via a Disproportionation Pathway

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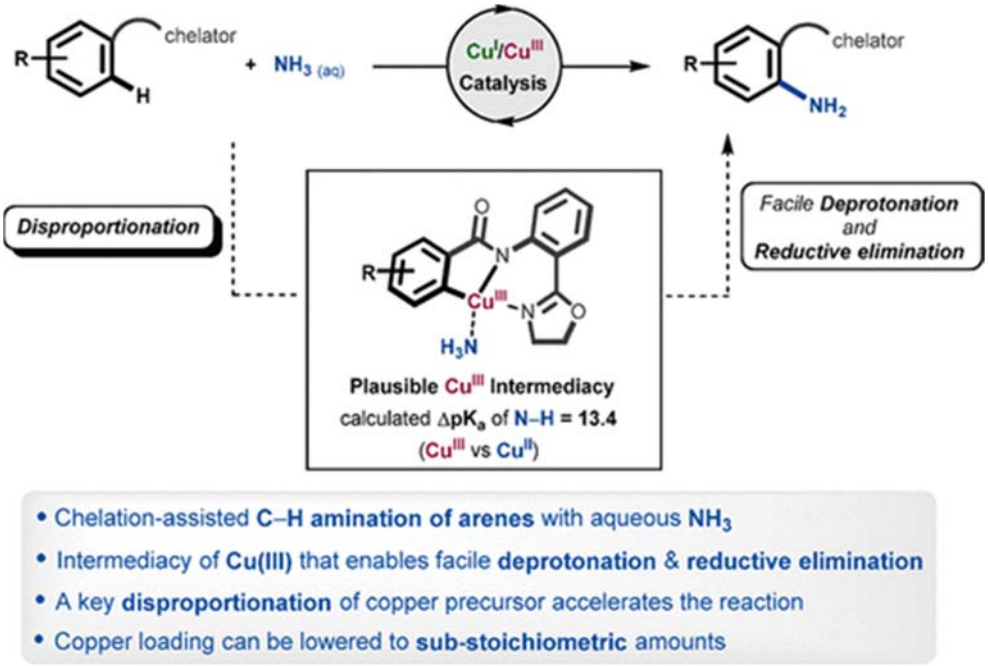
The direct amination of C−H bonds with ammonia is a challenge in synthetic chemistry. Herein, we present a copper-mediated approach that enables a chelation-assisted aromatic C−H bond amination using aqueous ammonia. A key strategy was to use soft low-valent Cu(I) species to avoid the strong coordination of ammonia. Mechanistic investigations suggest that the catalysis is initiated by a facile deprotonation of bound ammonia, and the C−N coupling is achieved by subsequent reductive elimination of the resultant copper−amido intermediate from a Cu(III) intermediate that is readily generated by disproportionation of low-valent copper analogues. This mechanistic postulate was supported by a preliminary kinetic isotope effect study and computations. This new chelation-assisted, copper-mediated C−H bond amination with aqueous ammonia was successfully applied to a broad range of substrates to deliver primary anilines. Moreover, the mild conditions required for this transformation allowed the reaction to operate even under catalytic conditions to enable a late-stage application for the preparation of pharmaceutical agents.



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Total syntheses of (*rac*)- and (+)-Goniomitine via intramolecular imino-Stetter reaction

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Goniomitine, isolated from the root bark of Gonioma Malagasy, has interesting biological activity such as antiproliferative activity in several cancer cell lines. In addition, although it belongs to aspidosperma alkaloids, it possesses unique structural features such as aminal-containing tetracyclic core and β-hydroxyethyl side chain at the 3-position of the indole. These intriguing characters of the goniomitine sparked interest within the synthetic community and there have been seven asymmetric total syntheses of this natural product along with five total syntheses of (±)-goniomitine to date.
According to the proposed biosynthetic pathway, this natural product might be generated from vincadifformine through a series of fragmentation/rearrangement through a tryptophol intermediate bearing ethyl-3-piperidinium, which could be generated from the corresponding lactam, at the 2-position. Although biomimetic synthesis could significantly streamline the synthetic approach for the natural product, most of the previous total syntheses of goniomitine have been developed through a different synthetic strategy and the total synthesis of goniomitine, particularly the asymmetric total syntheses, have not been well developed based on this biogenetic synthetic route. As part of our interest in the total synthesis of indole alkaloids based on the cyanide-catalyzed imino-Stetter reaction, we envisioned that the proposed key intermediate, tryptophol bearing ethyl piperidinone ring at the 2-position, could be prepared via the cyanide-catalyzed imino-Stetter reaction of 2-aminocinnamic acid derivatives and aldehyde bearing a piperidinone ring. In this poster presentation, we will describe the highly concise total syntheses of (±)- and (+)-goniomitine using the cyanide-catalyzed imino-Stetter reaction as the key step.

Concise Total Synthesis of Phenanthroindolizidine and Phenanthroquinolizidine Alkaloids Using the Building Block Strategy

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Since phenanthroindolizidine and phenanthroquinolizidine alkaloids exhibit interesting biological activities, they have received increasing attention in the past decades. In addition to their interesting biological activities, these natural products display structural diversity; they possess the different number of methoxy groups around the phenanthrene ring and the different positions of the nitrogen atom in the indolizidine and quinolizidine rings, respectively. Thus, they have been considered synthetically challenging targets and many different synthetic routes have been developed. Despite these synthetic efforts, most previous approaches have been designed for the synthesis of each specific target molecule through an independent synthetic pathway, and there have been no general synthetic approaches to access these natural products. Thus, it is important to develop a novel synthetic route to approach the phenanthroindolizidine and phenanthroquinolizidine alkaloids with structural diversity.

Although these natural products exhibit the structural diversity, we recognized the structural similarity in these natural products.[1,2] Particularly, these two classes of natural products possess phenanthrene including a 1,2-dimethoxyphenyl ring structure, and have structurally similar pentacyclic skeletons, which could be constructed from the corresponding ortho-aza-terphenyl structures. Based on the structural similarity of these natural products, we envisioned that these natural products could be prepared via the iterative Suzuki-Miyaura reaction of three building blocks: aryl boronic acid, ortho-bromoaryl MIDA boronates, and pyridyl bromide with a suitable side-chain. In this poster presentation, we will describe the development of a general and concise synthetic route for phenanthroindolizidine and phenanthroquinolizidine alkaloids by the building block strategy.

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Diverted Approach to Access Site-Selctive Amidation of Carbonyl Compounds: Umpolung Reactivity of Iridium Nitrenoid

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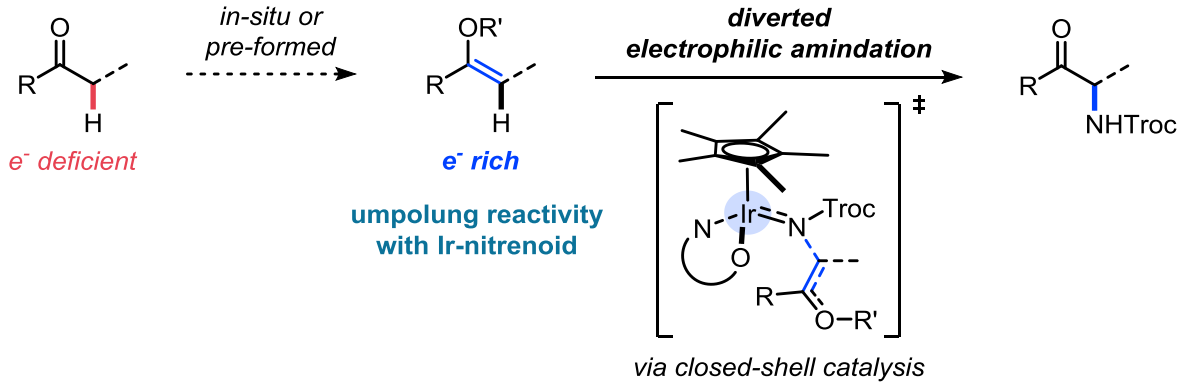
Amination to α-carbonyls have received great interest as a powerful tool for accessing nitrogen-containing molecules in synthetic and medicinal chemistry, because α-aminocarbonyls are common in bioactive molecules. In this regard, herein we describe the development of diverted C–H amination reaction of α-carbonyl compounds. In this reaction, the transient intermediate, electrophilic Ir-nitrenoid, was trapped by the nucleophilic attack of carbonyl compounds along with the high chemoselectivity. The origin of the high chemoselectivity toward carbonyl α-position was attributed to nucleophilic attack mode from enol tautomer based on the both experimental and computational results. By adopting the iridium system, the distinct mechanistic and experimental results was observed from previous radicaloid metal-catalyzed α-amidation reactions.



Dual-functional Fluorescent Molecular Rotor toward Microviscosity Imaging during Reticulophagy

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Autophagy of the endoplasmic reticulum (ER), termed reticulophagy, is a form of selective autophagy that is linked to the unfolded protein response for maintaining cell homeostasis.[1] Reticulophagy largely contributes to the protein quality control process in the ER; however, the accumulation of unfolded or misfolded proteins in the ER can lead to ER stress,[2-4] resulting in several pathophysiological processes and severe diseases such as tumorigenesis,[5] neurodegenerative diseases,[6] and diabetes.[7,8] Therefore, gaining a comprehensive understanding of the reticulophagy process could provide a promising approach for the diagnosis and therapy of these diseases.[9]

The current work describes a novel dual-functional fluorescent molecular rotor for imaging ER microviscosity during reticulophahy by a BODIPY-arsenicate fluorophore. The microenvitonment-sensitive, dual-functional fluorescent probe 1 was rationally designed to covalently bind to vicinal dithiol-containing proteins (VDPs) in the ER, and thus the selective binding of VDPs in the ER leads to reticulophagy initiation and microviscosity evaluation.

Probe 1 was able to induce intracellular reticulophagy while also allowing for quantification of the local viscosity changes of the ER in live cells, thereby providing a quantitative method to monitor the dynamic autophagic processes in the live cells. Due to the molecular rotor (BODIPY) and a phenylarsenicate moiety, we could explore the dynamic changes of the microenvironment in suborganelles during the formation of autolysosome. Furthermore, probe 1 was able to specifically label VDPs in the nascent proteins in the ER, which could result in ER stress because of the accumulation of misfolded or unfolded VDPs. Therefore, probe 1 could be a promising tool for the study of ER autophagy.

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Organic Functionalization on Polydiacetylenes System for Sensing Applications

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Polydiacetylenes (PDAs), which are generated from polymerization of diacetylene monomers are emerging systems for various sensing applications.[1] 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 addition, further studies for stepwise color change (blue-red-yellows) of PDA vesicle have been achieved. Although general PDA shows blue-red color transitions, the alkyl chain length-controlled (*e.g.*, methyl and *n*-octyl) showed interesting and reversible red-yellow color transition by temperature increase.[3]
Lastly, the installation of *tert*-amine in the PDA system will be presented. The chemical handle of amine group in PDA-liposome strongly enhanced ATP detection limits. And the positional controls of amine groups in PDA system also studied.[4] The synthetic procedures for diacetylene monomers along with color changes of PDA-liposome will be discussed.

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Enhancing the Performance and Stability of Perovskite Solar Cells by Applying Multifunctional Pt(II) Complex

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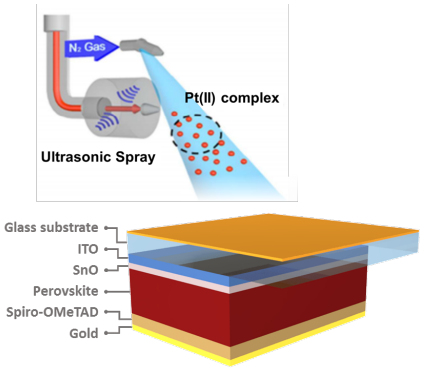
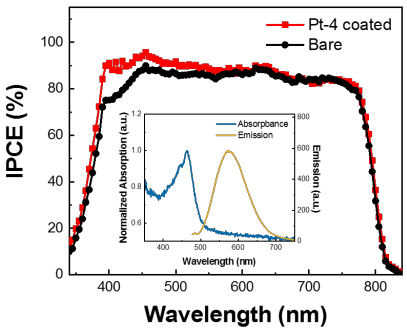
Perovskite solar cells have been regarded as one of the most promising photovoltaics due to the rapid growth of efficiency from 3.8% to 22.1%.[1] Because their most available range of light is limited to the visible region, a concept of frequency conversion has been presented as a strategy to further improve the power conversion efficiency (PCE) of the perovskite solar cells.[2] On the other hand, they usually have relatively low stability against ultraviolet light, water, and heat, making it difficult to withstand outdoor conditions. Therefore, it is important to develop a new system that can enhance both the performance and the stability of the perovskite solar cells.

Here, we present a stable Pt(II) complex with high emission quantum efficiency and easily tunable ligands. We have designed and synthesized the complex and applied it as a photon down-shifting layer. The optical properties and the solubility of the compound was successfully adjusted by ligand tuning. The thin and less-aggregated layer of the complex was fabricated by using the ultrasonic spray deposition (USD) method. With this additional layer, the perovskite solar cells showed the enhanced J_{SC} and PCE values, which was corresponding to the increased stability against ultraviolet irradiation. Furthermore, thanks to the hydrophobic fluoroalkyl groups attached to the ligands, the significantly improved humidity-stability for the devices was also observed.





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A Highly Stable Donor-Acceptor Type Oxazepine-Containing Fluorophore and Its Applications in Bio-imaging

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Oxazepines are unsaturated seven-membered heterocyles containing an oxygen and a nitrogen. It has been reported that some oxazepines show interesting biological activities such as antitumor, anti-inflammation, antimicrobiotic acitivites.[1] Especially, medicinally important drugs including Amoxapine, Loxapine, and Nitroxazepine have distinctive structural features consisting of oxazepine backbone with hybridization of two benzene rings.

In this work, we developed a new donor–acceptor type napthalene-based oxazepine fluoropore, **OXN-1**, which exhibits high chemcial stability in harsh conditions.[2] Its exceptional structural stabilities and photophysical properties were thoroughly examined and further explained by quantum chemical calculations. Its bioimaging capabilities for cells with low cytotoxicity were verified. In addition, its deep tissue imaging capability with two-photon microscopy (TPM) was evaluated. These findings may present **OXN-1** as a new promising fluorescent probe in biomedicinal application.

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Ultrasonic Spray Chemistry: In-situ Synthesis of Thin-Film Conjugated Microporous Polymers and Their Energy Storage Applications

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Conjugated microporous polymers (CMP) are potential energy storage materials owing to their rigid and cross-linked microporous structures. However, the fabrication of nano- and microstructured CMP films for practical applications is currently limited by processing challenges. We report ultrasonic spray chemistry (USC) as an effective method for synthesizing CMP films. The combined effect of ultrasonic cavitation and nebulization in USC provides enough energy to initiate chemical reactions. Thus, USC simultaneously achieves oxidative C–C coupling polymerization and fabrication of thin films. The reaction yield, porosity, and capacitance of the prepared CMP films were strongly dependent on the applied ultrasonic frequency (120 and 180 kHz). Furthermore, USC was used to prepare highly conductive, 3D porous electrodes by a layer-by-layer sequential deposition of CMP and single-walled carbon nanotubes. These supercapacitors demonstrated high specific capacitances (755.7 F/g and 61.3 mF/cm2 at 10 mV/s) with high cycling stability of 95% retention after 20,000 cycles.

Molecular Design Strategy toward Robust Organic Dyes in Thin-Film Photoanodes

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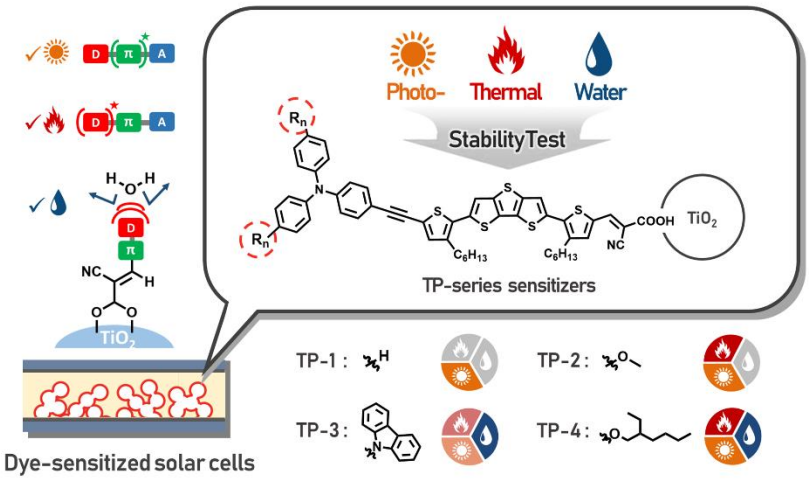
Dye-sensitized solar cells (DSSCs) have attracted attentions because of application to building integrated photo voltaic (BIPV) system. It has several advantages, especially very high efficiency at low illumination. However, there have been still stability issues and molecular strategy for rigid stability 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**.



Control of Electronic Coupling for Retarding Back Electron Transfer in Molecular Solar Cells

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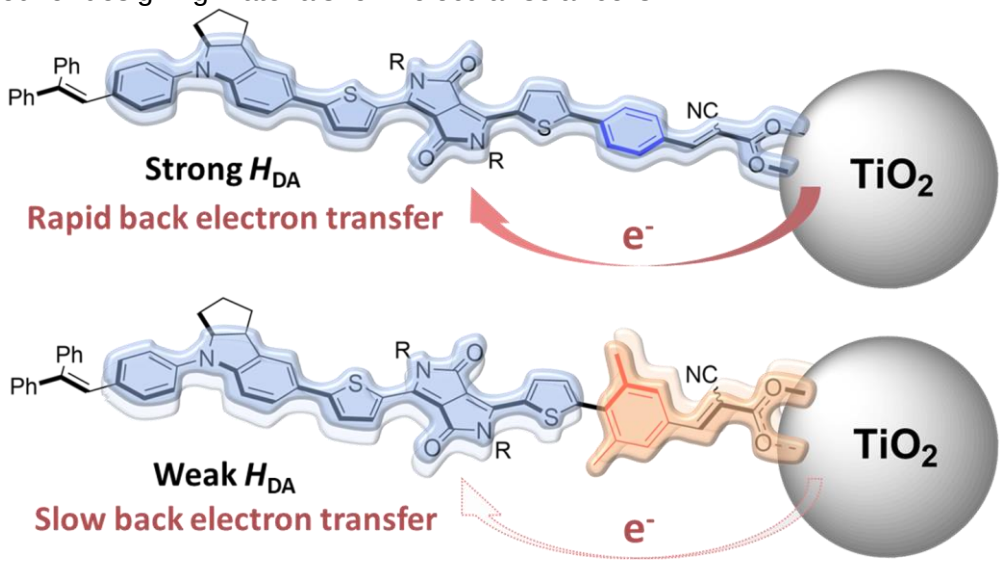
In molecular solar cells, it is general design strategy of light harvesting materials to have strong electronic coupling (H_{DA}) between electron donor and acceptor for rapid electron transfer and enhancing light harvesting ability. However, strong H_{DA} can promote undesired charge recombination reaction such as back electron transfer from semiconductor to oxidized molecules. Herein, we showed that weak H_{DA} material could enhanced power conversion efficiency (PCE) through efficiently retarding back electron transfer compared with strong H_{DA} materials. We synthesized four sensitizers and controlled magnitude of H_{DA} by geometric torsion of π-spacers (Fig. 1). A planar phenyl spacer (DD-DPP-Ph) that supports strong H_{DA} of 3787 cm^{-1}; and a tolyl spacer (DD-DPP-MP) prevents planarization and decreases H_{DA} of 3314 cm^{-1}; and a twisted xylyl spacer (DD-DPP-DMP) fully distorts π-conjugation and have weak H_{DA} of 984 cm^{-1} without a significant change in absorption spectra. In device results, the weak H_{DA} of DD-DPP-DMP showed *ca.* 36% enhanced PCE (8.6%) with high J_{SC} (17.71 mA/cm^2) owing to reduced back electron transfer compared with those of the strong H_{DA} DD-DPP-Ph. In addition, we introduced bulky donor unit into weak H_{DA} of sensitizer (bTPA-DPP-DMP) to maximize PCE. As a result, bTPA-DPP-DMP gave a PCE of 9.3% and a 10% PCE are achieved using co-sensitization with D35. Collectively, the results showed that a strong H_{DA} induced rapid back electron transfer, resulting poor device performances. In contrast, a weak H_{DA} efficiently retarded back electron transfer, and enhanced PCE. These findings should be considered for designing materials for molecular solar cells



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Chemiluminescent Probe for the In Vitro and In Vivo Imaging of Cancers Over-Expressing NQO1

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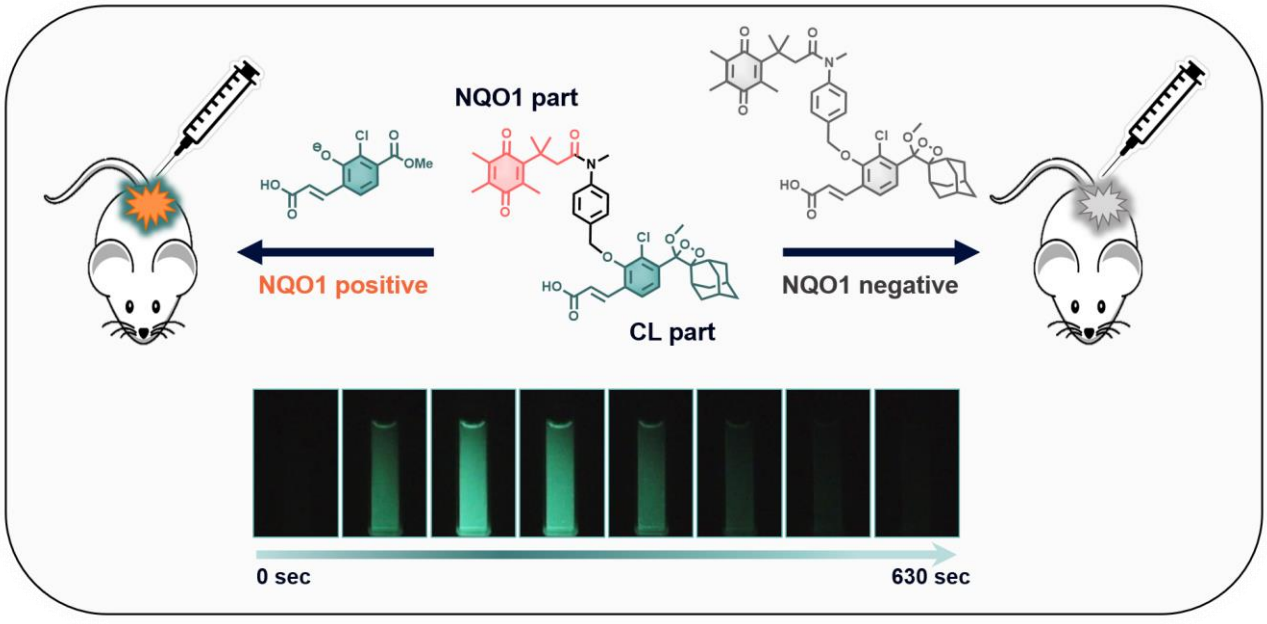
Abstract
Activatable(turn-on) probes that permit the rapid, sensitive, selective, and accurate identification of cancer-associated biomarkers can help drive advances in cancer research. Herein, a NAD(P)H:quinone oxidoreductase-1(NQO1)-specific chemiluminescent probe 1 is reported that allows the differentiation between cancer subtypes. Probe1 incorporates an NQO1-specific trimethyl-locked quinone trigger moiety covalently tethered to a phenoxy-dioxetane moiety through a para-aminobenzyl alcohol linker. Bio-reduction of the quinone to the corresponding hydroquinone results in a chemiluminescent signal. As inferred from a combination of in vitro cell culture analyses and in vivo mice studies, the probe is safe, cell permeable, and capable of producing a “turn-on” luminescence response in an NQO1-positive A549 lung cancer model. On this basis, probe 1 can be used to identify cancerous cells and tissues characterized by elevated NQO1 levels



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Function and oxygen tolerance of initiator-transfer agent-terminator (iniferter) in photomediated reversible addition-fragmentation chain transfer (photo-RAFT)

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Photomediated reversible addition-fragmentation chain transfer (photo-RAFT) polymerization is a practical tool for control the well-defined polymerization under mild condition with the advantages of temporal and spatial control. An innovative point that RAFT agents use as visible light initiator-transfer agent-terminator (iniferter) denotes the polymerization technique without the need for photocatalysts or initiators. However, the research of the comparison of RAFT iniferter polymerization and photoinduced electron/energy transfer (PET)-RAFT polymerization which uses photocatalysts had not been well established. Moreover, each iniferter as RAFT agent show different potential for oxygen tolerance. In this study, we investigated the function of iniferter in photo-RAFT polymerization and compared the abilities of iniferter and photocatalysts in the visible light region, and studied the oxygen tolerance in RAFT iniferter polymerization.

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A Two-Photon Fluorescence Probe for Monitoring hNQO1 Enzyme Activity in Human Colon Tissues.

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Human NAD(P)H:quinone oxidoreductase 1 (hNQO1, DT-diaphorase, Vitamin K reductase, E.C.1.6.99.2.) as a flavoenzyme catalyzes two- or four-electron reduction of endogenous and exogenous quinones to their hydroquinone forms.[1] Reductions catalyzed by hNQO1 play an important role in cell protecting, detoxification and antioxidant cycle.[1,2] In particular, hNQO1 is over-expressed in tumour cells compared with normal cells of the same origin.[3] 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.[4]

In this work, ratiometric two-photon fluorescence probe was designed for quantitative analysis of hNQO1 activity related to human cancer and normal tissues. Using fluorescence microscopy, the hNQO1 activity can be measured without homogenates of the tissue. Moreover, 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.[5] Two-photon microscopy (TPM) employs two near-infrared photons as the excitation source, offers a number of advantages including greater penetration depth (> 500 μm), localization of excitation with minimum background signal, and longer observation times.[6]

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.

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Polarity- and Viscosity-Sensitive, Deep-Red Emissive Probe for Lipid Droplets

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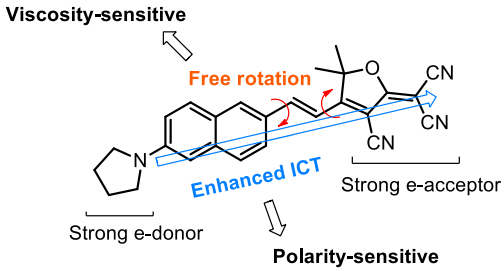
Lipid droplet (LD), a dynamic intracellular organelle play central roles in energy homeostasis, lipid metabolism, and are associated with various human diseases such as cancer, insulin resistance and neurodegenerative disease.[1] Therefore, it is important to develop a viable tool for studying LD-related biological processes. LD provides a more hydrophobic and viscous environment compared to that of cytosol, therefore, fluorescent dye that distinguish one of these differences have potential as LD probes.

Here, we disclosed a rational approach to develop the deep-red emitting probe that emits strong fluorescence not only in a highly viscous environment but also in a non-polar environment, two characteristics that LDs offer. The probe is proven to be efficient for the detection of LDs, as demonstrated in *cellulo* imaging studies on HeLa cells under starvation and under an excess level of oleic acid, and also for 3T3-L1 cells that differentiate into an adipocyte-like phenotype.[2]



Scheme 1. Both viscosity- and polarity-sensitive fluorescent probe.

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Evaluation of the mutagenicity of 2,7-diaminofluorene and 2,7-diaminocarbazole derivatives in the AMES test

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Daclatasvir, a well-known HCV NS5A protein inhibitor reported by Bristol-Myers Squibb (BMS) in 2010, exhibits high antiviral activities against HCV.[1] In spite of its extreme potency, daclatasvir loses its control over mutated NS5A proteins such as the ones with L31V and Y93H, since the proteins became resistant to daclatasvir after its exposure, causing the antiviral activities to drop by 15,000 times.[2] Numerous NS5A inhibitors have been introduced from many pharmaceutical companies maintaining proline-valine-carbamate motif from daclatasvir with the aim of solving resistance problem.[3] From our continued effort in the development of efficient HCV NS5A inhibitors, we discovered that fluorene or carbazole can be employed as a core structure of NS5A inhibitor connected through amide bonds to retain proline-valine-carbamate motif. Both 2,7-diaminofluorene and 2,7-diaminocarbazole appeared to be proper starting materials because they have amino groups already installed, allowing for straightforward amide bond formation with proline. However, amide bond can be easily cleaved via various metabolic pathways in our body system. Also the metabolites, which contain aniline, have been known as a mutagen.[4,5] Adduct between DNA base and electrophilic aniline metabolite is one cause of mutations.[6]

To avoid the mutagenesis issue, we introduced various functional groups at the C9 or N9 position of 2,7-diaminofluorene or 2,7-diaminocarbazole, respectively. We have found that some fluorene derivatives equipped with 9,9-dialkyl groups can be free from mutation problem. Likewise in carbazole cases some compounds having long alkyl groups were found to be non-mutagenic. We discovered that 2,7-diaminofluorene and 2,7-diaminocarbazole moieties can be employed in drug discovery without necessarily causing mutation problems through proper modification at the C9 or N9 position.

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

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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 N_2 or O_2 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.

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Selective Monitoring and Imaging of Eosinophil Peroxidase Activity with a J-Aggregating Probe

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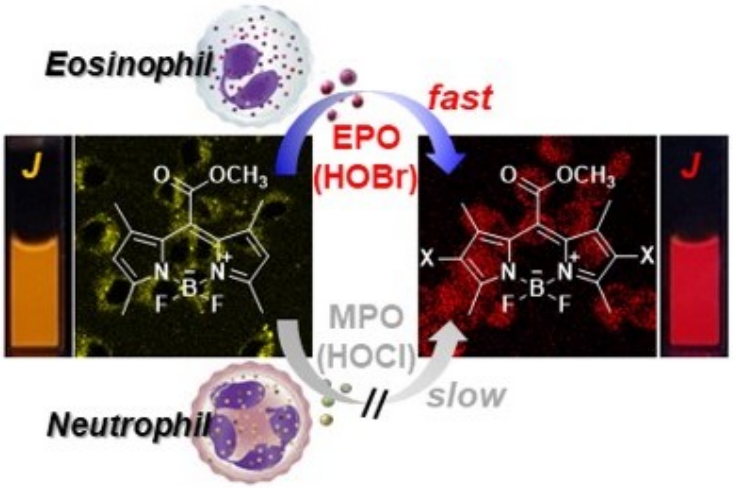
Eosinophil peroxidase (EPO) produces the cytotoxic agent HOBr via the oxidation of bromide (Br^-) using hydrogen peroxide. EPO has been closely related to various diseases due to their important roles in immunological and pathological functions. Therefore, it is a very valuable research to develop a method for the selective monitoring and imaging of EPO activity. In this presentation, a *meso*-ester BODIPY-based fluorescent probe **1** for the sensitive and selective detection of HOBr generated by EPO was developed. Probe **1** can be converted to the dibrominated compound **3** with high kinetic selectivity for HOBr over HOCl (>1200:1). The self-assembled aggregates of compound **3** showed emissive J-aggregates, which can offer fluorogenic detection of HOBr (EPO) over HOCl (MPO). Probe **1** can be successfully applied to the EPO activity assays, fluorescence imaging of EPO activity, the portable fluorescent indicator strips, and immune response detection in mice.[1]



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Water-Induced Hydrophobic Chiral Amplification

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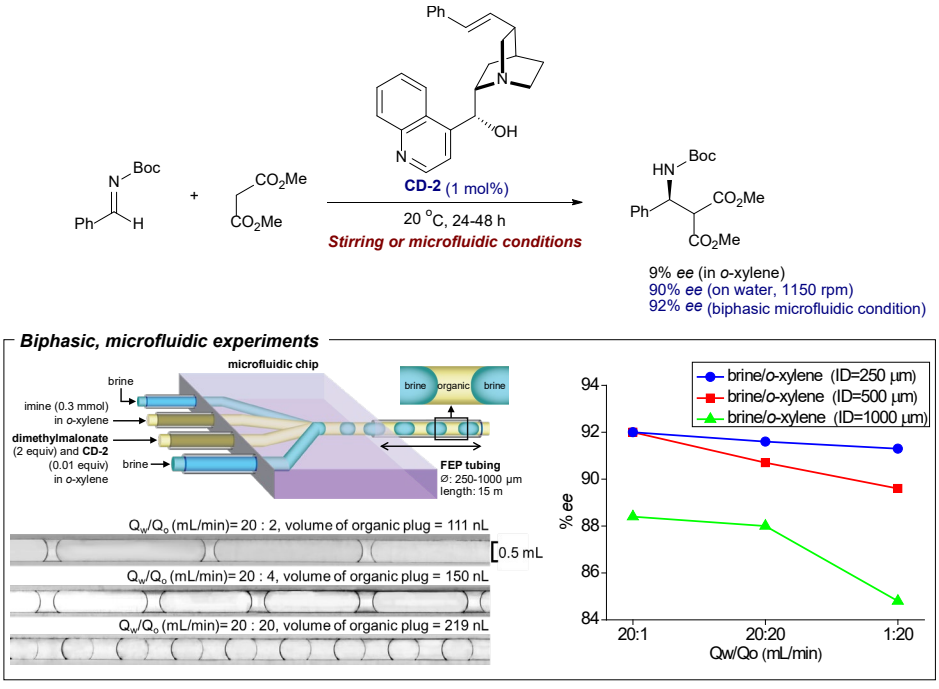
Homochirality is a fundamental component of molecular recognition in biological systems. Most theories for biological homochirality require a chiral amplification mechanism that acts to enhance a small initial asymmetry. We have found that water can induce the chirality amplification in a catalytic asymmetric reaction.[1] Under on-water conditions, the enantioselectivity of a catalytic reaction can be significantly enhanced in the confined hydrophobic spaces of organic droplets surrounded by water. More significantly, this chirality amplification can be further increased by decreasing the droplet size. The droplet size effect on the enantioselectivity was quantified by using the biphasic microfluidic technique. Although in-depth mechanistic studies are still needed in order to fully understand the role of water, we can conclude that this water-induced chirality amplification can be attributed to the hydrophobically induced confinement effect. This remarkable observation could provide some inspiration for developing new strategies to enhance enantioselectivity and thus has the potential to open a new chapter in the field of asymmetric catalysis. In addition, our discovery that the enantioselectivity can be greatly amplified in the confined cavities of water cages could help unlock secrets of homochirality which is a fundamental component of molecular recognition in biological systems.



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Quantitative Detection of Intracellular Polarity Distribution

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Intracellular polarity is important parameter that promotes various cellular processes such as activation of the immune response, local membrane growth, differentiation, and vector transport of molecules across the cell layer.[1] Abnormal polarity is direct linked to diabetes, neurological diseases and cancer.[2,3] Various ICT-based probes fluorescent probes have been reported for detecting intracellular polarity.[4,5] However, such an ICT-based probes have disadvantages that the fluorescence efficiency decreases sharply as the environmental polarity increases, so the range of fluorescence that can be observed is limited and detection is possible only in a lipophilic environment. In addition, reported probes can detect only the specific region in cells. So, these probes are difficult to observe the distribution of polarity entire the cell.

Here, we developed a new ratiometric probe that overcomes the limitations described above. In this probe were combined with two kind of polarity probes and it could measure a wide range of polarity quantitatively. The fluorescence intensity ratio was dramatically changed F_{yellow} and F_{red} depending on the polarity and showed a high correlation with the E_T^N value. In particular, this probe could observe the intracellular polarity distribution due to staining of various organelles in the cells, it has been confirmed that the polarity of lysosomes is the highest region in the cells

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A Gallium-Based Chiral Solvating Agent Enables the Use of ^{1}H NMR Spectroscopy to Differentiate Chiral Alcohols

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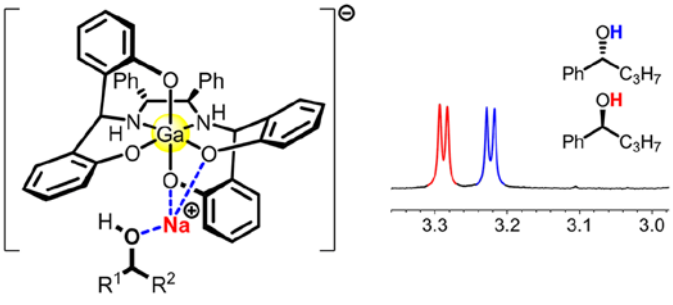
The chirality of molecules is an exceptionally important property and a large community in organic chemistry is dedicated to preparing and characterizing chiral molecules for a variety of applications. Chiral high-pressure liquid chromatography (HPLC) and gas chromatography (GC) are the most frequently used methods for chiral analysis. In addition, NMR spectroscopy can be a complementary analytical technique for chiral analysis. Especially with chiral solvating agent, operationally simple and convenient chiral analysis can be accomplished utilizing non-covalent interactions to convert chiral analytes to diastereomeric mixtures.

This useful technique was successfully demonstrated for a variety of substrates with chiral amines and carboxylic acids being the most commonly targeted substrates. The emphasis on these species is not surprising, because the majority of chiral solvating agents employ non-covalent interactions such as hydrogen-bonds and electrostatic attractions for structural recognition. Substrates that form relatively weak hydrogen-bonds and are less strongly coordinating such as alcohols are more challenging to study.

Here we developed a Ga-based chiral anionic metal complex for ^{1}H NMR chiral analysis of alcohols. Utilizing the optical pK_a value, the Ga complex was able to differentiate ^{1}H NMR signals of each (*R*)- and (*S*)-enantiomer of alcohols measured at room temperature. Furthermore, this direct ^{1}H NMR chiral analysis of alcohols was used to rapidly determine enantiomeric excess and conversion in a kinetic resolution and an asymmetric synthesis.

^{1}H NMR chiral analysis of alcohols at room temperature



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NQO1 Probe Using Chemiluminescence for Cancer Cells and Mouse Model Imaging

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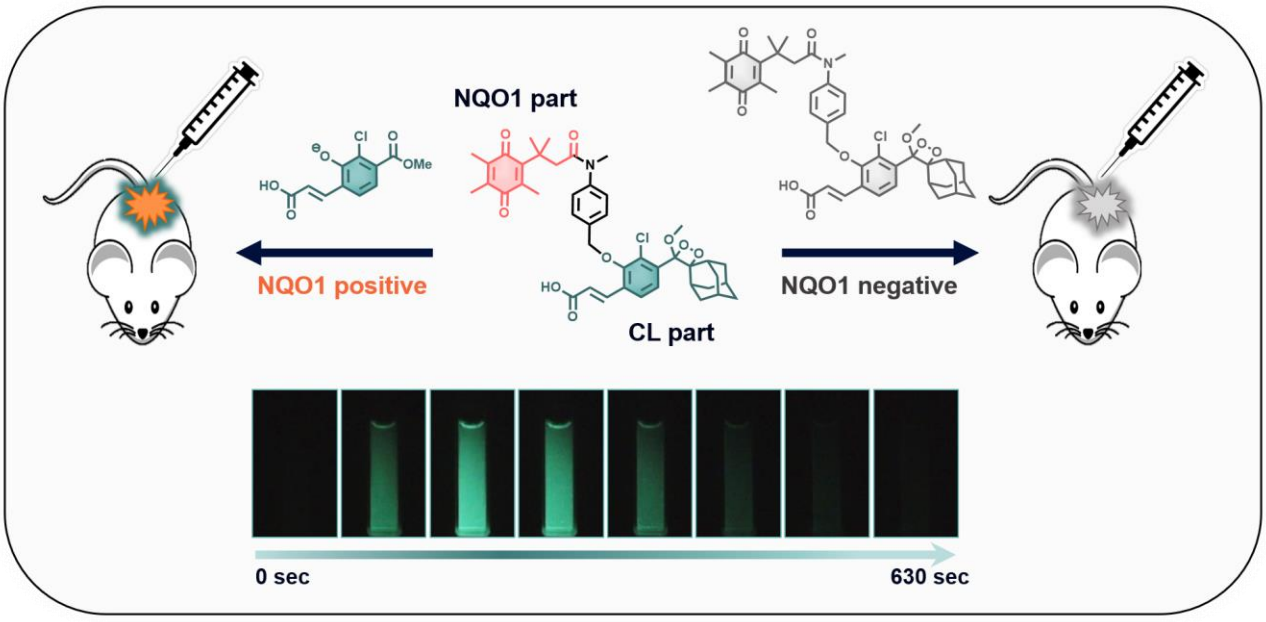
Abstract
Activatable(turn-on) probes that permit the rapid, sensitive, selective, and accurate identification of cancer-associated biomarkers can help drive advances in cancer research. Herein, a NAD(P)H:quinone oxidoreductase-1(NQO1)-specific chemiluminescent probe 1 is reported that allows the differentiation between cancer subtypes. Probe1 incorporates an NQO1-specific trimethyl-locked quinone trigger moiety covalently tethered to a phenoxy-dioxetane moiety through a para-aminobenzyl alcohol linker. Bio-reduction of the quinone to the corresponding hydroquinone results in a chemiluminescent signal. As inferred from a combination of in vitro cell culture analyses and in vivo mice studies, the probe is safe, cell permeable, and capable of producing a “turn-on” luminescence response in an NQO1-positive A549 lung cancer model. On this basis, probe 1 can be used to identify cancerous cells and tissues characterized by elevated NQO1 levels



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BODIPY-Containing Polymers for Use as Dopant-Free Hole Transporting Materials for Durable Perovskite Solar Cells

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Recently, device instability of perovskite solar cells (PSCs) provokes a critical issue despite their outstanding power conversion efficiency (PCE). To improve the device stability without a PCE drop, dopant-free hole transporting materials (HTMs) are needed to protect the air-sensitive perovskite layer from extrinsic factors, which induce its degradation. In this work, we developed novel polymers of benzo[1,2-b:4,5-b′]-dithiophene (BDT) and 4,4-difluoro-4-bora-3a,4a-diaza-*s*-indacene (BODIPY) for use as HTMs without dopants. The pBDT−BODIPY polymer allows individual “dialing” of the highest occupied molecular orbital (HOMO) or lowest unoccupied molecular orbital (LUMO) values with small modifications to the molecular structure, enabling study of the impact of the frontier molecular orbital on PSC performance. Different alkyl chains on BDT can minutely adjust the HOMO value, and *meso*-substituents on BODIPYs can selectively alter the LUMO value of the resulting polymers. Application of pBDT−BODIPY polymer into the perovskite solar cell as an HTM leads to a high PCE value (16.02%) and exceptional solar cell stability shown by the fact that over 80% of its original PCE value was maintained after 10 days under ambient air conditions.

Helical Living Supramolecular Polymerization from Achiral Bisporphyrin Derivative

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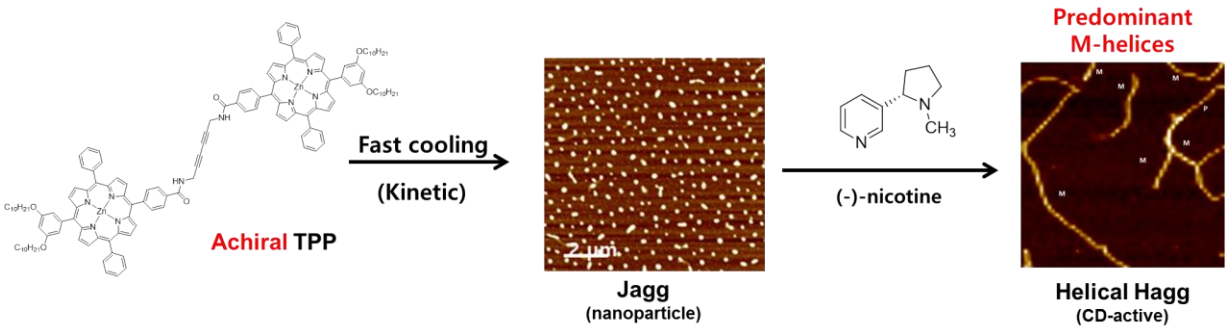
Recently, controllable supramolecular polymerization has attracted attention in the field of supramolecular chemistry. We designed a series of bisporphyrin derivatives (**DPP**, **TPP**, **mTPP**) to investigate the influence of substituent of porphyrin unit on their assembling behavior. All three bisporphyrin derivatives showed the formation of self-assembled structure in methylcyclohexane (MCH) at low temperature (273 K). The absorption spectra of **DPP** and **mTPP** exhibited red-shifted absorption than their monomeric state, indicating the formation of head-to-tail porphyrin aggregates (J-aggregate; J_{Agg}). Meanwhile, **TPP** showed two different types of aggregation modes which were dependent of the cooling procedure. When the hot solution of **TPP** was slowly cooled down, the bathochromic shift of absorption band was observed, indicating formation of co-facially stacked porphyrin aggregates (H-aggregate; H_{Agg}). On the other hand, **TPP** showed J-aggregates formation under fast cooling condition. The kinetically obtained J_{Agg} of **TPP** was gradually transformed to H_{Agg}. The atomic force microscopy (AFM) observation of **DPP**, **mTPP** and J_{Agg} of **TPP** showed the formation of nanoparticles. The growth of fibrous assembly of **TPP** was confirmed by AFM measurement. Under careful observation, the fibrous H_{Agg} was observed as a single-strand of helical assembly and the helicity of the helices was randomly oriented as M- or P-helices. To control the helicity of the H_{Agg}, we considered the chiral-auxiliary approach to the growth of helical H_{Agg}. We chose (-)-nicotine as chiral guest to be used, showing 1:1 binding mode to J_{Agg} of **TPP**. As different equivalent amount of (-)-nicotine added to the **TPP** solution, the H_{Agg} which transformed from J_{Agg} showed clear chiral-activity in the CD spectra. Furthermore, AFM images from the chiral-guest added **TPP** showed predominant M-helices over P-helices. We successfully achieved the controlled helicity of helical supramolecular polymer from achiral bisporphyrin derivative through small amount of chiral-auxiliary.



Synthesis and photophysical property of pH-sensitive fluorescein derivatives

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Development of pH probes for intracellular pH detection is very important since changes in pH play an important role in physiological function. Fluorescein and its derivatives are one of the most widely used in modern biochemical, biological, medicinal, photochemical research due to their excellent photophysical properties. Fluorescein has different light absorption and fluorescence properties depending on pH since it has several acidic groups. In this study, we synthesized 4',5'-diaminofluorescein and 4',5'-bis(dimethylamino)fluorescein. 4`,5`-Diaminofluorescein exhibited low fluorescecen in all pH regions. Interestingly, however, 4',5'-bis(dimethylamino)fluorescein showed high fluorescence only in the pH 3–6 region. We will discuss their pH-dependent photophysical properties in detail.

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γ-Aminobutyric acid Nanobelt Formation via Spontaneous Self-Assembly

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The formation of amyloid β fibrils under conditions found inside living organisms has inspired chemists to develop well-defined nano-/micro-sized functional materials with amyloid-like peptides.[1] Commonly used in studies of this nature, $(FKFE)_n$ peptides are one of several representative building blocks; they are known to self-assemble spontaneously, forming the bilayer structure, and eventually, well-defined superstructures.[2] However, the inherent structural complexities of peptides, such as backbone flexibility and ill-defined secondary structures, remain crucial hurdles in their effective application as building block molecules.

Herein, we introduce a γ-amino acid building block, β-benzyl γ-aminobutyric acid (γ-Phe), which is simple, cost-effective, and designed to mimic a fragment of the bilayer structure of amphipathic $(FKFE)_n$ peptides. The functional groups of phenylalanine, lysine, and glutamic acid all include this single γ-amino acid. In addition, β-benzyl would be the smallest building block to have all of the amphipathic advantages. (S)-γ-Phe was synthesized in an enantiopure form. It was found that through a spontaneous self-assembly process, this building block forms a well-defined nanobelt with interesting photoluminescence properties. This nanobelt was characterized via scanning electron microscopy (SEM), transmission electron microscopy (TEM), and powder X-ray diffraction. The molecular packing structure was successfully analyzed. Furthermore, distinct broad emission peaks at approximately 400 nm imply the existence of π–π interactions in the nanobelt, differentiating it from the raw powder of γ-Phe.

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Synthesizing Square-plate Foldecture Without Macrodipole

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Macrodipole of helical peptides plays an important role on protein folding[1]. Synthesis of foldecture[2], a self-assembly of helical peptide foldamer exposing in an immediate hydrophilic environment, also seems to be supported by macrodipole. However, since helical peptides always have macrodipole due to their nature, it was hard to show whether foldecture can be synthesized without macrodipole. Here, we have synthesized a helical foldamer **f1** which has similiar shape of α/β-peptide but having less macrodipole (figure 1a). Following standard foldecture synthesis process, foldamer **f1** self-assembled in a homogeneous foldecture **F1** with a well-defined morphology. Powder X-ray diffraction pattern of foldecture **F1** shows multiple sharp peaks which indicates clear packing structure and was used to solve molecular structure (figure 2a). Based on **F1** structure, it is clear that macrodipole doesn't affect on fast nucleation of foldecture but stable helical molecule having distinct intermolecular hydrogen bond system is the main key.

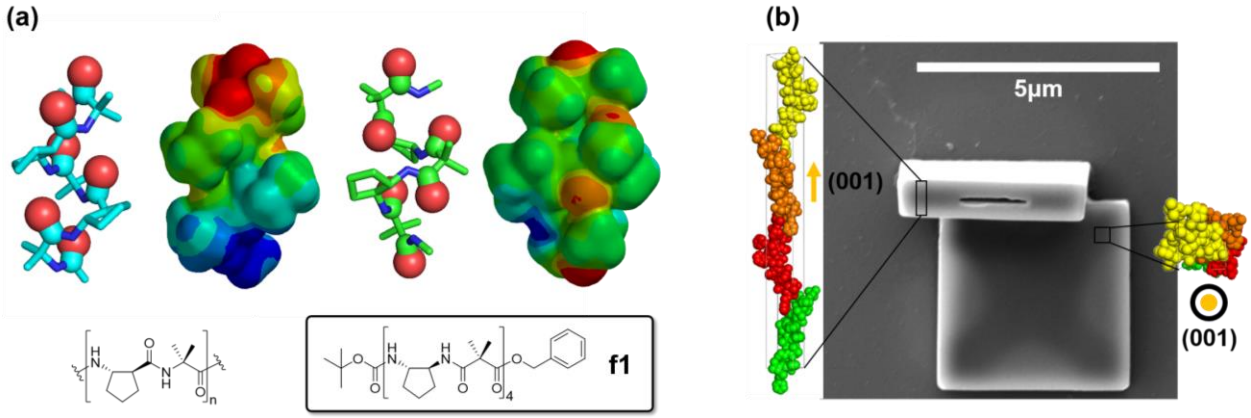

Figure 1 (a) Molecular structure and electrostatic potential map of α/β-peptide(cyan) and foldamer **f1**(green). (b) SEM image of foldecuture **F1** and unit cell packing model. Each color of molecules indicates the asymmetric unit of the crystal structure.

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Facile Fabrication of Multilayer Dye-Sensitized Solar Cells by Ultrasonic Spray-Coating Technology.

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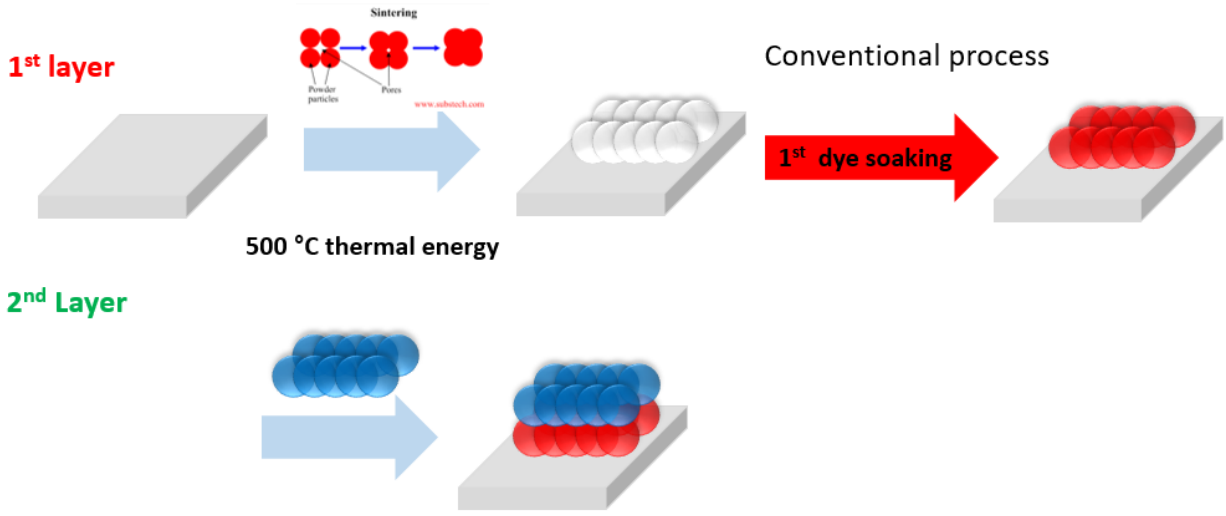
Dye-Sensitized Solar Cells(DSSCs) brings a lot of attentions due to their unique characters such as colorful, transparency, and flexibility. For enhancing power conversion efficiency(PCE) of DSSCs, broadening light absorption range of device is important. For this aim, the sensitizers need to capture broad range of the solar spectrum. However, individual sensitizers can only absorb relatively narrow range of the wavelength. For overcoming this issue, an additional scattering layer has been introduced to improve light harvesting. However, this additional layer cannot broaden the absorption range of devices which is mainly determined by sensitizers and reduce the transparency of device. From this reason, many researches are focus on developing the device structures which can containing more than one sensitizer such as dye cocktail and multilayer system. These methods can cover more broad range of absorption by employing more than one sensitizers which absorb different range of wavelength. However, there are severe recombination problem between sensitizers and its device fabrication processes are complex. For overcoming these limitations, sensitizers should be separated in different level of TiO_2 film. In this research, we employed Ultrasonic Spray-Coating Technology for coating discrete sensitized photo anode[1]. As a result, we achieved 6.4% of efficiency in multilayer system from 4.4% of single layer system.



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Monitoring Mitochondrial Response to Oxidative Stress via An Intramolecular Energy Transfer based Iridium(III) photosensitizer.

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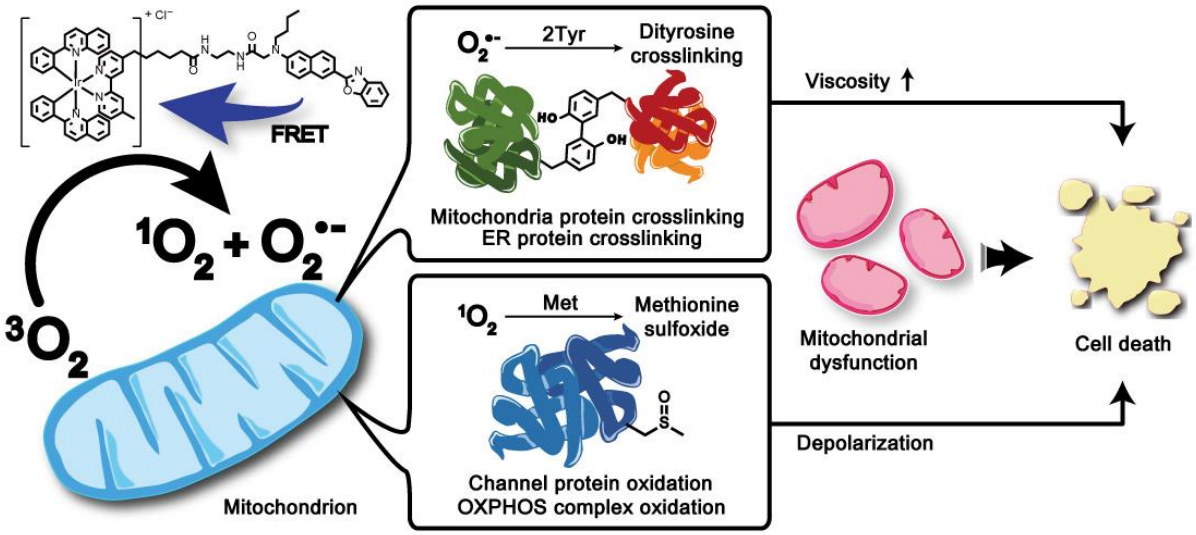
Mitochondrial oxidative stress induced by reactive oxygen species (ROS) change micro-physiological characteristics and cause mitochondrial dysfunction and apoptosis. Recently, there have been lots of reports that mitochondrial dysfunction is associated with various human diseases. Thus, this study developed an mitochondria-localized iridium(III) photosensitizer, Ir-OA, incorporating energy donor. The Ir-OA enables to trigger photoinduced cell death by enhanced ROS generation even under extremely low light dose (<0.17 J/cm2). Importantly, we have demonstrated the effect of photosensitizers on mitochondrial proteins in detail by analyzing protein oxidation and crosslinking. As results, the proteins related with mitochondrial channel and OXPHOS complexes were oxidized by photoactivation of Ir-OA. Correspondingly, the mitochondrial depolarization has been observed by the ratiometric imaging with Ir-OA which has a variable FRET efficiency depending on polarity. In addition, we have verified mitochondrial proteins are crosslinked by the Ir-OA, which cause increase of viscosity around mitochondria. By utilizing PLIM technique, local viscosity change has been monitored. The mitochondrial micro-environment change induced by protein modification accelerates cell killing effects of photosensitizers by disturbing physiological functions. This study present comprehensive underlying mechanism from mitochondrial oxidative stress to cell death through proteins dysfunctions and microenvironment changes.



Flexibility Controls of Metal-Organic Frameworks by Metal Cation Exchanges and Regioisomerisms

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Metal-organic frameworks (MOFs, or also called PCPs, Porous Coordination Polymers) are organic-inorganic hybrid materials consisting of multitopic coordinating ligands and metal clusters (or ions). Generally, MOFs have three-dimensional frameworks with permanent porosity, and in some specific cases, they show structural flexible. The flexibility of MOFs (i.e., structural changes of MOF frameworks) is changed by external stimuli such as pressure, guest molecular contact, solvent, etc. Recently, we have revealed that the position of functional groups and electronic density of ligands are also directly related with the flexibility changes of MOFs. Among the various combination of functionalities, only NH_2-Cl, NH_2-Br, NH_2-OMe, OMe-OMe displayed the flexibility changes by the position of functional groups (i.e., regioisomeric of functional group).[1-3]
Herein, we have performed and expanded our functional group-regioisomerism research to metal cation effect on the flexibility of MOFs. Using *para*- and *ortho*- NH_2-Cl functionalized ligands, we have successfully prepared three MOFs with different metal salts (cobalt, copper, and zinc) but with identical structures. Their structural analysis along with gas adsorption changes will be discussed in this presentation.

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Improvement for dehalogenation via organic photoredox catalyst: Approaching ppm-level visible-light-driven reductive dehalogenation

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Abstracting halogen atom from halide species and generating free-radical to produce reactive site have proven to be an important step in chemical synthesis. Hence, many researchers have improved this dehalogenation process into more efficient, simple, and environmentally friendly way. Adoption of photocatalytic process has risen to prominence, as it is inexpensive and a sustainable way to induce chemical reactions. Conventionally, inorganic photocatalysts such as iridium or ruthenium complexes were adopted in dehalogenation process. Unfortunately, their potential hazards and toxicity were of concerns, thus many researchers have thrived to develop organic photocatalytic system. Nevertheless, there still have been limitations such as high catalyst loading relative to organohalides, UV-light irradiation, requisites for harsh condition, and difficulties in reducing electron-rich organohalides. So here in we present purely organic photocatalyst designed, which successfully activate facile dehalogenation even in ppm level catalyst loading and mild conditions for the most aryl halides including even aryl chlorides and electron-rich aryl bromides, which have so far been reported to be difficult to reduce.

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Elevated Stability and Efficiency of Organic Solar Cells via Electric Double Layer Formation usin Ir(III) Complex

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Ionic material-based electrical double layer (EDLs) has enhanced the performance of optoelectronic devices, because they permit facile control of charge injection/extraction barriers. Nevertheless, the correlation between mobile ion kinetics and EDLs formation in polymer solar cells (PSCs) remains unclear. Here, we present a simple and effective method for universal interfacial energy level adjustment, using iridium(III) complexes with different cations (Ir-Li+, Ir-Na+, and Ir-K+). The effects of the ionic kinetics of Ir(III) complexes and EDLs formation on energy level tuning are investigated by measuring the turn-on voltage in light-emitting electrochemical cells, and the current density, conduction band shift, and electron mobility in PSCs. Ionic mobility plays a critical role in the formation of EDLs, which affects the device performance. Furthermore, PSCs containing Ir(III) complexes exhibit great enhancement in ultraviolet (UV) light stability, owing to the strong UV light absorption capacity of the Ir(III) complexes.

Study of β-Peptide Foldamers containing Tetrahydrothiophene : Fine Tuning of the Secondary Structure Derived by Single Atom Change

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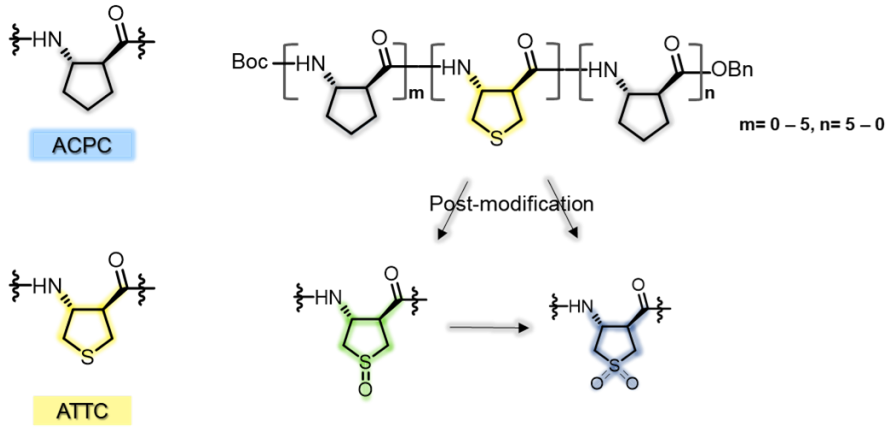
Foldamers, conformationally well-ordered synthetic oligomers that proved highly valuable because they mimic the structure and function of natural biomolecules. Therefore, these artificial molecules may afford significantly improved biomaterials and pharmaceuticals. In particular, foldamers containing heteroatoms in the backbone were of great interest as they increase the stability and biological activity.[1]

In this study, we tried to employ the simple strategy using bioisosteres to compare the folding propensity and chemical properties of the foldamer attained from small changes. We considered two factors to design this system, one is the stability of the backbone structure of the foldamer and the other is choosing of the bioisostere. Therefore, we choose *trans*-ACPC hexamer as a foldamer backbone according to its ability to form stable 12-helical secondary structure reported by Gellman *et al*. Next, thioether was chosen as a bioisostere, since it is one of the abundant functional group in nature and widely observed in protein sequence (i.e. methionine). Additional advantages for the thioether is that it could be post-modification to sulfoxide and sulfone through chemical conversion. Replacing the C4 carbon in the cyclopentane ring of (1*S*, 2*S*)-2-Aminocyclopentane-1-carboxylic acid (ACPC) with sulfur, (3*S*, 4*R*)-4-Aminotetrahydrothiophene-3-carboxylic acid (ATTC) is generated. These two structurally related building blocks are used to assemble a series of hexamers where the position of the ATTC in the sequence is varied systematically. We found that ATTC could act as an ACPC bioisostere in a foldamer level. However, thioether in ATTC was oxidized into sulfoxide and sulfone groups with remaining 12-helical secondary structure.



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Chemical strategies to modify amyloidogenic peptides by iridium(III) complexes: Coordination and photo-induced oxidation

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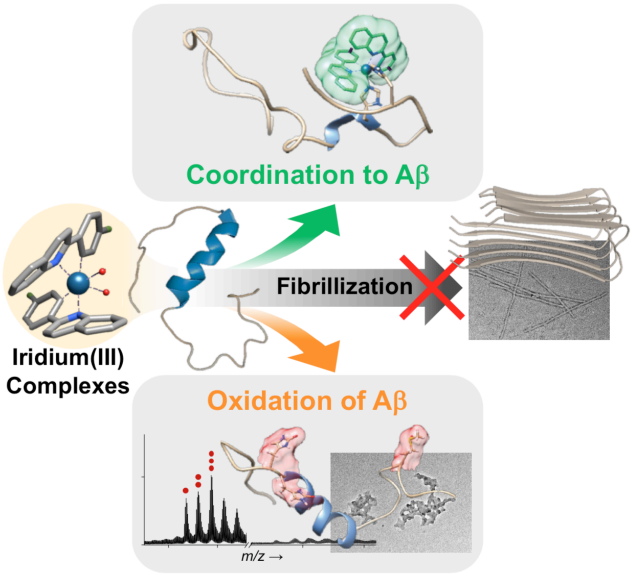
Amyloidogenic peptides are considered central pathological contributors towards neurodegeneration as observed in neurodegenerative disorders [*e.g.*, amyloid-β (Aβ) peptides in Alzheimer's disease (AD)]; however, their roles in the pathologies of the diseases have not been fully elucidated since they are a challenging target to be studied due to their heterogeneous nature and intrinsically disordered structure. Chemical approaches to modify amyloidogenic peptides would be valuable in advancing our molecular-level understanding of their involvement in neurodegeneration. Herein, we report effective chemical strategies for modifications of Aβ peptides (*i.e.*, coordination and coordination-/photo-mediated oxidation) implemented by a single Ir(III) complex in a photo-dependent manner. Such peptide variations can be achieved by our rationally designed Ir(III) complexes (**Ir-Me**, **Ir-H**, **Ir-F**, and **Ir-F2**) leading to significantly modulating the aggregation pathways of two main Aβ isoforms, $A\beta_{40}$ and $A\beta_{42}$, as well as the production of toxic Aβ species. Overall, we demonstrate chemical tactics for modifications of amyloidogenic peptides in an effective and manageable manner utilizing the coordination capacities and photophysical properties of transition metal complexes.



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Combination of Ir(III) Complex and Cancer-Environment-Customized Nanogel for Efficient Photodynamic Therapy

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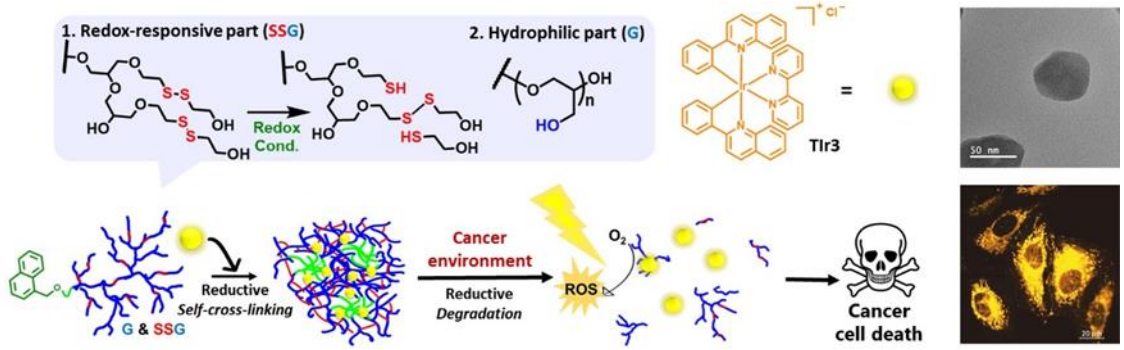
Ir(III) complexes have attracted much attentions in PDT due to their outstanding advantages in ROS generation efficiency, luminescence lifetime and photo-stability. However, the use of Ir(III) complexes has been limited because of their high cytotoxicity. Herein, we provide self-cross-linked nanogel consist of disulfide containing hyperbranched polyether for enhancing biocompatibility, loading capacity and cancer selectivity of iridium complexes. The size of nanogel was around 60 nm and it releases iridium complex fast in reductive condition. IrNG is internalized into cancer cells via ATP-dependent endocytosis and generates ROS inside of the cancer cells. Therefore, the cytotoxicity of IrNG was similar with that of TIr3 under light irradiation, but higher cell viability without light because of nanogel protection.



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2-Fluorenyl-1,2,3-triazole-labeled 2'-deoxynucleosides for potential SNP probes

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Fluorene is a widely used fluorophore, because it has a good quantum yield and is less bulky than other fluorophores. We have continuously used fluorene for synthesizing fluorescent nucleosides. Especially $\mathbf{U}^{\mathbf{FL}}$, fluorene of which is linked by ethynyl group to uridine base showed good photophysical properties and displayed differences in fluorescence intensity on duplex formation with their matched and mismatched complementary target. Therefore $\mathbf{U}^{\mathbf{FL}}$ can be applicable as an SNP (single nucleotide polymorphism) probe. In this study we synthesized 2-fluorenyl-1,2,3-triazole-labeled-2'-deoxynucleosides ($\mathbf{A}^{\mathbf{FT}}$, $\mathbf{U}^{\mathbf{FT}}$, $\mathbf{G}^{\mathbf{FT}}$, and $\mathbf{C}^{\mathbf{FT}}$), fluorene of which is linked by triazole group to bases of each nucleosides. We dissolved each modified nucleosides in 13 different solvents to investigate the solvatochromicity and inserted $\mathbf{U}^{\mathbf{FT}}$ in the central position of oligodeoxynucleotides to examine the potential for SNP probe.

A molecularly imprinted synthetic foldamer as a stereospecific and selective receptor for tartaric acid

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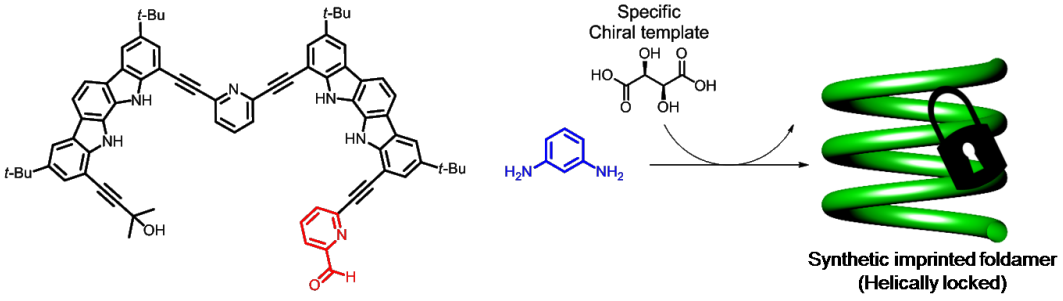
In recent years, synthetic receptors based on aromatic foldamers have been attracted much attention, partly owing to their tunable and modular features including precise positioning of functional groups and controlling the size and shape of the binding cavity.[1] Of great challenge is, however, to design an binding cavity complementary to a target guest at an atomic level. Combining the concepts of molecular imprinting, dynamic covalent synthesis and post-folding modification, we here describe an alternative strategy for the development of a synthetic receptor that exhibits an enzyme-like specificity and selectivity towards a specific guest. A short oligomer bearing an aldehyde functional group can be elongated to give a longer oligomer via the formation of imine bonds only in the presence of a specific diamine and guest, which in-situ undergoes the post-folding modification to afford a kinetically stable receptor of a helical structure containing a binding cavity. Details including syntheses and binding studies will be described.



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THF-containing amino acid revisited: Effects of ATFC as an alternative of ACPC in foldamer

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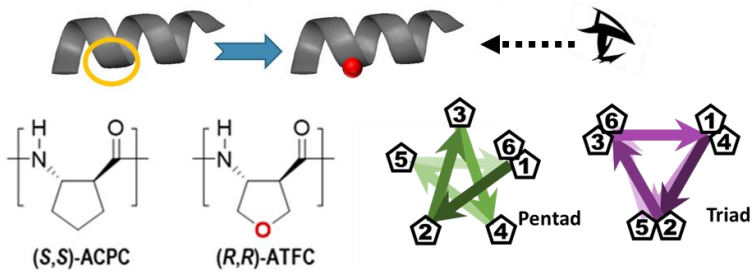
A little perturbation was given to a known 12-helical *β*-peptide as the model foldamer. Here, we have synthesized a cyclic *β*-amino acid ATFC ((*R*,*R*)-4-aminotetrahydrofuran-3-carboxylic acid) as an oxygen-containing analogue of ACPC ((*S*,*S*)-2-aminocyclopentanecarboxylic acid). We compared the self-assembly behavior and single crystal structures of a series of foldamers consist a single ATFC and five ACPC, to relate the helical backbone geometry depending on the ATFC position. Although all the oxygen-bearing foldamers maintained 12-membered helix in both solid and solution state, the scaffolds of the foldamers in their single crystal state were categorized to two distinct geometries, star-shape (tight form) and triangular-shape (loose form), named after their sidechain distribution from the top-view. Moreover, we expanded the scope of this study to find the tendency for the ATFC-containing foldamers' self-assembly behavior. The result suggests that the conformation-determining information of the *β*-peptide foldamers with 5-membered cyclic sidechains are stored in the peptides' primary structures. This strategy to connect the sequence and structure of the synthetic oligopeptides can be a guideline for designing and utilizing novel peptide foldamers.



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A Benzopyronin-based Two-photon Ratiometric Fluorescent Probe with Complete Spectral Separation for Imaging of Lysosomal Bisulfite

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Bisulfite (HSO_3^-), which equilibrates with sulfite (SO_3^{2-}) and sulfur dioxide (SO_2) in aqueous media, can be produced endogenously during oxidation of of hydrogen sulfide (H_2S) or sulfur-containing amino acids by reactive oxygen species (ROS) and also during decomposition of sulfinyl pyruvate to pyruvate in cells.[1] Besides, being important organelles, lysosomes act as a digestive compartment in eukaryotic cells and play various vital roles in regulating cellular metabolic processes including enzyme degradation, immunological stress and cellular apoptosis.[2] Therefore, detection of bisulfite in lysosomes is a subject of significant interest. In our continuous efforts to develop fluorescent probe for redox related species, this time we introduced a lysosome-targeting, two-photon excitable, and ratiometric signaling (near-infrared/green) fluorescent probe that detects bisulfite through a fast 1,6-conjugate addition reaction. The probe shows excellent selectivity toward bisulfite over other biologically relevant species. Notably, the probe allows ratiometric fluorescence imaging of lysosomal bisulfite with complete spectral separation under one-photon as well as two-photon excitation conditions.

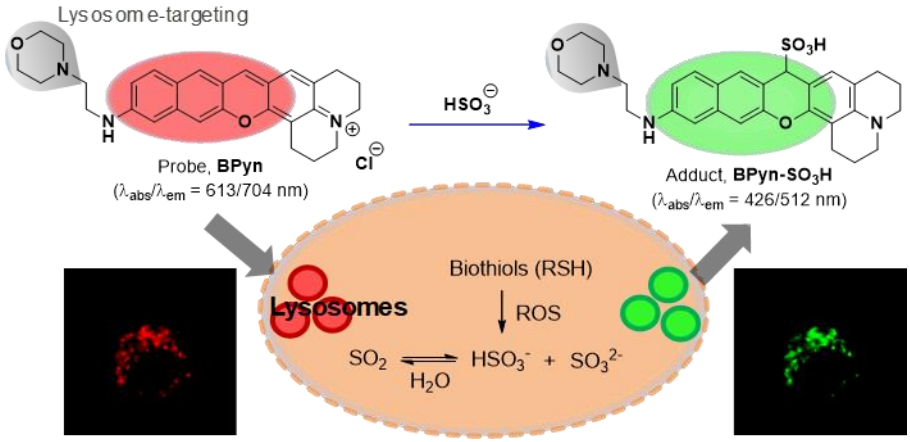

Fig. 1. Schematic illustration of two-photon lysosomal bisulfite probe, **BPyn** reacting with bisulfite.

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Foldectures from the Self-Assembly of α/β-Foldamers with Conformational change from 11-helix to 14/15-helix

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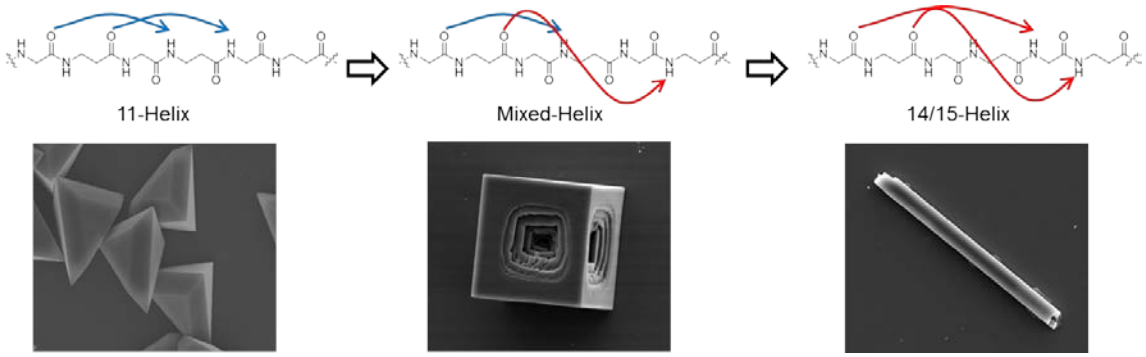
The α-helix and the 3_{10} helix are two common constituents of protein in nature.[1] 3_{10}-Helices have been proposed to be intermediates in the folding/unfolding of α-helices. The design of the helix is very important to understand the formation mechanism. Self-assembly of micro-sized architectures has the potential to provide the basis for new technology. We used α/β-foldamers composed of α-amino acid (2-aminoisobutyric acid, Aib) and β-amino acid (*trans*-2 aminocyclopentane carboxylic acid, ACPC) in a 1:1-alternating β-peptide foldamers. These foldamers are reported to display two helical conformations, the 11-helix and the 14/15-helix.[2] This phenomenon is similar to structural changes with the 3_{10}-helix and 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.[3-6] 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 foldectures 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 understanding the interaction of helix-type that makes up the protein.



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Substrate synthesis and structural analysis of peptidoglycan peptidase3, a bacterial cell-shape determining protein

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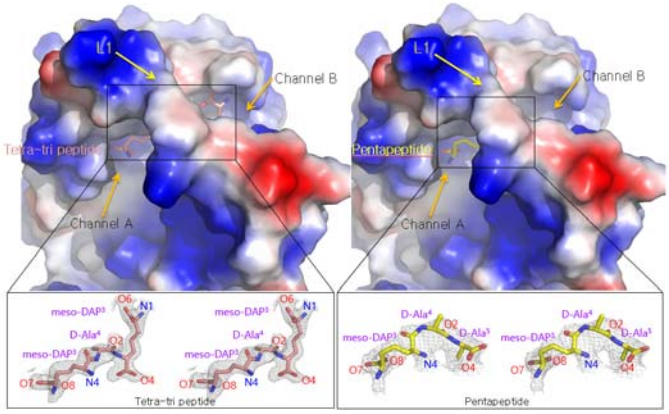
Helicobacter pylori and *Campylobacter jejuni*, which are known to be helical shaped Gram-negative bacteria, colonize the human mucus layer of the gastrointestinal tract and cause various gastrointestinal diseases such as chronic gastritis, peptic ulcer, gastroenteritis and gastric adenocarcinoma in humans.[1,2] In the pathogenesis and gut colonization, the helical shape of *H. pylori* and *C. jejuni* is believed to be a very important factor in their motility improvement.[3] Recently, a series of genes associated with maintaining the helical cell shape in these bacteria have been identified, most of which have been found to encode for either endo- or exoproteases that act on the peptide chains of peptidoglycan.[4] These proteases are referred to as cell shape determining (Csd) proteins or peptidoglycan peptides (Pgp). According to recent studies, inhibition of proteins responsible for the helical cell morphology could be useful in interference with the bacterial virulence and lifestyle, hence a very attractive therapeutic target.[5] However, their catalytic processes and substrate recognition are largely unknown. In this study, we describe the synthesis of two substrates for Pgp3, one of the Csd proteins, and the analysis of the Pgp3-substrate complex structures of the active site of Pgp3 in high resolution.



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A p27 Activator Identified via Forward Chemical Genetics Selectively Kills Leukemia Cells

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Forward chemical genetics is a highly useful strategy to explore the biological systems for chemists. In this strategy, compounds that induce a desired phenotypic change can be identified from screening a chemical library. Since it requires no hypotheses regarding the molecular basis of the phenotype in question, any genes or proteins that support this phenomenon are analyzed afterwards. The unbiased nature of the inquiry can lead to novel target proteins that could serve as novel drug targets or biomarkers, while discovering compounds that modulate those target proteins.

Here, I will discuss (1) discovery of a small-molecule p27 activator that selectively kill leukemia cells, (2) identification of the target associated with the compound which may lead to the malignant behaviour of leukemia, and (3) subsequent biological studies, through forward chemical genetics. This molecule could be developed as a novel class of anti-leukemia agent, as well as a molecular tool that can provide valuable information about the role of the target in leukemia.

Development of a fluorescent sensor array for pH sensing

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Owing to its high sensitivity and great applicability fluorometric sensors have been widely used especially for chemical sensing. Understanding of structure photophysical relationship of given fluorophore and development of supramolecular chemistry synergistically allowed to discover multiple different useful fluorescent sensors via incorporation of a chelator or functional moiety on the specific position. Intermolecular interactions between analytes and fluorophore, such as coordination or chemical reaction of certain analytes with chelator or functional moiety of the fluorescent sensor, induce perturbation of photophysical properties of given fluorophore which is used as a signal for the analysis. Despite continued enthusiastic efforts, however, it is still challenging to develop highly specific and sensitive fluorescent sensors. More importantly, many possible false positive/negative signals could be produced with single fluorescent sensors for certain analytes, reducing the accuracy of the analysis. Here we present a fluorescent sensor array for pH sensing system. Based on pKa value of the functional group, we designed 14 different fluorescent compounds responding with the pH changes via incorporation of pH sensitive functional groups on C-1 position of Kaleidolizine. Simple spotting of the fluorescent compounds on cellulose filter paper allowed us to generate an single array. By analyzing fluorescence pattern changes of the array, we successfully monitored the pH differences of the samples.

Development of multi-color fluorogenic tetrazine probes based on indolizine

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Recently, modification of tetrazine (Tz) to fluorophore is getting attention because of its unique fluorescence quenching effect. Since they only emit the fluorescence when they interact with biooorthogonal reaction partner, tetrazine probe allow us to get high contrast fluorescence image for Trans-cylcooctene(TCO) modified targets. Although several different approaches have been pursued, it is still challenging to develop multi-color fluorogenic tetrazine probes especially for multiplexing purpose. Here we present development of multi-color fluorogenic tetrazine probes via utilizing the color-tunable property of Kaleidolizine (KIz).

Asymmetric Synthesis of *cis*-5-Aminomethyl-3-(4-methoxyphenyl)-dihydrofuran-2(3H)-one

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The asymmetric synthesis of (2*R*,5*S*)-5-aminomethyl-3-(4-methoxyphenyl)dihydrofuran-2(3H)-one as ths most potent selective inactivator of monoamine B was successfully achieved by applying a newly developed synthetic method toward γ-aminomethyl-γ-lactone from intramolecular aziridine-ring opening in 63% overall yield from commercial starting material.

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Synthesis of Dihydrobenzoxazine-fused Spirooxazoline-4-ones via [3+2] Cycloaddition of Azaoxyallyl Cations with Vinyl Benzoxazinanones

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N,O-heterocycles are well-known privileged structural motifs commonly found in many natural products and synthetic pharmaceutical compounds which exhibit important biological activities, such as antifungal, antiviral, and anticancer properties.[1] On the other hand, spirocyclic compounds, which are constructed from two perpendicular rings connected by a single atomic center, are privileged structural scaffolds that display several unique characteristics related to their inherent rigidity.[2]

A novel [3+2] cycloaddition reaction between *in situ* generated azaoxyallyl cations and a variety of vinyl benzoxazinanones has also been developed. This reaction provides an attractive method for the synthesis of spirooxazoline-4-ones based on dihydrobenzoxazines, which were obtained in good yield (up to 98% yield) with high diastereoselectivity (up to >20:1). This efficient [3+2] cycloaddition reaction, which provides an attractive method for the synthesis of various spiro-bis-*N,O*-heterocycles, can be used as tool to provide building blocks for the synthesis of useful α-substituted carbonyl compounds.

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Synthesis of Diarylmethylamines via Lewis Acid-catalyzed Friedel–Crafts Reactions of Donor–Acceptor Aziridines with *N*,*N*-dialkylanilines

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The diarylmethylamine motif is the structural basis for a large number of small molecules with distinctive and desirable biological properties, which widely presented in many natural products and biologically active compounds and is used extensively in syntheses of the drug targets for the treatment of various diseases.[1]

We have reported here the efficient and mild synthesis of diarylmethylamine derivatives using a $Yb(OTf)_3$ catalyzed Friedel−Crafts reaction of D−A aziridines with *N,N*-dialkylanilines which constructed a biologically important diarylmethylamine derivatives in high yields (up to 88% yield). This method is suitable for the synthesis of various diarylmethylamine derivatives and includes an expanded electron-rich arene scope, including dimethoxybenzene.

References

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Progress toward total synthesis of (-)-platensimycin by internal H-bonding mediated intramolecular Diels-Alder reaction

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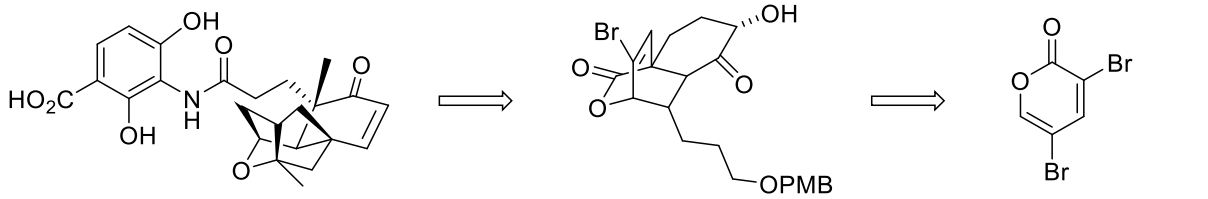
Abstract

We have investigated 3,5-dibromo-2-pyrone towards target-oriented synthesis, utilizing its peculiar reactivity as a neutral diene and the selective maneuverability of the two bromine groups. Such efforts have resulted in successful syntheses of an array of biologically important natural products.[1]

Inspired by our recent success on internal hydrogen bonding mediated asymmetric Diels-Alder reaction, we have launched a program inventing a new route that allows an efficient synthesis of (-)-platensimycin. Included in the new route are C3-selective Sonogashira coupling reaction of 3,5-dibromo-2-pyrone, chemo-selective hydrogenation and intramolecular Diels-Alder cyclization. Presented herein is our recent progress toward total synthesis of (-)-platensimycin.



(-)-platensimycin **2-pyrone IMDA adduct** **3,5-dibromo-2-pyrone**

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Stereoselective Strecker and Allylation Reactions using Aldimines Catalyzed by Chiral Oxazaborolidinium Ions

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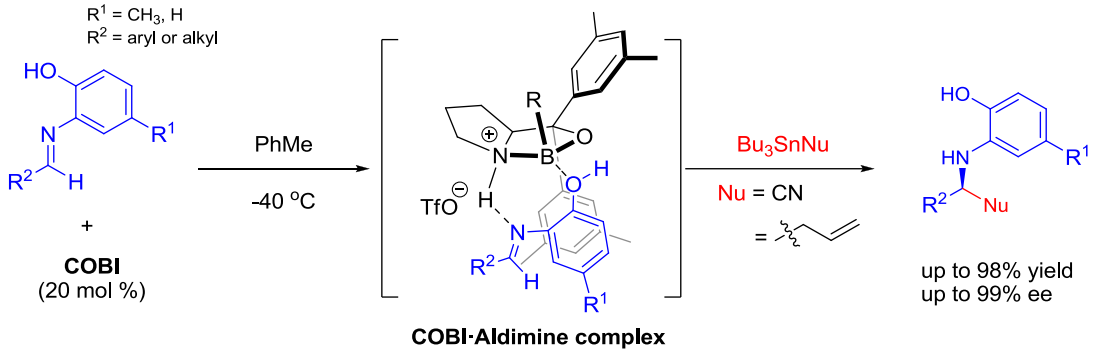
Stereoselective Strecker[1] and allylation[2] reactions of aldimines catalyzed by chiral oxazaborolidinium ion (COBI) using tributyltin cyanide and allyltributylstannane have been researched. Chiral *α*-aminonitriles and homoallylic amines are very important building blocks for enantioselective bio-active materials like *β*-amino acids. Various *α*-aminonitriles and homoallylic amines were synthesized in high yield (up to 98%) with high enantioselectivity (up to 99% ee). Additionally, a rational mechanistic model for the complex of COBI and aldimine is provided to account for these enantioselective reactions.



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Asymmetric Total Synthesis of (-)-Cynometrine Derivatives

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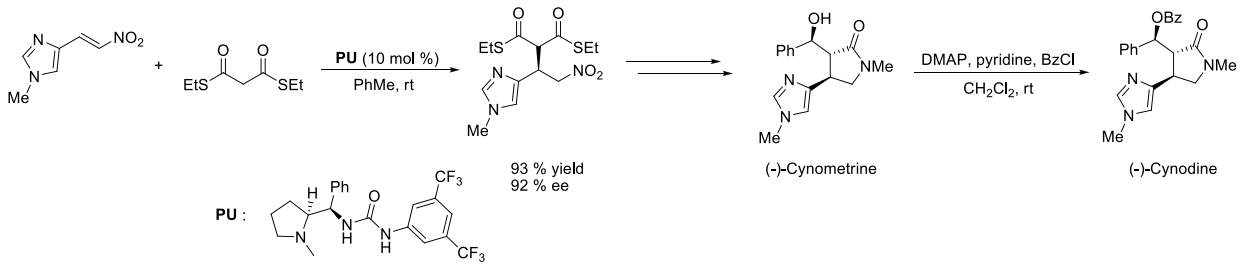
Asymmetric total synthesis of natural product (-)-cynometrine, known for antitussive and analgesic properties is described. From the heterocyclic nitroolefin and dithiomalonate, key intermediate of the natural products was synthesized. In the presence of proline-derived bifunctional organocatalyst, Michael adduct which has a chiral center possessing suitable functional groups with required stereochemistry was prepared through a Michael addition. Plausible reaction mechanism of organocatalysis is suggested. (-)-Cynodine is also synthesized from (-)-cynometrine by benzoylation.



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Copper(I)-catalyzed Cyclization Reactions of Ethyl (*E*)-*α*-Ethynyl-*β*-Aryl-*α*,*β*-Unsaturated Esters with *N*-Sulfonyl Azides: Synthesis of 1-Aminonaphthalene, 3-Aminobenzofuran, and 3-Aminothiobenzofuran Derivatives

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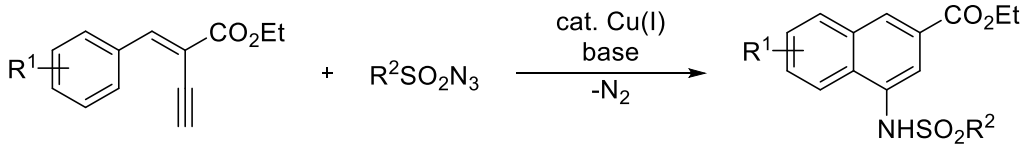
The structural motif of 1-aminonaphthalenes exists broadly in biologically active compounds used as a protein kinase and angiogenesis inhibitors for the treatment of cancer, Mcl-1 inhibitors, p38 inhibitors, and BRAF inhibitors. Accordingly, development of efficient synthetic method for functionalized 1-aminonaphthalene derivatives is of great importance.

A synthetic method for ethyl 4-(alkyl or arylsulfonamido)-2-naphthoates from ethyl (*E*)-*α*-ethynyl-*β*-aryl-*α*,*β*-unsaturated esters (**1**) and *N*-sulfonyl azides (**2**) in the presence of 2,6-lutidine in THF at 60 ^{o}C for 3 h was developed in one step, in which a copper(I)-catalyzed 1,3-dipolar cycloaddition, ketenimine formation, and 6π-electrocyclization followed by [1,3]-H shift tandem reaction took place. This method enabled efficient synthesis of a wide range of 1-aminonaphthalene and 3-aminobenzofuran and 3-aminobenzothiophene derivatives with the release of molecular nitrogen.



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Rh(II)/Pd(0)/Ru(II) Ternary Catalysis for One-pot Synthesis of Spiroheterocycles

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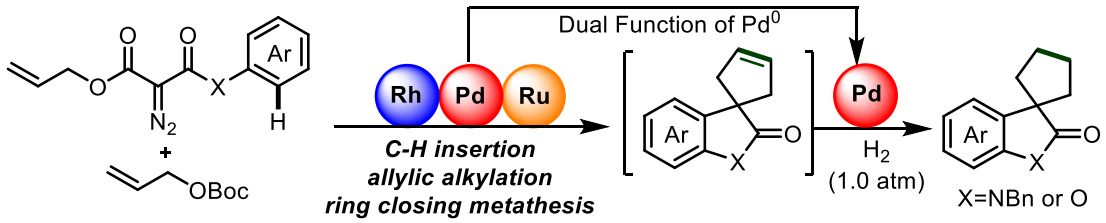
One-pot multi-catalytic reaction is one of the most efficient and environmentally benign synthetic strategies, wherein multiple bond formation could be achieved with minimization of waste generation and consumption of energy.[1] Challenges are ensuring the redox-compatibility, in particular, between the transition metal catalysts and achieving the balanced kinetics in selective activation of the substrates. Otherwise, the catalysts could be deactivated to decrease reaction efficiency. Recently, numbers of one-pot dual transition metal catalysis have been successfully developed.[2] However, a more complexed and challenging triple transition metal catalytic system has been far less explored.[3] Quite recently, we have demonstrated for the first time the compatibility between Rh(II) and Pd(0) catalysts.[4] In present work, we envisioned the ternary Rh(II)/Pd(0)/Ru(II) catalytic reaction for the construction of C-3 spirocyclic indolin-2-ones and benzofuran-2-ones. It may involve multi-step catalytic molecular transformations, *i.e.*, the Rh(II)-catalyzed C(sp^2)-H insertion/Pd(0)-catalyzed allylic alkylation/Ru(II)-catalyzed ring closing metathesis (RCM). Moreover, without addition of additional Pd(0) source, hydrogenation of olefin constructed by RCM could be performed implying the dual function of the Pd(0) catalyst.



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Aerobic Oxidation Approaches to Indoles: A Tandem Cross Coupling of Amines- Intramolecular Mannich-Oxidation Sequence

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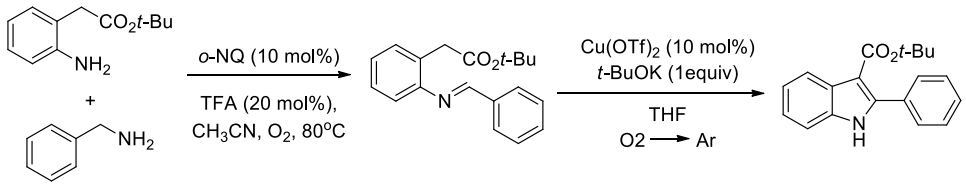
A tandem aerobic oxidation protocol has been developed for the facile synthesis of indole-3-caboxylates. Two readily available starting materials, anilines and benzyl amines, were efficiently cross-coupled under the *ortho*-naphthoquinone-catalyzed aerobic oxidation conditions to the corresponding 2-arylmethyleneaminophenylacetates that in turn smoothly underwent the Cu(II)-catalyzed intramolecular Mannich reaction. The resultant indoline derivatives were readily oxidized under air to give indole-3-carboxylates, providing a ready access to indole derivatives from two simple amine derivatives.



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Ligand-Controlled Stereodivergent Palladium Catalysis for Stereoselective Synthesis of Spiro-Furanindolines

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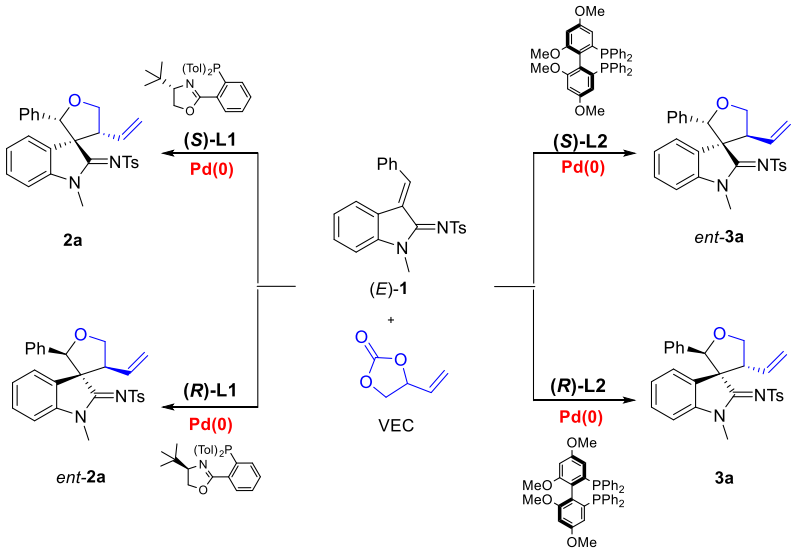
Stereodivergent (enantiodivergent and diastereodivergent) catalysis is one of the most fascinating yet challenging synthetic chemistry, because it can allow access to the possible stereoisomers having two or more stereogenic centers.[1] Although the use of different catalysts has been extensively studied for the stereodivergent catalytic reactions,[2] switching solvents or additives often achieved controlling the stereochemical outcomes.[3] Nevertheless, an efficient catalytic strategy to control both the enantio- and diastereoselectivities has not been developed yet. In present work, we have investigated the transition-metal-catalyzed ligand-controlled stereodivergent dipolar cycloaddition reactions. The zwitterionic alkoxy π-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 to afford one of the possible stereoisomeric spiro-furanindolines selectively.



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Studies of aerobic oxidative cyclization: Synthesis of 2-phenylisoquinolin-1(2*H*)-one

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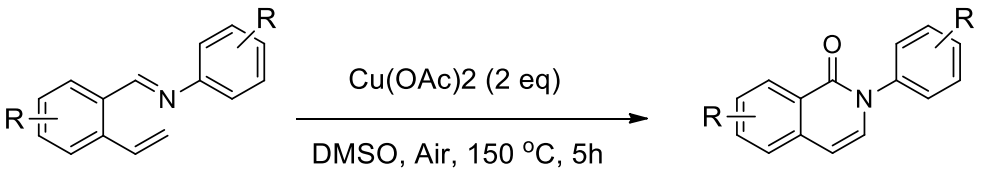
Isoquinolin-1(2*H*)-ones, one of the nitrogen-containing heterocycles, are important structural components present in potent drugs and biologically active natural products. The development of new effective methods for the synthesis of the isoquinolin-1(2*H*)-one is an important research area in medicinal chemistry.

In this study, we present an intramolecular aerobic aza-cyclization reaction of 2-vinyl-*N*-phenylbenzylimine to 2-phenylisoquinolin-1(2*H*)-one. We found a facile reaction condition to synthesize isoquinolin-1(2*H*)-ones. Now, we have found that $Cu(OAc)_2$ as an oxidant, DMSO as solvent, a high temperature of 150 ^{o}C, were necessary to synthesis the isoquinolin-1(2*H*)-one.

The development of new effective synthesis of isoquinolin-1(2*H*)-one is in progress.



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Nickel-catalyzed decarboxylative coupling reactions for the synthsis of 1,3-enynes

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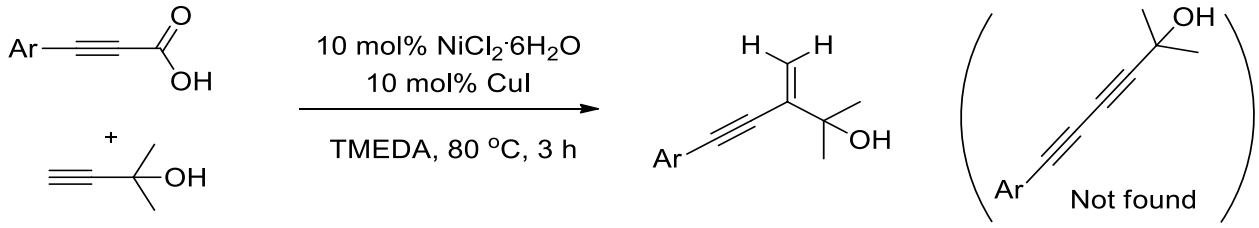
Conjugated 1,3-enynes are important structural units in synthetic chemistry, material science and bioactive product synthesis. [1]A number of synthetic methods have been reported for the preparation of 1,3-enynes, [2-3]including Wittig reaction with propargyl aldehydes, dehydration of propargyl alcohols.

We developed the synthesis of gem-1,3-enyne via Ni/Cu catalyzed decarboxylative dimerization of alkynoic acid and terminal alkyne. We found that the decarboxylation of alkynoic acid provided predominantly gem-1,3-enyne instead of 1,3-diyne which was known to be formed from the coupling of terminal alkynes. A variety of gem-1,3-diynes were obtained with good yields from the reaction of substituted aryl propiolic acids and terminal alkynes such as 2-methylbut-3-yn-2-ol, pent-4-yn-1-ol, 1-phenylpro-2-yn-1-ol, 1-entynylcychohexanol and ethynylcyclohexane. This catalytic system exhibited excellent regioselectivity and high functional group tolerance. It was found that nickel catalyst suppressed the pathway of the coupling of alkynes which was dominated by copper catalyst. This result was completely different from the previous reports [4-5]which 1,3-diyne was formed from the hetero cross coupling of two different alkynes in the presence of Ni/Cu or Cu catalyst.



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Synthetic Utility of *N*-Benzoyloxyamides as an Alternative Precursor of Acylnitrenoids for γ-Lactam Formation

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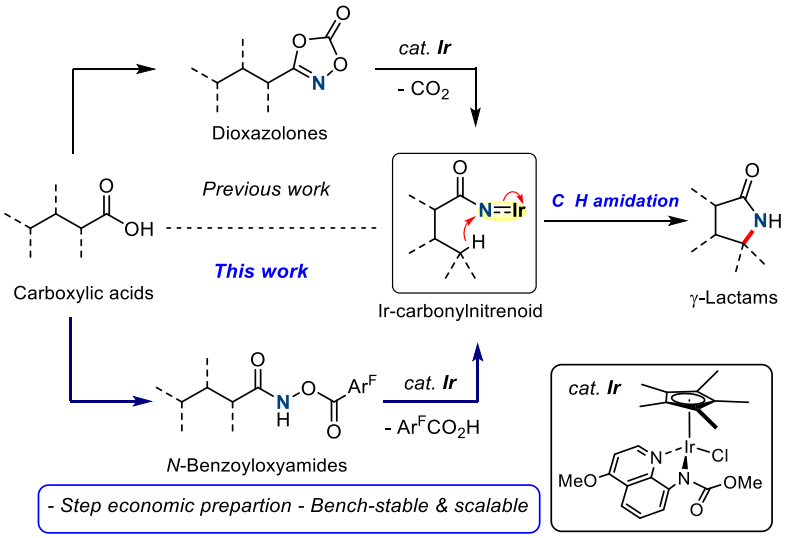
Cyclic amides are ubiquitous in alkaloid natural products and biologically active compounds. In particular, γ-lactams are a privileged scaffold being widely present in important pharmaceutical agents. Therefore, the development of efficient and selective synthetic routes to this 5-membered amide starting from readily available compounds is of great interest.

Recently, we showed that (pentamethyl)cyclopentadienyl (Cp*)-based Ir complexes with engineered bidentate ligands display an unprecedented performance in catalytic C−H amidation of dioxazolones with effective suppression of such side pathway. Herein, we present a new entry of acylnitrenoid precursors for γ-lactam synthesis via an intramolecular C−H amidation reaction. Upon the action of Ir catalysis, *N*-benzoyloxyamides serve as efficient substrates to afford 5-membered amides. Mechanistic studies revealed that the generation of a putative Ir-carbonylnitrenoid via N−O bond cleavage is facilitated by the chelation of counter cations. This protocol offers a convenient and step-economic route to γ-lactams starting from the corresponding carboxylic acids.



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Synthetic Studies towards Vertine and Its Analogues

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Vertine was first isolated from Decodon verticillatus (L.) Ell by Ferris in 1962 and classified as a member of the Lythraceae alkaloids. Vertine has a unique structure; it has a strained 12-membered macrolactone structure incorporating biaryl and quinolizidine. It exhibits a wide range of biological activities such as anti-inflammatory, sedative, antispasmodic actions, and glucose level regulation in blood. Despite these biological activities, only one total synthesis of vertine has been reported to date.[1]

Recently, our group developed highly concise total syntheses of phenanthroindolizidine and phenanthroquinolizidine alkaloids via iterative Suzuki-Miyaura reaction using ortho-bromophenyl MIDA boronate as a key building block.[2] We recognized that vertine also has ortho-aza-terphenyl structure and quinolizidine structure. Based on the structural similarity, we envisioned that vertine could be synthesized by the similar strategy. The Suzuki-Miyaura reaction of ortho-bromophenyl MIDA boronate with phenyl boronic acid followed by the second Suzuki-Miyarua reaction of the resulting biphenyl MIDA boronate with 2-pyridyl bromide afforded the desired ortho-aza-terphenyl compound. Subsequently, the quinolizidine structure with stereogenic centers was derived from pyridine scaffolds.[3] Then macrolactone structure could be prepared via macro ring formation reaction. In this poster presentation, we will describe the progress in the total synthesis of vertine and its analogues via building block strategy

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General Strategy for Synthesis of Corynanthe Family via Intramolecular Imino-Stetter Reaction Followed by Functionalization of Pyridine Ring

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Corynanthe alkaloids, isolated from old plants of the Catharanthus roseus, have unique structure originated from skeleton of the secologanin. These alkaloids are valuable because they have various pharmacological activities. For this reason, many synthetic methods of Corynanthe have been developed over a long time. One of the most common methods to access the core indoloquinolizine structure is C-3 functionalization of imines or amides derived from tryptamine via either Pictet-Spengler reaction or Bischler-Napieralski reaction. However, these methods generally require additional steps to generate the six-membered D-ring.

Recently, our group developed the methods to acess indole-3-acetic acid derivatives bearing a pyridyl moiety at the 2-position via the cyanide-catalyzed intramolecular imino-Stetter reaction of aldimine obtained from 2-aminocinnnamic acid derivatives and various pyridinecarbaldehydes.1 In this poster presentation, we disclose our efforts via the functionalization of the pyridinium ring of 2-pyridyl indole-3-acetic acid derivatives to construct the piperidine ring present in Corynanthe alkaloids. This approach allowed us to develope general synthetic protocol toward Corynanthe family.

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Development of Novel Protocols for Synthesis of 2-Arylquinolines from 2-Aminochalcones *via* Nucleophile-catalyzed Dehydrative Cyclization

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2-Substituted quinolines are important scaffolds found in biologically active natural products and pharmaceuticals, as well as key building blocks in materials science. Due to their importance, considerable effort has been made for the development of novel protocols for the synthesis of 2-arylquinolines. Among the protocols developed, the intramolecular cyclization of (*E*)-2-aminochalcones is one of the conventional methods. However, (*E*)-2-aminochalcones cannot undergo the dehydrative cyclization due to its restricted configuration of the double bond, and thus, most of the previous methods have been developed based on the conversion (*E*)-alkene into (*Z*)-isomer *via* either photoisomerisation or the use of a stoichiometric amount of chemical reagents, such as I_2 and PhSeCl, in the presence of a base.

We hypothesized that 2-arylquinolines could be prepared from 2-aminochalcones using a nucleophilic catalyst. Conjugate addition of the nucleophile to 2-aminochalcones would provide their saturated ketones bearing the nucleophile at the *β*-position. Conformational change from *s*-trans to *s*-cis about the C_{α}-C_{β} single bond allows the proximity of the two functional groups, and following condensation reaction would afford dihydroquinoline intermediates. Subsequent elimination of the nucleophile could provide the desired 2-arylquinolines. Based on this hypothesis, we developed a series of protocols for 2-arylquinolines starting from 2-aminochalcones in the presence of a nucleophile catalyst. Furthermore, we expanded this synthetic method to prepare 2-arylquinolines *via* palladium-catalyzed Heck reaction between 2-iodoaniline and *β*-chloropropiophenone, more readily available starting materials. In this poster presentation, the recent progress of 2-arylquinoline synthesis from 2-aminochalcone *via* dehydrative cyclization will be disclosed.

Development of A Novel Synthetic Method for Construction of Unsymmetrical Bisindole Compounds

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The dimeric indole compounds are class of the important structural motifs founded in indole natural products. Among the various dimeric species of indole, the bisindole structure in which two indoles are directly connected by single bond is the privileged scaffold. They exhibit widespread biological activities such as inhibition of protein kinase, cytotoxicity against tumor cell and cytotoxicity against human breast cancer. Because of these useful properties, they have attracted a lot of attention from the synthetic and medicinal communities. To date, several synthetic protocols of these useful structures have been reported in literatures. However, these reported methods have been applicable to a very limited scope of dimeric species. Particularly there have been few methods to access unsymmetric dimeric indole structures. In these reasons, the development of new efficient synthetic protocol is still in need.

Very recently, our group developed novel method to construct dimeric compound of indole via the cyanide catalyzed imino-Stetter reaction from 2-aminocinnamic acid and indole-2-carboxaldehyde.[1] When aldimines derived from 2-aminoccianmic acid derivatives and protected indole-2-carboxaldehydes were treated with catalytic amount of cyanide, the desired dimeric compounds were obtained. We further attempted to extend this protocol to the synthesis of dimeric indole compounds bearing different substituents at each indole moiety. The 2-aminocinnamic acid derivatives and indole-2-carboxaldehyde derivatives bearing different substituents gave the unsymmetric dimeric indole compounds. Herein we describe a novel synthetic method to construct unsymmetric dimeric indole compounds.

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Cu-catalyzed aerobic oxidative synthesis of sulfonamides from sulfonyl hydrazides and amines

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An environmentally friendly route for sulfonamides has been developed. The oxidative coupling of sulfonyl hydrazides and amines was catalyzed by $CuBr_2$ to produce various sulfonamides with the water and nitrogen gas as byproducts. Preliminary experiments revealed that the sulfonyl radical is likely to be involved in the reaction mechanism.
Previously reported sulfonamides synthesis use superstoichiometric amounts of TBHP and their scope is limited to aromatic sulfonyl hydrazides. This is less attractive. But our group describe a Cu-catalyzed aerobic oxidative synthesis of sulfonamides from sulfonyl hydrazides and amines. The developed sulfonamide synthesis fulfills the requirement for green and sustainable chemistry because only Cu catalyst is required without any additive or base, and water and nitrogen gas are produced as byproducts. In addition, the result of applying to aliphatic sulfonyl hydrazides was good.
In order to understand the mechanism of the present protocol, several experiments were carried out. First, When oxidative coupling without copper or under N_2, sulfonamide was not produced. Second, using TEMPO did not produce product. This imply that this reaction is radical pathway. In addition, the use of sodium benzenesulfinate produced product in 27% yield. These observations imply that the developed oxidative coupling proceeds through the benzenesulfonyl radical. When 4-(benzoyloxy)morpholine was employed instead of morpholine, the corresponding sulfonamide was efficiently produced, suggesting the copper amine complex might be involved in the reaction pathway.[1]

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Oxidation Potential Tunable Organic Molecules and Their Catalytic Application to Aerobic Dehydrogenation of Tetrahydroquinolines

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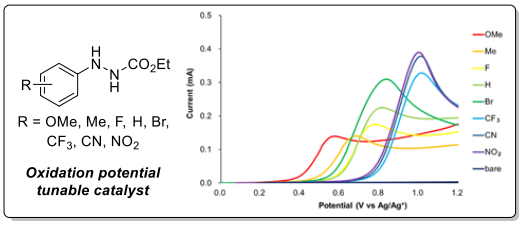

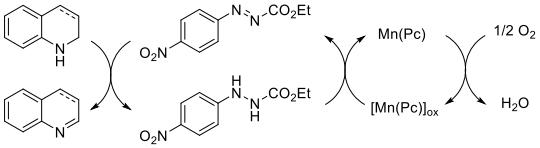

Redox-active organic molecules including quinones and nitroxyl radicals have been employed as substrate-selective catalysts. However, these redox-active organic molecules exhibited limited redox potentials because the synthesis of their derivatives having various electronic environments was quite restricted.

Recently, our group reported that the aerobic oxidation of di-*tert*-butyl hydrazodicarboxylate was catalyzed by CuI and DMAP and the developed catalytic system could facilitate the dehydrogenation of tetrahydroquinoline.[1] On the basis of this results, we envisioned that alkyl 2-phenyl hydrazocarboxylates can be utilized as oxidation potential tunable catalysts due to two reasons. First, the electronic modification of alkyl 2-phenyl hydrazocarboxylates would be easy by changing the substituent on the 2-phenyl group. Second, various alkyl 2-phenyl hydrazocarboxylates, which have substituents on 2-phenyl group, is readily accessible from the coupling of phenyl hydrazide and alkyl chloroformate

Various alkyl 2-phenyl hydrazocarboxylates, which has substituents such as OMe, Me, F, H, Br, CH_3, CN, and NO_2 on para-position of 2-phenyl group, were synthesized and their electrochemical oxidation potentials were determined by linear sweep voltammetry (LSV). The observed oxidation potentials of the alkyl 2-phenyl hydrazocarboxylates strongly depended on the class of substituent and correlated with Hammett constants. On the basis of this result, we could develop a coupled catalytic system for the aerobic dehydrogenation of 1,2,3,4-tetrahydroquinolines using a Mn(Pc) and ethyl 2-(4-nitrophenyl)hydrazocarboxylate redox couple.[2]

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Stereoselective Cycloadditions for a Series of N-Heterocycles: Beyond Corey-Chaykovsky Reactions

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Cyclopropane-containing systems, especially cyclopropane fused N-heterocycles, are common structural motives in many natural products, pharmacophore, and functional molecules. Besides, a three-membered ring can undergo a variety of transformations, such as ring openings, ring expansions, or cycloadditions resulting in furnishing complex structures. However, the synthetic approach of cyclopropanes has mostly relied on the carbene transformation using an expensive rhodium catalyst. Notably, stereoselective cyclopropanation under the catalyst-free conditions remains an unexplored field.

Recently, we discovered that N-aromatic zwitterions could serve as a 1,5-dipole for the construction of medium-sized heterocycles via [5 + n] cycloadditions with electrophilic partners. Based on our previous results, in this symposium, we will discuss diastereo- and enantioselective cyclopropanations through catalyst-free reactions between quinolinium zwitterions and various 1C coupling partners (sulfonium and sulfoxonium ylides). Interestingly, depending on the nature of coupling ylides, a variety of cycloadducts can be prepared stereoselectively.

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Radical Cation Cyclopropanation Reaction using Iron(III)-polypyridyl Complex

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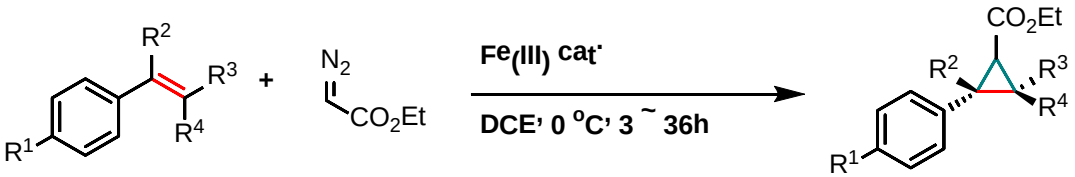
Various cyclopropanation of diazo reagent with electron-rich alkene have been studied for its reaction through metal carbenoid of Ru, Rh and Fe.[1] However, the redox reaction through a single electron transfer has been rarely reported. The Bauld group reported radical cation mediated cyclopropanation using ammonium radical cation salt which can oxidize stilbene type substrate.[2] After that, the Ferreira group reported the chromium photocatalyzed cyclopropanation reaction of alkene, which was transformed to the radical cation intermediate by single electron oxidation process.[3a] Iron catalysis is advantageous when compared to other transition metal reactions in that it is sustainable, cheap, and environmentally friendly in organic reactions. In addition, it is meaningful that the cyclopropanation reaction through the single electron transfer reaction using an iron catalyst has not been known yet. Iron(III)-polypyridyl complexes also have the adequate potential ($E_{1/2}$ = +0.82~1.10 V) to oxidize electron-rich alkenes such as anethole and stilbene ($E_{1/2}$ = +1.10~1.61 V) to form alkene radical cation intermediates.[3b] Under optimal condition of Fe(III)-polylyridyl complex, various cyclopropanes were synthesized from anetholes or stilbenes with different diazo esters. The mechanism of the radical cation cyclopropanation reaction was investigated by DFT calculation and several mechanistic experiments. Fe(III) catalyst oxidize anethole or stilbene to corresponding radical cation intermediate by single electron transfer, and the resulting radical cation reacts with a nucleophilic diazo ester. Simultaneous loss of N_2 affords a long-bonded cyclopropane radical cation. This reaction can be green and effective method using inexpensive iron to afford a radical cation cyclopropanation reaction.



R^1 = OAlkyl, H
R^2, R^3 = Alkyl
R^4 = Alkyl, Ar

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Photocatalytic Benzylic C-H bond Activation for Regioselective Construction of Cyclic Ethers and Lactones

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Visible-light-induced intramolecular benzylic C−O bond formation was developed using 2,4,6-triphenylpyrylium tetrafluoroborate (TPT), which allows the regioselective construction of 5- and 6- membered cyclic ethers and lactones. The reaction is supposed to proceed through the single-electron oxidation of the phenyl group, followed by the formation of a benzylic radical, thus preventing a competing 1,5-hydrogen abstraction pathway. Detailed mechanistic studies suggest that molecular oxygen is used to trap the benzylic radical intermediate to form benzyl alcohol, which undergoes intramolecular cyclization. This new method serves as a powerful platform by providing efficient access to cyclic ethers and lactones with a unified protocol.

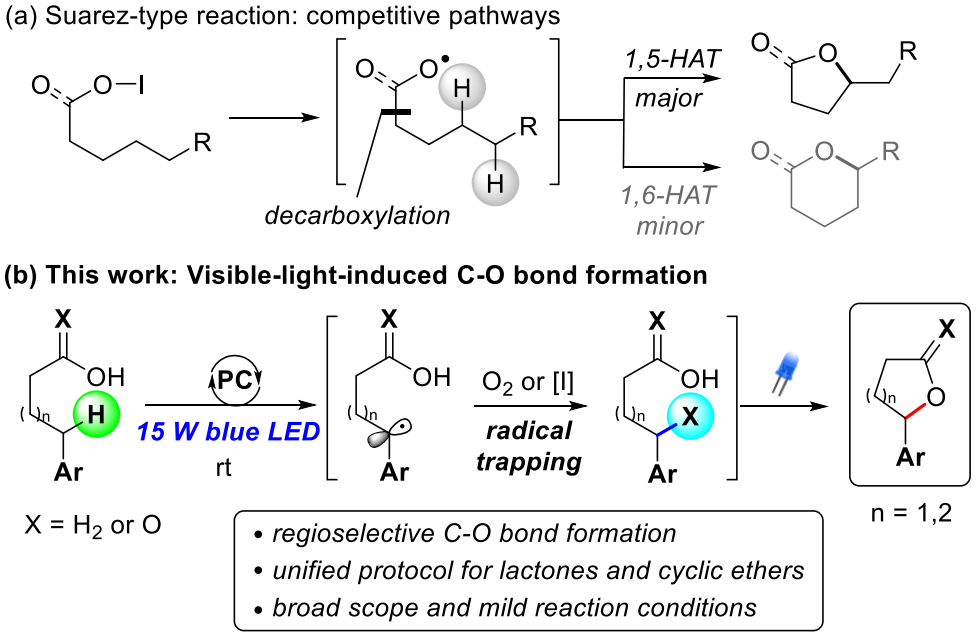

Figure 1. Regioselective photocatalytic construction of lactones and cyclic ethers

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Radical Translocation of N-Alkoxyheteroarenium Salts Driven by Photocatalysis of Quinolinone

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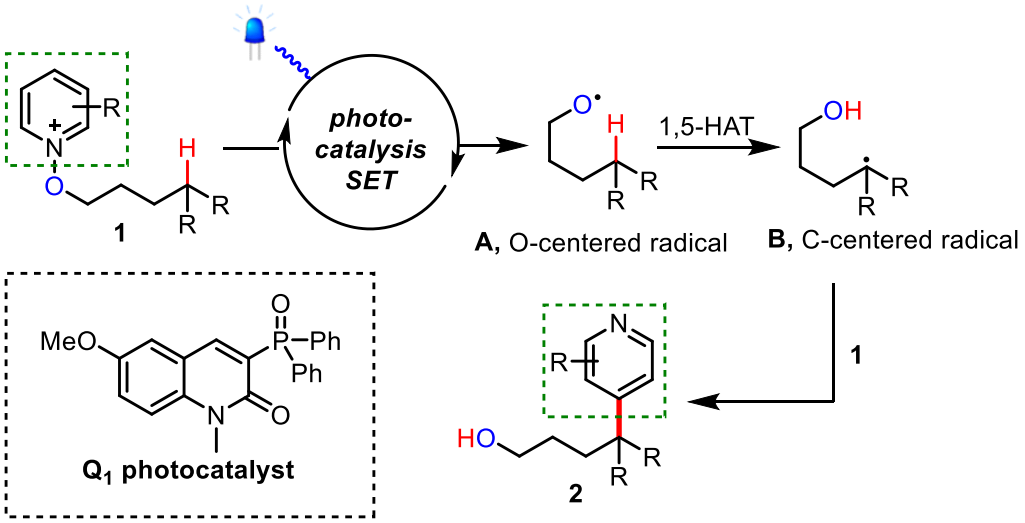
Metal-free, visible-light-induced site-selective heteroarylation of remote C(sp^3)–H bonds has been accomplished through the design of a class of N-alkoxyheteroarenium salts serving as both alkoxy radical precursors and heteroaryl sources. This strategy features a photoredox radical cascade process involving a sequential fragmentation of an N-alkoxyheteroarenium, a 1,5-HAT reaction, and a pyridylation process in a controllable and site-selective manner. The current transformation is well suited for late-stage functionalization of complex bioactive molecules.



- Remote C-H heteroarylation
- Broad scope
- Quinolinone as a photocatalyst
- Late-stage functionalization

References

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Ligand-controlled Regio- and Stereoselective Synthesis of 1,3-Oxazolidines and 1,3-Oxazepines *via* Pd-Catalyzed Decarboxylative [3+2]/[5+2] Cycloaddition

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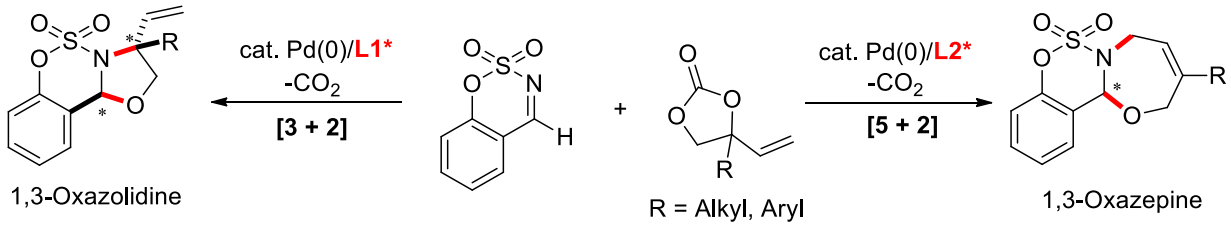
Divergent catalysis is an attractive and powerful strategy for rapid construction of different valuable molecules from common substrate. Over the past decades, the catalytic regiodivergent cycloaddition reactions have been successfully accomplished and demonstrated their potentials for the efficient manner to various heterocyclic framworks.[1] The typical approaches to catalytic divergent cycloadditions are to use substrates bearing different substituents to provide structurally dissimilar metal-ligated reactive dipoles, wherein each of the intermediates undergoes cycloadditions with a dipole to afford variant cyclic adducts.[2] On the other hand, examples of regiodivergent cycloadditions of identical substrates controlled by adjusting the catalytic conditions such as ligands are scarce because it is inherently difficult to predict and control the reactivity of variable reaction intermediate. In this study, we have developed ligand-controlled asymmetric divergent [3+2] and [5+2] cycloadditions to afford enantiomerically enriched 1,3-oxazolidine and 1,3-oxazepine derivatives, which are found in a tremendous range of natural products and bioactive molecules,[3] starting from common vinyl ethylene carbonates (VECs) and sulfate-derived cyclic imines. In catalytic processes, zwitterionic π-allyl Pd(II) species generated from VECs and Pd catalyst, which can act as 1,3- or 1,5-dipole equivalent, have been successfully controlled by different phosphine ligands.



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Selective *N*- or *O*-alkylation of 4,5-naphthalene-1-phenylpyrazol-3-one

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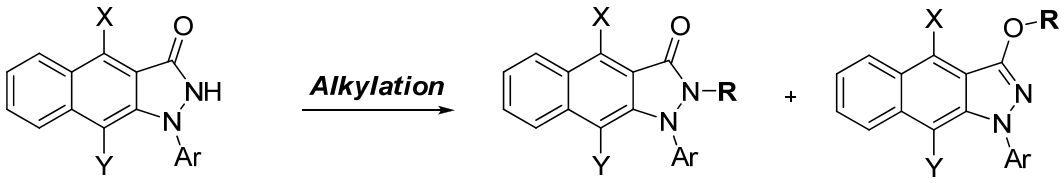
Pyrazolone is known as an interesting chemical moiety because of its importance for the synthesis of a variety of physiologically active compounds. Previously we have synthesized various 4, 5-naphthalene-fused 1-substituted pyrazol-3-one derivatives for pharmaceutically important compounds and found that there is a certain tendency between the structure of its derivatives and biological evaluation. The difficulty often encountered in the alkylation of 1-substituted pyrazolone compounds is that O-alkylated and N-alkylated products are formed simultaneously. In order to further investigate the structure-activity relationship (SAR) between O-analog and N-analog, there is a need to develop a highly selective synthesis method for N-alkylated or O-alkylated compounds. However, although studies on the C- and O-alkylation of 1,3-dicarbonyl compounds have been reported, there have been no reports on the O- and N-alkylation of pyrazolones to date. Thus, we needed to study the factors that can control the ratio of O- or N-alkylated adducts. Herein, we report optimal conditions for the selective synthesis of O- or N-alkylated adducts in the alkylation of 4,5-naphthalene-1-phenylpyrazol-3-one derivatives. It would be converted to naphthoquinone-conjugated pyrazolones or pyrazoles, which are expected to have potent anti-inflammatory activity.



N-alkylated product　　O-alkylated product

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Synthetic studies for the 1,4-dialkoxy-2-haloacetylnaphthalene derivatives as a precursor of AGEs Breaker

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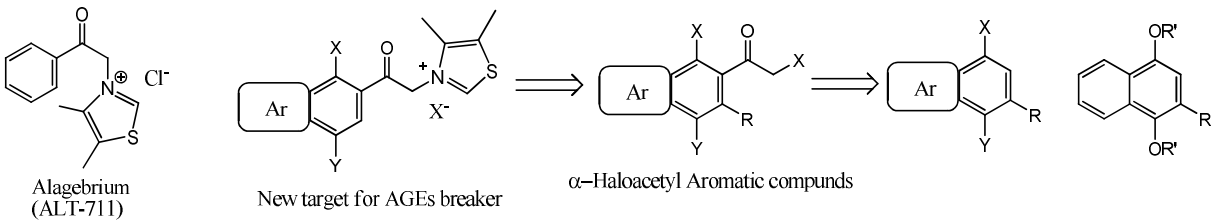
Advanced glycation end products, namely AGEs, are proteins or lipids that become glycated as a result of exposure of sugars. They can be a factor in aging and in the development or worsening of many degenerative diseases, such as diabetes, atherosclerosis, chronic renal failure, and Alzheimer's diseases. Compounds that are thought to break some existing AGE crossllinks include Alagebrium (ALT-711). N-Phenyl acetyl thiazolium salt, a core structure of alagebrium, could be synthesized from the reaction of N-phenyl acetyl halide and thiazole.

Previously we have prepared several 1,4-dimethoxy-2-haloacetylnaphthalene derivatives which are precursors of a potent candidate of AGEs breaker, such as naphthalene analog of alagebrium. However, it was often difficult to introduce haloacetyl moiety at the 2-position in 1,4-dialkoxynaphthalene. Therefore, in order to successfully develop a new AGEs breaker, it has been necessary to develop an efficient synthesis method of 1,4-dialkoxy-2-haloacetylnaphthalene. In this work, we describe several routes for various 1,4-dialkoxy-2-haloacetylnaphthalene derivatives; 1) acetylation of 1,4-dialkoxynaphthalene and α-bromination, 2) chloroacetylation of 1,4-dialkoxylnaphthalene 3) bromination of 1,4-dialkoxynaphthalene, lithiation, acetylation and α-bromination etc.



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Iron-polypyridyl Catalyzed Oxidative Alkenylation of Tertiary Aniline with Vinyl Sulfone

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The direct alkenylation reaction of an α-amino C(sp^3)-H bond of tertiary aniline with (*E*)-1,2-bis(arylsulfonyl)ethylene was achieved using iron-polypyridyl complex and oxidant. Photoredox radical alkenylation of α-amino acids and *N*-aryl amines was investigated by MacMillan using Ir(III) catalyst, and Inoue also reported the related protocol employing benzophenone under metal-free and photo-irradiation condition.[1a] In the context of an increasing interest in iron redox catalysis, oxidative transformation of amines by iron catalysts have been mostly limited in the iminium formation due to the uncontrollable oxidative property.[2] As a mild single-electron-transfer (SET) oxidation condition for the formation of α-aminoalkyl radical species, polypyridyl ligands were introduced to iron salts, based on electron donating effect of ligand to metal center. Iron-polypyridyl complex successfully generated the nucleophilic α-aminoalkyl radical species, which was reactive to (*E*)-1,2-bis(arylsulfonyl)ethylene as electron-deficient alkene. After α-aminoalkyl radical is trapped by vinyl sulfone, elimination of β-sulfonyl radical would provide the allyl amine product. The derived allyl amine products containing a sulfonyl group were further converted in a single step to the pyrrole derivative *via* cyclization and aromatization steps with ethyl isocyanoacetate.[1b]

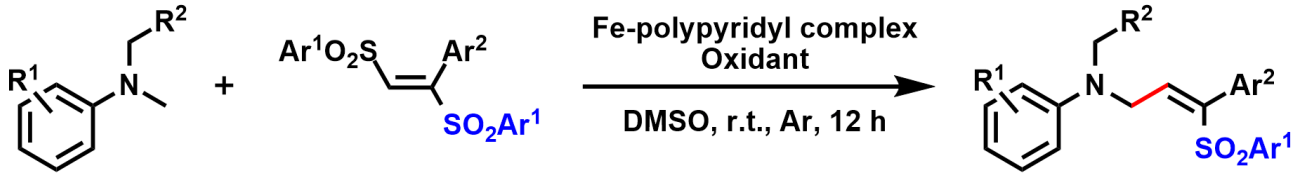

Figure 1. Oxidative alkenylation of tertiary anilines

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Synthesis of Cyclic Carbonate from CO_2 and Epoxide Catalyzed by Heteroleptic Fe(II)-iminopyridine Complexes

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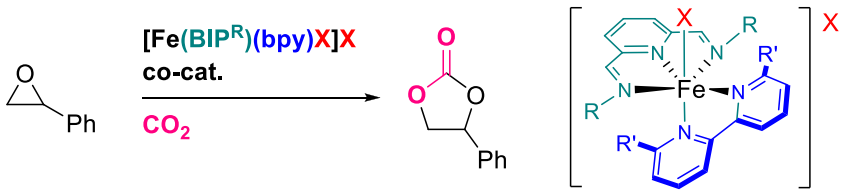
A wide range of metal and organocatalyst have investigated in the synthesis of cyclic carbonates from epoxides. Of all them, Iron is non-toxic, earth-abundant metal and Lewis-acidic metal as coupling epoxide with CO_2. So, many groups have been reported based on iron catalysts conversion of epoxide into cyclic carbonate. In the synthesis of cyclic carbonates from epoxides, the epoxide ring opening can be facilitated by a Lewis-acidic metal catalysts and nucleophiles.[1] In previous studies, our groups developed one-component complexes having hydrogen bond donor as activating epoxides and halide as nucleophiles.[2] While studies on epoxide activations have been active, CO_2 activations have been few reported. Accordingly, many groups have been introduced a Brønsted-acidic organocatalysts having an OH or NH group as CO_2 activator. CO_2 activation is possible by Lewis bases such as amine, alcohol, N-hetero aromatic compounds.[3] Due to the electrophilic nature of the carbon atoms of CO_2, electron-rich nucleophiles participate in forming the CO_2-adduct. And the solubility of CO_2 is increased in the reaction system by forming CO_2-adduct. In order to improve these activities, Fe(II) complexes containing N-hetero aromatic compound were designed. Hence, N-hetero aromatic compound of complexes activates CO_2 by forming a zwitterionic salt of base- CO_2.[4] In this work, a new multifunctional Fe(II) complexes were designed to synthesize cyclic carbonate under mild conditions by introducing Lewis base. The heteroleptic Fe(II) complexes are capable of CO_2 activation by Lewis base-derived ligand and epoxide activation as hydrogen bonding donor are developed. As a result, we could synthesize styrene oxide to cyclic carbonate under CO_2, low temperature, time and solvent-free condition, and it was possible to make more efficient reaction using additive.



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Proposed Total Synthesis of Type I Dimeric Securinega Alkaloids

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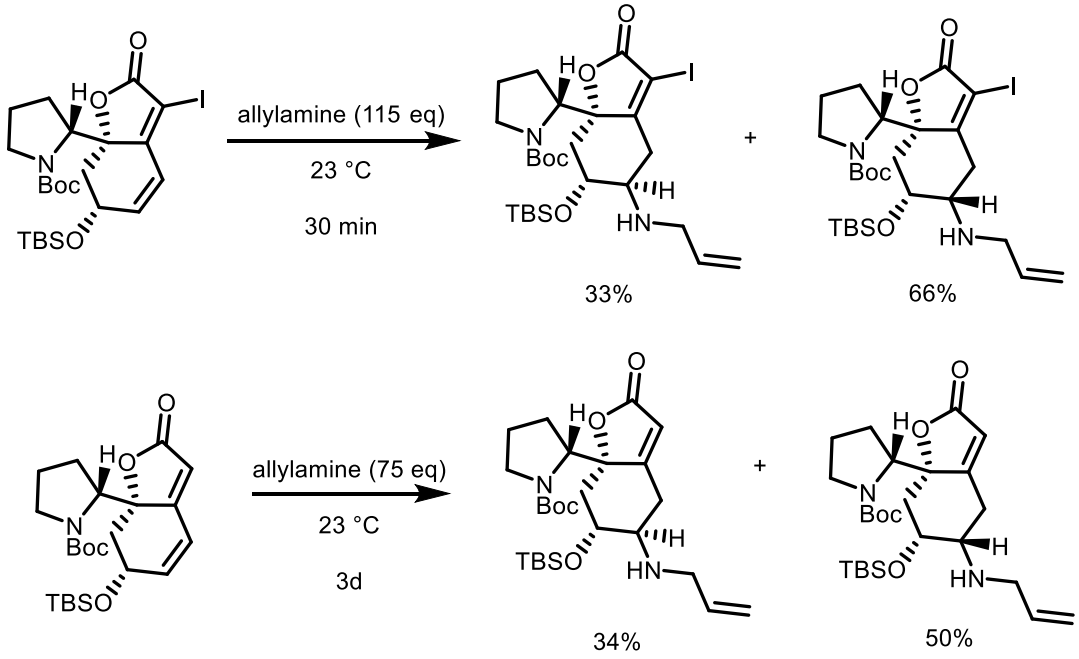
Securinega alkaloids consist of complex tetracyclic framework containing α,β-γ,δ-unsaturated butenolide. Molecular structure of dimeric securinega alkaloid is composed of various connection modes between securinega monomers. Type I dimeric securinega alkaloids refer to dimeric securinega alkaloids in which the monomeric units are connected by a conjugate addition of the heteroatom.[1]

During studies toward the total synthesis of fluggenine D, we observed a 1,6-conjugate addition of the methoxide moiety to the alpha-iodinated α,β-γ,δ-unsaturated butenolide. On the other hand, substrates without the alpha iodine did not show such electrophilicity.

Based on these observations, we reasoned that electrophilicity of alpha-iodinated unsaturated butenolide would serve as promising precursor for type I dimeric securinega alkaloid such as norsecurinamine B.

From experiments using methanol and allylamine as nucleophiles, increased electrophilicity exerted by the iodide group at the α position of the α,β-γ,δ-unsaturated butenolide was observed. Addition of methanol to the δ position of the unsaturated butenolide occurred only for substrate with the alpha iodide. On the other hand, addition of allylamine occurred for both substrates with and without the alpha iodide. However, we observed drastic difference in reaction kinetics.



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Co(III)/Ag(I)-Catalyzed γ-selective C–H Allylation/Hydroamination Cascade for the Synthesis of 3,4-Dihydroisoquinolines

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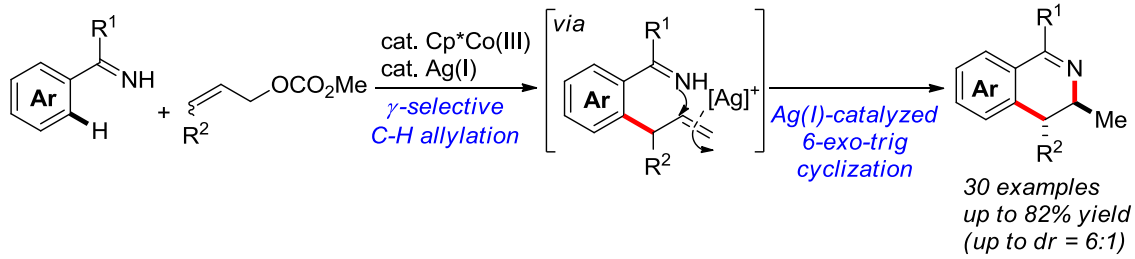
Introduction of useful functional groups via transition metal catalyzed direct C−H bond activations offers remarkable atom- and step-economy in organic synthesis.[1] Direct C−H allylations catalyzed by various transition metals such as Rh(III), Ru(II), Co(III) and Mn(I) have been extensively studied since the allyl moiety is an versatile functional group.[2] Nevertheless, transition metal-catalyzed direct C−H allylation still suffers from formidable issues such as poor α/γ selectivity, olefin migration and low reactivity in the case of allyl reagents in which alkyl or aryl substituents are present at α- or γ-position.[3] In addition, cascade reactions involving direct C−H allylation toward the synthesis of valuable heterocycles have been rarely studied. Herein, we report Cp*Co(III)-catalyzed γ-selective C–H allylation and cascading Ag(I)-catalyzed intramolecular hydroamination to access *trans*-3,4-dihydroisoquinolines, which are ubiquitous scaffolds that found in many natural products and commercial drugs, starting from NH ketimines and allyl carbonates. For an efficient γ-selective allylation, the conformation of γ-alkyl substituent of allyl carbonates has proven to be crucial.



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Construction of *β*-chiral dialkyl boron compounds via Copper-Catalyzed Enantioselective Reduction

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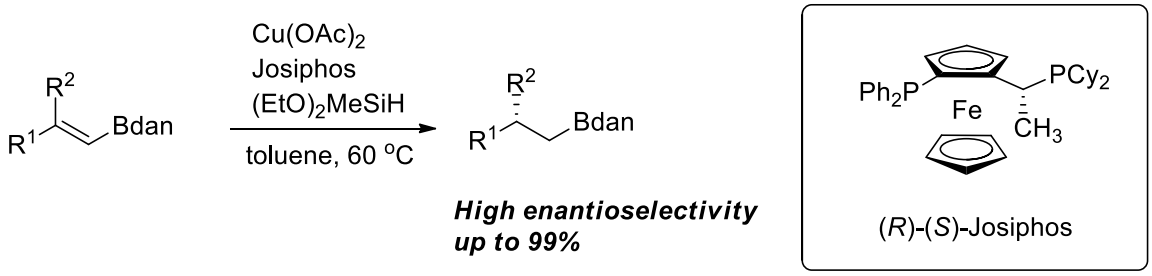
Highly enantioselective reduction of *β,β*-disubstituted alkenylboramide compounds employing copper catalyst and hydrosilanes was investigated. In the presence of a copper(Ⅱ) catalyst with chiral Josiphos ligand, a range of alkenylboramide compounds with primary or secondary alkyl, silyl and aryl substituent(R^1) produced chiral disubstituted boramide compounds in good yield with high enantioselectivity up to 99% ee.



Towards the Synthesis of Fluvirosaones A and B

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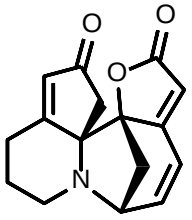
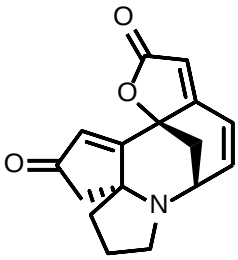
Securinega alkaloids have gained interests from synthetic community due to its characteristic bridged tetracyclic structure and diverse bioactivities, serving as a testing ground of new synthetic methods.[1] Although numerous synthetic pathways for monomeric *Securinega* alkaloids have been accomplished, synthetic strategies toward rearranged *Securinega* alkaloids are underdeveloped. Fluvirosaones A and B are *Securinega* alkaloids isolated from *Flueggea virosa* which bear unique pentacyclic structure. Fluvirosaone A has additional three carbon unit from its biogenetic precursor, securinine alkaloid. However, fluvirosaone B has rearranged carbon skeleton similar to secu'amamine A with additional three carbon unit.[2] In this poster, we report our recent synthetic progress towards fluvirosaones A and B.



Fluvirosaone A



Fluvirosaone B

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Studies Toward the Total Synthesis of Cinnamacrin C and Cinnafragrin D

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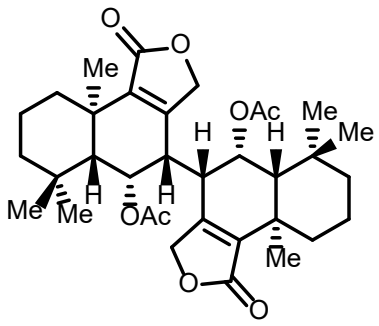
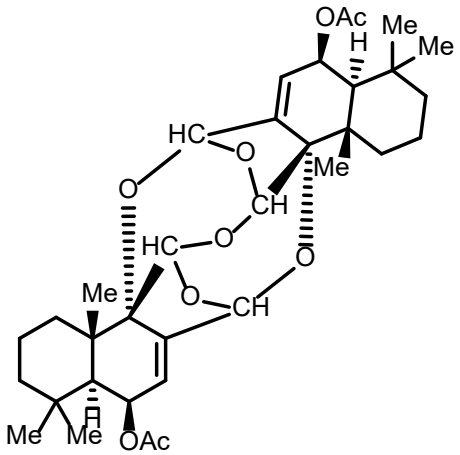
Drimane-type cinnamacrin C and cinnafragrin D were isolated from *Cinnamosma macrocarpa* by Yoshinori Asakawa and coworkers in 2007.1 Our group's continued interests toward dimeric natural products prompted us to embark on a synthetic program aimed at chemical synthesis of cinnamacrin C and cinnafragrin D. in this poster, we present our current research progress on this daunting and complex natural products.



Cinnamacrin C



Cinnafragrin D

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Formal Synthesis of (−)-Cephalotaxine via Construction of Azaspiranic Backbone using Proline Ester Enolate Claisen Rearrangement

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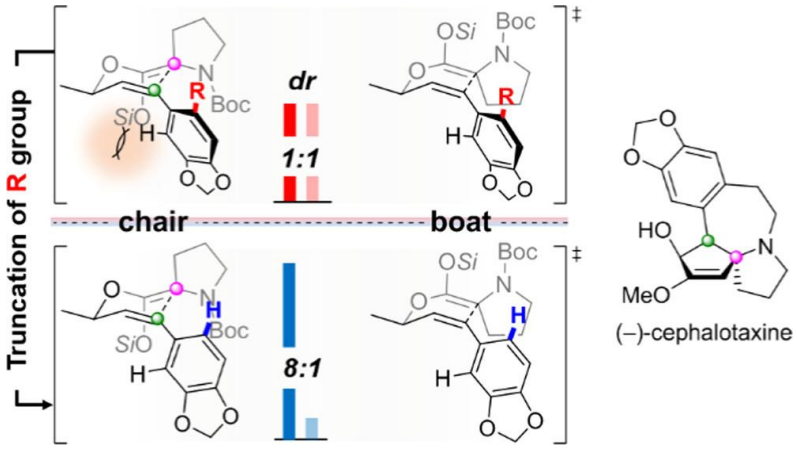
Cephalotaxus alkaloids exhibit potent cytotoxic activity against various human cancer cell lines.[1] Its azaspiranic tetracyclic backbone is structurally intriguing, which has attracted attention as synthetic target for last three decades. Recently, we have achieved a concise formal total synthesis of (−)-cephalotaxine, a parent structure of Cephalotaxus alkaloids, via an ester enolate Claisen rearrangement (EECR). The EECR of α-amino acids has been utilized as a powerful strategy for the synthesis of complex nitrogen-containing molecules because this transformation can deliver densely functionalized amino acids with a defined stereochemistry.[2] A series of EECRs of proline allyl esters were examined to obtain the desired relative stereochemistry of an azaspiranic tetracyclic backbone. An unexpected reversal or low diastereoselectivity of (Z)-cinnamyl ester was observed. We discovered that the diastereoselectivity of EECR was shifted depending on the ortho-substitution pattern of the aromatic ring of the proline (Z)-cinnamyl ester substrate. This result represents a useful guide in aiding the prediction of stereochemical outcome of EECR of α-amino allylic esters.



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Asymmetric synthesis of Cα-Quaternary Proline via C to N to C Chirality Transfers: Application to the Total Synthesis of (–)-Amathaspiramide F

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Proline has been recognized as attractive substance in chemistry and biology owing to the distinct conformational properties. Thus, C→N→C chirality transfer strategy has been developed for the asymmetric synthesis of proline derivatives. However, the main limitation of this approach was the poor level of C→N chirality transfer. To overcome this circumstance, we decided to utilize conformationally restricted proline derivatives. Diastereomeric purity of quaternary ammonium salt was completely transferred to enantiomeric purity of α-carbon through [2,3]-Stevens rearrangement. An enantiopure synthesis of Cα-substituted prolines was successfully achieved via controlling the stereodynamics of proline by using a nitrogen-fused bicyclic system. This developed strategy was subsequently utilized in the total synthesis of (–)-amathaspiramide F.

Aminooxygenation of Ynamides with N-Hydroxybenzotriazoles

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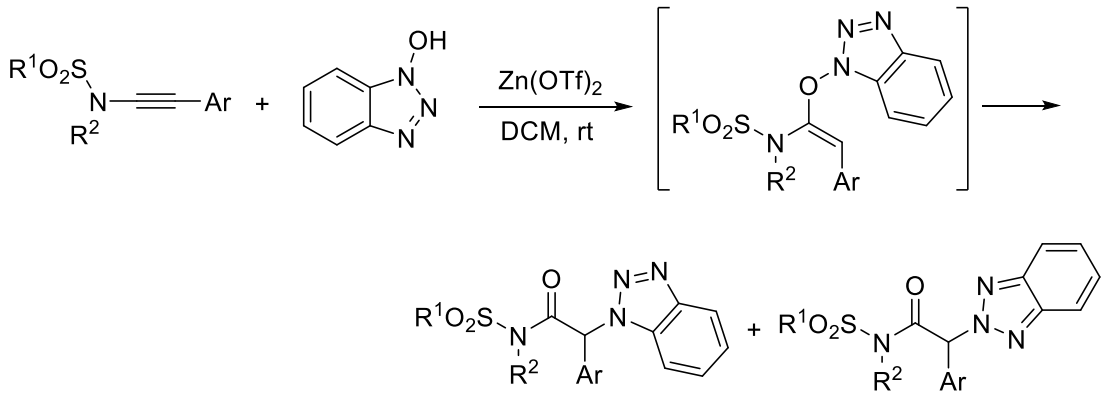
Aminooxygenation of alkynes provides one of the most direct routes to α-amino carbonyl compounds, which represent key motifs that are abundantly found in natural products and medicinal agents.[1] For example, Murakami and coworkers reported Rh-catalyzed denitrogenative hydration of triazole derivatives,[2a] and Shin and coworkers reported Au-catalyzed intramolecular aminooxygenation of hydroxylamine derivatives from alkynes.[2b] Besides these transition metal catalyzed routes, S_N2' addition of secondary amine to N-enoxypyridinium salts are known.[2c]

Herein, we report the reaction of ynamides with HOBt which underwent subsequent rearrangement into α-benzotriazolyl imides without isolation of the intermediate.[3] This process can be catalyzed by $Zn(OTf)_2$ (2.5 mol %), furnishing the desired α-triazolyl imides in up to 82 % yield at ambient temperature.



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Synthesis of cyclic amidines from quinolines via borane catalyzed dearomative hydrosilylation

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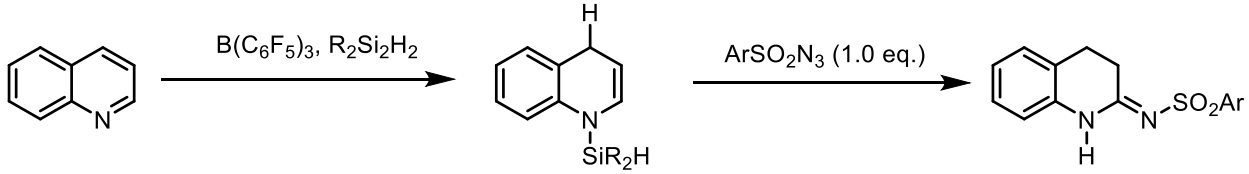
Amidine is one of the fundamental functional group in organic synthesis and pharmaceutical molecules. In particular, cyclic amidines are versatile structural motifs in various natural and synthetic compounds with wide range of bioactivities.[1] As a result, development of synthetic route to cyclic amidines has been investigated extensively. Among them, [2+3] cycloaddition of azide and enamine has garnered special attention since the resulting triazole intermediate can be utilized for various reaction pathways.[2] On the other hand, Borane catalyzed hydrosilylation of *N*-heterocycles had been developed by Chang and coworkers.[3] Mechanistic study revealed that there is a partially reduced endocyclic enamine intermediate that can be used as versatile building block.

Herein, a new synthetic route to cyclic amidines from readily available quinolines has been developed. Activation of the stable quinoline with borane catalyzed monohydrosilylation gave us the versatile silyl enamine intermediate. Subsequent addition of organic azides to the intermediate resulted in unique class of cyclic amidines, 3,4-dihydroquinolinimines.



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Synthesis of Spiro[oxindole-3,2′-pyrrolidine] Derivatives from Benzynes and Azomethine Ylides through 1,3-Dipolar Cycloaddition Reactions

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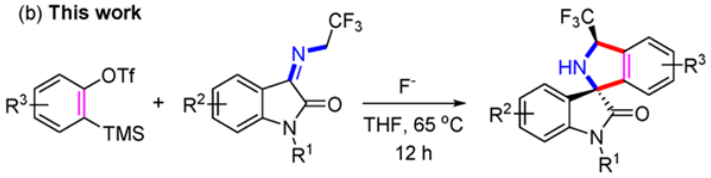
A novel synthetic strategy employing benzyne and azomethine ylides for the construction of spiro[oxindole-3,2′-pyrrolidine] derivatives has been achieved in good yields. The ketimines obtained from the condensation of isatins with $CF_3CH_2NH_2$ react with benzyne in the presence of weak bases such as TBAF or TBAT. This mild practical 1,3-dipolar cycloaddition provides an efficient route to access biologically active compounds.



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Thiol-Functionalization and -CH_2- Insertion on Dopamine for Poly(dopamine)-Coating Applications

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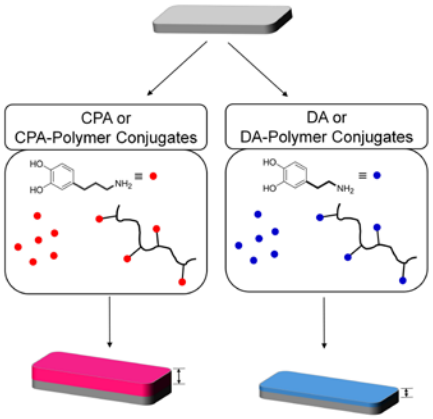
Dopamine is catecholamines derivatives organic molecules, and one of the important neurotransmitter in our nerve system. Although the biological activities in nervous system are the major role of dopamine, the utilization of dopamine molecules in the organic and surface chemistry have been emerging research field. The oxidation of catechol and cyclization promotes the self-polymerization to form thin, surface-adherent polydopamine films onto a wide range of inorganic and organic materials.
In this presentation, we will discuss our recent efforts to synthesize and derivatizing dopamine molecules. First, we have focused on the aliphatic amine part on dopamine molecules. The carbon chain length was elongated to three-carbons from two-carbons by CH_2 insertion. The modified dopamine (3C-DP) showed the better coating performance than the pristine dopamine.[1] The detail synthetic procedures along with coating properties will be presented. In addition, the terminal amino group was changed to thiol group to study the functional group effect. The thiol chemistry for dopamine also will be discussed.



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Regioisomerism of Functional Groups and Post-Synthetic Modification in Metal-Organic Frameworks

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Metal-organic frameworks are organic-inorganic hybrid materials consisting of multitopic coordinating ligands and metal clusters (or ions). The multitopic ligands could have additional functional group in their empty C-H bond sites, and various functional groups such as amino, nitro, halo, hydroxy, and additional aromatic rings have been successfully incorporated into MOFs through ligand functionalization. The chemical handles in MOFs could be converted to other functionalities in the solid-state manner, which called post-synthetic modification (PSM). Traditional organic transformations such as acylation from amino group, cyanation from bromo group have been accomplished through PSM strategy.[1]
Recently, we have successfully prepared several bifunctional MOFs with two chemical handles such as NH_2, NO_2, OMe, and Cl functionalities.[2-4] Besides the original studies were focused on the structural flexibility changes of MOFs with regioisomeric ligands, herein, PSM with two reactive chemical handles has been performed. The two functionalities, NH_2 and OH were successfully incorporated into MOFs with regioisomeric controls. The selective PSM were performed with positional changes. The detail synthetic procedures along with characterization will be discussed.

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Photochemical Triggers and Amine-Controls for Poly(dopamine) Coating

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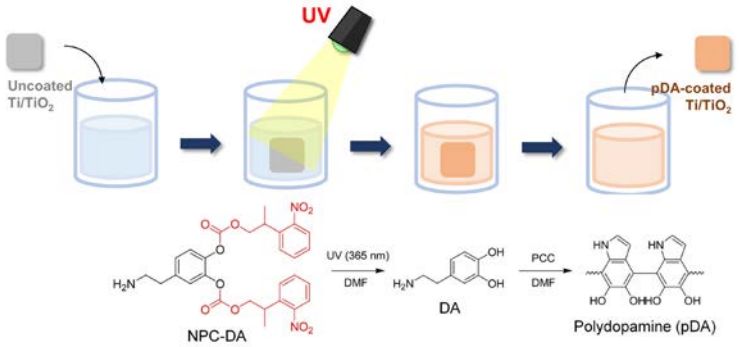
Dopamine is catecholamines derivatives organic molecules, and one of the important neurotransmitter in our nerve system. Dopamine is obtained by removing a carboxyl group from L-DOPA which is synthesized from our brain and kidney. Although the biological activities in nervous system are the major role of dopamine, the utilization of dopamine molecules in the organic and surface chemistry have been emerging research field. Dopamine has universal coating property with polymerization to poly(dopamine). Oxidation of catechol part to 1,2-hydroquinone and following cyclization is the main reaction for polymerization of dopamine. The oxidation could be promoted in the basic condition and with external oxidant.
In this presentation, we will discuss our recent efforts to control polymerization step by introducing photochemical protection/deprotection strategies. Protected dopamines with photolabile groups have been prepared, and the polymerization was initiated by UV-irradiation, and starting timing is perfectly controlled in this methodology.[1]
In addition, the amine part derivatizations on dopamine have been attempted. Since the polymerization of dopamine is containing cyclization of aliphatic amines, this step should be controlled by amine derivatives. Detail synthetic procedures along with coating properties will be discussed.



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Hemocompatible Sulfobetaine Polymer Coating with Poly((3-(Methacryloylamino)propyl)-Dimethyl(3-sulfopropyl)ammonium Hydroxide)

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As platelet adhesion and its excessive accumulation can cause blood coagulation, the inhibition of platelet adhesion/aggregation has been a critical issue for blood-contact medical devices.[1] For example, unnecessary blood coagulation on vascular stents can lead to blockage of blood flow and blood vessel destruction.[2] In addition, medical devices inserted into the body may lose their function. To solve this problem, we aim to develop the functional coating for preventing platelet adhesion/aggregation by grafting sulfobetaine zwitterionic polymer, poly((3-methacryloylamino)propyl-dimethyl(3-sulfopropyl)ammonium hydroxide) (poly(MPDSAH)) onto titanium dioxide substrates. The polymerization was carried out by activators regenerated by electron transfer for atom transfer radical polymerization (ARGET ATRP).[3] The polymer grafting process was developed as a substrate-independent manner by using polyphenol chemistry. The polymer grafting was characterized by ellipsometry, contact angle goniometry, and X-ray photoelectron spectroscopy. Compared to bare and polyphenol-coated substrates, poly(MPDSAH)-grafted substrate strongly inhibited platelet adhesion and aggregation, showing its antifouling capability and hemocompatibility.

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Success of photoinduced electron/energy transfer-reversible addition-fragmentation chain transfer (PET-RAFT) by using purely organic photocatalysts in the presence of oxygen

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Reversible addition-fragmentation chain transfer (RAFT) polymerization is a typical method of living radical polymerization which can control the polymerization degree and the molecular weight according to the reaction time and obtain the single molecular weight distribution. Recently, photoinduced electron/energy transfer (PET)-RAFT polymerization using photocatalysts showed the potential of oxygen tolerance. Most of the PET-RAFT polymerizations that currently exhibit the oxygen tolerance use transition metal-based catalysts such as $Ir(ppy)_3$, $Ru(bpy)_3Cl_2$, etc. However, it has the disadvantage that they must be purified to remove residual transition metals after reaction. To solve this problem, pure organic photocatalysts (e.g, Eosin Y, Fluorescein, etc.) have been studied recently. However, in this case, additional reducing agents are required to exhibit the oxygen tolerance. In this study, we discovered purely organic photocatalysts with light absorption in the visible light region, and succeeded in PET-RAFT polymerization with sufficient oxygen tolerance without additional reducing agents.

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A One-for-all Switchable Nanotheranostics: Photosensitizer Detecting Albumin In Vivo From the Disassembly of Nanovesicles

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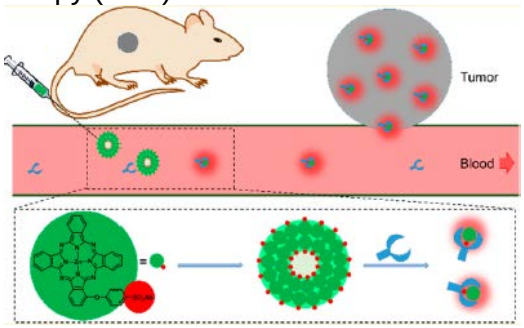
Theranostics that can indicate the expression of biomarkers and simultaneously transport therapeutic agents play a key role in basic biological studies as well as in treatment applications. Among many biomarkers, Albumin is one of the most promising candidates for potential disease diagnostics and it is used as a drug delivery carrier for many years. However, there are only few cases showing the specific interactions of exogenous probes with albumin in vivo, and slow fabrication processes and potential toxicity of the complexes were main problems of nanocompound delivery systems. In this study, we demonstrate a simplistic switchable nanotheranositc (NanoPcS) for both albumin detection and cancer treatment. Especially, the disassembly of injected NanoPcS causes the in vivo specific binding between albumin and PcS, and the binding is confirmed using an inducible transgenic mouse system. According to the results of fluorescence imaging and antitumor tests on different tumor models, NanoPcS has higher-level tumor-targeting ability and the potential for time-modulated, activatable photodynamic therapy (PDT).



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Rhodamine derivatives fluorescent probe for monitoring ATP in mitochondria and lysosomes

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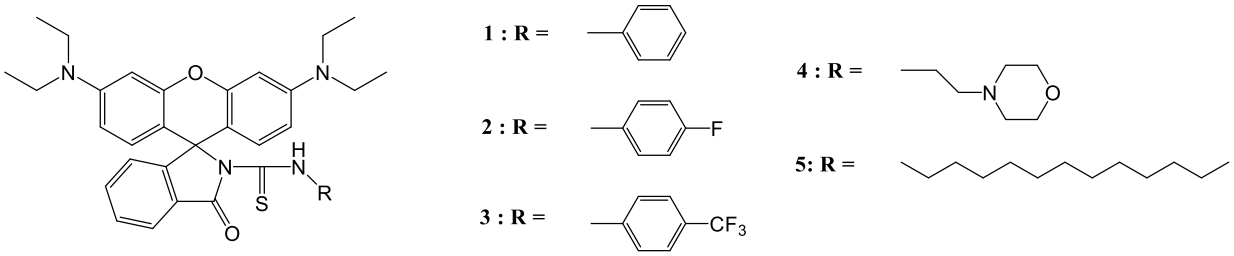
ATP is well known as an essential energy source in all living things and it plays key roles in variety of biological processes. In addition, low levels of ATP are indicators of Parkinson's disease, cardiovascular disease and ischemia. As a result, developing a fluorescent probe for detecting ATP selectively is a significant goal. Currently, we have developed colorimetric and fluorescent "turn-on" probe based on rhodamine derivatives, bearing thiourea groups, for the detection of adenosine-5′-triphosphate (ATP) through hydrogen bond interactions. Probes shows obvious color and fluorescence change with the presence of ATP. Moreover, these probes can be used to image ATP in HeLa cells. Because it was found to locate mainly in mitochondria, 2 and 5 can be employed to image ATP in mitochondria. On the other hand, probe 4, bearing a morpholine mainly locates to lysosomes and can be utilized to image ATP in lysosomes.



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Improvement of tumor targeting therapy using protein sequence reactive nanophotosensitizer complex

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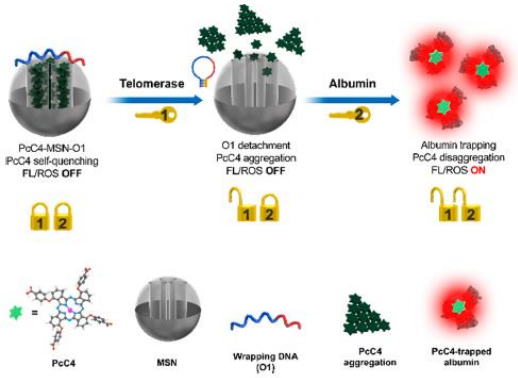
One of the difficulties in cancer treatment is the development of effective tumor targeting therapies that minimize side effects. Therefore, the idea of using an activatable photosensitizers (aPS) that only turns on by specific stimuli for photodynamic therapy (PDT) is being studied these days. In this paper, we introduce a protein sequence reactive aPS(PcC4-MSN-O1), which only turns on in the presence of two different protein targets. PcC4 has self-quenching photoactivity in the nanostructure of PcC4-MSNO1. However, the photoactivity is suddenly turned on when PcC4-MSN-O1 reacts with telomerase and albumin sequentially. Thus, PcC4-MSN-O1 shows obvious phototoxicity in cancer cells rather than normal cells. Also, when tested with xenograft mice model, accumulation in HeLa tumors was detected and a laser irradiation significantly inhibited tumor growth. Furthermore, PcC4-MSN-O1 shows the time-regulated activation of tumors and the quick excretion from the body.



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Phthalocyanine photosensitizers binding specifically to albumin dimers : natural advances enhancing PDT efficacy

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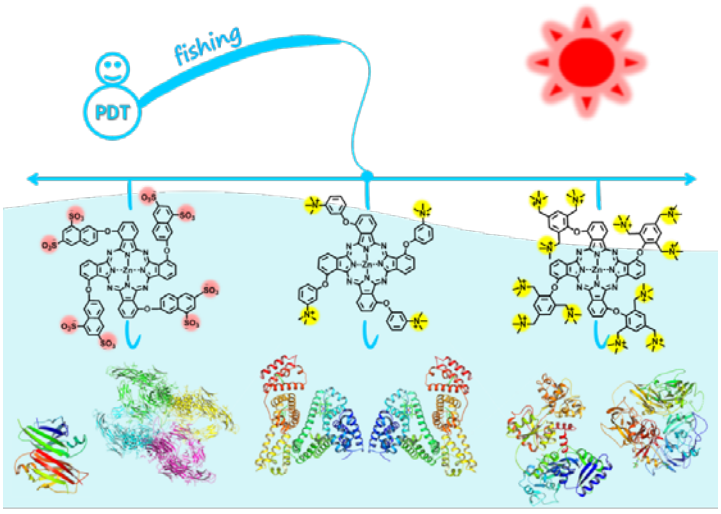
Target specific delivery of therapeutic operator is gaining attention in a field of cancer treatment. We came up with a green and competent way to deliver phthalocyanine-based photosensitizers for tumor targeting. In-vivo albumin was used as a natural carrier for these photosensitizers. Although other phthalocyanines did not show selectivity towards albumin dimer and monomer, positively-charged phthalocyanine $ZnPcN_4$ showed unique specific binding with albumin dimer. Gel assays, optical spectra and computational calculations were used to support this idea. These phthalocyanines effectively accumulate in tumor cells owing to the transport by albumin which is naturally occurring in human bodies so that unnatural additives are not needed. $ZnPcN_4$ indicates an exceptional phototherapeutic antitumor efficacy showing strong absorption in the far-red/near-infrared regions and generating high rate of reactive oxygen species.



Marine anti-fouling coating on solid surfaces using Carrageenan

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Non-specific adsorption on the surface of materials used in marine conditions causes various problems. For example, unwanted adsorption of marine organisms could disrupt marine ecosystems and increase fuel consumption. So, to solve it, the focus is on efforts to suppress the surface chemical composition of solid substrates. For example, polymer surface coatings have been frequently used to introduce marine antifouling properties to solid surfaces. Polysaccharides, PEG, and zwitterionic polymers are representatives that have been used in the preparation of marine antifouling surfaces. Here we report that the highly sulfated polysaccharide, carrageenan, could be a promising candidate for creating an excellent marine antifouling surface. Carrageenans were effectively introduced on solid surfaces via coordinate bond formation, and the resulting surfaces were found to be highly resistant to marine fouling organisms.

References

Biomedical Applications of solid surface by using Zirconium(IV)-Sulfated Polysaccharide Complexes

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Coating of solid substrate with ulvan, a sulfated polysaccharide, has been widely applied to medical implants because of its excellent anticoagulant properties. Coating a solid substrate with ulvan is accomplished primarily by covalent bond formation. However, this approach requires complex and time-consuming steps and adaptation since most studies are performed on specific substrates. In this study we aimed to develop an easy ulvan coating method that could circumvent the limitations of conventional ulvan coating methods. This approach consists of surface priming with tannic acid (TA) and ulvan grafting on the surface. The Zr^{IV}-mediated coordination formation between TA and ulvan allows easy deposition of ulvan on the solid surface without any derivatization. Using this method, the ulvan layer, which exhibits excellent resistance to protein adsorption and human platelet adhesion, has been successfully formed on the solid surface.

Design and synthesis of advanced Osmium-based electron-transfer mediator for Continuous glucose monitoring system(CGMS)

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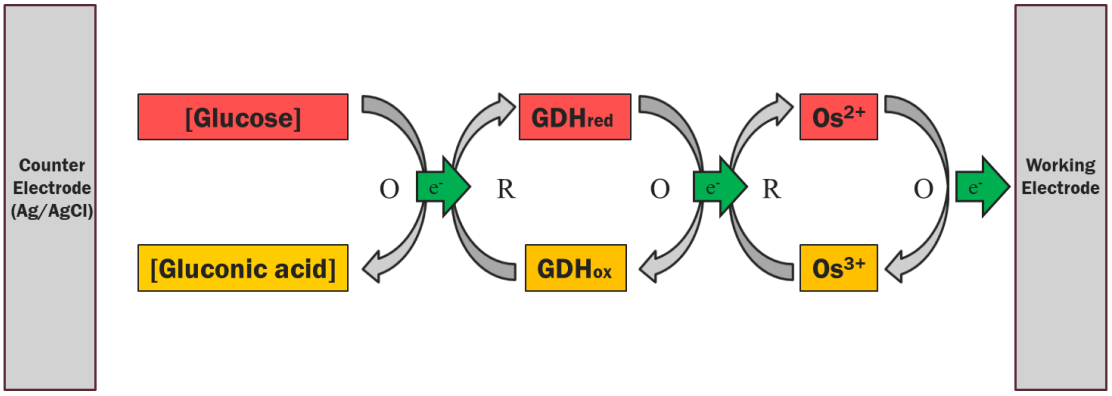
연속혈당측정기(Contiuous glucose monitoring system,CGMS)는 혈당을 측정하는 방법 중 하나로, 기존의 채혈식 혈당측정방식보다 여러가지 이점을 가지고 있다. 이전의 혈당측정기기 중 가장 널리 사용되고 있는 방법은 채혈한 혈액 샘플을 이용한 방법이었다. 하지만 연속혈당측정기는 채혈과정 없이 센서를 부착하는 것만으로 거의 동일한 수준의 연속적 혈당 측정이 가능하다. 이에 따라 연속혈당측정기가 적용된 새로운 혈당측정센서의 연구 및 개발이 활발하게 이뤄지고있다.

연속혈당측정기의 원리는 포도당의 산화반응을 이용한다. 포도당이 산화되면서 발생한 전자는 글루타민탈수소효소(Glutamate dehydrogenase,GDH)를 환원시키고, 이것이 다시 산화되면서 전자전달매개체로 전자이동이 일어난다. 이 때, 글루타민탈수소효소는 전극으로 전자의 직접적인 전달을 할 수 없기 때문에, 전자전달매개체를 통한 전극으로의 전자전달이 중요한 역할을 한다. 즉, 전자전달매개체의 산화환원 반응에 의해 전극에서 발생하는 전류로부터 포도당의 농도를 확인할 수 있다. 이 상관관계에 따라 체내 혈당 농도가 연속적으로 변화할 때, 그 신호를 해석하여 채혈 없이 실시간으로 혈당을 측정할 수 있게 된다. 우리는 연속혈당측정기에 적용할 오스뮴 기반의 새로운 전자전달매개체를 개발하고 있다. 이 전자전달매개체가 가져야 하는 특징은 산화환원반응에 대한 내구성, 정확도향상을 위한 적절한 포텐셜 튜닝, 빠른 에세이타임 등이 있다. 우리는 이러한 향상된 전기화학적 특징을 가지는 다양한 오스뮴 기반의 전자전달매개체를 개발 및 평가 하고 있다.



Aromatic Hybrid Foldamers as a Nucleophic Catalyst for the Resioselective Acylation of Monosaccharides

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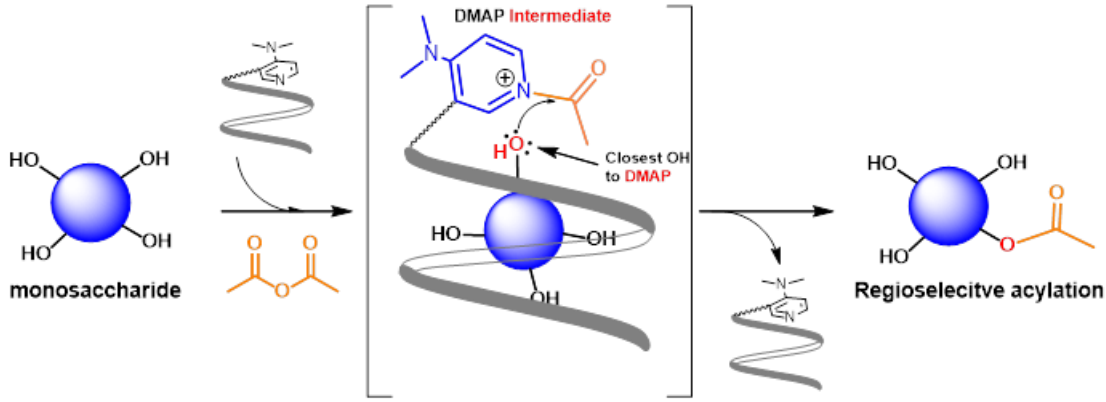
The regioselective acylation of polyols such as carbohydrates without repeating protection-deprotection processes is an important topic of researches in organic chemistry. Herein, we have designed and prepared new nucleophilic catalysts based on aromatic foldamers that can fold into helical conformations with an internal binding cavity. The aromatic foldamers consist of two different repeating subunits, indolocarbazole and naphthyridine , which are connected through ethynyl bonds. Upon folding into a helical conformation, the foldamers have been demonstrated to generate an internal cavity allowing for binding glucose.[1] To the end of the strand of these foldamers, 4-(*N,N*-dimethylamino)pyridine (DMAP) unit is incorporated to achieve the regioselective acylation of polyols. Details including syntheses and the results of acylations will be described in the presentation.



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Hypoxia-responsive theranostic prodrug based on anti-angiogenisis via COX-2 blockade

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Anti-angiogenesis, i.e., blocking the angiogenic pathway, has been considered as a significant strategy in current cancer therapy. However, the associated benefits have proven to be modest as tumor angiogenesis and regrowth persist, probably due to other ill-defined complex angiogenic mechanisms. Herein, we developed a cancer theranostic application consisted of indomethacin (IMC) incorporating system to mediate hypoxia responsive prodrug (**TA**) and diagnostic agent (**DA**). Cyclooxygenase 2 (COX-2) elevated expression in several cancer types is closely associated with severe tumor supporting vascularization factors. Utilizing COX-2 inhibition augmented the anti-angiogenetic induced hypoxia responsive prodrug activation well. Both in vitro and in vivo results proved that **DA** and **TA** exhibited specificity towards COX-2 positive (+ve) HeLa and A549 cancer cell lines and activation under hypoxic conditions. Compared with controls (R1, and anticancer drug SN-38), **TA** displayed prolonged tumor retention and enhanced therapeutic efficacy in xenograft mouse models at a reduced dosage. Our results considerably highlighted the importance of COX-2 blockade[1,2] mediated anti-angiogenesis in complementing the hypoxia-responsive drug delivery systems (DDSs) and could to valuable for the brisk development of more progressive antitumor therapeutics.

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Design and Synthesis of a New fluorescent TEMPO-FRIPS Reagent for Glycan Analysis

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Abstract

Glycans are very important because they are involved in various biological processes. There are many ways to analyze glycan, but mass spectrometry has been extensively used as a powerful tool because of its minimal sample consumption, high sensitivity, and short acquisition time. For glycan sequencing, linear or branched oligosaccharides are labelled with a mass tag reagent and analysed by positive-ion electrospray ionization with tandem mass spectrometry (ESI-MS/MS). Under low energy collision-induced dissociation (CID), the oligosaccharides provide fragments which have information about the glycan structure.

Free radical initiated peptide sequencing (FRIPS) produces the similar results obtained by electron capture dissociation (ECD) technique through collision induced dissociation (CID). The FRIPS demands introduction of a free-radical generation group into an analyte so that a radical species can be generated under CID conditions.

In our previous study, we have designed and synthesized a new tag reagent which is based on 2,2,6,6-tetramethylpiperidine-1-oxyl (TEMPO) radical. Furthermore, we have synthesized a tag reagent containing a new fluorescent structure in addition to the TEMPO moiety so that the mass tag allows FRIPS-MS analysis with easy detection ability during the chromatography.

Development of D-π-A Type Near-Infrared Probes for Diagnosis of Alzheimer's Disease

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Abstract

Alzheimer's disease (AD) is a neurodegenerative disorder, associated with aging, that gradually worsens over time and is characterized by dementia, disorientation, cognitive impairment, and irreversible memory decline. Clinical trial evidence shows that early recognition of cognitive impairment and clinical management at mild stages of AD delays the subsequent need for nursing home care. Consequently, it reduces the risk of misdiagnosis and inappropriate management.

Similar to protein fibrillogenesis, the formation and accumulation of amyloid-β (Aβ) plaques and tau aggregates in the brain are thought to be a critical pathological hallmark for early diagnosis of AD. Fluorescence imaging is an ideal method to detect these proteins due to its low cost, real time, and highly sensitive detection. During the past decade, several near-infrared (NIR) probes with diverse chemical structures have been designed to detect accumulation of proteins in the brain. However, their low specificity to Aβ or tau proteins was not suitable for clinical application. Therefore, the development of new near-infrared fluorescence probes targeting these protein aggregates selectively are needed for diagnosis of Alzheimer's disease, in particular, early disease progression.

In this presentation, we describe the synthesis of novel near-infrared fluorescence probes that selectively bind to Aβ and tau proteins. Based on our preliminary studies, we designed a series of compounds consisting of amino pyridine and dicyano indanes, which were synthesized by palladium-catalyzed Sonogashira coupling reactions and Knoevenagel condensations. Evaluation of the physicochemical properties of these probes and their biological efficacies against Aβ and tau proteins confirmed the possibility of their use as NIR fluorescent probes for early diagnosis of Alzheimer's diseases.

Ratiometric Two-Photon Probe for γ-Glutamyltransferase in Colon Cancer

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γ-Glutamyltransferase (GGT) is a cell-membrane-bound enzyme, which selectively hydrolyzes the cleavage of the γ-glutamyl bond in glutathione (GSH).[1] GGT has been shown to play an important role in cytoplasmic GSH and cysteine homeostasis involved in various physiological and pathological processes.[2] Actually, it has been discovered that overexpressed levels of GGT are connected with tumorigenesis in several human cancer cell, including ovarian and colon cancer.[3] Therefore, GGT has been recognized as a potential biomarker of malignant tumors.

In this respect, there is growing interest in fluorescent probes for GGT and various GGT activatable fluorescent probes have been developed for detection of GGT both in tumor cells and living animals.[4] However, only a handful of one-photon ratiometric fluorescent probe is known that is appropriate for biological imaging.

In this work, we developed a new ratiometric two-photon fluorescent probe for GGT by incorporating the γ-glu-substrate and benzothiazole fluorophore. This probe rapidly reacted with GGT and showed good selectivity for other biometabolites. Additionally, the probe showed a high quantum yield in physiological media, a marked shift of emission spectra, bright TPM imaging capability, and low cytotoxicity, thereby allowing sensitive analysis of GGT.

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H_2S_n Selective Two-Photon Fluorescence Probe for Parkinson's Disease

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Hydrogen polysulfide (H_2S_n, n>1) is primarily generated during the crosstalk between H_2S and reactive species (ROS and RNS) and it has received increasing attention in biochemical research.[1,2] H_2S_n is mostly generated in the mitochondria, and abnormal mitochondrial function and oxidative stress are directly related to many disorders including Parkinson's disease (PD).[3] Therefore, a marker that can directly observe mitochondrial H_2S_n could be used to implicate the abnormal mitochondrial function observed in many diseases.

A lot 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 selective probe, we observed mitochondrial H_2S_n is generated more in PD neuron than in normal neuron.

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Two-Photon Probe for Detection of Extracellular pH in Colon Cancer

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An imbalance of pH in tissues is directly linked to diseases such as cancer, renal failure, and ischemia.[1] The extracellular pH (pHe) of a cancer tissue is acidic while the intracellular pH (pHi) is basic in comparison to normal tissue,[2] as the buffering capacity of cancer tissues is decreased, and the production of lactic acid owing to the hypoxia is increased.[3] The acidified pHe could lead to various disorders such as tumor invasion, cancer metastasis, an increased rate of mutation, and a resistance to drugs.[4,5] Therefore, a pHe measurement is needed to specify the site of tumor invasion as well as for cancer diagnosis.

In this study, for an effective and accurate pHe analysis in cancer tissues, we designed two-photon probes (XBH1−3) to meet the following requirements: (i) the introduction of polar solubilizing units to stain the extracellular region, (ii) significant two-photon (TP) brightness along with emission color changes upon pH variations, and (iii) an appropriate pKa value for the pHe range of cancer tissues (6.0−7.0). These probes, based on benzimidazole and polar solubilizing groups, exhibited a strong two-photon-induced fluorescence and sensitive blue-to-green emission color changes with pKa values of 5.1−5.7. XBH1, containing a carboxylic acid, stained the extracellular region in neutral media; it entered the cell under acidic media, thereby allowing a precise measurement of the extra- and intra-cellular pH values in the acidified tissue. XBH2, containing the sulfonate peripheral unit, facilitated the monitoring of the pHe value only. Ratiometric TPM imaging revealed that the XBH1 labeling method can be used to directly monitor the pH values both inside and outside the cells in a colon cancer tissue; there is also the morphological aspect. This could be useful in the analysis of cancer-related diseases and drug development.

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Evaluation of Cell-Penetrating Ability of Bicyclic Peptoids

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Peptoids, oligomers of N-substituted glycines, are an attractive class of peptidomimetics with several desirable features such as ease of synthesis and proteolytic stability. Notably, it is well known that peptoids have better membrane permeability than native peptides. However, peptoids generally have relatively flexible structures, making it challenging for targeting intracellular proteins with high affinity and specificity. Macrocyclization has emerged as one strategy to solve these kinds of limitations. Macrocyclic peptoids are expected to have relatively rigid and preorganized structures compared to their linear counterparts, allowing them to bind more tightly to target proteins without major entropy penalty. Indeed, we recently demonstrated that monocyclic peptoids have better cell permeability compared to linear peptoids.[1] In addition, we previously developed highly efficient cyclization method for bicyclic peptoids which are expected to have improved conformational rigidity.[2] However, while the cell permeability of monocyclic peptoids was studied, that of bicyclic peptoids has not been explored yet.

Herein, we evaluated the cell permeability of bicyclic peptoids through a systematic investigation method for cell penetration. Halotag-labeled linear and bicyclic peptoids were synthesized priorly, and their penetration was monitered by confocal microscopy and FACS analysis. As expected, bicyclic peptoids showed highly improved membrane permeability than their linear counterparts indicating that they will serve as potential protein capture agents given their excellent cell permeability in addition to their conformational rigidity and proteolytic stability.

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Dual drug employed theranostic small molecule with selective cancer targeting for enhanced anticancer effect

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We reported the binary drug conjugated first small-molecule-based prodrug binary drug delivery system (BDDS) for the administration of two drugs (SN-38 and 5′-DFUR) in cancer cells. BDDS has a selective response to H_2O_2, over other bioanalytes. Due to conjugation with the IMC guiding unit, BDDS-specific uptake occurred with MIA Paca-2 cells [COX-2 (+ve)] over Caco-2 [COX-2 (−ve)] cells.[1] The cell viability assay explored that BDDS exhibited a significance effect on cancer-specific cell lines compared to SDDS, due to the synergistic effect of two drugs, SN-38 and 5′-DFUR, conjugated in BDDS. Hence, we expect it will offer a potential tool for small-molecule-based cancer specific multidrug-related combinational therapeutic approaches.

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Cancer-specific hNQO1-responsive fluorescent Off-On naphthalimides employed for imaging hNQO1 activity in living cells

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Human NAD(P)H:quinone oxidoreductase 1 (hNQO1) is a cancer-specific biomarker, which is overexpressed in cancer cells and also associated with a drug resistance factor of cancer. Herein, we presented hNQO1-responsive fluorescent Off-On naphthalimides **1** and **2** that could be employed for imaging hNQO1 activity in living cancer cells. Upon the presence of hNQO1 activity, the naphthalimides gave rise to a strong fluorescence Off-On change at 540 nm. In hNQO1-positive A549 cells, the naphthalimides showed a strong fluorescence image through a hNQO1-mediated enzymatic reaction, in contrast to hNQO1-negative H596 cells and hNQO1 inhibitor-pretreated A549 cells. We could propose that naphthalimides **1** and **2** can be used for a real-time monitoring of hNQO1 activity in living cancer cells.

Poly(2-oxazoline) based Smart Hydrogel for Multifunctional Stimuli-responsive Phase Transition

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Stimuli-responsive materials, which can respond to environmental stimuli such as temperature, pH, and electric fields, have attracted tremendous attention in various applications, including soft robotics, smart actuators and vehicles for drug delivery.[1-3] As an important class of soft materials, hydrogels particularly comprise stimuli-responsive components and can change their physical characteristics such as shape, transmittance or color under the influence of specific stimuli. Poly(2-alkyl-2-oxazoline)-based thermo-responsive hydrogels (**G-POx**s) containing methacrylate groups capable of photopolymerization was designed. **G-POx** with temperature-responsive properties of oxazoline undergoes a phase change at the lower critical solution temperature (LCST), which causes the hydrogel to change its volume accordingly. **G-POx** also contains a 4,4'-bipyridyl (viologen) unit, so the color changes from colorless to violet as the redox state changes. Using the swelling volume changes, thermo-responsive actuation have been achieved by combination of two differernt **G-POx**s having different LCST. Similarly, the shape of the hydrogel is also changed because the thermal transition temperature is changed as the redox state is changed. Such hydrogel actuators may provide new insights for the design and fabrication of intelligent soft materials.

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Regioisomeric Mixtures of Metal-Organic Frameworks

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The organic chemical handles in metal-organic frameworks (MOFs) could be installed through pre-functionalization on ligands. Various functional groups such as amino, nitro, halo, hydroxy, and additional aromatic rings have been successfully incorporated into MOFs. In case of the functional group has reactivity in the solvothermal synthetic conditions, and/or coordinating ability to metal cation, the post-synthetic modification (PSM) has been introduced. The target functionalities could be installed through solid state functionalization after MOF formation. Although, both pre-functionalization and PSM open up the various functionalization on MOFs, still the single functional group-containing MOFs are mainly studied in this field. Recently, we have successfully prepared several bifunctional MOFs with two chemical handles. The possible combinations from NH_2, NO_2, OMe, and Cl functionalities had been attempted, and only NH_2-NH_2 combination was failed to achieve MOF synthesis. Interestingly, the structural flexibility of MOFs was totally altered by the positional changes of MOFs, i.e., the functional group regioisomerism is directly related with the structural flexibility.[1-3]
Herein, our recent study for the regioisomeric mixture for MOF synthesis will be presented. Two regioisomeric ligands, BDC-2,3-$(OMe)_2$ and BDC-2,5-$(OMe)_2$ (BDC = benzene-1,4-dicarboxylic acid) were selected and ratio-controlled mixture of ligands were applied to solvothermal synthesis of MOFs. This solid, regioisomeric mixture of MOFs will allow the key information of MOF flexibility and fine-tuning of this organic/inorganic hybrid materials.

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Functional Group Controls in Metal-Organic Frameworks-Mixed Matrix Membranes (MOFs-MMMs)

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Metal-organic frameworks (MOFs) are crystalline three-dimensional porous materials, which is consisted of coordinating organic ligand and metal clusters. MOFs are interesting and emerging materials for a variety of applications such as molecular separation, molecular storage, sensors and catalysis based on their unique structural and functional conformation along with permanent porosity. However, the fragile character from their crystalline or powdery nature limits its precise application in a practical point of view. To address this handling problem on applications, the composite synthesis of MOFs with mixed matrix membranes (MMM) has been extensively studied. Recently we have introduced thiol-ene photo-click chemistry for covalently cross-linked MOF-MMM synthesis. This photo-click strategy allows a high MOF load (up to 60 wt%) without particle aggregation.[1]
In this presentation, we will present the additional functional group controls on MOF-MMM materials. Starting from the functionalized MOFs such as UiO-66-NH_2, UiO-66-NO_2, and UiO-66-Naph, the thiol-ene photo-click chemistry was successfully performed for fabrication of functionalized MOFs with MMM. The preparation of materials along with characterization will be discussed during the presentation.

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Installation of *o*-Carborane Cage to Metal-Organic Frameworks

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The general icosahedral carborane is $C_2B_{10}H_{12}$ cage type molecule, and it shows high thermal stability and chemical resistance, unique geometry and photochemical properties. Carboranes are utilized in a variety application such as heat-resistant polymers, catalysis, recovery of heavy metals from solution, and medical applications. In addition, the photochemical and electrochemical applications have been widely studied since the carborane cage has electron-deficient properties and affects the π-conjugation emission characteristics.[1,2]
Metal-Organic Frameworks (MOFs) are three-dimensional porous crystalline materials, which are consisted of metal clusters and multitopic organic ligands. Since MOFs are generally synthesized from solvothermal condition and shows structural rigidity, the introduction of carboranes into MOFs have been attempted by several research teams. Particularly, the benzene rings on MOF's ligand were replaced with carborane cages.[3-6] In this presentation, we will discuss our recent result about the synthesis of o-carborane-functionalized MOFs. The *o*-carborane-functionalized benzene-1,4-dicarboxylic acid ligand could be prepared from the phenyl acetylene moiety, and Zr-based UiO-66 was mainly attempted for this study. The detail synthetic procedures along with characterization data will be presented.

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Color Tuning of Metal-Organic Frameworks using Azo Compounds

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Metal-Organic Frameworks (MOFs, or PCPs, Porous Coordination Polymers) are three-dimensional porous crystalline materials, which are consisted of metal clusters and multitopic organic ligands such as bipyridyl or benzene dicarboxylic acids. Various applications such as gas storage, molecular separation, molecular delivery, and catalysis have been extensively studied using their unique porosity along with structural and chemical diversity.[1-2] Although the structural derivatization and functional group controls have been widely studied, the fundamental properties of MOFs such as morphology and color of crystals are still depending on the combination of metals and ligands.
Herein, we will present our recent efforts for color changes of MOFs using Azo compounds. Azo compounds have N=N bonds and generally shows unique colors from red to purple. The color of azo compound could be controlled by coupling partner for azo coupling reaction. We have prepared several azo compounds with dicarboxylic acids, and applied them to MOF synthesis. The detail synthetic procedures for azo-containing dicarboxylic acids along with characterization of MOFs will be discussed.

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A Cryptocyanine-Based Mitochondria-Targeted Photothermogenic Photosensitizer

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Cryptocyanine-based probes exhibit highly efficient photothermal conversion and represent a new class of photothermal agents for use in photothermal therapy (PTT). With the thermal susceptibility of mitochondria in mind, we have prepared a mitochondriatargeted, NIR-absorbing cryptocyanine probe (Mito-CCy) and evaluated its photophysical properties, photothermal conversion efficiency, biological compatibility, cytotoxicity, and mitochondrial localization in HeLa cells. Upon subjecting 0.5 mL of a PBS buffer solution (10 mM, pH 7.4, containing 50% DMSO) of Mito-CCy (0.5 mM) to 730 nm laser irradiation at 2.3 W/cm2, the temperature of the solution increased by 13.5 °C within 5 min. In contrast, the corresponding cryptocyanine (CCy) lacking the triarylphosphonium group gave rise to only an ~3.4 °C increase in solution temperature under otherwise identical conditions. Mito-CCy also exhibited high cytotoxicity in HeLa cells when subject to photoirradiation. This light-induced cytotoxicity is attributed to the endogenous production of reactive oxygen species (ROS) induced under conditions of local heating. ROS are known to interfere with the mitochondrial defense system and to trigger apoptosis. By targeting the mitochondria, the present sensitizer-based photothermogenic approach is rendered more effective. As such, the system reported here represents the vanguard of what might be a new generation of organelle-targeted photothermal therapeutics.

Zwitterionic Polymer Grafting by ARGET-ATRP using Ascorbic acid as a Reducing Agent

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In the medical industries, non-specific adsorption of proteins and bacteria on the surface is recognized as a problem to be solved.[1,3] For example, biofilm made from a pile of proteins and bacteria on the surface of medical tools can cause infection for hospitalized patients. As a strategy to solve the problems, we aim to develop an efficient antifouling coating. Sulfobetaine zwitterionic polymers were grafted on silicon dioxide (Si/SiO_2) via the process, *activators regenerated by electron transfer for atom transfer radical polymerization* (ARGET-ATRP)[2], using ascorbic acid as a reducing agent. The successful polymer grafting was characterized by ellipsometry and contact angle goniometry. We used 3-(methacryloylamino)propyl)-dimethyl(3-sulfopropyl)ammoniumhydroxide (MPDSAH)[4], as a zwitterionic monomer, which was reported to have antifouling effect when it is polymerized. The zwitterionic polymer can inhibit non-specific adsorption of proteins and bacteria by forming a thermodynamically stable hydration layer onto a surface. We examined the polymerization by measuring Cu^+ concentration in the reaction solution with UV-visible spectroscopy.[5] The degree of poly(MPDSAH) grafting onto Si/SiO_2 substrates was controlled over time. The optimal grafting condition was applicable to the environment where the reaction system was completely opened to air, showing that the polymerization system is oxygen-tolerant.

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Synthesis of Ergostenol, Cholestenol, Cholestenol amine and Their Hydrophilic Analogs as Anti-inflammatory Agents

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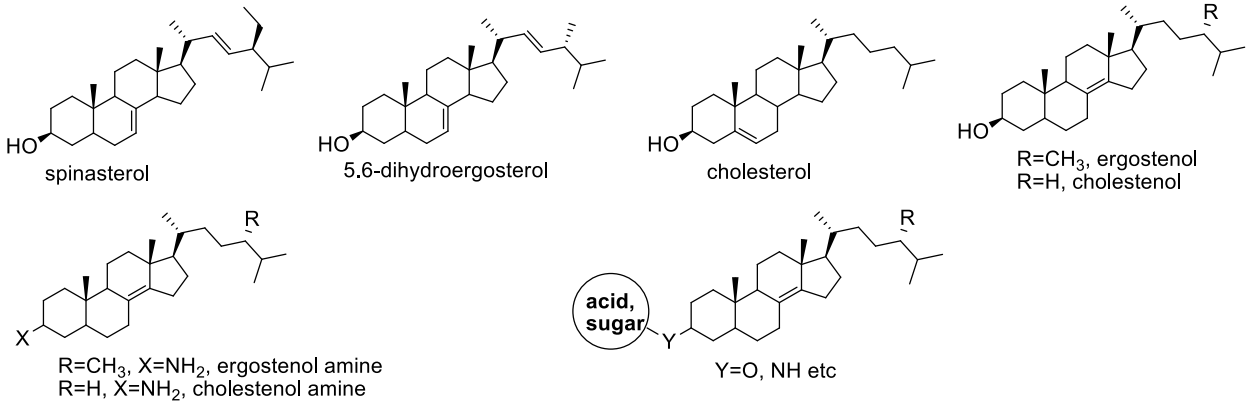
Natural spinasterol-glucose (3-O-β-D-glucopyanosylspinasterol) isolated from *Stewartia koreana* leaves was identified as a potent anti-inflammatory compound. [1-2] However, since the steroidal backbone cannot be easily obtained, we have developed 5,6-dihydroergosterol and $\Delta^{8(14)}$-ergostenol as new steroidal scaffolds that can be used instead of spinasterol, and studied the synthesis of their glycoside derivatives and their anti-inflammatory activity.

Recently we have found a new sterol, cholestenol (cholest-8(14)-en-3-ol) from 7-dehydrocholesterol, which is a regioisomer of cholesterol. Pd-catalyzed hydrogenation and subsequent allyllic isomerization of 7-dehydrocholesterol provides $\Delta^{8(14)}$-cholestenol [3]. Also, cholestenol azide was prepared by Mitsunobu reaction of cholestenol and the subsequent reduction gave cholestenol amine. We have synthesized some hydrophilic ergostenol and cholestenol derivatives combined with sugars or acids. These derivatives showed strong anti-inflammatory activity.



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Development of Azo-Based Turn-On Chemical Array System for Hydrazine Detection with Fluorescence Pattern Analysis

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Hydrazine is consisted with two nucleophilic nitrogen atoms as a chemical structure of N_2H_4, used as rocket fuel and synthesis of textile dyes, pharmaceuticals and pesticides. Although it is widely used in industry, hydrazine is carcinogenic and harmful to liver, kidneys and central nervous system. Consequently, spectrophotometric, titrimetric, voltammetric and chromatographic methods have been used to detect hydrazine, however, these methods have several drawbacks. To overcome limitation of conventional hydrazine detection methods, a facile turn-on chemical sensor array was developed for hydrazine detection by means of fluorescence pattern recognition. Taking advantage of the unique properties of the azo group, four different fluorogenic probes, SF-Azo 01–04, were designed and prepared. SF-Azo 01–04 displayed fluorescence enhancement of up to 800-fold upon reaction with hydrazine, and all probes exhibited excellent selectivity in the presence of various anions and nucleophiles. By employing the probes in a cellulose-paper-based array system, the hydrazine concentration was successfully determined by monitoring the change in fluorescent patterns.

Identification of Stapled Peptide Inhibitor of the GSK3β/Axin Protein-Protein Interaction

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Glycogen synthase kinase 3β (GSK3β) is a serine/threonine kinase that plays central roles in a diverse range of signaling pathways such as insulin, growth factor and Wnt signalling pathways. In Wnt signalling, GSK3β is recruited to a multiprotein complex through interaction with Axin in the absent of Wnt ligand, where it phosphorylates β-catenin, making it for ubiquitination and destruction. This canonical Wnt signalling engages tumour cell differentiation and tissue-invasive activity through an Axin2-dependent pathway that stabilizes the Snail1 zinc-transcription factor. Thus, developing a chemical modulator for controlling the function of Axin2 by inhibition of its binding partnet, GSK3β, can be a important therapeutic strategy for blocking invasive activity of tumor cell.

In this regard, we developed hydrocarbon-stapled peptide inhibitors for the GSK3β/Axin protein-protein interaction based on the co-crystal structure of GSK3β/Axin.[1] We confirmed that our novel stapled peptide inhibitor shows better cell pemeabillity and α-helical propensity than linear unstapled peptide. Expectedly, this stapled peptide decreased the level of Axin2 and Snail and showed suppression of invasive activity of tumor cell.

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Detection of chiral carboxylates using a naphthoimidazolium-cholesterol derivative as a ratiometric fluorescence based chemosensor

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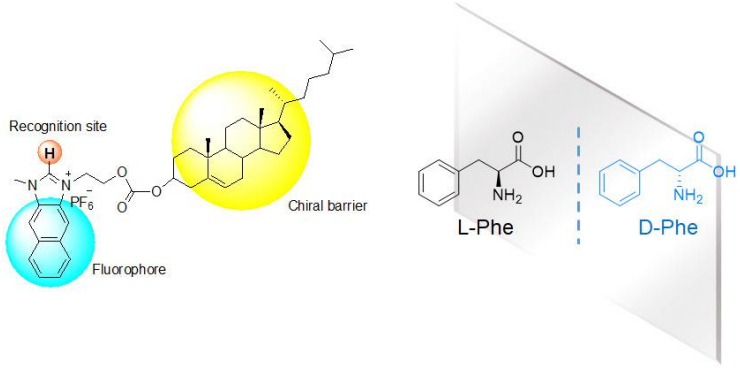
Fluorescence chemosensors to sense chiral molecules have been actively studied in recent years. In the current study, we report naphthoimidazolium-cholesterol derivative (NI-chol 1) as a fluorescence based chemosensor for chiral recognition, in which naphthoimidazolium serves not only as fluorophore but also as a recognition moiety for anions via imidazolium $(C\text{-}H)^{+}$--anion binding and the cholesterol unit acts as a chiral barrier. In particular, NI-chol 1 displayed unique and distinct ratiometric changes with Boc-D-Phe, on the other hand, Boc-L-Phe induced a negligible change. Furthermore, distinct downfield shift (from 9.64 ppm to 9.96 ppm) of the imidazolium C-H peak were observed for Boc-D-Phe (5 eq.) with severe broadening, which indicates strong ionic hydrogen bonding between the C-H proton and carboxylate.



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Aromatic Hybrid Foldamers Capable of Folding to Single and Double Helices

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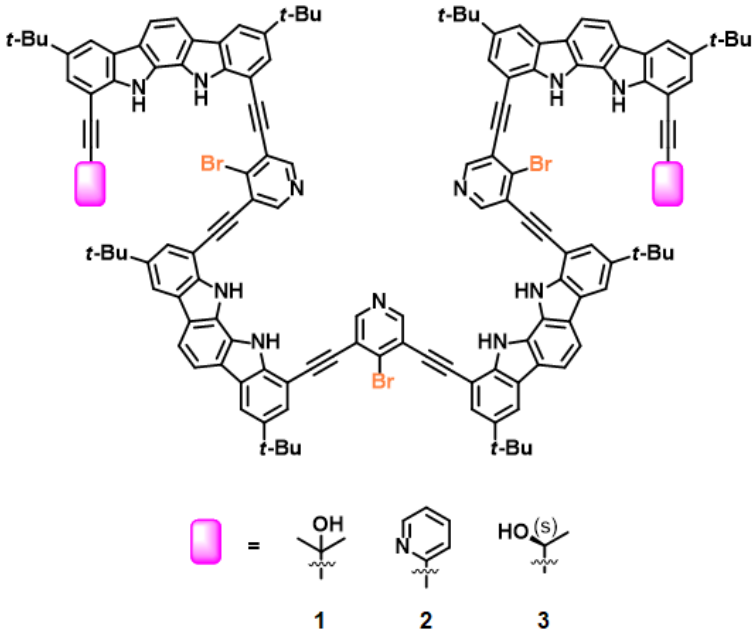
Recently, we have demonstrated that indolocarbazole-pyridine (IP) oligomers fold into a helical structure with an internal cavity and three water molecules are occupied in the internal cavity of IP heptamer.[1] Herein, we prepared new aromatic hybrid foldamers **1**–**3** that contained 4-bromopyridine subunits and can fold to helical conformations by intramolecular NH···Br···HN interactions. The three foldamers have different groups at the ends of the strands, dimethylcarbinol in **1**, 2-pyridine in **2** and (*S*)-methylcarbinol in **3**, that may control the stability and orientation of the helices. It has been demonstrated that the folding structures and aggregation states of the foldamers strongly depend on the polarity of the solvent and temperature. Details including synthesis and spectroscopic properties will be described in the presentation.



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β-Oxidation of Ynamides into *N,O*-Acetals by *m*CPBA: Application in Enantioselective Intermolecular Trans-Acetalization

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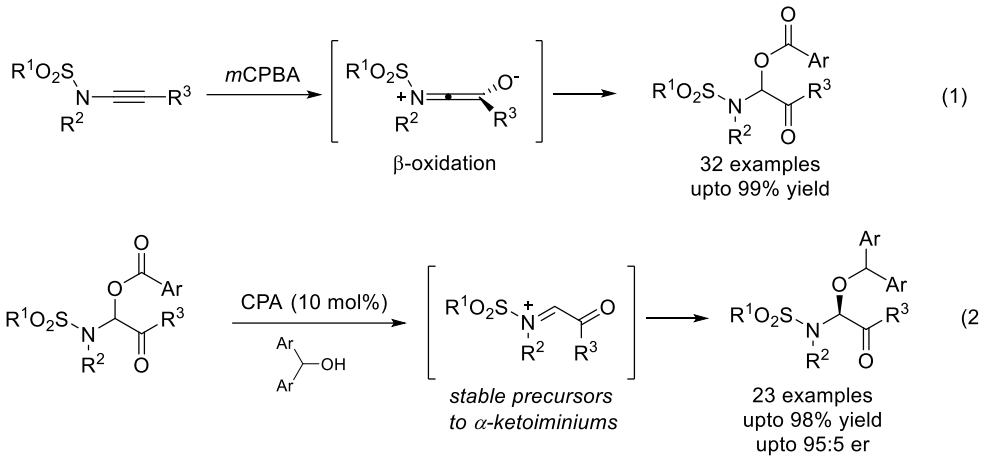
Ynamides are one of the most versatile building blocks in organic synthesis.[1] Recently, our group reported that pyridine-*N*-oxides or sulfoxides can oxidize ynamides at the α-position in the presence of Brønsted acid.[2] Given the success of this work, we further investigated the effects of stronger oxidants for ynamide oxidation. Interestingly, with *m*-CPBA as an oxidant, we observed the formation of *N,O*-acetals, which is thought to form via β-oxidation of ynamides (Eq. 1). Furthermore, we found that the initial *N,O*-acetal underwent an enantioselective intermolecular trans-acetalization in the presence of chiral phosphoric acid, forming enantio-enriched *N,O*-acetals (Eq. 2). While most chiral acetals are synthesized from the protonation of imines, this trans-acetalization protocol is unprecedented. The products *N,O*-acetals were configurationally stable and can be potentially useful synthetic intermediates to diols and amino alcohols.[3]



Scheme 1. β-Oxidation of ynamide followed by enantioselective trans-acetalization

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Macrocyclization of α-ABpeptoids and Conformational Studies

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Peptidomimetics foldamers that fold into well-defined conformations and incorporate diverse proteogenic and nonproteogenic side chains would be attractive alternatives to native peptides due to their proteolytic resistance.[1] For a decade, many efforts have been made to developed diverse peptidomimetic foldamers. Among them, peptoids are a class of peptidomimetics based on N-alkylated glycines. They can be easily synthesized by solid-phase method, and have better cell permeability than native peptides and great potential to interrogate protein functions and therapeutic candidates. However, peptoids are relatively flexible and have difficulty in forming the folding structures because of the lack of backbone chirality.

To address these limitations, we previously reported α-ABpeptoids (α-alkyl beta-peptoids) by inserting chiral methyl groups on carbonyl α-position.[2] Although the CD spectra of α-ABpeptoids with various side chains showed folding conformations, their crystal structures have not been revealed yet.[3] Macrocyclization is one of promising strategies to enhance conformational rigidity, therefore, it is considered that the possibility of forming crystal structures may be increased. Synthesized linear α-ABpeptoids in different lengths were macrocyclized and they have a characteristic CD spectra. Finally, the structure of cyclic α-ABpeptoids was solved through X-ray crystallography. It is the first time to confirm X-ray crystal structure of α-ABpeptoids.

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Lysosome Targeting Photodynamic Therapeutic Iridium complexes

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Iridium complexes with high biocompatibility under dark condition and effective cancer cell suppression via reactive oxygen species generation were synthesized and characterized. Basic photophysical properties were analyzed and in vitro cell tests were performed via MTT assay. Also, target motion of iridium series were investigated by confocal microscopy.

A selective fluorometric and colorimetric chemosensor based on conjugated polydiacetylenes for detection of Cd^{2+}

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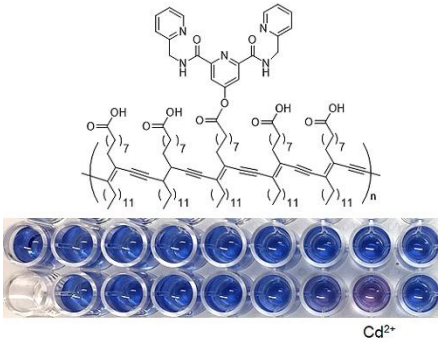
In recent years, pollution associated with the presence of heavy metal ions in the environment has been extensively investigated. Among the various heavy metal ions, cadmium (Ⅱ), is one of the most hazardous and carcinogenic metals, because of its widespread use in fields such as metal alloys, electroplating, stains, fertilizers, as well as in rechargeable batteries. As a result, a number of analytical techniques have been developed to detect Cd^{2+}, including atomic absorption spectrometry (AAS), inductively coupled plasma mass spectrometry (ICP-MS), fluorescent sensors and colorimetric assays. However, the application of these methods is restricted due to the complexity of sample preparation and instrumentation. Therefore, a rapid and convenient detection method for Cd^{2+} is imperative. In this regard, we present our findings involving the development of a simple and cost-effective sensor for naked-eye detection of Cd^{2+} that does not require an external power source.

Polydiacetylenes (PDAs) have received increasing attention as smart materials owing to their unique properties [1-3]. Upon addition of various stimuli, the blue PDAs can undergo a colorimetric transition from blue to red along with a change from non-fluorescent to fluorescent. The optical changes can be readily detected using the naked eye and by absorption and fluroescence spectrometers. These properties make PDAs excellent materials for use in platforms for sensing chemical or biological targets. In recent years, the number of biosensors and chemosensors based on the optical responses of polydiacetylenes have been reported. According to the approaches of inducing acceptors into a polymer matrix and the mechanism of optical changes, this context will comprehensively summarize the recent work on both biosensors and chemosensors based on the polydiacetylene platform.



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Ru−Catalyzed Deoxygenative Regioselective C8−H Arylation of Quinoline *N*−Oxides

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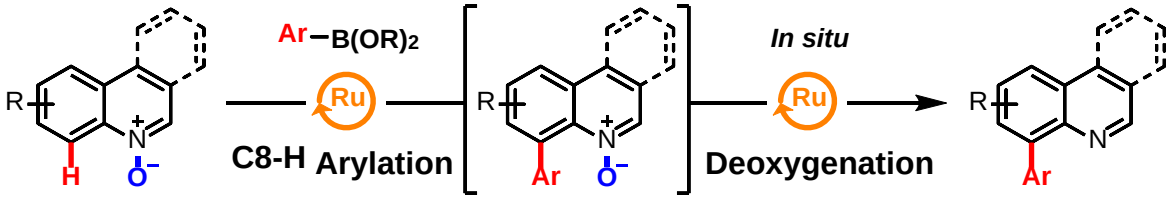
Quinoline is present in a broad range of natural and pharmaceutical compounds,[1] thus regioselective C−H functionalization on quinolines is of high interest to lead to value-added products.[2] Synthesis of quinoline derivatives via site-specific C−H bond activation has been scrutinized in recent years, albeit with limited substrate scope.[3] An alternative approach is to utilize quinoline *N*−oxides as the substrates, where *N*-oxide serves as an effective directing group to lead to the regioselective C−H bond activation.[4] In these procedures, an additional deoxygenation step is often required after the installation of the desired functional groups.[5]

Herein, we present the first example of Ru-catalyzed deoxygenative C8−H arylation of quinoline *N*-oxides by using arylboronic esters. (p-Cymene)Ru^{II} was found to effectively catalyze both C−H arylation and subsequent deoxygenation. The reaction is featured to display broad substrate scope and high functional group compatibility under mild conditions. Mechanistic studies revealed that it proceeds in a tandem process of arylation and then deoxygenation, wherein both steps were found to be catalytic with the ruthenium species.



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[5] (a) Aoyagi, Y.; Abe, T.; Ohta, A. *Synthesis* **1997**, *1997*, 891-894. (b) Singh, S. K.; Srinivasa Reddy, M.; Mangle, M.; Ravi Ganesh, K. *Tetrahedron* **2007**, *63*, 126-130. (c) Gupta, S.; Sureshbabu, P.; Singh, A. K.; Sabiah, S.; Kandasamy, J. *Tetrahedron Lett.* **2017**, *58*, 909-913.

A resorufin-based fluorescent turn-on probe responsive to nitroreductase activity and its application to bacterial detection

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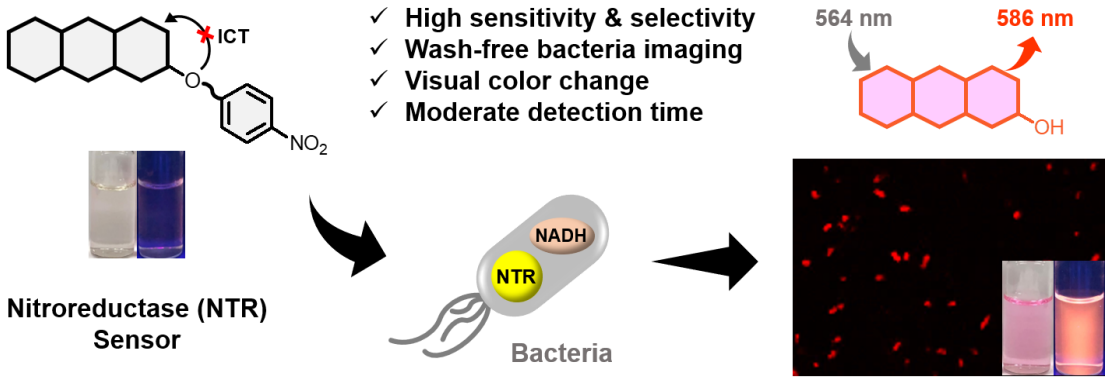
We present two resorufin-based fluorescent turn-on probes responsive to nitroreductase (NTR) activity (NTR probes **1** and **2**) and their use toward the detection of bacteria. The probes exhibit a fluorescence turn-on at 586 nm in response to NTR activity, which corresponds to a vivid pink color. These optical changes are based on the NTR-mediated reduction of the nitro groups in the probes, which results in the production of highly fluorescent resorufin. The detection ability, mechanism, and enzyme kinetics of the probes for NTR activity have been thoroughly investigated. The enzyme efficiencies of the probes were superior to those previously reported. In addition, NTR probe **1** exhibited an excellent detection ability for NTR with high selectivity and no background signal when compared to **2**. Moreover, NTR probe **1** was applicable for bacterial detection using a wash-free process because it gave rise to a fluorescence turn-on signal in response to bacterial NTR activity.



TCI · 세진시아이	LabNetwork with 대정화금(주)
ThermoFisher SCIENTIFIC	BRUKER
vacuubrand (주)수림교역 Vacuum Pump, Vacuum Controller	CENGAGE
영인크로매스 YOUNG IN Chromass	자유아카데미 상상아카데미 생각의힘
LG화학	(주) 이 우 과 학 교 역 IWOO Scientific Corporation

Biotage	LCB LegoChemBio
TORAY 도레이첨단소재	한국화합물은행 Korea Chemical Bank
BK Instruments Inc.	CAS® A DIVISION OF THE AMERICAN CHEMICAL SOCIETY
VORONOI / VORONOI BIO / B2S BIO	ALTOSS Analytic Total Solutions
Intocell into practice	Chong Kun Dang Pharm. Seoul, Korea
YONSUNG Fine Chemicals	

다차원 유기소재 연구단

Center for Multidimensional Organic Materials

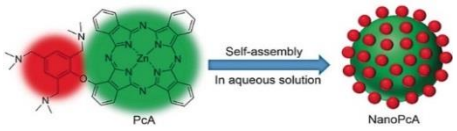
윤주영

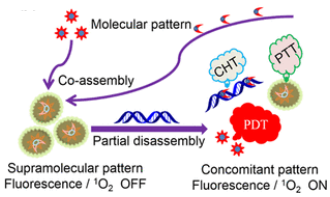
Office : 82-2-3277-2400, E-mail : jyoon@ewha.ac.kr
Homepage : home.ewha.ac.kr/~jyoon

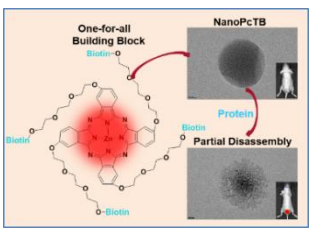
이화여대 다차원 유기소재 연구단(단장 윤주영)은 다양한 analyte에 대한 형광 이미징 프로브 및 화학센서를 개발하고 있다. 특정 표적을 인식하는 물질과 형광체를 결합하여 생체 내 이미징, 표적지향 약물전달 및 광열·광역학 치료가 가능한 물질을 개발하고, 새로운 다차원 의약 전달 및 광열·광역학 치료 시스템 연구를 활발히 진행하고 있다.

광열/ 광역학 치료제 개발

단일 화합물이 광역학 암 치료제 및 이미징 프로브 등의 다양한 역할을 수행하는 다기능 단일 분자 (“one-for-all”)를 개발하여 발표

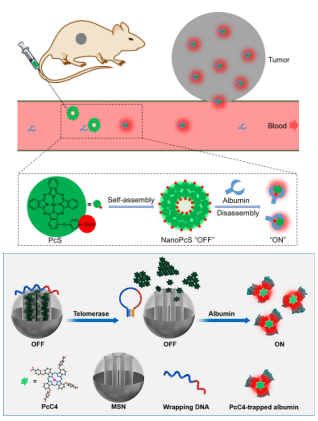






Angew. Chem. Int. Ed. **2018,** *57*, 9885.
ACS Nano **2018**, *12,* 681.
J. Am. Chem. Soc. **2017**, *139* , 10880.

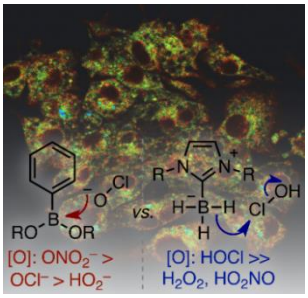
Albumin 감지와 암 치료가 동시에 가능한 switchable nanotheranostic 제시

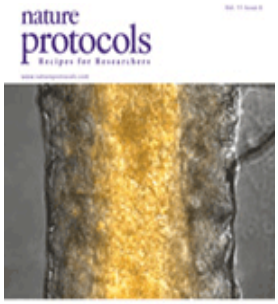


J. Am. Chem. Soc. **2019**, *141*, 1366.
ACS Nano **2019**, *13*, 6702.

생체 내 주요물질 감지

활성산소종 (reactive oxygen species), biothiols 및 금속 이온 등에 선택적인 형광 프로브 연구

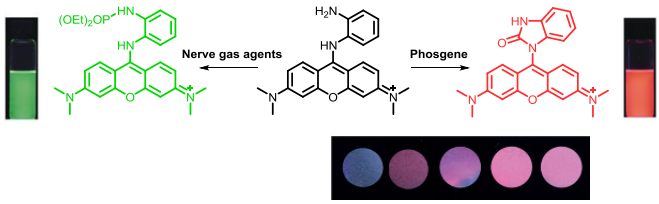




Angew. Chem. Int. Ed. **2018**, *57,* 1567.
Chem. **2018**, *4,* 1609.
Chem. Soc. Rev. **2018**, 47, 6900.
Angew. Chem. Int. Ed. **2017**, *56,* 5812.
Nat. Protoc. **2016**, *11*, 1219.

기능성 유기소재 개발

포스젠 가스를 색 또는 형광 변화로 검출할 수 있는 방법 제시



Angew. Chem. Int. Ed. **2016**, *55*, 4729.
ACS Appl. Mater. Interfaces **2016**, *8*, 22246.

http://cmca.kaist.ac.kr

멀티스케일 카이랄 구조체 연구센터
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 자기조립을 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.

제 1그룹
멀티스케일 카이랄성의 발현 및 상호전이원리 연구

이희승 (KAIST) | 김우연 (KAIST) | 이윤호 (KAIST) | 이해신 (KAIST)

제 2그룹
외부자극 기반 멀티스케일 카이랄성 유도

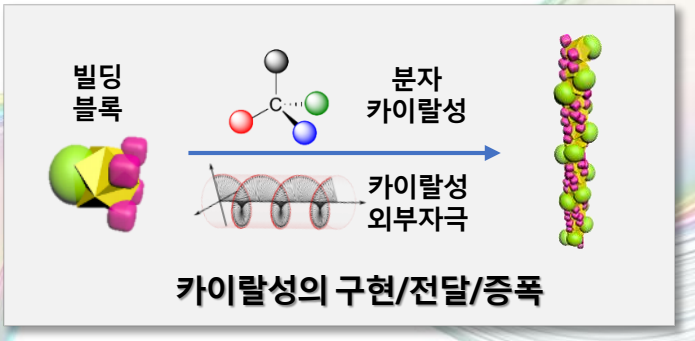
옥강민 (서강대) | 서명은 (KAIST) | 윤동기 (KAIST) | 한상우 (KAIST)

제 3그룹
멀티스케일 카이랄성을 이용한 입체선택성 전이 및 증폭

송현준 (KAIST) | 김병수 (연세대) | 한순규 (KAIST)

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



비대칭반응 촉매

능동형 광학재료

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

KAIST | 연세대학교 YONSEI UNIVERSITY | 서강대학교 SOGANG UNIVERSITY | 과학기술정보통신부 | NRF

細胞被包化 연구단
Center for Cell- Encapsulation Research

KAIST CHEMISTRY

Prof. Insung S. Choi
Department of Chemistry, KAIST

Office | 042) 350-2840
Lab | 042) 350-2880
E-mail | ischoi@kaist.ac.kr
Homepage | http://cisgroup.kaist.ac.kr

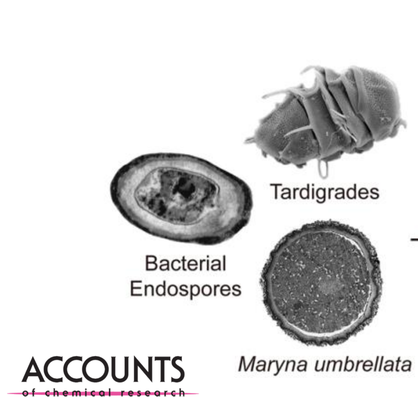
Post-doc (1); Researchers (4); Students (9); Staff (1)

JOB OPENING: POST-DOCS

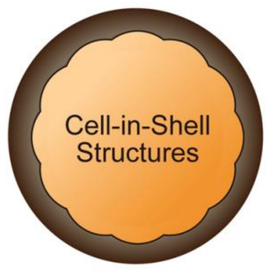
- *PHYSICAL ORGANIC CHEMISTS WITH CODING ABILITY*
- *COMPUTATIONAL CHEMISTS*
- *COMPUTER SCIENTISTS WITH INTEREST IN ORGANIC CHEMISTRY*
- *MOTIVATED PERSONS WITH MACHINE-LEARNING BACKGROUND*

Recent Work

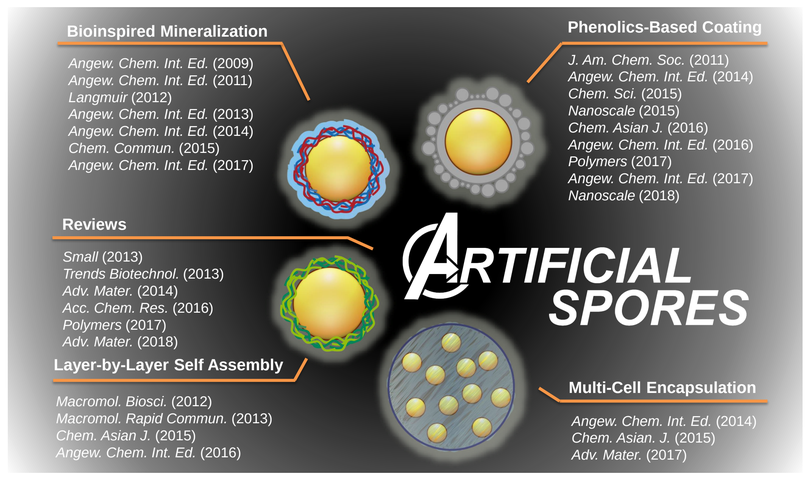
Cytospace: Cytointerfacial Chemistry



(a) *Concept Inspired by* *Cryptobiotic States*



(b) *Strategies Inspired by* *Natural Processes*



What is good about single-cell nanoencapsulation?

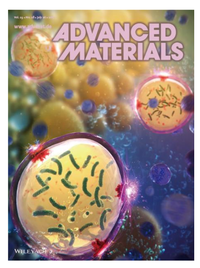
- ***Mechanical/Physical Stability:*** *Physical Protection*
- ***Selective Permeability:***
  Maintenance of Cell Viability (Gases, Nutrients, Etc.)
  Chemical/Biological Protection
- ***Controlled Degradability:***
  Stimulus-Responsive Shell-Degradation
  → *Chemically Controlled "Germination" of "Artificial Spores"*
- ***Chemical Functionalizability:*** *towards Applications*

2016

2016

2017

2017

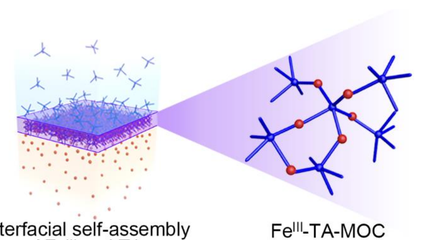


2018

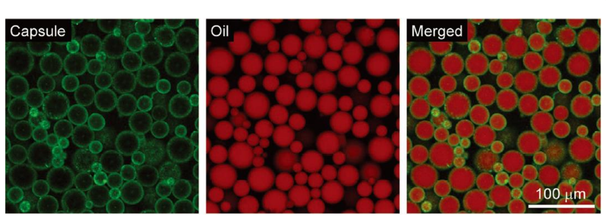
2018

2019

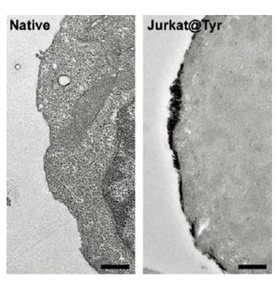
Interfacial Chemistry



Formation of Fe(III)-tannic acid complex at interface



Oil-water interfacial complex formation

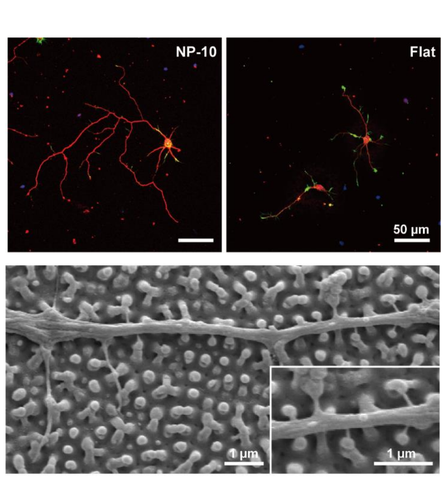


Enzymatic phenolic amine polymerization

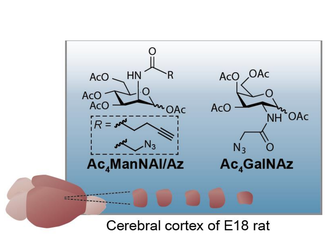
Publications

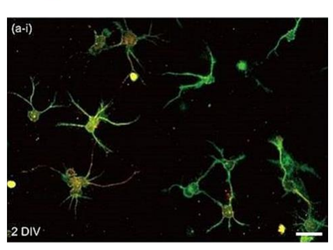
Chem. Commun. (2019)
Adv. Mater. (2018)
Langmuir (2018)
Nanoscale (2018)
Sci. Rep. (2017)
Adv. Mater. (2017)
Chem. Asian J. (2015)
Angew. Chem. Int. Ed. (2014)

Neurochemistry



Acceleration of axon development on the nanopillar structure





Metabolic labeling of sialic acids during development of cerebral neurons

Publications

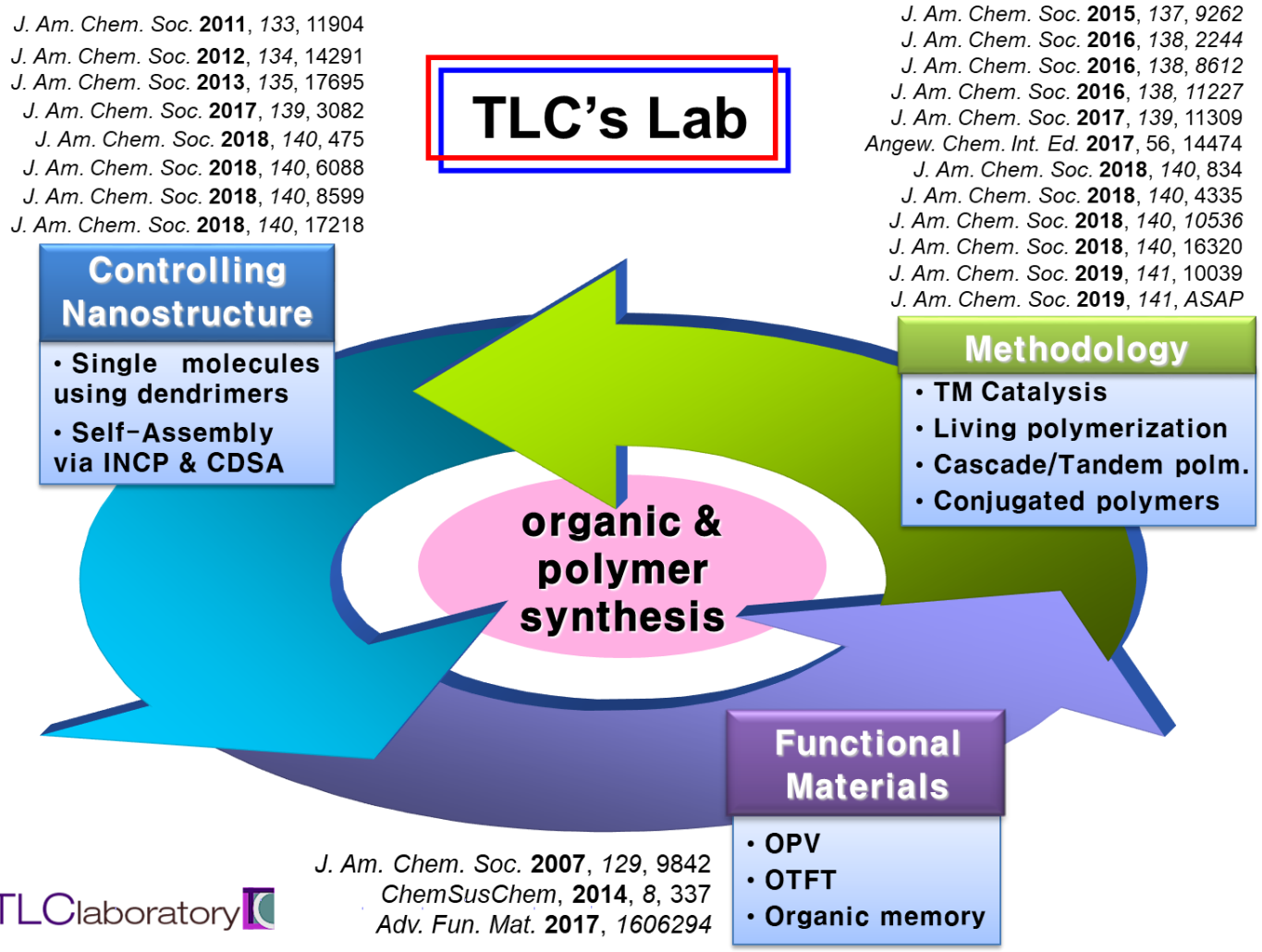
Chem. Asian J. (2018)
Adv. Healthcare Mater. (2018)
Small (2018)
Langmuir (2018)
ACS Chem. Neurosci. (2017)
Small (2016)
Nano Lett. (2016)
Proc. Natl. Acad. Sci. USA (2015)
Angew. Chem. Int. Ed. (2014)
Biomater. Sci. (2014)
J. Nanosci. Nanotechnol. (2014)
Angew. Chem. Int. Ed. (2012)
Angew. Chem. Int. Ed. (2012)
Biomaterials (2011)
Angew. Chem. Int. Ed. (2010)
Chem. Asian J. (2010)

Seoul National University
TLC laboratory

미래창조과학부
창의적연구진흥사업
Creative Research Initiatives

- 거대분자합성 연구단 @ 서울대학교 화학부 -

: 유기화학을 바탕으로 복잡하지만 정교한 다양한 거대분자/고분자를 창의적/선택적/고효율적 방법론으로 합성을 추구합니다.



[연구원 모집]

본 창의연구단에서 세계 선도적 연구를 주도적으로 수행할 창의적이고 역동적인 인재를 모십니다. 열정적인 연구원들의 많은 관심과 지원 부탁 드립니다.

1. **모집분야: 유기화학 전분야, 유기금속, 고분자화학**
2. **지원자격: 상기 분야의 박사학위 소지자**
3. **지원자 제출서류: CV 및 Research Summary (최태림 교수: tlc@snu.ac.kr)**

전남대학교 화학과 기초연구실 (이선우교수)

단일단계 합성법 개발 연구실

Single Step Synthesis Methodology Laboratory

한국연구재단
National Research Foundation of Korea

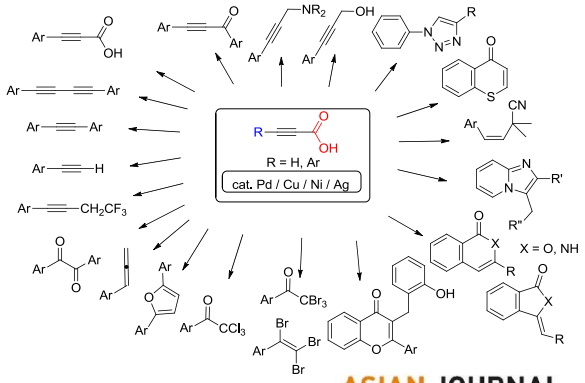
광주광역시 북구 용봉로 77 전남대 화학과
Tel) 062-530-3385; E-mail) sunwoo@chonnam.ac.kr

연구단 소개

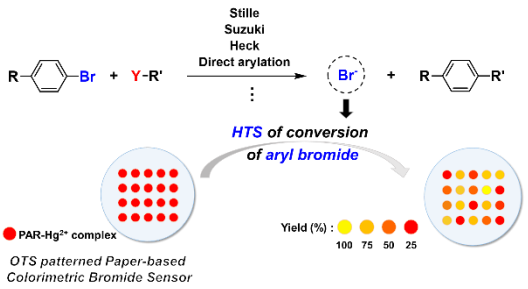
전남대 화학과 기초연구실이 수행하는 연구 과제는 유기물 합성, 리간드 디자인 및 합성, 그리고 촉매 제조 및 물성 조절에 대한 연구가 유기적으로 상호 작용하면서 복합적으로 진행되어야 하므로 단독 연구보다는 유기화학, 무기화학 및 촉매전문가들로 구성된 소규모 팀으로 진행한다. 따라서 본 연구실은 전이금속 촉매를 이용한 합성법 개발에 대한 경험과 전문 지식이 있는 연구책임자를 중심으로 유기화학 분야 2인(유기반응법 개발 전문가, 유기촉매를 이용한 합성법 전문가)과 촉매반응 분야 2인 (무기화학 분야 1인, 촉매화학 분야 1인)으로 구성하였다. 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 구심점으로 한 상호 유기적인 관계를 바탕으로 연구를 진행하고자 한다.

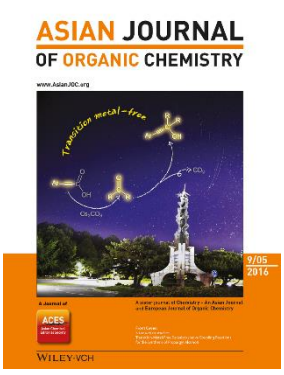
대표적 연구 내용 및 업적

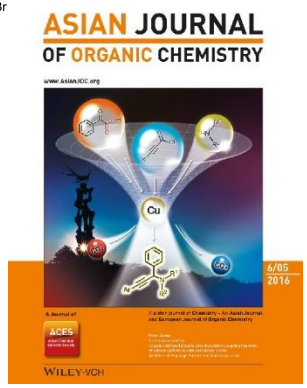
효율적 단일단계 합성법 개발

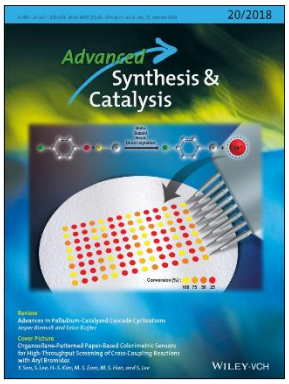


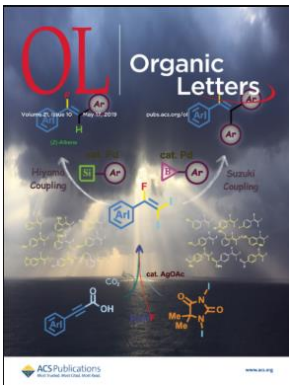
초고속 탐색법 개발











서강대학교 유기반응연구센터

3일 이내, 저렴한 가격

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◀ 보유장비 및 분석수가 안내 ▶

장비명	기준	단위	분석수가 (부가세 별도)			담당자
			대학	공공연구소	기업	
EA	CHNS		40,000	50,000	70,000	이혜경 R316 (02-705-8233)
	O		50,000	60,000	80,000	
GC-MS (저분해능 MS)	GC-MS (EI)	기본 (30분)	40,000	50,000	60,000	
		20분 추가	10,000	20,000	20,000	
UHR-MS (고분해능 MS)	MS		50,000	60,000	-	
Orbitrap-MS (고분해능 MS)	MS		-	-	70,000	박해진 R314 (02-705-8234)
500MHz NMR	1H	기본 (30분)	20,000	30,000	30,000	
	^{13}C, ^{31}P, ^{19}F	기본 (30분)	20,000	30,000	30,000	
		30분 추가	10,000	20,000	20,000	
	2D Kinetic exp.	기본 (30분)	20,000	30,000	30,000	
		30분 추가	10,000	20,000	20,000	
	Tube대여, 용매 sampling		20,000	20,000	20,000	
MALDI-TOF	MS		40,000	50,000	60,000	
	MS (30분, 본인사용)		50,000	60,000	70,000	
	MS/MS		45,000	55,000	75,000	
	Target 대여비		20,000	20,000	20,000	

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화합물 및 데이터 수집·관리

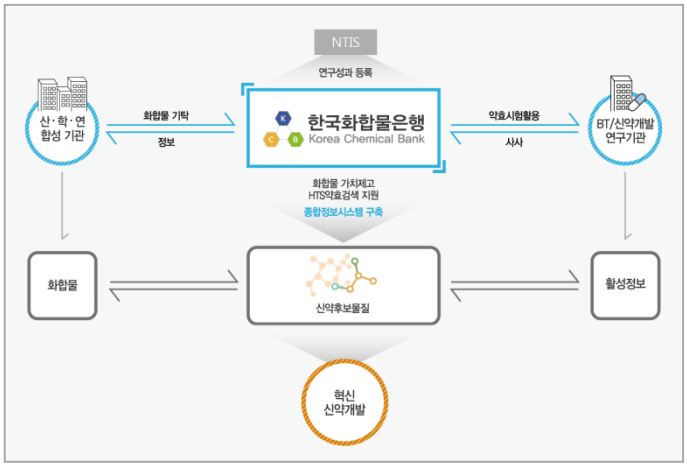
- 61만종 신약소재 화합물 보유
  - 고수준 신약소재 화합물 지속 확보 및 품질검증 (다양성 확대 및 가치제고)
- 650만건 이상의 화합물 활용 데이터 보유
  - 약효·독성·약물성 데이터 수집/표준화/통합 및 관리

화합물 및 데이터 활용지원

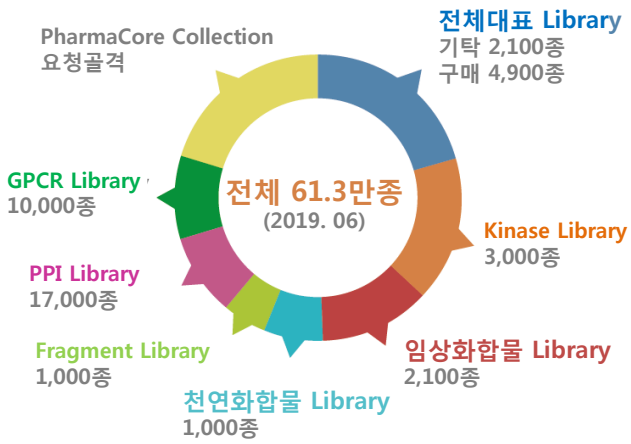
- 국내 신약개발 및 BT연구를 위한 화합물 활용 지원
- 화학정보학을 통한 화합물 선별 및 최적화 연구 지원
- 산·학·연 맞춤형 데이터 활용 지원
- 분자 표현자 정보 및 인공지능 기반 신약연구 지원

화합물 및 데이터, 예측모델의 공동활용 플랫폼

- 신약소재 화합물 및 데이터 공동활용 플랫폼 구축
- 인공지능 신약개발 예측모델의 공동활용 플랫폼 구축
- 화합물 통합 데이터베이스 및 공공 포털사이트 구축
- 웹기반 사용자 서비스 구축



한국화합물은행 제공 라이브러리 종류



관리·유통 전담기관제도 및 의무기탁 규정

한국화합물은행은 국가연구개발사업 수행을 통해 창출된 연구성과 중 **화합물 및 관련 정보의 관리·유통 전담기관으로 지정되어 있습니다.**
(과학기술정보통신부 고시 제2017-7호)
『공동관리규정』 제25조13항 : 국가연구개발사업을 통하여 창출된 연구성과(화합물)는 전담기관에 의무적으로 기탁하여야 한다.

국가연구개발 우수성과 선정시 전담기관(한국화합물은행)에 기탁된 성과만 인정하도록『국가연구개발 과제평가 표준지침』에 명시.
(2016.12.09 개정)

화합물 및 데이터의 기탁, 활용 문의

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첫 구매 고객 이벤트

기존 **Affymetrix-USB** 바이오케미컬 제품은
2019년 8월 1일 부터 www.alfa.co.kr 웹사이트에서
새롭게 바뀐 **Thermo scientific** 브랜드로 만나 보실 수 있습니다!

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- **제품/구매 정보 :** www.alfa.co.kr
- **대상 제품번호 :** J1, 2, 3, 7으로 시작하는 제품

EVENT

www.Alfa.co.kr 웹사이트에서 Thermo scientific (구, Affymetrix-USB) 바이오케미컬 제품을 구매하신 고객 중 선착순 50분께 Starbucks 기프티콘을 드립니다.

이벤트 내용

이벤트 기간 2019년 8월 한달간

경 품 스타벅스 기프티콘 (선착순 50명)

추가 이벤트 바이오케미컬 첫 구매 및 웹사이트 신규 가입 고객인 경우 USB(16GB) 추가 증정

※ 이벤트 당첨 고객은 개별 연락을 통해 안내 예정입니다.

더 많은 제품은 www.alfa.co.kr 에서 만나보세요.

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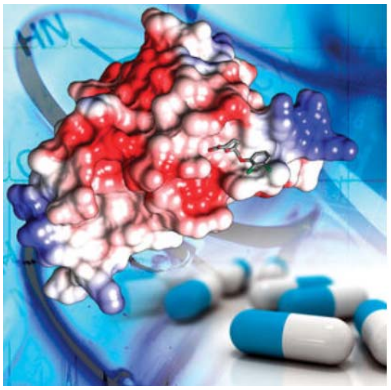
thermo scientific

Pharmaceutical Application of NMR and EPR



Lead Discovery

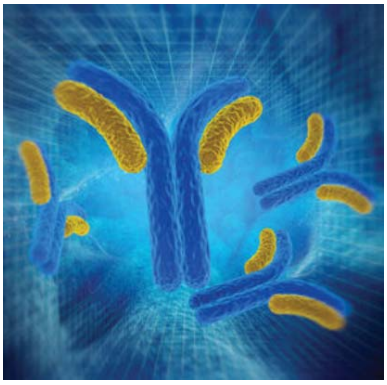
NMR, the most popular biophysical method for fragment-based screening, now with computer-aided tools to streamline data handling.

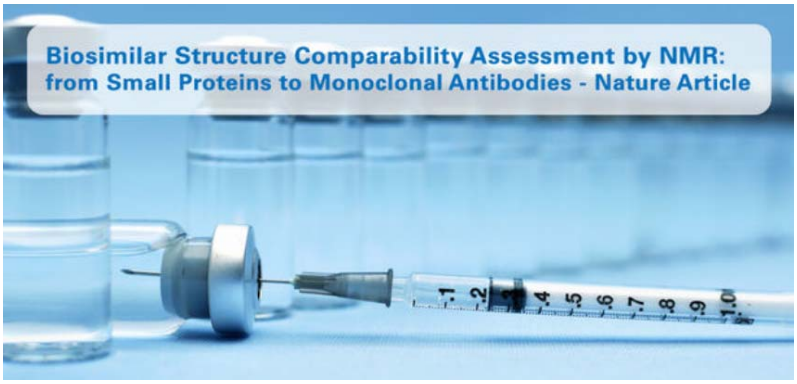
NMR fragment-based screening

Structures

Have you synthetized the right compound? Need to know the structure of an impurity? Proof of structure documentation, confidence before compound registration… NMR is what you need.

Complete Molecular Confidence Software





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InsightMR Portfolio

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Potency determination, absolute concentration of API, quantification of impurities in a mixture?
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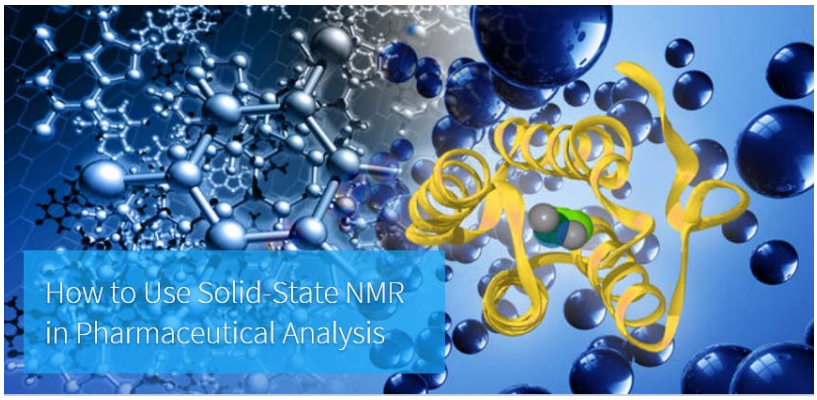
Quantification



Biologics Analysis

NMR provides unique information about high order structure of biological molecules (biologic drugs and biosimilars).

Quality Assessment of Biologics Drugs

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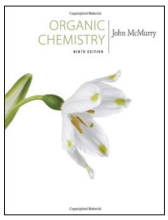
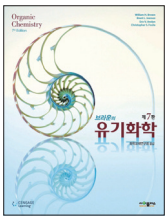
맥머리의 유기화학 9판



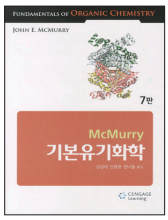
저 자 : McMurry
판 수 : 9
발 행 일 : 2017
페 이 지 : 1224
I S B N : 9788962184297

브라운의 유기화학 7판



저 자 : Brown
판 수 : 7
발 행 : 2016
페 이 지 : 1288
I S B N : 9788992603836

McMurry 기본유기화학 7판



저 자 : McMurry
판 수 : 7
발 행 : 2011
페 이 지 : 736
I S B N : 9788962181616

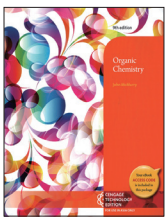
맥머리의 유기화학강의 9판

저 자 : McMurry
판 수 : 9
발 행 : 2016
페 이 지 : 480
I S B N : 9788962184396

파비아의 분광학강의 5판

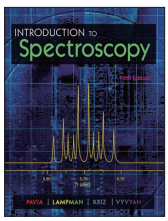
저 자 : Pavia
판 수 : 5
발 행 일 : 2017
페 이 지 : 772
I S B N : 9788962184389

Organic Chemistry 9/e



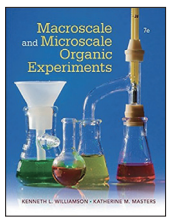
저 자 : McMurry
판 수 : 9
발 행 일 : 2016
페 이 지 : 1054
I S B N : 9789814773683

Introduction to Spectroscopy 5/e



저 자 : Pavia
판 수 : 5
발 행 일 : 2015
페 이 지 : 784
I S B N : 9781285460123

Macroscale and Microscale Organic Experiments 7/e

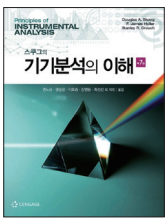


저 자 : Williamson
판 수 : 7
발 행 일 : 2017
페 이 지 : 842
I S B N : 9781305577190

Principles of Instrumental Analysis 7/e

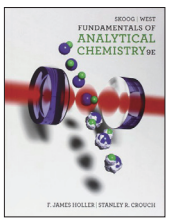
저 자 : Skoog
판 수 : 7
발 행 일 : 2019
페 이 지 : 988
I S B N : 9789814834346

스쿠그의 기기분석의 이해 7판



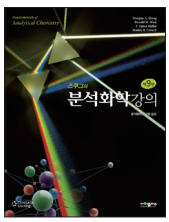
저 자 : Skoog
판 수 : 7
발 행 : 2018
페 이 지 : 921
I S B N : 9788962184242

Fundamentals of Analytical Chemistry 9/e



저 자 : Skoog
판 수 : 9
발 행 일 : 2014
페 이 지 : 1072
I S B N : 9780495558286

스쿠그의 분석화학강의 9판



저 자 : Skoog
판 수 : 9
발 행 : 2016
페 이 지 : 1056
I S B N : 9788962184587

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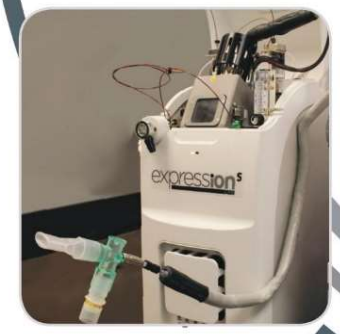

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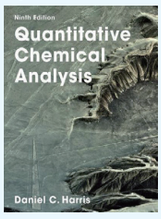
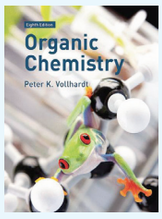


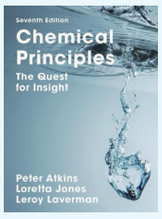
저　　자: Harris
출 판 사: Macmillan
출판년도: 2015년
쪽　　수: 928쪽
ISBN: 9781319154141

Organic Chemistry 8/e



저　　자: Vollhardt 외
출 판 사: Macmillan
출판년도: 2018년
쪽　　수: 1200쪽
ISBN: 9781319187712

Chemical Principles: The Quest for Insight 7/e

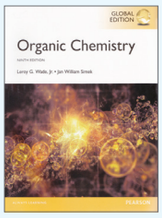


저　　자: Atkins 외
출 판 사: Macmillan
출판년도: 2016년
ISBN: 9781319154196

Organic Chemistry 5/e

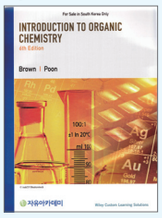
저　　자: Smith 외
출 판 사: McGraw-Hill
출판년도: 2016년
쪽　　수: 1344쪽
ISBN: 9781259254888

Organic Chemistry 9/e



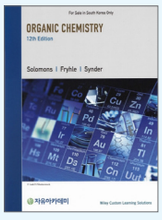
저　　자: Wade 외
출 판 사: Pearson
출판년도: 2017년
쪽　　수: 1,400쪽
ISBN: 9781292151106

Introduction to Organic Chemistry 6/e



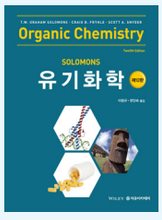
저　　자: Brown 외
출 판 사: Wiley
출판년도: 2016년
쪽　　수: 623쪽
ISBN: 9781119923152

Organic Chemistry 12/e



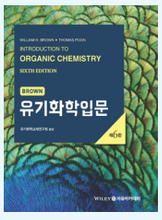
저　　자: Solomons 외
출 판 사: Wiley
출판년도: 2016년
쪽　　수: 1124쪽
ISBN: 9781118875766

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
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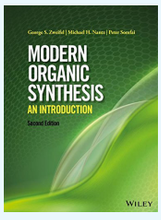


저　　자: Zweifel
출 판 사: Wiley
출판년도: 2017년
쪽　　수: 416쪽
ISBN: 9781119086536

현대 유기 합성 제2판

저　　자: Zweifel 외
역　　자: 강한영, 김병문, 안덕근, 이효원, 장두옥, 전철호
출판년도: 2018년
쪽　　수: 400쪽
ISBN: 9791158081645

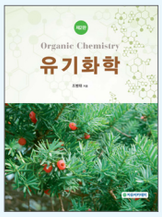
생명과학자를 위한 Yoon's 유기화학

저　　자: 윤용진 외
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

유기화학 제2판



저　　자: 조병태
출판년도: 2017년
쪽　　수: 656쪽
ISBN: 9791158081355

유기화학 반응 메커니즘의 단계별 접근법

저　　자: Moloney
역　　자: 이창윤
출판년도: 2017년
쪽　　수: 256쪽
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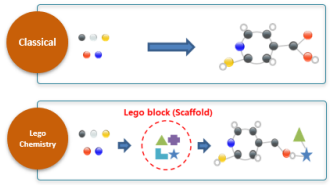
설립일	2006. 5. 2
상장일	2013. 5. 10 (코스닥)
업종	의학 및 약학연구개발업
대표이사	김용주
자본금	60억원
임직원수	94명
본사	대전 대덕구 문평서로 826

회사소개

㈜ 레고켐 바이오는 의약화학(medicinal chemistry)을 기반으로 한 합성신약(항생제, 항응혈제, 항암제) 연구개발을 중심축으로 ADC 원천기술을 통해 바이오 신약분야로 확장하고 있는 신약연구개발전문기업이다.

주요기술



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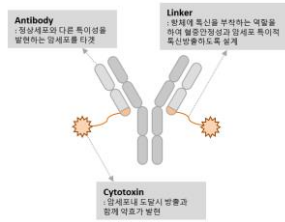
- 고유의 약물유사성(druglikeness)이 검증된 약 20여 종의 중간핵심구조(Scaffold) 보유. 중간핵심구조를 활용하여 지속적으로 새로운 pipeline을 확장 예정.



Conjuall

- 항체-약물 결합체 ADC 원천기술로써 기존 1세대 ADC 기술의 문제점을 극복한 단일물질 구현과 링커 의 안정성을 개선한 차세대원천기술
- 차세대 ADC 원천기술을 다양한 항체를 활용하여 구현되고 있으며, 기존 기술들과 비교하여 차별성 검증

회사연혁

2006년 회사설립

2011년 항응혈제(FXa 저해제미국FDA 임상1상 허가

2012년 아시아 유망 바이오 기업상 선정

2013년 코스닥 시장 상장

2014년 K-BrainPower 선정

2015년 2015년도 국제공동기술개발사업(한-프) 선정

2016년 그람음성균 항생제 LCB10-0200 글로벌 임상을 위한 JV 설립

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그람음성균 항생제 미국 NIH 국책과제 선정

2018년 Delpazolid(LCB01-0371) 미국 FDA 신속심사 선정

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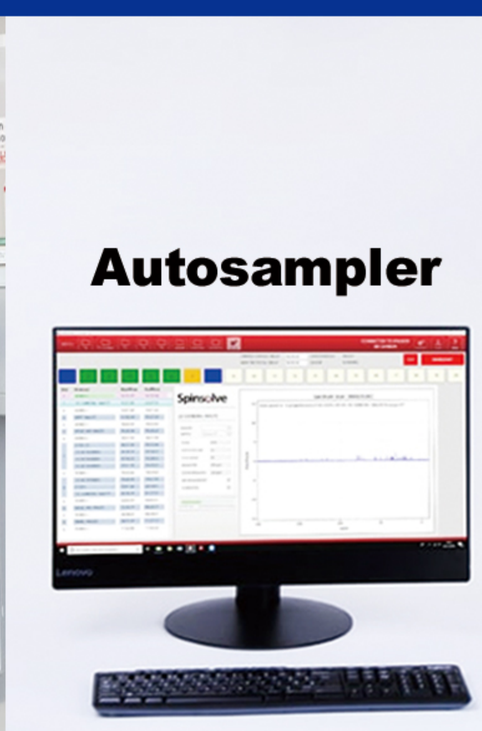

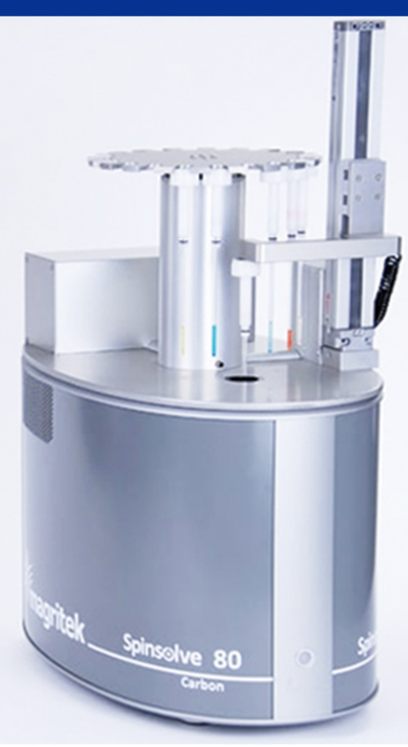

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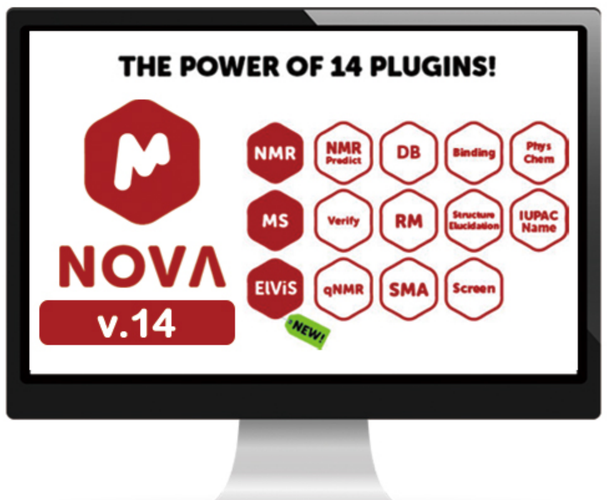

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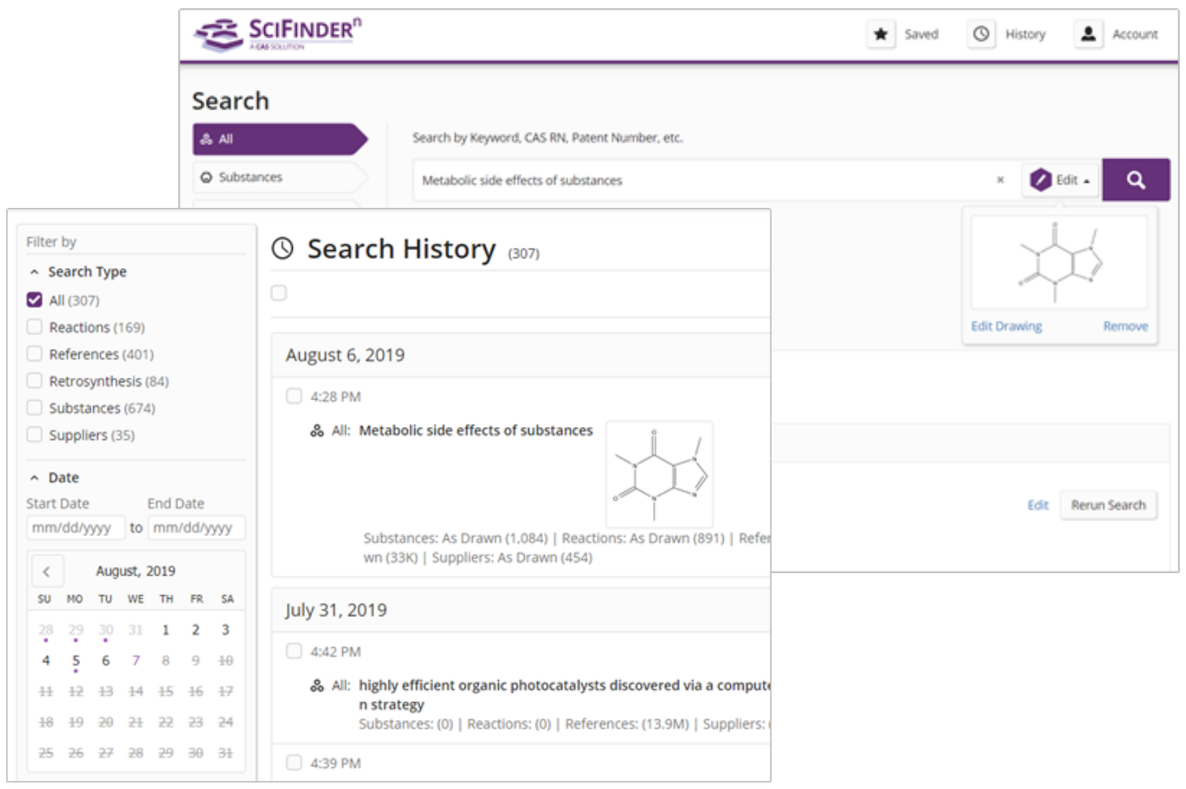

- 화학 구조식과 키워드를 함께 검색
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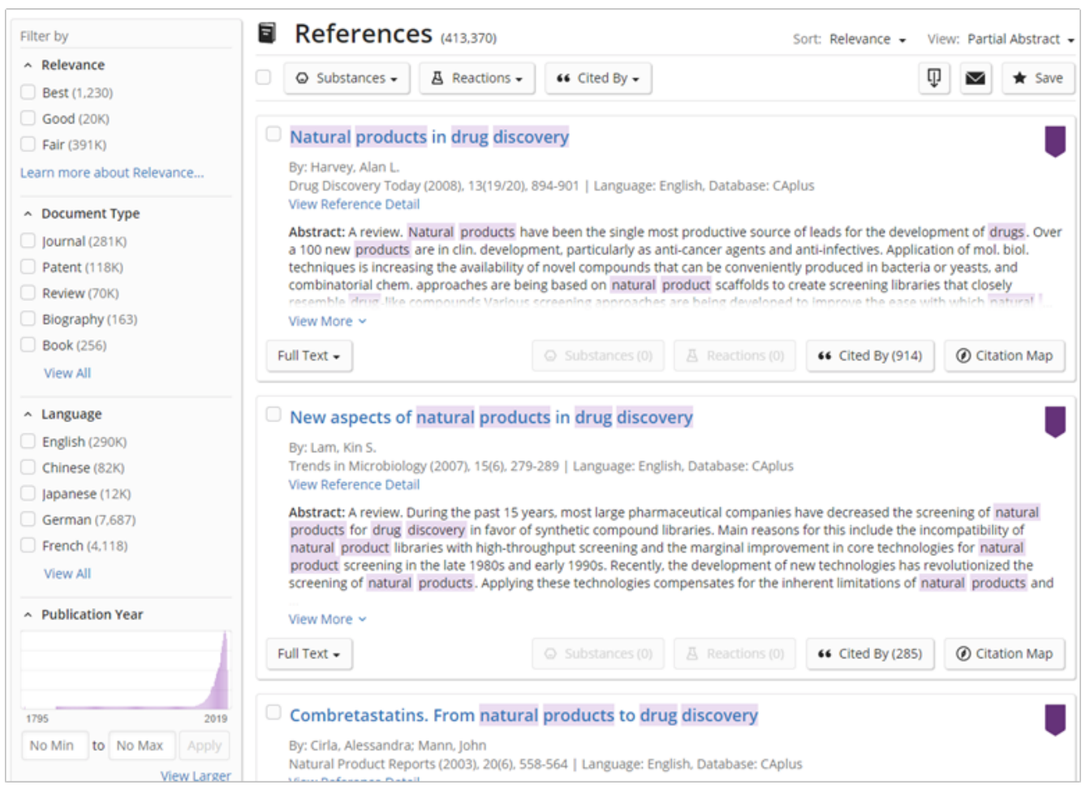
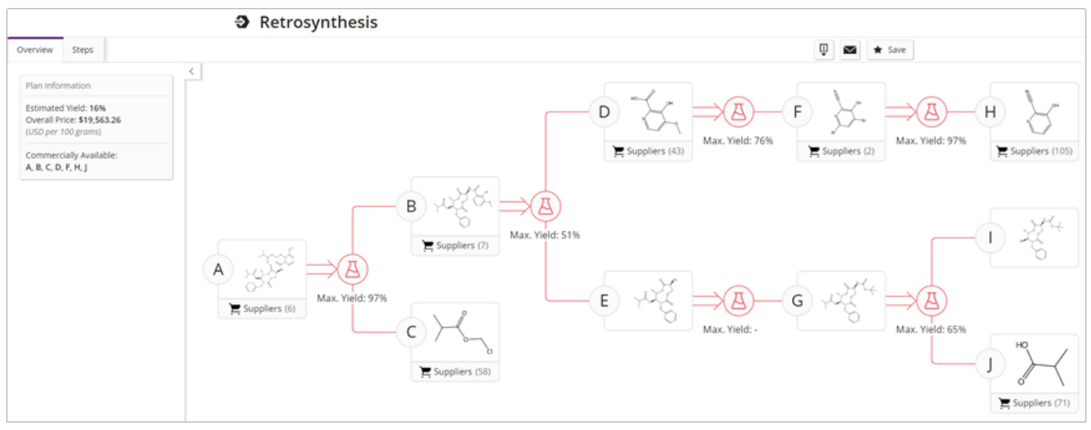
연관성 높은 결과



- Relevancy engine 탑재로 연관성 높은 문헌 순으로 결과 확인
- 강력하고, 종합적인 검색 필터를 통해 원하는 결과를 빠르게 검색
- 직관적인 결과 확인을 위해 디자인된 포맷
- 연구 동향 분석을 통해 연구 공개 속도에 발 맞춥니다

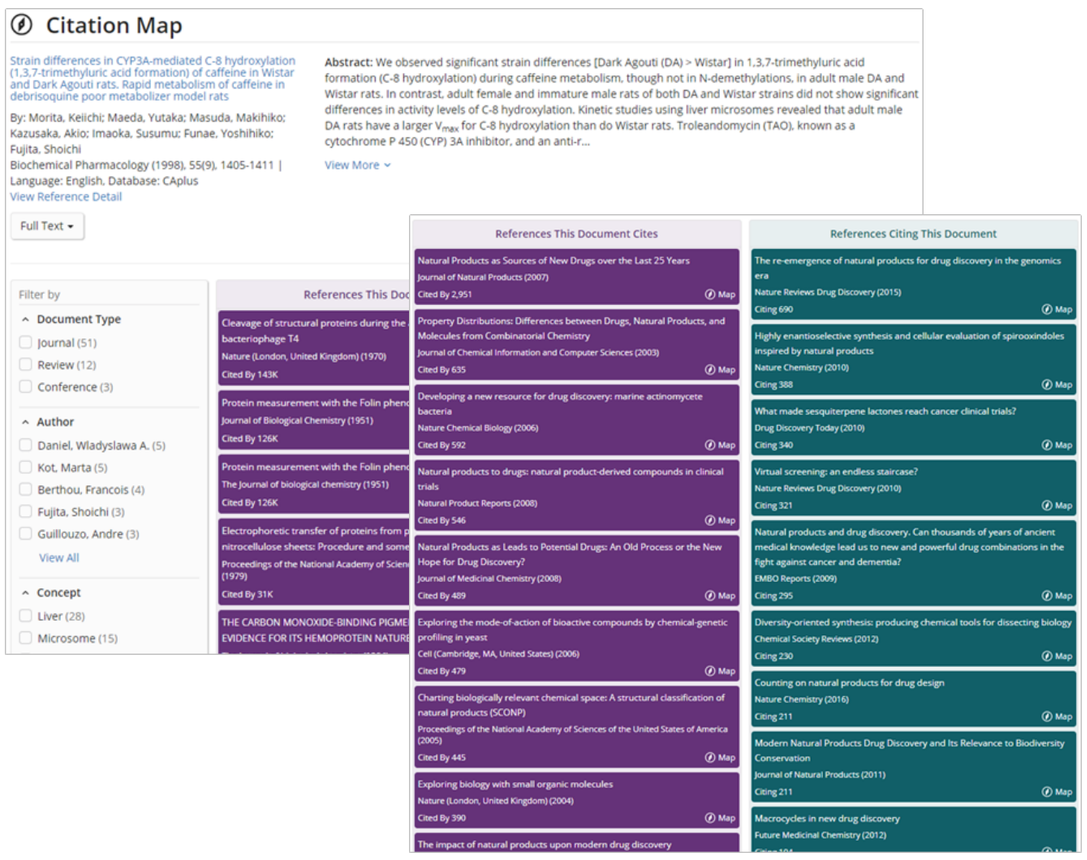
Retrosynthesis 레트로 합성



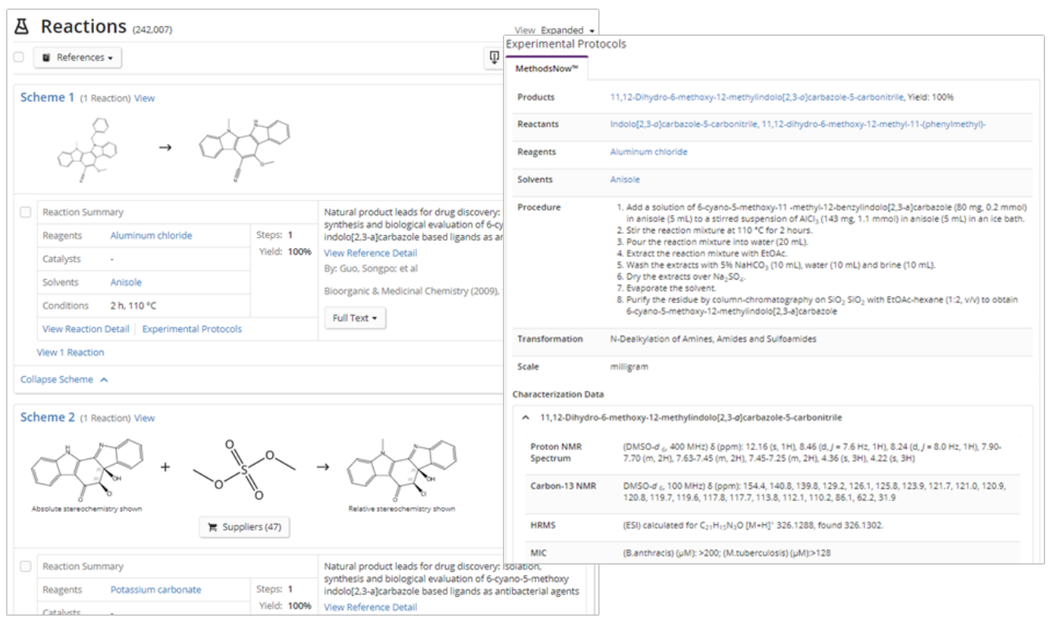
- CAS의 반응식 정보를 기반으로 한 레트로 합성법 확인
- 예측 수율과 가격 정보 확인
- 물질 판매처 정보 확인

Citation Mapping

- 상호 호환 검색 가능한 Map으로 중요 연구결과를 빠르게 확인
- "Family tree"를 통해 중요 자료를 찾기 용이
- 잠재 협력자, Funding sources, 경쟁업체 등 파악
- 놓칠 뻔 한 문헌을 Map을 통해 찾을 수 있음



단계별 합성법 제공



- CAS 과학자에 의해 요약된 합성법이 제공되어 시간 절약
- 단계별 실험방법을 연구실에서 바로 활용
- 반응식의 주요 화학물질 색인, 링크를 통한 추가 정보 확인

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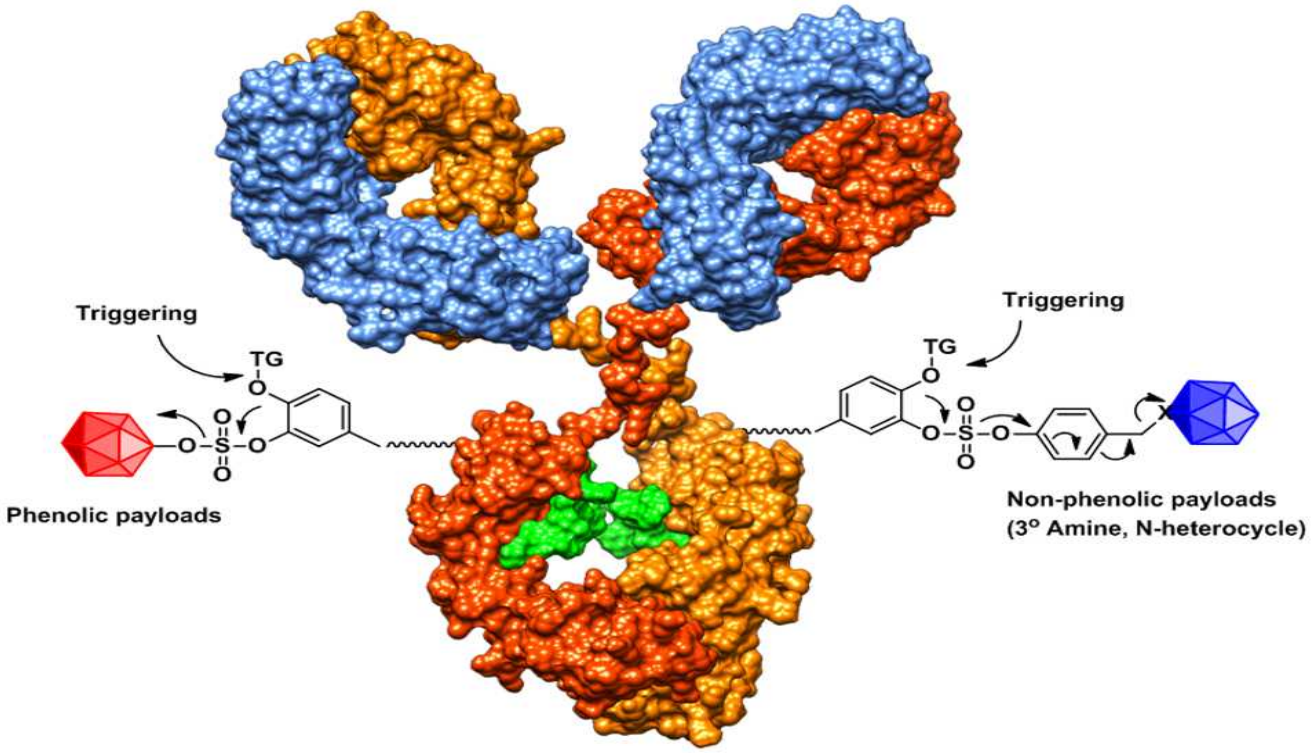

Summary of Characteristics

Synthesis	Efficient Convergent Synthesis
Stability	Highly Stable
Triggering Method	Chemical or Enzymatic
Conjugatable Functional Groups	Phenol, 3° Amine, N-heterocycles > Alcohol
Representative Payloads	**Toxins** Amanitins, Doxorubicin(oids), Pancratistatin, Tubulysin B, PBDs, Duocarmycinoids **Biopolymers** DNA/RNA, protein/oligopeptide

Patent	Region
Compounds Comprising Cleavable Linker And Uses Thereof	Korea/ USA/PCT
Benzodiazepine Dimers and Uses Related Thereto	USA
Compounds Comprising Beta-Galactoside Self-Immolati ve Linker	Korea/ PCT

Paper
Bioconjugate Chem. **2019**, 30, 1957–1968.
Bioconjugate Chem. **2019**, 30, 1969–1978.

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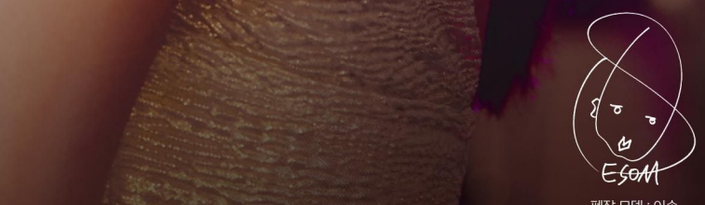

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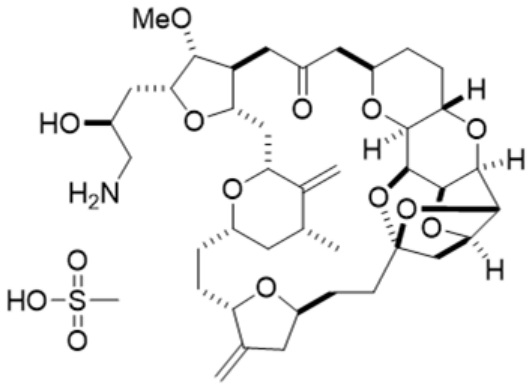

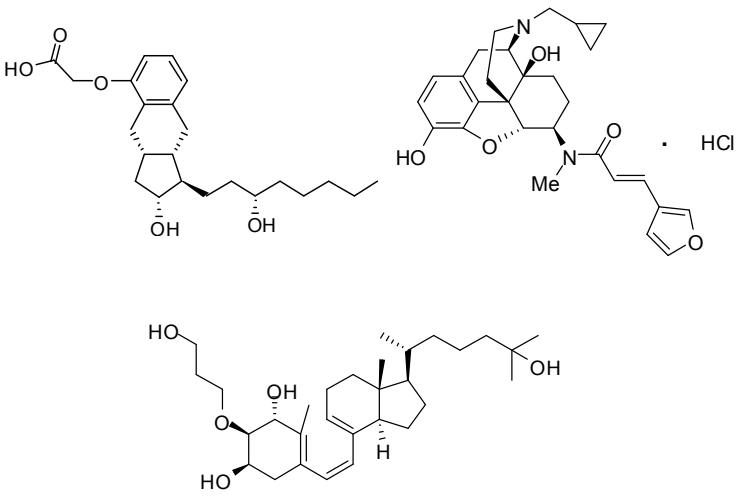

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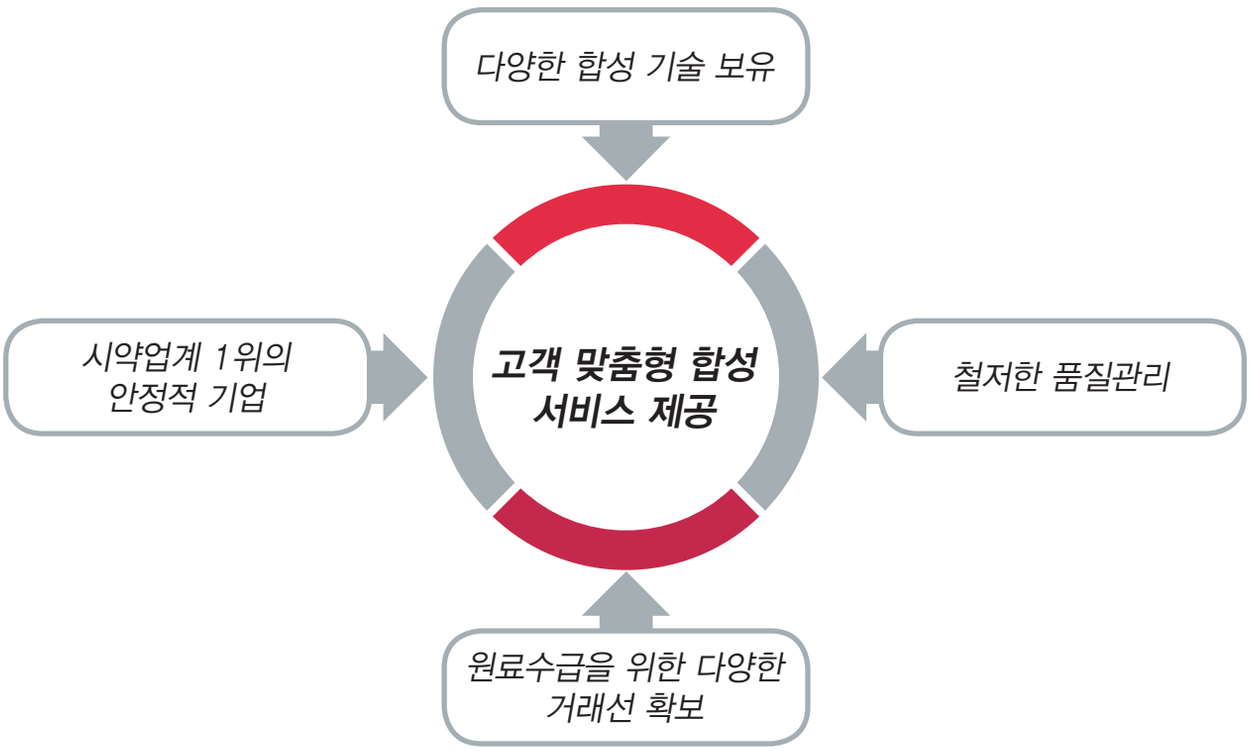


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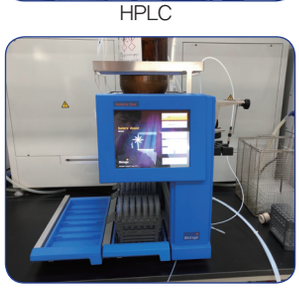
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